



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 03:43 pm BST

PDB ID : 9GR1 / pdb_00009gr1
EMDB ID : EMD-51517
Title : E. coli 70S-TEC complex in delivery state
Authors : Webster, M.W.; Weixlbaumer, A.
Deposited on : 2024-09-10
Resolution : 3.17 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:

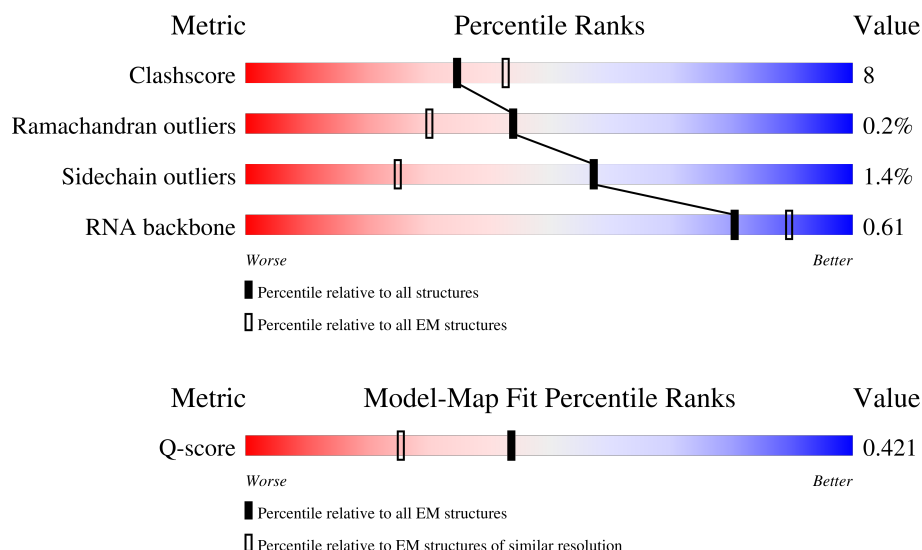
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 3.17 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	14465 (2.67 - 3.67)

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	0	55	
2	1	46	
3	2	65	

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Mol	Chain	Length	Quality of chain
4	3	38	
5	A	1542	
6	B	241	
7	C	233	
8	D	206	
9	E	167	
10	F	135	
11	G	179	
12	H	130	
13	I	130	
14	J	103	
15	K	129	
16	L	124	
17	M	118	
18	N	101	
19	O	89	
20	P	82	
21	Q	84	
22	R	75	
23	S	92	
24	T	87	
25	U	71	
26	X	16	
27	Z	76	
28	a	2925	

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Mol	Chain	Length	Quality of chain
29	b	119	
30	c	273	
31	d	209	
32	e	201	
33	f	179	
34	g	177	
35	h	149	
36	i	142	
37	j	123	
38	k	144	
39	l	136	
40	m	127	
41	n	117	
42	o	115	
43	p	118	
44	q	103	
45	r	110	
46	s	100	
47	t	104	
48	u	94	
49	v	85	
50	w	78	
51	x	63	
52	y	59	
53	z	57	

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Mol	Chain	Length	Quality of chain
54	4	10	
55	Y	77	

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
28	3TD	a	1919	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 142297 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1513	Total	C	N	O	P	0	0
			32478	14493	5961	10511	1513		

- Molecule 6 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 7 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 10 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 11 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 12 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	116	Total	C	N	O	S	0	0
			902	558	183	156	5		

- Molecule 17 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 20 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 21 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 22 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	55	Total	C	N	O	S	0	0
			455	288	86	81			

- Molecule 23 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 24 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 25 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 26 is a RNA chain called mRNA in ribosome channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	13	Total	C	N	O	P	0	0
			271	122	44	92	13		

- Molecule 27 is a RNA chain called Phe-NH-tRNA(Phe) A-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Z	76	Total	C	N	O	P	S	0	0
			1624	724	290	533	76	1		

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2748	Total	C	N	O	P	0	0
			59025	26336	10876	19065	2748		

- Molecule 29 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 30 is a protein called 50S ribosomal protein L2.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 32 is a protein called 50S ribosomal protein L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 35 is a protein called 50S ribosomal protein L9.

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

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	77	ILE	VAL	conflict	UNP A0A140N711

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	n	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 42 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

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

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

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

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 53 is a protein called 50S ribosomal protein L32.

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

- Molecule 54 is a RNA chain called mRNA in SD-aSD duplex.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	10	Total	C	N	O	P	0	0
			223	99	48	66	10		

- Molecule 55 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	Y	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	A	48	Total	K	0
			48	48	
57	a	112	Total	K	0
			112	112	
57	b	1	Total	K	0
			1	1	
57	c	4	Total	K	0
			4	4	
57	d	1	Total	K	0
			1	1	
57	e	1	Total	K	0
			1	1	
57	f	1	Total	K	0
			1	1	

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

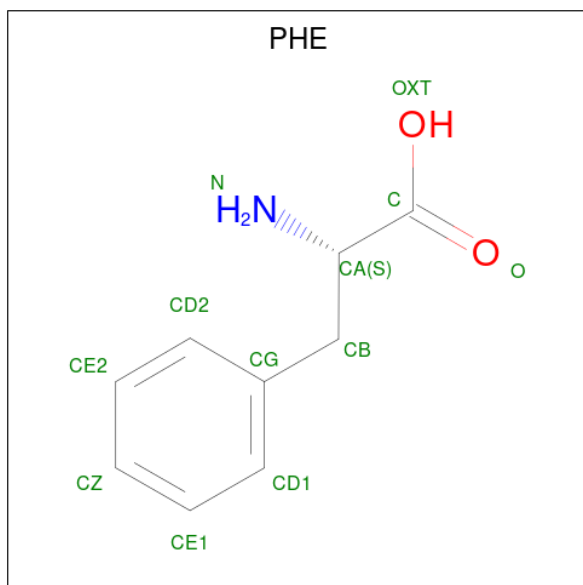
Mol	Chain	Residues	Atoms		AltConf
58	A	95	Total	Mg	0
			95	95	
58	N	1	Total	Mg	0
			1	1	
58	a	254	Total	Mg	0
			254	254	
58	b	5	Total	Mg	0
			5	5	
58	c	1	Total	Mg	0
			1	1	
58	d	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
58	k	1	Total	Mg	0
			1	1	
58	z	1	Total	Mg	0
			1	1	
58	Y	1	Total	Mg	0
			1	1	

- Molecule 59 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).

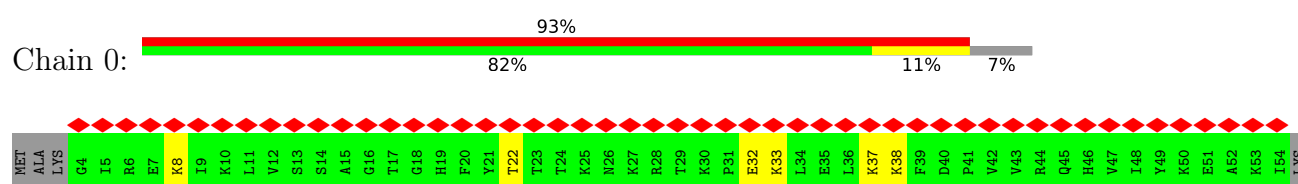


Mol	Chain	Residues	Atoms				AltConf
59	a	1	Total	C	N	O	0
			11	9	1	1	

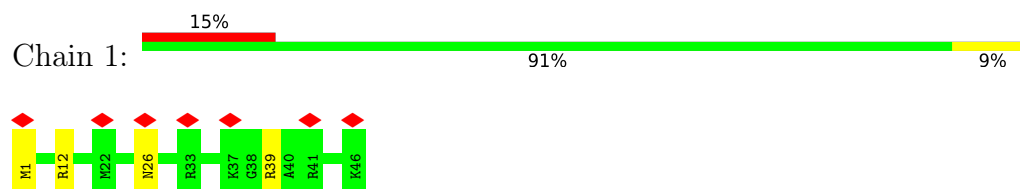
3 Residue-property plots [i](#)

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

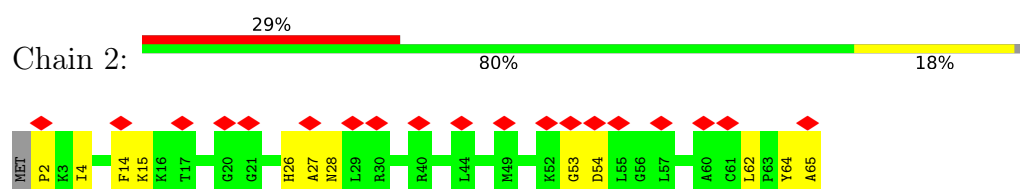
- Molecule 1: 50S ribosomal protein L33



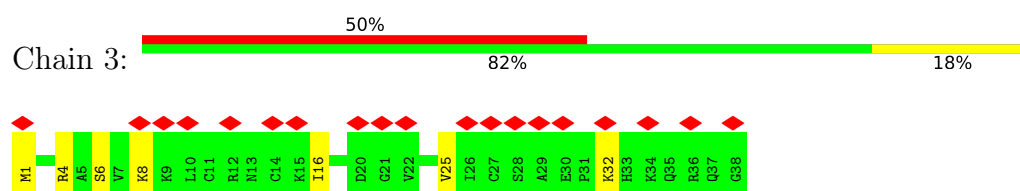
- Molecule 2: 50S ribosomal protein L34



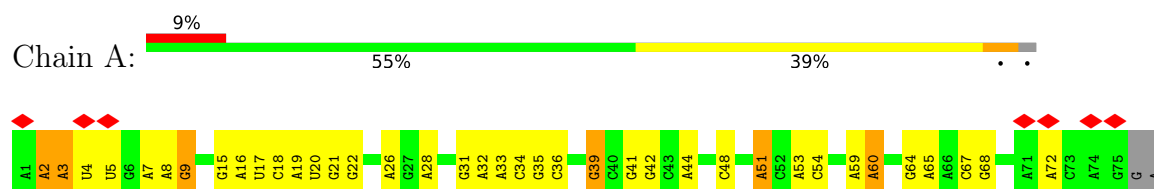
- Molecule 3: 50S ribosomal protein L35

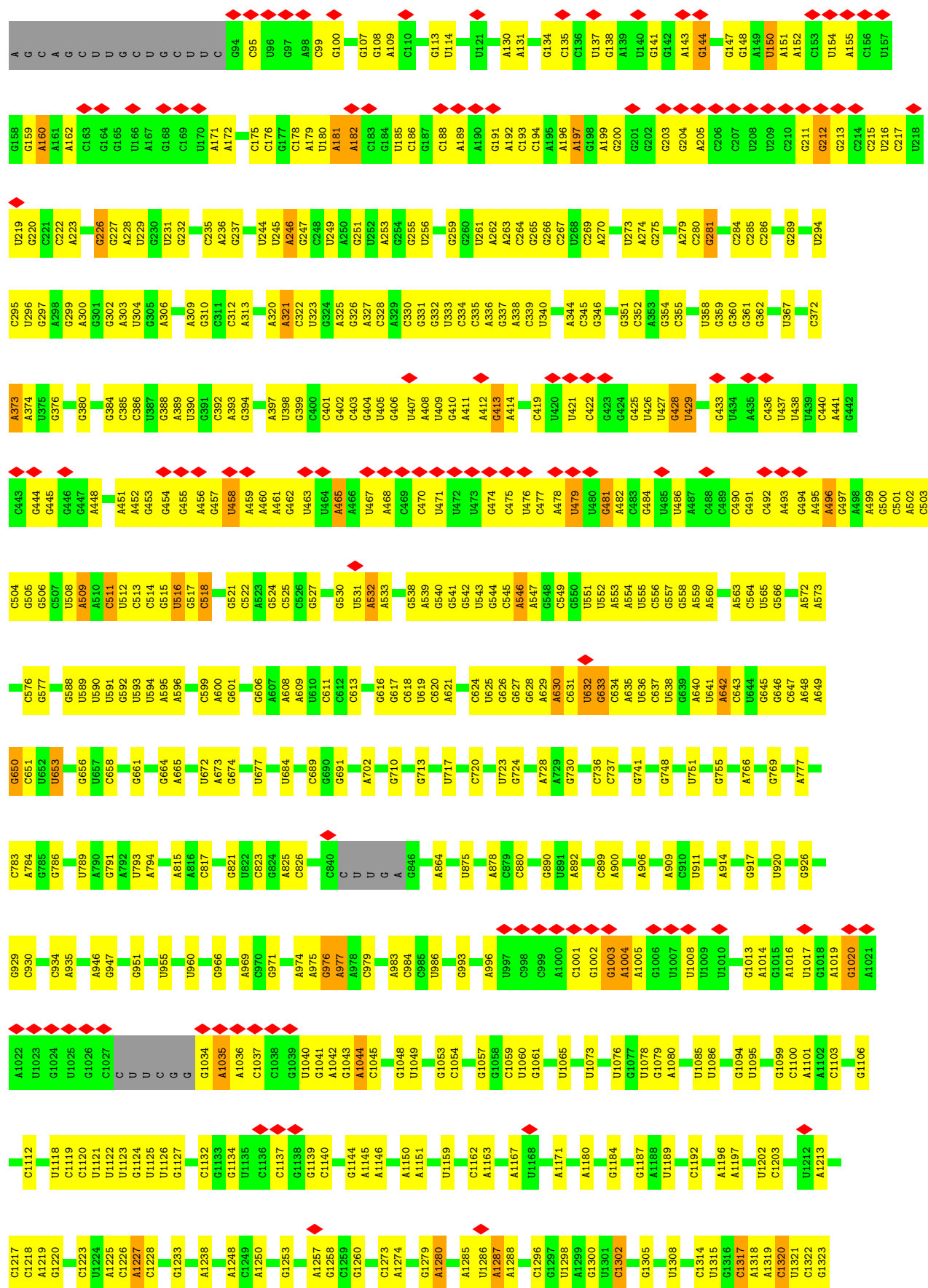


- Molecule 4: 50S ribosomal protein L36



- Molecule 5: 16S ribosomal RNA

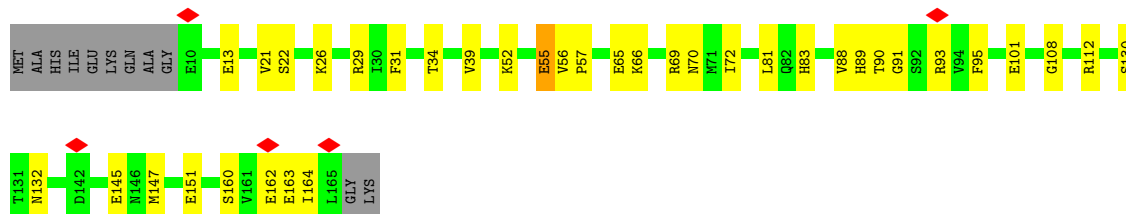






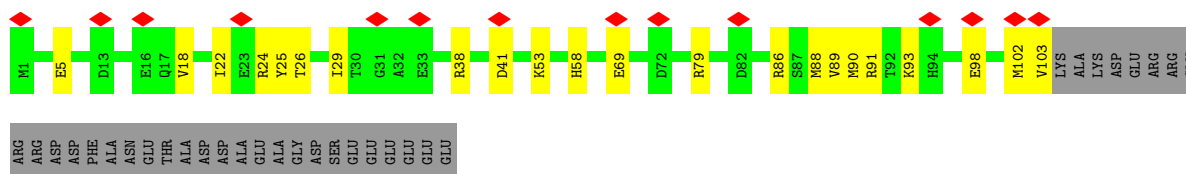
- Molecule 9: Small ribosomal subunit protein uS5

Chain E: 71% 22% 7%



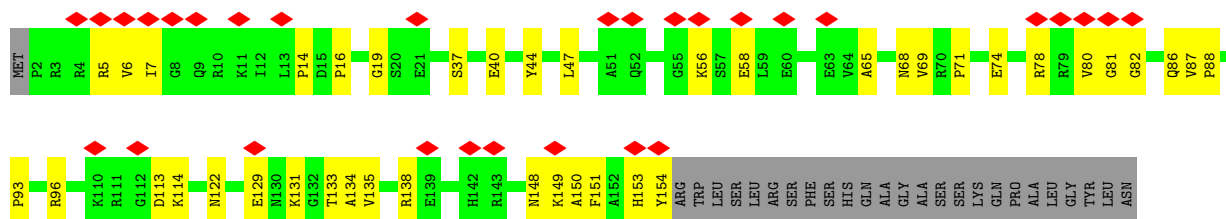
- Molecule 10: Small ribosomal subunit protein bS6, fully modified isoform

Chain F: 10% 60% 16% 24%



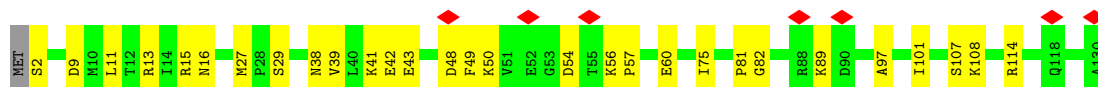
- Molecule 11: Small ribosomal subunit protein uS7

Chain G: 17% 63% 23% 15%



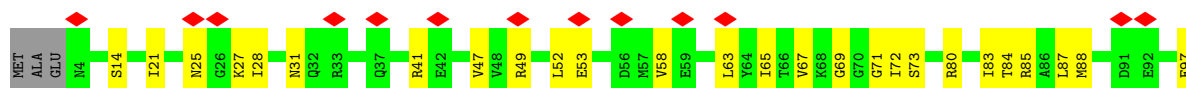
- Molecule 12: Small ribosomal subunit protein uS8

Chain H: 5% 77% 22%



- Molecule 13: Small ribosomal subunit protein uS9

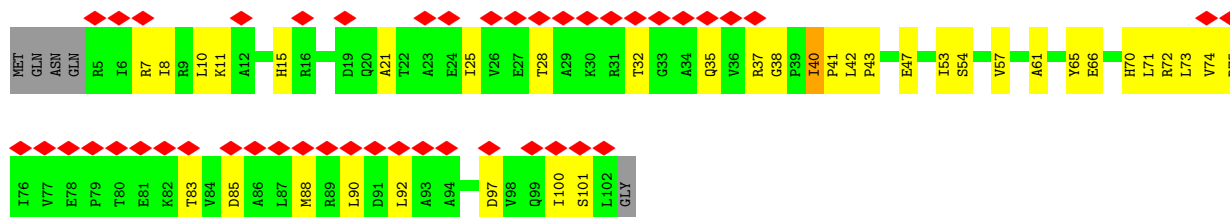
Chain I: 12% 71% 27%





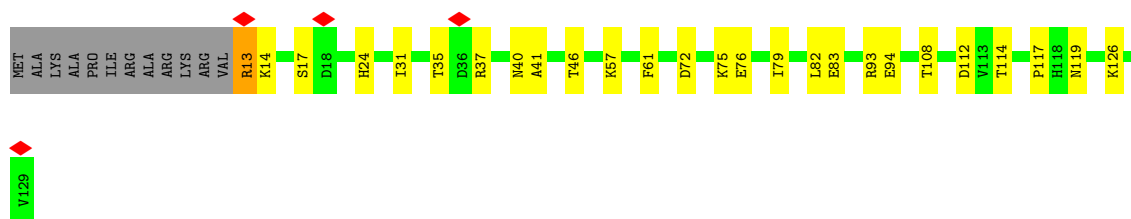
- Molecule 14: Small ribosomal subunit protein uS10

Chain J: 44% 59% 35% 5%



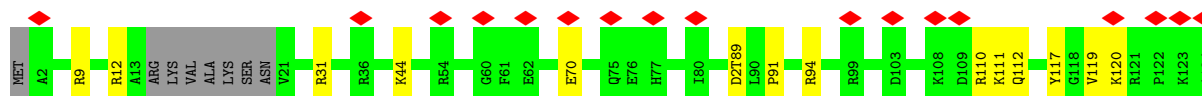
- Molecule 15: Small ribosomal subunit protein uS11

Chain K: 71% 19% 9%



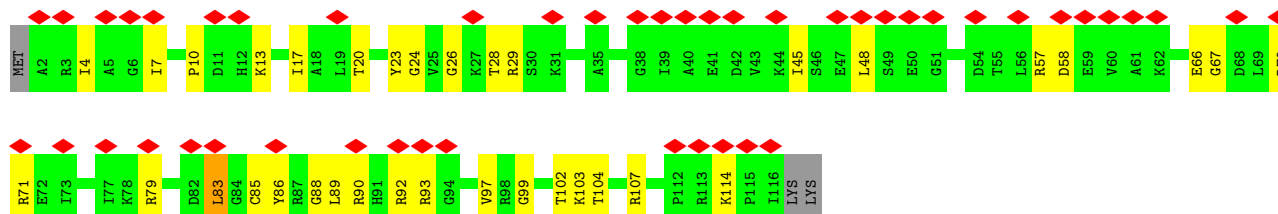
- Molecule 16: Small ribosomal subunit protein uS12

Chain L: 14% 82% 11% 6%



- Molecule 17: Small ribosomal subunit protein uS13

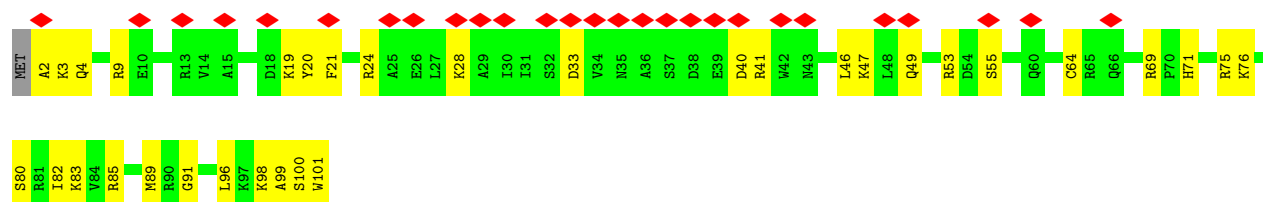
Chain M: 40% 68% 29% 2%



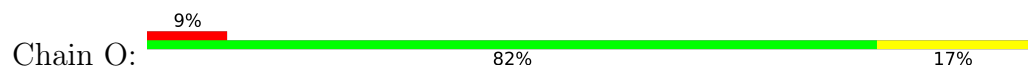
- Molecule 18: Small ribosomal subunit protein uS14

Chain N: 27% 66% 33% 2%

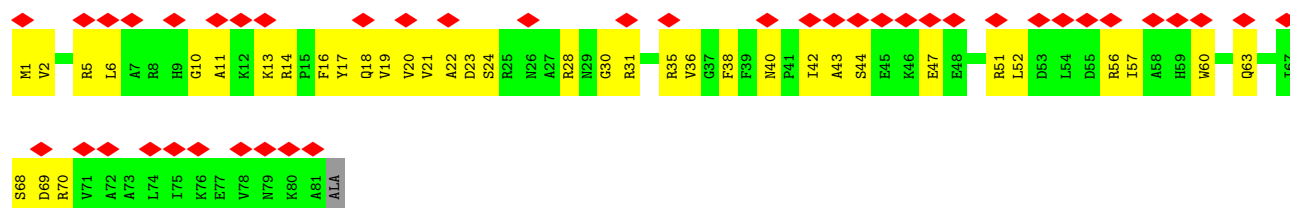




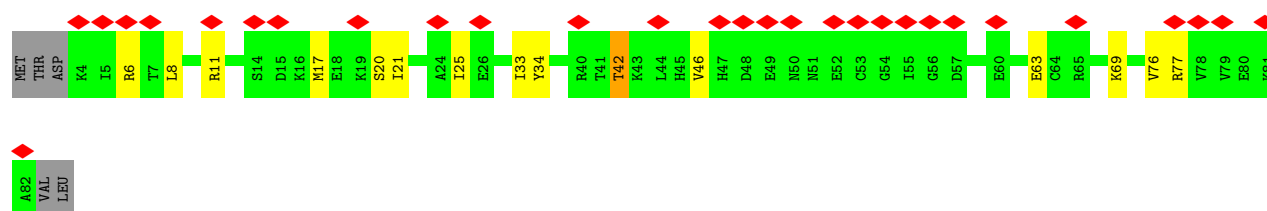
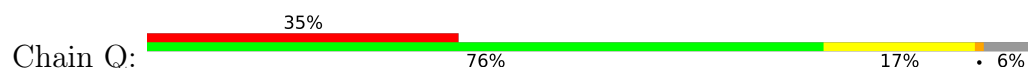
- Molecule 19: Small ribosomal subunit protein uS15



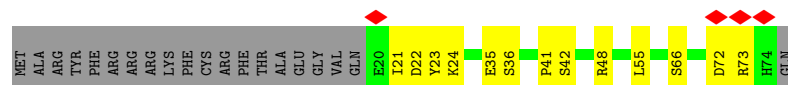
- Molecule 20: 30S ribosomal protein S16



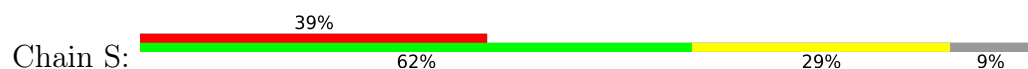
- Molecule 21: Small ribosomal subunit protein uS17

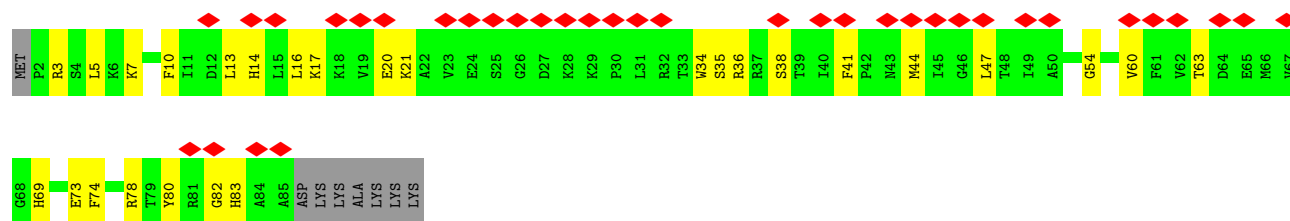


- Molecule 22: Small ribosomal subunit protein bS18

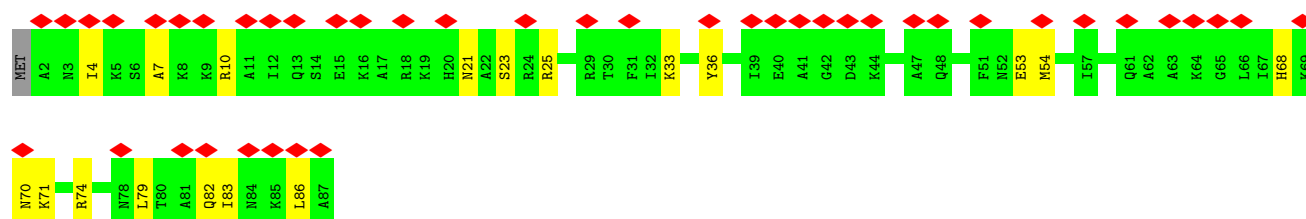
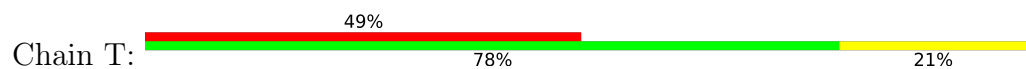


- Molecule 23: 30S ribosomal protein S19

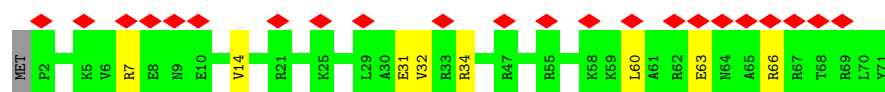
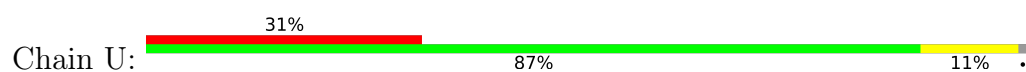




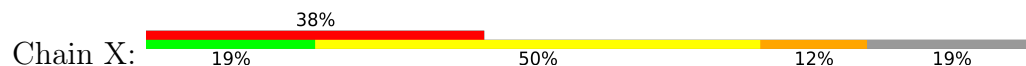
- Molecule 24: Small ribosomal subunit protein bS20



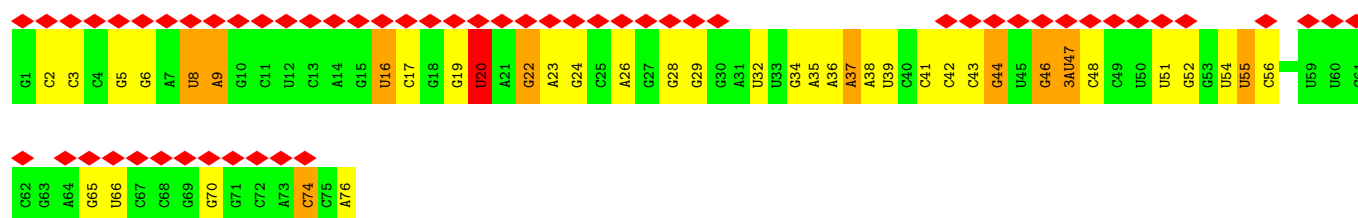
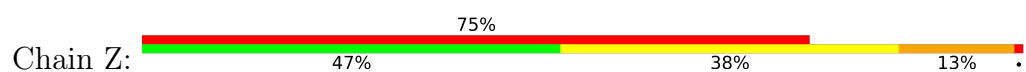
- Molecule 25: Small ribosomal subunit protein bS21



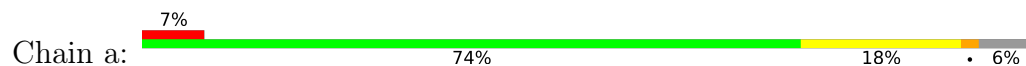
- Molecule 26: mRNA in ribosome channel



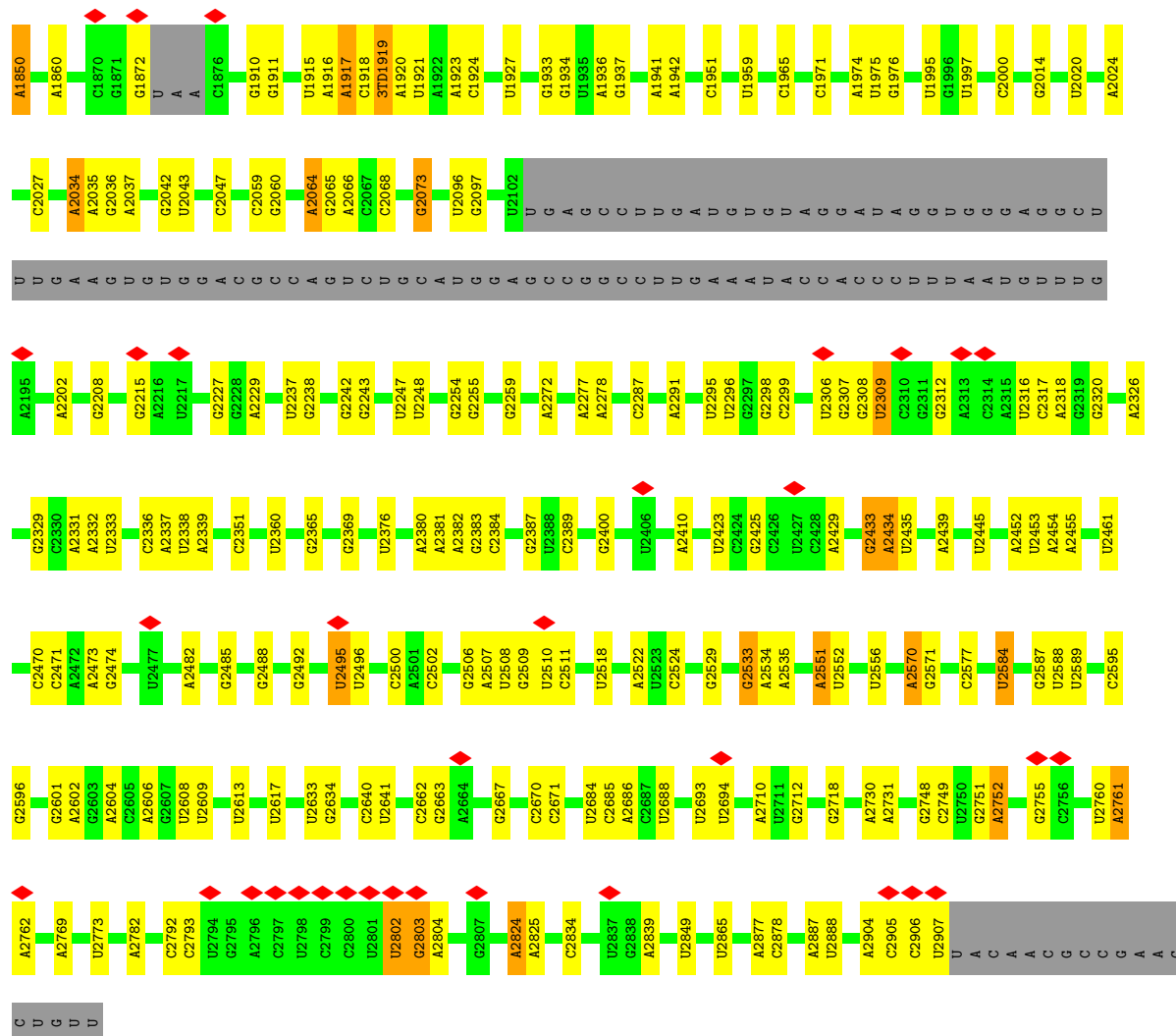
- Molecule 27: Phe-NH-tRNA(Phe) A-site



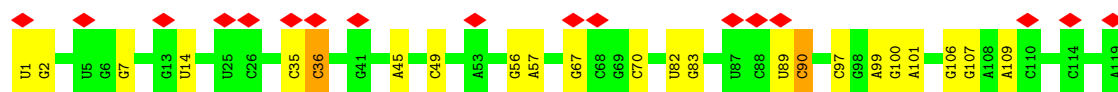
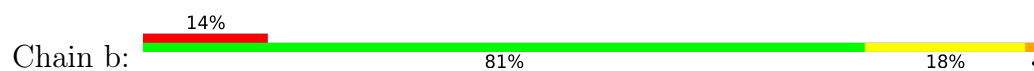
- Molecule 28: 23S ribosomal RNA



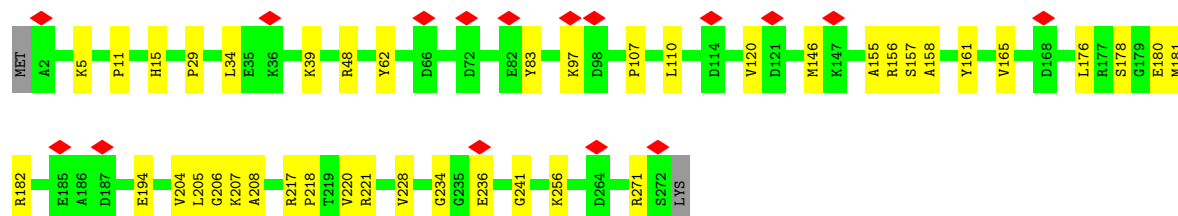
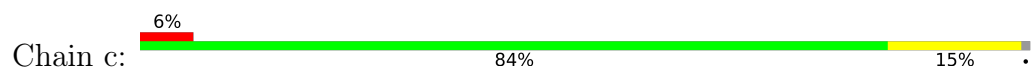




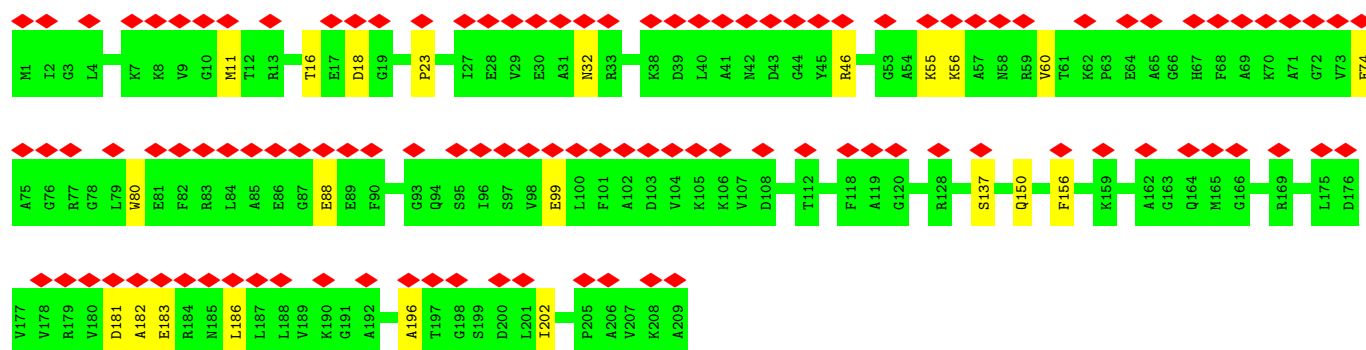
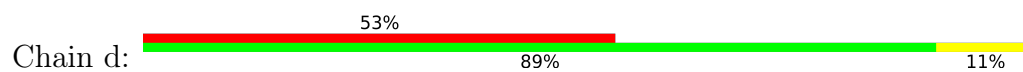
• Molecule 29: 5S ribosomal RNA



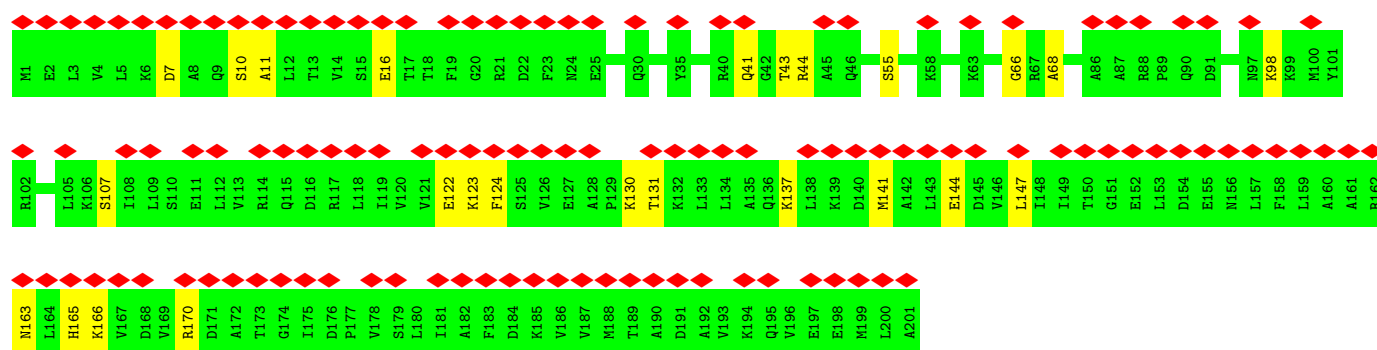
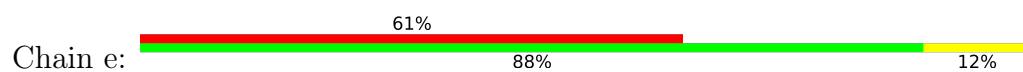
• Molecule 30: 50S ribosomal protein L2



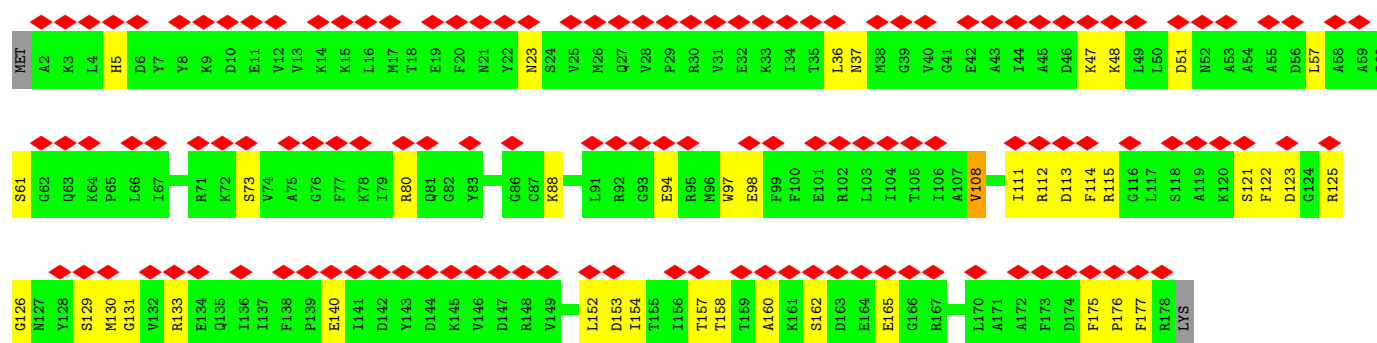
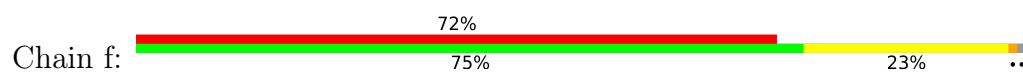
• Molecule 31: Large ribosomal subunit protein uL3



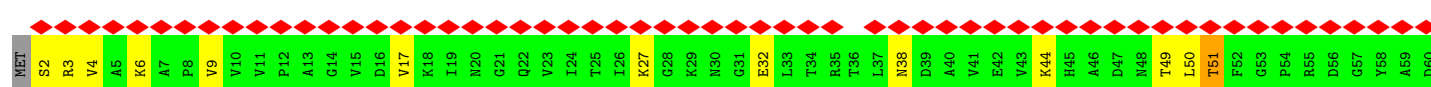
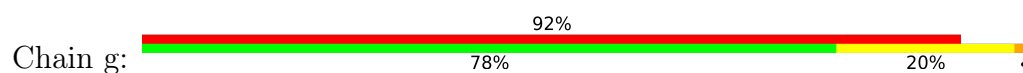
• Molecule 32: 50S ribosomal protein L4



• Molecule 33: 50S ribosomal protein L5

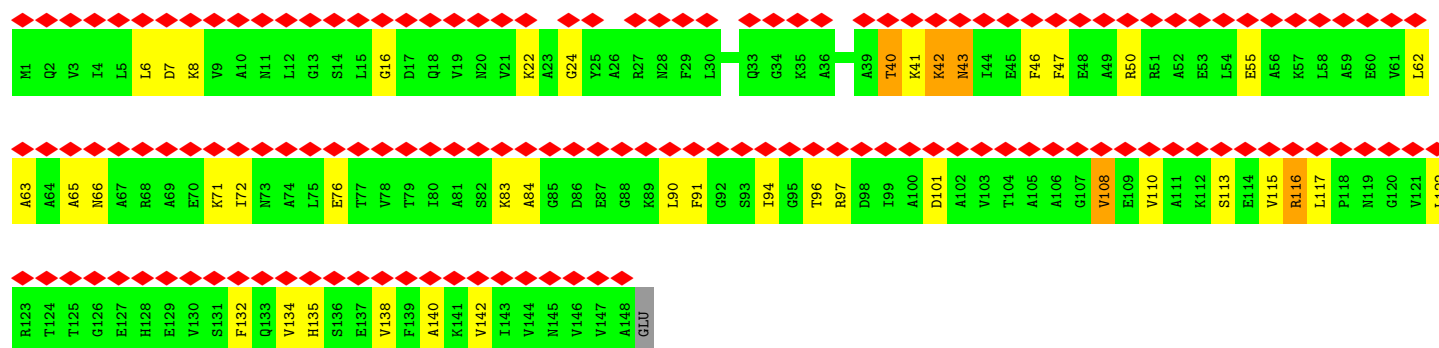


• Molecule 34: 50S ribosomal protein L6

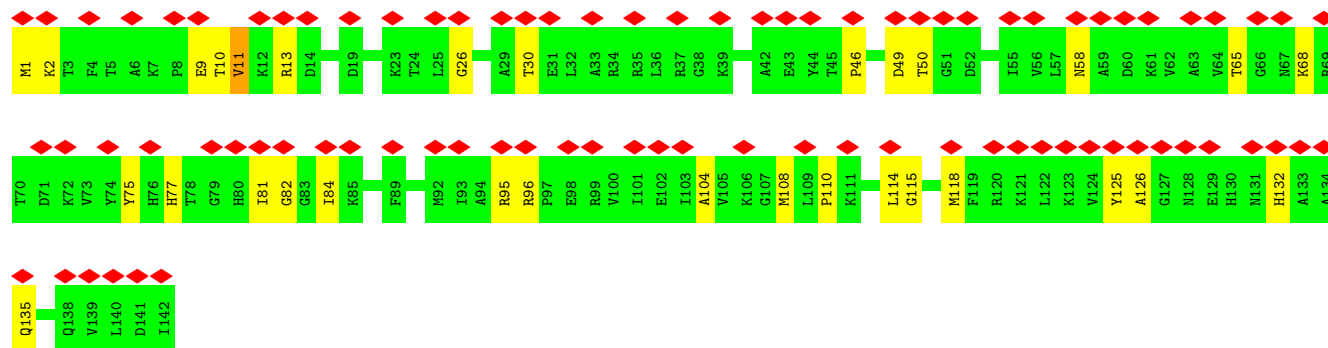
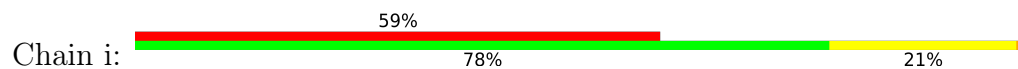




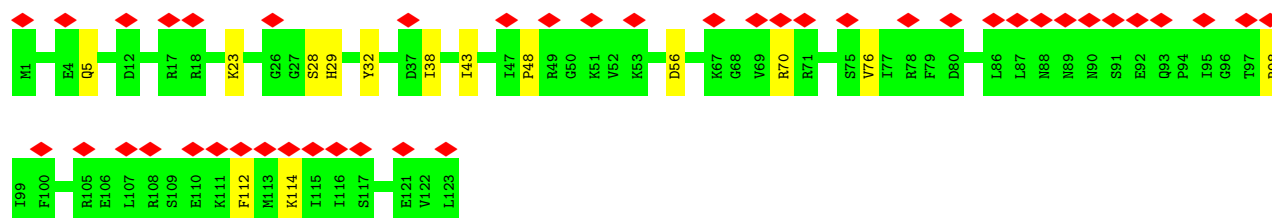
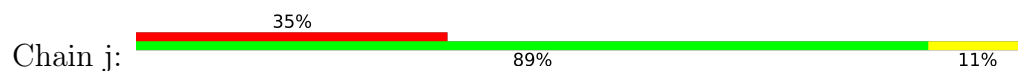
• Molecule 35: 50S ribosomal protein L9



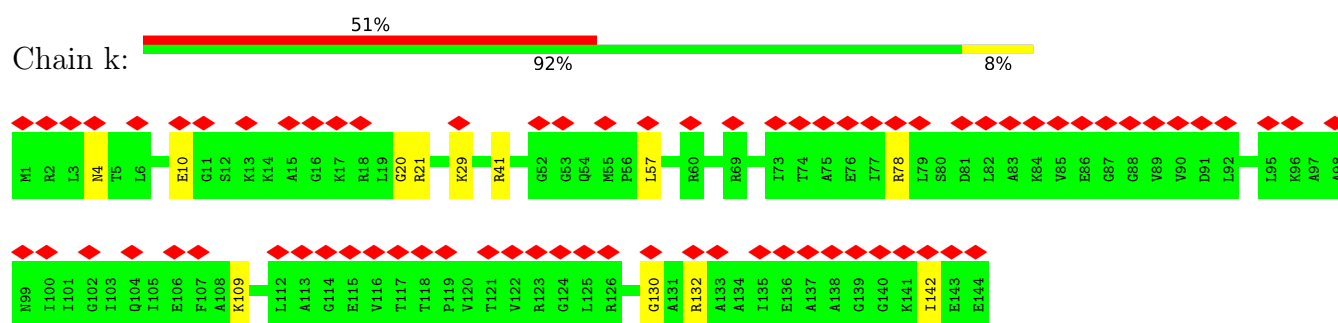
• Molecule 36: 50S ribosomal protein L13



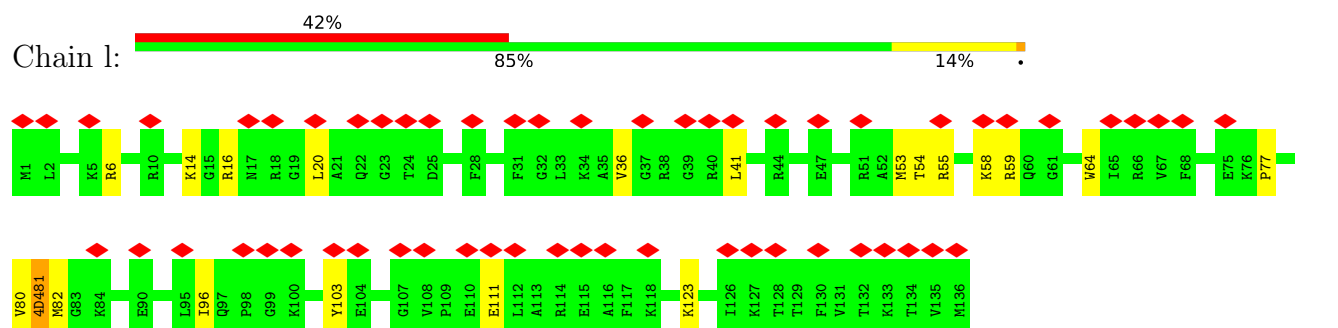
• Molecule 37: 50S ribosomal protein L14



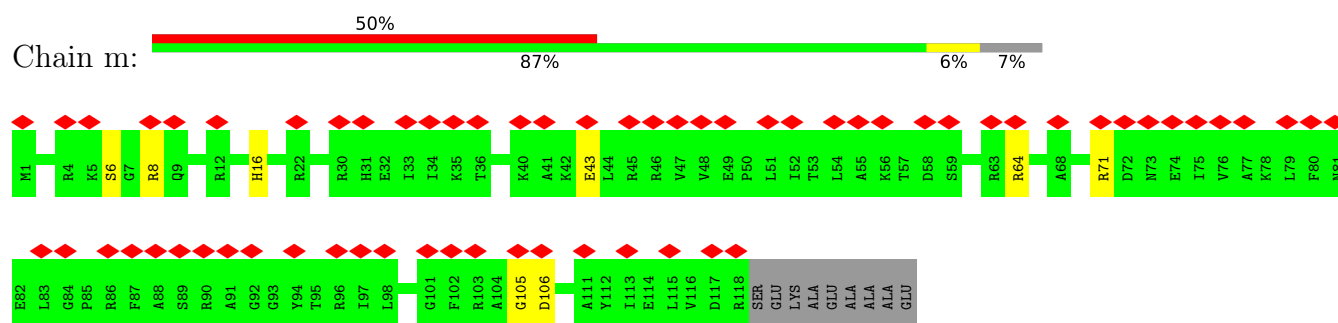
• Molecule 38: 50S ribosomal protein L15



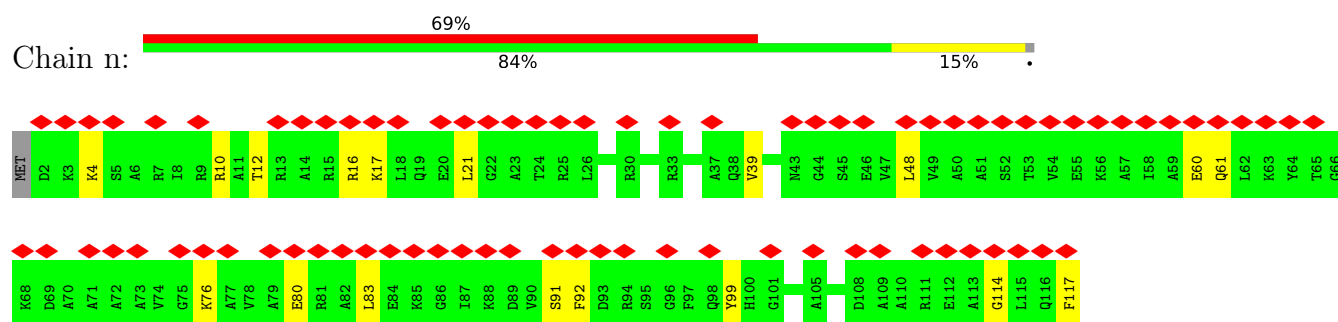
• Molecule 39: 50S ribosomal protein L16



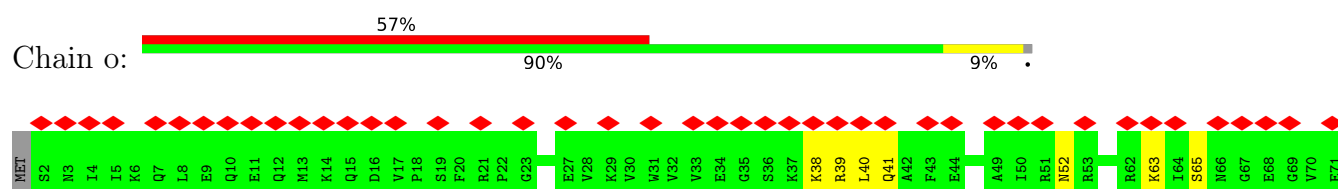
• Molecule 40: 50S ribosomal protein L17

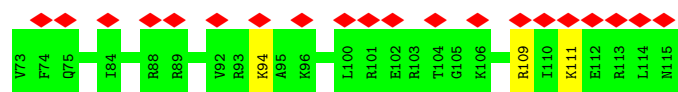


• Molecule 41: 50S ribosomal protein L18

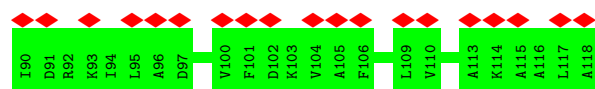
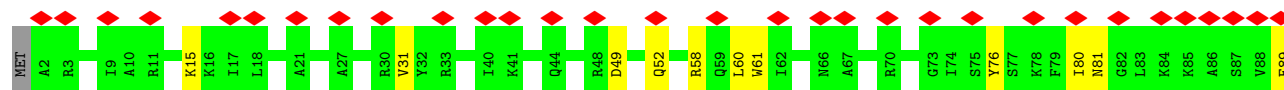
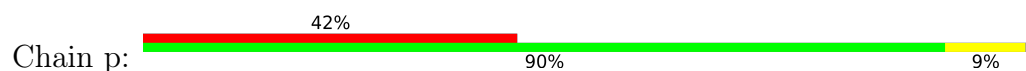


• Molecule 42: 50S ribosomal protein L19

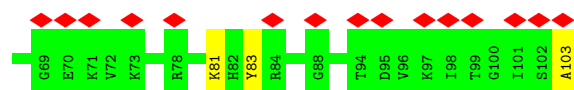
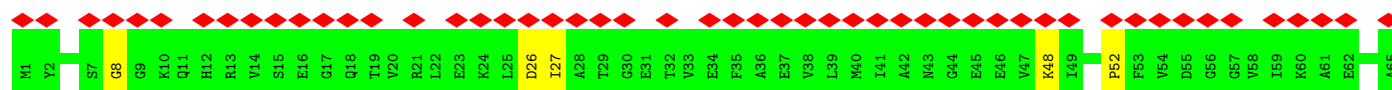
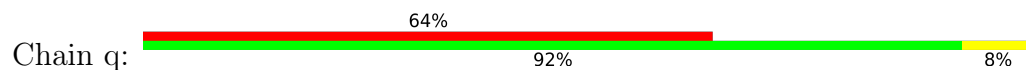




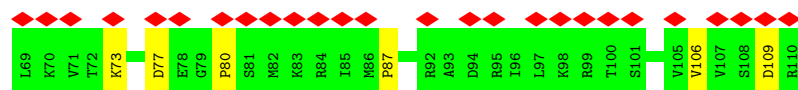
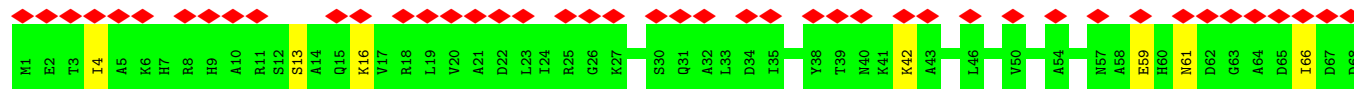
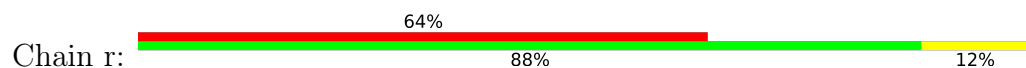
- Molecule 43: 50S ribosomal protein L20



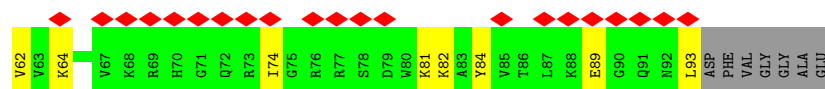
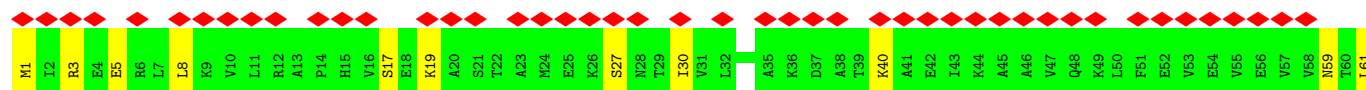
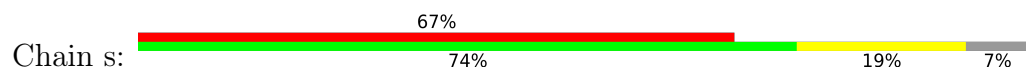
- Molecule 44: 50S ribosomal protein L21



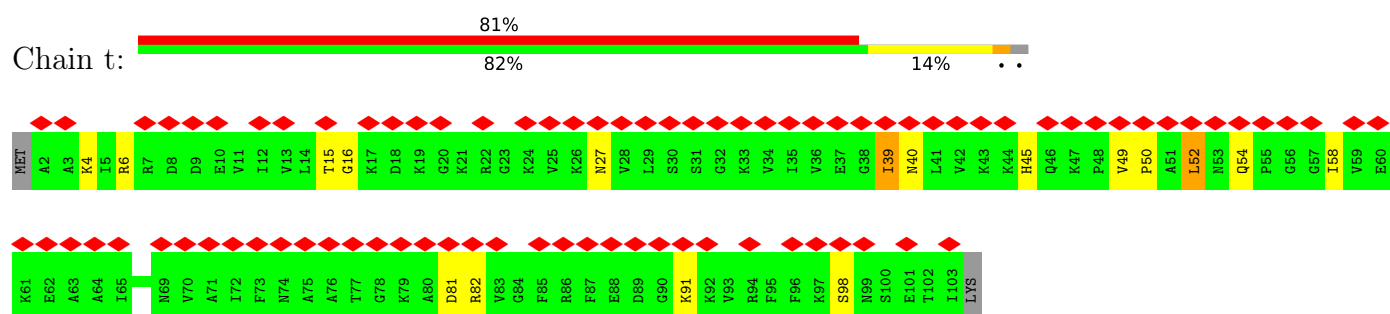
- Molecule 45: 50S ribosomal protein L22



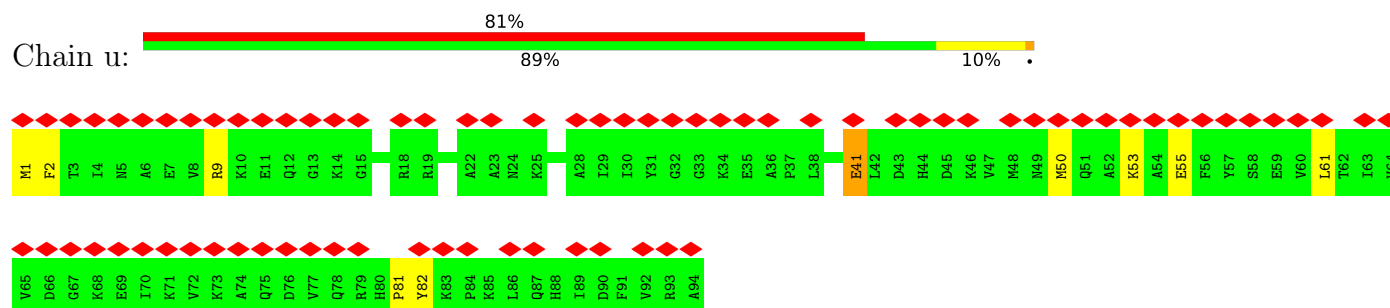
- Molecule 46: 50S ribosomal protein L23



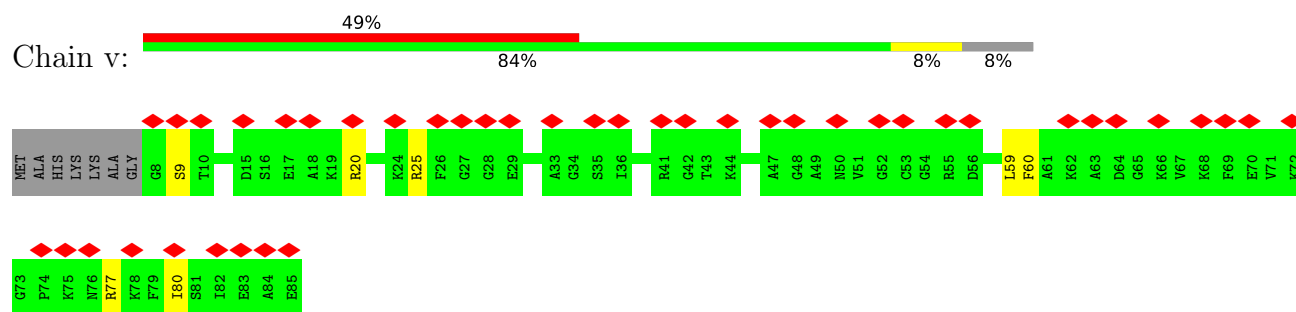
- Molecule 47: 50S ribosomal protein L24



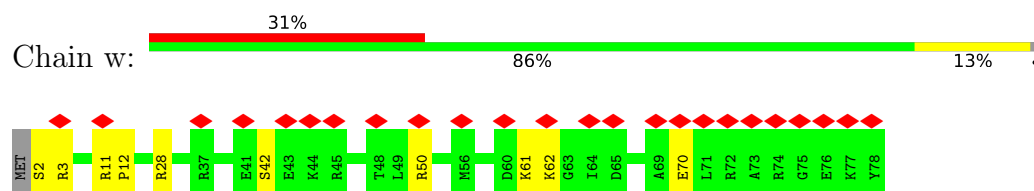
• Molecule 48: 50S ribosomal protein L25



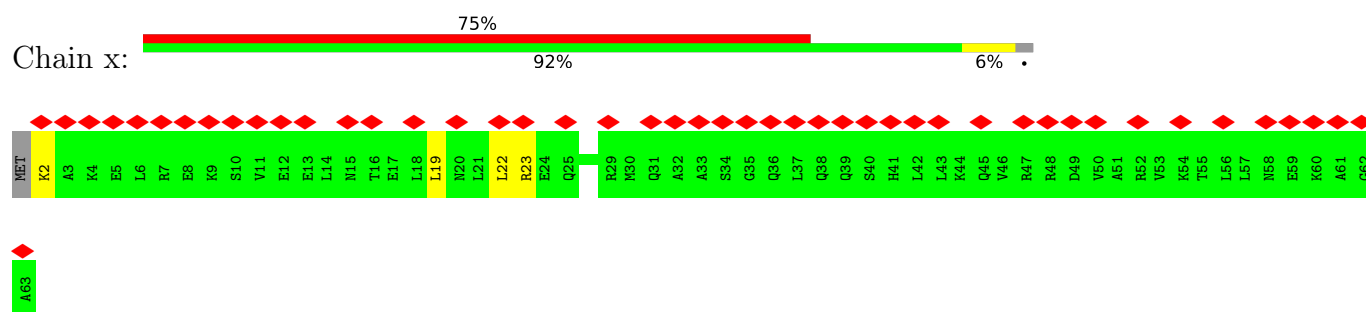
• Molecule 49: 50S ribosomal protein L27



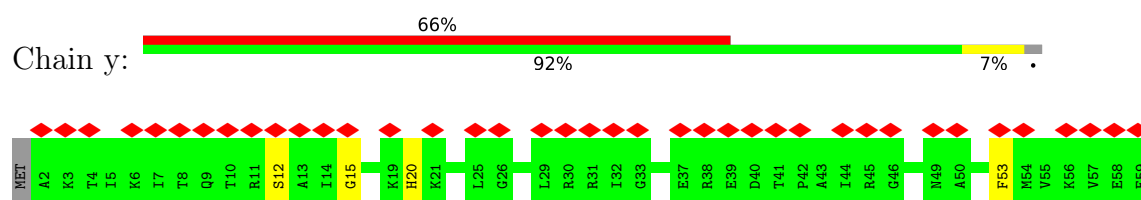
• Molecule 50: 50S ribosomal protein L28



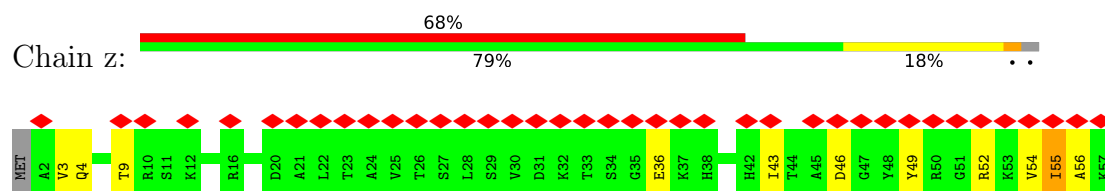
• Molecule 51: 50S ribosomal protein L29



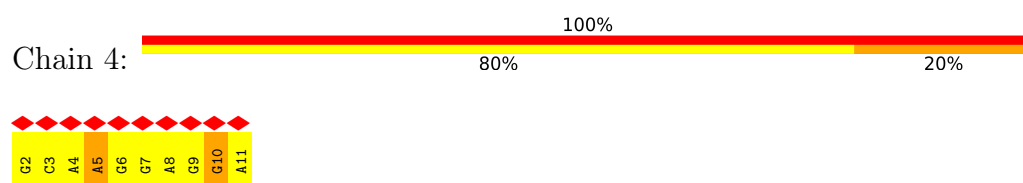
• Molecule 52: 50S ribosomal protein L30



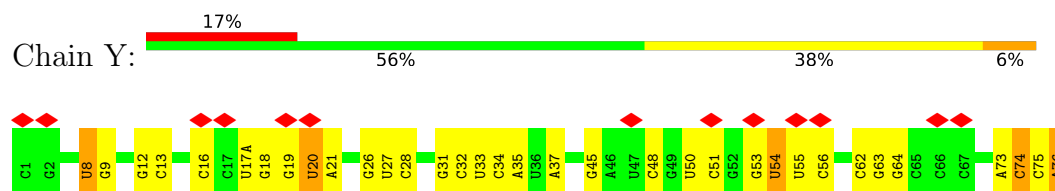
- Molecule 53: 50S ribosomal protein L32



- Molecule 54: mRNA in SD-aSD duplex



- Molecule 55: tRNA(fmet) P-site



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39139	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.147	Depositor
Minimum map value	-0.078	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	673.28, 673.28, 673.28	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D2T, OMC, MEQ, MG, 5MU, UR3, 2MA, OMG, H2U, G7M, PSU, 2MG, ZN, 4SU, 4D4, 1MG, MA6, 7MG, MIA, 6MZ, 4OC, K, OMU, 3AU, 3TD, 5MC

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	0	0.29	0/424	0.37	0/565
2	1	0.38	0/380	0.42	0/498
3	2	0.35	0/513	0.39	0/676
4	3	0.34	0/303	0.36	0/397
5	A	0.29	1/36083 (0.0%)	0.32	7/56274 (0.0%)
6	B	0.20	0/1784	0.33	0/2403
7	C	0.24	0/1651	0.31	0/2225
8	D	0.18	0/1665	0.36	0/2227
9	E	0.30	0/1165	0.34	0/1568
10	F	0.25	0/858	0.32	0/1160
11	G	0.20	0/1219	0.31	0/1635
12	H	0.28	0/989	0.31	0/1326
13	I	0.22	0/1034	0.33	0/1375
14	J	0.26	0/796	0.36	0/1077
15	K	0.27	0/893	0.40	0/1205
16	L	0.27	0/904	0.38	0/1211
17	M	0.19	0/900	0.29	0/1204
18	N	0.23	0/817	0.30	0/1088
19	O	0.25	0/722	0.24	0/964
20	P	0.18	0/653	0.48	0/877
21	Q	0.26	0/650	0.35	0/871
22	R	0.30	0/462	0.36	0/621
23	S	0.20	0/685	0.33	0/922
24	T	0.22	0/676	0.31	0/895
25	U	0.20	0/597	0.26	0/792
26	X	0.33	0/301	0.84	1/465 (0.2%)
27	Z	0.16	0/1584	0.20	0/2463
28	a	0.47	0/65531	0.41	1/102222 (0.0%)
29	b	0.37	0/2850	0.31	0/4444
30	c	0.35	0/2121	0.39	0/2852
31	d	0.35	0/1576	0.39	0/2119

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.33	0/1571	0.37	0/2113
33	f	0.23	0/1434	0.29	0/1926
34	g	0.26	0/1343	0.32	0/1816
35	h	0.27	0/1112	0.40	0/1503
36	i	0.34	0/1152	0.36	0/1551
37	j	0.34	0/955	0.38	0/1279
38	k	0.34	0/1062	0.39	0/1413
39	l	0.34	0/1081	0.39	0/1443
40	m	0.35	0/958	0.42	0/1281
41	n	0.27	0/902	0.34	0/1209
42	o	0.34	0/929	0.35	0/1242
43	p	0.35	0/960	0.38	0/1278
44	q	0.34	0/829	0.37	0/1107
45	r	0.34	0/864	0.36	0/1156
46	s	0.31	0/744	0.35	0/994
47	t	0.29	0/787	0.32	0/1051
48	u	0.31	0/766	0.34	0/1025
49	v	0.33	0/593	0.35	0/785
50	w	0.34	0/635	0.37	0/848
51	x	0.28	0/502	0.26	0/667
52	y	0.32	0/453	0.32	0/605
53	z	0.35	0/450	0.42	0/599
54	4	0.13	0/251	0.23	0/391
55	Y	0.18	0/1725	0.27	0/2687
All	All	0.38	1/152844 (0.0%)	0.37	9/228590 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1407	5MC	O3'-P	16.30	1.85	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1495	U	P-O3'-C3'	11.69	137.74	120.20
5	A	1495	U	OP2-P-O3'	-11.53	73.40	108.00
5	A	1407	5MC	O3'-P-O5'	10.72	120.08	104.00
26	X	21	C	O3'-P-O5'	-9.80	89.30	104.00
5	A	1495	U	O3'-P-O5'	8.59	116.88	104.00
28	a	2433	G	P-O3'-C3'	-6.88	109.88	120.20
5	A	1495	U	OP1-P-O3'	6.22	126.66	108.00
5	A	1407	5MC	P-O3'-C3'	-6.09	111.06	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1407	5MC	OP1-P-O3'	-5.68	90.95	108.00

There are no chirality outliers.

There are no planarity outliers.

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	0	417	0	451	6	0
2	1	377	0	417	5	0
3	2	504	0	572	10	0
4	3	302	0	340	10	0
5	A	32478	0	16356	766	0
6	B	1753	0	1780	23	0
7	C	1624	0	1696	31	0
8	D	1643	0	1707	116	0
9	E	1152	0	1196	41	0
10	F	839	0	833	21	0
11	G	1203	0	1254	31	0
12	H	979	0	1031	25	0
13	I	1022	0	1070	35	0
14	J	786	0	828	36	0
15	K	877	0	887	20	0
16	L	902	0	952	22	0
17	M	891	0	952	78	0
18	N	805	0	844	40	0
19	O	714	0	734	35	0
20	P	643	0	661	42	0
21	Q	641	0	682	14	0
22	R	455	0	478	12	0
23	S	668	0	693	43	0
24	T	670	0	719	31	0
25	U	589	0	629	3	0
26	X	271	0	139	20	0
27	Z	1624	0	823	56	0
28	a	59025	0	29690	579	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	b	2549	0	1291	14	0
30	c	2082	0	2153	56	0
31	d	1566	0	1618	16	0
32	e	1552	0	1619	18	0
33	f	1410	0	1444	101	0
34	g	1323	0	1370	57	0
35	h	1101	0	1142	32	0
36	i	1129	0	1162	45	0
37	j	946	0	1023	17	0
38	k	1053	0	1129	13	0
39	l	1075	0	1154	24	0
40	m	945	0	989	6	0
41	n	892	0	923	36	0
42	o	917	0	962	13	0
43	p	947	0	1019	8	0
44	q	816	0	839	6	0
45	r	857	0	922	12	0
46	s	738	0	807	23	0
47	t	779	0	831	26	0
48	u	753	0	780	7	0
49	v	586	0	596	10	0
50	w	625	0	652	9	0
51	x	501	0	531	4	0
52	y	449	0	488	6	0
53	z	444	0	458	9	0
54	4	223	0	108	39	0
55	Y	1645	0	842	47	0
56	3	1	0	0	0	0
57	A	48	0	0	0	0
57	a	112	0	0	0	0
57	b	1	0	0	0	0
57	c	4	0	0	0	0
57	d	1	0	0	0	0
57	e	1	0	0	0	0
57	f	1	0	0	0	0
58	A	95	0	0	0	0
58	N	1	0	0	0	0
58	Y	1	0	0	0	0
58	a	254	0	0	0	0
58	b	5	0	0	0	0
58	c	1	0	0	0	0
58	d	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	k	1	0	0	0	0
58	z	1	0	0	0	0
59	a	11	0	8	2	0
All	All	142297	0	95274	1844	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 8.

All (1844) 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)
17:M:71:ARG:NH1	33:f:115:ARG:HD2	1.24	1.41
5:A:1532:U:C4	5:A:1533:C:N4	1.90	1.39
17:M:71:ARG:CZ	33:f:115:ARG:HD2	1.57	1.35
27:Z:74:C:N4	28:a:2511:C:O2'	1.59	1.34
5:A:1054:C:N4	27:Z:34:G:C8	2.03	1.25
28:a:2309:U:O4'	33:f:131:GLY:HA3	1.37	1.25
19:O:88:ARG:NH2	28:a:716:U:OP2	1.69	1.24
17:M:67:GLY:HA3	33:f:113:ASP:OD1	1.37	1.21
5:A:262:A:H4'	24:T:70:ASN:CB	1.75	1.16
28:a:483:A:C8	47:t:45:HIS:HD2	1.67	1.13
5:A:1496:C:H4'	28:a:1924:C:O2'	1.46	1.13
13:I:129:LYS:NZ	55:Y:34:C:OP2	1.82	1.13
19:O:63:ARG:NH2	28:a:717:A:H4'	1.62	1.13
17:M:71:ARG:NH1	33:f:115:ARG:CD	2.11	1.12
28:a:2307:G:O4'	33:f:123:ASP:HA	1.49	1.11
27:Z:76:A:O2'	28:a:2510:U:H1'	1.50	1.11
5:A:1381:U:O3'	54:4:2:G:C1'	1.94	1.08
7:C:162:ILE:HD12	26:X:24:A:H4'	1.33	1.08
5:A:19:A:N1	5:A:917:G:C6	2.21	1.08
5:A:1537:U:C4	54:4:10:G:H5''	1.88	1.07
28:a:2308:G:H4'	33:f:129:SER:O	1.52	1.07
5:A:545:C:H5'	8:D:69:GLU:HG3	1.37	1.06
28:a:2307:G:H4'	33:f:122:PHE:O	1.56	1.05
5:A:1381:U:O2'	54:4:2:G:C1'	1.99	1.05
5:A:1381:U:H5''	54:4:3:C:H1'	1.38	1.04
19:O:56:LEU:HD21	28:a:717:A:C2	1.91	1.04
5:A:1400:C:C4	55:Y:34:C:C2	2.44	1.04
17:M:7:ILE:HG22	33:f:112:ARG:NH1	1.71	1.03
28:a:2533:G:OP1	34:g:172:LYS:NZ	1.90	1.03
5:A:508:U:H4'	8:D:51:TYR:CD2	1.93	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:911:U:OP2	16:L:94:ARG:NH2	1.92	1.03
5:A:1492:A:H5''	16:L:44:LYS:CG	1.87	1.03
5:A:1382:C:OP1	54:4:2:G:O2'	1.75	1.03
28:a:2309:U:H5	33:f:153:ASP:CG	1.67	1.03
5:A:1381:U:O3'	54:4:2:G:H1'	1.59	1.02
5:A:1492:A:H5''	16:L:44:LYS:HG3	1.38	1.02
28:a:483:A:C8	47:t:45:HIS:CD2	2.47	1.02
5:A:345:C:OP1	42:o:39:ARG:NE	1.93	1.01
5:A:1318:A:H5''	23:S:3:ARG:NH1	1.74	1.01
5:A:1381:U:O3'	54:4:2:G:C2'	2.09	1.01
17:M:71:ARG:NH2	33:f:115:ARG:HH11	1.59	1.00
5:A:323:U:H5''	24:T:21:ASN:ND2	1.76	1.00
5:A:545:C:H5'	8:D:69:GLU:CG	1.91	1.00
28:a:2309:U:C6	33:f:153:ASP:OD1	2.15	0.99
5:A:19:A:C6	5:A:917:G:C6	2.50	0.99
5:A:262:A:C4'	24:T:70:ASN:HB2	1.92	0.98
5:A:545:C:C5'	8:D:69:GLU:HG3	1.94	0.97
5:A:1532:U:N3	5:A:1533:C:N4	2.12	0.97
19:O:60:VAL:HG21	28:a:717:A:C8	1.98	0.97
17:M:71:ARG:NE	33:f:115:ARG:NH1	2.13	0.97
28:a:2307:G:C4'	33:f:122:PHE:O	2.13	0.96
5:A:8:A:H61	8:D:202:GLU:HB3	1.29	0.96
27:Z:76:A:C2	28:a:2587:G:N3	2.34	0.96
5:A:1060:U:H4'	14:J:53:ILE:HG13	1.45	0.96
17:M:71:ARG:CZ	33:f:115:ARG:CD	2.41	0.96
5:A:1359:C:OP2	18:N:75:ARG:NE	1.98	0.95
28:a:2663:G:P	34:g:158:LYS:NZ	2.40	0.95
5:A:1484:C:O2'	28:a:1965:C:H5'	1.66	0.94
28:a:2307:G:C1'	33:f:123:ASP:HA	1.96	0.94
28:a:731:G:C6	30:c:207:LYS:HB2	2.03	0.94
5:A:19:A:C6	5:A:917:G:N1	2.36	0.94
5:A:1496:C:H4'	28:a:1924:C:HO2'	1.28	0.94
5:A:546:A:OP1	8:D:70:ARG:N	2.01	0.93
5:A:1054:C:C4	27:Z:34:G:O4'	2.20	0.93
5:A:262:A:H4'	24:T:70:ASN:HB2	0.97	0.93
5:A:1054:C:N3	27:Z:34:G:O4'	2.00	0.93
5:A:1492:A:H4'	16:L:44:LYS:NZ	1.85	0.92
17:M:71:ARG:CZ	33:f:115:ARG:NH1	2.32	0.92
5:A:626:G:H4'	20:P:38:PHE:CZ	2.05	0.92
5:A:1054:C:N3	27:Z:34:G:C1'	2.32	0.92
5:A:19:A:C2	5:A:917:G:C2	2.58	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1227:A:O2'	17:M:114:LYS:HG3	1.70	0.92
28:a:1140:G:N3	36:i:108:MET:HE2	1.85	0.92
5:A:1381:U:O2'	54:4:2:G:H1'	1.71	0.91
19:O:63:ARG:HH22	28:a:717:A:H4'	1.30	0.91
5:A:1537:U:C4	54:4:10:G:C5'	2.51	0.91
28:a:483:A:C4	47:t:58:ILE:HD11	2.04	0.91
28:a:2309:U:C5	33:f:153:ASP:CG	2.48	0.91
5:A:1408:A:O2'	28:a:1920:A:N1	2.03	0.91
5:A:9:G:H5'	9:E:108:GLY:HA3	1.53	0.91
5:A:262:A:O2'	24:T:70:ASN:ND2	2.03	0.91
28:a:2755:G:H4'	34:g:4:VAL:HG23	1.52	0.91
5:A:1151:A:O4'	14:J:41:PRO:HB2	1.71	0.90
5:A:880:C:OP1	16:L:9:ARG:NH2	2.04	0.90
5:A:1014:A:H4'	23:S:14:HIS:CD2	2.06	0.90
5:A:1014:A:H4'	23:S:14:HIS:CG	2.07	0.90
28:a:2308:G:O4'	33:f:129:SER:HB2	1.70	0.90
5:A:1328:C:H5''	17:M:28:THR:HG21	1.52	0.89
5:A:18:C:OP1	9:E:132:ASN:ND2	2.06	0.88
5:A:955:U:HO2'	23:S:83:HIS:HD1	1.14	0.88
17:M:7:ILE:HG22	33:f:112:ARG:HH12	1.38	0.88
28:a:2309:U:C5	33:f:153:ASP:OD1	2.27	0.88
17:M:71:ARG:NE	33:f:115:ARG:CZ	2.36	0.88
19:O:88:ARG:NH1	28:a:716:U:C5	2.41	0.88
19:O:88:ARG:HH22	28:a:716:U:P	1.97	0.87
27:Z:26:A:H61	27:Z:44:G:H1	1.17	0.87
5:A:1381:U:C5'	54:4:3:C:H1'	2.04	0.87
28:a:1794:G:H5'	30:c:204:VAL:HG13	1.56	0.87
28:a:2068:C:OP1	55:Y:75:C:O2'	1.92	0.87
5:A:521:G:O5'	16:L:70:GLU:HG2	1.73	0.87
17:M:71:ARG:CZ	33:f:115:ARG:HH11	1.88	0.86
28:a:2534:A:N6	34:g:156:PRO:HG3	1.90	0.86
5:A:407:U:O2'	8:D:113:GLU:OE1	1.92	0.86
5:A:508:U:H4'	8:D:51:TYR:CE2	2.10	0.86
28:a:2663:G:OP2	34:g:158:LYS:NZ	2.08	0.86
28:a:2455:A:C2	59:a:3001:PHE:N	2.45	0.85
35:h:46:PHE:CZ	35:h:50:ARG:HD3	2.12	0.84
28:a:2309:U:H6	33:f:153:ASP:OD1	1.58	0.84
28:a:2670:C:H42	34:g:109:PHE:HA	1.41	0.84
5:A:1100:C:OP2	6:B:95:ARG:HD3	1.77	0.84
28:a:2380:A:C8	41:n:99:TYR:CD2	2.66	0.84
5:A:642:A:C8	12:H:107:SER:HA	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2307:G:O3'	33:f:121:SER:HA	1.77	0.84
5:A:1318:A:H5''	23:S:3:ARG:HH12	1.42	0.84
19:O:88:ARG:CZ	28:a:716:U:C5	2.61	0.83
5:A:1014:A:H4'	23:S:14:HIS:CE1	2.13	0.83
17:M:83:LEU:HD22	23:S:74:PHE:HE1	1.42	0.83
28:a:2663:G:P	34:g:158:LYS:HZ2	1.97	0.83
5:A:512:U:OP1	8:D:44:ARG:NH2	2.11	0.83
5:A:323:U:OP1	24:T:25:ARG:NH2	2.10	0.83
5:A:1400:C:C5	55:Y:34:C:N3	2.46	0.82
17:M:83:LEU:HD22	23:S:74:PHE:CE1	2.15	0.82
19:O:88:ARG:NH1	28:a:716:U:C6	2.47	0.82
28:a:813:U:H2'	38:k:21:ARG:HA	1.60	0.82
17:M:71:ARG:HH12	33:f:115:ARG:HD2	1.43	0.82
22:R:36:SER:HA	22:R:72:ASP:HB3	1.59	0.82
5:A:1532:U:O4	5:A:1533:C:N4	2.13	0.82
28:a:483:A:O4'	47:t:45:HIS:HB3	1.79	0.82
28:a:2259:G:H21	49:v:9:SER:HB3	1.43	0.82
5:A:1057:G:O2'	7:C:188:GLU:OE2	1.98	0.82
28:a:2309:U:C4'	33:f:131:GLY:HA3	2.09	0.82
5:A:642:A:N7	12:H:107:SER:HA	1.93	0.81
28:a:2309:U:O4'	33:f:131:GLY:CA	2.23	0.81
5:A:107:G:O6	24:T:10:ARG:NE	2.10	0.81
5:A:19:A:N6	5:A:917:G:O6	2.14	0.81
5:A:613:C:OP1	8:D:81:ARG:NH1	2.14	0.81
28:a:2024:A:H5'	53:z:9:THR:CG2	2.10	0.81
5:A:521:G:OP1	16:L:70:GLU:HA	1.81	0.80
28:a:2671:C:HO2'	34:g:111:HIS:HE2	1.02	0.80
5:A:263:A:P	24:T:74:ARG:HE	2.04	0.80
9:E:164:ILE:O	12:H:114:ARG:NH2	2.15	0.80
5:A:823:C:HO2'	12:H:2:SER:N	1.79	0.80
28:a:2488:G:O2'	39:l:123:LYS:O	1.98	0.79
28:a:2455:A:N3	59:a:3001:PHE:N	2.30	0.79
5:A:664:G:H22	5:A:741:G:H1	1.30	0.79
5:A:1538:C:N4	54:4:10:G:P	2.55	0.79
2:1:26:ASN:ND2	28:a:684:G:H5'	1.97	0.79
5:A:358:U:H2'	5:A:359:G:H8	1.48	0.79
33:f:158:THR:HG22	33:f:160:ALA:H	1.46	0.79
5:A:441:A:H61	5:A:493:A:H61	1.31	0.79
27:Z:76:A:O2'	28:a:2510:U:C1'	2.31	0.79
26:X:16:A:N6	55:Y:37:A:N1	2.31	0.79
5:A:1492:A:H5''	16:L:44:LYS:HG2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2308:G:H1'	33:f:129:SER:HB3	1.65	0.78
5:A:1537:U:C5	54:4:10:G:H5''	2.18	0.78
19:O:88:ARG:CZ	28:a:716:U:H5	1.96	0.78
5:A:1536:C:H5	54:4:10:G:N3	1.81	0.78
5:A:1233:G:OP1	13:I:119:ARG:NH1	2.15	0.78
28:a:2308:G:H5''	33:f:121:SER:OG	1.84	0.78
5:A:1054:C:N4	27:Z:34:G:N9	2.32	0.78
5:A:310:G:H5''	20:P:31:ARG:HB2	1.63	0.77
17:M:67:GLY:HA3	33:f:113:ASP:CG	2.10	0.77
5:A:18:C:P	9:E:132:ASN:HD21	2.07	0.77
5:A:339:C:OP2	37:j:98:ARG:NE	2.18	0.77
5:A:1328:C:H5''	17:M:28:THR:CG2	2.14	0.77
5:A:17:U:O2'	5:A:1079:G:H1'	1.83	0.77
5:A:1014:A:H5''	23:S:14:HIS:HB2	1.66	0.77
27:Z:56:C:OP2	39:l:59:ARG:NH1	2.18	0.77
5:A:8:A:N6	8:D:202:GLU:HB3	2.00	0.77
19:O:63:ARG:NH2	28:a:717:A:C4'	2.47	0.77
11:G:133:THR:HG22	11:G:134:ALA:H	1.50	0.76
27:Z:76:A:H2	28:a:2587:G:N3	1.77	0.76
5:A:8:A:H61	8:D:202:GLU:CB	1.99	0.76
26:X:18:G:N1	55:Y:35:A:C6	2.54	0.76
5:A:323:U:H5''	24:T:21:ASN:HD22	1.50	0.76
5:A:1517:G:C2	28:a:1924:C:H5'	2.21	0.76
9:E:101:GLU:OE1	9:E:101:GLU:N	2.17	0.76
28:a:1133:G:O4'	36:i:77:HIS:HD2	1.68	0.76
5:A:228:A:N3	20:P:1:MET:HE1	2.01	0.76
5:A:263:A:OP1	24:T:74:ARG:CD	2.34	0.76
5:A:8:A:N6	8:D:202:GLU:OE1	2.19	0.75
5:A:1492:A:H4'	16:L:44:LYS:HZ2	1.48	0.75
28:a:2316:U:O2'	33:f:37:ASN:ND2	2.19	0.75
5:A:1054:C:N3	27:Z:34:G:H1'	2.00	0.75
7:C:168:TYR:OH	9:E:55:GLU:CD	2.29	0.75
14:J:47:GLU:OE1	18:N:76:LYS:NZ	2.17	0.75
5:A:402:G:O3'	8:D:132:ILE:HD11	1.86	0.75
5:A:1400:C:C5	55:Y:34:C:C2	2.75	0.75
5:A:1409:C:H4'	28:a:1919:3TD:C10	2.16	0.75
17:M:85:CYS:HA	23:S:73:GLU:O	1.87	0.75
28:a:1651:G:O2'	40:m:106:ASP:OD2	2.05	0.75
5:A:1400:C:C5	55:Y:34:C:C4	2.74	0.74
28:a:2097:G:OP2	35:h:22:LYS:HD3	1.86	0.74
28:a:2671:C:O2	34:g:111:HIS:CD2	2.40	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2381:A:H4'	41:n:117:PHE:O	1.87	0.74
5:A:19:A:N1	5:A:917:G:N1	2.35	0.74
5:A:454:G:H2'	5:A:455:G:H8	1.53	0.74
5:A:1049:U:OP1	18:N:3:LYS:HG2	1.87	0.74
5:A:1409:C:C5'	28:a:1919:3TD:H10	2.18	0.74
28:a:1140:G:C2	36:i:108:MET:HE2	2.23	0.74
28:a:2307:G:O2'	33:f:121:SER:C	2.30	0.74
30:c:120:VAL:HB	35:h:91:PHE:HB3	1.70	0.74
28:a:284:U:H3	28:a:356:G:H1	1.36	0.73
5:A:784:A:H4'	28:a:1839:C:OP1	1.89	0.73
29:b:7:G:OP1	41:n:4:LYS:NZ	2.20	0.73
5:A:1496:C:O2'	28:a:1924:C:H4'	1.89	0.73
19:O:63:ARG:HH21	28:a:717:A:H4'	1.51	0.73
28:a:2307:G:H1'	33:f:123:ASP:CA	2.19	0.73
5:A:702:A:C6	28:a:1850:A:C6	2.77	0.73
5:A:1409:C:H4'	28:a:1919:3TD:H10A	1.71	0.73
28:a:335:C:H5''	47:t:82:ARG:HD3	1.71	0.73
28:a:2308:G:H5'	33:f:121:SER:HB3	1.71	0.73
28:a:2380:A:C4	41:n:99:TYR:CE1	2.76	0.73
5:A:19:A:N1	5:A:917:G:C5	2.56	0.72
28:a:2671:C:C2'	34:g:111:HIS:HE2	2.01	0.72
5:A:8:A:C2	9:E:112:ARG:NH2	2.58	0.72
5:A:1228:C:P	17:M:114:LYS:HZ3	2.11	0.72
28:a:1616:A:C6	45:r:87:PRO:HB3	2.24	0.72
5:A:545:C:P	8:D:69:GLU:HG3	2.29	0.72
28:a:2773:U:P	36:i:95:ARG:HH12	2.12	0.72
5:A:1054:C:C4	27:Z:34:G:C8	2.77	0.72
26:X:18:G:C2	55:Y:35:A:C2	2.77	0.72
28:a:1794:G:C5'	30:c:204:VAL:HG13	2.20	0.72
28:a:2096:U:H5''	35:h:24:GLY:HA3	1.71	0.72
5:A:825:A:O2'	12:H:9:ASP:OD1	2.04	0.72
5:A:909:A:O2'	5:A:1413:A:O2'	2.04	0.72
7:C:168:TYR:HH	9:E:55:GLU:CD	1.98	0.72
35:h:84:ALA:HB2	35:h:90:LEU:HD23	1.71	0.71
5:A:518:C:O2'	5:A:1492:A:N6	2.23	0.71
5:A:492:C:H2'	5:A:493:A:H8	1.54	0.71
8:D:68:LEU:O	8:D:72:PHE:HB2	1.90	0.71
26:X:16:A:C6	55:Y:37:A:C2	2.79	0.71
5:A:390:U:H4'	20:P:28:ARG:HH12	1.56	0.71
5:A:1226:C:OP1	17:M:90:ARG:NH2	2.23	0.71
19:O:40:GLN:OE1	28:a:718:A:H1'	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:56:C:H5''	39:l:59:ARG:HH12	1.55	0.71
28:a:2761:A:N1	34:g:67:THR:HG21	2.06	0.71
7:C:131:ARG:HH11	9:E:55:GLU:CD	1.99	0.71
17:M:71:ARG:NH2	33:f:115:ARG:NH1	2.35	0.71
5:A:1330:U:H4'	17:M:23:TYR:CE1	2.26	0.71
9:E:65:GLU:OE1	9:E:69:ARG:NH2	2.24	0.71
11:G:37:SER:HB3	13:I:41:ARG:HD3	1.72	0.70
15:K:72:ASP:OD1	15:K:75:LYS:NZ	2.25	0.70
28:a:2307:G:C1'	33:f:123:ASP:CA	2.68	0.70
28:a:2663:G:P	34:g:158:LYS:HZ3	2.07	0.70
32:e:10:SER:OG	32:e:11:ALA:N	2.22	0.70
33:f:73:SER:HB2	55:Y:56:C:O4'	1.92	0.70
5:A:784:A:C5'	28:a:1839:C:OP1	2.39	0.70
5:A:1233:G:P	13:I:119:ARG:HH12	2.14	0.70
5:A:1492:A:H4'	16:L:44:LYS:HZ3	1.56	0.70
28:a:2671:C:O2	34:g:111:HIS:HD2	1.74	0.70
34:g:86:LYS:HG2	34:g:132:VAL:HG22	1.73	0.70
5:A:401:C:O2'	5:A:621:A:N3	2.22	0.70
28:a:2320:G:O2'	33:f:125:ARG:NH2	2.25	0.70
7:C:168:TYR:OH	9:E:55:GLU:OE2	2.10	0.70
5:A:1400:C:C6	55:Y:34:C:N3	2.60	0.69
5:A:17:U:HO2'	5:A:1079:G:C2'	2.04	0.69
20:P:19:VAL:HG13	20:P:36:VAL:HG23	1.74	0.69
14:J:88:MET:N	14:J:88:MET:SD	2.65	0.69
28:a:1724:A:N6	28:a:1740:G:O2'	2.25	0.69
28:a:2533:G:H4'	34:g:175:LYS:HB3	1.73	0.69
5:A:259:G:P	24:T:82:GLN:HE22	2.16	0.69
5:A:1123:U:O2'	14:J:38:GLY:HA2	1.93	0.69
5:A:545:C:O5'	8:D:69:GLU:HG3	1.92	0.69
5:A:616:G:HO2'	20:P:47:GLU:CD	2.01	0.69
5:A:1382:C:P	54:4:2:G:O2'	2.51	0.69
17:M:71:ARG:HE	33:f:115:ARG:NH1	1.88	0.69
14:J:7:ARG:HB2	14:J:101:SER:HB3	1.72	0.69
5:A:229:U:O2'	20:P:23:ASP:OD2	2.11	0.69
28:a:2308:G:H1'	33:f:129:SER:CB	2.23	0.69
5:A:702:A:N6	28:a:1850:A:C6	2.60	0.69
5:A:1054:C:C2	27:Z:34:G:O4'	2.45	0.69
5:A:1517:G:C4	28:a:1924:C:OP1	2.46	0.69
28:a:1140:G:O2'	36:i:104:ALA:O	2.11	0.69
28:a:2473:A:H4'	39:l:55:ARG:CD	2.22	0.69
46:s:3:ARG:NH1	46:s:5:GLU:OE1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:619:U:O2	8:D:130:VAL:HA	1.93	0.69
28:a:1133:G:O4'	36:i:77:HIS:CD2	2.46	0.69
5:A:930:C:P	54:4:4:A:H5''	2.31	0.68
5:A:1381:U:H5'	54:4:3:C:O2	1.92	0.68
5:A:454:G:H2'	5:A:455:G:C8	2.28	0.68
33:f:80:ARG:NH2	55:Y:56:C:C4	2.61	0.68
5:A:1060:U:O2'	14:J:54:SER:HB2	1.92	0.68
5:A:1517:G:N9	28:a:1924:C:OP1	2.26	0.68
20:P:5:ARG:HH12	20:P:22:ALA:HB3	1.58	0.68
44:q:48:LYS:HE2	44:q:103:ALA:HB1	1.74	0.68
5:A:263:A:OP1	24:T:74:ARG:HD3	1.91	0.68
28:a:2382:A:O2'	41:n:91:SER:OG	2.04	0.68
5:A:684:U:O2'	15:K:40:ASN:HB3	1.93	0.68
5:A:403:C:H5'	8:D:132:ILE:HG13	1.76	0.68
5:A:1371:G:O3'	13:I:71:GLY:HA3	1.94	0.68
17:M:7:ILE:HG22	33:f:112:ARG:HH11	1.58	0.68
33:f:73:SER:HB2	55:Y:56:C:C1'	2.24	0.68
35:h:83:LYS:HE2	35:h:91:PHE:HB2	1.75	0.68
5:A:438:U:OP1	8:D:148:LYS:NZ	2.18	0.68
22:R:35:GLU:N	22:R:35:GLU:OE1	2.25	0.68
5:A:323:U:H3	5:A:327:A:H62	1.39	0.68
7:C:168:TYR:OH	9:E:55:GLU:OE1	2.10	0.68
5:A:1054:C:C4	27:Z:34:G:C1'	2.75	0.68
5:A:1060:U:OP1	18:N:85:ARG:NH2	2.25	0.68
7:C:131:ARG:NH1	9:E:55:GLU:CD	2.52	0.68
5:A:16:A:N3	5:A:1080:A:O2'	2.22	0.67
5:A:955:U:O2'	23:S:83:HIS:ND1	2.16	0.67
15:K:37:ARG:NH1	15:K:83:GLU:OE2	2.28	0.67
28:a:2024:A:H5'	53:z:9:THR:HG21	1.75	0.67
5:A:627:G:OP1	20:P:51:ARG:NH2	2.25	0.67
5:A:642:A:C5	12:H:107:SER:HA	2.29	0.67
5:A:1060:U:C4'	14:J:53:ILE:HG13	2.23	0.67
28:a:2308:G:C5'	33:f:121:SER:HB3	2.24	0.67
5:A:1537:U:C5	54:4:10:G:C5'	2.75	0.67
28:a:2380:A:C5	41:n:99:TYR:CD1	2.82	0.67
28:a:2755:G:C4	34:g:3:ARG:HD2	2.30	0.67
5:A:1014:A:H5''	23:S:14:HIS:CB	2.25	0.67
28:a:1341:G:OP1	46:s:17:SER:OG	2.10	0.67
28:a:1831:A:N3	30:c:15:HIS:NE2	2.41	0.67
28:a:2338:U:N3	41:n:16:ARG:HG3	2.09	0.67
28:a:2752:A:OP1	34:g:70:ALA:HB1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:40:GLN:NE2	28:a:717:A:N3	2.40	0.67
28:a:100:U:O2	47:t:91:LYS:NZ	2.16	0.67
28:a:2380:A:C4	41:n:99:TYR:CZ	2.82	0.67
34:g:2:SER:OG	34:g:3:ARG:N	2.26	0.67
5:A:1014:A:H4'	23:S:14:HIS:ND1	2.09	0.67
5:A:492:C:H2'	5:A:493:A:C8	2.29	0.67
8:D:150:LYS:NZ	8:D:177:LYS:O	2.28	0.67
28:a:1117:G:O2'	28:a:1118:G:O5'	2.12	0.67
36:i:9:GLU:HG2	36:i:10:THR:HG23	1.77	0.67
5:A:147:G:H2'	5:A:148:G:C8	2.31	0.66
5:A:339:C:OP2	37:j:98:ARG:NH2	2.28	0.66
28:a:2308:G:H4'	33:f:129:SER:C	2.21	0.66
27:Z:76:A:O3'	28:a:2589:U:O4	2.09	0.66
5:A:1187:G:N3	18:N:100:SER:OG	2.27	0.66
15:K:94:GLU:OE1	15:K:94:GLU:N	2.24	0.66
28:a:1342:U:OP1	46:s:84:TYR:OH	2.12	0.66
28:a:2380:A:N9	41:n:99:TYR:CE2	2.63	0.66
28:a:2670:C:N4	34:g:109:PHE:HA	2.11	0.66
5:A:617:G:H4'	20:P:44:SER:OG	1.96	0.66
5:A:1409:C:H2'	5:A:1410:A:H8	1.61	0.66
34:g:44:LYS:HB2	34:g:51:THR:HG22	1.78	0.66
5:A:19:A:C2	5:A:917:G:C4	2.84	0.65
5:A:150:U:H3	5:A:171:A:H62	1.42	0.65
5:A:1014:A:H4'	23:S:14:HIS:NE2	2.09	0.65
46:s:8:LEU:HD13	51:x:22:LEU:HB3	1.78	0.65
5:A:7:A:N1	9:E:95:PHE:CE2	2.64	0.65
5:A:455:G:H2'	5:A:456:A:H8	1.60	0.65
17:M:67:GLY:CA	33:f:113:ASP:OD1	2.30	0.65
23:S:44:MET:HB2	23:S:47:LEU:HD21	1.79	0.65
5:A:1226:C:P	17:M:90:ARG:HH22	2.18	0.65
28:a:2308:G:C5'	33:f:121:SER:CB	2.75	0.65
5:A:404:G:H5'	8:D:119:SER:OG	1.96	0.65
9:E:13:GLU:HG2	9:E:39:VAL:HG12	1.79	0.65
11:G:113:ASP:OD2	11:G:122:ASN:ND2	2.30	0.65
17:M:71:ARG:CZ	33:f:115:ARG:CZ	2.75	0.65
5:A:19:A:N6	5:A:917:G:C6	2.65	0.64
8:D:14:ARG:HG3	8:D:56:ARG:HH22	1.61	0.64
8:D:95:GLU:HA	8:D:100:ASN:HD22	1.61	0.64
28:a:2384:C:OP1	41:n:17:LYS:NZ	2.22	0.64
4:3:8:LYS:NZ	28:a:2471:C:OP1	2.30	0.64
5:A:427:U:OP1	8:D:13:ARG:NH2	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1329:A:H4'	17:M:24:GLY:O	1.97	0.64
28:a:278:A:OP2	28:a:361:G:N2	2.31	0.64
5:A:1328:C:OP1	17:M:28:THR:OG1	2.09	0.64
28:a:2773:U:OP1	36:i:95:ARG:NH1	2.29	0.64
5:A:392:C:O5'	20:P:13:LYS:NZ	2.31	0.64
5:A:909:A:C2'	5:A:1413:A:HO2'	2.10	0.64
28:a:1343:G:O2'	46:s:59:ASN:ND2	2.30	0.64
28:a:2308:G:C1'	33:f:129:SER:CB	2.75	0.64
36:i:1:MET:SD	36:i:2:LYS:N	2.71	0.64
27:Z:76:A:N6	28:a:2588:U:H4'	2.13	0.64
35:h:71:LYS:HZ2	35:h:71:LYS:HB3	1.63	0.64
5:A:1319:A:OP1	23:S:3:ARG:HB2	1.98	0.63
5:A:501:C:H2'	5:A:502:A:H8	1.62	0.63
54:4:4:A:H2'	54:4:5:A:H8	1.62	0.63
5:A:203:G:H1'	5:A:465:A:H61	1.62	0.63
28:a:2259:G:N2	49:v:9:SER:HB3	2.13	0.63
5:A:826:C:O2	12:H:16:ASN:ND2	2.32	0.63
5:A:1014:A:C4'	23:S:14:HIS:CD2	2.81	0.63
5:A:1014:A:C5'	23:S:14:HIS:CG	2.82	0.63
5:A:1401:G:OP1	26:X:18:G:O2'	2.13	0.63
5:A:1538:C:H41	54:4:10:G:P	2.20	0.63
28:a:2671:C:O2'	34:g:111:HIS:NE2	2.03	0.63
23:S:3:ARG:HH11	23:S:10:PHE:HB2	1.63	0.63
28:a:2369:G:H4'	49:v:60:PHE:CZ	2.33	0.63
5:A:312:C:H2'	5:A:313:A:H8	1.63	0.63
35:h:63:ALA:HA	35:h:66:ASN:HD22	1.63	0.63
5:A:689:C:OP1	15:K:46:THR:OG1	2.14	0.63
5:A:1464:U:H2'	5:A:1465:A:H8	1.64	0.63
8:D:87:GLY:HA3	8:D:197:GLU:HG3	1.80	0.63
28:a:483:A:H1'	47:t:58:ILE:CG1	2.29	0.63
5:A:212:G:H2'	5:A:213:G:H8	1.63	0.62
5:A:1322:C:H5''	17:M:99:GLY:HA3	1.80	0.62
21:Q:76:VAL:HG12	21:Q:77:ARG:HG2	1.81	0.62
28:a:483:A:N3	47:t:58:ILE:HD11	2.14	0.62
5:A:404:G:OP1	8:D:119:SER:HB2	1.99	0.62
28:a:2380:A:N1	41:n:92:PHE:CD2	2.67	0.62
5:A:19:A:C2	5:A:917:G:N3	2.66	0.62
28:a:2308:G:H5'	33:f:121:SER:CB	2.30	0.62
26:X:18:G:N1	55:Y:35:A:N1	2.47	0.62
5:A:677:U:H3	5:A:713:G:H22	1.47	0.62
5:A:1447:A:OP1	5:A:1448:C:N4	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:66:LYS:O	9:E:70:ASN:ND2	2.32	0.62
28:a:2380:A:N1	41:n:92:PHE:HD2	1.98	0.62
5:A:179:A:H61	5:A:196:A:H62	1.45	0.62
5:A:521:G:O5'	16:L:70:GLU:CG	2.48	0.62
5:A:539:A:H2'	5:A:540:G:H8	1.64	0.62
28:a:483:A:N9	47:t:45:HIS:HD2	1.95	0.62
5:A:19:A:H5''	9:E:91:GLY:HA3	1.82	0.62
5:A:419:C:H1'	8:D:40:GLN:OE1	1.99	0.62
5:A:1371:G:OP1	13:I:14:SER:OG	2.18	0.62
14:J:85:ASP:HA	14:J:88:MET:HE1	1.81	0.62
27:Z:76:A:O2'	28:a:2510:U:O2'	2.17	0.62
5:A:246:A:N6	5:A:281:G:C2	2.68	0.62
5:A:512:U:O4'	8:D:41:HIS:NE2	2.33	0.62
5:A:1397:C:P	9:E:29:ARG:HH22	2.23	0.62
27:Z:26:A:N6	27:Z:44:G:H1	1.91	0.62
5:A:1203:C:OP1	18:N:2:ALA:N	2.33	0.61
28:a:2380:A:C8	41:n:99:TYR:CE2	2.87	0.61
5:A:545:C:H5'	8:D:69:GLU:HG2	1.82	0.61
5:A:909:A:C2'	5:A:1413:A:O2'	2.48	0.61
28:a:783:A:P	30:c:217:ARG:HH22	2.22	0.61
28:a:2755:G:H4'	34:g:4:VAL:CG2	2.28	0.61
55:Y:62:C:H2'	55:Y:63:G:H8	1.65	0.61
5:A:259:G:OP1	24:T:82:GLN:NE2	2.29	0.61
5:A:929:G:OP2	54:4:3:C:H5'	1.99	0.61
28:a:483:A:H5'	47:t:45:HIS:HB3	1.81	0.61
8:D:95:GLU:HG3	8:D:191:LEU:HD11	1.82	0.61
5:A:309:A:H2'	5:A:310:G:H8	1.66	0.61
5:A:1391:U:H2'	5:A:1392:G:C8	2.36	0.61
5:A:197:A:N1	5:A:220:G:O2'	2.32	0.61
5:A:402:G:H4'	8:D:132:ILE:HD11	1.82	0.61
5:A:1407:5MC:C1'	28:a:1923:A:H1'	2.31	0.61
19:O:88:ARG:NH2	28:a:715:G:H3'	2.16	0.61
28:a:26:G:OP1	45:r:80:PRO:HB3	2.01	0.61
29:b:82:U:O3'	52:y:20:HIS:HE1	1.84	0.61
5:A:459:A:H2'	5:A:460:A:H8	1.65	0.61
5:A:702:A:C5	28:a:1850:A:C5	2.89	0.61
15:K:114:THR:HG21	25:U:32:VAL:HG21	1.81	0.61
5:A:17:U:O4'	5:A:1080:A:O4'	2.19	0.61
5:A:508:U:C4'	8:D:51:TYR:CD2	2.78	0.61
5:A:21:G:H2'	5:A:22:G:C8	2.35	0.61
5:A:246:A:N6	5:A:281:G:N2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:335:C:H2'	5:A:336:A:H8	1.66	0.61
5:A:1329:A:OP1	17:M:29:ARG:HB2	2.01	0.61
28:a:1132:U:H4'	36:i:81:ILE:HD11	1.81	0.61
5:A:310:G:OP1	20:P:31:ARG:N	2.34	0.60
11:G:78:ARG:NH1	54:4:2:G:O6	2.33	0.60
28:a:2671:C:C2'	34:g:111:HIS:NE2	2.63	0.60
48:u:9:ARG:HG2	48:u:41:GLU:HG2	1.83	0.60
5:A:17:U:H2'	5:A:18:C:C6	2.35	0.60
5:A:358:U:H2'	5:A:359:G:C8	2.35	0.60
5:A:626:G:H4'	20:P:38:PHE:CE1	2.36	0.60
5:A:672:U:P	10:F:79:ARG:HH12	2.24	0.60
6:B:130:THR:O	6:B:132:LYS:N	2.33	0.60
28:a:920:A:H5''	29:b:97:C:O2'	2.01	0.60
28:a:731:G:O6	30:c:207:LYS:HB2	2.02	0.60
28:a:1133:G:C4	36:i:77:HIS:CG	2.89	0.60
28:a:2662:C:H5'	34:g:160:LYS:HZ3	1.66	0.60
5:A:1407:5MC:H1'	28:a:1923:A:H1'	1.82	0.60
5:A:1414:U:H2'	5:A:1415:G:H8	1.66	0.60
28:a:2309:U:C5	33:f:152:LEU:C	2.80	0.60
5:A:530:G:C4	27:Z:35:A:H1'	2.37	0.60
5:A:499:A:H61	8:D:2:ALA:N	2.00	0.60
5:A:552:U:N3	5:A:553:A:N7	2.49	0.60
5:A:1001:C:H2'	5:A:1002:G:H8	1.67	0.60
5:A:1014:A:C4'	23:S:14:HIS:CG	2.83	0.60
15:K:13:ARG:NH2	15:K:76:GLU:OE1	2.33	0.60
5:A:545:C:OP1	8:D:69:GLU:CD	2.45	0.60
28:a:1790:C:OP1	30:c:221:ARG:NH2	2.34	0.60
28:a:2802:U:H4'	28:a:2803:G:H5'	1.84	0.60
5:A:539:A:H2'	5:A:540:G:C8	2.37	0.60
11:G:47:LEU:HD13	11:G:58:GLU:HB3	1.82	0.60
28:a:2308:G:H5''	33:f:121:SER:CB	2.32	0.60
2:1:26:ASN:CG	28:a:684:G:H5'	2.27	0.60
5:A:458:U:H3	5:A:474:G:H1	1.50	0.60
5:A:1217:C:OP2	18:N:9:ARG:NH2	2.27	0.59
7:C:130:PHE:O	7:C:134:MET:HG3	2.02	0.59
28:a:2534:A:C6	34:g:156:PRO:HG3	2.36	0.59
5:A:263:A:P	24:T:74:ARG:NE	2.73	0.59
5:A:556:C:H2'	5:A:557:G:H8	1.67	0.59
5:A:18:C:H4'	5:A:1078:U:O2	2.02	0.59
5:A:1048:G:H4'	18:N:3:LYS:HD2	1.84	0.59
17:M:90:ARG:HB2	17:M:97:VAL:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:i:125:TYR:HH	36:i:132:HIS:HE2	1.50	0.59
5:A:499:A:N6	8:D:2:ALA:N	2.51	0.59
5:A:1048:G:OP1	18:N:4:GLN:N	2.30	0.59
5:A:1257:A:C2	18:N:21:PHE:CE1	2.90	0.59
32:e:144:GLU:HG2	32:e:166:LYS:HE3	1.85	0.59
28:a:2309:U:H5	33:f:153:ASP:OD2	1.86	0.59
5:A:717:U:H4'	15:K:119:ASN:OD1	2.01	0.59
5:A:1061:G:C5'	14:J:61:ALA:HB2	2.33	0.59
33:f:73:SER:CB	55:Y:56:C:H1'	2.33	0.59
43:p:89:GLU:HG3	44:q:52:PRO:HB3	1.84	0.59
11:G:150:ALA:HA	15:K:61:PHE:HB3	1.85	0.59
20:P:52:LEU:HD21	20:P:57:ILE:HG13	1.85	0.59
28:a:1133:G:H5'	36:i:84:ILE:HB	1.84	0.59
31:d:156:PHE:CE1	36:i:81:ILE:HD13	2.37	0.59
7:C:24:ALA:HB1	7:C:28:GLU:HG2	1.84	0.59
28:a:786:G:C6	30:c:228:VAL:HG11	2.38	0.59
28:a:2473:A:N6	28:a:2485:G:O2'	2.36	0.59
30:c:120:VAL:CG2	35:h:91:PHE:HB3	2.33	0.59
5:A:1400:C:N3	55:Y:34:C:O2	2.36	0.58
27:Z:22:G:H2'	27:Z:23:A:H8	1.68	0.58
5:A:154:U:H2'	5:A:155:A:H8	1.68	0.58
5:A:1463:U:OP1	42:o:109:ARG:HD2	2.03	0.58
19:O:36:ILE:CG2	28:a:717:A:H1'	2.33	0.58
26:X:19:U:N3	27:Z:37:MIA:C2	2.66	0.58
28:a:2662:C:H5'	34:g:160:LYS:NZ	2.18	0.58
5:A:17:U:H2'	5:A:18:C:H6	1.69	0.58
5:A:151:A:N7	5:A:171:A:N6	2.52	0.58
5:A:455:G:H2'	5:A:456:A:C8	2.38	0.58
5:A:1412:C:H2'	5:A:1413:A:C8	2.39	0.58
8:D:43:ALA:O	8:D:45:LYS:NZ	2.35	0.58
17:M:66:GLU:OE1	17:M:70:ARG:NH2	2.36	0.58
28:a:2380:A:C1'	41:n:99:TYR:CE2	2.86	0.58
5:A:407:U:H2'	5:A:408:A:H8	1.68	0.58
13:I:47:VAL:HG13	13:I:80:ARG:HD3	1.85	0.58
8:D:105:MET:SD	8:D:180:GLY:HA3	2.43	0.58
29:b:36:C:N4	29:b:49:C:O2	2.36	0.58
5:A:477:C:H2'	5:A:478:A:C4	2.38	0.58
5:A:909:A:H2	5:A:1413:A:N3	2.02	0.58
9:E:88:VAL:HG22	9:E:93:ARG:HG2	1.84	0.58
5:A:459:A:H2'	5:A:460:A:C8	2.38	0.58
11:G:78:ARG:NH1	54:4:2:G:N1	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:866:G:H4'	29:b:101:A:H4'	1.83	0.58
28:a:917:C:O2	29:b:100:G:H4'	2.04	0.58
28:a:1133:G:N9	36:i:77:HIS:CD2	2.72	0.58
33:f:175:PHE:O	33:f:177:PHE:N	2.36	0.58
5:A:1464:U:P	42:o:109:ARG:HH12	2.27	0.58
17:M:92:ARG:HD3	28:a:890:C:C6	2.39	0.58
5:A:1373:G:OP1	13:I:41:ARG:NH2	2.37	0.58
6:B:129:LEU:HB2	6:B:134:ALA:HB2	1.85	0.58
14:J:11:LYS:HB2	14:J:97:ASP:HB3	1.86	0.58
28:a:958:G:C4'	39:l:82:MET:HE1	2.34	0.58
28:a:2308:G:C1'	33:f:129:SER:HB2	2.33	0.58
35:h:16:GLY:HA2	35:h:47:PHE:CE2	2.39	0.58
1:O:32:GLU:OE1	1:O:32:GLU:N	2.23	0.58
5:A:538:G:H2'	5:A:539:A:H8	1.69	0.58
5:A:1535:C:H4'	5:A:1536:C:H5'	1.86	0.58
5:A:376:G:OP1	20:P:68:SER:OG	2.18	0.57
5:A:702:A:C6	28:a:1850:A:C5	2.92	0.57
14:J:28:THR:HG21	14:J:90:LEU:HD22	1.85	0.57
28:a:875:C:H4'	39:l:64:TRP:NE1	2.19	0.57
44:q:26:ASP:O	44:q:27:ILE:HD13	2.04	0.57
5:A:15:G:O2'	9:E:22:SER:OG	2.13	0.57
5:A:691:G:O6	15:K:57:LYS:NZ	2.34	0.57
5:A:1319:A:P	23:S:3:ARG:HB2	2.44	0.57
28:a:2663:G:OP1	34:g:158:LYS:HD2	2.04	0.57
28:a:2803:G:O2'	28:a:2804:A:H5''	2.04	0.57
5:A:628:G:H2'	5:A:629:A:C8	2.39	0.57
13:I:25:ASN:OD1	13:I:27:LYS:NZ	2.36	0.57
28:a:321:U:OP2	32:e:130:LYS:HA	2.04	0.57
28:a:2308:G:C1'	33:f:129:SER:HB3	2.32	0.57
28:a:2259:G:H21	49:v:9:SER:CB	2.13	0.57
5:A:398:U:H2'	5:A:399:G:H8	1.70	0.57
5:A:460:A:H2'	5:A:461:A:H8	1.70	0.57
5:A:1414:U:O2	5:A:1487:G:N2	2.37	0.57
8:D:126:ASN:ND2	8:D:141:ASP:OD1	2.36	0.57
21:Q:11:ARG:HB2	21:Q:11:ARG:HH11	1.69	0.57
5:A:407:U:H2'	5:A:408:A:C8	2.39	0.57
5:A:590:U:H2'	5:A:591:U:H6	1.69	0.57
5:A:1381:U:O3'	54:4:2:G:H2'	2.01	0.57
28:a:570:U:O4	44:q:81:LYS:NZ	2.38	0.57
5:A:451:A:N7	5:A:481:G:N1	2.52	0.57
5:A:460:A:H2'	5:A:461:A:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:17:SER:HA	15:K:79:ILE:HA	1.86	0.57
33:f:140:GLU:OE1	33:f:140:GLU:N	2.38	0.57
5:A:26:A:H61	5:A:558:G:H1'	1.70	0.57
5:A:402:G:O2'	8:D:132:ILE:HD12	2.05	0.57
5:A:1040:U:H2'	5:A:1041:G:H8	1.70	0.57
17:M:17:ILE:O	17:M:20:THR:OG1	2.23	0.57
26:X:16:A:N6	55:Y:37:A:C2	2.73	0.57
5:A:16:A:H4'	9:E:21:VAL:HA	1.86	0.57
27:Z:55:PSU:OP1	39:l:54:THR:HG21	2.04	0.57
6:B:129:LEU:HD13	6:B:133:GLU:HG3	1.86	0.57
5:A:1400:C:N3	55:Y:34:C:C2	2.73	0.56
27:Z:76:A:C6	28:a:2588:U:O4'	2.58	0.56
28:a:883:G:H1	28:a:897:U:H3	1.53	0.56
28:a:1823:A:H5'	30:c:157:SER:OG	2.04	0.56
28:a:2307:G:H1'	33:f:123:ASP:HB3	1.85	0.56
5:A:312:C:H2'	5:A:313:A:C8	2.39	0.56
11:G:78:ARG:NH1	54:4:2:G:C6	2.73	0.56
26:X:16:A:N6	55:Y:37:A:C6	2.73	0.56
28:a:2298:G:OP1	41:n:10:ARG:HD2	2.05	0.56
28:a:2671:C:HO2'	34:g:111:HIS:CE1	2.17	0.56
33:f:108:VAL:HG11	33:f:176:PRO:HG2	1.86	0.56
41:n:76:LYS:O	41:n:80:GLU:HG3	2.04	0.56
5:A:1124:G:H3'	14:J:37:ARG:CZ	2.34	0.56
28:a:1142:C:H5'	36:i:26:GLY:HA3	1.88	0.56
33:f:73:SER:HB2	55:Y:56:C:H1'	1.87	0.56
5:A:28:A:O2'	5:A:296:U:OP1	2.23	0.56
5:A:986:U:H1'	23:S:54:GLY:O	2.05	0.56
5:A:1124:G:H3'	14:J:37:ARG:NH2	2.19	0.56
5:A:1329:A:H5''	17:M:26:GLY:H	1.69	0.56
13:I:130:ARG:CZ	55:Y:33:U:C5	2.89	0.56
19:O:63:ARG:HH21	28:a:717:A:C4'	2.14	0.56
5:A:253:A:OP1	21:Q:69:LYS:NZ	2.35	0.56
5:A:501:C:H2'	5:A:502:A:C8	2.40	0.56
5:A:1320:C:H1'	23:S:73:GLU:HG2	1.86	0.56
14:J:40:ILE:HB	14:J:73:LEU:HB3	1.87	0.56
28:a:1821:A:OP1	30:c:156:ARG:N	2.39	0.56
28:a:2383:G:H4'	41:n:21:LEU:HD11	1.87	0.56
5:A:1228:C:OP1	17:M:107:ARG:NH2	2.34	0.56
28:a:1245:C:H1'	38:k:4:ASN:O	2.04	0.56
30:c:120:VAL:CB	35:h:91:PHE:HB3	2.36	0.56
3:2:4:ILE:HD11	28:a:594:A:C2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:137:U:O2	5:A:226:G:O6	2.23	0.56
5:A:222:C:H2'	5:A:223:A:H8	1.71	0.56
5:A:1014:A:C5'	23:S:14:HIS:CD2	2.89	0.56
5:A:1061:G:H5'	14:J:61:ALA:HB2	1.88	0.56
5:A:1305:G:N2	5:A:1331:G:H1'	2.21	0.56
28:a:2380:A:C5	41:n:99:TYR:CG	2.94	0.56
28:a:2533:G:P	34:g:172:LYS:NZ	2.78	0.56
3:2:26:HIS:HA	28:a:2365:G:OP1	2.05	0.56
5:A:263:A:OP1	24:T:74:ARG:NE	2.39	0.56
5:A:1328:C:C5'	17:M:28:THR:HG21	2.29	0.56
5:A:1532:U:H3	5:A:1533:C:H42	1.53	0.56
5:A:508:U:C4'	8:D:51:TYR:CE2	2.88	0.56
8:D:58:LYS:NZ	8:D:69:GLU:OE2	2.36	0.56
27:Z:37:MIA:H2'	27:Z:38:A:O4'	2.05	0.56
45:r:59:GLU:OE1	45:r:66:ILE:HB	2.06	0.56
11:G:133:THR:O	11:G:135:VAL:N	2.37	0.56
23:S:41:PHE:H	23:S:44:MET:HE1	1.71	0.56
39:l:77:PRO:HG2	39:l:80:VAL:HG21	1.88	0.56
4:3:4:ARG:HB3	28:a:2470:C:OP1	2.06	0.55
5:A:34:C:H2'	5:A:35:G:H8	1.71	0.55
5:A:1397:C:OP2	9:E:29:ARG:NH2	2.39	0.55
28:a:971:G:O3'	52:y:15:GLY:HA2	2.06	0.55
5:A:490:C:H2'	5:A:491:G:H8	1.70	0.55
5:A:1329:A:H5'	17:M:29:ARG:HD2	1.88	0.55
20:P:14:ARG:HA	20:P:42:ILE:HD12	1.88	0.55
26:X:20:U:C4	27:Z:36:A:N1	2.74	0.55
5:A:323:U:O4	5:A:327:A:N7	2.40	0.55
5:A:1078:U:O4'	9:E:89:HIS:HE1	1.88	0.55
5:A:1517:G:C8	28:a:1924:C:OP1	2.59	0.55
8:D:85:ASN:HB2	8:D:88:GLU:CD	2.30	0.55
11:G:40:GLU:OE2	13:I:41:ARG:NH1	2.37	0.55
28:a:2533:G:H4'	34:g:175:LYS:CB	2.37	0.55
5:A:64:G:H4'	5:A:65:A:H3'	1.88	0.55
19:O:36:ILE:HG21	28:a:717:A:H1'	1.89	0.55
21:Q:11:ARG:HB2	21:Q:11:ARG:NH1	2.21	0.55
28:a:2380:A:H1'	41:n:99:TYR:CZ	2.41	0.55
17:M:92:ARG:NE	28:a:890:C:C5	2.75	0.55
33:f:162:SER:OG	33:f:165:GLU:OE1	2.24	0.55
5:A:946:A:H2'	5:A:947:G:C8	2.42	0.55
28:a:1793:A:O3'	30:c:205:LEU:HB2	2.06	0.55
28:a:1802:C:P	30:c:182:ARG:HH12	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:u:1:MET:SD	48:u:2:PHE:N	2.80	0.55
17:M:92:ARG:CD	28:a:890:C:C6	2.90	0.55
28:a:2749:C:O2'	34:g:139:GLN:O	2.23	0.55
31:d:55:LYS:HD3	31:d:60:VAL:HG22	1.89	0.55
9:E:162:GLU:OE1	9:E:162:GLU:N	2.37	0.55
28:a:1602:C:OP1	46:s:81:LYS:NZ	2.29	0.55
5:A:15:G:N7	5:A:1396:A:C2	2.75	0.55
5:A:1014:A:H5''	23:S:14:HIS:CG	2.42	0.55
19:O:60:VAL:HG22	28:a:717:A:O4'	2.07	0.54
28:a:483:A:H1'	47:t:58:ILE:HG13	1.89	0.54
28:a:2551:A:H2'	28:a:2552:U:C6	2.42	0.54
5:A:147:G:H2'	5:A:148:G:H8	1.73	0.54
5:A:159:G:N2	5:A:162:A:OP2	2.40	0.54
5:A:429:U:H3'	8:D:9:LEU:HD12	1.90	0.54
5:A:546:A:H8	8:D:68:LEU:HD22	1.71	0.54
5:A:410:G:OP1	8:D:26:ARG:NH1	2.35	0.54
28:a:1366:G:P	50:w:50:ARG:HH12	2.30	0.54
34:g:84:THR:HG23	34:g:134:LYS:HD3	1.90	0.54
10:F:24:ARG:HG3	10:F:24:ARG:HH11	1.73	0.54
11:G:93:PRO:HA	11:G:96:ARG:HD2	1.88	0.54
36:i:125:TYR:OH	36:i:132:HIS:NE2	2.35	0.54
5:A:339:C:P	37:j:98:ARG:HE	2.30	0.54
5:A:1486:G:H2'	5:A:1487:G:O4'	2.07	0.54
10:F:38:ARG:NH1	10:F:98:GLU:O	2.39	0.54
28:a:2307:G:H1'	33:f:123:ASP:CB	2.37	0.54
5:A:543:U:OP1	8:D:14:ARG:HG2	2.08	0.54
28:a:731:G:C5	30:c:207:LYS:HB2	2.40	0.54
28:a:1436:A:H2'	28:a:1437:G:C8	2.43	0.54
28:a:2663:G:OP1	34:g:158:LYS:NZ	2.25	0.54
30:c:29:PRO:HG2	30:c:34:LEU:HD11	1.89	0.54
37:j:43:ILE:HD12	37:j:56:ASP:HB2	1.89	0.54
5:A:19:A:H2'	5:A:20:U:C6	2.43	0.54
28:a:990:A:P	52:y:12:SER:HB3	2.48	0.54
28:a:1801:G:O2'	30:c:180:GLU:OE2	2.23	0.54
28:a:2380:A:H1'	41:n:99:TYR:OH	2.07	0.54
5:A:1407:5MC:O2'	28:a:1923:A:C8	2.59	0.54
7:C:162:ILE:CD1	26:X:24:A:H4'	2.23	0.54
19:O:40:GLN:NE2	28:a:717:A:C2	2.63	0.54
29:b:83:G:H4'	52:y:53:PHE:CG	2.43	0.54
5:A:784:A:C4'	28:a:1839:C:OP1	2.55	0.54
14:J:10:LEU:HB2	14:J:72:ARG:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:35:THR:HG22	15:K:41:ALA:HA	1.89	0.54
15:K:117:PRO:HB2	15:K:119:ASN:O	2.08	0.54
27:Z:51:U:H2'	27:Z:52:G:H8	1.73	0.54
28:a:2752:A:OP1	34:g:70:ALA:CB	2.55	0.54
5:A:269:C:H2'	5:A:270:A:C8	2.43	0.53
5:A:339:C:OP2	37:j:98:ARG:CZ	2.55	0.53
5:A:556:C:H2'	5:A:557:G:C8	2.43	0.53
27:Z:20:H2U:H61	27:Z:20:H2U:OP1	2.08	0.53
28:a:784:A:N7	30:c:220:VAL:HG21	2.23	0.53
28:a:1367:A:OP1	50:w:3:ARG:HD2	2.09	0.53
30:c:165:VAL:HG21	30:c:181:MET:HE1	1.88	0.53
5:A:8:A:H61	8:D:202:GLU:CA	2.21	0.53
5:A:19:A:C2	5:A:917:G:N1	2.76	0.53
5:A:1318:A:OP1	23:S:7:LYS:HE2	2.08	0.53
5:A:1372:U:OP1	13:I:73:SER:N	2.40	0.53
5:A:1409:C:H5''	28:a:1919:3TD:H10	1.91	0.53
5:A:1436:U:H2'	5:A:1437:A:C8	2.43	0.53
5:A:1517:G:H1'	28:a:1923:A:O3'	2.07	0.53
8:D:95:GLU:HA	8:D:100:ASN:ND2	2.23	0.53
26:X:20:U:O4	27:Z:36:A:N1	2.41	0.53
28:a:2473:A:H4'	39:l:55:ARG:HD2	1.89	0.53
5:A:362:G:P	16:L:31:ARG:NH2	2.82	0.53
5:A:656:G:O2'	19:O:28:GLN:OE1	2.24	0.53
5:A:1340:A:O2'	55:Y:31:G:O2'	2.04	0.53
28:a:24:G:O2'	45:r:77:ASP:HB3	2.08	0.53
28:a:786:G:H5'	28:a:787:G:OP1	2.07	0.53
5:A:545:C:P	8:D:69:GLU:CG	2.96	0.53
5:A:1048:G:H5''	18:N:3:LYS:HD2	1.88	0.53
28:a:483:A:C5'	47:t:45:HIS:HB3	2.39	0.53
28:a:731:G:C5	30:c:207:LYS:HD2	2.43	0.53
28:a:958:G:O4'	39:l:82:MET:HE1	2.09	0.53
28:a:1343:G:O3'	46:s:59:ASN:HB3	2.08	0.53
28:a:1756:A:C8	42:o:94:LYS:HE2	2.43	0.53
28:a:2751:G:O2'	34:g:67:THR:HB	2.08	0.53
5:A:346:G:P	42:o:41:GLN:HE21	2.31	0.53
13:I:85:ARG:HA	13:I:88:MET:HE2	1.90	0.53
16:L:110:ARG:HB3	16:L:119:VAL:HG21	1.91	0.53
28:a:2755:G:C5	34:g:3:ARG:HD2	2.43	0.53
5:A:512:U:P	8:D:44:ARG:NH2	2.82	0.53
5:A:673:A:H2'	5:A:674:G:C8	2.43	0.53
5:A:1422:G:H4'	37:j:48:PRO:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:483:A:H1'	47:t:58:ILE:HG12	1.91	0.53
28:a:1133:G:C2	36:i:77:HIS:HB3	2.43	0.53
28:a:1484:G:H1'	28:a:1511:A:H61	1.74	0.53
28:a:1802:C:C5'	30:c:146:MET:HE1	2.38	0.53
4:3:32:LYS:HE2	28:a:2482:A:H5'	1.89	0.53
5:A:1103:C:O2	6:B:106:THR:HG21	2.08	0.53
7:C:35:SER:OG	7:C:59:ARG:NH2	2.41	0.53
10:F:22:ILE:O	10:F:26:THR:HG23	2.08	0.53
10:F:90:MET:HE1	22:R:23:TYR:CZ	2.44	0.53
23:S:3:ARG:HH21	23:S:7:LYS:HB3	1.74	0.53
28:a:1132:U:C4'	36:i:81:ILE:HD11	2.39	0.53
28:a:1141:G:O3'	36:i:26:GLY:HA3	2.08	0.53
28:a:2670:C:N4	34:g:108:GLY:O	2.41	0.53
50:w:62:LYS:NZ	50:w:70:GLU:OE2	2.41	0.53
5:A:875:U:O2'	12:H:15:ARG:HD2	2.08	0.53
13:I:97:GLU:N	13:I:97:GLU:OE1	2.40	0.53
19:O:56:LEU:HD21	28:a:717:A:N1	2.23	0.53
24:T:4:ILE:HG22	24:T:7:ALA:H	1.73	0.53
27:Z:5:G:H2'	27:Z:6:G:H8	1.74	0.53
34:g:80:THR:OG1	34:g:81:GLU:N	2.41	0.53
39:l:53:MET:HE1	39:l:103:TYR:CG	2.44	0.53
8:D:196:ASN:OD1	8:D:197:GLU:N	2.42	0.53
49:v:59:LEU:HD12	49:v:80:ILE:HD12	1.90	0.53
1:0:8:LYS:HE3	28:a:2425:G:P	2.49	0.53
5:A:505:G:H2'	5:A:506:G:H8	1.74	0.53
5:A:617:G:C5'	20:P:44:SER:OG	2.57	0.53
4:3:16:ILE:HD13	4:3:25:VAL:HG22	1.89	0.52
20:P:56:ARG:HA	20:P:56:ARG:HE	1.74	0.52
5:A:613:C:P	8:D:81:ARG:NH1	2.82	0.52
5:A:1125:U:P	14:J:37:ARG:HH21	2.32	0.52
18:N:89:MET:HA	18:N:89:MET:HE2	1.90	0.52
28:a:329:G:O6	47:t:16:GLY:CA	2.56	0.52
28:a:495:G:O2'	45:r:61:ASN:ND2	2.39	0.52
42:o:63:LYS:HE2	42:o:65:SER:HB2	1.91	0.52
5:A:634:C:H2'	5:A:635:A:H8	1.72	0.52
5:A:974:A:OP1	18:N:71:HIS:HB3	2.09	0.52
14:J:21:ALA:HB1	14:J:92:LEU:HD13	1.92	0.52
28:a:337:C:OP1	47:t:4:LYS:HE3	2.10	0.52
5:A:227:G:O2'	20:P:63:GLN:OE1	2.22	0.52
5:A:1118:U:O3'	13:I:85:ARG:NH2	2.32	0.52
5:A:1250:A:O3'	13:I:69:GLY:HA2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1400:C:N4	55:Y:34:C:N1	2.57	0.52
11:G:86:GLN:HB2	11:G:148:ASN:ND2	2.25	0.52
14:J:42:LEU:HB2	14:J:71:LEU:HB3	1.91	0.52
26:X:18:G:C2	55:Y:35:A:N1	2.77	0.52
53:z:52:ARG:CZ	53:z:54:VAL:HG12	2.40	0.52
54:4:3:C:H2'	54:4:4:A:H8	1.73	0.52
5:A:769:G:H4'	5:A:1513:A:H4'	1.91	0.52
20:P:18:GLN:HE21	20:P:35:ARG:HD2	1.73	0.52
28:a:2307:G:H4'	33:f:122:PHE:C	2.33	0.52
5:A:297:G:N2	5:A:300:A:OP2	2.30	0.52
5:A:509:A:H5'	8:D:52:GLY:HA2	1.92	0.52
17:M:7:ILE:CG2	33:f:112:ARG:HH12	2.18	0.52
5:A:1228:C:N4	17:M:103:LYS:O	2.41	0.52
5:A:1323:G:H2'	5:A:1324:A:C8	2.44	0.52
7:C:134:MET:HE2	7:C:168:TYR:HD2	1.73	0.52
17:M:71:ARG:CD	33:f:115:ARG:CZ	2.87	0.52
20:P:1:MET:HG3	20:P:2:VAL:H	1.73	0.52
32:e:123:LYS:HE3	32:e:124:PHE:H	1.74	0.52
42:o:39:ARG:HG2	42:o:40:LEU:N	2.25	0.52
1:0:37:LYS:HZ2	1:0:37:LYS:HB3	1.75	0.52
5:A:1373:G:OP2	13:I:73:SER:OG	2.27	0.52
47:t:52:LEU:O	47:t:54:GLN:NE2	2.43	0.52
5:A:294:U:H2'	5:A:295:C:H6	1.75	0.52
5:A:672:U:OP1	10:F:79:ARG:NH1	2.42	0.52
13:I:84:THR:HG23	13:I:98:LEU:HD13	1.92	0.52
17:M:58:ASP:OD1	17:M:58:ASP:N	2.43	0.52
17:M:92:ARG:HB3	28:a:890:C:O4'	2.09	0.52
28:a:875:C:H4'	39:l:64:TRP:HE1	1.74	0.52
28:a:2306:U:O2'	33:f:123:ASP:O	2.19	0.52
35:h:7:ASP:OD1	35:h:8:LYS:N	2.41	0.52
14:J:40:ILE:HG13	14:J:73:LEU:HD23	1.90	0.52
28:a:12:U:O2	28:a:12:U:H2'	2.09	0.52
28:a:2320:G:H4'	33:f:125:ARG:NH1	2.25	0.52
27:Z:23:A:H2'	27:Z:24:G:H8	1.75	0.51
28:a:363:G:H2'	28:a:364:C:C6	2.45	0.51
28:a:1601:U:OP1	46:s:40:LYS:N	2.33	0.51
28:a:2318:A:H4'	33:f:157:THR:OG1	2.11	0.51
5:A:1061:G:H5'	14:J:61:ALA:CB	2.41	0.51
5:A:1412:C:H2'	5:A:1413:A:H8	1.75	0.51
10:F:41:ASP:OD1	10:F:58:HIS:NE2	2.41	0.51
28:a:766:A:C6	30:c:208:ALA:HB1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:s:30:ILE:HD13	46:s:93:LEU:HD23	1.92	0.51
55:Y:26:G:H1	55:Y:45:G:H22	1.59	0.51
5:A:1228:C:OP1	17:M:114:LYS:NZ	2.43	0.51
5:A:1536:C:O2'	5:A:1537:U:H5'	2.10	0.51
8:D:100:ASN:OD1	8:D:111:ARG:NH1	2.22	0.51
11:G:80:VAL:O	11:G:82:GLY:N	2.44	0.51
17:M:10:PRO:HG2	17:M:13:LYS:HE2	1.92	0.51
28:a:1735:G:H2'	28:a:1736:G:H8	1.75	0.51
28:a:2307:G:O4'	33:f:122:PHE:O	2.27	0.51
28:a:2752:A:P	34:g:70:ALA:CB	2.98	0.51
45:r:73:LYS:HB2	45:r:106:VAL:HB	1.92	0.51
5:A:384:G:H2'	5:A:385:C:C6	2.45	0.51
23:S:17:LYS:O	23:S:21:LYS:HG2	2.10	0.51
28:a:654:U:OP1	28:a:656:A:N6	2.44	0.51
28:a:2064:A:OP2	32:e:66:GLY:HA2	2.09	0.51
28:a:2584:PSU:OP1	31:d:137:SER:OG	2.24	0.51
5:A:441:A:N6	5:A:493:A:H61	2.05	0.51
5:A:444:G:H2'	5:A:445:G:H8	1.76	0.51
5:A:544:G:OP1	8:D:59:GLN:HG3	2.10	0.51
5:A:546:A:P	8:D:69:GLU:H	2.33	0.51
21:Q:17:MET:HB2	21:Q:20:SER:HB2	1.92	0.51
28:a:1133:G:C8	36:i:77:HIS:CD2	2.98	0.51
5:A:616:G:O2'	20:P:47:GLU:CD	2.54	0.51
5:A:1373:G:OP2	13:I:73:SER:CB	2.59	0.51
6:B:139:ARG:NE	6:B:139:ARG:HA	2.26	0.51
12:H:38:ASN:O	12:H:42:GLU:HG3	2.11	0.51
17:M:92:ARG:CZ	28:a:890:C:C5	2.93	0.51
5:A:216:U:H2'	5:A:217:C:C6	2.46	0.51
5:A:544:G:H5''	8:D:59:GLN:HE21	1.76	0.51
5:A:552:U:C2	5:A:553:A:C8	2.99	0.51
5:A:1530:G:H2'	5:A:1531:A:C8	2.45	0.51
11:G:5:ARG:NH1	11:G:7:ILE:O	2.43	0.51
5:A:674:G:P	10:F:86:ARG:HH22	2.33	0.51
6:B:85:LEU:O	6:B:87:CYS:N	2.43	0.51
19:O:60:VAL:HG21	28:a:717:A:N9	2.25	0.51
27:Z:43:C:H2'	27:Z:44:G:C8	2.46	0.51
28:a:809:U:OP2	38:k:41:ARG:NH2	2.43	0.51
28:a:1133:G:C8	36:i:77:HIS:NE2	2.78	0.51
28:a:2338:U:O4'	41:n:12:THR:HB	2.11	0.51
5:A:134:G:H2'	5:A:135:C:O4'	2.11	0.51
5:A:325:A:H2'	5:A:326:G:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:538:G:H2'	5:A:539:A:C8	2.46	0.51
14:J:65:TYR:HB3	18:N:96:LEU:HD11	1.92	0.51
27:Z:37:MIA:H8	27:Z:37:MIA:O5'	2.11	0.51
28:a:1793:A:H4'	30:c:205:LEU:HB2	1.92	0.51
46:s:8:LEU:HD13	51:x:22:LEU:CB	2.40	0.51
5:A:403:C:C5'	8:D:132:ILE:HG13	2.41	0.51
5:A:500:G:H2'	5:A:501:C:C6	2.46	0.51
5:A:1150:A:O2'	14:J:41:PRO:O	2.20	0.51
5:A:1532:U:C5	5:A:1533:C:N4	2.70	0.51
8:D:102:VAL:HG13	8:D:114:ALA:HB1	1.93	0.51
26:X:18:G:N2	55:Y:35:A:C4	2.79	0.51
28:a:2320:G:O2'	33:f:125:ARG:CZ	2.59	0.51
28:a:2671:C:H2'	34:g:111:HIS:CD2	2.46	0.51
5:A:244:U:O4	5:A:906:A:H1'	2.11	0.50
5:A:1382:C:H5'	54:4:2:G:H1'	1.93	0.50
5:A:1436:U:H2'	5:A:1437:A:H8	1.75	0.50
11:G:150:ALA:HA	15:K:61:PHE:CB	2.40	0.50
17:M:71:ARG:NH2	33:f:115:ARG:HD2	2.18	0.50
23:S:3:ARG:NH1	23:S:10:PHE:HB2	2.25	0.50
28:a:139:U:H5''	28:a:140:C:H5	1.75	0.50
28:a:1738:U:H2'	28:a:1739:G:O4'	2.10	0.50
28:a:2024:A:H5'	53:z:9:THR:HG22	1.89	0.50
45:r:4:ILE:HG12	45:r:106:VAL:HG22	1.92	0.50
5:A:355:C:O2'	5:A:388:G:N3	2.38	0.50
5:A:728:A:C8	19:O:54:ARG:CZ	2.94	0.50
5:A:1003:G:N2	5:A:1037:C:O2	2.33	0.50
5:A:1381:U:H5''	54:4:3:C:C1'	2.27	0.50
5:A:1409:C:H4'	28:a:1919:3TD:H10	1.91	0.50
28:a:2332:A:H2'	28:a:2333:U:C6	2.46	0.50
28:a:2380:A:N7	41:n:99:TYR:CG	2.79	0.50
28:a:2688:U:H4'	37:j:76:VAL:CG2	2.41	0.50
2:1:12:ARG:NH2	28:a:465:G:OP1	2.42	0.50
5:A:500:G:H2'	5:A:501:C:H6	1.76	0.50
28:a:813:U:C4	38:k:21:ARG:CZ	2.94	0.50
5:A:154:U:H2'	5:A:155:A:C8	2.46	0.50
5:A:405:U:H3	5:A:499:A:H62	1.60	0.50
5:A:1106:G:H5''	7:C:172:ARG:HG2	1.94	0.50
6:B:148:LEU:HD22	6:B:151:ILE:HD11	1.94	0.50
8:D:13:ARG:HG2	8:D:33:LYS:O	2.11	0.50
13:I:52:LEU:HD13	13:I:58:VAL:HA	1.94	0.50
28:a:282:A:H2'	28:a:283:G:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:294:U:H2'	5:A:295:C:C6	2.46	0.50
5:A:478:A:H2'	5:A:479:U:O4'	2.11	0.50
11:G:129:GLU:HB2	11:G:131:LYS:HD3	1.94	0.50
15:K:93:ARG:NH2	15:K:112:ASP:OD2	2.37	0.50
23:S:35:SER:HG	23:S:38:SER:HG	1.50	0.50
28:a:1798:U:H2'	28:a:1799:G:C8	2.47	0.50
28:a:2710:A:O2'	40:m:64:ARG:HD3	2.11	0.50
35:h:72:ILE:HG13	35:h:108:VAL:HG11	1.92	0.50
5:A:8:A:N6	8:D:202:GLU:CB	2.68	0.50
5:A:362:G:OP1	16:L:31:ARG:NH2	2.45	0.50
5:A:1407:5MC:O4'	28:a:1923:A:H1'	2.12	0.50
5:A:1438:G:H5''	24:T:33:LYS:NZ	2.26	0.50
28:a:2308:G:P	33:f:121:SER:HA	2.52	0.50
55:Y:73:A:H5'	55:Y:74:C:H5'	1.93	0.50
5:A:546:A:P	8:D:69:GLU:HB2	2.51	0.50
5:A:636:U:OP1	21:Q:6:ARG:NE	2.44	0.50
5:A:1464:U:OP2	42:o:109:ARG:NH1	2.33	0.50
5:A:1537:U:C5	54:4:10:G:H5'	2.47	0.50
27:Z:76:A:O2'	28:a:2510:U:O2	2.26	0.50
28:a:1367:A:O2'	50:w:11:ARG:NH2	2.41	0.50
5:A:976:G:OP2	5:A:1358:U:O2'	2.28	0.50
26:X:20:U:N3	27:Z:36:A:C2	2.80	0.50
28:a:1029:A:C2	28:a:2492:G:H5'	2.47	0.50
28:a:1407:U:H2'	28:a:1408:U:C6	2.47	0.50
28:a:2309:U:C5'	33:f:131:GLY:HA3	2.42	0.50
28:a:2380:A:N9	41:n:99:TYR:CZ	2.78	0.50
28:a:2551:A:H4'	37:j:29:HIS:CE1	2.47	0.50
5:A:36:C:OP1	16:L:120:LYS:HE3	2.12	0.50
5:A:625:U:H4'	20:P:16:PHE:CE2	2.46	0.50
13:I:49:ARG:HB3	13:I:53:GLU:OE2	2.12	0.50
17:M:71:ARG:CZ	33:f:115:ARG:NE	2.75	0.50
28:a:780:G:H5''	30:c:48:ARG:HD2	1.94	0.50
5:A:591:U:H2'	5:A:592:G:H8	1.77	0.49
5:A:1112:C:O2	7:C:179:ARG:HG2	2.12	0.49
7:C:12:LEU:HD11	18:N:91:GLY:HA2	1.93	0.49
27:Z:76:A:C4	28:a:2588:U:H1'	2.47	0.49
28:a:329:G:O6	47:t:16:GLY:HA2	2.11	0.49
28:a:1936:A:H2'	28:a:1937:G:O4'	2.12	0.49
28:a:2096:U:H5''	35:h:24:GLY:CA	2.41	0.49
28:a:2381:A:C4'	41:n:117:PHE:O	2.59	0.49
29:b:106:G:H2'	29:b:107:G:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:19:A:N3	5:A:917:G:C2	2.78	0.49
5:A:511:C:O3'	8:D:44:ARG:NH2	2.45	0.49
7:C:10:ILE:HD13	18:N:98:LYS:HD3	1.92	0.49
9:E:151:GLU:OE2	9:E:151:GLU:N	2.31	0.49
10:F:90:MET:HE1	22:R:23:TYR:CE2	2.48	0.49
28:a:1141:G:O3'	36:i:26:GLY:CA	2.61	0.49
28:a:1268:G:N7	45:r:16:LYS:HE3	2.27	0.49
33:f:94:GLU:O	33:f:98:GLU:HG3	2.12	0.49
5:A:900:A:H4'	28:a:1834:C:C5'	2.42	0.49
28:a:1831:A:O2'	30:c:15:HIS:CD2	2.65	0.49
5:A:41:G:H2'	5:A:42:G:H8	1.78	0.49
5:A:636:U:H5''	21:Q:6:ARG:HG2	1.95	0.49
5:A:730:G:O6	19:O:51:HIS:NE2	2.42	0.49
5:A:1400:C:N4	55:Y:34:C:H1'	2.27	0.49
28:a:1372:C:H2'	28:a:1373:G:O4'	2.12	0.49
28:a:2602:A:H5''	30:c:234:GLY:HA3	1.95	0.49
54:4:4:A:H2'	54:4:5:A:C8	2.46	0.49
5:A:36:C:OP1	16:L:120:LYS:CE	2.61	0.49
5:A:185:U:H2'	5:A:186:C:C6	2.47	0.49
5:A:563:A:H2	16:L:12:ARG:NH1	2.10	0.49
8:D:85:ASN:O	8:D:88:GLU:HG2	2.13	0.49
9:E:83:HIS:HB3	12:H:97:ALA:HB3	1.93	0.49
28:a:2247:U:H2'	28:a:2248:U:C6	2.48	0.49
28:a:1798:U:H2'	28:a:1799:G:H8	1.77	0.49
5:A:108:G:H5'	5:A:109:A:H5''	1.94	0.49
5:A:530:G:N3	27:Z:35:A:O2'	2.35	0.49
5:A:1356:G:H2'	5:A:1357:A:C8	2.48	0.49
8:D:70:ARG:O	8:D:74:ASN:ND2	2.45	0.49
8:D:125:VAL:HG23	8:D:143:VAL:HG22	1.93	0.49
24:T:54:MET:HE2	24:T:79:LEU:HD12	1.94	0.49
28:a:2309:U:O2'	33:f:133:ARG:NH1	2.46	0.49
5:A:2:A:H2'	5:A:3:A:C4	2.48	0.49
5:A:403:C:H2'	5:A:404:G:C8	2.47	0.49
5:A:440:C:C2	5:A:441:A:C8	3.01	0.49
8:D:100:ASN:O	8:D:104:ARG:HG2	2.13	0.49
28:a:997:C:N4	36:i:2:LYS:HD3	2.28	0.49
5:A:403:C:H5''	8:D:133:ALA:H	1.77	0.49
5:A:1126:U:H5	14:J:7:ARG:NH1	2.11	0.49
5:A:1400:C:C4	55:Y:34:C:N1	2.79	0.49
5:A:1517:G:C2	28:a:1924:C:C5'	2.95	0.49
7:C:22:TRP:HB3	7:C:59:ARG:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:483:A:N3	47:t:58:ILE:CD1	2.76	0.49
28:a:1134:U:O4'	36:i:75:TYR:CG	2.65	0.49
28:a:2662:C:C5'	34:g:160:LYS:NZ	2.76	0.49
29:b:83:G:H4'	52:y:53:PHE:CD2	2.48	0.49
31:d:183:GLU:H	31:d:183:GLU:CD	2.19	0.49
5:A:35:G:H2'	5:A:36:C:C6	2.48	0.49
5:A:261:U:OP1	24:T:71:LYS:NZ	2.45	0.49
5:A:512:U:P	8:D:44:ARG:HH21	2.36	0.49
5:A:632:U:H5'	5:A:633:G:C8	2.47	0.49
5:A:1220:G:O3'	23:S:36:ARG:HD3	2.13	0.49
5:A:1223:C:P	23:S:78:ARG:HH21	2.36	0.49
10:F:69:GLU:OE1	10:F:69:GLU:N	2.43	0.49
20:P:69:ASP:OD1	20:P:70:ARG:N	2.45	0.49
21:Q:25:ILE:HB	21:Q:42:THR:HG23	1.94	0.49
28:a:956:G:OP2	39:l:16:ARG:NH1	2.46	0.49
5:A:1103:C:OP1	6:B:95:ARG:NH2	2.46	0.48
23:S:3:ARG:NH2	23:S:7:LYS:HE2	2.28	0.48
28:a:590:U:H2'	28:a:591:U:C6	2.48	0.48
33:f:130:MET:HE3	33:f:130:MET:HB2	1.79	0.48
47:t:49:VAL:O	47:t:54:GLN:HG3	2.13	0.48
5:A:736:C:H5''	10:F:90:MET:HG2	1.95	0.48
5:A:930:C:P	54:4:4:A:C5'	2.99	0.48
5:A:1073:U:O2'	6:B:105:LYS:HE2	2.13	0.48
28:a:84:A:H5''	47:t:6:ARG:HD3	1.95	0.48
28:a:766:A:C6	30:c:208:ALA:CB	2.96	0.48
28:a:1143:U:H4'	28:a:1144:A:O4'	2.13	0.48
28:a:1800:U:OP2	30:c:271:ARG:NH1	2.45	0.48
5:A:8:A:C6	8:D:202:GLU:OE1	2.66	0.48
5:A:408:A:OP1	8:D:110:THR:HG21	2.14	0.48
5:A:1034:G:O2'	5:A:1035:A:H5'	2.13	0.48
5:A:1358:U:OP1	18:N:75:ARG:HB2	2.13	0.48
5:A:143:A:H5''	5:A:144:G:H5'	1.94	0.48
5:A:502:A:H2'	5:A:503:C:C6	2.48	0.48
8:D:185:LYS:HG3	8:D:186:PRO:HD2	1.95	0.48
13:I:31:ASN:HD21	13:I:67:VAL:HG22	1.78	0.48
14:J:53:ILE:HD11	14:J:61:ALA:HB1	1.95	0.48
5:A:544:G:P	8:D:59:GLN:NE2	2.87	0.48
5:A:1100:C:C5	6:B:95:ARG:CZ	2.97	0.48
5:A:1329:A:O3'	17:M:24:GLY:CA	2.62	0.48
8:D:188:ARG:NH2	8:D:195:ILE:O	2.46	0.48
11:G:133:THR:HG22	11:G:134:ALA:N	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:40:GLN:HE22	28:a:717:A:H2	1.50	0.48
28:a:1569:G:OP2	30:c:83:TYR:OH	2.27	0.48
3:2:62:LEU:HB3	3:2:65:ALA:HB2	1.95	0.48
5:A:19:A:H5'	9:E:90:THR:HG22	1.96	0.48
5:A:255:G:H2'	5:A:256:U:C6	2.48	0.48
5:A:339:C:H2'	5:A:340:U:H6	1.77	0.48
5:A:878:A:H5''	12:H:81:PRO:HB2	1.94	0.48
5:A:1400:C:C2	55:Y:34:C:O2	2.67	0.48
9:E:56:VAL:HB	9:E:57:PRO:HD3	1.96	0.48
10:F:5:GLU:OE2	22:R:24:LYS:NZ	2.45	0.48
28:a:329:G:C6	47:t:16:GLY:HA2	2.49	0.48
51:x:19:LEU:O	51:x:23:ARG:HG3	2.14	0.48
5:A:502:A:H2'	5:A:503:C:H6	1.78	0.48
5:A:878:A:OP1	12:H:82:GLY:N	2.32	0.48
27:Z:23:A:H2'	27:Z:24:G:C8	2.48	0.48
28:a:1484:G:H1'	28:a:1511:A:N6	2.28	0.48
28:a:2495:U:H4'	28:a:2496:U:OP1	2.14	0.48
28:a:2670:C:H42	34:g:109:PHE:CA	2.19	0.48
5:A:590:U:H2'	5:A:591:U:C6	2.48	0.48
5:A:1013:G:N2	5:A:1016:A:OP2	2.44	0.48
5:A:1014:A:H5'	23:S:14:HIS:CD2	2.49	0.48
5:A:1162:C:H2'	5:A:1163:A:C8	2.49	0.48
28:a:1185:U:H2'	28:a:1186:U:C6	2.49	0.48
5:A:826:C:H4'	12:H:13:ARG:HG2	1.96	0.48
5:A:892:A:HO2'	5:A:1415:G:HO2'	1.59	0.48
5:A:977:A:O2'	5:A:979:C:OP2	2.31	0.48
8:D:62:ARG:HH21	8:D:68:LEU:HA	1.77	0.48
11:G:14:PRO:HB2	11:G:19:GLY:HA2	1.95	0.48
28:a:483:A:O4'	47:t:45:HIS:CB	2.56	0.48
5:A:178:C:O2	5:A:179:A:H8	1.97	0.48
5:A:320:A:H2'	5:A:321:A:C8	2.49	0.48
5:A:337:G:H2'	5:A:338:A:H8	1.77	0.48
5:A:1061:G:H5''	14:J:61:ALA:HB2	1.96	0.48
12:H:11:LEU:HD22	12:H:75:ILE:HD11	1.96	0.48
28:a:172:A:H2'	28:a:173:A:C8	2.49	0.48
28:a:1342:U:C2'	46:s:61:LEU:HD22	2.44	0.48
5:A:8:A:N6	8:D:202:GLU:O	2.47	0.47
5:A:259:G:OP1	24:T:36:TYR:HE1	1.96	0.47
5:A:411:A:H4'	5:A:412:A:H5'	1.96	0.47
12:H:39:VAL:O	12:H:43:GLU:HG2	2.14	0.47
26:X:20:U:O4	27:Z:36:A:C6	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:76:A:C2'	28:a:2510:U:HO2'	2.25	0.47
28:a:1049:G:N2	28:a:1112:G:O2'	2.43	0.47
28:a:2308:G:O4'	33:f:129:SER:CB	2.53	0.47
28:a:1133:G:OP1	36:i:82:GLY:N	2.45	0.47
28:a:2307:G:O2'	33:f:121:SER:O	2.32	0.47
35:h:46:PHE:CZ	35:h:50:ARG:CD	2.93	0.47
35:h:132:PHE:HB2	35:h:140:ALA:HB3	1.96	0.47
5:A:339:C:H2'	5:A:340:U:C6	2.49	0.47
5:A:624:C:H4'	20:P:10:GLY:HA2	1.96	0.47
5:A:899:C:HO2'	28:a:1834:C:P	2.37	0.47
5:A:1298:U:C5	11:G:114:LYS:HD2	2.49	0.47
5:A:1329:A:O3'	17:M:24:GLY:C	2.58	0.47
19:O:17:ARG:NE	19:O:18:ASP:OD2	2.32	0.47
28:a:1802:C:H5''	30:c:146:MET:HE1	1.95	0.47
28:a:2686:A:C2	31:d:23:PRO:HB3	2.49	0.47
34:g:27:LYS:NZ	34:g:32:GLU:OE2	2.44	0.47
34:g:63:ALA:O	34:g:67:THR:HG22	2.15	0.47
39:l:6:ARG:HG3	39:l:6:ARG:HH11	1.79	0.47
47:t:81:ASP:OD2	47:t:98:SER:OG	2.32	0.47
5:A:545:C:P	8:D:69:GLU:CD	2.97	0.47
5:A:592:G:H2'	5:A:593:U:C6	2.49	0.47
5:A:1415:G:C6	5:A:1486:G:C6	3.03	0.47
5:A:1536:C:C5	54:4:10:G:N3	2.72	0.47
40:m:8:ARG:HD2	40:m:43:GLU:HG2	1.96	0.47
55:Y:26:G:H1	55:Y:45:G:N2	2.12	0.47
4:3:8:LYS:CE	28:a:2471:C:OP1	2.63	0.47
5:A:178:C:O2	5:A:178:C:H2'	2.15	0.47
5:A:212:G:H2'	5:A:213:G:C8	2.47	0.47
5:A:259:G:P	24:T:82:GLN:NE2	2.85	0.47
5:A:563:A:H4'	5:A:566:G:O2'	2.14	0.47
5:A:930:C:OP1	54:4:4:A:H5''	2.14	0.47
5:A:1483:A:O2'	28:a:1951:C:O2'	2.13	0.47
8:D:73:ARG:O	8:D:77:LYS:HG2	2.15	0.47
20:P:23:ASP:OD1	20:P:24:SER:N	2.48	0.47
28:a:865:A:H4'	29:b:100:G:N3	2.30	0.47
28:a:935:A:H5'	28:a:936:U:OP2	2.14	0.47
28:a:1133:G:C5'	36:i:84:ILE:HB	2.43	0.47
28:a:1793:A:O2'	30:c:206:GLY:N	2.45	0.47
35:h:94:ILE:HB	35:h:122:LEU:HB2	1.96	0.47
5:A:1477:U:H2'	5:A:1478:U:C6	2.49	0.47
6:B:100:MET:HE3	6:B:100:MET:HB2	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:102:MET:HE1	22:R:24:LYS:O	2.15	0.47
20:P:5:ARG:HG2	20:P:5:ARG:HH11	1.79	0.47
28:a:483:A:C4'	47:t:45:HIS:HB3	2.44	0.47
28:a:1133:G:C4	36:i:77:HIS:CD2	3.02	0.47
35:h:97:ARG:NH1	35:h:101:ASP:OD1	2.48	0.47
39:l:36:VAL:HG13	48:u:82:TYR:CD2	2.50	0.47
5:A:8:A:N6	8:D:202:GLU:CA	2.78	0.47
5:A:67:C:H2'	5:A:68:G:C8	2.49	0.47
5:A:392:C:C5'	20:P:13:LYS:NZ	2.77	0.47
5:A:560:A:H5'	5:A:566:G:N2	2.30	0.47
5:A:1180:A:OP1	13:I:105:THR:OG1	2.27	0.47
17:M:88:GLY:O	17:M:92:ARG:HG3	2.14	0.47
18:N:64:CYS:HB2	18:N:80:SER:HB3	1.97	0.47
28:a:271:G:O2'	28:a:272:A:O5'	2.31	0.47
28:a:859:G:H2'	28:a:860:G:O4'	2.15	0.47
28:a:1341:G:P	46:s:17:SER:HG	2.33	0.47
28:a:2434:A:H2'	28:a:2434:A:N3	2.28	0.47
33:f:73:SER:HB3	55:Y:56:C:H1'	1.96	0.47
39:l:111:GLU:CD	39:l:111:GLU:H	2.23	0.47
5:A:285:C:H2'	5:A:286:C:C6	2.50	0.47
5:A:600:A:H2'	5:A:601:G:H8	1.80	0.47
5:A:1329:A:H4'	17:M:24:GLY:C	2.40	0.47
8:D:4:TYR:HE2	8:D:11:LEU:HD21	1.80	0.47
28:a:1368:A:OP1	50:w:2:SER:OG	2.26	0.47
28:a:1802:C:OP2	30:c:182:ARG:NH1	2.26	0.47
34:g:9:VAL:HG22	34:g:50:LEU:HB2	1.95	0.47
3:2:4:ILE:HD11	28:a:594:A:H2	1.79	0.47
5:A:429:U:H5'	8:D:9:LEU:HD12	1.96	0.47
5:A:544:G:OP1	8:D:59:GLN:NE2	2.48	0.47
5:A:1189:U:OP1	18:N:98:LYS:NZ	2.41	0.47
12:H:50:LYS:NZ	12:H:60:GLU:OE2	2.46	0.47
27:Z:2:C:H2'	27:Z:3:C:C6	2.50	0.47
28:a:1511:A:HO2'	28:a:1512:G:H8	1.60	0.47
4:3:8:LYS:HE2	28:a:2471:C:OP1	2.14	0.47
5:A:1321:U:H5''	17:M:86:TYR:CE1	2.50	0.47
28:a:1780:U:H2'	28:a:1786:A:N6	2.30	0.47
28:a:1822:U:O2'	30:c:158:ALA:O	2.19	0.47
30:c:5:LYS:HE3	30:c:5:LYS:HB3	1.68	0.47
5:A:15:G:O2'	9:E:22:SER:CB	2.63	0.46
5:A:28:A:H5'	8:D:73:ARG:NH2	2.30	0.46
5:A:107:G:N7	24:T:10:ARG:NH2	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:335:C:H2'	5:A:336:A:C8	2.49	0.46
5:A:1329:A:O2'	17:M:24:GLY:HA2	2.15	0.46
8:D:161:LEU:O	8:D:164:GLN:HG2	2.15	0.46
10:F:88:MET:SD	10:F:90:MET:HE2	2.55	0.46
19:O:6:GLU:H	19:O:6:GLU:CD	2.23	0.46
19:O:56:LEU:CD2	28:a:717:A:C2	2.82	0.46
55:Y:62:C:H2'	55:Y:63:G:C8	2.48	0.46
5:A:551:U:H2'	5:A:552:U:H6	1.80	0.46
5:A:1225:A:H2'	5:A:1226:C:C5	2.50	0.46
18:N:83:LYS:HD2	18:N:83:LYS:HA	1.65	0.46
28:a:2331:A:H2'	28:a:2332:A:C8	2.50	0.46
28:a:2380:A:C6	41:n:99:TYR:CD1	3.04	0.46
35:h:71:LYS:HE3	35:h:108:VAL:HG13	1.97	0.46
35:h:135:HIS:HB3	35:h:138:VAL:HG12	1.97	0.46
53:z:36:GLU:OE2	53:z:46:ASP:HB2	2.16	0.46
5:A:17:U:O2'	5:A:1079:G:C1'	2.59	0.46
5:A:53:A:N6	5:A:359:G:O6	2.47	0.46
5:A:151:A:C5	5:A:152:A:C8	3.04	0.46
5:A:236:A:H2'	5:A:237:G:C8	2.51	0.46
5:A:303:A:H2'	5:A:304:U:O4'	2.15	0.46
5:A:427:U:O2'	5:A:541:G:OP1	2.33	0.46
5:A:522:C:H5''	16:L:117:TYR:OH	2.16	0.46
5:A:564:C:H1'	21:Q:33:ILE:O	2.14	0.46
5:A:1314:C:H2'	5:A:1315:U:C6	2.49	0.46
5:A:1317:C:OP2	18:N:28:LYS:HD3	2.16	0.46
8:D:124:MET:HE2	8:D:127:GLY:HA2	1.96	0.46
28:a:1592:A:H2'	28:a:1593:A:C8	2.50	0.46
28:a:1818:C:H3'	30:c:62:TYR:CZ	2.50	0.46
31:d:46:ARG:NH2	31:d:88:GLU:O	2.46	0.46
54:4:3:C:H2'	54:4:4:A:C8	2.50	0.46
5:A:269:C:H2'	5:A:270:A:H8	1.80	0.46
5:A:737:C:OP1	10:F:91:ARG:N	2.32	0.46
5:A:1001:C:H2'	5:A:1002:G:C8	2.50	0.46
5:A:1125:U:P	14:J:37:ARG:NH2	2.89	0.46
5:A:1228:C:P	17:M:107:ARG:HH12	2.37	0.46
20:P:6:LEU:HD13	20:P:17:TYR:CG	2.49	0.46
28:a:1671:A:O4'	37:j:5:GLN:HG3	2.15	0.46
28:a:2533:G:C4'	34:g:175:LYS:HB3	2.44	0.46
55:Y:53:G:H2'	55:Y:54:5MU:H6	1.80	0.46
3:2:54:ASP:HB3	38:k:57:LEU:HD22	1.98	0.46
5:A:191:G:H2'	5:A:192:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:215:C:H2'	5:A:216:U:C6	2.51	0.46
5:A:338:A:H2'	5:A:339:C:H6	1.80	0.46
5:A:544:G:OP1	8:D:59:GLN:CD	2.58	0.46
5:A:1368:A:H5''	18:N:101:TRP:HZ2	1.81	0.46
5:A:1400:C:N4	55:Y:34:C:C1'	2.79	0.46
28:a:282:A:H2'	28:a:283:G:C8	2.50	0.46
28:a:898:A:C6	28:a:899:C:H1'	2.51	0.46
28:a:1163:C:O2'	44:q:8:GLY:HA2	2.15	0.46
30:c:107:PRO:HD2	30:c:110:LEU:HD22	1.98	0.46
35:h:62:LEU:O	35:h:66:ASN:ND2	2.48	0.46
5:A:191:G:H2'	5:A:192:A:H8	1.78	0.46
7:C:131:ARG:HD2	9:E:55:GLU:OE1	2.15	0.46
10:F:18:VAL:O	10:F:22:ILE:HG13	2.16	0.46
13:I:130:ARG:NH2	55:Y:35:A:OP2	2.42	0.46
28:a:1117:G:HO2'	28:a:1118:G:P	2.38	0.46
28:a:2036:G:C8	31:d:150:MEQ:HE3	2.51	0.46
5:A:409:U:N3	5:A:433:G:N1	2.58	0.46
28:a:2299:C:OP2	41:n:10:ARG:HD3	2.16	0.46
28:a:2381:A:O2'	41:n:117:PHE:O	2.25	0.46
28:a:2595:C:H2'	28:a:2596:G:C8	2.51	0.46
33:f:158:THR:HG22	33:f:160:ALA:N	2.22	0.46
5:A:513:C:H2'	5:A:514:C:C6	2.51	0.46
5:A:532:A:N6	7:C:156:ARG:HH12	2.13	0.46
5:A:631:C:H5''	5:A:632:U:O5'	2.15	0.46
6:B:128:LYS:HE3	6:B:129:LEU:HD23	1.97	0.46
11:G:68:ASN:O	11:G:138:ARG:NH2	2.49	0.46
28:a:628:A:H2'	38:k:78:ARG:NH2	2.31	0.46
28:a:2380:A:N3	41:n:99:TYR:CE1	2.84	0.46
28:a:2383:G:O3'	41:n:17:LYS:HE2	2.15	0.46
5:A:199:A:H2'	5:A:200:G:C8	2.51	0.46
5:A:505:G:H2'	5:A:506:G:C8	2.51	0.46
5:A:1073:U:H4'	6:B:105:LYS:HE2	1.98	0.46
5:A:1287:A:H2'	5:A:1288:A:C8	2.51	0.46
5:A:1415:G:C2	5:A:1416:G:C8	3.04	0.46
14:J:15:HIS:HB3	14:J:70:HIS:CE1	2.50	0.46
21:Q:8:LEU:HB3	21:Q:25:ILE:HD12	1.97	0.46
28:a:276:U:H2'	28:a:277:G:C8	2.51	0.46
28:a:920:A:H4'	29:b:97:C:O2	2.15	0.46
28:a:2552:U:O2	37:j:23:LYS:NZ	2.49	0.46
49:v:25:ARG:HA	49:v:25:ARG:HD2	1.80	0.46
5:A:249:U:O2	5:A:275:G:O6	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:401:C:OP1	8:D:74:ASN:OD1	2.34	0.46
5:A:508:U:C5'	8:D:51:TYR:CD2	2.99	0.46
5:A:1043:G:O2'	5:A:1044:A:O5'	2.30	0.46
5:A:1321:U:C5'	17:M:86:TYR:CE1	2.99	0.46
6:B:64:LYS:HA	6:B:64:LYS:HD3	1.74	0.46
7:C:73:PRO:HG3	7:C:105:GLU:OE1	2.15	0.46
27:Z:51:U:H2'	27:Z:52:G:C8	2.50	0.46
28:a:1801:G:C5	30:c:176:LEU:HD13	2.51	0.46
3:2:64:TYR:HH	28:a:594:A:HO2'	1.58	0.45
5:A:26:A:N6	5:A:558:G:H1'	2.30	0.45
5:A:231:U:H2'	5:A:232:G:H8	1.81	0.45
5:A:592:G:C6	5:A:648:A:C6	3.04	0.45
27:Z:5:G:H2'	27:Z:6:G:C8	2.51	0.45
27:Z:76:A:O2'	28:a:2510:U:C2'	2.63	0.45
28:a:542:C:H2'	28:a:543:A:C8	2.52	0.45
28:a:1024:G:O6	36:i:68:LYS:NZ	2.34	0.45
28:a:1277:A:O4'	40:m:16:HIS:CE1	2.69	0.45
5:A:44:A:OP1	20:P:11:ALA:HA	2.16	0.45
5:A:599:C:H2'	5:A:600:A:H8	1.81	0.45
5:A:1162:C:H2'	5:A:1163:A:H8	1.81	0.45
8:D:76:TYR:CE2	8:D:204:TYR:HB3	2.51	0.45
35:h:65:ALA:HB1	35:h:135:HIS:HB2	1.97	0.45
5:A:413:G:H1'	5:A:428:G:N2	2.31	0.45
5:A:1218:C:H2'	5:A:1219:A:C8	2.51	0.45
5:A:1328:C:OP1	17:M:28:THR:HG21	2.16	0.45
15:K:126:LYS:HE2	15:K:126:LYS:HB2	1.58	0.45
28:a:1916:A:C2	28:a:1923:A:C6	3.03	0.45
28:a:2535:A:H5'	34:g:157:TYR:CE1	2.52	0.45
28:a:2834:C:H5''	31:d:56:LYS:HE3	1.98	0.45
28:a:2906:C:H2'	28:a:2907:U:O4'	2.16	0.45
3:2:27:ALA:O	3:2:28:ASN:HB2	2.17	0.45
5:A:193:C:H2'	5:A:194:C:C6	2.51	0.45
5:A:384:G:C2	5:A:385:C:C4	3.04	0.45
5:A:544:G:O5'	8:D:59:GLN:NE2	2.49	0.45
19:O:88:ARG:NE	28:a:716:U:H5	2.13	0.45
27:Z:65:G:H2'	27:Z:66:U:C6	2.52	0.45
28:a:2014:G:OP1	45:r:42:LYS:N	2.34	0.45
32:e:7:ASP:CG	32:e:122:GLU:H	2.25	0.45
35:h:42:LYS:O	35:h:43:ASN:C	2.59	0.45
37:j:114:LYS:HE2	37:j:114:LYS:HB2	1.73	0.45
5:A:34:C:H2'	5:A:35:G:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:346:G:OP2	42:o:41:GLN:NE2	2.44	0.45
5:A:419:C:N3	5:A:425:G:N1	2.65	0.45
5:A:564:C:H5'	21:Q:34:TYR:CD1	2.51	0.45
5:A:1329:A:H5''	17:M:26:GLY:N	2.32	0.45
5:A:1422:G:H5'	37:j:48:PRO:HG3	1.98	0.45
8:D:174:ASP:HB3	8:D:179:GLU:HG2	1.98	0.45
12:H:48:ASP:OD1	12:H:49:PHE:N	2.46	0.45
28:a:595:U:H2'	28:a:596:U:C6	2.52	0.45
28:a:2849:U:H5''	42:o:52:ASN:O	2.17	0.45
5:A:263:A:OP2	24:T:74:ARG:NE	2.50	0.45
5:A:530:G:O2'	27:Z:35:A:H4'	2.17	0.45
5:A:1227:A:H4'	17:M:114:LYS:HE2	1.99	0.45
5:A:1302:C:C5	17:M:17:ILE:HG13	2.52	0.45
12:H:89:LYS:HE3	12:H:89:LYS:HB3	1.76	0.45
27:Z:2:C:H2'	27:Z:3:C:H6	1.81	0.45
28:a:2255:OMG:HM23	28:a:2255:OMG:H1'	1.76	0.45
36:i:13:ARG:NH2	36:i:49:ASP:O	2.44	0.45
38:k:10:GLU:H	38:k:10:GLU:CD	2.25	0.45
5:A:335:C:C2	5:A:336:A:C8	3.05	0.45
21:Q:21:ILE:HG13	21:Q:46:VAL:HB	1.99	0.45
28:a:1340:G:O3'	46:s:17:SER:HB2	2.16	0.45
28:a:2295:U:H2'	28:a:2296:U:C6	2.51	0.45
28:a:2570:A:N1	37:j:28:SER:OG	2.38	0.45
5:A:504:C:C2	5:A:542:G:N2	2.85	0.45
14:J:66:GLU:HB3	18:N:99:ALA:HB2	1.99	0.45
28:a:1388:C:H2'	28:a:1389:A:C8	2.52	0.45
55:Y:27:U:H2'	55:Y:28:C:H6	1.81	0.45
4:3:1:MET:HE2	4:3:1:MET:HB2	1.92	0.45
5:A:59:A:H3'	5:A:331:G:H22	1.82	0.45
5:A:160:A:H1'	5:A:344:A:C5	2.52	0.45
5:A:175:C:H2'	5:A:176:C:H6	1.81	0.45
5:A:337:G:C2	5:A:338:A:C5	3.04	0.45
5:A:452:A:H2'	5:A:453:G:O4'	2.16	0.45
5:A:720:C:H5''	22:R:41:PRO:HA	1.99	0.45
7:C:134:MET:HE2	7:C:168:TYR:CD2	2.51	0.45
11:G:71:PRO:O	11:G:96:ARG:HG2	2.17	0.45
28:a:1821:A:OP2	30:c:155:ALA:N	2.47	0.45
28:a:2255:OMG:N7	39:l:81:4D4:NH1	2.57	0.45
36:i:11:VAL:HG21	36:i:50:THR:HA	1.99	0.45
5:A:60:A:OP1	5:A:331:G:N1	2.34	0.45
5:A:508:U:H4'	8:D:51:TYR:HD2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:751:U:OP1	19:O:17:ARG:NH1	2.50	0.45
5:A:784:A:H5'	28:a:1839:C:OP1	2.16	0.45
5:A:1060:U:P	18:N:85:ARG:HH12	2.40	0.45
6:B:117:LEU:HB3	6:B:141:LEU:HD23	1.99	0.45
7:C:50:ALA:O	7:C:70:THR:OG1	2.35	0.45
8:D:103:TYR:HD2	8:D:104:ARG:HD2	1.80	0.45
28:a:628:A:H2'	38:k:78:ARG:CZ	2.48	0.45
28:a:1250:G:OP1	32:e:44:ARG:NH1	2.49	0.45
28:a:1722:U:H2'	28:a:1723:G:O4'	2.16	0.45
28:a:2601:G:H5'	30:c:241:GLY:HA3	1.99	0.45
35:h:113:SER:O	35:h:116:ARG:NH2	2.50	0.45
5:A:262:A:H5'	24:T:68:HIS:HB3	1.99	0.44
5:A:593:U:H2'	5:A:594:U:C6	2.51	0.44
5:A:710:G:OP1	10:F:53:LYS:HD2	2.16	0.44
5:A:1144:G:N2	5:A:1146:A:H62	2.16	0.44
5:A:1308:U:OP1	17:M:97:VAL:HG22	2.16	0.44
5:A:1371:G:P	13:I:14:SER:OG	2.75	0.44
5:A:1492:A:OP1	16:L:44:LYS:N	2.43	0.44
20:P:21:VAL:HG11	20:P:60:TRP:NE1	2.31	0.44
28:a:1141:G:O2'	36:i:26:GLY:HA3	2.16	0.44
28:a:2259:G:N2	49:v:9:SER:CB	2.78	0.44
28:a:2307:G:C4'	33:f:122:PHE:C	2.88	0.44
28:a:2535:A:H4'	34:g:157:TYR:CD2	2.52	0.44
3:2:2:PRO:HD2	28:a:669:U:O2	2.17	0.44
5:A:16:A:N1	5:A:920:U:C2	2.85	0.44
12:H:29:SER:HB3	12:H:57:PRO:HB2	1.99	0.44
28:a:858:G:H2'	28:a:859:G:C8	2.52	0.44
28:a:1257:U:C5	32:e:68:ALA:HA	2.52	0.44
37:j:38:ILE:HD11	37:j:112:PHE:HZ	1.82	0.44
46:s:74:ILE:HD12	46:s:74:ILE:HA	1.85	0.44
5:A:19:A:H2'	5:A:20:U:H6	1.81	0.44
5:A:402:G:O3'	8:D:132:ILE:CD1	2.63	0.44
5:A:1493:A:H2'	28:a:1917:A:N6	2.32	0.44
13:I:28:ILE:HG12	13:I:63:LEU:HD22	1.99	0.44
28:a:572:G:H2'	28:a:2034:6MZ:N7	2.33	0.44
28:a:725:C:H2'	28:a:726:U:O4'	2.17	0.44
33:f:73:SER:CB	55:Y:56:C:C1'	2.93	0.44
43:p:49:ASP:HA	43:p:52:GLN:HB2	1.99	0.44
53:z:55:ILE:HG13	53:z:56:ALA:O	2.16	0.44
5:A:783:C:H4'	28:a:1838:C:OP1	2.17	0.44
19:O:60:VAL:CG2	28:a:717:A:C8	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:76:A:N6	28:a:2588:U:C4'	2.81	0.44
33:f:36:LEU:HD22	33:f:154:ILE:HG12	1.99	0.44
5:A:634:C:H2'	5:A:635:A:C8	2.51	0.44
5:A:658:C:H1'	19:O:22:THR:HG21	1.99	0.44
5:A:1381:U:H5'	54:4:3:C:H1'	1.96	0.44
28:a:958:G:N7	39:l:14:LYS:NZ	2.58	0.44
28:a:1268:G:O6	45:r:13:SER:HB3	2.18	0.44
28:a:2000:C:H5	37:j:32:TYR:OH	2.00	0.44
32:e:137:LYS:O	32:e:141:MET:HG3	2.16	0.44
35:h:46:PHE:CE1	35:h:50:ARG:HD3	2.53	0.44
35:h:96:THR:HG22	35:h:117:LEU:CD1	2.47	0.44
5:A:380:G:N1	5:A:384:G:O6	2.51	0.44
5:A:521:G:P	16:L:70:GLU:HG2	2.57	0.44
5:A:1019:A:H2'	5:A:1020:G:O4'	2.18	0.44
6:B:12:ALA:HA	6:B:208:ARG:HH11	1.81	0.44
7:C:110:GLU:HB2	7:C:144:LEU:HD22	1.99	0.44
9:E:34:THR:HG22	9:E:52:LYS:HG2	2.00	0.44
22:R:21:ILE:HG21	22:R:55:LEU:HD23	1.98	0.44
28:a:1601:U:OP2	46:s:40:LYS:HD2	2.17	0.44
33:f:47:LYS:HB2	33:f:47:LYS:HE2	1.57	0.44
5:A:246:A:C6	5:A:281:G:N2	2.86	0.44
5:A:425:G:H2'	5:A:426:U:C6	2.53	0.44
5:A:1048:G:C4'	18:N:3:LYS:HD2	2.47	0.44
5:A:1060:U:C5'	14:J:53:ILE:HG13	2.48	0.44
5:A:1119:C:OP1	13:I:85:ARG:NH1	2.50	0.44
5:A:1273:C:H2'	5:A:1274:A:O4'	2.18	0.44
7:C:14:ILE:HG22	7:C:15:VAL:HG13	2.00	0.44
8:D:170:TRP:CE3	8:D:186:PRO:HB3	2.53	0.44
9:E:151:GLU:H	9:E:151:GLU:CD	2.22	0.44
12:H:27:MET:HE2	12:H:27:MET:HB3	1.94	0.44
20:P:1:MET:HG3	20:P:2:VAL:N	2.32	0.44
22:R:48:ARG:HE	22:R:48:ARG:HB3	1.68	0.44
28:a:582:U:O3'	43:p:31:VAL:HG13	2.17	0.44
2:1:39:ARG:NH2	28:a:468:G:N7	2.46	0.44
5:A:564:C:C4	5:A:565:U:C4	3.06	0.44
5:A:702:A:C5	28:a:1850:A:C4	3.06	0.44
5:A:1220:G:H4'	23:S:34:TRP:O	2.18	0.44
5:A:1226:C:H6	17:M:102:THR:OG1	2.01	0.44
5:A:1406:U:O2	28:a:1923:A:O2'	2.31	0.44
8:D:8:LYS:HB3	8:D:21:LEU:HB3	2.00	0.44
28:a:493:G:H2'	28:a:494:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1133:G:C4'	36:i:84:ILE:HB	2.47	0.44
28:a:1849:A:O3'	28:a:1850:A:H8	2.01	0.44
28:a:2237:U:H2'	28:a:2238:G:C8	2.53	0.44
28:a:2298:G:P	41:n:10:ARG:HD2	2.58	0.44
28:a:2380:A:C1'	41:n:99:TYR:CZ	3.00	0.44
28:a:2671:C:O2	34:g:109:PHE:HB3	2.18	0.44
32:e:10:SER:HG	32:e:11:ALA:N	2.15	0.44
5:A:653:U:H5'	12:H:56:LYS:NZ	2.33	0.44
5:A:1040:U:H2'	5:A:1041:G:C8	2.51	0.44
5:A:1408:A:N6	5:A:1494:G:O6	2.51	0.44
9:E:81:LEU:HB3	9:E:147:MET:SD	2.57	0.44
14:J:25:ILE:HD13	14:J:25:ILE:HA	1.82	0.44
27:Z:9:A:N6	27:Z:22:G:N7	2.66	0.44
28:a:358:U:H2'	28:a:359:G:C8	2.53	0.44
28:a:1134:U:H4'	36:i:75:TYR:CE1	2.53	0.44
28:a:1603:G:OP1	46:s:62:VAL:HB	2.18	0.44
28:a:1802:C:H5'	30:c:146:MET:HE1	2.00	0.44
28:a:2308:G:C4'	33:f:129:SER:HB2	2.48	0.44
31:d:74:GLU:H	31:d:74:GLU:CD	2.26	0.44
5:A:181:A:H1'	5:A:182:A:N7	2.33	0.43
5:A:402:G:H4'	8:D:132:ILE:CD1	2.47	0.43
5:A:606:G:N2	5:A:632:U:OP1	2.35	0.43
5:A:611:C:H42	5:A:629:A:H61	1.66	0.43
5:A:645:G:C2	5:A:646:G:C8	3.05	0.43
5:A:736:C:H2'	5:A:737:C:C6	2.52	0.43
5:A:1329:A:C5'	17:M:26:GLY:H	2.30	0.43
8:D:15:GLU:HG2	8:D:60:LYS:HG3	2.00	0.43
17:M:71:ARG:HH21	33:f:115:ARG:HH11	1.52	0.43
17:M:93:ARG:HH12	23:S:80:TYR:HE2	1.66	0.43
28:a:659:U:H2'	28:a:660:U:C6	2.53	0.43
28:a:2306:U:HO2'	33:f:123:ASP:C	2.20	0.43
43:p:58:ARG:HA	43:p:61:TRP:CE3	2.53	0.43
3:2:14:PHE:O	3:2:15:LYS:HD3	2.18	0.43
5:A:393:A:C2	5:A:394:G:C8	3.06	0.43
5:A:628:G:C2	5:A:629:A:C5	3.06	0.43
5:A:642:A:H2'	5:A:643:C:C6	2.53	0.43
5:A:689:C:OP1	15:K:46:THR:CB	2.67	0.43
5:A:1127:G:H5'	5:A:1280:A:O2'	2.18	0.43
5:A:1192:C:OP2	7:C:4:LYS:NZ	2.35	0.43
13:I:129:LYS:HZ2	55:Y:33:U:P	2.41	0.43
18:N:40:ASP:OD1	18:N:41:ARG:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:143:C:H4'	46:s:1:MET:O	2.19	0.43
28:a:191:A:H2'	28:a:192:C:C6	2.53	0.43
28:a:1916:A:C2	28:a:1923:A:C5	3.06	0.43
46:s:89:GLU:OE1	46:s:89:GLU:HA	2.18	0.43
5:A:19:A:C5	5:A:917:G:N1	2.83	0.43
5:A:204:G:H2'	5:A:205:A:H8	1.82	0.43
5:A:630:A:H8	5:A:630:A:OP2	2.01	0.43
5:A:1538:C:N4	54:4:10:G:OP2	2.51	0.43
11:G:56:LYS:HE2	11:G:56:LYS:HB2	1.79	0.43
28:a:813:U:OP2	38:k:20:GLY:C	2.61	0.43
28:a:1030:A:N6	28:a:1127:G:H2'	2.34	0.43
28:a:1153:A:O3'	43:p:81:ASN:HB2	2.17	0.43
32:e:147:LEU:HD11	32:e:170:ARG:HG3	2.00	0.43
34:g:2:SER:O	34:g:6:LYS:HG2	2.17	0.43
35:h:115:VAL:O	35:h:116:ARG:NH1	2.51	0.43
37:j:38:ILE:HD11	37:j:112:PHE:CZ	2.53	0.43
5:A:228:A:C2	20:P:1:MET:SD	3.11	0.43
5:A:299:G:H2'	5:A:300:A:C8	2.54	0.43
5:A:402:G:C3'	8:D:132:ILE:HD11	2.48	0.43
5:A:632:U:H5'	5:A:633:G:H8	1.80	0.43
17:M:79:ARG:NH2	23:S:69:HIS:NE2	2.67	0.43
28:a:879:A:H2	28:a:902:A:N7	2.15	0.43
35:h:65:ALA:CB	35:h:135:HIS:HB2	2.48	0.43
41:n:60:GLU:HG3	41:n:61:GLN:OE1	2.18	0.43
41:n:83:LEU:HD11	41:n:114:GLY:HA3	2.00	0.43
5:A:864:A:H4'	9:E:90:THR:HG23	2.00	0.43
5:A:1202:U:H1'	18:N:69:ARG:HD2	2.00	0.43
5:A:1415:G:C5	5:A:1486:G:N1	2.86	0.43
8:D:177:LYS:H	8:D:177:LYS:HG2	1.62	0.43
11:G:149:LYS:HE3	15:K:61:PHE:CZ	2.53	0.43
28:a:853:C:H2'	28:a:854:U:C6	2.54	0.43
28:a:958:G:H4'	39:l:82:MET:HE1	2.00	0.43
28:a:1268:G:C5	45:r:16:LYS:HE3	2.53	0.43
28:a:1818:C:H3'	30:c:62:TYR:CE1	2.54	0.43
28:a:1821:A:C2	30:c:178:SER:HB3	2.54	0.43
28:a:2749:C:O2	34:g:139:GLN:NE2	2.51	0.43
5:A:262:A:H4'	24:T:70:ASN:HB3	1.88	0.43
5:A:402:G:C4'	8:D:132:ILE:HD11	2.47	0.43
5:A:600:A:H2'	5:A:601:G:C8	2.54	0.43
5:A:637:C:H2'	5:A:638:U:C6	2.53	0.43
5:A:951:G:O6	17:M:104:THR:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:95:GLU:OE1	8:D:100:ASN:ND2	2.49	0.43
20:P:20:VAL:HG12	20:P:35:ARG:HG3	2.00	0.43
25:U:31:GLU:OE2	25:U:34:ARG:NH2	2.50	0.43
28:a:1183:U:H2'	28:a:1184:G:C8	2.52	0.43
28:a:1748:A:H2'	28:a:1749:U:C6	2.53	0.43
28:a:1829:U:OP2	30:c:221:ARG:HD2	2.18	0.43
33:f:111:ILE:HB	33:f:114:PHE:HB2	1.99	0.43
36:i:114:LEU:HG	36:i:118:MET:HE3	2.01	0.43
38:k:132:ARG:HG3	38:k:142:ILE:HD13	2.00	0.43
42:o:38:LYS:HE2	42:o:38:LYS:HB3	1.66	0.43
3:2:53:GLY:O	28:a:836:G:H4'	2.19	0.43
5:A:219:U:H2'	5:A:220:G:H8	1.84	0.43
5:A:517:G:N2	5:A:530:G:OP1	2.42	0.43
23:S:16:LEU:O	23:S:20:GLU:HG2	2.19	0.43
36:i:46:PRO:HD3	43:p:60:LEU:HD13	2.00	0.43
5:A:323:U:C5'	24:T:21:ASN:HD22	2.27	0.43
5:A:653:U:O4'	12:H:56:LYS:HE3	2.19	0.43
11:G:16:PRO:HD2	11:G:44:TYR:OH	2.18	0.43
17:M:92:ARG:CB	28:a:890:C:O4'	2.66	0.43
28:a:1140:G:N2	36:i:108:MET:HE2	2.34	0.43
28:a:1810:A:C2	50:w:28:ARG:HD2	2.54	0.43
28:a:2309:U:H5''	33:f:131:GLY:HA3	2.01	0.43
31:d:11:MET:HE2	31:d:11:MET:HB3	1.94	0.43
34:g:164:TYR:HB2	34:g:167:GLU:HB2	2.01	0.43
35:h:110:VAL:HG11	35:h:132:PHE:CD2	2.53	0.43
35:h:110:VAL:HG11	35:h:132:PHE:CE2	2.54	0.43
48:u:55:GLU:CD	48:u:55:GLU:H	2.27	0.43
5:A:444:G:H2'	5:A:445:G:C8	2.54	0.43
5:A:1442:G:H2'	5:A:1443:C:C6	2.54	0.43
5:A:1537:U:H2'	5:A:1538:C:O4'	2.19	0.43
6:B:4:VAL:HG21	6:B:212:LEU:HD21	1.99	0.43
11:G:82:GLY:HA2	26:X:12:A:H4'	2.01	0.43
14:J:8:ILE:HB	14:J:74:VAL:HB	2.00	0.43
14:J:32:THR:O	14:J:83:THR:OG1	2.34	0.43
28:a:1245:C:O2	38:k:4:ASN:HA	2.18	0.43
28:a:1705:G:H2'	28:a:1706:C:C6	2.54	0.43
28:a:2380:A:C4	41:n:99:TYR:CD1	3.07	0.43
36:i:95:ARG:HG2	36:i:96:ARG:HG2	2.01	0.43
5:A:427:U:OP2	5:A:428:G:O2'	2.18	0.43
5:A:481:G:H21	5:A:482:A:H61	1.66	0.43
5:A:608:A:C2	5:A:609:A:H1'	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:900:A:H4'	28:a:1834:C:H5'	2.01	0.43
5:A:1409:C:C4'	28:a:1919:3TD:H10	2.47	0.43
17:M:4:ILE:HG23	17:M:57:ARG:HG2	2.00	0.43
28:a:2277:A:H2'	28:a:2278:A:C8	2.53	0.43
28:a:2317:C:H5''	33:f:88:LYS:HD2	2.01	0.43
28:a:2518:U:H4'	36:i:81:ILE:HG21	2.00	0.43
28:a:2792:C:H2'	28:a:2793:C:C6	2.54	0.43
31:d:99:GLU:HG2	31:d:182:ALA:HB2	2.00	0.43
46:s:93:LEU:HD12	46:s:93:LEU:HA	1.83	0.43
55:Y:50:U:H2'	55:Y:51:C:C6	2.53	0.43
1:O:38:LYS:HE3	1:O:38:LYS:HB3	1.77	0.42
5:A:19:A:OP1	9:E:130:SER:OG	2.35	0.42
5:A:1004:A:H2'	5:A:1005:A:O4'	2.18	0.42
8:D:7:PRO:HB2	8:D:10:LYS:HB3	2.01	0.42
20:P:5:ARG:NH1	20:P:22:ALA:HB3	2.30	0.42
28:a:641:U:H2'	28:a:642:C:C6	2.54	0.42
28:a:1810:A:H3'	28:a:1811:A:C8	2.54	0.42
47:t:50:PRO:HA	47:t:54:GLN:HE21	1.83	0.42
5:A:17:U:O2'	5:A:1079:G:O2'	1.98	0.42
5:A:235:C:H1'	21:Q:63:GLU:OE2	2.18	0.42
5:A:501:C:O2	5:A:549:C:O2'	2.37	0.42
5:A:564:C:H5'	21:Q:34:TYR:HD1	1.84	0.42
5:A:595:A:O2'	5:A:640:A:N6	2.52	0.42
5:A:636:U:H2'	5:A:637:C:H6	1.84	0.42
5:A:1381:U:O3'	54:4:2:G:O2'	2.35	0.42
5:A:1400:C:H42	55:Y:34:C:H1'	1.83	0.42
18:N:98:LYS:HB3	18:N:98:LYS:HE3	1.83	0.42
28:a:2:G:H2'	28:a:3:U:C6	2.54	0.42
28:a:6:A:O2'	36:i:135:GLN:OE1	2.26	0.42
28:a:1007:C:O2	36:i:30:THR:HG21	2.18	0.42
28:a:1342:U:OP1	46:s:19:LYS:NZ	2.37	0.42
28:a:1541:U:H2'	28:a:1542:G:H8	1.84	0.42
28:a:2604:A:N7	30:c:236:GLU:HB2	2.35	0.42
28:a:2684:U:O2'	28:a:2685:C:H5'	2.19	0.42
28:a:2751:G:O2'	34:g:67:THR:CB	2.66	0.42
33:f:57:LEU:O	33:f:61:SER:OG	2.35	0.42
36:i:58:ASN:HA	36:i:126:ALA:O	2.19	0.42
5:A:15:G:C8	5:A:1396:A:C2	3.08	0.42
5:A:262:A:C2'	24:T:70:ASN:HD22	2.24	0.42
5:A:333:U:C2	5:A:334:C:C5	3.07	0.42
5:A:1220:G:P	18:N:53:ARG:HH12	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:105:MET:HG2	8:D:107:PHE:CE2	2.54	0.42
10:F:98:GLU:OE1	10:F:98:GLU:N	2.36	0.42
13:I:21:ILE:HA	13:I:21:ILE:HD13	1.81	0.42
13:I:83:ILE:O	13:I:87:LEU:HD12	2.20	0.42
15:K:24:HIS:HB3	15:K:31:ILE:HB	2.00	0.42
23:S:44:MET:HB2	23:S:47:LEU:CD2	2.48	0.42
28:a:646:A:H2'	28:a:647:C:O4'	2.18	0.42
28:a:875:C:H4'	39:l:64:TRP:CD1	2.54	0.42
28:a:1143:U:H5	36:i:65:THR:HG1	1.66	0.42
28:a:1609:C:N4	28:a:1624:G:OP2	2.39	0.42
30:c:161:TYR:HB3	30:c:194:GLU:HG2	2.00	0.42
31:d:80:TRP:CD1	31:d:202:ILE:HD11	2.55	0.42
32:e:41:GLN:HG2	32:e:43:THR:HG23	2.01	0.42
36:i:110:PRO:O	36:i:115:GLY:HA3	2.20	0.42
5:A:35:G:H2'	5:A:36:C:H6	1.84	0.42
5:A:171:A:O2'	5:A:172:A:O4'	2.27	0.42
5:A:461:A:H2'	5:A:462:G:H8	1.85	0.42
5:A:513:C:H2'	5:A:514:C:H6	1.82	0.42
5:A:620:C:C2	8:D:132:ILE:HD13	2.55	0.42
5:A:1054:C:C4	27:Z:34:G:N9	2.86	0.42
5:A:1059:C:O3'	18:N:85:ARG:NH1	2.45	0.42
5:A:1409:C:H2'	5:A:1410:A:C8	2.46	0.42
5:A:1462:C:H2'	5:A:1463:U:C6	2.55	0.42
28:a:1791:A:H4'	30:c:218:PRO:HB3	2.01	0.42
1:0:33:LYS:HA	1:0:33:LYS:HD2	1.82	0.42
5:A:236:A:H2'	5:A:237:G:H8	1.85	0.42
5:A:546:A:C8	8:D:68:LEU:CD2	3.02	0.42
5:A:554:A:H2'	5:A:555:U:C6	2.55	0.42
5:A:617:G:H5''	20:P:44:SER:OG	2.19	0.42
5:A:636:U:H2'	5:A:637:C:C6	2.55	0.42
6:B:139:ARG:HA	6:B:139:ARG:CZ	2.50	0.42
12:H:43:GLU:HG3	12:H:101:ILE:HD13	2.02	0.42
20:P:40:ASN:HB3	20:P:43:ALA:HB2	2.01	0.42
28:a:744:A:H2'	28:a:745:A:C8	2.54	0.42
28:a:835:A:H2'	28:a:836:G:C8	2.54	0.42
28:a:960:U:N3	29:b:90:C:OP1	2.52	0.42
28:a:1821:A:OP1	30:c:155:ALA:HA	2.19	0.42
28:a:2712:G:H1'	40:m:71:ARG:CZ	2.49	0.42
28:a:2904:A:H2'	28:a:2905:C:O4'	2.18	0.42
5:A:180:U:C2'	5:A:181:A:H5'	2.49	0.42
5:A:376:G:C2	5:A:389:A:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:475:C:H2'	5:A:476:U:C6	2.54	0.42
5:A:591:U:C2	5:A:592:G:C8	3.08	0.42
5:A:593:U:N3	5:A:594:U:O4	2.53	0.42
5:A:892:A:O2'	5:A:1415:G:O2'	2.33	0.42
5:A:1049:U:P	18:N:3:LYS:HG2	2.60	0.42
8:D:103:TYR:HE1	8:D:110:THR:HA	1.84	0.42
13:I:63:LEU:HD23	13:I:65:ILE:HD11	2.02	0.42
22:R:21:ILE:N	22:R:21:ILE:HD13	2.34	0.42
28:a:786:G:N1	30:c:228:VAL:HG11	2.35	0.42
28:a:2020:U:O2'	53:z:4:GLN:O	2.36	0.42
47:t:39:ILE:HG22	47:t:40:ASN:N	2.35	0.42
4:3:6:SER:CB	28:a:2470:C:H5''	2.50	0.42
4:3:6:SER:HB3	28:a:2470:C:H5''	2.01	0.42
5:A:592:G:C5	5:A:593:U:C4	3.07	0.42
5:A:983:A:H5'	5:A:984:C:OP2	2.20	0.42
5:A:1368:A:OP1	13:I:113:ARG:NH2	2.51	0.42
5:A:1408:A:O3'	28:a:1920:A:H2	2.02	0.42
6:B:135:LEU:HA	6:B:138:THR:HG22	2.02	0.42
17:M:23:TYR:CE2	17:M:70:ARG:HG3	2.54	0.42
17:M:92:ARG:HG2	28:a:890:C:C1'	2.49	0.42
28:a:639:A:OP1	38:k:130:GLY:HA3	2.19	0.42
28:a:880:A:N7	28:a:901:A:H2	2.18	0.42
29:b:1:U:H2'	29:b:2:G:C8	2.54	0.42
31:d:16:THR:OG1	31:d:18:ASP:OD1	2.28	0.42
35:h:40:THR:O	35:h:41:LYS:C	2.63	0.42
53:z:43:ILE:HG22	53:z:49:TYR:HB2	2.02	0.42
5:A:19:A:C2	5:A:917:G:C5	3.07	0.42
5:A:310:G:OP1	20:P:30:GLY:CA	2.68	0.42
11:G:47:LEU:HB3	11:G:58:GLU:HG2	2.02	0.42
11:G:131:LYS:HE2	11:G:131:LYS:HB2	1.86	0.42
23:S:5:LEU:HD23	23:S:5:LEU:HA	1.78	0.42
28:a:2338:U:C2	41:n:16:ARG:HG3	2.54	0.42
28:a:2534:A:H3'	34:g:157:TYR:OH	2.19	0.42
5:A:15:G:N2	9:E:22:SER:O	2.46	0.42
5:A:53:A:C6	5:A:359:G:C6	3.08	0.42
5:A:702:A:N7	28:a:1850:A:C4	2.88	0.42
5:A:1086:U:H3	5:A:1099:G:H22	1.66	0.42
5:A:1124:G:N2	5:A:1125:U:O4	2.33	0.42
8:D:128:ARG:HD2	8:D:128:ARG:N	2.35	0.42
10:F:25:TYR:O	10:F:29:ILE:HD12	2.20	0.42
11:G:74:GLU:O	11:G:88:PRO:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:41:LYS:HD2	12:H:48:ASP:HA	2.02	0.42
25:U:63:GLU:HA	25:U:66:ARG:HD2	2.02	0.42
28:a:964:G:N2	39:l:82:MET:HE2	2.35	0.42
28:a:1329:A:H2'	28:a:1330:A:O4'	2.20	0.42
28:a:1452:G:C6	28:a:1453:C:N4	2.88	0.42
5:A:494:G:O2'	5:A:496:A:H1'	2.19	0.42
5:A:1463:U:H2'	5:A:1464:U:C6	2.55	0.42
23:S:80:TYR:CZ	23:S:82:GLY:HA2	2.55	0.42
28:a:155:A:H2'	28:a:156:A:C8	2.54	0.42
5:A:175:C:H2'	5:A:176:C:C6	2.55	0.41
5:A:373:A:C2	5:A:374:A:C8	3.08	0.41
5:A:736:C:O2'	10:F:89:VAL:O	2.34	0.41
5:A:1076:U:OP1	6:B:174:LYS:NZ	2.46	0.41
5:A:1120:C:H2'	5:A:1121:U:C6	2.55	0.41
8:D:48:LEU:HD11	8:D:52:GLY:HA3	2.02	0.41
15:K:82:LEU:HD23	15:K:82:LEU:HA	1.93	0.41
27:Z:28:G:H2'	27:Z:29:G:H8	1.85	0.41
28:a:2454:A:N3	55:Y:76:A:H2	2.17	0.41
5:A:33:A:H2'	5:A:34:C:C6	2.55	0.41
5:A:1333:A:H2'	5:A:1334:G:O4'	2.20	0.41
8:D:27:ALA:O	8:D:30:THR:OG1	2.34	0.41
11:G:80:VAL:HG21	11:G:154:TYR:HE2	1.84	0.41
20:P:13:LYS:HA	20:P:13:LYS:HD3	1.81	0.41
28:a:1746:A:H3'	28:a:1747:A:H8	1.84	0.41
28:a:1919:3TD:O5'	28:a:1919:3TD:H6	2.20	0.41
34:g:155:GLU:H	34:g:155:GLU:HG3	1.71	0.41
43:p:76:TYR:CZ	43:p:80:ILE:HG13	2.56	0.41
4:3:32:LYS:HG2	28:a:2482:A:H5'	2.02	0.41
5:A:7:A:N1	9:E:95:PHE:HE2	2.16	0.41
5:A:338:A:H2'	5:A:339:C:C6	2.55	0.41
5:A:436:C:H2'	5:A:437:U:C6	2.55	0.41
5:A:458:U:H2'	5:A:459:A:C8	2.55	0.41
5:A:1296:C:H4'	5:A:1302:C:N4	2.36	0.41
5:A:1305:G:H22	5:A:1331:G:H1'	1.85	0.41
11:G:87:VAL:HG13	11:G:151:PHE:O	2.20	0.41
28:a:320:A:H2'	32:e:131:THR:OG1	2.21	0.41
28:a:568:U:OP1	38:k:29:LYS:HD2	2.20	0.41
28:a:1796:A:H2'	28:a:1797:C:C6	2.56	0.41
50:w:3:ARG:O	50:w:12:PRO:HD3	2.20	0.41
5:A:9:G:N7	5:A:558:G:O2'	2.54	0.41
5:A:99:C:O2'	5:A:100:G:H8	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:336:A:H2'	5:A:337:G:H8	1.84	0.41
5:A:625:U:H2'	5:A:626:G:C8	2.55	0.41
5:A:1248:A:H2	13:I:72:ILE:HD11	1.84	0.41
28:a:1810:A:N1	50:w:28:ARG:HD2	2.35	0.41
28:a:1846:C:O3'	30:c:256:LYS:HE2	2.20	0.41
28:a:2752:A:O2'	34:g:66:GLY:HA3	2.20	0.41
41:n:39:VAL:HG12	41:n:48:LEU:HD12	2.01	0.41
2:l:1:MET:HE1	28:a:754:A:O5'	2.21	0.41
5:A:461:A:H2'	5:A:462:G:C8	2.56	0.41
5:A:1409:C:H5''	28:a:1919:3TD:C10	2.50	0.41
8:D:150:LYS:HG3	8:D:178:MET:SD	2.60	0.41
20:P:1:MET:HE3	20:P:2:VAL:HG23	2.02	0.41
28:a:2014:G:H5''	45:r:42:LYS:HB2	2.02	0.41
28:a:2307:G:O4'	33:f:123:ASP:CA	2.40	0.41
28:a:2309:U:C5	33:f:153:ASP:N	2.89	0.41
48:u:2:PHE:HZ	48:u:53:LYS:HD2	1.85	0.41
54:4:6:G:C2	54:4:7:G:N7	2.89	0.41
5:A:409:U:O4	5:A:433:G:O6	2.38	0.41
5:A:470:C:H2'	5:A:471:U:C6	2.55	0.41
5:A:588:G:C5	5:A:589:U:C4	3.09	0.41
5:A:702:A:N6	28:a:1850:A:N1	2.68	0.41
13:I:112:GLU:OE2	13:I:115:LYS:NZ	2.46	0.41
26:X:20:U:C4	27:Z:36:A:C2	3.09	0.41
27:Z:41:C:H2'	27:Z:42:C:C6	2.56	0.41
28:a:323:C:O2	32:e:163:ASN:ND2	2.51	0.41
28:a:654:U:P	28:a:656:A:H61	2.44	0.41
28:a:1207:A:C4	32:e:165:HIS:CE1	3.08	0.41
28:a:1756:A:C8	42:o:94:LYS:CE	3.03	0.41
33:f:48:LYS:HA	33:f:51:ASP:OD2	2.20	0.41
39:l:20:LEU:HD13	48:u:81:PRO:HG2	2.02	0.41
5:A:524:G:H2'	5:A:525:C:C6	2.56	0.41
5:A:646:G:C5	5:A:647:C:C5	3.09	0.41
8:D:15:GLU:HG3	8:D:60:LYS:NZ	2.36	0.41
27:Z:41:C:H2'	27:Z:42:C:H6	1.86	0.41
28:a:1:G:H2'	28:a:2:G:C8	2.56	0.41
28:a:694:C:H5''	30:c:39:LYS:HB2	2.03	0.41
28:a:2254:G:O2'	28:a:2500:C:OP1	2.39	0.41
28:a:2316:U:O2	33:f:37:ASN:OD1	2.39	0.41
28:a:2731:A:O3'	37:j:70:ARG:NH1	2.54	0.41
5:A:19:A:C4	5:A:917:G:C2	3.09	0.41
5:A:228:A:N3	20:P:1:MET:CE	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:253:A:N6	5:A:274:A:N1	2.68	0.41
7:C:12:LEU:CD1	18:N:91:GLY:HA2	2.50	0.41
10:F:93:LYS:HE3	10:F:93:LYS:HB3	1.75	0.41
17:M:45:ILE:HA	17:M:48:LEU:HG	2.03	0.41
22:R:22:ASP:OD2	22:R:24:LYS:HE2	2.21	0.41
28:a:1776:C:O2	30:c:11:PRO:HB2	2.20	0.41
35:h:71:LYS:HB3	35:h:71:LYS:NZ	2.30	0.41
5:A:51:A:N7	5:A:114:U:O2'	2.48	0.41
5:A:113:G:H2'	5:A:114:U:C6	2.56	0.41
5:A:284:C:C2	5:A:285:C:C5	3.09	0.41
5:A:302:G:N3	5:A:556:C:H4'	2.35	0.41
5:A:539:A:OP2	16:L:112:GLN:NE2	2.39	0.41
5:A:563:A:H2'	5:A:563:A:N3	2.36	0.41
5:A:1121:U:H2'	5:A:1122:U:C6	2.56	0.41
5:A:1409:C:C5'	28:a:1919:3TD:C10	2.95	0.41
7:C:10:ILE:CD1	18:N:98:LYS:HD3	2.51	0.41
8:D:118:VAL:HG22	8:D:123:ILE:HG13	2.03	0.41
9:E:26:LYS:HB2	9:E:26:LYS:HE3	1.79	0.41
9:E:31:PHE:HE2	26:X:24:A:N7	2.19	0.41
24:T:83:ILE:O	24:T:86:LEU:HB2	2.21	0.41
28:a:786:G:C6	30:c:228:VAL:CG1	3.03	0.41
28:a:1189:G:H5'	44:q:83:TYR:CE1	2.56	0.41
28:a:1342:U:OP2	46:s:82:LYS:NZ	2.48	0.41
28:a:1492:A:N1	30:c:97:LYS:HE3	2.36	0.41
28:a:2824:A:O2'	31:d:196:ALA:HB2	2.20	0.41
29:b:14:U:OP2	29:b:70:C:O2'	2.32	0.41
39:l:41:LEU:HG	39:l:96:ILE:HG13	2.01	0.41
54:4:4:A:O2'	54:4:5:A:H5'	2.20	0.41
55:Y:53:G:H2'	55:Y:54:5MU:C6	2.56	0.41
1:0:22:THR:HG21	28:a:2423:U:H4'	2.02	0.41
5:A:455:G:N2	5:A:478:A:H2	2.19	0.41
5:A:515:G:H2'	5:A:516:PSU:H6	1.85	0.41
5:A:538:G:C2	5:A:539:A:C5	3.09	0.41
5:A:649:A:H2'	5:A:650:G:O4'	2.21	0.41
5:A:1150:A:H4'	14:J:43:PRO:HG3	2.03	0.41
5:A:1438:G:H5''	24:T:33:LYS:HZ3	1.86	0.41
5:A:1538:C:C4	54:4:10:G:OP2	2.73	0.41
18:N:33:ASP:O	18:N:41:ARG:NH2	2.39	0.41
19:O:36:ILE:HG23	28:a:717:A:H1'	2.01	0.41
20:P:6:LEU:HD22	20:P:17:TYR:HB3	2.03	0.41
28:a:479:A:N3	28:a:481:G:H5''	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:636:C:H2'	28:a:637:C:C6	2.56	0.41
28:a:1022:A:C2	28:a:1143:U:C2	3.09	0.41
28:a:1601:U:H2'	28:a:1602:C:C6	2.56	0.41
28:a:1643:A:H2'	28:a:1644:G:O4'	2.20	0.41
28:a:2306:U:H2'	28:a:2307:G:C8	2.55	0.41
31:d:32:ASN:N	31:d:32:ASN:HD22	2.19	0.41
36:i:104:ALA:O	36:i:108:MET:HG3	2.21	0.41
5:A:17:U:C2	5:A:18:C:C5	3.08	0.40
5:A:264:C:H2'	5:A:265:G:O4'	2.21	0.40
5:A:273:U:H2'	5:A:274:A:H5'	2.03	0.40
5:A:538:G:H5''	16:L:111:LYS:HB2	2.02	0.40
5:A:625:U:H2'	5:A:626:G:H8	1.85	0.40
5:A:1202:U:N3	18:N:82:ILE:HG21	2.36	0.40
5:A:1435:G:H2'	5:A:1436:U:C6	2.56	0.40
7:C:6:HIS:CG	18:N:89:MET:HB3	2.56	0.40
7:C:49:LYS:HE3	7:C:49:LYS:HB3	1.81	0.40
18:N:24:ARG:HD2	18:N:55:SER:OG	2.21	0.40
19:O:73:LYS:HA	19:O:73:LYS:HD2	1.84	0.40
28:a:340:A:H2'	28:a:341:C:O4'	2.20	0.40
28:a:347:A:H2'	28:a:348:A:C8	2.56	0.40
28:a:391:A:H1'	28:a:411:G:O4'	2.20	0.40
28:a:990:A:OP2	52:y:12:SER:HB3	2.21	0.40
28:a:1207:A:O2'	32:e:165:HIS:CE1	2.74	0.40
28:a:2640:C:H2'	28:a:2641:U:C6	2.56	0.40
32:e:123:LYS:HE3	32:e:124:PHE:N	2.36	0.40
33:f:5:HIS:HB2	33:f:97:TRP:CD1	2.56	0.40
5:A:261:U:P	24:T:71:LYS:NZ	2.94	0.40
5:A:321:A:H2'	5:A:322:C:C6	2.56	0.40
14:J:35:GLN:OE1	14:J:35:GLN:N	2.53	0.40
18:N:46:LEU:HD13	23:S:13:LEU:HD13	2.03	0.40
18:N:47:LYS:HA	18:N:47:LYS:HD2	1.90	0.40
28:a:247:G:H4'	28:a:386:G:C5	2.56	0.40
28:a:609:U:C5'	32:e:98:LYS:HE3	2.52	0.40
28:a:647:C:H2'	28:a:649:G:C8	2.56	0.40
28:a:1044:G:C6	28:a:1045:C:C4	3.09	0.40
28:a:2020:U:H1'	53:z:3:VAL:HG21	2.04	0.40
28:a:2760:U:H1'	28:a:2761:A:H5''	2.03	0.40
31:d:181:ASP:HB3	31:d:186:LEU:HB2	2.02	0.40
48:u:2:PHE:CD1	48:u:50:MET:HE3	2.57	0.40
5:A:138:G:C6	5:A:226:G:C5	3.10	0.40
5:A:385:C:C2	5:A:386:C:C5	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1120:C:H2'	5:A:1121:U:H6	1.87	0.40
5:A:1180:A:P	13:I:99:ARG:HH22	2.44	0.40
11:G:65:ALA:O	11:G:69:VAL:HG23	2.22	0.40
24:T:53:GLU:H	24:T:53:GLU:CD	2.29	0.40
28:a:361:G:HO2'	28:a:362:A:H8	1.67	0.40
28:a:372:G:O4'	50:w:61:LYS:NZ	2.55	0.40
28:a:783:A:P	30:c:217:ARG:NH2	2.92	0.40
28:a:783:A:OP2	30:c:217:ARG:NH2	2.54	0.40
28:a:878:C:H2'	28:a:879:A:O4'	2.22	0.40
28:a:1604:U:OP2	46:s:64:LYS:NZ	2.55	0.40
28:a:1735:G:H2'	28:a:1736:G:C8	2.55	0.40
28:a:2336:C:OP1	49:v:77:ARG:CZ	2.68	0.40
33:f:126:GLY:O	33:f:158:THR:HB	2.21	0.40
39:l:6:ARG:HG3	39:l:6:ARG:NH1	2.37	0.40
42:o:111:LYS:HB3	42:o:111:LYS:HE3	1.78	0.40
55:Y:63:G:H2'	55:Y:64:G:H8	1.86	0.40
5:A:244:U:H4'	5:A:245:U:H5''	2.04	0.40
5:A:789:U:O2'	5:A:791:G:N7	2.55	0.40
5:A:899:C:O2'	28:a:1833:G:O3'	2.40	0.40
5:A:1124:G:O2'	5:A:1145:A:C6	2.75	0.40
5:A:1330:U:P	17:M:24:GLY:H	2.44	0.40
5:A:1410:A:H2'	5:A:1411:C:H6	1.87	0.40
6:B:100:MET:HA	6:B:107:VAL:HG21	2.03	0.40
6:B:130:THR:O	6:B:130:THR:OG1	2.36	0.40
7:C:131:ARG:HD3	7:C:168:TYR:OH	2.22	0.40
8:D:87:GLY:HA3	8:D:197:GLU:CG	2.48	0.40
8:D:114:ALA:O	8:D:118:VAL:HG23	2.21	0.40
9:E:72:ILE:HD13	9:E:145:GLU:HB2	2.03	0.40
12:H:108:LYS:HD2	12:H:108:LYS:HA	1.81	0.40
28:a:118:A:N3	28:a:178:G:H1'	2.37	0.40
28:a:1181:G:H2'	28:a:1182:U:C6	2.56	0.40
28:a:1343:G:H1'	46:s:59:ASN:HB3	2.04	0.40
28:a:1927:U:O2'	55:Y:12:G:H1'	2.21	0.40
28:a:2042:G:H2'	28:a:2043:U:O4'	2.22	0.40
28:a:2360:U:O3'	49:v:20:ARG:HG2	2.22	0.40
43:p:15:LYS:HE3	43:p:15:LYS:HB3	1.86	0.40
5:A:39:G:C4	5:A:404:G:N2	2.89	0.40
5:A:358:U:C2	5:A:359:G:C8	3.09	0.40
5:A:360:G:H2'	5:A:361:G:C8	2.56	0.40
5:A:505:G:C2	5:A:506:G:C5	3.10	0.40
5:A:555:U:H2'	5:A:556:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1504:G:H4'	5:A:1505:G:C4	2.57	0.40
9:E:160:SER:OG	9:E:163:GLU:HG3	2.21	0.40
18:N:19:LYS:HD3	18:N:20:TYR:CE1	2.57	0.40
22:R:24:LYS:HE2	22:R:24:LYS:HB2	1.96	0.40
28:a:896:U:H2'	28:a:897:U:O4'	2.22	0.40
28:a:1289:A:N7	40:m:105:GLY:HA3	2.36	0.40
28:a:1435:A:H2'	28:a:1436:A:O4'	2.22	0.40
28:a:2369:G:H4'	49:v:60:PHE:CE1	2.57	0.40
28:a:2762:A:O2'	34:g:38:ASN:ND2	2.42	0.40
51:x:2:LYS:O	51:x:2:LYS:HG3	2.21	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	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
6	B	222/241 (92%)	210 (95%)	9 (4%)	3 (1%)	9	36
7	C	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
8	D	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
9	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
10	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
11	G	151/179 (84%)	136 (90%)	13 (9%)	2 (1%)	9	38
12	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
13	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	J	96/103 (93%)	88 (92%)	7 (7%)	1 (1%)	12	43
15	K	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
16	L	111/124 (90%)	107 (96%)	3 (3%)	1 (1%)	14	45
17	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
18	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
19	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
20	P	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
21	Q	77/84 (92%)	70 (91%)	7 (9%)	0	100	100
22	R	53/75 (71%)	51 (96%)	1 (2%)	1 (2%)	6	30
23	S	82/92 (89%)	74 (90%)	8 (10%)	0	100	100
24	T	84/87 (97%)	84 (100%)	0	0	100	100
25	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
30	c	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
31	d	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
32	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
33	f	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
34	g	174/177 (98%)	160 (92%)	13 (8%)	1 (1%)	21	53
35	h	146/149 (98%)	134 (92%)	10 (7%)	2 (1%)	9	36
36	i	140/142 (99%)	140 (100%)	0	0	100	100
37	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
38	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
39	l	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
40	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
41	n	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
42	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
43	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
44	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
45	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
46	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
47	t	100/104 (96%)	96 (96%)	3 (3%)	1 (1%)	12	43
48	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
50	w	75/78 (96%)	75 (100%)	0	0	100	100
51	x	60/63 (95%)	60 (100%)	0	0	100	100
52	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
53	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5515/5843 (94%)	5313 (96%)	190 (3%)	12 (0%)	44	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	87	CYS
6	B	131	LYS
11	G	81	GLY
14	J	57	VAL
34	g	126	PRO
6	B	86	SER
35	h	42	LYS
35	h	76	GLU
11	G	153	HIS
22	R	73	ARG
47	t	39	ILE
16	L	91	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	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
6	B	186/199 (94%)	179 (96%)	7 (4%)	29	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	C	170/190 (90%)	166 (98%)	4 (2%)	43	67
8	D	172/173 (99%)	172 (100%)	0	100	100
9	E	119/126 (94%)	118 (99%)	1 (1%)	73	80
10	F	90/116 (78%)	89 (99%)	1 (1%)	65	77
11	G	126/147 (86%)	125 (99%)	1 (1%)	73	80
12	H	104/105 (99%)	103 (99%)	1 (1%)	68	78
13	I	105/107 (98%)	105 (100%)	0	100	100
14	J	86/90 (96%)	83 (96%)	3 (4%)	32	61
15	K	90/99 (91%)	87 (97%)	3 (3%)	33	62
16	L	96/103 (93%)	96 (100%)	0	100	100
17	M	93/96 (97%)	91 (98%)	2 (2%)	45	68
18	N	83/84 (99%)	82 (99%)	1 (1%)	63	76
19	O	76/77 (99%)	75 (99%)	1 (1%)	61	75
20	P	65/65 (100%)	65 (100%)	0	100	100
21	Q	73/78 (94%)	72 (99%)	1 (1%)	59	74
22	R	48/65 (74%)	46 (96%)	2 (4%)	26	56
23	S	72/79 (91%)	70 (97%)	2 (3%)	38	64
24	T	65/66 (98%)	64 (98%)	1 (2%)	57	73
25	U	60/61 (98%)	57 (95%)	3 (5%)	22	52
30	c	216/218 (99%)	216 (100%)	0	100	100
31	d	163/163 (100%)	163 (100%)	0	100	100
32	e	165/165 (100%)	162 (98%)	3 (2%)	51	71
33	f	148/150 (99%)	146 (99%)	2 (1%)	59	74
34	g	137/138 (99%)	131 (96%)	6 (4%)	25	55
35	h	113/114 (99%)	105 (93%)	8 (7%)	13	41
36	i	116/116 (100%)	115 (99%)	1 (1%)	70	79
37	j	104/104 (100%)	104 (100%)	0	100	100
38	k	103/103 (100%)	102 (99%)	1 (1%)	68	78
39	l	108/108 (100%)	107 (99%)	1 (1%)	70	79
40	m	98/103 (95%)	97 (99%)	1 (1%)	68	78
41	n	86/87 (99%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	o	99/100 (99%)	99 (100%)	0	100	100
43	p	89/90 (99%)	89 (100%)	0	100	100
44	q	84/84 (100%)	84 (100%)	0	100	100
45	r	93/93 (100%)	92 (99%)	1 (1%)	65	77
46	s	80/84 (95%)	79 (99%)	1 (1%)	61	75
47	t	83/85 (98%)	80 (96%)	3 (4%)	31	60
48	u	78/78 (100%)	76 (97%)	2 (3%)	40	66
49	v	58/63 (92%)	58 (100%)	0	100	100
50	w	67/68 (98%)	66 (98%)	1 (2%)	57	73
51	x	54/55 (98%)	54 (100%)	0	100	100
52	y	48/49 (98%)	48 (100%)	0	100	100
53	z	47/48 (98%)	46 (98%)	1 (2%)	47	69
All	All	4585/4765 (96%)	4519 (99%)	66 (1%)	57	74

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	4	VAL
6	B	8	ASP
6	B	10	LEU
6	B	36	ASN
6	B	80	VAL
6	B	127	ASP
6	B	146	ASN
7	C	44	THR
7	C	53	SER
7	C	121	THR
7	C	192	THR
9	E	55	GLU
10	F	103	VAL
11	G	6	VAL
12	H	54	ASP
14	J	40	ILE
14	J	75	ASP
14	J	100	ILE
15	K	13	ARG
15	K	14	LYS
15	K	108	THR

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Mol	Chain	Res	Type
17	M	83	LEU
17	M	89	LEU
18	N	49	GLN
19	O	80	GLN
21	Q	42	THR
22	R	42	SER
22	R	66	SER
23	S	60	VAL
23	S	63	THR
24	T	23	SER
25	U	7	ARG
25	U	14	VAL
25	U	60	LEU
32	e	16	GLU
32	e	55	SER
32	e	107	SER
33	f	23	ASN
33	f	108	VAL
34	g	17	VAL
34	g	49	THR
34	g	51	THR
34	g	67	THR
34	g	81	GLU
34	g	92	VAL
35	h	6	LEU
35	h	40	THR
35	h	43	ASN
35	h	55	GLU
35	h	108	VAL
35	h	116	ARG
35	h	134	VAL
35	h	142	VAL
36	i	11	VAL
38	k	109	LYS
39	l	58	LYS
40	m	6	SER
45	r	109	ASP
46	s	27	SER
47	t	15	THR
47	t	27	ASN
47	t	52	LEU
48	u	41	GLU

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Mol	Chain	Res	Type
48	u	61	LEU
50	w	42	SER
53	z	55	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
6	B	227	GLN
7	C	190	HIS
8	D	59	GLN
9	E	77	ASN
9	E	89	HIS
10	F	17	GLN
12	H	38	ASN
13	I	110	GLN
14	J	58	ASN
15	K	118	HIS
17	M	14	HIS
18	N	43	ASN
18	N	60	GLN
20	P	18	GLN
21	Q	50	ASN
23	S	14	HIS
24	T	61	GLN
24	T	70	ASN
24	T	82	GLN
25	U	9	ASN
25	U	56	HIS
30	c	86	ASN
30	c	134	ASN
30	c	153	GLN
31	d	49	GLN
32	e	9	GLN
32	e	90	GLN
32	e	92	HIS
33	f	5	HIS
33	f	37	ASN
34	g	38	ASN
34	g	104	ASN
35	h	66	ASN
36	i	76	HIS
37	j	3	GLN

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Mol	Chain	Res	Type
37	j	29	HIS
38	k	104	GLN
41	n	116	GLN
42	o	41	GLN
45	r	9	HIS
47	t	45	HIS
47	t	46	GLN
48	u	5	ASN
51	x	20	ASN
51	x	58	ASN
52	y	20	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	X	12/16 (75%)	5 (41%)	0
27	Z	75/76 (98%)	13 (17%)	1 (1%)
28	a	2742/2925 (93%)	260 (9%)	0
29	b	118/119 (99%)	10 (8%)	0
5	A	1508/1542 (97%)	191 (12%)	5 (0%)
54	4	9/10 (90%)	5 (55%)	0
55	Y	76/77 (98%)	12 (15%)	0
All	All	4540/4765 (95%)	496 (10%)	6 (0%)

All (496) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	2	A
5	A	3	A
5	A	4	U
5	A	5	U
5	A	9	G
5	A	31	G
5	A	32	A
5	A	39	G
5	A	48	C
5	A	51	A
5	A	54	C
5	A	60	A
5	A	72	A
5	A	95	C

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Mol	Chain	Res	Type
5	A	130	A
5	A	131	A
5	A	141	G
5	A	144	G
5	A	150	U
5	A	160	A
5	A	181	A
5	A	182	A
5	A	188	C
5	A	189	A
5	A	197	A
5	A	211	G
5	A	212	G
5	A	226	G
5	A	246	A
5	A	247	G
5	A	251	G
5	A	266	G
5	A	267	C
5	A	279	A
5	A	280	C
5	A	281	G
5	A	289	G
5	A	306	A
5	A	321	A
5	A	328	C
5	A	330	C
5	A	332	G
5	A	351	G
5	A	352	C
5	A	354	G
5	A	367	U
5	A	372	C
5	A	373	A
5	A	397	A
5	A	406	G
5	A	413	G
5	A	414	A
5	A	421	U
5	A	422	C
5	A	428	G
5	A	429	U

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Mol	Chain	Res	Type
5	A	448	A
5	A	457	G
5	A	458	U
5	A	463	U
5	A	465	A
5	A	467	U
5	A	468	A
5	A	479	U
5	A	481	G
5	A	484	G
5	A	486	U
5	A	495	A
5	A	496	A
5	A	497	G
5	A	509	A
5	A	511	C
5	A	518	C
5	A	531	U
5	A	532	A
5	A	533	A
5	A	546	A
5	A	547	A
5	A	559	A
5	A	572	A
5	A	573	A
5	A	576	C
5	A	577	G
5	A	596	A
5	A	618	C
5	A	630	A
5	A	632	U
5	A	633	G
5	A	642	A
5	A	650	G
5	A	651	C
5	A	653	U
5	A	661	G
5	A	665	A
5	A	723	U
5	A	724	G
5	A	748	G
5	A	755	G

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Mol	Chain	Res	Type
5	A	777	A
5	A	793	U
5	A	794	A
5	A	815	A
5	A	817	C
5	A	821	G
5	A	890	G
5	A	914	A
5	A	926	G
5	A	934	C
5	A	935	A
5	A	960	U
5	A	966	2MG
5	A	969	A
5	A	971	G
5	A	975	A
5	A	976	G
5	A	977	A
5	A	993	G
5	A	996	A
5	A	1003	G
5	A	1004	A
5	A	1008	U
5	A	1017	U
5	A	1020	G
5	A	1035	A
5	A	1036	A
5	A	1042	A
5	A	1044	A
5	A	1045	C
5	A	1053	G
5	A	1065	U
5	A	1085	U
5	A	1094	G
5	A	1095	U
5	A	1101	A
5	A	1132	C
5	A	1134	G
5	A	1137	C
5	A	1139	G
5	A	1140	C
5	A	1159	U

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Mol	Chain	Res	Type
5	A	1167	A
5	A	1171	A
5	A	1184	G
5	A	1196	A
5	A	1197	A
5	A	1213	A
5	A	1227	A
5	A	1238	A
5	A	1253	G
5	A	1258	G
5	A	1260	G
5	A	1279	G
5	A	1280	A
5	A	1285	A
5	A	1286	U
5	A	1287	A
5	A	1300	G
5	A	1302	C
5	A	1317	C
5	A	1320	C
5	A	1338	G
5	A	1346	A
5	A	1353	G
5	A	1363	A
5	A	1370	G
5	A	1378	C
5	A	1379	G
5	A	1398	A
5	A	1408	A
5	A	1419	G
5	A	1432	G
5	A	1441	A
5	A	1442	G
5	A	1446	A
5	A	1453	G
5	A	1487	G
5	A	1492	A
5	A	1494	G
5	A	1496	C
5	A	1497	G
5	A	1503	A
5	A	1506	U

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Mol	Chain	Res	Type
5	A	1517	G
5	A	1529	G
5	A	1530	G
5	A	1534	A
5	A	1535	C
5	A	1536	C
5	A	1537	U
5	A	1538	C
5	A	1541	U
26	X	13	U
26	X	16	A
26	X	22	A
26	X	23	C
26	X	24	A
27	Z	8	4SU
27	Z	9	A
27	Z	16	H2U
27	Z	17	C
27	Z	19	G
27	Z	20	H2U
27	Z	22	G
27	Z	44	G
27	Z	46	7MG
27	Z	47	3AU
27	Z	48	C
27	Z	70	G
27	Z	74	C
28	a	10	A
28	a	15	G
28	a	34	U
28	a	42	A
28	a	71	A
28	a	74	A
28	a	75	G
28	a	101	A
28	a	102	U
28	a	118	A
28	a	119	A
28	a	120	U
28	a	125	A
28	a	136	G
28	a	139	U

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Mol	Chain	Res	Type
28	a	140	C
28	a	142	A
28	a	163	C
28	a	165	A
28	a	181	A
28	a	196	A
28	a	215	G
28	a	216	A
28	a	221	A
28	a	222	A
28	a	248	G
28	a	272	A
28	a	276	U
28	a	277	G
28	a	278	A
28	a	279	A
28	a	281	C
28	a	287	G
28	a	311	A
28	a	329	G
28	a	330	A
28	a	345	A
28	a	361	G
28	a	367	G
28	a	386	G
28	a	405	U
28	a	411	G
28	a	412	A
28	a	481	G
28	a	491	G
28	a	505	A
28	a	509	C
28	a	530	G
28	a	531	C
28	a	532	A
28	a	565	A
28	a	575	U
28	a	577	A
28	a	605	A
28	a	617	U
28	a	629	A
28	a	639	A

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Mol	Chain	Res	Type
28	a	647	C
28	a	648	U
28	a	649	G
28	a	655	U
28	a	656	A
28	a	657	A
28	a	688	U
28	a	719	C
28	a	732	A
28	a	749	5MU
28	a	766	A
28	a	767	C
28	a	777	G
28	a	778	G
28	a	784	A
28	a	786	G
28	a	787	G
28	a	807	G
28	a	814	C
28	a	829	U
28	a	830	U
28	a	848	U
28	a	861	G
28	a	884	G
28	a	886	U
28	a	887	C
28	a	890	C
28	a	892	C
28	a	893	G
28	a	897	U
28	a	898	A
28	a	899	C
28	a	901	A
28	a	912	A
28	a	916	G
28	a	933	U
28	a	948	C
28	a	963	C
28	a	976	G
28	a	985	A
28	a	986	A
28	a	987	C

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Mol	Chain	Res	Type
28	a	998	A
28	a	1014	U
28	a	1015	C
28	a	1024	G
28	a	1035	U
28	a	1042	A
28	a	1049	G
28	a	1110	U
28	a	1112	G
28	a	1113	A
28	a	1114	G
28	a	1118	G
28	a	1124	G
28	a	1134	U
28	a	1137	C
28	a	1144	A
28	a	1173	G
28	a	1255	A
28	a	1258	G
28	a	1273	G
28	a	1274	A
28	a	1302	G
28	a	1303	A
28	a	1354	U
28	a	1367	A
28	a	1381	U
28	a	1385	A
28	a	1413	U
28	a	1418	G
28	a	1430	C
28	a	1436	A
28	a	1454	G
28	a	1455	A
28	a	1484	G
28	a	1495	C
28	a	1510	A
28	a	1511	A
28	a	1512	G
28	a	1517	A
28	a	1531	G
28	a	1536	U
28	a	1537	A

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Mol	Chain	Res	Type
28	a	1538	C
28	a	1539	G
28	a	1568	A
28	a	1571	A
28	a	1580	U
28	a	1585	A
28	a	1587	C
28	a	1610	A
28	a	1649	U
28	a	1650	U
28	a	1651	G
28	a	1676	G
28	a	1717	G
28	a	1731	U
28	a	1732	C
28	a	1740	G
28	a	1746	A
28	a	1766	C
28	a	1775	A
28	a	1802	C
28	a	1803	A
28	a	1810	A
28	a	1818	C
28	a	1831	A
28	a	1849	A
28	a	1850	A
28	a	1860	A
28	a	1872	G
28	a	1910	G
28	a	1911	G
28	a	1917	A
28	a	1918	C
28	a	1933	G
28	a	1934	G
28	a	1941	A
28	a	1942	A
28	a	1959	U
28	a	1971	C
28	a	1974	A
28	a	1975	U
28	a	1976	G
28	a	1995	U

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Mol	Chain	Res	Type
28	a	1997	U
28	a	2027	C
28	a	2035	A
28	a	2037	A
28	a	2047	C
28	a	2059	C
28	a	2060	G
28	a	2064	A
28	a	2065	G
28	a	2066	A
28	a	2073	G7M
28	a	2202	A
28	a	2208	G
28	a	2215	G
28	a	2227	G
28	a	2229	A
28	a	2242	G
28	a	2243	G
28	a	2272	A
28	a	2287	C
28	a	2291	A
28	a	2309	U
28	a	2312	G
28	a	2326	A
28	a	2329	G
28	a	2337	A
28	a	2339	A
28	a	2351	C
28	a	2376	U
28	a	2387	G
28	a	2389	C
28	a	2400	G
28	a	2410	A
28	a	2429	A
28	a	2433	G
28	a	2434	A
28	a	2435	U
28	a	2439	A
28	a	2445	U
28	a	2452	A
28	a	2474	G
28	a	2495	U

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Mol	Chain	Res	Type
28	a	2506	G
28	a	2509	G
28	a	2522	A
28	a	2524	C
28	a	2529	G
28	a	2533	G
28	a	2551	A
28	a	2570	A
28	a	2571	G
28	a	2577	C
28	a	2606	A
28	a	2613	U
28	a	2617	U
28	a	2633	U
28	a	2634	G
28	a	2667	G
28	a	2693	U
28	a	2694	U
28	a	2718	G
28	a	2730	A
28	a	2748	G
28	a	2752	A
28	a	2761	A
28	a	2769	A
28	a	2782	A
28	a	2802	U
28	a	2803	G
28	a	2824	A
28	a	2825	A
28	a	2839	A
28	a	2865	U
28	a	2877	A
28	a	2878	C
28	a	2887	A
28	a	2888	U
29	b	35	C
29	b	36	C
29	b	45	A
29	b	56	G
29	b	57	A
29	b	67	G
29	b	89	U

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Mol	Chain	Res	Type
29	b	90	C
29	b	99	A
29	b	109	A
54	4	5	A
54	4	8	A
54	4	9	G
54	4	10	G
54	4	11	A
55	Y	8	4SU
55	Y	9	G
55	Y	13	C
55	Y	16	C
55	Y	17(A)	U
55	Y	18	G
55	Y	19	G
55	Y	20	H2U
55	Y	21	A
55	Y	48	C
55	Y	74	C
55	Y	76	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	641	U
5	A	766	A
5	A	786	G
5	A	1035	A
5	A	1535	C
27	Z	19	G

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

53 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
28	PSU	a	748	28,58	18,21,22	1.10	2 (11%)	22,30,33	1.60	3 (13%)
28	PSU	a	1921	28	18,21,22	1.04	1 (5%)	22,30,33	1.84	4 (18%)
5	MA6	A	1519	5	23,26,27	1.38	5 (21%)	34,38,41	2.87	13 (38%)
55	OMC	Y	32	55	19,22,23	3.01	8 (42%)	26,31,34	0.90	2 (7%)
5	4OC	A	1402	5	20,23,24	2.98	8 (40%)	26,32,35	0.94	1 (3%)
28	PSU	a	1915	28	18,21,22	1.01	1 (5%)	22,30,33	1.78	3 (13%)
27	5MU	Z	54	27	19,22,23	1.38	5 (26%)	28,32,35	2.09	6 (21%)
28	OMU	a	2556	57,28,58	19,22,23	3.07	7 (36%)	26,31,34	1.66	4 (15%)
55	4SU	Y	8	55	18,21,22	4.19	8 (44%)	26,30,33	2.26	5 (19%)
5	5MC	A	1407	5	18,22,23	0.83	1 (5%)	26,32,35	0.58	0
27	4SU	Z	8	27	18,21,22	4.19	8 (44%)	26,30,33	2.25	4 (15%)
55	H2U	Y	20	55	18,21,22	3.11	5 (27%)	21,30,33	1.97	5 (23%)
39	4D4	l	81	39	9,11,12	0.54	0	8,13,15	1.03	1 (12%)
31	MEQ	d	150	31	8,9,10	0.82	0	5,10,12	0.76	0
28	5MU	a	749	28	19,22,23	0.72	0	28,32,35	0.56	0
27	H2U	Z	20	27	18,21,22	3.13	5 (27%)	21,30,33	1.99	5 (23%)
28	2MG	a	2449	28	23,26,27	0.78	0	32,38,41	0.57	0
5	2MG	A	1516	5	23,26,27	0.65	0	32,38,41	0.62	0
28	PSU	a	957	28	18,21,22	1.07	1 (5%)	22,30,33	1.79	2 (9%)
27	PSU	Z	32	27	18,21,22	1.07	1 (5%)	22,30,33	1.77	5 (22%)
28	1MG	a	747	28	22,26,27	2.59	6 (27%)	33,39,42	2.07	7 (21%)
27	PSU	Z	55	27	18,21,22	1.10	1 (5%)	22,30,33	1.81	5 (22%)
28	2MA	a	2507	57,28,58	22,25,26	3.74	11 (50%)	33,37,40	2.78	12 (36%)
28	5MU	a	1943	57,28	19,22,23	0.81	0	28,32,35	0.46	0
28	OMC	a	2502	28,58	19,22,23	0.81	1 (5%)	26,31,34	0.66	0
27	7MG	Z	46	27	20,25,27	3.36	10 (50%)	27,37,42	2.11	8 (29%)
28	PSU	a	2508	57,28	18,21,22	1.03	1 (5%)	22,30,33	1.87	4 (18%)
16	D2T	L	89	16	7,9,10	1.36	1 (14%)	6,11,13	1.79	2 (33%)
5	PSU	A	516	5	18,21,22	0.99	1 (5%)	22,30,33	1.71	5 (22%)
28	OMG	a	2255	57,28,55	23,26,27	0.71	0	33,38,41	0.53	0
55	5MU	Y	54	55	19,22,23	1.39	5 (26%)	28,32,35	2.07	6 (21%)
5	5MC	A	967	5	18,22,23	0.76	0	26,32,35	0.61	0
28	6MZ	a	1620	28	22,25,26	2.86	5 (22%)	30,36,39	2.72	11 (36%)
28	2MG	a	1837	28	23,26,27	0.69	0	32,38,41	0.56	0
28	PSU	a	2584	28	18,21,22	1.07	2 (11%)	22,30,33	1.77	3 (13%)
27	3AU	Z	47	27	18,21,29	3.38	8 (44%)	26,30,43	1.64	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	MIA	Z	37	27	21,24,32	1.74	4 (19%)	31,35,47	2.13	10 (32%)
28	6MZ	a	2034	28	22,25,26	2.81	6 (27%)	30,36,39	2.84	11 (36%)
5	MA6	A	1518	5	23,26,27	1.37	5 (21%)	34,38,41	2.81	14 (41%)
28	3TD	a	1919	28	18,22,23	4.02	7 (38%)	22,32,35	1.79	3 (13%)
27	H2U	Z	16	27	18,21,22	3.06	5 (27%)	21,30,33	2.09	5 (23%)
5	G7M	A	527	5	23,26,27	2.61	9 (39%)	35,39,42	2.63	11 (31%)
5	2MG	A	1207	57,5	23,26,27	0.56	0	32,38,41	0.54	0
28	5MC	a	1966	57,28	18,22,23	0.81	0	26,32,35	0.53	0
28	H2U	a	2453	28	18,21,22	0.63	0	21,30,33	1.07	3 (14%)
28	G7M	a	2073	57,28	23,26,27	2.67	9 (39%)	35,39,42	1.69	9 (25%)
28	PSU	a	2609	28	18,21,22	1.08	1 (5%)	22,30,33	1.89	4 (18%)
28	PSU	a	2608	28	18,21,22	1.05	1 (5%)	22,30,33	1.85	3 (13%)
5	2MG	A	966	5	23,26,27	0.57	0	32,38,41	0.55	0
27	PSU	Z	39	27	18,21,22	1.05	1 (5%)	22,30,33	1.80	5 (22%)
55	PSU	Y	55	55	18,21,22	1.12	1 (5%)	22,30,33	1.76	4 (18%)
28	PSU	a	2461	28	18,21,22	1.10	1 (5%)	22,30,33	1.84	4 (18%)
5	UR3	A	1498	5	19,22,23	2.57	6 (31%)	26,32,35	1.37	3 (11%)

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
28	PSU	a	748	28,58	-	1/7/25/26	0/2/2/2
28	PSU	a	1921	28	-	0/7/25/26	0/2/2/2
5	MA6	A	1519	5	-	3/11/29/30	0/3/3/3
55	OMC	Y	32	55	-	3/9/27/28	0/2/2/2
5	4OC	A	1402	5	-	0/9/29/30	0/2/2/2
28	PSU	a	1915	28	-	0/7/25/26	0/2/2/2
27	5MU	Z	54	27	-	0/7/25/26	0/2/2/2
28	OMU	a	2556	57,28,58	-	0/9/27/28	0/2/2/2
55	4SU	Y	8	55	-	2/7/25/26	0/2/2/2
5	5MC	A	1407	5	-	0/7/25/26	0/2/2/2
27	4SU	Z	8	27	-	2/7/25/26	0/2/2/2
55	H2U	Y	20	55	-	7/7/38/39	0/2/2/2
39	4D4	l	81	39	-	6/11/12/14	-
31	MEQ	d	150	31	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	5MU	a	749	28	-	0/7/25/26	0/2/2/2
27	H2U	Z	20	27	-	2/7/38/39	0/2/2/2
28	2MG	a	2449	28	-	0/9/27/28	0/3/3/3
5	2MG	A	1516	5	-	0/9/27/28	0/3/3/3
28	PSU	a	957	28	-	0/7/25/26	0/2/2/2
27	PSU	Z	32	27	-	0/7/25/26	0/2/2/2
28	1MG	a	747	28	-	0/7/25/26	0/3/3/3
27	PSU	Z	55	27	-	0/7/25/26	0/2/2/2
28	2MA	a	2507	57,28,58	-	2/7/25/26	0/3/3/3
28	5MU	a	1943	57,28	-	0/7/25/26	0/2/2/2
28	OMC	a	2502	28,58	-	0/9/27/28	0/2/2/2
27	7MG	Z	46	27	-	2/7/34/38	0/3/3/3
28	PSU	a	2508	57,28	-	0/7/25/26	0/2/2/2
16	D2T	L	89	16	-	3/7/12/14	-
5	PSU	A	516	5	-	0/7/25/26	0/2/2/2
28	OMG	a	2255	57,28,55	-	1/9/27/28	0/3/3/3
55	5MU	Y	54	55	-	0/7/25/26	0/2/2/2
5	5MC	A	967	5	-	0/7/25/26	0/2/2/2
28	6MZ	a	1620	28	-	0/9/27/28	0/3/3/3
28	2MG	a	1837	28	-	0/9/27/28	0/3/3/3
28	PSU	a	2584	28	-	0/7/25/26	0/2/2/2
27	3AU	Z	47	27	-	2/7/25/35	0/2/2/2
27	MIA	Z	37	27	-	0/7/25/34	0/3/3/3
28	6MZ	a	2034	28	-	2/9/27/28	0/3/3/3
5	MA6	A	1518	5	-	0/11/29/30	0/3/3/3
28	3TD	a	1919	28	-	2/7/25/26	0/2/2/2
27	H2U	Z	16	27	-	0/7/38/39	0/2/2/2
5	G7M	A	527	5	-	0/7/25/26	0/3/3/3
5	2MG	A	1207	57,5	-	0/9/27/28	0/3/3/3
28	5MC	a	1966	57,28	-	0/7/25/26	0/2/2/2
28	H2U	a	2453	28	-	0/7/38/39	0/2/2/2
28	G7M	a	2073	57,28	-	2/7/25/26	0/3/3/3
28	PSU	a	2609	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2608	28	-	0/7/25/26	0/2/2/2
5	2MG	A	966	5	-	0/9/27/28	0/3/3/3
27	PSU	Z	39	27	-	0/7/25/26	0/2/2/2
55	PSU	Y	55	55	-	0/7/25/26	0/2/2/2
28	PSU	a	2461	28	-	0/7/25/26	0/2/2/2
5	UR3	A	1498	5	-	0/7/25/26	0/2/2/2

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1919	3TD	C6-C5	12.08	1.49	1.35
28	a	1620	6MZ	C6-N6	11.66	1.46	1.34
28	a	2034	6MZ	C6-N6	11.18	1.46	1.34
28	a	2507	2MA	C4-N3	10.44	1.47	1.34
27	Z	20	H2U	C2-N1	9.70	1.49	1.35
55	Y	20	H2U	C2-N1	9.64	1.49	1.35
55	Y	8	4SU	C4-N3	9.58	1.47	1.37
27	Z	8	4SU	C4-N3	9.42	1.47	1.37
27	Z	16	H2U	C2-N1	9.37	1.49	1.35
28	a	1919	3TD	C2-N1	8.61	1.48	1.37
27	Z	8	4SU	C2-N1	7.98	1.51	1.38
55	Y	8	4SU	C2-N1	7.72	1.50	1.38
27	Z	47	3AU	C2-N1	7.32	1.50	1.38
27	Z	47	3AU	C6-C5	6.98	1.51	1.35
27	Z	8	4SU	C2-N3	6.66	1.49	1.38
55	Y	8	4SU	C2-N3	6.58	1.49	1.38
27	Z	20	H2U	C2-N3	6.52	1.49	1.38
55	Y	20	H2U	C2-N3	6.50	1.49	1.38
27	Z	47	3AU	C2-N3	6.50	1.49	1.38
27	Z	16	H2U	C2-N3	6.48	1.49	1.38
55	Y	32	OMC	C2-N3	6.43	1.49	1.36
28	a	2507	2MA	C6-N1	6.34	1.44	1.35
5	A	527	G7M	C4-N3	6.32	1.49	1.34
5	A	1402	4OC	C4-N3	6.31	1.43	1.32
5	A	1498	UR3	C2-N1	6.28	1.47	1.38
28	a	747	1MG	C2-N3	6.27	1.45	1.34
28	a	2507	2MA	C2-N3	6.26	1.45	1.34
28	a	2556	OMU	C2-N3	6.26	1.49	1.38
27	Z	8	4SU	C6-C5	6.05	1.49	1.35
55	Y	8	4SU	C6-C5	6.05	1.49	1.35
27	Z	46	7MG	C2-N3	6.05	1.47	1.33
5	A	1402	4OC	C6-C5	6.04	1.49	1.35
28	a	747	1MG	C4-N3	6.02	1.48	1.34
27	Z	37	MIA	C6-N6	5.98	1.49	1.34
27	Z	46	7MG	C4-N3	5.97	1.48	1.34
28	a	2073	G7M	C2-N2	5.94	1.48	1.34
55	Y	32	OMC	C6-C5	5.91	1.48	1.35
28	a	2556	OMU	C2-N1	5.90	1.47	1.38
28	a	747	1MG	C2-N2	5.88	1.44	1.34
28	a	2507	2MA	C2-N1	5.84	1.44	1.34
5	A	1498	UR3	C6-C5	5.75	1.48	1.35
55	Y	8	4SU	C5-C4	5.71	1.49	1.42
27	Z	8	4SU	C5-C4	5.68	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Z	46	7MG	C4-N9	5.66	1.44	1.37
5	A	1402	4OC	C2-N3	5.66	1.47	1.36
28	a	2073	G7M	C4-N3	5.56	1.47	1.34
28	a	1919	3TD	C6-N1	5.44	1.45	1.36
5	A	527	G7M	C2-N3	5.44	1.46	1.33
55	Y	8	4SU	C4-S4	-5.41	1.58	1.68
28	a	2073	G7M	C5-N7	-5.34	1.33	1.39
27	Z	8	4SU	C4-S4	-5.33	1.58	1.68
55	Y	32	OMC	C4-N3	5.25	1.45	1.34
28	a	2556	OMU	C6-C5	5.24	1.47	1.35
27	Z	47	3AU	C4-N3	5.19	1.47	1.38
28	a	2556	OMU	O4-C4	-5.18	1.14	1.24
27	Z	20	H2U	C4-N3	5.03	1.46	1.37
27	Z	16	H2U	C4-N3	4.95	1.46	1.37
55	Y	20	H2U	C4-N3	4.92	1.46	1.37
27	Z	46	7MG	C2-N2	4.89	1.45	1.34
27	Z	46	7MG	C5-C4	4.88	1.44	1.37
55	Y	32	OMC	C4-N4	4.86	1.45	1.33
28	a	2073	G7M	C2-N3	4.83	1.44	1.33
5	A	527	G7M	C5-N7	-4.80	1.33	1.39
5	A	527	G7M	C2-N2	4.76	1.45	1.34
28	a	2507	2MA	C5-C6	4.71	1.54	1.41
5	A	1402	4OC	C4-N4	4.68	1.45	1.35
5	A	1498	UR3	C2-N3	4.53	1.47	1.39
55	Y	32	OMC	C2-N1	4.53	1.49	1.40
28	a	2556	OMU	O2-C2	-4.46	1.14	1.23
27	Z	46	7MG	C2-N1	4.39	1.48	1.37
27	Z	46	7MG	C5-C6	4.34	1.53	1.42
28	a	2507	2MA	C4-N9	-3.99	1.28	1.37
28	a	1919	3TD	C2-N3	3.93	1.47	1.38
28	a	2507	2MA	C5-N7	-3.87	1.31	1.39
28	a	2556	OMU	C4-N3	3.70	1.45	1.38
28	a	2034	6MZ	C5-N7	-3.69	1.32	1.39
28	a	747	1MG	C5-N7	-3.67	1.32	1.39
5	A	1402	4OC	C5-C4	3.65	1.48	1.40
27	Z	46	7MG	C6-N1	3.59	1.45	1.38
5	A	527	G7M	C5-C6	3.59	1.53	1.43
55	Y	55	PSU	C6-C5	3.58	1.39	1.35
28	a	2507	2MA	C8-N7	3.58	1.38	1.31
5	A	1402	4OC	C2-N1	3.49	1.47	1.40
27	Z	55	PSU	C6-C5	3.46	1.39	1.35
27	Z	46	7MG	O6-C6	-3.45	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1402	4OC	O2-C2	-3.44	1.17	1.23
5	A	1518	MA6	C5-C4	-3.42	1.32	1.39
28	a	2073	G7M	O6-C6	-3.41	1.17	1.23
28	a	1620	6MZ	C5-N7	-3.38	1.32	1.39
27	Z	32	PSU	C6-C5	3.37	1.39	1.35
28	a	2073	G7M	C5-C6	3.36	1.52	1.43
27	Z	39	PSU	C6-C5	3.36	1.39	1.35
27	Z	47	3AU	C6-N1	3.33	1.46	1.38
28	a	2556	OMU	C6-N1	3.30	1.45	1.38
27	Z	8	4SU	C6-N1	3.28	1.45	1.38
5	A	1519	MA6	C5-C4	-3.26	1.32	1.39
55	Y	8	4SU	C6-N1	3.24	1.45	1.38
55	Y	8	4SU	O2-C2	-3.20	1.17	1.23
27	Z	46	7MG	C5-N7	3.14	1.44	1.35
55	Y	32	OMC	C6-N1	3.14	1.45	1.38
28	a	1921	PSU	C6-C5	3.08	1.38	1.35
28	a	748	PSU	C6-C5	2.99	1.38	1.35
27	Z	8	4SU	O2-C2	-2.98	1.17	1.23
5	A	516	PSU	C6-C5	2.96	1.38	1.35
28	a	2508	PSU	C6-C5	2.95	1.38	1.35
28	a	2461	PSU	C6-C5	2.91	1.38	1.35
28	a	957	PSU	C6-C5	2.90	1.38	1.35
28	a	747	1MG	C5-C6	2.88	1.52	1.45
28	a	1915	PSU	C6-C5	2.87	1.38	1.35
5	A	1402	4OC	C6-N1	2.85	1.44	1.38
27	Z	47	3AU	O4-C4	-2.83	1.19	1.24
5	A	1498	UR3	O2-C2	-2.78	1.17	1.22
27	Z	47	3AU	C5-C4	2.75	1.49	1.43
5	A	527	G7M	C2-N1	2.71	1.44	1.37
5	A	1498	UR3	O4-C4	-2.69	1.17	1.23
27	Z	54	5MU	C6-C5	2.67	1.39	1.34
55	Y	32	OMC	O2-C2	-2.67	1.18	1.23
5	A	527	G7M	O6-C6	-2.66	1.18	1.23
28	a	2034	6MZ	C8-N9	-2.65	1.32	1.37
5	A	1498	UR3	C6-N1	2.64	1.44	1.38
28	a	2034	6MZ	C5-C4	-2.63	1.34	1.39
28	a	1620	6MZ	C5-C4	-2.61	1.34	1.39
27	Z	37	MIA	C5-N7	-2.61	1.34	1.39
5	A	1518	MA6	C6-N6	2.61	1.44	1.36
55	Y	54	5MU	C4-N3	-2.61	1.34	1.38
28	a	747	1MG	O6-C6	-2.61	1.17	1.23
55	Y	54	5MU	C6-C5	2.60	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Z	54	5MU	C4-N3	-2.59	1.34	1.38
5	A	1519	MA6	C5-N7	-2.59	1.34	1.39
28	a	2609	PSU	C6-C5	2.59	1.38	1.35
28	a	2608	PSU	C6-C5	2.58	1.38	1.35
27	Z	47	3AU	O2-C2	-2.55	1.18	1.23
5	A	1519	MA6	C6-N6	2.54	1.44	1.36
28	a	2584	PSU	C6-C5	2.51	1.38	1.35
28	a	1919	3TD	O4-C4	-2.50	1.17	1.23
28	a	2507	2MA	C6-N6	-2.47	1.27	1.34
27	Z	37	MIA	C4-N9	-2.43	1.32	1.37
28	a	2034	6MZ	C6-N1	-2.42	1.31	1.35
28	a	2073	G7M	C2-N1	2.38	1.43	1.37
28	a	1620	6MZ	C8-N9	-2.36	1.33	1.37
55	Y	54	5MU	C6-N1	-2.36	1.34	1.38
5	A	527	G7M	C6-N1	2.36	1.43	1.38
27	Z	16	H2U	O2-C2	-2.36	1.18	1.23
28	a	1919	3TD	C1'-C5	2.36	1.55	1.50
55	Y	32	OMC	C5-C4	2.35	1.48	1.42
5	A	1518	MA6	C8-N9	-2.35	1.33	1.37
5	A	1518	MA6	C5-N7	-2.34	1.34	1.39
55	Y	20	H2U	O2-C2	-2.34	1.18	1.23
28	a	1620	6MZ	C6-N1	-2.31	1.31	1.35
5	A	1519	MA6	C8-N9	-2.31	1.33	1.37
27	Z	20	H2U	O2-C2	-2.31	1.18	1.23
28	a	2034	6MZ	C2-N1	2.30	1.38	1.33
27	Z	54	5MU	C6-N1	-2.28	1.34	1.38
55	Y	54	5MU	C2-N1	2.26	1.42	1.38
28	a	2584	PSU	O4'-C1'	-2.25	1.40	1.43
55	Y	20	H2U	O4-C4	-2.23	1.18	1.23
5	A	527	G7M	C4-N9	-2.22	1.32	1.38
28	a	1919	3TD	C4-N3	2.21	1.45	1.40
5	A	1518	MA6	C4-N9	-2.20	1.32	1.37
27	Z	20	H2U	O4-C4	-2.18	1.18	1.23
28	a	2507	2MA	C5-C4	-2.18	1.34	1.39
28	a	2507	2MA	C8-N9	-2.17	1.33	1.37
5	A	1519	MA6	C4-N9	-2.16	1.32	1.37
27	Z	54	5MU	C4-C5	2.15	1.48	1.44
27	Z	16	H2U	O4-C4	-2.14	1.18	1.23
55	Y	54	5MU	C4-C5	2.14	1.48	1.44
27	Z	37	MIA	C5-C4	-2.13	1.35	1.39
28	a	2073	G7M	C6-N1	2.12	1.42	1.38
28	a	2073	G7M	C4-N9	-2.12	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Z	54	5MU	C2-N1	2.10	1.41	1.38
28	a	2502	OMC	C4-N3	-2.09	1.30	1.34
5	A	1407	5MC	C4-N3	-2.06	1.30	1.34
28	a	748	PSU	O4'-C1'	-2.01	1.41	1.43
16	L	89	D2T	CB1-SB	-2.01	1.75	1.79

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1519	MA6	N1-C6-N6	-9.37	106.84	117.08
5	A	1518	MA6	N1-C6-N6	-8.90	107.36	117.08
28	a	2507	2MA	C1'-N9-C8	-8.83	107.21	127.14
55	Y	8	4SU	C4-N3-C2	-7.98	119.59	127.34
27	Z	8	4SU	C4-N3-C2	-7.85	119.72	127.34
27	Z	16	H2U	C4-N3-C2	-7.28	119.75	125.79
27	Z	46	7MG	C5-C4-N3	-7.12	120.45	127.80
28	a	2034	6MZ	C4-C5-C6	6.98	122.22	116.81
28	a	2507	2MA	C4-N9-C1'	6.94	143.13	126.59
27	Z	20	H2U	C4-N3-C2	-6.89	120.07	125.79
55	Y	20	H2U	C4-N3-C2	-6.77	120.17	125.79
5	A	527	G7M	C1'-N9-C8	-6.70	104.10	126.74
28	a	1620	6MZ	C4-C5-C6	6.63	121.95	116.81
5	A	527	G7M	C1'-N9-C4	6.62	146.16	126.50
28	a	2034	6MZ	C5-C4-N3	-6.22	118.64	126.75
28	a	1620	6MZ	C5-C4-N3	-6.16	118.71	126.75
5	A	1519	MA6	N1-C2-N3	-5.96	119.27	128.60
28	a	2507	2MA	N9-C8-N7	-5.92	105.82	113.91
28	a	1919	3TD	N1-C2-N3	5.90	120.79	116.14
5	A	527	G7M	CN7-N7-C5	5.85	134.04	126.77
5	A	1518	MA6	N1-C2-N3	-5.81	119.52	128.60
27	Z	8	4SU	C5-C4-N3	5.75	120.03	114.69
55	Y	8	4SU	C5-C4-N3	5.66	119.94	114.69
28	a	747	1MG	C5-C4-N3	-5.61	119.36	128.46
28	a	747	1MG	C1'-N9-C4	-5.45	110.32	126.50
27	Z	37	MIA	C5-C4-N3	-5.42	119.68	126.75
27	Z	37	MIA	N3-C2-N1	-5.31	120.30	128.60
28	a	1620	6MZ	N1-C2-N3	-5.27	120.36	128.60
28	a	747	1MG	C1'-N9-C8	5.20	141.49	126.70
27	Z	54	5MU	C4-N3-C2	-5.19	120.63	127.35
5	A	1518	MA6	N9-C8-N7	-5.18	106.83	113.91
28	a	2461	PSU	N1-C2-N3	5.09	120.89	115.13
55	Y	54	5MU	C4-N3-C2	-5.07	120.79	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2556	OMU	C4-N3-C2	-5.04	119.93	126.58
28	a	2609	PSU	N1-C2-N3	5.01	120.80	115.13
28	a	1620	6MZ	C9-N6-C6	5.00	127.18	122.87
28	a	2034	6MZ	N3-C4-N9	4.97	135.27	127.08
28	a	2508	PSU	N1-C2-N3	4.94	120.73	115.13
28	a	2034	6MZ	C9-N6-C6	4.93	127.12	122.87
28	a	957	PSU	C4-N3-C2	-4.93	119.23	126.34
5	A	1519	MA6	C5-C6-N6	4.93	133.89	125.30
5	A	1519	MA6	N9-C8-N7	-4.92	107.18	113.91
28	a	2034	6MZ	N1-C2-N3	-4.91	120.92	128.60
27	Z	47	3AU	C4-N3-C2	-4.89	120.13	126.58
5	A	1498	UR3	C4-N3-C2	-4.85	120.00	124.56
28	a	1921	PSU	C4-N3-C2	-4.83	119.38	126.34
28	a	2608	PSU	C4-N3-C2	-4.83	119.39	126.34
28	a	1915	PSU	C4-N3-C2	-4.80	119.42	126.34
28	a	2609	PSU	C4-N3-C2	-4.77	119.46	126.34
27	Z	54	5MU	N3-C2-N1	4.74	121.19	114.89
28	a	2608	PSU	N1-C2-N3	4.72	120.48	115.13
28	a	2584	PSU	C4-N3-C2	-4.71	119.56	126.34
28	a	1921	PSU	N1-C2-N3	4.69	120.45	115.13
27	Z	54	5MU	C5-C4-N3	4.69	119.31	115.31
28	a	2508	PSU	C4-N3-C2	-4.68	119.60	126.34
28	a	957	PSU	N1-C2-N3	4.66	120.41	115.13
5	A	527	G7M	CN7-N7-C8	-4.65	117.66	124.84
55	Y	54	5MU	C5-C4-N3	4.64	119.28	115.31
28	a	1620	6MZ	N3-C4-N9	4.64	134.72	127.08
55	Y	54	5MU	N3-C2-N1	4.62	121.03	114.89
55	Y	55	PSU	C4-N3-C2	-4.59	119.73	126.34
27	Z	55	PSU	C4-N3-C2	-4.58	119.74	126.34
27	Z	39	PSU	C4-N3-C2	-4.57	119.76	126.34
5	A	1518	MA6	C5-C6-N6	4.54	133.20	125.30
27	Z	39	PSU	N1-C2-N3	4.53	120.26	115.13
28	a	2461	PSU	C4-N3-C2	-4.48	119.89	126.34
28	a	2034	6MZ	N9-C8-N7	-4.48	107.79	113.91
27	Z	32	PSU	C4-N3-C2	-4.46	119.91	126.34
28	a	748	PSU	C4-N3-C2	-4.46	119.91	126.34
28	a	2073	G7M	C2-N3-C4	4.46	120.25	112.30
28	a	1915	PSU	N1-C2-N3	4.46	120.18	115.13
27	Z	55	PSU	N1-C2-N3	4.44	120.16	115.13
28	a	2584	PSU	N1-C2-N3	4.44	120.16	115.13
27	Z	32	PSU	N1-C2-N3	4.39	120.11	115.13
27	Z	54	5MU	O4-C4-C5	-4.35	119.86	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	46	7MG	C2-N3-C4	4.33	120.01	112.30
55	Y	55	PSU	N1-C2-N3	4.28	119.98	115.13
27	Z	37	MIA	N9-C8-N7	-4.28	108.06	113.91
5	A	516	PSU	C4-N3-C2	-4.26	120.19	126.34
55	Y	54	5MU	O4-C4-C5	-4.25	119.97	124.90
5	A	527	G7M	C2-N3-C4	4.22	119.82	112.30
5	A	516	PSU	N1-C2-N3	4.22	119.91	115.13
28	a	2556	OMU	N3-C2-N1	4.16	120.41	114.89
5	A	1519	MA6	C2-N1-C6	4.16	121.58	111.75
28	a	748	PSU	N1-C2-N3	4.14	119.82	115.13
5	A	1519	MA6	C5-C4-N3	-4.10	121.40	126.75
5	A	1518	MA6	C2-N1-C6	4.05	121.31	111.75
27	Z	47	3AU	N3-C2-N1	3.99	120.19	114.89
5	A	527	G7M	C5-C6-N1	3.98	120.10	111.79
28	a	747	1MG	N9-C4-N3	3.97	133.92	125.94
5	A	1518	MA6	C5-C4-N3	-3.92	121.64	126.75
28	a	1919	3TD	C4-N3-C2	-3.91	120.37	124.61
55	Y	8	4SU	N3-C2-N1	3.85	119.99	114.89
28	a	2507	2MA	CM2-C2-N1	3.83	123.12	117.15
28	a	2073	G7M	C5-C6-N1	3.82	119.76	111.79
5	A	527	G7M	C5-C4-N3	-3.82	120.83	128.15
28	a	2073	G7M	C5-C4-N3	-3.75	120.97	128.15
28	a	1620	6MZ	N9-C8-N7	-3.71	108.84	113.91
27	Z	8	4SU	N3-C2-N1	3.68	119.77	114.89
5	A	1518	MA6	C1'-N9-C8	-3.67	118.84	127.14
28	a	747	1MG	C2-N3-C4	3.67	120.22	111.98
5	A	527	G7M	O6-C6-C5	-3.64	119.84	128.06
27	Z	54	5MU	C5-C6-N1	-3.64	119.59	123.34
28	a	2507	2MA	N3-C2-N1	-3.59	119.11	125.72
28	a	2507	2MA	C4-N9-C8	3.59	109.61	105.73
28	a	1620	6MZ	C2-N3-C4	3.51	120.03	111.75
27	Z	8	4SU	C5-C4-S4	-3.47	120.00	124.47
27	Z	37	MIA	C2-N3-C4	3.47	119.94	111.75
5	A	1518	MA6	C5-N7-C8	3.41	108.36	103.51
28	a	2034	6MZ	C6-C5-N7	-3.41	128.70	132.39
55	Y	54	5MU	C5-C6-N1	-3.37	119.87	123.34
5	A	1518	MA6	C4-N9-C8	3.37	109.38	105.73
55	Y	8	4SU	C5-C4-S4	-3.34	120.16	124.47
5	A	1519	MA6	C2-N3-C4	3.33	119.62	111.75
28	a	2034	6MZ	C2-N3-C4	3.33	119.62	111.75
27	Z	16	H2U	N3-C2-N1	3.32	120.17	116.65
28	a	1620	6MZ	C6-C5-N7	-3.32	128.80	132.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1519	MA6	C5-N7-C8	3.29	108.18	103.51
28	a	2034	6MZ	C5-N7-C8	3.29	108.18	103.51
55	Y	20	H2U	N3-C2-N1	3.27	120.11	116.65
27	Z	37	MIA	C5-N7-C8	3.27	108.15	103.51
27	Z	47	3AU	C5-C4-N3	3.24	119.69	114.84
27	Z	37	MIA	N3-C4-N9	3.23	132.40	127.08
28	a	2508	PSU	O2-C2-N1	-3.22	119.25	122.79
5	A	1519	MA6	C1'-N9-C8	-3.21	119.89	127.14
5	A	1518	MA6	C2-N3-C4	3.18	119.25	111.75
28	a	2073	G7M	O6-C6-C5	-3.13	120.99	128.06
27	Z	20	H2U	N3-C2-N1	3.09	119.92	116.65
27	Z	46	7MG	O6-C6-C5	-3.06	120.21	127.24
5	A	527	G7M	N9-C4-N3	3.06	132.09	125.94
28	a	2507	2MA	C5-N7-C8	3.06	107.85	103.51
28	a	2507	2MA	C5-C4-N9	3.04	109.31	105.78
28	a	2556	OMU	C5-C4-N3	2.99	119.32	114.84
5	A	1519	MA6	C4-N9-C8	2.99	108.97	105.73
27	Z	16	H2U	C5-C4-N3	2.95	119.96	116.65
5	A	516	PSU	O2-C2-N1	-2.95	119.55	122.79
28	a	2461	PSU	C6-N1-C2	-2.93	119.69	122.68
5	A	527	G7M	C2-N1-C6	-2.90	119.81	125.10
28	a	2034	6MZ	C4-N9-C8	2.89	108.86	105.73
28	a	2073	G7M	C2-N1-C6	-2.83	119.94	125.10
27	Z	46	7MG	C2-N1-C6	-2.82	119.95	125.10
27	Z	47	3AU	O4-C4-C5	-2.82	120.20	125.16
27	Z	20	H2U	C5-C6-N1	2.78	120.78	111.61
27	Z	20	H2U	C5-C4-N3	2.77	119.76	116.65
55	Y	20	H2U	C5-C6-N1	2.75	120.67	111.61
28	a	2034	6MZ	C4-N9-C1'	-2.70	120.15	126.59
27	Z	32	PSU	O2-C2-N1	-2.69	119.83	122.79
5	A	1498	UR3	C6-N1-C2	-2.66	119.41	121.79
27	Z	55	PSU	O2-C2-N1	-2.66	119.86	122.79
5	A	1519	MA6	C4-C5-C6	2.65	118.84	115.88
5	A	1518	MA6	C4-C5-C6	2.64	118.84	115.88
28	a	1620	6MZ	C5-N7-C8	2.64	107.26	103.51
28	a	2507	2MA	C4-C5-N7	-2.64	107.40	110.62
27	Z	46	7MG	N9-C4-N3	2.63	129.40	125.47
27	Z	16	H2U	C5-C6-N1	2.62	120.26	111.61
55	Y	55	PSU	O2-C2-N1	-2.61	119.92	122.79
27	Z	16	H2U	O2-C2-N1	-2.59	119.86	123.11
5	A	1402	4OC	C6-C5-C4	2.59	120.12	116.96
55	Y	20	H2U	C5-C4-N3	2.58	119.55	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2508	PSU	C6-N1-C2	-2.57	120.05	122.68
28	a	1921	PSU	O2-C2-N1	-2.56	119.97	122.79
28	a	2609	PSU	C6-N1-C2	-2.55	120.08	122.68
27	Z	54	5MU	O2-C2-N1	-2.51	119.46	122.79
27	Z	46	7MG	C5-C4-N9	2.49	110.15	106.68
28	a	2073	G7M	N9-C4-N3	2.49	130.93	125.94
28	a	1919	3TD	C6-C5-C4	2.47	119.93	118.22
27	Z	39	PSU	O2-C2-N1	-2.47	120.07	122.79
28	a	747	1MG	N9-C8-N7	-2.47	108.75	113.39
27	Z	46	7MG	C5-C6-N1	2.45	119.61	112.31
5	A	516	PSU	C6-N1-C2	-2.43	120.20	122.68
28	a	2556	OMU	O4-C4-C5	-2.43	120.89	125.16
27	Z	32	PSU	C6-N1-C2	-2.41	120.22	122.68
16	L	89	D2T	OD2-CG-CB	2.40	118.34	113.15
27	Z	37	MIA	C1'-N9-C8	-2.38	121.77	127.14
28	a	1915	PSU	O2-C2-N1	-2.37	120.18	122.79
27	Z	55	PSU	C6-C5-C4	2.34	119.84	118.20
28	a	2584	PSU	O4'-C1'-C2'	2.32	108.42	105.14
5	A	1518	MA6	C4-C5-N7	-2.30	107.82	110.62
5	A	1519	MA6	N3-C4-N9	2.29	130.86	127.08
16	L	89	D2T	O-C-CA	-2.29	118.78	124.78
28	a	2507	2MA	N6-C6-N1	2.29	120.27	117.03
27	Z	37	MIA	C4-C5-N7	-2.28	107.84	110.62
28	a	747	1MG	C5-C6-N1	2.28	119.32	114.91
28	a	2453	H2U	C5-C4-N3	-2.28	114.09	116.65
28	a	2608	PSU	C6-C5-C4	2.27	119.78	118.20
28	a	2453	H2U	C4-N3-C2	2.26	127.67	125.79
5	A	516	PSU	O4'-C1'-C2'	2.26	108.33	105.14
55	Y	8	4SU	O2-C2-N1	-2.26	119.78	122.79
27	Z	47	3AU	O2-C2-N1	-2.25	119.80	122.79
39	l	81	4D4	O-C-CA	-2.24	118.90	124.78
27	Z	37	MIA	C6-C5-C4	2.23	120.19	117.18
27	Z	39	PSU	C6-C5-C4	2.23	119.75	118.20
5	A	1518	MA6	N3-C4-N9	2.22	130.74	127.08
5	A	1498	UR3	C1'-N1-C2	2.21	120.72	116.99
28	a	2461	PSU	O2-C2-N3	-2.20	117.67	121.82
27	Z	39	PSU	C6-N1-C2	-2.20	120.43	122.68
5	A	1519	MA6	C4-C5-N7	-2.20	107.94	110.62
28	a	2073	G7M	N2-C2-N1	2.19	121.38	116.71
28	a	748	PSU	C6-N1-C2	-2.19	120.44	122.68
5	A	527	G7M	N9-C8-N7	-2.19	106.80	112.21
28	a	2507	2MA	C6-C5-N7	2.17	136.06	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1518	MA6	C4-N9-C1'	2.17	131.76	126.59
28	a	1620	6MZ	C4-N9-C8	2.16	108.07	105.73
28	a	2609	PSU	O2-C2-N1	-2.15	120.43	122.79
28	a	2073	G7M	CN7-N7-C5	2.14	129.43	126.77
27	Z	37	MIA	C4-N9-C8	2.13	108.03	105.73
27	Z	20	H2U	O2-C2-N1	-2.12	120.45	123.11
28	a	2453	H2U	O2-C2-N3	-2.11	117.56	121.50
27	Z	55	PSU	C6-N1-C2	-2.10	120.54	122.68
28	a	2073	G7M	N9-C8-N7	-2.09	107.03	112.21
55	Y	55	PSU	C6-N1-C2	-2.09	120.54	122.68
55	Y	20	H2U	O2-C2-N1	-2.08	120.50	123.11
55	Y	32	OMC	O2-C2-N3	-2.06	118.97	122.33
55	Y	32	OMC	C1'-N1-C2	2.05	122.99	118.42
55	Y	54	5MU	C1'-N1-C2	2.03	121.25	117.57
27	Z	46	7MG	C4-C5-N7	2.03	110.08	106.13
28	a	2507	2MA	C5-C4-N3	-2.01	124.93	127.19
27	Z	32	PSU	C6-C5-C4	2.01	119.60	118.20
28	a	1921	PSU	C6-C5-C4	2.00	119.60	118.20
28	a	1620	6MZ	C4-N9-C1'	-2.00	121.82	126.59

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	Z	46	7MG	O4'-C4'-C5'-O5'
39	l	81	4D4	NH1-CZ-NE-CD
55	Y	20	H2U	O4'-C1'-N1-C6
55	Y	32	OMC	C1'-C2'-O2'-CM2
28	a	2034	6MZ	O4'-C4'-C5'-O5'
28	a	2255	OMG	C1'-C2'-O2'-CM2
27	Z	46	7MG	C3'-C4'-C5'-O5'
27	Z	47	3AU	O4'-C4'-C5'-O5'
55	Y	20	H2U	O4'-C4'-C5'-O5'
28	a	2034	6MZ	C3'-C4'-C5'-O5'
31	d	150	MEQ	OE1-CD-CG-CB
31	d	150	MEQ	NE2-CD-CG-CB
27	Z	8	4SU	C3'-C4'-C5'-O5'
27	Z	8	4SU	O4'-C4'-C5'-O5'
27	Z	47	3AU	C3'-C4'-C5'-O5'
55	Y	8	4SU	C3'-C4'-C5'-O5'
55	Y	8	4SU	O4'-C4'-C5'-O5'
5	A	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	A	1519	MA6	C3'-C4'-C5'-O5'
28	a	1919	3TD	O4'-C4'-C5'-O5'
5	A	1519	MA6	C5-C6-N6-C10
39	l	81	4D4	NH2-CZ-NE-CD
55	Y	20	H2U	C3'-C4'-C5'-O5'
28	a	2073	G7M	C4'-C5'-O5'-P
55	Y	20	H2U	C4'-C5'-O5'-P
39	l	81	4D4	OB-CB-CG-CD
39	l	81	4D4	CG-CD-NE-CZ
39	l	81	4D4	NE-CD-CG-CB
16	L	89	D2T	CA-CB-SB-CB1
28	a	2507	2MA	C4'-C5'-O5'-P
16	L	89	D2T	SB-CB-CG-OD2
55	Y	32	OMC	C2'-C1'-N1-C6
28	a	1919	3TD	C3'-C4'-C5'-O5'
16	L	89	D2T	CG-CB-SB-CB1
27	Z	20	H2U	C2'-C1'-N1-C2
28	a	748	PSU	O4'-C1'-C5-C6
55	Y	32	OMC	C2'-C1'-N1-C2
55	Y	20	H2U	C2'-C1'-N1-C6
55	Y	20	H2U	O4'-C1'-N1-C2
55	Y	20	H2U	C2'-C1'-N1-C2
27	Z	20	H2U	O4'-C4'-C5'-O5'
28	a	2073	G7M	O4'-C4'-C5'-O5'
28	a	2507	2MA	O4'-C4'-C5'-O5'
39	l	81	4D4	O-C-CA-CB

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1407	5MC	4	0
39	l	81	4D4	1	0
31	d	150	MEQ	1	0
27	Z	20	H2U	1	0
27	Z	55	PSU	1	0
5	A	516	PSU	1	0
28	a	2255	OMG	2	0
55	Y	54	5MU	2	0
28	a	2584	PSU	1	0
27	Z	37	MIA	3	0
28	a	2034	6MZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	1919	3TD	9	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 530 ligands modelled in this entry, 529 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
59	PHE	a	3001	-	10,11,12	0.43	0	10,13,15	0.30	0

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
59	PHE	a	3001	-	-	0/5/6/8	0/1/1/1

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	a	3001	PHE	2	0

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
5	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1532:U	O3'	1533:C	P	3.52
1	A	1407:5MC	O3'	1408:A	P	1.85

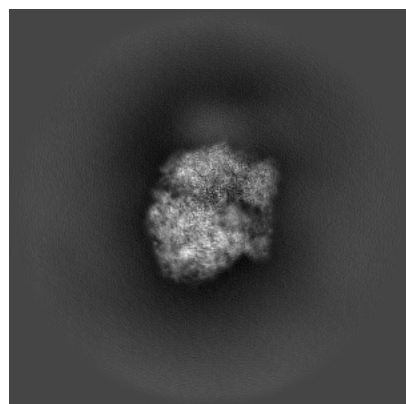
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51517. These allow visual inspection of the internal detail of the map and identification of artifacts.

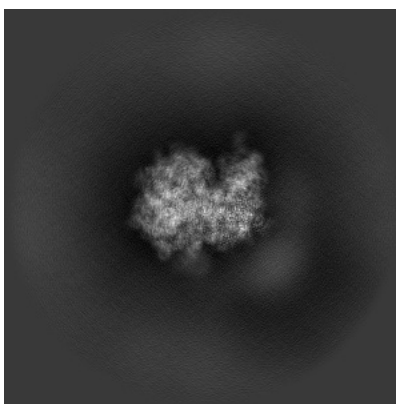
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

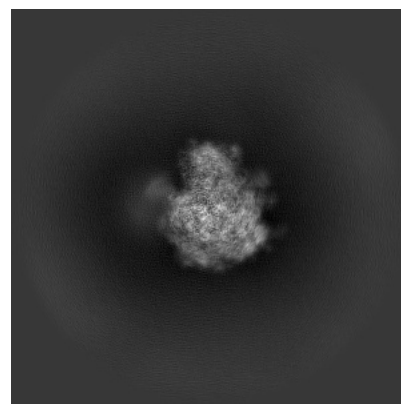
6.1.1 Primary map



X

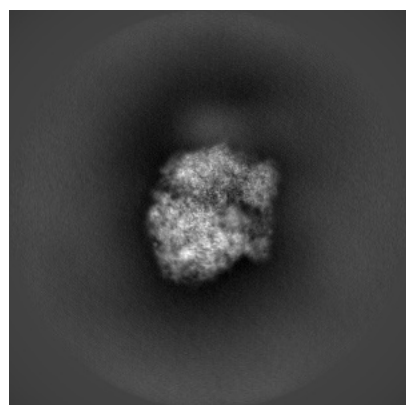


Y

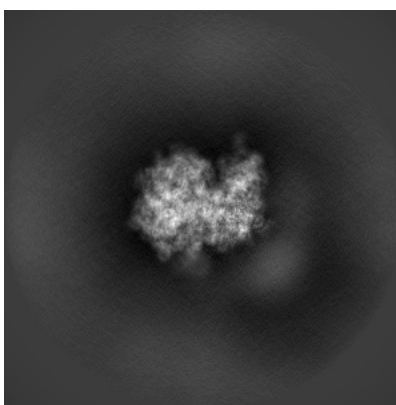


Z

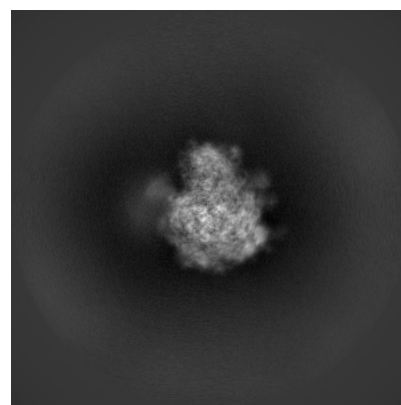
6.1.2 Raw map



X



Y

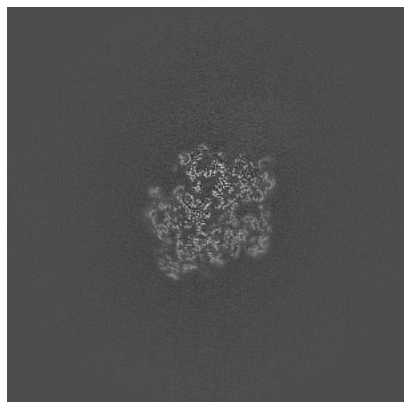


Z

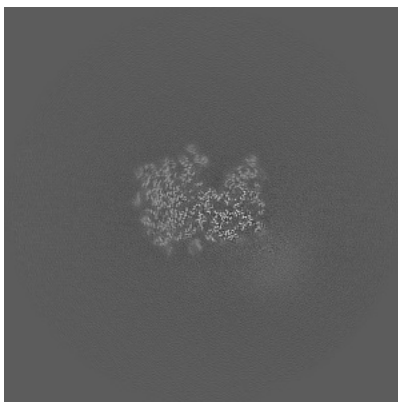
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

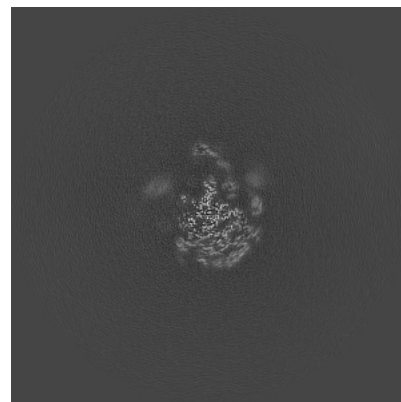
6.2.1 Primary map



X Index: 320

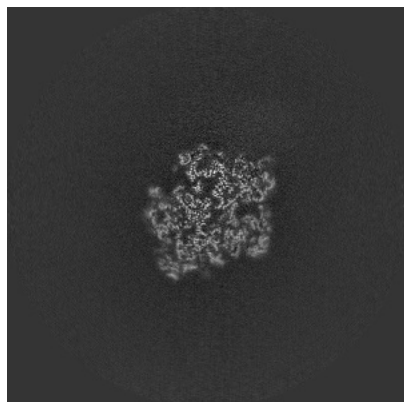


Y Index: 320

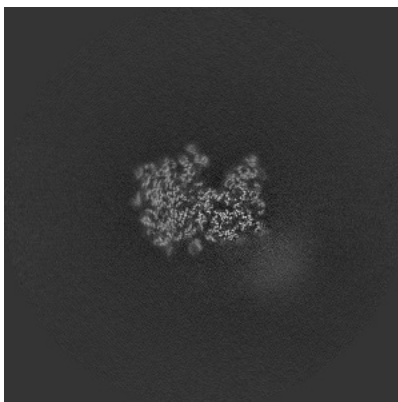


Z Index: 320

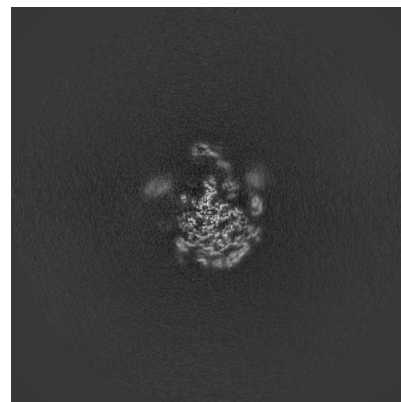
6.2.2 Raw map



X Index: 320



Y Index: 320

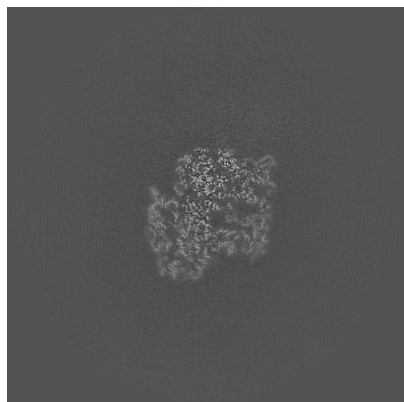


Z Index: 320

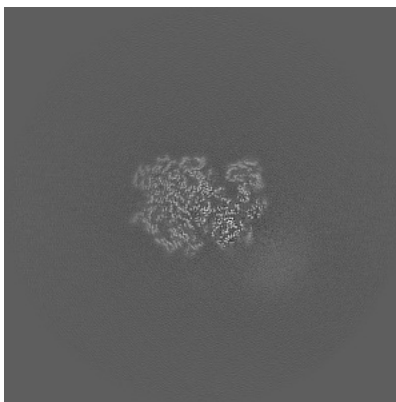
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

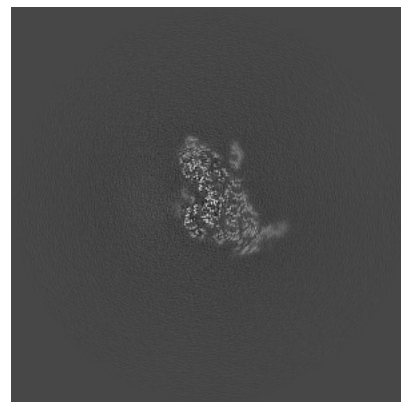
6.3.1 Primary map



X Index: 309

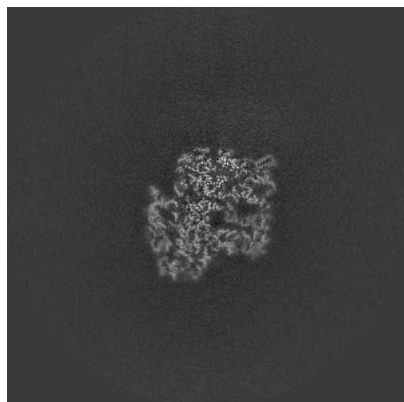


Y Index: 310

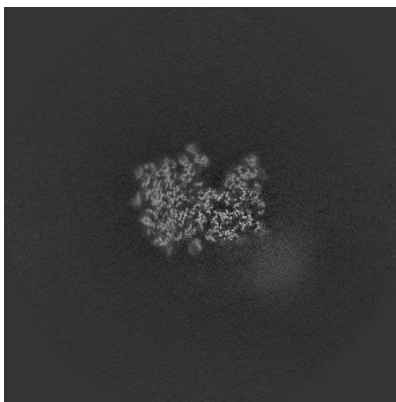


Z Index: 377

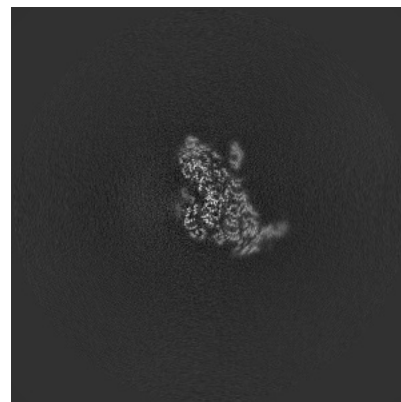
6.3.2 Raw map



X Index: 310



Y Index: 320

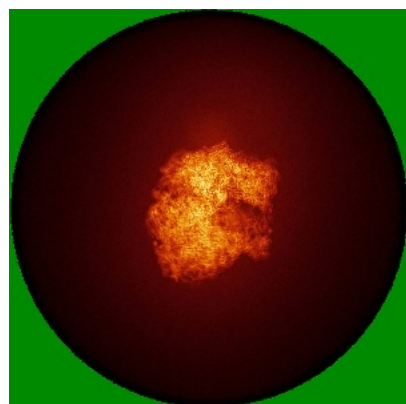


Z Index: 377

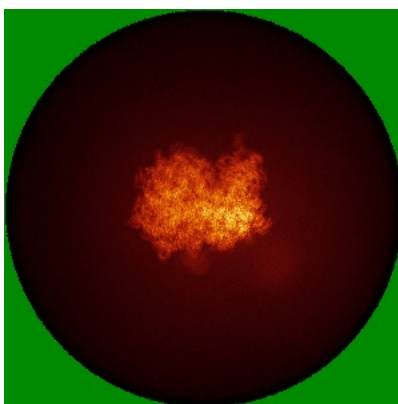
The images above show the largest variance slices of the map in three orthogonal directions.

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

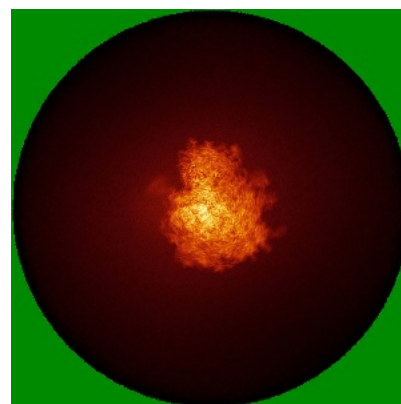
6.4.1 Primary map



X

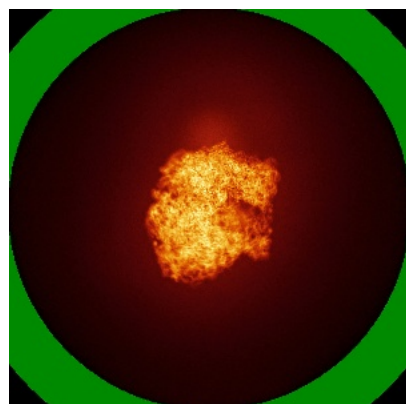


Y

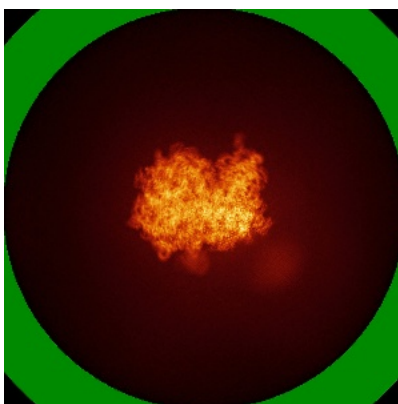


Z

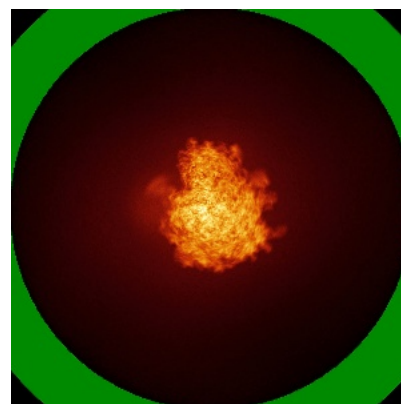
6.4.2 Raw map



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.

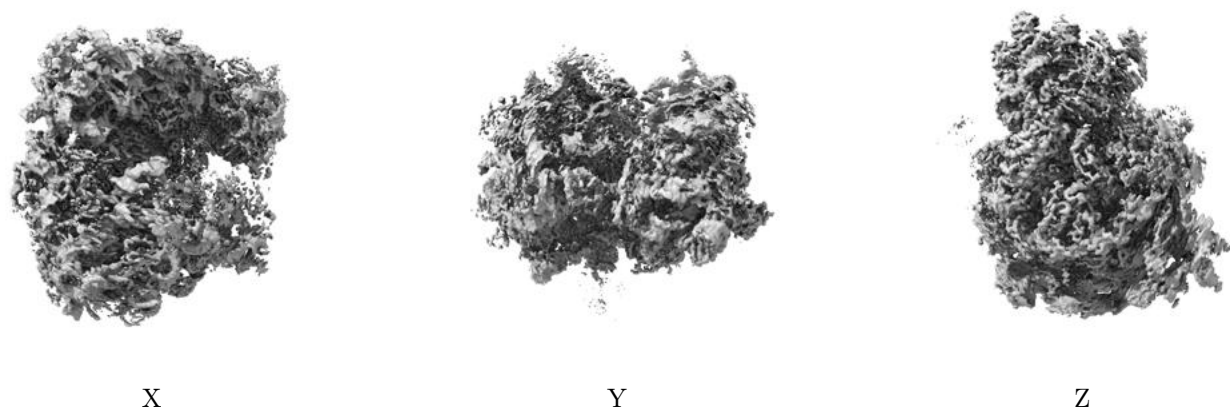
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

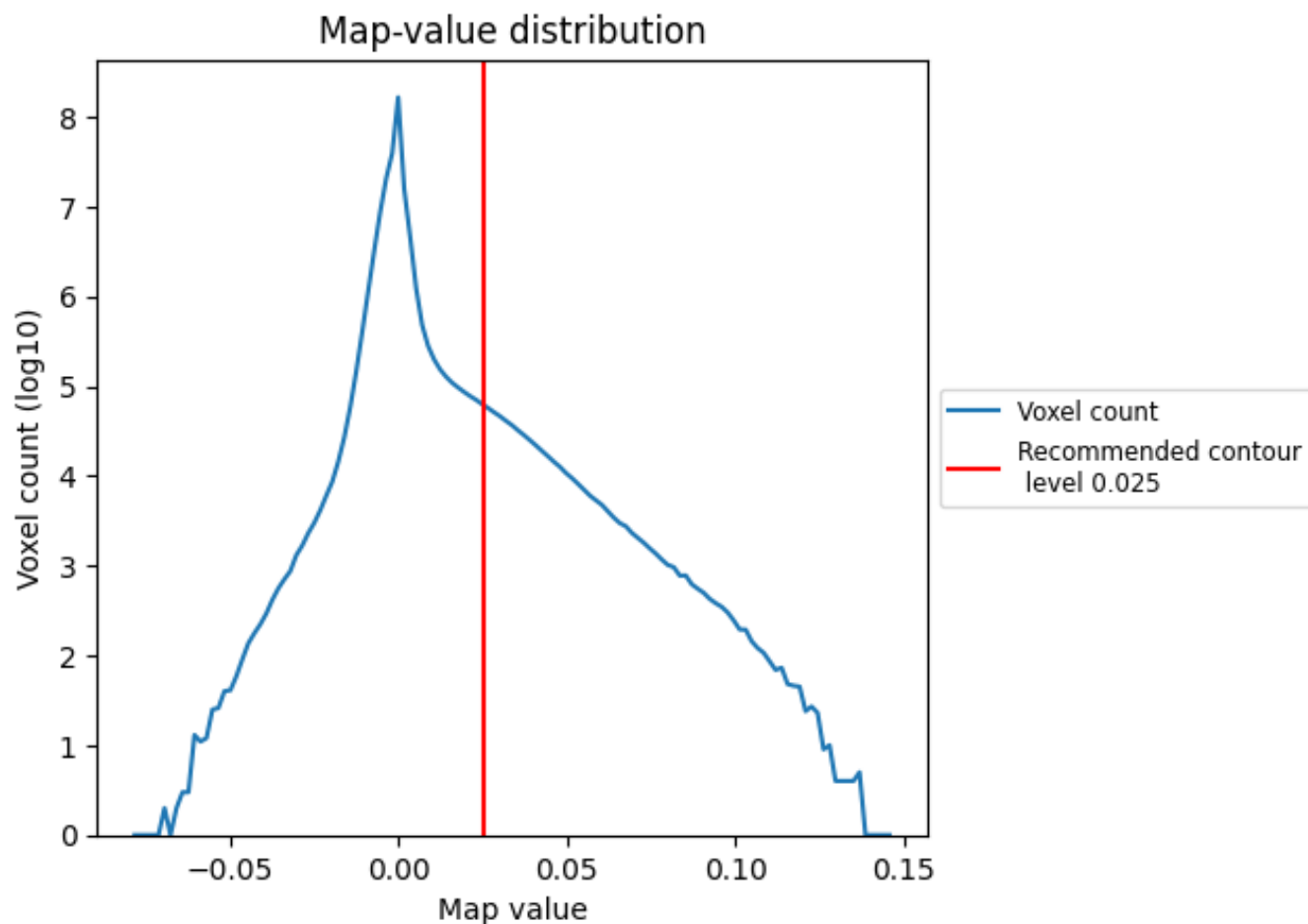
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

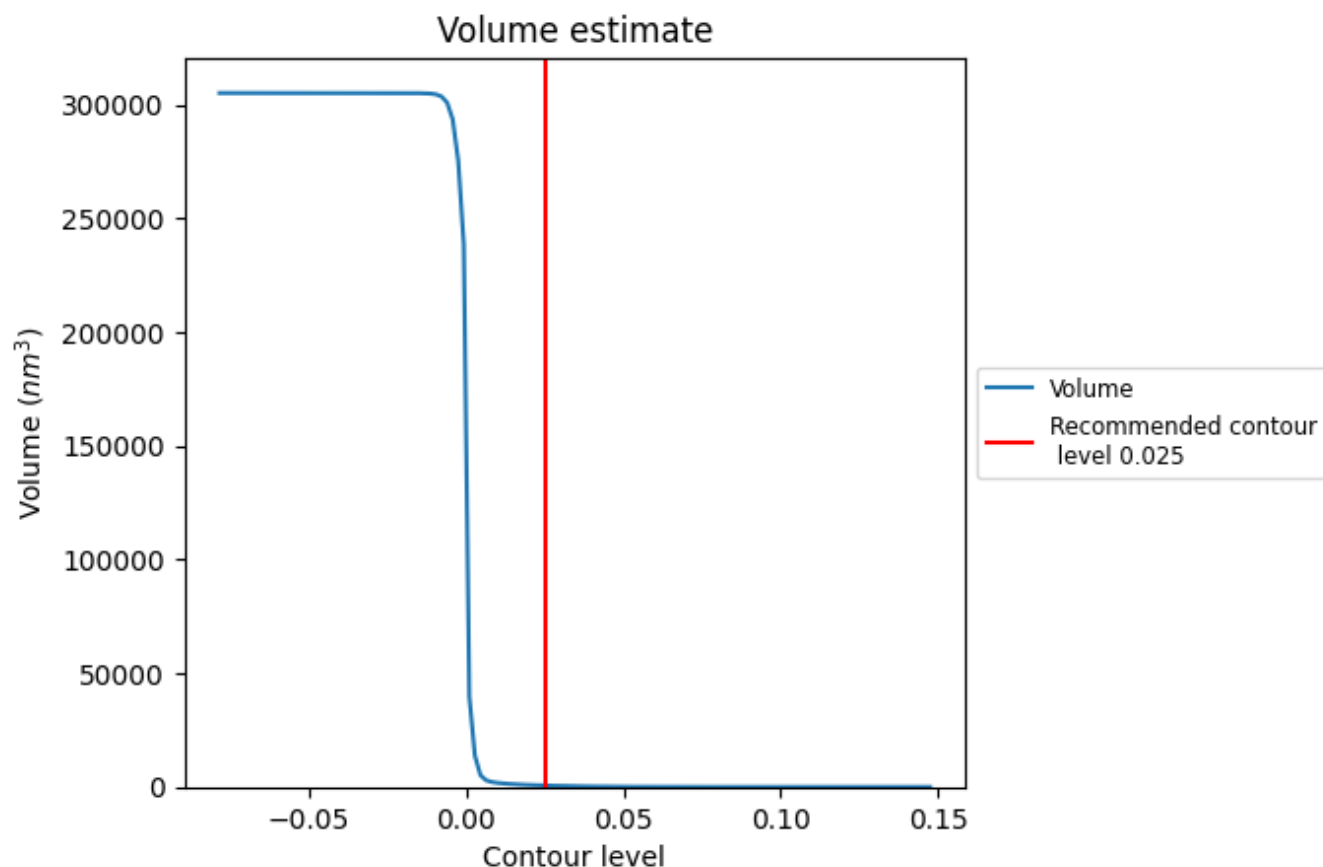
This section contains the results of statistical analysis of the map.

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.

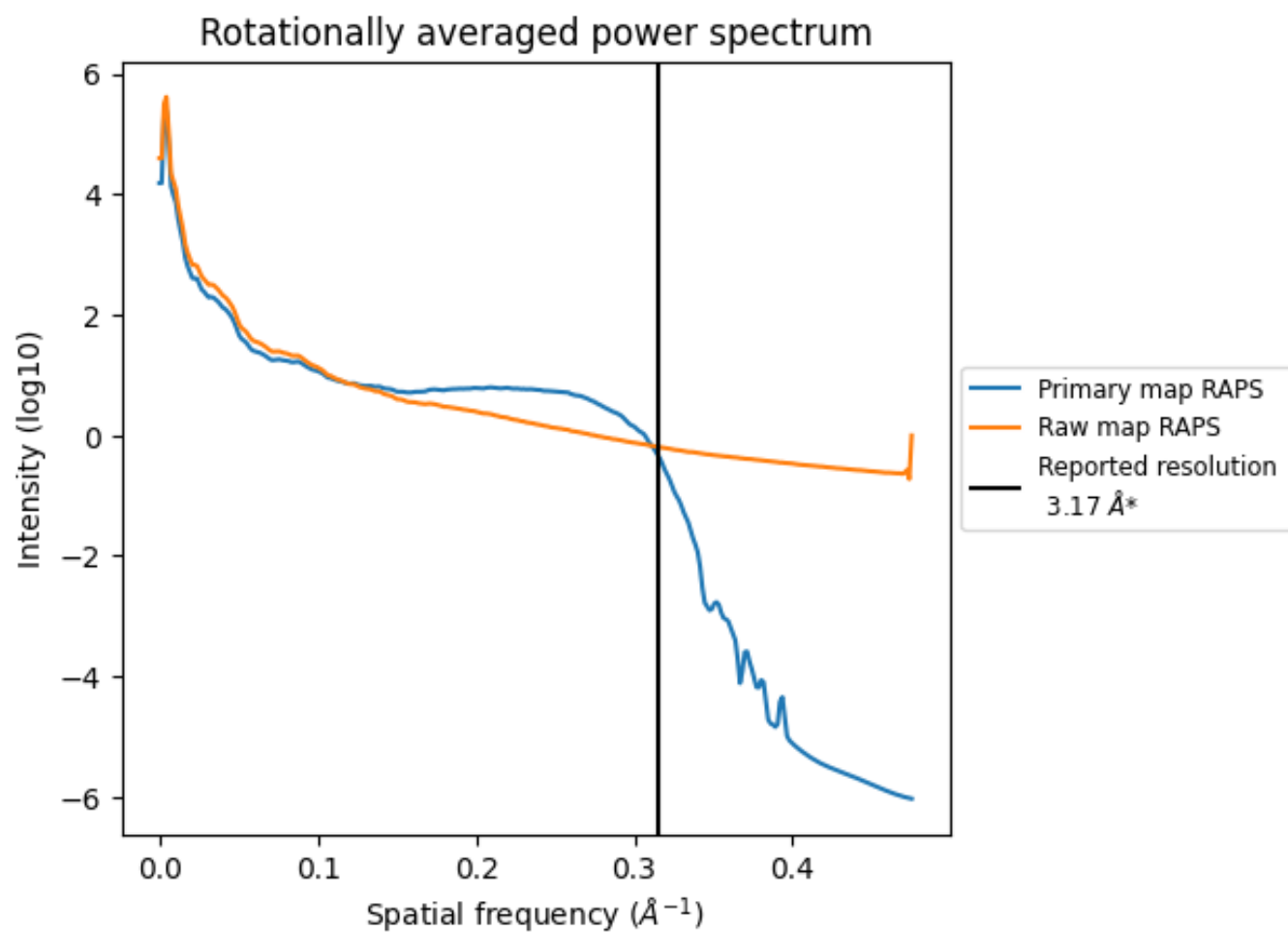
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 631 nm^3 ; this corresponds to an approximate mass of 570 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 ⓘ

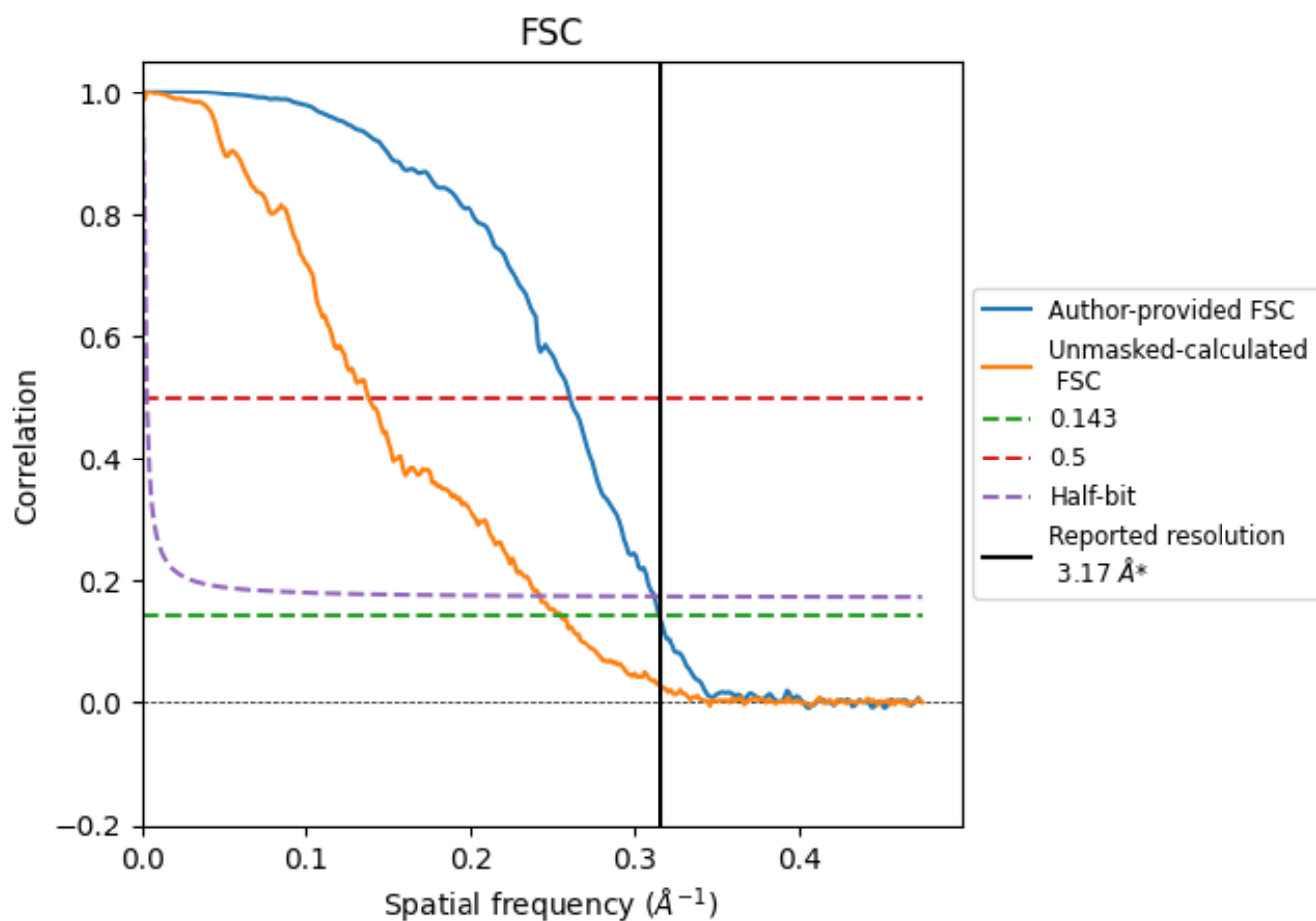


*Reported resolution corresponds to spatial frequency of 0.315 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.315 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

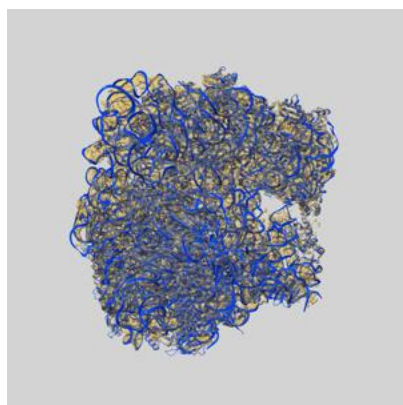
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.17	3.84	3.21
Unmasked-calculated*	3.92	7.25	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.17 by more than 10 %

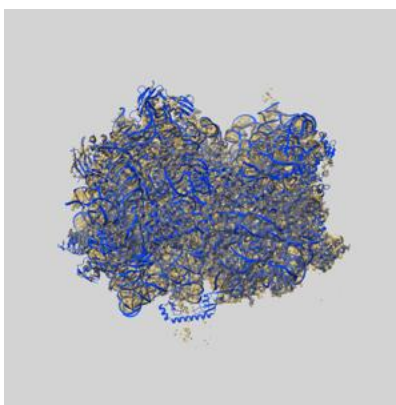
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51517 and PDB model 9GR1. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

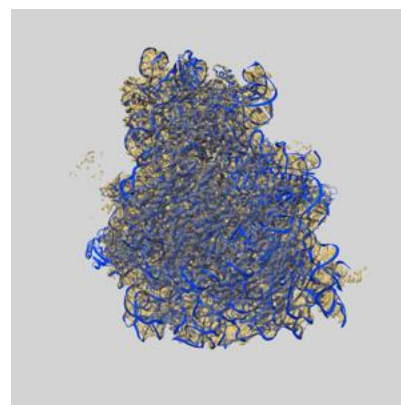
9.1 Map-model overlay [i](#)



X



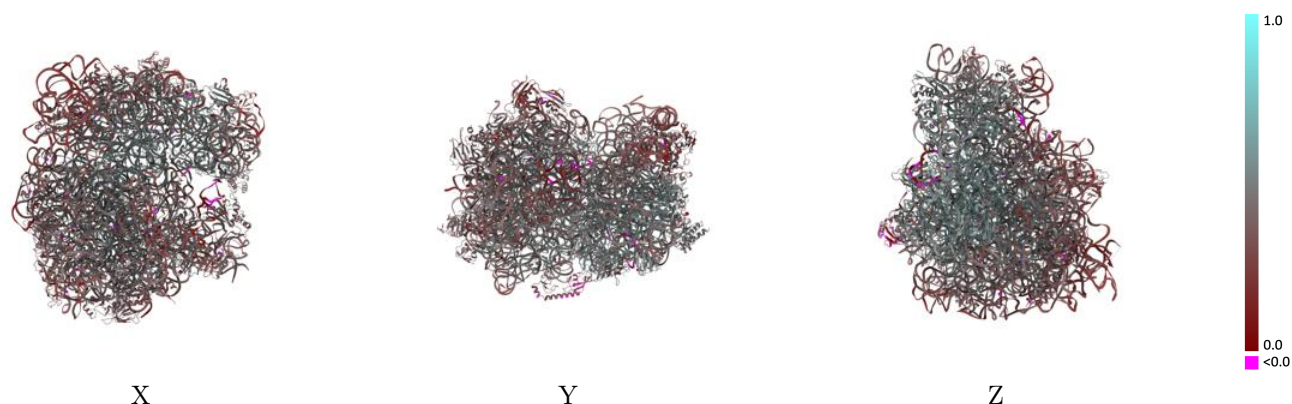
Y



Z

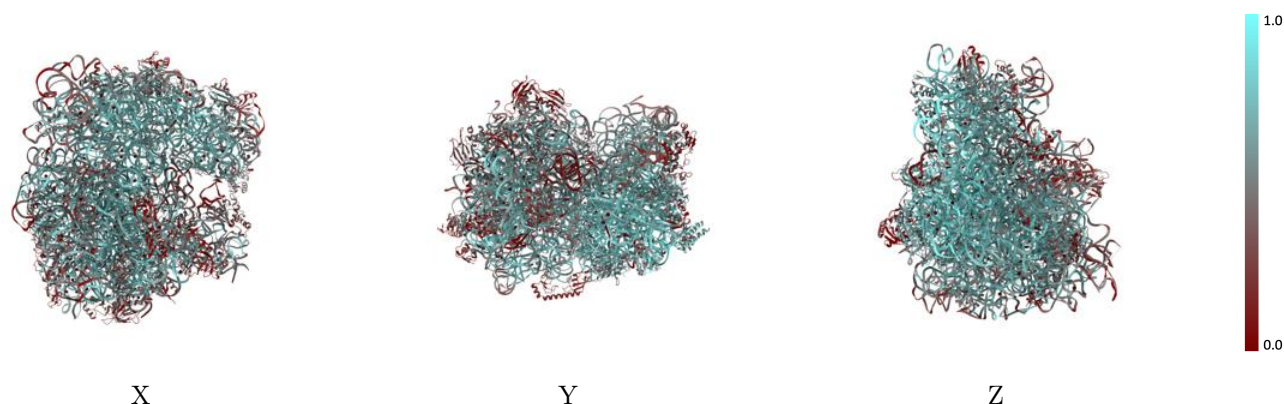
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



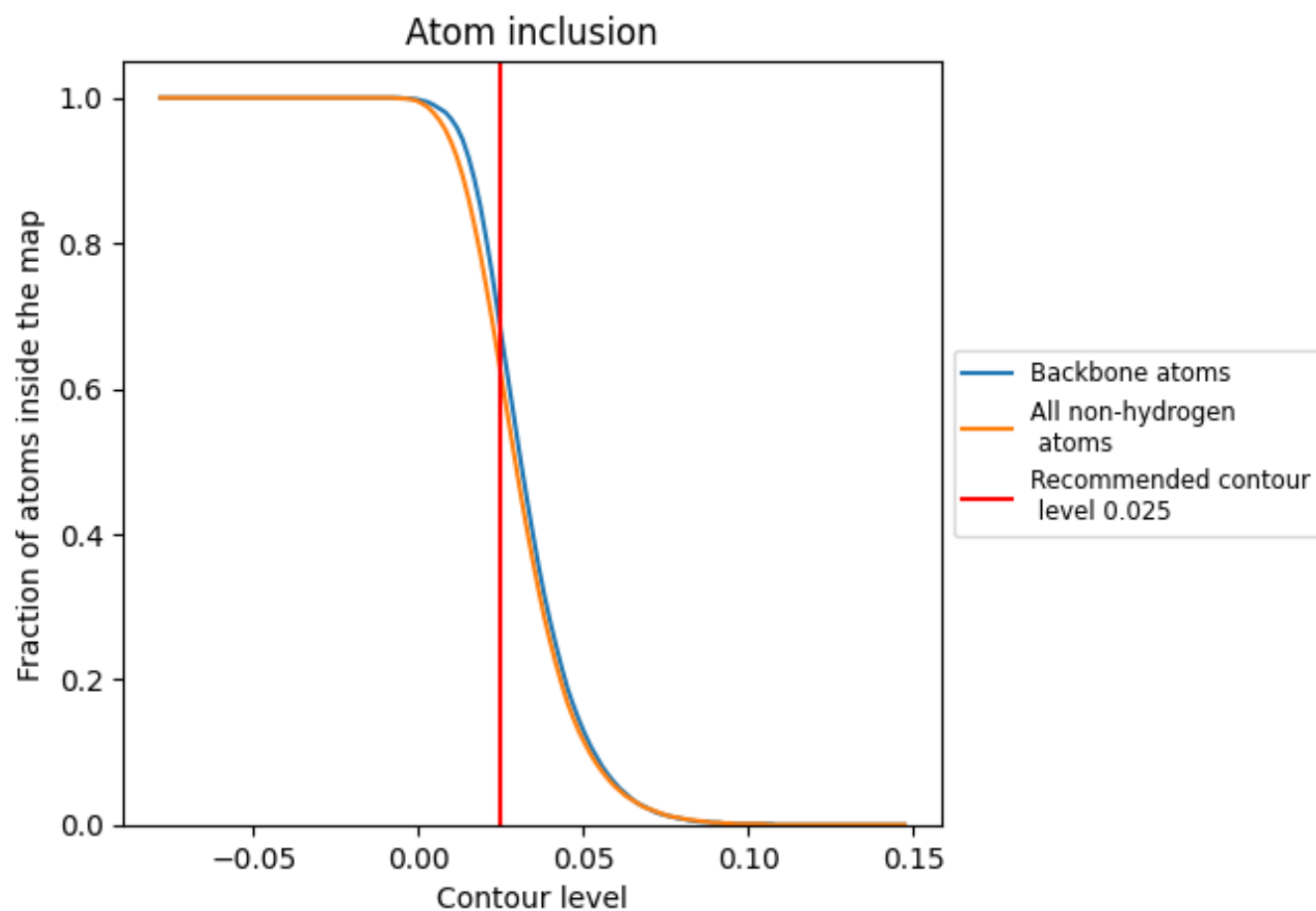
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 62% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6190	 0.4210
0	 0.0390	 0.3730
1	 0.5580	 0.4810
2	 0.4890	 0.4880
3	 0.4200	 0.4080
4	 0.0990	 0.1170
A	 0.7280	 0.4270
B	 0.6860	 0.4950
C	 0.5820	 0.4940
D	 0.3010	 0.3440
E	 0.6720	 0.5250
F	 0.6410	 0.5020
G	 0.5770	 0.4630
H	 0.6650	 0.5190
I	 0.6540	 0.5010
J	 0.4110	 0.4280
K	 0.7020	 0.5210
L	 0.5830	 0.4940
M	 0.4820	 0.4510
N	 0.5340	 0.4640
O	 0.6420	 0.5090
P	 0.3960	 0.3770
Q	 0.4780	 0.4130
R	 0.7180	 0.5230
S	 0.4290	 0.4080
T	 0.4210	 0.3530
U	 0.5010	 0.4110
X	 0.4980	 0.4400
Y	 0.6020	 0.4140
Z	 0.3090	 0.3770
a	 0.6990	 0.4200
b	 0.5960	 0.3880
c	 0.6740	 0.5320
d	 0.3700	 0.4050
e	 0.3260	 0.3840



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Chain	Atom inclusion	Q-score
f	 0.2900	 0.3580
g	 0.1180	 0.2880
h	 0.0410	 0.1850
i	 0.3680	 0.3960
j	 0.4650	 0.4520
k	 0.3990	 0.4280
l	 0.4550	 0.4530
m	 0.4050	 0.4000
n	 0.2860	 0.3450
o	 0.3660	 0.3860
p	 0.4540	 0.4170
q	 0.3200	 0.4040
r	 0.3590	 0.4090
s	 0.2920	 0.3690
t	 0.1750	 0.2940
u	 0.2340	 0.3460
v	 0.4140	 0.4330
w	 0.4990	 0.4510
x	 0.2560	 0.2910
y	 0.3300	 0.3700
z	 0.3430	 0.3950