



Full wwPDB EM Validation Report ⓘ

Jul 6, 2026 – 02:34 pm BST

PDB ID : 9HIG / pdb_00009hig
EMDB ID : EMD-52192
Title : Cryo-EM composite structure of 70S ribosome of marine cold bacterium *Pseudalteromonas translucida* (P. haloplanktis)TAC125.
Authors : Singh, V.; Godsora, B.K.J.; Emmerich, A.G.; Majumdar, S.; Sanyal, S.
Deposited on : 2024-11-26
Resolution : 2.36 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.dev133
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) : 2.50

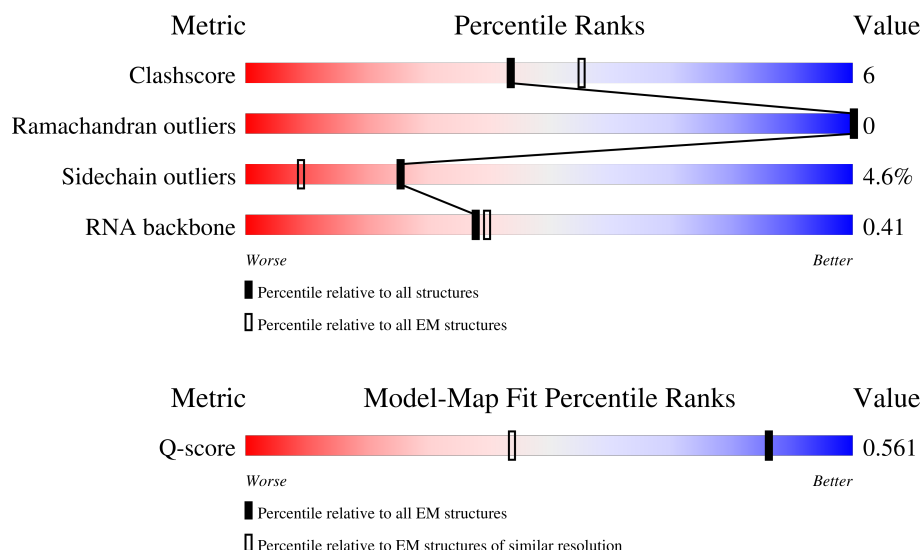
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.36 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	4686 (1.86 - 2.86)

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	A	1528	
2	B	242	
3	C	233	

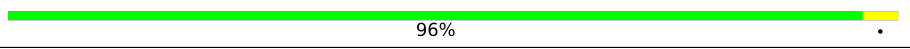
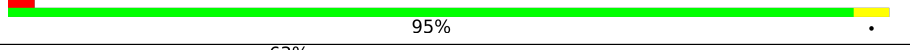
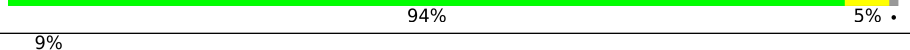
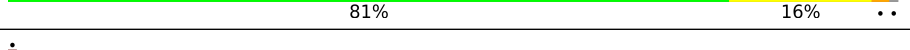
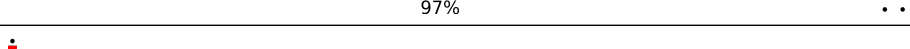
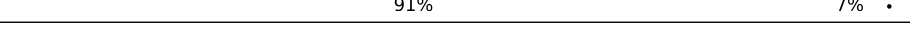
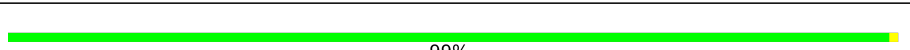
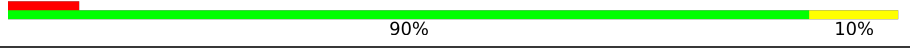
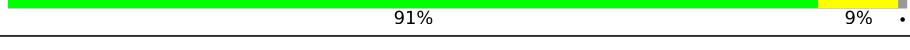
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Mol	Chain	Length	Quality of chain
4	D	206	
5	E	168	
6	F	113	
7	G	156	
8	H	130	
9	I	129	
10	J	103	
11	K	128	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	85	
18	R	75	
19	S	96	
20	T	86	
21	U	71	
22	W	18	
23	X	4	
24	a	2889	
25	b	117	
26	0	51	
27	1	44	
28	2	66	

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Mol	Chain	Length	Quality of chain
29	3	44	
30	c	274	
31	d	211	
32	e	201	
33	g	177	
34	h	150	
35	i	142	
36	j	122	
37	k	144	
38	l	137	
39	m	133	
40	n	116	
41	o	119	
42	p	120	
43	q	103	
44	r	110	
45	s	100	
46	t	104	
47	u	204	
48	v	85	
49	w	95	
50	x	63	
51	y	60	
52	z	56	
53	f	179	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 132798 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1426	Total	C	N	O	P	0	0
			30595	13652	5602	9915	1426		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	214	Total	C	N	O	S	0	0
			1668	1058	297	306	7		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	202	Total	C	N	O	S	0	0
			1553	988	283	279	3		

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	154	Total	C	N	O	S	0	0
			1200	759	212	228	1		

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	153	Total	C	N	O	S	0	0
			1126	701	213	206	6		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	103	Total	C	N	O	S	0	0
			834	526	149	154	5		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	128	Total	C	N	O	S	0	0
			689	420	136	132	1		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	129	Total	C	N	O	S	0	0
			979	620	176	180	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	124	Total	C	N	O	S	0	0
			911	567	178	165	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	94	Total	C	N	O	0	0
			602	371	115	116		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	116	Total	C	N	O	S	0	0
			864	533	170	159	2		

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	82	Total	C	N	O	S	0	0
			638	395	129	112	2		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	112	Total	C	N	O	S	0	0
			867	535	175	155	2		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	97	Total	C	N	O	S	0	0
			774	480	156	134	4		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			717	451	138	128			

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	79	Total	C	N	O	S	0	0
			634	402	123	108	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	78	Total	C	N	O	S	0	0
			633	402	118	111	2		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	52	Total	C	N	O	0	0
			417	266	75	76		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	79	Total	C	N	O	S	0	0
			586	373	104	105	4		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	79	Total	C	N	O	S	0	0
			622	388	126	106	2		

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	42	Total	C	N	O	S	0	0
			267	166	51	49	1		

- Molecule 22 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	18	Total	C	N	O	P	0	0
			385	172	71	124	18		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	4	Total	C	N	O	P	0	0
			87	39	17	27	4		

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	2708	Total	C	N	O	P	0	0
			58077	25934	10643	18792	2708		

- Molecule 25 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	116	Total	C	N	O	P	0	0
			2476	1107	448	805	116		

- Molecule 26 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	0	51	Total	C	N	O	S	0	0
			420	270	76	71	3		

- Molecule 27 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	44	Total	C	N	O	S	0	0
			356	220	84	50	2		

- Molecule 28 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	65	Total	C	N	O	S	0	0
			531	338	113	77	3		

- Molecule 29 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	38	Total	C	N	O	S	0	0
			298	189	60	46	3		

- Molecule 30 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	253	Total	C	N	O	S	0	0
			1941	1197	396	343	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	210	Total	C	N	O	S	0	0
			1551	967	288	292	4		

- Molecule 32 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	201	Total	C	N	O	S	0	0
			1537	969	278	288	2		

- Molecule 33 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	168	Total	C	N	O	S	0	0
			1277	803	231	242	1		

- Molecule 34 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	149	Total	C	N	O	S	0	0
			1072	678	179	214	1		

- Molecule 35 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	141	Total	C	N	O	S	0	0
			1115	714	198	199	4		

- Molecule 36 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	121	Total	C	N	O	S	0	0
			932	584	179	165	4		

- Molecule 37 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	144	Total	C	N	O	S	0	0
			1052	653	204	192	3		

- Molecule 38 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	134	Total	C	N	O	S	0	0
			1078	681	212	180	5		

- Molecule 39 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	120	Total	C	N	O	S	0	0
			946	586	191	164	5		

- Molecule 40 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	108	Total	C	N	O	S	0	0
			805	498	158	148	1		

- Molecule 41 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	116	Total	C	N	O		0	0
			908	566	179	163			

- Molecule 42 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	p	118	Total	C	N	O	0	0
			945	599	190	156		

- Molecule 43 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	103	Total	C	N	O	S	0	0
			810	510	152	146	2		

- Molecule 44 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	110	Total	C	N	O	S	0	0
			843	526	158	155	4		

- Molecule 45 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	97	Total	C	N	O	S	0	0
			759	481	135	142	1		

- Molecule 46 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	t	103	Total	C	N	O	0	0
			769	482	141	146		

- Molecule 47 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	u	96	Total	C	N	O	0	0
			769	482	138	149		

- Molecule 48 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	v	78	Total	C	N	O	0	0
			595	368	116	111		

- Molecule 49 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	77	Total	C	N	O	S	0	0
			620	385	129	104	2		

- Molecule 50 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	63	Total	C	N	O	S	0	0
			496	303	97	93	3		

- Molecule 51 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	y	57	Total	C	N	O	S	0	0
			442	274	86	79	3		

- Molecule 52 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	55	Total	C	N	O	S	0	0
			427	255	91	80	1		

- Molecule 53 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	f	178	Total	C	N	O	S	0	0
			987	606	197	183	1		

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	47	Total	Mg	0
			47	47	
54	D	1	Total	Mg	0
			1	1	
54	F	1	Total	Mg	0
			1	1	
54	N	1	Total	Mg	0
			1	1	
54	S	1	Total	Mg	0
			1	1	
54	a	230	Total	Mg	0
			230	230	

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Mol	Chain	Residues	Atoms		AltConf
54	b	3	Total 3	Mg 3	0
54	c	3	Total 3	Mg 3	0
54	d	1	Total 1	Mg 1	0
54	e	1	Total 1	Mg 1	0

- Molecule 55 is water.

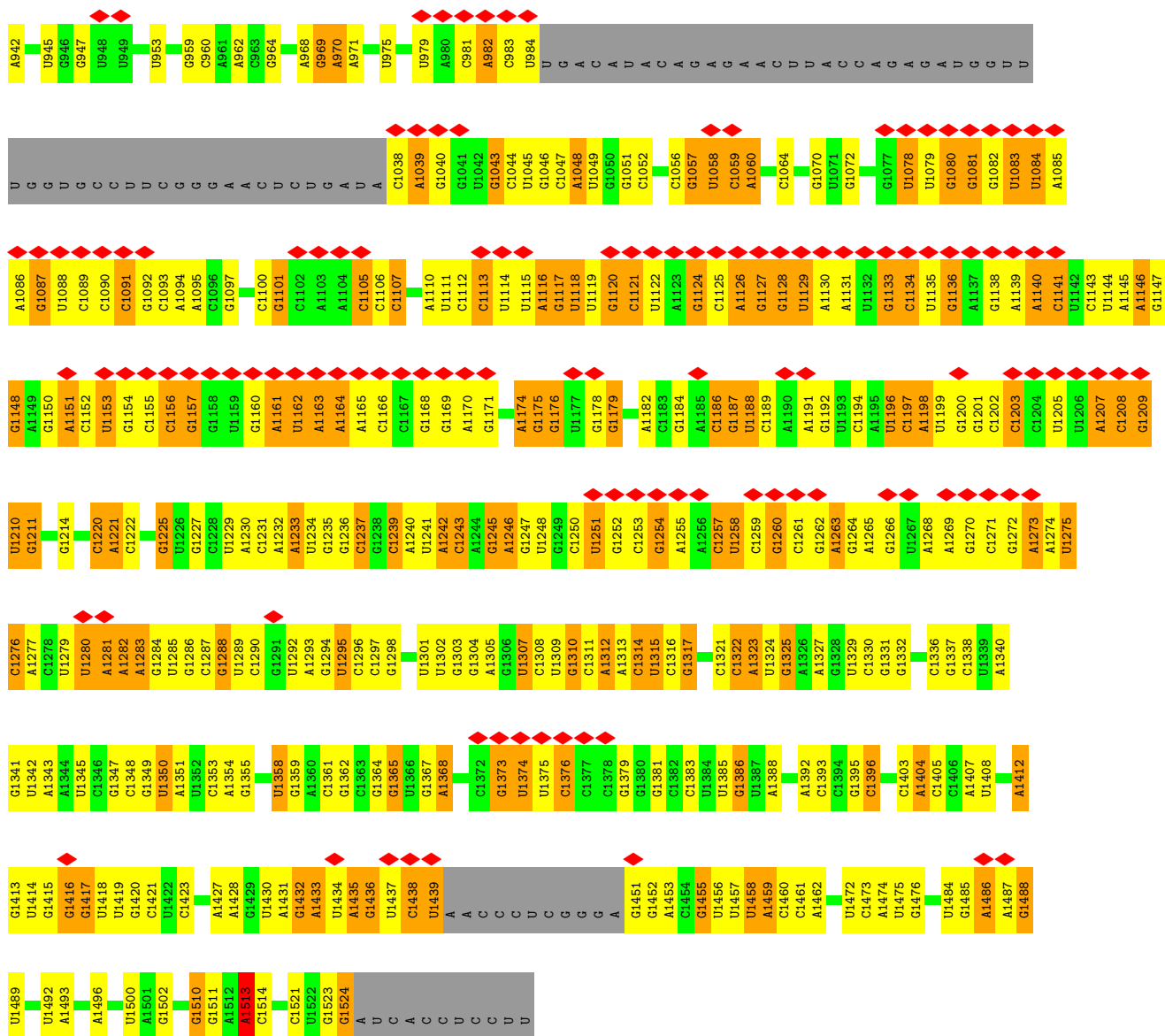
Mol	Chain	Residues	Atoms		AltConf
55	A	2	Total 2	O 2	0
55	a	22	Total 22	O 22	0
55	c	1	Total 1	O 1	0
55	m	1	Total 1	O 1	0
55	z	1	Total 1	O 1	0

3 Residue-property plots

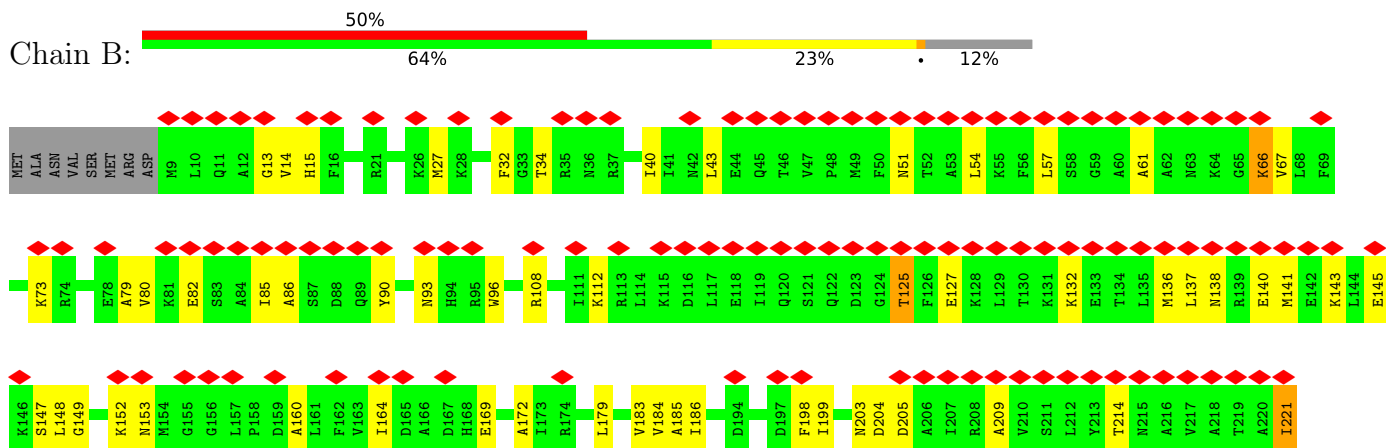
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

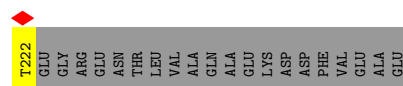
• Molecule 1: 16S rRNA



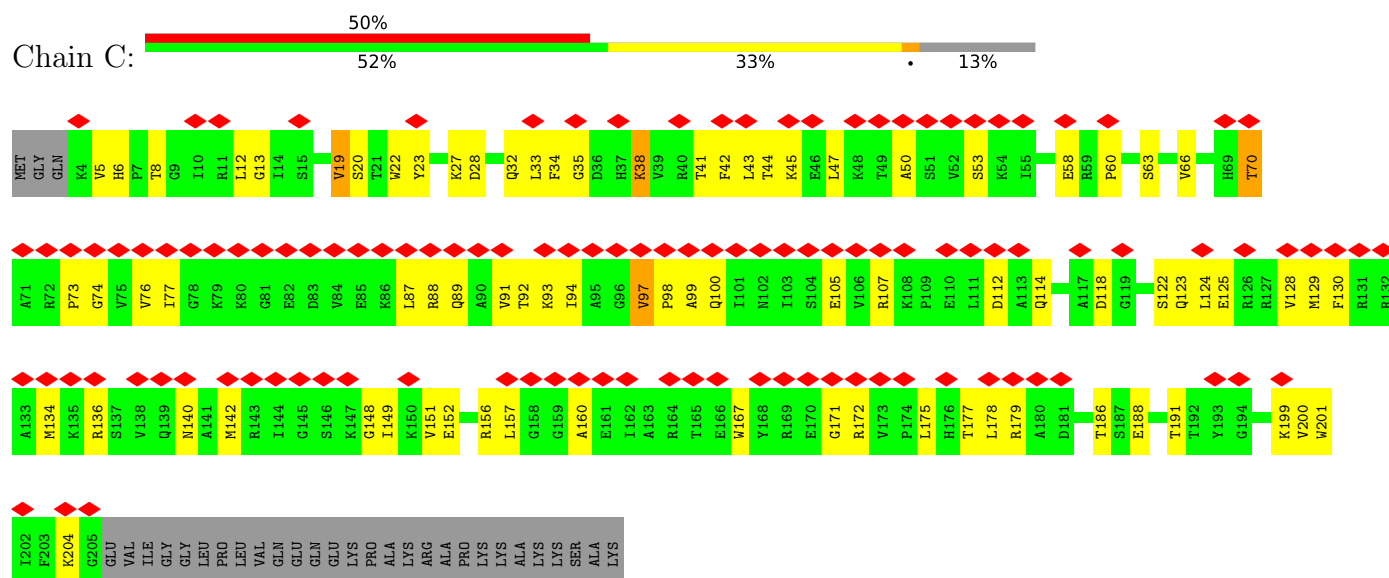


• Molecule 2: Small ribosomal subunit protein uS2

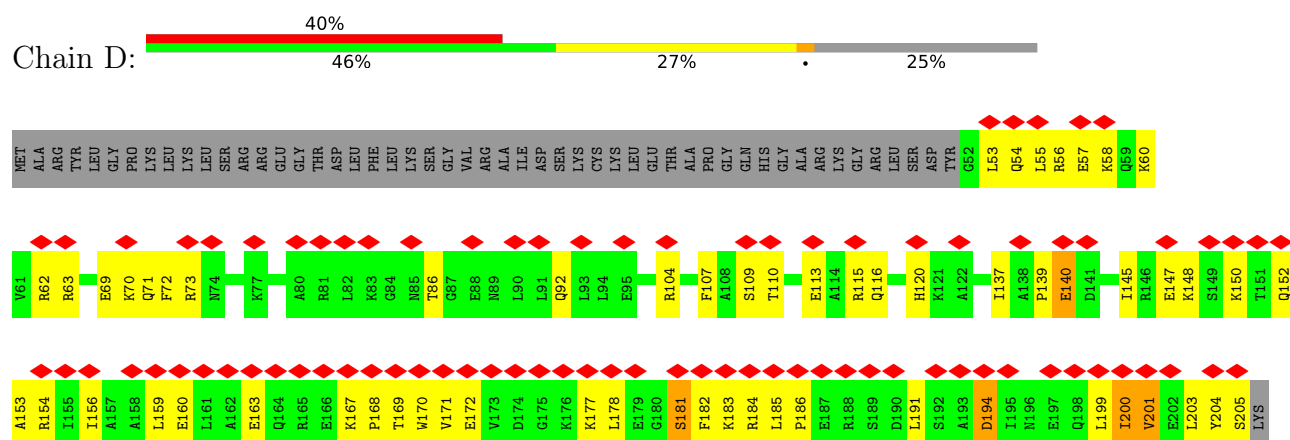




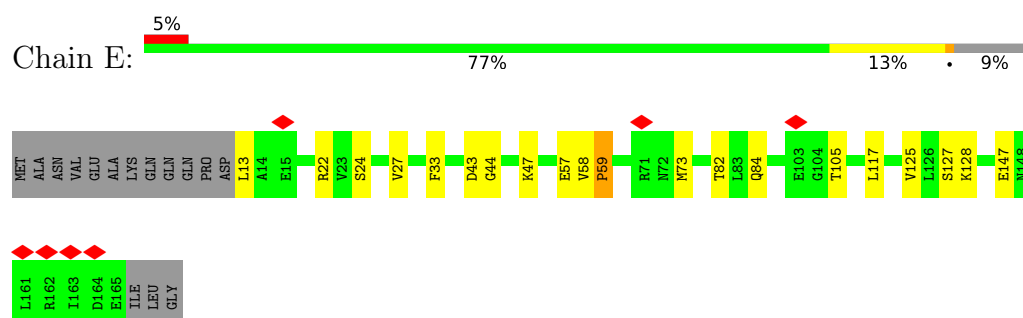
• Molecule 3: Small ribosomal subunit protein uS3



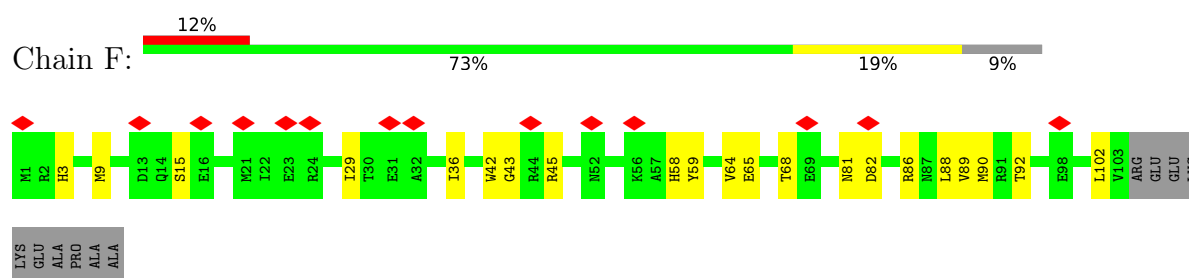
• Molecule 4: Small ribosomal subunit protein uS4



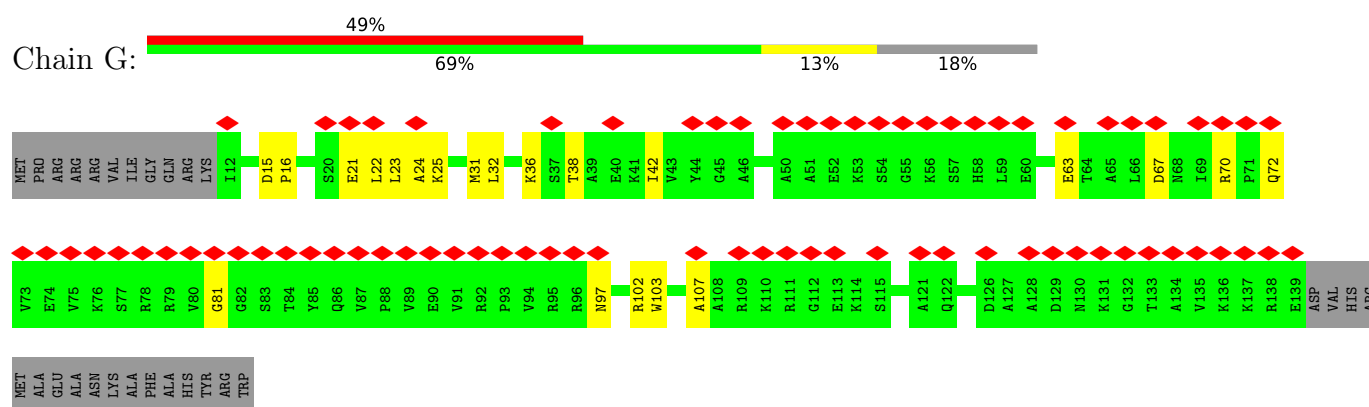
• Molecule 5: Small ribosomal subunit protein uS5



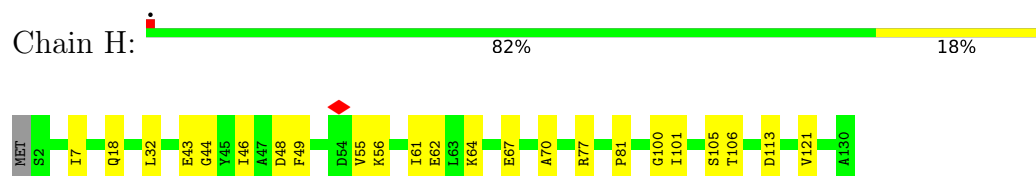
• Molecule 6: Small ribosomal subunit protein bS6



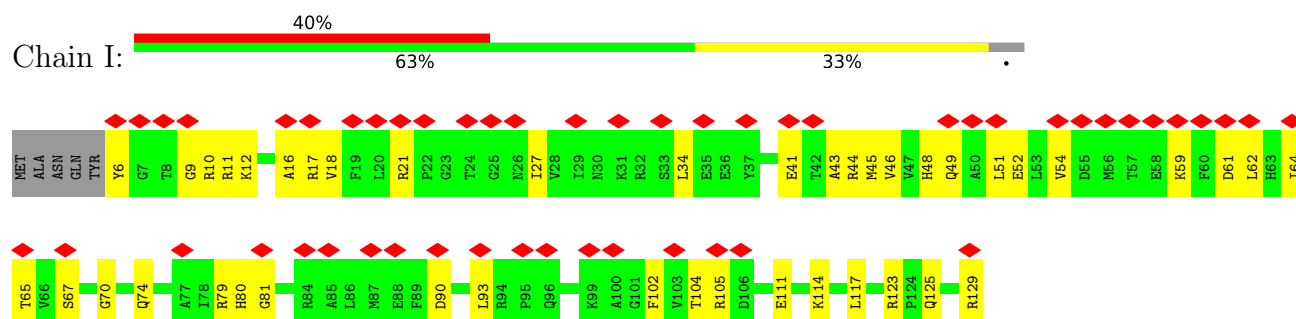
• Molecule 7: Small ribosomal subunit protein uS7



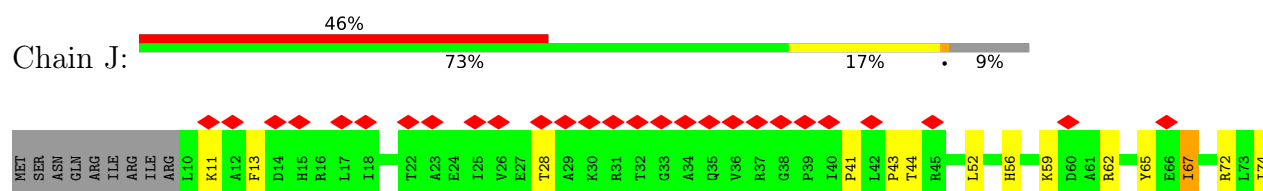
• Molecule 8: Small ribosomal subunit protein uS8

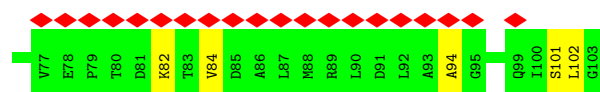


• Molecule 9: Small ribosomal subunit protein uS9

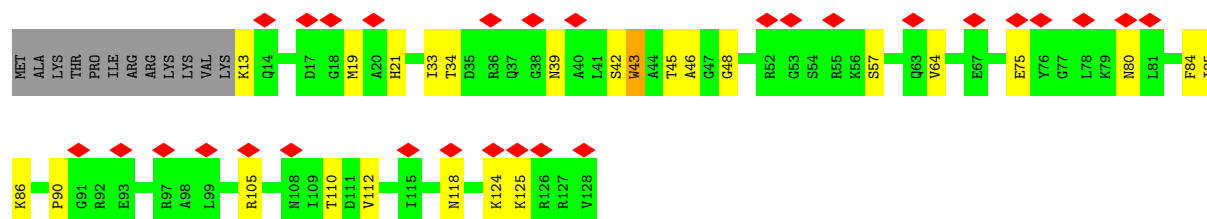


• Molecule 10: Small ribosomal subunit protein uS10

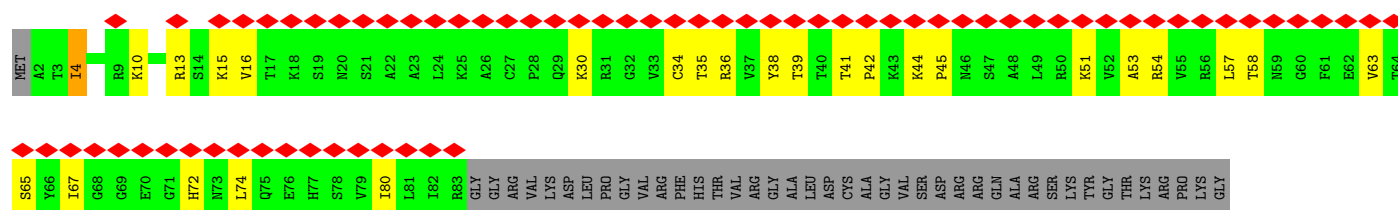




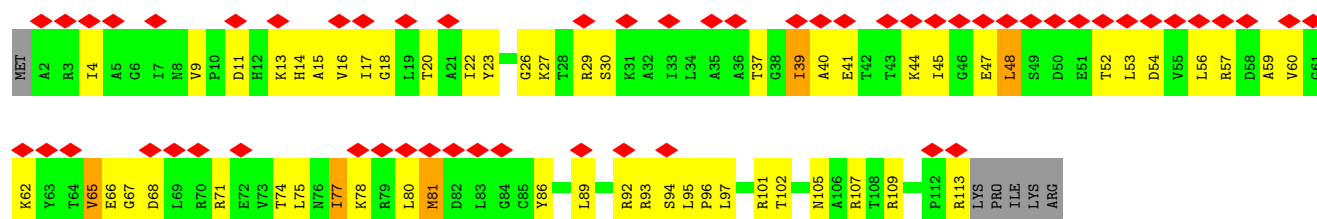
- Molecule 11: Small ribosomal subunit protein uS11



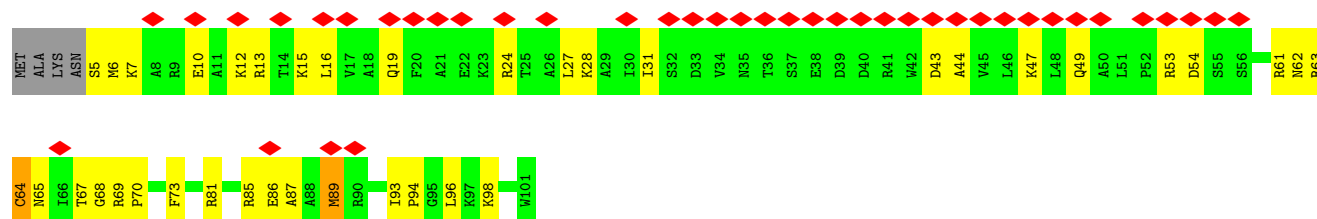
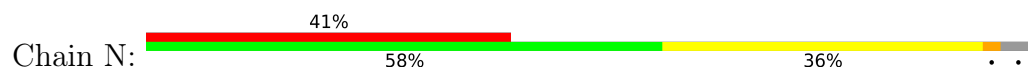
- Molecule 12: Small ribosomal subunit protein uS12



- Molecule 13: Small ribosomal subunit protein uS13



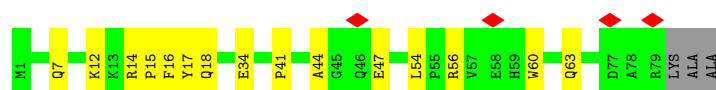
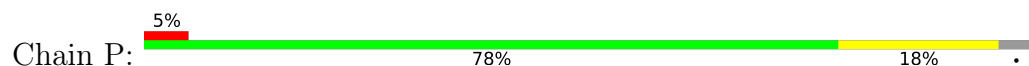
- Molecule 14: Small ribosomal subunit protein uS14



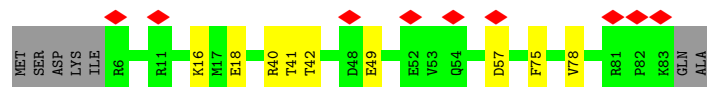
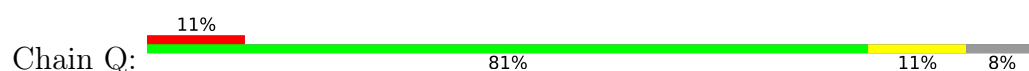
- Molecule 15: Small ribosomal subunit protein uS15



- Molecule 16: Small ribosomal subunit protein bS16



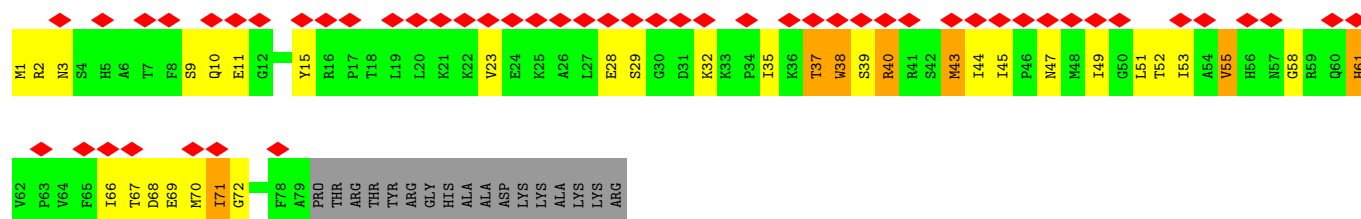
- Molecule 17: Small ribosomal subunit protein uS17



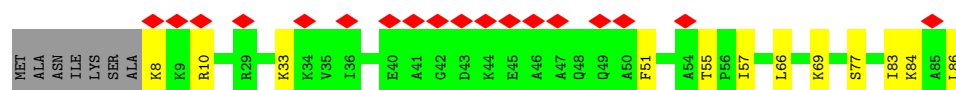
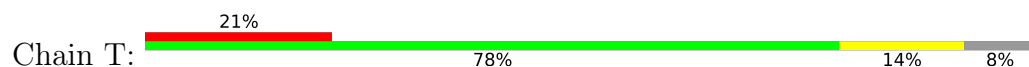
- Molecule 18: Small ribosomal subunit protein bS18



- Molecule 19: Small ribosomal subunit protein uS19

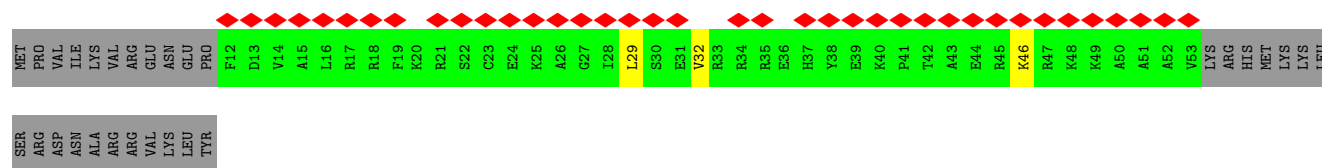


- Molecule 20: Small ribosomal subunit protein bS20

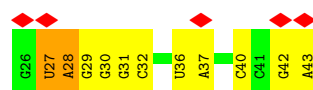
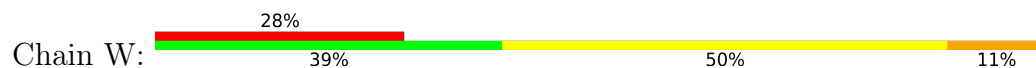


- Molecule 21: Small ribosomal subunit protein bS21





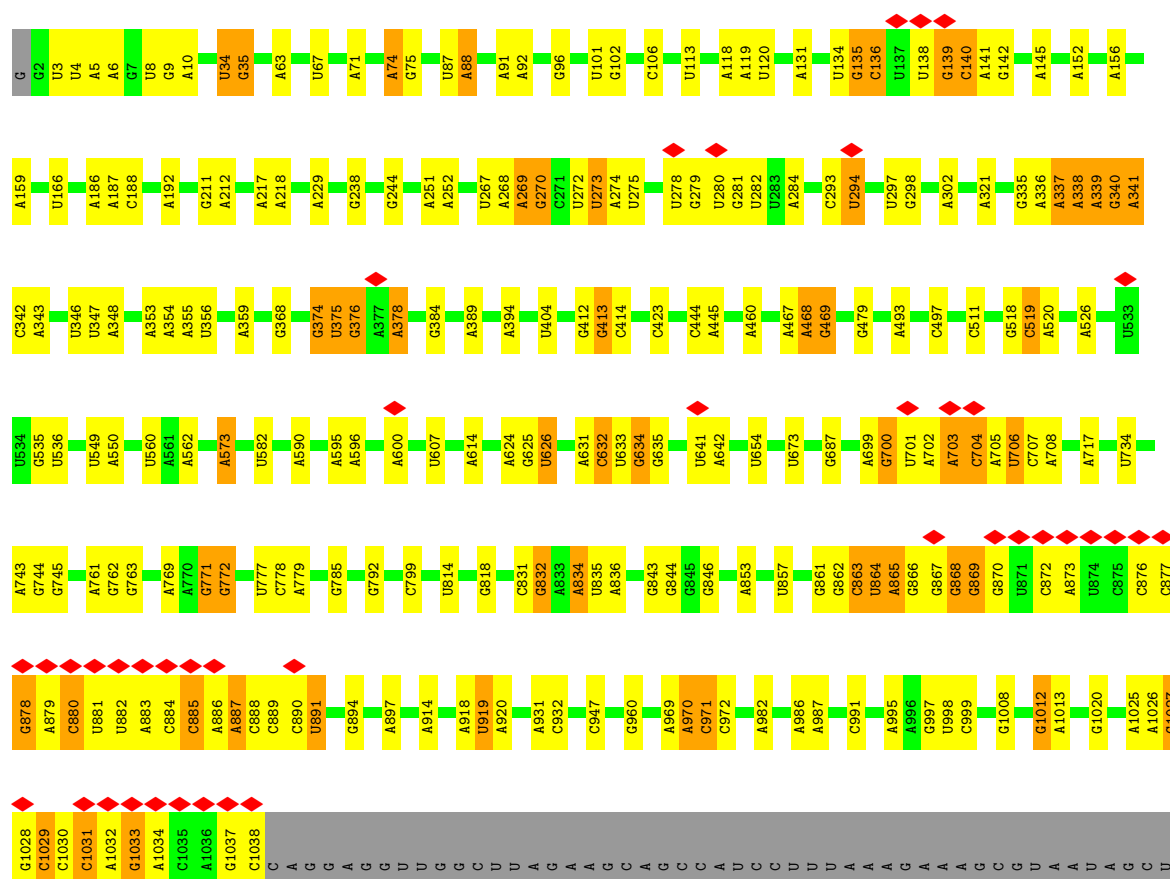
• Molecule 22: P-site tRNA-fMet



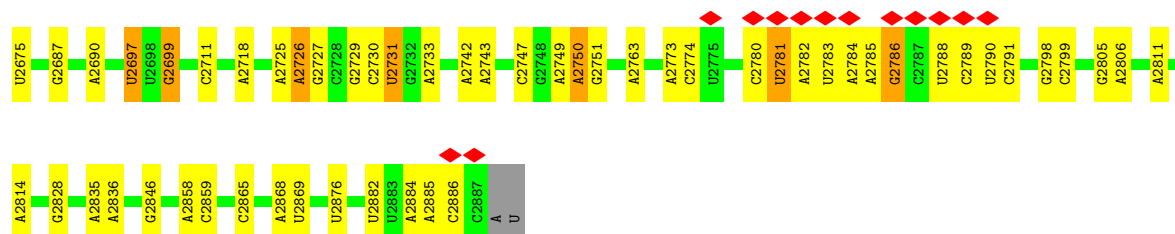
• Molecule 23: mRNA



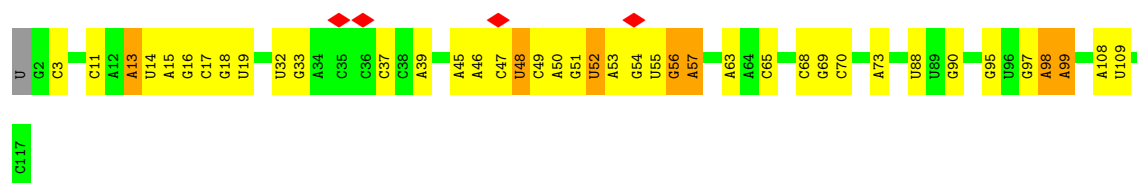
• Molecule 24: 23S rRNA



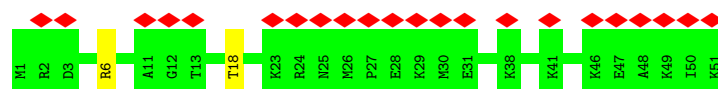
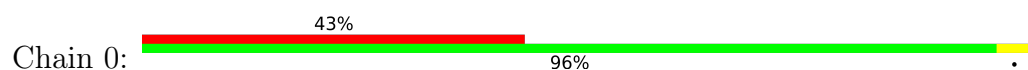




• Molecule 25: 5S rRNA



• Molecule 26: Large ribosomal subunit protein bL33



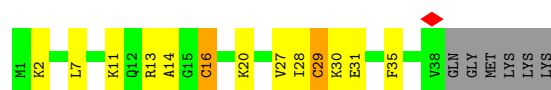
• Molecule 27: Large ribosomal subunit protein bL34



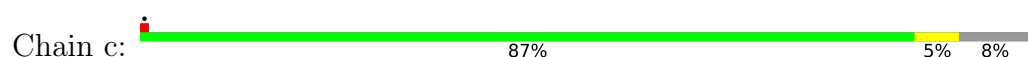
• Molecule 28: Large ribosomal subunit protein bL35



• Molecule 29: Large ribosomal subunit protein bL36



• Molecule 30: Large ribosomal subunit protein uL2





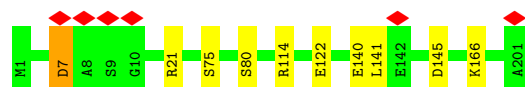
- Molecule 31: Large ribosomal subunit protein uL3

Chain d: 96%



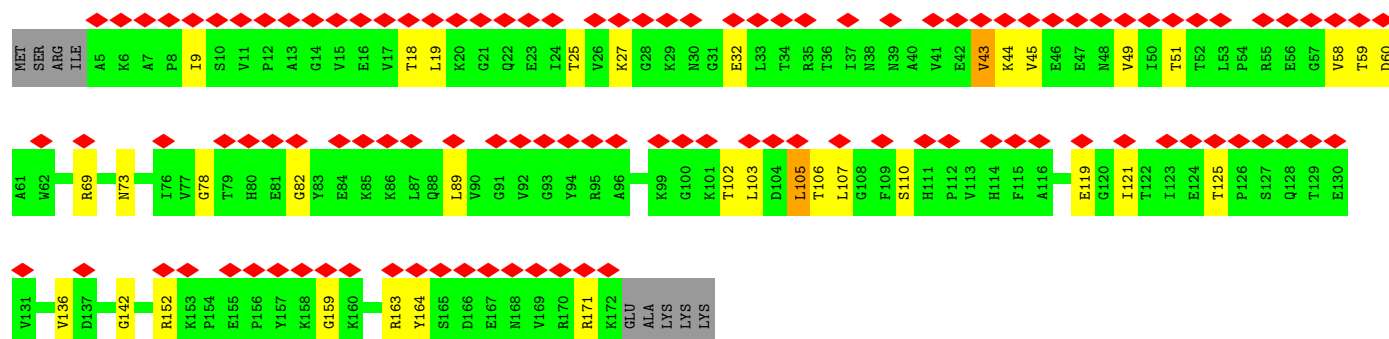
- Molecule 32: Large ribosomal subunit protein uL4

Chain e: 95%



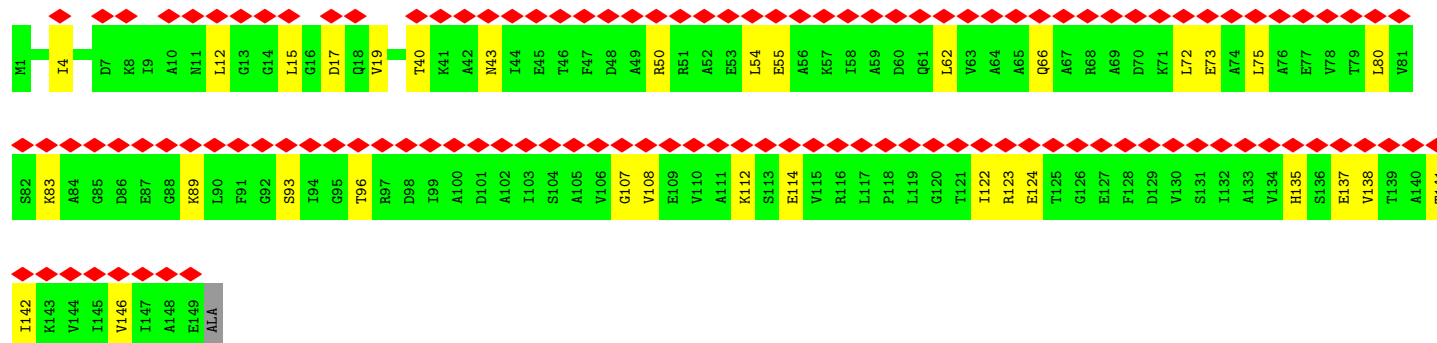
- Molecule 33: Large ribosomal subunit protein uL6

Chain g: 63% 75% 19% 5%

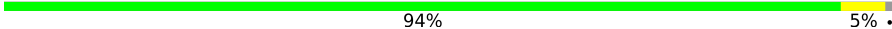


- Molecule 34: Large ribosomal subunit protein bL9

Chain h: 81% 77% 22%



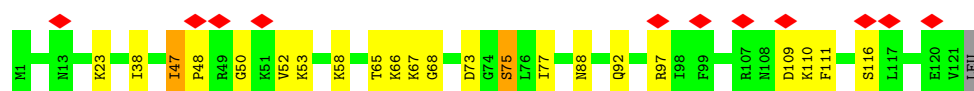
- Molecule 35: Large ribosomal subunit protein uL13

Chain i:  94% 5%

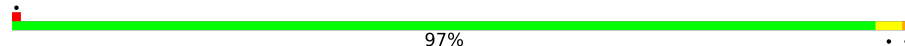


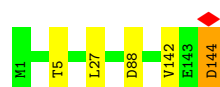
- Molecule 36: Large ribosomal subunit protein uL14

Chain j:  9% 81% 16% ..



- Molecule 37: Large ribosomal subunit protein uL15

Chain k:  97% ..



- Molecule 38: Large ribosomal subunit protein uL16

Chain l:  91% 7% .



- Molecule 39: Large ribosomal subunit protein bL17

Chain m:  84% 5% 10%



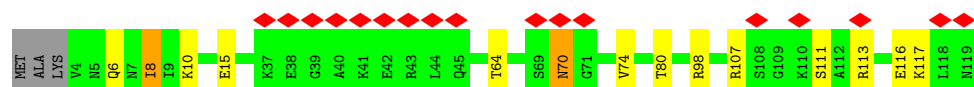
- Molecule 40: Large ribosomal subunit protein uL18

Chain n:  73% 19% 7%

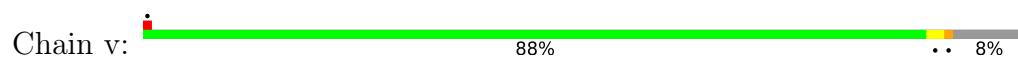


- Molecule 41: Large ribosomal subunit protein bL19

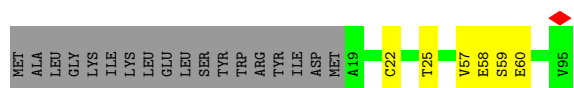
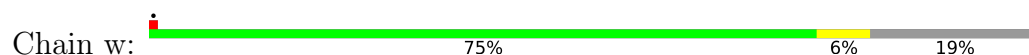
Chain o:  14% 86% 10% ..



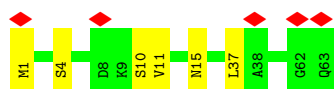
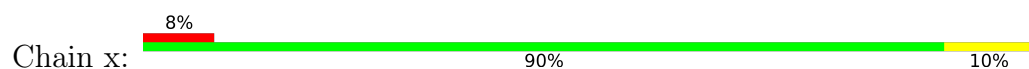
- Molecule 48: Large ribosomal subunit protein bL27



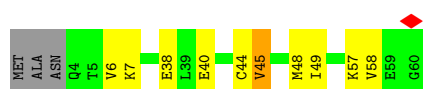
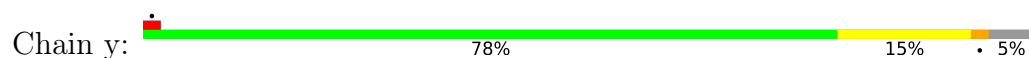
- Molecule 49: Large ribosomal subunit protein bL28



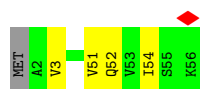
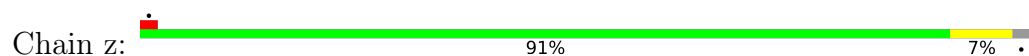
- Molecule 50: Large ribosomal subunit protein uL29



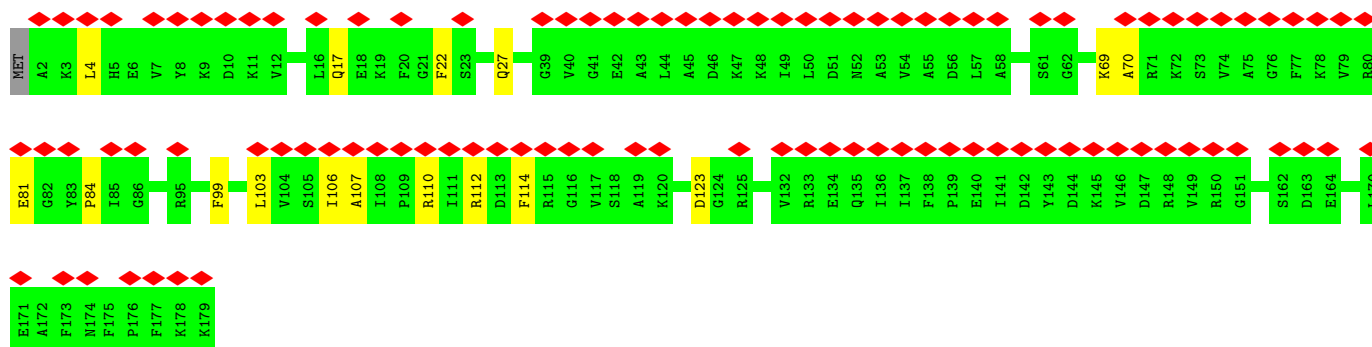
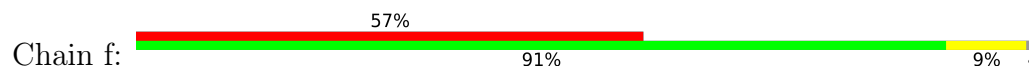
- Molecule 51: Large ribosomal subunit protein uL30



- Molecule 52: Large ribosomal subunit protein bL32



- Molecule 53: Large ribosomal subunit protein uL5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	360324	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 ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	33.362	Depositor
Minimum map value	-7.716	Depositor
Average map value	-0.010	Depositor
Map value standard deviation	1.018	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, OMU, 2MA, 5MC, H2U, 2MG, 5MU, MG, UR3, OMG, G7M, MA6, 4OC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/34100	0.36	0/53181
2	B	0.23	0/1699	0.38	0/2296
3	C	0.23	0/1580	0.39	0/2134
4	D	0.27	0/1215	0.53	1/1642 (0.1%)
5	E	0.36	0/1138	0.47	1/1530 (0.1%)
6	F	0.33	0/851	0.32	0/1154
7	G	0.23	0/692	0.41	0/953
8	H	0.41	0/990	0.38	0/1327
9	I	0.28	0/923	0.43	0/1239
10	J	0.32	0/611	0.44	0/839
11	K	0.27	0/881	0.45	1/1191 (0.1%)
12	L	0.18	0/646	0.28	0/869
13	M	0.26	0/875	0.51	0/1174
14	N	0.27	0/785	0.43	0/1048
15	O	0.35	0/727	0.26	0/969
16	P	0.42	0/645	0.41	0/863
17	Q	0.36	0/645	0.38	0/868
18	R	0.44	0/423	0.41	0/572
19	S	0.20	0/598	0.38	0/808
20	T	0.34	0/629	0.42	0/837
21	U	0.13	0/270	0.19	0/369
22	W	0.31	0/430	0.38	0/668
23	X	0.44	0/97	0.36	0/149
24	a	0.37	0/64816	0.39	0/101081
25	b	0.29	0/2770	0.33	0/4315
26	0	0.15	0/427	0.35	0/566
27	1	0.33	0/359	0.35	0/471
28	2	0.30	0/542	0.44	0/714
29	3	0.30	0/300	0.54	0/395
30	c	0.29	0/1978	0.39	0/2659
31	d	0.32	0/1573	0.43	0/2116
32	e	0.30	0/1556	0.38	0/2095

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.14	0/1296	0.28	0/1755
34	h	0.15	0/1081	0.38	0/1467
35	i	0.33	0/1139	0.38	0/1535
36	j	0.27	0/941	0.37	0/1262
37	k	0.30	0/1062	0.40	0/1413
38	l	0.31	0/1098	0.39	0/1465
39	m	0.34	0/960	0.42	0/1285
40	n	0.25	0/813	0.46	0/1095
41	o	0.29	0/917	0.36	0/1229
42	p	0.35	0/958	0.32	0/1279
43	q	0.33	0/822	0.45	0/1097
44	r	0.33	0/852	0.38	0/1143
45	s	0.29	0/767	0.45	0/1028
46	t	0.28	0/775	0.43	0/1037
47	u	0.28	0/781	0.37	0/1054
48	v	0.31	0/603	0.45	0/804
49	w	0.30	0/629	0.43	0/842
50	x	0.24	0/497	0.30	0/663
51	y	0.32	0/445	0.45	0/596
52	z	0.31	0/433	0.42	0/577
53	f	0.13	0/997	0.33	0/1373
All	All	0.36	0/143637	0.38	3/215091 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
30	c	0	1
37	k	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	59	PRO	CA-N-CD	-7.26	101.83	112.00
11	K	43	TRP	N-CA-CB	-5.23	108.21	114.17
4	D	140	GLU	CA-CB-CG	5.13	124.37	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	c	232	HIS	Peptide
37	k	27	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30595	0	15410	430	0
2	B	1668	0	1690	39	0
3	C	1553	0	1609	57	0
4	D	1200	0	1203	57	0
5	E	1126	0	1179	12	0
6	F	834	0	831	10	0
7	G	689	0	440	15	0
8	H	979	0	1039	14	0
9	I	911	0	897	34	0
10	J	602	0	463	12	0
11	K	864	0	864	18	0
12	L	638	0	684	15	0
13	M	867	0	924	42	0
14	N	774	0	814	31	0
15	O	717	0	744	3	0
16	P	634	0	658	14	0
17	Q	633	0	658	7	0
18	R	417	0	440	7	0
19	S	586	0	577	31	0
20	T	622	0	664	9	0
21	U	267	0	210	1	0
22	W	385	0	196	7	0
23	X	87	0	44	0	0
24	a	58077	0	29220	366	0
25	b	2476	0	1251	21	0
26	0	420	0	443	1	0
27	1	356	0	406	1	0
28	2	531	0	585	4	0
29	3	298	0	340	13	0
30	c	1941	0	1995	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	d	1551	0	1579	4	0
32	e	1537	0	1602	6	0
33	g	1277	0	1322	17	0
34	h	1072	0	1086	19	0
35	i	1115	0	1154	3	0
36	j	932	0	1005	16	0
37	k	1052	0	1122	2	0
38	l	1078	0	1136	4	0
39	m	946	0	994	3	0
40	n	805	0	827	16	0
41	o	908	0	949	11	0
42	p	945	0	1005	3	0
43	q	810	0	836	8	0
44	r	843	0	894	1	0
45	s	759	0	799	10	0
46	t	769	0	792	3	0
47	u	769	0	771	4	0
48	v	595	0	603	1	0
49	w	620	0	654	4	0
50	x	496	0	525	3	0
51	y	442	0	475	7	0
52	z	427	0	424	1	0
53	f	987	0	597	12	0
54	A	47	0	0	0	0
54	D	1	0	0	0	0
54	F	1	0	0	0	0
54	N	1	0	0	0	0
54	S	1	0	0	0	0
54	a	230	0	0	0	0
54	b	3	0	0	0	0
54	c	3	0	0	0	0
54	d	1	0	0	0	0
54	e	1	0	0	0	0
55	A	2	0	0	0	0
55	a	22	0	0	4	0
55	c	1	0	0	0	0
55	m	1	0	0	0	0
55	z	1	0	0	0	0
All	All	132798	0	87629	1356	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1356) 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)
24:a:1926:5MU:C5	24:a:1926:5MU:C4	1.81	1.67
24:a:284:A:N6	24:a:335:G:H1	1.56	1.02
1:A:1298:G:H22	1:A:1329:U:H3	1.06	0.99
1:A:1304:G:H1	1:A:1323:A:H2	1.06	0.98
24:a:1400:G:O6	24:a:1567:A:N1	1.97	0.97
24:a:1902:U:N3	24:a:1928:C:N4	2.14	0.96
1:A:1243:C:N4	1:A:1285:U:N3	2.13	0.95
24:a:1389:G:H22	24:a:1582:G:H1	1.11	0.95
24:a:1902:U:H3	24:a:1928:C:N4	1.65	0.94
1:A:441:G:H21	1:A:481:A:H62	1.01	0.92
2:B:141:MET:N	2:B:141:MET:SD	2.45	0.89
16:P:12:LYS:H	16:P:12:LYS:HD2	1.35	0.89
1:A:441:G:N2	1:A:481:A:H62	1.68	0.89
1:A:947:G:H1	1:A:1221:A:H2	1.21	0.88
10:J:65:TYR:HB3	14:N:96:LEU:HD11	1.56	0.88
24:a:1425:A:H2	24:a:1536:G:H1	1.17	0.88
1:A:1240:A:N1	1:A:1288:G:C6	2.43	0.87
1:A:1243:C:N4	1:A:1285:U:H3	1.73	0.86
1:A:1304:G:N1	1:A:1323:A:C2	2.43	0.86
1:A:1264:G:N2	1:A:1307:U:O2	2.09	0.86
7:G:31:MET:HE3	7:G:32:LEU:H	1.40	0.85
1:A:1310:G:H21	1:A:1355:G:H22	1.26	0.84
1:A:1304:G:O6	1:A:1323:A:N1	2.11	0.84
1:A:441:G:H21	1:A:481:A:N6	1.74	0.84
24:a:2457:G:H21	24:a:2463:A:H62	1.26	0.83
24:a:1425:A:C2	24:a:1536:G:N1	2.46	0.83
1:A:1243:C:N4	1:A:1285:U:C4	2.48	0.82
24:a:284:A:N1	24:a:335:G:N2	2.25	0.82
1:A:1430:U:O4	1:A:1459:A:N6	2.13	0.81
24:a:2781:U:H3	24:a:2786:G:H1	1.11	0.81
1:A:431:U:OP1	4:D:154:ARG:NH2	2.14	0.81
24:a:701:U:O2	24:a:704:C:N4	2.14	0.80
1:A:1302:U:O4	1:A:1325:G:N2	2.13	0.80
1:A:1129:U:N3	1:A:1131:A:N7	2.29	0.80
25:b:33:G:H1	25:b:50:A:H2	1.25	0.80
41:o:6:GLN:HE21	41:o:8:ILE:HB	1.47	0.80
24:a:1416:A:N6	24:a:1546:U:O4	2.15	0.80
24:a:275:U:N3	24:a:346:U:O4	2.12	0.79
24:a:2781:U:O2	24:a:2786:G:N2	2.15	0.79
6:F:3:HIS:ND1	6:F:65:GLU:OE2	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:56:ARG:O	4:D:56:ARG:NE	2.15	0.79
1:A:1064:C:N4	1:A:1087:G:O6	2.16	0.78
1:A:1350:U:H3	1:A:1362:G:H22	1.26	0.78
24:a:284:A:H61	24:a:335:G:H1	0.82	0.78
24:a:1026:A:H61	24:a:1101:G:H22	1.31	0.78
32:e:7:ASP:OD1	32:e:7:ASP:N	2.17	0.77
1:A:500:G:N3	1:A:502:U:O2'	2.17	0.77
1:A:928:A:N6	1:A:1374:U:O4	2.18	0.77
24:a:1390:A:N6	24:a:1581:U:O4	2.18	0.77
51:y:40:GLU:OE2	51:y:40:GLU:N	2.16	0.77
1:A:55:A:H62	1:A:351:G:H21	1.32	0.77
1:A:1248:U:O4	1:A:1280:U:N3	2.18	0.77
24:a:1399:C:H2'	24:a:1400:G:H21	1.49	0.77
1:A:1304:G:N1	1:A:1323:A:H2	1.82	0.76
24:a:9:G:H8	24:a:2785:A:H61	1.33	0.76
13:M:57:ARG:O	13:M:57:ARG:NH1	2.19	0.76
1:A:400:G:N1	1:A:489:A:N7	2.34	0.76
24:a:1400:G:C6	24:a:1567:A:N1	2.53	0.76
1:A:64:G:H4'	1:A:65:A:H5'	1.68	0.76
1:A:1240:A:C2	1:A:1288:G:N1	2.54	0.76
1:A:927:C:O2	1:A:929:C:N4	2.19	0.76
24:a:1858:G:H2'	24:a:1859:G:C8	2.21	0.75
1:A:1174:A:H62	9:I:104:THR:HB	1.50	0.75
3:C:151:VAL:HG12	3:C:200:VAL:HA	1.69	0.75
19:S:32:LYS:HA	19:S:51:LEU:HB3	1.69	0.75
24:a:1389:G:N2	24:a:1582:G:H1	1.84	0.75
1:A:1156:C:N3	1:A:1170:A:N6	2.34	0.75
1:A:1157:G:H22	1:A:1168:G:H1	1.33	0.75
24:a:869:G:N1	24:a:881:U:N3	2.34	0.74
1:A:1309:U:OP2	19:S:3:ASN:ND2	2.20	0.74
4:D:145:ILE:HG13	4:D:177:LYS:HE2	1.67	0.74
24:a:2289:G:N1	24:a:2297:U:O4	2.16	0.74
1:A:711:U:O3'	11:K:118:ASN:ND2	2.20	0.74
24:a:1400:G:H1	24:a:1567:A:H61	1.33	0.74
24:a:701:U:O2'	24:a:703:A:N7	2.21	0.74
1:A:508:C:N4	1:A:509:G:O6	2.21	0.74
1:A:1052:C:O3'	14:N:85:ARG:NH2	2.20	0.74
3:C:70:THR:HG21	3:C:76:VAL:HG21	1.68	0.73
9:I:111:GLU:N	9:I:111:GLU:OE1	2.21	0.73
8:H:48:ASP:OD1	8:H:49:PHE:N	2.21	0.73
34:h:112:LYS:NZ	34:h:114:GLU:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:GLY:HA2	3:C:38:LYS:HZ1	1.51	0.73
19:S:10:GLN:HA	19:S:37:THR:HG23	1.71	0.73
24:a:881:U:O4	24:a:883:A:N6	2.22	0.73
1:A:189:C:N4	20:T:86:LEU:O	2.21	0.73
24:a:1902:U:O2	24:a:1928:C:N3	2.21	0.73
1:A:514:A:H2	1:A:523:G:H22	1.37	0.73
9:I:46:VAL:O	9:I:79:ARG:NH2	2.22	0.73
4:D:170:TRP:HB3	4:D:183:LYS:HZ3	1.53	0.72
24:a:1401:A:N6	24:a:1565:U:O4	2.22	0.72
24:a:2641:U:O2	24:a:2650:A:N7	2.22	0.72
25:b:39:A:H1'	25:b:47:C:H42	1.55	0.72
2:B:140:GLU:N	2:B:140:GLU:OE1	2.23	0.72
3:C:125:GLU:OE1	3:C:125:GLU:N	2.22	0.72
1:A:612:C:O2	1:A:616:A:N6	2.22	0.71
24:a:2727:G:H1	24:a:2747:C:H5	1.38	0.71
1:A:337:U:O2'	1:A:340:G:O6	2.07	0.71
19:S:35:ILE:HG21	19:S:71:ILE:HB	1.72	0.71
24:a:886:A:H2'	24:a:887:A:H8	1.54	0.71
24:a:1467:U:H3	24:a:1486:G:H1	0.76	0.71
1:A:696:A:N1	24:a:1831:G:O2'	2.24	0.71
1:A:881:G:H3'	1:A:882:A:H5''	1.73	0.71
24:a:1902:U:C4	24:a:1928:C:N4	2.57	0.71
25:b:18:G:H1	25:b:65:C:H5	1.38	0.71
1:A:456:G:H22	1:A:465:U:H1'	1.56	0.71
14:N:63:ARG:HH11	14:N:63:ARG:HB2	1.55	0.71
1:A:1438:C:O2'	1:A:1439:U:O4'	2.09	0.70
1:A:1342:U:O2'	1:A:1368:A:N6	2.24	0.70
47:u:14:GLU:N	47:u:14:GLU:OE2	2.24	0.70
1:A:346:C:O2'	1:A:348:G:OP1	2.08	0.70
24:a:272:U:HO2'	24:a:273:U:H6	1.39	0.70
1:A:1373:G:H2'	1:A:1374:U:H4'	1.71	0.70
29:3:27:VAL:HB	29:3:35:PHE:HB2	1.73	0.70
1:A:1251:U:H3	1:A:1272:G:H21	1.37	0.70
1:A:1412:A:H2	1:A:1476:G:H21	1.39	0.69
5:E:57:GLU:N	5:E:57:GLU:OE2	2.25	0.69
24:a:1851:A:N6	24:a:1861:A:OP2	2.23	0.69
1:A:947:G:N1	1:A:1221:A:C2	2.50	0.69
47:u:56:GLU:N	47:u:56:GLU:OE1	2.25	0.69
9:I:21:ARG:O	9:I:61:ASP:N	2.24	0.69
24:a:1457:G:O2'	24:a:1496:C:N4	2.24	0.69
1:A:1240:A:N1	1:A:1288:G:O6	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1304:G:C6	1:A:1323:A:N1	2.60	0.69
1:A:1322:C:H2'	1:A:1323:A:H8	1.56	0.69
1:A:486:C:N3	1:A:487:A:N6	2.40	0.69
3:C:118:ASP:OD1	3:C:122:SER:OG	2.10	0.69
1:A:1150:G:N2	1:A:1175:G:OP2	2.25	0.69
24:a:1467:U:O2	24:a:1486:G:N2	2.19	0.69
16:P:34:GLU:OE2	16:P:60:TRP:NE1	2.21	0.68
34:h:80:LEU:HD13	34:h:146:VAL:HG22	1.76	0.68
1:A:477:C:H5''	1:A:478:G:H5''	1.75	0.68
2:B:149:GLY:HA2	2:B:152:LYS:HD3	1.75	0.68
1:A:1260:G:N2	1:A:1265:A:N1	2.42	0.68
24:a:412:G:H2'	24:a:413:G:H5'	1.74	0.68
24:a:375:U:OP1	24:a:378:A:N6	2.22	0.68
36:j:50:GLY:O	36:j:53:LYS:NZ	2.27	0.68
1:A:1458:U:OP1	41:o:113:ARG:NH2	2.26	0.68
24:a:1709:G:H21	24:a:1723:A:H62	1.40	0.68
1:A:1487:A:H2'	1:A:1488:G:H8	1.59	0.68
13:M:81:MET:SD	13:M:81:MET:N	2.61	0.67
9:I:114:LYS:HB2	9:I:117:LEU:HD22	1.74	0.67
41:o:70:ASN:OD1	41:o:70:ASN:N	2.28	0.67
1:A:1264:G:N2	1:A:1308:C:O4'	2.28	0.67
4:D:110:THR:HG23	4:D:113:GLU:H	1.57	0.67
4:D:183:LYS:H	4:D:183:LYS:HD3	1.59	0.67
43:q:28:GLU:N	43:q:28:GLU:OE1	2.27	0.67
1:A:1124:G:N2	1:A:1141:C:OP1	2.28	0.67
1:A:1151:A:H5'	1:A:1152:C:H5'	1.75	0.67
13:M:48:LEU:O	13:M:52:THR:OG1	2.11	0.67
41:o:6:GLN:NE2	41:o:8:ILE:HB	2.09	0.67
1:A:1305:A:H61	1:A:1322:C:H42	1.43	0.67
24:a:2196:A:N6	24:a:2198:U:OP1	2.25	0.67
25:b:48:U:OP2	40:n:10:ARG:NH1	2.28	0.66
1:A:1197:C:H2'	1:A:1198:A:H5'	1.76	0.66
1:A:1199:U:O4	1:A:1200:G:N1	2.28	0.66
24:a:1027:G:N2	24:a:1102:G:OP2	2.29	0.66
24:a:1037:G:H1	24:a:1094:U:H3	1.43	0.66
1:A:600:G:N2	1:A:625:C:O2'	2.28	0.66
1:A:832:A:N1	1:A:833:G:O6	2.29	0.66
13:M:53:LEU:HD12	13:M:56:LEU:HD13	1.76	0.66
24:a:868:G:H21	24:a:883:A:H61	1.43	0.66
40:n:34:HIS:ND1	40:n:52:THR:OG1	2.27	0.66
17:Q:40:ARG:HG2	17:Q:40:ARG:HH11	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:1425:A:N1	24:a:1536:G:O6	2.28	0.66
24:a:1702:C:O2'	24:a:1729:A:N1	2.24	0.66
24:a:1840:U:O4	24:a:2074:G:O2'	2.09	0.66
24:a:1992:A:N7	55:a:3201:HOH:O	2.29	0.66
24:a:863:C:H42	24:a:886:A:H61	1.42	0.66
1:A:1452:G:N7	1:A:1453:A:N6	2.43	0.66
4:D:170:TRP:HZ2	4:D:186:PRO:HB3	1.60	0.66
24:a:1843:A:O2'	24:a:1871:G:N2	2.29	0.65
24:a:1425:A:H2	24:a:1536:G:N1	1.92	0.65
24:a:1856:U:H3'	24:a:1857:A:H8	1.61	0.65
4:D:150:LYS:HA	4:D:150:LYS:HE2	1.77	0.65
13:M:27:LYS:HE2	13:M:27:LYS:HA	1.77	0.65
1:A:527:A:C4	1:A:529:A:H2'	2.31	0.65
1:A:1184:G:H5'	3:C:5:VAL:HG11	1.79	0.65
1:A:1310:G:N2	1:A:1355:G:H22	1.95	0.65
24:a:1025:A:H61	24:a:1102:G:H1	1.45	0.65
1:A:608:C:O2	1:A:621:G:N2	2.30	0.65
1:A:1043:G:H1'	1:A:1209:G:H21	1.62	0.65
1:A:1260:G:N2	1:A:1266:G:O6	2.29	0.65
14:N:10:GLU:HA	14:N:13:ARG:HG2	1.79	0.65
24:a:1967:C:O2'	24:a:1969:U:OP2	2.15	0.65
1:A:499:G:N2	1:A:505:C:OP2	2.30	0.64
8:H:67:GLU:OE1	8:H:67:GLU:N	2.30	0.64
4:D:194:ASP:N	4:D:194:ASP:OD1	2.31	0.64
1:A:25:C:O2'	1:A:26:A:O5'	2.13	0.64
24:a:1392:A:N6	24:a:1579:U:O4	2.31	0.64
1:A:407:G:N2	1:A:422:G:O2'	2.31	0.64
1:A:1039:A:H61	1:A:1208:C:H42	1.46	0.64
19:S:45:ILE:H	19:S:61:HIS:CE1	2.16	0.64
24:a:1025:A:N6	24:a:1102:G:H1	1.96	0.64
1:A:1221:A:H5''	13:M:102:THR:HG21	1.79	0.64
11:K:33:ILE:HD11	11:K:42:SER:HB2	1.79	0.64
4:D:56:ARG:HE	4:D:56:ARG:C	2.06	0.64
1:A:174:A:H8	1:A:174:A:OP2	1.81	0.64
7:G:63:GLU:O	7:G:67:ASP:N	2.28	0.64
1:A:555:U:O2	12:L:15:LYS:NZ	2.29	0.63
1:A:1303:G:H22	1:A:1324:U:H3	1.45	0.63
13:M:107:ARG:NH2	13:M:113:ARG:O	2.28	0.63
3:C:188:GLU:OE1	3:C:188:GLU:N	2.32	0.63
13:M:4:ILE:HD12	13:M:9:VAL:HG11	1.80	0.63
49:w:57:VAL:HG12	49:w:59:SER:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:16:LEU:HD13	14:N:54:ASP:HB3	1.79	0.63
53:f:110:ARG:O	53:f:112:ARG:NH1	2.30	0.63
1:A:1524:G:O6	21:U:46:LYS:NZ	2.31	0.63
25:b:13:A:H8	25:b:69:G:H21	1.47	0.63
1:A:648:G:H1	1:A:748:C:H5	1.46	0.63
1:A:1240:A:C2	1:A:1288:G:C6	2.87	0.63
9:I:105:ARG:HG3	9:I:105:ARG:HH11	1.63	0.63
24:a:1839:A:N6	24:a:1875:G:O2'	2.32	0.63
24:a:1852:U:O2'	24:a:1861:A:N3	2.32	0.63
1:A:1080:G:O6	1:A:1091:C:O2'	2.10	0.62
1:A:1202:C:H3'	1:A:1203:C:H5''	1.81	0.62
24:a:1394:A:N1	24:a:1578:A:N6	2.46	0.62
24:a:1425:A:N1	24:a:1536:G:C6	2.67	0.62
53:f:70:ALA:HB3	53:f:81:GLU:HA	1.81	0.62
24:a:339:A:H2'	24:a:340:G:H4'	1.81	0.62
25:b:97:G:O2'	25:b:98:A:H5'	2.00	0.62
1:A:1113:C:H41	1:A:1174:A:H5''	1.64	0.62
45:s:67:THR:HG22	45:s:76:ARG:HG3	1.82	0.62
1:A:1415:G:N1	1:A:1417:G:O6	2.33	0.62
19:S:70:MET:N	19:S:70:MET:SD	2.72	0.62
9:I:52:GLU:N	9:I:52:GLU:OE1	2.31	0.62
24:a:1902:U:C2	24:a:1928:C:N3	2.68	0.62
51:y:7:LYS:NZ	51:y:38:GLU:OE2	2.25	0.62
1:A:1126:A:OP2	1:A:1128:G:H5''	1.99	0.62
1:A:1210:U:H3'	1:A:1211:G:H8	1.65	0.62
1:A:1263:A:H2'	1:A:1264:G:C8	2.35	0.62
26:0:18:THR:HG23	28:2:35:THR:HG23	1.82	0.62
2:B:112:LYS:HE2	2:B:112:LYS:N	2.15	0.62
53:f:69:LYS:HA	53:f:84:PRO:HA	1.80	0.62
22:W:28:A:H61	22:W:40:C:H42	1.48	0.62
13:M:44:LYS:HB2	13:M:47:GLU:HG3	1.82	0.61
24:a:293:C:H3'	24:a:294:U:H4'	1.82	0.61
24:a:2514:G:OP2	33:g:171:ARG:NH2	2.33	0.61
1:A:942:A:H2	1:A:1227:G:H22	1.49	0.61
17:Q:18:GLU:N	17:Q:18:GLU:OE2	2.29	0.61
31:d:75:GLU:OE2	31:d:75:GLU:N	2.34	0.61
24:a:868:G:C6	24:a:879:A:H5''	2.35	0.61
24:a:1842:G:N2	24:a:1873:U:H3	1.98	0.61
1:A:947:G:O6	1:A:1221:A:N1	2.33	0.61
24:a:141:A:H2'	24:a:142:G:H8	1.66	0.61
24:a:2645:A:OP1	24:a:2647:A:N6	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:57:ARG:HH22	13:M:59:ALA:HB2	1.66	0.61
24:a:2298:C:H2'	24:a:2299:G:H8	1.65	0.61
1:A:621:G:O2'	1:A:622:G:O5'	2.18	0.61
1:A:1107:C:O5'	3:C:179:ARG:NH2	2.34	0.61
24:a:1026:A:N6	24:a:1101:G:H22	1.98	0.61
24:a:1353:G:N7	55:a:3203:HOH:O	2.31	0.61
7:G:25:LYS:HB3	7:G:102:ARG:HH12	1.64	0.60
4:D:185:LEU:HD22	4:D:186:PRO:HD2	1.81	0.60
41:o:107:ARG:HD2	41:o:111:SER:HB2	1.83	0.60
1:A:918:G:H1	1:A:1385:U:H5	1.50	0.60
13:M:17:ILE:O	13:M:20:THR:OG1	2.17	0.60
13:M:94:SER:O	13:M:109:ARG:NH1	2.31	0.60
24:a:2289:G:O6	24:a:2292:G:N2	2.33	0.60
30:c:133:ARG:O	30:c:167:ARG:NH1	2.34	0.60
1:A:55:A:H62	1:A:351:G:N2	1.99	0.60
3:C:22:TRP:NE1	3:C:32:GLN:OE1	2.34	0.60
53:f:103:LEU:HA	53:f:107:ALA:HB3	1.84	0.60
24:a:1031:C:H1'	24:a:1033:G:H21	1.65	0.60
1:A:971:A:N3	1:A:1317:G:N2	2.50	0.60
2:B:13:GLY:HA3	2:B:209:ALA:HB2	1.84	0.60
3:C:6:HIS:CE1	3:C:8:THR:HG22	2.36	0.60
5:E:22:ARG:NE	5:E:33:PHE:HD2	2.00	0.60
24:a:2194:U:H4'	24:a:2195:G:H5'	1.83	0.60
1:A:1082:G:O2'	1:A:1162:U:OP1	2.20	0.60
7:G:103:TRP:O	7:G:107:ALA:N	2.27	0.60
19:S:29:SER:HB3	19:S:49:ILE:HG22	1.84	0.60
24:a:865:A:O2'	24:a:866:G:H3'	2.02	0.60
1:A:1243:C:H42	1:A:1285:U:H3	1.32	0.59
5:E:117:LEU:HD13	5:E:125:VAL:HG21	1.84	0.59
1:A:24:U:O2'	1:A:519:C:O2'	2.16	0.59
1:A:512:C:H5'	1:A:524:G:H21	1.66	0.59
1:A:947:G:N1	1:A:1221:A:H2	1.96	0.59
3:C:38:LYS:HB2	3:C:94:ILE:HD11	1.84	0.59
12:L:35:THR:HG22	12:L:36:ARG:HG3	1.83	0.59
24:a:141:A:H2'	24:a:142:G:C8	2.36	0.59
24:a:866:G:C2	24:a:886:A:H1'	2.36	0.59
3:C:34:PHE:O	3:C:38:LYS:NZ	2.35	0.59
33:g:18:THR:OG1	33:g:27:LYS:NZ	2.35	0.59
1:A:222:A:H5'	16:P:63:GLN:HE22	1.67	0.59
7:G:31:MET:SD	7:G:36:LYS:HB2	2.42	0.59
13:M:101:ARG:HD3	13:M:105:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:1538:U:H2'	24:a:1539:G:C8	2.37	0.59
24:a:2526:A:H8	24:a:2750:A:H61	1.49	0.59
33:g:107:LEU:O	33:g:152:ARG:NH2	2.36	0.59
14:N:49:GLN:OE1	14:N:49:GLN:N	2.30	0.59
2:B:132:LYS:NZ	2:B:136:MET:H	2.00	0.59
29:3:11:LYS:HZ2	29:3:14:ALA:HB2	1.68	0.59
1:A:1144:U:C4	1:A:1145:A:N1	2.71	0.59
24:a:2462:U:O2'	24:a:2464:U:OP2	2.15	0.59
24:a:2781:U:O4	24:a:2786:G:O6	2.20	0.59
32:e:122:GLU:H	32:e:122:GLU:CD	2.10	0.59
1:A:8:A:H62	4:D:205:SER:HB2	1.68	0.58
3:C:128:VAL:HG22	3:C:129:MET:H	1.67	0.58
7:G:16:PRO:HD3	7:G:24:ALA:HB2	1.83	0.58
14:N:67:THR:HG22	14:N:68:GLY:H	1.66	0.58
34:h:40:THR:OG1	34:h:43:ASN:OD1	2.22	0.58
1:A:26:A:C2	1:A:552:G:N2	2.69	0.58
24:a:869:G:H1'	24:a:870:G:C8	2.38	0.58
24:a:1842:G:H22	24:a:1873:U:H3	1.51	0.58
52:z:52:GLN:NE2	52:z:54:ILE:O	2.36	0.58
29:3:11:LYS:HE2	29:3:13:ARG:HB2	1.85	0.58
1:A:1275:U:H3'	1:A:1276:C:H2'	1.84	0.58
24:a:1467:U:O4	24:a:1486:G:O6	2.21	0.58
24:a:2293:G:N7	24:a:2294:A:N6	2.52	0.58
40:n:59:GLU:OE1	40:n:60:THR:HG23	2.04	0.58
24:a:2641:U:C2	24:a:2650:A:N7	2.72	0.58
27:1:40:LYS:NZ	27:1:40:LYS:HB3	2.19	0.58
45:s:54:GLU:HB2	45:s:88:LYS:HB3	1.85	0.58
5:E:159:ARG:HH22	8:H:101:ILE:HD11	1.69	0.58
13:M:71:ARG:O	13:M:74:THR:OG1	2.21	0.58
24:a:1843:A:H8	24:a:1872:A:H62	1.52	0.58
25:b:33:G:N1	25:b:50:A:H2	1.99	0.58
25:b:56:G:N3	53:f:27:GLN:NE2	2.52	0.58
1:A:1153:U:O5'	1:A:1176:G:N2	2.35	0.57
9:I:90:ASP:HB3	9:I:93:LEU:HB2	1.85	0.57
12:L:53:ALA:HB2	12:L:67:ILE:HD11	1.85	0.57
40:n:83:ASP:OD2	40:n:83:ASP:N	2.33	0.57
24:a:273:U:H2'	24:a:274:A:H8	1.69	0.57
24:a:861:G:H21	24:a:890:C:H41	1.52	0.57
38:l:76:ASN:HB2	38:l:91:GLU:HG3	1.84	0.57
45:s:27:ASN:O	45:s:27:ASN:ND2	2.35	0.57
1:A:499:G:O2'	1:A:500:G:O5'	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:G:C6	1:A:1221:A:N1	2.72	0.57
1:A:1057:G:H4'	1:A:1058:U:OP1	2.03	0.57
1:A:1150:G:C5	1:A:1151:A:H1'	2.40	0.57
1:A:1457:U:H3'	41:o:113:ARG:HH12	1.69	0.57
1:A:174:A:H2'	1:A:175:C:H5'	1.86	0.57
1:A:1427:A:H2'	1:A:1428:A:C8	2.38	0.57
24:a:269:A:O2'	24:a:270:G:H8	1.86	0.57
24:a:890:C:H3'	24:a:891:U:H5''	1.86	0.57
24:a:1398:G:O2'	24:a:1399:C:O4'	2.21	0.57
1:A:457:U:H3	1:A:464:C:H42	1.53	0.57
11:K:34:THR:OG1	11:K:39:ASN:N	2.37	0.57
1:A:1287:C:H2'	1:A:1288:G:C8	2.39	0.57
24:a:1101:G:N1	24:a:1102:G:O6	2.38	0.57
29:3:31:GLU:OE2	29:3:31:GLU:N	2.37	0.57
17:Q:40:ARG:HG2	17:Q:40:ARG:NH1	2.20	0.57
24:a:1854:C:N3	24:a:1857:A:N6	2.53	0.57
1:A:406:A:O2'	1:A:422:G:N1	2.38	0.57
1:A:786:A:H1'	1:A:788:A:N7	2.20	0.57
13:M:89:LEU:O	13:M:92:ARG:HG2	2.05	0.57
24:a:1715:U:O2'	24:a:1717:C:OP2	2.22	0.57
34:h:122:ILE:H	34:h:122:ILE:HD12	1.70	0.57
1:A:1116:A:H3'	1:A:1117:G:H5''	1.87	0.57
4:D:152:GLN:HB3	4:D:154:ARG:NH2	2.20	0.57
1:A:1196:U:H4'	1:A:1197:C:H5''	1.87	0.56
24:a:1422:A:H2	24:a:1539:G:H22	1.53	0.56
24:a:1832:A:H61	24:a:1880:C:H42	1.52	0.56
1:A:540:G:P	4:D:69:GLU:HB2	2.45	0.56
1:A:933:C:H2'	1:A:934:G:H8	1.70	0.56
13:M:93:ARG:H	13:M:93:ARG:HD2	1.70	0.56
33:g:159:GLY:O	33:g:163:ARG:NH1	2.38	0.56
3:C:105:GLU:O	3:C:107:ARG:NH1	2.38	0.56
6:F:9:MET:HE2	6:F:86:ARG:HB2	1.86	0.56
8:H:43:GLU:HG2	8:H:101:ILE:HG12	1.86	0.56
18:R:31:ASN:OD1	18:R:31:ASN:N	2.38	0.56
24:a:832:G:H8	24:a:834:A:N6	2.03	0.56
24:a:1341:A:H61	24:a:2197:A:H62	1.53	0.56
24:a:1415:C:H42	24:a:1547:A:N6	2.03	0.56
24:a:1576:U:H2'	24:a:1577:U:C2	2.40	0.56
24:a:1719:C:O2'	24:a:1720:U:O2	2.24	0.56
25:b:49:C:H2'	25:b:50:A:C8	2.41	0.56
29:3:2:LYS:HE2	29:3:35:PHE:HE1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:U:H2'	1:A:168:G:C8	2.41	0.56
1:A:1145:A:O2'	1:A:1146:A:H5''	2.05	0.56
18:R:70:TYR:HB3	18:R:71:THR:HG23	1.87	0.56
22:W:28:A:N6	22:W:40:C:H42	2.04	0.56
24:a:1400:G:O2'	24:a:1401:A:O4'	2.11	0.56
24:a:1840:U:OP2	24:a:1840:U:H3'	2.04	0.56
25:b:45:A:H2'	25:b:46:A:O4'	2.05	0.56
34:h:72:LEU:HD11	34:h:141:THR:HA	1.88	0.56
1:A:1321:C:H2'	1:A:1322:C:C6	2.41	0.56
1:A:148:G:C2	1:A:149:A:C8	2.94	0.56
4:D:57:GLU:HA	4:D:60:LYS:NZ	2.21	0.56
16:P:44:ALA:N	16:P:47:GLU:OE2	2.31	0.56
1:A:406:A:N6	1:A:426:A:N7	2.54	0.56
4:D:57:GLU:HB3	4:D:58:LYS:NZ	2.21	0.56
24:a:861:G:N2	24:a:890:C:H41	2.04	0.56
24:a:1538:U:H2'	24:a:1539:G:H8	1.71	0.56
25:b:98:A:O2'	25:b:99:A:H8	1.89	0.56
1:A:439:A:H2'	1:A:440:G:C8	2.40	0.55
14:N:24:ARG:O	14:N:28:LYS:N	2.28	0.55
14:N:63:ARG:HB2	14:N:63:ARG:NH1	2.21	0.55
11:K:80:ASN:HA	11:K:105:ARG:HB2	1.88	0.55
14:N:64:CYS:SG	14:N:65:ASN:N	2.78	0.55
29:3:28:ILE:HD12	29:3:28:ILE:O	2.06	0.55
1:A:1124:G:H8	1:A:1134:C:H42	1.53	0.55
4:D:170:TRP:CZ2	4:D:186:PRO:HB3	2.41	0.55
24:a:1567:A:C2	24:a:1568:G:H1'	2.42	0.55
1:A:1210:U:H3'	1:A:1211:G:C8	2.41	0.55
1:A:1315:U:O4	1:A:1316:C:N4	2.40	0.55
14:N:62:ASN:HD22	14:N:73:PHE:HE2	1.50	0.55
43:q:55:ASN:OD1	43:q:56:GLY:N	2.39	0.55
1:A:126:G:OP1	1:A:599:U:O2'	2.22	0.55
1:A:1338:C:O3'	9:I:123:ARG:HG3	2.06	0.55
9:I:129:ARG:NH2	22:W:32:C:OP2	2.37	0.55
16:P:12:LYS:HD2	16:P:12:LYS:N	2.14	0.55
24:a:843:G:H2'	24:a:844:G:C8	2.42	0.55
1:A:1305:A:N6	1:A:1322:C:H42	2.04	0.55
2:B:184:VAL:HG22	2:B:198:PHE:HB2	1.88	0.55
24:a:2196:A:H2'	24:a:2196:A:N3	2.22	0.55
24:a:2587:A:H8	24:a:2588:G:N7	2.04	0.55
1:A:834:C:H2'	1:A:835:C:C2	2.42	0.55
1:A:903:C:HO2'	1:A:904:U:H6	1.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:LYS:HD2	4:D:148:LYS:O	2.06	0.55
24:a:890:C:O5'	24:a:891:U:H5''	2.06	0.55
24:a:2289:G:O2'	24:a:2291:C:OP1	2.23	0.55
1:A:1124:G:OP2	1:A:1134:C:N4	2.30	0.55
3:C:148:GLY:HA2	3:C:171:GLY:HA3	1.89	0.55
31:d:6:VAL:H	31:d:33:ASN:HD21	1.53	0.55
4:D:160:GLU:HA	4:D:163:GLU:CD	2.32	0.55
20:T:51:PHE:O	20:T:55:THR:OG1	2.17	0.55
24:a:1787:A:H2'	24:a:1788:A:C8	2.40	0.55
1:A:1084:U:O2'	1:A:1086:A:N6	2.36	0.55
1:A:1348:C:H2'	1:A:1349:G:H8	1.72	0.55
2:B:137:LEU:HD22	2:B:138:ASN:H	1.72	0.55
40:n:62:LYS:O	40:n:62:LYS:HD3	2.07	0.55
1:A:411:G:O2'	1:A:535:G:OP1	2.26	0.54
1:A:1106:C:H42	3:C:177:THR:HA	1.72	0.54
7:G:70:ARG:O	7:G:72:GLN:N	2.40	0.54
15:O:88:ARG:O	15:O:89:ARG:NH1	2.41	0.54
24:a:1840:U:H5'	24:a:2218:U:H4'	1.89	0.54
43:q:39:LEU:HA	43:q:49:ILE:HG21	1.88	0.54
1:A:1417:G:H2'	1:A:1417:G:N3	2.23	0.54
3:C:156:ARG:NH2	3:C:160:ALA:O	2.33	0.54
25:b:56:G:O2'	25:b:57:A:O4'	2.23	0.54
32:e:21:ARG:O	32:e:114:ARG:NH2	2.40	0.54
1:A:161:A:O2'	1:A:162:A:O4'	2.23	0.54
1:A:832:A:C6	1:A:833:G:O6	2.60	0.54
24:a:91:A:H1'	24:a:92:A:C8	2.42	0.54
24:a:139:G:H5'	45:s:2:ILE:HB	1.89	0.54
3:C:41:THR:O	3:C:45:LYS:N	2.39	0.54
11:K:21:HIS:HD2	11:K:84:PHE:HB2	1.72	0.54
24:a:1419:C:H42	24:a:1543:C:H42	1.54	0.54
1:A:1308:C:H41	19:S:1:MET:HB2	1.72	0.54
19:S:11:GLU:O	19:S:15:TYR:N	2.41	0.54
24:a:2405:C:OP1	28:2:35:THR:OG1	2.24	0.54
6:F:81:ASN:OD1	6:F:82:ASP:N	2.41	0.54
24:a:1595:A:H2	24:a:1608:U:H3	1.54	0.54
45:s:14:PRO:HG3	45:s:96:VAL:HB	1.89	0.54
1:A:525:U:H5'	1:A:526:A:H3'	1.90	0.54
1:A:1239:C:H42	1:A:1289:U:H3	1.54	0.54
24:a:869:G:O6	24:a:881:U:O4	2.26	0.54
24:a:1351:G:N7	55:a:3204:HOH:O	2.34	0.54
7:G:31:MET:HE3	7:G:32:LEU:N	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:j:65:THR:OG1	36:j:67:LYS:O	2.25	0.54
1:A:527:A:H1'	1:A:529:A:H5''	1.89	0.53
1:A:983:C:O2'	1:A:984:U:O4'	2.22	0.53
9:I:18:VAL:HG11	9:I:81:GLY:O	2.08	0.53
24:a:1149:G:OP1	43:q:24:LYS:NZ	2.41	0.53
1:A:318:G:N2	1:A:321:A:OP2	2.40	0.53
1:A:707:G:H2'	1:A:708:G:C8	2.44	0.53
4:D:148:LYS:HD2	4:D:148:LYS:C	2.32	0.53
45:s:4:GLU:N	45:s:4:GLU:OE2	2.40	0.53
1:A:521:G:OP2	1:A:521:G:N2	2.41	0.53
1:A:1038:C:N4	1:A:1207:A:OP2	2.42	0.53
24:a:869:G:N2	24:a:881:U:O2	2.40	0.53
24:a:1025:A:N1	24:a:1102:G:N2	2.54	0.53
24:a:1537:C:H2'	24:a:1538:U:O2	2.07	0.53
24:a:1871:G:O3'	24:a:1872:A:H8	1.90	0.53
4:D:69:GLU:N	4:D:69:GLU:OE1	2.41	0.53
9:I:117:LEU:CD1	9:I:123:ARG:HH12	2.22	0.53
24:a:4:U:H2'	24:a:5:A:H8	1.73	0.53
33:g:9:ILE:HD13	33:g:73:ASN:HB2	1.89	0.53
34:h:15:LEU:HD13	34:h:55:GLU:HG2	1.88	0.53
34:h:62:LEU:HD12	34:h:62:LEU:H	1.73	0.53
1:A:392:U:H2'	1:A:393:G:C8	2.43	0.53
1:A:1105:C:P	1:A:1107:C:H41	2.32	0.53
24:a:2454:A:H2'	24:a:2455:G:O4'	2.08	0.53
34:h:137:GLU:CD	34:h:137:GLU:H	2.16	0.53
24:a:269:A:HO2'	24:a:270:G:H8	1.57	0.53
24:a:1428:C:H2'	24:a:1429:A:C8	2.43	0.53
1:A:43:C:O3'	16:P:12:LYS:NZ	2.42	0.53
1:A:286:G:N2	1:A:602:A:H61	2.06	0.53
1:A:396:G:OP2	4:D:70:LYS:NZ	2.41	0.53
1:A:933:C:H2'	1:A:934:G:C8	2.44	0.53
1:A:507:C:O2'	1:A:526:A:OP2	2.24	0.53
24:a:1858:G:N7	24:a:1860:G:N2	2.57	0.53
1:A:1264:G:H22	1:A:1307:U:H2'	1.74	0.52
2:B:73:LYS:NZ	2:B:205:ASP:OD1	2.38	0.52
19:S:69:GLU:OE2	19:S:72:GLY:HA3	2.10	0.52
24:a:1395:A:N6	24:a:1577:U:O4	2.43	0.52
24:a:1567:A:OP2	24:a:1568:G:N2	2.42	0.52
25:b:56:G:O2'	25:b:57:A:O5'	2.26	0.52
3:C:88:ARG:NE	3:C:99:ALA:O	2.42	0.52
24:a:1428:C:H2'	24:a:1429:A:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:1900:A:O2'	24:a:1950:U:O4	2.26	0.52
24:a:2292:G:H4'	24:a:2293:G:O5'	2.09	0.52
24:a:2312:A:H2'	24:a:2313:A:C8	2.44	0.52
38:l:60:ARG:NH1	38:l:61:GLN:HA	2.24	0.52
4:D:57:GLU:HB3	4:D:58:LYS:HZ3	1.74	0.52
10:J:41:PRO:HA	10:J:72:ARG:O	2.09	0.52
1:A:1302:U:H2'	1:A:1303:G:C8	2.45	0.52
2:B:203:ASN:OD1	2:B:204:ASP:N	2.42	0.52
10:J:82:LYS:C	10:J:84:VAL:H	2.17	0.52
24:a:1899:A:N6	24:a:1905:A:N7	2.58	0.52
1:A:1048:A:N6	1:A:1201:G:C5	2.77	0.52
1:A:1303:G:H5''	13:M:97:LEU:HD21	1.91	0.52
24:a:1856:U:H5''	24:a:1857:A:C8	2.44	0.52
24:a:1902:U:H5	24:a:1903:A:C4	2.27	0.52
7:G:81:GLY:HA3	7:G:97:ASN:HA	1.92	0.52
13:M:93:ARG:HD2	13:M:93:ARG:N	2.24	0.52
1:A:470:G:H2'	1:A:471:C:C5	2.45	0.52
24:a:1902:U:N3	24:a:1928:C:C4	2.68	0.52
43:q:51:VAL:HG22	43:q:53:PHE:H	1.74	0.52
1:A:1112:C:H2'	1:A:1113:C:H5''	1.91	0.52
1:A:1432:G:O6	1:A:1433:A:N6	2.43	0.52
4:D:62:ARG:HB2	4:D:72:PHE:HE2	1.74	0.52
9:I:34:LEU:HD13	9:I:34:LEU:O	2.10	0.52
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.42	0.52
30:c:98:ASP:OD1	30:c:98:ASP:N	2.42	0.52
1:A:465:U:N3	1:A:466:G:N7	2.57	0.52
1:A:1312:A:N3	14:N:53:ARG:NH2	2.58	0.52
9:I:18:VAL:HA	9:I:64:ILE:HG22	1.92	0.52
1:A:1282:A:H2'	1:A:1283:A:C8	2.45	0.52
24:a:1575:A:N3	24:a:1576:U:H5	2.08	0.52
24:a:1705:U:H4'	24:a:1705:U:OP1	2.09	0.52
24:a:2288:G:N7	53:f:123:ASP:HA	2.25	0.52
1:A:1114:U:O2'	1:A:1148:G:N2	2.41	0.51
1:A:1302:U:H2'	1:A:1303:G:H8	1.73	0.51
13:M:16:VAL:HG13	13:M:41:GLU:HB3	1.92	0.51
19:S:39:SER:HB2	19:S:68:ASP:H	1.74	0.51
24:a:337:A:H5''	24:a:338:A:H5''	1.92	0.51
24:a:1162:A:H2'	24:a:1163:U:C6	2.45	0.51
24:a:2697:U:OP1	24:a:2699:G:H4'	2.11	0.51
4:D:60:LYS:HA	4:D:63:ARG:NH1	2.25	0.51
24:a:1566:A:H3'	24:a:1567:A:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:G:O2'	1:A:42:G:H8	1.94	0.51
13:M:4:ILE:HB	13:M:9:VAL:HG21	1.91	0.51
46:t:103:THR:O	46:t:103:THR:OG1	2.29	0.51
13:M:67:GLY:O	13:M:71:ARG:NE	2.44	0.51
24:a:1860:G:OP1	24:a:1862:G:O2'	2.24	0.51
1:A:904:U:H2'	1:A:905:C:C6	2.45	0.51
1:A:1245:G:H2'	1:A:1246:A:C8	2.46	0.51
1:A:1415:G:H2'	1:A:1416:G:N7	2.24	0.51
2:B:79:ALA:HB1	2:B:214:THR:HG21	1.93	0.51
2:B:169:GLU:OE1	2:B:172:ALA:HB3	2.10	0.51
13:M:14:HIS:O	13:M:18:GLY:N	2.32	0.51
19:S:69:GLU:HG2	19:S:72:GLY:H	1.74	0.51
25:b:56:G:H5'	25:b:57:A:C6	2.45	0.51
5:E:58:VAL:HB	5:E:59:PRO:HD2	1.93	0.51
19:S:29:SER:OG	19:S:47:ASN:O	2.19	0.51
19:S:35:ILE:HG21	19:S:71:ILE:H	1.76	0.51
33:g:78:GLY:HA2	33:g:82:GLY:HA2	1.92	0.51
24:a:1566:A:H2'	24:a:1567:A:O4'	2.10	0.51
24:a:1580:A:H2'	24:a:1581:U:O4'	2.10	0.51
24:a:2346:C:H2'	24:a:2347:G:H5'	1.91	0.51
1:A:489:A:H4'	1:A:490:A:H5'	1.92	0.51
1:A:934:G:H22	1:A:1337:G:N2	2.08	0.51
1:A:1117:G:H4'	1:A:1117:G:OP1	2.08	0.51
1:A:1121:C:H2'	1:A:1276:C:H5'	1.92	0.51
1:A:1125:C:H2'	1:A:1126:A:C8	2.46	0.51
1:A:1285:U:C4	1:A:1286:G:C6	2.98	0.51
13:M:37:THR:HG21	13:M:57:ARG:HE	1.76	0.51
14:N:15:LYS:O	14:N:19:GLN:N	2.43	0.51
24:a:74:A:O2'	24:a:88:A:OP2	2.23	0.51
24:a:281:G:H2'	24:a:282:U:C6	2.46	0.51
24:a:1155:U:H2'	24:a:1156:C:O4'	2.10	0.51
1:A:529:A:H8	1:A:529:A:P	2.34	0.51
1:A:1058:U:O2'	1:A:1060:A:OP2	2.17	0.51
2:B:132:LYS:HZ3	2:B:136:MET:H	1.59	0.51
18:R:71:THR:O	18:R:71:THR:OG1	2.15	0.51
24:a:1835:G:N1	24:a:1878:G:O6	2.40	0.51
24:a:2457:G:C2	24:a:2459:U:H2'	2.46	0.51
40:n:105:LEU:HD12	40:n:106:ALA:N	2.25	0.51
1:A:400:G:O2'	1:A:401:U:OP1	2.27	0.51
1:A:500:G:H4'	1:A:501:C:H5'	1.92	0.51
1:A:1227:G:H5''	9:I:125:GLN:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:C:H2'	1:A:1260:G:H8	1.76	0.51
24:a:1423:G:H1	24:a:1538:U:H5	1.59	0.51
40:n:15:ARG:NE	40:n:87:GLU:OE1	2.40	0.51
1:A:44:A:O5'	16:P:12:LYS:NZ	2.44	0.50
1:A:400:G:H2'	1:A:401:U:O4'	2.11	0.50
1:A:1083:U:O4'	1:A:1164:A:N6	2.44	0.50
1:A:1106:C:H2'	3:C:179:ARG:HH21	1.76	0.50
4:D:170:TRP:CB	4:D:183:LYS:HZ3	2.22	0.50
1:A:286:G:H21	1:A:602:A:H61	1.59	0.50
1:A:636:A:N3	8:H:105:SER:OG	2.45	0.50
1:A:1124:G:N7	1:A:1125:C:N4	2.60	0.50
24:a:519:C:H5	24:a:2005:G:H1	1.58	0.50
24:a:1096:G:H21	24:a:1097:A:H62	1.57	0.50
24:a:1419:C:N4	24:a:1543:C:H42	2.09	0.50
45:s:89:GLU:OE2	45:s:90:GLY:N	2.44	0.50
1:A:172:A:N6	1:A:174:A:H62	2.10	0.50
1:A:490:A:O2'	1:A:491:G:H2'	2.12	0.50
1:A:1260:G:N3	1:A:1260:G:H2'	2.25	0.50
11:K:19:MET:HE3	11:K:21:HIS:CE1	2.46	0.50
14:N:31:ILE:HD11	14:N:44:ALA:HB3	1.93	0.50
24:a:1459:A:H3'	24:a:1460:G:H8	1.75	0.50
24:a:2586:C:H2'	24:a:2587:A:O4'	2.11	0.50
19:S:32:LYS:HB3	19:S:51:LEU:HD23	1.93	0.50
24:a:890:C:H3'	24:a:891:U:C5'	2.41	0.50
24:a:1401:A:C8	24:a:1402:U:H5	2.29	0.50
29:3:11:LYS:HD3	29:3:14:ALA:H	1.75	0.50
1:A:1091:C:H4'	1:A:1163:A:C6	2.46	0.50
2:B:82:GLU:HA	2:B:85:ILE:HB	1.94	0.50
3:C:118:ASP:O	3:C:122:SER:N	2.37	0.50
24:a:876:C:H5''	24:a:877:C:H5''	1.93	0.50
24:a:1415:C:H42	24:a:1547:A:H61	1.58	0.50
24:a:1702:C:H4'	24:a:1704:G:C4	2.46	0.50
24:a:1858:G:H2'	24:a:1859:G:H8	1.74	0.50
29:3:13:ARG:CZ	29:3:13:ARG:HA	2.41	0.50
1:A:1141:C:H4'	9:I:6:TYR:CD2	2.47	0.50
1:A:1416:G:H4'	36:j:48:PRO:HG3	1.94	0.50
4:D:147:GLU:O	4:D:150:LYS:HG2	2.12	0.50
10:J:59:LYS:HE2	10:J:62:ARG:NH2	2.27	0.50
11:K:45:THR:HG23	11:K:46:ALA:O	2.12	0.50
24:a:1341:A:H61	24:a:2197:A:N6	2.09	0.50
24:a:1466:U:N3	24:a:1488:A:O2'	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:U:H3	1:A:98:A:H62	1.59	0.50
1:A:716:A:H61	1:A:727:A:H61	1.59	0.50
1:A:833:G:C5	1:A:834:C:N4	2.79	0.50
1:A:1279:U:H5''	1:A:1281:A:OP2	2.11	0.50
1:A:1435:A:H1'	1:A:1436:G:N7	2.27	0.50
3:C:42:PHE:HA	3:C:45:LYS:HB3	1.92	0.50
29:3:13:ARG:HA	29:3:13:ARG:NE	2.26	0.50
30:c:108:LYS:O	30:c:108:LYS:NZ	2.41	0.50
1:A:549:U:H2'	1:A:550:C:C6	2.47	0.50
24:a:835:U:H2'	24:a:836:A:H8	1.77	0.50
24:a:1455:G:H2'	24:a:1456:A:C8	2.47	0.50
24:a:2789:C:H2'	24:a:2790:U:C6	2.45	0.50
25:b:52:U:H1'	25:b:53:A:C2	2.47	0.50
1:A:1174:A:N7	9:I:104:THR:OG1	2.40	0.50
24:a:2298:C:H2'	24:a:2299:G:C8	2.46	0.50
39:m:45:ARG:O	39:m:49:GLU:HG3	2.12	0.50
5:E:150:ASN:OD1	5:E:150:ASN:N	2.45	0.49
7:G:15:ASP:CG	7:G:22:LEU:HA	2.36	0.49
24:a:187:A:H2'	24:a:188:C:C6	2.47	0.49
24:a:1571:U:O4'	24:a:1574:G:N1	2.45	0.49
1:A:1124:G:H1	1:A:1140:A:H5'	1.77	0.49
1:A:1157:G:H22	1:A:1168:G:H22	1.60	0.49
1:A:1322:C:H2'	1:A:1323:A:C8	2.42	0.49
1:A:1349:G:C4	1:A:1364:G:N2	2.81	0.49
24:a:268:A:O2'	24:a:269:A:H5'	2.12	0.49
24:a:868:G:H21	24:a:883:A:N6	2.09	0.49
24:a:878:G:H3'	24:a:879:A:H8	1.77	0.49
24:a:884:C:H3'	24:a:885:C:H4'	1.95	0.49
24:a:1498:U:O4	24:a:1717:C:N3	2.45	0.49
24:a:2012:C:H2'	24:a:2013:A:C8	2.47	0.49
1:A:1143:C:H2'	1:A:1144:U:C6	2.47	0.49
1:A:1262:G:N2	1:A:1322:C:H4'	2.27	0.49
1:A:1472:U:H2'	1:A:1473:C:C6	2.48	0.49
2:B:51:ASN:HA	2:B:54:LEU:HB2	1.95	0.49
1:A:1485:G:H2'	1:A:1486:A:C8	2.47	0.49
24:a:278:U:H2'	24:a:279:G:C8	2.47	0.49
24:a:1896:C:H5	24:a:1905:A:H62	1.60	0.49
1:A:478:G:H4'	1:A:479:U:H5'	1.94	0.49
1:A:832:A:N1	1:A:833:G:C6	2.81	0.49
4:D:60:LYS:H	4:D:60:LYS:HD2	1.77	0.49
8:H:44:GLY:O	8:H:64:LYS:NZ	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:A:H5'	1:A:567:A:H8	1.76	0.49
1:A:1232:A:N6	1:A:1331:G:N3	2.61	0.49
24:a:34:U:O2'	24:a:35:G:OP1	2.28	0.49
24:a:866:G:N1	24:a:886:A:N3	2.61	0.49
24:a:872:C:N4	24:a:876:C:OP1	2.45	0.49
1:A:461:U:OP2	1:A:462:A:N6	2.45	0.49
1:A:1124:G:C8	1:A:1125:C:C4	3.01	0.49
2:B:61:ALA:HB1	2:B:221:ILE:HD13	1.95	0.49
24:a:280:U:H2'	24:a:281:G:C8	2.47	0.49
1:A:470:G:H2'	1:A:471:C:C6	2.48	0.49
1:A:701:U:H4'	11:K:21:HIS:CE1	2.48	0.49
1:A:1385:U:HO2'	1:A:1386:G:H8	1.61	0.49
17:Q:49:GLU:OE1	17:Q:49:GLU:N	2.42	0.49
24:a:918:A:N3	24:a:919:U:H1'	2.28	0.49
24:a:1031:C:O2	24:a:1033:G:N2	2.46	0.49
3:C:19:VAL:HG12	3:C:20:SER:OG	2.13	0.49
9:I:49:GLN:HE21	9:I:79:ARG:NH2	2.11	0.49
10:J:52:LEU:HB2	14:N:81:ARG:HD2	1.95	0.49
17:Q:16:LYS:HB3	17:Q:16:LYS:HZ2	1.78	0.49
24:a:135:G:H3'	24:a:136:C:H4'	1.94	0.49
51:y:40:GLU:H	51:y:40:GLU:CD	2.15	0.49
1:A:508:C:C2	1:A:533:A:H1'	2.48	0.49
19:S:52:THR:OG1	19:S:53:ILE:HG13	2.12	0.49
24:a:3:U:H2'	24:a:4:U:C6	2.48	0.49
24:a:2195:G:O2'	24:a:2196:A:OP2	2.25	0.49
2:B:127:GLU:HB3	2:B:132:LYS:HB3	1.94	0.48
9:I:9:GLY:H	9:I:16:ALA:HB3	1.78	0.48
9:I:10:ARG:C	9:I:105:ARG:HH12	2.21	0.48
13:M:54:ASP:O	13:M:57:ARG:HD2	2.13	0.48
24:a:862:G:H1	24:a:888:C:H41	1.61	0.48
1:A:503:A:N1	1:A:504:A:N6	2.61	0.48
24:a:869:G:C6	24:a:881:U:N3	2.81	0.48
1:A:332:A:H5''	36:j:97:ARG:NH1	2.27	0.48
1:A:689:A:H2'	1:A:690:A:C8	2.48	0.48
1:A:1257:C:H2'	1:A:1258:U:C5	2.48	0.48
4:D:104:ARG:HH21	4:D:191:LEU:HD12	1.78	0.48
11:K:33:ILE:HD12	11:K:33:ILE:O	2.14	0.48
14:N:87:ALA:HB3	14:N:93:ILE:HD11	1.95	0.48
22:W:27:U:HO2'	22:W:28:A:H8	1.59	0.48
24:a:886:A:C4	24:a:887:A:N7	2.82	0.48
43:q:39:LEU:HB3	43:q:49:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:y:44:CYS:SG	51:y:48:MET:HE3	2.53	0.48
1:A:934:G:H1	1:A:1337:G:H22	1.61	0.48
2:B:147:SER:OG	2:B:148:LEU:N	2.46	0.48
3:C:112:ASP:HA	3:C:204:LYS:NZ	2.28	0.48
4:D:53:LEU:HB3	4:D:199:LEU:HD21	1.94	0.48
6:F:29:ILE:HD13	6:F:64:VAL:HG11	1.96	0.48
24:a:771:G:H5'	24:a:772:G:OP1	2.14	0.48
24:a:2781:U:N3	24:a:2786:G:N1	2.28	0.48
53:f:4:LEU:H	53:f:4:LEU:HD12	1.78	0.48
24:a:879:A:H2'	24:a:880:C:C6	2.48	0.48
1:A:392:U:H2'	1:A:393:G:H8	1.78	0.48
1:A:524:G:H1	12:L:45:PRO:HG3	1.79	0.48
1:A:1156:C:H2'	1:A:1157:G:H8	1.77	0.48
1:A:1458:U:H2'	1:A:1459:A:C8	2.49	0.48
2:B:132:LYS:HZ1	2:B:136:MET:HG3	1.78	0.48
2:B:141:MET:O	2:B:145:GLU:HG3	2.13	0.48
13:M:22:ILE:HD12	13:M:65:VAL:HG22	1.96	0.48
13:M:89:LEU:HA	13:M:92:ARG:HE	1.77	0.48
4:D:57:GLU:HA	4:D:60:LYS:HZ3	1.77	0.48
13:M:101:ARG:HD3	13:M:105:ASN:ND2	2.28	0.48
24:a:1709:G:N2	24:a:1723:A:H62	2.11	0.48
53:f:17:GLN:NE2	53:f:22:PHE:O	2.47	0.48
1:A:1314:C:OP1	19:S:2:ARG:NH1	2.47	0.48
3:C:152:GLU:OE1	3:C:167:TRP:HB2	2.14	0.48
24:a:705:A:O2'	24:a:706:U:H6	1.96	0.48
46:t:90:ASP:OD1	46:t:91:GLY:N	2.45	0.48
1:A:486:C:H2'	1:A:487:A:C8	2.49	0.48
11:K:33:ILE:HD11	11:K:42:SER:CB	2.44	0.48
24:a:1708:U:H3'	24:a:1709:G:H5''	1.96	0.48
40:n:84:LYS:NZ	40:n:84:LYS:HB3	2.29	0.48
1:A:165:A:H2'	1:A:166:C:H6	1.79	0.48
1:A:1106:C:H2'	3:C:179:ARG:HE	1.79	0.48
1:A:1434:U:H5''	1:A:1435:A:OP1	2.14	0.48
29:3:11:LYS:HZ2	29:3:14:ALA:CB	2.27	0.48
1:A:1241:U:C4	1:A:1242:A:C6	3.02	0.47
2:B:96:TRP:CZ2	2:B:172:ALA:HB2	2.49	0.47
1:A:1144:U:N3	1:A:1145:A:N1	2.62	0.47
2:B:14:VAL:HB	2:B:43:LEU:HD21	1.95	0.47
4:D:183:LYS:HD3	4:D:183:LYS:N	2.26	0.47
24:a:337:A:H3'	24:a:338:A:C5'	2.44	0.47
30:c:167:ARG:HG3	30:c:172:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:G:OP2	1:A:1353:C:O2'	2.32	0.47
7:G:15:ASP:HB3	7:G:21:GLU:O	2.14	0.47
24:a:573:A:H62	24:a:1233:C:H5	1.63	0.47
24:a:700:G:H3'	24:a:701:U:H6	1.78	0.47
24:a:1567:A:N3	24:a:1568:G:H1'	2.29	0.47
24:a:1865:G:H2'	24:a:1866:C:C6	2.49	0.47
24:a:2798:G:H2'	24:a:2799:C:H6	1.79	0.47
24:a:412:G:C2'	24:a:413:G:H5'	2.41	0.47
40:n:31:THR:HG23	40:n:34:HIS:H	1.79	0.47
1:A:1039:A:N6	1:A:1208:C:H42	2.12	0.47
1:A:1452:G:N7	1:A:1453:A:C6	2.83	0.47
6:F:42:TRP:HB2	6:F:59:TYR:HB2	1.96	0.47
6:F:90:MET:HE3	18:R:61:ARG:NH1	2.29	0.47
24:a:595:A:H2'	24:a:596:A:C8	2.49	0.47
24:a:880:C:H2'	24:a:881:U:O4'	2.14	0.47
1:A:221:G:O2'	16:P:63:GLN:NE2	2.48	0.47
1:A:1078:U:H5'	1:A:1087:G:H1'	1.95	0.47
1:A:1169:G:N1	1:A:1170:A:N7	2.62	0.47
3:C:118:ASP:O	3:C:122:SER:OG	2.32	0.47
10:J:67:ILE:HD11	14:N:96:LEU:HB2	1.96	0.47
24:a:1455:G:H1	24:a:1501:G:H1	1.61	0.47
24:a:1909:G:H2'	24:a:1910:U:O4'	2.14	0.47
36:j:68:GLY:HA3	36:j:77:ILE:O	2.14	0.47
42:p:36:PHE:O	42:p:40:THR:HG23	2.14	0.47
1:A:412:C:H5''	1:A:533:A:N3	2.30	0.47
1:A:1157:G:N2	1:A:1168:G:H22	2.12	0.47
1:A:1236:G:N7	1:A:1237:C:N4	2.61	0.47
1:A:1324:U:C4	1:A:1325:G:C6	3.03	0.47
1:A:1404:A:H62	1:A:1484:U:H3	1.62	0.47
3:C:60:PRO:HG2	10:J:94:ALA:HB1	1.96	0.47
4:D:170:TRP:HD1	4:D:184:ARG:HD2	1.79	0.47
11:K:13:LYS:HD2	11:K:75:GLU:OE2	2.14	0.47
13:M:29:ARG:HG3	13:M:62:LYS:HE2	1.97	0.47
24:a:342:C:H2'	24:a:343:A:H8	1.80	0.47
24:a:1417:G:H22	24:a:1545:A:H8	1.63	0.47
24:a:1739:C:OP1	41:o:98:ARG:NH1	2.47	0.47
24:a:2276:U:H2'	24:a:2277:U:C6	2.50	0.47
36:j:38:ILE:HD11	36:j:111:PHE:HZ	1.80	0.47
47:u:36:GLY:O	47:u:97:ARG:NH1	2.47	0.47
24:a:1309:A:N6	24:a:1634:U:O2	2.48	0.47
1:A:229:C:H2'	1:A:230:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:U:H3	1:A:1200:G:N2	2.13	0.47
1:A:1412:A:N6	1:A:1476:G:O2'	2.45	0.47
1:A:1451:G:N7	1:A:1452:G:N1	2.63	0.47
24:a:1861:A:OP1	24:a:1863:A:H1'	2.15	0.47
25:b:33:G:N1	25:b:50:A:C2	2.57	0.47
1:A:971:A:H1'	1:A:1317:G:C2	2.50	0.47
4:D:58:LYS:HG2	4:D:200:ILE:HD13	1.97	0.47
11:K:46:ALA:O	11:K:48:GLY:N	2.46	0.47
13:M:15:ALA:HB3	13:M:41:GLU:HA	1.97	0.47
24:a:687:G:O2'	24:a:1619:A:N3	2.45	0.47
24:a:1012:G:OP2	24:a:1120:A:O2'	2.27	0.47
24:a:1402:U:H2'	24:a:1403:G:O4'	2.15	0.47
24:a:1543:C:H2'	24:a:1544:C:C6	2.50	0.47
24:a:1894:G:H1	24:a:1910:U:H3	1.63	0.47
24:a:2643:C:H2'	24:a:2644:G:O4'	2.14	0.47
43:q:46:LYS:N	43:q:46:LYS:HD2	2.30	0.47
1:A:359:U:H5'	1:A:360:A:OP1	2.15	0.46
1:A:535:G:H2'	1:A:536:G:C8	2.50	0.46
1:A:535:G:H2'	1:A:536:G:H8	1.78	0.46
24:a:914:A:H2	51:y:44:CYS:HG	1.59	0.46
24:a:914:A:N1	55:a:3205:HOH:O	2.35	0.46
24:a:2288:G:O2'	24:a:2290:U:OP2	2.21	0.46
24:a:2517:G:H5''	24:a:2518:U:H5	1.80	0.46
1:A:1048:A:C6	1:A:1201:G:C5	3.04	0.46
19:S:43:MET:HE3	19:S:43:MET:HB3	1.85	0.46
42:p:66:ASN:O	42:p:70:ARG:HG3	2.15	0.46
50:x:11:VAL:O	50:x:15:ASN:ND2	2.46	0.46
1:A:41:G:HO2'	1:A:42:G:H8	1.61	0.46
1:A:835:C:H2'	1:A:836:U:O4'	2.14	0.46
7:G:31:MET:HE1	7:G:36:LYS:N	2.31	0.46
12:L:34:CYS:HB3	12:L:80:ILE:HD11	1.97	0.46
17:Q:75:PHE:HZ	17:Q:78:VAL:HG23	1.78	0.46
24:a:1401:A:H2'	24:a:1402:U:H6	1.80	0.46
1:A:341:G:H2'	1:A:342:G:O4'	2.15	0.46
1:A:400:G:H22	1:A:431:U:H3	1.63	0.46
1:A:487:A:H1'	1:A:488:G:C8	2.50	0.46
1:A:1134:C:O2'	1:A:1138:G:O6	2.33	0.46
16:P:15:PRO:HG2	16:P:41:PRO:HG2	1.97	0.46
24:a:1104:C:N4	24:a:1105:U:O4	2.48	0.46
24:a:1840:U:O3'	24:a:1841:U:H6	1.98	0.46
24:a:2518:U:OP1	24:a:2650:A:O2'	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:g:43:VAL:O	33:g:44:LYS:HD2	2.16	0.46
34:h:50:ARG:O	34:h:54:LEU:N	2.48	0.46
1:A:926:G:C6	1:A:928:A:N6	2.83	0.46
12:L:4:ILE:HD13	12:L:4:ILE:HA	1.65	0.46
14:N:67:THR:HG22	14:N:68:GLY:N	2.29	0.46
24:a:1461:G:N1	24:a:1494:A:O2'	2.32	0.46
24:a:1897:G:H5'	24:a:1898:U:C5'	2.44	0.46
34:h:75:LEU:HD13	34:h:107:GLY:HA2	1.97	0.46
13:M:23:TYR:HB3	13:M:65:VAL:O	2.15	0.46
24:a:1568:G:H5''	24:a:1569:C:C5	2.51	0.46
1:A:108:G:H1	20:T:10:ARG:HD3	1.80	0.46
3:C:89:GLN:O	3:C:93:LYS:NZ	2.35	0.46
3:C:178:LEU:H	3:C:178:LEU:HD23	1.80	0.46
24:a:707:C:H2'	24:a:708:A:C8	2.51	0.46
1:A:400:G:C6	1:A:489:A:N7	2.84	0.46
1:A:1100:C:OP1	3:C:172:ARG:NH2	2.49	0.46
2:B:93:ASN:OD1	2:B:93:ASN:C	2.58	0.46
9:I:45:MET:HA	9:I:48:HIS:NE2	2.31	0.46
16:P:54:LEU:HD23	16:P:54:LEU:HA	1.70	0.46
19:S:38:TRP:HE3	19:S:38:TRP:H	1.64	0.46
24:a:354:A:H2	24:a:412:G:H21	1.64	0.46
24:a:868:G:O2'	24:a:869:G:N7	2.46	0.46
24:a:1392:A:H2'	24:a:1393:U:C6	2.51	0.46
30:c:121:ASP:OD1	30:c:121:ASP:N	2.48	0.46
1:A:1309:U:H2'	1:A:1310:G:C8	2.51	0.46
2:B:137:LEU:HA	2:B:140:GLU:OE2	2.16	0.46
24:a:347:U:H2'	24:a:348:A:C8	2.51	0.46
34:h:73:GLU:HG2	34:h:142:ILE:HB	1.97	0.46
1:A:1293:A:N3	1:A:1294:G:N1	2.63	0.46
1:A:1373:G:C5	1:A:1374:U:H1'	2.51	0.46
2:B:57:LEU:O	2:B:61:ALA:HB2	2.16	0.46
2:B:66:LYS:NZ	2:B:90:TYR:OH	2.49	0.46
4:D:172:GLU:HG2	4:D:181:SER:HB3	1.97	0.46
4:D:178:LEU:HD23	4:D:178:LEU:H	1.80	0.46
24:a:2302:C:H2'	24:a:2303:G:O4'	2.16	0.46
30:c:133:ARG:NH1	34:h:123:ARG:HH12	2.13	0.46
31:d:31:THR:HG23	31:d:32:PRO:HD2	1.98	0.46
1:A:623:A:N6	1:A:624:A:N3	2.61	0.45
2:B:67:VAL:HG22	2:B:160:ALA:HB3	1.97	0.45
11:K:125:LYS:H	11:K:125:LYS:HG3	1.55	0.45
20:T:69:LYS:HB2	20:T:69:LYS:NZ	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:8:U:O2'	24:a:9:G:H5'	2.16	0.45
24:a:282:U:H3	24:a:338:A:N6	2.13	0.45
25:b:14:U:OP2	25:b:70:C:O2'	2.34	0.45
25:b:56:G:H3'	25:b:57:A:C2	2.50	0.45
32:e:166:LYS:HA	32:e:166:LYS:HD3	1.71	0.45
33:g:27:LYS:HE2	33:g:27:LYS:HB2	1.67	0.45
34:h:112:LYS:HG2	34:h:114:GLU:H	1.81	0.45
1:A:209:C:HO2'	1:A:210:U:C5'	2.28	0.45
1:A:504:A:HO2'	1:A:536:G:HO2'	1.64	0.45
9:I:18:VAL:HG23	9:I:64:ILE:HG22	1.97	0.45
24:a:970:A:H3'	24:a:971:C:H5'	1.98	0.45
24:a:1401:A:N1	24:a:1566:A:N6	2.64	0.45
24:a:2231:G:H2'	24:a:2232:A:C8	2.51	0.45
25:b:33:G:H22	25:b:50:A:H2	1.64	0.45
40:n:2:ASP:HB3	40:n:5:THR:HG23	1.97	0.45
1:A:1120:G:H8	1:A:1275:U:H3	1.63	0.45
3:C:35:GLY:CA	3:C:38:LYS:HZ1	2.23	0.45
3:C:87:LEU:O	3:C:91:VAL:N	2.37	0.45
6:F:90:MET:HE1	18:R:23:TYR:CE1	2.52	0.45
9:I:114:LYS:N	9:I:114:LYS:HD3	2.31	0.45
24:a:1127:U:H4'	24:a:1128:A:O4'	2.15	0.45
3:C:47:LEU:HD11	3:C:50:ALA:HB2	1.99	0.45
24:a:1546:U:H4'	24:a:1547:A:O5'	2.17	0.45
33:g:119:GLU:H	33:g:119:GLU:HG3	1.56	0.45
51:y:57:LYS:HB3	51:y:57:LYS:HE3	1.72	0.45
1:A:934:G:H1	1:A:1337:G:N2	2.14	0.45
1:A:1161:A:H2'	1:A:1162:U:H3'	1.99	0.45
1:A:1416:G:O2'	1:A:1417:G:N3	2.40	0.45
3:C:88:ARG:HH22	3:C:98:PRO:HB3	1.80	0.45
4:D:153:ALA:H	4:D:154:ARG:NH1	2.15	0.45
19:S:53:ILE:HD12	19:S:55:VAL:O	2.15	0.45
24:a:4:U:H2'	24:a:5:A:C8	2.51	0.45
24:a:342:C:H2'	24:a:343:A:C8	2.50	0.45
24:a:864:U:O2'	24:a:865:A:O4'	2.33	0.45
24:a:1492:U:H2'	24:a:1493:A:C8	2.52	0.45
24:a:1860:G:O2'	24:a:1861:A:OP2	2.33	0.45
1:A:11:G:H1	1:A:23:C:H5	1.65	0.45
1:A:1262:G:H22	1:A:1322:C:H4'	1.82	0.45
24:a:1501:G:O2'	24:a:1502:A:H5''	2.16	0.45
45:s:1:MET:HB3	45:s:1:MET:HE3	1.73	0.45
1:A:1236:G:C8	1:A:1237:C:C5	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1287:C:H2'	1:A:1288:G:H8	1.81	0.45
2:B:140:GLU:HA	2:B:143:LYS:HB3	1.98	0.45
24:a:272:U:O2'	24:a:273:U:H6	1.96	0.45
1:A:595:G:N2	1:A:632:U:O2	2.49	0.45
1:A:1502:G:H1	1:A:1521:C:H5	1.63	0.45
1:A:1510:2MG:N2	1:A:1513:MA6:OP2	2.50	0.45
20:T:33:LYS:HD3	20:T:33:LYS:HA	1.71	0.45
24:a:869:G:O6	24:a:881:U:C4	2.70	0.45
1:A:439:A:H2'	1:A:440:G:H8	1.80	0.45
1:A:524:G:N1	12:L:45:PRO:HG3	2.32	0.45
1:A:981:C:C2	1:A:982:A:C8	3.05	0.45
3:C:22:TRP:HE3	14:N:94:PRO:HB3	1.82	0.45
14:N:6:MET:SD	14:N:6:MET:N	2.85	0.45
19:S:35:ILE:CG2	19:S:71:ILE:H	2.30	0.45
24:a:2058:A:H2'	24:a:2059:C:C6	2.52	0.45
50:x:37:LEU:HD12	50:x:37:LEU:HA	1.80	0.45
1:A:1258:U:H2'	1:A:1259:C:C6	2.52	0.45
3:C:22:TRP:CD1	3:C:32:GLN:OE1	2.70	0.45
24:a:704:C:H2'	24:a:705:A:C8	2.51	0.45
24:a:2454:A:OP2	24:a:2461:A:N6	2.50	0.45
25:b:33:G:O6	25:b:50:A:N1	2.50	0.45
1:A:1187:G:H3'	1:A:1188:U:H5''	1.99	0.44
24:a:1774:A:OP2	30:c:221:ARG:NH1	2.50	0.44
1:A:934:G:N2	1:A:1337:G:N2	2.65	0.44
1:A:1285:U:C4	1:A:1286:G:N1	2.85	0.44
2:B:185:ALA:C	2:B:186:ILE:HD13	2.42	0.44
8:H:18:GLN:NE2	8:H:70:ALA:HB1	2.33	0.44
9:I:79:ARG:HD3	9:I:102:PHE:CD1	2.53	0.44
24:a:707:C:H2'	24:a:708:A:H8	1.83	0.44
24:a:2293:G:N2	24:a:2295:C:OP2	2.46	0.44
24:a:2789:C:H2'	24:a:2790:U:H6	1.82	0.44
37:k:88:ASP:OD2	37:k:88:ASP:N	2.50	0.44
1:A:1126:A:OP2	1:A:1128:G:H8	2.01	0.44
1:A:1156:C:H6	1:A:1156:C:OP2	2.00	0.44
3:C:134:MET:HE2	3:C:134:MET:HB2	1.79	0.44
6:F:45:ARG:HH12	6:F:102:LEU:HD11	1.83	0.44
24:a:5:A:H2'	24:a:6:A:C8	2.52	0.44
24:a:632:C:H2'	24:a:634:G:C8	2.51	0.44
24:a:1489:C:O2'	24:a:1490:A:O4'	2.35	0.44
34:h:83:LYS:HE3	34:h:83:LYS:HB3	1.86	0.44
1:A:488:G:H2'	1:A:490:A:N3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:C:P	9:I:10:ARG:HH21	2.40	0.44
1:A:1294:G:C4	1:A:1296:C:H1'	2.52	0.44
2:B:32:PHE:HD2	2:B:40:ILE:HD11	1.82	0.44
4:D:70:LYS:HE3	4:D:71:GLN:HG3	1.99	0.44
8:H:46:ILE:HD12	8:H:61:ILE:HG23	2.00	0.44
22:W:27:U:O2'	22:W:28:A:H8	2.01	0.44
24:a:1535:U:H1'	24:a:1536:G:H5'	2.00	0.44
33:g:9:ILE:HD11	33:g:69:ARG:HG3	2.00	0.44
41:o:10:LYS:NZ	41:o:10:LYS:HB2	2.32	0.44
50:x:1:MET:HE3	50:x:1:MET:HB3	1.76	0.44
1:A:208:G:O2'	1:A:209:C:O4'	2.28	0.44
1:A:1194:C:O2'	1:A:1197:C:OP2	2.34	0.44
1:A:1301:U:C5	1:A:1302:U:C5	3.05	0.44
24:a:761:A:H2'	24:a:761:A:N3	2.33	0.44
24:a:1029:C:C2'	24:a:1098:G:H1	2.31	0.44
24:a:2641:U:N3	24:a:2650:A:C8	2.80	0.44
37:k:144:ASP:OD1	37:k:144:ASP:N	2.30	0.44
1:A:400:G:N2	1:A:431:U:H3	2.16	0.44
1:A:534:G:N2	1:A:536:G:N7	2.65	0.44
1:A:623:A:C5	1:A:624:A:H1'	2.53	0.44
2:B:108:ARG:O	2:B:112:LYS:HE3	2.18	0.44
34:h:123:ARG:O	34:h:124:GLU:HG3	2.17	0.44
40:n:55:LYS:C	40:n:55:LYS:HD2	2.43	0.44
1:A:667:A:H2'	1:A:668:G:C8	2.52	0.44
1:A:1230:A:O5'	1:A:1230:A:H8	2.01	0.44
4:D:183:LYS:N	4:D:183:LYS:CD	2.81	0.44
16:P:56:ARG:HA	16:P:56:ARG:HD2	1.63	0.44
24:a:1706:G:N3	24:a:1706:G:H2'	2.33	0.44
38:l:39:ARG:HB3	38:l:99:PRO:HD3	2.00	0.44
40:n:73:VAL:HG21	40:n:105:LEU:HD11	2.00	0.44
53:f:106:ILE:C	53:f:110:ARG:HH21	2.25	0.44
1:A:1275:U:O4	10:J:43:PRO:HD2	2.18	0.44
1:A:1313:A:H5'	19:S:2:ARG:NH1	2.33	0.44
1:A:1351:A:N6	1:A:1361:C:H42	2.16	0.44
3:C:23:TYR:HD1	3:C:23:TYR:H	1.66	0.44
3:C:186:THR:HG22	3:C:199:LYS:HA	2.00	0.44
11:K:57:SER:O	11:K:90:PRO:HG2	2.17	0.44
18:R:35:GLU:OE2	18:R:35:GLU:N	2.51	0.44
24:a:1354:U:O2'	24:a:2197:A:H8	2.01	0.44
24:a:1898:U:N3	24:a:1899:A:N7	2.66	0.44
32:e:140:GLU:C	32:e:140:GLU:OE2	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:89:LYS:HB2	34:h:124:GLU:HB3	1.99	0.44
48:v:38:VAL:HG13	48:v:59:ILE:HB	1.99	0.44
1:A:549:U:H2'	1:A:550:C:H6	1.83	0.44
1:A:1127:G:H3'	1:A:1128:G:H4'	1.99	0.44
1:A:1152:C:N4	1:A:1175:G:O5'	2.51	0.44
9:I:18:VAL:HG23	9:I:64:ILE:CG2	2.48	0.44
9:I:41:GLU:C	9:I:43:ALA:H	2.25	0.44
11:K:86:LYS:NZ	11:K:112:VAL:HG13	2.33	0.44
24:a:1029:C:H2'	24:a:1098:G:H1	1.83	0.44
1:A:688:A:H2'	1:A:689:A:O4'	2.18	0.43
1:A:1253:C:H2'	1:A:1254:G:C8	2.53	0.43
1:A:1457:U:H2'	1:A:1458:U:C5	2.53	0.43
2:B:90:TYR:HE2	2:B:153:ASN:HB2	1.83	0.43
4:D:163:GLU:HA	4:D:167:LYS:NZ	2.32	0.43
12:L:10:LYS:HD3	12:L:13:ARG:HH22	1.83	0.43
14:N:6:MET:HE2	14:N:7:LYS:NZ	2.32	0.43
24:a:1027:G:C6	24:a:1029:C:H1'	2.52	0.43
24:a:1852:U:H2'	24:a:1853:C:C6	2.53	0.43
24:a:1897:G:H5'	24:a:1898:U:H5''	2.00	0.43
29:3:30:LYS:HA	29:3:30:LYS:HD3	1.64	0.43
45:s:39:THR:HG22	45:s:41:ALA:H	1.81	0.43
1:A:527:A:H8	1:A:530:C:O4'	2.01	0.43
1:A:1059:C:H42	1:A:1186:C:H41	1.64	0.43
1:A:1110:A:O2'	1:A:1111:U:H5'	2.17	0.43
1:A:1220:C:O2'	1:A:1221:A:O5'	2.35	0.43
1:A:1351:A:H61	1:A:1361:C:N4	2.16	0.43
12:L:30:LYS:HA	12:L:30:LYS:HD3	1.81	0.43
13:M:11:ASP:OD1	13:M:11:ASP:N	2.50	0.43
14:N:12:LYS:HE2	14:N:16:LEU:HD11	1.98	0.43
24:a:3:U:N3	24:a:2886:C:O2	2.51	0.43
24:a:341:A:H2'	24:a:342:C:C6	2.53	0.43
24:a:631:A:H2'	24:a:632:C:O4'	2.18	0.43
24:a:1389:G:H22	24:a:1582:G:H22	1.66	0.43
24:a:1704:G:H1	24:a:1728:G:H1	1.65	0.43
24:a:1860:G:H4'	24:a:1862:G:H4'	2.00	0.43
1:A:1202:C:C4	1:A:1203:C:C5	3.07	0.43
3:C:27:LYS:HD3	3:C:27:LYS:HA	1.78	0.43
5:E:47:LYS:NZ	5:E:73:MET:HB3	2.33	0.43
20:T:83:ILE:C	20:T:84:LYS:HD3	2.44	0.43
24:a:1026:A:N1	24:a:1101:G:N2	2.66	0.43
24:a:2364:G:H2'	24:a:2365:U:O2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:2646:G:H2'	24:a:2647:A:O4'	2.19	0.43
1:A:28:A:H2'	1:A:29:U:O4'	2.18	0.43
3:C:123:GLN:HG3	3:C:136:ARG:HH21	1.84	0.43
24:a:1415:C:N4	24:a:1547:A:H61	2.16	0.43
24:a:2773:A:H2'	24:a:2774:C:C6	2.52	0.43
33:g:73:ASN:OD1	33:g:73:ASN:C	2.61	0.43
1:A:413:C:O2'	1:A:414:U:O5'	2.37	0.43
1:A:929:C:H5	1:A:1374:U:O2	2.01	0.43
4:D:109:SER:N	4:D:113:GLU:OE1	2.34	0.43
4:D:139:PRO:HA	4:D:182:PHE:HB3	2.00	0.43
14:N:43:ASP:O	14:N:47:LYS:N	2.47	0.43
24:a:880:C:H3'	24:a:881:U:C6	2.54	0.43
24:a:1421:A:H3'	24:a:1422:A:H8	1.84	0.43
24:a:2457:G:C6	24:a:2459:U:H5''	2.54	0.43
24:a:2725:A:H2'	24:a:2726:A:C8	2.53	0.43
1:A:427:G:C2	1:A:428:C:H1'	2.53	0.43
1:A:1436:G:H2'	1:A:1437:U:O4'	2.19	0.43
4:D:154:ARG:CD	4:D:154:ARG:H	2.32	0.43
6:F:36:ILE:HG13	6:F:64:VAL:HG12	2.00	0.43
19:S:69:GLU:H	19:S:69:GLU:CD	2.27	0.43
24:a:338:A:H4'	24:a:339:A:O5'	2.17	0.43
24:a:2539:U:H2'	24:a:2540:U:C6	2.53	0.43
36:j:47:ILE:HD13	36:j:47:ILE:HA	1.84	0.43
46:t:48:LYS:HG3	46:t:49:PRO:HD2	1.99	0.43
1:A:165:A:H2'	1:A:166:C:C6	2.54	0.43
1:A:945:U:H3	1:A:1225:G:H1	1.66	0.43
11:K:124:LYS:HE2	11:K:124:LYS:HB3	1.64	0.43
24:a:2197:A:H2	24:a:2197:A:OP2	2.02	0.43
24:a:2647:A:H3'	24:a:2648:G:H8	1.84	0.43
1:A:488:G:H21	1:A:490:A:H1'	1.83	0.43
1:A:531:G:H2'	1:A:532:G:H5'	2.00	0.43
1:A:611:G:H21	16:P:14:ARG:NH1	2.16	0.43
1:A:938:G:C2	1:A:939:A:C8	3.06	0.43
1:A:1436:G:C6	1:A:1437:U:C2	3.07	0.43
1:A:1458:U:P	41:o:113:ARG:HH22	2.42	0.43
4:D:137:ILE:HD13	4:D:137:ILE:HA	1.91	0.43
10:J:52:LEU:HB3	14:N:81:ARG:HH11	1.84	0.43
10:J:102:LEU:HD12	10:J:102:LEU:HA	1.75	0.43
12:L:38:TYR:OH	12:L:54:ARG:NE	2.52	0.43
24:a:1719:C:O2'	24:a:1720:U:O4'	2.36	0.43
1:A:448:G:N2	1:A:473:G:H22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:H1	1:A:1365:G:N2	2.15	0.43
13:M:86:TYR:HA	13:M:89:LEU:HD13	2.01	0.43
22:W:28:A:H61	22:W:40:C:N4	2.14	0.43
1:A:1136:G:N3	1:A:1136:G:H2'	2.34	0.43
1:A:1310:G:N2	1:A:1314:C:H41	2.16	0.43
2:B:179:LEU:HD23	2:B:179:LEU:HA	1.82	0.43
4:D:107:PHE:HB3	4:D:177:LYS:HZ1	1.84	0.43
24:a:467:A:H4'	24:a:468:A:OP1	2.19	0.43
24:a:1809:G:O2'	30:c:253:THR:HG21	2.18	0.43
40:n:62:LYS:HD3	40:n:62:LYS:C	2.44	0.43
49:w:57:VAL:HG11	49:w:60:GLU:HG3	2.00	0.43
1:A:902:A:H2'	1:A:903:C:H5'	2.01	0.42
1:A:979:U:H3	1:A:1214:G:H1	1.65	0.42
1:A:1110:A:N1	1:A:1179:G:O6	2.52	0.42
1:A:1118:U:H1'	1:A:1120:G:OP1	2.19	0.42
1:A:1303:G:H1	1:A:1324:U:H3	1.67	0.42
20:T:66:LEU:HA	20:T:66:LEU:HD23	1.76	0.42
24:a:1162:A:H2'	24:a:1163:U:H6	1.83	0.42
24:a:1852:U:H4'	24:a:1861:A:C2	2.54	0.42
24:a:2648:G:H2'	24:a:2649:G:O4'	2.18	0.42
45:s:6:ARG:HD2	45:s:6:ARG:HA	1.60	0.42
1:A:871:A:H5''	8:H:81:PRO:O	2.18	0.42
1:A:1160:G:H21	1:A:1165:A:H62	1.67	0.42
1:A:1258:U:H2'	1:A:1259:C:H6	1.83	0.42
1:A:1310:G:H1	1:A:1314:C:H5	1.66	0.42
1:A:1436:G:H22	1:A:1455:G:H1'	1.83	0.42
9:I:70:GLY:O	9:I:74:GLN:HG3	2.19	0.42
24:a:654:U:H1'	28:2:2:ALA:HA	2.01	0.42
24:a:1394:A:H1'	24:a:1395:A:C2	2.54	0.42
24:a:1570:U:O3'	24:a:1574:G:N2	2.52	0.42
24:a:2289:G:H2'	24:a:2293:G:OP1	2.19	0.42
34:h:93:SER:HB2	34:h:123:ARG:HE	1.83	0.42
44:r:109:ASP:OD2	44:r:109:ASP:C	2.61	0.42
1:A:286:G:H21	1:A:602:A:N6	2.17	0.42
1:A:514:A:OP2	12:L:44:LYS:NZ	2.51	0.42
1:A:1272:G:H2'	1:A:1273:A:C2	2.54	0.42
2:B:125:THR:OG1	2:B:127:GLU:HG2	2.19	0.42
3:C:66:VAL:HG12	3:C:100:GLN:O	2.20	0.42
3:C:88:ARG:CZ	3:C:99:ALA:H	2.32	0.42
4:D:169:THR:HG22	4:D:184:ARG:NH2	2.35	0.42
9:I:27:ILE:HG12	9:I:62:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:8:LYS:O	20:T:8:LYS:HD3	2.19	0.42
24:a:1464:G:H2'	24:a:1465:U:C5	2.54	0.42
36:j:58:LYS:HE3	36:j:58:LYS:HB3	1.88	0.42
1:A:332:A:H5''	36:j:97:ARG:HH12	1.84	0.42
1:A:448:G:N2	1:A:473:G:H1	2.17	0.42
1:A:1082:G:H1'	1:A:1162:U:C6	2.55	0.42
1:A:1313:A:H5'	19:S:2:ARG:HH12	1.85	0.42
20:T:8:LYS:HA	20:T:8:LYS:HE3	2.02	0.42
24:a:374:G:H3'	24:a:378:A:N6	2.33	0.42
24:a:1856:U:H5''	24:a:1857:A:N7	2.34	0.42
24:a:2647:A:H3'	24:a:2648:G:C8	2.55	0.42
24:a:2790:U:H2'	24:a:2791:C:H6	1.83	0.42
31:d:18:GLU:CD	31:d:18:GLU:H	2.27	0.42
1:A:931:A:N6	1:A:1340:A:H61	2.17	0.42
2:B:86:ALA:O	2:B:222:THR:OG1	2.35	0.42
8:H:100:GLY:C	8:H:101:ILE:HD12	2.45	0.42
24:a:625:G:H2'	24:a:626:U:C6	2.54	0.42
24:a:866:G:N3	24:a:886:A:H1'	2.34	0.42
24:a:2295:C:O2'	24:a:2296:A:H5''	2.18	0.42
28:2:9:ARG:HD2	28:2:9:ARG:HA	1.75	0.42
33:g:19:LEU:HD21	33:g:45:VAL:HB	2.02	0.42
1:A:27:G:H2'	1:A:28:A:N3	2.35	0.42
1:A:609:G:C2	1:A:610:G:C8	3.08	0.42
1:A:1162:U:O2'	1:A:1163:A:N7	2.52	0.42
1:A:1295:U:C4	1:A:1330:C:H5	2.38	0.42
3:C:74:GLY:HA2	3:C:77:ILE:HD12	2.00	0.42
3:C:130:PHE:HE2	3:C:157:LEU:HD13	1.84	0.42
17:Q:57:ASP:OD1	17:Q:57:ASP:N	2.49	0.42
22:W:27:U:C4	22:W:42:G:C2	3.07	0.42
24:a:339:A:N6	24:a:340:G:N3	2.64	0.42
24:a:1388:C:H2'	24:a:1389:G:C8	2.55	0.42
24:a:1398:G:N3	24:a:1398:G:H2'	2.34	0.42
24:a:1840:U:H5	24:a:2074:G:H21	1.67	0.42
36:j:109:ASP:OD2	36:j:109:ASP:N	2.48	0.42
1:A:24:U:O2'	1:A:520:C:O4'	2.38	0.42
1:A:40:C:H2'	1:A:41:G:H5'	2.01	0.42
1:A:489:A:H4'	1:A:490:A:C5'	2.50	0.42
1:A:1457:U:H2'	1:A:1458:U:C6	2.55	0.42
13:M:39:ILE:HG22	13:M:40:ALA:H	1.84	0.42
24:a:1832:A:N6	24:a:1880:C:H42	2.15	0.42
36:j:88:ASN:HD21	36:j:92:GLN:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:66:ASN:C	40:n:66:ASN:OD1	2.62	0.42
53:f:114:PHE:CD2	53:f:114:PHE:C	2.97	0.42
1:A:701:U:H4'	11:K:21:HIS:ND1	2.34	0.42
1:A:1056:C:H2'	1:A:1057:G:C8	2.55	0.42
1:A:1080:G:C2	1:A:1081:G:H1'	2.55	0.42
4:D:104:ARG:HA	4:D:104:ARG:HD2	1.90	0.42
7:G:16:PRO:HD2	7:G:21:GLU:O	2.20	0.42
13:M:75:LEU:HA	13:M:78:LYS:HB3	2.01	0.42
41:o:15:GLU:H	41:o:15:GLU:HG3	1.62	0.42
1:A:404:G:H5''	1:A:405:A:OP2	2.20	0.42
1:A:485:A:O2'	1:A:486:C:O5'	2.37	0.42
1:A:1133:G:H3'	1:A:1133:G:N3	2.35	0.42
1:A:1199:U:C4	1:A:1200:G:N1	2.87	0.42
1:A:1246:A:OP2	1:A:1246:A:H8	2.02	0.42
1:A:1404:A:H2'	1:A:1405:C:O4'	2.20	0.42
3:C:12:LEU:HD13	3:C:13:GLY:N	2.35	0.42
13:M:27:LYS:HA	13:M:27:LYS:CE	2.49	0.42
24:a:139:G:O2'	24:a:140:C:H3'	2.19	0.42
33:g:58:VAL:HG12	33:g:60:ASP:H	1.84	0.42
36:j:53:LYS:N	36:j:53:LYS:HD2	2.34	0.42
1:A:1283:A:H8	1:A:1283:A:OP2	2.03	0.42
8:H:113:ASP:N	8:H:113:ASP:OD1	2.52	0.42
24:a:869:G:H1'	24:a:870:G:N7	2.35	0.42
24:a:2271:G:H4'	24:a:2272:A:O4'	2.20	0.42
34:h:4:ILE:HD13	34:h:4:ILE:HA	1.83	0.42
1:A:462:A:N7	1:A:463:C:O2'	2.54	0.41
1:A:484:G:O6	1:A:485:A:N6	2.53	0.41
2:B:27:MET:HB3	2:B:27:MET:HE3	1.82	0.41
2:B:132:LYS:NZ	2:B:136:MET:HG3	2.35	0.41
2:B:132:LYS:HZ1	2:B:137:LEU:H	1.68	0.41
3:C:92:THR:OG1	3:C:97:VAL:O	2.32	0.41
4:D:154:ARG:H	4:D:154:ARG:HD3	1.85	0.41
11:K:42:SER:O	11:K:43:TRP:HB3	2.20	0.41
24:a:278:U:H2'	24:a:279:G:H8	1.85	0.41
24:a:1389:G:N2	24:a:1582:G:H22	2.18	0.41
35:i:114:LEU:HG	35:i:118:MET:HE3	2.02	0.41
53:f:17:GLN:C	53:f:17:GLN:OE1	2.63	0.41
6:F:43:GLY:C	6:F:58:HIS:HD2	2.27	0.41
8:H:48:ASP:HB3	8:H:62:GLU:OE2	2.20	0.41
9:I:105:ARG:HG3	9:I:105:ARG:NH1	2.34	0.41
12:L:10:LYS:HD3	12:L:13:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:39:SER:N	19:S:68:ASP:O	2.53	0.41
24:a:831:C:H42	24:a:920:A:H61	1.68	0.41
35:i:90:ASP:OD1	35:i:90:ASP:N	2.53	0.41
1:A:540:G:OP1	4:D:70:LYS:N	2.53	0.41
1:A:1214:G:H21	19:S:32:LYS:HD2	1.85	0.41
5:E:158:LYS:HB3	5:E:158:LYS:HE3	1.89	0.41
24:a:986:A:H2'	24:a:987:A:C8	2.54	0.41
24:a:2516:A:C8	24:a:2517:G:N2	2.89	0.41
1:A:548:A:H2'	1:A:549:U:C6	2.56	0.41
1:A:607:C:N4	1:A:621:G:H1	2.19	0.41
1:A:698:A:C4	1:A:699:G:C8	3.08	0.41
1:A:1170:A:H2'	1:A:1171:G:C8	2.55	0.41
3:C:73:PRO:HG3	3:C:105:GLU:HB2	2.01	0.41
3:C:149:ILE:HG13	3:C:201:TRP:O	2.20	0.41
5:E:127:SER:O	5:E:128:LYS:HG3	2.20	0.41
24:a:368:G:N7	24:a:376:G:O6	2.52	0.41
24:a:1577:U:H2'	24:a:1578:A:C5	2.54	0.41
24:a:2731:U:OP1	33:g:142:GLY:HA3	2.20	0.41
24:a:2790:U:H2'	24:a:2791:C:C6	2.56	0.41
39:m:49:GLU:O	39:m:53:THR:HG22	2.20	0.41
1:A:167:U:H2'	1:A:168:G:H8	1.84	0.41
1:A:499:G:H3'	1:A:529:A:OP2	2.21	0.41
1:A:504:A:N3	1:A:537:U:H1'	2.35	0.41
1:A:1270:G:C2	1:A:1271:C:H1'	2.55	0.41
3:C:53:SER:O	3:C:114:GLN:HG2	2.20	0.41
3:C:142:MET:HE2	3:C:142:MET:HB2	1.80	0.41
4:D:156:ILE:HD12	4:D:159:LEU:HD23	2.03	0.41
10:J:82:LYS:C	10:J:84:VAL:N	2.78	0.41
14:N:13:ARG:NE	14:N:54:ASP:OD2	2.49	0.41
24:a:1844:U:H5	24:a:1871:G:H21	1.69	0.41
36:j:66:LYS:HE3	36:j:66:LYS:HB3	1.65	0.41
36:j:110:LYS:HE3	36:j:110:LYS:HB2	1.74	0.41
1:A:754:U:H3	24:a:702:A:H62	1.68	0.41
1:A:1156:C:H2'	1:A:1157:G:C8	2.54	0.41
1:A:1247:G:N2	1:A:1350:U:O2'	2.54	0.41
1:A:1456:U:H2'	1:A:1457:U:O4'	2.20	0.41
1:A:1472:U:H2'	1:A:1473:C:H6	1.84	0.41
4:D:116:GLN:OE1	4:D:120:HIS:HB2	2.20	0.41
13:M:13:LYS:O	13:M:45:ILE:HG12	2.19	0.41
13:M:66:GLU:C	13:M:68:ASP:H	2.29	0.41
14:N:13:ARG:HE	14:N:54:ASP:CG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:7:GLN:O	16:P:17:TYR:HD2	2.04	0.41
24:a:467:A:N3	24:a:469:G:H5''	2.35	0.41
24:a:1486:G:O6	24:a:1488:A:N6	2.53	0.41
25:b:33:G:C2	25:b:51:G:C2	3.08	0.41
29:3:20:LYS:HB3	29:3:20:LYS:HE2	1.87	0.41
33:g:106:THR:O	33:g:107:LEU:HD13	2.21	0.41
34:h:123:ARG:C	34:h:124:GLU:HG3	2.45	0.41
39:m:72:ASP:O	39:m:76:VAL:HG23	2.21	0.41
1:A:451:U:N3	1:A:470:G:O6	2.53	0.41
1:A:1233:A:H2'	1:A:1234:U:H5''	2.02	0.41
2:B:90:TYR:CE2	2:B:153:ASN:HB2	2.56	0.41
3:C:58:GLU:C	3:C:60:PRO:HD3	2.45	0.41
12:L:39:THR:HG23	12:L:42:PRO:HG2	2.02	0.41
24:a:337:A:H3'	24:a:338:A:H5''	2.02	0.41
30:c:125:LYS:HB3	30:c:125:LYS:NZ	2.36	0.41
35:i:130:HIS:CE1	35:i:132:HIS:HB2	2.55	0.41
40:n:64:THR:O	40:n:66:ASN:N	2.48	0.41
53:f:99:PHE:CD2	53:f:99:PHE:C	2.99	0.41
1:A:553:A:H4'	1:A:554:A:H3'	2.02	0.41
1:A:1324:U:OP1	13:M:26:GLY:HA3	2.21	0.41
5:E:159:ARG:NH2	8:H:101:ILE:HD11	2.35	0.41
9:I:11:ARG:HG3	9:I:12:LYS:H	1.85	0.41
12:L:10:LYS:HE3	12:L:10:LYS:HB3	1.73	0.41
14:N:86:GLU:O	14:N:89:MET:HB3	2.21	0.41
19:S:44:ILE:HG23	19:S:45:ILE:HG12	2.03	0.41
24:a:280:U:O4	24:a:340:G:N2	2.54	0.41
40:n:10:ARG:HE	40:n:90:ALA:HB1	1.86	0.41
1:A:166:C:H2'	1:A:167:U:C6	2.56	0.41
1:A:470:G:O2'	1:A:471:C:O5'	2.30	0.41
1:A:514:A:H2	1:A:523:G:N2	2.11	0.41
1:A:552:G:OP2	1:A:553:A:O2'	2.35	0.41
1:A:612:C:C2	1:A:616:A:N6	2.80	0.41
1:A:970:A:OP1	14:N:61:ARG:NH2	2.50	0.41
1:A:1040:G:H21	1:A:1210:U:H1'	1.85	0.41
1:A:1043:G:C2	1:A:1044:C:C5	3.08	0.41
1:A:1157:G:N2	1:A:1168:G:H1	2.09	0.41
1:A:1284:G:N2	1:A:1367:G:O4'	2.50	0.41
1:A:1375:U:H4'	1:A:1376:C:C5	2.56	0.41
9:I:17:ARG:NH1	9:I:65:THR:OG1	2.54	0.41
24:a:339:A:H62	24:a:340:G:H21	1.69	0.41
24:a:1391:U:H3	24:a:1580:A:H62	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:1500:A:N6	24:a:1501:G:O6	2.54	0.41
29:3:16:CYS:SG	29:3:29:CYS:HB2	2.61	0.41
32:e:145:ASP:OD1	32:e:145:ASP:C	2.63	0.41
33:g:27:LYS:HG3	33:g:32:GLU:HG3	2.02	0.41
36:j:23:LYS:HB2	36:j:23:LYS:HE3	1.93	0.41
43:q:28:GLU:H	43:q:28:GLU:CD	2.27	0.41
1:A:1125:C:O2'	1:A:1126:A:O4'	2.27	0.41
1:A:1285:U:O3'	7:G:38:THR:HG21	2.21	0.41
3:C:63:SER:OG	3:C:98:PRO:HB2	2.21	0.41
4:D:167:LYS:HD3	4:D:167:LYS:HA	1.65	0.41
5:E:84:GLN:HG3	5:E:149:MET:HE3	2.02	0.41
13:M:26:GLY:O	13:M:30:SER:HB2	2.21	0.41
16:P:16:PHE:HE2	16:P:18:GLN:HE21	1.68	0.41
19:S:39:SER:HB2	19:S:67:THR:N	2.36	0.41
1:A:159:G:N1	1:A:161:A:OP1	2.54	0.40
1:A:1125:C:C4	1:A:1126:A:C6	3.09	0.40
1:A:1263:A:H2'	1:A:1264:G:H8	1.85	0.40
3:C:38:LYS:CB	3:C:94:ILE:HD11	2.50	0.40
4:D:54:GLN:HB2	4:D:203:LEU:HD13	2.03	0.40
4:D:86:THR:HG21	4:D:201:VAL:HG11	2.03	0.40
8:H:55:VAL:HG13	8:H:56:LYS:HG3	2.03	0.40
14:N:47:LYS:HD2	14:N:47:LYS:HA	1.69	0.40
14:N:69:ARG:HA	14:N:70:PRO:HD3	1.93	0.40
19:S:40:ARG:HE	19:S:40:ARG:HB3	1.67	0.40
19:S:49:ILE:HD12	19:S:58:GLY:N	2.36	0.40
24:a:6:A:N1	24:a:2882:U:H5	2.19	0.40
24:a:1952:C:H5''	24:a:1953:A:H2'	2.03	0.40
24:a:2306:U:H5'	24:a:2307:A:OP2	2.21	0.40
49:w:58:GLU:OE2	49:w:58:GLU:O	2.38	0.40
1:A:158:G:C6	1:A:164:G:C6	3.08	0.40
1:A:1336:C:H2'	1:A:1337:G:C8	2.56	0.40
1:A:1403:C:O2'	1:A:1404:A:H5'	2.20	0.40
1:A:1407:A:O2'	1:A:1408:U:H6	2.04	0.40
5:E:43:ASP:OD1	5:E:44:GLY:N	2.55	0.40
10:J:65:TYR:HD1	14:N:98:LYS:HA	1.87	0.40
13:M:96:PRO:HB3	13:M:109:ARG:HH22	1.86	0.40
24:a:273:U:C2	24:a:274:A:C8	3.09	0.40
38:l:60:ARG:HD2	38:l:60:ARG:O	2.21	0.40
41:o:116:GLU:HG3	41:o:117:LYS:N	2.36	0.40
1:A:208:G:H2'	1:A:209:C:C6	2.56	0.40
1:A:531:G:C2'	1:A:532:G:H5'	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:G:N2	1:A:1358:U:C2	2.89	0.40
1:A:1039:A:H61	1:A:1208:C:N4	2.14	0.40
1:A:1045:U:O2'	1:A:1048:A:OP2	2.32	0.40
1:A:1301:U:C4	1:A:1327:A:C8	3.10	0.40
3:C:140:ASN:HD22	3:C:140:ASN:C	2.29	0.40
4:D:168:PRO:O	4:D:171:VAL:HG23	2.21	0.40
12:L:39:THR:OG1	12:L:51:LYS:HG2	2.22	0.40
24:a:273:U:H2'	24:a:274:A:C8	2.52	0.40
24:a:280:U:H2'	24:a:281:G:H8	1.85	0.40
24:a:297:U:H2'	24:a:298:G:O4'	2.21	0.40
24:a:835:U:H2'	24:a:836:A:C8	2.56	0.40
24:a:868:G:O2'	24:a:869:G:OP1	2.39	0.40
24:a:1502:A:N1	24:a:1503:C:N4	2.70	0.40
24:a:2587:A:C8	24:a:2588:G:N7	2.89	0.40
24:a:2730:C:H2'	24:a:2731:U:C6	2.57	0.40
24:a:2798:G:H2'	24:a:2799:C:C6	2.57	0.40
1:A:1086:A:H4'	1:A:1101:G:H22	1.85	0.40
1:A:1282:A:O2'	1:A:1283:A:O5'	2.35	0.40
4:D:73:ARG:HD3	4:D:204:TYR:HE1	1.86	0.40
4:D:139:PRO:C	4:D:140:GLU:OE2	2.64	0.40
7:G:23:LEU:HD12	7:G:23:LEU:HA	1.93	0.40
9:I:51:LEU:HD23	9:I:51:LEU:HA	1.84	0.40
13:M:77:ILE:HD13	13:M:80:LEU:HD21	2.03	0.40
13:M:97:LEU:HD23	13:M:97:LEU:H	1.85	0.40
18:R:26:LEU:HD22	18:R:68:LEU:HD21	2.02	0.40
19:S:39:SER:HB3	19:S:66:ILE:HD12	2.02	0.40
24:a:341:A:H8	24:a:341:A:O5'	2.05	0.40
24:a:700:G:H5''	24:a:701:U:H5	1.86	0.40
24:a:864:U:HO2'	24:a:865:A:H8	1.64	0.40
24:a:1096:G:H21	24:a:1097:A:N6	2.19	0.40
24:a:1476:A:H2'	24:a:1477:A:C8	2.56	0.40
24:a:1842:G:H2'	24:a:1843:A:H5''	2.03	0.40
24:a:2780:C:C2	24:a:2781:U:C5	3.09	0.40
33:g:89:LEU:HD21	33:g:105:LEU:HD21	2.04	0.40
36:j:73:ASP:OD1	36:j:75:SER:OG	2.39	0.40
42:p:22:LYS:HB2	42:p:22:LYS:HE2	1.91	0.40
47:u:98:ILE:HD12	47:u:98:ILE:C	2.47	0.40
49:w:22:CYS:SG	49:w:25:THR:OG1	2.66	0.40
1:A:1227:G:O5'	1:A:1227:G:H8	2.04	0.40
3:C:42:PHE:HE1	3:C:91:VAL:HG22	1.86	0.40
9:I:34:LEU:CD1	9:I:44:ARG:HE	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.90	0.40
24:a:2313:A:H2'	24:a:2314:U:C6	2.57	0.40
30:c:266:LYS:H	30:c:266:LYS:HG2	1.78	0.40
51:y:45:VAL:O	51:y:49:ILE:HG13	2.22	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	
2	B	212/242 (88%)	192 (91%)	20 (9%)	0	100	100
3	C	200/233 (86%)	182 (91%)	18 (9%)	0	100	100
4	D	152/206 (74%)	128 (84%)	24 (16%)	0	100	100
5	E	151/168 (90%)	144 (95%)	7 (5%)	0	100	100
6	F	101/113 (89%)	97 (96%)	4 (4%)	0	100	100
7	G	126/156 (81%)	114 (90%)	12 (10%)	0	100	100
8	H	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
9	I	122/129 (95%)	104 (85%)	18 (15%)	0	100	100
10	J	92/103 (89%)	77 (84%)	15 (16%)	0	100	100
11	K	114/128 (89%)	99 (87%)	15 (13%)	0	100	100
12	L	80/124 (64%)	76 (95%)	4 (5%)	0	100	100
13	M	110/118 (93%)	95 (86%)	15 (14%)	0	100	100
14	N	95/101 (94%)	87 (92%)	8 (8%)	0	100	100
15	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	P	77/82 (94%)	73 (95%)	4 (5%)	0	100	100
17	Q	76/85 (89%)	71 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	50/75 (67%)	48 (96%)	2 (4%)	0	100	100
19	S	77/96 (80%)	69 (90%)	8 (10%)	0	100	100
20	T	77/86 (90%)	74 (96%)	3 (4%)	0	100	100
21	U	40/71 (56%)	40 (100%)	0	0	100	100
26	0	49/51 (96%)	46 (94%)	3 (6%)	0	100	100
27	1	42/44 (96%)	42 (100%)	0	0	100	100
28	2	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
29	3	36/44 (82%)	30 (83%)	6 (17%)	0	100	100
30	c	251/274 (92%)	239 (95%)	12 (5%)	0	100	100
31	d	208/211 (99%)	196 (94%)	12 (6%)	0	100	100
32	e	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
33	g	166/177 (94%)	156 (94%)	10 (6%)	0	100	100
34	h	147/150 (98%)	131 (89%)	16 (11%)	0	100	100
35	i	139/142 (98%)	139 (100%)	0	0	100	100
36	j	119/122 (98%)	111 (93%)	8 (7%)	0	100	100
37	k	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
38	l	132/137 (96%)	126 (96%)	6 (4%)	0	100	100
39	m	118/133 (89%)	112 (95%)	6 (5%)	0	100	100
40	n	106/116 (91%)	93 (88%)	13 (12%)	0	100	100
41	o	114/119 (96%)	108 (95%)	6 (5%)	0	100	100
42	p	116/120 (97%)	113 (97%)	3 (3%)	0	100	100
43	q	101/103 (98%)	89 (88%)	12 (12%)	0	100	100
44	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
45	s	95/100 (95%)	87 (92%)	8 (8%)	0	100	100
46	t	101/104 (97%)	94 (93%)	7 (7%)	0	100	100
47	u	94/204 (46%)	92 (98%)	2 (2%)	0	100	100
48	v	76/85 (89%)	69 (91%)	7 (9%)	0	100	100
49	w	75/95 (79%)	70 (93%)	5 (7%)	0	100	100
50	x	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
51	y	55/60 (92%)	54 (98%)	1 (2%)	0	100	100
52	z	53/56 (95%)	48 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	f	176/179 (98%)	166 (94%)	10 (6%)	0	100	100
All	All	5307/5945 (89%)	4935 (93%)	372 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	B	177/200 (88%)	168 (95%)	9 (5%)	21	26
3	C	162/191 (85%)	151 (93%)	11 (7%)	14	16
4	D	124/176 (70%)	117 (94%)	7 (6%)	19	23
5	E	117/129 (91%)	110 (94%)	7 (6%)	17	21
6	F	91/98 (93%)	86 (94%)	5 (6%)	19	24
7	G	18/128 (14%)	17 (94%)	1 (6%)	19	23
8	H	104/105 (99%)	99 (95%)	5 (5%)	23	29
9	I	86/106 (81%)	82 (95%)	4 (5%)	23	30
10	J	39/91 (43%)	31 (80%)	8 (20%)	1	1
11	K	86/97 (89%)	83 (96%)	3 (4%)	32	42
12	L	71/103 (69%)	62 (87%)	9 (13%)	4	4
13	M	90/96 (94%)	83 (92%)	7 (8%)	11	12
14	N	81/84 (96%)	77 (95%)	4 (5%)	22	28
15	O	76/77 (99%)	74 (97%)	2 (3%)	40	54
16	P	65/66 (98%)	65 (100%)	0	100	100
17	Q	70/76 (92%)	68 (97%)	2 (3%)	37	49
18	R	44/64 (69%)	40 (91%)	4 (9%)	9	9
19	S	60/82 (73%)	50 (83%)	10 (17%)	2	2
20	T	62/68 (91%)	60 (97%)	2 (3%)	34	46
21	U	16/63 (25%)	14 (88%)	2 (12%)	4	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	0	45/47 (96%)	44 (98%)	1 (2%)	45	59
27	1	35/35 (100%)	35 (100%)	0	100	100
28	2	55/56 (98%)	54 (98%)	1 (2%)	51	66
29	3	33/38 (87%)	30 (91%)	3 (9%)	9	9
30	c	198/216 (92%)	195 (98%)	3 (2%)	57	72
31	d	158/159 (99%)	156 (99%)	2 (1%)	61	76
32	e	159/159 (100%)	155 (98%)	4 (2%)	42	55
33	g	135/143 (94%)	122 (90%)	13 (10%)	8	7
34	h	108/114 (95%)	100 (93%)	8 (7%)	13	14
35	i	118/119 (99%)	116 (98%)	2 (2%)	53	68
36	j	102/103 (99%)	98 (96%)	4 (4%)	28	39
37	k	107/107 (100%)	104 (97%)	3 (3%)	38	51
38	l	110/113 (97%)	107 (97%)	3 (3%)	39	52
39	m	100/110 (91%)	96 (96%)	4 (4%)	28	37
40	n	76/85 (89%)	72 (95%)	4 (5%)	20	25
41	o	95/99 (96%)	90 (95%)	5 (5%)	20	25
42	p	90/91 (99%)	88 (98%)	2 (2%)	45	59
43	q	85/85 (100%)	81 (95%)	4 (5%)	23	30
44	r	89/89 (100%)	89 (100%)	0	100	100
45	s	81/83 (98%)	78 (96%)	3 (4%)	30	40
46	t	80/88 (91%)	76 (95%)	4 (5%)	22	27
47	u	83/175 (47%)	79 (95%)	4 (5%)	23	29
48	v	62/67 (92%)	60 (97%)	2 (3%)	34	46
49	w	66/83 (80%)	66 (100%)	0	100	100
50	x	54/55 (98%)	52 (96%)	2 (4%)	30	40
51	y	50/52 (96%)	47 (94%)	3 (6%)	17	21
52	z	45/47 (96%)	43 (96%)	2 (4%)	25	33
53	f	25/150 (17%)	25 (100%)	0	100	100
All	All	4083/4868 (84%)	3895 (95%)	188 (5%)	25	31

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	15	HIS
2	B	34	THR
2	B	66	LYS
2	B	80	VAL
2	B	125	THR
2	B	164	ILE
2	B	183	VAL
2	B	199	ILE
2	B	221	ILE
3	C	19	VAL
3	C	28	ASP
3	C	33	LEU
3	C	38	LYS
3	C	43	LEU
3	C	44	THR
3	C	70	THR
3	C	97	VAL
3	C	124	LEU
3	C	175	LEU
3	C	191	THR
4	D	55	LEU
4	D	92	GLN
4	D	115	ARG
4	D	181	SER
4	D	194	ASP
4	D	200	ILE
4	D	201	VAL
5	E	13	LEU
5	E	24	SER
5	E	27	VAL
5	E	82	THR
5	E	105	THR
5	E	147	GLU
5	E	150	ASN
6	F	15	SER
6	F	68	THR
6	F	88	LEU
6	F	89	VAL
6	F	92	THR
7	G	42	ILE
8	H	7	ILE
8	H	32	LEU
8	H	77	ARG

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Mol	Chain	Res	Type
8	H	106	THR
8	H	121	VAL
9	I	54	VAL
9	I	59	LYS
9	I	67	SER
9	I	80	HIS
10	J	11	LYS
10	J	13	PHE
10	J	28	THR
10	J	44	THR
10	J	56	HIS
10	J	67	ILE
10	J	74	ILE
10	J	101	SER
11	K	64	VAL
11	K	85	ILE
11	K	110	THR
12	L	4	ILE
12	L	16	VAL
12	L	41	THR
12	L	57	LEU
12	L	58	THR
12	L	63	VAL
12	L	65	SER
12	L	72	HIS
12	L	74	LEU
13	M	39	ILE
13	M	48	LEU
13	M	60	VAL
13	M	65	VAL
13	M	77	ILE
13	M	81	MET
13	M	95	LEU
14	N	5	SER
14	N	27	LEU
14	N	64	CYS
14	N	89	MET
15	O	4	SER
15	O	76	THR
17	Q	41	THR
17	Q	42	THR
18	R	28	THR

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Mol	Chain	Res	Type
18	R	31	ASN
18	R	34	THR
18	R	47	THR
19	S	9	SER
19	S	23	VAL
19	S	28	GLU
19	S	37	THR
19	S	38	TRP
19	S	40	ARG
19	S	43	MET
19	S	55	VAL
19	S	61	HIS
19	S	71	ILE
20	T	57	ILE
20	T	77	SER
21	U	29	LEU
21	U	32	VAL
26	0	6	ARG
28	2	39	SER
29	3	7	LEU
29	3	16	CYS
29	3	29	CYS
30	c	118	SER
30	c	130	LEU
30	c	258	THR
31	d	59	SER
31	d	130	SER
32	e	7	ASP
32	e	75	SER
32	e	80	SER
32	e	141	LEU
33	g	25	THR
33	g	43	VAL
33	g	49	VAL
33	g	51	THR
33	g	59	THR
33	g	102	THR
33	g	103	LEU
33	g	105	LEU
33	g	110	SER
33	g	121	ILE
33	g	125	THR

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Mol	Chain	Res	Type
33	g	136	VAL
33	g	164	TYR
34	h	12	LEU
34	h	17	ASP
34	h	19	VAL
34	h	66	GLN
34	h	96	THR
34	h	108	VAL
34	h	135	HIS
34	h	138	VAL
35	i	5	VAL
35	i	34	LEU
36	j	47	ILE
36	j	52	VAL
36	j	75	SER
36	j	116	SER
37	k	5	THR
37	k	142	VAL
37	k	144	ASP
38	l	58	VAL
38	l	67	ARG
38	l	81	VAL
39	m	6	SER
39	m	36	THR
39	m	53	THR
39	m	65	LEU
40	n	27	VAL
40	n	51	SER
40	n	57	ILE
40	n	73	VAL
41	o	8	ILE
41	o	64	THR
41	o	70	ASN
41	o	74	VAL
41	o	80	THR
42	p	77	SER
42	p	115	GLU
43	q	1	MET
43	q	47	ILE
43	q	51	VAL
43	q	75	VAL
45	s	39	THR

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Mol	Chain	Res	Type
45	s	53	VAL
45	s	93	LEU
46	t	25	VAL
46	t	38	GLU
46	t	71	VAL
46	t	73	ILE
47	u	11	GLU
47	u	45	THR
47	u	73	SER
47	u	83	ARG
48	v	10	THR
48	v	38	VAL
50	x	4	SER
50	x	10	SER
51	y	6	VAL
51	y	45	VAL
51	y	58	VAL
52	z	3	VAL
52	z	51	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	42	ASN
2	B	63	ASN
2	B	153	ASN
5	E	72	ASN
5	E	81	ASN
5	E	124	ASN
5	E	153	GLN
6	F	17	GLN
10	J	70	HIS
13	M	8	ASN
13	M	105	ASN
16	P	63	GLN
19	S	3	ASN
19	S	56	HIS
27	l	16	HIS
30	c	58	HIS
31	d	33	ASN
32	e	115	GLN
33	g	128	GLN

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Mol	Chain	Res	Type
34	h	33	GLN
34	h	135	HIS
37	k	38	GLN
38	l	46	GLN
40	n	21	GLN
41	o	6	GLN
41	o	56	ASN
44	r	23	GLN
46	t	47	GLN
49	w	40	ASN
49	w	53	HIS
51	y	51	GLN
53	f	27	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1422/1528 (93%)	435 (30%)	15 (1%)
22	W	17/18 (94%)	8 (47%)	0
23	X	3/4 (75%)	0	0
24	a	2703/2889 (93%)	515 (19%)	0
25	b	115/117 (98%)	25 (21%)	0
All	All	4260/4556 (93%)	983 (23%)	15 (0%)

All (983) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	14	U
1	A	25	C
1	A	26	A
1	A	31	G
1	A	32	A
1	A	33	A
1	A	35	G
1	A	37	U
1	A	39	G
1	A	42	G
1	A	43	C
1	A	44	A
1	A	47	C

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Mol	Chain	Res	Type
1	A	48	C
1	A	51	A
1	A	56	U
1	A	60	A
1	A	62	U
1	A	65	A
1	A	68	G
1	A	100	G
1	A	103	C
1	A	110	C
1	A	112	G
1	A	121	U
1	A	131	C
1	A	139	G
1	A	149	A
1	A	154	A
1	A	156	U
1	A	160	A
1	A	161	A
1	A	162	A
1	A	169	C
1	A	170	U
1	A	174	A
1	A	175	C
1	A	177	G
1	A	181	A
1	A	188	A
1	A	190	G
1	A	197	A
1	A	203	C
1	A	206	C
1	A	207	G
1	A	208	G
1	A	210	U
1	A	239	U
1	A	241	G
1	A	245	G
1	A	252	A
1	A	257	A
1	A	260	G
1	A	261	C
1	A	266	C

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Mol	Chain	Res	Type
1	A	278	C
1	A	283	G
1	A	294	A
1	A	301	U
1	A	315	A
1	A	321	A
1	A	322	C
1	A	323	A
1	A	324	C
1	A	325	G
1	A	333	C
1	A	337	U
1	A	339	C
1	A	341	G
1	A	346	C
1	A	348	G
1	A	352	U
1	A	353	G
1	A	358	A
1	A	359	U
1	A	361	U
1	A	366	C
1	A	367	A
1	A	376	A
1	A	378	G
1	A	379	C
1	A	391	A
1	A	392	U
1	A	400	G
1	A	401	U
1	A	402	G
1	A	404	G
1	A	405	A
1	A	406	A
1	A	407	G
1	A	408	A
1	A	409	A
1	A	412	C
1	A	413	C
1	A	414	U
1	A	415	U
1	A	416	C

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Mol	Chain	Res	Type
1	A	418	G
1	A	421	U
1	A	423	U
1	A	424	A
1	A	425	A
1	A	427	G
1	A	428	C
1	A	429	A
1	A	430	C
1	A	431	U
1	A	443	G
1	A	447	A
1	A	448	G
1	A	451	U
1	A	452	A
1	A	454	C
1	A	455	A
1	A	457	U
1	A	458	U
1	A	460	A
1	A	461	U
1	A	462	A
1	A	463	C
1	A	465	U
1	A	470	G
1	A	471	C
1	A	472	U
1	A	473	G
1	A	474	U
1	A	478	G
1	A	480	U
1	A	481	A
1	A	482	C
1	A	486	C
1	A	488	G
1	A	490	A
1	A	492	A
1	A	499	G
1	A	500	G
1	A	501	C
1	A	504	A
1	A	505	C

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Mol	Chain	Res	Type
1	A	506	U
1	A	507	C
1	A	508	C
1	A	509	G
1	A	510	U
1	A	511	G
1	A	512	C
1	A	513	C
1	A	514	A
1	A	515	G
1	A	517	A
1	A	519	C
1	A	522	C
1	A	524	G
1	A	525	U
1	A	526	A
1	A	527	A
1	A	529	A
1	A	530	C
1	A	531	G
1	A	533	A
1	A	534	G
1	A	535	G
1	A	541	A
1	A	558	C
1	A	566	A
1	A	567	A
1	A	568	A
1	A	569	G
1	A	570	C
1	A	571	G
1	A	576	C
1	A	578	G
1	A	606	C
1	A	612	C
1	A	615	A
1	A	622	G
1	A	623	A
1	A	624	A
1	A	625	C
1	A	626	U
1	A	647	A

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Mol	Chain	Res	Type
1	A	659	A
1	A	669	A
1	A	674	C
1	A	676	G
1	A	689	A
1	A	690	A
1	A	712	A
1	A	717	U
1	A	718	G
1	A	723	A
1	A	747	A
1	A	749	G
1	A	755	G
1	A	758	C
1	A	771	A
1	A	772	G
1	A	774	A
1	A	775	A
1	A	776	A
1	A	788	A
1	A	790	C
1	A	803	G
1	A	809	A
1	A	811	C
1	A	812	G
1	A	834	C
1	A	838	G
1	A	839	G
1	A	851	A
1	A	852	A
1	A	856	U
1	A	857	A
1	A	865	A
1	A	878	G
1	A	882	A
1	A	883	G
1	A	884	U
1	A	893	A
1	A	895	G
1	A	896	G
1	A	899	A
1	A	904	U

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Mol	Chain	Res	Type
1	A	907	A
1	A	908	A
1	A	919	G
1	A	928	A
1	A	931	A
1	A	934	G
1	A	953	U
1	A	962	A
1	A	964	G
1	A	968	A
1	A	969	G
1	A	970	A
1	A	975	U
1	A	982	A
1	A	1039	A
1	A	1043	G
1	A	1046	G
1	A	1047	C
1	A	1048	A
1	A	1051	G
1	A	1057	G
1	A	1058	U
1	A	1059	C
1	A	1060	A
1	A	1070	G
1	A	1072	G
1	A	1078	U
1	A	1079	U
1	A	1080	G
1	A	1081	G
1	A	1083	U
1	A	1084	U
1	A	1085	A
1	A	1087	G
1	A	1088	U
1	A	1089	C
1	A	1090	C
1	A	1091	C
1	A	1093	C
1	A	1094	A
1	A	1095	A
1	A	1097	G

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Mol	Chain	Res	Type
1	A	1101	G
1	A	1105	C
1	A	1107	C
1	A	1113	C
1	A	1115	U
1	A	1116	A
1	A	1117	G
1	A	1118	U
1	A	1119	U
1	A	1120	G
1	A	1121	C
1	A	1122	U
1	A	1124	G
1	A	1126	A
1	A	1127	G
1	A	1128	G
1	A	1129	U
1	A	1130	A
1	A	1133	G
1	A	1134	C
1	A	1135	U
1	A	1136	G
1	A	1139	A
1	A	1140	A
1	A	1141	C
1	A	1146	A
1	A	1147	G
1	A	1148	G
1	A	1151	A
1	A	1153	U
1	A	1154	G
1	A	1155	C
1	A	1156	C
1	A	1157	G
1	A	1161	A
1	A	1162	U
1	A	1163	A
1	A	1164	A
1	A	1166	C
1	A	1174	A
1	A	1175	G
1	A	1176	G

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Mol	Chain	Res	Type
1	A	1178	G
1	A	1179	G
1	A	1182	A
1	A	1186	C
1	A	1187	G
1	A	1188	U
1	A	1189	C
1	A	1191	A
1	A	1192	G
1	A	1196	U
1	A	1197	C
1	A	1198	A
1	A	1203	C
1	A	1205	U
1	A	1207	A
1	A	1208	C
1	A	1209	G
1	A	1210	U
1	A	1211	G
1	A	1220	C
1	A	1221	A
1	A	1222	C
1	A	1225	G
1	A	1229	U
1	A	1231	C
1	A	1233	A
1	A	1235	G
1	A	1237	C
1	A	1239	C
1	A	1242	A
1	A	1243	C
1	A	1245	G
1	A	1246	A
1	A	1250	C
1	A	1251	U
1	A	1252	G
1	A	1254	G
1	A	1255	A
1	A	1257	C
1	A	1258	U
1	A	1260	G
1	A	1261	C

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Mol	Chain	Res	Type
1	A	1263	A
1	A	1268	A
1	A	1269	A
1	A	1273	A
1	A	1274	A
1	A	1275	U
1	A	1276	C
1	A	1277	A
1	A	1280	U
1	A	1281	A
1	A	1282	A
1	A	1283	A
1	A	1288	G
1	A	1290	C
1	A	1292	U
1	A	1295	U
1	A	1297	C
1	A	1307	U
1	A	1310	G
1	A	1311	C
1	A	1312	A
1	A	1314	C
1	A	1315	U
1	A	1317	G
1	A	1322	C
1	A	1323	A
1	A	1325	G
1	A	1332	G
1	A	1341	G
1	A	1343	A
1	A	1345	U
1	A	1350	U
1	A	1354	A
1	A	1358	U
1	A	1359	G
1	A	1365	G
1	A	1368	A
1	A	1373	G
1	A	1374	U
1	A	1376	C
1	A	1379	G
1	A	1381	G

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Mol	Chain	Res	Type
1	A	1383	C
1	A	1386	G
1	A	1388	A
1	A	1392	A
1	A	1393	C
1	A	1395	G
1	A	1396	4OC
1	A	1404	A
1	A	1412	A
1	A	1413	G
1	A	1414	U
1	A	1416	G
1	A	1417	G
1	A	1418	U
1	A	1419	U
1	A	1420	G
1	A	1421	C
1	A	1423	C
1	A	1431	A
1	A	1432	G
1	A	1433	A
1	A	1435	A
1	A	1436	G
1	A	1438	C
1	A	1439	U
1	A	1455	G
1	A	1458	U
1	A	1459	A
1	A	1460	C
1	A	1461	C
1	A	1462	A
1	A	1474	A
1	A	1475	U
1	A	1486	A
1	A	1489	U
1	A	1493	A
1	A	1496	A
1	A	1500	U
1	A	1511	G
1	A	1513	MA6
1	A	1514	C
1	A	1523	G

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Mol	Chain	Res	Type
1	A	1524	G
22	W	27	U
22	W	28	A
22	W	29	G
22	W	30	G
22	W	31	G
22	W	36	U
22	W	37	A
22	W	43	A
24	a	10	A
24	a	34	U
24	a	35	G
24	a	63	A
24	a	67	U
24	a	71	A
24	a	74	A
24	a	75	G
24	a	87	U
24	a	88	A
24	a	96	G
24	a	101	U
24	a	102	G
24	a	106	C
24	a	113	U
24	a	118	A
24	a	119	A
24	a	120	U
24	a	131	A
24	a	134	U
24	a	135	G
24	a	136	C
24	a	138	U
24	a	139	G
24	a	140	C
24	a	145	A
24	a	152	A
24	a	156	A
24	a	159	A
24	a	166	U
24	a	186	A
24	a	192	A
24	a	211	G

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Mol	Chain	Res	Type
24	a	212	A
24	a	217	A
24	a	218	A
24	a	229	A
24	a	238	G
24	a	244	G
24	a	251	A
24	a	252	A
24	a	267	U
24	a	269	A
24	a	270	G
24	a	273	U
24	a	294	U
24	a	302	A
24	a	321	A
24	a	336	A
24	a	337	A
24	a	338	A
24	a	339	A
24	a	340	G
24	a	341	A
24	a	353	A
24	a	355	A
24	a	356	U
24	a	359	A
24	a	374	G
24	a	375	U
24	a	376	G
24	a	378	A
24	a	384	G
24	a	389	A
24	a	394	A
24	a	404	U
24	a	413	G
24	a	414	C
24	a	423	C
24	a	444	C
24	a	445	A
24	a	460	A
24	a	468	A
24	a	469	G
24	a	479	G

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Mol	Chain	Res	Type
24	a	493	A
24	a	497	C
24	a	511	C
24	a	518	G
24	a	519	C
24	a	520	A
24	a	526	A
24	a	535	G
24	a	536	U
24	a	549	U
24	a	550	A
24	a	560	U
24	a	562	A
24	a	573	A
24	a	582	U
24	a	590	A
24	a	600	A
24	a	607	U
24	a	614	A
24	a	624	A
24	a	626	U
24	a	632	C
24	a	633	U
24	a	634	G
24	a	635	G
24	a	641	U
24	a	642	A
24	a	673	U
24	a	699	A
24	a	700	G
24	a	703	A
24	a	704	C
24	a	706	U
24	a	717	A
24	a	734	U
24	a	743	A
24	a	744	G
24	a	745	G
24	a	762	G
24	a	763	G
24	a	769	A
24	a	771	G

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Mol	Chain	Res	Type
24	a	772	G
24	a	777	U
24	a	778	C
24	a	779	A
24	a	785	G
24	a	792	G
24	a	799	C
24	a	814	U
24	a	818	G
24	a	832	G
24	a	834	A
24	a	846	G
24	a	853	A
24	a	857	U
24	a	863	C
24	a	864	U
24	a	865	A
24	a	867	G
24	a	868	G
24	a	869	G
24	a	873	A
24	a	878	G
24	a	880	C
24	a	882	U
24	a	885	C
24	a	887	A
24	a	889	C
24	a	891	U
24	a	894	G
24	a	897	A
24	a	919	U
24	a	931	A
24	a	932	C
24	a	947	C
24	a	960	G
24	a	969	A
24	a	970	A
24	a	971	C
24	a	972	C
24	a	982	A
24	a	991	C
24	a	995	A

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Mol	Chain	Res	Type
24	a	997	G
24	a	998	U
24	a	999	C
24	a	1008	G
24	a	1012	G
24	a	1013	A
24	a	1020	G
24	a	1027	G
24	a	1028	G
24	a	1029	C
24	a	1030	C
24	a	1031	C
24	a	1032	A
24	a	1033	G
24	a	1034	A
24	a	1038	C
24	a	1096	G
24	a	1097	A
24	a	1098	G
24	a	1101	G
24	a	1102	G
24	a	1106	G
24	a	1116	U
24	a	1118	U
24	a	1119	A
24	a	1121	C
24	a	1128	A
24	a	1134	U
24	a	1169	G
24	a	1188	G
24	a	1225	C
24	a	1231	U
24	a	1235	A
24	a	1238	G
24	a	1250	A
24	a	1253	G
24	a	1254	A
24	a	1271	C
24	a	1282	G
24	a	1283	A
24	a	1299	A
24	a	1303	C

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Mol	Chain	Res	Type
24	a	1322	U
24	a	1327	C
24	a	1328	G
24	a	1334	U
24	a	1347	A
24	a	1361	U
24	a	1364	G
24	a	1365	A
24	a	1366	A
24	a	1369	A
24	a	1376	U
24	a	1377	A
24	a	1378	U
24	a	1389	G
24	a	1394	A
24	a	1395	A
24	a	1398	G
24	a	1399	C
24	a	1400	G
24	a	1401	A
24	a	1410	C
24	a	1411	G
24	a	1419	C
24	a	1424	C
24	a	1429	A
24	a	1434	G
24	a	1435	U
24	a	1440	A
24	a	1444	C
24	a	1449	G
24	a	1452	A
24	a	1454	U
24	a	1457	G
24	a	1459	A
24	a	1464	G
24	a	1465	U
24	a	1466	U
24	a	1467	U
24	a	1470	U
24	a	1471	U
24	a	1472	A
24	a	1473	G

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Mol	Chain	Res	Type
24	a	1474	G
24	a	1475	U
24	a	1476	A
24	a	1485	C
24	a	1494	A
24	a	1495	A
24	a	1496	C
24	a	1503	C
24	a	1536	G
24	a	1537	C
24	a	1539	G
24	a	1541	U
24	a	1544	C
24	a	1546	U
24	a	1553	A
24	a	1556	A
24	a	1561	C
24	a	1566	A
24	a	1568	G
24	a	1569	C
24	a	1570	U
24	a	1571	U
24	a	1572	C
24	a	1573	A
24	a	1576	U
24	a	1578	A
24	a	1579	U
24	a	1580	A
24	a	1584	A
24	a	1595	A
24	a	1601	A
24	a	1604	C
24	a	1634	U
24	a	1635	U
24	a	1636	G
24	a	1661	G
24	a	1677	A
24	a	1679	U
24	a	1680	U
24	a	1700	A
24	a	1701	U
24	a	1703	U

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Mol	Chain	Res	Type
24	a	1704	G
24	a	1705	U
24	a	1706	G
24	a	1707	A
24	a	1709	G
24	a	1710	A
24	a	1711	G
24	a	1713	C
24	a	1714	U
24	a	1715	U
24	a	1716	G
24	a	1717	C
24	a	1718	U
24	a	1720	U
24	a	1721	C
24	a	1728	G
24	a	1731	G
24	a	1741	G
24	a	1742	U
24	a	1743	G
24	a	1747	A
24	a	1748	G
24	a	1749	G
24	a	1758	A
24	a	1767	U
24	a	1776	A
24	a	1785	C
24	a	1786	A
24	a	1787	A
24	a	1794	A
24	a	1801	C
24	a	1806	A
24	a	1807	C
24	a	1814	A
24	a	1815	C
24	a	1832	A
24	a	1833	A
24	a	1834	G
24	a	1835	G
24	a	1836	U
24	a	1837	U
24	a	1839	A

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Mol	Chain	Res	Type
24	a	1840	U
24	a	1845	G
24	a	1854	C
24	a	1857	A
24	a	1858	G
24	a	1860	G
24	a	1861	A
24	a	1863	A
24	a	1864	A
24	a	1865	G
24	a	1866	C
24	a	1872	A
24	a	1873	U
24	a	1875	G
24	a	1876	A
24	a	1893	G
24	a	1897	G
24	a	1898	U
24	a	1900	A
24	a	1901	C
24	a	1902	U
24	a	1903	A
24	a	1904	U
24	a	1905	A
24	a	1906	A
24	a	1907	C
24	a	1909	G
24	a	1911	C
24	a	1914	A
24	a	1917	G
24	a	1925	A
24	a	1928	C
24	a	1934	C
24	a	1942	U
24	a	1954	C
24	a	1957	A
24	a	1958	U
24	a	1959	G
24	a	1969	U
24	a	1978	U
24	a	1980	U
24	a	2010	C

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Mol	Chain	Res	Type
24	a	2018	A
24	a	2020	A
24	a	2023	C
24	a	2026	U
24	a	2030	C
24	a	2042	C
24	a	2043	G
24	a	2046	A
24	a	2047	A
24	a	2048	G
24	a	2049	A
24	a	2050	C
24	a	2051	C
24	a	2056	G7M
24	a	2074	G
24	a	2179	U
24	a	2180	C
24	a	2182	A
24	a	2188	G
24	a	2195	G
24	a	2196	A
24	a	2197	A
24	a	2198	U
24	a	2199	C
24	a	2210	A
24	a	2223	G
24	a	2224	G
24	a	2253	A
24	a	2268	C
24	a	2269	A
24	a	2272	A
24	a	2273	A
24	a	2289	G
24	a	2290	U
24	a	2291	C
24	a	2293	G
24	a	2295	C
24	a	2296	A
24	a	2298	C
24	a	2300	U
24	a	2304	G
24	a	2307	A

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Mol	Chain	Res	Type
24	a	2310	G
24	a	2312	A
24	a	2326	G
24	a	2330	A
24	a	2332	C
24	a	2335	C
24	a	2341	A
24	a	2348	U
24	a	2351	A
24	a	2362	A
24	a	2364	G
24	a	2368	G
24	a	2370	C
24	a	2376	G
24	a	2387	U
24	a	2388	C
24	a	2391	A
24	a	2410	A
24	a	2413	G
24	a	2414	G
24	a	2415	A
24	a	2418	A
24	a	2419	A
24	a	2420	A
24	a	2426	U
24	a	2433	A
24	a	2447	C
24	a	2458	U
24	a	2461	A
24	a	2462	U
24	a	2476	U
24	a	2487	G
24	a	2490	G
24	a	2503	A
24	a	2505	C
24	a	2514	G
24	a	2515	A
24	a	2516	A
24	a	2517	G
24	a	2532	A
24	a	2537	OMU
24	a	2543	C

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Mol	Chain	Res	Type
24	a	2550	A
24	a	2551	A
24	a	2558	C
24	a	2562	A
24	a	2570	U
24	a	2587	A
24	a	2588	G
24	a	2589	U
24	a	2594	U
24	a	2598	U
24	a	2600	U
24	a	2614	U
24	a	2624	A
24	a	2641	U
24	a	2644	G
24	a	2645	A
24	a	2646	G
24	a	2647	A
24	a	2648	G
24	a	2649	G
24	a	2658	G
24	a	2667	G
24	a	2674	U
24	a	2675	U
24	a	2687	G
24	a	2690	A
24	a	2697	U
24	a	2699	G
24	a	2711	C
24	a	2718	A
24	a	2726	A
24	a	2729	G
24	a	2731	U
24	a	2733	A
24	a	2742	A
24	a	2743	A
24	a	2749	A
24	a	2750	A
24	a	2751	G
24	a	2763	A
24	a	2781	U
24	a	2782	A

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Mol	Chain	Res	Type
24	a	2783	U
24	a	2784	A
24	a	2786	G
24	a	2788	U
24	a	2805	G
24	a	2806	A
24	a	2811	A
24	a	2814	A
24	a	2828	G
24	a	2835	A
24	a	2836	A
24	a	2846	G
24	a	2858	A
24	a	2859	C
24	a	2865	C
24	a	2868	A
24	a	2869	U
24	a	2876	U
24	a	2884	A
24	a	2885	A
25	b	3	C
25	b	11	C
25	b	13	A
25	b	15	A
25	b	16	G
25	b	17	C
25	b	19	U
25	b	32	U
25	b	37	C
25	b	48	U
25	b	52	U
25	b	54	G
25	b	55	U
25	b	56	G
25	b	57	A
25	b	63	A
25	b	68	C
25	b	73	A
25	b	88	U
25	b	90	G
25	b	95	G
25	b	98	A

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Mol	Chain	Res	Type
25	b	99	A
25	b	108	A
25	b	109	U

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	43	C
1	A	338	A
1	A	400	G
1	A	489	A
1	A	499	G
1	A	567	A
1	A	688	A
1	A	1057	G
1	A	1092	G
1	A	1147	G
1	A	1175	G
1	A	1413	G
1	A	1416	G
1	A	1418	U
1	A	1488	G

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

15 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	$\# Z > 2$
1	4OC	A	1396	1	20,23,24	2.95	8 (40%)	26,32,35	1.31	4 (15%)
24	OMC	a	2483	24,54	19,22,23	2.88	8 (42%)	26,31,34	0.86	1 (3%)
1	2MG	A	1510	1	23,26,27	2.72	9 (39%)	32,38,41	3.13	11 (34%)
24	2MG	a	1820	24	23,26,27	2.70	9 (39%)	32,38,41	3.14	13 (40%)
24	OMG	a	2236	24	23,26,27	2.33	8 (34%)	33,38,41	2.44	11 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	G7M	a	2056	24	23,26,27	2.57	8 (34%)	35,39,42	1.88	8 (22%)
24	H2U	a	2434	24	18,21,22	2.95	5 (27%)	21,30,33	2.27	5 (23%)
1	UR3	A	1492	1	19,22,23	2.92	7 (36%)	26,32,35	1.33	3 (11%)
1	2MG	A	959	1	23,26,27	2.78	9 (39%)	32,38,41	3.56	10 (31%)
1	MA6	A	1513	1	23,26,27	1.41	4 (17%)	34,38,41	4.45	14 (41%)
24	5MU	a	1926	24	19,22,23	7.61	8 (42%)	28,32,35	3.41	10 (35%)
24	2MA	a	2488	24,54	22,25,26	3.72	8 (36%)	33,37,40	2.40	10 (30%)
24	OMU	a	2537	24	19,22,23	3.20	8 (42%)	26,31,34	1.72	5 (19%)
1	5MC	A	960	1	18,22,23	3.71	7 (38%)	26,32,35	0.98	1 (3%)
24	2MG	a	2430	24	23,26,27	2.59	9 (39%)	32,38,41	3.00	14 (43%)

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
1	4OC	A	1396	1	-	4/9/29/30	0/2/2/2
24	OMC	a	2483	24,54	-	0/9/27/28	0/2/2/2
1	2MG	A	1510	1	-	1/9/27/28	0/3/3/3
24	2MG	a	1820	24	-	0/9/27/28	0/3/3/3
24	OMG	a	2236	24	-	0/9/27/28	0/3/3/3
24	G7M	a	2056	24	-	1/7/25/26	0/3/3/3
24	H2U	a	2434	24	-	0/7/38/39	0/2/2/2
1	UR3	A	1492	1	-	0/7/25/26	0/2/2/2
1	2MG	A	959	1	-	2/9/27/28	0/3/3/3
1	MA6	A	1513	1	-	6/11/29/30	0/3/3/3
24	5MU	a	1926	24	-	0/7/25/26	0/2/2/2
24	2MA	a	2488	24,54	-	1/7/25/26	0/3/3/3
24	OMU	a	2537	24	-	2/9/27/28	0/2/2/2
1	5MC	A	960	1	-	0/7/25/26	0/2/2/2
24	2MG	a	2430	24	-	1/9/27/28	0/3/3/3

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	1926	5MU	C4-C5	22.16	1.81	1.44
24	a	1926	5MU	C6-N1	16.30	1.65	1.38
24	a	1926	5MU	C6-C5	-12.61	1.13	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	2488	2MA	C4-N3	11.48	1.48	1.34
24	a	1926	5MU	C4-N3	-11.25	1.18	1.38
1	A	960	5MC	C6-C5	9.17	1.49	1.34
24	a	2434	H2U	C2-N1	8.78	1.48	1.35
24	a	2537	OMU	C2-N1	7.53	1.50	1.38
24	a	2537	OMU	C2-N3	7.48	1.51	1.38
1	A	1492	UR3	C2-N1	7.43	1.49	1.38
1	A	959	2MG	C2-N3	7.34	1.46	1.31
24	a	2488	2MA	C2-N3	7.13	1.46	1.34
24	a	1820	2MG	C2-N3	6.94	1.45	1.31
1	A	1510	2MG	C2-N3	6.87	1.45	1.31
1	A	960	5MC	C4-N4	6.71	1.51	1.34
1	A	1492	UR3	C6-C5	6.68	1.50	1.35
24	a	2483	OMC	C2-N3	6.67	1.49	1.36
1	A	960	5MC	C2-N3	6.66	1.49	1.36
24	a	2434	H2U	C2-N3	6.40	1.49	1.38
24	a	2483	OMC	C6-C5	6.25	1.49	1.35
24	a	2430	2MG	C2-N3	6.12	1.43	1.31
1	A	1396	4OC	C4-N3	6.06	1.43	1.32
24	a	2537	OMU	C6-C5	6.04	1.49	1.35
1	A	959	2MG	C4-N3	5.97	1.48	1.34
1	A	1510	2MG	C4-N3	5.95	1.48	1.34
24	a	1820	2MG	C4-N3	5.92	1.48	1.34
1	A	1396	4OC	C6-C5	5.92	1.48	1.35
24	a	2056	G7M	C4-N3	5.91	1.48	1.34
24	a	2236	OMG	C4-N3	5.89	1.48	1.34
24	a	2056	G7M	C5-N7	-5.88	1.32	1.39
1	A	960	5MC	C4-N3	5.88	1.44	1.34
1	A	1396	4OC	C2-N3	5.63	1.47	1.36
24	a	2430	2MG	C4-N3	5.49	1.47	1.34
1	A	1492	UR3	C2-N3	5.38	1.49	1.39
1	A	959	2MG	C2-N2	5.21	1.45	1.33
1	A	1510	2MG	C2-N2	5.03	1.44	1.33
24	a	1820	2MG	C2-N2	4.97	1.44	1.33
24	a	2056	G7M	C2-N3	4.95	1.45	1.33
24	a	2488	2MA	C6-N1	4.91	1.42	1.35
24	a	2488	2MA	C2-N1	4.88	1.42	1.34
24	a	2236	OMG	C2-N3	4.84	1.44	1.33
24	a	2488	2MA	C6-N6	-4.76	1.22	1.34
1	A	959	2MG	C2-N1	4.71	1.44	1.36
24	a	2430	2MG	C2-N2	4.66	1.43	1.33
1	A	1510	2MG	C2-N1	4.53	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	2434	H2U	C4-N3	4.47	1.45	1.37
1	A	960	5MC	C6-N1	4.47	1.45	1.38
24	a	2483	OMC	C4-N3	4.47	1.43	1.34
24	a	1820	2MG	C2-N1	4.47	1.43	1.36
24	a	2236	OMG	C2-N2	4.34	1.44	1.34
24	a	2488	2MA	C5-C6	4.33	1.53	1.41
24	a	2056	G7M	C2-N2	4.30	1.44	1.34
1	A	1396	4OC	C4-N4	4.25	1.44	1.35
1	A	1396	4OC	C2-N1	4.23	1.49	1.40
24	a	1926	5MU	O2-C2	-4.21	1.15	1.23
24	a	2430	2MG	C2-N1	4.03	1.43	1.36
24	a	1926	5MU	C2-N3	4.03	1.45	1.38
24	a	2537	OMU	C4-N3	4.01	1.45	1.38
24	a	2483	OMC	C2-N1	3.99	1.48	1.40
1	A	1396	4OC	C5-C4	3.79	1.48	1.40
24	a	1926	5MU	C2-N1	3.60	1.44	1.38
1	A	1510	2MG	C5-N7	-3.52	1.32	1.39
1	A	1492	UR3	O4-C4	-3.44	1.16	1.23
1	A	959	2MG	C5-N7	-3.43	1.32	1.39
24	a	2056	G7M	C5-C6	3.43	1.52	1.43
24	a	2236	OMG	C5-N7	-3.41	1.32	1.39
24	a	2483	OMC	C4-N4	3.38	1.41	1.33
24	a	2488	2MA	C5-N7	-3.37	1.32	1.39
24	a	2430	2MG	C5-N7	-3.27	1.32	1.39
24	a	2483	OMC	O2-C2	-3.25	1.17	1.23
24	a	2430	2MG	O6-C6	-3.24	1.17	1.23
24	a	1820	2MG	C5-N7	-3.21	1.32	1.39
1	A	960	5MC	C2-N1	3.20	1.46	1.40
1	A	1513	MA6	C5-C4	-3.20	1.33	1.39
1	A	1513	MA6	C5-N7	-3.15	1.33	1.39
24	a	2056	G7M	O6-C6	-3.13	1.17	1.23
1	A	1396	4OC	O2-C2	-3.11	1.18	1.23
24	a	2430	2MG	C4-N9	-3.08	1.30	1.38
24	a	2434	H2U	O2-C2	-3.08	1.17	1.23
24	a	2483	OMC	C6-N1	3.07	1.45	1.38
24	a	2236	OMG	O6-C6	-3.06	1.17	1.23
24	a	2537	OMU	O4-C4	-2.95	1.18	1.24
24	a	1820	2MG	O6-C6	-2.88	1.18	1.23
24	a	2488	2MA	CM2-C2	2.79	1.57	1.49
24	a	2537	OMU	C6-N1	2.78	1.44	1.38
1	A	1510	2MG	O6-C6	-2.71	1.18	1.23
1	A	1396	4OC	C6-N1	2.66	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	959	2MG	O6-C6	-2.56	1.18	1.23
1	A	1492	UR3	O2-C2	-2.53	1.17	1.22
24	a	2537	OMU	C5-C4	2.52	1.49	1.43
24	a	1926	5MU	O4-C4	-2.52	1.18	1.23
24	a	2236	OMG	C4-N9	-2.50	1.31	1.38
24	a	2430	2MG	C5-C6	2.45	1.53	1.44
1	A	1510	2MG	C4-N9	-2.45	1.31	1.38
1	A	960	5MC	O2-C2	-2.42	1.19	1.23
24	a	2236	OMG	C2-N1	2.42	1.43	1.37
24	a	1820	2MG	C5-C6	2.42	1.53	1.44
24	a	1820	2MG	C4-N9	-2.36	1.31	1.38
1	A	1492	UR3	C6-N1	2.30	1.43	1.38
1	A	1513	MA6	C6-N6	2.28	1.43	1.36
1	A	959	2MG	C4-N9	-2.28	1.32	1.38
1	A	1492	UR3	C5-C4	2.28	1.49	1.43
1	A	1513	MA6	C8-N9	-2.27	1.33	1.37
1	A	959	2MG	C6-N1	2.27	1.43	1.38
24	a	2236	OMG	C5-C6	2.26	1.52	1.44
1	A	1510	2MG	C6-N1	2.22	1.43	1.38
1	A	1510	2MG	C5-C6	2.21	1.52	1.44
24	a	1820	2MG	C6-N1	2.20	1.42	1.38
24	a	2434	H2U	O4-C4	-2.19	1.18	1.23
24	a	2056	G7M	C4-N9	-2.18	1.32	1.38
1	A	959	2MG	C5-C6	2.15	1.52	1.44
24	a	2056	G7M	C2-N1	2.11	1.42	1.37
24	a	2483	OMC	C5-C4	2.10	1.47	1.42
24	a	2537	OMU	O2-C2	-2.08	1.19	1.23
24	a	2430	2MG	C6-N1	2.05	1.42	1.38

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1513	MA6	N1-C6-N6	-15.95	99.64	117.08
1	A	959	2MG	C1'-N9-C8	-12.07	92.35	126.70
1	A	959	2MG	C1'-N9-C4	10.97	159.08	126.50
1	A	1513	MA6	C1'-N9-C8	-10.20	104.11	127.14
24	a	1926	5MU	C5-C4-N3	10.08	123.92	115.31
1	A	1510	2MG	C1'-N9-C8	-9.53	99.57	126.70
24	a	1820	2MG	C1'-N9-C8	-9.45	99.79	126.70
1	A	1513	MA6	C4-N9-C1'	9.31	148.77	126.59
1	A	1510	2MG	C1'-N9-C4	8.85	152.80	126.50
24	a	1926	5MU	C5-C6-N1	-8.61	114.48	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	1820	2MG	C1'-N9-C4	8.61	152.07	126.50
1	A	1513	MA6	C5-C6-N6	8.56	140.21	125.30
24	a	2430	2MG	C1'-N9-C8	-8.33	102.97	126.70
24	a	2488	2MA	C5-C4-N3	-7.88	118.32	127.19
24	a	2434	H2U	C4-N3-C2	-7.80	119.32	125.79
24	a	2430	2MG	C1'-N9-C4	7.51	148.81	126.50
24	a	1926	5MU	C4-N3-C2	-7.16	118.08	127.35
24	a	2430	2MG	C2-N3-C4	6.86	120.54	112.04
24	a	2236	OMG	C1'-N9-C8	-6.83	107.24	126.70
24	a	1820	2MG	C2-N3-C4	6.49	120.08	112.04
1	A	1510	2MG	C2-N3-C4	6.37	119.94	112.04
1	A	959	2MG	C2-N3-C4	6.20	119.72	112.04
24	a	2236	OMG	C1'-N9-C4	6.04	144.43	126.50
1	A	1513	MA6	N1-C2-N3	-5.76	119.59	128.60
24	a	2488	2MA	N3-C4-N9	5.39	134.47	126.99
24	a	2537	OMU	C4-N3-C2	-5.22	119.69	126.58
1	A	1513	MA6	C5-C4-N3	-5.16	120.02	126.75
1	A	959	2MG	C5-C4-N3	-5.15	120.10	128.46
1	A	1492	UR3	C4-N3-C2	-4.86	119.99	124.56
24	a	1926	5MU	N3-C2-N1	4.82	121.30	114.89
24	a	2236	OMG	C5-C4-N3	-4.75	120.76	128.46
1	A	1510	2MG	C5-C4-N3	-4.74	120.77	128.46
24	a	1820	2MG	C5-C4-N3	-4.74	120.77	128.46
24	a	1820	2MG	C2-N1-C6	-4.71	119.05	124.48
24	a	2056	G7M	C2-N3-C4	4.65	120.59	112.30
24	a	2430	2MG	C2-N1-C6	-4.64	119.14	124.48
24	a	1926	5MU	C5M-C5-C6	-4.56	116.76	122.85
1	A	1510	2MG	C2-N1-C6	-4.48	119.33	124.48
1	A	959	2MG	C2-N1-C6	-4.38	119.43	124.48
24	a	2488	2MA	N9-C8-N7	-4.35	107.96	113.91
24	a	2236	OMG	C2-N3-C4	4.31	119.98	112.30
24	a	2056	G7M	C5-C6-N1	4.30	120.77	111.79
24	a	2056	G7M	C5-C4-N3	-4.28	119.94	128.15
1	A	1513	MA6	N9-C8-N7	-4.21	108.15	113.91
24	a	2434	H2U	N3-C2-N1	4.18	121.08	116.65
24	a	2430	2MG	C5-C4-N3	-4.09	121.83	128.46
24	a	2488	2MA	C4-N9-C1'	-3.67	117.84	126.59
1	A	1513	MA6	C2-N1-C6	3.66	120.40	111.75
24	a	1926	5MU	O4-C4-C5	-3.65	120.68	124.90
1	A	1513	MA6	C2-N3-C4	3.59	120.24	111.75
24	a	1926	5MU	C6-C5-C4	3.58	121.03	118.03
24	a	2537	OMU	N3-C2-N1	3.57	119.63	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	2056	G7M	CN7-N7-C5	3.54	131.17	126.77
24	a	2537	OMU	C5-C4-N3	3.54	120.14	114.84
1	A	960	5MC	C5-C6-N1	-3.52	119.72	123.34
1	A	1513	MA6	C5-N7-C8	3.38	108.32	103.51
1	A	1396	4OC	O2-C2-N3	-3.38	116.83	122.33
24	a	2430	2MG	N9-C8-N7	-3.36	107.07	113.39
24	a	2236	OMG	C2-N1-C6	-3.33	119.03	125.10
1	A	1513	MA6	C4-C5-C6	3.32	119.60	115.88
24	a	2056	G7M	C2-N1-C6	-3.32	119.05	125.10
1	A	959	2MG	N9-C4-N3	3.31	132.58	125.94
24	a	2056	G7M	O6-C6-C5	-3.31	120.59	128.06
24	a	2488	2MA	C5-N7-C8	3.30	108.20	103.51
24	a	1820	2MG	N9-C8-N7	-3.23	107.30	113.39
24	a	2236	OMG	N9-C8-N7	-3.21	107.34	113.39
24	a	1926	5MU	C5M-C5-C4	3.13	122.22	118.77
24	a	2537	OMU	O4-C4-C5	-3.12	119.67	125.16
24	a	2430	2MG	C5-C6-N1	3.03	120.89	113.19
24	a	2430	2MG	CM2-N2-C2	-3.03	117.17	123.86
24	a	2056	G7M	N9-C4-N3	3.00	131.96	125.94
24	a	2488	2MA	C1'-N9-C8	3.00	133.90	127.14
24	a	2434	H2U	C5-C4-N3	2.92	119.93	116.65
24	a	1820	2MG	CM2-N2-C2	-2.89	117.47	123.86
24	a	2236	OMG	C5-C6-N1	2.89	120.53	113.19
1	A	959	2MG	N9-C8-N7	-2.89	107.95	113.39
1	A	1510	2MG	CM2-N2-C2	-2.86	117.54	123.86
24	a	1820	2MG	C5-C6-N1	2.84	120.40	113.19
1	A	1510	2MG	N9-C8-N7	-2.84	108.05	113.39
24	a	2488	2MA	N3-C2-N1	-2.82	120.53	125.72
24	a	2434	H2U	O2-C2-N1	-2.82	119.57	123.11
1	A	1513	MA6	C5-C4-N9	2.80	109.04	105.78
24	a	2430	2MG	N1-C2-N3	-2.73	119.73	123.95
1	A	1510	2MG	C5-C6-N1	2.73	120.11	113.19
24	a	2430	2MG	C6-C5-N7	2.72	135.31	130.25
24	a	2488	2MA	C6-C5-C4	2.72	120.84	117.18
24	a	2056	G7M	CN7-N7-C8	-2.69	120.68	124.84
1	A	1510	2MG	O6-C6-C5	-2.66	119.55	126.60
1	A	959	2MG	O6-C6-C5	-2.65	119.56	126.60
1	A	1513	MA6	C4-C5-N7	-2.65	107.39	110.62
24	a	2434	H2U	C5-C6-N1	2.58	120.12	111.61
24	a	1926	5MU	O2-C2-N1	-2.54	119.41	122.79
1	A	1396	4OC	C1'-N1-C2	2.51	124.03	118.42
24	a	2236	OMG	O6-C6-C5	-2.50	119.97	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	959	2MG	C5-C6-N1	2.48	119.49	113.19
24	a	2430	2MG	C4-C5-N7	-2.47	106.81	110.72
1	A	1510	2MG	N1-C2-N3	-2.46	120.14	123.95
24	a	1926	5MU	O4-C4-N3	-2.46	115.41	120.12
24	a	1820	2MG	O6-C6-C5	-2.39	120.27	126.60
24	a	2236	OMG	N9-C4-N3	2.38	130.73	125.94
1	A	1396	4OC	CM4-N4-C4	-2.37	117.83	122.45
24	a	1820	2MG	N1-C2-N3	-2.36	120.30	123.95
1	A	1513	MA6	N3-C4-N9	2.34	130.94	127.08
24	a	2488	2MA	C4-N9-C8	2.33	108.26	105.73
24	a	1820	2MG	C8-N7-C5	2.32	108.45	104.24
1	A	959	2MG	N1-C2-N3	-2.31	120.39	123.95
24	a	2236	OMG	C8-N7-C5	2.28	108.36	104.24
24	a	2430	2MG	O6-C6-C5	-2.25	120.63	126.60
24	a	1820	2MG	N9-C4-N3	2.25	130.45	125.94
1	A	1510	2MG	N9-C4-N3	2.25	130.45	125.94
1	A	1396	4OC	C6-C5-C4	2.25	119.71	116.96
24	a	2483	OMC	O2-C2-N3	-2.24	118.69	122.33
24	a	2430	2MG	C8-N7-C5	2.22	108.26	104.24
24	a	2430	2MG	C5-C4-N9	2.22	109.66	105.63
24	a	1820	2MG	C4-C5-N7	-2.14	107.33	110.72
24	a	2488	2MA	CM2-C2-N3	2.11	120.44	117.15
24	a	2236	OMG	C4-C5-N7	-2.06	107.47	110.72
1	A	1492	UR3	C1'-N1-C2	2.05	120.44	116.99
1	A	1492	UR3	C6-N1-C2	-2.04	119.96	121.79
24	a	2537	OMU	C1'-N1-C2	2.01	121.21	117.57

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	959	2MG	O4'-C1'-N9-C8
1	A	959	2MG	O4'-C1'-N9-C4
1	A	1396	4OC	O4'-C1'-N1-C2
1	A	1396	4OC	O4'-C1'-N1-C6
1	A	1513	MA6	O4'-C4'-C5'-O5'
1	A	1513	MA6	C3'-C4'-C5'-O5'
1	A	1513	MA6	C5-C6-N6-C10
24	a	2537	OMU	C3'-C4'-C5'-O5'
1	A	1396	4OC	O4'-C4'-C5'-O5'
24	a	2537	OMU	O4'-C4'-C5'-O5'
1	A	1396	4OC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	1513	MA6	N1-C6-N6-C10
1	A	1513	MA6	C5-C6-N6-C9
1	A	1510	2MG	O4'-C4'-C5'-O5'
24	a	2488	2MA	O4'-C4'-C5'-O5'
1	A	1513	MA6	C4'-C5'-O5'-P
24	a	2430	2MG	C3'-C4'-C5'-O5'
24	a	2056	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1510	2MG	1	0
1	A	1513	MA6	1	0
24	a	1926	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 289 ligands modelled in this entry, 289 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

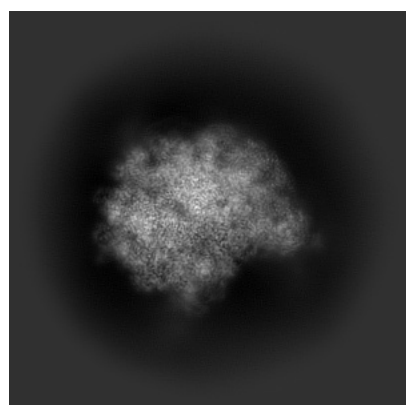
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52192. These allow visual inspection of the internal detail of the map and identification of artifacts.

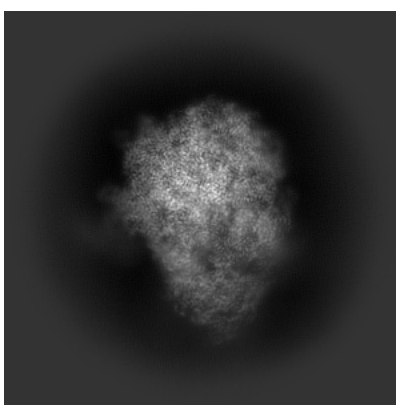
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

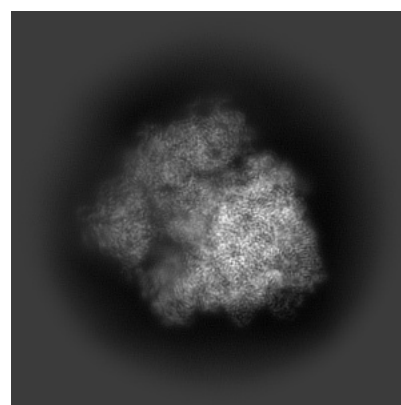
6.1.1 Primary map



X



Y

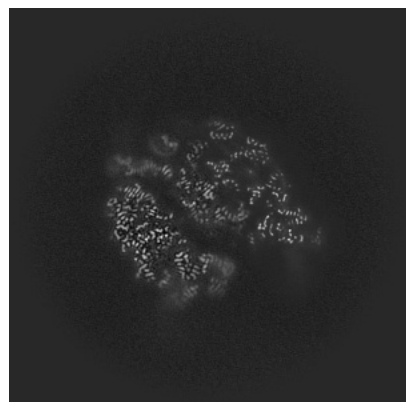


Z

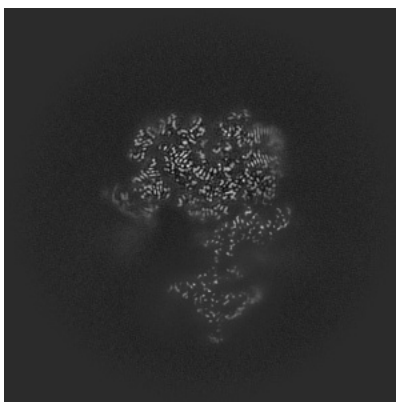
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

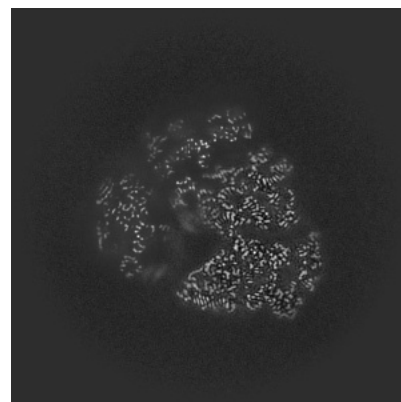
6.2.1 Primary map



X Index: 256



Y Index: 256

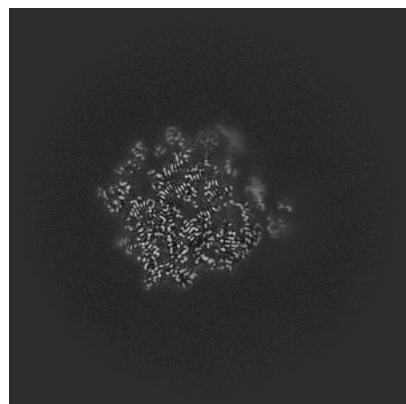


Z Index: 256

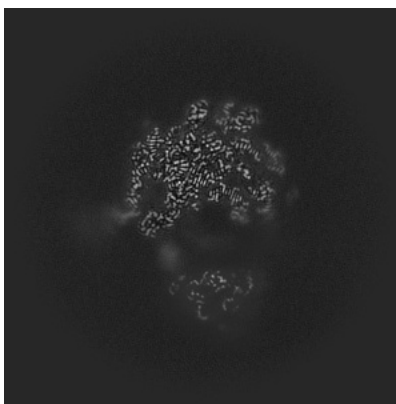
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

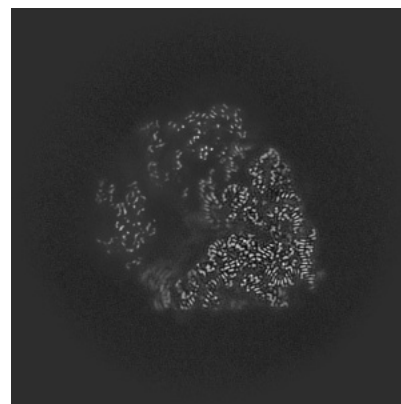
6.3.1 Primary map



X Index: 306



Y Index: 205

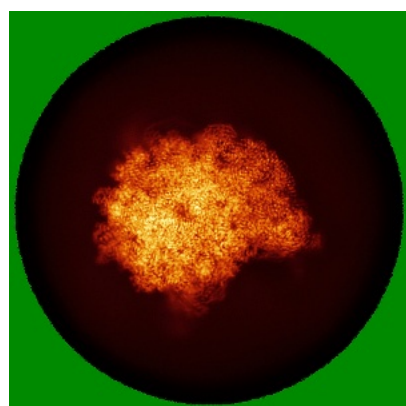


Z Index: 244

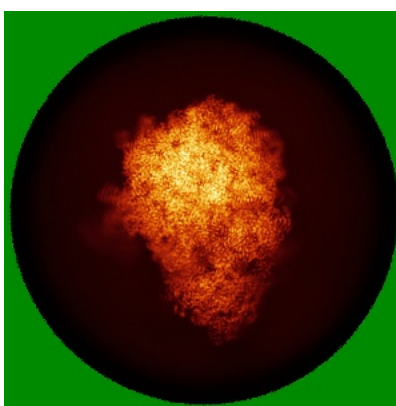
The images above show the largest variance slices of the map in three orthogonal directions.

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

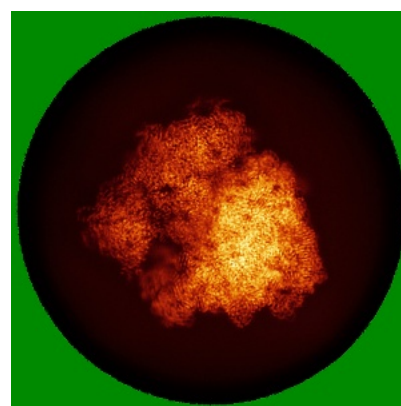
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

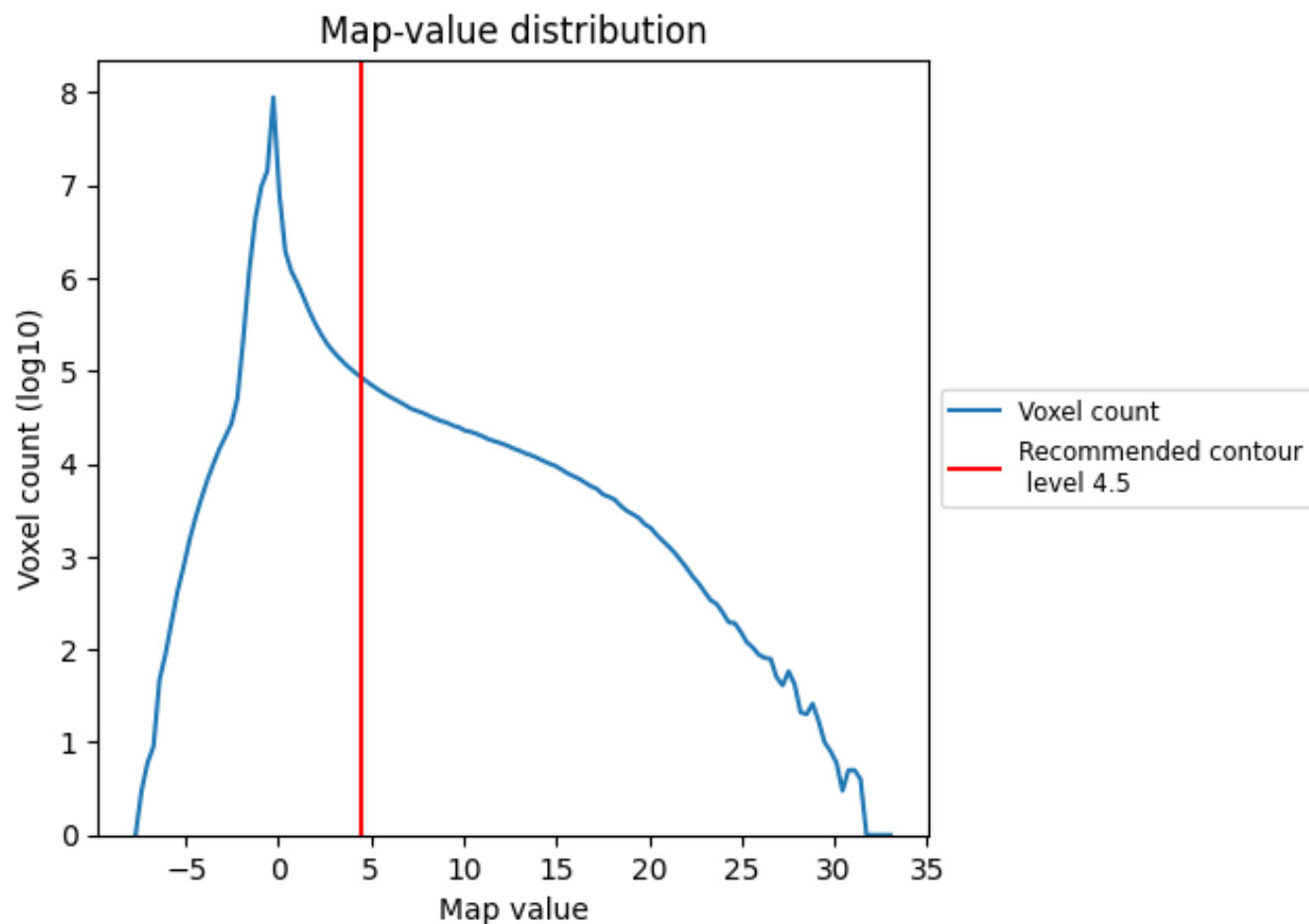
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

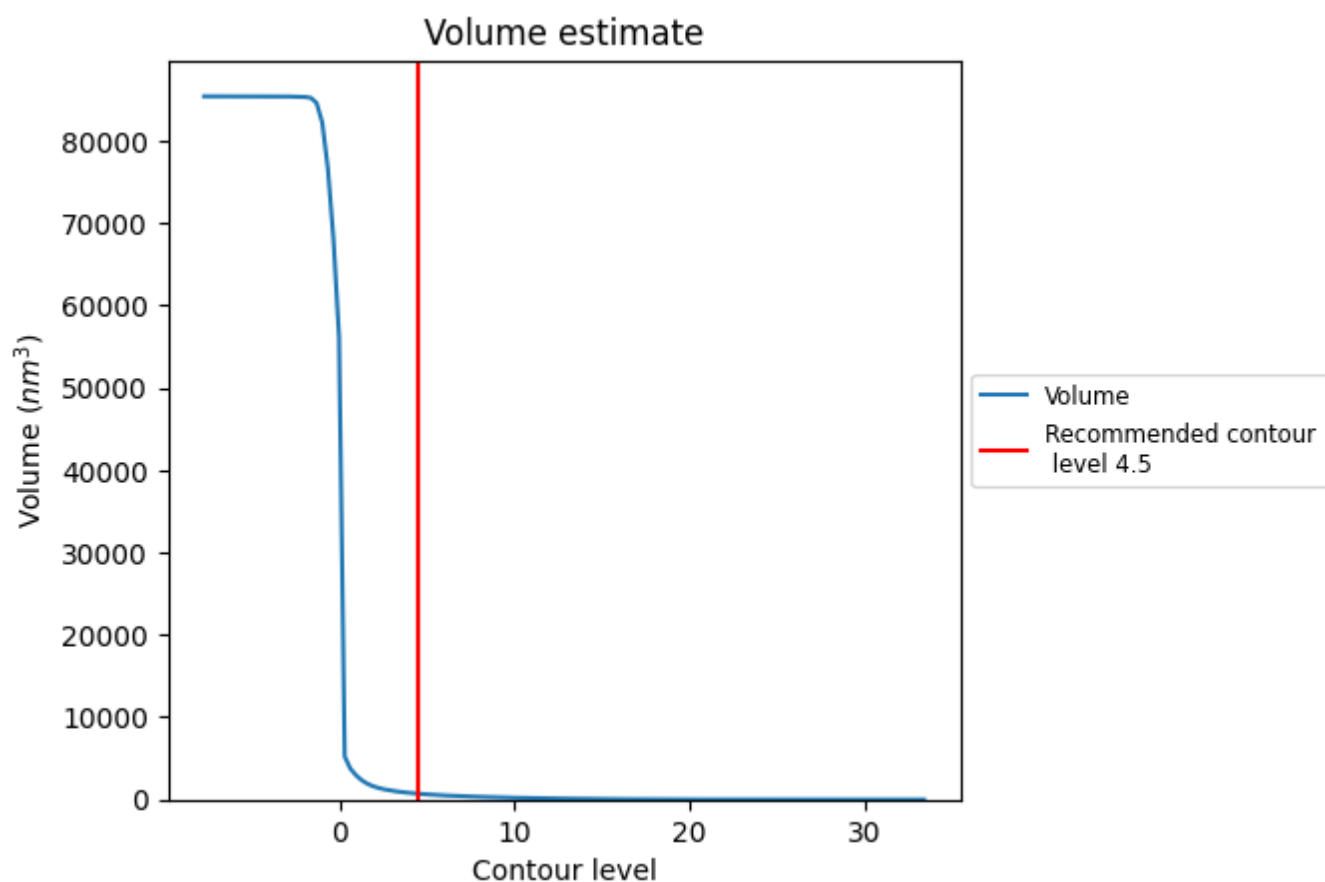
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

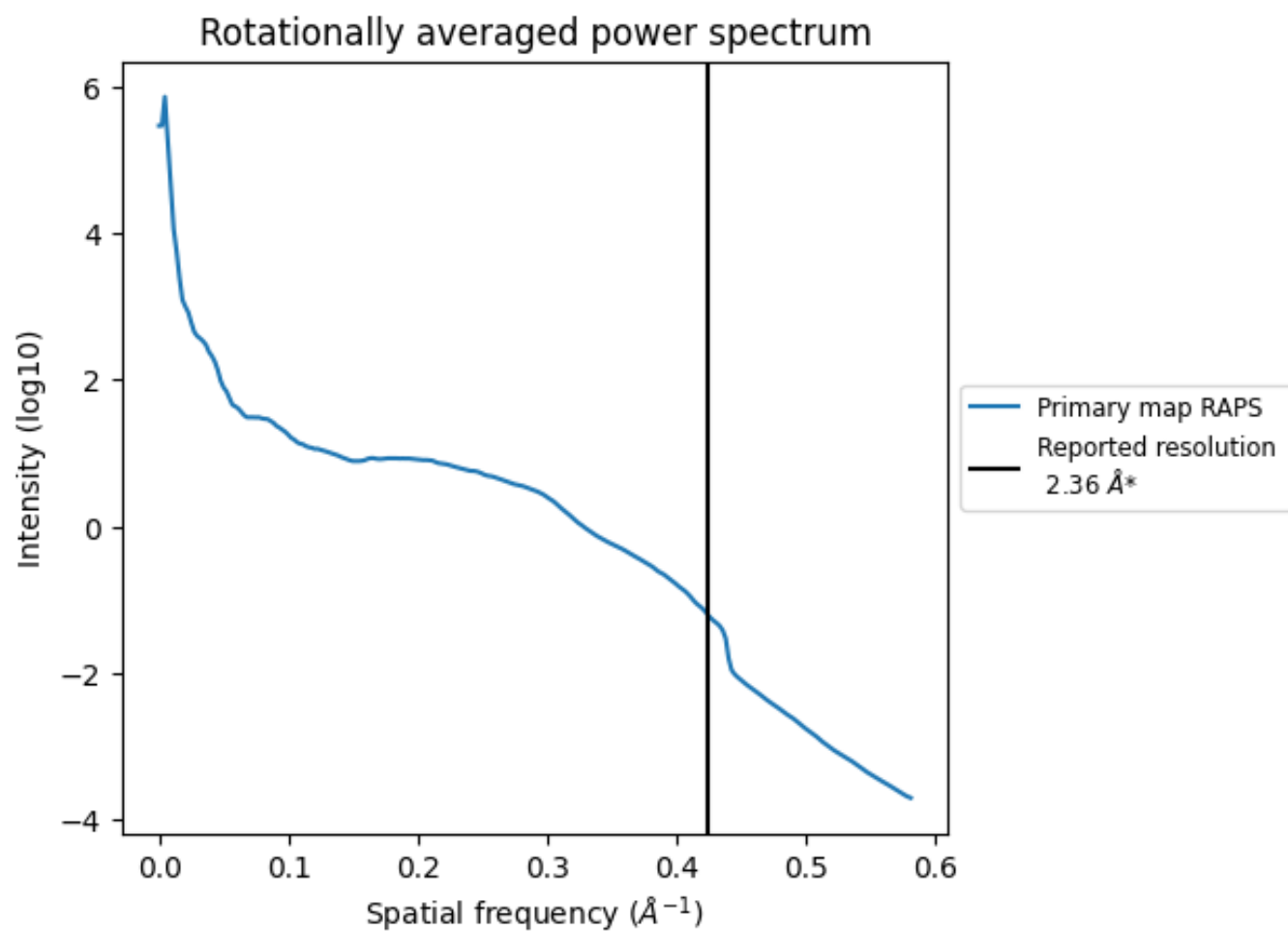
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 710 nm^3 ; this corresponds to an approximate mass of 642 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 0.424 Å⁻¹

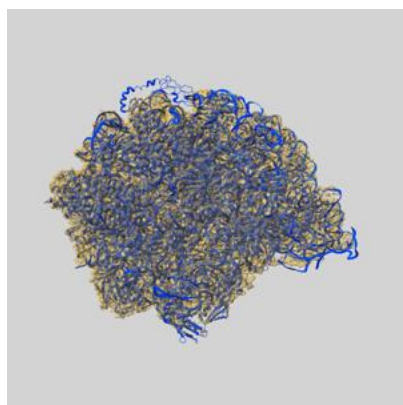
8 Fourier-Shell correlation

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

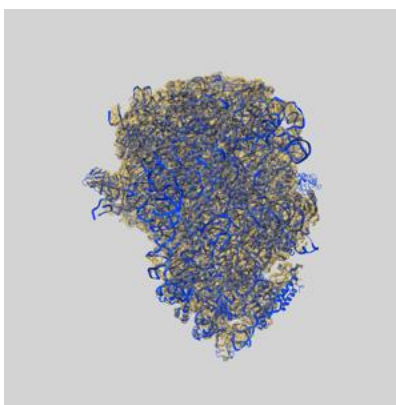
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52192 and PDB model 9HIG. Per-residue inclusion information can be found in section [3](#) on page [14](#).

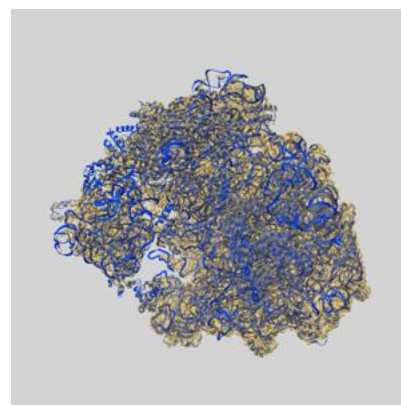
9.1 Map-model overlay [i](#)



X



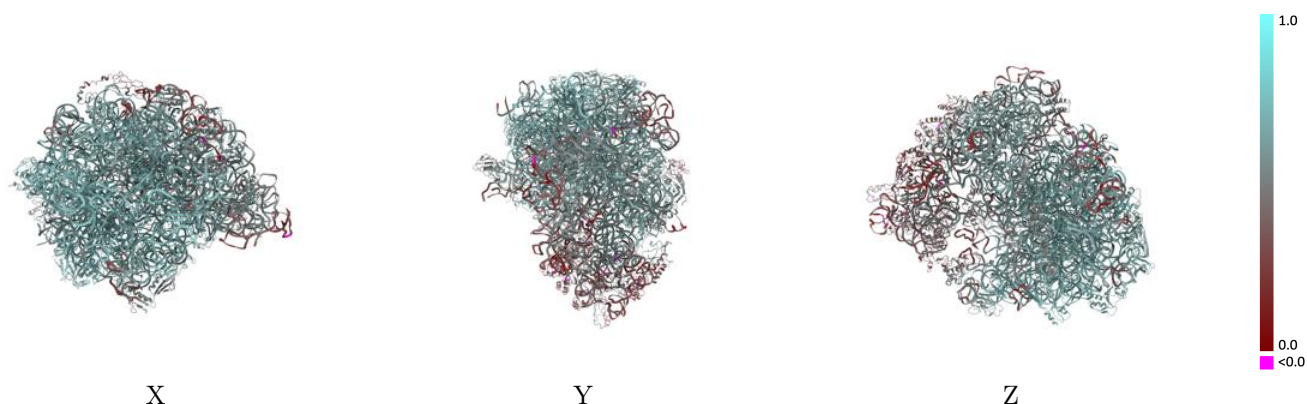
Y



Z

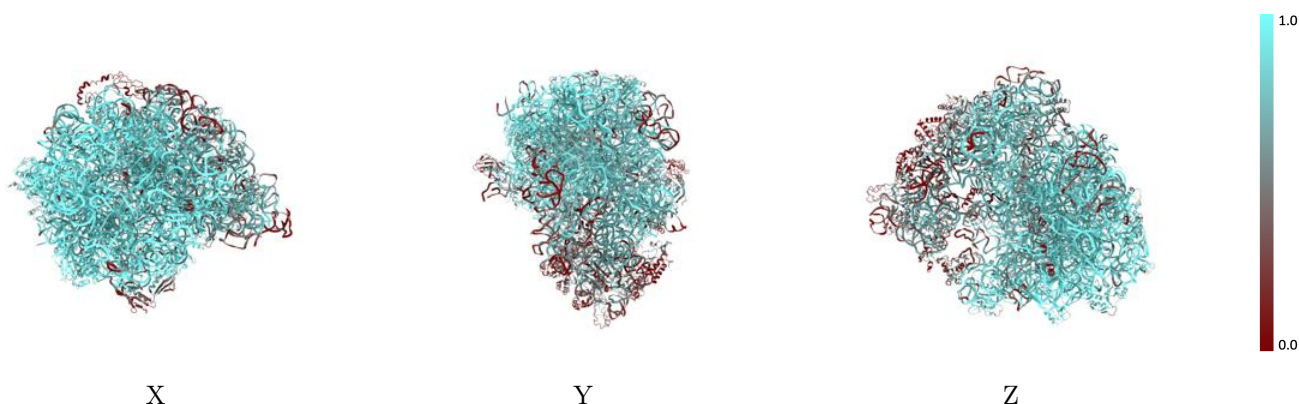
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



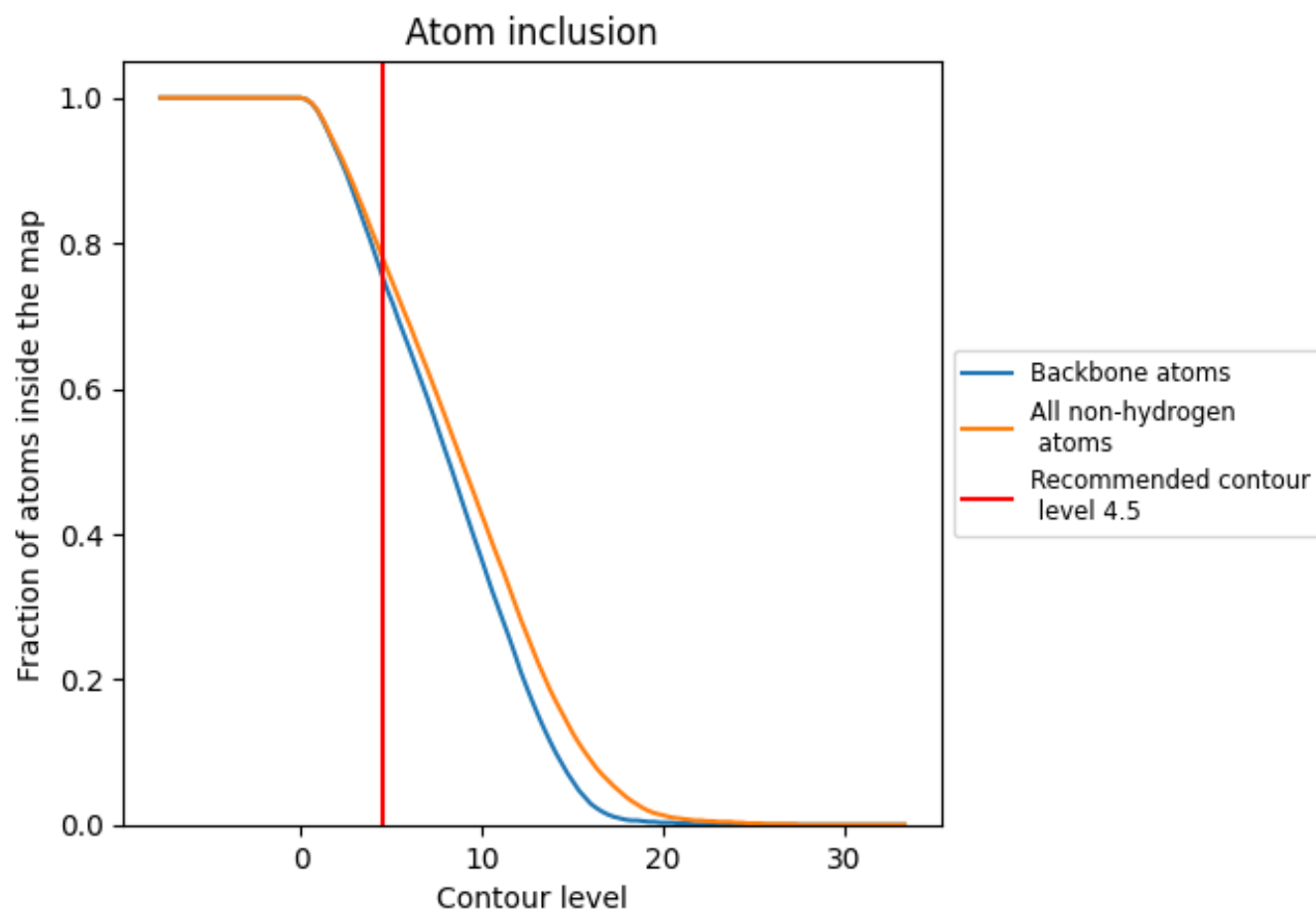
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 78% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7830	 0.5610
0	 0.5080	 0.6220
1	 0.9850	 0.6850
2	 0.9750	 0.6730
3	 0.7930	 0.5430
A	 0.6630	 0.4730
B	 0.3370	 0.4300
C	 0.3330	 0.3640
D	 0.3840	 0.3830
E	 0.6760	 0.5610
F	 0.6190	 0.5450
G	 0.3810	 0.3730
H	 0.7430	 0.5900
I	 0.4880	 0.4080
J	 0.4620	 0.4340
K	 0.5350	 0.4720
L	 0.1360	 0.3620
M	 0.4050	 0.3850
N	 0.4620	 0.3920
O	 0.6430	 0.5660
P	 0.7160	 0.5540
Q	 0.6880	 0.5690
R	 0.7340	 0.5670
S	 0.2970	 0.3120
T	 0.5990	 0.5110
U	 0.1600	 0.4730
W	 0.5560	 0.4840
X	 0.6670	 0.5280
a	 0.9150	 0.6150
b	 0.9230	 0.5620
c	 0.9320	 0.6580
d	 0.9440	 0.6590
e	 0.9070	 0.6490
f	 0.3830	 0.4490
g	 0.3200	 0.4870



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Chain	Atom inclusion	Q-score
h	 0.1710	 0.3980
i	 0.9550	 0.6650
j	 0.8140	 0.6380
k	 0.9420	 0.6570
l	 0.9440	 0.6560
m	 0.9760	 0.6690
n	 0.8200	 0.5550
o	 0.7820	 0.6260
p	 0.9750	 0.6790
q	 0.9170	 0.6420
r	 0.9330	 0.6560
s	 0.8540	 0.6110
t	 0.8520	 0.6190
u	 0.8720	 0.6170
v	 0.9520	 0.6620
w	 0.9460	 0.6510
x	 0.7810	 0.5910
y	 0.9420	 0.6440
z	 0.9490	 0.6590