



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:55 AM UTC

PDB ID : 9E0P / pdb\_00009e0p  
EMDB ID : EMD-47365  
Title : M. smegmatis methylated 70S ribosome structure  
Authors : Nandi, S.; Conn, G.L.  
Deposited on : 2024-10-18  
Resolution : 3.17 Å(reported)  
Based on initial model : 5ZEB

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

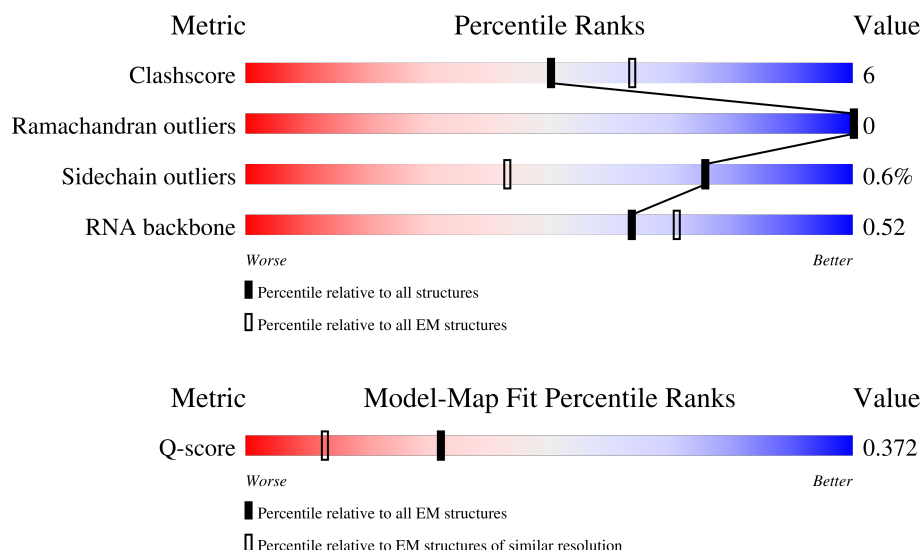
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





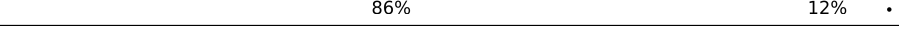
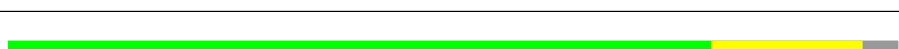



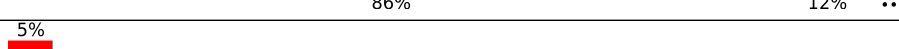


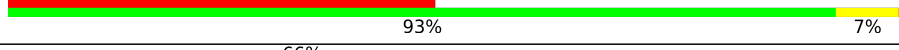
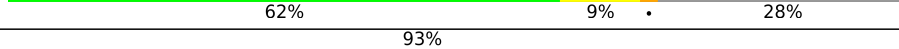

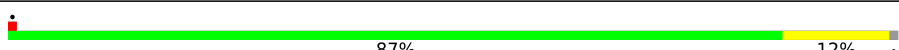


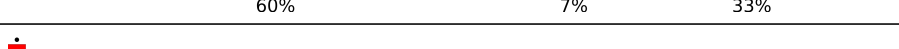







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14465 ( 2.67 - 3.67 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	61	
2	2	75	
3	3	57	

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Mol	Chain	Length	Quality of chain
4	4	55	
5	5	47	
6	6	64	
7	7	37	
8	8	24	
9	A	3120	
10	B	118	
11	C	278	
12	D	217	
13	E	215	
14	F	187	
15	G	179	
16	H	151	
17	I	174	
18	J	142	
19	K	147	
20	L	122	
21	M	147	
22	N	138	
23	O	174	
24	P	127	
25	Q	113	
26	R	129	
27	S	103	
28	T	153	



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Mol	Chain	Length	Quality of chain
29	U	100	
30	V	105	
31	W	215	
32	X	88	
33	Y	64	
34	Z	77	
35	a	1528	
36	b	277	
37	c	275	
38	d	201	
39	e	214	
40	f	96	
41	g	156	
42	h	132	
43	i	150	
44	j	101	
45	k	138	
46	l	124	
47	m	124	
48	n	61	
49	o	89	
50	p	156	
51	q	98	
52	r	84	
53	s	93	

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Mol	Chain	Length	Quality of chain
54	t	86	 90% 8%
55	u	33	 85% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	OMC	a	1392	-	-	X	-

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 148821 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	60	Total	C	N	O	0	0
			483	298	97	88		

- Molecule 2 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	66	Total	C	N	O	S	0	0
			510	316	93	96	5		

- Molecule 3 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 4 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	50	Total	C	N	O	S	0	0
			416	254	86	72	4		

- Molecule 5 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	45	Total	C	N	O	S	0	0
			372	222	96	53	1		

- Molecule 6 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	6	63	Total	C	N	O	0	0
			502	302	115	85		

- Molecule 7 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	37	Total	C	N	O	S	0	0
			298	181	66	46	5		

- Molecule 8 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	8	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 9 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	3102	Total	C	N	O	P	0	0
			66624	29695	12253	21574	3102		

- Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	117	Total	C	N	O	P	0	0
			2501	1116	462	806	117		

- Molecule 11 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	273	Total	C	N	O	S	0	0
			2097	1290	435	368	4		

- Molecule 12 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 13 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	207	Total	C	N	O	S	0	0
			1548	955	292	299	2		

- Molecule 14 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	181	Total	C	N	O	S	0	0
			1437	903	269	259	6		

- Molecule 15 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 18 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 19 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	147	Total	C	N	O	S	0	0
			1138	727	208	201	2		

- Molecule 20 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	121	Total	C	N	O	S	0	0
			930	580	178	169	3		

- Molecule 21 is a protein called Large ribosomal subunit protein uL15.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 22 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	134	Total	C	N	O	S	0	0
			1074	680	211	181	2		

- Molecule 23 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	117	Total	C	N	O	S	0	0
			919	577	178	162	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	126	Total	C	N	O		0	0
			956	586	199	171			

- Molecule 25 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 26 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	124	Total	C	N	O		0	0
			988	613	203	172			

- Molecule 27 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	102	Total	C	N	O		0	0
			768	487	140	141			

- Molecule 28 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	T	114	Total	C	N	O	0	0
			873	543	171	159		

- Molecule 29 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	U	94	Total	C	N	O	0	0
			739	469	135	135		

- Molecule 30 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	97	Total	C	N	O	S	0	0
			731	456	137	136	2		

- Molecule 31 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	W	188	Total	C	N	O	0	0
			1407	869	251	287		

- Molecule 32 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	X	82	Total	C	N	O	0	0
			604	372	127	105		

- Molecule 33 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 34 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	63	Total	C	N	O	S	0	0
			527	322	102	102	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	1506	Total	C	N	O	P	0	0
			32342	14405	5921	10510	1506		

- Molecule 36 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	228	Total	C	N	O	S	0	0
			1793	1132	322	330	9		

- Molecule 37 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	210	Total	C	N	O	S	0	0
			1672	1043	324	300	5		

- Molecule 38 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	200	Total	C	N	O	S	0	0
			1641	1028	316	295	2		

- Molecule 39 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	198	Total	C	N	O	S	0	0
			1433	885	282	262	4		

- Molecule 40 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	96	Total	C	N	O	S	0	0
			771	486	138	145	2		

- Molecule 41 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	156	Total	C	N	O	S	0	0
			1240	773	242	222	3		

- Molecule 42 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	130	Total	C	N	O	S	0	0
			1003	629	188	185	1		

- Molecule 43 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	126	Total	C	N	O	S	0	0
			994	630	194	170			

- Molecule 44 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	97	Total	C	N	O	S	0	0
			775	488	143	141	3		

- Molecule 45 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	117	Total	C	N	O	S	0	0
			871	539	173	158	1		

- Molecule 46 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	122	Total	C	N	O	S	0	0
			958	594	197	165	2		

- Molecule 47 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	116	Total	C	N	O	S	0	0
			935	572	191	169	3		

- Molecule 48 is a protein called Small ribosomal subunit protein uS14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	n	60	Total	C	N	O	S	0	0
			477	302	97	73	5		

- Molecule 49 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	o	87	Total	C	N	O	0	0
			709	443	143	123		

- Molecule 50 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	p	113	Total	C	N	O	0	0
			891	570	162	159		

- Molecule 51 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	q	92	Total	C	N	O	S	0	0
			730	458	138	132	2		

- Molecule 52 is a protein called Small ribosomal subunit protein bS18B.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	r	64	Total	C	N	O	S	0	0
			512	319	102	88	3		

- Molecule 53 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	78	Total	C	N	O	S	0	0
			630	405	117	107	1		

- Molecule 54 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	t	84	Total	C	N	O	0	0
			655	399	138	118		

- Molecule 55 is a protein called Conserved domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	u	32	Total	C	N	O	S	0	0
			280	172	71	36	1		


- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	2	1	Total 1	Mg 1	0
56	3	1	Total 1	Mg 1	0
56	A	109	Total 109	Mg 109	0
56	B	3	Total 3	Mg 3	0
56	D	1	Total 1	Mg 1	0
56	a	23	Total 23	Mg 23	0
56	j	1	Total 1	Mg 1	0

### 3 Residue-property plots [i](#)


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

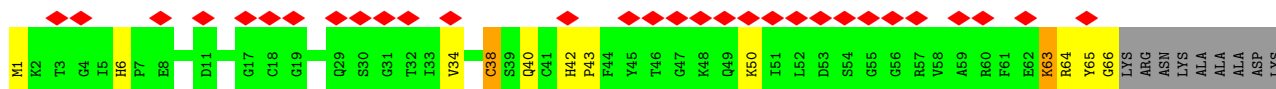
- Molecule 1: Large ribosomal subunit protein uL30

Chain 1: 




- Molecule 2: Large ribosomal subunit protein bL31

Chain 2: 



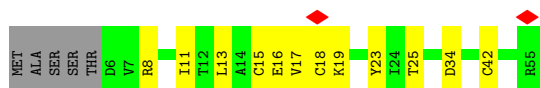
- Molecule 3: Large ribosomal subunit protein bL32

Chain 3: 




- Molecule 4: Large ribosomal subunit protein bL33A

Chain 4: 




- Molecule 5: Large ribosomal subunit protein bL34

Chain 5: 




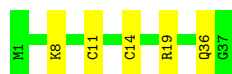
- Molecule 6: Large ribosomal subunit protein bL35

Chain 6:  86% 12% .




- Molecule 7: 50S ribosomal protein L36

Chain 7:  86% 14%



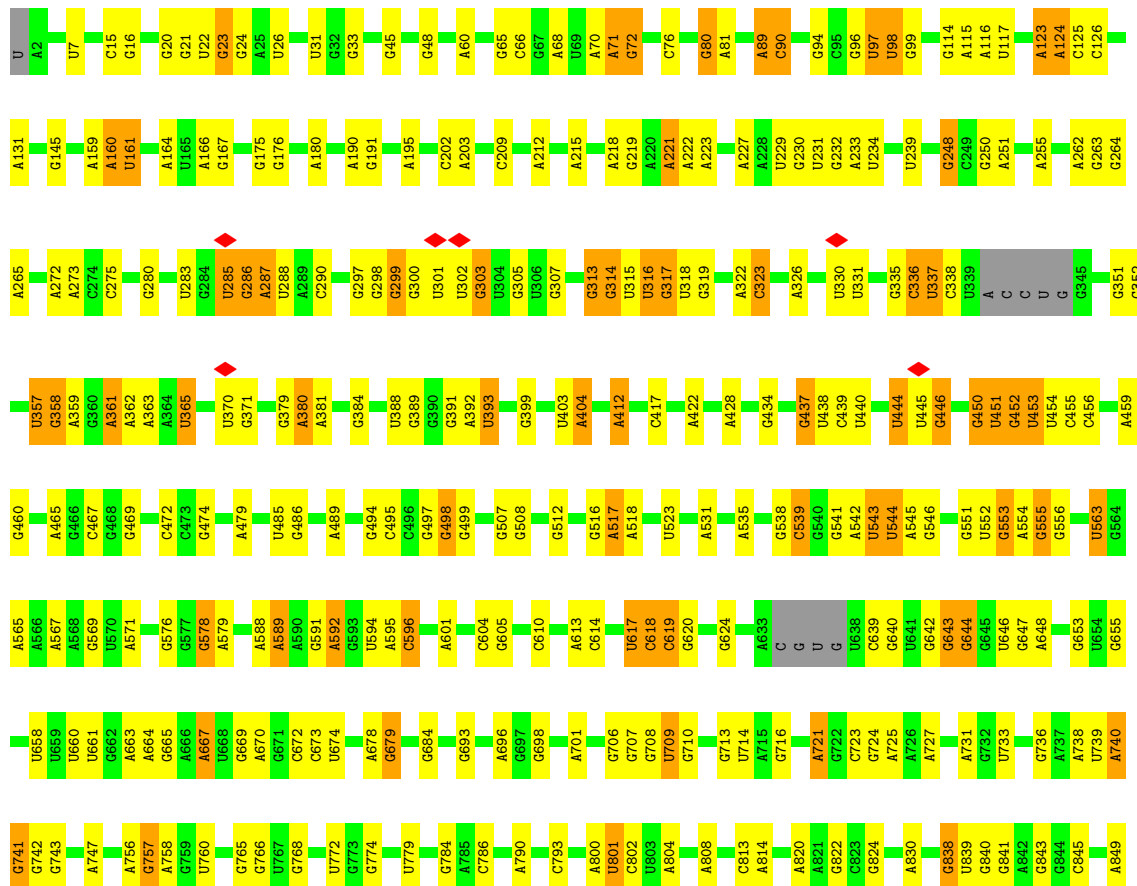
- Molecule 8: 50S ribosomal protein bL37

Chain 8:  79% 17% .



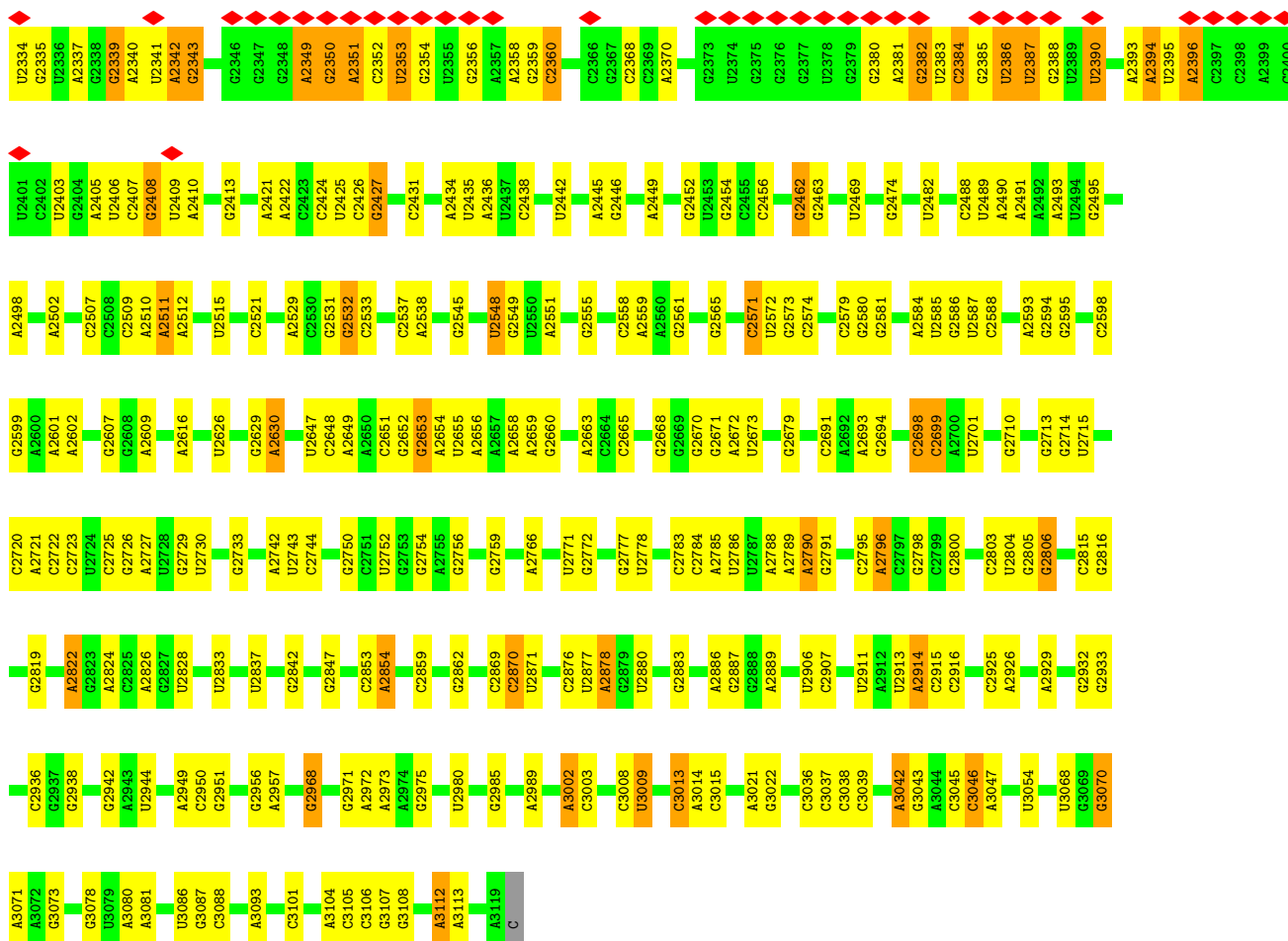
- Molecule 9: 23S rRNA

Chain A:  63% 29% 7% .

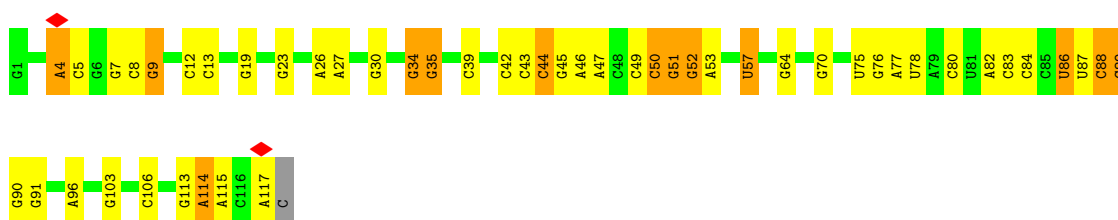




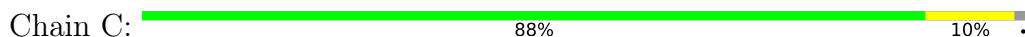




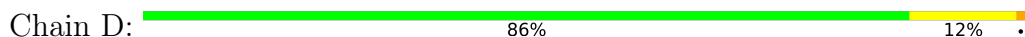
- Molecule 10: 5S rRNA



- Molecule 11: Large ribosomal subunit protein uL2

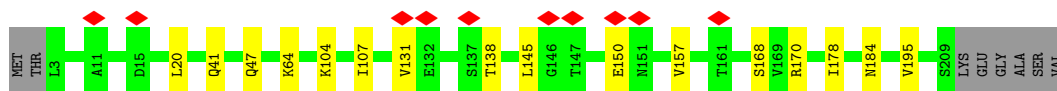
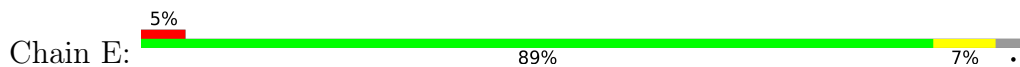


- Molecule 12: Large ribosomal subunit protein uL3

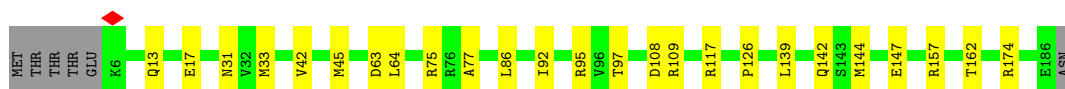
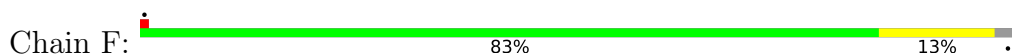




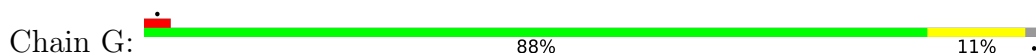
- Molecule 13: Large ribosomal subunit protein uL4



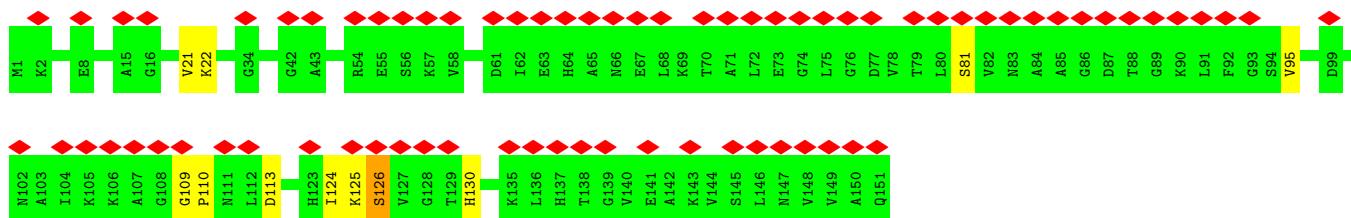
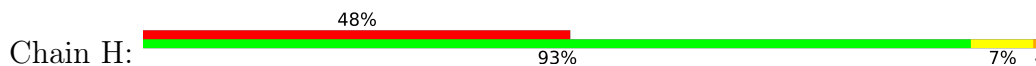
- Molecule 14: Large ribosomal subunit protein uL5



- Molecule 15: Large ribosomal subunit protein uL6

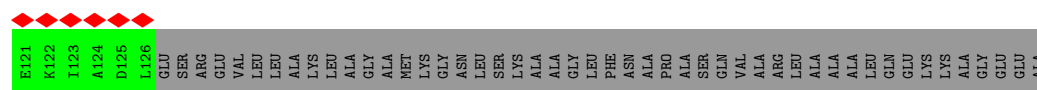


- Molecule 16: 50S ribosomal protein L9

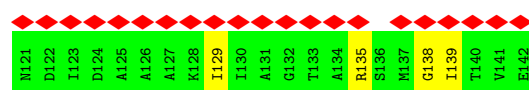
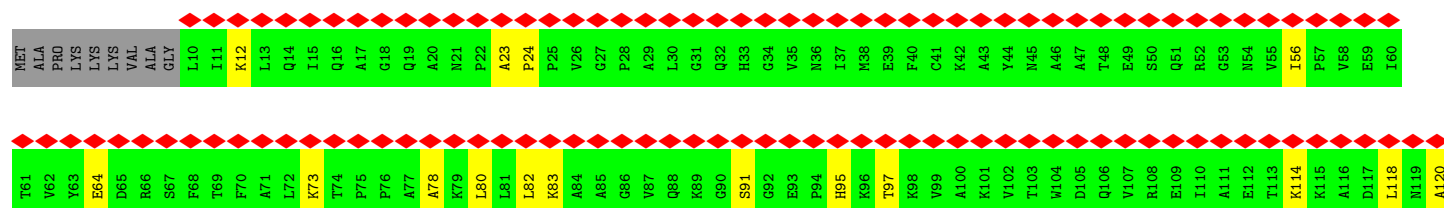
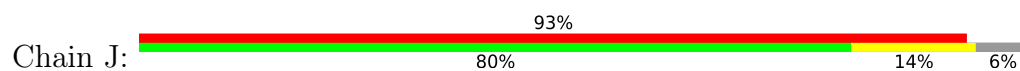


- Molecule 17: Large ribosomal subunit protein uL10





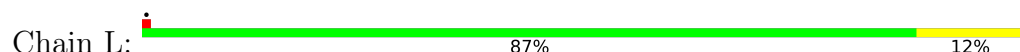
- Molecule 18: Large ribosomal subunit protein uL11



- Molecule 19: Large ribosomal subunit protein uL13



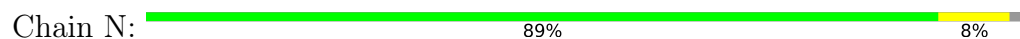
- Molecule 20: Large ribosomal subunit protein uL14




- Molecule 21: Large ribosomal subunit protein uL15

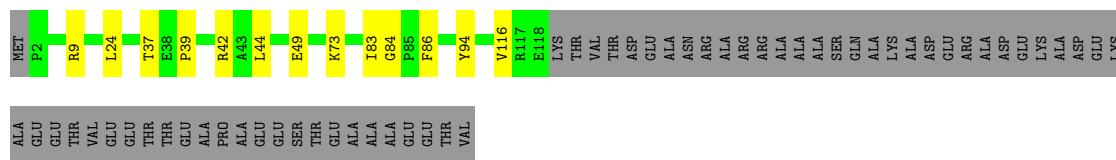


- Molecule 22: Large ribosomal subunit protein uL16




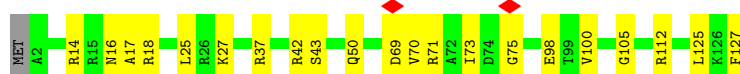
- Molecule 23: Large ribosomal subunit protein bL17

Chain O:  60% 7% 33%




- Molecule 24: Large ribosomal subunit protein uL18

Chain P:  83% 17%




- Molecule 25: Large ribosomal subunit protein bL19

Chain Q:  86% 14%



- Molecule 26: Large ribosomal subunit protein bL20

Chain R:  81% 16%



- Molecule 27: Large ribosomal subunit protein bL21

Chain S:  89% 10%



- Molecule 28: Large ribosomal subunit protein uL22

Chain T:  67% 8% 25%

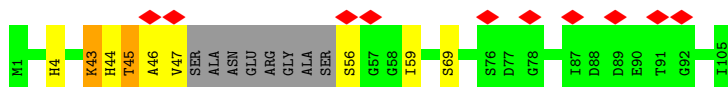
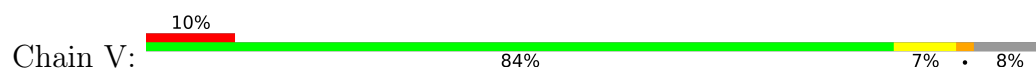


- Molecule 29: Large ribosomal subunit protein uL23

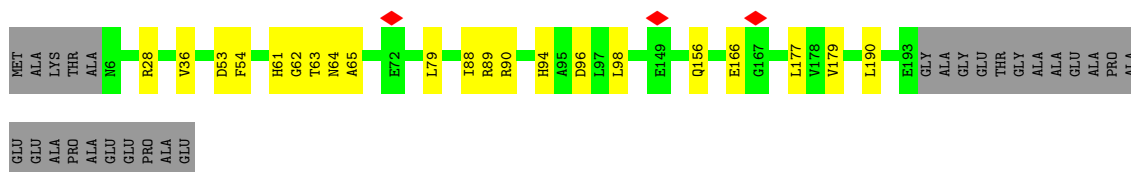
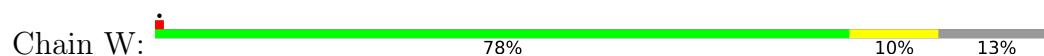
Chain U:  86% 8% 6%



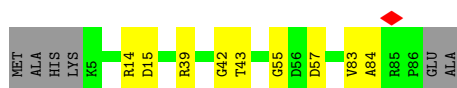
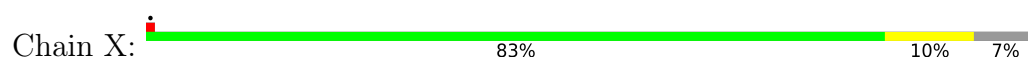
- Molecule 30: Large ribosomal subunit protein uL24



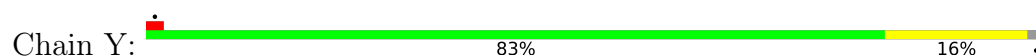
- Molecule 31: Large ribosomal subunit protein bL25



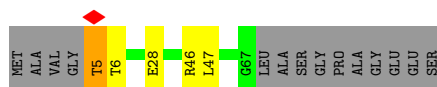
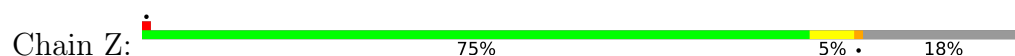
- Molecule 32: Large ribosomal subunit protein bL27



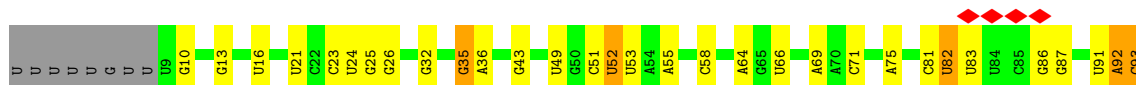
- Molecule 33: Large ribosomal subunit protein bL28

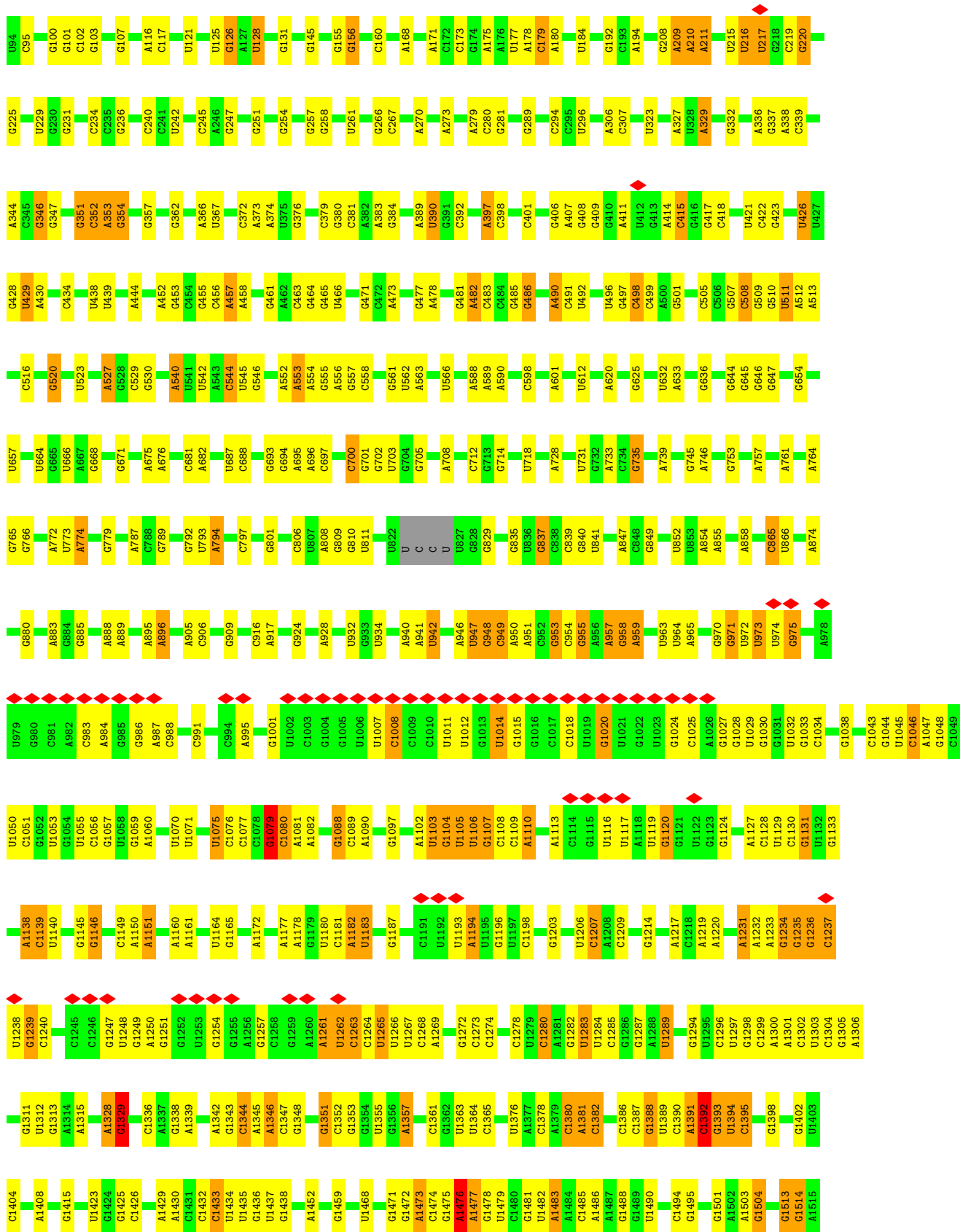


- Molecule 34: Large ribosomal subunit protein uL29



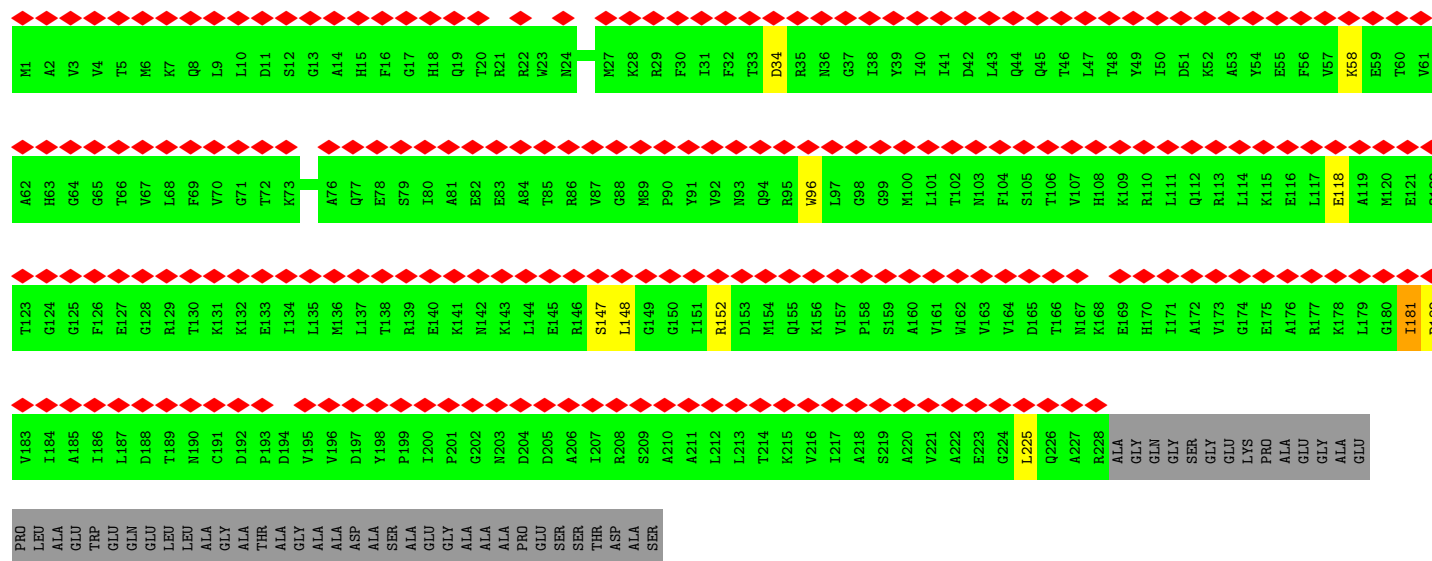
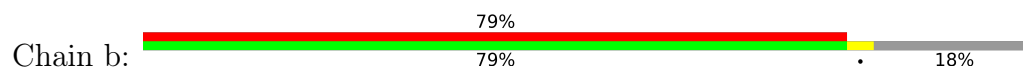
- Molecule 35: 16S rRNA



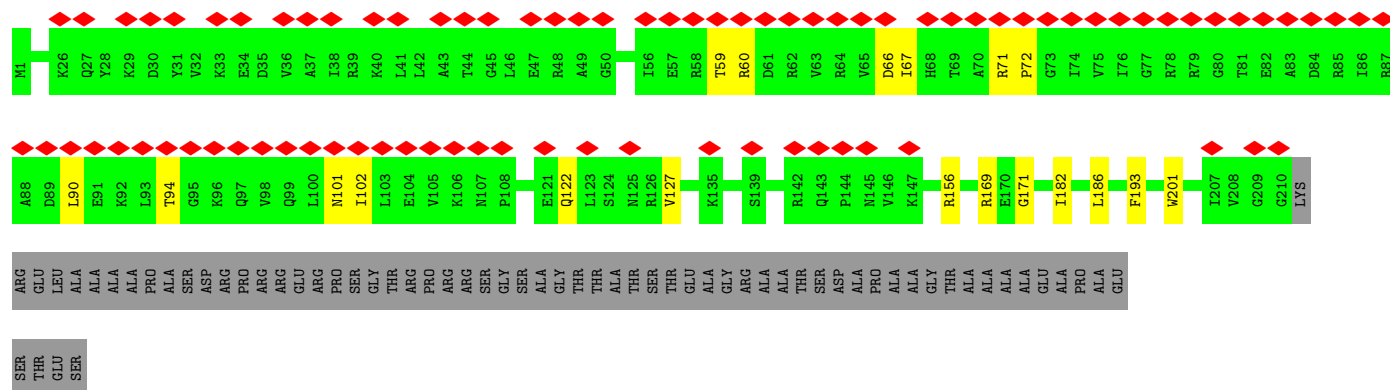




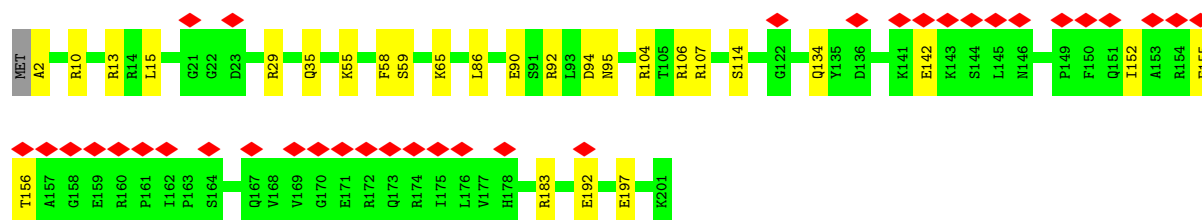
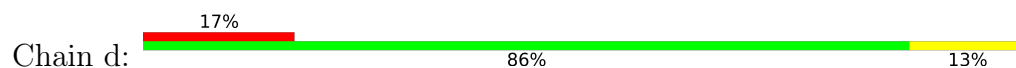
• Molecule 36: Small ribosomal subunit protein uS2



• Molecule 37: Small ribosomal subunit protein uS3

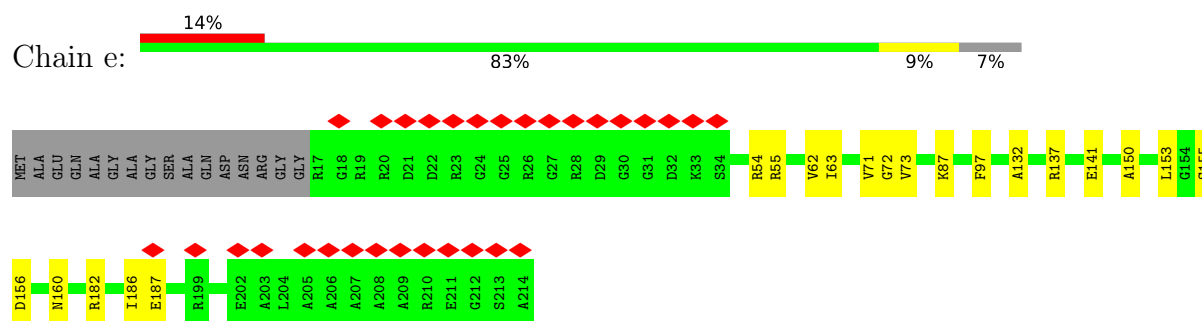


• Molecule 38: Small ribosomal subunit protein uS4

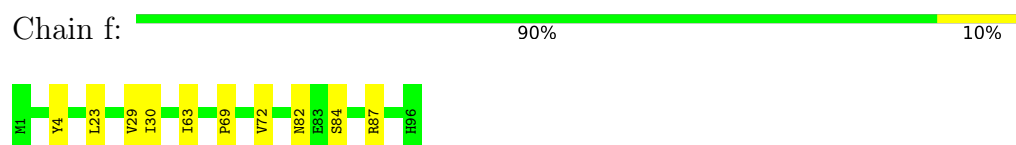




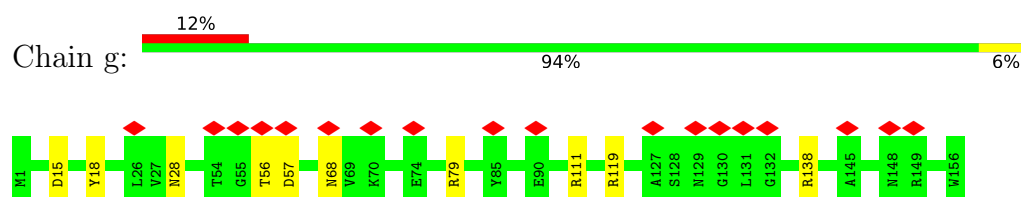
- Molecule 39: Small ribosomal subunit protein uS5



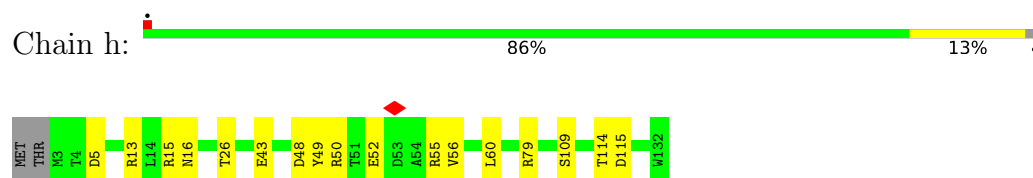
- Molecule 40: Small ribosomal subunit protein bS6



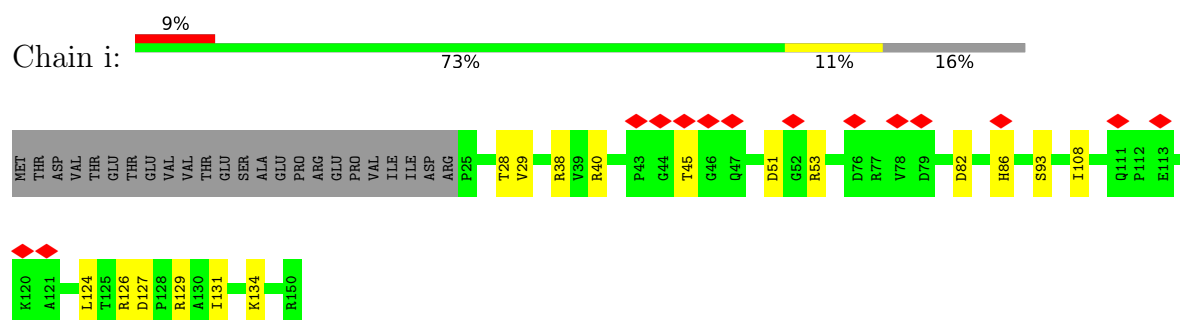
- Molecule 41: Small ribosomal subunit protein uS7



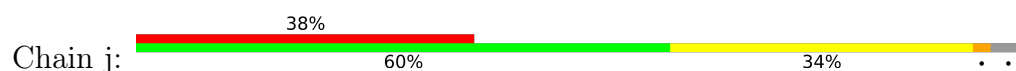
- Molecule 42: Small ribosomal subunit protein uS8

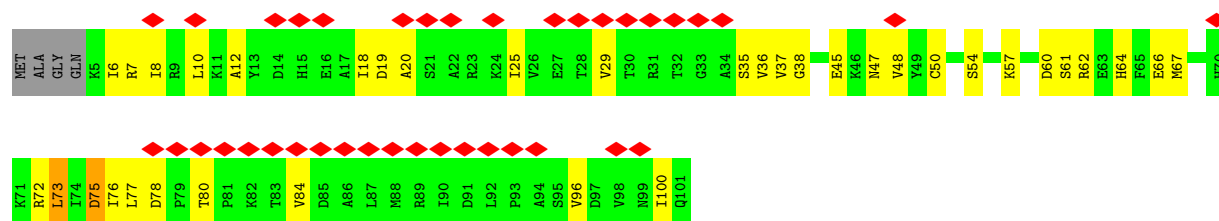


- Molecule 43: Small ribosomal subunit protein uS9



- Molecule 44: Small ribosomal subunit protein uS10





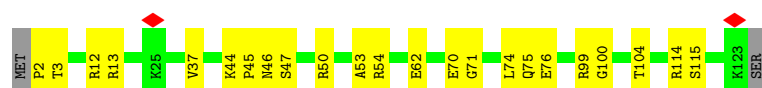
- Molecule 45: Small ribosomal subunit protein uS11

Chain k: 79% 6% 15%



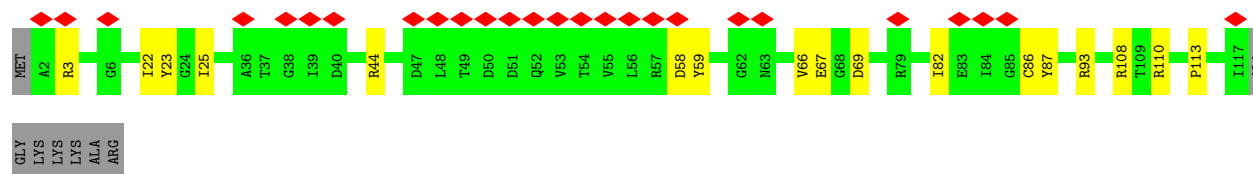
- Molecule 46: Small ribosomal subunit protein uS12

Chain l: 80% 19% .



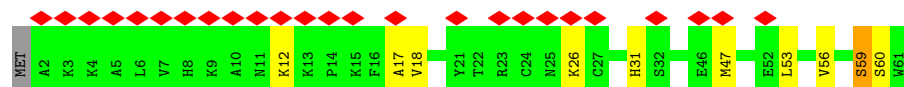
- Molecule 47: Small ribosomal subunit protein uS13

Chain m: 21% 80% 14% 6%



- Molecule 48: Small ribosomal subunit protein uS14B

Chain n: 41% 82% 15% ..



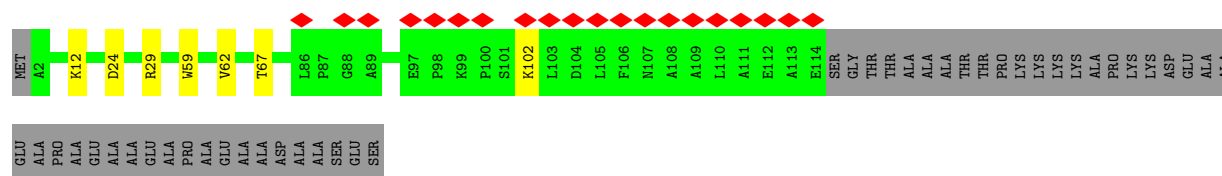
- Molecule 49: Small ribosomal subunit protein uS15

Chain o: 91% 7% .

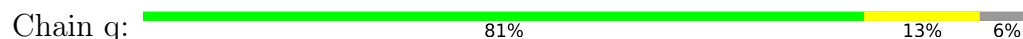


- Molecule 50: Small ribosomal subunit protein bS16

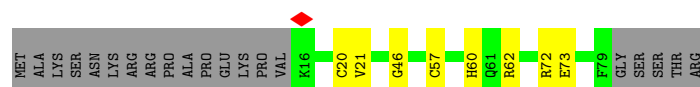
Chain p: 13% 68% . 28%



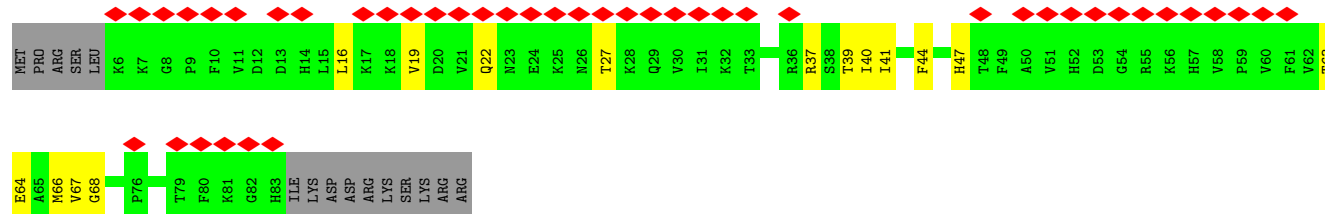
- Molecule 51: Small ribosomal subunit protein uS17



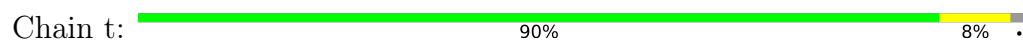
- Molecule 52: Small ribosomal subunit protein bS18B



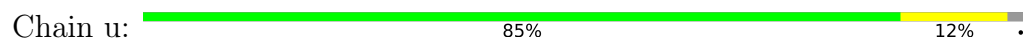
- Molecule 53: Small ribosomal subunit protein uS19



- Molecule 54: Small ribosomal subunit protein bS20



- Molecule 55: Conserved domain protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	443500	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 ( $e^-/\text{\AA}^2$ )	52.51	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.012	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	427.6, 427.6, 427.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.069, 1.069, 1.069	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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	0.08	0/486	0.25	0/651
2	2	0.15	0/520	0.29	0/698
3	3	0.11	0/427	0.23	0/572
4	4	0.14	0/424	0.32	0/567
5	5	0.12	0/375	0.33	0/493
6	6	0.09	0/507	0.30	0/672
7	7	0.14	0/302	0.31	0/401
8	8	0.11	0/191	0.24	0/247
9	A	0.09	1/74575 (0.0%)	0.21	0/116352
10	B	0.09	0/2797	0.20	0/4357
11	C	0.10	0/2140	0.26	0/2879
12	D	0.09	0/1609	0.23	0/2165
13	E	0.09	0/1571	0.26	0/2125
14	F	0.10	0/1459	0.31	0/1962
15	G	0.09	0/1369	0.22	0/1848
16	H	0.10	0/1027	0.22	0/1398
17	I	0.11	0/925	0.26	0/1246
18	J	0.09	0/1006	0.23	0/1364
19	K	0.10	0/1165	0.22	0/1578
20	L	0.10	0/938	0.27	0/1257
21	M	0.09	0/1091	0.23	0/1457
22	N	0.10	0/1100	0.26	0/1482
23	O	0.09	0/936	0.27	0/1256
24	P	0.10	0/966	0.21	0/1298
25	Q	0.11	0/921	0.25	0/1236
26	R	0.10	0/1000	0.23	0/1341
27	S	0.07	0/778	0.21	0/1048
28	T	0.10	0/887	0.30	0/1204
29	U	0.09	0/749	0.25	0/1006
30	V	0.14	0/737	0.30	0/987
31	W	0.08	0/1422	0.24	0/1941
32	X	0.10	0/613	0.32	0/821

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Y	0.10	0/478	0.24	0/641
34	Z	0.10	0/530	0.26	0/708
35	a	0.08	0/36179	0.25	14/56454 (0.0%)
36	b	0.10	0/1822	0.23	0/2457
37	c	0.10	0/1696	0.27	0/2276
38	d	0.10	0/1672	0.23	0/2251
39	e	0.09	0/1449	0.25	0/1949
40	f	0.11	0/782	0.24	0/1059
41	g	0.10	0/1260	0.27	0/1701
42	h	0.08	0/1018	0.24	0/1375
43	i	0.09	0/1012	0.26	0/1362
44	j	0.14	0/789	0.37	0/1069
45	k	0.09	0/889	0.26	0/1201
46	l	0.10	0/969	0.34	0/1294
47	m	0.11	0/942	0.27	0/1260
48	n	0.11	0/488	0.28	0/650
49	o	0.09	0/718	0.27	0/963
50	p	0.10	0/908	0.25	0/1226
51	q	0.08	0/741	0.25	0/993
52	r	0.11	0/517	0.34	0/691
53	s	0.10	0/647	0.27	0/871
54	t	0.09	0/658	0.24	0/875
55	u	0.12	0/280	0.27	0/359
All	All	0.09	1/161457 (0.0%)	0.23	14/241594 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2144	OMC	O3'-P	-11.80	1.43	1.61

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	1329	G	OP1-P-OP2	-13.54	79.00	119.60
35	a	1328	A	OP1-P-O3'	-12.37	70.89	108.00
35	a	1328	A	OP2-P-O3'	9.71	137.12	108.00
35	a	1329	G	O5'-P-OP2	-9.70	78.90	108.00
35	a	1079	G	OP2-P-O3'	-8.83	81.52	108.00
35	a	1289	U	OP1-P-O3'	-8.80	81.59	108.00
35	a	1079	G	OP1-P-O3'	-8.54	82.39	108.00
35	a	1104	G	OP2-P-O3'	-8.32	83.03	108.00
35	a	1289	U	OP2-P-O3'	-8.24	83.27	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	1104	G	OP1-P-O3'	-8.22	83.33	108.00
35	a	1329	G	O5'-P-OP1	7.08	129.25	108.00
35	a	1390	C	P-O3'-C3'	-5.90	111.35	120.20
35	a	1390	C	O3'-P-O5'	5.88	112.83	104.00
35	a	1476	A	C3'-C2'-O2'	5.23	118.55	110.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	483	0	513	8	0
2	2	510	0	501	9	0
3	3	423	0	463	5	0
4	4	416	0	422	8	0
5	5	372	0	406	8	0
6	6	502	0	541	7	0
7	7	298	0	322	4	0
8	8	189	0	205	5	0
9	A	66624	0	33524	642	0
10	B	2501	0	1273	40	0
11	C	2097	0	2149	25	0
12	D	1587	0	1630	20	0
13	E	1548	0	1573	17	0
14	F	1437	0	1470	19	0
15	G	1348	0	1399	13	0
16	H	1018	0	988	10	0
17	I	918	0	959	23	0
18	J	990	0	1021	16	0
19	K	1138	0	1178	5	0
20	L	930	0	989	11	0
21	M	1078	0	1151	9	0
22	N	1074	0	1116	8	0
23	O	919	0	959	10	0
24	P	956	0	991	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Q	907	0	938	10	0
26	R	988	0	1038	20	0
27	S	768	0	820	7	0
28	T	873	0	909	10	0
29	U	739	0	785	5	0
30	V	731	0	782	12	0
31	W	1407	0	1423	14	0
32	X	604	0	622	7	0
33	Y	470	0	484	9	0
34	Z	527	0	538	2	0
35	a	32342	0	16273	351	0
36	b	1793	0	1839	8	0
37	c	1672	0	1722	10	0
38	d	1641	0	1668	24	0
39	e	1433	0	1490	16	0
40	f	771	0	797	6	0
41	g	1240	0	1293	6	0
42	h	1003	0	1039	11	0
43	i	994	0	1050	14	0
44	j	775	0	808	47	0
45	k	871	0	885	5	0
46	l	958	0	1045	17	0
47	m	935	0	986	12	0
48	n	477	0	503	9	0
49	o	709	0	747	5	0
50	p	891	0	935	6	0
51	q	730	0	774	9	0
52	r	512	0	543	5	0
53	s	630	0	640	17	0
54	t	655	0	707	6	0
55	u	280	0	342	8	0
56	2	1	0	0	0	0
56	3	1	0	0	0	0
56	A	109	0	0	0	0
56	B	3	0	0	0	0
56	D	1	0	0	0	0
56	a	23	0	0	0	0
56	j	1	0	0	0	0
All	All	148821	0	100168	1325	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 (1325) 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)
9:A:313:G:O2'	9:A:314:G:O5'	1.83	0.96
35:a:1231:A:N6	35:a:1269:A:C6	2.34	0.95
9:A:2350:G:O2'	9:A:2351:A:O5'	1.84	0.94
9:A:1533:U:OP1	9:A:1536:A:N6	2.02	0.93
35:a:865:C:O2'	35:a:866:U:O4'	1.87	0.91
9:A:2795:C:HO2'	12:D:156:THR:HG1	1.08	0.90
35:a:1236:G:N2	35:a:1240:C:O2	2.05	0.90
9:A:2482:U:O2'	9:A:2651:C:OP2	1.91	0.89
35:a:1104:G:O2'	35:a:1105:U:OP2	1.91	0.89
35:a:1392:OMC:HN41	35:a:1475:G:H1	1.17	0.89
35:a:1027:G:O2'	35:a:1196:G:O2'	1.88	0.89
9:A:1710:A:N6	9:A:1716:A:OP2	2.06	0.88
35:a:1264:C:O2'	35:a:1265:U:OP1	1.90	0.88
9:A:451:U:O2'	9:A:452:G:O5'	1.90	0.88
9:A:2350:G:HO2'	9:A:2351:A:P	1.96	0.87
30:V:47:VAL:HA	30:V:56:SER:HA	1.54	0.87
35:a:219:C:O2'	35:a:381:C:OP1	1.93	0.87
13:E:150:GLU:OE2	13:E:195:VAL:HB	1.74	0.87
31:W:63:THR:O	31:W:64:ASN:ND2	2.08	0.86
9:A:2151:A:H2'	9:A:2152:A:C8	2.11	0.86
9:A:965:U:N3	9:A:1043:G:O6	2.09	0.85
9:A:2178:G:O2'	9:A:2180:U:O4	1.93	0.85
9:A:2216:G:N2	9:A:2220:C:O2'	2.09	0.85
35:a:83:U:O2	35:a:86:G:O6	1.94	0.85
9:A:2088:C:O2'	9:A:2089:C:OP1	1.95	0.84
9:A:1996:U:OP2	9:A:2001:A:N6	2.10	0.84
9:A:1092:G:OP1	9:A:1302:G:O2'	1.95	0.83
35:a:21:U:O2	35:a:1059:G:N2	2.11	0.83
9:A:1125:C:OP2	9:A:1126:U:O2'	1.96	0.83
35:a:1415:G:O2'	35:a:1452:A:N6	2.11	0.83
35:a:1386:C:O2	35:a:1483:A:N6	2.12	0.83
35:a:209:A:O2'	35:a:210:A:O5'	1.95	0.83
9:A:661:U:O2'	9:A:1063:G:N2	2.11	0.83
9:A:2333:G:O2'	9:A:2343:G:OP2	1.96	0.83
35:a:178:A:O2'	35:a:208:G:O6	1.97	0.83
35:a:1076:C:O2	35:a:1151:A:O2'	1.97	0.82
26:R:50:ARG:O	26:R:54:LYS:NZ	2.12	0.82
35:a:954:C:O3'	44:j:62:ARG:NH2	2.13	0.82
9:A:114:G:OP2	9:A:116:A:O2'	1.95	0.82
35:a:1232:A:OP2	35:a:1268:C:N4	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1010:U:O2'	9:A:1011:A:OP1	1.97	0.82
9:A:1202:A:O2'	17:I:51:VAL:O	1.97	0.82
20:L:97:ARG:NH1	35:a:339:C:OP2	2.12	0.82
9:A:908:A:OP2	9:A:2294:A:O2'	1.97	0.81
9:A:1899:G:OP2	9:A:1974:A:N6	2.14	0.81
48:n:53:LEU:HD23	48:n:56:VAL:HG11	1.62	0.81
9:A:1044:U:OP2	9:A:1045:C:N4	2.13	0.81
9:A:2580:G:N2	9:A:2586:G:O6	2.14	0.80
35:a:566:U:O2	35:a:735:G:O6	1.99	0.80
9:A:660:U:O2	9:A:2254:A:N6	2.12	0.80
9:A:2049:C:O4'	55:u:29:ARG:NH2	2.14	0.80
10:B:49:C:OP2	24:P:42:ARG:NH1	2.13	0.80
9:A:1181:G:O2'	18:J:91:SER:O	2.00	0.80
9:A:1249:G:O6	9:A:2248:C:O2'	1.99	0.80
35:a:401:C:O2'	35:a:601:A:N3	2.15	0.79
9:A:1730:U:O2'	9:A:1731:A:OP2	1.99	0.79
35:a:644:G:O2'	35:a:646:G:OP2	2.00	0.79
35:a:948:G:O2'	35:a:949:C:OP1	2.01	0.79
9:A:160:A:O2'	9:A:161:U:OP1	2.00	0.79
9:A:222:A:O2'	9:A:508:G:N3	2.15	0.79
35:a:32:G:O2'	35:a:296:U:OP1	2.01	0.79
9:A:176:G:OP2	9:A:176:G:N2	2.14	0.79
9:A:2279:C:N4	9:A:2723:C:O2	2.16	0.79
9:A:1146:A:N3	9:A:2710:G:O2'	2.15	0.79
9:A:2031:G:OP2	9:A:2032:A:O2'	2.01	0.79
35:a:254:G:O2'	51:q:33:GLN:O	2.01	0.78
35:a:1494:C:N4	35:a:1495:G:O6	2.16	0.78
9:A:571:A:H4'	30:V:46:ALA:HA	1.64	0.78
9:A:1500:A:O2'	9:A:1511:U:O2	2.01	0.78
4:4:19:LYS:NZ	4:4:42:CYS:SG	2.56	0.78
35:a:1233:A:N1	35:a:1336:C:O2'	2.16	0.78
9:A:2555:G:O2'	32:X:43:THR:OG1	2.00	0.78
9:A:1163:A:OP1	9:A:1164:A:O2'	2.01	0.78
35:a:1363:U:O2	35:a:1365:C:N4	2.17	0.78
9:A:21:G:O2'	28:T:85:GLU:O	2.02	0.78
9:A:159:A:N1	9:A:160:A:N6	2.32	0.78
9:A:2819:G:N2	9:A:2822:A:OP2	2.15	0.78
35:a:1138:A:OP1	35:a:1139:C:N4	2.17	0.77
9:A:1716:A:N3	9:A:1797:C:O2'	2.17	0.77
35:a:527:A:OP2	38:d:2:ALA:N	2.17	0.77
9:A:191:G:O2'	9:A:917:A:N3	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2176:A:N3	9:A:2784:C:O2'	2.18	0.77
9:A:283:U:O2	9:A:303:G:O6	2.03	0.77
9:A:693:G:N2	9:A:698:G:O3'	2.17	0.77
35:a:1203:G:OP1	35:a:1303:U:O2'	2.01	0.77
9:A:255:A:O2'	9:A:472:C:OP2	2.02	0.77
35:a:975:G:N7	35:a:1194:A:N6	2.32	0.77
10:B:44:C:O2	10:B:47:A:N6	2.18	0.77
4:4:25:THR:OG1	9:A:2510:A:N6	2.18	0.77
10:B:49:C:O2'	10:B:50:C:O5'	2.01	0.76
9:A:15:C:N4	9:A:16:G:O6	2.18	0.76
9:A:1507:G:O2'	9:A:1508:A:O5'	2.03	0.76
35:a:485:G:O2'	35:a:486:G:OP1	2.03	0.76
9:A:1466:C:O2'	9:A:1791:A:O2'	2.02	0.76
9:A:1915:G:OP2	9:A:1916:A:O2'	2.04	0.76
9:A:361:A:O2'	9:A:362:A:O4'	2.02	0.76
35:a:953:G:O2'	35:a:1348:G:O2'	2.02	0.76
1:1:11:SER:OG	9:A:1107:G:OP2	2.00	0.76
9:A:2255:A:N3	9:A:2679:G:O2'	2.18	0.76
9:A:2699:C:O2'	9:A:2701:U:OP2	2.03	0.76
35:a:1043:C:OP2	35:a:1044:G:O2'	2.00	0.76
35:a:1482:U:O2'	35:a:1483:A:OP2	2.04	0.76
9:A:610:C:O2	9:A:646:U:O2'	2.04	0.76
11:C:146:GLU:OE2	11:C:190:ARG:N	2.19	0.76
35:a:173:C:O2'	35:a:1430:A:O2'	2.03	0.76
9:A:1173:G:O2'	9:A:1174:G:O5'	2.00	0.76
9:A:1938:G:N2	9:A:1955:A:OP2	2.12	0.76
35:a:1109:C:O2'	35:a:1110:A:O5'	2.03	0.75
35:a:102:C:O2'	35:a:379:C:OP1	2.04	0.75
9:A:159:A:N3	9:A:2431:C:O2'	2.19	0.75
9:A:624:G:O2'	9:A:648:A:N6	2.20	0.75
9:A:1105:C:O2'	9:A:1118:A:N3	2.20	0.75
35:a:1299:C:N4	48:n:17:ALA:O	2.20	0.75
9:A:1695:U:O2	9:A:1949:C:N4	2.16	0.75
35:a:16:U:O2	35:a:26:G:O6	2.04	0.75
35:a:806:C:O2	42:h:16:ASN:ND2	2.19	0.75
35:a:1131:G:O2'	44:j:73:LEU:O	2.00	0.75
9:A:1000:C:OP2	9:A:1002:C:N4	2.20	0.75
35:a:1231:A:N3	35:a:1353:G:O2'	2.19	0.75
6:6:16:ARG:NH1	6:6:59:ASN:OD1	2.19	0.74
35:a:1106:U:O2'	35:a:1107:G:OP1	2.05	0.74
35:a:1198:C:OP1	48:n:31:HIS:ND1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:613:A:O2'	9:A:2267:C:O2	2.04	0.74
35:a:75:A:N6	35:a:95:C:O2	2.20	0.74
35:a:463:C:OP2	35:a:464:G:O2'	2.06	0.74
35:a:858:A:O5'	42:h:15:ARG:NH1	2.21	0.74
46:l:71:GLY:O	46:l:99:ARG:NH1	2.20	0.74
9:A:2132:U:H2'	9:A:2133:G:C8	2.22	0.74
9:A:1136:C:O2'	9:A:1238:G:N2	2.21	0.74
9:A:3078:G:N2	9:A:3081:A:OP2	2.19	0.74
14:F:13:GLN:NE2	14:F:17:GLU:OE1	2.21	0.74
17:I:48:THR:OG1	17:I:83:LYS:NZ	2.20	0.74
35:a:545:U:OP2	35:a:546:G:O2'	2.05	0.74
9:A:736:G:O2'	9:A:2573:G:O2'	2.06	0.73
35:a:1376:U:HO2'	35:a:1485:C:HO2'	1.33	0.73
9:A:1570:C:N4	9:A:1598:U:O4	2.20	0.73
9:A:485:U:O2'	9:A:2454:G:N2	2.20	0.73
9:A:2693:A:OP1	22:N:120:ARG:NH2	2.21	0.73
35:a:49:U:OP1	35:a:307:C:O2'	2.05	0.73
35:a:880:G:N2	35:a:883:A:OP2	2.21	0.73
6:6:31:HIS:NE2	9:A:2616:A:OP2	2.22	0.73
9:A:1221:A:OP2	9:A:1222:C:N4	2.22	0.73
9:A:1454:G:OP2	29:U:81:ARG:NH1	2.21	0.73
35:a:829:G:O3'	36:b:58:LYS:NZ	2.22	0.73
9:A:2538:A:OP1	14:F:95:ARG:NH1	2.22	0.73
35:a:1107:G:H5''	44:j:77:LEU:HD12	1.71	0.73
9:A:2173:G:O2'	35:a:1402:G:O2'	1.94	0.72
9:A:2907:C:O2	20:L:76:TYR:OH	2.05	0.72
21:M:80:VAL:O	21:M:84:ASN:ND2	2.20	0.72
9:A:1197:C:O2'	18:J:135:ARG:NH1	2.22	0.72
10:B:4:A:O2'	10:B:23:G:N2	2.21	0.72
35:a:1231:A:C6	35:a:1269:A:C6	2.78	0.72
9:A:1094:G:HO2'	9:A:1274:A:HO2'	1.32	0.72
9:A:272:A:N3	9:A:456:C:O2'	2.22	0.72
8:8:21:ARG:NH2	9:A:1100:C:N3	2.38	0.72
9:A:2017:C:OP1	11:C:259:LYS:NZ	2.20	0.72
9:A:2159:G:H1	9:A:2186:C:HO2'	1.38	0.72
15:G:150:ARG:NE	15:G:163:VAL:O	2.23	0.72
35:a:1032:U:O4	35:a:1181:C:O2'	2.07	0.72
9:A:2043:C:O2'	9:A:2195:U:OP2	2.08	0.71
35:a:1206:U:O2'	35:a:1207:C:OP1	2.07	0.71
35:a:705:G:OP1	35:a:835:G:N2	2.24	0.71
35:a:1108:C:C5	44:j:77:LEU:HD13	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:s:22:GLN:NE2	53:s:27:THR:O	2.23	0.71
9:A:1083:G:O4'	9:A:2491:A:N6	2.24	0.71
10:B:47:A:OP1	24:P:14:ARG:NE	2.23	0.71
9:A:2177:A:O2'	9:A:2783:C:O2	2.08	0.71
9:A:3013:C:O2'	9:A:3113:A:N6	2.23	0.71
9:A:1031:G:HO2'	10:B:96:A:HO2'	1.37	0.71
10:B:26:A:O2'	10:B:113:G:O2'	2.05	0.71
1:1:24:ARG:NH2	9:A:1044:U:O4	2.24	0.71
9:A:1033:A:N3	10:B:80:C:O2'	2.22	0.71
16:H:126:SER:O	16:H:130:HIS:NE2	2.24	0.71
43:i:126:ARG:NH2	43:i:127:ASP:O	2.23	0.71
53:s:63:THR:OG1	53:s:66:MET:SD	2.48	0.71
9:A:1479:G:OP1	33:Y:2:ALA:N	2.24	0.71
9:A:964:C:N4	9:A:965:U:O4	2.24	0.71
9:A:2132:U:H2'	9:A:2133:G:H8	1.54	0.70
9:A:2663:A:O2'	9:A:2824:A:OP1	2.08	0.70
9:A:2870:C:OP2	9:A:2956:G:O2'	2.06	0.70
9:A:3086:U:OP2	9:A:3087:G:O2'	2.06	0.70
35:a:1097:G:N2	35:a:1161:A:N3	2.40	0.70
7:7:11:CYS:SG	7:7:14:CYS:N	2.63	0.70
9:A:1493:A:O2'	9:A:1494:U:OP2	2.09	0.70
9:A:2024:G:N2	9:A:2027:A:OP2	2.24	0.70
44:j:8:ILE:HG23	44:j:73:LEU:HD12	1.73	0.70
9:A:2048:G:O2'	55:u:29:ARG:NH2	2.24	0.70
35:a:229:U:O2'	50:p:24:ASP:OD1	2.09	0.70
9:A:2815:C:N4	9:A:2816:G:O6	2.25	0.70
9:A:2975:G:N2	9:A:2975:G:OP1	2.23	0.70
35:a:1297:U:O2'	35:a:1342:A:N3	2.23	0.70
9:A:974:G:O2'	9:A:975:U:O5'	2.10	0.70
9:A:723:C:O2	9:A:733:U:O2'	2.09	0.69
35:a:636:G:N1	35:a:731:U:O4	2.26	0.69
20:L:97:ARG:NH2	35:a:338:A:OP1	2.24	0.69
35:a:654:G:O6	35:a:696:A:N1	2.25	0.69
35:a:1232:A:N3	35:a:1352:C:O2'	2.24	0.69
9:A:993:G:O2'	9:A:1015:A:N6	2.24	0.69
35:a:24:U:O2'	35:a:553:A:N6	2.25	0.69
9:A:2299:C:OP2	9:A:2462:G:N2	2.24	0.69
37:c:66:ASP:OD2	37:c:101:ASN:ND2	2.25	0.69
9:A:336:C:O2'	9:A:337:U:OP1	2.11	0.69
40:f:82:ASN:OD1	40:f:84:SER:OG	2.11	0.69
35:a:352:C:O2'	35:a:353:A:O5'	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:601:A:N3	9:A:673:C:O2'	2.24	0.69
11:C:72:LYS:O	11:C:119:SER:OG	2.11	0.69
35:a:657:U:O2	35:a:757:A:O2'	2.10	0.69
35:a:1231:A:C6	35:a:1269:A:N6	2.61	0.69
35:a:1106:U:N3	44:j:84:VAL:HG22	2.08	0.68
9:A:1092:G:O2'	9:A:1093:A:OP2	2.10	0.68
9:A:248:G:O2'	9:A:2656:A:OP1	2.07	0.68
9:A:2394:A:O2'	9:A:2396:A:OP1	2.04	0.68
35:a:508:C:N4	46:l:46:ASN:OD1	2.27	0.68
35:a:957:A:N6	44:j:50:CYS:SG	2.67	0.68
9:A:539:C:N4	9:A:542:A:OP2	2.24	0.68
9:A:2065:A:C5	35:a:682:A:C6	2.81	0.68
14:F:42:VAL:HG12	14:F:97:THR:HG22	1.76	0.68
35:a:23:C:OP1	39:e:155:SER:OG	2.12	0.68
9:A:2151:A:H2'	9:A:2152:A:H8	1.56	0.68
35:a:397:A:N7	35:a:527:A:O2'	2.25	0.68
35:a:1329:G:N2	35:a:1357:A:OP2	2.23	0.68
9:A:2713:G:O2'	9:A:2714:G:O4'	2.11	0.68
52:r:46:GLY:O	52:r:72:ARG:NH1	2.27	0.67
9:A:89:A:O2'	9:A:90:C:OP1	2.10	0.67
9:A:980:C:O2'	9:A:981:U:O5'	2.10	0.67
35:a:121:U:O2	35:a:236:G:O6	2.11	0.67
35:a:676:A:N3	35:a:766:G:O2'	2.27	0.67
35:a:1355:U:OP1	43:i:93:SER:N	2.27	0.67
35:a:746:A:N6	35:a:793:U:C2	2.62	0.67
35:a:1247:G:N2	35:a:1250:A:OP2	2.27	0.67
9:A:313:G:HO2'	9:A:314:G:P	2.16	0.67
53:s:64:GLU:N	53:s:64:GLU:OE1	2.28	0.67
16:H:124:ILE:HG22	16:H:125:LYS:H	1.59	0.67
35:a:1504:G:OP2	55:u:11:ARG:NH2	2.27	0.67
9:A:2137:A:N6	35:a:1392:OMC:O2	2.28	0.67
9:A:190:A:O2'	9:A:793:C:O2	2.12	0.67
9:A:619:C:OP1	9:A:653:G:N2	2.23	0.67
9:A:1063:G:O6	9:A:1090:G:N2	2.28	0.67
9:A:1201:G:N2	9:A:1204:A:OP2	2.28	0.67
35:a:258:G:OP1	54:t:85:LYS:NZ	2.27	0.67
35:a:1110:A:O2'	43:i:40:ARG:NH1	2.27	0.67
9:A:1886:A:N3	9:A:1888:C:N4	2.43	0.67
9:A:2883:G:N2	9:A:2886:A:OP2	2.28	0.67
9:A:3037:C:O2	9:A:3104:A:O2'	2.13	0.67
35:a:1108:C:N4	44:j:77:LEU:HD22	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1363:G:OP1	26:R:2:ALA:N	2.28	0.66
35:a:746:A:N7	35:a:793:U:O4	2.29	0.66
37:c:169:ARG:NH2	37:c:171:GLY:O	2.28	0.66
9:A:273:A:O2'	9:A:455:C:O2	2.13	0.66
35:a:1206:U:HO2'	35:a:1207:C:P	2.18	0.66
44:j:66:GLU:N	44:j:66:GLU:OE1	2.27	0.66
9:A:2847:G:OP1	9:A:3047:A:O2'	2.09	0.66
9:A:2163:U:OP1	9:A:2828:U:O2'	2.13	0.66
9:A:2588:C:O3'	32:X:55:GLY:N	2.27	0.66
35:a:1392:OMC:N4	35:a:1475:G:H1	1.92	0.66
17:I:26:THR:O	17:I:78:ALA:HB3	1.96	0.66
9:A:2300:A:N3	9:A:2658:A:O2'	2.26	0.66
35:a:718:U:OP1	40:f:4:TYR:OH	2.14	0.66
35:a:1231:A:N6	35:a:1269:A:C5	2.61	0.66
35:a:35:G:O4'	35:a:306:A:O2'	2.14	0.65
35:a:1391:A:H3'	35:a:1392:OMC:H6	1.59	0.65
1:1:21:GLU:OE2	9:A:964:C:O2'	2.13	0.65
9:A:2629:G:O2'	9:A:2630:A:OP1	2.13	0.65
35:a:16:U:O2'	35:a:896:A:OP1	2.13	0.65
9:A:26:U:O2	9:A:1329:G:O2'	2.14	0.65
9:A:1202:A:N6	17:I:79:ILE:O	2.29	0.65
18:J:91:SER:HG	18:J:97:THR:HG1	1.44	0.65
43:i:51:ASP:OD1	43:i:86:HIS:ND1	2.30	0.65
9:A:935:A:N3	9:A:1060:U:O2'	2.29	0.65
9:A:1914:G:N2	9:A:2201:A:O2'	2.23	0.65
35:a:103:G:OP1	35:a:131:G:N2	2.29	0.65
35:a:1046:C:O2'	35:a:1047:A:O5'	2.13	0.65
35:a:1231:A:C5	35:a:1269:A:N6	2.65	0.65
9:A:219:G:N1	9:A:516:G:OP2	2.29	0.65
9:A:541:G:N2	9:A:546:G:OP2	2.30	0.65
9:A:1202:A:H61	17:I:78:ALA:HB1	1.61	0.65
9:A:1569:A:N7	9:A:1603:G:N2	2.44	0.65
10:B:86:U:H1'	10:B:88:C:N4	2.12	0.65
35:a:261:U:OP2	54:t:71:GLN:NE2	2.30	0.65
9:A:451:U:HO2'	9:A:452:G:P	2.19	0.65
2:2:64:ARG:HE	53:s:67:VAL:HG22	1.61	0.64
9:A:33:G:N3	9:A:538:G:O2'	2.31	0.64
9:A:921:C:O2	9:A:2668:G:O2'	2.14	0.64
35:a:1183:U:OP2	44:j:54:SER:OG	2.11	0.64
10:B:30:G:OP1	24:P:14:ARG:NH1	2.31	0.64
26:R:73:ASP:O	26:R:114:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:i:127:ASP:OD2	43:i:129:ARG:NH1	2.31	0.64
9:A:747:A:N6	9:A:768:G:O2'	2.30	0.64
9:A:808:A:O2'	9:A:1468:A:N3	2.29	0.64
31:W:61:HIS:O	31:W:65:ALA:HB2	1.96	0.64
9:A:2854:A:N3	9:A:3112:A:O2'	2.29	0.64
53:s:66:MET:SD	53:s:66:MET:N	2.71	0.64
9:A:709:U:O2'	13:E:184:ASN:ND2	2.31	0.64
35:a:380:G:N2	35:a:383:A:OP2	2.31	0.64
35:a:1300:A:O2'	53:s:68:GLY:O	2.10	0.64
3:3:41:ARG:NH1	9:A:3036:C:O2	2.31	0.63
1:1:42:GLN:NE2	9:A:1042:A:N3	2.45	0.63
9:A:1938:G:H21	9:A:1956:A:H62	1.45	0.63
9:A:2445:A:O3'	11:C:188:ARG:NH2	2.32	0.63
10:B:27:A:OP1	24:P:71:ARG:NH2	2.31	0.63
9:A:1631:A:C8	9:A:1632:G:C8	2.86	0.63
16:H:95:VAL:HG11	16:H:124:ILE:HG21	1.79	0.63
41:g:68:ASN:O	41:g:138:ARG:NH2	2.30	0.63
9:A:1339:G:O2'	9:A:1340:A:O4'	2.14	0.63
9:A:2075:G:O2'	9:A:2076:A:OP2	2.14	0.63
48:n:26:LYS:NZ	48:n:47:MET:SD	2.72	0.63
46:l:54:ARG:NE	46:l:62:GLU:OE2	2.30	0.63
43:i:51:ASP:O	43:i:53:ARG:NH1	2.31	0.63
14:F:63:ASP:OD2	14:F:157:ARG:NH2	2.31	0.63
44:j:77:LEU:HD23	44:j:78:ASP:N	2.14	0.63
9:A:669:G:O2'	9:A:1369:A:OP1	2.17	0.63
25:Q:48:ARG:NE	25:Q:59:THR:OG1	2.32	0.63
9:A:2065:A:C6	35:a:682:A:N6	2.68	0.62
44:j:48:VAL:HG23	44:j:48:VAL:O	1.98	0.62
9:A:617:U:N3	9:A:2245:C:O2	2.32	0.62
38:d:59:SER:O	38:d:106:ARG:NH1	2.31	0.62
9:A:417:C:O2	30:V:69:SER:OG	2.10	0.62
9:A:1437:A:N1	9:A:1448:C:O2'	2.32	0.62
35:a:948:G:HO2'	35:a:949:C:P	2.22	0.62
9:A:614:C:N4	9:A:3003:C:OP2	2.26	0.62
9:A:1825:C:N4	9:A:1840:G:OP2	2.33	0.62
35:a:697:C:O2'	35:a:714:G:O4'	2.16	0.62
10:B:26:A:HO2'	10:B:113:G:HO2'	1.47	0.62
47:m:86:CYS:SG	47:m:87:TYR:N	2.73	0.62
9:A:565:A:N6	9:A:588:A:OP1	2.33	0.61
9:A:202:C:OP2	9:A:203:A:O2'	2.14	0.61
9:A:2316:G:O2'	9:A:2421:A:N1	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:1474:C:H2'	35:a:1475:G:C8	2.34	0.61
37:c:71:ARG:NH2	37:c:72:PRO:O	2.33	0.61
4:4:8:ARG:NE	9:A:2509:C:OP2	2.32	0.61
9:A:2907:C:N3	9:A:2951:G:O2'	2.32	0.61
44:j:8:ILE:HG21	44:j:10:LEU:HD23	1.81	0.61
9:A:543:U:O2'	9:A:544:U:OP1	2.18	0.61
9:A:2006:A:OP2	11:C:222:ARG:NH1	2.33	0.61
9:A:2072:G:O2'	9:A:2311:G:O2'	2.18	0.61
9:A:2973:A:O2'	15:G:63:ARG:NH1	2.34	0.61
28:T:97:GLN:OE1	28:T:99:ARG:NH2	2.33	0.61
5:5:19:HIS:NE2	9:A:552:U:O2	2.34	0.61
35:a:988:C:O2'	35:a:1018:C:O2'	2.18	0.61
9:A:1067:G:O6	9:A:1086:C:N4	2.34	0.61
35:a:1209:C:OP1	47:m:108:ARG:NH1	2.33	0.61
22:N:55:ASN:ND2	31:W:190:LEU:O	2.34	0.61
35:a:1108:C:H41	44:j:77:LEU:HD22	1.63	0.61
9:A:380:A:N1	9:A:404:A:O2'	2.26	0.60
9:A:1112:C:OP2	26:R:54:LYS:NZ	2.30	0.60
35:a:874:A:O2'	35:a:1398:G:O2'	2.18	0.60
9:A:1224:G:N1	9:A:1225:G:O6	2.34	0.60
5:5:11:ASN:ND2	9:A:885:G:OP1	2.34	0.60
9:A:724:G:N2	9:A:727:A:OP2	2.30	0.60
9:A:1531:C:O2'	9:A:1532:G:OP1	2.17	0.60
9:A:2805:G:N2	9:A:2805:G:OP2	2.35	0.60
35:a:1472:G:H2'	35:a:1473:A:C8	2.36	0.60
13:E:138:THR:HG21	13:E:168:SER:CB	2.31	0.60
35:a:1351:G:OP2	43:i:134:LYS:NZ	2.34	0.60
20:L:54:ARG:NH2	35:a:1404:C:OP1	2.34	0.60
35:a:100:G:OP1	54:t:16:ARG:NH1	2.34	0.60
5:5:14:ARG:NH2	9:A:885:G:OP2	2.35	0.60
9:A:160:A:H2	9:A:2442:U:O4'	1.85	0.59
18:J:91:SER:OG	18:J:97:THR:OG1	2.14	0.59
9:A:159:A:C6	9:A:160:A:N6	2.68	0.59
9:A:404:A:OP1	13:E:170:ARG:NE	2.35	0.59
9:A:2193:A:H2'	9:A:2196:G:H21	1.67	0.59
9:A:2349:A:N6	9:A:2385:G:O3'	2.35	0.59
35:a:66:U:O2'	35:a:379:C:O2	2.20	0.59
9:A:2648:C:O2	9:A:2653:G:O2'	2.21	0.59
35:a:257:G:O6	35:a:270:A:N6	2.34	0.59
35:a:970:G:O2'	35:a:971:G:OP1	2.21	0.59
35:a:1474:C:H2'	35:a:1475:G:H8	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:392:A:O2'	9:A:393:U:OP2	2.19	0.59
9:A:1099:A:OP2	9:A:1100:C:N4	2.36	0.59
9:A:1870:U:O2'	9:A:1872:A:OP2	2.10	0.59
35:a:1055:U:O4	35:a:1056:C:N4	2.36	0.59
9:A:1177:G:OP1	18:J:73:LYS:NZ	2.35	0.59
9:A:2916:C:O2	9:A:3068:U:O2'	2.19	0.59
20:L:4:GLN:OE1	20:L:23:ARG:NH2	2.36	0.59
35:a:664:U:O2'	45:k:50:VAL:O	2.15	0.59
35:a:1070:U:O2'	35:a:1071:U:O4'	2.20	0.59
35:a:529:C:N4	35:a:530:G:O6	2.36	0.59
35:a:558:C:O2'	35:a:708:A:N3	2.30	0.59
35:a:1105:U:OP1	44:j:35:SER:OG	2.09	0.59
9:A:2147:U:N3	9:A:2148:C:N4	2.50	0.59
10:B:49:C:HO2'	10:B:50:C:C5'	2.16	0.59
9:A:679:G:OP2	21:M:24:ARG:NH1	2.35	0.58
9:A:1071:G:O2'	9:A:2498:A:N1	2.31	0.58
9:A:2021:G:O6	9:A:2031:G:N2	2.35	0.58
21:M:89:GLN:NE2	21:M:90:GLY:O	2.36	0.58
35:a:1387:C:O2'	35:a:1388:G:H5'	2.02	0.58
9:A:265:A:N6	9:A:359:A:N7	2.52	0.58
9:A:1173:G:HO2'	9:A:1174:G:C5'	2.13	0.58
44:j:72:ARG:O	44:j:73:LEU:HD13	2.03	0.58
9:A:1911:U:O2'	11:C:14:ARG:NH1	2.34	0.58
31:W:89:ARG:O	31:W:90:ARG:NH2	2.36	0.58
34:Z:28:GLU:OE2	34:Z:46:ARG:NH1	2.37	0.58
35:a:25:G:H21	35:a:896:A:H62	1.52	0.58
9:A:218:A:N3	9:A:234:U:O2'	2.36	0.58
9:A:365:U:O2	9:A:437:G:O6	2.22	0.58
35:a:745:G:H1	35:a:792:G:HO2'	1.50	0.58
35:a:1007:U:O2'	35:a:1008:C:O5'	2.22	0.58
35:a:1476:A:H2'	35:a:1477:A:C8	2.38	0.58
9:A:551:G:N2	9:A:554:A:OP2	2.31	0.58
14:F:126:PRO:O	14:F:174:ARG:NH1	2.37	0.58
20:L:88:LYS:N	20:L:92:ASP:O	2.35	0.58
9:A:672:C:OP1	26:R:33:ARG:NH1	2.36	0.57
9:A:1552:A:O2'	9:A:1618:C:N4	2.37	0.57
9:A:2942:G:O2'	9:A:3068:U:OP1	2.22	0.57
35:a:1180:U:OP1	44:j:57:LYS:NZ	2.30	0.57
2:2:64:ARG:NE	53:s:67:VAL:HG22	2.19	0.57
9:A:1930:C:OP2	9:A:1931:A:O2'	2.18	0.57
35:a:849:G:O2'	35:a:855:A:N1	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:j:8:ILE:CG2	44:j:73:LEU:HD12	2.34	0.57
35:a:23:C:OP1	39:e:160:ASN:ND2	2.37	0.57
38:d:134:GLN:O	50:p:102:LYS:NZ	2.38	0.57
46:l:37:VAL:HG12	46:l:53:ALA:HB2	1.85	0.57
53:s:22:GLN:OE1	53:s:47:HIS:ND1	2.35	0.57
31:W:94:HIS:NE2	31:W:96:ASP:OD1	2.36	0.57
9:A:2489:U:OP2	9:A:2490:A:O2'	2.20	0.57
35:a:1128:C:O2	43:i:38:ARG:NE	2.38	0.57
35:a:1234:G:O2'	35:a:1235:G:O5'	2.22	0.57
9:A:1649:C:N4	9:A:1790:A:OP2	2.36	0.57
35:a:69:A:N6	35:a:216:U:O4'	2.38	0.57
35:a:1107:G:O5'	44:j:76:ILE:O	2.22	0.57
35:a:1392:OMC:H3'	35:a:1393:G:H8	1.69	0.57
42:h:13:ARG:NH2	42:h:26:THR:O	2.37	0.57
9:A:723:C:O3'	9:A:743:G:N2	2.37	0.57
9:A:1971:C:OP1	25:Q:93:ARG:NE	2.37	0.57
35:a:438:U:O2'	35:a:439:U:O2	2.21	0.57
9:A:1541:G:N2	9:A:1631:A:H62	2.03	0.57
35:a:510:G:O2'	35:a:511:U:OP1	2.22	0.57
10:B:9:G:OP1	24:P:37:ARG:NH2	2.38	0.56
23:O:49:GLU:OE1	23:O:94:TYR:N	2.38	0.56
35:a:1394:U:H2'	35:a:1395:C:C6	2.40	0.56
9:A:981:U:O2'	9:A:982:A:OP2	2.23	0.56
9:A:1176:G:OP1	18:J:12:LYS:NZ	2.33	0.56
9:A:1249:G:O2'	9:A:2249:G:O2'	2.24	0.56
12:D:27:THR:OG1	12:D:196:GLY:O	2.23	0.56
30:V:47:VAL:HA	30:V:56:SER:CA	2.29	0.56
8:8:10:ASP:OD2	9:A:1252:G:N2	2.37	0.56
9:A:65:G:N2	9:A:71:A:O4'	2.39	0.56
9:A:2409:U:O4	9:A:2410:A:N6	2.39	0.56
9:A:2601:A:O2'	24:P:127:PHE:O	2.19	0.56
25:Q:23:ASP:OD1	25:Q:89:GLY:N	2.37	0.56
22:N:58:ILE:HD12	22:N:106:LEU:HD21	1.86	0.56
35:a:562:U:O4	35:a:563:A:N6	2.39	0.56
4:4:15:CYS:SG	4:4:16:GLU:N	2.78	0.56
53:s:16:LEU:HD13	53:s:41:ILE:HG21	1.88	0.56
9:A:2065:A:N7	35:a:682:A:C6	2.74	0.56
24:P:98:GLU:N	24:P:98:GLU:OE1	2.37	0.56
44:j:64:HIS:O	48:n:60:SER:N	2.39	0.56
9:A:389:G:H21	9:A:412:A:H61	1.53	0.56
9:A:3008:C:O2'	12:D:38:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:1289:U:O2'	47:m:110:ARG:NE	2.35	0.56
14:F:108:ASP:OD1	14:F:109:ARG:N	2.38	0.55
25:Q:2:ASN:O	25:Q:5:ASP:N	2.38	0.55
2:2:1:MET:SD	2:2:6:HIS:NE2	2.79	0.55
9:A:931:C:OP1	9:A:1300:G:O2'	2.14	0.55
35:a:561:G:N1	35:a:739:A:OP2	2.35	0.55
9:A:1203:A:N3	17:I:51:VAL:HG22	2.22	0.55
35:a:1264:C:O2'	35:a:1265:U:P	2.64	0.55
9:A:1112:C:OP1	26:R:53:ARG:NH2	2.39	0.55
13:E:20:LEU:O	13:E:20:LEU:HD12	2.07	0.55
35:a:995:A:N6	35:a:1001:G:O6	2.39	0.55
41:g:15:ASP:OD2	41:g:18:TYR:N	2.36	0.55
9:A:1568:C:N4	9:A:1604:G:O2'	2.39	0.55
9:A:2015:U:OP2	11:C:272:ARG:NH1	2.37	0.55
44:j:37:VAL:HG22	44:j:38:GLY:H	1.70	0.55
9:A:698:G:N3	9:A:772:U:O2'	2.40	0.55
23:O:37:THR:HG22	23:O:39:PRO:HD2	1.88	0.55
24:P:43:SER:O	24:P:112:ARG:NH1	2.40	0.55
35:a:1102:A:N6	35:a:1103:U:O4	2.40	0.55
9:A:604:C:O2'	28:T:25:ARG:NH1	2.40	0.55
9:A:869:U:O2'	9:A:1387:A:N1	2.39	0.55
9:A:2303:A:OP1	33:Y:19:SER:OG	2.25	0.55
9:A:3038:C:OP1	23:O:42:ARG:NH1	2.37	0.55
9:A:3042:A:OP1	12:D:201:ARG:NH1	2.39	0.54
14:F:63:ASP:OD2	14:F:142:GLN:NE2	2.40	0.54
35:a:1038:G:H4'	37:c:186:LEU:HD11	1.88	0.54
9:A:263:G:O2'	9:A:517:A:N3	2.41	0.54
9:A:531:A:OP1	13:E:47:GLN:N	2.41	0.54
35:a:481:G:OP1	46:l:114:ARG:NH2	2.39	0.54
24:P:18:ARG:NH1	24:P:105:GLY:O	2.40	0.54
9:A:1336:A:OP1	27:S:91:ARG:NH1	2.41	0.54
9:A:2051:U:O2'	9:A:2194:A:OP2	2.24	0.54
25:Q:22:GLY:N	25:Q:46:VAL:O	2.41	0.54
35:a:225:G:O2'	51:q:10:THR:O	2.25	0.54
9:A:1940:A:N6	9:A:1954:C:O2'	2.40	0.54
19:K:13:ARG:NH2	19:K:49:ASP:O	2.41	0.54
6:6:7:HIS:NE2	9:A:251:A:OP1	2.39	0.54
9:A:1380:A:N6	9:A:2238:A:OP2	2.41	0.54
9:A:479:A:O2'	9:A:498:G:OP1	2.19	0.54
9:A:1173:G:C2'	9:A:1174:G:O5'	2.55	0.54
9:A:2204:G:O2'	9:A:2206:C:OP2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2454:G:O2'	33:Y:30:ASN:O	2.22	0.54
9:A:357:U:H4'	9:A:358:G:O5'	2.08	0.54
9:A:1010:U:HO2'	9:A:1011:A:P	2.29	0.54
9:A:1046:C:O2'	9:A:1287:C:O2	2.23	0.54
13:E:157:VAL:HG12	13:E:178:ILE:HG13	1.90	0.54
7:7:19:ARG:NH1	9:A:2980:U:OP2	2.39	0.53
9:A:977:G:O2'	10:B:78:U:O2	2.25	0.53
9:A:2515:U:O2'	9:A:2598:C:O2	2.26	0.53
11:C:186:ASP:N	11:C:186:ASP:OD1	2.41	0.53
9:A:1248:U:O2	12:D:159:ARG:NH1	2.40	0.53
9:A:1456:G:OP1	9:A:1512:U:N3	2.40	0.53
44:j:12:ALA:HB2	44:j:18:ILE:HD12	1.90	0.53
9:A:1668:C:O2'	9:A:1764:A:N3	2.37	0.53
35:a:1057:G:N2	35:a:1060:A:OP2	2.33	0.53
53:s:19:VAL:HG13	53:s:47:HIS:CD2	2.44	0.53
9:A:1043:G:N2	9:A:1044:U:O4	2.42	0.53
35:a:323:U:O4	35:a:327:A:N7	2.41	0.53
35:a:1214:G:O2'	35:a:1348:G:OP1	2.26	0.53
9:A:97:U:OP1	9:A:98:U:O2'	2.16	0.53
9:A:1847:U:O4	9:A:1848:A:N6	2.41	0.53
35:a:92:A:O2'	35:a:93:C:O5'	2.27	0.53
35:a:145:G:O6	35:a:171:A:N1	2.42	0.53
35:a:1471:G:C2'	35:a:1472:G:H5'	2.39	0.53
45:k:45:ASP:OD1	45:k:49:ASN:N	2.40	0.53
35:a:746:A:N7	35:a:793:U:C4	2.77	0.53
9:A:1035:G:N2	9:A:2493:A:O4'	2.42	0.53
9:A:571:A:H4'	30:V:46:ALA:CA	2.36	0.53
35:a:496:U:OP2	35:a:497:G:N2	2.42	0.53
35:a:1278:C:OP1	47:m:44:ARG:NH2	2.42	0.53
17:I:9:ALA:O	17:I:13:ILE:HG13	2.09	0.52
35:a:177:U:O4	35:a:209:A:N7	2.41	0.52
35:a:1234:G:HO2'	35:a:1235:G:C5'	2.21	0.52
44:j:61:SER:O	48:n:59:SER:OG	2.20	0.52
6:6:13:ARG:NH1	9:A:250:G:OP2	2.42	0.52
9:A:81:A:OP1	30:V:4:HIS:NE2	2.43	0.52
9:A:190:A:H3'	9:A:191:G:H21	1.74	0.52
9:A:672:C:H4'	26:R:31:LEU:HD13	1.91	0.52
35:a:485:G:O2'	35:a:486:G:P	2.67	0.52
40:f:87:ARG:NH1	52:r:73:GLU:O	2.42	0.52
9:A:66:C:O2	9:A:70:A:O2'	2.26	0.52
9:A:81:A:N1	9:A:96:G:O2'	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1787:A:O2'	11:C:63:ARG:NH1	2.43	0.52
9:A:1880:U:O2'	9:A:2911:U:OP1	2.26	0.52
9:A:576:G:O2'	9:A:579:A:N6	2.42	0.52
9:A:1137:U:OP1	9:A:1153:U:O2'	2.25	0.52
9:A:1533:U:O2	9:A:1803:A:O2'	2.21	0.52
35:a:1120:G:O2'	44:j:77:LEU:HD11	2.09	0.52
9:A:981:U:O2'	9:A:982:A:P	2.67	0.52
35:a:81:C:H3'	35:a:82:U:H5''	1.90	0.52
35:a:671:G:N2	35:a:676:A:OP2	2.41	0.52
35:a:1387:C:O2	35:a:1503:A:O2'	2.27	0.52
54:t:45:ASP:OD1	54:t:46:LYS:N	2.42	0.52
35:a:1233:A:O2'	44:j:45:GLU:OE1	2.27	0.52
1:1:16:ARG:NH2	9:A:1086:C:OP2	2.42	0.52
9:A:2452:G:N2	33:Y:34:GLN:OE1	2.39	0.52
9:A:2733:G:N1	9:A:2804:U:O4	2.43	0.52
35:a:101:G:N2	35:a:379:C:O3'	2.42	0.52
35:a:1478:G:O5'	35:a:1478:G:H8	1.92	0.52
9:A:2329:G:O6	9:A:2407:C:N4	2.43	0.52
7:7:8:LYS:NZ	9:A:2691:C:OP1	2.43	0.52
9:A:223:A:N7	9:A:507:G:O2'	2.43	0.52
35:a:418:C:O2	38:d:35:GLN:NE2	2.43	0.52
9:A:2033:U:O4	11:C:35:ARG:NH2	2.42	0.51
9:A:2048:G:N3	55:u:29:ARG:NH1	2.59	0.51
10:B:34:G:O2'	10:B:35:G:O5'	2.25	0.51
10:B:82:A:N1	10:B:91:G:O6	2.43	0.51
35:a:483:C:O2'	35:a:490:A:N6	2.43	0.51
38:d:15:LEU:HD11	38:d:58:PHE:HD2	1.75	0.51
6:6:47:ARG:NH1	9:A:725:A:OP2	2.43	0.51
10:B:70:G:H22	10:B:103:G:H1	1.57	0.51
31:W:62:GLY:O	31:W:63:THR:OG1	2.28	0.51
31:W:166:GLU:N	31:W:166:GLU:OE1	2.41	0.51
35:a:1264:C:HO2'	35:a:1265:U:P	2.33	0.51
10:B:30:G:N2	14:F:33:MET:SD	2.84	0.51
10:B:88:C:H2'	10:B:89:C:O4'	2.11	0.51
37:c:67:ILE:HG13	37:c:102:ILE:HG23	1.91	0.51
9:A:830:A:OP1	49:o:64:ARG:NH1	2.43	0.51
35:a:1109:C:O2'	35:a:1110:A:P	2.68	0.51
9:A:2328:G:C6	9:A:2408:G:C2	2.98	0.51
9:A:2670:G:N2	9:A:2673:U:O2	2.42	0.51
19:K:129:ASP:OD1	19:K:129:ASP:N	2.43	0.51
35:a:1380:C:OP2	39:e:54:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:r:57:CYS:SG	52:r:60:HIS:ND1	2.78	0.51
53:s:19:VAL:HG11	53:s:44:PHE:HD1	1.75	0.51
8:8:18:HIS:HB3	10:B:86:U:C5	2.46	0.51
9:A:736:G:N2	9:A:739:U:OP2	2.43	0.51
9:A:2135:U:H2'	9:A:2142:A:N1	2.25	0.51
9:A:643:G:O2'	9:A:644:G:OP1	2.19	0.51
9:A:2015:U:OP1	11:C:271:ARG:NH1	2.42	0.51
10:B:90:G:H2'	10:B:91:G:H8	1.75	0.51
9:A:1212:U:N3	9:A:1215:U:OP2	2.39	0.51
9:A:1777:U:OP2	9:A:1778:A:O2'	2.14	0.51
9:A:1899:G:N2	9:A:1980:G:OP2	2.36	0.51
9:A:2018:G:O4'	9:A:2426:C:O2'	2.29	0.51
35:a:1311:G:O2'	47:m:23:TYR:O	2.29	0.51
16:H:113:ASP:OD1	16:H:113:ASP:N	2.40	0.51
9:A:123:A:O2'	9:A:124:A:O4'	2.25	0.51
9:A:2150:U:H2'	9:A:2152:A:OP2	2.11	0.51
9:A:2975:G:OP2	15:G:3:ARG:NH1	2.43	0.51
35:a:439:U:O2'	38:d:114:SER:O	2.29	0.51
9:A:2242:G:O2'	26:R:34:LYS:NZ	2.32	0.50
15:G:2:SER:OG	15:G:3:ARG:N	2.44	0.50
35:a:125:U:N3	35:a:128:U:O4	2.44	0.50
35:a:501:G:N7	46:l:50:ARG:NH2	2.56	0.50
44:j:47:ASN:ND2	44:j:67:MET:O	2.40	0.50
9:A:1224:G:H3'	17:I:76:PRO:HB2	1.93	0.50
9:A:2752:U:O2'	9:A:2754:G:OP1	2.24	0.50
35:a:294:C:OP1	35:a:590:A:O2'	2.29	0.50
9:A:159:A:N7	9:A:166:A:C6	2.80	0.50
9:A:2929:A:O2'	9:A:3073:G:OP1	2.25	0.50
10:B:7:G:N2	24:P:50:GLN:OE1	2.42	0.50
35:a:632:U:O4	35:a:733:A:N7	2.44	0.50
35:a:1257:G:N2	35:a:1263:C:O2	2.37	0.50
36:b:118:GLU:OE1	36:b:152:ARG:NH2	2.44	0.50
42:h:5:ASP:OD2	42:h:79:ARG:NH2	2.45	0.50
9:A:543:U:H2'	9:A:543:U:O2	2.10	0.50
17:I:27:GLU:HA	17:I:78:ALA:HB3	1.93	0.50
35:a:1119:U:H2'	35:a:1119:U:O2	2.10	0.50
49:o:39:LEU:HD23	49:o:56:LEU:HB2	1.92	0.50
9:A:2474:G:O2'	9:A:2720:C:OP1	2.20	0.50
22:N:67:ASN:ND2	22:N:105:GLU:OE2	2.42	0.50
9:A:1628:A:H4'	9:A:1630:U:OP1	2.12	0.50
26:R:43:LEU:HD13	27:S:76:HIS:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:1392:OMC:O2	35:a:1392:OMC:H2'	2.11	0.50
38:d:92:ARG:NH1	38:d:94:ASP:OD2	2.45	0.50
9:A:2328:G:C6	9:A:2408:G:N1	2.80	0.50
27:S:43:VAL:HG13	27:S:48:VAL:HG12	1.93	0.50
35:a:1478:G:H2'	35:a:1479:U:C6	2.47	0.50
9:A:2077:C:H42	9:A:2106:A:H61	1.60	0.50
9:A:2537:C:OP1	14:F:75:ARG:NH1	2.45	0.50
9:A:2880:U:O2	9:A:2889:A:N7	2.45	0.50
9:A:1203:A:C4	17:I:51:VAL:HG22	2.46	0.49
9:A:2085:C:O2'	9:A:2086:U:O5'	2.30	0.49
38:d:95:ASN:OD1	38:d:106:ARG:NE	2.44	0.49
9:A:813:C:O2'	9:A:849:A:N6	2.45	0.49
9:A:1426:G:OP2	9:A:1426:G:N2	2.41	0.49
9:A:2139:U:C4	9:A:2140:A:C6	3.01	0.49
9:A:2199:G:N3	55:u:33:LYS:NZ	2.51	0.49
40:f:23:LEU:HD22	40:f:63:ILE:HD11	1.94	0.49
43:i:28:THR:OG1	43:i:29:VAL:N	2.41	0.49
44:j:25:ILE:O	44:j:29:VAL:HG22	2.12	0.49
9:A:89:A:HO2'	9:A:90:C:P	2.31	0.49
9:A:1070:G:O2'	9:A:2490:A:OP2	2.28	0.49
36:b:181:ILE:N	36:b:182:PRO:CD	2.75	0.49
39:e:182:ARG:NH2	42:h:43:GLU:OE1	2.44	0.49
9:A:958:A:N6	9:A:1053:G:O6	2.45	0.49
9:A:1259:U:OP2	19:K:65:SER:OG	2.25	0.49
9:A:1272:C:OP1	26:R:92:ARG:NH2	2.44	0.49
9:A:1540:U:C5	9:A:1629:G:C8	3.00	0.49
9:A:2163:U:O4'	9:A:2815:C:O2'	2.21	0.49
35:a:1261:A:C4	44:j:6:ILE:HG23	2.48	0.49
48:n:53:LEU:HD23	48:n:56:VAL:CG1	2.38	0.49
9:A:380:A:O2'	9:A:381:A:O4'	2.22	0.49
18:J:23:ALA:HB3	18:J:24:PRO:HD3	1.94	0.49
35:a:928:A:O2'	35:a:1315:A:N3	2.43	0.49
38:d:197:GLU:OE2	39:e:137:ARG:NH2	2.46	0.49
51:q:22:THR:OG1	51:q:77:MET:SD	2.69	0.49
9:A:2157:G:H5''	55:u:26:VAL:HG21	1.94	0.49
35:a:409:G:OP1	38:d:104:ARG:NH2	2.46	0.49
35:a:1105:U:O5'	44:j:35:SER:HB3	2.12	0.49
9:A:1436:C:O3'	28:T:18:ARG:NH2	2.46	0.49
9:A:2698:C:H2'	9:A:2698:C:O2	2.11	0.49
35:a:216:U:O2'	35:a:217:U:OP2	2.26	0.49
35:a:242:U:OP1	46:l:13:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:1106:U:OP2	44:j:77:LEU:O	2.29	0.49
35:a:1312:U:O4	35:a:1313:G:N1	2.45	0.49
46:l:75:GLN:OE1	46:l:76:GLU:N	2.45	0.49
9:A:131:A:N6	9:A:145:G:O6	2.45	0.49
38:d:94:ASP:OD1	38:d:95:ASN:N	2.45	0.49
39:e:71:VAL:O	39:e:97:PHE:N	2.46	0.49
41:g:56:THR:OG1	41:g:57:ASP:N	2.46	0.49
9:A:993:G:N2	9:A:1015:A:OP2	2.43	0.49
20:L:102:VAL:HB	20:L:106:LEU:HD12	1.93	0.49
35:a:417:G:N2	35:a:520:G:O3'	2.44	0.49
1:l:24:ARG:CZ	9:A:1044:U:O4	2.61	0.49
9:A:664:A:OP2	27:S:81:LYS:NZ	2.45	0.49
9:A:1058:A:N3	9:A:1305:G:O2'	2.39	0.49
9:A:1679:A:O2'	9:A:1680:A:OP2	2.22	0.49
9:A:2796:A:OP2	12:D:155:ALA:N	2.38	0.49
9:A:2842:G:N3	12:D:160:VAL:HG21	2.28	0.49
10:B:8:C:OP1	24:P:18:ARG:NH2	2.44	0.49
13:E:131:VAL:HG11	13:E:138:THR:HG22	1.94	0.49
23:O:24:LEU:HB3	23:O:44:LEU:HD22	1.95	0.49
35:a:987:A:N6	35:a:1008:C:O4'	2.46	0.49
35:a:1080:C:OP2	36:b:96:TRP:N	2.39	0.49
9:A:2244:A:N6	9:A:2259:G:O6	2.46	0.48
9:A:2515:U:O2	9:A:2598:C:O2'	2.30	0.48
18:J:95:HIS:NE2	18:J:135:ARG:O	2.46	0.48
31:W:156:GLN:HB3	31:W:177:LEU:HD13	1.94	0.48
35:a:1432:C:N4	35:a:1433:C:N4	2.60	0.48
9:A:403:U:O2'	9:A:422:A:N3	2.45	0.48
9:A:535:A:N1	9:A:542:A:O2'	2.28	0.48
9:A:958:A:N6	9:A:1053:G:C6	2.82	0.48
35:a:1106:U:OP2	44:j:78:ASP:O	2.31	0.48
44:j:80:THR:O	44:j:84:VAL:HG23	2.13	0.48
9:A:698:G:O2'	9:A:772:U:O2	2.31	0.48
9:A:2314:U:OP2	9:A:2315:U:O2'	2.28	0.48
9:A:2424:C:OP1	33:Y:48:ARG:NH2	2.44	0.48
14:F:86:LEU:HD22	14:F:92:ILE:HD11	1.95	0.48
22:N:130:ARG:NH2	31:W:88:ILE:O	2.47	0.48
35:a:625:G:O2'	51:q:43:ARG:NH2	2.46	0.48
35:a:753:G:O6	35:a:787:A:N6	2.46	0.48
35:a:772:A:O2'	35:a:774:A:N7	2.37	0.48
9:A:667:A:OP2	9:A:2723:C:O2'	2.29	0.48
25:Q:26:ASN:OD1	25:Q:26:ASN:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:11:SER:HB2	1:1:31:ILE:HD11	1.96	0.48
9:A:3070:G:O3'	9:A:3087:G:N2	2.47	0.48
13:E:138:THR:HG21	13:E:168:SER:OG	2.13	0.48
35:a:1011:U:O2'	35:a:1012:U:O5'	2.27	0.48
12:D:110:ALA:O	12:D:182:VAL:HG12	2.13	0.48
35:a:746:A:N6	35:a:793:U:N3	2.61	0.48
35:a:983:C:N4	35:a:984:A:H62	2.12	0.48
44:j:19:ASP:OD1	44:j:20:ALA:N	2.47	0.48
14:F:117:ARG:O	47:m:3:ARG:NH2	2.47	0.48
16:H:124:ILE:O	16:H:125:LYS:HB2	2.14	0.48
35:a:126:G:N7	51:q:17:ARG:NH2	2.61	0.48
9:A:723:C:N4	9:A:724:G:O6	2.47	0.48
9:A:1042:A:C2	9:A:1043:G:N7	2.82	0.48
9:A:2131:G:H2'	9:A:2132:U:H5'	1.95	0.48
9:A:160:A:C2	9:A:2442:U:O4'	2.66	0.48
9:A:2925:C:O2'	23:O:73:LYS:NZ	2.33	0.48
9:A:2054:C:H1'	9:A:2152:A:H1'	1.96	0.48
12:D:160:VAL:HG12	12:D:160:VAL:O	2.13	0.48
52:r:20:CYS:SG	52:r:21:VAL:N	2.86	0.48
9:A:166:A:N6	9:A:167:G:N3	2.62	0.47
9:A:1337:G:N2	9:A:1340:A:OP2	2.47	0.47
9:A:2054:C:O2	9:A:2151:A:H2	1.97	0.47
9:A:2075:G:HO2'	9:A:2076:A:P	2.36	0.47
9:A:2349:A:H61	9:A:2386:U:P	2.37	0.47
12:D:118:SER:OG	12:D:173:ASP:OD1	2.31	0.47
17:I:110:MET:SD	17:I:111:ASP:N	2.87	0.47
25:Q:47:ILE:O	25:Q:96:LEU:N	2.41	0.47
35:a:540:A:C6	39:e:153:LEU:HD13	2.49	0.47
35:a:888:A:O2'	35:a:889:A:O4'	2.29	0.47
30:V:59:ILE:HG23	30:V:59:ILE:O	2.14	0.47
32:X:15:ASP:OD1	32:X:15:ASP:C	2.58	0.47
35:a:636:G:O2'	49:o:28:GLN:OE1	2.27	0.47
8:8:4:ARG:NH2	9:A:1078:G:O6	2.48	0.47
9:A:963:U:H2'	9:A:964:C:O4'	2.14	0.47
9:A:980:C:HO2'	9:A:981:U:P	2.34	0.47
9:A:2137:A:C2	35:a:1478:G:C8	3.01	0.47
18:J:138:GLY:O	18:J:139:ILE:HD13	2.14	0.47
26:R:77:ASN:OD1	26:R:78:ARG:N	2.47	0.47
35:a:408:G:O3'	38:d:104:ARG:NH1	2.47	0.47
35:a:498:C:O2	46:l:47:SER:OG	2.30	0.47
35:a:1234:G:O2'	35:a:1235:G:P	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:907:A:N3	9:A:2295:C:O2'	2.41	0.47
33:Y:19:SER:OG	33:Y:20:HIS:N	2.46	0.47
35:a:64:A:OP1	35:a:107:G:N2	2.47	0.47
9:A:670:A:OP1	9:A:1370:U:O2'	2.32	0.47
9:A:1127:A:O2'	9:A:1128:A:O4'	2.25	0.47
9:A:1224:G:N3	9:A:1224:G:H2'	2.29	0.47
9:A:1518:A:O2'	9:A:1692:G:O2'	2.29	0.47
35:a:745:G:N1	35:a:792:G:O2'	2.38	0.47
39:e:63:ILE:HD12	39:e:73:VAL:HG12	1.95	0.47
43:i:108:ILE:HD11	43:i:124:LEU:HD22	1.95	0.47
4:4:17:VAL:HG23	4:4:18:CYS:N	2.29	0.47
35:a:429:U:OP1	38:d:13:ARG:NH1	2.48	0.47
35:a:1107:G:N3	35:a:1107:G:H2'	2.30	0.47
9:A:1350:G:O3'	9:A:1351:G:O4'	2.32	0.47
9:A:1532:G:O2'	9:A:1533:U:O5'	2.30	0.47
9:A:1631:A:H8	9:A:1632:G:C8	2.30	0.47
9:A:1888:C:O2	9:A:2217:U:O2'	2.25	0.47
9:A:2130:G:H5''	9:A:2153:G:C8	2.50	0.47
9:A:2730:U:OP2	9:A:2800:G:N1	2.43	0.47
11:C:73:ASP:OD2	11:C:190:ARG:NH1	2.45	0.47
35:a:1353:G:P	43:i:131:ILE:HG21	2.54	0.47
9:A:239:U:O2'	9:A:716:G:O2'	2.31	0.47
9:A:1248:U:N3	9:A:2249:G:OP1	2.46	0.47
9:A:2219:U:O2	20:L:3:GLN:NE2	2.45	0.47
9:A:2233:G:OP1	28:T:48:GLN:NE2	2.47	0.47
10:B:34:G:HO2'	10:B:35:G:P	2.37	0.47
10:B:84:C:N3	10:B:89:C:N4	2.62	0.47
35:a:959:A:O2'	35:a:963:U:O4	2.33	0.47
9:A:1927:C:O2'	9:A:3080:A:N3	2.43	0.47
9:A:2094:G:C4'	9:A:2095:G:OP1	2.63	0.47
12:D:62:VAL:HG21	12:D:77:PRO:HB2	1.96	0.47
15:G:116:ILE:HD11	15:G:152:LEU:HD11	1.97	0.47
24:P:16:ASN:OD1	24:P:17:ALA:N	2.48	0.47
9:A:830:A:C2	49:o:56:LEU:HD21	2.50	0.47
9:A:1788:G:OP2	11:C:63:ARG:NH1	2.48	0.47
9:A:2511:A:O2'	9:A:2512:A:O5'	2.32	0.47
9:A:2713:G:HO2'	9:A:2714:G:C4'	2.27	0.47
11:C:105:ILE:HG22	11:C:106:ILE:N	2.30	0.47
24:P:100:VAL:HG22	24:P:125:LEU:HD12	1.97	0.47
28:T:7:PHE:N	28:T:8:PRO:HD3	2.30	0.47
35:a:984:A:N6	35:a:1020:G:O6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b:225:LEU:O	36:b:225:LEU:HD13	2.15	0.47
9:A:65:G:N2	9:A:71:A:O5'	2.48	0.46
9:A:222:A:N1	9:A:495:C:O2'	2.45	0.46
9:A:1499:A:O2'	9:A:1519:C:O2	2.33	0.46
26:R:91:ASP:OD1	26:R:94:ASN:ND2	2.46	0.46
38:d:15:LEU:HD11	38:d:58:PHE:CD2	2.50	0.46
39:e:137:ARG:NE	39:e:141:GLU:OE2	2.48	0.46
2:2:50:LYS:HG3	47:m:69:ASP:OD1	2.14	0.46
9:A:80:G:O2'	9:A:81:A:O4'	2.32	0.46
9:A:779:U:O2'	9:A:1057:C:OP1	2.19	0.46
11:C:143:HIS:ND1	11:C:194:GLY:O	2.44	0.46
26:R:89:GLU:O	27:S:13:GLN:NE2	2.42	0.46
35:a:71:C:O2'	35:a:168:A:N3	2.41	0.46
35:a:175:A:OP1	54:t:56:ARG:NH1	2.48	0.46
51:q:63:ASP:OD1	51:q:64:GLU:N	2.48	0.46
53:s:39:THR:C	53:s:40:ILE:HD13	2.40	0.46
9:A:742:G:C2	9:A:743:G:N7	2.84	0.46
9:A:790:A:OP1	13:E:64:LYS:NZ	2.45	0.46
9:A:1185:A:O2'	9:A:1186:G:O5'	2.31	0.46
10:B:75:U:H1'	31:W:36:VAL:HG11	1.97	0.46
35:a:1303:U:OP2	35:a:1304:C:O2'	2.15	0.46
35:a:1305:G:O2'	35:a:1344:C:O2'	2.06	0.46
9:A:2914:A:OP1	23:O:9:ARG:NH2	2.46	0.46
29:U:24:ILE:HD12	29:U:29:TYR:CD2	2.51	0.46
34:Z:5:THR:OG1	34:Z:6:THR:N	2.47	0.46
35:a:794:A:HO2'	35:a:1494:C:C2'	2.22	0.46
9:A:710:G:H5''	13:E:107:ILE:HD11	1.97	0.46
9:A:1202:A:N6	17:I:78:ALA:HB1	2.29	0.46
35:a:35:G:N2	35:a:52:U:OP1	2.47	0.46
35:a:336:A:N6	35:a:337:G:O6	2.49	0.46
51:q:69:GLY:N	51:q:72:ASP:OD2	2.45	0.46
9:A:16:G:OP1	26:R:23:GLY:N	2.49	0.46
9:A:2565:G:N2	9:A:2598:C:O3'	2.48	0.46
16:H:124:ILE:HG22	16:H:125:LYS:N	2.29	0.46
35:a:687:U:C2	35:a:688:C:C5	3.04	0.46
35:a:1296:C:N4	35:a:1306:A:N1	2.64	0.46
46:l:44:LYS:N	46:l:45:PRO:CD	2.79	0.46
35:a:647:G:OP1	35:a:712:C:O2'	2.29	0.46
35:a:1012:U:O2	35:a:1012:U:O4'	2.33	0.46
35:a:1075:U:OP1	35:a:1088:G:N2	2.49	0.46
36:b:34:ASP:OD1	36:b:34:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:c:122:GLN:O	37:c:127:VAL:HG22	2.16	0.46
38:d:86:LEU:HD23	38:d:192:GLU:HG2	1.97	0.46
9:A:209:C:O2'	9:A:1481:C:O2	2.33	0.46
9:A:439:C:C2	9:A:440:U:C5	3.03	0.46
9:A:2062:G:O6	9:A:2120:A:N6	2.49	0.46
9:A:2804:U:O2'	9:A:2805:G:O4'	2.29	0.46
13:E:145:LEU:HG	13:E:150:GLU:OE1	2.16	0.46
35:a:810:G:H21	36:b:181:ILE:HG21	1.80	0.46
35:a:1105:U:O2	44:j:29:VAL:HG21	2.16	0.46
38:d:183:ARG:O	38:d:183:ARG:NH1	2.49	0.46
9:A:974:G:HO2'	9:A:975:U:P	2.39	0.46
9:A:1137:U:O2'	9:A:1139:A:N7	2.41	0.46
9:A:2571:C:N3	9:A:2595:G:N2	2.64	0.46
35:a:58:C:P	35:a:351:G:H21	2.39	0.46
35:a:234:C:O3'	51:q:87:ARG:NH2	2.49	0.46
9:A:2007:C:O2'	11:C:209:ALA:HB2	2.16	0.46
9:A:2135:U:H2'	9:A:2142:A:C2	2.51	0.46
9:A:2351:A:N6	9:A:2384:C:O2	2.47	0.46
9:A:2796:A:OP1	9:A:2798:G:O2'	2.27	0.46
14:F:86:LEU:HD22	14:F:92:ILE:CD1	2.46	0.46
35:a:184:U:O3'	54:t:84:ASN:ND2	2.49	0.46
35:a:906:C:O2'	35:a:1486:A:N7	2.41	0.46
35:a:1237:C:O2	35:a:1237:C:C2'	2.64	0.46
5:5:13:ARG:NH2	9:A:1493:A:OP1	2.49	0.45
9:A:619:C:C2'	9:A:619:C:O2	2.63	0.45
9:A:1025:A:N3	9:A:2488:C:O2'	2.43	0.45
9:A:1637:G:HO2'	9:A:1805:G:HO2'	1.64	0.45
31:W:53:ASP:OD1	31:W:54:PHE:N	2.49	0.45
9:A:486:G:OP1	33:Y:32:ASN:ND2	2.48	0.45
9:A:2788:A:O2'	9:A:2789:A:O4'	2.23	0.45
16:H:21:VAL:HG22	16:H:22:LYS:H	1.81	0.45
18:J:120:ALA:HB2	18:J:129:ILE:HD12	1.97	0.45
28:T:42:ILE:HG22	28:T:43:LEU:N	2.32	0.45
35:a:1182:A:O2'	35:a:1183:U:OP2	2.32	0.45
37:c:59:THR:OG1	37:c:60:ARG:N	2.50	0.45
9:A:71:A:H4'	9:A:72:G:O5'	2.16	0.45
9:A:323:C:H2'	9:A:323:C:O2	2.15	0.45
9:A:1628:A:N3	9:A:1630:U:N3	2.63	0.45
9:A:1913:G:N7	11:C:14:ARG:NH2	2.64	0.45
9:A:2040:G:OP1	11:C:217:LYS:NZ	2.49	0.45
24:P:73:ILE:HG22	24:P:75:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y:39:VAL:HG12	33:Y:41:ARG:O	2.17	0.45
35:a:1032:U:O2	35:a:1187:G:O6	2.33	0.45
35:a:1106:U:O2	35:a:1106:U:O4'	2.34	0.45
47:m:66:VAL:HG12	47:m:67:GLU:N	2.32	0.45
7:7:36:GLN:NE2	9:A:1149:G:N3	2.64	0.45
9:A:2065:A:C5	35:a:682:A:N6	2.85	0.45
9:A:2386:U:OP1	9:A:2393:A:O2'	2.31	0.45
18:J:114:LYS:HG2	18:J:118:LEU:HD23	1.98	0.45
35:a:254:G:O6	35:a:273:A:N6	2.49	0.45
35:a:1353:G:OP2	43:i:131:ILE:HG21	2.17	0.45
9:A:592:A:O2'	9:A:596:C:O2'	2.31	0.45
18:J:64:GLU:N	18:J:64:GLU:OE1	2.49	0.45
35:a:1376:U:O2'	35:a:1485:C:O2'	2.10	0.45
42:h:50:ARG:NE	42:h:52:GLU:OE2	2.46	0.45
1:1:8:GLN:HB2	1:1:28:LEU:HD13	1.99	0.45
9:A:389:G:H21	9:A:412:A:N6	2.15	0.45
9:A:589:A:N7	9:A:592:A:N6	2.65	0.45
9:A:894:U:H5''	11:C:49:ILE:HD12	1.99	0.45
9:A:1329:G:O6	9:A:1350:G:C2	2.70	0.45
9:A:2548:U:O2'	9:A:2561:G:OP1	2.35	0.45
9:A:2944:U:O2	9:A:2944:U:H2'	2.17	0.45
9:A:3043:G:O2'	9:A:3045:C:OP2	2.18	0.45
10:B:89:C:H2'	10:B:90:G:O4'	2.16	0.45
12:D:28:VAL:HG22	12:D:193:LEU:HD22	1.98	0.45
35:a:793:U:OP1	35:a:885:G:O2'	2.35	0.45
9:A:2133:G:H1	9:A:2145:C:H42	1.65	0.45
9:A:2150:U:O2'	9:A:2151:A:OP1	2.29	0.45
37:c:156:ARG:NH2	37:c:193:PHE:O	2.49	0.45
47:m:108:ARG:NH2	47:m:113:PRO:O	2.48	0.45
6:6:24:ARG:NH2	9:A:2584:A:OP1	2.47	0.45
9:A:1089:C:H2'	9:A:1090:G:O4'	2.17	0.45
35:a:444:A:N6	35:a:471:G:O6	2.50	0.45
9:A:1083:G:H4'	9:A:2495:G:H22	1.81	0.45
9:A:1675:U:O2'	9:A:1676:G:N7	2.50	0.45
9:A:2014:G:OP1	11:C:256:ARG:NH2	2.50	0.45
9:A:2971:G:H5'	15:G:71:THR:HG21	1.99	0.45
15:G:18:THR:HG23	15:G:25:SER:HB2	1.99	0.45
18:J:78:ALA:O	18:J:82:LEU:HD23	2.17	0.45
28:T:42:ILE:HG22	28:T:43:LEU:H	1.82	0.45
35:a:390:U:O3'	50:p:29:ARG:NH2	2.48	0.45
44:j:12:ALA:HB2	44:j:96:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:j:60:ASP:OD1	44:j:60:ASP:N	2.49	0.45
2:2:42:HIS:N	2:2:43:PRO:HD2	2.32	0.45
9:A:814:A:N3	9:A:1851:G:O2'	2.42	0.45
9:A:1549:G:O2'	9:A:1550:G:O5'	2.32	0.45
9:A:2350:G:H1'	9:A:2351:A:OP1	2.17	0.45
9:A:2579:C:H2'	9:A:2580:G:O4'	2.17	0.45
9:A:2771:U:OP2	9:A:2790:A:O2'	2.35	0.45
10:B:76:G:O3'	31:W:28:ARG:NH1	2.48	0.45
29:U:6:ASP:O	29:U:8:ARG:N	2.45	0.45
35:a:811:U:O2	35:a:837:G:O6	2.35	0.45
35:a:1378:C:O2	35:a:1381:A:O2'	2.35	0.45
42:h:55:ARG:O	42:h:56:VAL:C	2.60	0.45
9:A:21:G:C2	9:A:22:U:C5	3.06	0.44
9:A:335:G:H2'	9:A:336:C:O4'	2.17	0.44
9:A:1130:C:N3	19:K:27:ARG:NH1	2.65	0.44
9:A:1332:G:C6	9:A:1347:G:C6	3.05	0.44
9:A:2772:G:O6	9:A:2785:A:N6	2.50	0.44
9:A:2859:C:O2	12:D:40:ARG:NH2	2.50	0.44
18:J:80:LEU:HD23	18:J:83:LYS:HE3	1.99	0.44
47:m:58:ASP:OD1	47:m:59:TYR:N	2.50	0.44
50:p:59:TRP:HA	50:p:62:VAL:HG22	1.99	0.44
9:A:357:U:H1'	9:A:358:G:OP2	2.16	0.44
9:A:2044:U:OP2	11:C:222:ARG:NE	2.48	0.44
49:o:42:HIS:NE2	49:o:49:ASP:OD2	2.50	0.44
9:A:964:C:N4	9:A:965:U:C4	2.85	0.44
9:A:1640:A:O2'	9:A:1641:U:H5''	2.18	0.44
9:A:1698:A:N1	9:A:1777:U:O2'	2.48	0.44
9:A:2065:A:C8	35:a:682:A:C5	3.06	0.44
9:A:2342:A:N1	9:A:2390:U:O2'	2.48	0.44
9:A:3009:U:O2	12:D:69:GLN:NE2	2.49	0.44
12:D:58:SER:O	12:D:62:VAL:HG23	2.17	0.44
30:V:43:LYS:HZ2	30:V:45:THR:HA	1.82	0.44
31:W:79:LEU:N	31:W:98:LEU:O	2.51	0.44
35:a:354:G:H2'	35:a:354:G:N3	2.31	0.44
35:a:523:U:OP2	38:d:10:ARG:NH2	2.45	0.44
35:a:1220:A:O2'	35:a:1280:C:N4	2.47	0.44
35:a:1486:A:N3	35:a:1486:A:H2'	2.31	0.44
16:H:95:VAL:CG1	16:H:124:ILE:HG21	2.47	0.44
32:X:14:ARG:O	32:X:15:ASP:OD1	2.35	0.44
35:a:83:U:O2	35:a:86:G:C6	2.68	0.44
35:a:323:U:H3	35:a:327:A:H62	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:544:C:OP1	46:l:12:ARG:NE	2.43	0.44
35:a:1236:G:H2'	35:a:1239:G:H21	1.82	0.44
35:a:1513:G:O2'	35:a:1514:G:OP1	2.22	0.44
46:l:2:PRO:O	46:l:3:THR:OG1	2.35	0.44
9:A:980:C:H42	9:A:1024:A:H62	1.65	0.44
9:A:2048:G:H21	55:u:29:ARG:HH11	1.66	0.44
9:A:2298:U:O2'	9:A:2300:A:OP2	2.25	0.44
14:F:147:GLU:N	14:F:147:GLU:OE1	2.50	0.44
23:O:83:ILE:O	23:O:86:PHE:N	2.46	0.44
29:U:20:SER:O	29:U:24:ILE:HG12	2.17	0.44
35:a:794:A:O3'	35:a:1494:C:O2'	2.36	0.44
35:a:895:A:H4'	35:a:896:A:O5'	2.18	0.44
45:k:121:ASP:OD1	45:k:123:THR:OG1	2.35	0.44
9:A:316:U:H1'	9:A:317:G:OP1	2.18	0.44
9:A:663:A:N3	9:A:663:A:H2'	2.32	0.44
9:A:714:U:O2	9:A:714:U:C2'	2.65	0.44
9:A:2065:A:C8	35:a:682:A:C4	3.06	0.44
10:B:50:C:H2'	10:B:51:G:O4'	2.18	0.44
35:a:700:C:O3'	52:r:62:ARG:NH2	2.51	0.44
35:a:934:U:H4'	35:a:946:A:H61	1.82	0.44
35:a:1105:U:H3	44:j:29:VAL:HG21	1.83	0.44
35:a:1393:G:H2'	35:a:1393:G:N3	2.32	0.44
40:f:29:VAL:HG13	40:f:30:ILE:N	2.33	0.44
9:A:756:A:H2'	9:A:757:G:O4'	2.18	0.44
9:A:947:U:OP2	9:A:1061:G:N1	2.41	0.44
9:A:2008:A:O2'	11:C:207:GLY:N	2.51	0.44
9:A:2137:A:H2	35:a:1478:G:C8	2.35	0.44
35:a:380:G:N1	35:a:384:G:O6	2.50	0.44
9:A:388:U:H2'	9:A:389:G:O4'	2.17	0.44
9:A:1886:A:N1	9:A:1894:A:N6	2.66	0.44
9:A:2287:C:N4	9:A:2725:C:O2	2.45	0.44
25:Q:13:ARG:NH1	25:Q:80:ILE:O	2.49	0.44
35:a:1478:G:H2'	35:a:1479:U:H6	1.83	0.44
9:A:2138:C:H3'	9:A:2139:U:C5	2.53	0.44
9:A:2599:G:N2	9:A:2602:A:OP2	2.42	0.44
9:A:2877:U:OP2	9:A:2878:A:O2'	2.32	0.44
12:D:85:ARG:O	12:D:209:ARG:NH2	2.47	0.44
35:a:958:G:O2'	35:a:959:A:OP2	2.26	0.44
35:a:1051:C:OP1	39:e:55:ARG:NH2	2.51	0.44
39:e:62:VAL:O	39:e:63:ILE:HD13	2.18	0.44
9:A:701:A:OP2	9:A:713:G:N1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:883:G:H22	9:A:1494:U:C1'	2.30	0.43
9:A:1111:G:OP1	26:R:50:ARG:NE	2.41	0.43
9:A:2750:G:OP2	15:G:154:ARG:NH2	2.42	0.43
15:G:12:PRO:HG2	15:G:81:THR:HG21	2.00	0.43
35:a:155:G:H2'	35:a:156:G:C1'	2.48	0.43
35:a:598:C:N4	35:a:601:A:OP2	2.51	0.43
38:d:152:ILE:O	38:d:156:THR:HG22	2.18	0.43
44:j:48:VAL:O	44:j:48:VAL:CG2	2.65	0.43
9:A:221:A:H61	9:A:232:G:H1'	1.82	0.43
9:A:2199:G:H2'	9:A:2200:U:O4'	2.18	0.43
14:F:45:MET:HE2	14:F:64:LEU:HG	2.00	0.43
15:G:20:ASN:OD1	15:G:20:ASN:N	2.51	0.43
35:a:1392:OMC:C4	35:a:1393:G:N7	2.85	0.43
37:c:90:LEU:O	37:c:94:THR:HG22	2.18	0.43
9:A:618:C:OP1	9:A:653:G:N1	2.51	0.43
9:A:1112:C:O2	27:S:12:LYS:NZ	2.43	0.43
9:A:1640:A:O2'	9:A:1641:U:OP1	2.37	0.43
14:F:77:ALA:HB2	14:F:92:ILE:HD12	2.00	0.43
35:a:179:C:H2'	35:a:179:C:O2	2.18	0.43
38:d:90:GLU:OE1	38:d:95:ASN:ND2	2.51	0.43
5:5:14:ARG:NH1	9:A:801:U:O4'	2.44	0.43
9:A:2157:G:C5'	55:u:26:VAL:HG21	2.48	0.43
9:A:2425:U:O2'	9:A:2427:G:OP1	2.34	0.43
35:a:415:C:O2	35:a:415:C:O4'	2.35	0.43
39:e:155:SER:O	39:e:156:ASP:C	2.61	0.43
9:A:262:A:N3	9:A:518:A:O2'	2.40	0.43
9:A:822:G:O6	9:A:840:G:C2	2.71	0.43
35:a:942:U:O2	35:a:942:U:O4'	2.36	0.43
35:a:1263:C:N4	44:j:100:ILE:HG21	2.33	0.43
38:d:15:LEU:HD13	38:d:55:LYS:HA	2.00	0.43
51:q:90:LEU:O	51:q:91:VAL:HG13	2.18	0.43
53:s:19:VAL:HG11	53:s:44:PHE:CD1	2.53	0.43
3:3:28:VAL:HG13	9:A:3107:G:O3'	2.19	0.43
9:A:643:G:C2'	9:A:644:G:OP1	2.66	0.43
9:A:727:A:OP1	21:M:72:ARG:NH1	2.52	0.43
9:A:863:G:OP1	28:T:95:ARG:NH2	2.45	0.43
9:A:1938:G:N2	9:A:1956:A:H62	2.14	0.43
15:G:77:VAL:HA	15:G:80:VAL:HG22	2.00	0.43
35:a:1298:G:C4	35:a:1300:A:OP2	2.72	0.43
44:j:75:ASP:C	44:j:76:ILE:HG23	2.44	0.43
9:A:45:G:N2	9:A:176:G:OP2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:740:A:C4	9:A:741:G:C8	3.06	0.43
9:A:1128:A:O2'	9:A:1271:C:O2	2.36	0.43
9:A:1402:A:N6	9:A:1867:G:O4'	2.51	0.43
9:A:2587:U:O2	32:X:39:ARG:NH1	2.52	0.43
9:A:2880:U:C2	9:A:2889:A:N7	2.86	0.43
10:B:52:G:O2'	10:B:53:A:O5'	2.32	0.43
18:J:118:LEU:CD1	18:J:129:ILE:HG21	2.49	0.43
35:a:764:A:N6	35:a:779:G:O6	2.52	0.43
35:a:954:C:H3'	35:a:955:G:H5''	2.01	0.43
9:A:76:C:O2'	9:A:428:A:N3	2.41	0.43
9:A:800:A:H1'	9:A:804:A:N6	2.33	0.43
9:A:1084:U:H4'	9:A:1085:G:OP2	2.19	0.43
9:A:1225:G:OP2	17:I:78:ALA:N	2.51	0.43
9:A:1516:G:H2'	9:A:1517:U:O4'	2.19	0.43
9:A:2532:G:N3	9:A:2532:G:H2'	2.34	0.43
26:R:31:LEU:HD12	26:R:34:LYS:HD3	2.01	0.43
35:a:496:U:O4	35:a:513:A:N7	2.52	0.43
35:a:1391:A:C6	35:a:1392:OMC:C4	3.06	0.43
38:d:142:GLU:OE1	38:d:142:GLU:N	2.48	0.43
9:A:287:A:N7	9:A:299:G:O2'	2.41	0.43
9:A:927:C:O2'	9:A:1340:A:O2'	2.29	0.43
9:A:2051:U:H5''	9:A:2052:G:H5'	2.01	0.43
9:A:2087:C:H2'	9:A:2088:C:C1'	2.48	0.43
9:A:2328:G:C5	9:A:2408:G:N2	2.87	0.43
9:A:2756:G:N2	9:A:2887:G:O2'	2.51	0.43
23:O:116:VAL:HG23	23:O:116:VAL:O	2.17	0.43
31:W:177:LEU:HD11	31:W:179:VAL:O	2.18	0.43
35:a:527:A:OP1	38:d:65:LYS:NZ	2.49	0.43
35:a:965:A:O2'	35:a:1029:U:O3'	2.37	0.43
35:a:1046:C:C2'	35:a:1047:A:O5'	2.66	0.43
44:j:7:ARG:HA	44:j:8:ILE:HB	2.01	0.43
2:2:38:CYS:O	2:2:40:GLN:N	2.43	0.43
9:A:516:G:C2'	9:A:517:A:O5'	2.67	0.43
9:A:552:U:C2'	9:A:553:G:O5'	2.67	0.43
9:A:592:A:HO2'	9:A:596:C:HO2'	1.61	0.43
9:A:858:A:N6	9:A:870:G:O6	2.52	0.43
9:A:911:U:C2	9:A:912:C:C5	3.07	0.43
9:A:1115:G:OP2	26:R:58:ARG:NH1	2.51	0.43
9:A:1177:G:OP2	9:A:1178:U:H3'	2.18	0.43
9:A:2339:G:N1	9:A:2387:U:O4	2.52	0.43
9:A:2351:A:N3	9:A:2396:A:O2'	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2862:G:O2'	9:A:3002:A:N6	2.52	0.43
9:A:3054:U:O2'	12:D:60:ARG:NH1	2.51	0.43
10:B:39:C:O2'	10:B:46:A:N1	2.48	0.43
23:O:83:ILE:O	23:O:84:GLY:C	2.62	0.43
35:a:376:G:OP1	50:p:67:THR:OG1	2.34	0.43
35:a:1088:G:H2'	35:a:1088:G:N3	2.33	0.43
35:a:1160:A:O2'	35:a:1161:A:O4'	2.37	0.43
35:a:1299:C:H42	48:n:18:VAL:HA	1.84	0.43
35:a:1357:A:O2'	41:g:28:ASN:O	2.36	0.43
9:A:740:A:O2'	9:A:741:G:OP2	2.33	0.42
9:A:1414:G:N1	9:A:1858:A:OP2	2.47	0.42
9:A:2558:C:O3'	24:P:27:LYS:NZ	2.50	0.42
9:A:2691:C:O2	22:N:124:LYS:NZ	2.51	0.42
35:a:211:A:N1	35:a:220:G:O2'	2.46	0.42
35:a:407:A:OP1	38:d:107:ARG:NH1	2.52	0.42
35:a:840:G:N1	35:a:852:U:OP2	2.46	0.42
35:a:1046:C:H42	35:a:1172:A:H62	1.67	0.42
35:a:1231:A:N6	35:a:1269:A:N1	2.66	0.42
35:a:1338:G:H2'	35:a:1339:A:C8	2.53	0.42
39:e:132:ALA:HB2	39:e:150:ALA:HB3	2.00	0.42
9:A:959:U:H2'	9:A:960:G:N9	2.34	0.42
9:A:1087:G:N2	9:A:1103:C:OP1	2.41	0.42
9:A:1380:A:P	9:A:1382:U:H1'	2.59	0.42
9:A:1401:A:N6	9:A:1444:U:O2	2.52	0.42
10:B:83:C:N4	10:B:84:C:N4	2.68	0.42
35:a:374:A:N1	35:a:390:U:O2'	2.52	0.42
35:a:671:G:OP2	45:k:37:ASN:ND2	2.52	0.42
35:a:681:C:OP1	35:a:682:A:O2'	2.26	0.42
35:a:958:G:N2	35:a:1345:A:OP2	2.47	0.42
9:A:992:C:N4	9:A:1017:G:O6	2.53	0.42
9:A:1168:A:H2'	9:A:1169:A:O4'	2.19	0.42
9:A:1224:G:H2'	9:A:1225:G:OP1	2.19	0.42
9:A:1225:G:H5'	17:I:76:PRO:O	2.19	0.42
9:A:1227:C:O3'	9:A:1228:A:O4'	2.37	0.42
9:A:2245:C:O2	9:A:2245:C:H2'	2.19	0.42
9:A:2469:U:O2'	9:A:2660:G:OP2	2.28	0.42
9:A:2804:U:H2'	9:A:2805:G:O4'	2.19	0.42
27:S:68:THR:OG1	27:S:69:LYS:N	2.52	0.42
35:a:1231:A:H2'	35:a:1232:A:C8	2.54	0.42
42:h:48:ASP:OD1	42:h:49:TYR:N	2.51	0.42
9:A:316:U:H4'	9:A:317:G:OP2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:469:G:OP1	33:Y:24:ARG:NH2	2.52	0.42
9:A:541:G:N3	9:A:545:A:O2'	2.52	0.42
9:A:576:G:C2	9:A:578:G:OP2	2.73	0.42
9:A:1224:G:H5''	17:I:77:THR:H	1.84	0.42
9:A:2088:C:O2'	9:A:2089:C:P	2.77	0.42
9:A:2593:A:N6	9:A:2594:G:O6	2.53	0.42
9:A:465:A:N6	9:A:486:G:O6	2.52	0.42
9:A:1092:G:O4'	9:A:1301:G:N2	2.50	0.42
9:A:1203:A:OP1	17:I:9:ALA:HB1	2.20	0.42
9:A:1444:U:OP2	9:A:1445:C:N4	2.30	0.42
9:A:1630:U:C4	9:A:1631:A:C8	3.08	0.42
32:X:83:VAL:HG22	32:X:84:ALA:H	1.83	0.42
35:a:426:U:OP1	38:d:29:ARG:NH2	2.53	0.42
35:a:1076:C:H2'	35:a:1077:C:C6	2.55	0.42
53:s:63:THR:H	53:s:66:MET:HB2	1.84	0.42
2:2:64:ARG:O	2:2:65:TYR:C	2.61	0.42
5:5:36:ASN:ND2	9:A:555:G:OP1	2.52	0.42
9:A:280:G:C6	9:A:307:G:C6	3.08	0.42
9:A:1173:G:O4'	17:I:29:ARG:HG2	2.19	0.42
9:A:2030:C:H2'	9:A:2031:G:O4'	2.19	0.42
9:A:2330:U:C4	9:A:2331:U:C4	3.08	0.42
9:A:2359:G:H3'	9:A:2360:C:H5''	2.01	0.42
13:E:41:GLN:OE1	13:E:184:ASN:ND2	2.53	0.42
13:E:41:GLN:NE2	13:E:184:ASN:OD1	2.52	0.42
20:L:80:ASP:OD2	25:Q:61:ARG:NH2	2.50	0.42
21:M:55:MET:O	21:M:60:ARG:NH1	2.52	0.42
22:N:58:ILE:HG23	22:N:108:TYR:CE1	2.54	0.42
42:h:50:ARG:O	42:h:60:LEU:HD12	2.20	0.42
9:A:22:U:C2'	9:A:23:G:O5'	2.68	0.42
9:A:2754:G:OP2	9:A:2759:G:N2	2.53	0.42
9:A:2876:C:H2'	9:A:2877:U:O4'	2.20	0.42
9:A:2968:G:N2	15:G:144:GLN:OE1	2.52	0.42
35:a:1345:A:O2'	35:a:1346:A:OP1	2.35	0.42
35:a:1408:A:N1	35:a:1459:G:O6	2.53	0.42
44:j:7:ARG:HG2	44:j:76:ILE:HG12	2.02	0.42
9:A:563:U:H3	9:A:567:A:H62	1.67	0.42
9:A:619:C:O2	9:A:619:C:H2'	2.20	0.42
10:B:57:U:O4'	14:F:31:ASN:ND2	2.50	0.42
30:V:47:VAL:HG13	30:V:56:SER:N	2.35	0.42
35:a:25:G:H5'	35:a:553:A:H61	1.85	0.42
35:a:327:A:O2'	35:a:329:A:OP2	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:1053:U:OP1	39:e:87:LYS:NZ	2.45	0.42
35:a:1105:U:H2'	44:j:76:ILE:HG22	2.00	0.42
35:a:1261:A:C4'	35:a:1262:U:OP1	2.67	0.42
35:a:1273:C:C2	35:a:1274:C:C5	3.08	0.42
5:5:7:THR:HG22	9:A:802:C:H1'	2.01	0.42
9:A:860:G:N2	9:A:868:C:N3	2.68	0.42
9:A:923:G:O6	21:M:43:ARG:NH1	2.53	0.42
9:A:1202:A:H4'	17:I:13:ILE:HG12	2.02	0.42
9:A:1493:A:O2'	9:A:1495:G:OP2	2.37	0.42
9:A:2006:A:H2'	9:A:2007:C:O4'	2.20	0.42
10:B:114:A:H2'	10:B:115:A:C8	2.55	0.42
16:H:109:GLY:N	16:H:110:PRO:CD	2.82	0.42
22:N:14:HIS:O	22:N:15:PRO:C	2.63	0.42
35:a:25:G:N2	35:a:896:A:H62	2.16	0.42
35:a:357:G:OP1	35:a:366:A:O2'	2.33	0.42
35:a:865:C:H2'	35:a:866:U:C6	2.54	0.42
35:a:1472:G:H2'	35:a:1473:A:H8	1.81	0.42
36:b:147:SER:O	36:b:148:LEU:HD22	2.19	0.42
46:l:70:GLU:N	46:l:70:GLU:OE1	2.52	0.42
9:A:2149:C:H2'	9:A:2150:U:C6	2.55	0.42
35:a:389:A:O2'	35:a:390:U:OP1	2.33	0.42
35:a:1079:G:O2'	35:a:1080:C:OP1	2.21	0.42
35:a:1261:A:O4'	44:j:100:ILE:HD12	2.20	0.42
44:j:72:ARG:C	44:j:73:LEU:HD13	2.45	0.42
47:m:82:ILE:O	47:m:93:ARG:NH2	2.53	0.42
9:A:450:G:H3'	9:A:451:U:C5	2.54	0.41
9:A:983:C:N3	9:A:1027:C:O2'	2.46	0.41
10:B:42:C:N3	14:F:97:THR:OG1	2.52	0.41
35:a:52:U:O2	35:a:52:U:O4'	2.35	0.41
35:a:693:G:H2'	35:a:694:G:C8	2.55	0.41
35:a:1364:U:O2'	41:g:79:ARG:O	2.29	0.41
46:l:100:GLY:N	46:l:104:THR:OG1	2.43	0.41
47:m:22:ILE:HD12	47:m:25:ILE:HD12	2.02	0.41
9:A:159:A:N6	9:A:166:A:N3	2.68	0.41
9:A:1011:A:H3'	9:A:1012:C:H5''	2.03	0.41
9:A:2932:G:C2	9:A:2933:G:N7	2.88	0.41
9:A:3038:C:OP1	23:O:42:ARG:NH2	2.50	0.41
12:D:114:VAL:HG21	12:D:198:ILE:HB	2.02	0.41
20:L:105:GLU:OE2	20:L:105:GLU:N	2.50	0.41
30:V:46:ALA:O	30:V:56:SER:HA	2.19	0.41
35:a:501:G:O2'	35:a:516:C:O2'	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:905:A:O2'	35:a:1382:C:OP2	2.38	0.41
35:a:1475:G:N3	35:a:1476:A:N7	2.68	0.41
42:h:114:THR:OG1	42:h:115:ASP:N	2.52	0.41
4:4:13:LEU:N	4:4:23:TYR:O	2.54	0.41
9:A:72:G:H2'	9:A:72:G:N3	2.35	0.41
9:A:422:A:O2'	13:E:170:ARG:NH2	2.54	0.41
9:A:438:U:C5	9:A:439:C:C5	3.08	0.41
9:A:713:G:N7	13:E:104:LYS:NZ	2.69	0.41
9:A:1203:A:N7	17:I:50:THR:HG23	2.35	0.41
9:A:1982:G:O6	9:A:2212:A:N6	2.53	0.41
9:A:2488:C:H2'	9:A:2489:U:O4'	2.20	0.41
18:J:56:ILE:O	18:J:56:ILE:HG23	2.20	0.41
35:a:991:C:OP1	48:n:12:LYS:NZ	2.48	0.41
5:5:42:ARG:NH2	9:A:556:G:N7	2.65	0.41
9:A:160:A:C2'	9:A:161:U:OP1	2.68	0.41
9:A:963:U:C2	9:A:1050:A:N3	2.88	0.41
9:A:1105:C:H2'	9:A:1106:A:O4'	2.20	0.41
9:A:2352:C:H3'	9:A:2353:U:H5''	2.03	0.41
10:B:34:G:O2'	10:B:35:G:P	2.78	0.41
19:K:43:THR:HG22	26:R:100:VAL:HG13	2.01	0.41
20:L:10:VAL:HG12	20:L:12:ASP:OD1	2.20	0.41
35:a:482:A:OP1	46:l:115:SER:OG	2.34	0.41
35:a:588:A:C6	35:a:589:A:H1'	2.56	0.41
8:8:4:ARG:NH1	9:A:2679:G:O3'	2.54	0.41
9:A:285:U:H3'	9:A:286:G:H4'	2.01	0.41
9:A:926:U:O4	21:M:24:ARG:NH1	2.54	0.41
9:A:965:U:C4	9:A:1043:G:O6	2.73	0.41
9:A:2128:G:O2'	9:A:2152:A:N1	2.45	0.41
9:A:2358:A:O2'	9:A:2382:G:O2'	2.30	0.41
9:A:2777:G:O4'	9:A:2806:G:O2'	2.32	0.41
30:V:43:LYS:HG2	30:V:45:THR:HG23	2.02	0.41
35:a:1089:C:C2	35:a:1090:A:C8	3.09	0.41
35:a:1282:G:N2	35:a:1283:U:O4	2.54	0.41
45:k:56:SER:HA	45:k:59:VAL:HG12	2.01	0.41
53:s:19:VAL:HG11	53:s:44:PHE:HA	2.02	0.41
3:3:16:ARG:NH2	9:A:1379:G:OP1	2.53	0.41
9:A:959:U:H2'	9:A:960:G:O4'	2.20	0.41
9:A:1239:C:H3'	9:A:1240:G:H5''	2.03	0.41
13:E:150:GLU:OE2	13:E:195:VAL:CB	2.58	0.41
35:a:1014:U:H2'	35:a:1015:G:C8	2.56	0.41
35:a:1145:G:H3'	35:a:1146:G:H5''	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:g:111:ARG:O	41:g:119:ARG:NE	2.53	0.41
9:A:444:U:OP1	9:A:446:G:H4'	2.21	0.41
9:A:472:C:H2'	9:A:472:C:O2	2.19	0.41
9:A:843:G:O2'	11:C:10:THR:HG21	2.20	0.41
9:A:1112:C:P	26:R:54:LYS:HZ1	2.42	0.41
9:A:2047:C:H2'	9:A:2048:G:H8	1.86	0.41
9:A:2133:G:H2'	9:A:2134:G:C8	2.55	0.41
9:A:2137:A:H2	35:a:1478:G:N7	2.18	0.41
9:A:2869:C:O2	9:A:2869:C:O4'	2.37	0.41
35:a:455:G:N2	35:a:457:A:N3	2.68	0.41
35:a:934:U:O3'	35:a:946:A:N6	2.53	0.41
35:a:972:U:H3'	35:a:973:U:H5''	2.03	0.41
35:a:1272:G:C2	35:a:1273:C:C6	3.08	0.41
46:l:74:LEU:HD23	46:l:104:THR:HG22	2.02	0.41
9:A:379:G:O2'	9:A:404:A:N1	2.40	0.41
9:A:1475:G:N1	9:A:2438:C:N3	2.69	0.41
9:A:2548:U:H5''	9:A:2549:G:H5''	2.02	0.41
10:B:42:C:H2'	10:B:43:C:O4'	2.21	0.41
11:C:147:LEU:HD11	11:C:155:LEU:HD21	2.03	0.41
35:a:620:A:N3	42:h:109:SER:OG	2.46	0.41
39:e:186:ILE:HG22	39:e:187:GLU:N	2.36	0.41
3:3:5:LYS:NZ	9:A:2279:C:OP1	2.51	0.41
4:4:34:ASP:N	4:4:34:ASP:OD1	2.54	0.41
6:6:38:THR:HG21	9:A:2572:U:P	2.60	0.41
9:A:336:C:HO2'	9:A:337:U:P	2.40	0.41
9:A:820:A:N6	9:A:840:G:O2'	2.54	0.41
9:A:1146:A:OP2	9:A:1244:A:N6	2.50	0.41
9:A:1201:G:H5''	17:I:16:GLN:HG2	2.03	0.41
9:A:1403:C:O2	9:A:1403:C:O4'	2.39	0.41
9:A:1694:C:H2'	9:A:1694:C:O2	2.21	0.41
9:A:2161:A:H62	9:A:2164:U:H5	1.68	0.41
9:A:3046:C:O2	9:A:3046:C:O4'	2.36	0.41
35:a:598:C:O2	50:p:12:LYS:NZ	2.53	0.41
35:a:694:G:H2'	35:a:695:A:C8	2.56	0.41
44:j:77:LEU:HD23	44:j:78:ASP:CB	2.51	0.41
9:A:159:A:N3	9:A:159:A:H2'	2.35	0.41
9:A:391:G:N2	9:A:412:A:OP1	2.54	0.41
9:A:1938:G:N2	9:A:1939:U:O4	2.54	0.41
9:A:2216:G:O2'	9:A:2221:A:N6	2.54	0.41
15:G:90:ILE:O	15:G:130:THR:OG1	2.37	0.41
35:a:946:A:H3'	35:a:947:U:C5'	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:1338:G:N3	44:j:48:VAL:HG21	2.36	0.41
9:A:467:C:O2'	9:A:2456:C:OP1	2.38	0.40
9:A:674:U:OP1	26:R:14:ARG:NH1	2.54	0.40
9:A:882:U:H2'	9:A:883:G:H8	1.86	0.40
9:A:2594:G:H2'	9:A:2595:G:O4'	2.21	0.40
9:A:2804:U:C2'	9:A:2805:G:O4'	2.69	0.40
11:C:106:ILE:HG22	11:C:106:ILE:O	2.22	0.40
16:H:81:SER:O	16:H:81:SER:OG	2.36	0.40
17:I:12:ASP:OD1	17:I:12:ASP:C	2.64	0.40
21:M:126:ALA:O	21:M:147:LEU:N	2.54	0.40
25:Q:41:VAL:HG22	35:a:346:G:H4'	2.03	0.40
40:f:69:PRO:HA	40:f:72:VAL:HG22	2.03	0.40
3:3:16:ARG:NH2	9:A:1381:G:OP2	2.50	0.40
9:A:721:A:C8	21:M:77:VAL:HG21	2.55	0.40
9:A:824:G:C6	9:A:838:G:C6	3.10	0.40
9:A:2166:C:OP2	9:A:2167:U:O2'	2.15	0.40
9:A:2803:C:O4'	12:D:144:VAL:HG11	2.20	0.40
9:A:2805:G:OP2	9:A:2805:G:C2	2.74	0.40
32:X:42:GLY:N	32:X:57:ASP:OD2	2.50	0.40
35:a:444:A:C6	35:a:471:G:C6	3.09	0.40
35:a:555:G:O2'	35:a:801:G:OP2	2.15	0.40
46:l:37:VAL:HG12	46:l:53:ALA:CB	2.51	0.40
4:4:11:ILE:HD11	4:4:25:THR:HG23	2.03	0.40
9:A:160:A:O2'	9:A:161:U:P	2.80	0.40
9:A:453:U:H2'	9:A:454:U:N1	2.36	0.40
9:A:563:U:O4	9:A:567:A:N7	2.54	0.40
9:A:571:A:O3'	30:V:46:ALA:HA	2.21	0.40
9:A:872:G:N3	9:A:872:G:H2'	2.36	0.40
9:A:1743:G:OP2	9:A:1744:A:O2'	2.20	0.40
14:F:42:VAL:HG23	14:F:162:THR:HB	2.03	0.40
24:P:69:ASP:OD1	24:P:70:VAL:N	2.54	0.40
29:U:55:ASP:N	29:U:85:LYS:O	2.48	0.40
35:a:953:G:O2'	35:a:1348:G:O3'	2.39	0.40
37:c:182:ILE:HD11	37:c:201:TRP:HB3	2.03	0.40
39:e:71:VAL:HG22	39:e:72:GLY:N	2.36	0.40
2:2:63:LYS:CD	53:s:64:GLU:HG2	2.51	0.40
2:2:66:GLY:N	53:s:44:PHE:O	2.53	0.40
9:A:543:U:H3'	9:A:544:U:C5'	2.51	0.40
9:A:1172:A:C4	17:I:29:ARG:HD2	2.56	0.40
9:A:1475:G:O6	9:A:2438:C:O2	2.39	0.40
9:A:1534:C:O2	9:A:1534:C:C2'	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2234:G:H5'	28:T:49:ALA:HB3	2.03	0.40
9:A:2435:U:O2	9:A:2435:U:H2'	2.20	0.40
9:A:2743:U:O4'	9:A:2766:A:N6	2.54	0.40
9:A:2949:A:HO2'	9:A:2950:C:P	2.45	0.40
10:B:19:G:H22	10:B:64:G:H22	1.68	0.40
10:B:76:G:H2'	10:B:77:A:O4'	2.20	0.40
35:a:1011:U:O2	35:a:1012:U:N3	2.50	0.40
35:a:1131:G:H2'	35:a:1131:G:N3	2.36	0.40
35:a:1249:G:O2'	35:a:1250:A:O4'	2.34	0.40
9:A:1202:A:H1'	17:I:52:ALA:HB2	2.03	0.40
12:D:7:LEU:HD12	12:D:207:VAL:HG13	2.03	0.40
14:F:139:LEU:HD23	14:F:144:MET:HB2	2.04	0.40
35:a:1329:G:O2'	43:i:131:ILE:HD13	2.22	0.40
43:i:45:THR:N	43:i:82:ASP:OD1	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
2	2	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
3	3	52/57 (91%)	52 (100%)	0	0	100	100
4	4	48/55 (87%)	39 (81%)	9 (19%)	0	100	100
5	5	43/47 (92%)	42 (98%)	1 (2%)	0	100	100
6	6	61/64 (95%)	57 (93%)	4 (7%)	0	100	100
7	7	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
8	8	21/24 (88%)	21 (100%)	0	0	100	100
11	C	271/278 (98%)	256 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	D	212/217 (98%)	204 (96%)	8 (4%)	0	100	100
13	E	205/215 (95%)	190 (93%)	15 (7%)	0	100	100
14	F	179/187 (96%)	170 (95%)	9 (5%)	0	100	100
15	G	174/179 (97%)	170 (98%)	4 (2%)	0	100	100
16	H	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
17	I	124/174 (71%)	116 (94%)	8 (6%)	0	100	100
18	J	131/142 (92%)	124 (95%)	7 (5%)	0	100	100
19	K	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
20	L	119/122 (98%)	108 (91%)	11 (9%)	0	100	100
21	M	143/147 (97%)	135 (94%)	8 (6%)	0	100	100
22	N	132/138 (96%)	130 (98%)	2 (2%)	0	100	100
23	O	115/174 (66%)	106 (92%)	9 (8%)	0	100	100
24	P	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
25	Q	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
26	R	122/129 (95%)	121 (99%)	1 (1%)	0	100	100
27	S	100/103 (97%)	100 (100%)	0	0	100	100
28	T	112/153 (73%)	109 (97%)	3 (3%)	0	100	100
29	U	92/100 (92%)	84 (91%)	8 (9%)	0	100	100
30	V	93/105 (89%)	88 (95%)	5 (5%)	0	100	100
31	W	186/215 (86%)	175 (94%)	11 (6%)	0	100	100
32	X	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
33	Y	61/64 (95%)	61 (100%)	0	0	100	100
34	Z	61/77 (79%)	61 (100%)	0	0	100	100
36	b	226/277 (82%)	216 (96%)	10 (4%)	0	100	100
37	c	208/275 (76%)	199 (96%)	9 (4%)	0	100	100
38	d	198/201 (98%)	196 (99%)	2 (1%)	0	100	100
39	e	196/214 (92%)	185 (94%)	11 (6%)	0	100	100
40	f	94/96 (98%)	90 (96%)	4 (4%)	0	100	100
41	g	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
42	h	128/132 (97%)	122 (95%)	6 (5%)	0	100	100
43	i	124/150 (83%)	123 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	j	95/101 (94%)	83 (87%)	12 (13%)	0	100	100
45	k	115/138 (83%)	109 (95%)	6 (5%)	0	100	100
46	l	120/124 (97%)	107 (89%)	13 (11%)	0	100	100
47	m	114/124 (92%)	109 (96%)	5 (4%)	0	100	100
48	n	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
49	o	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
50	p	111/156 (71%)	106 (96%)	5 (4%)	0	100	100
51	q	90/98 (92%)	85 (94%)	5 (6%)	0	100	100
52	r	62/84 (74%)	56 (90%)	6 (10%)	0	100	100
53	s	76/93 (82%)	71 (93%)	5 (7%)	0	100	100
54	t	82/86 (95%)	81 (99%)	1 (1%)	0	100	100
55	u	30/33 (91%)	30 (100%)	0	0	100	100
All	All	5989/6653 (90%)	5702 (95%)	287 (5%)	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	
1	1	53/54 (98%)	51 (96%)	2 (4%)	29	59
2	2	57/63 (90%)	54 (95%)	3 (5%)	20	50
3	3	43/46 (94%)	43 (100%)	0	100	100
4	4	48/52 (92%)	48 (100%)	0	100	100
5	5	35/36 (97%)	35 (100%)	0	100	100
6	6	53/54 (98%)	53 (100%)	0	100	100
7	7	35/35 (100%)	35 (100%)	0	100	100
8	8	18/19 (95%)	18 (100%)	0	100	100
11	C	214/218 (98%)	211 (99%)	3 (1%)	59	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	D	160/163 (98%)	158 (99%)	2 (1%)	61	75
13	E	165/173 (95%)	165 (100%)	0	100	100
14	F	150/156 (96%)	150 (100%)	0	100	100
15	G	148/150 (99%)	148 (100%)	0	100	100
16	H	90/116 (78%)	89 (99%)	1 (1%)	65	77
17	I	89/120 (74%)	86 (97%)	3 (3%)	32	61
18	J	102/108 (94%)	102 (100%)	0	100	100
19	K	120/120 (100%)	120 (100%)	0	100	100
20	L	99/100 (99%)	98 (99%)	1 (1%)	68	78
21	M	112/114 (98%)	112 (100%)	0	100	100
22	N	112/116 (97%)	112 (100%)	0	100	100
23	O	96/138 (70%)	96 (100%)	0	100	100
24	P	93/94 (99%)	92 (99%)	1 (1%)	65	77
25	Q	100/100 (100%)	100 (100%)	0	100	100
26	R	97/99 (98%)	97 (100%)	0	100	100
27	S	82/83 (99%)	81 (99%)	1 (1%)	63	76
28	T	90/117 (77%)	90 (100%)	0	100	100
29	U	82/85 (96%)	82 (100%)	0	100	100
30	V	81/86 (94%)	78 (96%)	3 (4%)	30	59
31	W	154/168 (92%)	154 (100%)	0	100	100
32	X	59/63 (94%)	59 (100%)	0	100	100
33	Y	50/51 (98%)	50 (100%)	0	100	100
34	Z	58/66 (88%)	56 (97%)	2 (3%)	32	61
36	b	191/218 (88%)	190 (100%)	1 (0%)	81	83
37	c	171/212 (81%)	171 (100%)	0	100	100
38	d	175/176 (99%)	174 (99%)	1 (1%)	78	82
39	e	139/147 (95%)	139 (100%)	0	100	100
40	f	85/85 (100%)	85 (100%)	0	100	100
41	g	132/132 (100%)	132 (100%)	0	100	100
42	h	106/108 (98%)	106 (100%)	0	100	100
43	i	102/125 (82%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	j	88/90 (98%)	85 (97%)	3 (3%)	32	61
45	k	91/105 (87%)	91 (100%)	0	100	100
46	l	103/105 (98%)	103 (100%)	0	100	100
47	m	99/104 (95%)	99 (100%)	0	100	100
48	n	49/50 (98%)	48 (98%)	1 (2%)	48	69
49	o	75/77 (97%)	75 (100%)	0	100	100
50	p	92/118 (78%)	92 (100%)	0	100	100
51	q	78/83 (94%)	78 (100%)	0	100	100
52	r	55/72 (76%)	55 (100%)	0	100	100
53	s	69/84 (82%)	68 (99%)	1 (1%)	59	74
54	t	69/70 (99%)	69 (100%)	0	100	100
55	u	30/31 (97%)	30 (100%)	0	100	100
All	All	4944/5355 (92%)	4915 (99%)	29 (1%)	76	82

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	21	GLU
1	1	50	VAL
2	2	34	VAL
2	2	38	CYS
2	2	63	LYS
11	C	147	LEU
11	C	248	SER
11	C	257	THR
12	D	156	THR
12	D	201	ARG
16	H	126	SER
17	I	50	THR
17	I	51	VAL
17	I	79	ILE
20	L	91	ASN
24	P	25	LEU
27	S	26	LYS
30	V	43	LYS
30	V	44	HIS
30	V	45	THR
34	Z	5	THR

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Mol	Chain	Res	Type
34	Z	47	LEU
36	b	181	ILE
38	d	155	GLU
44	j	36	VAL
44	j	73	LEU
44	j	75	ASP
48	n	59	SER
53	s	37	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
5	5	9	GLN
5	5	36	ASN
6	6	25	GLN
6	6	63	ASN
11	C	233	HIS
13	E	83	GLN
13	E	151	ASN
14	F	13	GLN
19	K	40	HIS
21	M	127	ASN
23	O	31	HIS
23	O	61	HIS
24	P	53	ASN
25	Q	40	GLN
26	R	39	GLN
27	S	90	HIS
27	S	92	GLN
29	U	41	GLN
31	W	61	HIS
31	W	91	ASN
31	W	126	GLN
36	b	167	ASN
37	c	145	ASN
42	h	29	HIS
45	k	86	HIS
46	l	105	GLN
46	l	112	GLN
48	n	11	ASN
49	o	50	HIS
52	r	61	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	116/118 (98%)	19 (16%)	2 (1%)
35	a	1504/1528 (98%)	276 (18%)	0
9	A	3096/3120 (99%)	545 (17%)	27 (0%)
All	All	4716/4766 (98%)	840 (17%)	29 (0%)

All (840) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	7	U
9	A	20	G
9	A	23	G
9	A	24	G
9	A	31	U
9	A	48	G
9	A	60	A
9	A	68	A
9	A	71	A
9	A	72	G
9	A	80	G
9	A	89	A
9	A	90	C
9	A	94	G
9	A	97	U
9	A	98	U
9	A	99	G
9	A	115	A
9	A	117	U
9	A	123	A
9	A	124	A
9	A	125	C
9	A	126	C
9	A	160	A
9	A	161	U
9	A	164	A
9	A	175	G
9	A	180	A
9	A	195	A
9	A	212	A
9	A	215	A
9	A	221	A
9	A	227	A

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Mol	Chain	Res	Type
9	A	229	U
9	A	230	G
9	A	231	U
9	A	233	A
9	A	248	G
9	A	264	G
9	A	275	C
9	A	285	U
9	A	286	G
9	A	287	A
9	A	288	U
9	A	290	C
9	A	297	G
9	A	298	G
9	A	299	G
9	A	300	G
9	A	301	U
9	A	302	U
9	A	303	G
9	A	305	G
9	A	313	G
9	A	314	G
9	A	315	U
9	A	317	G
9	A	318	U
9	A	319	G
9	A	322	A
9	A	323	C
9	A	326	A
9	A	330	U
9	A	331	U
9	A	336	C
9	A	337	U
9	A	338	C
9	A	351	G
9	A	352	G
9	A	357	U
9	A	358	G
9	A	361	A
9	A	363	A
9	A	365	U
9	A	370	U

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Mol	Chain	Res	Type
9	A	371	G
9	A	380	A
9	A	384	G
9	A	393	U
9	A	399	G
9	A	404	A
9	A	412	A
9	A	434	G
9	A	437	G
9	A	444	U
9	A	445	U
9	A	446	G
9	A	450	G
9	A	451	U
9	A	452	G
9	A	453	U
9	A	459	A
9	A	460	G
9	A	474	G
9	A	489	A
9	A	494	G
9	A	497	G
9	A	498	G
9	A	499	G
9	A	512	G
9	A	517	A
9	A	523	U
9	A	539	C
9	A	543	U
9	A	544	U
9	A	553	G
9	A	555	G
9	A	563	U
9	A	569	G
9	A	578	G
9	A	589	A
9	A	591	G
9	A	592	A
9	A	594	U
9	A	595	A
9	A	596	C
9	A	605	G

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Mol	Chain	Res	Type
9	A	617	U
9	A	618	C
9	A	619	C
9	A	620	G
9	A	639	C
9	A	640	G
9	A	642	G
9	A	644	G
9	A	647	G
9	A	655	G
9	A	658	U
9	A	665	G
9	A	667	A
9	A	678	A
9	A	679	G
9	A	684	G
9	A	696	A
9	A	706	G
9	A	707	G
9	A	708	G
9	A	709	U
9	A	721	A
9	A	731	A
9	A	738	A
9	A	740	A
9	A	741	G
9	A	757	G
9	A	758	A
9	A	760	U
9	A	765	G
9	A	766	G
9	A	774	G
9	A	784	G
9	A	786	C
9	A	801	U
9	A	838	G
9	A	839	U
9	A	841	G
9	A	845	C
9	A	862	U
9	A	863	G
9	A	868	C

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Mol	Chain	Res	Type
9	A	872	G
9	A	890	G
9	A	897	A
9	A	898	A
9	A	899	G
9	A	904	A
9	A	920	G
9	A	921	C
9	A	927	C
9	A	942	U
9	A	961	U
9	A	972	A
9	A	974	G
9	A	975	U
9	A	981	U
9	A	982	A
9	A	994	A
9	A	1001	C
9	A	1002	C
9	A	1008	G
9	A	1009	U
9	A	1011	A
9	A	1012	C
9	A	1014	G
9	A	1025	A
9	A	1029	C
9	A	1045	C
9	A	1046	C
9	A	1047	A
9	A	1048	A
9	A	1049	G
9	A	1063	G
9	A	1076	A
9	A	1078	G
9	A	1079	C
9	A	1085	G
9	A	1092	G
9	A	1098	A
9	A	1101	A
9	A	1114	G
9	A	1127	A
9	A	1130	C

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Mol	Chain	Res	Type
9	A	1131	G
9	A	1138	A
9	A	1144	A
9	A	1151	U
9	A	1164	A
9	A	1172	A
9	A	1173	G
9	A	1174	G
9	A	1178	U
9	A	1181	G
9	A	1184	U
9	A	1185	A
9	A	1186	G
9	A	1188	A
9	A	1189	G
9	A	1191	A
9	A	1201	G
9	A	1202	A
9	A	1203	A
9	A	1205	G
9	A	1206	A
9	A	1207	G
9	A	1208	U
9	A	1209	G
9	A	1212	U
9	A	1213	A
9	A	1215	U
9	A	1223	U
9	A	1225	G
9	A	1226	U
9	A	1228	A
9	A	1230	G
9	A	1240	G
9	A	1251	A
9	A	1253	C
9	A	1260	C
9	A	1261	A
9	A	1293	G
9	A	1326	G
9	A	1335	G
9	A	1344	A
9	A	1351	G

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Mol	Chain	Res	Type
9	A	1353	G
9	A	1359	G
9	A	1371	G
9	A	1380	A
9	A	1384	G
9	A	1386	G
9	A	1387	A
9	A	1389	U
9	A	1415	A
9	A	1416	A
9	A	1429	C
9	A	1440	C
9	A	1444	U
9	A	1448	C
9	A	1456	G
9	A	1465	C
9	A	1474	A
9	A	1480	A
9	A	1493	A
9	A	1494	U
9	A	1495	G
9	A	1499	A
9	A	1500	A
9	A	1507	G
9	A	1508	A
9	A	1510	A
9	A	1522	G
9	A	1531	C
9	A	1532	G
9	A	1534	C
9	A	1540	U
9	A	1541	G
9	A	1543	A
9	A	1550	G
9	A	1551	U
9	A	1552	A
9	A	1553	C
9	A	1554	U
9	A	1562	C
9	A	1564	A
9	A	1565	A
9	A	1568	C

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Mol	Chain	Res	Type
9	A	1570	C
9	A	1571	C
9	A	1574	G
9	A	1579	C
9	A	1580	A
9	A	1581	C
9	A	1587	G
9	A	1593	U
9	A	1594	G
9	A	1595	G
9	A	1599	U
9	A	1600	G
9	A	1601	G
9	A	1603	G
9	A	1605	G
9	A	1606	G
9	A	1625	G
9	A	1629	G
9	A	1630	U
9	A	1631	A
9	A	1632	G
9	A	1640	A
9	A	1641	U
9	A	1648	A
9	A	1649	C
9	A	1672	C
9	A	1676	G
9	A	1679	A
9	A	1680	A
9	A	1681	U
9	A	1703	G
9	A	1713	U
9	A	1716	A
9	A	1717	U
9	A	1724	G
9	A	1728	U
9	A	1731	A
9	A	1737	A
9	A	1753	C
9	A	1754	G
9	A	1767	U
9	A	1789	A

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Mol	Chain	Res	Type
9	A	1798	U
9	A	1803	A
9	A	1816	C
9	A	1826	A
9	A	1852	A
9	A	1864	U
9	A	1866	C
9	A	1870	U
9	A	1871	G
9	A	1872	A
9	A	1892	G
9	A	1933	G
9	A	1973	C
9	A	1975	A
9	A	1981	U
9	A	1990	A
9	A	1998	C
9	A	2001	A
9	A	2017	C
9	A	2018	G
9	A	2025	C
9	A	2026	A
9	A	2033	U
9	A	2046	A
9	A	2052	G
9	A	2064	A
9	A	2065	A
9	A	2066	G
9	A	2075	G
9	A	2076	A
9	A	2083	A
9	A	2085	C
9	A	2086	U
9	A	2088	C
9	A	2089	C
9	A	2091	U
9	A	2092	U
9	A	2093	G
9	A	2094	G
9	A	2095	G
9	A	2096	G
9	A	2107	G

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Mol	Chain	Res	Type
9	A	2130	G
9	A	2134	G
9	A	2135	U
9	A	2137	A
9	A	2138	C
9	A	2139	U
9	A	2140	A
9	A	2141	U
9	A	2142	A
9	A	2144	OMC
9	A	2151	A
9	A	2153	G
9	A	2154	G
9	A	2161	A
9	A	2163	U
9	A	2179	U
9	A	2187	U
9	A	2188	G
9	A	2190	A
9	A	2191	C
9	A	2194	A
9	A	2195	U
9	A	2196	G
9	A	2215	U
9	A	2216	G
9	A	2217	U
9	A	2221	A
9	A	2239	A
9	A	2245	C
9	A	2246	U
9	A	2247	A
9	A	2254	A
9	A	2255	A
9	A	2256	G
9	A	2257	A
9	A	2267	C
9	A	2276	G
9	A	2279	C
9	A	2280	G
9	A	2283	A
9	A	2284	A
9	A	2285	G

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Mol	Chain	Res	Type
9	A	2286	A
9	A	2315	U
9	A	2320	C
9	A	2328	G
9	A	2331	U
9	A	2333	G
9	A	2334	U
9	A	2335	G
9	A	2337	A
9	A	2339	G
9	A	2340	A
9	A	2341	U
9	A	2342	A
9	A	2343	G
9	A	2349	A
9	A	2350	G
9	A	2351	A
9	A	2353	U
9	A	2354	G
9	A	2356	G
9	A	2360	C
9	A	2368	C
9	A	2370	A
9	A	2380	G
9	A	2382	G
9	A	2383	U
9	A	2384	C
9	A	2386	U
9	A	2387	U
9	A	2388	G
9	A	2390	U
9	A	2394	A
9	A	2395	U
9	A	2396	A
9	A	2403	U
9	A	2405	A
9	A	2406	U
9	A	2408	G
9	A	2413	G
9	A	2422	A
9	A	2427	G
9	A	2434	A

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Mol	Chain	Res	Type
9	A	2436	A
9	A	2446	G
9	A	2449	A
9	A	2462	G
9	A	2463	G
9	A	2502	A
9	A	2507	C
9	A	2511	A
9	A	2521	C
9	A	2529	A
9	A	2531	G
9	A	2532	G
9	A	2533	C
9	A	2545	G
9	A	2548	U
9	A	2551	A
9	A	2559	A
9	A	2571	C
9	A	2574	C
9	A	2581	G
9	A	2585	U
9	A	2607	G
9	A	2609	A
9	A	2626	U
9	A	2630	A
9	A	2647	U
9	A	2649	A
9	A	2652	G
9	A	2653	G
9	A	2654	A
9	A	2655	U
9	A	2659	A
9	A	2665	C
9	A	2671	G
9	A	2672	A
9	A	2694	G
9	A	2698	C
9	A	2699	C
9	A	2715	U
9	A	2721	A
9	A	2722	C
9	A	2726	G

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Mol	Chain	Res	Type
9	A	2727	A
9	A	2729	G
9	A	2742	A
9	A	2744	C
9	A	2778	U
9	A	2786	U
9	A	2790	A
9	A	2791	G
9	A	2796	A
9	A	2806	G
9	A	2822	A
9	A	2826	A
9	A	2833	U
9	A	2837	U
9	A	2853	C
9	A	2854	A
9	A	2870	C
9	A	2871	U
9	A	2878	A
9	A	2906	U
9	A	2913	U
9	A	2914	A
9	A	2915	C
9	A	2926	A
9	A	2936	C
9	A	2938	G
9	A	2957	A
9	A	2968	G
9	A	2972	A
9	A	2985	G
9	A	2989	A
9	A	3002	A
9	A	3009	U
9	A	3013	C
9	A	3014	A
9	A	3015	C
9	A	3021	A
9	A	3022	G
9	A	3039	C
9	A	3042	A
9	A	3046	C
9	A	3070	G

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Mol	Chain	Res	Type
9	A	3071	A
9	A	3088	C
9	A	3093	A
9	A	3101	C
9	A	3105	C
9	A	3106	C
9	A	3108	G
9	A	3112	A
10	B	4	A
10	B	5	C
10	B	9	G
10	B	12	C
10	B	13	C
10	B	35	G
10	B	44	C
10	B	45	G
10	B	50	C
10	B	51	G
10	B	52	G
10	B	57	U
10	B	86	U
10	B	87	U
10	B	88	C
10	B	89	C
10	B	106	C
10	B	114	A
10	B	117	A
35	a	10	G
35	a	13	G
35	a	35	G
35	a	36	A
35	a	43	G
35	a	51	C
35	a	52	U
35	a	53	U
35	a	55	A
35	a	82	U
35	a	87	G
35	a	91	U
35	a	92	A
35	a	93	C
35	a	116	A

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Mol	Chain	Res	Type
35	a	117	C
35	a	126	G
35	a	128	U
35	a	156	G
35	a	160	C
35	a	179	C
35	a	180	A
35	a	192	G
35	a	194	A
35	a	209	A
35	a	210	A
35	a	211	A
35	a	215	U
35	a	216	U
35	a	217	U
35	a	220	G
35	a	231	G
35	a	240	C
35	a	245	C
35	a	247	G
35	a	251	G
35	a	266	G
35	a	267	C
35	a	279	A
35	a	280	C
35	a	281	G
35	a	289	G
35	a	329	A
35	a	332	G
35	a	344	A
35	a	346	G
35	a	347	G
35	a	351	G
35	a	352	C
35	a	353	A
35	a	354	G
35	a	362	G
35	a	367	U
35	a	372	C
35	a	373	A
35	a	390	U
35	a	392	C

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Mol	Chain	Res	Type
35	a	397	A
35	a	398	C
35	a	406	G
35	a	411	A
35	a	414	A
35	a	415	C
35	a	421	U
35	a	422	C
35	a	423	G
35	a	426	U
35	a	428	G
35	a	429	U
35	a	430	A
35	a	434	C
35	a	452	A
35	a	453	G
35	a	456	C
35	a	457	A
35	a	458	A
35	a	461	G
35	a	465	G
35	a	466	U
35	a	473	A
35	a	477	G
35	a	478	A
35	a	482	A
35	a	486	G
35	a	490	A
35	a	491	C
35	a	492	U
35	a	498	C
35	a	499	C
35	a	505	C
35	a	507	G
35	a	508	C
35	a	509	G
35	a	511	U
35	a	512	A
35	a	520	G
35	a	527	A
35	a	540	A
35	a	542	U

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Mol	Chain	Res	Type
35	a	544	C
35	a	552	A
35	a	553	A
35	a	554	A
35	a	556	A
35	a	557	G
35	a	612	U
35	a	633	A
35	a	645	G
35	a	666	U
35	a	668	G
35	a	675	A
35	a	700	C
35	a	701	G
35	a	702	G
35	a	703	U
35	a	728	A
35	a	735	G
35	a	761	A
35	a	765	G
35	a	773	U
35	a	774	A
35	a	789	G
35	a	794	A
35	a	797	C
35	a	808	A
35	a	809	G
35	a	837	G
35	a	839	C
35	a	841	U
35	a	847	A
35	a	854	A
35	a	865	C
35	a	896	A
35	a	909	G
35	a	916	C
35	a	917	A
35	a	924	G
35	a	932	U
35	a	940	A
35	a	941	A
35	a	942	U

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Mol	Chain	Res	Type
35	a	947	U
35	a	948	G
35	a	949	C
35	a	950	A
35	a	951	A
35	a	953	G
35	a	955	G
35	a	957	A
35	a	958	G
35	a	959	A
35	a	964	U
35	a	971	G
35	a	973	U
35	a	974	U
35	a	975	G
35	a	986	G
35	a	1008	C
35	a	1014	U
35	a	1020	G
35	a	1024	G
35	a	1025	C
35	a	1028	G
35	a	1030	G
35	a	1033	G
35	a	1034	C
35	a	1045	U
35	a	1046	C
35	a	1048	G
35	a	1050	U
35	a	1075	U
35	a	1079	G
35	a	1080	C
35	a	1081	A
35	a	1082	A
35	a	1088	G
35	a	1103	U
35	a	1105	U
35	a	1106	U
35	a	1107	G
35	a	1110	A
35	a	1113	A
35	a	1116	U

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Mol	Chain	Res	Type
35	a	1117	U
35	a	1120	G
35	a	1124	G
35	a	1127	A
35	a	1129	U
35	a	1130	C
35	a	1131	G
35	a	1133	G
35	a	1138	A
35	a	1139	C
35	a	1140	U
35	a	1146	G
35	a	1149	C
35	a	1150	A
35	a	1151	A
35	a	1164	U
35	a	1165	G
35	a	1177	A
35	a	1178	A
35	a	1182	A
35	a	1183	U
35	a	1193	U
35	a	1194	A
35	a	1207	C
35	a	1217	A
35	a	1219	A
35	a	1231	A
35	a	1234	G
35	a	1235	G
35	a	1236	G
35	a	1237	C
35	a	1238	U
35	a	1239	G
35	a	1248	U
35	a	1251	G
35	a	1254	G
35	a	1261	A
35	a	1262	U
35	a	1263	C
35	a	1265	U
35	a	1266	U
35	a	1267	U

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Mol	Chain	Res	Type
35	a	1280	C
35	a	1283	U
35	a	1284	U
35	a	1285	C
35	a	1287	G
35	a	1294	G
35	a	1301	A
35	a	1302	C
35	a	1328	A
35	a	1329	G
35	a	1343	G
35	a	1344	C
35	a	1346	A
35	a	1347	C
35	a	1351	G
35	a	1357	A
35	a	1361	C
35	a	1380	C
35	a	1381	A
35	a	1382	C
35	a	1388	G
35	a	1389	U
35	a	1391	A
35	a	1392	OMC
35	a	1393	G
35	a	1394	U
35	a	1395	C
35	a	1423	U
35	a	1425	G
35	a	1426	C
35	a	1429	A
35	a	1433	C
35	a	1434	U
35	a	1435	U
35	a	1436	G
35	a	1437	U
35	a	1438	G
35	a	1468	U
35	a	1473	A
35	a	1476	A
35	a	1477	A
35	a	1481	G

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Mol	Chain	Res	Type
35	a	1483	A
35	a	1488	G
35	a	1490	U
35	a	1501	G
35	a	1504	G
35	a	1513	G
35	a	1514	G
35	a	1516	U
35	a	1518	A

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	89	A
9	A	313	G
9	A	316	U
9	A	336	C
9	A	357	U
9	A	451	U
9	A	643	G
9	A	948	G
9	A	970	G
9	A	974	G
9	A	980	C
9	A	981	U
9	A	1010	U
9	A	1044	U
9	A	1084	U
9	A	1224	G
9	A	1261	A
9	A	1264	C
9	A	1473	G
9	A	1507	G
9	A	1531	C
9	A	1730	U
9	A	2088	C
9	A	2094	G
9	A	2150	U
9	A	2350	G
9	A	2381	A
10	B	34	G
10	B	86	U

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

2 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	$\# Z  > 2$
9	OMC	A	2144	9	19,22,23	0.84	0	25,31,34	1.25	2 (8%)
35	OMC	a	1392	35	19,22,23	0.94	0	25,31,34	1.03	2 (8%)

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
9	OMC	A	2144	9	-	3/9/27/28	0/2/2/2
35	OMC	a	1392	35	-	6/9/27/28	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2144	OMC	C2'-C1'-N1	-4.04	106.57	114.24
9	A	2144	OMC	O2-C2-N3	-2.60	118.23	122.33
35	a	1392	OMC	O2-C2-N3	-2.37	118.59	122.33
35	a	1392	OMC	O4'-C1'-C2'	-2.15	102.88	106.59

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	2144	OMC	C1'-C2'-O2'-CM2
9	A	2144	OMC	O4'-C4'-C5'-O5'
35	a	1392	OMC	C1'-C2'-O2'-CM2
35	a	1392	OMC	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
9	A	2144	OMC	C3'-C4'-C5'-O5'
35	a	1392	OMC	C3'-C4'-C5'-O5'
35	a	1392	OMC	O4'-C4'-C5'-O5'
35	a	1392	OMC	C2'-C1'-N1-C6
35	a	1392	OMC	C2'-C1'-N1-C2

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	a	1392	OMC	8	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 139 ligands modelled in this entry, 139 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

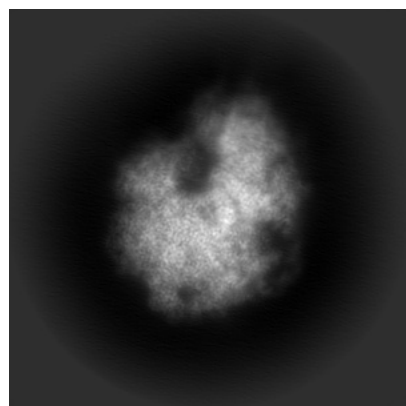
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47365. These allow visual inspection of the internal detail of the map and identification of artifacts.

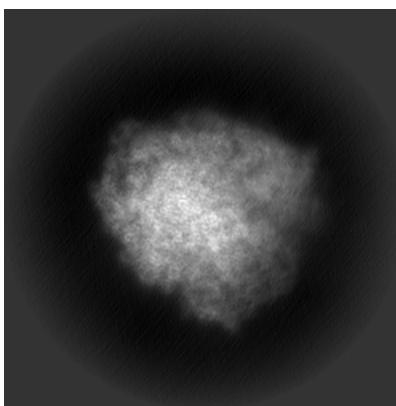
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

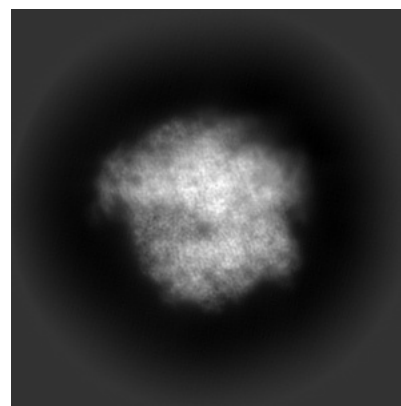
#### 6.1.1 Primary map



X

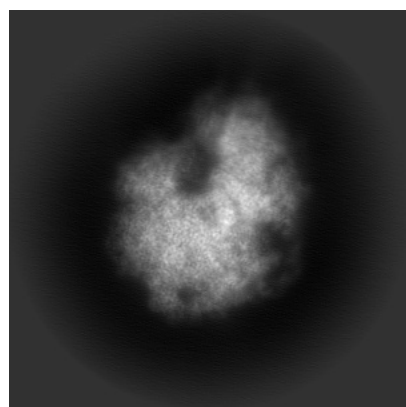


Y

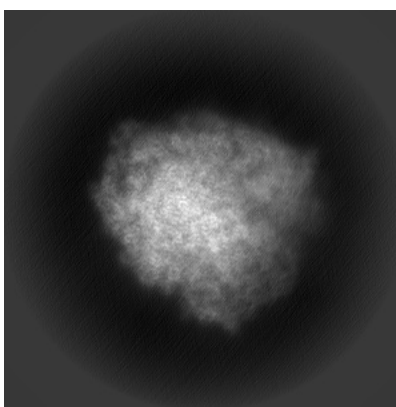


Z

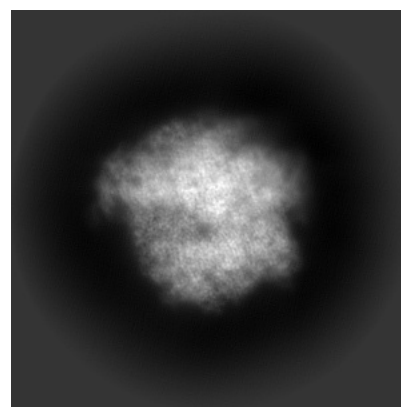
#### 6.1.2 Raw map



X



Y

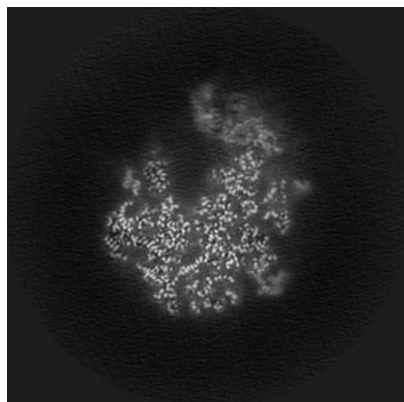


Z

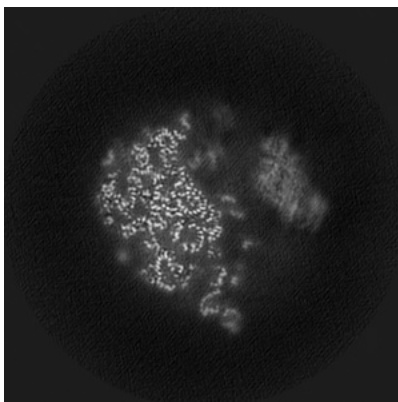
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

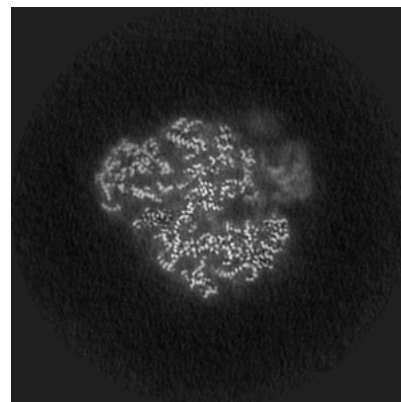
### 6.2.1 Primary map



X Index: 200

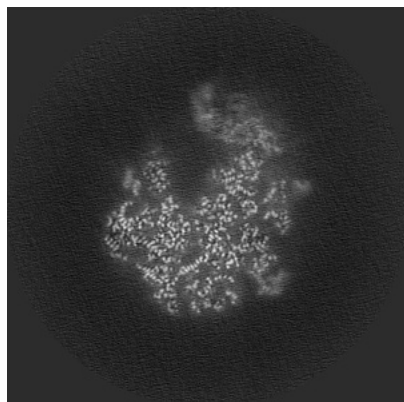


Y Index: 200

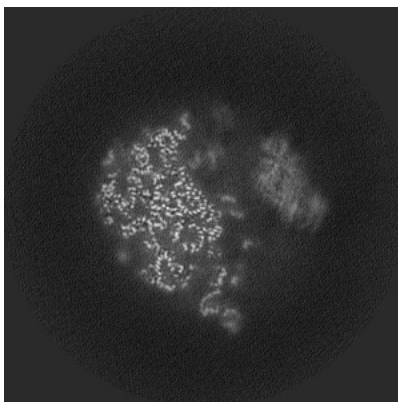


Z Index: 200

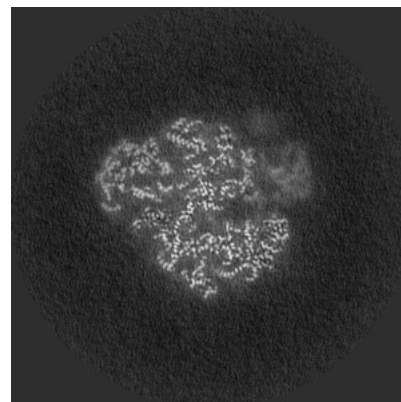
### 6.2.2 Raw map



X Index: 200



Y Index: 200

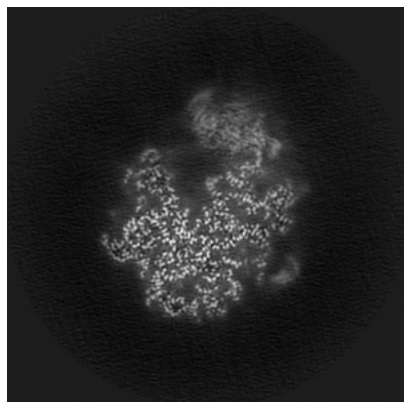


Z Index: 200

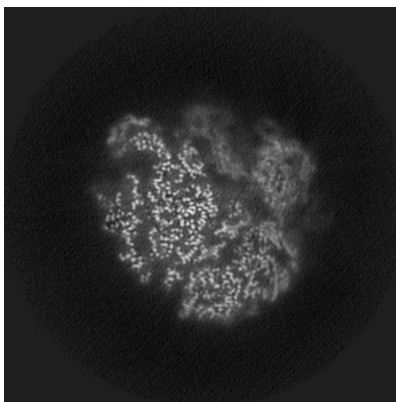
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

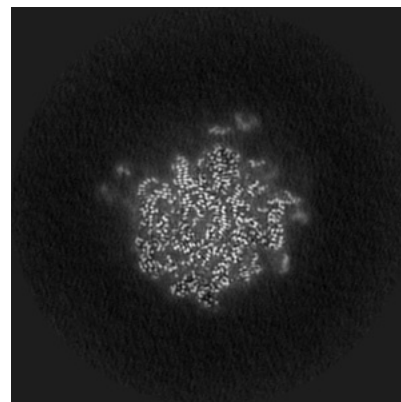
### 6.3.1 Primary map



X Index: 209

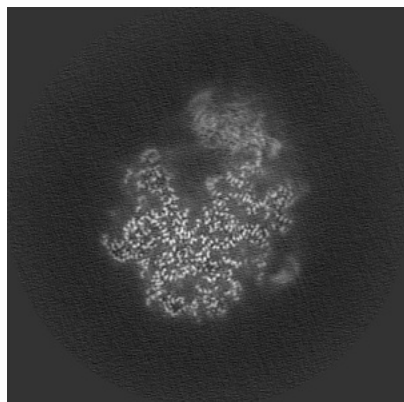


Y Index: 217

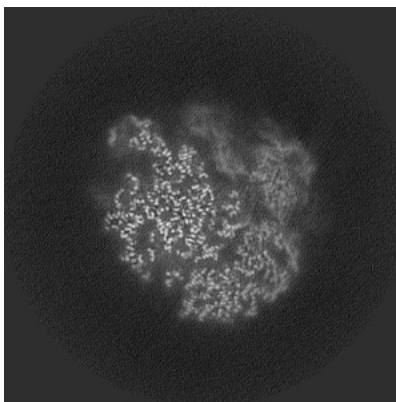


Z Index: 175

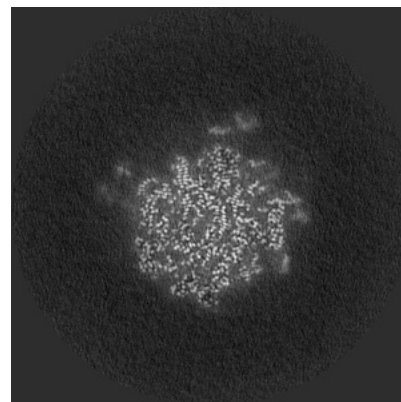
### 6.3.2 Raw map



X Index: 209



Y Index: 219



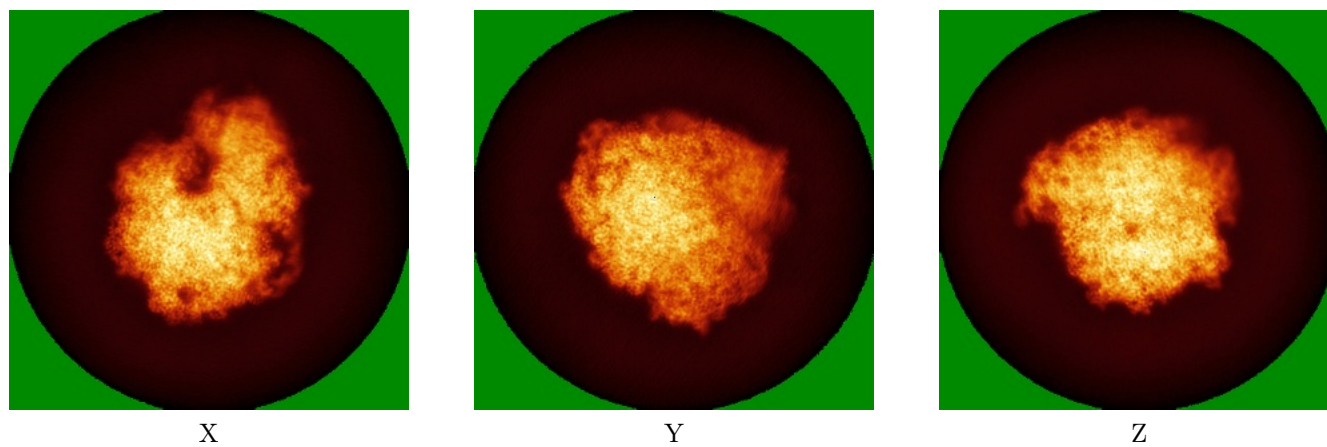
Z Index: 175

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

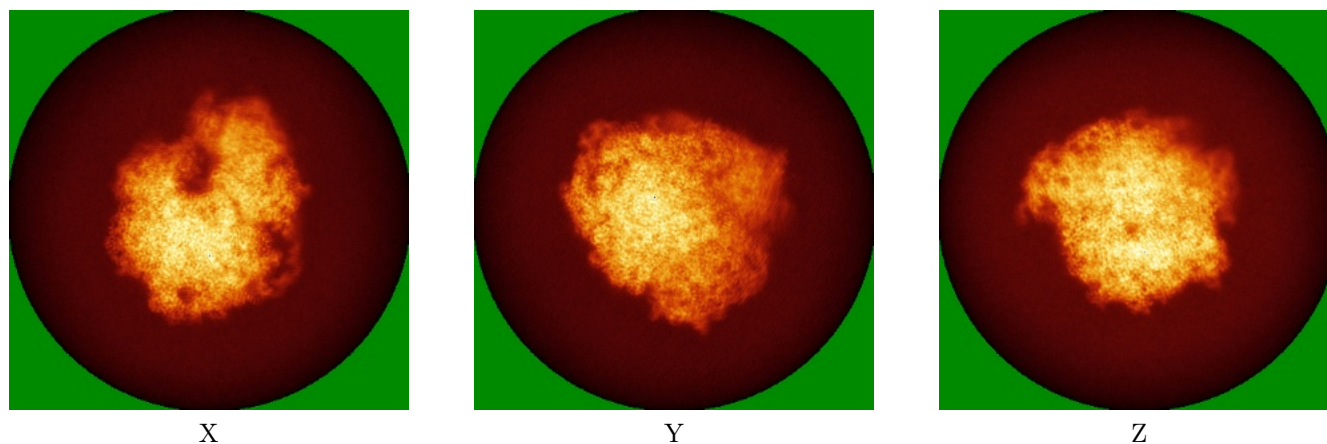


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

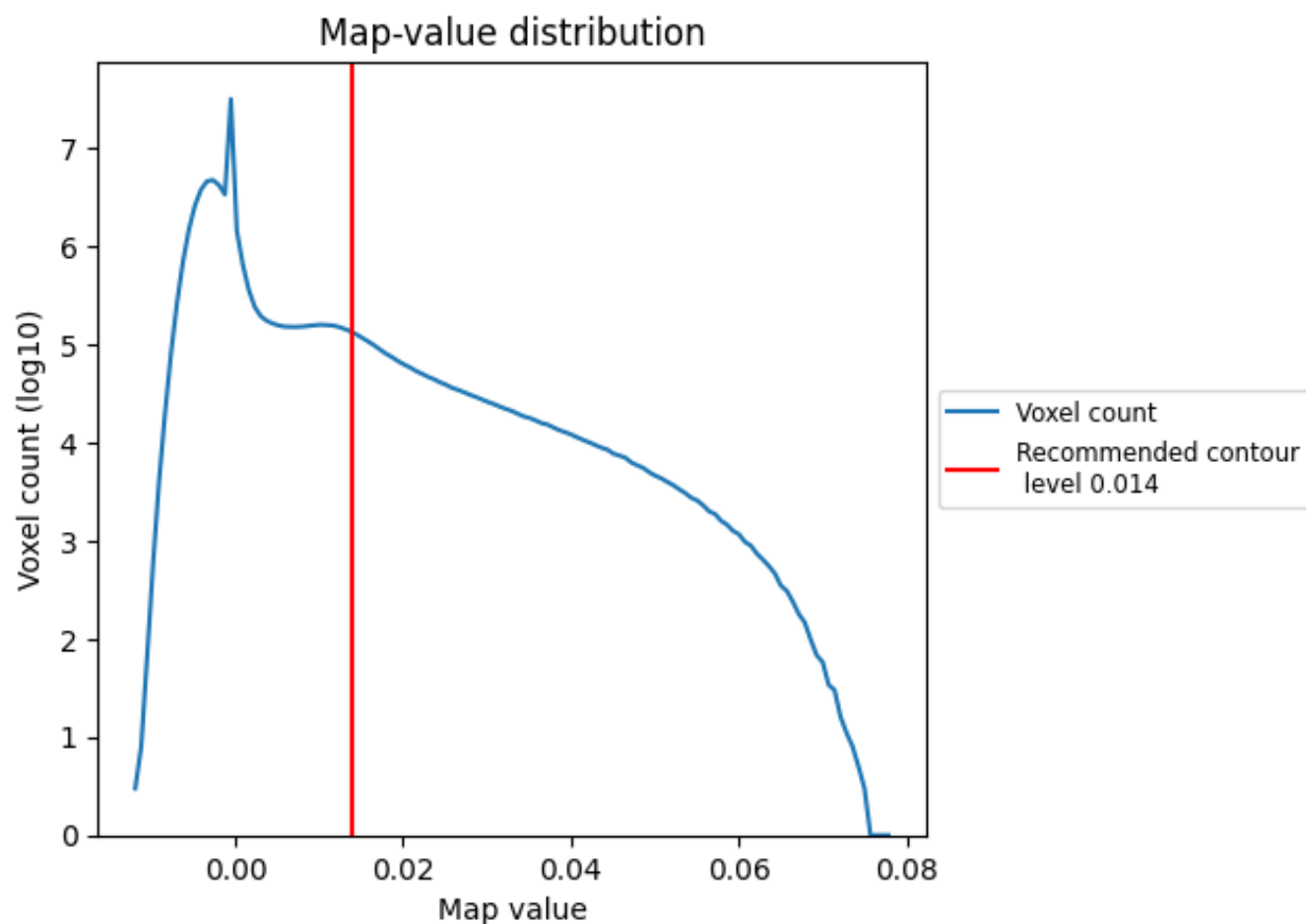
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

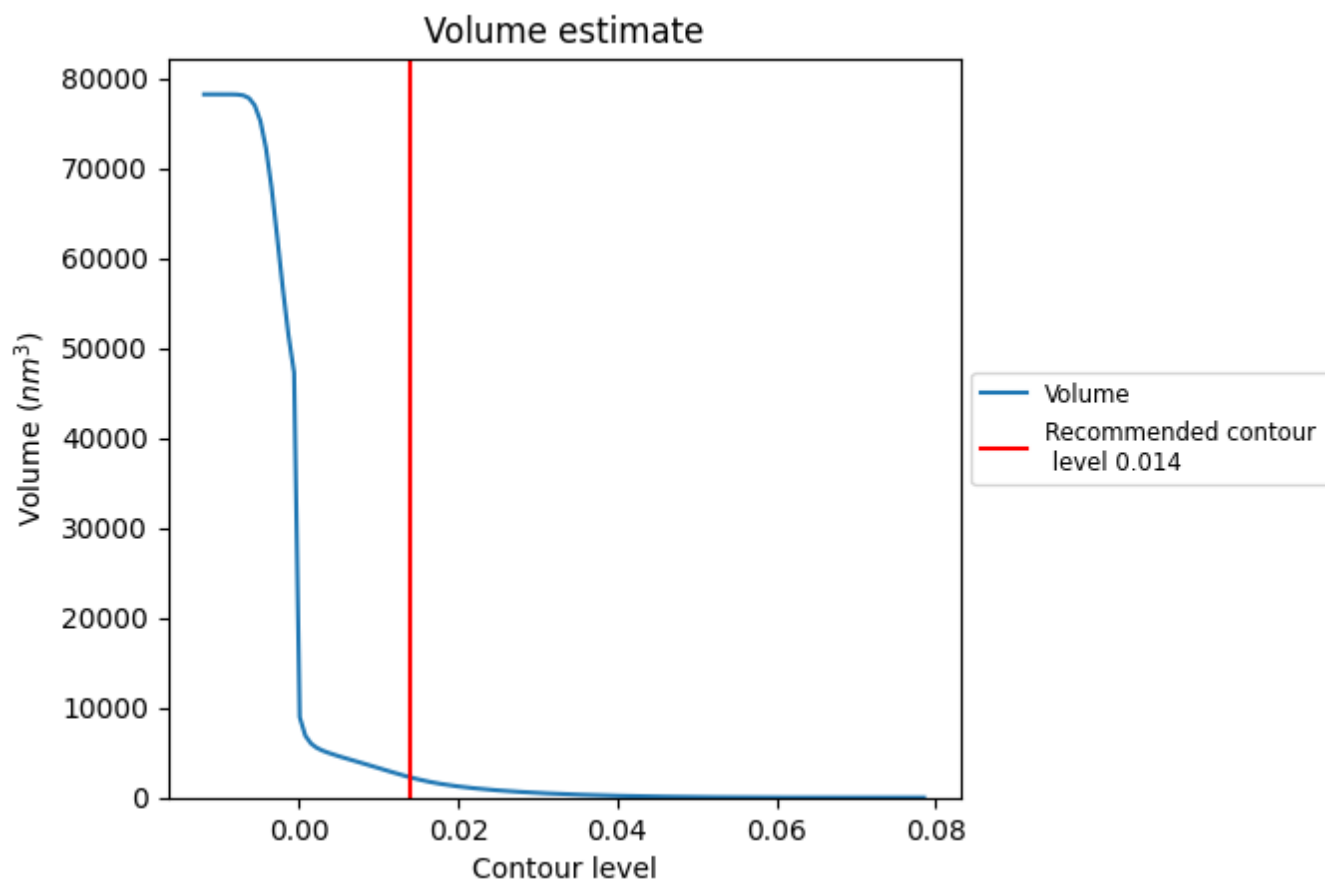
This section contains the results of statistical analysis of the map.

### 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.

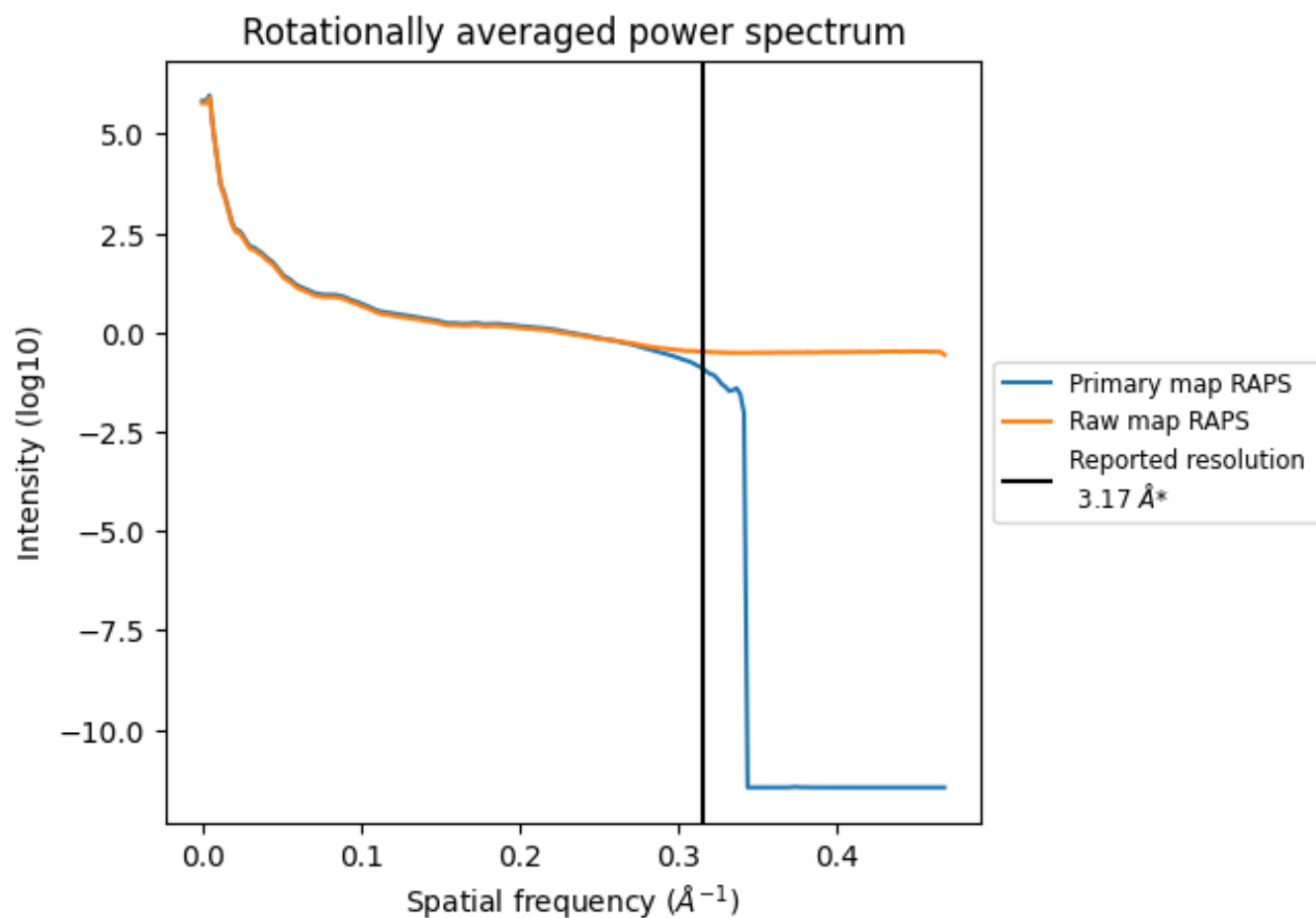
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2250 nm<sup>3</sup>; this corresponds to an approximate mass of 2032 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

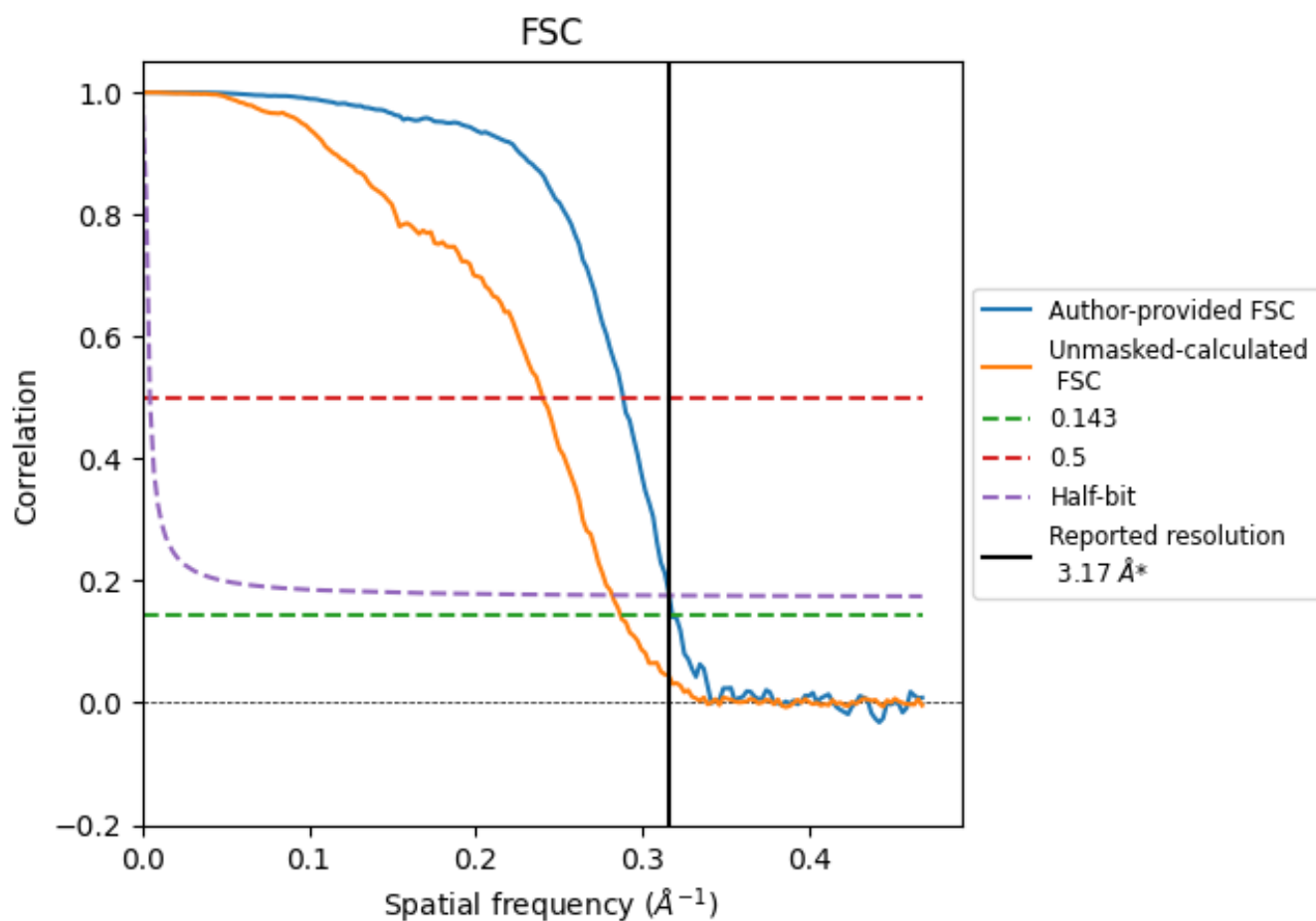


\*Reported resolution corresponds to spatial frequency of 0.315  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



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

## 8.2 Resolution estimates [i](#)

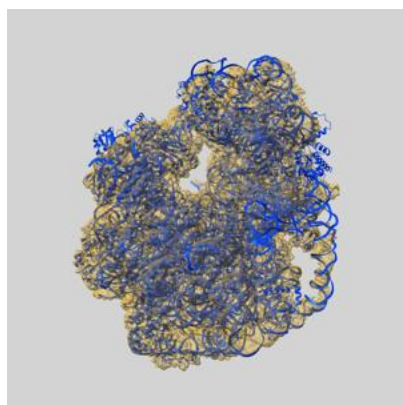
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.15	3.47	3.16
Unmasked-calculated*	3.49	4.16	3.55

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.49 differs from the reported value 3.17 by more than 10 %

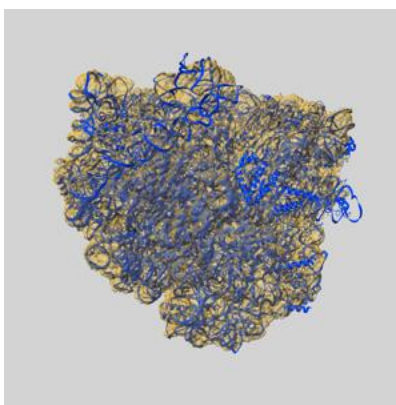
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47365 and PDB model 9E0P. Per-residue inclusion information can be found in section [3](#) on page [15](#).

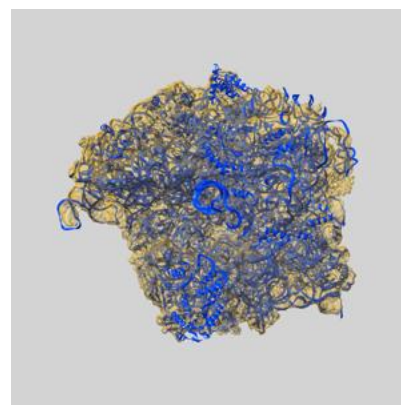
### 9.1 Map-model overlay [i](#)



X



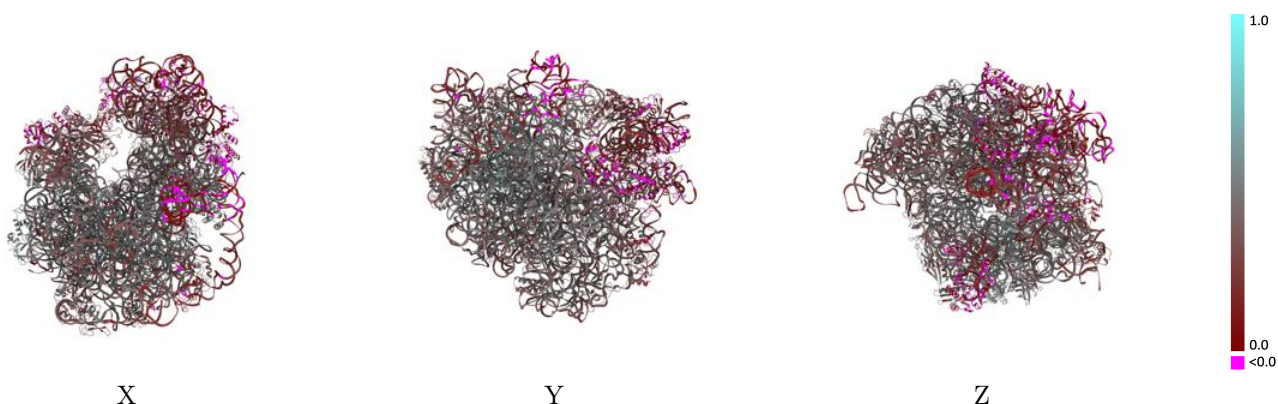
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



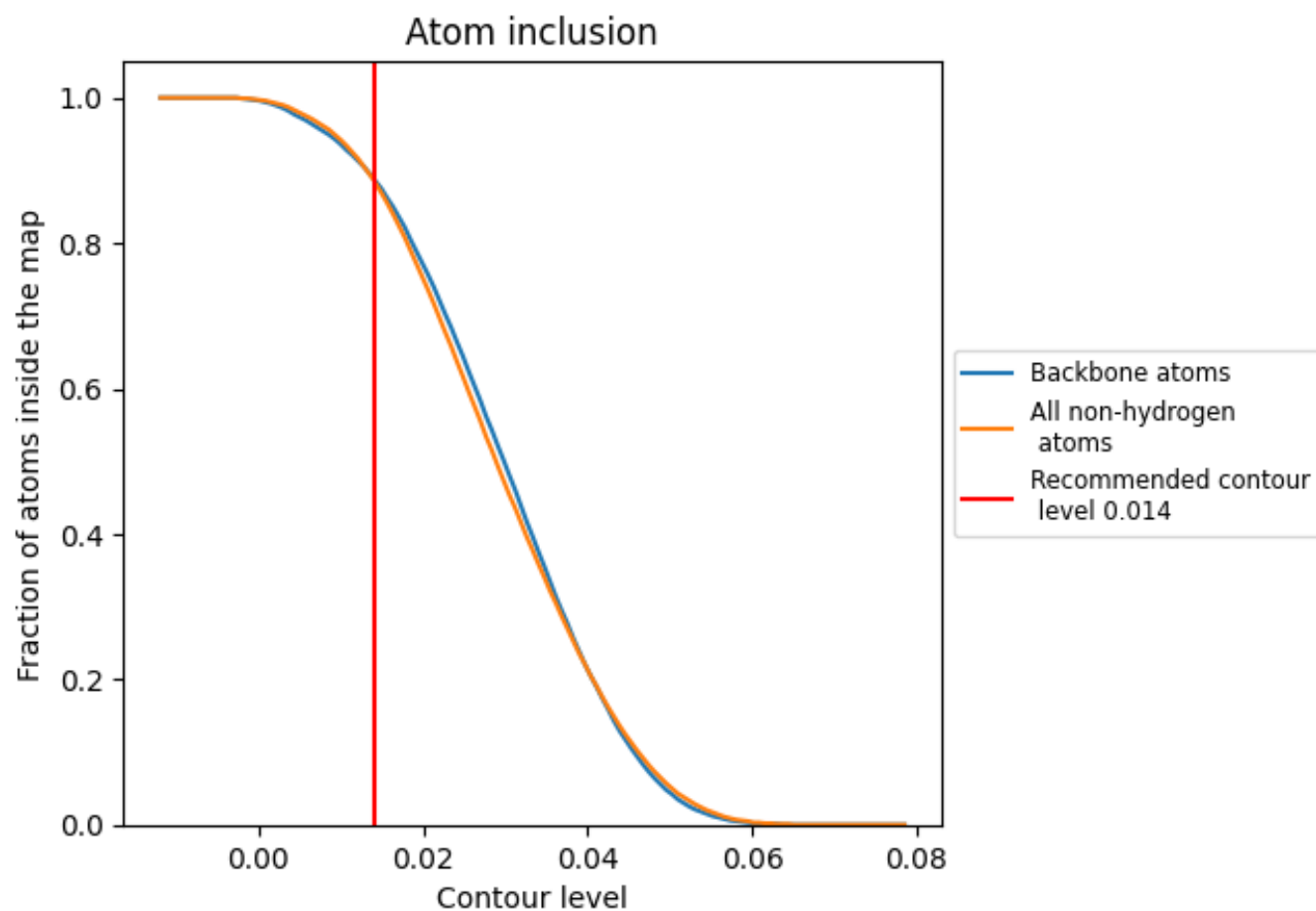
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ











































The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8870	 0.3720
1	 0.9210	 0.4740
2	 0.5040	 0.1460
3	 0.9500	 0.4830
4	 0.9110	 0.3850
5	 0.9970	 0.5070
6	 0.9900	 0.4520
7	 0.9900	 0.4590
8	 0.9940	 0.4960
A	 0.9420	 0.4010
B	 0.9290	 0.3500
C	 0.9900	 0.4990
D	 0.9290	 0.4540
E	 0.8500	 0.3870
F	 0.8470	 0.3290
G	 0.8270	 0.3920
H	 0.4310	 0.3210
I	 0.0660	 0.0320
J	 0.0100	 0.0950
K	 0.9500	 0.4860
L	 0.9220	 0.3920
M	 0.8950	 0.4110
N	 0.9710	 0.4720
O	 0.9440	 0.4170
P	 0.8600	 0.3420
Q	 0.9060	 0.3600
R	 0.9590	 0.5060
S	 0.9010	 0.5090
T	 0.9510	 0.4740
U	 0.9090	 0.4180
V	 0.7940	 0.3720
W	 0.8120	 0.4000
X	 0.9640	 0.4490
Y	 0.9780	 0.5000
Z	 0.8720	 0.4160



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Chain	Atom inclusion	Q-score
a	 0.9290	 0.3480
b	 0.0370	 0.0480
c	 0.5200	 0.2050
d	 0.7340	 0.3370
e	 0.7740	 0.3550
f	 0.9020	 0.4230
g	 0.8150	 0.2290
h	 0.9330	 0.4500
i	 0.8220	 0.1900
j	 0.5280	 -0.0010
k	 0.9040	 0.4200
l	 0.9010	 0.3650
m	 0.7170	 0.2640
n	 0.4800	 0.0360
o	 0.9470	 0.4540
p	 0.7730	 0.3750
q	 0.9320	 0.4430
r	 0.9030	 0.3880
s	 0.3650	 0.0560
t	 0.9120	 0.4010
u	 0.9770	 0.3920