



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:44 PM UTC

PDB ID : 5V93 / pdb_00005v93
EMDB ID : EMD-8645
Title : Cryo-EM structure of the 70S ribosome from Mycobacterium tuberculosis bound with Capreomycin
Authors : Yang, K.; Chang, J.-Y.; Cui, Z.; Li, X.; Meng, R.; Duan, L.; Thongchol, J.; Jakana, J.; Huwe, C.; Sacchettini, J.; Zhang, J.
Deposited on : 2017-03-22
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

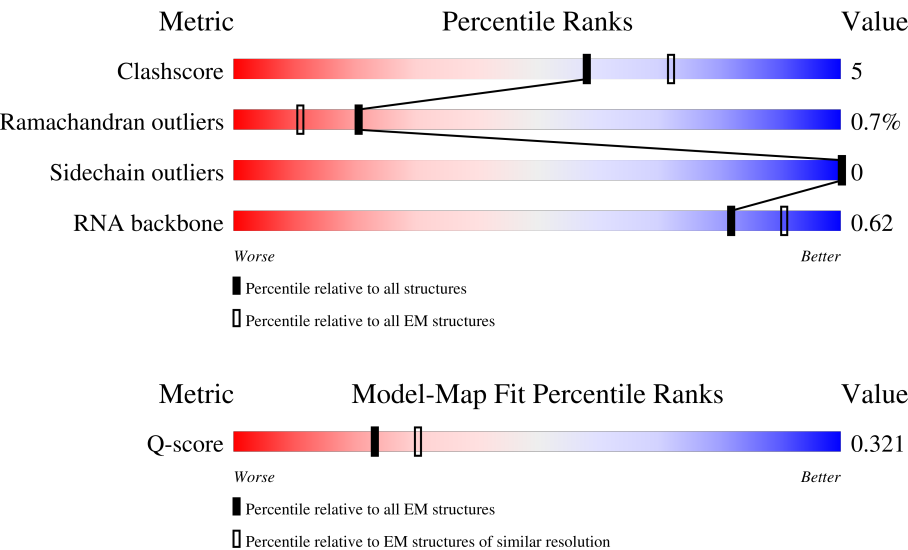
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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

Mol	Chain	Length	Quality of chain
1	0	57	42% 84% 9% 7%
2	1	55	25% 78% 7% 13%
3	2	47	15% 79% 11% 11%

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Mol	Chain	Length	Quality of chain
4	3	64	
5	4	37	
6	6	80	
7	A	3138	
8	B	115	
9	C	280	
10	D	217	
11	E	223	
12	F	187	
13	G	179	
14	H	152	
15	J	147	
16	K	122	
17	L	146	
18	M	138	
19	N	180	
20	O	122	
21	P	113	
22	Q	129	
23	R	104	
24	S	197	
25	T	100	
26	U	105	
27	V	215	
28	W	86	

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Mol	Chain	Length	Quality of chain
29	X	64	
30	Y	77	
31	Z	65	
32	a	1537	
33	b	6	
34	c	274	
35	d	201	
36	e	220	
37	f	96	
38	g	156	
39	h	132	
40	i	151	
41	j	101	
42	k	139	
43	l	124	
44	m	124	
45	n	61	
46	o	89	
47	p	162	
48	q	135	
49	r	84	
50	s	93	
51	t	86	
52	x	33	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 143579 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	53	Total	C	N	O	0	0
			421	262	93	66		

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			400	245	84	67	4		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	42	Total	C	N	O	S	0	0
			358	212	94	51	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1	VAL	MET	conflict	UNP A0A1L6JUG3

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	62	Total	C	N	O	0	0
			494	298	112	84		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			299	182	66	47	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	VAL	MET	conflict	UNP A0A1L6JSF4

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	45	Total	C	N	O	S	0	0
			345	214	60	66	5		

- Molecule 7 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	3118	Total	C	N	O	P	0	0
			66956	29845	12340	21653	3118		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	115	Total	C	N	O	P	0	0
			2458	1097	456	790	115		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	272	Total	C	N	O	S	0	0
			2088	1277	437	369	5		

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	213	Total	C	N	O	S	0	0
			1590	985	307	292	6		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	207	Total	C	N	O	S	0	0
			1552	958	303	289	2		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	170	Total	C	N	O	S	0	0
			1335	834	254	242	5		

- Molecule 13 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	174	Total	C	N	O	S	0	0
			1330	836	249	244	1		

- Molecule 14 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	47	Total	C	N	O	S	0	0
			350	220	64	65	1		

- Molecule 15 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	146	Total	C	N	O	S	0	0
			1143	724	217	199	3		

- Molecule 16 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	121	Total	C	N	O	S	0	0
			934	585	179	168	2		

- Molecule 17 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	142	Total	C	N	O	S	0	0
			1060	656	215	187	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	VAL	MET	conflict	UNP A0A0T7M0A0

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	134	Total	C	N	O	S	0	0
			1072	679	215	177	1		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	116	Total	C	N	O	S	0	0
			908	574	175	158	1		

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	116	Total	C	N	O		0	0
			886	541	188	157			

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	112	Total	C	N	O	S	0	0
			907	573	174	159	1		

- Molecule 22 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	122	Total	C	N	O		0	0
			980	608	205	167			

- Molecule 23 is a protein called LSU ribosomal protein L21p.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	98	Total	C	N	O		0	0
			742	472	136	134			

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	113	Total	C	N	O		0	0
			860	533	178	149			

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	T	98	Total	C	N	O	0	0
			759	480	141	138		

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	90	Total	C	N	O	S	0
			699	430	138	129	2	0

- Molecule 27 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	V	177	Total	C	N	O		0
			1319	822	243	254		0

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	W	74	Total	C	N	O	0	0
			546	336	111	99		

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	X	63	Total	C	N	O	S	0
			476	289	101	81	5	0

- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Y	65	Total	C	N	O	S	0
			541	331	106	103	1	0

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Z	59	Total	C	N	O	0	0
			476	293	101	82		

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1519	Total	C	N	O	P	0	0
			32610	14525	5961	10605	1519		

- Molecule 33 is a protein called Capreomycin.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	b	6	Total	C	N	O	0	0
			46	25	14	7		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	207	Total	C	N	O	S	0	0
			1654	1030	322	298	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	1	VAL	MET	conflict	UNP A0A045H4H6

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	201	Total	C	N	O	S	0	0
			1658	1041	317	297	3		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	160	Total	C	N	O	S	0	0
			1149	726	214	206	3		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	95	Total	C	N	O	S	0	0
			757	480	133	141	3		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	152	Total	C	N	O	S	0	0
			1193	742	234	215	2		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	130	Total	C	N	O	S	0	0
			999	627	187	184	1		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	127	Total	C	N	O	S	0	0
			993	628	195	170			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	99	Total	C	N	O	S	0	0
			789	496	146	144	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	1	VAL	MET	conflict	UNP A0A045HTN2

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	117	Total	C	N	O	S	0	0
			873	540	175	158			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	123	Total	C	N	O	S	0	0
			967	599	198	167	3		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	113	Total	C	N	O	S	0	0
			919	562	190	164	3		

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	59	Total	C	N	O	S	0	0
			463	291	95	72	5		

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	87	Total	C	N	O	S	0	0
			718	449	144	125			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	85	Total	C	N	O	S	0	0
			688	438	130	119	1		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	94	Total	C	N	O	S	0	0
			763	477	151	132	3		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	63	Total	C	N	O	S	0	0
			497	309	96	89	3		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	81	Total	C	N	O	S	0	0
			657	421	123	112	1		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	t	82	Total	C	N	O	0	0
			631	381	137	113		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	1	VAL	MET	conflict	UNP A0A045GXQ2

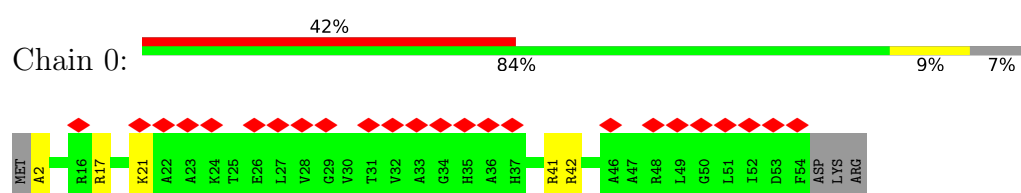
- Molecule 52 is a protein called Mitochondrial domain of uncharacterised function (DUF1713).

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	31	Total	C	N	O	S	0	0
			271	166	69	35	1		

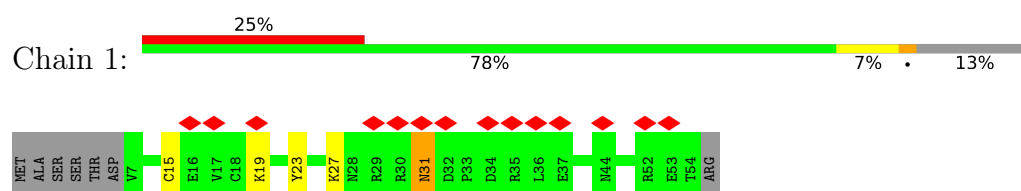
3 Residue-property plots [i](#)

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

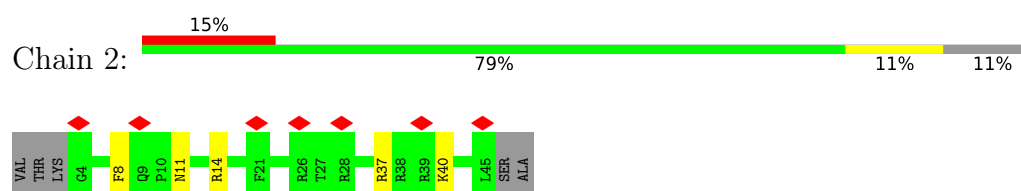
- Molecule 1: 50S ribosomal protein L32



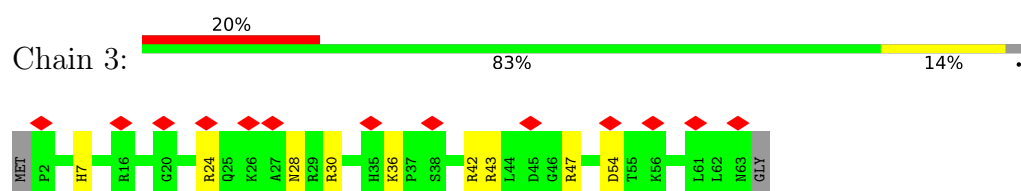
- Molecule 2: 50S ribosomal protein L33



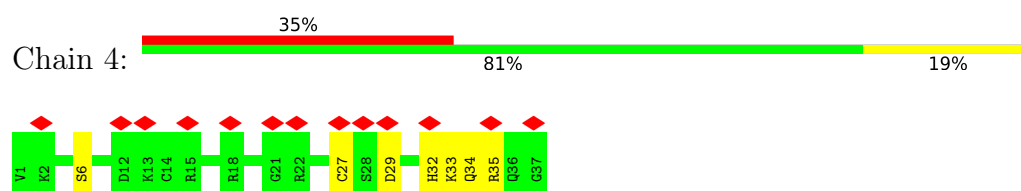
- Molecule 3: 50S ribosomal protein L34



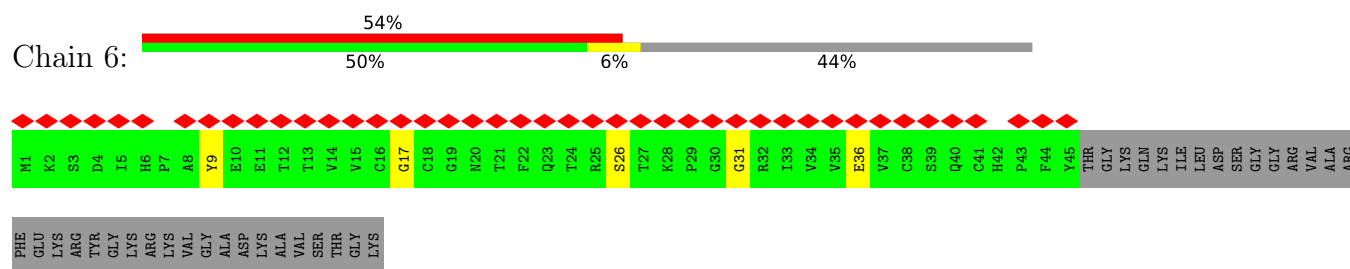
- Molecule 4: 50S ribosomal protein L35



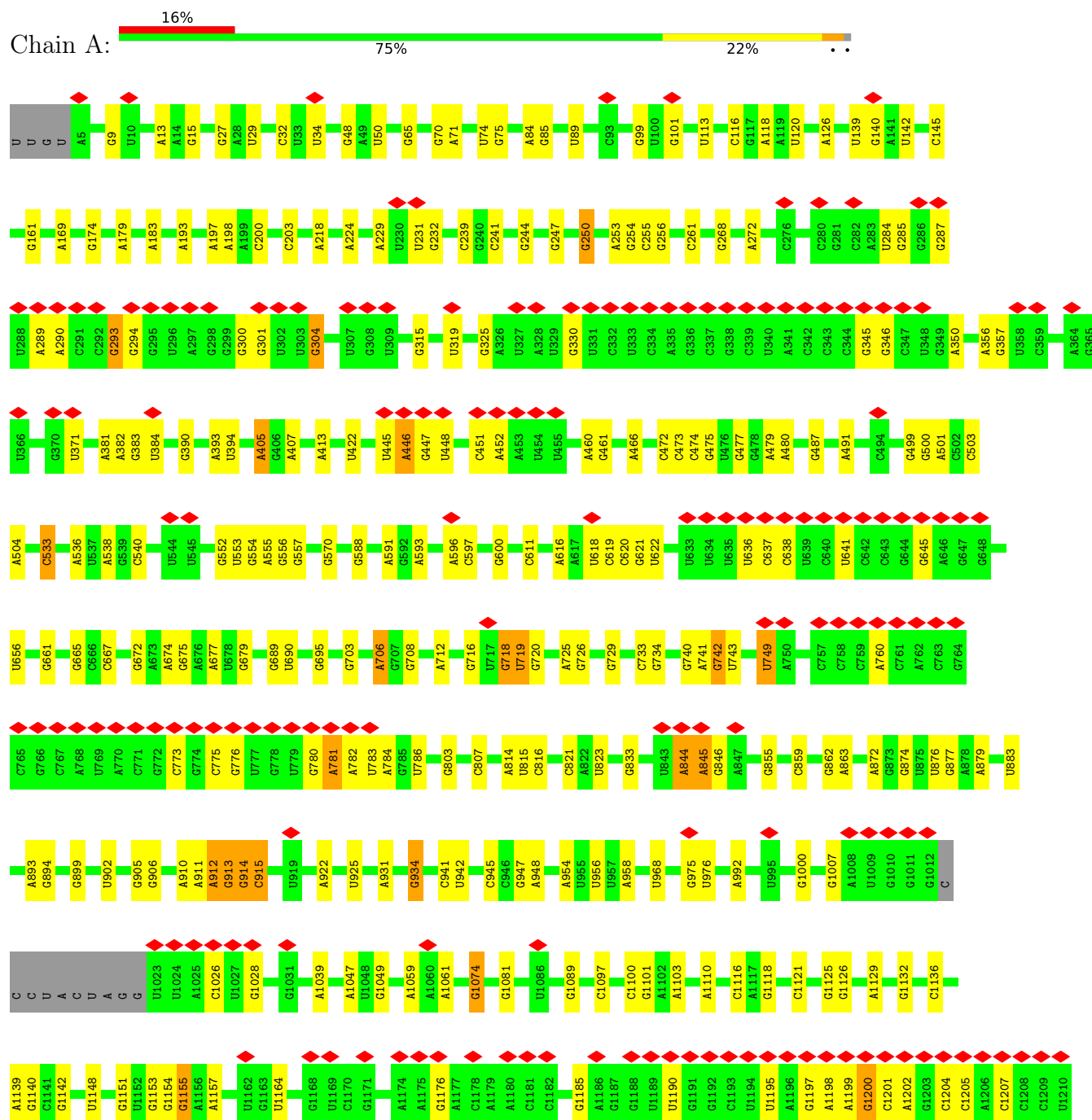
- Molecule 5: 50S ribosomal protein L36

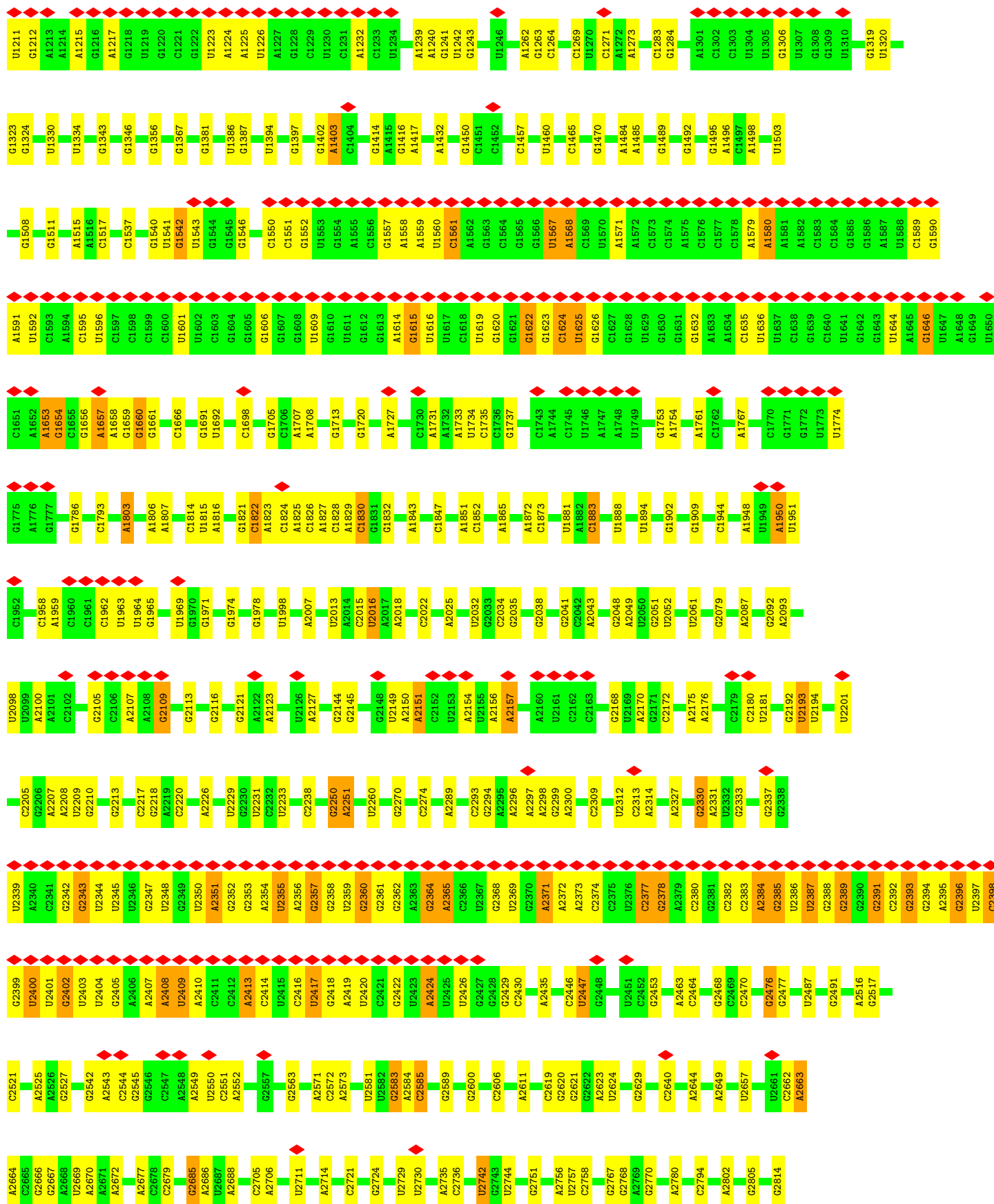


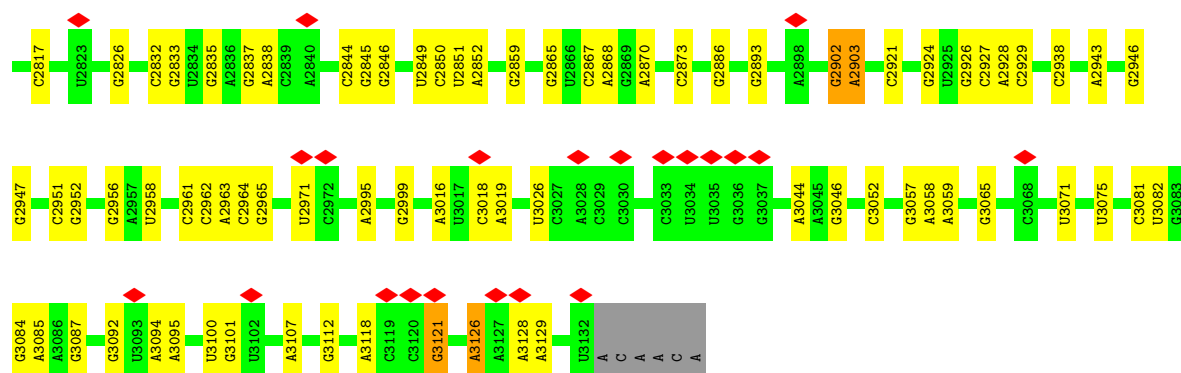
- Molecule 6: 50S ribosomal protein L31



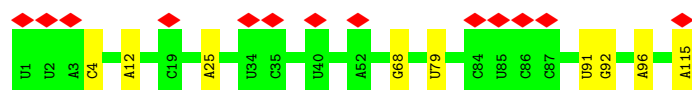
- Molecule 7: 23S rRNA



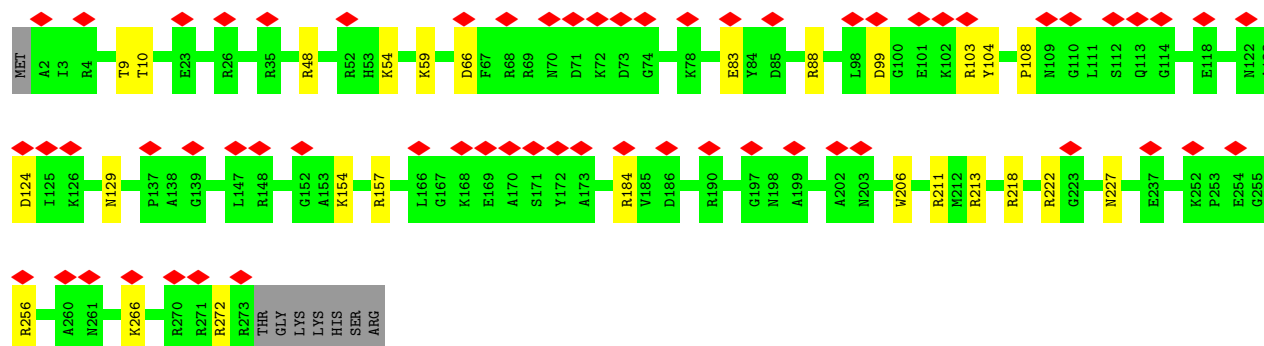
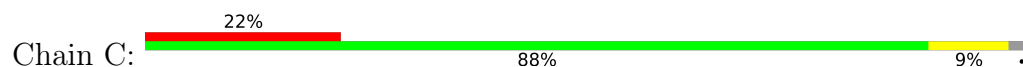




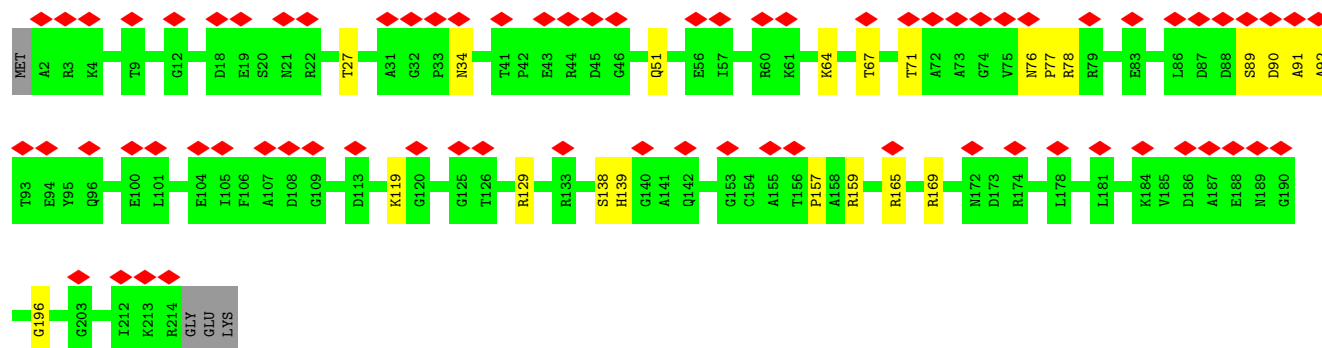
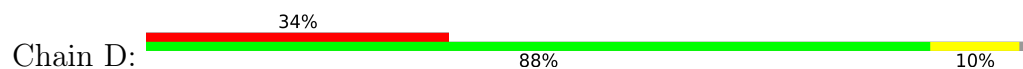
• Molecule 8: 5S rRNA



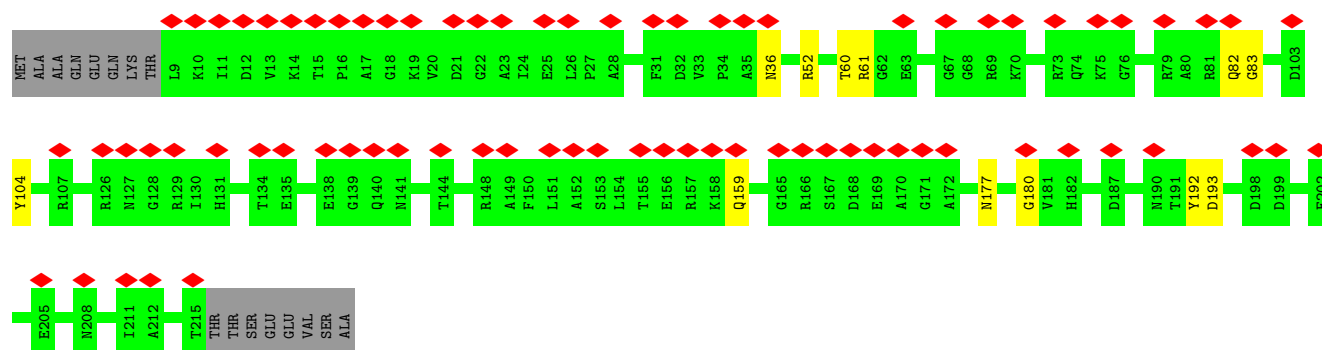
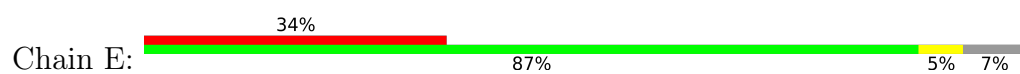
• Molecule 9: 50S ribosomal protein L2



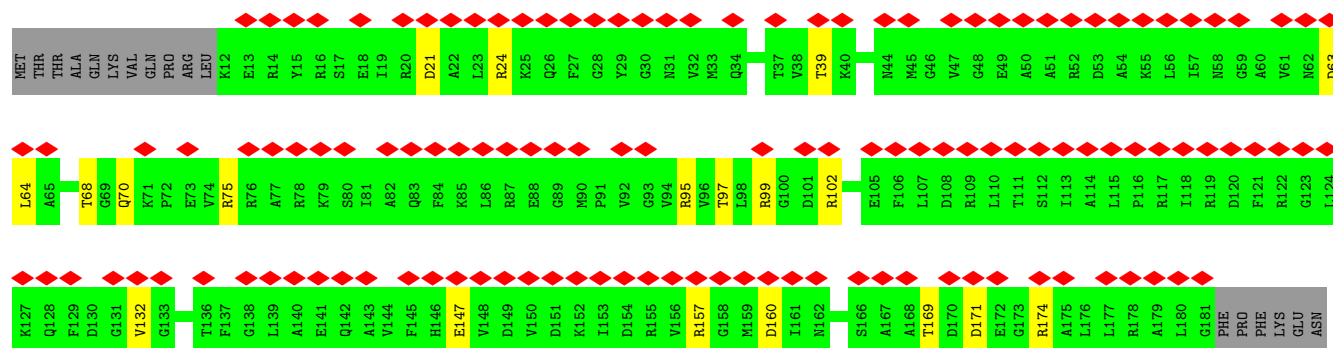
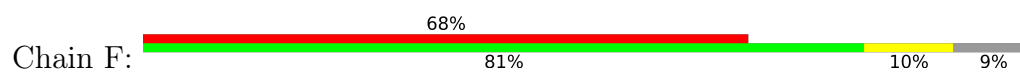
• Molecule 10: 50S ribosomal protein L3



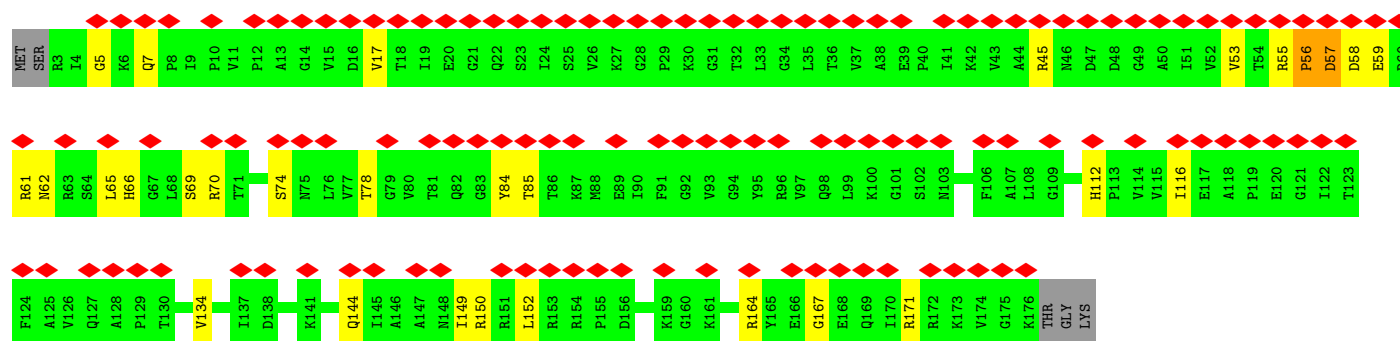
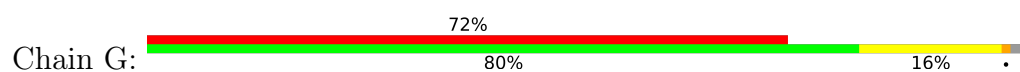
• Molecule 11: 50S ribosomal protein L4



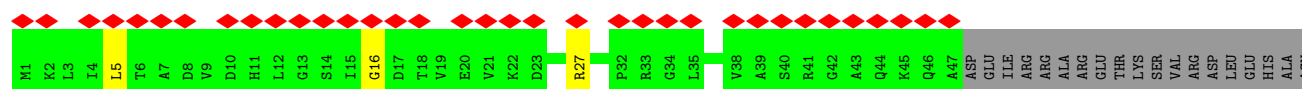
• Molecule 12: 50S ribosomal protein L5



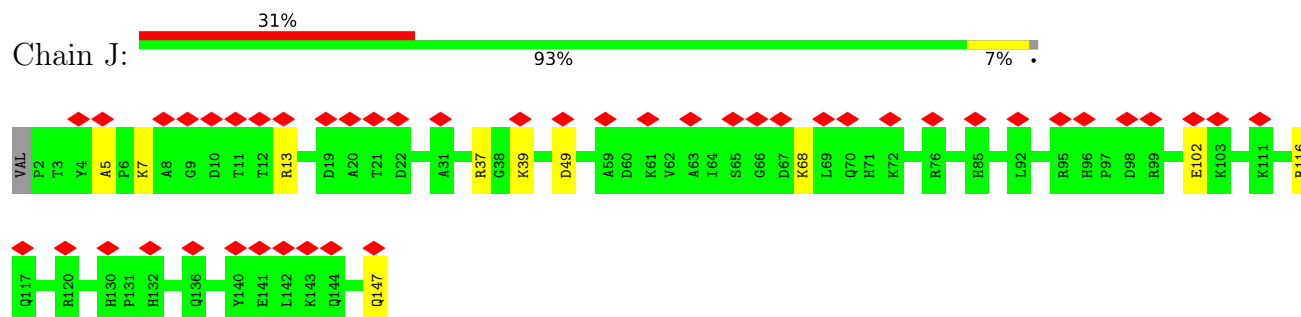
• Molecule 13: 50S ribosomal protein L6



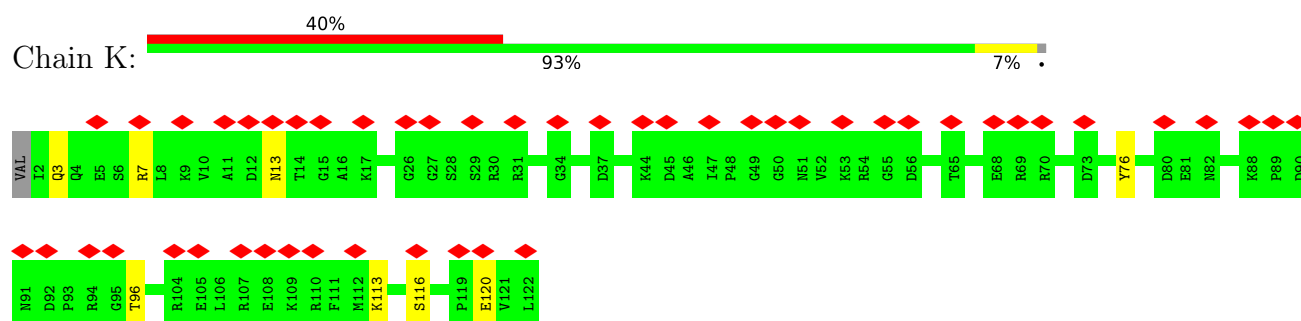
• Molecule 14: 50S ribosomal protein L9



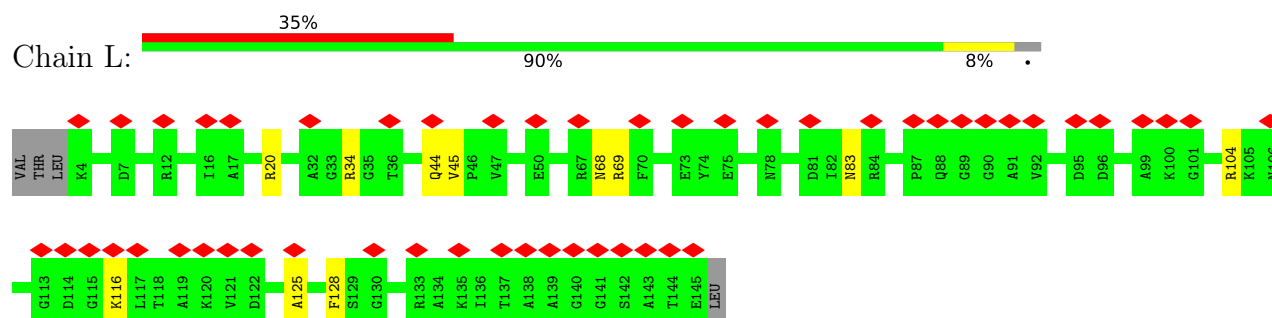
- Molecule 15: 50S ribosomal protein L13



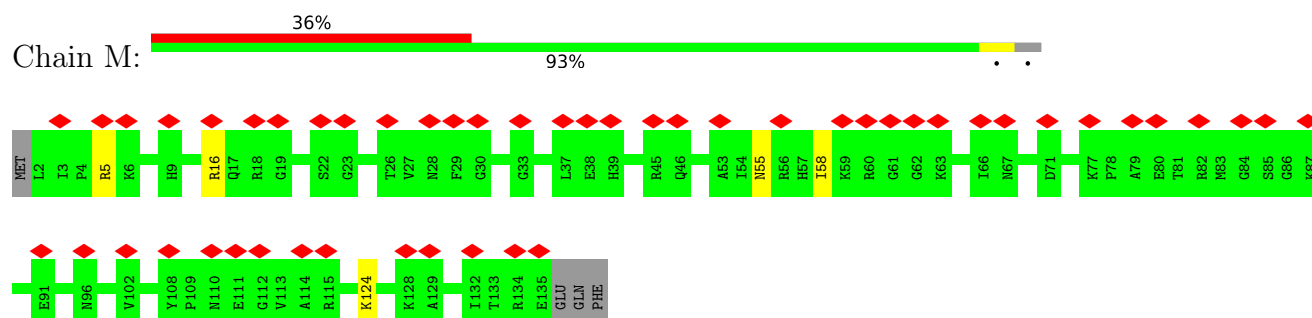
- Molecule 16: 50S ribosomal protein L14



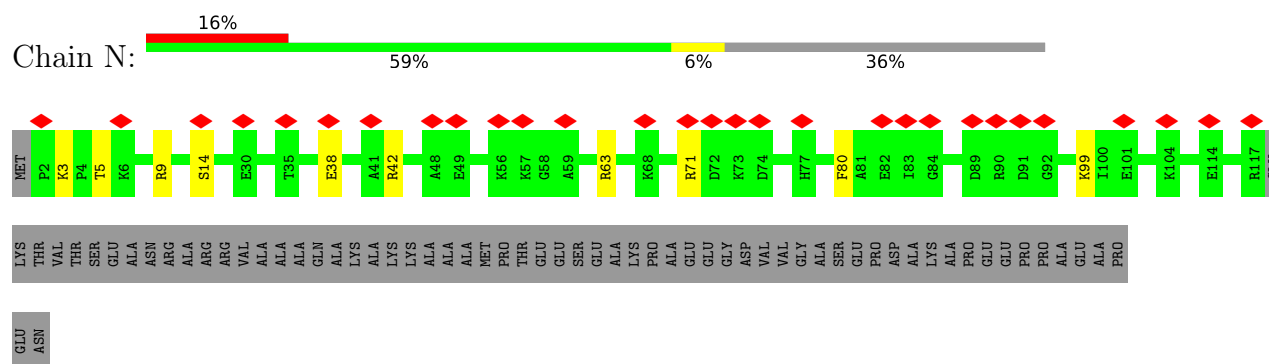
- Molecule 17: 50S ribosomal protein L15



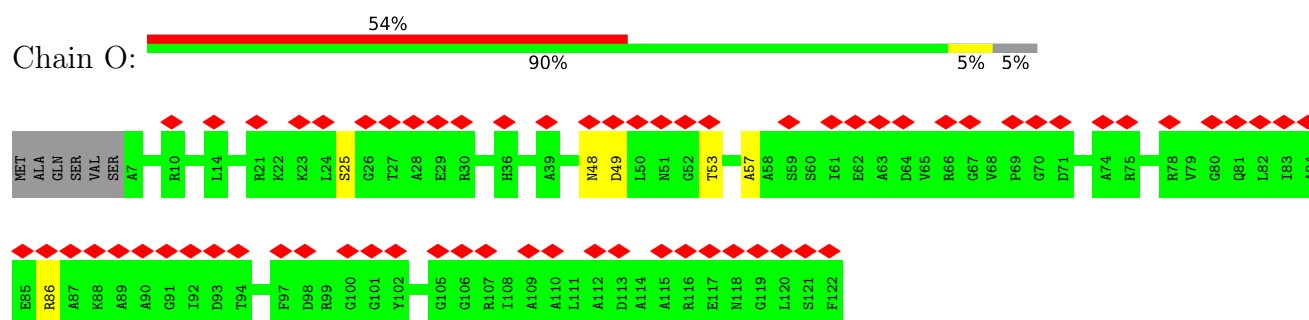
- Molecule 18: 50S ribosomal protein L16



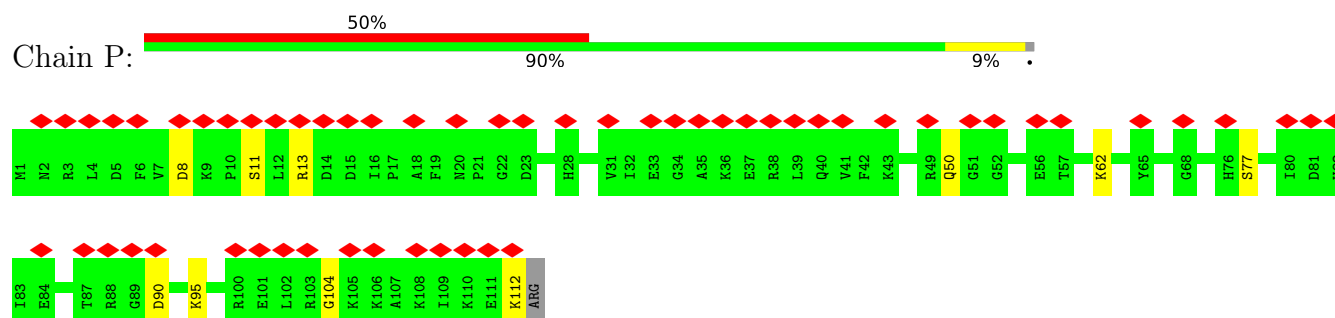
- Molecule 19: 50S ribosomal protein L17



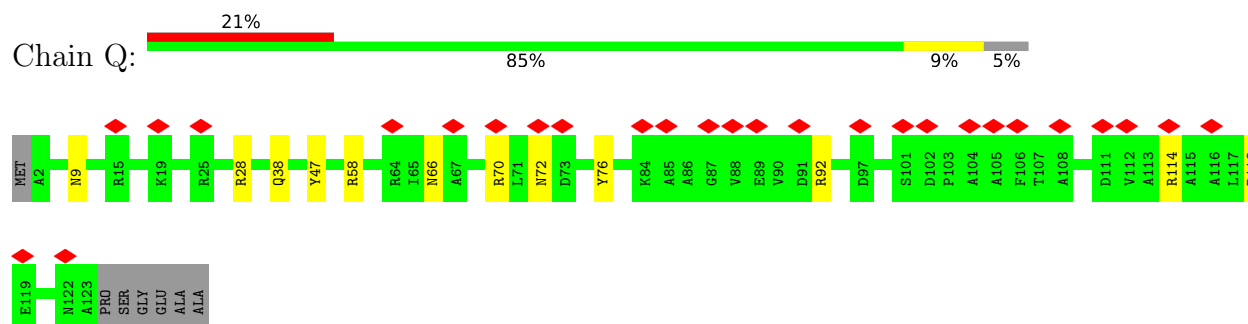
- Molecule 20: 50S ribosomal protein L18



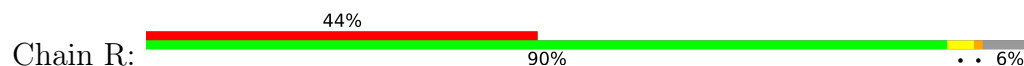
- Molecule 21: 50S ribosomal protein L19

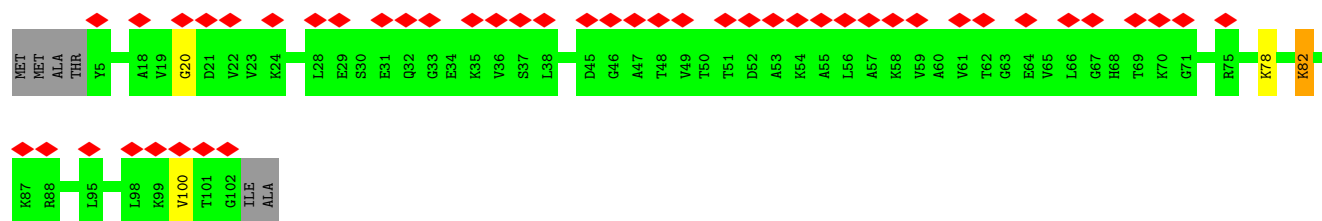


- Molecule 22: 50S ribosomal protein L20

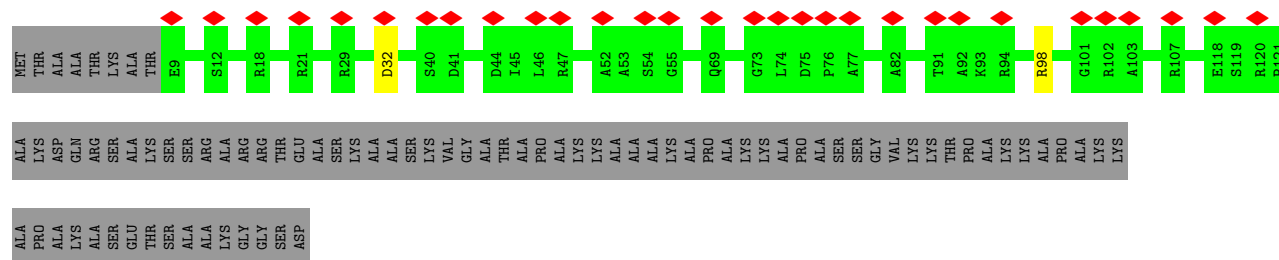


- Molecule 23: LSU ribosomal protein L21p

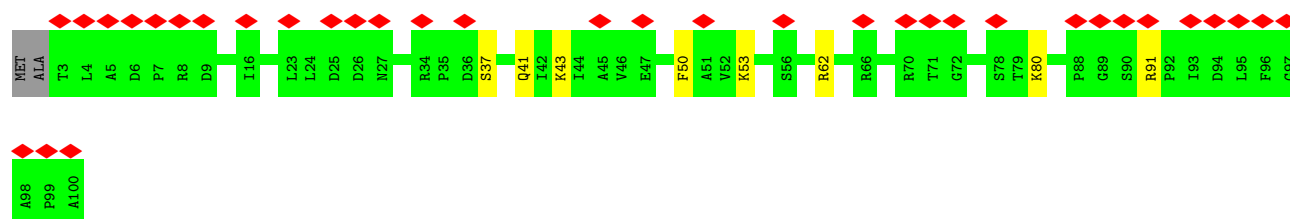
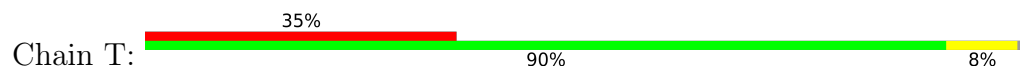




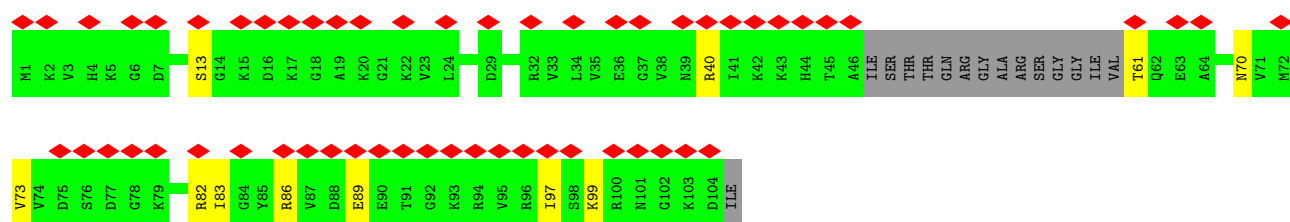
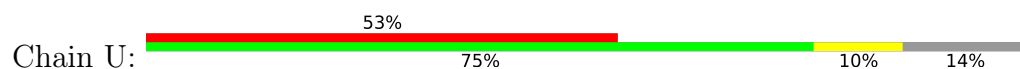
• Molecule 24: 50S ribosomal protein L22



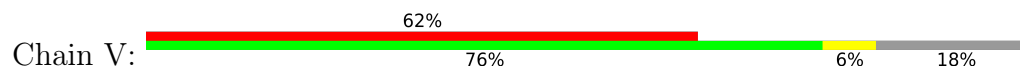
• Molecule 25: 50S ribosomal protein L23



• Molecule 26: 50S ribosomal protein L24

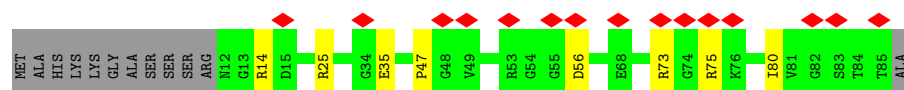
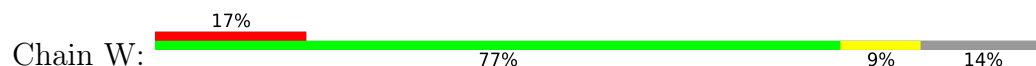


• Molecule 27: 50S ribosomal protein L25

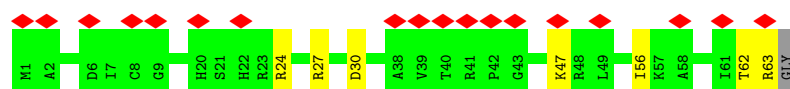
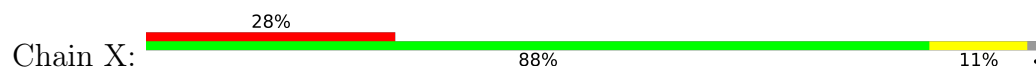




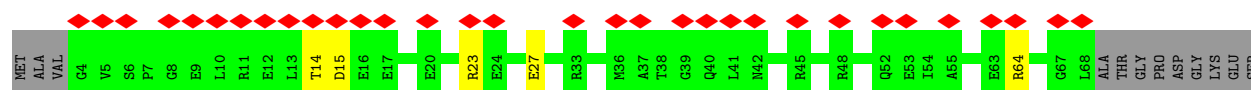
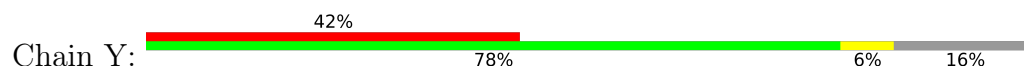
• Molecule 28: 50S ribosomal protein L27



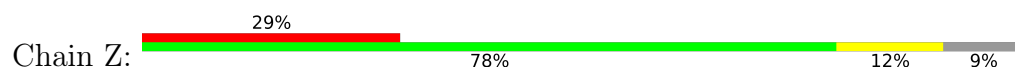
• Molecule 29: 50S ribosomal protein L28



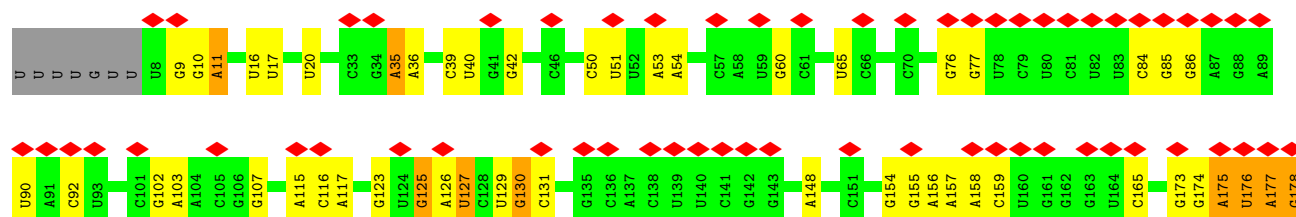
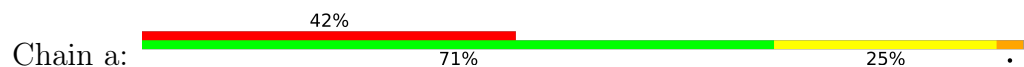
• Molecule 30: 50S ribosomal protein L29



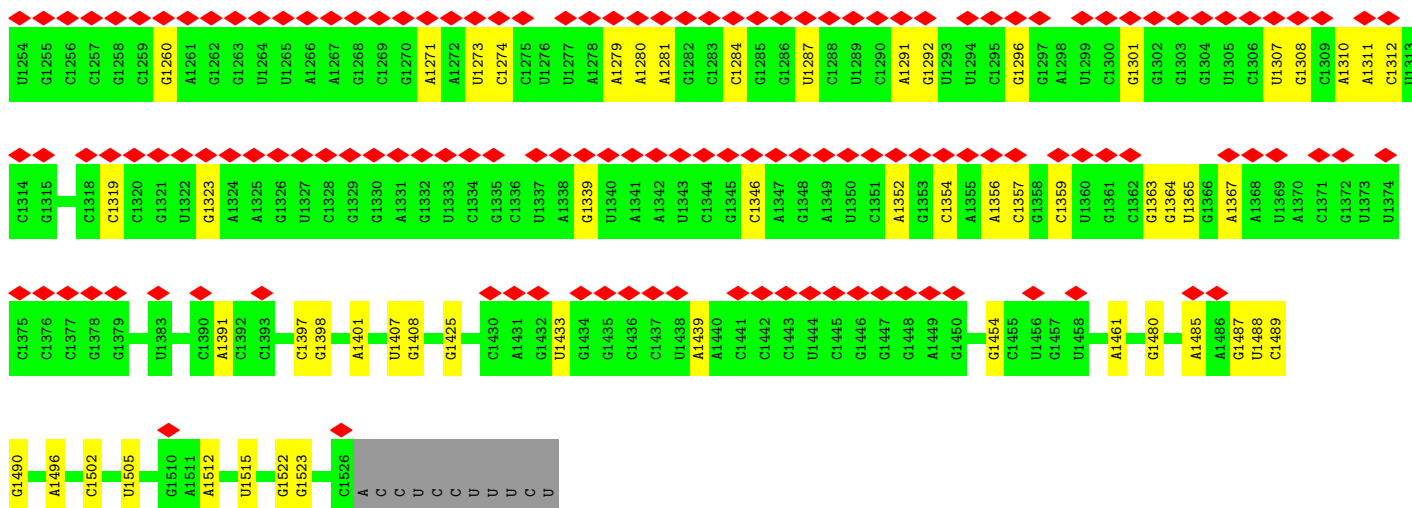
• Molecule 31: 50S ribosomal protein L30



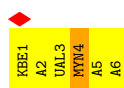
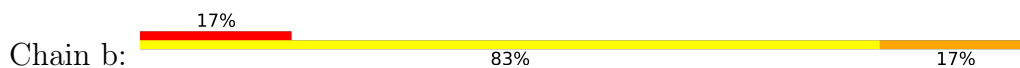
• Molecule 32: 16S rRNA



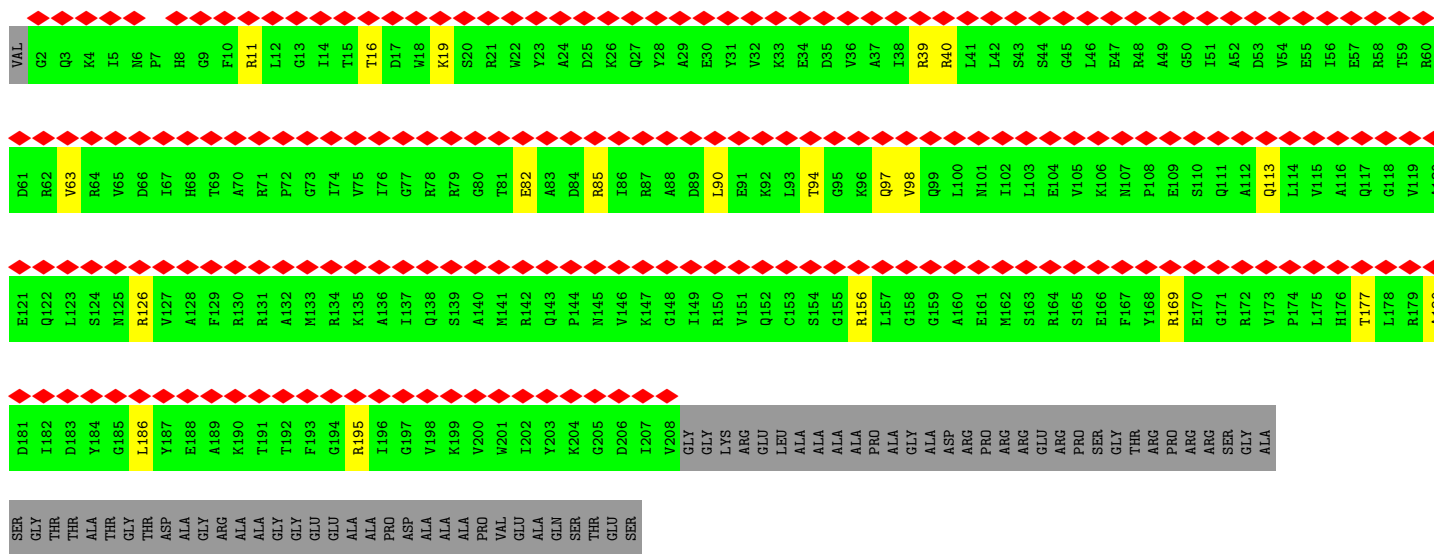
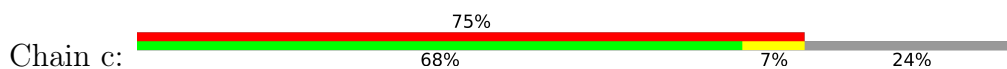




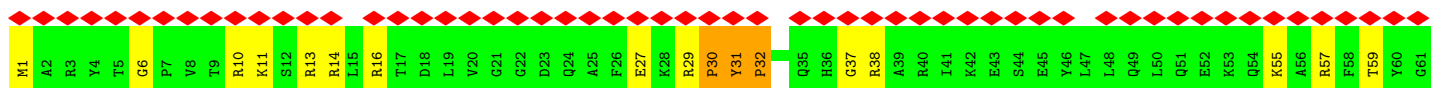
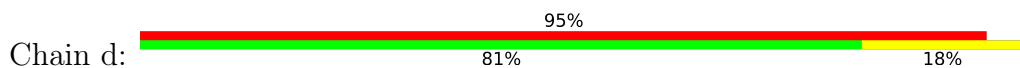
• Molecule 33: Capreomycin



• Molecule 34: 30S ribosomal protein S3

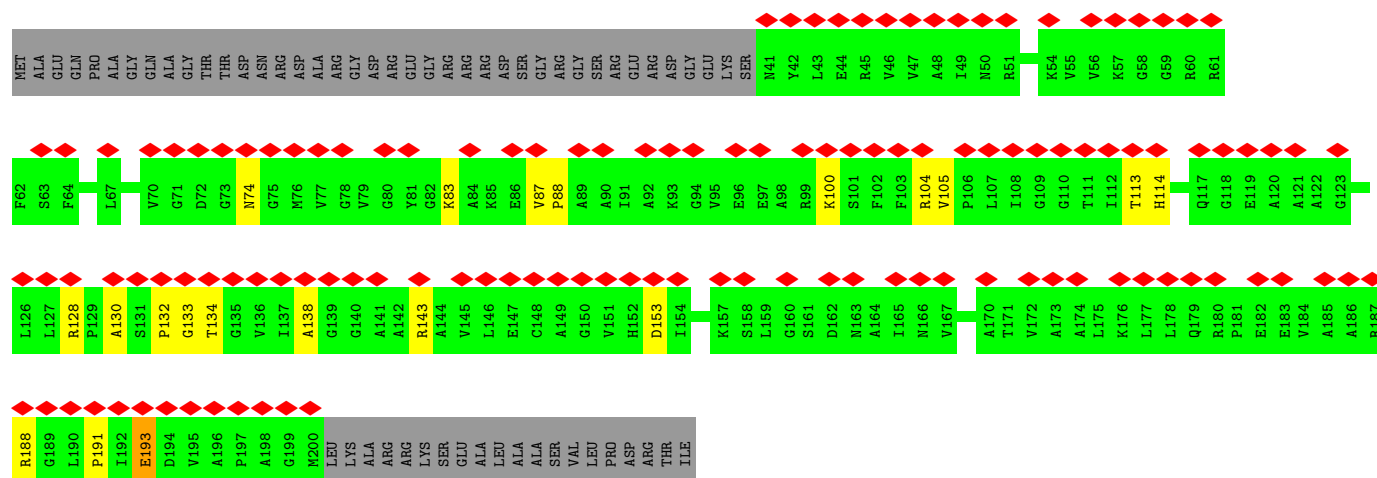


• Molecule 35: 30S ribosomal protein S4

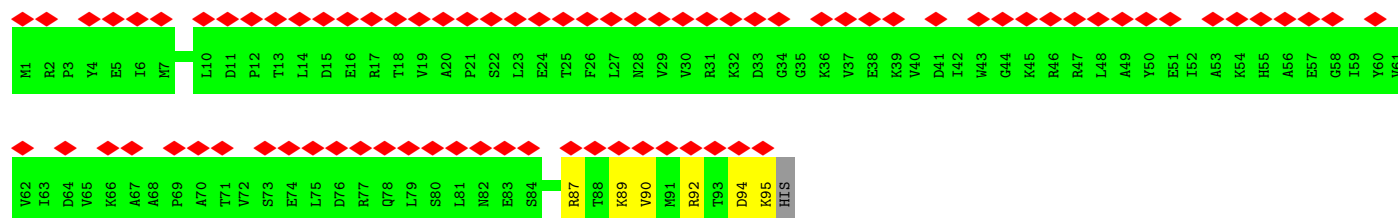
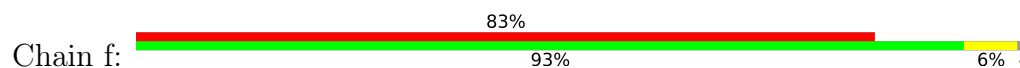




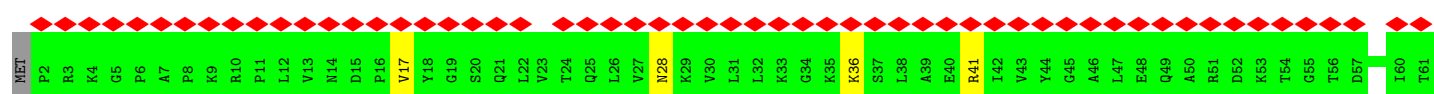
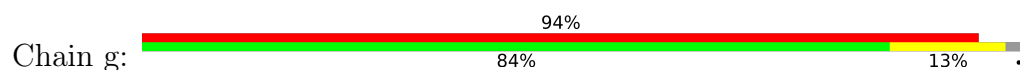
• Molecule 36: 30S ribosomal protein S5

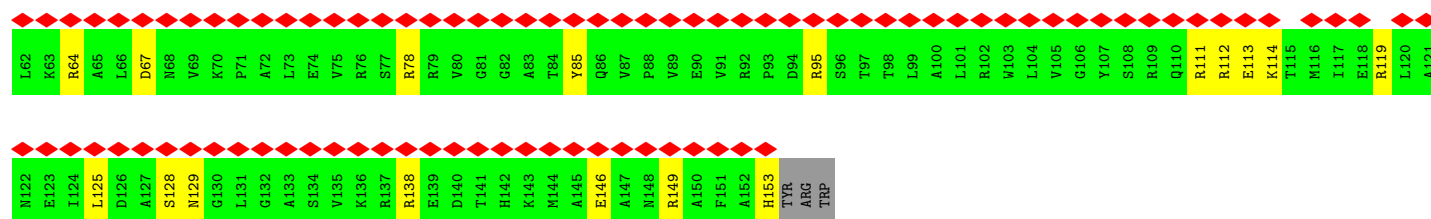


• Molecule 37: 30S ribosomal protein S6

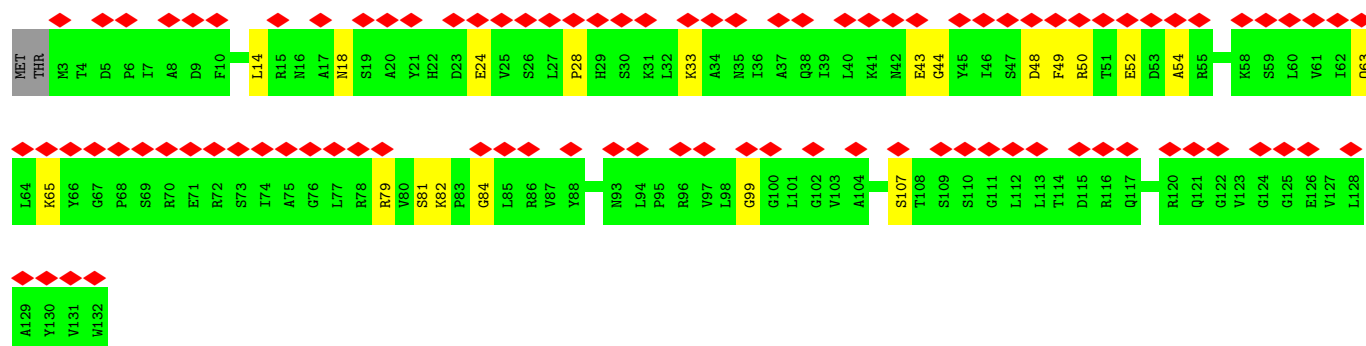
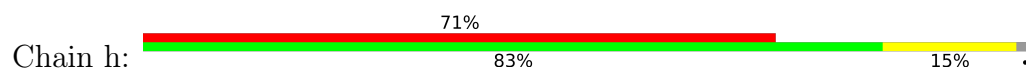


• Molecule 38: 30S ribosomal protein S7

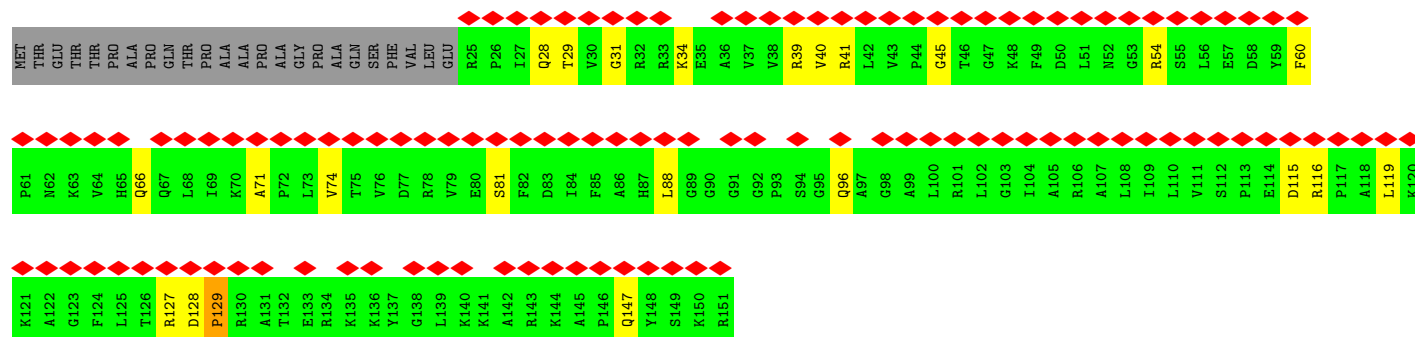
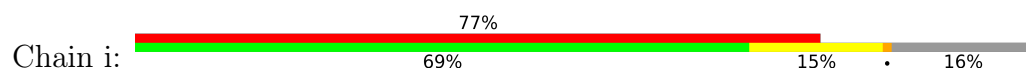




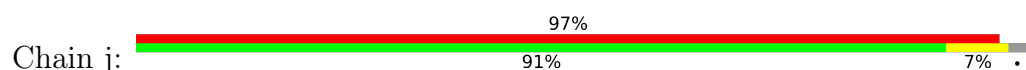
• Molecule 39: 30S ribosomal protein S8



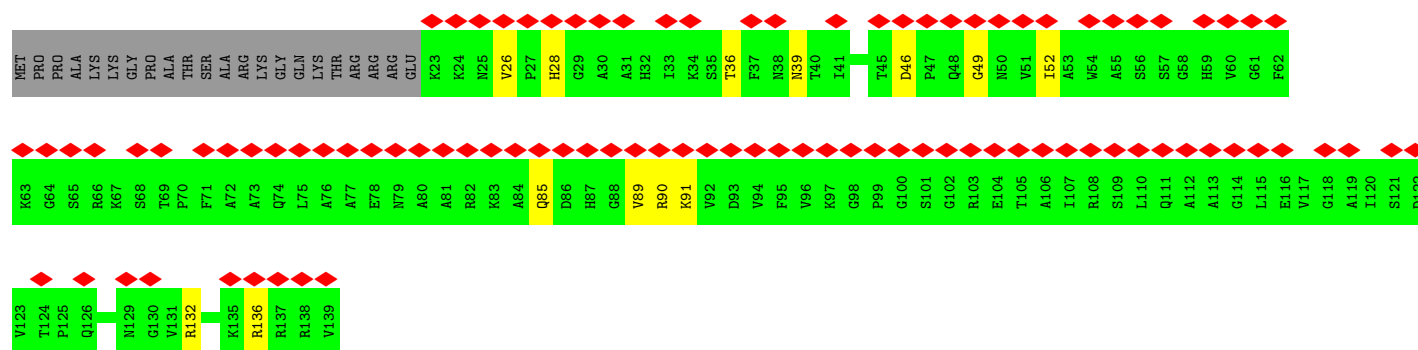
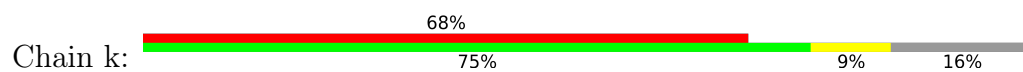
• Molecule 40: 30S ribosomal protein S9



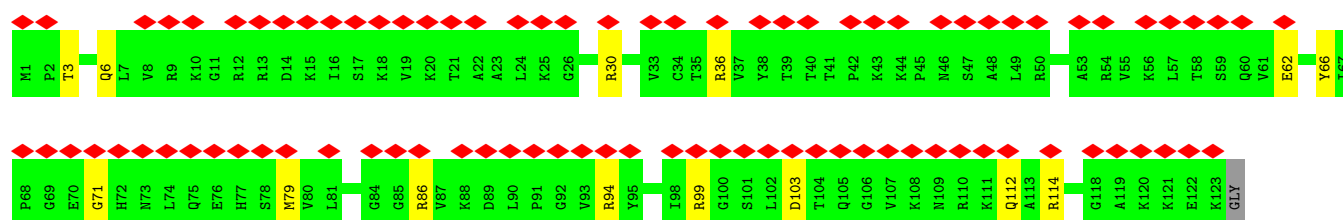
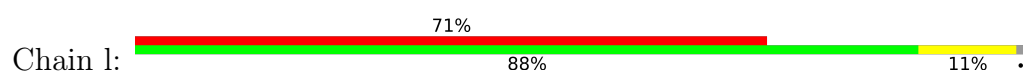
• Molecule 41: 30S ribosomal protein S10



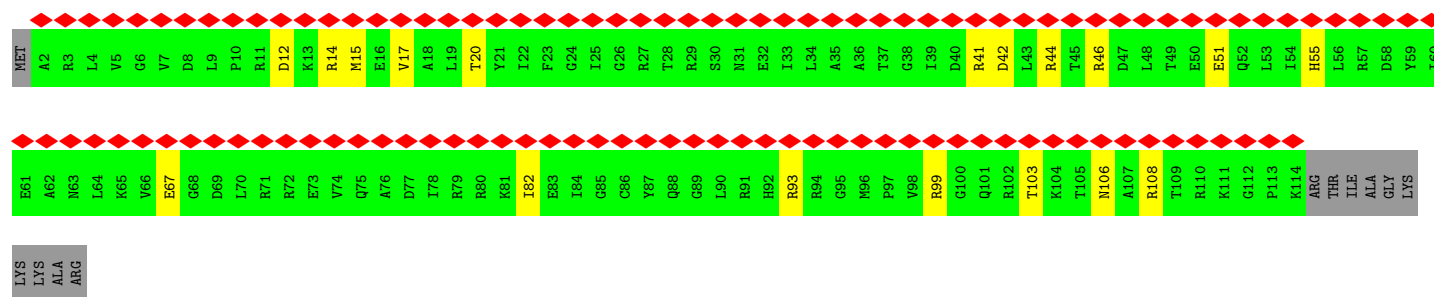
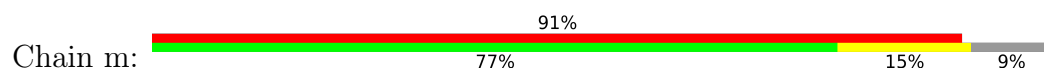
• Molecule 42: 30S ribosomal protein S11



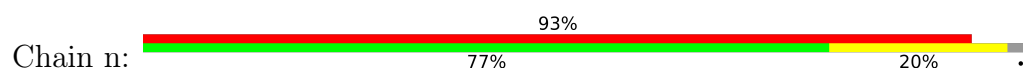
• Molecule 43: 30S ribosomal protein S12



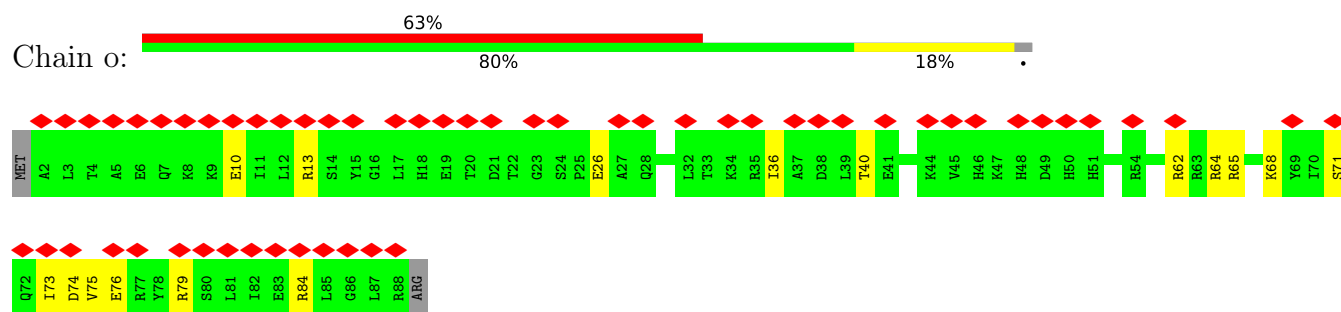
• Molecule 44: 30S ribosomal protein S13



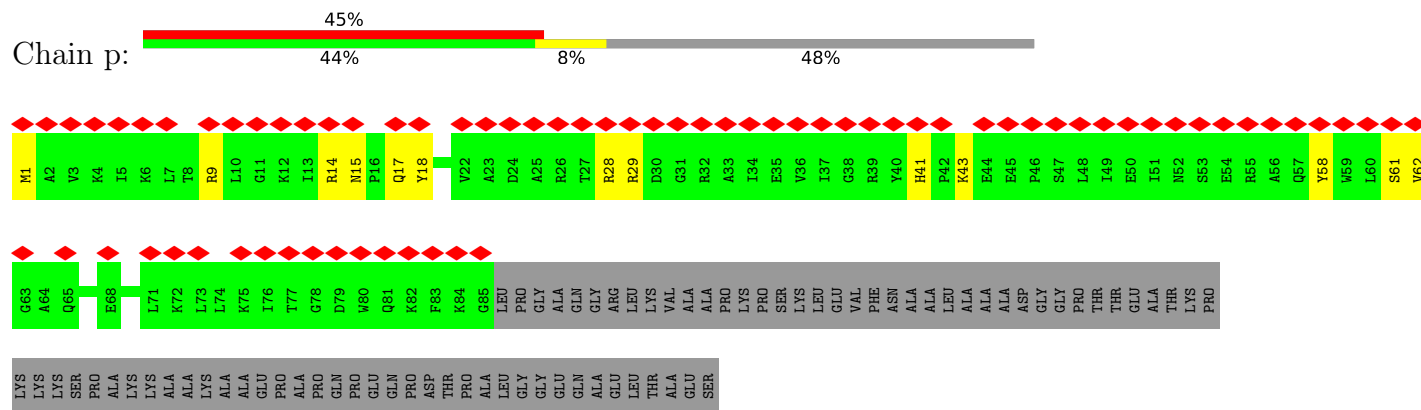
• Molecule 45: 30S ribosomal protein S14 type Z



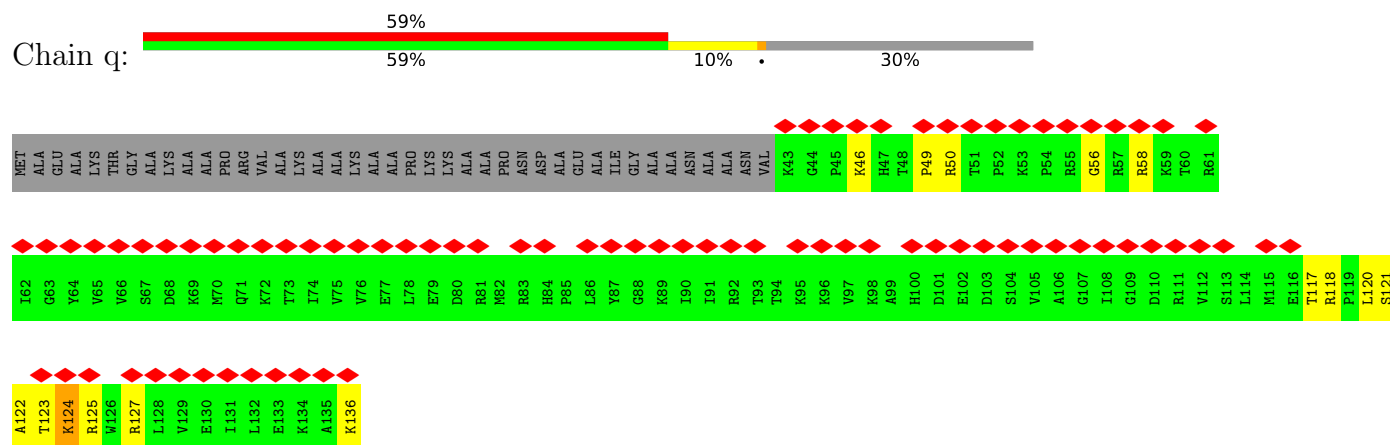
• Molecule 46: 30S ribosomal protein S15



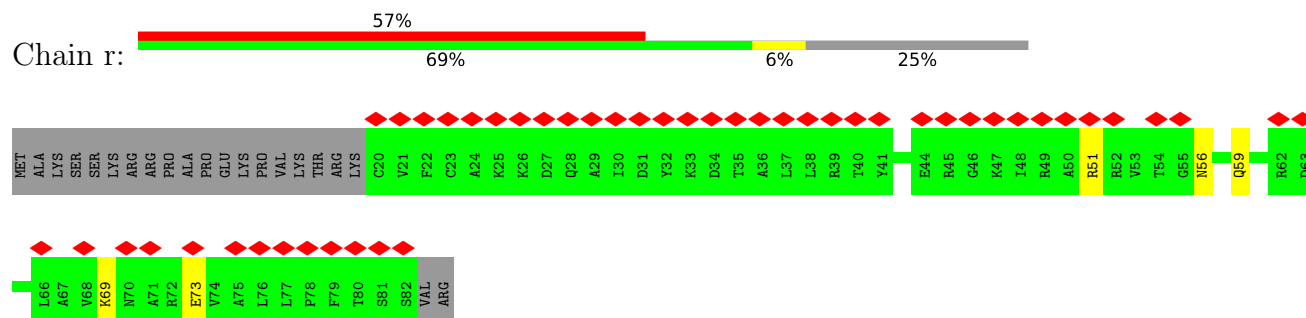
• Molecule 47: 30S ribosomal protein S16



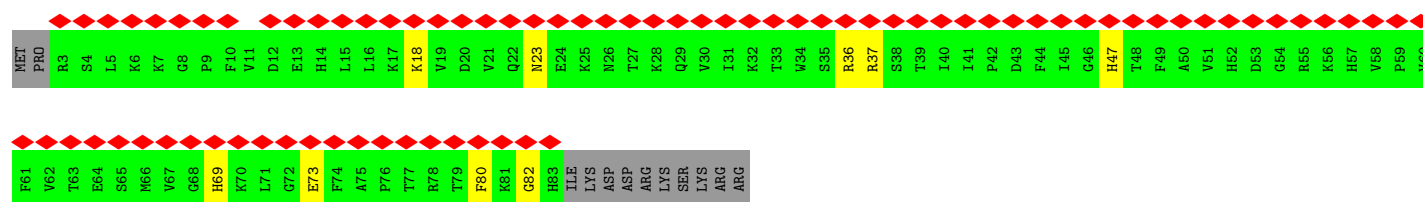
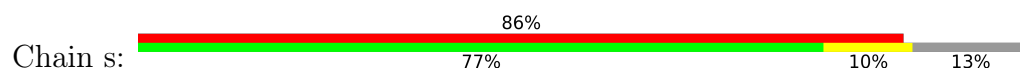
• Molecule 48: 30S ribosomal protein S17



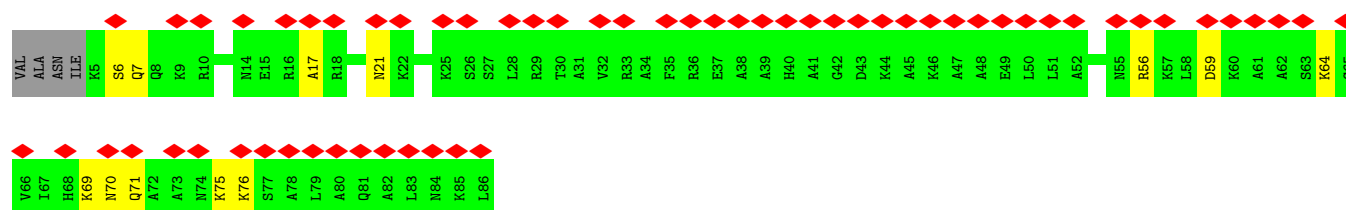
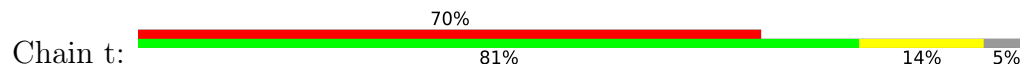
• Molecule 49: 30S ribosomal protein S18



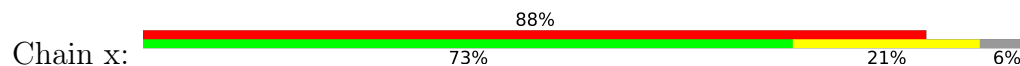
• Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20



- Molecule 52: Mitochondrial domain of uncharacterised function (DUF1713)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184330	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	400.0, 400.0, 400.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.25, 1.25, 1.25	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: KBE, UAL, MYN, DPP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.54	0/427	0.63	0/570
2	1	0.51	0/407	0.65	0/543
3	2	0.69	0/361	0.73	0/473
4	3	0.61	0/499	0.64	0/664
5	4	0.51	0/303	0.68	0/402
6	6	0.31	0/353	0.61	0/478
7	A	0.47	0/74973	0.51	0/116979
8	B	0.37	0/2749	0.43	0/4284
9	C	0.60	0/2129	0.69	0/2861
10	D	0.50	0/1613	0.65	0/2174
11	E	0.52	0/1575	0.63	0/2129
12	F	0.40	0/1352	0.63	0/1817
13	G	0.36	0/1351	0.59	0/1824
14	H	0.37	0/353	0.60	0/474
15	J	0.50	0/1170	0.62	0/1584
16	K	0.55	0/944	0.65	0/1268
17	L	0.53	0/1073	0.71	1/1432 (0.1%)
18	M	0.49	0/1098	0.63	0/1481
19	N	0.55	0/925	0.65	0/1242
20	O	0.42	0/895	0.60	0/1202
21	P	0.39	0/922	0.55	0/1236
22	Q	0.59	0/992	0.67	0/1329
23	R	0.44	0/751	0.61	0/1009
24	S	0.55	0/874	0.63	0/1186
25	T	0.45	0/770	0.63	0/1038
26	U	0.33	0/705	0.51	0/941
27	V	0.30	0/1336	0.49	0/1820
28	W	0.50	0/551	0.57	0/735
29	X	0.56	0/484	0.73	0/648
30	Y	0.46	0/544	0.58	0/727
31	Z	0.55	0/480	0.66	0/645
32	a	0.57	0/36501	0.56	0/56956

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	1.17	0/4	1.50	0/4
34	c	0.45	0/1678	0.57	0/2254
35	d	0.54	0/1691	0.70	1/2279 (0.0%)
36	e	0.65	0/1165	0.78	1/1578 (0.1%)
37	f	0.59	0/767	0.70	0/1036
38	g	0.48	0/1210	0.65	0/1631
39	h	0.65	0/1014	0.74	0/1369
40	i	0.48	0/1011	0.68	0/1356
41	j	0.44	0/803	0.63	0/1086
42	k	0.56	0/891	0.73	1/1204 (0.1%)
43	l	0.60	0/978	0.79	0/1306
44	m	0.44	0/927	0.66	0/1239
45	n	0.52	0/472	0.79	0/627
46	o	0.67	0/727	0.72	0/973
47	p	0.59	0/701	0.70	0/944
48	q	0.55	0/775	0.70	2/1035 (0.2%)
49	r	0.58	0/502	0.67	0/674
50	s	0.41	0/674	0.61	0/906
51	t	0.68	0/633	0.69	0/838
52	x	0.60	0/271	0.90	0/348
All	All	0.51	0/156354	0.56	6/234838 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	e	105	VAL	N-CA-C	7.75	115.30	108.63
35	d	31	TYR	C-N-CD	-5.63	101.91	125.00
42	k	52	ILE	N-CA-C	-5.35	106.45	111.48
17	L	45	VAL	N-CA-C	5.25	113.14	108.63
48	q	122	ALA	CA-C-N	5.00	131.09	121.54
48	q	122	ALA	C-N-CA	5.00	131.09	121.54

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	0	421	0	461	6	0
2	1	400	0	413	4	0
3	2	358	0	390	5	0
4	3	494	0	533	8	0
5	4	299	0	326	6	0
6	6	345	0	332	3	0
7	A	66956	0	33720	430	0
8	B	2458	0	1253	6	0
9	C	2088	0	2123	21	0
10	D	1590	0	1633	14	0
11	E	1552	0	1593	9	0
12	F	1335	0	1372	12	0
13	G	1330	0	1390	21	0
14	H	350	0	367	2	0
15	J	1143	0	1173	8	0
16	K	934	0	993	6	0
17	L	1060	0	1119	7	0
18	M	1072	0	1115	5	0
19	N	908	0	956	12	0
20	O	886	0	924	3	0
21	P	907	0	947	7	0
22	Q	980	0	1028	8	0
23	R	742	0	799	3	0
24	S	860	0	903	2	0
25	T	759	0	809	7	0
26	U	699	0	738	6	0
27	V	1319	0	1365	7	0
28	W	546	0	567	5	0
29	X	476	0	496	5	0
30	Y	541	0	551	3	0
31	Z	476	0	509	6	0
32	a	32610	0	16406	296	0
33	b	46	0	43	5	0
34	c	1654	0	1694	15	0
35	d	1658	0	1683	39	0
36	e	1149	0	1207	12	0
37	f	757	0	796	6	0
38	g	1193	0	1256	12	0
39	h	999	0	1034	11	0
40	i	993	0	1052	18	0
41	j	789	0	821	8	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	k	873	0	887	11	0
43	l	967	0	1056	10	0
44	m	919	0	961	11	0
45	n	463	0	491	11	0
46	o	718	0	760	11	0
47	p	688	0	726	12	0
48	q	763	0	824	10	0
49	r	497	0	517	4	0
50	s	657	0	671	7	0
51	t	631	0	681	10	0
52	x	271	0	329	6	0
All	All	143579	0	94793	957	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 5.

All (957) 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)
7:A:1540:G:N3	7:A:1829:A:C2	2.26	1.04
7:A:1540:G:H1	7:A:1828:C:N4	1.58	1.02
7:A:2343:G:N1	7:A:2420:U:O2	1.95	0.98
35:d:32:PRO:HG2	35:d:38:ARG:HG2	1.53	0.90
7:A:1540:G:N2	7:A:1829:A:C4	2.42	0.88
32:a:243:U:O4	32:a:886:C:N4	2.08	0.86
32:a:117:A:N6	32:a:238:G:O6	2.08	0.86
7:A:2339:U:O2	7:A:2424:A:N6	2.09	0.86
7:A:1540:G:C2	7:A:1829:A:C2	2.64	0.85
40:i:45:GLY:O	40:i:81:SER:OG	1.95	0.85
7:A:1540:G:H1	7:A:1828:C:H42	1.13	0.84
32:a:10:G:O6	36:e:128:ARG:NH2	2.11	0.84
32:a:1433:U:O2	32:a:1454:G:N1	2.10	0.84
5:4:27:CYS:HG	5:4:32:HIS:HE2	1.25	0.83
7:A:1959:A:N1	7:A:1969:U:O4	2.11	0.83
17:L:83:ASN:ND2	17:L:116:LYS:O	2.11	0.83
7:A:1830:C:OP1	25:T:53:LYS:NZ	2.10	0.82
32:a:995:A:C2	32:a:1029:C:N4	2.47	0.82
32:a:913:U:O2'	32:a:1072:G:O2'	1.97	0.82
13:G:78:THR:OG1	13:G:84:TYR:OH	1.95	0.82
7:A:1492:G:O2'	7:A:2453:G:O2'	1.98	0.82
7:A:2373:A:N6	7:A:2392:C:O2'	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:245:A:N1	32:a:277:G:O2'	2.13	0.81
32:a:253:G:OP1	48:q:124:LYS:NZ	2.13	0.81
32:a:708:C:O2'	32:a:725:G:O4'	1.97	0.81
39:h:44:GLY:O	39:h:65:LYS:NZ	2.14	0.81
7:A:2016:U:O2	7:A:2846:G:O2'	1.99	0.81
32:a:342:U:O2	32:a:345:G:C6	2.35	0.80
32:a:563:A:OP1	52:x:6:LYS:NZ	2.14	0.80
7:A:733:C:O2	7:A:743:U:O2'	2.00	0.80
32:a:1046:A:N3	34:c:156:ARG:NH2	2.30	0.80
35:d:32:PRO:CG	35:d:38:ARG:HG2	2.12	0.80
3:2:14:ARG:NH2	7:A:899:G:OP2	2.14	0.80
7:A:976:U:O4	7:A:1061:A:N7	2.14	0.80
7:A:2289:A:N6	7:A:2852:A:O2'	2.15	0.80
47:p:9:ARG:NH2	47:p:18:TYR:OH	2.14	0.80
32:a:535:G:OP2	35:d:11:LYS:NZ	2.15	0.79
38:g:146:GLU:OE1	38:g:149:ARG:NH1	2.16	0.79
32:a:1311:A:N6	32:a:1352:A:N1	2.30	0.79
32:a:477:U:O2'	32:a:478:A:O4'	2.01	0.79
32:a:1287:U:O2'	44:m:14:ARG:NH1	2.16	0.78
7:A:1754:A:O2'	7:A:1793:C:O2	2.02	0.78
7:A:2312:U:OP2	7:A:2476:G:O2'	2.00	0.78
32:a:458:G:OP2	32:a:459:G:N2	2.16	0.78
7:A:2677:A:O2'	7:A:2838:A:OP1	2.01	0.78
32:a:1307:U:O2'	32:a:1352:A:N3	2.17	0.78
7:A:2384:A:O2'	7:A:2385:G:O4'	2.02	0.77
7:A:70:G:HO2'	7:A:113:U:HO2'	1.23	0.77
7:A:1540:G:C4	7:A:1829:A:C2	2.73	0.77
7:A:2032:U:OP2	9:C:272:ARG:NH2	2.17	0.77
32:a:1310:A:N3	50:s:37:ARG:NH1	2.32	0.77
7:A:350:A:N6	7:A:445:U:O4	2.17	0.77
10:D:67:THR:O	10:D:71:THR:OG1	2.02	0.77
32:a:405:G:O2'	35:d:111:GLN:NE2	2.16	0.77
32:a:1241:C:N4	32:a:1280:A:OP2	2.18	0.77
7:A:1110:A:O2'	7:A:2274:C:O2'	2.02	0.76
7:A:2386:U:O2'	7:A:2387:U:O4'	2.03	0.76
7:A:2606:C:N4	7:A:2620:G:O6	2.18	0.76
32:a:499:C:O2	32:a:501:A:N6	2.18	0.76
32:a:148:A:N6	32:a:165:C:O2	2.18	0.76
4:3:7:HIS:NE2	7:A:253:A:OP1	2.18	0.76
32:a:192:A:N6	48:q:56:GLY:O	2.19	0.76
32:a:1043:U:O2	32:a:1198:G:O6	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1152:G:O6	32:a:1168:A:N6	2.15	0.76
32:a:254:G:O6	32:a:265:G:O6	2.04	0.76
4:3:43:ARG:NH2	7:A:2600:G:N7	2.34	0.76
7:A:1000:G:OP1	18:M:5:ARG:NH2	2.19	0.76
7:A:2859:G:OP1	10:D:129:ARG:NH2	2.19	0.76
7:A:3100:U:OP2	7:A:3101:G:O2'	2.02	0.76
7:A:874:G:O2'	7:A:877:G:O2'	2.03	0.75
32:a:1398:G:H22	32:a:1489:C:H42	1.32	0.75
7:A:1126:G:OP2	22:Q:58:ARG:NH1	2.20	0.75
7:A:477:G:O6	7:A:479:A:O2'	2.03	0.75
44:m:42:ASP:OD1	44:m:44:ARG:NH1	2.18	0.75
38:g:64:ARG:NE	38:g:128:SER:O	2.20	0.75
7:A:1136:C:OP1	15:J:39:LYS:NZ	2.20	0.75
8:B:92:G:O6	27:V:19:LYS:NZ	2.17	0.75
32:a:770:C:O2	42:k:132:ARG:NH2	2.20	0.75
32:a:1502:C:OP1	52:x:8:ARG:NH1	2.20	0.75
19:N:5:THR:O	19:N:9:ARG:NH2	2.20	0.74
32:a:436:U:C2	32:a:486:A:N6	2.54	0.74
32:a:613:A:OP1	35:d:69:ARG:NH2	2.19	0.74
7:A:821:C:O2	7:A:1485:A:O2'	2.05	0.74
32:a:1397:C:O2	32:a:1512:A:O2'	2.04	0.74
7:A:1786:G:O2'	7:A:1974:G:N2	2.20	0.74
32:a:259:G:OP1	51:t:75:LYS:NZ	2.20	0.74
16:K:13:ASN:ND2	16:K:96:THR:OG1	2.20	0.74
7:A:2051:G:OP1	9:C:88:ARG:NH2	2.21	0.74
1:0:41:ARG:NH1	7:A:3121:G:N3	2.34	0.74
46:o:68:LYS:O	46:o:71:SER:OG	2.02	0.74
32:a:261:G:OP2	51:t:71:GLN:NE2	2.21	0.74
32:a:1039:G:OP1	45:n:3:LYS:N	2.21	0.73
39:h:79:ARG:NH1	39:h:81:SER:O	2.21	0.73
7:A:1567:U:O2'	7:A:1568:A:OP2	2.06	0.73
7:A:2359:U:O2'	7:A:2409:U:O4	2.05	0.73
7:A:2378:G:O6	7:A:2387:U:O2	2.07	0.73
13:G:55:ARG:HH11	13:G:56:PRO:HD2	1.52	0.73
7:A:1201:C:OP1	7:A:1204:C:N4	2.21	0.73
7:A:2049:A:OP2	9:C:54:LYS:NZ	2.21	0.73
32:a:681:G:OP2	42:k:39:ASN:ND2	2.20	0.73
7:A:2757:U:O4'	7:A:2780:A:N6	2.22	0.73
7:A:910:A:OP1	9:C:218:ARG:NH2	2.21	0.73
7:A:1540:G:C2	7:A:1829:A:C4	2.77	0.73
7:A:197:A:N6	7:A:200:C:OP2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:107:G:OP1	47:p:28:ARG:NE	2.22	0.72
7:A:2025:A:O2'	9:C:206:TRP:O	2.08	0.72
7:A:536:A:O4'	7:A:538:A:N6	2.23	0.72
7:A:460:A:N6	7:A:491:A:OP2	2.22	0.72
28:W:25:ARG:NH2	28:W:35:GLU:OE2	2.23	0.72
7:A:3026:U:O2'	7:A:3044:A:N3	2.23	0.72
31:Z:2:SER:N	31:Z:39:ASP:OD1	2.23	0.72
13:G:17:VAL:O	13:G:45:ARG:NH2	2.23	0.71
5:4:6:SER:O	5:4:34:GLN:NE2	2.24	0.71
32:a:931:A:O3'	38:g:95:ARG:NH2	2.24	0.71
35:d:31:TYR:N	35:d:32:PRO:HD3	2.05	0.71
32:a:174:G:OP1	51:t:56:ARG:NH2	2.24	0.71
32:a:1108:G:H21	40:i:127:ARG:HH12	1.37	0.71
33:b:4:MYN:N1	33:b:6:ALA:O	2.24	0.71
35:d:104:ARG:NH2	35:d:159:GLU:OE1	2.24	0.71
40:i:60:PHE:O	40:i:66:GLN:NE2	2.18	0.71
32:a:65:U:O2'	32:a:378:C:O2	2.09	0.71
35:d:13:ARG:NH2	35:d:32:PRO:O	2.23	0.71
1:0:17:ARG:NH2	7:A:1394:U:OP1	2.23	0.71
7:A:2013:U:OP2	7:A:2018:A:N6	2.22	0.71
7:A:2688:A:OP1	7:A:2735:A:O2'	2.07	0.70
32:a:654:A:N7	37:f:95:LYS:NZ	2.39	0.70
7:A:1140:G:N3	15:J:147:GLN:NE2	2.38	0.70
7:A:1414:G:N2	7:A:1417:A:OP2	2.25	0.70
32:a:492:C:OP1	43:l:114:ARG:NH1	2.23	0.70
32:a:664:G:O3'	37:f:87:ARG:NH2	2.24	0.70
32:a:1398:G:O3'	52:x:16:LYS:NZ	2.22	0.70
7:A:775:C:N4	7:A:776:G:O6	2.25	0.70
7:A:1540:G:N2	7:A:1828:C:N3	2.39	0.70
32:a:1139:C:O2'	40:i:28:GLN:NE2	2.24	0.70
45:n:41:ARG:O	45:n:45:ARG:NH1	2.24	0.70
7:A:1136:C:OP1	15:J:37:ARG:NH1	2.24	0.70
32:a:460:U:OP1	32:a:462:C:N4	2.24	0.70
43:l:36:ARG:NH1	43:l:62:GLU:OE2	2.24	0.70
32:a:177:A:O2'	32:a:178:G:O4'	2.09	0.70
7:A:1707:A:OP2	7:A:1761:A:N6	2.25	0.70
32:a:995:A:H2	32:a:1029:C:N4	1.90	0.70
49:r:51:ARG:NE	49:r:56:ASN:O	2.24	0.69
32:a:507:U:O2	32:a:524:A:N7	2.24	0.69
32:a:420:U:O4	34:c:126:ARG:NH1	2.25	0.69
4:3:47:ARG:NH2	7:A:734:G:OP1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:289:A:N1	7:A:300:G:N2	2.40	0.69
32:a:1072:G:N7	36:e:83:LYS:NZ	2.40	0.69
32:a:1291:A:N7	38:g:112:ARG:NH2	2.40	0.69
7:A:703:G:OP1	11:E:36:ASN:ND2	2.26	0.69
19:N:38:GLU:OE2	19:N:42:ARG:NH2	2.26	0.69
3:2:11:ASN:ND2	7:A:899:G:OP1	2.25	0.69
7:A:2218:G:O2'	7:A:2220:C:OP2	2.11	0.69
32:a:1312:C:N3	50:s:36:ARG:NH1	2.40	0.69
7:A:2354:A:OP1	7:A:2402:G:N2	2.26	0.69
7:A:2343:G:C2	7:A:2420:U:O2	2.45	0.69
32:a:1002:G:O6	32:a:1013:G:O6	2.11	0.68
7:A:2172:C:OP2	52:x:28:ARG:NE	2.26	0.68
32:a:11:A:N6	35:d:197:GLU:O	2.26	0.68
32:a:518:G:O2'	32:a:526:A:N1	2.22	0.68
7:A:2814:G:O2'	7:A:2817:C:OP2	2.10	0.68
32:a:756:G:H1	32:a:803:G:HO2'	1.35	0.68
32:a:1138:A:O2'	40:i:41:ARG:NH2	2.26	0.68
7:A:193:A:O2'	7:A:807:C:O2	2.10	0.68
35:d:31:TYR:N	35:d:32:PRO:CD	2.56	0.68
2:1:15:CYS:O	2:1:19:LYS:N	2.27	0.68
32:a:223:U:OP1	51:t:69:LYS:NZ	2.27	0.68
7:A:244:G:O2'	7:A:256:G:O6	2.12	0.68
7:A:718:G:N2	11:E:193:ASP:OD1	2.27	0.68
7:A:2399:G:N2	7:A:2400:U:O4	2.27	0.68
15:J:13:ARG:NH2	15:J:49:ASP:O	2.27	0.68
2:1:23:TYR:OH	7:A:2585:C:O2'	2.10	0.68
32:a:129:U:O2	32:a:228:U:O4	2.12	0.67
7:A:2149:U:O2	7:A:2157:A:N6	2.26	0.67
32:a:683:U:OP1	42:k:136:ARG:NH1	2.27	0.67
7:A:2372:A:N1	7:A:2393:G:O2'	2.23	0.67
7:A:3084:G:O2'	7:A:3101:G:N2	2.28	0.67
7:A:740:G:O2'	7:A:742:G:O2'	2.13	0.67
7:A:1397:G:N2	7:A:2251:A:OP2	2.26	0.67
32:a:175:A:O2'	32:a:177:A:OP1	2.13	0.67
32:a:490:A:N6	32:a:538:A:O5'	2.27	0.67
32:a:1367:A:OP1	38:g:36:LYS:NZ	2.28	0.67
7:A:708:G:N3	7:A:786:U:O2'	2.28	0.67
7:A:1948:A:N3	7:A:1950:A:O2'	2.28	0.67
32:a:567:A:N6	32:a:750:A:OP1	2.28	0.67
7:A:1176:G:N2	7:A:1239:A:O2'	2.28	0.67
7:A:2233:U:O2	16:K:3:GLN:NE2	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2711:U:OP1	7:A:2767:G:N2	2.28	0.67
7:A:2865:G:O2'	7:A:3019:A:N1	2.23	0.67
4:3:28:ASN:O	4:3:36:LYS:NZ	2.27	0.67
7:A:1511:G:N2	7:A:1807:A:N1	2.42	0.67
7:A:2870:A:O2'	7:A:3046:G:O2'	2.13	0.66
13:G:7:GLN:O	13:G:70:ARG:NH1	2.27	0.66
32:a:674:G:N2	42:k:49:GLY:O	2.28	0.66
26:U:13:SER:OG	26:U:70:ASN:OD1	2.12	0.66
4:3:43:ARG:NH1	7:A:2600:G:OP2	2.28	0.66
43:l:86:ARG:NH1	43:l:94:ARG:O	2.28	0.66
7:A:1199:A:N7	7:A:1225:A:O2'	2.28	0.66
7:A:2552:A:OP1	12:F:95:ARG:NH1	2.28	0.66
48:q:117:THR:O	48:q:125:ARG:NE	2.28	0.66
7:A:945:C:C2	7:A:1324:G:N2	2.63	0.66
7:A:2100:A:N6	7:A:2113:G:O2'	2.27	0.66
35:d:31:TYR:H	35:d:32:PRO:HD3	1.58	0.66
7:A:844:A:O2'	7:A:845:A:OP1	2.13	0.66
11:E:52:ARG:NH1	11:E:104:TYR:OH	2.29	0.66
32:a:986:G:O2'	32:a:987:A:N7	2.28	0.66
7:A:1659:G:H1	7:A:1814:C:H42	1.41	0.66
7:A:2470:C:OP2	29:X:27:ARG:NH2	2.29	0.65
36:e:134:THR:N	36:e:153:ASP:OD1	2.29	0.65
31:Z:47:ILE:O	31:Z:50:VAL:C	2.40	0.65
35:d:57:ARG:NH1	35:d:64:GLU:OE1	2.29	0.65
7:A:1713:G:O2'	7:A:1753:G:O6	2.11	0.65
7:A:3071:U:O4	7:A:3118:A:N6	2.28	0.65
32:a:633:A:N3	39:h:107:SER:OG	2.25	0.65
7:A:2418:G:OP2	7:A:2419:A:N6	2.29	0.65
32:a:226:G:N2	47:p:62:VAL:O	2.30	0.65
27:V:47:LEU:H	27:V:48:PRO:HD2	1.62	0.65
7:A:1200:G:O2'	7:A:1205:C:N4	2.28	0.65
7:A:2293:C:O2'	7:A:2742:U:O5'	2.15	0.65
7:A:272:A:OP2	7:A:315:G:N1	2.30	0.65
7:A:1540:G:C4	7:A:1829:A:N1	2.65	0.64
12:F:64:LEU:O	12:F:68:THR:OG1	2.12	0.64
7:A:1211:U:OP2	7:A:1212:G:N1	2.30	0.64
32:a:400:C:O2'	32:a:612:A:N3	2.28	0.64
7:A:1197:G:N2	7:A:1224:A:O2'	2.31	0.64
46:o:73:ILE:O	48:q:136:LYS:NZ	2.30	0.64
7:A:2392:C:O2'	7:A:2393:G:O4'	2.12	0.64
7:A:3058:A:OP1	10:D:169:ARG:NE	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1381:G:O6	17:L:20:ARG:NH2	2.31	0.64
25:T:50:PHE:O	25:T:91:ARG:NH2	2.31	0.64
7:A:203:C:OP1	29:X:24:ARG:NH1	2.29	0.64
32:a:870:C:OP1	39:h:82:LYS:NZ	2.21	0.64
38:g:114:LYS:O	38:g:119:ARG:NE	2.31	0.63
7:A:1139:A:N3	7:A:1283:C:O2	2.31	0.63
32:a:342:U:O2	32:a:345:G:O6	2.15	0.63
44:m:82:ILE:O	44:m:93:ARG:NH2	2.30	0.63
7:A:241:C:O2'	7:A:726:G:O2'	2.17	0.63
14:H:27:ARG:NH1	29:X:56:ILE:O	2.31	0.63
32:a:1188:A:O2'	32:a:1189:A:OP1	2.12	0.63
7:A:250:G:O2'	7:A:2670:A:OP1	2.17	0.63
13:G:85:THR:OG1	13:G:134:VAL:O	2.13	0.62
32:a:1487:G:N7	33:b:5:DPP:N	2.43	0.62
38:g:67:ASP:O	38:g:138:ARG:NH1	2.32	0.62
1:O:21:LYS:NZ	24:S:32:ASP:OD2	2.32	0.62
10:D:34:ASN:OD1	10:D:78:ARG:NE	2.32	0.62
32:a:295:U:O2'	32:a:547:C:O2	2.16	0.62
32:a:986:G:N7	32:a:1205:A:N6	2.47	0.62
40:i:29:THR:OG1	40:i:40:VAL:O	2.12	0.62
7:A:140:G:N2	7:A:1540:G:H1'	2.14	0.62
7:A:1656:G:O2'	7:A:1815:U:O4	2.15	0.62
7:A:2330:G:O2'	7:A:2435:A:N1	2.28	0.62
22:Q:28:ARG:NH1	22:Q:38:GLN:OE1	2.32	0.62
7:A:2544:C:OP2	7:A:2545:G:O2'	2.10	0.62
7:A:1731:A:H2	7:A:1816:A:HO2'	1.47	0.62
7:A:2364:G:O2'	7:A:2365:A:O4'	2.16	0.62
7:A:1951:U:O4	7:A:1978:G:O6	2.18	0.62
7:A:2154:A:N6	32:a:1401:A:O2'	2.33	0.62
7:A:2192:G:O2'	7:A:2194:U:O4	2.15	0.62
8:B:91:U:O2'	31:Z:51:ARG:NH1	2.32	0.62
32:a:203:U:O2	32:a:204:G:N2	2.31	0.62
7:A:2893:G:N2	7:A:2903:A:OP2	2.33	0.61
32:a:389:U:O2'	47:p:29:ARG:NE	2.32	0.61
7:A:3075:U:O4	7:A:3112:G:O6	2.17	0.61
32:a:254:G:O6	32:a:265:G:C6	2.53	0.61
32:a:261:G:O2'	51:t:70:ASN:ND2	2.33	0.61
32:a:1128:A:N3	32:a:1129:A:O2'	2.32	0.61
32:a:1260:G:N2	32:a:1319:C:O4'	2.34	0.61
7:A:2926:G:OP1	7:A:2951:C:N4	2.33	0.61
32:a:1213:G:OP1	50:s:36:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1457:C:N4	7:A:1883:C:O2'	2.32	0.61
32:a:131:C:N3	47:p:1:MET:N	2.43	0.61
7:A:3081:C:OP1	21:P:50:GLN:NE2	2.34	0.61
32:a:11:A:N3	36:e:143:ARG:NH1	2.49	0.61
32:a:1308:G:N1	32:a:1311:A:OP2	2.33	0.61
19:N:38:GLU:OE2	19:N:99:LYS:NZ	2.33	0.61
7:A:1450:G:O6	7:A:1465:C:N4	2.34	0.61
7:A:1540:G:N1	7:A:1828:C:N4	2.25	0.61
7:A:2371:A:O2'	7:A:2396:G:N2	2.34	0.61
21:P:13:ARG:NH1	21:P:77:SER:O	2.33	0.61
32:a:1398:G:N2	32:a:1489:C:H42	1.99	0.61
7:A:1155:G:OP2	7:A:1263:G:O2'	2.18	0.60
7:A:2446:C:N4	7:A:2447:U:O4	2.34	0.60
7:A:2928:A:N6	19:N:3:LYS:O	2.34	0.60
51:t:17:ALA:O	51:t:21:ASN:ND2	2.34	0.60
7:A:29:U:O2	7:A:1346:G:O2'	2.19	0.60
7:A:382:A:N7	26:U:82:ARG:NH1	2.49	0.60
18:M:55:ASN:O	18:M:58:ILE:C	2.44	0.60
7:A:2226:A:OP1	16:K:7:ARG:NH2	2.33	0.60
42:k:36:THR:OG1	42:k:39:ASN:N	2.34	0.60
42:k:85:GLN:OE1	42:k:90:ARG:NH1	2.34	0.60
7:A:1121:C:OP1	23:R:78:LYS:NZ	2.33	0.60
32:a:1043:U:C2	32:a:1198:G:O6	2.55	0.60
47:p:17:GLN:OE1	47:p:41:HIS:NE2	2.35	0.60
7:A:823:U:OP1	9:C:59:LYS:NZ	2.33	0.60
7:A:3057:G:O2'	7:A:3059:A:OP2	2.11	0.60
32:a:609:C:N4	32:a:612:A:OP2	2.34	0.60
32:a:772:A:O2'	32:a:1515:U:O2	2.19	0.60
34:c:11:ARG:NE	34:c:180:ALA:O	2.35	0.60
46:o:36:ILE:O	46:o:40:THR:OG1	2.19	0.60
7:A:716:G:N2	7:A:719:U:O2	2.33	0.59
32:a:11:A:N6	35:d:200:SER:OG	2.36	0.59
34:c:82:GLU:OE1	34:c:85:ARG:NE	2.34	0.59
7:A:474:C:O2'	7:A:477:G:N2	2.35	0.59
7:A:1537:C:C4	7:A:1832:G:N2	2.70	0.59
7:A:2662:C:O2	7:A:2667:G:O2'	2.19	0.59
37:f:89:LYS:NZ	49:r:73:GLU:OE1	2.22	0.59
7:A:1540:G:N1	7:A:1829:A:C6	2.70	0.59
32:a:530:A:OP2	43:l:112:GLN:NE2	2.33	0.59
36:e:138:ALA:O	36:e:143:ARG:NH1	2.34	0.59
7:A:504:A:O2'	7:A:2100:A:OP1	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:976:U:C4	7:A:1061:A:N7	2.70	0.59
7:A:992:A:O2'	8:B:96:A:N3	2.35	0.59
32:a:180:A:N1	32:a:204:G:N1	2.51	0.59
7:A:1832:G:OP2	25:T:43:LYS:NZ	2.28	0.59
32:a:155:G:N2	32:a:158:A:OP2	2.35	0.59
1:0:2:ALA:N	7:A:2850:C:HO2'	2.01	0.59
47:p:14:ARG:O	47:p:43:LYS:NZ	2.32	0.59
23:R:20:GLY:N	23:R:100:VAL:O	2.35	0.59
50:s:23:ASN:OD1	50:s:47:HIS:NE2	2.34	0.58
7:A:247:G:N2	7:A:473:C:O2'	2.36	0.58
7:A:948:A:OP2	7:A:1319:G:N2	2.35	0.58
7:A:1546:G:H1	7:A:1822:C:H42	1.48	0.58
27:V:11:VAL:HG11	27:V:45:LEU:HD23	1.85	0.58
32:a:968:A:N1	32:a:1359:C:O2'	2.30	0.58
44:m:17:VAL:O	44:m:20:THR:OG1	2.15	0.58
32:a:102:G:OP1	32:a:324:A:N6	2.36	0.58
32:a:261:G:H5''	51:t:71:GLN:HE22	1.69	0.58
6:6:9:TYR:O	6:6:26:SER:OG	2.15	0.58
7:A:330:G:O2'	7:A:446:A:OP2	2.10	0.58
7:A:2956:G:H4'	21:P:95:LYS:HG3	1.86	0.58
32:a:1053:U:O4	32:a:1186:U:O4	2.21	0.58
44:m:12:ASP:OD1	44:m:46:ARG:NH2	2.36	0.58
4:3:24:ARG:NH2	4:3:54:ASP:OD2	2.37	0.58
7:A:2331:A:O4'	7:A:2435:A:N6	2.37	0.58
32:a:632:U:O2'	32:a:633:A:O5'	2.21	0.58
7:A:552:G:N2	7:A:555:A:OP2	2.33	0.58
7:A:968:U:O2'	7:A:1323:G:N3	2.37	0.58
7:A:1540:G:C2	7:A:1829:A:N3	2.70	0.58
7:A:1215:A:O2'	7:A:1232:A:N6	2.35	0.57
32:a:457:G:N2	32:a:465:U:O2	2.36	0.57
41:j:50:CYS:O	45:n:41:ARG:NH2	2.37	0.57
7:A:2360:G:OP1	7:A:2413:A:N6	2.37	0.57
12:F:171:ASP:OD1	12:F:174:ARG:NH2	2.36	0.57
26:U:40:ARG:HD2	26:U:61:THR:HB	1.86	0.57
32:a:1056:U:O4'	32:a:1182:G:N2	2.37	0.57
7:A:2928:A:N6	19:N:5:THR:OG1	2.37	0.57
7:A:2527:G:N2	7:A:2584:A:OP1	2.38	0.57
32:a:1056:U:N3	32:a:1182:G:O4'	2.37	0.57
32:a:53:A:O2'	32:a:359:G:N2	2.38	0.57
7:A:749:U:O2	7:A:749:U:O2'	2.23	0.57
7:A:914:G:O2'	7:A:915:C:O5'	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1540:G:C2	7:A:1829:A:C5	2.93	0.57
7:A:356:A:N6	7:A:357:G:O6	2.37	0.56
7:A:503:C:O2	7:A:2098:U:O2'	2.21	0.56
7:A:2408:A:OP1	7:A:2410:A:N6	2.37	0.56
20:O:49:ASP:OD2	20:O:53:THR:OG1	2.21	0.56
32:a:537:G:O3'	35:d:1:MET:N	2.37	0.56
7:A:1148:U:OP1	7:A:1164:U:O2'	2.23	0.56
32:a:586:G:O2'	32:a:632:U:O4	2.10	0.56
32:a:1065:G:OP1	36:e:100:LYS:NZ	2.38	0.56
32:a:1196:A:N3	34:c:195:ARG:NH2	2.52	0.56
40:i:31:GLY:O	40:i:39:ARG:NH2	2.38	0.56
6:6:17:GLY:N	6:6:36:GLU:O	2.37	0.56
7:A:1081:G:OP1	18:M:16:ARG:NE	2.36	0.56
7:A:1962:C:HO2'	7:A:1965:G:H1	1.52	0.56
28:W:47:PRO:O	28:W:73:ARG:NH2	2.38	0.56
7:A:9:G:N2	7:A:2867:C:O2	2.37	0.56
7:A:2378:G:O6	7:A:2388:G:N2	2.39	0.56
7:A:1902:G:O2'	7:A:2229:U:O4	2.23	0.56
35:d:29:ARG:HB3	35:d:30:PRO:HD2	1.87	0.56
32:a:155:G:O2'	32:a:157:A:N7	2.35	0.56
32:a:837:U:O2'	32:a:838:U:O4'	2.24	0.56
32:a:437:U:OP1	35:d:117:HIS:NE2	2.39	0.55
32:a:1171:A:OP2	40:i:116:ARG:NH2	2.35	0.55
7:A:883:U:O2'	7:A:1403:A:N1	2.39	0.55
32:a:629:C:N4	32:a:630:G:O6	2.39	0.55
7:A:2380:C:O2'	7:A:2385:G:N2	2.39	0.55
32:a:413:A:OP2	32:a:427:G:N1	2.38	0.55
34:c:63:VAL:HB	34:c:98:VAL:HG23	1.87	0.55
7:A:638:C:N4	7:A:641:U:O4	2.38	0.55
35:d:32:PRO:HB3	35:d:37:GLY:C	2.31	0.55
7:A:285:G:O2'	7:A:289:A:OP1	2.23	0.55
35:d:197:GLU:O	35:d:200:SER:OG	2.22	0.55
7:A:1660:G:C6	7:A:1661:G:C5	2.94	0.55
11:E:159:GLN:NE2	11:E:180:GLY:O	2.39	0.55
7:A:1622:G:O2'	7:A:1623:G:O4'	2.24	0.55
40:i:127:ARG:HB3	40:i:129:PRO:HD3	1.88	0.55
5:4:29:ASP:OD1	13:G:171:ARG:NH2	2.40	0.55
32:a:759:A:N3	32:a:1505:U:O2'	2.40	0.55
7:A:556:G:O2'	7:A:925:U:O2'	2.25	0.55
43:l:3:THR:O	43:l:6:GLN:N	2.40	0.55
32:a:999:C:H6	32:a:999:C:O5'	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:h:82:LYS:O	39:h:84:GLY:N	2.40	0.54
43:l:79:MET:N	43:l:103:ASP:OD2	2.39	0.54
7:A:667:C:O2	7:A:679:G:N2	2.40	0.54
7:A:2644:A:OP2	7:A:2649:A:N6	2.38	0.54
7:A:2999:G:O2'	13:G:144:GLN:NE2	2.40	0.54
32:a:967:A:OP2	41:j:57:LYS:NZ	2.35	0.54
7:A:1540:G:C2	7:A:1829:A:C6	2.94	0.54
7:A:1571:A:OP2	7:A:1632:G:N1	2.38	0.54
10:D:138:SER:OG	10:D:139:HIS:N	2.41	0.54
32:a:578:G:N2	32:a:746:G:N7	2.55	0.54
32:a:971:A:N7	32:a:1352:A:N6	2.55	0.54
7:A:466:A:N6	7:A:487:G:O6	2.41	0.54
7:A:1873:C:O3'	7:A:2947:G:N2	2.40	0.54
30:Y:23:ARG:NH1	30:Y:27:GLU:OE2	2.40	0.54
32:a:212:C:N4	32:a:215:U:C4	2.76	0.54
7:A:139:U:N3	7:A:142:U:OP2	2.39	0.54
7:A:844:A:OP2	46:o:64:ARG:NH2	2.40	0.54
7:A:2217:C:N4	7:A:2218:G:O6	2.40	0.54
7:A:145:C:H5''	25:T:41:GLN:HE21	1.72	0.54
32:a:212:C:O2	32:a:216:A:N6	2.41	0.54
32:a:1097:G:O2'	34:c:169:ARG:NH1	2.40	0.54
46:o:10:GLU:OE2	46:o:13:ARG:NH1	2.41	0.54
7:A:2549:A:O2'	7:A:2550:U:O4'	2.24	0.54
16:K:113:LYS:O	16:K:116:SER:OG	2.15	0.54
32:a:173:G:OP2	51:t:64:LYS:NZ	2.37	0.54
32:a:459:G:HO2'	32:a:463:U:H3	1.56	0.54
42:k:36:THR:N	42:k:39:ASN:O	2.39	0.54
7:A:1958:C:N3	7:A:1971:G:N2	2.55	0.54
39:h:14:LEU:O	39:h:18:ASN:ND2	2.40	0.54
13:G:112:HIS:O	13:G:112:HIS:ND1	2.41	0.54
35:d:91:SER:OG	35:d:131:ARG:NE	2.40	0.54
40:i:71:ALA:O	40:i:74:VAL:N	2.40	0.54
44:m:51:GLU:OE2	44:m:55:HIS:NE2	2.40	0.54
7:A:2517:G:N7	28:W:14:ARG:NH2	2.50	0.53
25:T:37:SER:O	25:T:80:LYS:NZ	2.35	0.53
32:a:392:A:OP1	47:p:14:ARG:NH2	2.39	0.53
32:a:1240:A:O2'	40:i:54:ARG:NH1	2.39	0.53
32:a:410:A:N7	35:d:29:ARG:NH2	2.54	0.53
7:A:2052:U:OP2	9:C:157:ARG:NE	2.40	0.53
7:A:2551:C:OP1	12:F:75:ARG:NE	2.38	0.53
9:C:184:ARG:NH2	9:C:266:LYS:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:86:ARG:HD3	26:U:97:ILE:HD13	1.89	0.53
38:g:78:ARG:HH11	38:g:153:HIS:HB3	1.74	0.53
1:0:2:ALA:N	7:A:2850:C:O2	2.42	0.53
27:V:47:LEU:H	27:V:48:PRO:CD	2.21	0.53
32:a:884:U:OP2	32:a:899:A:N6	2.41	0.53
4:3:30:ARG:NH1	7:A:2657:U:O4	2.40	0.53
7:A:945:C:N3	7:A:1324:G:C2	2.76	0.53
7:A:2386:U:O2'	7:A:2387:U:O5'	2.27	0.53
32:a:450:A:N6	32:a:472:G:O4'	2.41	0.53
32:a:648:U:OP1	46:o:62:ARG:NH1	2.41	0.53
42:k:46:ASP:O	42:k:49:GLY:N	2.40	0.53
7:A:2296:A:N6	7:A:2297:A:N1	2.57	0.53
7:A:2832:C:N4	7:A:2833:G:O6	2.42	0.53
7:A:2927:C:O2	19:N:14:SER:OG	2.16	0.53
10:D:64:LYS:O	10:D:67:THR:OG1	2.17	0.53
31:Z:47:ILE:O	31:Z:50:VAL:O	2.26	0.53
32:a:179:G:N2	32:a:223:U:O5'	2.42	0.53
32:a:655:G:O2'	32:a:657:G:OP2	2.08	0.53
32:a:1339:G:N7	40:i:34:LYS:NZ	2.55	0.53
3:2:37:ARG:NH1	7:A:555:A:OP1	2.41	0.53
7:A:1402:G:N2	7:A:1852:C:O4'	2.42	0.53
7:A:2079:G:OP1	9:C:256:ARG:NH1	2.38	0.53
7:A:2372:A:O2'	7:A:2397:U:N3	2.41	0.53
20:O:57:ALA:O	20:O:86:ARG:NH1	2.40	0.53
7:A:1026:C:H2'	7:A:1026:C:O2	2.09	0.53
32:a:409:G:O2'	32:a:431:A:N6	2.41	0.53
32:a:1128:A:O2'	32:a:1129:A:O4'	2.26	0.53
7:A:872:A:O2'	7:A:1894:U:OP1	2.24	0.52
32:a:410:A:N1	32:a:427:G:O2'	2.39	0.52
2:1:27:LYS:HE2	2:1:31:ASN:HD22	1.74	0.52
7:A:706:A:N6	7:A:784:A:O4'	2.42	0.52
7:A:1157:A:N3	7:A:2724:G:O2'	2.33	0.52
7:A:1540:G:H2'	7:A:1541:U:C6	2.44	0.52
9:C:124:ASP:O	9:C:129:ASN:ND2	2.39	0.52
13:G:116:ILE:HD11	13:G:149:ILE:HD13	1.92	0.52
7:A:1731:A:H2	7:A:1816:A:O2'	1.91	0.52
7:A:2041:G:OP1	9:C:48:ARG:NH1	2.42	0.52
32:a:835:C:N4	32:a:837:U:O4	2.38	0.52
5:4:27:CYS:SG	5:4:32:HIS:NE2	2.66	0.52
7:A:1414:G:O2'	7:A:1416:G:N7	2.27	0.52
7:A:2368:G:N1	7:A:2396:G:OP1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:62:THR:OG1	29:X:63:ARG:N	2.43	0.52
35:d:32:PRO:HB3	35:d:38:ARG:N	2.24	0.52
36:e:74:ASN:O	36:e:104:ARG:NH1	2.43	0.52
7:A:947:G:N1	7:A:1320:U:OP2	2.38	0.52
7:A:2092:G:O2'	7:A:2121:G:N2	2.41	0.52
7:A:2339:U:C2	7:A:2424:A:N6	2.76	0.52
8:B:12:A:N1	8:B:68:G:O2'	2.35	0.52
17:L:125:ALA:HB3	17:L:128:PHE:CE1	2.45	0.52
7:A:161:G:N2	7:A:169:A:OP2	2.39	0.52
7:A:1049:G:OP1	31:Z:18:LYS:NZ	2.43	0.52
10:D:157:PRO:O	10:D:159:ARG:N	2.41	0.52
7:A:1047:A:N3	8:B:79:U:O2'	2.43	0.52
7:A:3092:G:N2	7:A:3095:A:OP2	2.41	0.52
32:a:802:C:O2'	32:a:894:A:N6	2.40	0.52
7:A:2629:G:N1	7:A:2663:A:OP1	2.43	0.52
32:a:827:G:OP1	49:r:59:GLN:NE2	2.43	0.51
32:a:982:G:O2'	32:a:1009:G:N2	2.43	0.51
7:A:48:G:N2	7:A:179:A:OP2	2.39	0.51
7:A:1540:G:C2	7:A:1828:C:N3	2.78	0.51
7:A:2399:G:O2'	7:A:2408:A:OP2	2.14	0.51
32:a:988:C:N3	32:a:1037:A:O2'	2.41	0.51
7:A:760:A:N6	7:A:781:A:O5'	2.44	0.51
7:A:934:G:N2	7:A:958:A:OP1	2.42	0.51
7:A:2359:U:O2'	7:A:2359:U:O2	2.27	0.51
7:A:2926:G:N1	7:A:2958:U:OP2	2.42	0.51
7:A:893:A:N3	9:C:213:ARG:NH1	2.58	0.51
7:A:1624:C:O2'	7:A:1625:U:OP1	2.26	0.51
7:A:2902:G:O2'	7:A:2903:A:O5'	2.18	0.51
15:J:5:ALA:O	15:J:7:LYS:N	2.44	0.51
32:a:883:G:N2	32:a:900:A:OP2	2.44	0.51
7:A:2751:G:OP1	10:D:165:ARG:NE	2.44	0.51
7:A:405:A:OP2	11:E:177:ASN:ND2	2.42	0.51
7:A:905:G:N1	7:A:2309:C:OP1	2.43	0.51
7:A:1139:A:C2	7:A:1283:C:O2	2.63	0.51
10:D:76:ASN:HD22	10:D:77:PRO:N	2.09	0.51
7:A:1540:G:C6	7:A:1828:C:N4	2.57	0.51
32:a:1172:A:N3	40:i:127:ARG:NH2	2.58	0.51
32:a:1181:U:OP1	41:j:53:ARG:NH2	2.44	0.51
7:A:1540:G:C6	7:A:1829:A:C6	2.98	0.51
7:A:2402:G:O6	7:A:2408:A:N3	2.44	0.51
12:F:21:ASP:OD1	12:F:24:ARG:NH2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:57:ASP:O	13:G:59:GLU:N	2.44	0.51
35:d:55:LYS:O	35:d:59:THR:OG1	2.20	0.51
7:A:451:C:N3	7:A:452:A:N6	2.59	0.51
35:d:99:ARG:NH1	35:d:187:ASP:OD2	2.42	0.51
35:d:115:HIS:O	35:d:141:ARG:NH1	2.37	0.51
7:A:2388:G:N2	7:A:2389:G:O6	2.44	0.50
12:F:70:GLN:NE2	12:F:97:THR:O	2.45	0.50
32:a:616:G:O3'	47:p:17:GLN:NE2	2.44	0.50
7:A:862:G:N2	7:A:863:A:N7	2.59	0.50
7:A:945:C:N3	7:A:1324:G:N2	2.60	0.50
7:A:1560:U:H3'	7:A:1561:C:C5	2.46	0.50
7:A:2844:C:N4	7:A:2845:G:O6	2.45	0.50
9:C:83:GLU:OE1	9:C:104:TYR:OH	2.25	0.50
7:A:2378:G:C6	7:A:2387:U:O2	2.64	0.50
35:d:32:PRO:HG3	35:d:38:ARG:HA	1.93	0.50
7:A:1653:A:O2'	7:A:1654:G:OP1	2.28	0.50
32:a:77:G:N2	32:a:92:C:N3	2.60	0.50
47:p:58:TYR:O	47:p:61:SER:OG	2.17	0.50
7:A:1283:C:C5	7:A:1284:G:C5	2.99	0.50
7:A:1567:U:O2'	7:A:1568:A:P	2.69	0.50
27:V:151:PRO:HB3	27:V:179:VAL:HG12	1.92	0.50
32:a:508:G:N2	32:a:524:A:OP2	2.43	0.50
7:A:229:A:N6	7:A:499:G:N3	2.58	0.50
37:f:92:ARG:NH1	37:f:94:ASP:OD1	2.45	0.50
37:f:92:ARG:NH1	37:f:95:LYS:O	2.43	0.50
7:A:2468:G:O2'	29:X:30:ASP:O	2.29	0.50
32:a:1425:G:O2'	32:a:1461:A:N6	2.45	0.50
39:h:24:GLU:OE1	39:h:63:GLN:NE2	2.37	0.50
7:A:611:C:O2	7:A:656:U:O2'	2.29	0.50
7:A:616:A:N7	15:J:116:ARG:NH1	2.59	0.50
7:A:1100:C:OP1	7:A:1118:G:N1	2.39	0.50
7:A:2583:G:O2'	7:A:2619:C:O2	2.26	0.50
20:O:25:SER:O	20:O:48:ASN:ND2	2.43	0.50
32:a:476:G:H3'	32:a:477:U:C5'	2.42	0.50
7:A:976:U:N3	7:A:1061:A:N7	2.59	0.49
32:a:178:G:N2	32:a:205:G:N7	2.59	0.49
32:a:1144:G:O4'	41:j:72:ARG:NH2	2.45	0.49
35:d:30:PRO:HG2	35:d:32:PRO:HD2	1.94	0.49
7:A:1944:C:HO2'	7:A:3094:A:HO2'	1.45	0.49
12:F:39:THR:O	12:F:99:ARG:NE	2.45	0.49
46:o:74:ASP:OD1	46:o:75:VAL:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2357:G:N1	7:A:2416:C:O4'	2.44	0.49
43:l:71:GLY:O	43:l:99:ARG:NH1	2.41	0.49
32:a:1143:U:O2'	41:j:72:ARG:NH2	2.45	0.49
32:a:771:G:N1	32:a:792:U:OP2	2.44	0.49
32:a:1048:G:N3	34:c:195:ARG:NH2	2.55	0.49
7:A:1537:C:N4	7:A:1832:G:N2	2.61	0.49
32:a:1367:A:O2'	38:g:28:ASN:O	2.28	0.49
36:e:113:THR:OG1	36:e:114:HIS:N	2.46	0.49
7:A:1223:U:N3	7:A:1226:U:OP2	2.46	0.49
7:A:1540:G:C2	7:A:1829:A:N1	2.81	0.49
7:A:1615:G:C2	7:A:1616:U:C5	3.00	0.48
32:a:952:A:N6	32:a:1214:G:O4'	2.46	0.48
34:c:113:GLN:NE2	34:c:186:LEU:O	2.46	0.48
7:A:261:C:O2	7:A:725:A:O2'	2.29	0.48
7:A:2193:U:O4	7:A:2794:C:N4	2.46	0.48
32:a:85:G:N2	32:a:86:G:O6	2.46	0.48
32:a:944:G:N3	32:a:963:C:O2'	2.45	0.48
7:A:1692:U:O4'	19:N:63:ARG:NH1	2.44	0.48
7:A:2685:G:N2	7:A:2688:A:OP2	2.47	0.48
7:A:2873:C:O2'	10:D:51:GLN:NE2	2.47	0.48
32:a:126:A:H5''	32:a:127:U:H5'	1.96	0.48
32:a:154:G:N2	32:a:159:C:O2	2.45	0.48
32:a:264:G:N2	32:a:266:C:O4'	2.46	0.48
32:a:1407:U:H2'	32:a:1408:G:H8	1.78	0.48
42:k:36:THR:OG1	42:k:39:ASN:O	2.31	0.48
7:A:553:U:O4	7:A:554:G:N1	2.46	0.48
7:A:1470:G:N7	25:T:62:ARG:NH2	2.58	0.48
7:A:2149:U:O4	7:A:2156:A:O2'	2.20	0.48
7:A:2833:G:O2'	7:A:2835:G:O6	2.30	0.48
32:a:997:G:O5'	32:a:1018:U:N3	2.45	0.48
7:A:1580:A:O2'	7:A:1624:C:N4	2.47	0.48
17:L:125:ALA:HB3	17:L:128:PHE:HE1	1.78	0.48
32:a:997:G:H2'	32:a:998:A:O4'	2.13	0.48
44:m:15:MET:N	44:m:41:ARG:O	2.44	0.48
7:A:140:G:H21	7:A:1540:G:H1'	1.78	0.48
7:A:877:G:N3	7:A:879:A:N6	2.62	0.48
14:H:5:LEU:O	14:H:16:GLY:N	2.40	0.48
35:d:32:PRO:HG2	35:d:38:ARG:CG	2.34	0.48
7:A:2943:A:O2'	7:A:3087:G:OP1	2.28	0.48
32:a:446:G:HO2'	32:a:447:A:P	2.34	0.48
13:G:59:GLU:HB2	13:G:62:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:x:21:LEU:O	52:x:24:THR:C	2.57	0.48
32:a:508:G:N1	32:a:524:A:OP2	2.46	0.48
7:A:942:U:O2'	7:A:1356:G:O2'	2.31	0.47
7:A:1190:U:O2'	7:A:1199:A:N3	2.46	0.47
7:A:2170:A:N3	7:A:2207:A:N6	2.62	0.47
32:a:1007:G:OP2	50:s:18:LYS:NZ	2.41	0.47
50:s:69:HIS:ND1	50:s:73:GLU:OE1	2.45	0.47
7:A:1737:G:N2	9:C:99:ASP:O	2.46	0.47
7:A:2035:G:OP2	9:C:154:LYS:NZ	2.47	0.47
32:a:427:G:OP2	35:d:10:ARG:NH2	2.41	0.47
7:A:913:G:O4'	9:C:227:ASN:ND2	2.47	0.47
7:A:1185:G:N2	7:A:1232:A:C8	2.81	0.47
32:a:1407:U:O2	32:a:1480:G:N2	2.47	0.47
32:a:1488:U:N3	32:a:1489:C:H5	2.10	0.47
32:a:485:G:O2'	32:a:486:A:O5'	2.27	0.47
1:0:42:ARG:NH2	19:N:38:GLU:OE1	2.48	0.47
7:A:1733:A:O4'	7:A:1815:U:O2'	2.31	0.47
7:A:2250:G:O2'	7:A:2251:A:O5'	2.22	0.47
7:A:2921:C:O2	16:K:76:TYR:OH	2.32	0.47
13:G:5:GLY:O	13:G:70:ARG:NH2	2.46	0.47
31:Z:11:SER:OG	31:Z:12:THR:N	2.38	0.47
32:a:361:G:O3'	43:l:30:ARG:NH1	2.45	0.47
32:a:412:G:O3'	32:a:427:G:N2	2.46	0.47
32:a:756:G:N2	32:a:804:U:OP2	2.47	0.47
7:A:480:A:O2'	7:A:499:G:OP1	2.31	0.47
7:A:2378:G:N2	7:A:2387:U:O2'	2.45	0.47
32:a:533:G:O2'	35:d:14:ARG:NH2	2.48	0.47
32:a:1301:G:N7	44:m:99:ARG:NH2	2.62	0.47
7:A:407:A:N6	7:A:422:U:O4'	2.47	0.47
7:A:1660:G:C6	7:A:1661:G:N7	2.82	0.47
7:A:1826:C:H2'	7:A:1827:A:C8	2.50	0.47
7:A:2092:G:HO2'	7:A:2093:A:H8	1.61	0.47
7:A:2354:A:C2	7:A:2402:G:O6	2.68	0.47
32:a:361:G:N2	32:a:364:U:OP2	2.41	0.47
32:a:1210:C:OP2	45:n:9:LYS:NZ	2.46	0.47
51:t:59:ASP:OD2	51:t:76:LYS:NZ	2.43	0.47
32:a:421:C:O2'	32:a:422:G:N2	2.48	0.47
32:a:677:U:O4	32:a:694:G:O2'	2.32	0.47
7:A:588:G:N1	7:A:591:A:OP2	2.46	0.47
7:A:1121:C:OP1	22:Q:47:TYR:OH	2.30	0.47
9:C:66:ASP:OD2	9:C:103:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1284:C:OP1	38:g:41:ARG:NH1	2.43	0.47
7:A:533:C:OP1	11:E:52:ARG:NE	2.48	0.46
32:a:409:G:N1	32:a:430:A:OP2	2.42	0.46
32:a:860:G:O2'	32:a:866:A:N1	2.38	0.46
35:d:27:GLU:O	35:d:29:ARG:NH1	2.48	0.46
7:A:618:U:O2'	7:A:2274:C:OP1	2.29	0.46
7:A:912:A:H2'	7:A:913:G:H4'	1.97	0.46
7:A:954:A:O3'	7:A:2666:G:O2'	2.31	0.46
12:F:70:GLN:OE1	12:F:102:ARG:NH2	2.48	0.46
32:a:1158:G:N1	32:a:1161:A:OP2	2.42	0.46
7:A:2963:A:O2'	7:A:2965:G:N7	2.38	0.46
22:Q:72:ASN:O	22:Q:114:ARG:NH2	2.48	0.46
32:a:196:C:O2'	48:q:50:ARG:NH2	2.43	0.46
32:a:848:G:OP2	32:a:864:U:N3	2.43	0.46
7:A:1074:G:O6	7:A:1101:G:N2	2.48	0.46
7:A:2364:G:O2'	7:A:2365:A:O5'	2.33	0.46
32:a:206:A:C3'	32:a:207:A:H5'	2.45	0.46
32:a:826:G:O6	32:a:845:C:N4	2.48	0.46
32:a:968:A:O2'	45:n:41:ARG:NH1	2.47	0.46
34:c:11:ARG:O	34:c:16:THR:OG1	2.29	0.46
7:A:1195:U:N3	7:A:1198:A:OP2	2.49	0.46
7:A:2542:G:O2'	12:F:160:ASP:OD2	2.33	0.46
12:F:132:VAL:O	12:F:169:THR:N	2.49	0.46
18:M:55:ASN:O	18:M:58:ILE:O	2.33	0.46
32:a:631:A:H2'	32:a:632:U:O4'	2.15	0.46
32:a:1489:C:O2	32:a:1489:C:H2'	2.15	0.46
7:A:1269:C:OP2	15:J:68:LYS:NZ	2.49	0.46
7:A:1734:U:OP2	7:A:1735:C:N4	2.42	0.46
32:a:1365:U:OP1	40:i:96:GLN:N	2.44	0.46
35:d:6:GLY:O	35:d:107:ARG:NH2	2.45	0.46
7:A:27:G:O2'	7:A:600:G:N2	2.45	0.46
7:A:1824:C:O2	7:A:1825:A:C8	2.69	0.46
7:A:1827:A:H2'	7:A:1828:C:C6	2.51	0.46
7:A:2377:C:O2	7:A:2378:G:N7	2.48	0.46
30:Y:14:THR:O	30:Y:64:ARG:NH1	2.48	0.46
32:a:501:A:O2'	32:a:533:G:N2	2.49	0.46
32:a:507:U:C2	32:a:524:A:N7	2.84	0.46
5:4:27:CYS:HG	5:4:32:HIS:CE1	2.29	0.46
7:A:32:C:N4	7:A:536:A:OP2	2.49	0.46
7:A:239:C:O2	7:A:712:A:O2'	2.33	0.46
13:G:164:ARG:NH2	13:G:167:GLY:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:90:ASP:HB2	21:P:112:LYS:HD3	1.97	0.46
22:Q:76:TYR:HH	22:Q:92:ARG:HE	1.62	0.46
32:a:969:G:OP1	45:n:32:ALA:N	2.49	0.46
32:a:1218:C:OP1	44:m:103:THR:OG1	2.30	0.46
32:a:1308:G:O2'	32:a:1310:A:N7	2.39	0.46
7:A:2327:A:N6	7:A:2468:G:O6	2.49	0.46
7:A:3085:A:OP2	7:A:3101:G:N1	2.40	0.46
10:D:89:SER:OG	10:D:90:ASP:N	2.48	0.46
13:G:55:ARG:HD2	13:G:56:PRO:HD2	1.97	0.46
32:a:830:U:C4	32:a:840:G:O6	2.69	0.46
32:a:868:U:O4	32:a:869:A:N6	2.48	0.46
32:a:952:A:O2'	32:a:977:C:O2'	2.25	0.46
7:A:1540:G:N2	7:A:1829:A:N3	2.62	0.46
7:A:2721:C:N3	18:M:124:LYS:NZ	2.62	0.46
13:G:53:VAL:O	13:G:66:HIS:NE2	2.49	0.46
32:a:263:C:H1'	48:q:118:ARG:HE	1.80	0.46
3:2:8:PHE:O	7:A:1847:C:O2'	2.33	0.45
7:A:1129:A:OP2	7:A:1284:G:N1	2.42	0.45
7:A:1657:A:H4'	7:A:1658:A:H5'	1.98	0.45
27:V:104:VAL:HB	27:V:133:ALA:O	2.15	0.45
32:a:368:G:OP2	32:a:387:G:N2	2.47	0.45
32:a:572:G:OP1	46:o:65:ARG:NH1	2.49	0.45
10:D:27:THR:OG1	10:D:196:GLY:O	2.26	0.45
32:a:886:C:C5	32:a:887:G:N7	2.83	0.45
6:6:31:GLY:N	12:F:147:GLU:OE2	2.50	0.45
11:E:60:THR:OG1	11:E:61:ARG:N	2.48	0.45
32:a:438:U:O2'	35:d:126:ASN:ND2	2.48	0.45
13:G:74:SER:O	13:G:78:THR:OG1	2.34	0.45
32:a:60:G:O6	32:a:355:A:N6	2.49	0.45
7:A:255:C:C5	7:A:256:G:N7	2.85	0.45
7:A:877:G:OP1	24:S:98:ARG:NH2	2.50	0.45
13:G:57:ASP:OD1	13:G:57:ASP:N	2.48	0.45
32:a:1489:C:C2	32:a:1490:G:N3	2.84	0.45
34:c:90:LEU:HG	34:c:94:THR:HG23	1.97	0.45
7:A:2038:G:O6	7:A:2048:G:N2	2.49	0.45
12:F:63:ASP:OD2	12:F:157:ARG:NH2	2.50	0.45
7:A:145:C:C5'	25:T:41:GLN:HE21	2.30	0.45
7:A:833:G:O2'	7:A:855:G:N2	2.49	0.45
7:A:1660:G:C5	7:A:1661:G:N7	2.85	0.45
7:A:2351:A:N1	7:A:2352:G:N2	2.64	0.45
7:A:2669:U:N3	7:A:2672:A:OP2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2938:C:O2	19:N:71:ARG:NH2	2.49	0.45
32:a:189:U:O2	32:a:194:G:N2	2.41	0.45
32:a:1398:G:H1	32:a:1489:C:H42	1.65	0.45
7:A:1330:U:H1'	22:Q:9:ASN:HD21	1.82	0.45
36:e:87:VAL:HB	36:e:88:PRO:HD3	1.99	0.45
7:A:2354:A:C2	7:A:2402:G:C6	3.05	0.45
7:A:3018:C:N4	15:J:102:GLU:OE2	2.50	0.45
32:a:1487:G:O4'	33:b:6:ALA:HA	2.17	0.45
7:A:2354:A:N6	7:A:2407:A:OP2	2.40	0.44
9:C:9:THR:OG1	9:C:10:THR:N	2.50	0.44
32:a:510:C:H2'	32:a:511:A:O4'	2.17	0.44
32:a:665:G:H2'	32:a:666:A:C8	2.52	0.44
35:d:94:ASP:OD1	35:d:95:ASN:N	2.50	0.44
7:A:689:G:H3'	7:A:690:U:H5'	1.99	0.44
7:A:2022:C:OP1	9:C:222:ARG:NH2	2.51	0.44
32:a:1271:A:O2'	32:a:1274:C:N4	2.51	0.44
7:A:2946:G:N3	19:N:71:ARG:NH1	2.63	0.44
32:a:1273:U:OP2	32:a:1274:C:N4	2.44	0.44
35:d:32:PRO:CG	35:d:38:ARG:CG	2.89	0.44
39:h:28:PRO:O	39:h:33:LYS:NZ	2.29	0.44
7:A:254:G:C2	7:A:255:C:C2	3.05	0.44
7:A:1489:G:N1	7:A:1503:U:OP2	2.47	0.44
7:A:1559:A:H61	7:A:1644:U:H2'	1.82	0.44
7:A:2150:A:OP2	7:A:2156:A:N6	2.46	0.44
7:A:2961:C:P	10:D:119:LYS:HZ3	2.40	0.44
32:a:212:C:C4	32:a:215:U:N3	2.85	0.44
32:a:1107:U:O2	32:a:1176:G:N2	2.50	0.44
34:c:40:ARG:NH1	45:n:26:LYS:O	2.45	0.44
7:A:13:A:O2'	7:A:15:G:N7	2.49	0.44
7:A:284:U:O2	7:A:304:G:O6	2.36	0.44
32:a:125:G:O6	32:a:192:A:O2'	2.35	0.44
32:a:457:G:C2	32:a:465:U:O2	2.71	0.44
7:A:116:C:O2'	7:A:126:A:N3	2.48	0.44
7:A:674:A:OP2	23:R:82:LYS:NZ	2.50	0.44
13:G:65:LEU:O	13:G:69:SER:OG	2.32	0.44
22:Q:66:ASN:OD1	22:Q:70:ARG:NE	2.51	0.44
32:a:39:C:H2'	32:a:40:U:O4'	2.18	0.44
32:a:808:C:N4	32:a:810:G:N3	2.66	0.44
32:a:969:G:C2	32:a:1354:C:C2	3.06	0.44
47:p:15:ASN:OD1	47:p:43:LYS:NZ	2.31	0.44
7:A:390:G:N1	7:A:393:A:OP2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1614:A:H3'	7:A:1615:G:H5''	2.00	0.44
7:A:2151:A:O2'	33:b:2:DPP:N	2.49	0.44
7:A:2487:U:N3	7:A:2491:G:OP2	2.51	0.44
7:A:2768:G:O2'	7:A:2770:G:OP2	2.28	0.44
46:o:26:GLU:OE2	46:o:84:ARG:NH1	2.49	0.44
7:A:325:G:N2	7:A:451:C:O2	2.51	0.44
7:A:1619:U:H2'	7:A:1620:G:C8	2.53	0.44
32:a:117:A:O2'	32:a:311:C:O2'	2.32	0.44
32:a:175:A:H1'	32:a:176:U:H3'	2.00	0.44
32:a:1054:C:OP2	32:a:1055:G:O2'	2.32	0.44
36:e:191:PRO:O	36:e:193:GLU:N	2.42	0.44
7:A:1803:A:OP1	9:C:211:ARG:NH2	2.45	0.44
7:A:2061:U:OP2	9:C:222:ARG:NH1	2.47	0.44
32:a:123:G:O3'	48:q:58:ARG:NH1	2.45	0.44
32:a:1281:A:N1	32:a:1364:G:O2'	2.43	0.44
32:a:495:C:H1'	32:a:501:A:H2'	2.00	0.43
39:h:48:ASP:OD1	39:h:49:PHE:N	2.50	0.43
46:o:76:GLU:OE2	46:o:79:ARG:NH2	2.51	0.43
5:4:33:LYS:O	5:4:35:ARG:NH1	2.52	0.43
7:A:667:C:N4	7:A:675:G:OP1	2.50	0.43
7:A:1132:G:N2	7:A:1283:C:N3	2.66	0.43
7:A:1334:U:O2'	11:E:192:TYR:OH	2.25	0.43
7:A:1542:G:C6	7:A:1543:U:C4	3.05	0.43
7:A:2802:A:OP1	7:A:2886:G:O2'	2.31	0.43
32:a:35:A:H2'	32:a:36:A:C8	2.52	0.43
35:d:90:GLU:HG3	35:d:183:ARG:HB2	1.99	0.43
7:A:2238:C:O2'	7:A:2927:C:OP2	2.24	0.43
7:A:1658:A:H61	7:A:1815:U:H3	1.66	0.43
7:A:2342:G:H3'	7:A:2343:G:H5''	2.00	0.43
32:a:428:U:H3	32:a:430:A:N6	2.16	0.43
39:h:50:ARG:NH2	39:h:52:GLU:OE2	2.49	0.43
7:A:2398:C:O2'	7:A:2408:A:N7	2.45	0.43
32:a:268:U:H2'	32:a:269:A:C8	2.52	0.43
32:a:665:G:H2'	32:a:666:A:H8	1.84	0.43
32:a:748:U:H2'	32:a:749:G:O4'	2.18	0.43
32:a:1044:G:N2	32:a:1049:G:O6	2.51	0.43
32:a:1488:U:C2	32:a:1489:C:H5	2.36	0.43
7:A:845:A:H2'	7:A:846:G:O4'	2.18	0.43
7:A:1495:G:N2	7:A:1498:A:OP2	2.46	0.43
7:A:2374:C:N4	7:A:2391:G:N7	2.67	0.43
7:A:2571:A:OP2	28:W:75:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2581:U:O2'	7:A:2611:A:O2'	2.15	0.43
32:a:597:G:N2	32:a:623:U:OP1	2.46	0.43
32:a:1020:C:HO2'	32:a:1026:G:N2	2.16	0.43
32:a:1242:A:N6	32:a:1346:C:O2'	2.48	0.43
7:A:1579:A:C6	7:A:1626:G:N1	2.87	0.43
7:A:2180:C:H5'	7:A:2181:U:H2'	2.00	0.43
7:A:2343:G:H2'	7:A:2344:U:C6	2.53	0.43
32:a:17:U:N3	32:a:20:U:OP2	2.43	0.43
32:a:493:A:OP1	43:l:114:ARG:N	2.52	0.43
32:a:551:A:O5'	32:a:557:G:N2	2.51	0.43
45:n:16:PHE:O	45:n:19:ARG:N	2.38	0.43
7:A:1822:C:O2	7:A:1823:A:C8	2.72	0.43
32:a:1312:C:O2	50:s:36:ARG:NH2	2.52	0.43
42:k:26:VAL:HB	42:k:89:VAL:HB	2.00	0.43
7:A:65:G:O6	7:A:89:U:O4	2.37	0.43
7:A:729:G:N7	17:L:104:ARG:NH2	2.64	0.43
7:A:1557:G:O6	7:A:1646:G:O2'	2.32	0.43
7:A:2337:G:N2	7:A:2426:U:O2	2.47	0.43
32:a:974:U:O4	32:a:1215:C:N4	2.52	0.43
7:A:345:G:H2'	7:A:346:G:C8	2.54	0.43
7:A:1007:G:N1	7:A:1028:G:N3	2.67	0.43
7:A:2354:A:C5	7:A:2402:G:N1	2.87	0.43
17:L:68:ASN:OD1	17:L:69:ARG:N	2.52	0.42
32:a:454:U:O4	32:a:468:G:O6	2.37	0.42
32:a:1363:G:H2'	32:a:1364:G:H8	1.83	0.42
8:B:4:C:O2'	8:B:25:A:N6	2.46	0.42
32:a:446:G:N2	32:a:478:A:C8	2.86	0.42
32:a:692:C:OP1	32:a:693:A:O2'	2.33	0.42
32:a:941:C:OP1	44:m:108:ARG:N	2.53	0.42
33:b:4:MYN:N	33:b:6:ALA:O	2.52	0.42
40:i:128:ASP:N	40:i:129:PRO:HD3	2.34	0.42
7:A:1865:A:N1	7:A:1872:A:N6	2.68	0.42
17:L:34:ARG:NH2	17:L:44:GLN:HE21	2.17	0.42
32:a:1140:U:H4'	40:i:39:ARG:HD2	2.01	0.42
7:A:2429:G:H2'	7:A:2430:C:O4'	2.19	0.42
32:a:323:G:N2	32:a:326:A:OP2	2.51	0.42
32:a:643:U:O4	32:a:743:G:O2'	2.36	0.42
42:k:28:HIS:ND1	42:k:91:LYS:O	2.53	0.42
7:A:1561:C:H6	7:A:1561:C:O5'	2.02	0.42
32:a:206:A:H3'	32:a:207:A:H5'	2.01	0.42
32:a:533:G:O3'	35:d:14:ARG:NH2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1131:G:N2	32:a:1135:G:O6	2.53	0.42
48:q:121:SER:O	48:q:123:THR:N	2.52	0.42
7:A:1540:G:C5	7:A:1829:A:N1	2.87	0.42
7:A:2098:U:C4	7:A:2116:G:O6	2.73	0.42
7:A:3082:U:OP1	21:P:95:LYS:NZ	2.53	0.42
26:U:73:VAL:HG21	26:U:83:ILE:HD11	2.01	0.42
32:a:177:A:H2'	32:a:178:G:N3	2.34	0.42
32:a:380:C:H2'	32:a:381:A:O4'	2.19	0.42
7:A:2105:G:N2	7:A:2109:G:O6	2.48	0.42
32:a:260:U:N3	32:a:263:C:OP2	2.50	0.42
32:a:477:U:HO2'	32:a:478:A:H8	1.64	0.42
35:d:71:TYR:HA	35:d:85:LEU:HD21	2.00	0.42
7:A:2833:G:N1	7:A:2837:G:O6	2.53	0.42
7:A:3052:C:N3	7:A:3065:G:N2	2.67	0.42
7:A:3052:C:OP1	19:N:42:ARG:NH2	2.53	0.42
35:d:16:ARG:NH1	35:d:31:TYR:HB3	2.35	0.42
3:2:40:LYS:NZ	7:A:557:G:OP2	2.40	0.42
7:A:381:A:N6	7:A:382:A:N1	2.68	0.42
7:A:622:U:O4	7:A:661:G:O6	2.38	0.42
7:A:1614:A:C6	7:A:1615:G:C8	3.07	0.42
32:a:969:G:N2	32:a:1354:C:O2	2.53	0.42
32:a:1120:C:N4	32:a:1136:G:O6	2.53	0.42
40:i:115:ASP:O	40:i:119:LEU:N	2.41	0.42
7:A:1666:C:O2'	7:A:1806:A:OP2	2.36	0.42
7:A:2098:U:O4	7:A:2116:G:O6	2.38	0.42
13:G:150:ARG:C	13:G:152:LEU:H	2.27	0.42
21:P:8:ASP:O	21:P:11:SER:OG	2.33	0.42
7:A:1283:C:OP1	22:Q:92:ARG:NH2	2.53	0.41
7:A:1484:A:OP2	7:A:1508:G:N1	2.52	0.41
32:a:412:G:H5'	32:a:413:A:H5''	2.01	0.41
32:a:477:U:O2'	32:a:478:A:O5'	2.38	0.41
32:a:900:A:H2'	32:a:901:A:O4'	2.20	0.41
34:c:19:LYS:N	45:n:51:GLY:O	2.51	0.41
41:j:66:GLU:OE2	41:j:68:ARG:NE	2.45	0.41
4:3:42:ARG:NE	7:A:2589:G:O6	2.45	0.41
7:A:383:G:OP2	26:U:99:LYS:NZ	2.50	0.41
7:A:1116:C:O2'	7:A:1129:A:N3	2.51	0.41
32:a:727:U:O2'	37:f:90:VAL:O	2.31	0.41
32:a:1296:G:O6	32:a:1323:G:O2'	2.37	0.41
7:A:1197:G:N2	7:A:1202:A:N7	2.69	0.41
7:A:1707:A:H2'	7:A:1708:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2924:G:N1	7:A:2962:C:O2	2.53	0.41
16:K:120:GLU:OE2	21:P:62:LYS:NZ	2.44	0.41
32:a:573:U:OP2	32:a:749:G:N1	2.45	0.41
32:a:1068:G:N2	32:a:1071:A:OP2	2.44	0.41
7:A:293:G:N1	7:A:294:G:O6	2.53	0.41
7:A:1622:G:C2'	7:A:1623:G:O4'	2.68	0.41
7:A:2087:A:N7	7:A:2127:A:N6	2.68	0.41
27:V:138:ILE:H	27:V:139:PRO:HD2	1.85	0.41
30:Y:14:THR:OG1	30:Y:15:ASP:N	2.50	0.41
32:a:130:G:H1	47:p:1:MET:H3	1.67	0.41
32:a:179:G:N2	32:a:222:G:O2'	2.53	0.41
32:a:451:A:H2'	32:a:452:G:O4'	2.21	0.41
32:a:1398:G:H22	32:a:1489:C:N4	2.09	0.41
7:A:2705:C:H2'	7:A:2706:A:H5'	2.03	0.41
10:D:76:ASN:HD22	10:D:76:ASN:C	2.29	0.41
19:N:63:ARG:HG2	19:N:80:PHE:CE2	2.56	0.41
32:a:891:G:N2	32:a:894:A:OP2	2.49	0.41
7:A:803:G:H5''	11:E:83:GLY:HA3	2.02	0.41
7:A:1153:G:OP2	7:A:1154:G:O2'	2.23	0.41
32:a:156:A:H2'	32:a:157:A:O4'	2.20	0.41
32:a:379:G:N2	32:a:382:A:OP2	2.51	0.41
32:a:1058:A:N1	32:a:1099:G:O2'	2.53	0.41
32:a:102:G:H2'	32:a:103:A:O4'	2.21	0.41
32:a:966:G:H4'	41:j:57:LYS:HB3	2.03	0.41
32:a:1308:G:N2	32:a:1311:A:O5'	2.47	0.41
38:g:125:LEU:O	38:g:129:ASN:ND2	2.54	0.41
51:t:6:SER:O	51:t:7:GLN:NE2	2.53	0.41
7:A:876:U:OP2	7:A:2849:U:O2'	2.38	0.41
7:A:1595:C:N4	7:A:1596:U:O4	2.54	0.41
13:G:59:GLU:O	13:G:61:ARG:N	2.46	0.41
32:a:725:G:O3'	49:r:69:LYS:NZ	2.54	0.41
32:a:998:A:C5	32:a:999:C:C2	3.09	0.41
36:e:130:ALA:O	36:e:133:GLY:N	2.54	0.41
7:A:472:C:C2	7:A:480:A:N6	2.88	0.41
7:A:814:A:O2'	7:A:902:U:O4	2.31	0.41
7:A:1635:C:H2'	7:A:1636:U:C6	2.55	0.41
7:A:2345:U:O4	7:A:2417:U:H2'	2.21	0.41
32:a:513:C:OP2	43:l:66:TYR:OH	2.38	0.41
32:a:830:U:O4	32:a:840:G:O6	2.38	0.41
32:a:893:A:H2'	32:a:894:A:O4'	2.20	0.41
32:a:942:A:OP2	44:m:106:ASN:ND2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1210:C:H2'	32:a:1211:A:C8	2.56	0.41
32:a:1489:C:C4	32:a:1490:G:C2	3.08	0.41
7:A:945:C:N4	7:A:1323:G:O6	2.54	0.41
7:A:2213:G:O4'	52:x:27:GLN:NE2	2.54	0.41
7:A:2355:U:O4	7:A:2385:G:N2	2.46	0.41
32:a:264:G:H4'	48:q:120:LEU:HA	2.03	0.41
32:a:406:G:O4'	35:d:111:GLN:NE2	2.53	0.41
38:g:111:ARG:O	38:g:113:GLU:N	2.54	0.41
41:j:68:ARG:NH1	45:n:57:GLN:OE1	2.54	0.41
7:A:636:U:OP2	7:A:637:C:N4	2.52	0.40
7:A:1343:G:N2	7:A:1367:G:O2'	2.54	0.40
7:A:1622:G:H2'	7:A:1623:G:O4'	2.20	0.40
13:G:56:PRO:HB2	13:G:57:ASP:H	1.69	0.40
34:c:39:ARG:NH2	45:n:52:GLU:OE1	2.54	0.40
36:e:188:ARG:NH1	39:h:43:GLU:OE1	2.52	0.40
40:i:45:GLY:C	40:i:81:SER:HG	2.20	0.40
7:A:844:A:HO2'	7:A:845:A:P	2.38	0.40
7:A:1484:A:N7	7:A:1508:G:N2	2.70	0.40
7:A:2624:U:O2'	28:W:56:ASP:OD1	2.39	0.40
7:A:2826:G:O6	7:A:2845:G:N1	2.54	0.40
32:a:721:G:H21	32:a:757:A:H5'	1.85	0.40
46:o:36:ILE:O	46:o:40:THR:CB	2.68	0.40
7:A:672:G:N2	7:A:2736:C:O2'	2.53	0.40
32:a:1102:A:N1	34:c:177:THR:OG1	2.47	0.40
2:1:27:LYS:CE	2:1:31:ASN:HD22	2.34	0.40
7:A:84:A:N1	7:A:99:G:O2'	2.52	0.40
7:A:1540:G:N2	7:A:1828:C:C2	2.81	0.40
7:A:3044:A:N6	7:A:3126:A:N7	2.69	0.40
32:a:76:G:H2'	32:a:77:G:O4'	2.21	0.40
32:a:193:U:OP1	48:q:127:ARG:NH1	2.54	0.40
32:a:548:G:H2'	32:a:549:G:O4'	2.22	0.40
32:a:578:G:N1	32:a:745:C:OP2	2.51	0.40
32:a:1488:U:C2	32:a:1489:C:C5	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	51/57 (90%)	49 (96%)	2 (4%)	0	100	100
2	1	46/55 (84%)	42 (91%)	3 (6%)	1 (2%)	5	31
3	2	40/47 (85%)	39 (98%)	1 (2%)	0	100	100
4	3	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
5	4	35/37 (95%)	26 (74%)	9 (26%)	0	100	100
6	6	43/80 (54%)	33 (77%)	10 (23%)	0	100	100
9	C	270/280 (96%)	248 (92%)	21 (8%)	1 (0%)	30	65
10	D	211/217 (97%)	182 (86%)	27 (13%)	2 (1%)	14	48
11	E	205/223 (92%)	181 (88%)	23 (11%)	1 (0%)	24	60
12	F	168/187 (90%)	152 (90%)	16 (10%)	0	100	100
13	G	172/179 (96%)	153 (89%)	16 (9%)	3 (2%)	7	36
14	H	45/152 (30%)	38 (84%)	7 (16%)	0	100	100
15	J	144/147 (98%)	135 (94%)	9 (6%)	0	100	100
16	K	119/122 (98%)	110 (92%)	9 (8%)	0	100	100
17	L	140/146 (96%)	130 (93%)	10 (7%)	0	100	100
18	M	132/138 (96%)	116 (88%)	16 (12%)	0	100	100
19	N	114/180 (63%)	105 (92%)	9 (8%)	0	100	100
20	O	114/122 (93%)	101 (89%)	13 (11%)	0	100	100
21	P	110/113 (97%)	96 (87%)	13 (12%)	1 (1%)	14	48
22	Q	120/129 (93%)	112 (93%)	7 (6%)	1 (1%)	16	52
23	R	96/104 (92%)	87 (91%)	8 (8%)	1 (1%)	12	45
24	S	111/197 (56%)	106 (96%)	5 (4%)	0	100	100
25	T	96/100 (96%)	88 (92%)	8 (8%)	0	100	100
26	U	86/105 (82%)	73 (85%)	12 (14%)	1 (1%)	10	42
27	V	175/215 (81%)	146 (83%)	26 (15%)	3 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	W	72/86 (84%)	57 (79%)	14 (19%)	1 (1%)	9	39
29	X	61/64 (95%)	55 (90%)	5 (8%)	1 (2%)	7	37
30	Y	63/77 (82%)	60 (95%)	3 (5%)	0	100	100
31	Z	57/65 (88%)	51 (90%)	6 (10%)	0	100	100
34	c	205/274 (75%)	189 (92%)	15 (7%)	1 (0%)	24	60
35	d	199/201 (99%)	180 (90%)	17 (8%)	2 (1%)	12	45
36	e	158/220 (72%)	138 (87%)	18 (11%)	2 (1%)	9	41
37	f	93/96 (97%)	81 (87%)	12 (13%)	0	100	100
38	g	150/156 (96%)	126 (84%)	22 (15%)	2 (1%)	9	41
39	h	128/132 (97%)	113 (88%)	13 (10%)	2 (2%)	7	37
40	i	125/151 (83%)	104 (83%)	18 (14%)	3 (2%)	4	30
41	j	97/101 (96%)	91 (94%)	5 (5%)	1 (1%)	12	45
42	k	115/139 (83%)	106 (92%)	9 (8%)	0	100	100
43	l	121/124 (98%)	98 (81%)	23 (19%)	0	100	100
44	m	111/124 (90%)	102 (92%)	8 (7%)	1 (1%)	14	48
45	n	57/61 (93%)	44 (77%)	12 (21%)	1 (2%)	6	34
46	o	85/89 (96%)	79 (93%)	6 (7%)	0	100	100
47	p	83/162 (51%)	75 (90%)	8 (10%)	0	100	100
48	q	92/135 (68%)	76 (83%)	13 (14%)	3 (3%)	3	24
49	r	61/84 (73%)	53 (87%)	8 (13%)	0	100	100
50	s	79/93 (85%)	73 (92%)	4 (5%)	2 (2%)	4	29
51	t	80/86 (93%)	77 (96%)	3 (4%)	0	100	100
52	x	29/33 (88%)	28 (97%)	1 (3%)	0	100	100
All	All	5224/6149 (85%)	4659 (89%)	528 (10%)	37 (1%)	20	54

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	G	56	PRO
13	G	58	ASP
27	V	47	LEU
9	C	108	PRO
22	Q	118	PRO
23	R	82	LYS

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Mol	Chain	Res	Type
27	V	114	GLY
28	W	80	ILE
29	X	47	LYS
35	d	32	PRO
36	e	193	GLU
38	g	85	TYR
39	h	54	ALA
39	h	99	GLY
44	m	67	GLU
48	q	124	LYS
10	D	91	ALA
10	D	92	ALA
13	G	57	ASP
26	U	89	GLU
40	i	88	LEU
48	q	49	PRO
50	s	82	GLY
11	E	82	GLN
48	q	46	LYS
34	c	97	GLN
35	d	30	PRO
40	i	147	GLN
50	s	80	PHE
2	l	31	ASN
36	e	132	PRO
45	n	30	PRO
27	V	60	GLY
38	g	17	VAL
40	i	129	PRO
41	j	79	PRO
21	P	104	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	43/47 (92%)	43 (100%)	0	100	100
2	1	45/51 (88%)	45 (100%)	0	100	100
3	2	36/40 (90%)	36 (100%)	0	100	100
4	3	53/54 (98%)	53 (100%)	0	100	100
5	4	35/35 (100%)	35 (100%)	0	100	100
6	6	40/66 (61%)	40 (100%)	0	100	100
9	C	212/219 (97%)	212 (100%)	0	100	100
10	D	163/166 (98%)	163 (100%)	0	100	100
11	E	159/172 (92%)	159 (100%)	0	100	100
12	F	139/155 (90%)	139 (100%)	0	100	100
13	G	143/147 (97%)	143 (100%)	0	100	100
14	H	36/121 (30%)	36 (100%)	0	100	100
15	J	120/121 (99%)	120 (100%)	0	100	100
16	K	100/101 (99%)	100 (100%)	0	100	100
17	L	106/110 (96%)	106 (100%)	0	100	100
18	M	110/114 (96%)	110 (100%)	0	100	100
19	N	94/139 (68%)	94 (100%)	0	100	100
20	O	88/93 (95%)	88 (100%)	0	100	100
21	P	98/99 (99%)	98 (100%)	0	100	100
22	Q	95/99 (96%)	95 (100%)	0	100	100
23	R	79/83 (95%)	79 (100%)	0	100	100
24	S	87/140 (62%)	87 (100%)	0	100	100
25	T	82/83 (99%)	82 (100%)	0	100	100
26	U	77/88 (88%)	77 (100%)	0	100	100
27	V	142/164 (87%)	142 (100%)	0	100	100
28	W	54/62 (87%)	54 (100%)	0	100	100
29	X	52/52 (100%)	52 (100%)	0	100	100
30	Y	58/66 (88%)	58 (100%)	0	100	100
31	Z	51/55 (93%)	51 (100%)	0	100	100
34	c	170/210 (81%)	170 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	d	177/177 (100%)	177 (100%)	0	100	100
36	e	114/159 (72%)	114 (100%)	0	100	100
37	f	84/85 (99%)	84 (100%)	0	100	100
38	g	127/131 (97%)	127 (100%)	0	100	100
39	h	106/108 (98%)	106 (100%)	0	100	100
40	i	102/120 (85%)	102 (100%)	0	100	100
41	j	89/90 (99%)	89 (100%)	0	100	100
42	k	90/107 (84%)	90 (100%)	0	100	100
43	l	105/105 (100%)	105 (100%)	0	100	100
44	m	96/104 (92%)	96 (100%)	0	100	100
45	n	46/47 (98%)	46 (100%)	0	100	100
46	o	77/79 (98%)	77 (100%)	0	100	100
47	p	72/125 (58%)	72 (100%)	0	100	100
48	q	84/105 (80%)	84 (100%)	0	100	100
49	r	53/72 (74%)	53 (100%)	0	100	100
50	s	73/85 (86%)	73 (100%)	0	100	100
51	t	62/65 (95%)	62 (100%)	0	100	100
52	x	29/31 (94%)	29 (100%)	0	100	100
All	All	4353/4947 (88%)	4353 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	31	ASN
4	3	35	HIS
5	4	34	GLN
9	C	96	HIS
9	C	227	ASN
10	D	76	ASN
10	D	139	HIS
13	G	144	GLN
15	J	130	HIS
17	L	44	GLN

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Mol	Chain	Res	Type
18	M	9	HIS
18	M	13	HIS
20	O	36	HIS
21	P	50	GLN
22	Q	9	ASN
23	R	86	HIS
25	T	27	ASN
25	T	41	GLN
26	U	44	HIS
26	U	67	HIS
27	V	8	GLN
27	V	58	HIS
27	V	62	ASN
28	W	46	HIS
30	Y	35	GLN
34	c	138	GLN
35	d	35	GLN
35	d	77	GLN
35	d	111	GLN
35	d	119	ASN
36	e	169	HIS
38	g	14	ASN
38	g	142	HIS
40	i	28	GLN
40	i	52	ASN
41	j	64	HIS
43	l	29	GLN
46	o	46	HIS
49	r	60	HIS
50	s	83	HIS
51	t	70	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	a	1518/1537 (98%)	114 (7%)	0
7	A	3116/3138 (99%)	273 (8%)	10 (0%)
8	B	114/115 (99%)	1 (0%)	0
All	All	4748/4790 (99%)	388 (8%)	10 (0%)

All (388) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	34	U
7	A	50	U
7	A	71	A
7	A	74	U
7	A	75	G
7	A	85	G
7	A	101	G
7	A	118	A
7	A	120	U
7	A	183	A
7	A	198	A
7	A	218	A
7	A	224	A
7	A	231	U
7	A	232	G
7	A	250	G
7	A	268	G
7	A	287	G
7	A	290	A
7	A	293	G
7	A	301	G
7	A	304	G
7	A	319	U
7	A	371	U
7	A	384	U
7	A	394	U
7	A	405	A
7	A	413	A
7	A	446	A
7	A	447	G
7	A	448	U
7	A	461	G
7	A	475	G
7	A	500	G
7	A	501	A
7	A	533	C
7	A	540	C
7	A	570	G
7	A	593	A
7	A	596	A
7	A	597	C
7	A	619	C
7	A	620	C

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Mol	Chain	Res	Type
7	A	621	G
7	A	645	G
7	A	665	G
7	A	677	A
7	A	695	G
7	A	706	A
7	A	718	G
7	A	719	U
7	A	720	G
7	A	741	A
7	A	742	G
7	A	749	U
7	A	773	C
7	A	780	G
7	A	781	A
7	A	782	A
7	A	783	U
7	A	815	U
7	A	816	C
7	A	845	A
7	A	859	C
7	A	894	G
7	A	906	G
7	A	911	A
7	A	912	A
7	A	913	G
7	A	914	G
7	A	915	C
7	A	922	A
7	A	931	A
7	A	934	G
7	A	941	C
7	A	956	U
7	A	975	G
7	A	1039	A
7	A	1059	A
7	A	1074	G
7	A	1089	G
7	A	1097	C
7	A	1103	A
7	A	1125	G
7	A	1142	G

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Mol	Chain	Res	Type
7	A	1151	G
7	A	1155	G
7	A	1200	G
7	A	1207	C
7	A	1217	A
7	A	1240	A
7	A	1241	G
7	A	1242	U
7	A	1243	G
7	A	1262	A
7	A	1264	C
7	A	1271	C
7	A	1273	A
7	A	1306	G
7	A	1386	U
7	A	1387	G
7	A	1403	A
7	A	1432	A
7	A	1460	U
7	A	1496	A
7	A	1515	A
7	A	1517	C
7	A	1542	G
7	A	1550	C
7	A	1551	C
7	A	1552	G
7	A	1558	A
7	A	1561	C
7	A	1567	U
7	A	1568	A
7	A	1580	A
7	A	1589	C
7	A	1590	G
7	A	1591	A
7	A	1592	U
7	A	1601	U
7	A	1606	G
7	A	1609	U
7	A	1615	G
7	A	1622	G
7	A	1625	U
7	A	1646	G

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Mol	Chain	Res	Type
7	A	1653	A
7	A	1654	G
7	A	1657	A
7	A	1660	G
7	A	1691	G
7	A	1698	C
7	A	1705	G
7	A	1720	G
7	A	1727	A
7	A	1767	A
7	A	1774	U
7	A	1803	A
7	A	1821	G
7	A	1822	C
7	A	1830	C
7	A	1843	A
7	A	1851	A
7	A	1881	U
7	A	1883	C
7	A	1888	U
7	A	1909	G
7	A	1950	A
7	A	1963	U
7	A	1964	U
7	A	1998	U
7	A	2007	A
7	A	2015	C
7	A	2016	U
7	A	2034	C
7	A	2043	A
7	A	2107	A
7	A	2109	G
7	A	2123	A
7	A	2144	G
7	A	2145	G
7	A	2151	A
7	A	2157	A
7	A	2168	G
7	A	2175	A
7	A	2176	A
7	A	2193	U
7	A	2201	U

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Mol	Chain	Res	Type
7	A	2205	C
7	A	2208	A
7	A	2209	U
7	A	2210	G
7	A	2231	U
7	A	2251	A
7	A	2260	U
7	A	2270	G
7	A	2294	G
7	A	2298	A
7	A	2299	G
7	A	2300	A
7	A	2313	C
7	A	2314	A
7	A	2330	G
7	A	2333	G
7	A	2343	G
7	A	2347	G
7	A	2348	U
7	A	2350	U
7	A	2351	A
7	A	2353	G
7	A	2355	U
7	A	2356	A
7	A	2357	G
7	A	2358	G
7	A	2360	G
7	A	2361	G
7	A	2362	G
7	A	2364	G
7	A	2365	A
7	A	2369	U
7	A	2371	A
7	A	2377	C
7	A	2378	G
7	A	2382	C
7	A	2383	C
7	A	2384	A
7	A	2385	G
7	A	2387	U
7	A	2389	G
7	A	2391	G

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Mol	Chain	Res	Type
7	A	2393	G
7	A	2394	G
7	A	2395	A
7	A	2396	G
7	A	2398	C
7	A	2400	U
7	A	2401	U
7	A	2402	G
7	A	2403	U
7	A	2404	U
7	A	2405	G
7	A	2408	A
7	A	2409	U
7	A	2413	A
7	A	2414	C
7	A	2417	U
7	A	2422	G
7	A	2424	A
7	A	2447	U
7	A	2463	A
7	A	2464	C
7	A	2476	G
7	A	2477	G
7	A	2516	A
7	A	2521	C
7	A	2525	A
7	A	2543	A
7	A	2563	G
7	A	2572	C
7	A	2573	A
7	A	2583	G
7	A	2585	C
7	A	2621	G
7	A	2623	A
7	A	2640	C
7	A	2663	A
7	A	2664	A
7	A	2679	C
7	A	2685	G
7	A	2686	A
7	A	2714	A
7	A	2729	U

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Mol	Chain	Res	Type
7	A	2730	U
7	A	2742	U
7	A	2744	U
7	A	2756	A
7	A	2758	C
7	A	2805	G
7	A	2851	U
7	A	2868	A
7	A	2903	A
7	A	2929	C
7	A	2952	G
7	A	2964	C
7	A	2971	U
7	A	2995	A
7	A	3016	A
7	A	3107	A
7	A	3121	G
7	A	3126	A
7	A	3128	A
7	A	3129	A
8	B	115	A
32	a	9	G
32	a	11	A
32	a	16	U
32	a	35	A
32	a	42	G
32	a	50	C
32	a	51	U
32	a	54	A
32	a	84	C
32	a	90	U
32	a	115	A
32	a	116	C
32	a	125	G
32	a	127	U
32	a	130	G
32	a	175	A
32	a	176	U
32	a	177	A
32	a	178	G
32	a	194	G
32	a	195	U

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Mol	Chain	Res	Type
32	a	206	A
32	a	207	A
32	a	247	C
32	a	249	U
32	a	265	G
32	a	266	C
32	a	278	A
32	a	279	C
32	a	280	G
32	a	288	G
32	a	327	U
32	a	328	A
32	a	329	C
32	a	351	C
32	a	366	U
32	a	397	C
32	a	405	G
32	a	410	A
32	a	411	U
32	a	412	G
32	a	413	A
32	a	421	C
32	a	422	G
32	a	428	U
32	a	436	U
32	a	437	U
32	a	447	A
32	a	460	U
32	a	475	G
32	a	477	U
32	a	478	A
32	a	509	C
32	a	518	G
32	a	522	U
32	a	523	A
32	a	524	A
32	a	538	A
32	a	564	A
32	a	567	A
32	a	568	G
32	a	624	G
32	a	633	A

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Mol	Chain	Res	Type
32	a	656	G
32	a	693	A
32	a	694	G
32	a	746	G
32	a	819	A
32	a	835	C
32	a	836	C
32	a	837	U
32	a	838	U
32	a	883	G
32	a	927	C
32	a	928	A
32	a	953	U
32	a	959	G
32	a	962	A
32	a	968	A
32	a	969	G
32	a	985	U
32	a	986	G
32	a	997	G
32	a	1018	U
32	a	1021	C
32	a	1022	U
32	a	1023	U
32	a	1044	G
32	a	1086	U
32	a	1092	A
32	a	1129	A
32	a	1131	G
32	a	1132	G
32	a	1151	U
32	a	1160	C
32	a	1175	U
32	a	1176	G
32	a	1188	A
32	a	1189	A
32	a	1205	A
32	a	1219	A
32	a	1230	A
32	a	1249	U
32	a	1250	G
32	a	1279	A

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Mol	Chain	Res	Type
32	a	1292	G
32	a	1356	A
32	a	1357	C
32	a	1391	A
32	a	1439	A
32	a	1485	A
32	a	1496	A
32	a	1522	G
32	a	1523	G

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	174	G
7	A	844	A
7	A	913	G
7	A	1567	U
7	A	1624	C
7	A	1653	A
7	A	2250	G
7	A	2364	G
7	A	2402	G
7	A	2902	G

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

5 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	$\# Z > 2$
33	MYN	b	4	33	8,11,12	9.00	6 (75%)	6,14,16	1.49	1 (16%)
33	DPP	b	5	33	4,5,6	0.95	0	1,5,7	0.02	0
33	UAL	b	3	33	6,8,9	3.73	5 (83%)	4,9,11	2.18	1 (25%)
33	DPP	b	2	33	4,5,6	0.49	0	1,5,7	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	KBE	b	1	33	8,8,9	1.24	1 (12%)	6,8,10	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	MYN	b	4	33	-	0/1/16/18	0/1/1/1
33	DPP	b	5	33	-	1/2/4/6	-
33	UAL	b	3	33	-	1/3/7/9	-
33	DPP	b	2	33	-	2/2/4/6	-
33	KBE	b	1	33	-	4/7/7/8	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	4	MYN	CZ-NE	18.54	1.52	1.34
33	b	4	MYN	CB-N1	11.35	1.62	1.47
33	b	4	MYN	CG-CB	-10.35	1.31	1.53
33	b	4	MYN	CD-NE	-5.99	1.34	1.46
33	b	3	UAL	C-CA	5.38	1.54	1.45
33	b	4	MYN	CZ-NZ	4.64	1.45	1.34
33	b	3	UAL	C1-N2	4.24	1.44	1.33
33	b	3	UAL	C1-N1	3.69	1.45	1.40
33	b	3	UAL	O2-C1	-3.38	1.19	1.24
33	b	3	UAL	CB-N1	3.25	1.44	1.35
33	b	4	MYN	CG-CD	2.40	1.59	1.52
33	b	1	KBE	CA-C	2.31	1.56	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	3	UAL	O-C-CA	-4.06	120.30	125.39
33	b	4	MYN	O-C-CA	-2.41	118.57	124.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	b	1	KBE	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
33	b	1	KBE	C-CA-CB-CG
33	b	2	DPP	N-CA-CB-NG
33	b	3	UAL	CA-CB-N1-C1
33	b	1	KBE	C-CA-CB-N
33	b	2	DPP	C-CA-CB-NG
33	b	5	DPP	C-CA-CB-NG
33	b	1	KBE	CE-CD-CG-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	b	4	MYN	2	0
33	b	5	DPP	1	0
33	b	2	DPP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

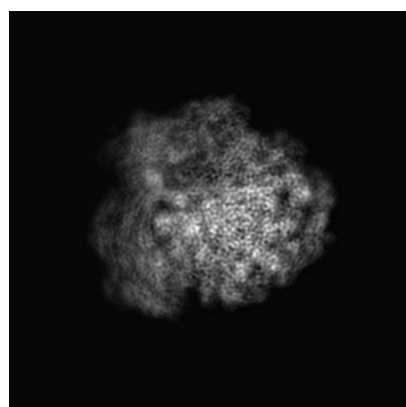
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8645. These allow visual inspection of the internal detail of the map and identification of artifacts.

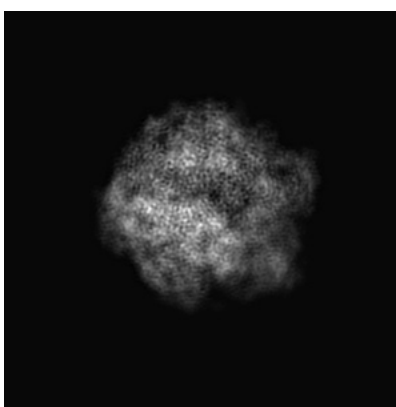
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

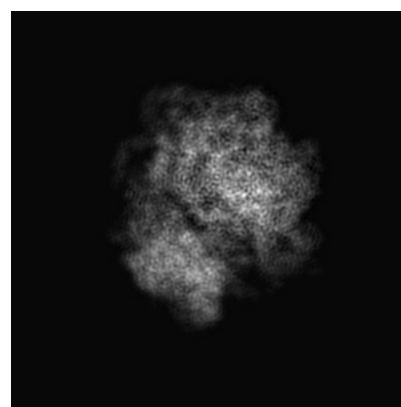
6.1.1 Primary map



X



Y

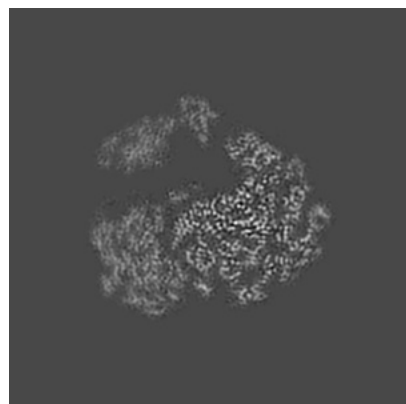


Z

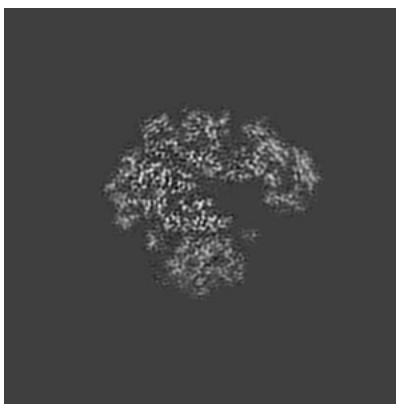
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

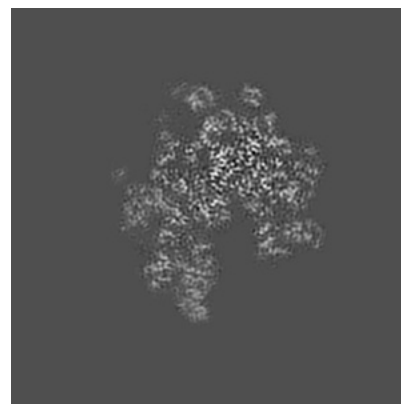
6.2.1 Primary map



X Index: 160



Y Index: 160

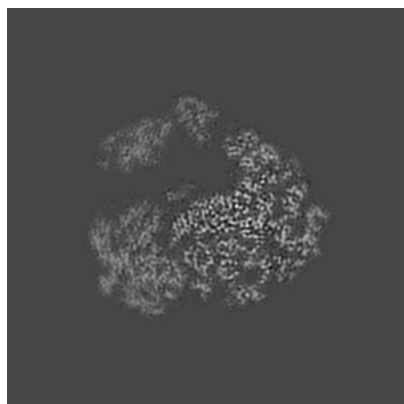


Z Index: 160

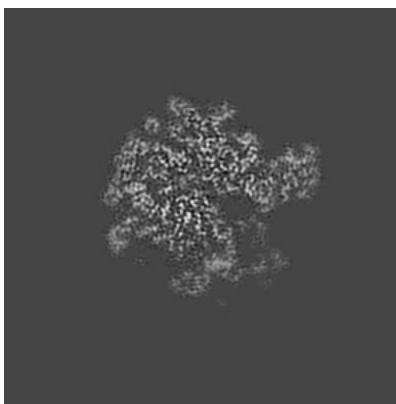
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

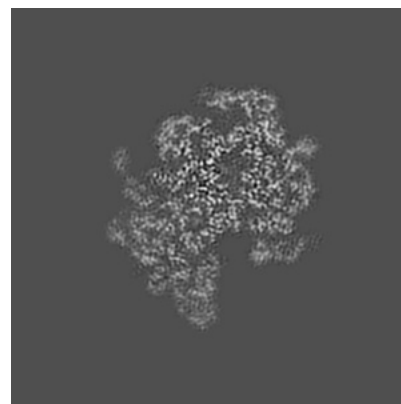
6.3.1 Primary map



X Index: 161



Y Index: 175

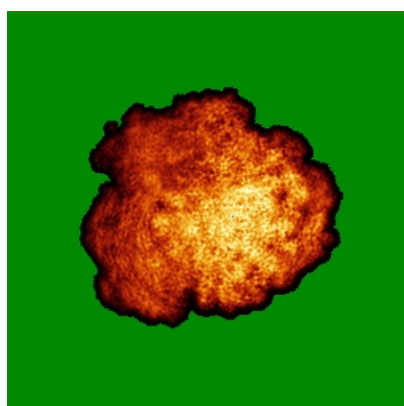


Z Index: 147

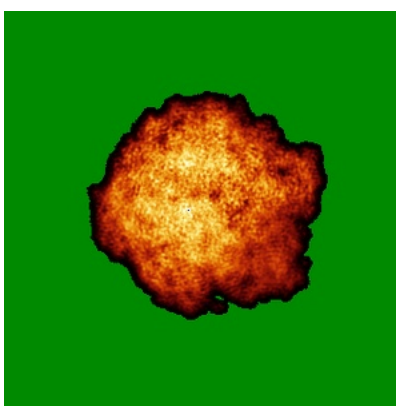
The images above show the largest variance slices of the map in three orthogonal directions.

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

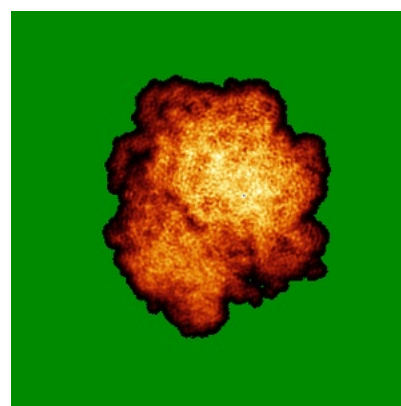
6.4.1 Primary map



X



Y

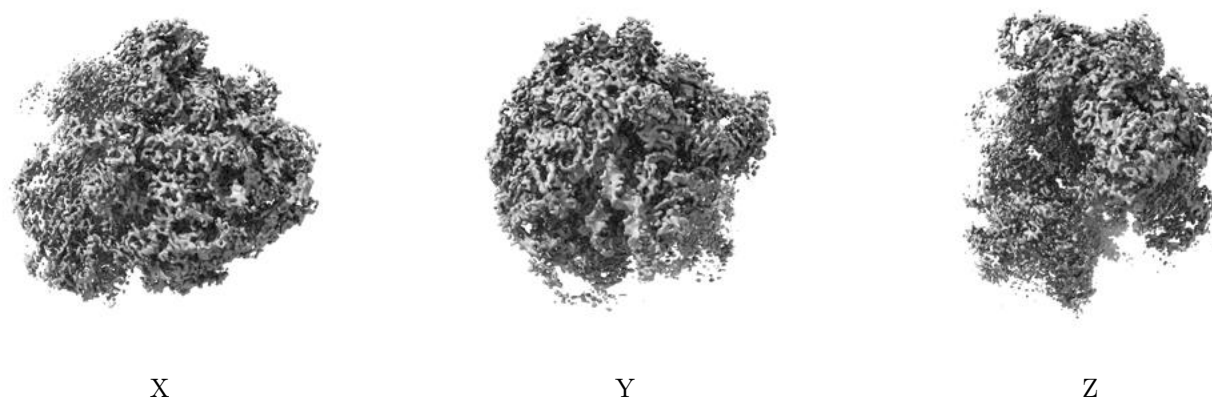


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

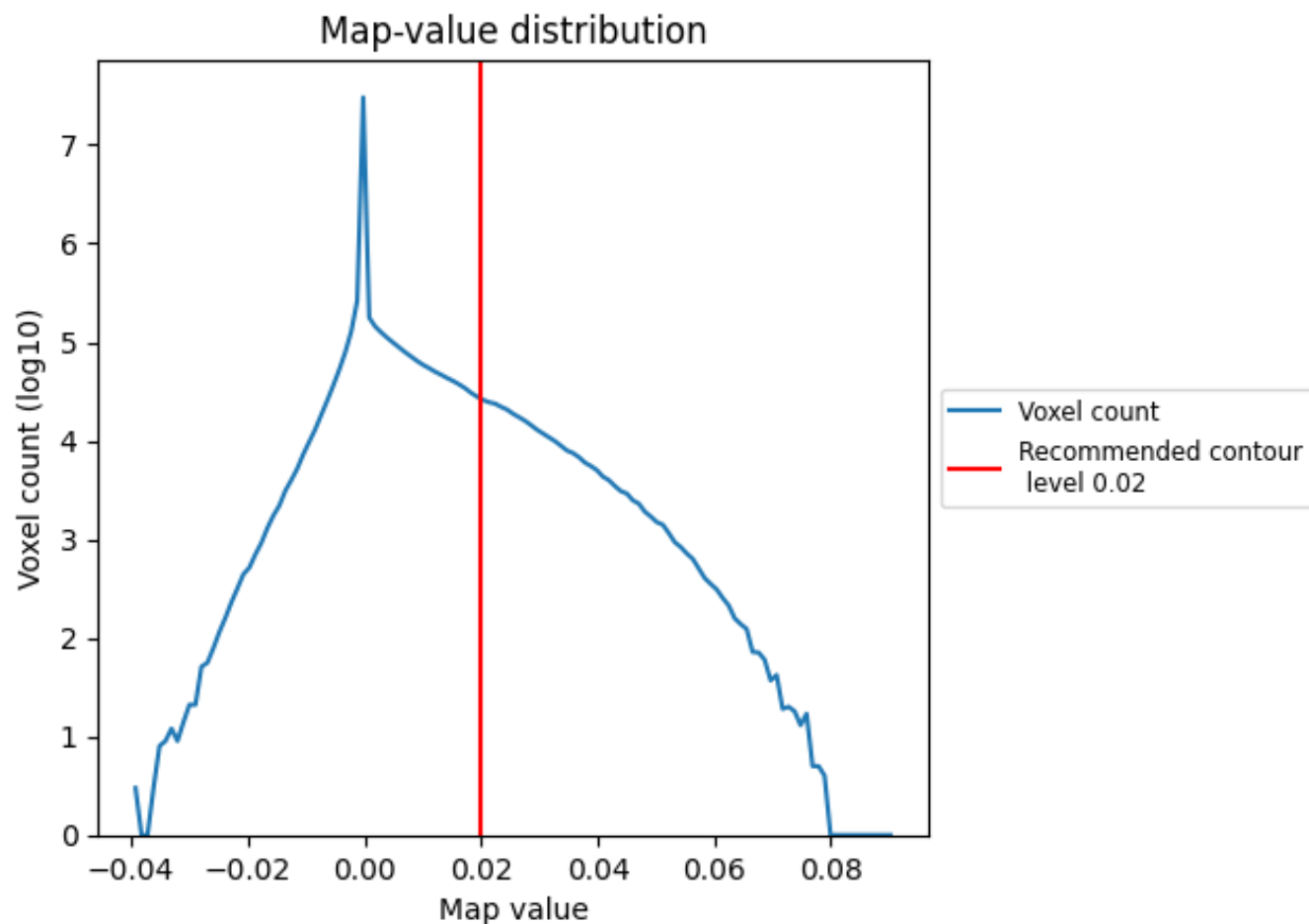
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

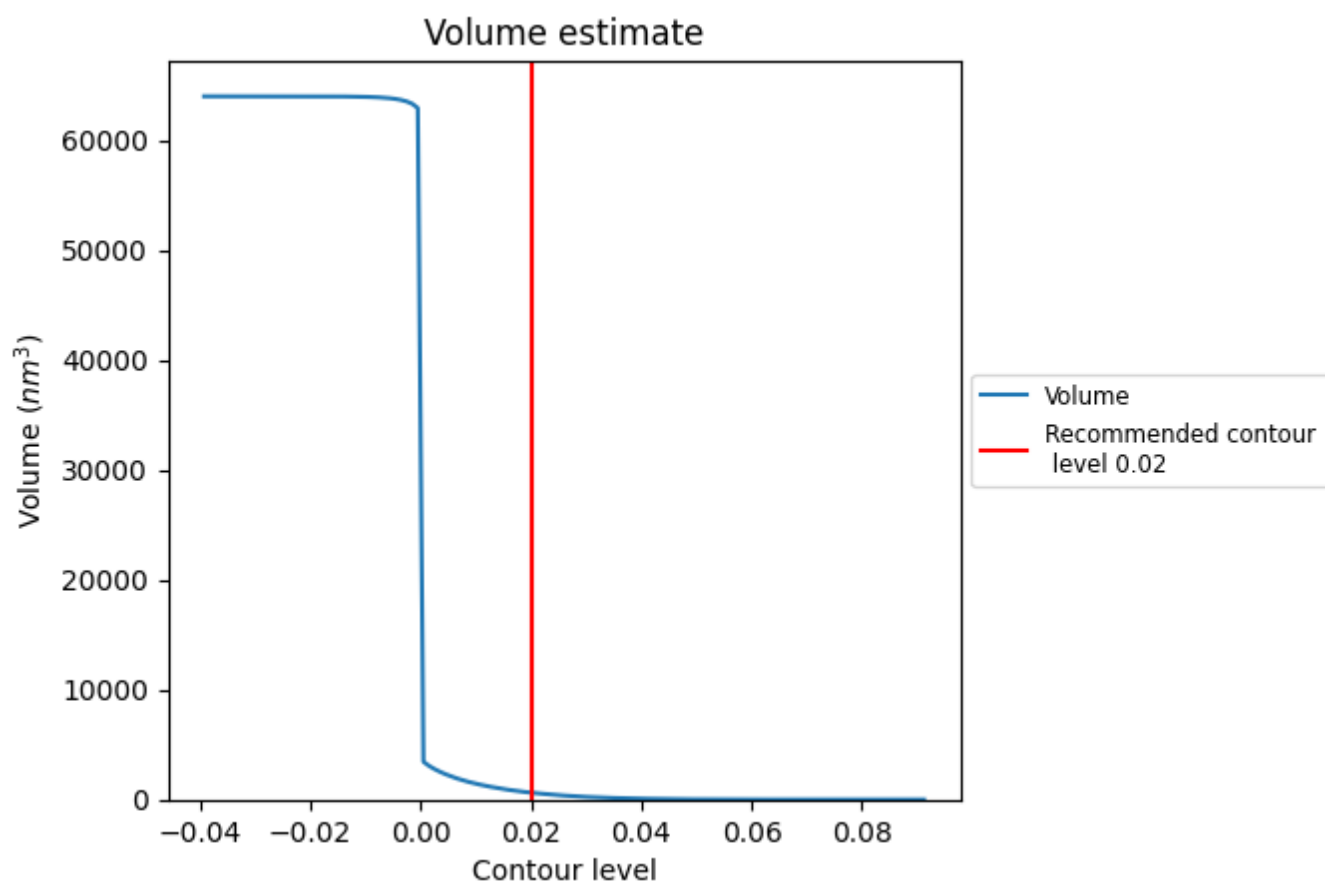
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

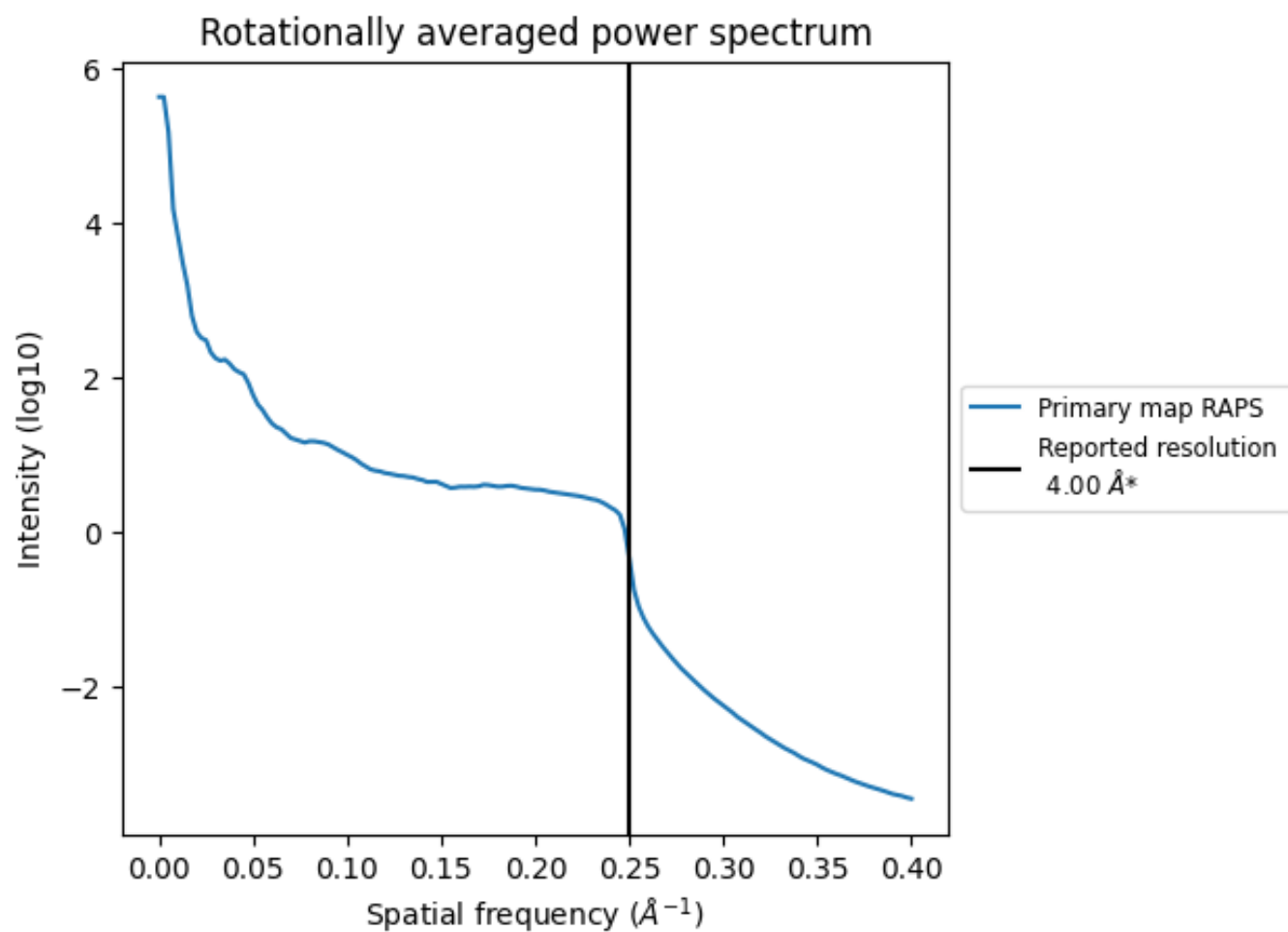
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 630 nm³; this corresponds to an approximate mass of 569 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 ⓘ

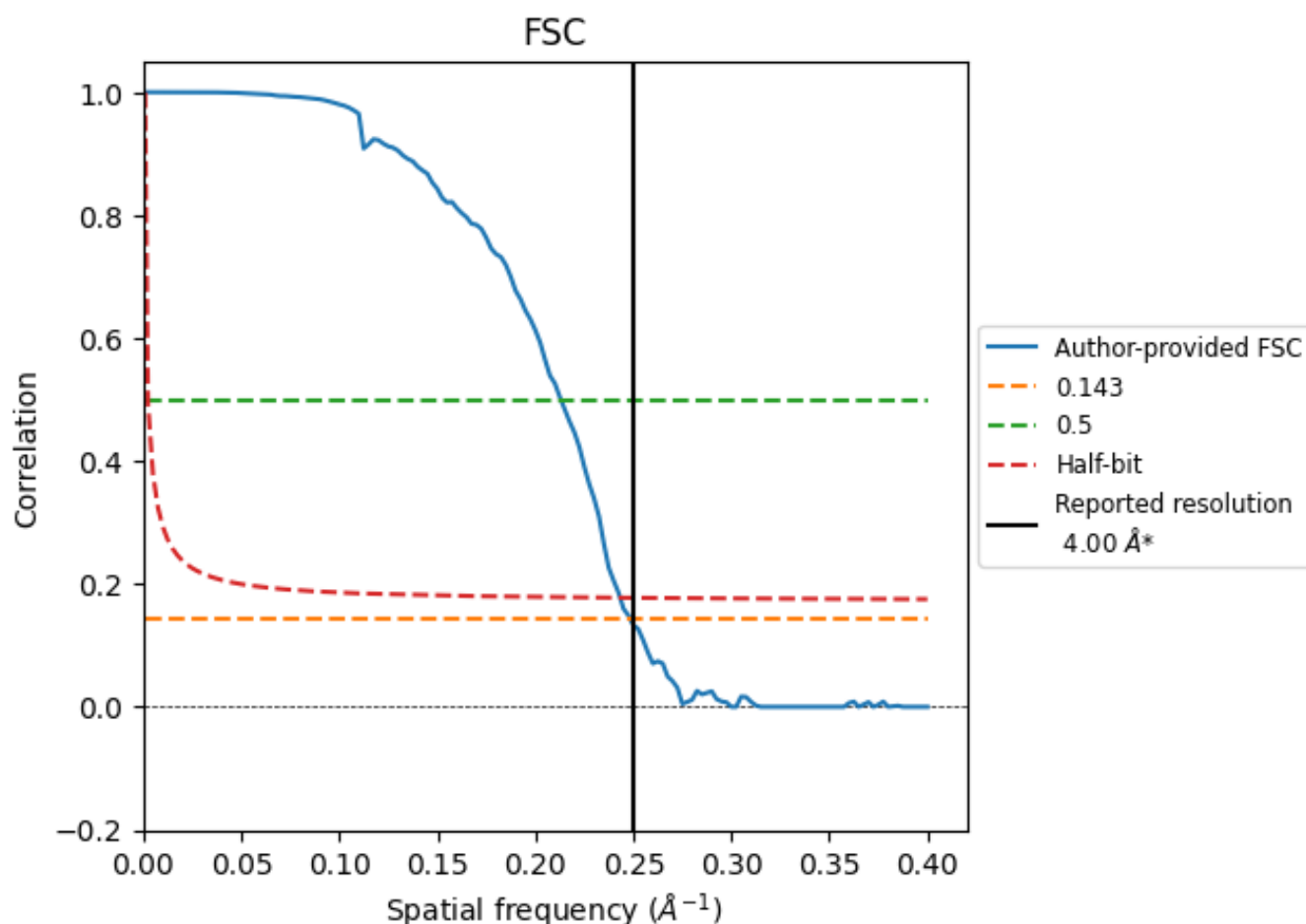


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

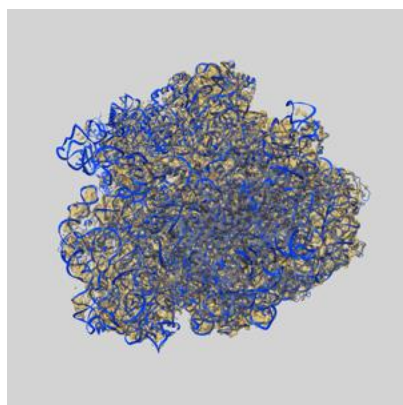
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.03	4.69	4.11
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

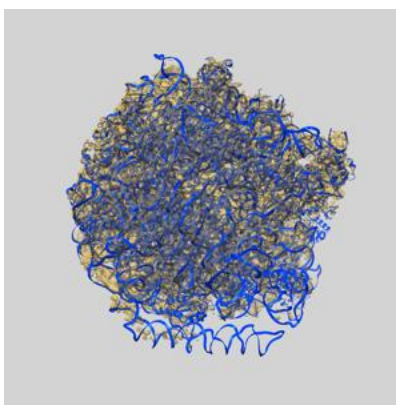
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8645 and PDB model 5V93. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

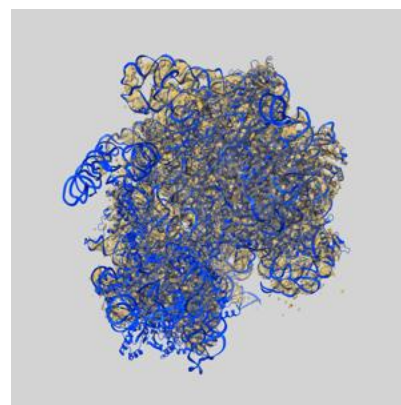
9.1 Map-model overlay [i](#)



X



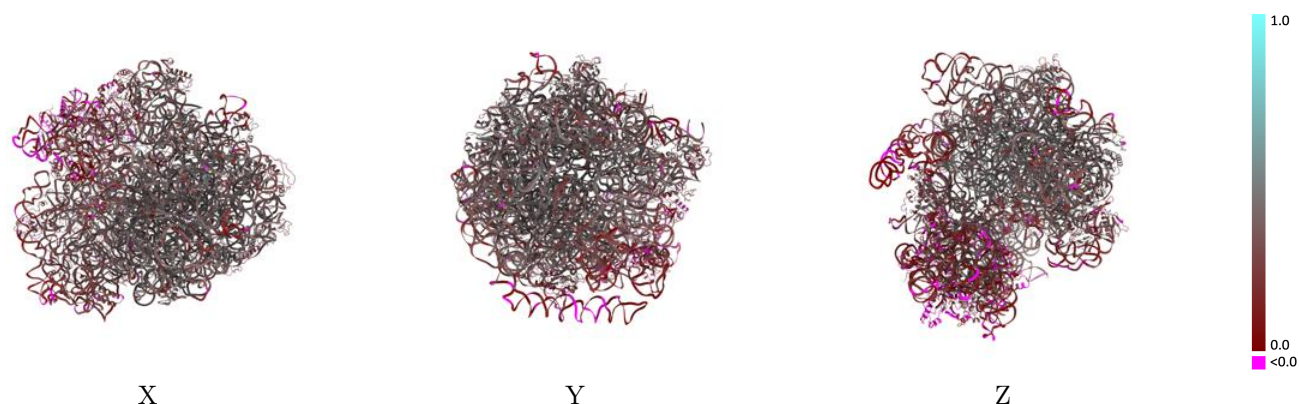
Y



Z

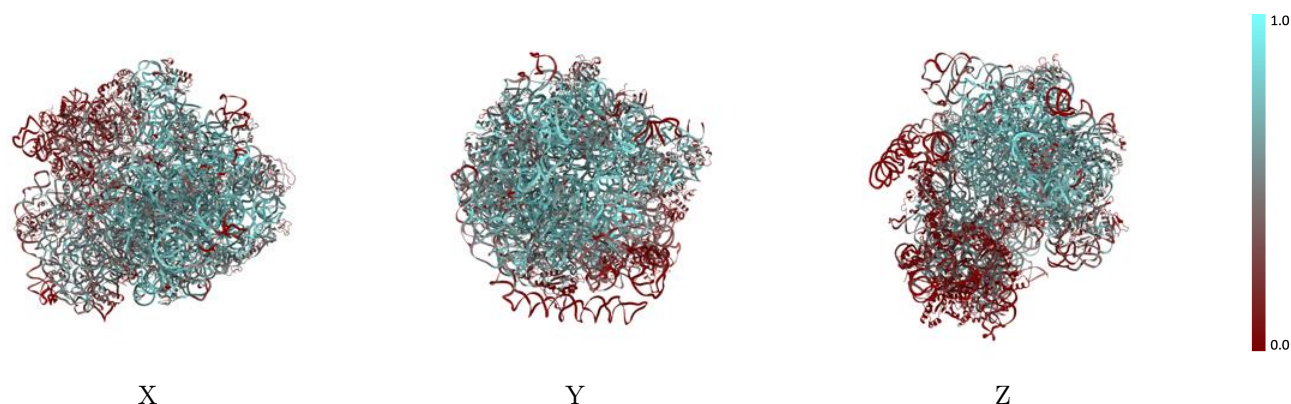
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



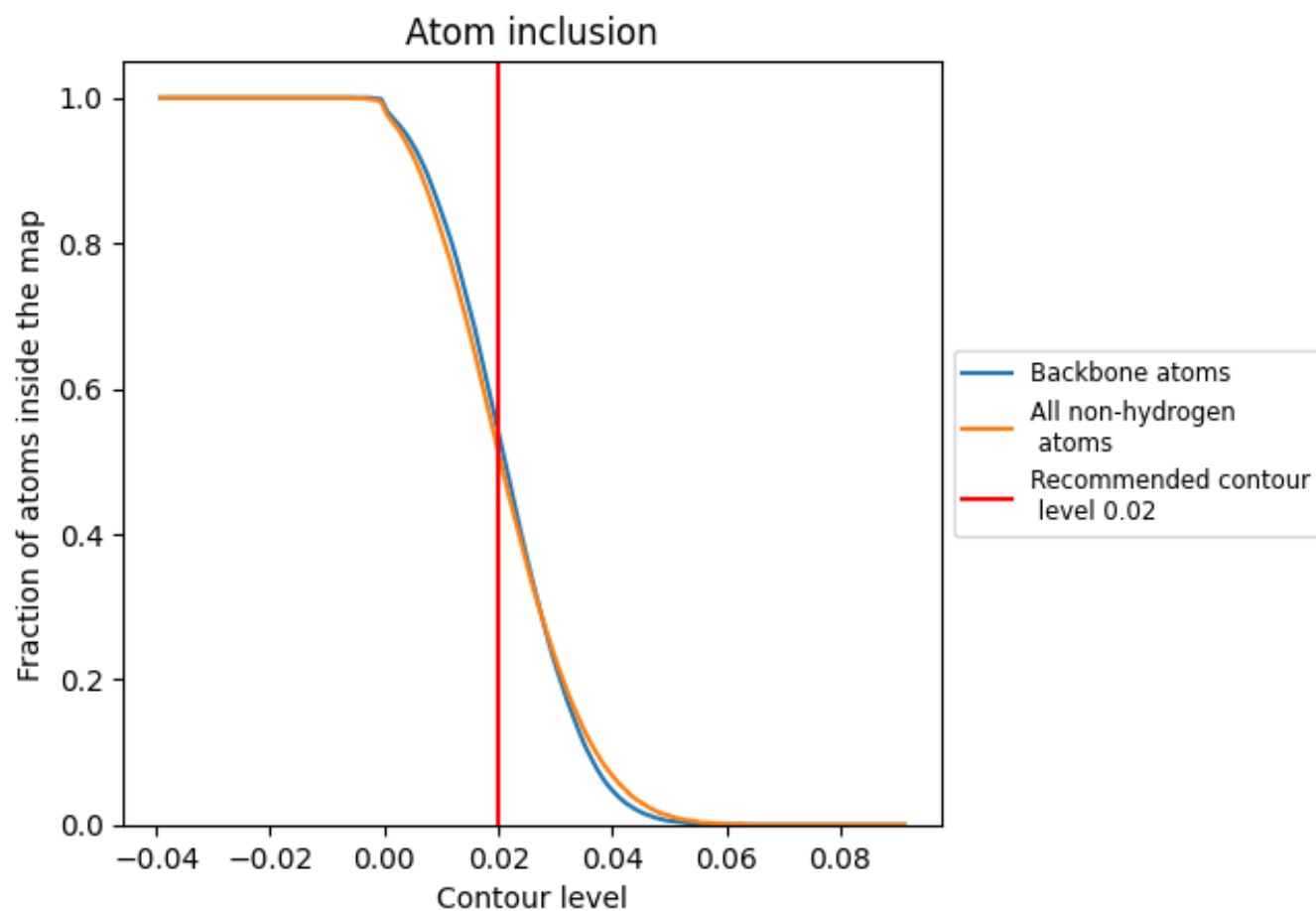
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 51% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5130	 0.3210
0	 0.4250	 0.3600
1	 0.5350	 0.3590
2	 0.6340	 0.4070
3	 0.5660	 0.3990
4	 0.4390	 0.3510
6	 0.0910	 0.2200
A	 0.6570	 0.3630
B	 0.6590	 0.3480
C	 0.5570	 0.4090
D	 0.4790	 0.3880
E	 0.4680	 0.3590
F	 0.2560	 0.2500
G	 0.2680	 0.2460
H	 0.2860	 0.3040
J	 0.4890	 0.3680
K	 0.4600	 0.3780
L	 0.4830	 0.3810
M	 0.4730	 0.3750
N	 0.5010	 0.3900
O	 0.3990	 0.3250
P	 0.3790	 0.3080
Q	 0.5670	 0.3850
R	 0.4130	 0.3680
S	 0.5370	 0.4020
T	 0.4290	 0.3670
U	 0.2940	 0.2910
V	 0.2430	 0.2840
W	 0.5610	 0.3990
X	 0.5160	 0.3840
Y	 0.4270	 0.3290
Z	 0.4970	 0.3880
a	 0.4450	 0.2670
b	 0.4570	 0.3910
c	 0.0250	 0.1190



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Chain	Atom inclusion	Q-score
d	 0.0990	 0.2030
e	 0.2600	 0.2930
f	 0.1760	 0.2570
g	 0.0690	 0.1210
h	 0.2600	 0.2900
i	 0.0860	 0.1390
j	 0.0420	 0.1090
k	 0.2000	 0.2630
l	 0.2620	 0.3030
m	 0.0500	 0.1350
n	 0.0470	 0.1870
o	 0.3110	 0.2850
p	 0.1960	 0.2400
q	 0.1790	 0.2420
r	 0.2390	 0.2460
s	 0.0430	 0.0960
t	 0.2580	 0.2440
x	 0.1940	 0.3030