



Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 03:28 pm GMT

PDB ID : 7ASP
EMDB ID : EMD-11903
Title : Staphylococcus aureus 70S after 50 minutes incubation at 37C
Authors : Camicata, G.; Bashan, A.; Yonath, A.
Deposited on : 2020-10-27
Resolution : 2.86 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

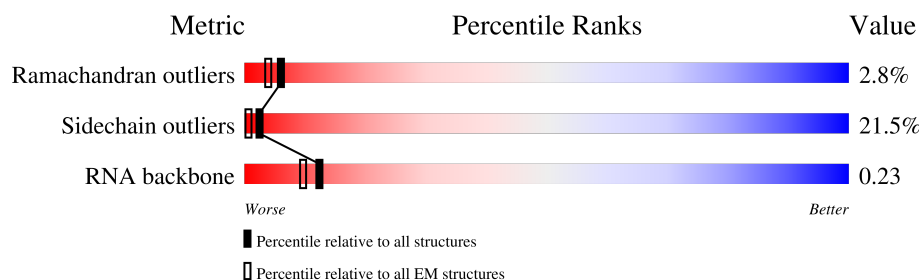
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	Y	2923	
2	X	1552	
3	3	114	
4	1	105	
4	A	105	
5	B	43	
6	2	64	
7	4	37	

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Mol	Chain	Length	Quality of chain
8	a	80	
9	b	114	
10	c	136	
11	C	274	
12	d	113	
13	D	215	
14	E	206	
15	e	60	
16	f	88	
17	g	83	
18	G	175	
19	H	145	
20	h	80	
21	I	122	
22	i	56	
23	j	78	
24	J	146	
25	k	202	
26	K	137	
27	L	120	
28	l	198	
29	m	156	
30	M	119	
31	n	95	
32	N	114	

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Mol	Chain	Length	Quality of chain
33	o	130	 5% 76% 22% .
34	O	116	 88% 12%
35	p	155	 26% 78% 21% ..
36	P	102	 78% 21% .
37	q	127	 26% 75% 24% .
38	Q	112	 90% 10%
39	R	89	 81% 18% .
40	S	103	 83% 17%
41	T	94	 82% 18%
42	U	79	 82% 16% .
43	V	49	 82% 16% .
44	W	67	 78% 22%
45	Z	47	 83% 17%
46	F	158	 92% 6% .

2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 128828 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y	2723	Total	C	N	O	P	0	0
			58376	26062	10687	18904	2723		

- Molecule 2 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	1447	Total	C	N	O	P	0	0
			31009	13847	5680	10037	1445		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	114	Total	C	N	O	P	0	0
			2430	1086	436	794	114		

- Molecule 4 is a protein called 50S ribosomal protein L33,50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	47	Total	C	N	O	S	0	0
			390	238	78	70	4		
4	1	58	Total	C	N	O		0	0
			449	280	85	84			

- Molecule 5 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 6 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4	37	Total	C	N	O	S	0	0
			295	186	60	44	5		

- Molecule 8 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	80	Total	C	N	O	S	0	0
			626	394	116	116			

- Molecule 9 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	114	Total	C	N	O	S	0	0
			826	507	158	159	2		

- Molecule 10 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	136	Total	C	N	O	S	0	0
			976	611	190	173	2		

- Molecule 11 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	274	Total	C	N	O	S	0	0
			2094	1303	415	371	5		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	113	Total	C	N	O	S	0	0
			828	510	168	149	1		

- Molecule 13 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 14 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 15 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	60	Total	C	N	O	S	0	0
			497	314	99	79	5		

- Molecule 16 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	88	Total	C	N	O	S	0	0
			713	441	148	123	1		

- Molecule 17 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	83	Total	C	N	O	S	0	0
			537	335	105	96	1		

- Molecule 18 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	G	165	Total	C	N	O	S	0	0
			1184	739	226	216	3		

- Molecule 19 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H	145	Total	C	N	O	S	0	0
			1143	714	208	218	3		

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	h	80	Total	C	N	O		
			520	327	97	96	0	0

- Molecule 21 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	I	122	Total	C	N	O	S		
			918	572	174	168	4	0	0

- Molecule 22 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	i	56	Total	C	N	O	S		
			458	292	88	76	2	0	0

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	j	77	Total	C	N	O	S		
			498	300	99	98	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	146	Total	C	N	O	S		
			1086	674	214	197	1	0	0

- Molecule 25 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	k	202	Total	C	N	O	S		
			1551	979	293	278	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	K	137	Total	C	N	O	S		
			1071	689	203	175	4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	L	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 28 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	l	198	Total	C	N	O		0	0
			1058	634	211	213			

- Molecule 29 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	m	156	Total	C	N	O	S	0	0
			1153	727	211	213	2		

- Molecule 30 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	M	119	Total	C	N	O		0	0
			882	549	174	159			

- Molecule 31 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	n	95	Total	C	N	O	S	0	0
			785	496	138	149	2		

- Molecule 32 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	N	114	Total	C	N	O		0	0
			889	563	175	151			

- Molecule 33 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	130	Total	C	N	O	S	0	0
			1007	639	180	184	4		

- Molecule 34 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	O	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 35 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	154	Total	C	N	O	S	0	0
			1155	719	219	214	3		

- Molecule 36 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	P	102	Total	C	N	O	S	0	0
			790	503	142	144	1		

- Molecule 37 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	q	127	Total	C	N	O	S	0	0
			975	605	194	175	1		

- Molecule 38 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Q	112	Total	C	N	O	S	0	0
			854	534	164	153	3		

- Molecule 39 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	R	89	Total	C	N	O	S	0	0
			715	453	127	131	4		

- Molecule 40 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	S	103	Total	C	N	O	S	0	0
			770	486	142	141	1		

- Molecule 41 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	T	94	Total	C	N	O	0	0
			722	463	130	129		

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	U	79	Total	C	N	O	0	0
			597	369	117	111		

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	V	49	Total	C	N	O	0	0
			379	234	82	63		

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	W	67	Total	C	N	O	0	0
			541	333	102	106		

- Molecule 45 is a protein called 50S ribosomalprotein L32p.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Z	47	Total	C	N	O	S	0	0
			355	219	76	58	2		

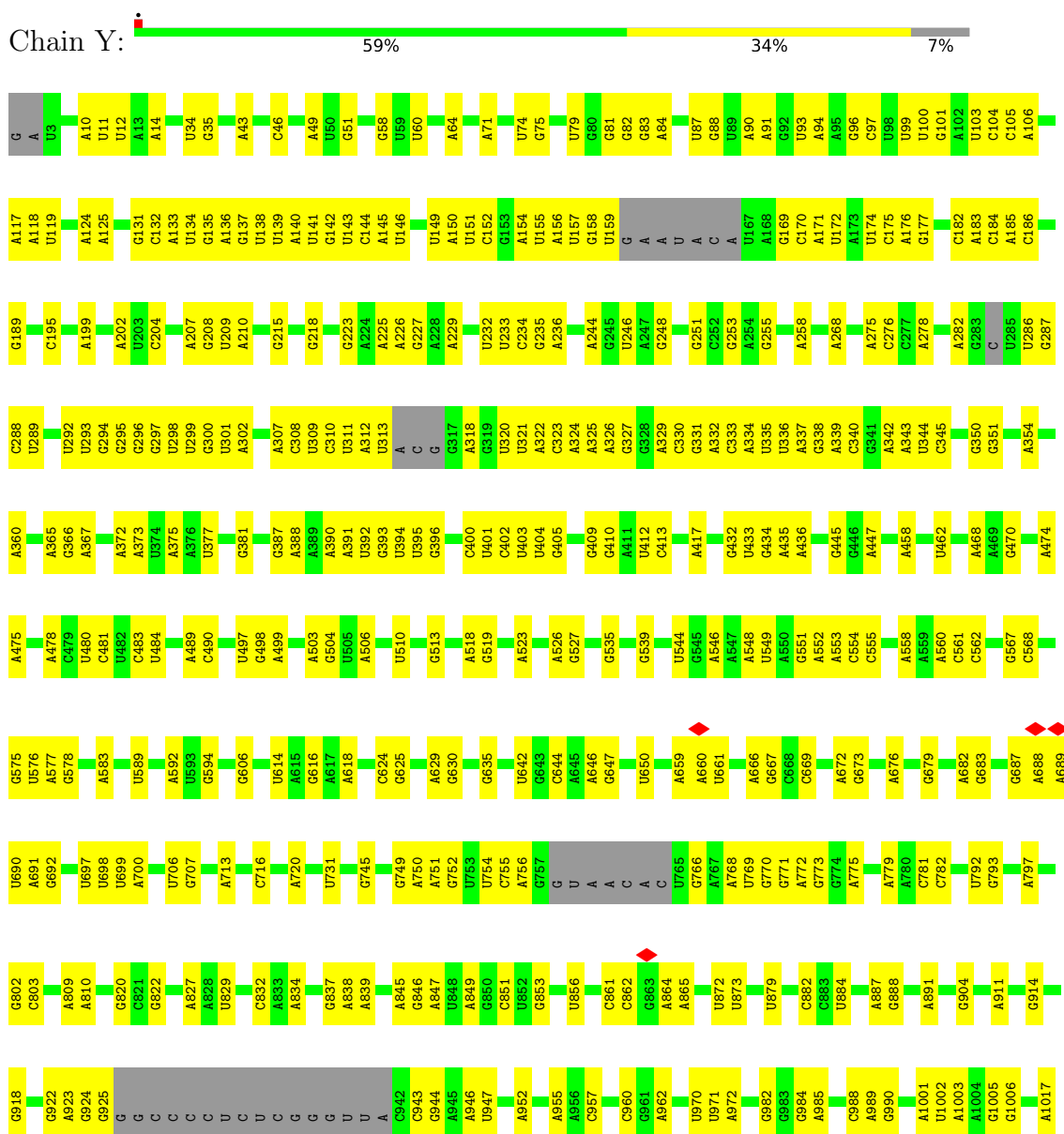
- Molecule 46 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	F	155	Total	C	N	O	0	0
			765	455	155	155		

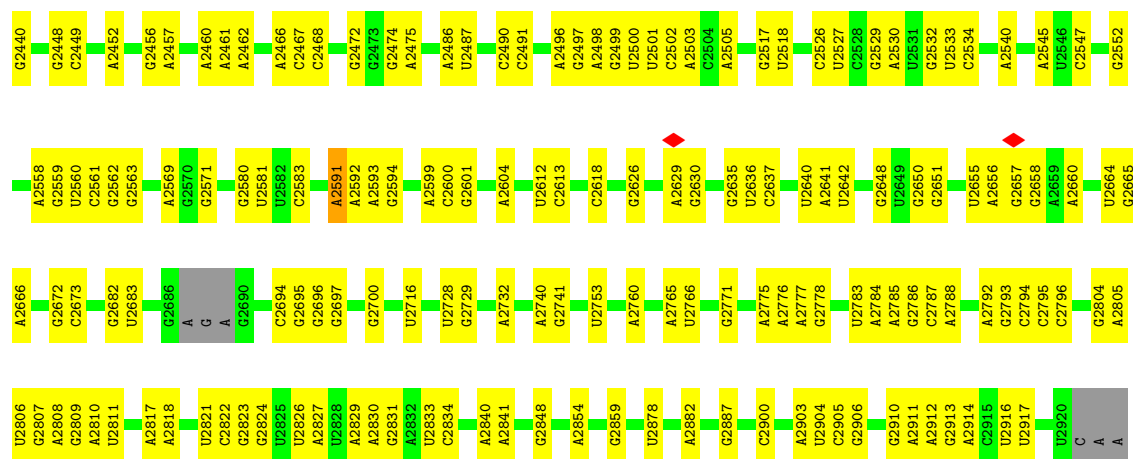
3 Residue-property plots

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

• Molecule 1: 23S rRNA

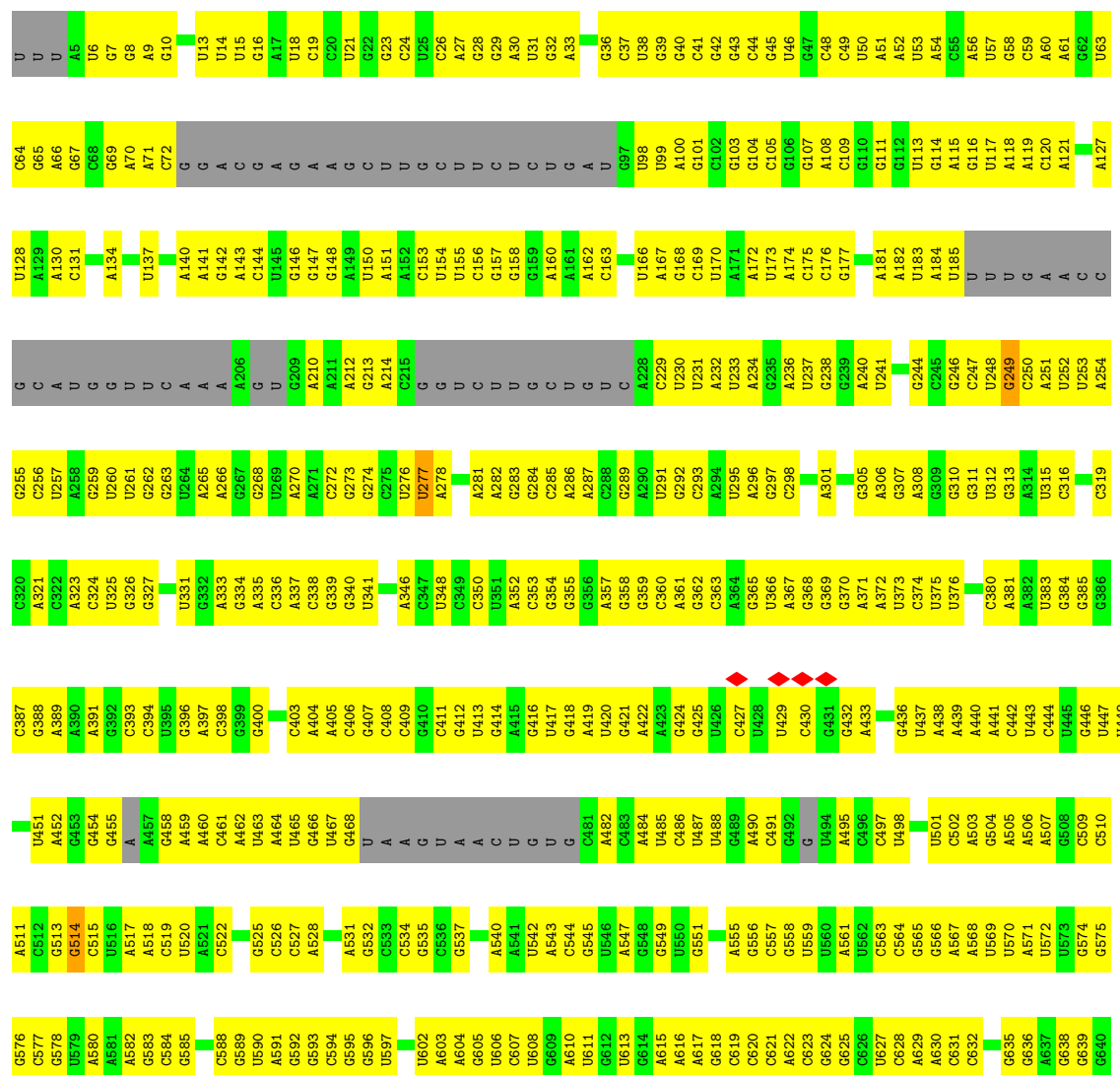


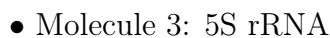




• Molecule 2: 16S rRNA

Chain X: 26% 66% 7%




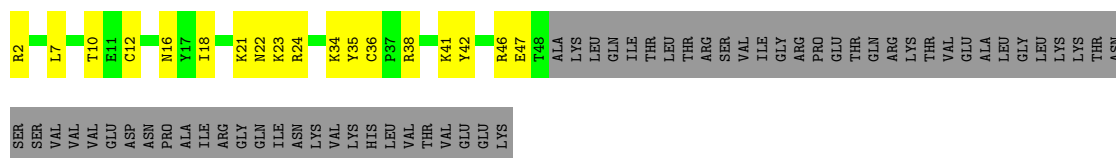


Chain 3:  59% 40%



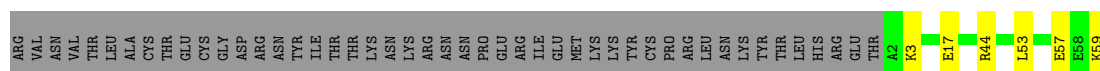
- Molecule 4: 50S ribosomal protein L33, 50S ribosomal protein L30

Chain A:  28% 17% 55%




- Molecule 4: 50S ribosomal protein L33, 50S ribosomal protein L30

Chain 1:  50% 6% 45%




- Molecule 5: 50S ribosomal protein L34

Chain B:  88% 12%




- Molecule 6: 50S ribosomal protein L35

Chain 2:  86% 14%



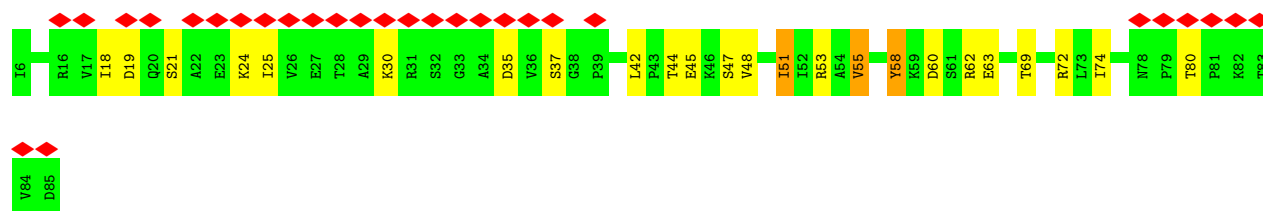
- Molecule 7: 50S ribosomal protein L36

Chain 4:  81% 19%

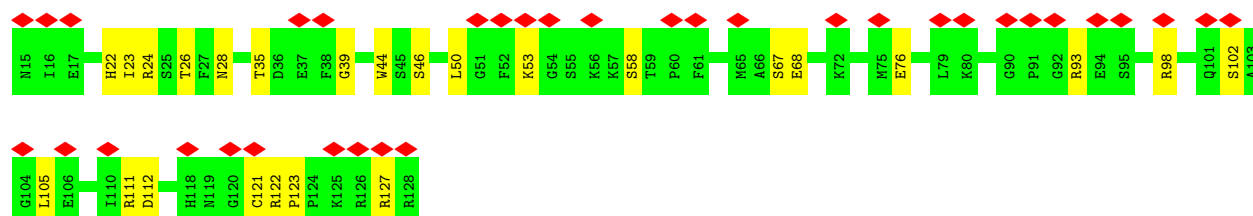
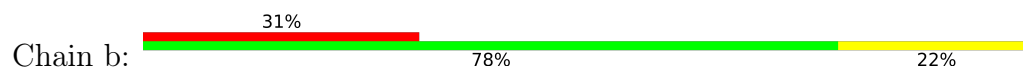


- Molecule 8: 30S ribosomal protein S10

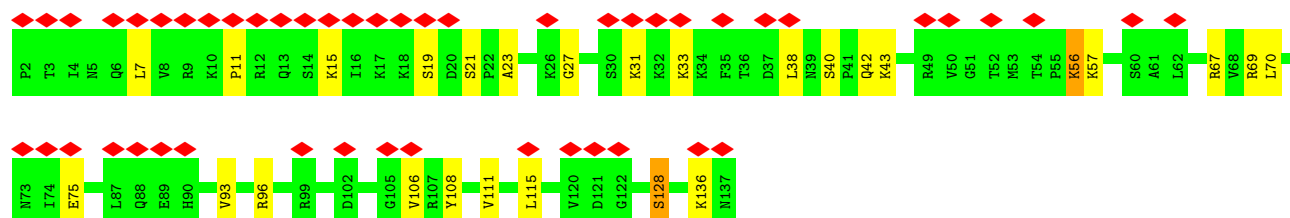
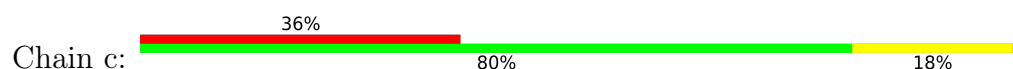
Chain a:  36% 70% 26%



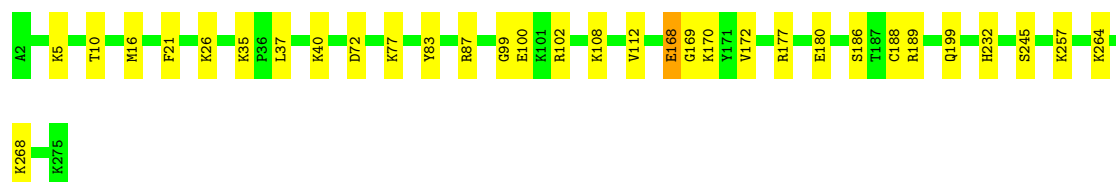
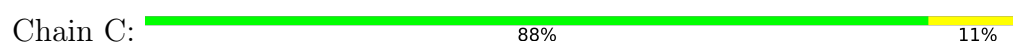
• Molecule 9: 30S ribosomal protein S11



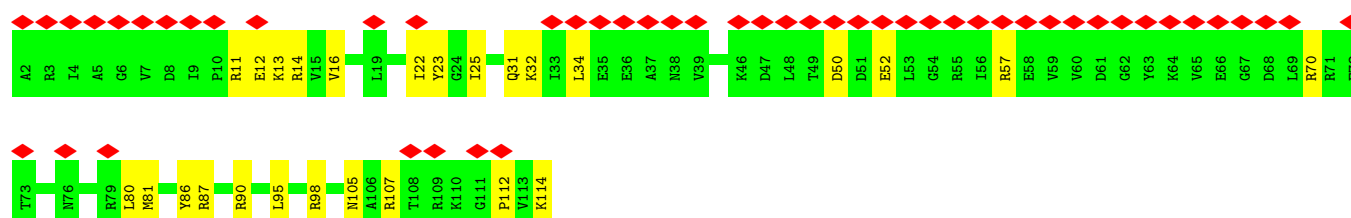
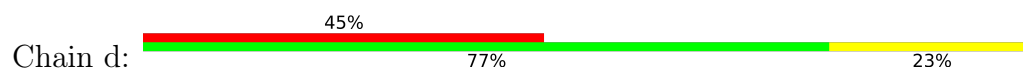
• Molecule 10: 30S ribosomal protein S12



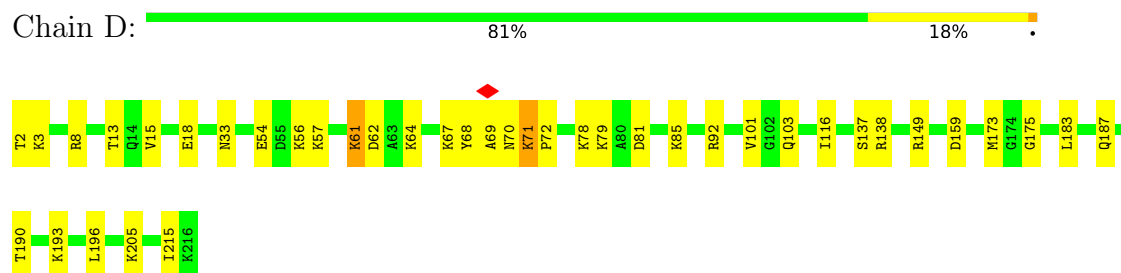
• Molecule 11: 50S ribosomal protein L2



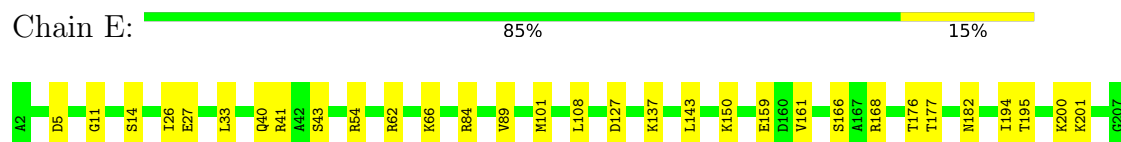
• Molecule 12: 30S ribosomal protein S13



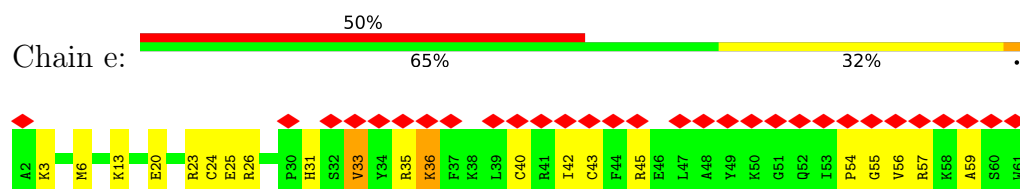
- Molecule 13: 50S ribosomal protein L3



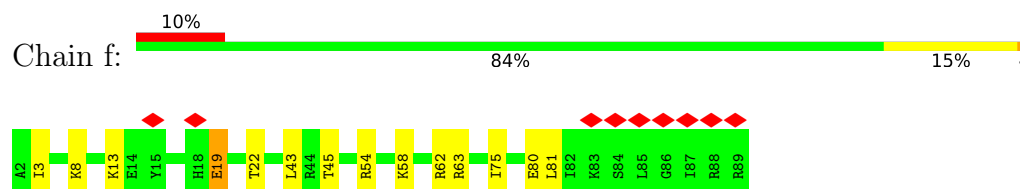
- Molecule 14: 50S ribosomal protein L4



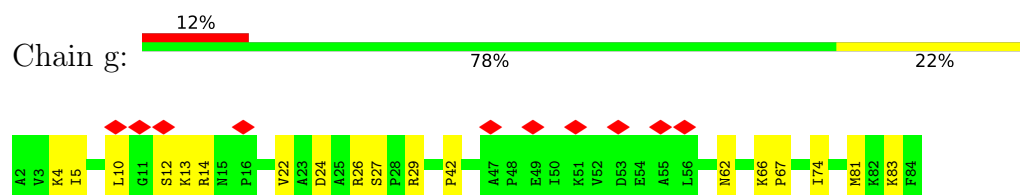
- Molecule 15: 30S ribosomal protein S14 type Z



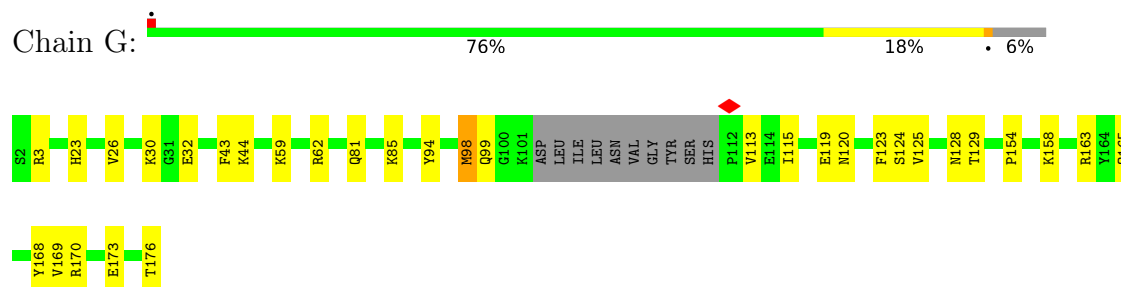
- Molecule 16: 30S ribosomal protein S15



- Molecule 17: 30S ribosomal protein S16

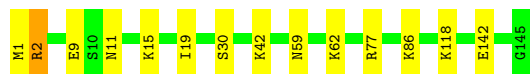


- Molecule 18: 50S ribosomal protein L6




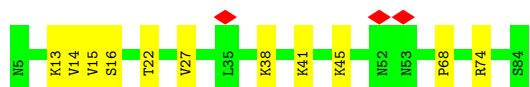
- Molecule 19: 50S ribosomal protein L13

Chain H:  90% 9%




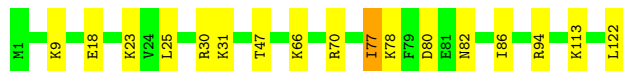
- Molecule 20: 30S ribosomal protein S17

Chain h:  86% 14%



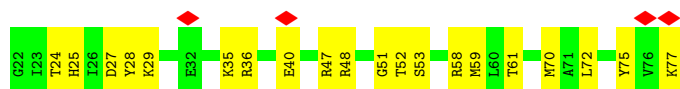
- Molecule 21: 50S ribosomal protein L14

Chain I:  86% 13%



- Molecule 22: 30S ribosomal protein S18

Chain i:  7% 64% 36%




- Molecule 23: 30S ribosomal protein S20

Chain j:  74% 23%




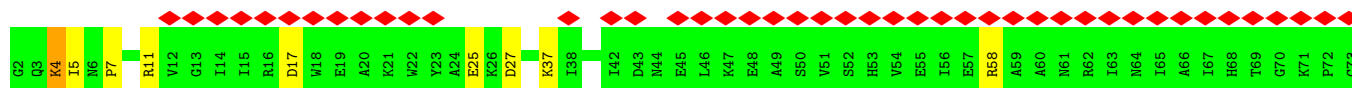
- Molecule 24: 50S ribosomal protein L15

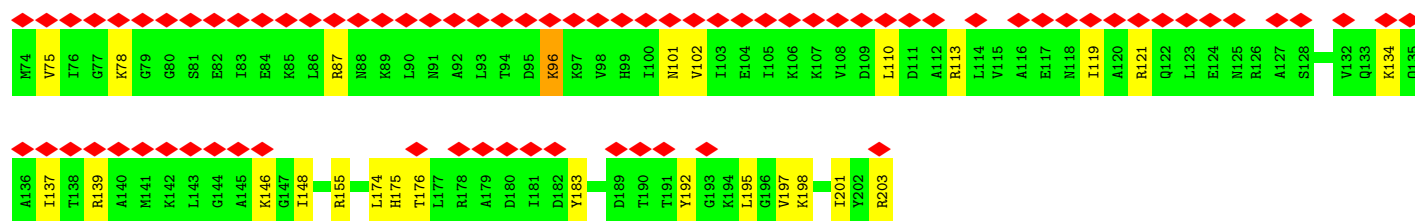
Chain J:  85% 14%



- Molecule 25: 30S ribosomal protein S3

Chain k:  60% 83% 16%





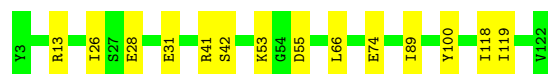
- Molecule 26: 50S ribosomal protein L16

Chain K: 86% 14%



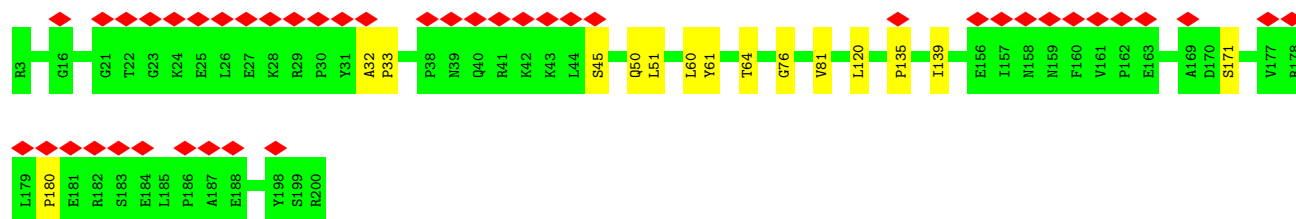
- Molecule 27: 50S ribosomal protein L17

Chain L: 88% 12%



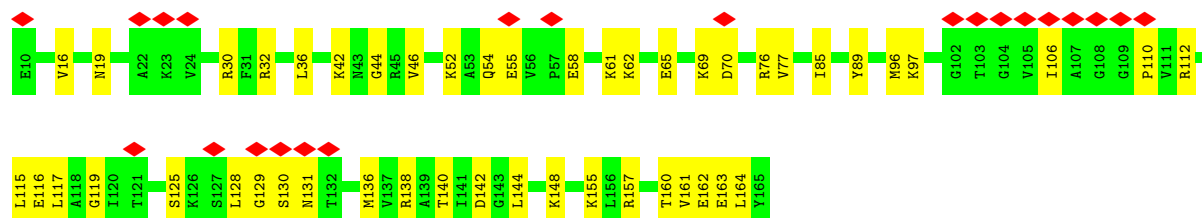
- Molecule 28: 30S ribosomal protein S4

Chain l: 22% 92% 8%



- Molecule 29: 30S ribosomal protein S5

Chain m: 14% 69% 31%

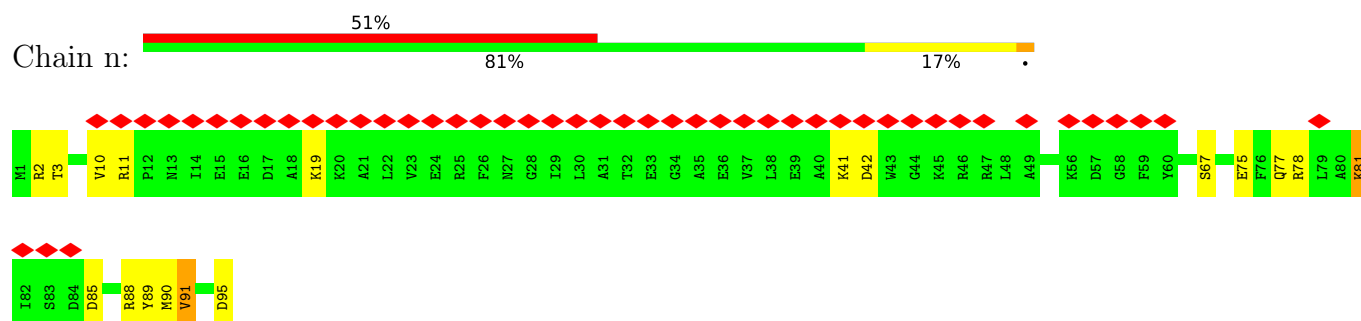


- Molecule 30: 50S ribosomal protein L18

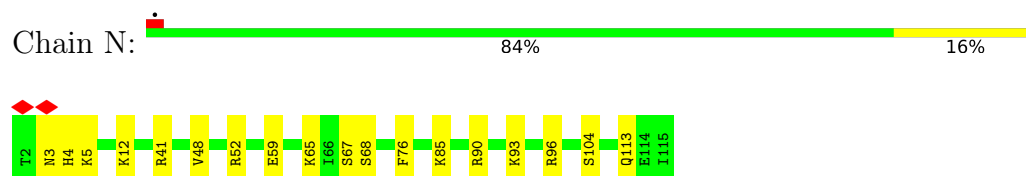
Chain M: 74% 25%



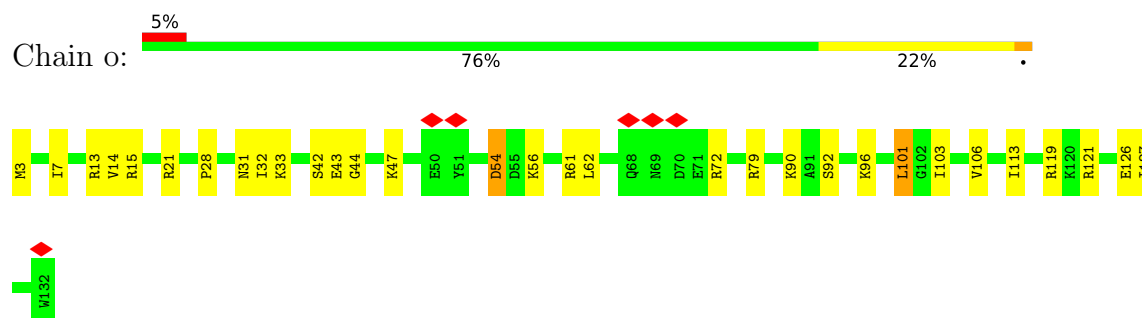
- Molecule 31: 30S ribosomal protein S6



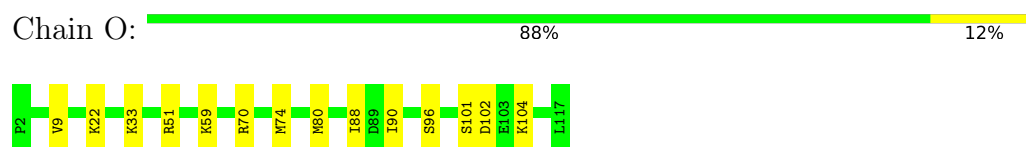
- Molecule 32: 50S ribosomal protein L19



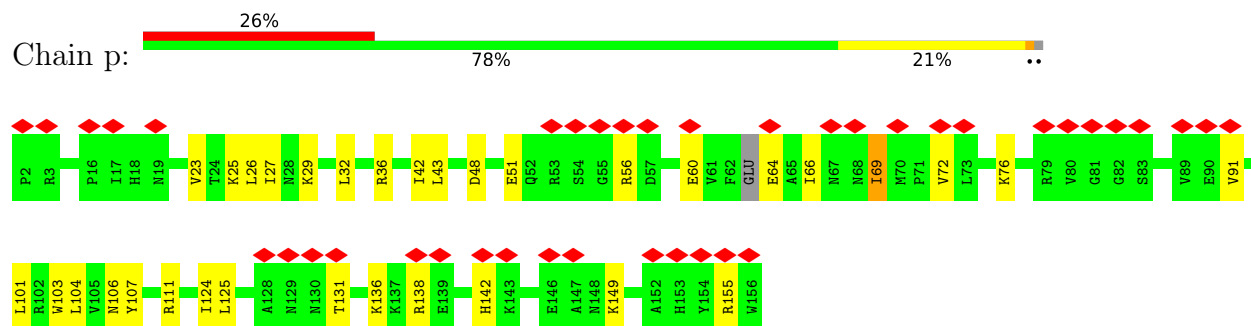
- Molecule 33: 30S ribosomal protein S8




- Molecule 34: 50S ribosomal protein L20

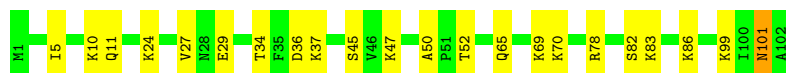


- Molecule 35: 30S ribosomal protein S7




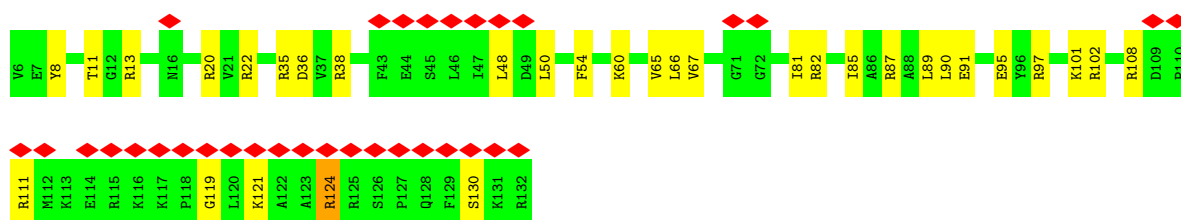
- Molecule 36: 50S ribosomal protein L21

Chain P:  78% 21% .




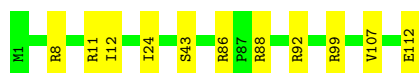
- Molecule 37: 30S ribosomal protein S9

Chain q:  26% 75% 24% .




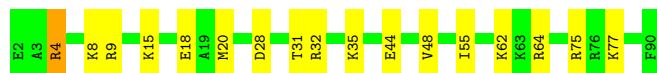
- Molecule 38: 50S ribosomal protein L22

Chain Q:  90% 10% .




- Molecule 39: 50S ribosomal protein L23

Chain R:  81% 18% .




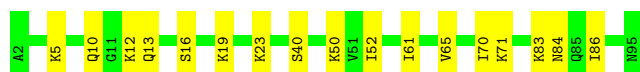
- Molecule 40: 50S ribosomal protein L24

Chain S:  83% 17% .




- Molecule 41: 50S ribosomal protein L25

Chain T:  82% 18% .



- Molecule 42: 50S ribosomal protein L27

Chain U:  82% 16% .



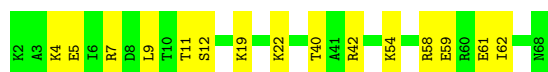
- Molecule 43: 50S ribosomal protein L28

Chain V: 82% 16% •



- Molecule 44: 50S ribosomal protein L29

Chain W: 78% 22%



- Molecule 45: 50S ribosomal protein L32p

Chain Z: 83% 17%



- Molecule 46: 50S ribosomal protein L5

Chain F: 92% 6% •



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	192105	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	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	0.076	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0045	Depositor
Map size (\AA)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.85, 0.85, 0.85	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	Y	0.21	0/65368	0.63	2/101922 (0.0%)
2	X	0.20	0/34716	0.64	6/54120 (0.0%)
3	3	0.21	0/2717	0.64	1/4232 (0.0%)
4	1	0.65	0/451	0.57	0/606
4	A	0.62	0/395	0.57	0/530
5	B	0.61	0/371	0.56	0/484
6	2	0.62	0/526	0.57	0/690
7	4	0.64	0/298	0.57	0/392
8	a	0.67	0/637	0.62	0/865
9	b	0.67	0/840	0.60	0/1137
10	c	0.68	0/991	0.60	0/1337
11	C	0.64	0/2129	0.60	0/2858
12	d	0.68	0/835	0.59	0/1123
13	D	0.65	0/1651	0.59	0/2215
14	E	0.64	0/1595	0.57	0/2154
15	e	0.63	0/507	0.58	0/674
16	f	0.65	0/721	0.56	0/964
17	g	0.71	0/541	0.62	0/733
18	G	0.69	0/1199	0.62	0/1621
19	H	0.64	0/1165	0.57	0/1570
20	h	0.72	0/527	0.60	0/721
21	I	0.65	0/925	0.58	0/1242
22	i	0.64	0/465	0.56	0/620
23	j	0.72	0/496	0.71	0/669
24	J	0.65	0/1100	0.59	0/1467
25	k	0.66	0/1573	0.59	0/2121
26	K	0.64	0/1095	0.58	0/1472
27	L	0.65	0/936	0.57	0/1253
28	l	0.78	0/1062	0.64	0/1465
29	m	0.67	0/1167	0.61	0/1576
30	M	0.66	0/891	0.59	0/1194
31	n	0.64	0/796	0.56	0/1069
32	N	0.64	0/901	0.56	0/1209
33	o	0.66	0/1019	0.59	0/1371

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	O	0.62	0/954	0.55	0/1264
35	p	0.67	0/1170	0.65	0/1580
36	P	0.64	0/800	0.57	0/1070
37	q	0.65	0/990	0.60	0/1332
38	Q	0.64	0/862	0.57	0/1161
39	R	0.64	0/723	0.56	0/966
40	S	0.66	0/779	0.59	0/1043
41	T	0.67	0/730	0.59	0/981
42	U	0.65	0/603	0.58	0/802
43	V	0.65	0/384	0.58	0/515
44	W	0.65	0/542	0.55	0/722
45	Z	0.65	0/361	0.59	0/482
46	F	0.84	0/763	0.83	0/1059
All	All	0.39	0/140267	0.62	9/210653 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	2591	A	C2'-C3'-O3'	7.59	126.20	109.50
3	3	26	C	C2'-C3'-O3'	7.59	126.20	109.50
2	X	1431	U	C2'-C3'-O3'	7.43	125.85	109.50
2	X	514	G	C2'-C3'-O3'	6.51	124.11	113.70
2	X	277	U	C2'-C3'-O3'	6.34	123.84	113.70
2	X	823	A	C2'-C3'-O3'	6.30	123.78	113.70
2	X	249	G	C2'-C3'-O3'	6.29	123.76	113.70
1	Y	1897	U	C2'-C3'-O3'	5.90	123.13	113.70
2	X	1016	A	C2'-C3'-O3'	5.63	122.70	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	1	56/105 (53%)	51 (91%)	5 (9%)	0	100	100
4	A	45/105 (43%)	41 (91%)	3 (7%)	1 (2%)	5	12
5	B	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
6	2	62/64 (97%)	48 (77%)	13 (21%)	1 (2%)	8	18
7	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	3	8
8	a	78/80 (98%)	51 (65%)	22 (28%)	5 (6%)	1	1
9	b	112/114 (98%)	85 (76%)	22 (20%)	5 (4%)	2	3
10	c	134/136 (98%)	101 (75%)	26 (19%)	7 (5%)	1	2
11	C	272/274 (99%)	230 (85%)	38 (14%)	4 (2%)	8	19
12	d	111/113 (98%)	88 (79%)	20 (18%)	3 (3%)	4	10
13	D	213/215 (99%)	179 (84%)	27 (13%)	7 (3%)	3	7
14	E	204/206 (99%)	181 (89%)	21 (10%)	2 (1%)	13	26
15	e	58/60 (97%)	44 (76%)	9 (16%)	5 (9%)	0	1
16	f	86/88 (98%)	73 (85%)	12 (14%)	1 (1%)	11	23
17	g	81/83 (98%)	54 (67%)	22 (27%)	5 (6%)	1	2
18	G	161/175 (92%)	126 (78%)	31 (19%)	4 (2%)	4	10
19	H	143/145 (99%)	125 (87%)	15 (10%)	3 (2%)	5	13
20	h	78/80 (98%)	60 (77%)	17 (22%)	1 (1%)	10	22
21	I	120/122 (98%)	105 (88%)	14 (12%)	1 (1%)	16	32
22	i	54/56 (96%)	42 (78%)	10 (18%)	2 (4%)	2	5
23	j	73/78 (94%)	56 (77%)	15 (20%)	2 (3%)	4	10
24	J	144/146 (99%)	123 (85%)	18 (12%)	3 (2%)	5	13
25	k	200/202 (99%)	159 (80%)	35 (18%)	6 (3%)	3	8
26	K	135/137 (98%)	119 (88%)	13 (10%)	3 (2%)	5	12
27	L	118/120 (98%)	108 (92%)	9 (8%)	1 (1%)	16	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	l	196/198 (99%)	154 (79%)	33 (17%)	9 (5%)	2	3
29	m	154/156 (99%)	116 (75%)	32 (21%)	6 (4%)	2	5
30	M	117/119 (98%)	98 (84%)	15 (13%)	4 (3%)	3	6
31	n	93/95 (98%)	72 (77%)	19 (20%)	2 (2%)	5	12
32	N	112/114 (98%)	100 (89%)	10 (9%)	2 (2%)	7	16
33	o	128/130 (98%)	88 (69%)	35 (27%)	5 (4%)	2	5
34	O	114/116 (98%)	108 (95%)	3 (3%)	3 (3%)	4	10
35	p	150/155 (97%)	127 (85%)	20 (13%)	3 (2%)	6	14
36	P	100/102 (98%)	84 (84%)	14 (14%)	2 (2%)	6	14
37	q	125/127 (98%)	98 (78%)	23 (18%)	4 (3%)	3	7
38	Q	110/112 (98%)	96 (87%)	13 (12%)	1 (1%)	14	29
39	R	87/89 (98%)	77 (88%)	8 (9%)	2 (2%)	5	11
40	S	101/103 (98%)	83 (82%)	14 (14%)	4 (4%)	2	4
41	T	92/94 (98%)	82 (89%)	8 (9%)	2 (2%)	5	12
42	U	77/79 (98%)	69 (90%)	6 (8%)	2 (3%)	4	10
43	V	47/49 (96%)	39 (83%)	6 (13%)	2 (4%)	2	4
44	W	65/67 (97%)	58 (89%)	6 (9%)	1 (2%)	8	19
45	Z	45/47 (96%)	38 (84%)	5 (11%)	2 (4%)	2	4
46	F	151/158 (96%)	110 (73%)	32 (21%)	9 (6%)	1	2
All	All	4878/5094 (96%)	4016 (82%)	724 (15%)	138 (3%)	6	9

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	a	63	GLU
10	c	57	LYS
12	d	95	LEU
13	D	71	LYS
17	g	66	LYS
28	l	32	ALA
35	p	155	ARG
40	S	51	ASN
46	F	74	ILE
46	F	85	ILE
46	F	132	VAL

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Mol	Chain	Res	Type
4	A	42	TYR
6	2	20	GLY
8	a	51	ILE
8	a	55	VAL
9	b	123	PRO
13	D	175	GLY
14	E	11	GLY
15	e	33	VAL
15	e	55	GLY
18	G	98	MET
18	G	173	GLU
21	I	77	ILE
22	i	24	THR
23	j	11	VAL
25	k	4	LYS
28	l	33	PRO
28	l	120	LEU
28	l	139	ILE
29	m	110	PRO
29	m	119	GLY
29	m	129	GLY
30	M	66	THR
34	O	102	ASP
42	U	28	ARG
46	F	81	GLU
10	c	136	LYS
11	C	169	GLY
12	d	105	ASN
15	e	59	ALA
19	H	11	ASN
19	H	59	ASN
25	k	25	GLU
27	L	100	TYR
28	l	76	GLY
28	l	81	VAL
29	m	44	GLY
29	m	77	VAL
30	M	26	ALA
33	o	44	GLY
36	P	101	ASN
37	q	124	ARG
40	S	6	GLY

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Mol	Chain	Res	Type
40	S	96	LYS
41	T	84	ASN
44	W	11	THR
45	Z	33	CYS
46	F	84	PRO
46	F	121	ALA
8	a	58	TYR
9	b	50	LEU
9	b	76	GLU
10	c	23	ALA
10	c	56	LYS
10	c	128	SER
11	C	168	GLU
13	D	61	LYS
13	D	62	ASP
14	E	89	VAL
15	e	36	LYS
15	e	54	PRO
16	f	19	GLU
17	g	62	ASN
18	G	165	GLN
22	i	51	GLY
25	k	7	PRO
25	k	17	ASP
25	k	78	LYS
25	k	96	LYS
26	K	80	GLU
26	K	85	ALA
31	n	81	LYS
32	N	3	ASN
32	N	67	SER
33	o	54	ASP
33	o	101	LEU
34	O	101	SER
35	p	131	THR
36	P	50	ALA
38	Q	11	ARG
39	R	32	ARG
41	T	65	VAL
45	Z	43	CYS
46	F	109	PRO
46	F	145	LYS

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Mol	Chain	Res	Type
12	d	112	PRO
13	D	69	ALA
13	D	72	PRO
20	h	68	PRO
23	j	56	LEU
24	J	2	LYS
24	J	53	GLY
24	J	106	LYS
26	K	14	ARG
28	l	171	SER
29	m	128	LEU
33	o	43	GLU
42	U	82	ARG
43	V	58	LYS
46	F	32	ASP
7	4	26	ILE
8	a	80	THR
9	b	46	SER
11	C	21	PHE
19	H	2	ARG
37	q	67	VAL
39	R	4	ARG
13	D	101	VAL
17	g	22	VAL
17	g	42	PRO
30	M	70	VAL
31	n	91	VAL
35	p	69	ILE
37	q	65	VAL
37	q	119	GLY
18	G	154	PRO
33	o	28	PRO
34	O	9	VAL
40	S	55	GLY
9	b	39	GLY
10	c	11	PRO
10	c	27	GLY
11	C	99	GLY
17	g	67	PRO
28	l	135	PRO
28	l	180	PRO
30	M	97	GLY

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Mol	Chain	Res	Type
43	V	57	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	1	52/97 (54%)	46 (88%)	6 (12%)	4	8
4	A	44/97 (45%)	27 (61%)	17 (39%)	0	0
5	B	39/39 (100%)	34 (87%)	5 (13%)	3	6
6	2	55/55 (100%)	47 (86%)	8 (14%)	2	4
7	4	35/35 (100%)	29 (83%)	6 (17%)	1	2
8	a	67/73 (92%)	45 (67%)	22 (33%)	0	0
9	b	85/90 (94%)	65 (76%)	20 (24%)	0	0
10	c	95/118 (80%)	73 (77%)	22 (23%)	0	0
11	C	221/221 (100%)	192 (87%)	29 (13%)	3	6
12	d	75/97 (77%)	52 (69%)	23 (31%)	0	0
13	D	173/173 (100%)	138 (80%)	35 (20%)	1	1
14	E	168/168 (100%)	139 (83%)	29 (17%)	1	2
15	e	51/52 (98%)	33 (65%)	18 (35%)	0	0
16	f	74/80 (92%)	60 (81%)	14 (19%)	1	1
17	g	36/70 (51%)	23 (64%)	13 (36%)	0	0
18	G	115/153 (75%)	86 (75%)	29 (25%)	0	0
19	H	122/123 (99%)	110 (90%)	12 (10%)	6	13
20	h	35/75 (47%)	25 (71%)	10 (29%)	0	0
21	I	100/100 (100%)	83 (83%)	17 (17%)	1	2
22	i	49/50 (98%)	31 (63%)	18 (37%)	0	0
23	j	37/65 (57%)	19 (51%)	18 (49%)	0	0
24	J	109/112 (97%)	89 (82%)	20 (18%)	1	1
25	k	151/164 (92%)	120 (80%)	31 (20%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	K	108/114 (95%)	92 (85%)	16 (15%)	2	4
27	L	96/101 (95%)	83 (86%)	13 (14%)	3	5
28	l	23/174 (13%)	17 (74%)	6 (26%)	0	0
29	m	120/122 (98%)	78 (65%)	42 (35%)	0	0
30	M	83/95 (87%)	55 (66%)	28 (34%)	0	0
31	n	82/83 (99%)	64 (78%)	18 (22%)	1	0
32	N	93/100 (93%)	77 (83%)	16 (17%)	1	2
33	o	107/111 (96%)	79 (74%)	28 (26%)	0	0
34	O	96/96 (100%)	85 (88%)	11 (12%)	4	8
35	p	114/131 (87%)	83 (73%)	31 (27%)	0	0
36	P	84/86 (98%)	63 (75%)	21 (25%)	0	0
37	q	96/105 (91%)	67 (70%)	29 (30%)	0	0
38	Q	89/91 (98%)	79 (89%)	10 (11%)	5	9
39	R	78/80 (98%)	62 (80%)	16 (20%)	1	1
40	S	81/88 (92%)	67 (83%)	14 (17%)	1	2
41	T	78/82 (95%)	63 (81%)	15 (19%)	1	1
42	U	59/62 (95%)	46 (78%)	13 (22%)	1	0
43	V	39/41 (95%)	31 (80%)	8 (20%)	1	1
44	W	58/60 (97%)	44 (76%)	14 (24%)	0	0
45	Z	35/43 (81%)	29 (83%)	6 (17%)	1	2
All	All	3607/4172 (86%)	2830 (78%)	777 (22%)	2	0

All (777) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	2	ARG
4	A	7	LEU
4	A	10	THR
4	A	12	CYS
4	A	16	ASN
4	A	18	ILE
4	A	21	LYS
4	A	22	ASN
4	A	23	LYS
4	A	24	ARG

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Mol	Chain	Res	Type
4	A	34	LYS
4	A	35	TYR
4	A	36	CYS
4	A	38	ARG
4	A	41	LYS
4	A	46	ARG
4	A	47	GLU
5	B	5	THR
5	B	11	ARG
5	B	15	LYS
5	B	25	THR
5	B	30	LYS
6	2	3	LYS
6	2	4	MET
6	2	12	LYS
6	2	26	ARG
6	2	35	ASN
6	2	46	LYS
6	2	53	SER
6	2	59	LYS
7	4	8	LYS
7	4	11	CYS
7	4	13	LYS
7	4	15	LYS
7	4	28	GLU
7	4	34	GLN
8	a	18	ILE
8	a	19	ASP
8	a	21	SER
8	a	24	LYS
8	a	25	ILE
8	a	30	LYS
8	a	35	ASP
8	a	37	SER
8	a	42	LEU
8	a	44	THR
8	a	45	GLU
8	a	47	SER
8	a	48	VAL
8	a	51	ILE
8	a	53	ARG
8	a	55	VAL

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Mol	Chain	Res	Type
8	a	58	TYR
8	a	60	ASP
8	a	62	ARG
8	a	69	THR
8	a	72	ARG
8	a	74	ILE
9	b	22	HIS
9	b	23	ILE
9	b	24	ARG
9	b	26	THR
9	b	28	ASN
9	b	35	THR
9	b	44	TRP
9	b	53	LYS
9	b	58	SER
9	b	67	SER
9	b	68	GLU
9	b	93	ARG
9	b	98	ARG
9	b	102	SER
9	b	105	LEU
9	b	111	ARG
9	b	112	ASP
9	b	121	CYS
9	b	122	ARG
9	b	127	ARG
10	c	7	LEU
10	c	15	LYS
10	c	19	SER
10	c	21	SER
10	c	31	LYS
10	c	33	LYS
10	c	38	LEU
10	c	40	SER
10	c	42	GLN
10	c	43	LYS
10	c	56	LYS
10	c	67	ARG
10	c	69	ARG
10	c	70	LEU
10	c	75	GLU
10	c	93	VAL

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Mol	Chain	Res	Type
10	c	96	ARG
10	c	106	VAL
10	c	108	TYR
10	c	111	VAL
10	c	115	LEU
10	c	128	SER
11	C	5	LYS
11	C	10	THR
11	C	16	MET
11	C	26	LYS
11	C	35	LYS
11	C	37	LEU
11	C	40	LYS
11	C	72	ASP
11	C	77	LYS
11	C	83	TYR
11	C	87	ARG
11	C	100	GLU
11	C	102	ARG
11	C	108	LYS
11	C	112	VAL
11	C	168	GLU
11	C	170	LYS
11	C	172	VAL
11	C	177	ARG
11	C	180	GLU
11	C	186	SER
11	C	188	CYS
11	C	189	ARG
11	C	199	GLN
11	C	232	HIS
11	C	245	SER
11	C	257	LYS
11	C	264	LYS
11	C	268	LYS
12	d	11	ARG
12	d	12	GLU
12	d	13	LYS
12	d	14	ARG
12	d	16	VAL
12	d	22	ILE
12	d	23	TYR

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Mol	Chain	Res	Type
12	d	25	ILE
12	d	31	GLN
12	d	32	LYS
12	d	34	LEU
12	d	50	ASP
12	d	52	GLU
12	d	57	ARG
12	d	70	ARG
12	d	80	LEU
12	d	81	MET
12	d	86	TYR
12	d	87	ARG
12	d	90	ARG
12	d	98	ARG
12	d	107	ARG
12	d	114	LYS
13	D	2	THR
13	D	3	LYS
13	D	8	ARG
13	D	13	THR
13	D	15	VAL
13	D	18	GLU
13	D	33	ASN
13	D	54	GLU
13	D	56	LYS
13	D	57	LYS
13	D	61	LYS
13	D	64	LYS
13	D	67	LYS
13	D	68	TYR
13	D	70	ASN
13	D	71	LYS
13	D	78	LYS
13	D	79	LYS
13	D	81	ASP
13	D	85	LYS
13	D	92	ARG
13	D	103	GLN
13	D	116	ILE
13	D	137	SER
13	D	138	ARG
13	D	149	ARG

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Mol	Chain	Res	Type
13	D	159	ASP
13	D	173	MET
13	D	183	LEU
13	D	187	GLN
13	D	190	THR
13	D	193	LYS
13	D	196	LEU
13	D	205	LYS
13	D	215	ILE
14	E	5	ASP
14	E	14	SER
14	E	26	ILE
14	E	27	GLU
14	E	33	LEU
14	E	40	GLN
14	E	41	ARG
14	E	43	SER
14	E	54	ARG
14	E	62	ARG
14	E	66	LYS
14	E	84	ARG
14	E	101	MET
14	E	108	LEU
14	E	127	ASP
14	E	137	LYS
14	E	143	LEU
14	E	150	LYS
14	E	159	GLU
14	E	161	VAL
14	E	166	SER
14	E	168	ARG
14	E	176	THR
14	E	177	THR
14	E	182	ASN
14	E	194	ILE
14	E	195	THR
14	E	200	LYS
14	E	201	LYS
15	e	3	LYS
15	e	6	MET
15	e	13	LYS
15	e	20	GLU

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Mol	Chain	Res	Type
15	e	23	ARG
15	e	24	CYS
15	e	25	GLU
15	e	26	ARG
15	e	31	HIS
15	e	33	VAL
15	e	35	ARG
15	e	36	LYS
15	e	40	CYS
15	e	42	ILE
15	e	43	CYS
15	e	45	ARG
15	e	56	VAL
15	e	57	ARG
16	f	3	ILE
16	f	8	LYS
16	f	13	LYS
16	f	19	GLU
16	f	22	THR
16	f	43	LEU
16	f	45	THR
16	f	54	ARG
16	f	58	LYS
16	f	62	ARG
16	f	63	ARG
16	f	75	ILE
16	f	80	GLU
16	f	81	LEU
17	g	4	LYS
17	g	5	ILE
17	g	10	LEU
17	g	12	SER
17	g	13	LYS
17	g	14	ARG
17	g	24	ASP
17	g	26	ARG
17	g	27	SER
17	g	29	ARG
17	g	74	ILE
17	g	81	MET
17	g	83	LYS
18	G	3	ARG

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Mol	Chain	Res	Type
18	G	23	HIS
18	G	26	VAL
18	G	30	LYS
18	G	32	GLU
18	G	43	PHE
18	G	44	LYS
18	G	59	LYS
18	G	62	ARG
18	G	81	GLN
18	G	85	LYS
18	G	94	TYR
18	G	98	MET
18	G	99	GLN
18	G	113	VAL
18	G	115	ILE
18	G	119	GLU
18	G	120	ASN
18	G	123	PHE
18	G	124	SER
18	G	125	VAL
18	G	128	ASN
18	G	129	THR
18	G	158	LYS
18	G	163	ARG
18	G	168	TYR
18	G	169	VAL
18	G	170	ARG
18	G	176	THR
19	H	1	MET
19	H	2	ARG
19	H	9	GLU
19	H	15	LYS
19	H	19	ILE
19	H	30	SER
19	H	42	LYS
19	H	62	LYS
19	H	77	ARG
19	H	86	LYS
19	H	118	LYS
19	H	142	GLU
20	h	13	LYS
20	h	14	VAL

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Mol	Chain	Res	Type
20	h	15	VAL
20	h	16	SER
20	h	22	THR
20	h	27	VAL
20	h	38	LYS
20	h	41	LYS
20	h	45	LYS
20	h	74	ARG
21	I	9	LYS
21	I	18	GLU
21	I	23	LYS
21	I	25	LEU
21	I	30	ARG
21	I	31	LYS
21	I	47	THR
21	I	66	LYS
21	I	70	ARG
21	I	77	ILE
21	I	78	LYS
21	I	80	ASP
21	I	82	ASN
21	I	86	ILE
21	I	94	ARG
21	I	113	LYS
21	I	122	LEU
22	i	25	HIS
22	i	27	ASP
22	i	28	TYR
22	i	29	LYS
22	i	35	LYS
22	i	36	ARG
22	i	40	GLU
22	i	47	ARG
22	i	48	ARG
22	i	52	THR
22	i	53	SER
22	i	58	ARG
22	i	59	MET
22	i	61	THR
22	i	70	MET
22	i	72	LEU
22	i	75	TYR

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Mol	Chain	Res	Type
22	i	77	LYS
23	j	5	LYS
23	j	6	SER
23	j	8	ILE
23	j	9	LYS
23	j	11	VAL
23	j	12	LYS
23	j	13	THR
23	j	14	THR
23	j	15	GLU
23	j	16	LYS
23	j	18	GLU
23	j	20	ARG
23	j	22	ILE
23	j	33	LYS
23	j	68	SER
23	j	75	LYS
23	j	78	LEU
23	j	79	MET
24	J	6	LEU
24	J	7	LYS
24	J	16	ARG
24	J	29	LYS
24	J	31	SER
24	J	33	ARG
24	J	42	SER
24	J	50	PHE
24	J	64	ARG
24	J	69	ILE
24	J	76	ILE
24	J	98	GLU
24	J	104	ASN
24	J	106	LYS
24	J	107	SER
24	J	120	LYS
24	J	123	VAL
24	J	127	LYS
24	J	129	SER
24	J	139	LYS
25	k	4	LYS
25	k	5	ILE
25	k	11	ARG

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Mol	Chain	Res	Type
25	k	27	ASP
25	k	37	LYS
25	k	58	ARG
25	k	75	VAL
25	k	87	ARG
25	k	96	LYS
25	k	101	ASN
25	k	102	VAL
25	k	110	LEU
25	k	113	ARG
25	k	119	ILE
25	k	121	ARG
25	k	134	LYS
25	k	137	ILE
25	k	139	ARG
25	k	146	LYS
25	k	148	ILE
25	k	155	ARG
25	k	174	LEU
25	k	175	HIS
25	k	176	THR
25	k	183	TYR
25	k	192	TYR
25	k	195	LEU
25	k	197	VAL
25	k	198	LYS
25	k	201	ILE
25	k	203	ARG
26	K	13	HIS
26	K	16	LYS
26	K	18	THR
26	K	38	THR
26	K	39	THR
26	K	45	ARG
26	K	54	MET
26	K	81	VAL
26	K	101	ARG
26	K	103	LEU
26	K	109	VAL
26	K	110	SER
26	K	122	SER
26	K	127	VAL

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Mol	Chain	Res	Type
26	K	130	LYS
26	K	137	LEU
27	L	13	ARG
27	L	26	ILE
27	L	28	GLU
27	L	31	GLU
27	L	41	ARG
27	L	42	SER
27	L	53	LYS
27	L	55	ASP
27	L	66	LEU
27	L	74	GLU
27	L	89	ILE
27	L	118	ILE
27	L	119	ILE
28	l	45	SER
28	l	50	GLN
28	l	51	LEU
28	l	60	LEU
28	l	61	TYR
28	l	64	THR
29	m	16	VAL
29	m	19	ASN
29	m	30	ARG
29	m	32	ARG
29	m	36	LEU
29	m	42	LYS
29	m	46	VAL
29	m	52	LYS
29	m	54	GLN
29	m	55	GLU
29	m	58	GLU
29	m	61	LYS
29	m	62	LYS
29	m	65	GLU
29	m	69	LYS
29	m	70	ASP
29	m	76	ARG
29	m	85	ILE
29	m	89	TYR
29	m	96	MET
29	m	97	LYS

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Mol	Chain	Res	Type
29	m	106	ILE
29	m	112	ARG
29	m	115	LEU
29	m	116	GLU
29	m	117	LEU
29	m	125	SER
29	m	130	SER
29	m	131	ASN
29	m	136	MET
29	m	138	ARG
29	m	140	THR
29	m	142	ASP
29	m	144	LEU
29	m	148	LYS
29	m	155	LYS
29	m	157	ARG
29	m	160	THR
29	m	161	VAL
29	m	162	GLU
29	m	163	GLU
29	m	164	LEU
30	M	9	LYS
30	M	10	VAL
30	M	11	ARG
30	M	12	LEU
30	M	13	LYS
30	M	22	LEU
30	M	28	LYS
30	M	30	ARG
30	M	31	LEU
30	M	37	ASN
30	M	41	TYR
30	M	44	ILE
30	M	49	LYS
30	M	53	LEU
30	M	57	SER
30	M	58	SER
30	M	59	LYS
30	M	68	THR
30	M	70	VAL
30	M	72	LEU
30	M	75	LYS

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Mol	Chain	Res	Type
30	M	87	LYS
30	M	90	LYS
30	M	99	TYR
30	M	100	LEU
30	M	105	VAL
30	M	117	LEU
30	M	119	PHE
31	n	2	ARG
31	n	3	THR
31	n	10	VAL
31	n	11	ARG
31	n	19	LYS
31	n	41	LYS
31	n	42	ASP
31	n	67	SER
31	n	75	GLU
31	n	77	GLN
31	n	78	ARG
31	n	81	LYS
31	n	85	ASP
31	n	88	ARG
31	n	89	TYR
31	n	90	MET
31	n	91	VAL
31	n	95	ASP
32	N	4	HIS
32	N	5	LYS
32	N	12	LYS
32	N	41	ARG
32	N	48	VAL
32	N	52	ARG
32	N	59	GLU
32	N	65	LYS
32	N	68	SER
32	N	76	PHE
32	N	85	LYS
32	N	90	ARG
32	N	93	LYS
32	N	96	ARG
32	N	104	SER
32	N	113	GLN
33	o	3	MET

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Mol	Chain	Res	Type
33	o	7	ILE
33	o	13	ARG
33	o	14	VAL
33	o	15	ARG
33	o	21	ARG
33	o	31	ASN
33	o	32	ILE
33	o	33	LYS
33	o	42	SER
33	o	47	LYS
33	o	54	ASP
33	o	56	LYS
33	o	61	ARG
33	o	62	LEU
33	o	72	ARG
33	o	79	ARG
33	o	90	LYS
33	o	92	SER
33	o	96	LYS
33	o	101	LEU
33	o	103	ILE
33	o	106	VAL
33	o	113	ILE
33	o	119	ARG
33	o	121	ARG
33	o	126	GLU
33	o	127	ILE
34	O	22	LYS
34	O	33	LYS
34	O	51	ARG
34	O	59	LYS
34	O	70	ARG
34	O	74	MET
34	O	80	MET
34	O	88	ILE
34	O	90	ILE
34	O	96	SER
34	O	104	LYS
35	p	23	VAL
35	p	25	LYS
35	p	26	LEU
35	p	27	ILE

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Mol	Chain	Res	Type
35	p	29	LYS
35	p	32	LEU
35	p	36	ARG
35	p	42	ILE
35	p	43	LEU
35	p	48	ASP
35	p	51	GLU
35	p	56	ARG
35	p	60	GLU
35	p	64	GLU
35	p	66	ILE
35	p	69	ILE
35	p	72	VAL
35	p	76	LYS
35	p	91	VAL
35	p	101	LEU
35	p	103	TRP
35	p	104	LEU
35	p	106	ASN
35	p	107	TYR
35	p	111	ARG
35	p	124	ILE
35	p	125	LEU
35	p	136	LYS
35	p	138	ARG
35	p	142	HIS
35	p	149	LYS
36	P	5	ILE
36	P	10	LYS
36	P	11	GLN
36	P	24	LYS
36	P	27	VAL
36	P	29	GLU
36	P	34	THR
36	P	36	ASP
36	P	37	LYS
36	P	45	SER
36	P	47	LYS
36	P	52	THR
36	P	65	GLN
36	P	69	LYS
36	P	70	LYS

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Mol	Chain	Res	Type
36	P	78	ARG
36	P	82	SER
36	P	83	LYS
36	P	86	LYS
36	P	99	LYS
36	P	101	ASN
37	q	8	TYR
37	q	11	THR
37	q	13	ARG
37	q	20	ARG
37	q	22	ARG
37	q	35	ARG
37	q	36	ASP
37	q	38	ARG
37	q	48	LEU
37	q	50	LEU
37	q	54	PHE
37	q	60	LYS
37	q	66	LEU
37	q	81	ILE
37	q	82	ARG
37	q	85	ILE
37	q	87	ARG
37	q	89	LEU
37	q	90	LEU
37	q	91	GLU
37	q	95	GLU
37	q	97	ARG
37	q	101	LYS
37	q	102	ARG
37	q	108	ARG
37	q	111	ARG
37	q	121	LYS
37	q	124	ARG
37	q	130	SER
38	Q	8	ARG
38	Q	12	ILE
38	Q	24	ILE
38	Q	43	SER
38	Q	86	ARG
38	Q	88	ARG
38	Q	92	ARG

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Mol	Chain	Res	Type
38	Q	99	ARG
38	Q	107	VAL
38	Q	112	GLU
39	R	4	ARG
39	R	8	LYS
39	R	9	ARG
39	R	15	LYS
39	R	18	GLU
39	R	20	MET
39	R	28	ASP
39	R	31	THR
39	R	35	LYS
39	R	44	GLU
39	R	48	VAL
39	R	55	ILE
39	R	62	LYS
39	R	64	ARG
39	R	75	ARG
39	R	77	LYS
40	S	2	HIS
40	S	7	ASP
40	S	10	LYS
40	S	22	LYS
40	S	29	LYS
40	S	32	ARG
40	S	43	LYS
40	S	45	GLN
40	S	60	GLU
40	S	66	SER
40	S	85	PHE
40	S	87	ASP
40	S	89	LYS
40	S	101	ILE
41	T	5	LYS
41	T	10	GLN
41	T	12	LYS
41	T	13	GLN
41	T	16	SER
41	T	19	LYS
41	T	23	LYS
41	T	40	SER
41	T	50	LYS

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Mol	Chain	Res	Type
41	T	52	ILE
41	T	61	ILE
41	T	70	ILE
41	T	71	LYS
41	T	83	LYS
41	T	86	ILE
42	U	18	THR
42	U	22	ARG
42	U	29	LEU
42	U	47	ARG
42	U	48	GLN
42	U	70	LYS
42	U	78	GLU
42	U	79	ARG
42	U	80	LYS
42	U	82	ARG
42	U	83	ASP
42	U	88	SER
42	U	92	VAL
43	V	22	LEU
43	V	26	LYS
43	V	29	TRP
43	V	38	ILE
43	V	45	LYS
43	V	47	VAL
43	V	58	LYS
43	V	60	THR
44	W	4	LYS
44	W	5	GLU
44	W	7	ARG
44	W	9	LEU
44	W	12	SER
44	W	19	LYS
44	W	22	LYS
44	W	40	THR
44	W	42	ARG
44	W	54	LYS
44	W	58	ARG
44	W	59	GLU
44	W	61	GLU
44	W	62	ILE
4	1	3	LYS

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Mol	Chain	Res	Type
4	1	17	GLU
4	1	44	ARG
4	1	53	LEU
4	1	57	GLU
4	1	59	LYS
45	Z	6	ARG
45	Z	7	ARG
45	Z	22	ILE
45	Z	23	SER
45	Z	27	MET
45	Z	37	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	22	ASN
8	a	56	HIS
8	a	67	GLN
11	C	128	ASN
11	C	133	GLN
11	C	226	ASN
11	C	232	HIS
13	D	70	ASN
13	D	143	HIS
13	D	200	ASN
14	E	40	GLN
14	E	162	ASN
16	f	5	GLN
16	f	42	HIS
16	f	68	ASN
18	G	23	HIS
22	i	25	HIS
24	J	27	ASN
25	k	6	ASN
25	k	118	ASN
26	K	25	ASN
26	K	35	GLN
27	L	106	GLN
28	l	67	GLN
29	m	83	HIS
30	M	43	GLN
31	n	69	ASN

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Mol	Chain	Res	Type
32	N	3	ASN
32	N	14	GLN
32	N	31	HIS
33	o	22	HIS
34	O	37	GLN
34	O	91	ASN
38	Q	61	ASN
40	S	64	HIS
41	T	13	GLN
41	T	38	ASN
41	T	84	ASN
43	V	34	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Y	2709/2923 (92%)	1004 (37%)	48 (1%)
2	X	1436/1552 (92%)	1029 (71%)	56 (3%)
3	3	113/114 (99%)	47 (41%)	2 (1%)
All	All	4258/4589 (92%)	2080 (48%)	106 (2%)

All (2080) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Y	10	A
1	Y	11	U
1	Y	12	U
1	Y	14	A
1	Y	34	U
1	Y	35	G
1	Y	43	A
1	Y	46	C
1	Y	49	A
1	Y	51	G
1	Y	58	G
1	Y	60	U
1	Y	64	A
1	Y	71	A
1	Y	74	U
1	Y	75	G
1	Y	79	U

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Mol	Chain	Res	Type
1	Y	81	G
1	Y	82	G
1	Y	83	G
1	Y	84	A
1	Y	87	U
1	Y	88	G
1	Y	90	A
1	Y	91	A
1	Y	93	U
1	Y	94	A
1	Y	96	G
1	Y	97	C
1	Y	99	U
1	Y	100	U
1	Y	101	G
1	Y	103	U
1	Y	104	C
1	Y	105	C
1	Y	106	A
1	Y	117	A
1	Y	118	A
1	Y	119	U
1	Y	124	A
1	Y	125	A
1	Y	131	G
1	Y	132	C
1	Y	133	A
1	Y	134	U
1	Y	135	G
1	Y	136	A
1	Y	137	G
1	Y	138	U
1	Y	140	A
1	Y	141	U
1	Y	142	G
1	Y	143	U
1	Y	144	C
1	Y	145	A
1	Y	146	U
1	Y	149	U
1	Y	150	A
1	Y	151	U

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Mol	Chain	Res	Type
1	Y	152	C
1	Y	154	A
1	Y	155	U
1	Y	156	A
1	Y	157	U
1	Y	158	G
1	Y	159	U
1	Y	169	G
1	Y	170	C
1	Y	171	A
1	Y	172	U
1	Y	174	U
1	Y	175	C
1	Y	176	A
1	Y	177	G
1	Y	182	C
1	Y	183	A
1	Y	184	C
1	Y	185	A
1	Y	186	C
1	Y	189	G
1	Y	195	C
1	Y	199	A
1	Y	202	A
1	Y	204	C
1	Y	207	A
1	Y	209	U
1	Y	210	A
1	Y	215	G
1	Y	218	G
1	Y	223	G
1	Y	225	A
1	Y	226	A
1	Y	227	G
1	Y	229	A
1	Y	232	U
1	Y	233	U
1	Y	234	C
1	Y	235	G
1	Y	236	A
1	Y	244	A
1	Y	246	U

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Mol	Chain	Res	Type
1	Y	248	G
1	Y	251	G
1	Y	253	G
1	Y	255	G
1	Y	258	A
1	Y	268	A
1	Y	275	A
1	Y	276	C
1	Y	278	A
1	Y	282	A
1	Y	286	U
1	Y	287	G
1	Y	288	C
1	Y	289	U
1	Y	292	U
1	Y	293	U
1	Y	294	G
1	Y	295	G
1	Y	296	G
1	Y	297	G
1	Y	298	U
1	Y	299	U
1	Y	300	G
1	Y	301	U
1	Y	302	A
1	Y	307	A
1	Y	308	C
1	Y	309	U
1	Y	310	C
1	Y	311	U
1	Y	312	A
1	Y	313	U
1	Y	318	A
1	Y	320	U
1	Y	321	U
1	Y	322	A
1	Y	323	C
1	Y	325	A
1	Y	326	A
1	Y	327	G
1	Y	329	A
1	Y	330	C

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Mol	Chain	Res	Type
1	Y	331	G
1	Y	332	A
1	Y	333	C
1	Y	334	A
1	Y	335	U
1	Y	336	U
1	Y	337	A
1	Y	338	G
1	Y	339	A
1	Y	340	C
1	Y	342	A
1	Y	343	A
1	Y	344	U
1	Y	345	C
1	Y	350	G
1	Y	351	G
1	Y	354	A
1	Y	360	A
1	Y	365	A
1	Y	366	G
1	Y	367	A
1	Y	372	A
1	Y	373	A
1	Y	375	A
1	Y	377	U
1	Y	381	G
1	Y	387	G
1	Y	388	A
1	Y	390	A
1	Y	391	A
1	Y	392	U
1	Y	393	G
1	Y	394	U
1	Y	395	U
1	Y	396	G
1	Y	400	C
1	Y	401	U
1	Y	402	C
1	Y	403	U
1	Y	404	U
1	Y	405	G
1	Y	409	G

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Mol	Chain	Res	Type
1	Y	410	G
1	Y	412	U
1	Y	413	C
1	Y	417	A
1	Y	432	G
1	Y	433	U
1	Y	434	G
1	Y	435	A
1	Y	436	A
1	Y	445	G
1	Y	447	A
1	Y	458	A
1	Y	462	U
1	Y	468	A
1	Y	470	G
1	Y	474	A
1	Y	475	A
1	Y	478	A
1	Y	480	U
1	Y	481	C
1	Y	483	C
1	Y	484	U
1	Y	489	A
1	Y	490	C
1	Y	497	U
1	Y	498	G
1	Y	499	A
1	Y	503	A
1	Y	504	G
1	Y	506	A
1	Y	510	U
1	Y	513	G
1	Y	518	A
1	Y	519	G
1	Y	523	A
1	Y	526	A
1	Y	527	G
1	Y	535	G
1	Y	539	G
1	Y	544	U
1	Y	546	A
1	Y	548	A

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Mol	Chain	Res	Type
1	Y	549	U
1	Y	551	G
1	Y	552	A
1	Y	553	A
1	Y	554	C
1	Y	555	C
1	Y	558	A
1	Y	560	A
1	Y	561	C
1	Y	562	C
1	Y	567	G
1	Y	568	C
1	Y	575	G
1	Y	576	U
1	Y	577	A
1	Y	578	G
1	Y	583	A
1	Y	589	U
1	Y	592	A
1	Y	594	G
1	Y	606	G
1	Y	614	U
1	Y	616	G
1	Y	618	A
1	Y	624	C
1	Y	625	G
1	Y	629	A
1	Y	630	G
1	Y	635	G
1	Y	642	U
1	Y	644	C
1	Y	646	A
1	Y	647	G
1	Y	650	U
1	Y	659	A
1	Y	660	A
1	Y	661	U
1	Y	666	A
1	Y	667	G
1	Y	669	C
1	Y	672	A
1	Y	673	G

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Mol	Chain	Res	Type
1	Y	676	A
1	Y	679	G
1	Y	682	A
1	Y	683	G
1	Y	687	G
1	Y	688	A
1	Y	689	A
1	Y	690	U
1	Y	691	A
1	Y	692	G
1	Y	697	U
1	Y	698	U
1	Y	699	U
1	Y	700	A
1	Y	706	U
1	Y	707	G
1	Y	713	A
1	Y	716	C
1	Y	720	A
1	Y	731	U
1	Y	745	G
1	Y	749	G
1	Y	750	A
1	Y	751	A
1	Y	752	G
1	Y	754	U
1	Y	755	C
1	Y	756	A
1	Y	766	G
1	Y	768	A
1	Y	769	U
1	Y	770	G
1	Y	771	G
1	Y	772	A
1	Y	773	G
1	Y	775	A
1	Y	779	A
1	Y	781	C
1	Y	782	C
1	Y	792	U
1	Y	793	G
1	Y	797	A

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Mol	Chain	Res	Type
1	Y	802	G
1	Y	803	C
1	Y	809	A
1	Y	810	A
1	Y	820	G
1	Y	822	G
1	Y	827	A
1	Y	829	U
1	Y	832	C
1	Y	834	A
1	Y	837	G
1	Y	838	A
1	Y	839	A
1	Y	845	A
1	Y	846	G
1	Y	847	A
1	Y	849	A
1	Y	851	C
1	Y	853	G
1	Y	856	U
1	Y	861	C
1	Y	862	C
1	Y	864	A
1	Y	865	A
1	Y	872	U
1	Y	873	U
1	Y	879	U
1	Y	882	C
1	Y	884	U
1	Y	887	A
1	Y	888	G
1	Y	891	A
1	Y	904	G
1	Y	911	A
1	Y	914	G
1	Y	918	G
1	Y	922	G
1	Y	923	A
1	Y	924	G
1	Y	925	G
1	Y	943	C
1	Y	944	G

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Mol	Chain	Res	Type
1	Y	946	A
1	Y	947	U
1	Y	952	A
1	Y	955	A
1	Y	957	C
1	Y	960	C
1	Y	962	A
1	Y	970	U
1	Y	971	U
1	Y	972	A
1	Y	982	G
1	Y	984	G
1	Y	985	A
1	Y	988	C
1	Y	989	A
1	Y	990	G
1	Y	1001	A
1	Y	1002	U
1	Y	1003	A
1	Y	1005	G
1	Y	1006	G
1	Y	1017	A
1	Y	1018	A
1	Y	1027	A
1	Y	1029	C
1	Y	1030	C
1	Y	1032	A
1	Y	1034	A
1	Y	1035	C
1	Y	1040	A
1	Y	1043	U
1	Y	1052	A
1	Y	1053	A
1	Y	1055	A
1	Y	1056	U
1	Y	1057	A
1	Y	1060	U
1	Y	1062	U
1	Y	1066	G
1	Y	1067	U
1	Y	1069	G
1	Y	1070	A

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Mol	Chain	Res	Type
1	Y	1077	U
1	Y	1078	G
1	Y	1082	C
1	Y	1083	G
1	Y	1086	G
1	Y	1089	C
1	Y	1090	A
1	Y	1091	G
1	Y	1092	A
1	Y	1093	C
1	Y	1095	A
1	Y	1096	C
1	Y	1097	U
1	Y	1098	A
1	Y	1099	G
1	Y	1150	A
1	Y	1152	U
1	Y	1154	G
1	Y	1155	A
1	Y	1156	G
1	Y	1158	G
1	Y	1159	A
1	Y	1160	C
1	Y	1167	C
1	Y	1169	G
1	Y	1170	A
1	Y	1171	A
1	Y	1172	A
1	Y	1176	U
1	Y	1177	A
1	Y	1178	C
1	Y	1179	C
1	Y	1180	G
1	Y	1181	G
1	Y	1185	U
1	Y	1186	A
1	Y	1194	U
1	Y	1195	A
1	Y	1198	G
1	Y	1201	G
1	Y	1205	U
1	Y	1208	A

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Mol	Chain	Res	Type
1	Y	1214	C
1	Y	1217	U
1	Y	1218	G
1	Y	1219	G
1	Y	1221	C
1	Y	1229	G
1	Y	1245	G
1	Y	1263	A
1	Y	1267	A
1	Y	1275	A
1	Y	1276	G
1	Y	1278	G
1	Y	1279	C
1	Y	1280	U
1	Y	1285	A
1	Y	1291	A
1	Y	1293	U
1	Y	1294	G
1	Y	1309	G
1	Y	1310	A
1	Y	1312	A
1	Y	1313	G
1	Y	1315	C
1	Y	1321	A
1	Y	1337	A
1	Y	1338	U
1	Y	1339	U
1	Y	1342	C
1	Y	1343	U
1	Y	1357	G
1	Y	1358	A
1	Y	1359	A
1	Y	1360	G
1	Y	1362	C
1	Y	1363	U
1	Y	1366	U
1	Y	1367	C
1	Y	1368	C
1	Y	1369	G
1	Y	1370	C
1	Y	1373	U
1	Y	1374	G

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Mol	Chain	Res	Type
1	Y	1389	U
1	Y	1396	A
1	Y	1399	C
1	Y	1400	C
1	Y	1402	A
1	Y	1405	G
1	Y	1416	U
1	Y	1417	G
1	Y	1421	A
1	Y	1422	A
1	Y	1423	C
1	Y	1425	G
1	Y	1429	G
1	Y	1430	A
1	Y	1440	A
1	Y	1446	U
1	Y	1447	A
1	Y	1448	U
1	Y	1449	A
1	Y	1450	A
1	Y	1451	U
1	Y	1452	C
1	Y	1453	G
1	Y	1460	U
1	Y	1461	C
1	Y	1462	G
1	Y	1463	A
1	Y	1464	U
1	Y	1465	G
1	Y	1468	G
1	Y	1471	A
1	Y	1472	C
1	Y	1473	G
1	Y	1474	C
1	Y	1477	U
1	Y	1478	A
1	Y	1479	G
1	Y	1480	G
1	Y	1481	A
1	Y	1482	U
1	Y	1483	A
1	Y	1484	G

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Mol	Chain	Res	Type
1	Y	1486	C
1	Y	1487	G
1	Y	1488	A
1	Y	1489	A
1	Y	1490	G
1	Y	1491	C
1	Y	1492	G
1	Y	1493	U
1	Y	1494	G
1	Y	1495	C
1	Y	1497	A
1	Y	1498	U
1	Y	1499	U
1	Y	1500	G
1	Y	1502	A
1	Y	1504	U
1	Y	1505	G
1	Y	1506	C
1	Y	1507	A
1	Y	1508	C
1	Y	1509	G
1	Y	1512	U
1	Y	1513	A
1	Y	1514	A
1	Y	1516	C
1	Y	1518	G
1	Y	1520	A
1	Y	1521	A
1	Y	1522	G
1	Y	1525	U
1	Y	1526	G
1	Y	1527	A
1	Y	1528	G
1	Y	1529	U
1	Y	1556	G
1	Y	1557	C
1	Y	1561	G
1	Y	1562	C
1	Y	1563	U
1	Y	1564	G
1	Y	1565	U
1	Y	1567	A

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Mol	Chain	Res	Type
1	Y	1569	G
1	Y	1570	G
1	Y	1571	G
1	Y	1572	G
1	Y	1573	A
1	Y	1574	G
1	Y	1578	A
1	Y	1579	C
1	Y	1589	U
1	Y	1590	C
1	Y	1591	G
1	Y	1592	A
1	Y	1593	G
1	Y	1595	C
1	Y	1596	G
1	Y	1597	U
1	Y	1598	U
1	Y	1599	G
1	Y	1601	U
1	Y	1602	U
1	Y	1603	U
1	Y	1604	C
1	Y	1607	A
1	Y	1608	C
1	Y	1609	U
1	Y	1610	G
1	Y	1611	C
1	Y	1612	C
1	Y	1613	G
1	Y	1614	A
1	Y	1616	A
1	Y	1626	A
1	Y	1627	G
1	Y	1628	A
1	Y	1629	U
1	Y	1630	A
1	Y	1631	G
1	Y	1635	A
1	Y	1636	U
1	Y	1637	A
1	Y	1638	G
1	Y	1639	G

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Mol	Chain	Res	Type
1	Y	1640	U
1	Y	1642	C
1	Y	1643	C
1	Y	1651	C
1	Y	1652	A
1	Y	1653	A
1	Y	1654	A
1	Y	1660	A
1	Y	1661	C
1	Y	1662	A
1	Y	1677	G
1	Y	1678	A
1	Y	1683	U
1	Y	1690	A
1	Y	1691	G
1	Y	1692	C
1	Y	1693	G
1	Y	1709	A
1	Y	1718	G
1	Y	1721	A
1	Y	1738	C
1	Y	1740	G
1	Y	1748	G
1	Y	1755	U
1	Y	1756	U
1	Y	1757	U
1	Y	1758	A
1	Y	1759	G
1	Y	1760	G
1	Y	1761	G
1	Y	1762	U
1	Y	1765	A
1	Y	1766	C
1	Y	1767	G
1	Y	1768	C
1	Y	1770	C
1	Y	1771	A
1	Y	1772	G
1	Y	1773	A
1	Y	1774	A
1	Y	1775	G
1	Y	1785	G

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Mol	Chain	Res	Type
1	Y	1788	U
1	Y	1789	A
1	Y	1790	G
1	Y	1791	G
1	Y	1796	A
1	Y	1800	A
1	Y	1806	U
1	Y	1807	A
1	Y	1811	A
1	Y	1814	A
1	Y	1818	A
1	Y	1827	C
1	Y	1828	U
1	Y	1829	A
1	Y	1839	G
1	Y	1842	A
1	Y	1843	U
1	Y	1844	G
1	Y	1856	A
1	Y	1866	G
1	Y	1870	C
1	Y	1871	U
1	Y	1874	A
1	Y	1875	A
1	Y	1876	G
1	Y	1877	G
1	Y	1878	U
1	Y	1879	U
1	Y	1880	A
1	Y	1882	G
1	Y	1883	A
1	Y	1884	G
1	Y	1885	G
1	Y	1886	A
1	Y	1887	G
1	Y	1889	G
1	Y	1890	G
1	Y	1892	U
1	Y	1893	A
1	Y	1894	G
1	Y	1896	U
1	Y	1897	U

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Mol	Chain	Res	Type
1	Y	1898	C
1	Y	1899	U
1	Y	1900	G
1	Y	1901	C
1	Y	1902	G
1	Y	1903	A
1	Y	1904	A
1	Y	1907	U
1	Y	1908	A
1	Y	1912	A
1	Y	1915	G
1	Y	1916	A
1	Y	1917	A
1	Y	1918	G
1	Y	1920	C
1	Y	1921	C
1	Y	1923	A
1	Y	1924	G
1	Y	1928	A
1	Y	1933	G
1	Y	1934	G
1	Y	1935	C
1	Y	1936	C
1	Y	1937	G
1	Y	1938	U
1	Y	1941	C
1	Y	1942	U
1	Y	1943	A
1	Y	1944	U
1	Y	1945	A
1	Y	1946	A
1	Y	1947	C
1	Y	1948	G
1	Y	1950	U
1	Y	1951	C
1	Y	1953	U
1	Y	1954	A
1	Y	1956	G
1	Y	1957	G
1	Y	1958	U
1	Y	1960	G
1	Y	1965	A

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Mol	Chain	Res	Type
1	Y	1967	U
1	Y	1978	U
1	Y	1982	U
1	Y	1990	C
1	Y	1991	G
1	Y	1992	C
1	Y	1994	C
1	Y	1997	A
1	Y	1998	A
1	Y	1999	G
1	Y	2002	G
1	Y	2004	A
1	Y	2011	U
1	Y	2012	G
1	Y	2013	G
1	Y	2015	C
1	Y	2016	A
1	Y	2017	C
1	Y	2018	U
1	Y	2020	U
1	Y	2024	A
1	Y	2033	C
1	Y	2050	A
1	Y	2054	G
1	Y	2058	A
1	Y	2059	G
1	Y	2060	A
1	Y	2063	C
1	Y	2070	C
1	Y	2077	C
1	Y	2082	C
1	Y	2083	G
1	Y	2087	A
1	Y	2088	G
1	Y	2089	A
1	Y	2096	G
1	Y	2103	U
1	Y	2120	G
1	Y	2124	U
1	Y	2125	U
1	Y	2127	G
1	Y	2128	G

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Mol	Chain	Res	Type
1	Y	2132	A
1	Y	2135	U
1	Y	2209	G
1	Y	2211	U
1	Y	2212	G
1	Y	2213	U
1	Y	2214	G
1	Y	2216	U
1	Y	2217	G
1	Y	2220	U
1	Y	2224	U
1	Y	2225	A
1	Y	2226	A
1	Y	2231	C
1	Y	2232	A
1	Y	2234	C
1	Y	2237	U
1	Y	2238	U
1	Y	2239	A
1	Y	2241	C
1	Y	2242	G
1	Y	2243	U
1	Y	2244	G
1	Y	2246	U
1	Y	2247	G
1	Y	2252	A
1	Y	2265	G
1	Y	2266	G
1	Y	2269	G
1	Y	2295	A
1	Y	2306	G
1	Y	2309	G
1	Y	2310	C
1	Y	2314	A
1	Y	2315	A
1	Y	2323	U
1	Y	2326	G
1	Y	2329	U
1	Y	2330	G
1	Y	2331	G
1	Y	2332	U
1	Y	2333	U

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Mol	Chain	Res	Type
1	Y	2334	G
1	Y	2335	G
1	Y	2336	A
1	Y	2337	A
1	Y	2338	A
1	Y	2339	U
1	Y	2340	C
1	Y	2345	A
1	Y	2346	U
1	Y	2347	A
1	Y	2348	G
1	Y	2352	G
1	Y	2354	A
1	Y	2360	A
1	Y	2362	A
1	Y	2374	C
1	Y	2377	C
1	Y	2381	A
1	Y	2388	A
1	Y	2395	C
1	Y	2398	G
1	Y	2400	U
1	Y	2401	C
1	Y	2410	G
1	Y	2412	C
1	Y	2413	U
1	Y	2417	U
1	Y	2419	A
1	Y	2425	U
1	Y	2433	C
1	Y	2434	A
1	Y	2437	G
1	Y	2440	G
1	Y	2448	G
1	Y	2449	C
1	Y	2452	A
1	Y	2456	G
1	Y	2457	A
1	Y	2460	A
1	Y	2461	A
1	Y	2462	A
1	Y	2466	A

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Mol	Chain	Res	Type
1	Y	2467	C
1	Y	2468	C
1	Y	2472	G
1	Y	2474	G
1	Y	2475	A
1	Y	2486	A
1	Y	2487	U
1	Y	2490	C
1	Y	2491	C
1	Y	2496	A
1	Y	2497	G
1	Y	2498	A
1	Y	2499	G
1	Y	2500	U
1	Y	2501	U
1	Y	2502	C
1	Y	2503	A
1	Y	2505	A
1	Y	2517	G
1	Y	2518	U
1	Y	2526	C
1	Y	2527	U
1	Y	2529	G
1	Y	2530	A
1	Y	2532	G
1	Y	2533	U
1	Y	2534	C
1	Y	2540	A
1	Y	2545	A
1	Y	2547	C
1	Y	2552	G
1	Y	2558	A
1	Y	2559	G
1	Y	2560	U
1	Y	2561	C
1	Y	2562	G
1	Y	2563	G
1	Y	2569	A
1	Y	2571	G
1	Y	2580	G
1	Y	2581	U
1	Y	2583	C

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Mol	Chain	Res	Type
1	Y	2591	A
1	Y	2592	A
1	Y	2593	A
1	Y	2594	G
1	Y	2599	A
1	Y	2600	C
1	Y	2601	G
1	Y	2604	A
1	Y	2612	U
1	Y	2613	C
1	Y	2618	C
1	Y	2626	G
1	Y	2629	A
1	Y	2630	G
1	Y	2635	G
1	Y	2636	U
1	Y	2637	C
1	Y	2640	U
1	Y	2641	A
1	Y	2642	U
1	Y	2648	G
1	Y	2650	G
1	Y	2651	G
1	Y	2655	U
1	Y	2656	A
1	Y	2657	G
1	Y	2658	G
1	Y	2660	A
1	Y	2665	G
1	Y	2666	A
1	Y	2672	G
1	Y	2673	C
1	Y	2682	G
1	Y	2683	U
1	Y	2694	C
1	Y	2695	G
1	Y	2696	G
1	Y	2697	G
1	Y	2700	G
1	Y	2716	U
1	Y	2728	U
1	Y	2729	G

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Mol	Chain	Res	Type
1	Y	2732	A
1	Y	2740	A
1	Y	2741	G
1	Y	2753	U
1	Y	2760	A
1	Y	2765	A
1	Y	2766	U
1	Y	2771	G
1	Y	2775	A
1	Y	2776	A
1	Y	2777	A
1	Y	2778	G
1	Y	2783	U
1	Y	2784	A
1	Y	2785	A
1	Y	2786	G
1	Y	2787	C
1	Y	2788	A
1	Y	2792	A
1	Y	2793	G
1	Y	2794	C
1	Y	2795	C
1	Y	2796	C
1	Y	2804	G
1	Y	2805	A
1	Y	2806	U
1	Y	2807	G
1	Y	2808	A
1	Y	2809	G
1	Y	2810	A
1	Y	2811	U
1	Y	2817	A
1	Y	2818	A
1	Y	2821	U
1	Y	2822	C
1	Y	2823	G
1	Y	2824	G
1	Y	2826	U
1	Y	2827	A
1	Y	2829	A
1	Y	2830	A
1	Y	2831	G

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Mol	Chain	Res	Type
1	Y	2833	U
1	Y	2834	C
1	Y	2840	A
1	Y	2841	A
1	Y	2848	G
1	Y	2854	A
1	Y	2859	G
1	Y	2878	U
1	Y	2882	A
1	Y	2887	G
1	Y	2900	C
1	Y	2903	A
1	Y	2904	U
1	Y	2905	C
1	Y	2906	G
1	Y	2911	A
1	Y	2912	A
1	Y	2913	G
1	Y	2914	A
1	Y	2916	U
1	Y	2917	U
2	X	6	U
2	X	7	G
2	X	8	G
2	X	9	A
2	X	10	G
2	X	13	U
2	X	14	U
2	X	15	U
2	X	16	G
2	X	18	U
2	X	19	C
2	X	21	U
2	X	23	G
2	X	24	C
2	X	26	C
2	X	27	A
2	X	28	G
2	X	29	G
2	X	30	A
2	X	31	U
2	X	32	G

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Mol	Chain	Res	Type
2	X	33	A
2	X	36	G
2	X	37	C
2	X	38	U
2	X	39	G
2	X	40	G
2	X	41	C
2	X	42	G
2	X	43	G
2	X	44	C
2	X	45	G
2	X	46	U
2	X	48	C
2	X	49	C
2	X	50	U
2	X	51	A
2	X	52	A
2	X	53	U
2	X	54	A
2	X	56	A
2	X	57	U
2	X	58	G
2	X	59	C
2	X	60	A
2	X	61	A
2	X	64	C
2	X	65	G
2	X	66	A
2	X	67	G
2	X	69	G
2	X	70	A
2	X	71	A
2	X	72	C
2	X	98	U
2	X	99	U
2	X	100	A
2	X	101	G
2	X	103	G
2	X	104	G
2	X	105	C
2	X	107	G
2	X	108	A

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Mol	Chain	Res	Type
2	X	109	C
2	X	111	G
2	X	113	U
2	X	114	G
2	X	115	A
2	X	116	G
2	X	117	U
2	X	118	A
2	X	119	A
2	X	120	C
2	X	121	A
2	X	127	A
2	X	128	U
2	X	130	A
2	X	131	C
2	X	134	A
2	X	137	U
2	X	140	A
2	X	141	A
2	X	142	G
2	X	143	A
2	X	144	C
2	X	146	G
2	X	147	G
2	X	148	G
2	X	150	U
2	X	151	A
2	X	153	C
2	X	154	U
2	X	155	U
2	X	156	C
2	X	157	G
2	X	158	G
2	X	160	A
2	X	162	A
2	X	163	C
2	X	166	U
2	X	167	A
2	X	168	G
2	X	169	C
2	X	170	U
2	X	172	A

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Mol	Chain	Res	Type
2	X	173	U
2	X	174	A
2	X	175	C
2	X	176	C
2	X	177	G
2	X	181	A
2	X	182	A
2	X	183	U
2	X	184	A
2	X	185	U
2	X	210	A
2	X	212	A
2	X	213	G
2	X	214	A
2	X	229	C
2	X	230	U
2	X	231	U
2	X	232	A
2	X	233	U
2	X	234	A
2	X	236	A
2	X	237	U
2	X	238	G
2	X	240	A
2	X	241	U
2	X	244	G
2	X	246	G
2	X	247	C
2	X	248	U
2	X	249	G
2	X	250	C
2	X	251	A
2	X	252	U
2	X	253	U
2	X	254	A
2	X	255	G
2	X	256	C
2	X	257	U
2	X	259	G
2	X	260	U
2	X	261	U
2	X	262	G

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Mol	Chain	Res	Type
2	X	263	G
2	X	265	A
2	X	266	A
2	X	268	G
2	X	270	A
2	X	272	C
2	X	273	G
2	X	274	G
2	X	276	U
2	X	278	A
2	X	281	A
2	X	282	A
2	X	283	G
2	X	284	G
2	X	285	C
2	X	286	A
2	X	287	A
2	X	289	G
2	X	291	U
2	X	292	G
2	X	293	C
2	X	295	U
2	X	296	A
2	X	297	G
2	X	298	C
2	X	301	A
2	X	305	G
2	X	306	A
2	X	307	G
2	X	308	A
2	X	310	G
2	X	311	G
2	X	312	U
2	X	313	G
2	X	315	U
2	X	316	C
2	X	319	C
2	X	321	A
2	X	323	A
2	X	324	C
2	X	325	U
2	X	326	G

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Mol	Chain	Res	Type
2	X	327	G
2	X	331	U
2	X	333	A
2	X	334	G
2	X	335	A
2	X	336	C
2	X	337	A
2	X	338	C
2	X	339	G
2	X	340	G
2	X	341	U
2	X	346	A
2	X	348	U
2	X	350	C
2	X	352	A
2	X	353	C
2	X	354	G
2	X	355	G
2	X	357	A
2	X	358	G
2	X	359	G
2	X	360	C
2	X	361	A
2	X	362	G
2	X	363	C
2	X	365	G
2	X	366	U
2	X	367	A
2	X	368	G
2	X	369	G
2	X	370	G
2	X	371	A
2	X	372	A
2	X	373	U
2	X	374	C
2	X	375	U
2	X	376	U
2	X	380	C
2	X	381	A
2	X	383	U
2	X	384	G
2	X	385	G

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Mol	Chain	Res	Type
2	X	387	C
2	X	388	G
2	X	389	A
2	X	391	A
2	X	393	C
2	X	394	C
2	X	396	G
2	X	397	A
2	X	398	C
2	X	400	G
2	X	403	C
2	X	404	A
2	X	405	A
2	X	406	C
2	X	407	G
2	X	408	C
2	X	409	C
2	X	411	C
2	X	412	G
2	X	413	U
2	X	414	G
2	X	416	G
2	X	417	U
2	X	418	G
2	X	419	A
2	X	420	U
2	X	421	G
2	X	422	A
2	X	424	G
2	X	425	G
2	X	427	C
2	X	429	U
2	X	430	C
2	X	432	G
2	X	433	A
2	X	436	G
2	X	437	U
2	X	438	A
2	X	439	A
2	X	440	A
2	X	441	A
2	X	442	C

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Mol	Chain	Res	Type
2	X	443	U
2	X	444	C
2	X	446	G
2	X	447	U
2	X	448	U
2	X	451	U
2	X	452	A
2	X	454	G
2	X	455	G
2	X	458	G
2	X	459	A
2	X	460	A
2	X	461	C
2	X	462	A
2	X	463	U
2	X	464	A
2	X	465	U
2	X	466	G
2	X	467	U
2	X	468	G
2	X	482	A
2	X	484	A
2	X	485	U
2	X	486	C
2	X	487	U
2	X	488	U
2	X	490	A
2	X	491	C
2	X	495	A
2	X	497	C
2	X	498	U
2	X	501	U
2	X	502	C
2	X	503	A
2	X	504	G
2	X	505	A
2	X	506	A
2	X	507	A
2	X	509	C
2	X	510	C
2	X	511	A
2	X	513	G

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Mol	Chain	Res	Type
2	X	514	G
2	X	515	C
2	X	517	A
2	X	518	A
2	X	519	C
2	X	520	U
2	X	522	C
2	X	525	G
2	X	526	C
2	X	527	C
2	X	528	A
2	X	531	A
2	X	532	G
2	X	534	C
2	X	535	G
2	X	537	G
2	X	540	A
2	X	542	U
2	X	543	A
2	X	544	C
2	X	545	G
2	X	547	A
2	X	549	G
2	X	551	G
2	X	555	A
2	X	556	G
2	X	557	C
2	X	558	G
2	X	559	U
2	X	561	A
2	X	563	C
2	X	564	C
2	X	565	G
2	X	566	G
2	X	567	A
2	X	568	A
2	X	569	U
2	X	570	U
2	X	571	A
2	X	572	U
2	X	574	G
2	X	575	G

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Mol	Chain	Res	Type
2	X	576	G
2	X	577	C
2	X	578	G
2	X	580	A
2	X	582	A
2	X	583	G
2	X	584	C
2	X	585	G
2	X	588	C
2	X	589	G
2	X	590	U
2	X	591	A
2	X	592	G
2	X	593	G
2	X	594	C
2	X	595	G
2	X	596	G
2	X	597	U
2	X	602	U
2	X	603	A
2	X	604	A
2	X	605	G
2	X	606	U
2	X	607	C
2	X	608	U
2	X	610	A
2	X	611	U
2	X	613	U
2	X	615	A
2	X	616	A
2	X	617	A
2	X	618	G
2	X	619	C
2	X	620	C
2	X	621	C
2	X	622	A
2	X	623	C
2	X	624	G
2	X	625	G
2	X	627	U
2	X	628	C
2	X	629	A

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Mol	Chain	Res	Type
2	X	630	A
2	X	631	C
2	X	632	C
2	X	635	G
2	X	636	G
2	X	638	G
2	X	639	G
2	X	641	U
2	X	642	C
2	X	643	A
2	X	644	U
2	X	645	U
2	X	647	G
2	X	648	A
2	X	649	A
2	X	650	A
2	X	651	C
2	X	652	U
2	X	653	G
2	X	656	A
2	X	657	A
2	X	659	C
2	X	662	G
2	X	663	A
2	X	664	G
2	X	665	U
2	X	666	G
2	X	667	C
2	X	668	A
2	X	669	G
2	X	670	A
2	X	671	A
2	X	672	G
2	X	673	A
2	X	674	G
2	X	675	G
2	X	677	A
2	X	679	G
2	X	681	G
2	X	682	G
2	X	683	A
2	X	685	U

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Mol	Chain	Res	Type
2	X	686	U
2	X	687	C
2	X	690	U
2	X	691	G
2	X	692	U
2	X	693	G
2	X	694	U
2	X	695	A
2	X	696	G
2	X	699	G
2	X	701	G
2	X	702	A
2	X	704	A
2	X	705	U
2	X	706	G
2	X	708	G
2	X	709	C
2	X	710	A
2	X	711	G
2	X	712	A
2	X	714	A
2	X	715	U
2	X	716	A
2	X	717	U
2	X	719	G
2	X	720	A
2	X	721	G
2	X	722	G
2	X	723	A
2	X	725	C
2	X	726	A
2	X	727	C
2	X	728	C
2	X	729	A
2	X	730	G
2	X	731	U
2	X	732	G
2	X	733	G
2	X	734	C
2	X	736	A
2	X	737	A
2	X	738	G

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Mol	Chain	Res	Type
2	X	739	G
2	X	740	C
2	X	741	G
2	X	743	C
2	X	744	U
2	X	746	U
2	X	747	C
2	X	748	U
2	X	749	G
2	X	750	G
2	X	751	U
2	X	752	C
2	X	753	U
2	X	757	A
2	X	758	C
2	X	759	U
2	X	761	A
2	X	763	G
2	X	765	U
2	X	766	G
2	X	767	A
2	X	768	U
2	X	769	G
2	X	770	U
2	X	771	G
2	X	772	C
2	X	773	G
2	X	774	A
2	X	776	A
2	X	779	G
2	X	780	U
2	X	781	G
2	X	782	G
2	X	783	G
2	X	784	G
2	X	785	A
2	X	786	U
2	X	787	C
2	X	788	A
2	X	789	A
2	X	791	C
2	X	793	G

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Mol	Chain	Res	Type
2	X	794	G
2	X	795	A
2	X	797	U
2	X	798	A
2	X	799	G
2	X	801	U
2	X	802	A
2	X	803	C
2	X	804	C
2	X	809	U
2	X	810	A
2	X	811	G
2	X	812	U
2	X	815	A
2	X	816	C
2	X	817	G
2	X	818	C
2	X	820	G
2	X	821	U
2	X	822	A
2	X	823	A
2	X	824	A
2	X	825	C
2	X	826	G
2	X	827	A
2	X	828	U
2	X	829	G
2	X	830	A
2	X	831	G
2	X	832	U
2	X	833	G
2	X	835	U
2	X	836	A
2	X	838	G
2	X	840	G
2	X	841	U
2	X	842	U
2	X	843	A
2	X	845	G
2	X	846	G
2	X	848	G
2	X	856	C

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Mol	Chain	Res	Type
2	X	857	C
2	X	858	C
2	X	860	U
2	X	861	U
2	X	863	G
2	X	864	U
2	X	865	G
2	X	868	G
2	X	870	A
2	X	871	G
2	X	872	C
2	X	874	A
2	X	878	C
2	X	879	A
2	X	880	U
2	X	882	A
2	X	883	A
2	X	885	C
2	X	887	C
2	X	888	U
2	X	889	C
2	X	890	C
2	X	891	G
2	X	892	C
2	X	893	C
2	X	894	U
2	X	895	G
2	X	896	G
2	X	897	G
2	X	898	G
2	X	899	A
2	X	900	G
2	X	901	U
2	X	902	A
2	X	904	G
2	X	905	A
2	X	906	C
2	X	908	G
2	X	909	C
2	X	910	A
2	X	911	A
2	X	912	G

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Mol	Chain	Res	Type
2	X	913	G
2	X	915	U
2	X	916	G
2	X	923	A
2	X	924	A
2	X	926	G
2	X	927	G
2	X	928	A
2	X	929	A
2	X	932	G
2	X	933	A
2	X	934	C
2	X	935	G
2	X	936	G
2	X	937	G
2	X	940	C
2	X	943	G
2	X	944	C
2	X	945	A
2	X	946	C
2	X	948	A
2	X	949	G
2	X	951	G
2	X	953	U
2	X	954	G
2	X	955	G
2	X	956	A
2	X	958	C
2	X	959	A
2	X	960	U
2	X	961	G
2	X	962	U
2	X	963	G
2	X	964	G
2	X	965	U
2	X	966	U
2	X	967	U
2	X	968	A
2	X	970	U
2	X	971	U
2	X	972	C
2	X	974	A

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Mol	Chain	Res	Type
2	X	975	A
2	X	977	C
2	X	978	A
2	X	979	A
2	X	981	G
2	X	982	C
2	X	983	G
2	X	984	A
2	X	986	G
2	X	987	A
2	X	991	U
2	X	992	U
2	X	993	A
2	X	994	C
2	X	995	C
2	X	996	A
2	X	997	A
2	X	998	A
2	X	999	U
2	X	1000	C
2	X	1001	U
2	X	1002	U
2	X	1004	A
2	X	1005	C
2	X	1006	A
2	X	1008	C
2	X	1011	U
2	X	1013	G
2	X	1014	A
2	X	1015	C
2	X	1016	A
2	X	1017	A
2	X	1018	C
2	X	1019	U
2	X	1022	A
2	X	1023	G
2	X	1027	U
2	X	1029	G
2	X	1030	A
2	X	1032	C
2	X	1033	C
2	X	1034	U

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Mol	Chain	Res	Type
2	X	1052	A
2	X	1054	U
2	X	1061	U
2	X	1062	G
2	X	1063	G
2	X	1064	U
2	X	1065	G
2	X	1066	C
2	X	1067	A
2	X	1070	G
2	X	1071	U
2	X	1073	G
2	X	1075	C
2	X	1076	G
2	X	1077	U
2	X	1078	C
2	X	1079	A
2	X	1082	U
2	X	1083	C
2	X	1086	G
2	X	1087	U
2	X	1088	C
2	X	1089	G
2	X	1090	U
2	X	1091	G
2	X	1092	A
2	X	1093	G
2	X	1094	A
2	X	1095	U
2	X	1096	G
2	X	1098	U
2	X	1100	G
2	X	1101	G
2	X	1106	G
2	X	1107	U
2	X	1108	C
2	X	1109	C
2	X	1110	C
2	X	1111	G
2	X	1113	A
2	X	1114	A
2	X	1115	C

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Mol	Chain	Res	Type
2	X	1118	G
2	X	1120	G
2	X	1121	C
2	X	1122	A
2	X	1127	U
2	X	1128	U
2	X	1130	A
2	X	1131	G
2	X	1133	U
2	X	1134	U
2	X	1135	A
2	X	1136	G
2	X	1137	U
2	X	1138	U
2	X	1139	G
2	X	1141	C
2	X	1143	U
2	X	1144	C
2	X	1146	U
2	X	1147	U
2	X	1148	A
2	X	1149	A
2	X	1150	G
2	X	1151	U
2	X	1152	U
2	X	1153	G
2	X	1154	G
2	X	1155	G
2	X	1157	A
2	X	1158	C
2	X	1159	U
2	X	1160	C
2	X	1161	U
2	X	1163	A
2	X	1164	G
2	X	1165	U
2	X	1166	U
2	X	1167	G
2	X	1168	A
2	X	1169	C
2	X	1171	G
2	X	1172	C

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Mol	Chain	Res	Type
2	X	1173	C
2	X	1174	G
2	X	1175	G
2	X	1176	U
2	X	1178	A
2	X	1180	A
2	X	1181	A
2	X	1182	A
2	X	1185	G
2	X	1187	A
2	X	1188	G
2	X	1189	G
2	X	1190	A
2	X	1192	G
2	X	1193	G
2	X	1194	U
2	X	1195	G
2	X	1196	G
2	X	1197	G
2	X	1198	G
2	X	1200	U
2	X	1201	G
2	X	1202	A
2	X	1203	C
2	X	1204	G
2	X	1207	A
2	X	1208	A
2	X	1209	A
2	X	1211	C
2	X	1212	A
2	X	1213	U
2	X	1214	C
2	X	1216	U
2	X	1217	G
2	X	1218	C
2	X	1220	C
2	X	1221	C
2	X	1222	U
2	X	1223	U
2	X	1224	A
2	X	1226	G
2	X	1227	A

Continued on next page...

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Mol	Chain	Res	Type
2	X	1228	U
2	X	1230	U
2	X	1231	G
2	X	1232	G
2	X	1234	C
2	X	1235	U
2	X	1236	A
2	X	1237	C
2	X	1238	A
2	X	1239	C
2	X	1240	A
2	X	1241	C
2	X	1243	U
2	X	1244	G
2	X	1245	C
2	X	1246	U
2	X	1247	A
2	X	1249	A
2	X	1251	U
2	X	1252	G
2	X	1253	G
2	X	1256	A
2	X	1257	A
2	X	1258	U
2	X	1259	A
2	X	1261	A
2	X	1262	A
2	X	1267	C
2	X	1268	A
2	X	1269	G
2	X	1270	C
2	X	1271	G
2	X	1272	A
2	X	1273	A
2	X	1276	C
2	X	1277	G
2	X	1278	C
2	X	1279	G
2	X	1281	G
2	X	1282	G
2	X	1283	U
2	X	1284	C

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Mol	Chain	Res	Type
2	X	1285	A
2	X	1287	G
2	X	1288	C
2	X	1291	A
2	X	1292	U
2	X	1294	C
2	X	1296	A
2	X	1297	U
2	X	1298	A
2	X	1299	A
2	X	1302	U
2	X	1304	G
2	X	1309	C
2	X	1310	A
2	X	1311	G
2	X	1312	U
2	X	1313	U
2	X	1314	C
2	X	1315	G
2	X	1316	G
2	X	1318	U
2	X	1319	U
2	X	1322	A
2	X	1325	C
2	X	1326	U
2	X	1327	G
2	X	1328	C
2	X	1329	A
2	X	1330	A
2	X	1331	C
2	X	1332	U
2	X	1333	C
2	X	1334	G
2	X	1335	A
2	X	1339	C
2	X	1341	U
2	X	1342	G
2	X	1343	A
2	X	1344	A
2	X	1345	G
2	X	1346	C
2	X	1349	G

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Mol	Chain	Res	Type
2	X	1351	A
2	X	1352	U
2	X	1356	U
2	X	1357	A
2	X	1358	G
2	X	1359	U
2	X	1360	A
2	X	1361	A
2	X	1363	C
2	X	1369	U
2	X	1373	C
2	X	1374	A
2	X	1375	U
2	X	1376	G
2	X	1377	C
2	X	1379	A
2	X	1380	C
2	X	1382	G
2	X	1383	U
2	X	1384	G
2	X	1385	A
2	X	1386	A
2	X	1387	U
2	X	1388	A
2	X	1389	C
2	X	1390	G
2	X	1391	U
2	X	1392	U
2	X	1394	C
2	X	1397	G
2	X	1398	G
2	X	1399	U
2	X	1400	C
2	X	1401	U
2	X	1402	U
2	X	1403	G
2	X	1404	U
2	X	1406	C
2	X	1407	A
2	X	1408	C
2	X	1409	A
2	X	1410	C

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Mol	Chain	Res	Type
2	X	1412	G
2	X	1413	C
2	X	1414	C
2	X	1416	G
2	X	1418	C
2	X	1419	A
2	X	1420	C
2	X	1423	C
2	X	1427	A
2	X	1428	G
2	X	1429	A
2	X	1430	G
2	X	1431	U
2	X	1432	U
2	X	1435	U
2	X	1443	G
2	X	1444	A
2	X	1446	G
2	X	1447	C
2	X	1448	C
2	X	1449	G
2	X	1451	U
2	X	1452	G
2	X	1454	A
2	X	1455	G
2	X	1456	U
2	X	1457	A
2	X	1459	C
2	X	1460	C
2	X	1461	U
2	X	1462	U
2	X	1463	U
2	X	1465	A
2	X	1467	G
2	X	1468	A
2	X	1469	G
2	X	1471	U
2	X	1472	A
2	X	1473	G
2	X	1475	C
2	X	1476	G
2	X	1477	U

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Mol	Chain	Res	Type
2	X	1479	G
2	X	1481	A
2	X	1484	U
2	X	1485	G
2	X	1487	G
2	X	1490	A
2	X	1493	U
2	X	1496	U
2	X	1497	U
2	X	1498	G
2	X	1499	G
2	X	1500	G
2	X	1501	G
2	X	1504	A
2	X	1505	A
2	X	1507	U
2	X	1508	C
2	X	1510	U
2	X	1511	A
2	X	1512	A
2	X	1513	C
2	X	1514	A
2	X	1515	A
2	X	1516	G
2	X	1517	G
2	X	1518	U
2	X	1519	A
2	X	1522	C
2	X	1525	A
2	X	1526	U
2	X	1528	G
2	X	1529	G
2	X	1530	A
2	X	1531	A
2	X	1532	G
2	X	1534	U
2	X	1535	G
2	X	1537	G
2	X	1538	G
2	X	1540	U
2	X	1541	G
2	X	1542	G

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Mol	Chain	Res	Type
3	3	8	A
3	3	10	U
3	3	11	A
3	3	13	A
3	3	17	A
3	3	19	G
3	3	20	A
3	3	22	G
3	3	25	A
3	3	26	C
3	3	27	A
3	3	29	C
3	3	30	U
3	3	32	U
3	3	33	U
3	3	35	C
3	3	38	U
3	3	39	G
3	3	40	C
3	3	41	C
3	3	42	G
3	3	43	A
3	3	49	G
3	3	50	A
3	3	51	A
3	3	54	U
3	3	55	A
3	3	61	U
3	3	64	A
3	3	67	G
3	3	70	G
3	3	71	A
3	3	76	A
3	3	83	U
3	3	84	U
3	3	85	A
3	3	86	C
3	3	87	G
3	3	88	U
3	3	90	C
3	3	93	C
3	3	95	A

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Mol	Chain	Res	Type
3	3	96	G
3	3	100	A
3	3	102	A
3	3	105	G
3	3	106	U

All (106) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	Y	104	C
1	Y	139	U
1	Y	145	A
1	Y	149	U
1	Y	157	U
1	Y	174	U
1	Y	175	C
1	Y	208	G
1	Y	324	A
1	Y	338	G
1	Y	388	A
1	Y	402	C
1	Y	410	G
1	Y	434	G
1	Y	548	A
1	Y	660	A
1	Y	690	U
1	Y	770	G
1	Y	846	G
1	Y	872	U
1	Y	1029	C
1	Y	1154	G
1	Y	1186	A
1	Y	1357	G
1	Y	1368	C
1	Y	1474	C
1	Y	1477	U
1	Y	1479	G
1	Y	1491	C
1	Y	1506	C
1	Y	1560	A
1	Y	1610	G
1	Y	1635	A

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Mol	Chain	Res	Type
1	Y	1879	U
1	Y	1897	U
1	Y	1902	G
1	Y	1946	A
1	Y	2334	G
1	Y	2338	A
1	Y	2345	A
1	Y	2591	A
1	Y	2664	U
1	Y	2785	A
1	Y	2830	A
1	Y	2905	C
1	Y	2910	G
1	Y	2911	A
1	Y	2912	A
2	X	21	U
2	X	61	A
2	X	63	U
2	X	99	U
2	X	114	G
2	X	246	G
2	X	249	G
2	X	251	A
2	X	277	U
2	X	334	G
2	X	353	C
2	X	384	G
2	X	396	G
2	X	419	A
2	X	436	G
2	X	514	G
2	X	522	C
2	X	589	G
2	X	606	U
2	X	616	A
2	X	635	G
2	X	682	G
2	X	695	A
2	X	730	G
2	X	756	A
2	X	764	C
2	X	796	U

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Mol	Chain	Res	Type
2	X	823	A
2	X	826	G
2	X	828	U
2	X	884	G
2	X	895	G
2	X	927	G
2	X	935	G
2	X	970	U
2	X	1014	A
2	X	1016	A
2	X	1105	A
2	X	1117	A
2	X	1134	U
2	X	1160	C
2	X	1202	A
2	X	1207	A
2	X	1222	U
2	X	1251	U
2	X	1268	A
2	X	1311	G
2	X	1378	U
2	X	1379	A
2	X	1384	G
2	X	1401	U
2	X	1431	U
2	X	1462	U
2	X	1496	U
2	X	1507	U
2	X	1511	A
3	3	26	C
3	3	40	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.

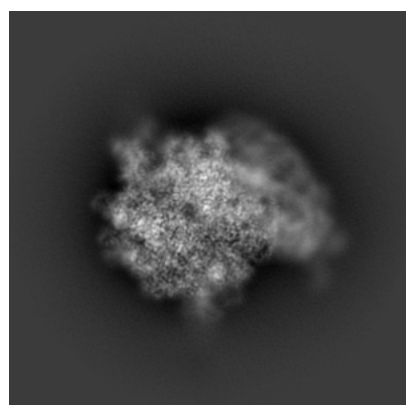
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11903. These allow visual inspection of the internal detail of the map and identification of artifacts.

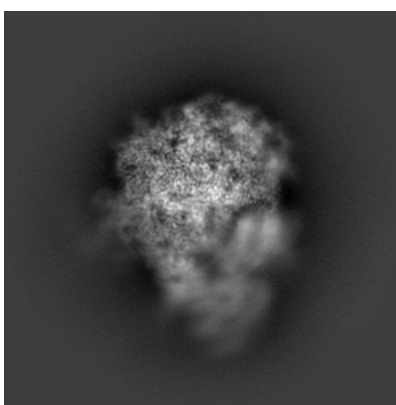
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

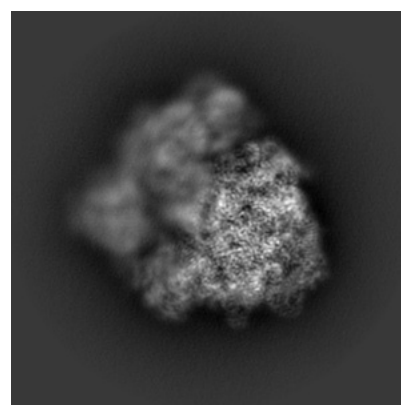
6.1.1 Primary map



X



Y

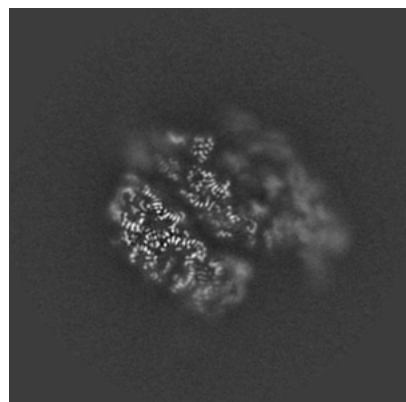


Z

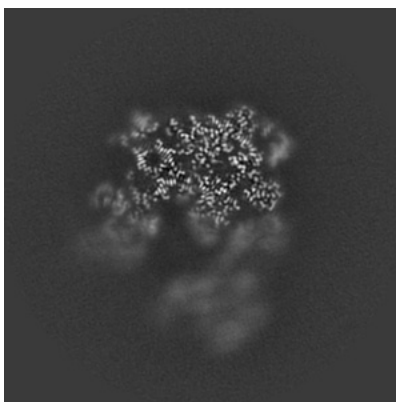
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

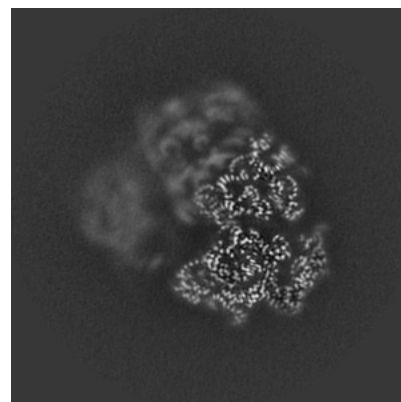
6.2.1 Primary map



X Index: 240



Y Index: 240

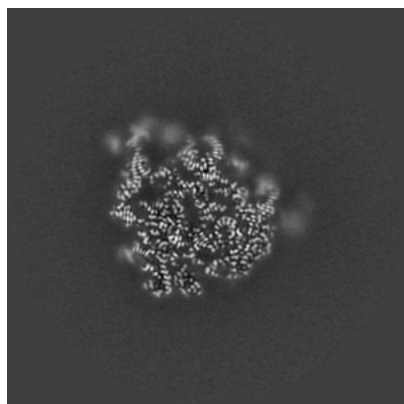


Z Index: 240

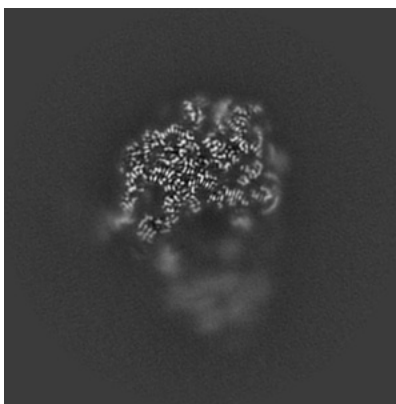
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

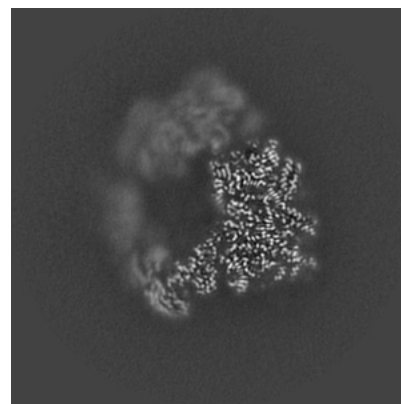
6.3.1 Primary map



X Index: 294



Y Index: 206

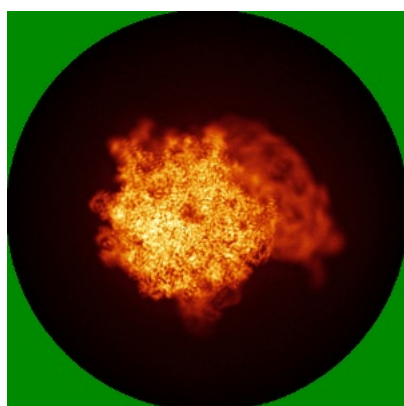


Z Index: 213

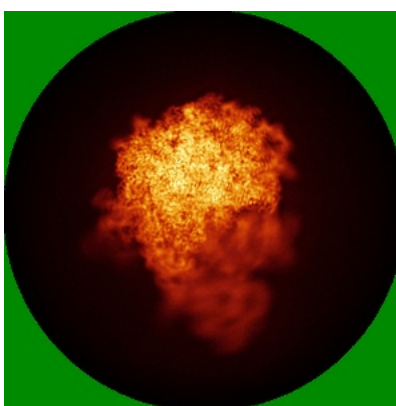
The images above show the largest variance slices of the map in three orthogonal directions.

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

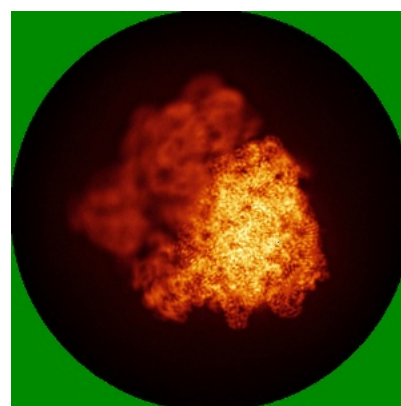
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

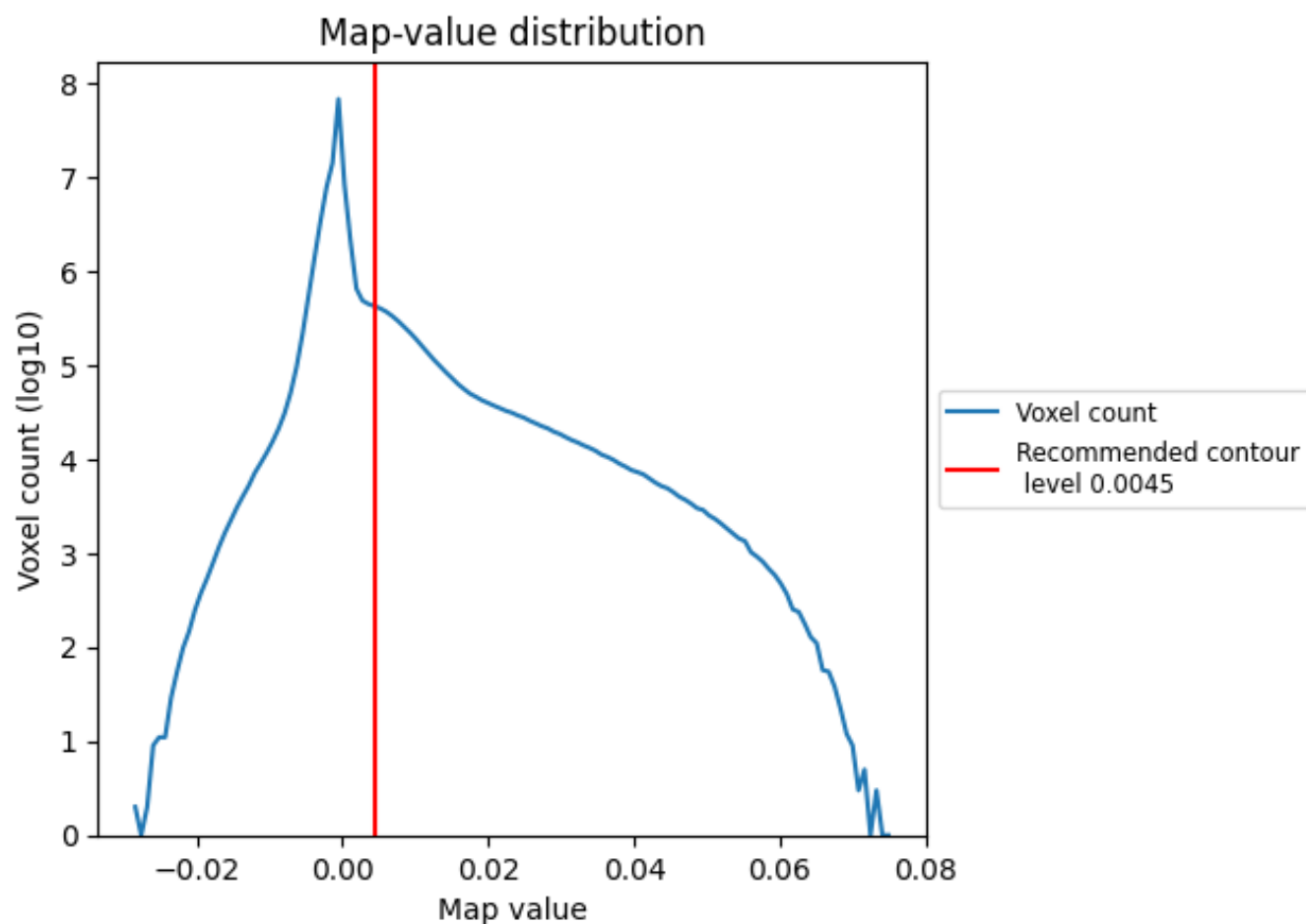
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

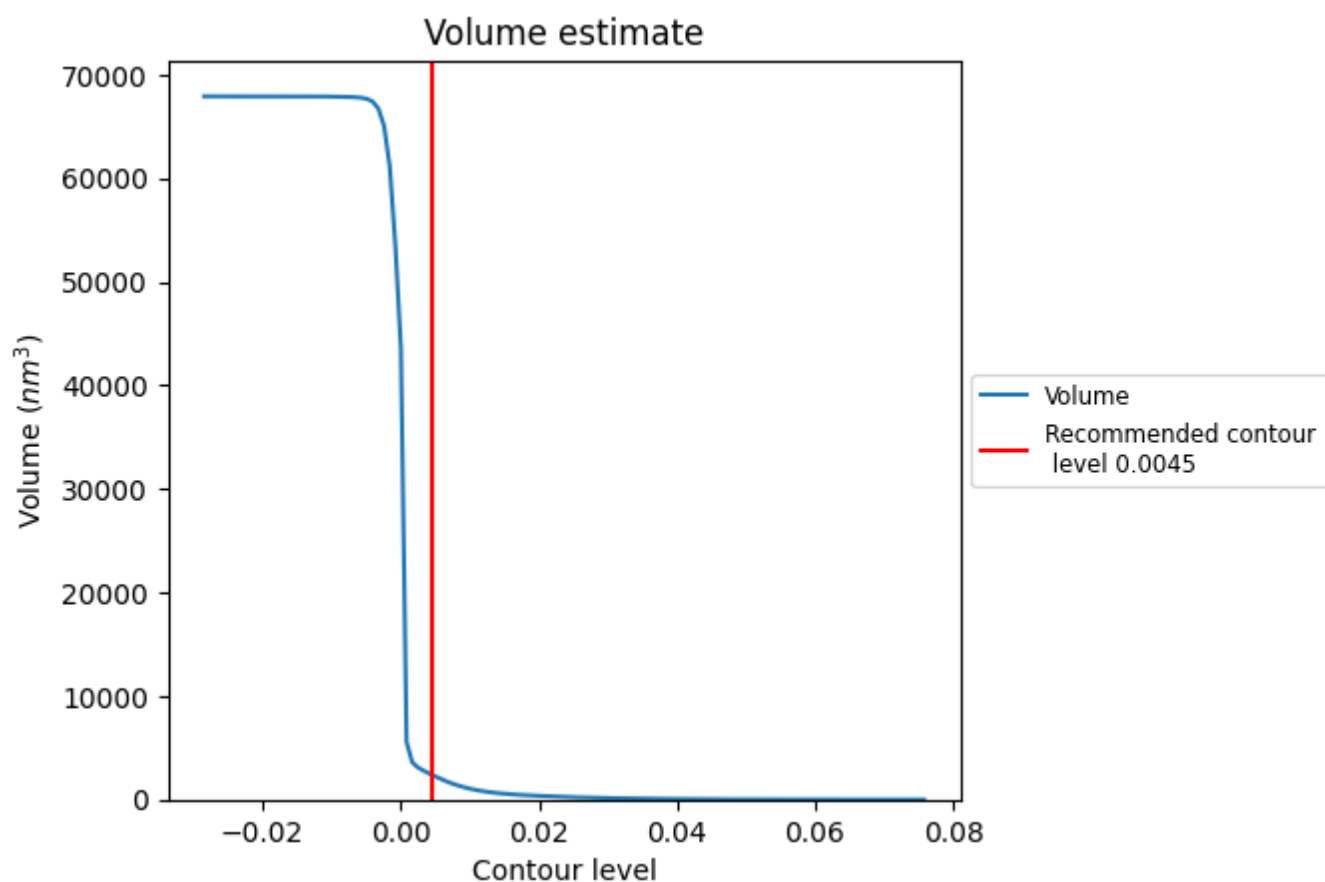
This section contains the results of statistical analysis of the map.

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.

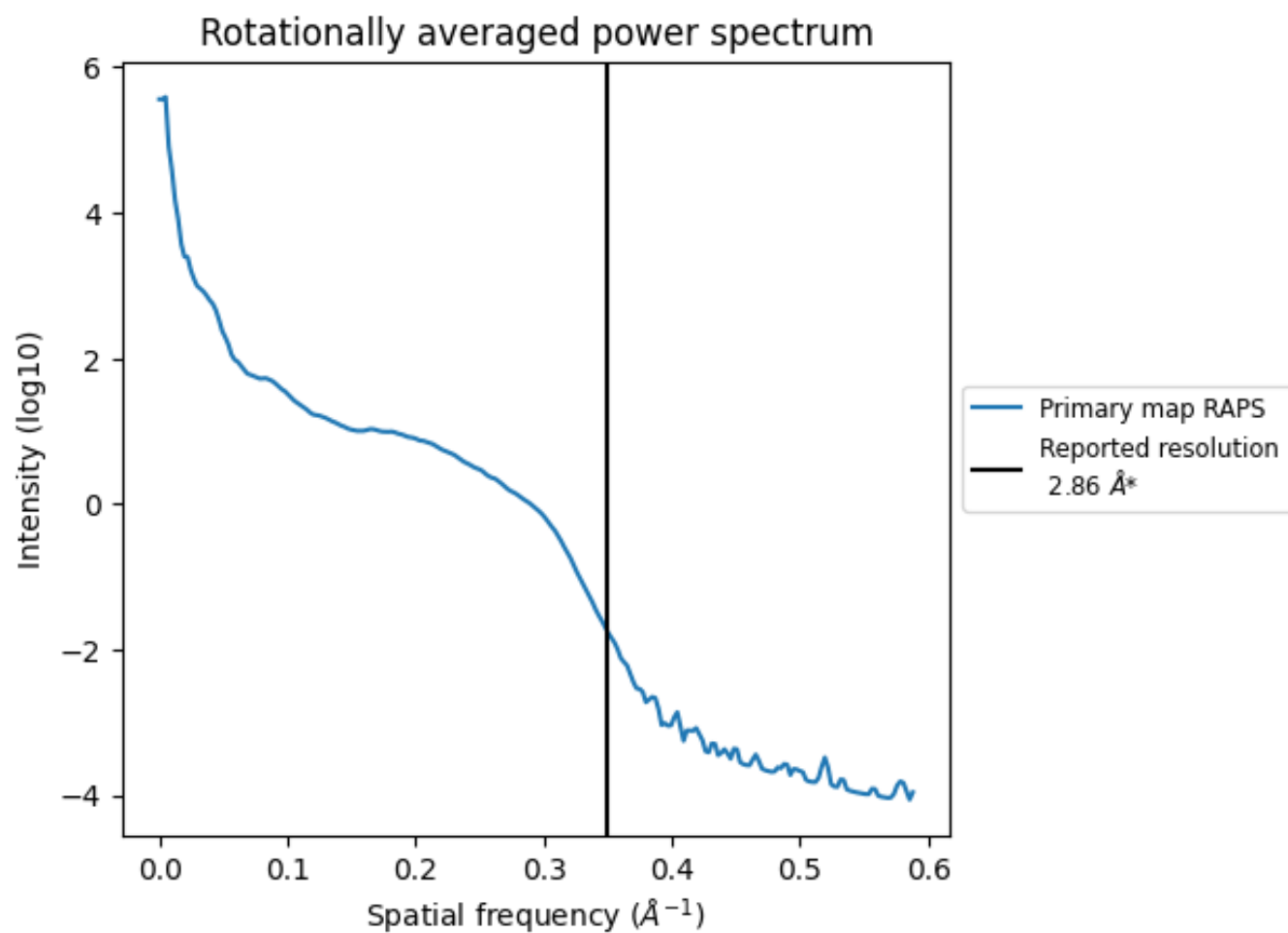
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2394 nm^3 ; this corresponds to an approximate mass of 2163 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 0.350 Å⁻¹

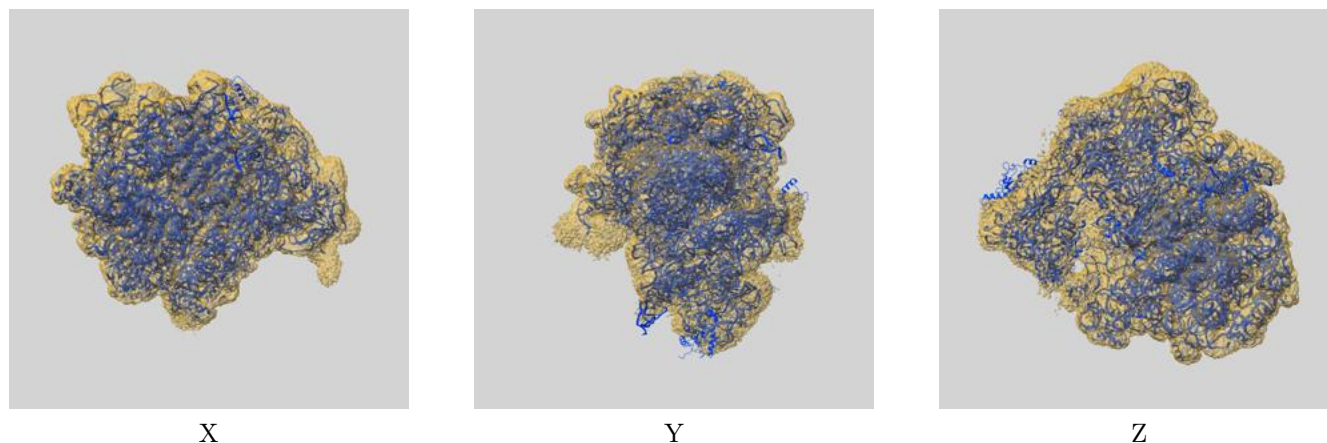
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11903 and PDB model 7ASP. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



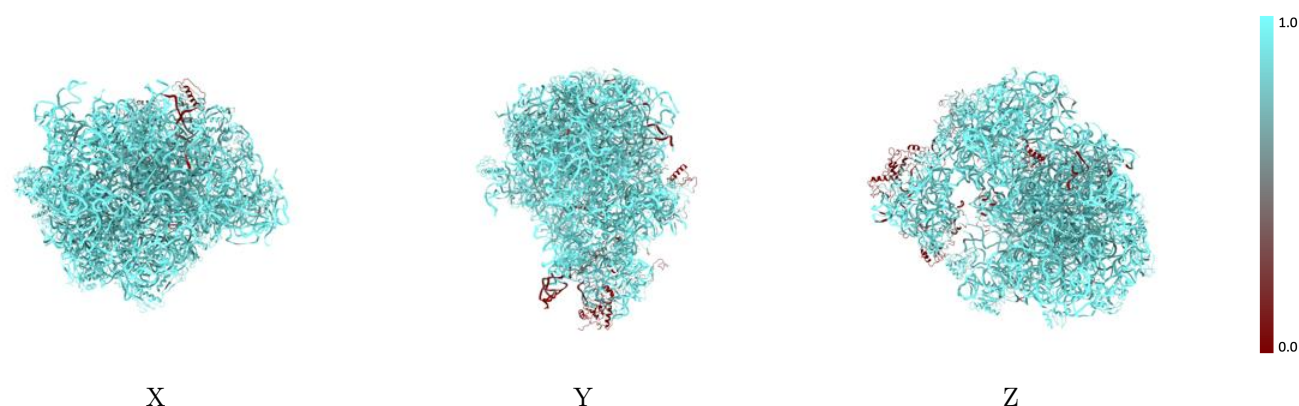
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



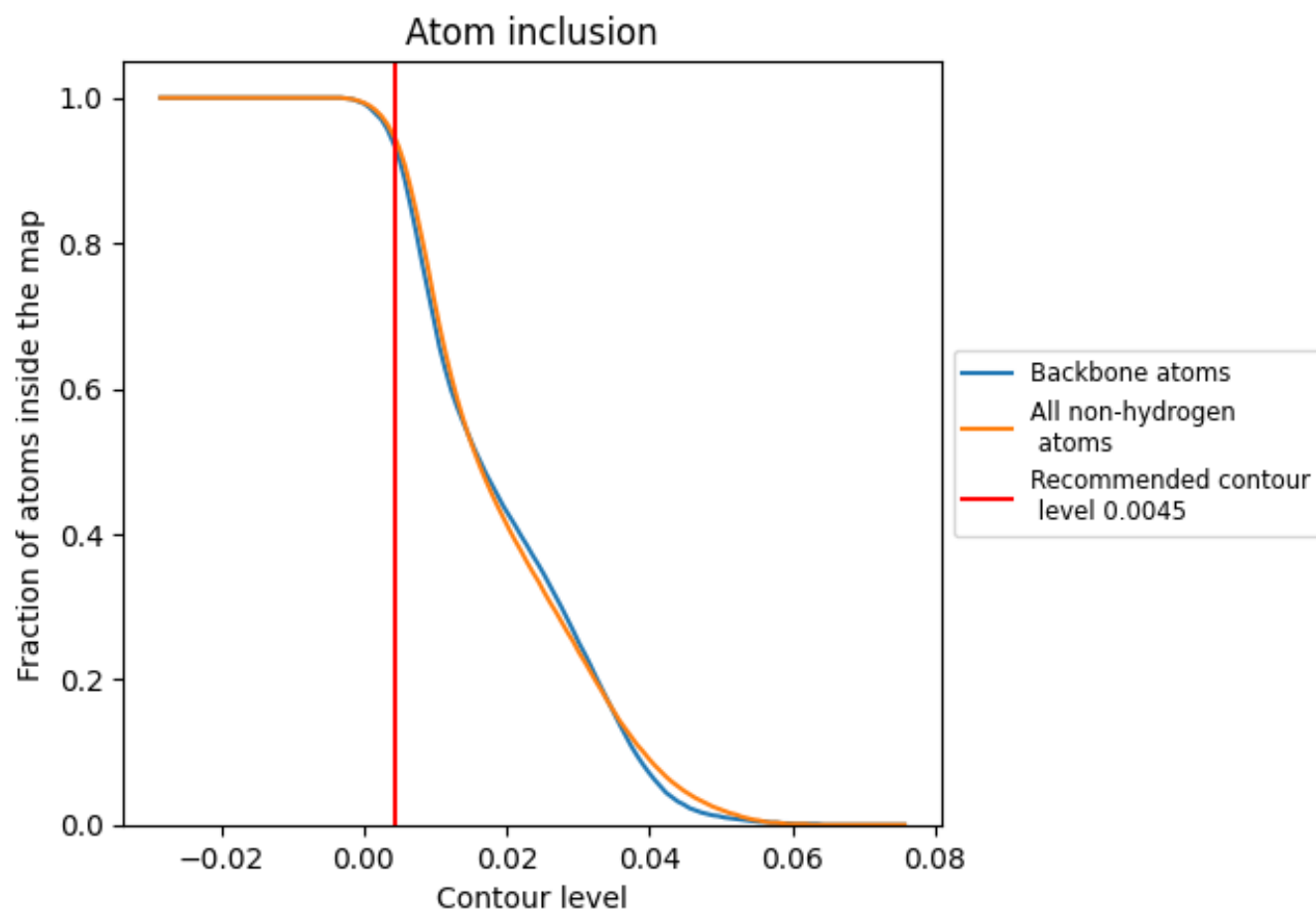
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0045).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 94% 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 (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9420	 0.3760
1	 0.9820	 0.5540
2	 0.9760	 0.5590
3	 0.9980	 0.4340
4	 0.9340	 0.5020
A	 0.8800	 0.4910
B	 0.9830	 0.5810
C	 0.9670	 0.5420
D	 0.9770	 0.5480
E	 0.9810	 0.5310
F	 0.9910	 0.3300
G	 0.9660	 0.2980
H	 0.9810	 0.5560
I	 0.9740	 0.5610
J	 0.9880	 0.5380
K	 0.9800	 0.5410
L	 0.9810	 0.5530
M	 0.9920	 0.4440
N	 0.9620	 0.5490
O	 0.9860	 0.5680
P	 0.9880	 0.5600
Q	 0.9710	 0.5490
R	 0.9830	 0.5250
S	 0.9800	 0.4750
T	 0.9450	 0.4880
U	 0.9670	 0.5580
V	 0.9780	 0.5240
W	 0.9890	 0.4400
X	 0.9560	 0.1800
Y	 0.9810	 0.4900
Z	 0.9850	 0.5060
a	 0.6290	 0.0890
b	 0.6160	 0.0970
c	 0.5690	 0.1800
d	 0.5130	 0.0780



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Chain	Atom inclusion	Q-score
e	 0.4830	 0.0600
f	 0.9010	 0.1860
g	 0.8350	 0.0730
h	 0.9060	 0.1110
i	 0.8730	 0.1350
j	 0.9780	 0.1810
k	 0.4020	 0.0840
l	 0.7630	 0.0860
m	 0.7940	 0.0820
n	 0.4670	 0.0870
o	 0.8880	 0.1140
p	 0.7240	 0.0840
q	 0.7210	 0.1080