



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:20 pm GMT

PDB ID : 6ENF
EMDB ID : EMD-3898
Title : Cryo-EM structure of a polyproline-stalled ribosome in the absence of EF-P
Authors : Huter, P.; Arenz, S.; Wilson, D.N.
Deposited on : 2017-10-04
Resolution : 3.20 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:

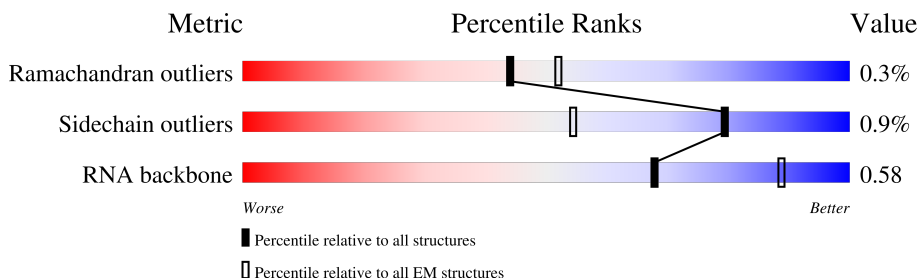
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	a	1539	
2	b	218	
3	c	206	
4	d	205	
5	e	157	
6	f	100	
7	g	151	
8	h	129	

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Mol	Chain	Length	Quality of chain
9	i	127	35% 98%
10	j	98	54% 99%
11	k	116	34% 99%
12	l	123	24% 98%
13	m	114	42% 97%
14	n	101	33% 100%
15	o	88	30% 100%
16	p	82	26% 99%
17	q	80	36% 98%
18	r	65	32% 100%
19	s	79	37% 100%
20	t	85	31% 100%
21	u	65	77% 100%
22	v	3	33% 67%
23	A	2903	10% 77% 18%
24	B	120	12% 80% 17%
25	C	271	15% 99%
26	D	209	16% 100%
27	E	201	35% 100%
28	F	177	48% 99%
29	G	176	58% 98%
30	J	142	16% 100%
31	K	122	22% 100%
32	L	143	20% 99%
33	M	136	21% 97%

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Mol	Chain	Length	Quality of chain
34	N	120	12% 99%
35	O	116	28% 100%
36	P	114	27% 99%
37	Q	117	13% 100%
38	R	103	33% 98%
39	S	110	18% 99%
40	T	93	32% 100%
41	U	102	48% 99%
42	V	94	36% 100%
43	W	78	17% 73% 23%
44	X	77	23% 99%
45	Y	63	48% 100%
46	Z	58	19% 100%
47	0	56	21% 100%
48	1	50	36% 100%
49	2	46	11% 100%
50	3	64	12% 95%
51	4	38	16% 100%
52	6	66	83% 100%
53	x	77	36% 61% 32% 6%

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 140797 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1539	33016	14725	6052	10700	1539	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	218	1704	1081	305	311	7	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	157	1141	709	218	208	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	100	817	515	148	148	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	151	1181	735	227	215	4	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	116	869	535	173	158	3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	123	955	590	196	165	4	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	114	883	546	178	156	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	n	101	799	498	165	133	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	p	82	649	406	128	114	1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	q	80	648	411	121	113	3	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	r	65	504	317	96	91	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	s	79	637	408	120	107	2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 22 is a RNA chain called RNA (5'-R(P*CP*CP*G)-3'), mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	v	3	Total	C	N	O	P	0	0
			63	28	11	21	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A	2807	Total	C	N	O	P	0	0
			60275	26888	11109	19471	2807		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 802133627
A	1847	G	A	conflict	GB 802133627
A	2069	A	G	conflict	GB 802133627

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1213441078

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

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

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

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

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	W	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

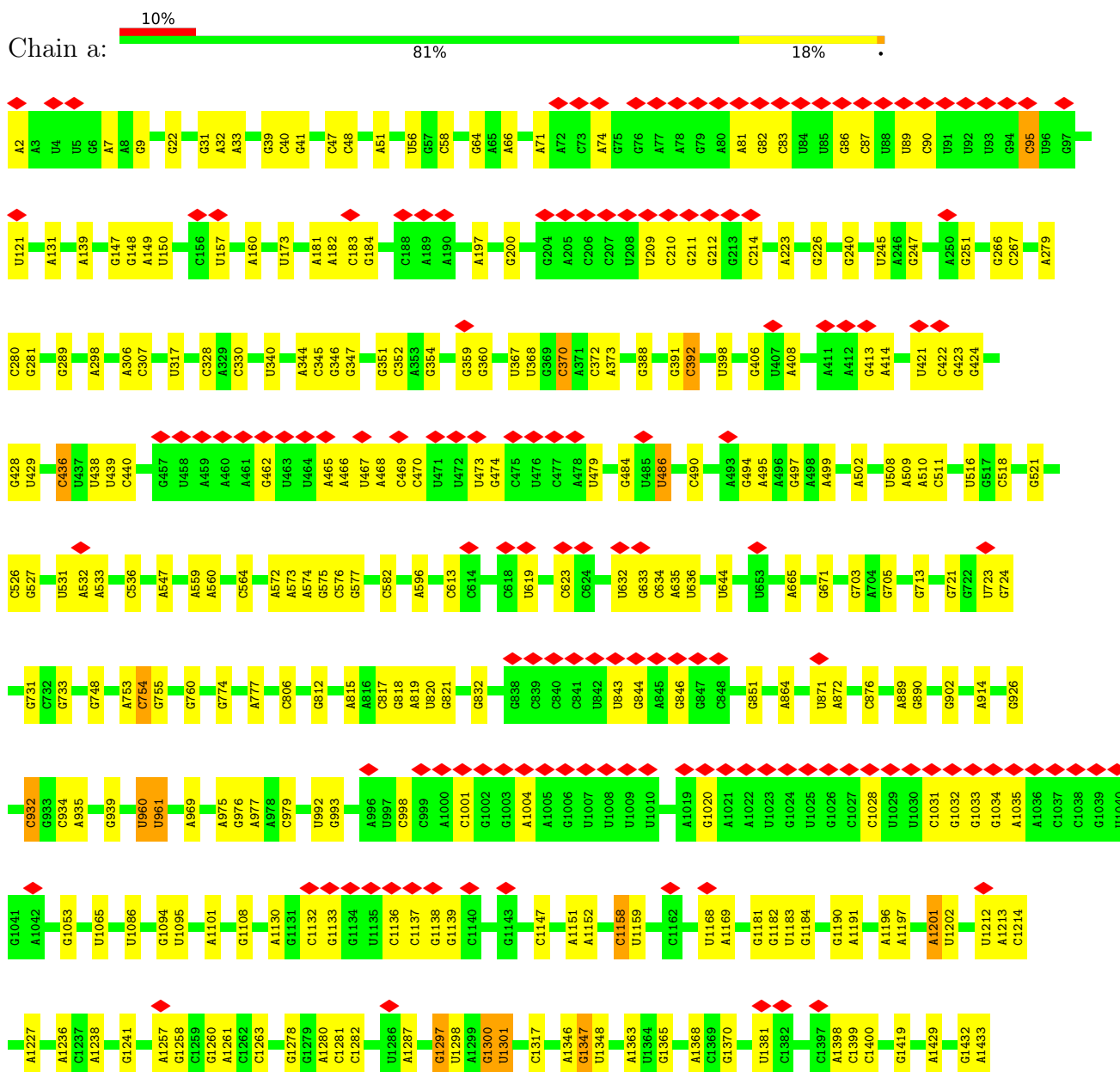
- Molecule 53 is a RNA chain called proline tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	x	77	1646	733	295	541	77	0	0

3 Residue-property plots

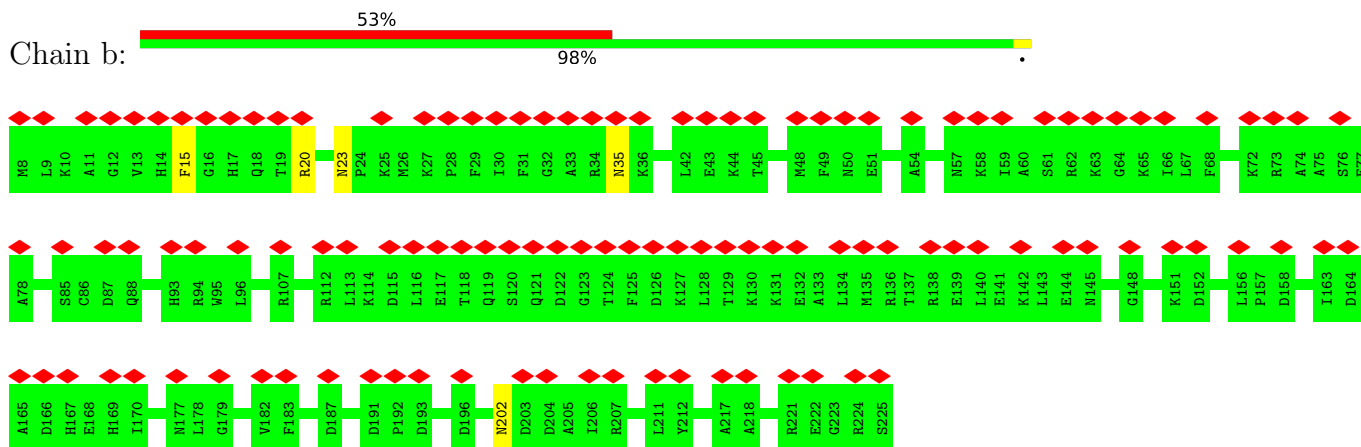
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S ribosomal RNA

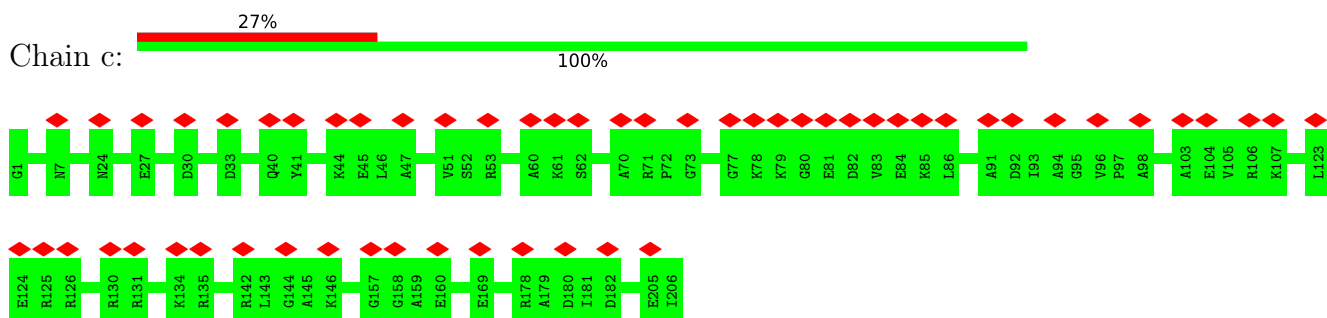




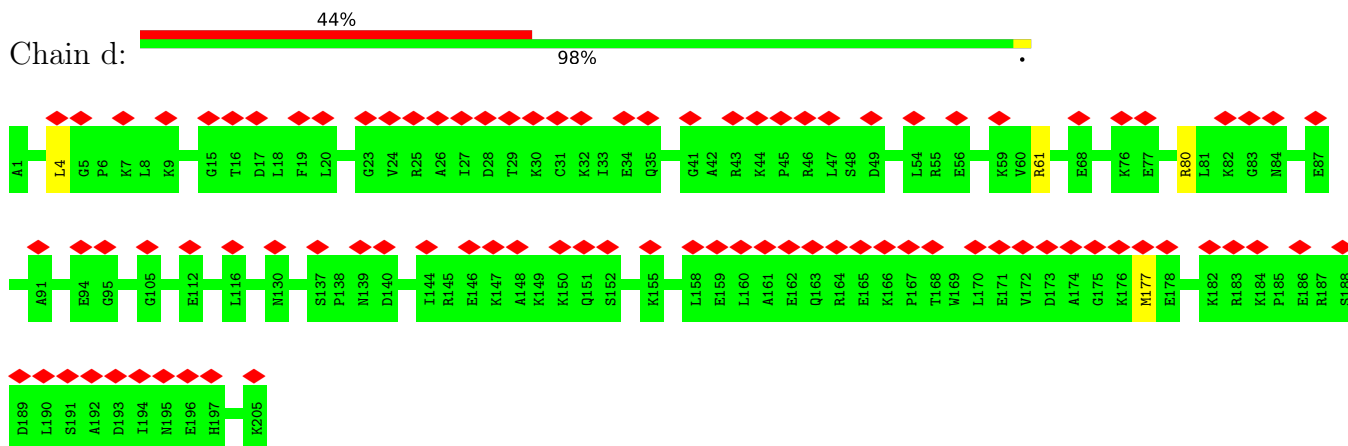
- Molecule 2: 30S ribosomal protein S2



- Molecule 3: 30S ribosomal protein S3

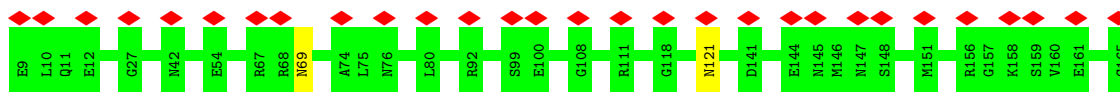


- Molecule 4: 30S ribosomal protein S4

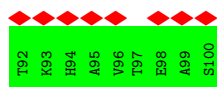
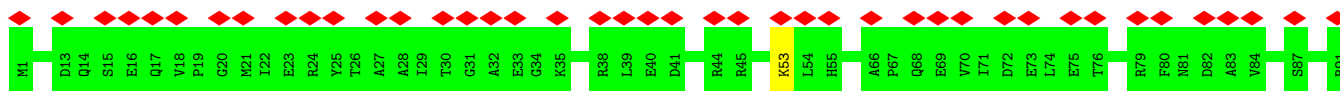


- Molecule 5: 30S ribosomal protein S5

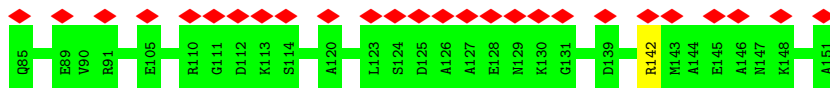
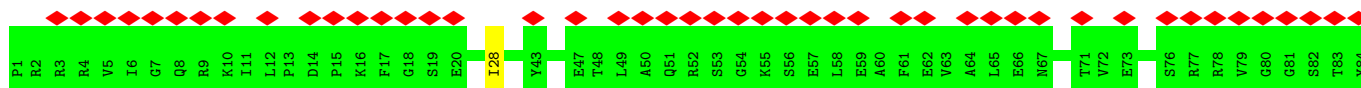




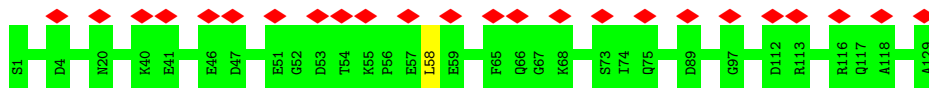
- Molecule 6: 30S ribosomal protein S6



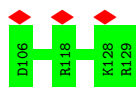
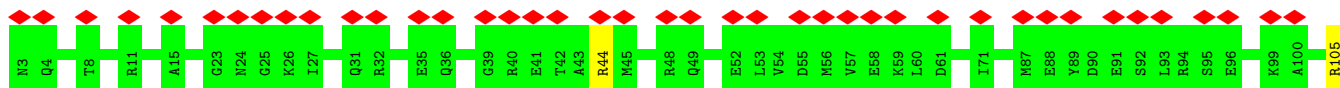
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

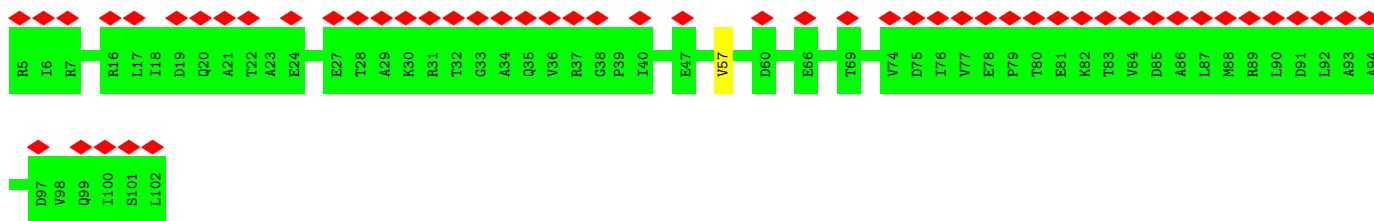


- Molecule 9: 30S ribosomal protein S9

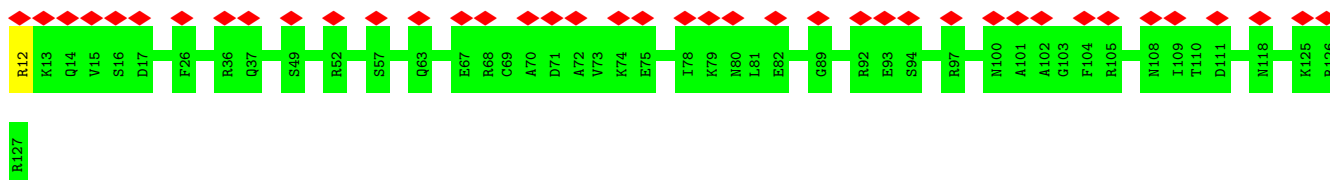


- Molecule 10: 30S ribosomal protein S10

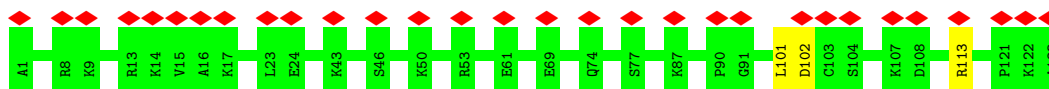




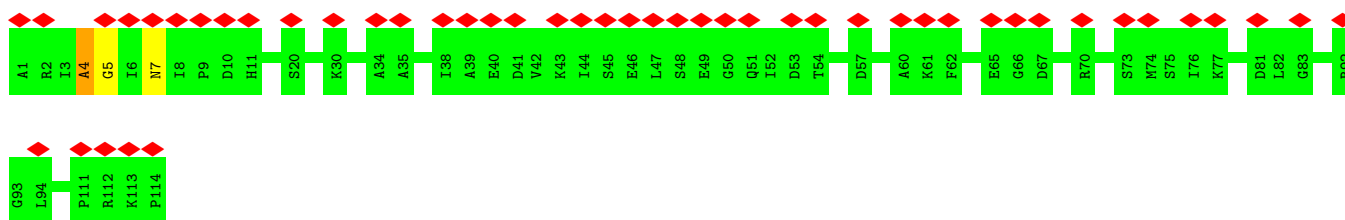
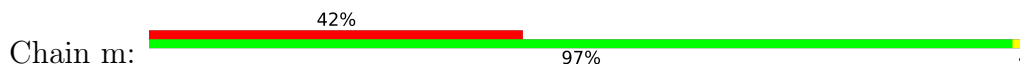
- Molecule 11: 30S ribosomal protein S11



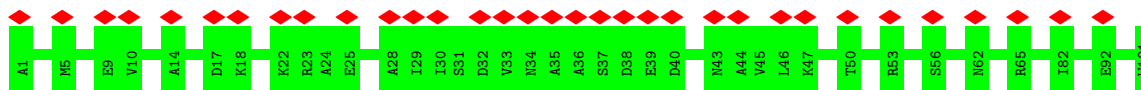
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

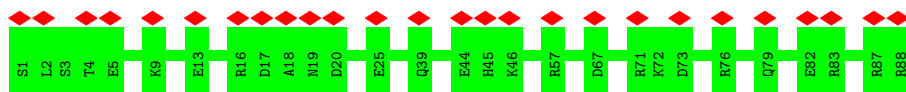


- Molecule 14: 30S ribosomal protein S14

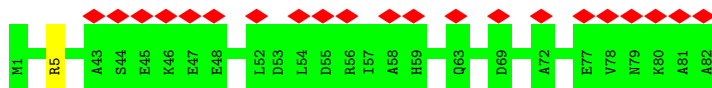


- Molecule 15: 30S ribosomal protein S15

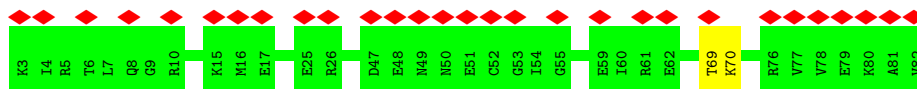




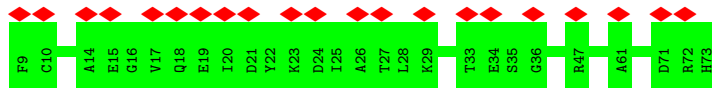
- Molecule 16: 30S ribosomal protein S16



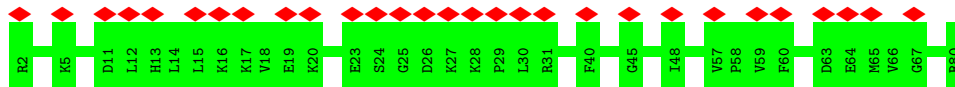
- Molecule 17: 30S ribosomal protein S17



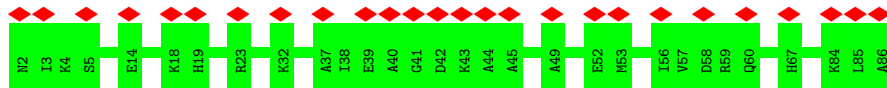
- Molecule 18: 30S ribosomal protein S18



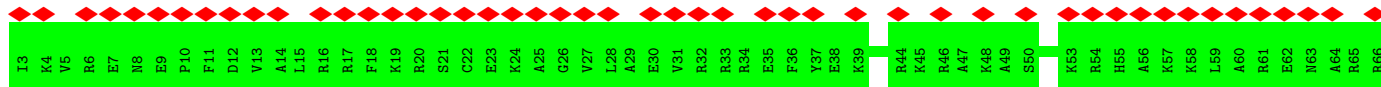
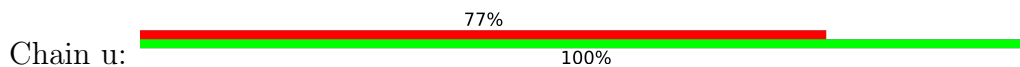
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

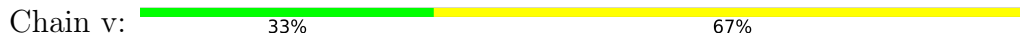


- Molecule 21: 30S ribosomal protein S21



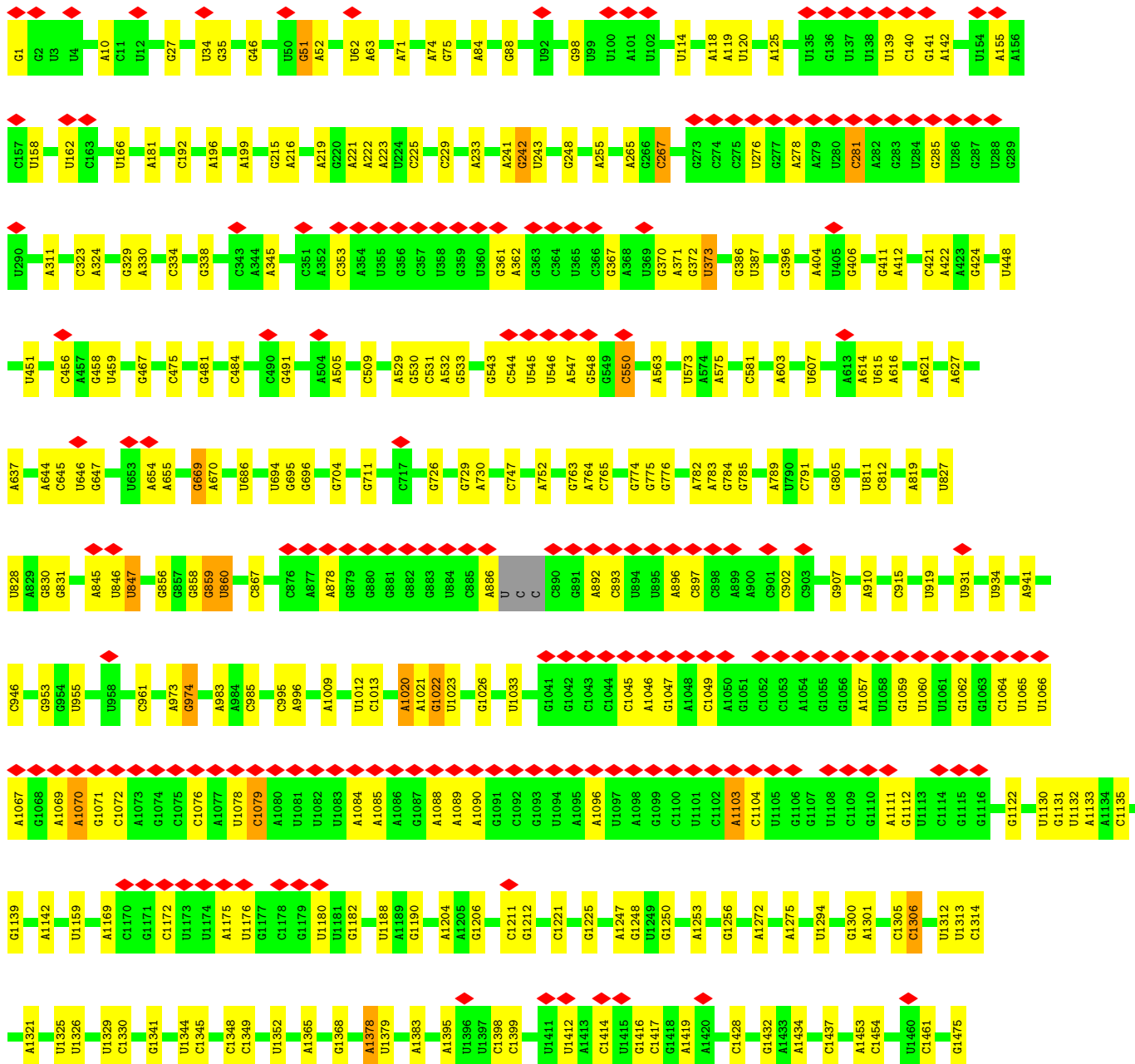
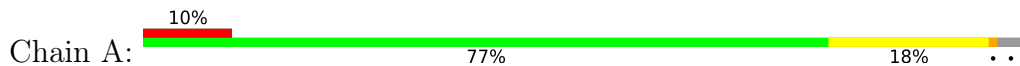
767

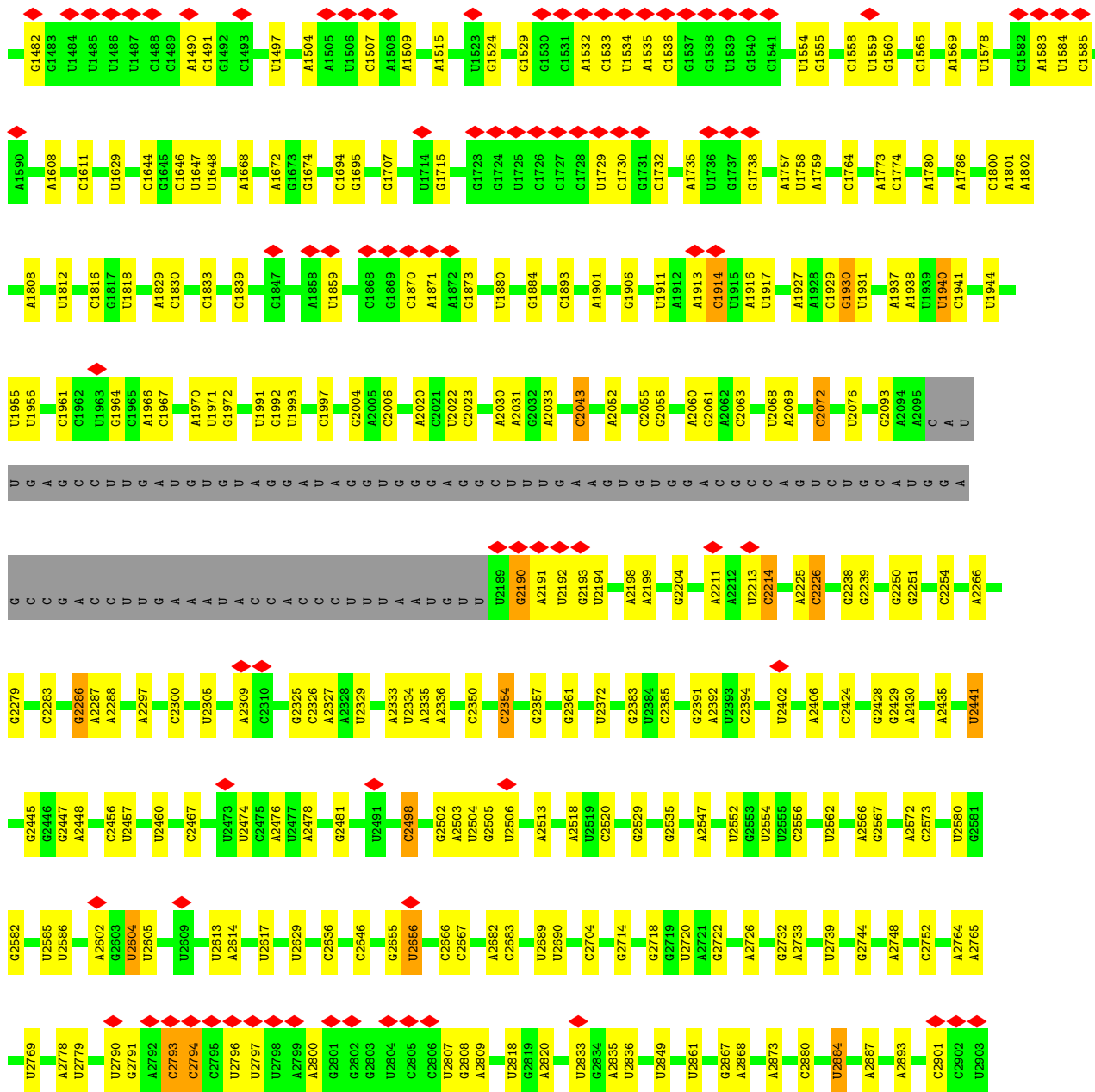
- Molecule 22: RNA (5'-R(P*CP*CP*G)-3'), mRNA



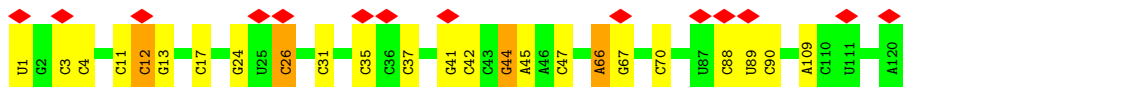
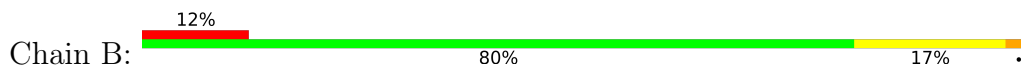
G16
C17
G18

- Molecule 23: 23S ribosomal RNA



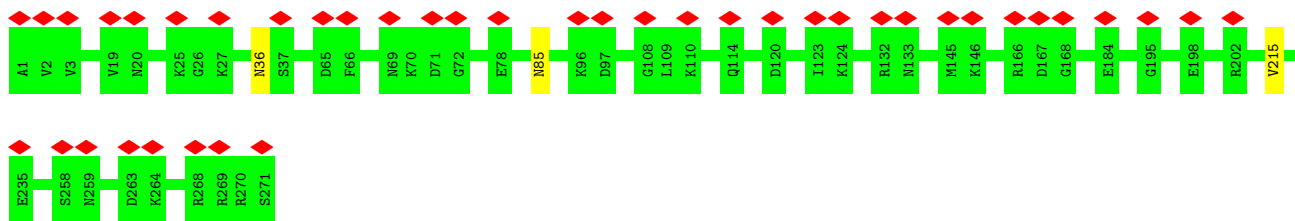


• Molecule 24: 5S ribosomal RNA

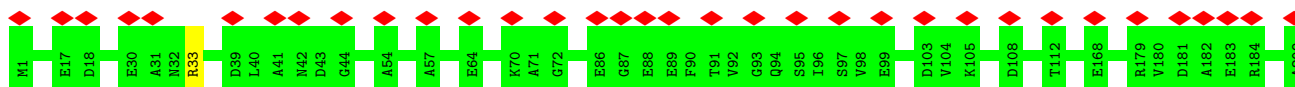


• Molecule 25: 50S ribosomal protein L2

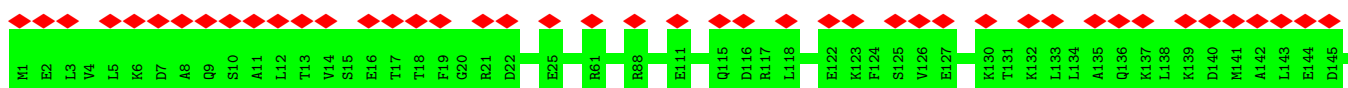




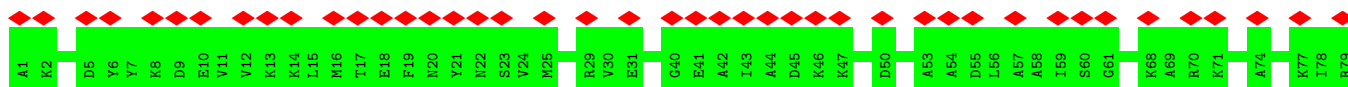
- Molecule 26: 50S ribosomal protein L3



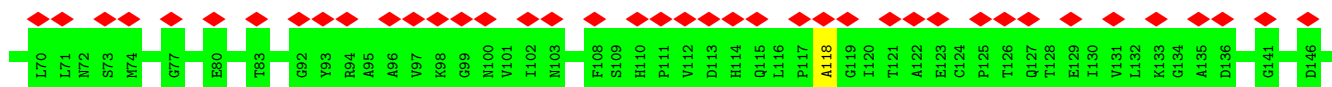
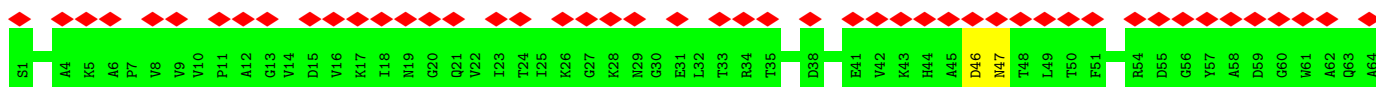
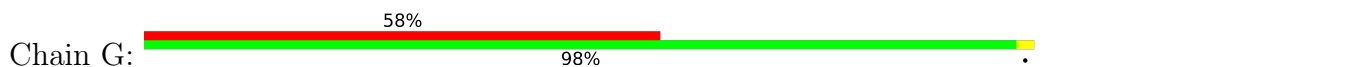
- Molecule 27: 50S ribosomal protein L4

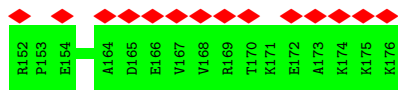


- Molecule 28: 50S ribosomal protein L5

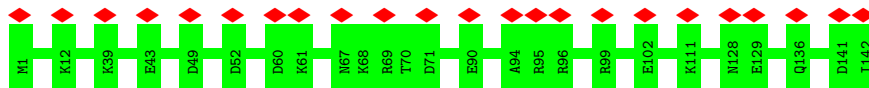


- Molecule 29: 50S ribosomal protein L6

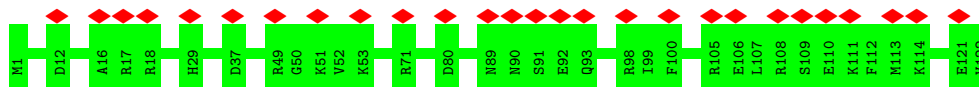




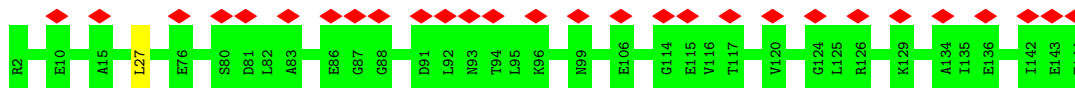
- Molecule 30: 50S ribosomal protein L13



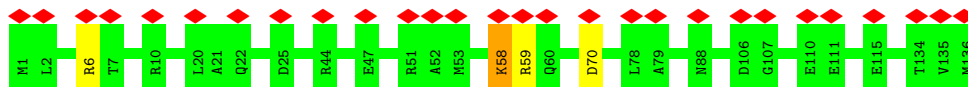
- Molecule 31: 50S ribosomal protein L14



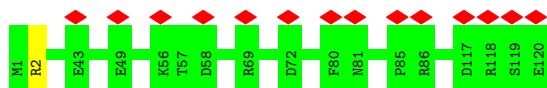
- Molecule 32: 50S ribosomal protein L15



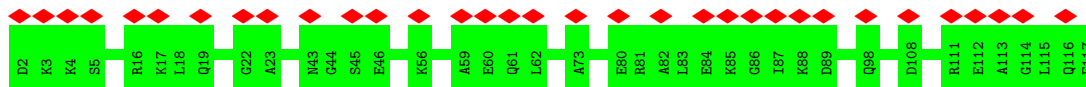
- Molecule 33: 50S ribosomal protein L16



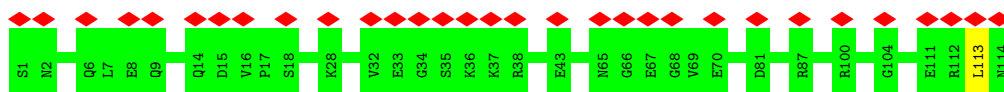
- Molecule 34: 50S ribosomal protein L17



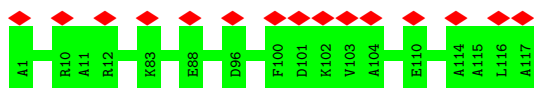
- Molecule 35: 50S ribosomal protein L18



- Molecule 36: 50S ribosomal protein L19



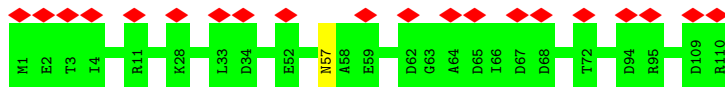
- Molecule 37: 50S ribosomal protein L20



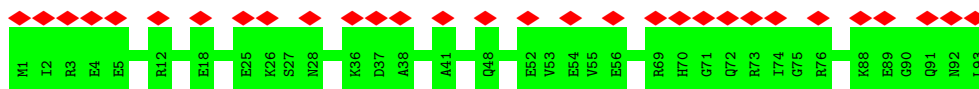
- Molecule 38: 50S ribosomal protein L21



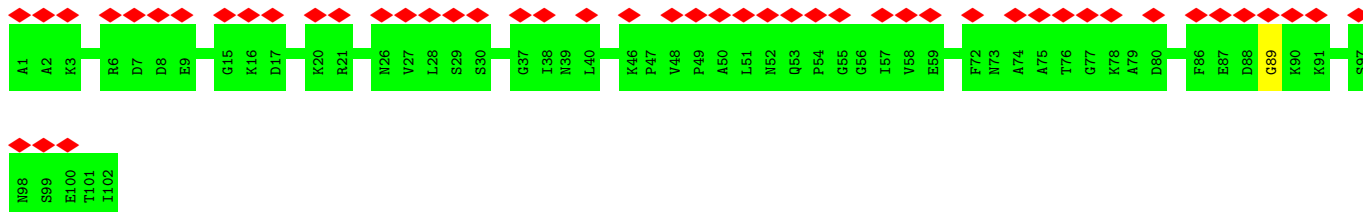
- Molecule 39: 50S ribosomal protein L22



- Molecule 40: 50S ribosomal protein L23

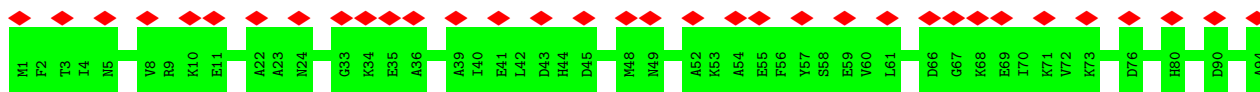


- Molecule 41: 50S ribosomal protein L24

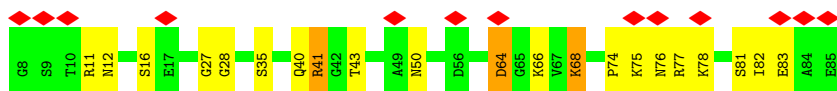
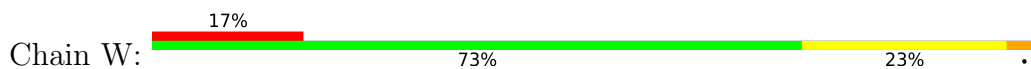


- Molecule 42: 50S ribosomal protein L25

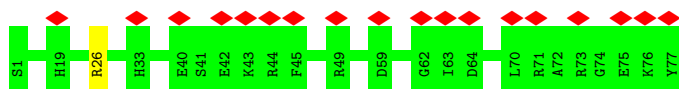




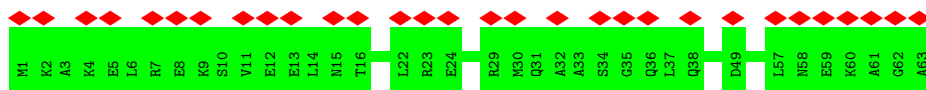
- Molecule 43: 50S ribosomal protein L27



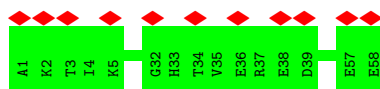
- Molecule 44: 50S ribosomal protein L28



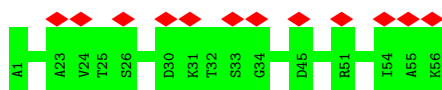
- Molecule 45: 50S ribosomal protein L29



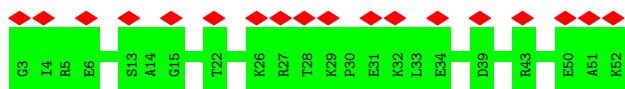
- Molecule 46: 50S ribosomal protein L30



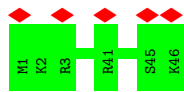
- Molecule 47: 50S ribosomal protein L32



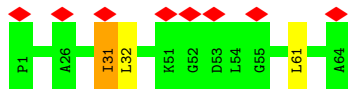
- Molecule 48: 50S ribosomal protein L33



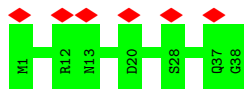
- Molecule 49: 50S ribosomal protein L34



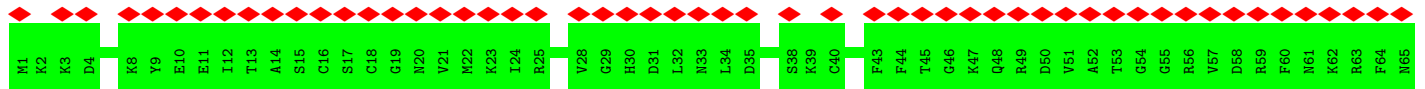
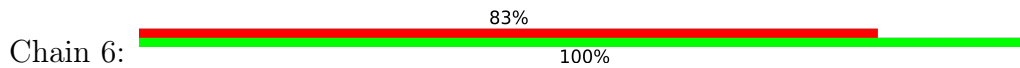
- Molecule 50: 50S ribosomal protein L35



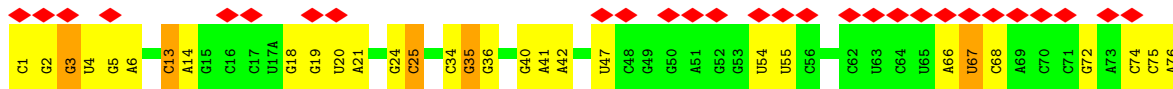
- Molecule 51: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L31



- Molecule 53: proline tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75089	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.633	Depositor
Minimum map value	-0.336	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.105	Depositor
Map size (\AA)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.084, 1.084, 1.084	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.29	1/36967 (0.0%)	0.99	74/57666 (0.1%)
2	b	0.27	0/1735	0.51	0/2338
3	c	0.26	0/1651	0.51	0/2225
4	d	0.26	0/1665	0.55	1/2227 (0.0%)
5	e	0.28	0/1154	0.57	0/1554
6	f	0.26	0/835	0.55	0/1128
7	g	0.26	0/1195	0.53	0/1602
8	h	0.26	0/989	0.54	1/1326 (0.1%)
9	i	0.27	0/1034	0.56	0/1375
10	j	0.25	0/796	0.59	0/1077
11	k	0.27	0/885	0.52	0/1195
12	l	0.29	0/969	0.59	0/1300
13	m	0.24	0/892	0.54	0/1193
14	n	0.24	0/811	0.50	0/1081
15	o	0.24	0/722	0.51	0/964
16	p	0.26	0/659	0.52	0/884
17	q	0.28	0/657	0.56	0/881
18	r	0.23	0/511	0.49	0/689
19	s	0.26	0/652	0.50	0/877
20	t	0.26	0/671	0.45	0/888
21	u	0.30	0/500	0.59	0/668
22	v	0.33	0/69	1.11	0/105
23	A	0.30	1/67511 (0.0%)	1.00	224/105319 (0.2%)
24	B	0.36	1/2876 (0.0%)	1.07	18/4483 (0.4%)
25	C	0.26	0/2121	0.52	1/2852 (0.0%)
26	D	0.26	0/1586	0.51	0/2134
27	E	0.25	0/1571	0.46	0/2113
28	F	0.27	0/1434	0.51	0/1926
29	G	0.25	0/1343	0.47	0/1816
30	J	0.25	0/1152	0.46	0/1551
31	K	0.26	0/947	0.51	0/1268
32	L	0.26	0/1054	0.55	0/1403
33	M	0.27	0/1093	0.55	1/1460 (0.1%)
34	N	0.25	0/973	0.53	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	O	0.24	0/902	0.45	0/1209
36	P	0.25	0/929	0.50	1/1242 (0.1%)
37	Q	0.25	0/960	0.42	0/1278
38	R	0.25	0/829	0.52	0/1107
39	S	0.24	0/864	0.50	0/1156
40	T	0.24	0/744	0.49	0/994
41	U	0.26	0/787	0.51	0/1051
42	V	0.25	0/766	0.49	0/1025
43	W	0.58	0/599	0.81	0/792
44	X	0.24	0/635	0.45	0/848
45	Y	0.23	0/510	0.45	0/677
46	Z	0.22	0/453	0.47	0/605
47	0	0.23	0/450	0.48	0/599
48	1	0.25	0/416	0.48	0/554
49	2	0.25	0/380	0.46	0/498
50	3	0.28	0/513	0.65	2/676 (0.3%)
51	4	0.26	0/303	0.51	0/397
52	6	0.26	0/531	0.48	0/709
53	x	0.38	0/1839	1.10	19/2866 (0.7%)
All	All	0.29	3/153090 (0.0%)	0.90	342/229152 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
5	e	0	1
6	f	0	1
7	g	0	1
10	j	0	1
12	l	0	1
13	m	0	1
17	q	0	1
28	F	0	2
29	G	0	2
33	M	0	1
38	R	0	1
All	All	0	14

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1	U	OP3-P	-10.59	1.48	1.61
23	A	1	G	OP3-P	-10.59	1.48	1.61
1	a	2	A	OP3-P	-10.49	1.48	1.61

All (342) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1507	C	N3-C2-O2	-11.99	113.51	121.90
1	a	582	C	N1-C2-O2	11.45	125.77	118.90
23	A	1507	C	N1-C2-O2	11.15	125.59	118.90
1	a	582	C	N3-C2-O2	-10.34	114.66	121.90
23	A	1914	C	N1-C2-O2	9.72	124.73	118.90
23	A	1956	U	N1-C2-O2	8.96	129.07	122.80
23	A	2580	U	N3-C2-O2	-8.93	115.95	122.20
1	a	979	C	N1-C2-O2	8.80	124.18	118.90
23	A	1313	U	N3-C2-O2	-8.68	116.13	122.20
23	A	1313	U	N1-C2-O2	8.55	128.79	122.80
1	a	440	C	N1-C2-O2	8.44	123.96	118.90
23	A	2604	U	N3-C2-O2	-8.34	116.36	122.20
23	A	1956	U	N3-C2-O2	-8.26	116.42	122.20
23	A	1313	U	C2-N1-C1'	8.25	127.59	117.70
23	A	1917	U	N3-C2-O2	-8.15	116.50	122.20
1	a	469	C	N1-C2-O2	8.14	123.78	118.90
23	A	860	U	N1-C2-O2	8.13	128.49	122.80
23	A	2604	U	N1-C2-O2	8.13	128.49	122.80
23	A	2605	U	C2-N1-C1'	8.05	127.36	117.70
23	A	2604	U	C2-N1-C1'	8.04	127.34	117.70
23	A	1917	U	C2-N1-C1'	7.99	127.28	117.70
23	A	1914	C	C2-N1-C1'	7.96	127.56	118.80
23	A	2580	U	N1-C2-O2	7.96	128.37	122.80
23	A	955	U	C2-N1-C1'	7.93	127.22	117.70
24	B	26	C	N1-C2-O2	7.93	123.66	118.90
23	A	1348	C	N1-C2-O2	7.90	123.64	118.90
23	A	1349	C	N1-C2-O2	7.82	123.59	118.90
23	A	1914	C	N3-C2-O2	-7.81	116.43	121.90
23	A	2354	C	N1-C2-O2	7.74	123.54	118.90
23	A	1774	C	N3-C2-O2	-7.74	116.48	121.90
23	A	2457	U	C2-N1-C1'	7.72	126.97	117.70
23	A	2063	C	N1-C2-O2	7.61	123.47	118.90
1	a	979	C	N3-C2-O2	-7.60	116.58	121.90
23	A	1917	U	N1-C2-O2	7.49	128.05	122.80
1	a	754	C	C2-N1-C1'	7.49	127.04	118.80
23	A	267	C	N1-C2-O2	7.43	123.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	867	C	N1-C2-O2	7.39	123.33	118.90
1	a	440	C	C6-N1-C2	-7.35	117.36	120.30
1	a	40	C	N1-C2-O2	7.28	123.27	118.90
23	A	1507	C	C6-N1-C2	-7.27	117.39	120.30
23	A	955	U	N3-C2-O2	-7.27	117.11	122.20
1	a	979	C	C6-N1-C2	-7.26	117.39	120.30
23	A	860	U	N3-C2-O2	-7.26	117.12	122.20
1	a	439	U	N1-C2-O2	7.26	127.88	122.80
23	A	2556	C	N1-C2-O2	7.25	123.25	118.90
23	A	1326	U	N3-C2-O2	-7.24	117.13	122.20
23	A	2457	U	N1-C2-O2	7.21	127.85	122.80
23	A	2457	U	N3-C2-O2	-7.18	117.17	122.20
1	a	979	C	C2-N1-C1'	7.12	126.63	118.80
1	a	440	C	N3-C2-O2	-7.11	116.92	121.90
23	A	550	C	C2-N1-C1'	7.10	126.61	118.80
1	a	1301	U	C2-N1-C1'	7.07	126.18	117.70
23	A	2072	C	C2-N1-C1'	7.06	126.56	118.80
23	A	2580	U	C2-N1-C1'	7.05	126.16	117.70
53	x	67	U	P-O3'-C3'	7.04	128.15	119.70
23	A	2474	U	N1-C2-O2	7.04	127.73	122.80
23	A	2190	G	C4-N9-C1'	6.99	135.59	126.50
1	a	392	C	C2-N1-C1'	6.95	126.45	118.80
23	A	1049	C	N1-C2-O2	6.95	123.07	118.90
23	A	1774	C	N1-C2-O2	6.95	123.07	118.90
1	a	436	C	N1-C2-O2	6.90	123.04	118.90
23	A	1914	C	C6-N1-C2	-6.88	117.55	120.30
23	A	860	U	C2-N1-C1'	6.85	125.92	117.70
23	A	1022	G	P-O3'-C3'	6.83	127.89	119.70
23	A	192	C	N1-C2-O2	6.83	123.00	118.90
1	a	436	C	N3-C2-O2	-6.80	117.14	121.90
53	x	3	G	P-O3'-C3'	6.79	127.85	119.70
23	A	2300	C	N1-C2-O2	6.78	122.97	118.90
23	A	955	U	N1-C2-O2	6.75	127.53	122.80
23	A	1159	U	N3-C2-O2	-6.75	117.47	122.20
23	A	242	G	P-O3'-C3'	6.70	127.74	119.70
23	A	2063	C	N3-C2-O2	-6.69	117.22	121.90
53	x	34	C	N1-C2-O2	6.69	122.92	118.90
1	a	439	U	N3-C2-O2	-6.68	117.53	122.20
1	a	1297	G	P-O3'-C3'	6.67	127.71	119.70
53	x	2	G	P-O3'-C3'	6.67	127.70	119.70
23	A	1326	U	N1-C2-O2	6.66	127.47	122.80
1	a	644	U	N3-C2-O2	-6.66	117.54	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1378	A	P-O3'-C3'	6.65	127.68	119.70
23	A	2605	U	N1-C2-O2	6.64	127.45	122.80
1	a	469	C	N3-C2-O2	-6.64	117.25	121.90
23	A	1349	C	N3-C2-O2	-6.62	117.27	121.90
23	A	1020	A	P-O3'-C3'	6.61	127.63	119.70
23	A	1049	C	N3-C2-O2	-6.58	117.29	121.90
4	d	4	LEU	CA-CB-CG	6.58	130.44	115.30
23	A	114	U	C2-N1-C1'	6.56	125.58	117.70
1	a	1201	A	P-O3'-C3'	6.54	127.55	119.70
23	A	2617	U	N3-C2-O2	-6.52	117.63	122.20
25	C	215	VAL	C-N-CA	6.52	138.00	121.70
23	A	2605	U	N3-C2-O2	-6.50	117.65	122.20
23	A	2474	U	C2-N1-C1'	6.48	125.48	117.70
1	a	1347	G	P-O3'-C3'	6.47	127.46	119.70
23	A	2063	C	C2-N1-C1'	6.46	125.90	118.80
23	A	2300	C	C2-N1-C1'	6.44	125.89	118.80
23	A	2474	U	N3-C2-O2	-6.43	117.70	122.20
1	a	307	C	N1-C2-O2	6.42	122.75	118.90
1	a	1158	C	C2-N1-C1'	6.42	125.86	118.80
23	A	1306	C	C2-N1-C1'	6.42	125.86	118.80
23	A	2072	C	C5-C6-N1	6.41	124.20	121.00
23	A	1930	G	P-O3'-C3'	6.40	127.38	119.70
23	A	2214	C	N1-C2-O2	6.40	122.74	118.90
23	A	62	U	C2-N1-C1'	6.40	125.38	117.70
23	A	2043	C	C2-N1-C1'	6.37	125.81	118.80
1	a	40	C	C2-N1-C1'	6.37	125.81	118.80
24	B	44	G	N1-C6-O6	-6.37	116.08	119.90
24	B	26	C	N3-C2-O2	-6.34	117.46	121.90
23	A	1349	C	C6-N1-C2	-6.33	117.77	120.30
23	A	2683	C	N1-C2-O2	6.33	122.69	118.90
23	A	2636	C	N1-C2-O2	6.30	122.68	118.90
23	A	2354	C	N3-C2-O2	-6.30	117.49	121.90
24	B	37	C	N1-C2-O2	6.29	122.67	118.90
1	a	486	U	N1-C2-O2	6.26	127.18	122.80
23	A	919	U	N1-C2-O2	6.26	127.18	122.80
23	A	1378	A	OP1-P-O3'	6.26	118.97	105.20
1	a	932	C	C2-N1-C1'	6.24	125.66	118.80
23	A	2063	C	C6-N1-C2	-6.23	117.81	120.30
23	A	1348	C	N3-C2-O2	-6.21	117.56	121.90
23	A	2226	C	N1-C2-O2	6.18	122.61	118.90
23	A	1294	U	N3-C2-O2	-6.17	117.88	122.20
24	B	3	C	P-O3'-C3'	6.16	127.09	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1159	U	N1-C2-O2	6.16	127.11	122.80
23	A	2617	U	N1-C2-O2	6.15	127.11	122.80
23	A	1070	A	P-O3'-C3'	6.14	127.06	119.70
1	a	1182	G	P-O3'-C3'	6.13	127.05	119.70
24	B	26	C	C2-N1-C1'	6.12	125.54	118.80
23	A	867	C	N3-C2-O2	-6.12	117.61	121.90
23	A	1398	C	C2-N1-C1'	6.12	125.53	118.80
23	A	1294	U	N1-C2-O2	6.12	127.08	122.80
23	A	166	U	N1-C2-O2	6.11	127.08	122.80
1	a	439	U	C2-N1-C1'	6.11	125.03	117.70
23	A	2072	C	C6-N1-C2	-6.11	117.86	120.30
23	A	2752	C	N1-C2-O2	6.07	122.54	118.90
1	a	440	C	C5-C6-N1	6.06	124.03	121.00
23	A	2354	C	C2-N1-C1'	6.03	125.43	118.80
23	A	2720	U	N3-C2-O2	-6.00	118.00	122.20
1	a	644	U	N1-C2-O2	6.00	127.00	122.80
23	A	902	C	N1-C2-O2	5.99	122.49	118.90
50	3	61	LEU	CA-CB-CG	5.99	129.07	115.30
23	A	2354	C	C6-N1-C2	-5.99	117.91	120.30
23	A	2456	C	C6-N1-C2	-5.98	117.91	120.30
23	A	1188	U	N1-C2-O2	5.97	126.98	122.80
23	A	267	C	N3-C2-O2	-5.97	117.72	121.90
23	A	1314	C	C2-N1-C1'	5.96	125.36	118.80
1	a	40	C	N3-C2-O2	-5.96	117.73	121.90
23	A	1079	C	N1-C2-O2	5.95	122.47	118.90
23	A	1940	U	P-O3'-C3'	5.93	126.82	119.70
1	a	1399	C	P-O3'-C3'	5.93	126.82	119.70
23	A	1893	C	N1-C2-O2	5.92	122.45	118.90
1	a	960	U	P-O3'-C3'	5.92	126.80	119.70
23	A	2796	U	N3-C2-O2	-5.92	118.06	122.20
24	B	17	C	C2-N1-C1'	5.91	125.30	118.80
23	A	919	U	N3-C2-O2	-5.90	118.07	122.20
23	A	2190	G	C8-N9-C1'	-5.90	119.33	127.00
23	A	669	G	C4-N9-C1'	5.89	134.15	126.50
1	a	1301	U	N1-C2-O2	5.87	126.91	122.80
1	a	1432	G	P-O3'-C3'	5.87	126.74	119.70
23	A	51	G	P-O3'-C3'	5.85	126.72	119.70
23	A	2372	U	N1-C2-O2	5.84	126.89	122.80
53	x	25	C	C5-C6-N1	5.84	123.92	121.00
23	A	166	U	N3-C2-O2	-5.84	118.11	122.20
23	A	2636	C	C2-N1-C1'	5.82	125.20	118.80
23	A	1326	U	C2-N1-C1'	5.82	124.68	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1158	C	N1-C2-O2	5.82	122.39	118.90
1	a	1301	U	N3-C2-O2	-5.82	118.13	122.20
53	x	3	G	OP1-P-O3'	5.81	117.99	105.20
23	A	2286	G	P-O3'-C3'	5.81	126.67	119.70
23	A	1103	A	C2-N3-C4	5.80	113.50	110.60
23	A	2556	C	N3-C2-O2	-5.78	117.85	121.90
23	A	859	G	P-O3'-C3'	5.77	126.62	119.70
23	A	2190	G	N3-C4-C5	-5.76	125.72	128.60
23	A	1306	C	C6-N1-C2	-5.75	118.00	120.30
1	a	1190	G	P-O3'-C3'	5.73	126.57	119.70
24	B	26	C	C6-N1-C2	-5.73	118.01	120.30
1	a	486	U	N3-C2-O2	-5.71	118.20	122.20
1	a	1300	G	P-O3'-C3'	5.71	126.55	119.70
36	P	113	LEU	CA-CB-CG	5.70	128.41	115.30
23	A	267	C	C6-N1-C2	-5.69	118.02	120.30
23	A	1893	C	N3-C2-O2	-5.69	117.91	121.90
1	a	1086	U	N1-C2-O2	5.69	126.78	122.80
1	a	760	G	N3-C2-N2	5.69	123.88	119.90
23	A	2467	C	N1-C2-O2	5.69	122.31	118.90
23	A	2704	C	N1-C2-O2	5.68	122.31	118.90
23	A	2190	G	N3-C4-N9	5.67	129.40	126.00
23	A	192	C	N3-C2-O2	-5.67	117.93	121.90
24	B	70	C	N1-C2-O2	5.67	122.30	118.90
1	a	392	C	C6-N1-C2	-5.66	118.04	120.30
23	A	1956	U	C2-N1-C1'	5.64	124.47	117.70
23	A	2394	C	N1-C2-O2	5.64	122.28	118.90
1	a	998	C	N1-C2-O2	5.63	122.28	118.90
23	A	1914	C	C5-C6-N1	5.62	123.81	121.00
24	B	31	C	N1-C2-O2	5.62	122.27	118.90
1	a	95	C	N1-C2-O2	5.59	122.26	118.90
23	A	1221	C	C2-N1-C1'	5.59	124.95	118.80
1	a	486	U	C2-N1-C1'	5.59	124.41	117.70
1	a	754	C	C6-N1-C1'	-5.58	114.10	120.80
1	a	469	C	C2-N1-C1'	5.57	124.93	118.80
33	M	70	ASP	CB-CG-OD1	5.56	123.31	118.30
23	A	62	U	N1-C2-O2	5.55	126.69	122.80
23	A	1103	A	C4-N9-C1'	5.55	136.29	126.30
23	A	2666	C	N1-C2-O2	5.55	122.23	118.90
24	B	11	C	C6-N1-C2	-5.55	118.08	120.30
23	A	2300	C	C6-N1-C2	-5.54	118.08	120.30
1	a	806	C	N1-C2-O2	5.54	122.22	118.90
23	A	985	C	C2-N1-C1'	5.54	124.89	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	582	C	C6-N1-C2	-5.52	118.09	120.30
23	A	2072	C	N1-C2-O2	5.52	122.21	118.90
1	a	340	U	N1-C2-O2	5.51	126.66	122.80
23	A	2720	U	N1-C2-O2	5.51	126.66	122.80
53	x	1	C	N1-C2-O2	5.50	122.20	118.90
53	x	13	C	P-O3'-C3'	5.49	126.29	119.70
53	x	35	G	C4'-C3'-O3'	5.48	123.96	113.00
53	x	55	U	C2-N1-C1'	5.48	124.28	117.70
1	a	40	C	C6-N1-C2	-5.47	118.11	120.30
1	a	1086	U	N3-C2-O2	-5.46	118.38	122.20
1	a	440	C	C2-N1-C1'	5.45	124.80	118.80
1	a	470	C	N1-C2-O2	5.45	122.17	118.90
1	a	473	U	C2-N1-C1'	5.43	124.22	117.70
23	A	2372	U	N3-C2-O2	-5.43	118.40	122.20
53	x	24	G	P-O3'-C3'	5.43	126.22	119.70
1	a	1498	U	C2-N1-C1'	5.42	124.20	117.70
1	a	1263	C	N1-C2-O2	5.42	122.15	118.90
23	A	1049	C	C6-N1-C2	-5.41	118.14	120.30
1	a	462	G	C4-N9-C1'	5.41	133.53	126.50
23	A	985	C	N1-C2-O2	5.40	122.14	118.90
23	A	2794	C	C2-N1-C1'	5.39	124.73	118.80
23	A	607	U	N3-C2-O2	-5.38	118.43	122.20
24	B	3	C	OP1-P-O3'	5.38	117.04	105.20
24	B	44	G	C5-C6-O6	5.38	131.82	128.60
23	A	2556	C	C2-N1-C1'	5.36	124.70	118.80
23	A	267	C	C2-N1-C1'	5.36	124.70	118.80
23	A	847	U	N3-C2-O2	-5.36	118.45	122.20
23	A	2884	U	C2-N1-C1'	5.35	124.12	117.70
23	A	1812	U	N1-C2-O2	5.34	126.54	122.80
23	A	1839	G	C4-N9-C1'	5.34	133.44	126.50
1	a	58	C	C6-N1-C2	-5.33	118.17	120.30
23	A	1812	U	N3-C2-O2	-5.33	118.47	122.20
23	A	1911	U	C2-N1-C1'	5.33	124.10	117.70
23	A	2605	U	C5-C6-N1	5.33	125.36	122.70
1	a	469	C	C6-N1-C2	-5.32	118.17	120.30
23	A	1314	C	C6-N1-C2	-5.32	118.17	120.30
53	x	24	G	OP1-P-O3'	5.32	116.90	105.20
23	A	2254	C	N1-C2-O2	5.32	122.09	118.90
24	B	47	C	N1-C2-O2	5.30	122.08	118.90
53	x	34	C	N3-C2-O2	-5.29	118.20	121.90
23	A	373	U	N3-C2-O2	-5.29	118.50	122.20
1	a	623	C	C6-N1-C2	-5.28	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1349	C	C2-N1-C1'	5.28	124.61	118.80
23	A	2076	U	C2-N1-C1'	5.28	124.04	117.70
23	A	114	U	N1-C2-O2	5.27	126.49	122.80
23	A	2467	C	N3-C2-O2	-5.26	118.22	121.90
23	A	974	G	C4-N9-C1'	5.25	133.33	126.50
23	A	2793	C	N1-C2-O2	5.25	122.05	118.90
53	x	55	U	N3-C2-O2	-5.25	118.53	122.20
23	A	2457	U	O4'-C1'-N1	5.23	112.39	108.20
53	x	35	G	C2'-C3'-O3'	5.23	122.06	113.70
1	a	961	U	N1-C2-O2	5.22	126.46	122.80
23	A	550	C	C6-N1-C2	-5.22	118.21	120.30
23	A	2796	U	N1-C2-O2	5.22	126.46	122.80
23	A	1880	U	N3-C2-O2	-5.22	118.55	122.20
23	A	2300	C	N3-C2-O2	-5.22	118.25	121.90
24	B	66	A	P-O3'-C3'	5.22	125.96	119.70
1	a	516	U	C2-N1-C1'	5.21	123.95	117.70
23	A	62	U	N3-C2-O2	-5.21	118.55	122.20
1	a	340	U	N3-C2-O2	-5.21	118.56	122.20
23	A	2043	C	C5-C6-N1	5.21	123.60	121.00
23	A	1830	C	C6-N1-C2	-5.21	118.22	120.30
23	A	1412	U	N1-C2-O2	5.19	126.43	122.80
23	A	2372	U	C2-N1-C1'	5.18	123.92	117.70
53	x	25	C	C6-N1-C2	-5.18	118.23	120.30
23	A	1294	U	C2-N1-C1'	5.17	123.90	117.70
24	B	12	C	C2-N1-C1'	5.17	124.48	118.80
23	A	1188	U	N3-C2-O2	-5.16	118.59	122.20
23	A	915	C	C2-N1-C1'	5.16	124.48	118.80
23	A	1417	C	C2-N1-C1'	5.16	124.48	118.80
1	a	370	C	C2-N1-C1'	5.16	124.47	118.80
23	A	2460	U	N1-C2-O2	5.16	126.41	122.80
23	A	1961	C	N1-C2-O2	5.15	121.99	118.90
23	A	1348	C	C2-N1-C1'	5.15	124.46	118.80
23	A	2214	C	N3-C2-O2	-5.14	118.30	121.90
23	A	2441	U	N3-C2-O2	-5.14	118.60	122.20
23	A	2656	U	C5-C6-N1	5.14	125.27	122.70
1	a	979	C	C5-C6-N1	5.14	123.57	121.00
23	A	669	G	C8-N9-C1'	-5.14	120.32	127.00
23	A	1774	C	C6-N1-C2	-5.14	118.25	120.30
23	A	2556	C	C6-N1-C2	-5.14	118.25	120.30
23	A	2667	C	N1-C2-O2	5.13	121.98	118.90
8	h	58	LEU	CA-CB-CG	5.13	127.10	115.30
23	A	2580	U	O4'-C1'-N1	5.12	112.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2552	U	C2-N1-C1'	5.12	123.85	117.70
23	A	1629	U	N3-C2-O2	-5.12	118.62	122.20
23	A	2226	C	C6-N1-C2	-5.12	118.25	120.30
23	A	1818	U	N1-C2-O2	5.12	126.38	122.80
1	a	754	C	N1-C2-O2	5.12	121.97	118.90
23	A	281	C	N1-C2-O2	5.12	121.97	118.90
23	A	550	C	C5-C6-N1	5.11	123.55	121.00
53	x	41	A	P-O3'-C3'	5.11	125.83	119.70
23	A	1839	G	N3-C4-N9	5.11	129.06	126.00
23	A	1412	U	C2-N1-C1'	5.10	123.82	117.70
23	A	1414	C	N1-C2-O2	5.10	121.96	118.90
53	x	34	C	C6-N1-C2	-5.10	118.26	120.30
23	A	1348	C	C6-N1-C2	-5.10	118.26	120.30
53	x	34	C	C2-N1-C1'	5.10	124.41	118.80
23	A	1103	A	N3-C4-N9	5.09	131.47	127.40
23	A	484	C	C6-N1-C2	-5.09	118.26	120.30
23	A	694	U	N1-C2-O2	5.09	126.36	122.80
23	A	1644	C	N1-C2-O2	5.09	121.95	118.90
1	a	307	C	N3-C2-O2	-5.09	118.34	121.90
1	a	490	C	C2-N1-C1'	5.09	124.40	118.80
23	A	1412	U	N3-C2-O2	-5.09	118.64	122.20
23	A	1830	C	C2-N1-C1'	5.09	124.39	118.80
23	A	2752	C	C6-N1-C2	-5.09	118.27	120.30
23	A	2460	U	N3-C2-O2	-5.08	118.64	122.20
23	A	1911	U	N3-C2-O2	-5.08	118.65	122.20
23	A	2329	U	C5-C6-N1	5.08	125.24	122.70
23	A	860	U	C5-C6-N1	5.07	125.24	122.70
23	A	1313	U	C6-N1-C1'	-5.07	114.10	121.20
23	A	955	U	O4'-C1'-N1	5.07	112.25	108.20
23	A	2498	C	N1-C2-O2	5.07	121.94	118.90
1	a	392	C	N1-C2-O2	5.06	121.94	118.90
23	A	1221	C	N1-C2-O2	5.06	121.94	118.90
23	A	1306	C	C5-C6-N1	5.05	123.53	121.00
23	A	158	U	N1-C2-O2	5.05	126.33	122.80
23	A	459	U	N1-C2-O2	5.05	126.33	122.80
23	A	1993	U	N3-C2-O2	-5.05	118.67	122.20
24	B	17	C	C6-N1-C2	-5.05	118.28	120.30
23	A	192	C	C6-N1-C2	-5.04	118.28	120.30
23	A	2498	C	C6-N1-C2	-5.04	118.28	120.30
23	A	2006	C	C2-N1-C1'	5.04	124.34	118.80
23	A	1305	C	C2-N1-C1'	5.04	124.34	118.80
23	A	2043	C	C6-N1-C2	-5.03	118.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2636	C	C6-N1-C2	-5.03	118.29	120.30
24	B	37	C	N3-C2-O2	-5.03	118.38	121.90
23	A	581	C	C5-C6-N1	5.03	123.52	121.00
23	A	1961	C	N3-C2-O2	-5.03	118.38	121.90
1	a	1147	C	N1-C2-O2	5.02	121.91	118.90
23	A	919	U	C2-N1-C1'	5.02	123.72	117.70
23	A	1818	U	C2-N1-C1'	5.02	123.72	117.70
23	A	166	U	C2-N1-C1'	5.01	123.72	117.70
23	A	1812	U	C2-N1-C1'	5.01	123.72	117.70
50	3	31	ILE	CG1-CB-CG2	-5.01	100.37	111.40
23	A	1398	C	C6-N1-C2	-5.01	118.30	120.30
23	A	353	C	C2-N1-C1'	5.00	124.31	118.80

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	F	173	ASP	Peptide
28	F	174	PHE	Peptide
29	G	118	ALA	Peptide
29	G	46	ASP	Peptide
33	M	58	LYS	Peptide
38	R	53	PHE	Peptide
2	b	15	PHE	Peptide
5	e	121	ASN	Peptide
6	f	53	LYS	Peptide
7	g	28	ILE	Peptide
10	j	57	VAL	Peptide
12	l	101	LEU	Peptide
13	m	4	ALA	Peptide
17	q	69	THR	Peptide

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	
2	b	216/218 (99%)	200 (93%)	16 (7%)	0	100	100
3	c	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
4	d	203/205 (99%)	185 (91%)	18 (9%)	0	100	100
5	e	155/157 (99%)	137 (88%)	18 (12%)	0	100	100
6	f	98/100 (98%)	82 (84%)	16 (16%)	0	100	100
7	g	149/151 (99%)	135 (91%)	14 (9%)	0	100	100
8	h	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
9	i	125/127 (98%)	108 (86%)	17 (14%)	0	100	100
10	j	96/98 (98%)	84 (88%)	12 (12%)	0	100	100
11	k	114/116 (98%)	98 (86%)	16 (14%)	0	100	100
12	l	121/123 (98%)	99 (82%)	21 (17%)	1 (1%)	19	58
13	m	112/114 (98%)	102 (91%)	8 (7%)	2 (2%)	8	41
14	n	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
15	o	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
16	p	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
17	q	78/80 (98%)	68 (87%)	9 (12%)	1 (1%)	12	47
18	r	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
19	s	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
20	t	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
21	u	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
25	C	269/271 (99%)	255 (95%)	14 (5%)	0	100	100
26	D	207/209 (99%)	196 (95%)	11 (5%)	0	100	100
27	E	199/201 (99%)	185 (93%)	14 (7%)	0	100	100
28	F	175/177 (99%)	165 (94%)	10 (6%)	0	100	100
29	G	174/176 (99%)	162 (93%)	11 (6%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
31	K	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
32	L	141/143 (99%)	124 (88%)	17 (12%)	0	100	100
33	M	134/136 (98%)	128 (96%)	4 (3%)	2 (2%)	10	44
34	N	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
35	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
36	P	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
37	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
38	R	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
39	S	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
40	T	91/93 (98%)	81 (89%)	10 (11%)	0	100	100
41	U	100/102 (98%)	83 (83%)	16 (16%)	1 (1%)	15	54
42	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
43	W	76/78 (97%)	55 (72%)	13 (17%)	8 (10%)	0	3
44	X	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
45	Y	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
46	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
47	0	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
48	1	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
49	2	44/46 (96%)	44 (100%)	0	0	100	100
50	3	62/64 (97%)	53 (86%)	7 (11%)	2 (3%)	4	26
51	4	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
52	6	64/66 (97%)	56 (88%)	8 (12%)	0	100	100
All	All	5435/5531 (98%)	4983 (92%)	434 (8%)	18 (0%)	44	74

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	W	27	GLY
50	3	31	ILE
12	l	102	ASP
17	q	70	LYS
33	M	59	ARG
43	W	28	GLY

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Mol	Chain	Res	Type
43	W	50	ASN
43	W	64	ASP
43	W	74	PRO
43	W	78	LYS
50	3	32	LEU
13	m	4	ALA
29	G	47	ASN
33	M	58	LYS
13	m	5	GLY
43	W	41	ARG
43	W	68	LYS
41	U	89	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/180 (100%)	176 (98%)	4 (2%)	52	79
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	169 (98%)	3 (2%)	60	83
5	e	114/119 (96%)	113 (99%)	1 (1%)	78	91
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	124/124 (100%)	123 (99%)	1 (1%)	81	93
8	h	104/104 (100%)	104 (100%)	0	100	100
9	i	105/105 (100%)	103 (98%)	2 (2%)	57	81
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	88 (99%)	1 (1%)	73	88
12	l	103/103 (100%)	102 (99%)	1 (1%)	76	90
13	m	92/92 (100%)	91 (99%)	1 (1%)	73	88
14	n	79/83 (95%)	79 (100%)	0	100	100
15	o	76/76 (100%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	p	65/65 (100%)	64 (98%)	1 (2%)	65	85
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	44 (100%)	0	100	100
25	C	216/216 (100%)	214 (99%)	2 (1%)	78	91
26	D	164/164 (100%)	163 (99%)	1 (1%)	86	94
27	E	165/165 (100%)	164 (99%)	1 (1%)	86	94
28	F	148/148 (100%)	148 (100%)	0	100	100
29	G	137/137 (100%)	137 (100%)	0	100	100
30	J	116/116 (100%)	116 (100%)	0	100	100
31	K	103/103 (100%)	103 (100%)	0	100	100
32	L	102/102 (100%)	101 (99%)	1 (1%)	76	90
33	M	109/109 (100%)	108 (99%)	1 (1%)	78	91
34	N	100/100 (100%)	99 (99%)	1 (1%)	76	90
35	O	86/86 (100%)	86 (100%)	0	100	100
36	P	99/99 (100%)	99 (100%)	0	100	100
37	Q	89/89 (100%)	89 (100%)	0	100	100
38	R	84/84 (100%)	83 (99%)	1 (1%)	71	88
39	S	93/93 (100%)	92 (99%)	1 (1%)	73	88
40	T	80/80 (100%)	80 (100%)	0	100	100
41	U	83/83 (100%)	83 (100%)	0	100	100
42	V	78/78 (100%)	78 (100%)	0	100	100
43	W	59/59 (100%)	43 (73%)	16 (27%)	0	1
44	X	67/67 (100%)	66 (98%)	1 (2%)	65	85
45	Y	55/55 (100%)	55 (100%)	0	100	100
46	Z	48/48 (100%)	48 (100%)	0	100	100
47	0	47/47 (100%)	47 (100%)	0	100	100
48	1	45/45 (100%)	45 (100%)	0	100	100
49	2	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	3	51/51 (100%)	51 (100%)	0	100	100
51	4	34/34 (100%)	34 (100%)	0	100	100
52	6	59/59 (100%)	59 (100%)	0	100	100
All	All	4502/4530 (99%)	4461 (99%)	41 (1%)	79	91

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	20	ARG
2	b	23	ASN
2	b	35	ASN
2	b	202	ASN
4	d	61	ARG
4	d	80	ARG
4	d	177	MET
5	e	69	ASN
7	g	142	ARG
9	i	44	ARG
9	i	105	ARG
11	k	12	ARG
12	l	113	ARG
13	m	7	ASN
16	p	5	ARG
25	C	36	ASN
25	C	85	ASN
26	D	33	ARG
27	E	156	ASN
32	L	27	LEU
33	M	6	ARG
34	N	2	ARG
38	R	43	ASN
39	S	57	ASN
43	W	11	ARG
43	W	12	ASN
43	W	16	SER
43	W	35	SER
43	W	40	GLN
43	W	41	ARG
43	W	43	THR
43	W	64	ASP
43	W	66	LYS

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Mol	Chain	Res	Type
43	W	68	LYS
43	W	75	LYS
43	W	76	ASN
43	W	77	ARG
43	W	81	SER
43	W	82	ILE
43	W	83	GLU
44	X	26	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	23	ASN
2	b	35	ASN
2	b	202	ASN
4	d	58	GLN
4	d	115	GLN
4	d	151	GLN
5	e	69	ASN
6	f	55	HIS
8	h	3	GLN
9	i	31	GLN
9	i	36	GLN
9	i	125	GLN
10	j	58	ASN
14	n	60	GLN
15	o	45	HIS
16	p	63	GLN
16	p	79	ASN
17	q	30	HIS
18	r	51	GLN
19	s	68	HIS
25	C	36	ASN
25	C	85	ASN
25	C	114	GLN
25	C	250	GLN
26	D	36	GLN
26	D	49	GLN
26	D	150	GLN
26	D	164	GLN
27	E	156	ASN
29	G	63	GLN

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Mol	Chain	Res	Type
29	G	138	GLN
30	J	40	HIS
30	J	47	HIS
31	K	3	GLN
35	O	38	GLN
36	P	11	GLN
37	Q	43	GLN
38	R	6	GLN
38	R	43	ASN
39	S	7	HIS
39	S	57	ASN
43	W	40	GLN
45	Y	58	ASN
48	1	45	HIS
52	6	41	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1538/1539 (99%)	267 (17%)	0
22	v	2/3 (66%)	2 (100%)	0
23	A	2804/2903 (96%)	477 (17%)	19 (0%)
24	B	119/120 (99%)	15 (12%)	1 (0%)
53	x	76/77 (98%)	24 (31%)	0
All	All	4539/4642 (97%)	785 (17%)	20 (0%)

All (785) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	7	A
1	a	9	G
1	a	22	G
1	a	31	G
1	a	32	A
1	a	33	A
1	a	39	G
1	a	41	G
1	a	47	C
1	a	48	C
1	a	51	A
1	a	56	U

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Mol	Chain	Res	Type
1	a	64	G
1	a	66	A
1	a	71	A
1	a	74	A
1	a	81	A
1	a	82	G
1	a	83	C
1	a	86	G
1	a	87	C
1	a	89	U
1	a	90	C
1	a	95	C
1	a	121	U
1	a	131	A
1	a	139	A
1	a	147	G
1	a	148	G
1	a	149	A
1	a	150	U
1	a	157	U
1	a	160	A
1	a	173	U
1	a	181	A
1	a	182	A
1	a	183	C
1	a	184	G
1	a	197	A
1	a	200	G
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	214	C
1	a	223	A
1	a	226	G
1	a	240	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	279	A

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Mol	Chain	Res	Type
1	a	280	C
1	a	281	G
1	a	289	G
1	a	298	A
1	a	306	A
1	a	317	U
1	a	328	C
1	a	330	C
1	a	344	A
1	a	345	C
1	a	346	G
1	a	347	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	359	G
1	a	360	G
1	a	367	U
1	a	368	U
1	a	370	C
1	a	372	C
1	a	373	A
1	a	388	G
1	a	391	G
1	a	392	C
1	a	398	U
1	a	406	G
1	a	408	A
1	a	413	G
1	a	414	A
1	a	421	U
1	a	422	C
1	a	423	G
1	a	424	G
1	a	428	G
1	a	429	U
1	a	436	C
1	a	438	U
1	a	465	A
1	a	466	A
1	a	467	U
1	a	468	A

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Mol	Chain	Res	Type
1	a	474	G
1	a	479	U
1	a	484	G
1	a	486	U
1	a	494	G
1	a	495	A
1	a	497	G
1	a	499	A
1	a	502	A
1	a	508	U
1	a	509	A
1	a	510	A
1	a	511	C
1	a	518	C
1	a	521	G
1	a	526	C
1	a	527	G
1	a	531	U
1	a	532	A
1	a	533	A
1	a	536	C
1	a	547	A
1	a	559	A
1	a	560	A
1	a	564	C
1	a	572	A
1	a	573	A
1	a	574	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	596	A
1	a	613	C
1	a	619	U
1	a	632	U
1	a	633	G
1	a	634	C
1	a	635	A
1	a	636	U
1	a	665	A
1	a	671	G
1	a	703	G

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Mol	Chain	Res	Type
1	a	705	G
1	a	713	G
1	a	721	G
1	a	723	U
1	a	724	G
1	a	731	G
1	a	733	G
1	a	748	G
1	a	753	A
1	a	754	C
1	a	755	G
1	a	774	G
1	a	777	A
1	a	812	G
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	820	U
1	a	821	G
1	a	832	G
1	a	843	U
1	a	844	G
1	a	846	G
1	a	851	G
1	a	864	A
1	a	871	U
1	a	872	A
1	a	876	C
1	a	889	A
1	a	890	G
1	a	902	G
1	a	914	A
1	a	926	G
1	a	932	C
1	a	934	C
1	a	935	A
1	a	939	G
1	a	960	U
1	a	961	U
1	a	969	A
1	a	975	A

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Mol	Chain	Res	Type
1	a	976	G
1	a	977	A
1	a	992	U
1	a	993	G
1	a	1001	C
1	a	1004	A
1	a	1020	G
1	a	1028	C
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1053	G
1	a	1065	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1108	G
1	a	1130	A
1	a	1132	C
1	a	1133	G
1	a	1136	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1151	A
1	a	1152	A
1	a	1158	C
1	a	1159	U
1	a	1168	U
1	a	1169	A
1	a	1181	G
1	a	1183	U
1	a	1184	G
1	a	1191	A
1	a	1196	A
1	a	1197	A
1	a	1201	A
1	a	1202	U
1	a	1212	U
1	a	1213	A

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Mol	Chain	Res	Type
1	a	1214	C
1	a	1227	A
1	a	1236	A
1	a	1238	A
1	a	1241	G
1	a	1257	A
1	a	1258	G
1	a	1260	G
1	a	1261	A
1	a	1278	G
1	a	1280	A
1	a	1281	C
1	a	1282	C
1	a	1287	A
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1301	U
1	a	1317	C
1	a	1346	A
1	a	1347	G
1	a	1348	U
1	a	1363	A
1	a	1365	G
1	a	1368	A
1	a	1370	G
1	a	1381	U
1	a	1398	A
1	a	1400	C
1	a	1419	G
1	a	1429	A
1	a	1433	A
1	a	1446	A
1	a	1452	C
1	a	1492	A
1	a	1499	A
1	a	1502	A
1	a	1503	A
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1534	A

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Mol	Chain	Res	Type
1	a	1535	C
1	a	1536	C
1	a	1539	C
22	v	17	C
22	v	18	G
23	A	10	A
23	A	27	G
23	A	34	U
23	A	35	G
23	A	46	G
23	A	51	G
23	A	52	A
23	A	63	A
23	A	71	A
23	A	74	A
23	A	75	G
23	A	84	A
23	A	88	G
23	A	98	G
23	A	118	A
23	A	119	A
23	A	120	U
23	A	125	A
23	A	139	U
23	A	140	C
23	A	141	G
23	A	142	A
23	A	155	A
23	A	162	U
23	A	181	A
23	A	196	A
23	A	199	A
23	A	215	G
23	A	216	A
23	A	219	A
23	A	221	A
23	A	222	A
23	A	223	A
23	A	225	C
23	A	229	C
23	A	233	A
23	A	241	A

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Mol	Chain	Res	Type
23	A	242	G
23	A	243	U
23	A	248	G
23	A	255	A
23	A	265	A
23	A	267	C
23	A	276	U
23	A	278	A
23	A	281	C
23	A	285	G
23	A	311	A
23	A	323	C
23	A	324	A
23	A	329	G
23	A	330	A
23	A	334	C
23	A	338	G
23	A	345	A
23	A	361	G
23	A	362	A
23	A	367	G
23	A	370	G
23	A	371	A
23	A	372	G
23	A	373	U
23	A	386	G
23	A	387	U
23	A	396	G
23	A	404	A
23	A	406	G
23	A	411	G
23	A	412	A
23	A	422	A
23	A	424	G
23	A	448	U
23	A	451	U
23	A	456	C
23	A	458	G
23	A	467	G
23	A	475	C
23	A	481	G
23	A	491	G

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Mol	Chain	Res	Type
23	A	505	A
23	A	509	C
23	A	529	A
23	A	530	G
23	A	531	C
23	A	532	A
23	A	533	G
23	A	543	G
23	A	544	C
23	A	545	U
23	A	546	U
23	A	547	A
23	A	548	G
23	A	550	C
23	A	563	A
23	A	573	U
23	A	575	A
23	A	603	A
23	A	614	A
23	A	615	U
23	A	616	A
23	A	621	A
23	A	627	A
23	A	637	A
23	A	644	A
23	A	645	C
23	A	646	U
23	A	647	G
23	A	654	A
23	A	655	A
23	A	669	G
23	A	670	A
23	A	686	U
23	A	695	G
23	A	696	G
23	A	704	G
23	A	711	G
23	A	726	G
23	A	729	G
23	A	730	A
23	A	747	C
23	A	752	A

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Mol	Chain	Res	Type
23	A	763	G
23	A	764	A
23	A	765	C
23	A	774	G
23	A	775	G
23	A	776	G
23	A	782	A
23	A	783	A
23	A	784	G
23	A	785	G
23	A	789	A
23	A	791	C
23	A	805	G
23	A	811	U
23	A	812	C
23	A	819	A
23	A	827	U
23	A	828	U
23	A	830	G
23	A	831	G
23	A	845	A
23	A	846	U
23	A	847	U
23	A	856	G
23	A	858	G
23	A	860	U
23	A	878	A
23	A	886	A
23	A	892	A
23	A	893	C
23	A	896	A
23	A	897	C
23	A	907	G
23	A	910	A
23	A	931	U
23	A	934	U
23	A	941	A
23	A	946	C
23	A	953	G
23	A	961	C
23	A	973	A
23	A	974	G

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Mol	Chain	Res	Type
23	A	983	A
23	A	995	C
23	A	996	A
23	A	1009	A
23	A	1012	U
23	A	1013	C
23	A	1021	A
23	A	1023	U
23	A	1026	G
23	A	1033	U
23	A	1045	C
23	A	1046	A
23	A	1047	G
23	A	1057	A
23	A	1059	G
23	A	1060	U
23	A	1062	G
23	A	1064	C
23	A	1065	U
23	A	1066	U
23	A	1067	A
23	A	1069	A
23	A	1070	A
23	A	1071	G
23	A	1072	C
23	A	1076	C
23	A	1078	U
23	A	1079	C
23	A	1084	A
23	A	1085	A
23	A	1088	A
23	A	1089	A
23	A	1090	A
23	A	1096	A
23	A	1103	A
23	A	1104	C
23	A	1111	A
23	A	1112	G
23	A	1122	G
23	A	1130	U
23	A	1131	G
23	A	1132	U

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Mol	Chain	Res	Type
23	A	1133	A
23	A	1135	C
23	A	1139	G
23	A	1142	A
23	A	1169	A
23	A	1172	C
23	A	1175	A
23	A	1176	U
23	A	1180	U
23	A	1204	A
23	A	1206	G
23	A	1211	C
23	A	1212	G
23	A	1225	G
23	A	1247	A
23	A	1248	G
23	A	1250	G
23	A	1253	A
23	A	1256	G
23	A	1272	A
23	A	1275	A
23	A	1300	G
23	A	1301	A
23	A	1306	C
23	A	1312	U
23	A	1321	A
23	A	1325	U
23	A	1329	U
23	A	1330	C
23	A	1341	G
23	A	1344	U
23	A	1345	C
23	A	1352	U
23	A	1365	A
23	A	1368	G
23	A	1378	A
23	A	1379	U
23	A	1383	A
23	A	1395	A
23	A	1416	G
23	A	1419	A
23	A	1428	C

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Mol	Chain	Res	Type
23	A	1434	A
23	A	1437	C
23	A	1453	A
23	A	1454	C
23	A	1461	C
23	A	1475	G
23	A	1482	G
23	A	1490	A
23	A	1491	G
23	A	1497	U
23	A	1504	A
23	A	1509	A
23	A	1515	A
23	A	1524	G
23	A	1529	G
23	A	1532	A
23	A	1533	C
23	A	1534	U
23	A	1535	A
23	A	1536	C
23	A	1554	U
23	A	1555	G
23	A	1558	C
23	A	1559	U
23	A	1560	G
23	A	1565	C
23	A	1569	A
23	A	1578	U
23	A	1583	A
23	A	1584	U
23	A	1585	C
23	A	1608	A
23	A	1611	C
23	A	1646	C
23	A	1647	U
23	A	1648	U
23	A	1668	A
23	A	1672	A
23	A	1674	G
23	A	1694	C
23	A	1695	G
23	A	1707	G

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Mol	Chain	Res	Type
23	A	1715	G
23	A	1729	U
23	A	1730	C
23	A	1732	C
23	A	1735	A
23	A	1738	G
23	A	1757	A
23	A	1758	U
23	A	1759	A
23	A	1764	C
23	A	1773	A
23	A	1780	A
23	A	1786	A
23	A	1800	C
23	A	1801	A
23	A	1802	A
23	A	1808	A
23	A	1816	C
23	A	1829	A
23	A	1833	C
23	A	1859	U
23	A	1870	C
23	A	1871	A
23	A	1873	G
23	A	1884	G
23	A	1901	A
23	A	1906	G
23	A	1913	A
23	A	1914	C
23	A	1916	A
23	A	1927	A
23	A	1929	G
23	A	1930	G
23	A	1931	U
23	A	1937	A
23	A	1938	A
23	A	1940	U
23	A	1941	C
23	A	1944	U
23	A	1955	U
23	A	1964	G
23	A	1966	A

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Mol	Chain	Res	Type
23	A	1967	C
23	A	1970	A
23	A	1971	U
23	A	1972	G
23	A	1991	U
23	A	1992	G
23	A	1997	C
23	A	2004	G
23	A	2020	A
23	A	2022	U
23	A	2023	C
23	A	2030	A
23	A	2031	A
23	A	2033	A
23	A	2043	C
23	A	2052	A
23	A	2055	C
23	A	2056	G
23	A	2060	A
23	A	2061	G
23	A	2068	U
23	A	2069	A
23	A	2072	C
23	A	2093	G
23	A	2190	G
23	A	2191	A
23	A	2192	U
23	A	2193	G
23	A	2194	U
23	A	2198	A
23	A	2199	A
23	A	2204	G
23	A	2211	A
23	A	2213	U
23	A	2214	C
23	A	2225	A
23	A	2226	C
23	A	2238	G
23	A	2239	G
23	A	2250	G
23	A	2251	G
23	A	2266	A

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Mol	Chain	Res	Type
23	A	2279	G
23	A	2283	C
23	A	2287	A
23	A	2288	A
23	A	2297	A
23	A	2305	U
23	A	2309	A
23	A	2325	G
23	A	2327	A
23	A	2333	A
23	A	2334	U
23	A	2335	A
23	A	2336	A
23	A	2350	C
23	A	2354	C
23	A	2357	G
23	A	2361	G
23	A	2383	G
23	A	2385	C
23	A	2392	A
23	A	2402	U
23	A	2406	A
23	A	2424	C
23	A	2428	G
23	A	2429	G
23	A	2430	A
23	A	2435	A
23	A	2441	U
23	A	2445	G
23	A	2447	G
23	A	2448	A
23	A	2476	A
23	A	2478	A
23	A	2481	G
23	A	2498	C
23	A	2502	G
23	A	2503	A
23	A	2504	U
23	A	2505	G
23	A	2506	U
23	A	2513	A
23	A	2518	A

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Mol	Chain	Res	Type
23	A	2520	C
23	A	2529	G
23	A	2535	G
23	A	2547	A
23	A	2554	U
23	A	2562	U
23	A	2566	A
23	A	2567	G
23	A	2572	A
23	A	2573	C
23	A	2582	G
23	A	2585	U
23	A	2586	U
23	A	2602	A
23	A	2604	U
23	A	2613	U
23	A	2614	A
23	A	2629	U
23	A	2646	C
23	A	2655	G
23	A	2656	U
23	A	2682	A
23	A	2689	U
23	A	2690	U
23	A	2714	G
23	A	2718	G
23	A	2722	G
23	A	2726	A
23	A	2732	G
23	A	2733	A
23	A	2739	U
23	A	2744	G
23	A	2748	A
23	A	2764	A
23	A	2765	A
23	A	2769	U
23	A	2778	A
23	A	2779	U
23	A	2790	U
23	A	2791	G
23	A	2793	C
23	A	2794	C

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Mol	Chain	Res	Type
23	A	2797	U
23	A	2800	A
23	A	2807	U
23	A	2808	G
23	A	2809	A
23	A	2818	U
23	A	2820	A
23	A	2833	U
23	A	2835	A
23	A	2836	U
23	A	2849	U
23	A	2861	U
23	A	2867	G
23	A	2868	A
23	A	2873	A
23	A	2880	C
23	A	2884	U
23	A	2887	A
23	A	2893	A
23	A	2901	C
24	B	4	C
24	B	12	C
24	B	13	G
24	B	24	G
24	B	26	C
24	B	35	C
24	B	41	G
24	B	42	C
24	B	44	G
24	B	45	A
24	B	67	G
24	B	88	C
24	B	89	U
24	B	90	C
24	B	109	A
53	x	3	G
53	x	4	U
53	x	5	G
53	x	6	A
53	x	13	C
53	x	14	A
53	x	18	G

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Mol	Chain	Res	Type
53	x	19	G
53	x	20	U
53	x	21	A
53	x	25	C
53	x	35	G
53	x	36	G
53	x	40	G
53	x	42	A
53	x	47	U
53	x	54	U
53	x	66	A
53	x	67	U
53	x	68	C
53	x	72	G
53	x	74	C
53	x	75	C
53	x	76	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	A	51	G
23	A	242	G
23	A	421	C
23	A	859	G
23	A	1020	A
23	A	1022	G
23	A	1070	A
23	A	1182	G
23	A	1190	G
23	A	1300	G
23	A	1378	A
23	A	1399	C
23	A	1432	G
23	A	1930	G
23	A	1940	U
23	A	2286	G
23	A	2326	C
23	A	2391	G
23	A	2808	G
24	B	66	A

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 monosaccharides 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.

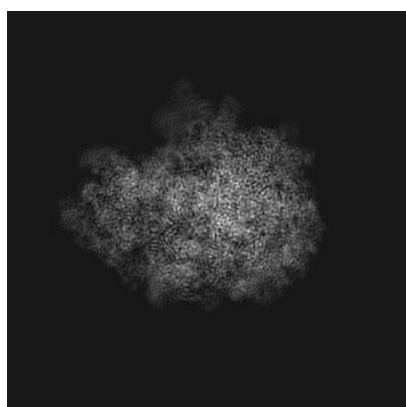
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3898. These allow visual inspection of the internal detail of the map and identification of artifacts.

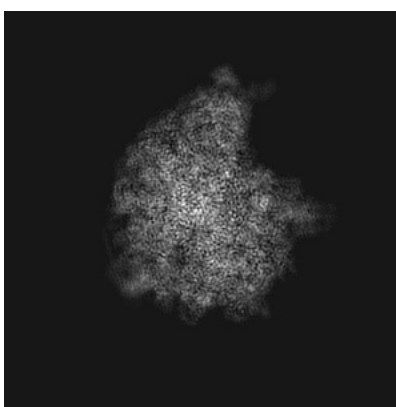
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

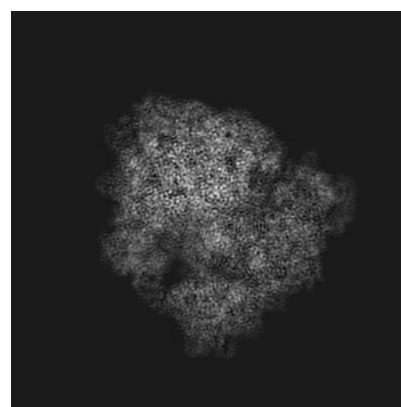
6.1.1 Primary map



X



Y

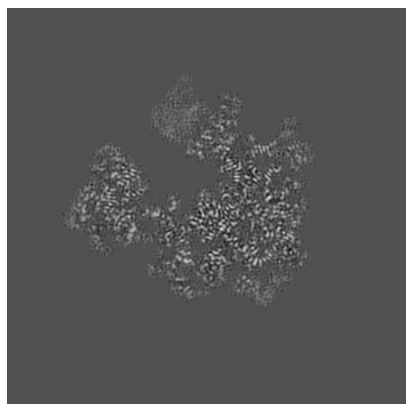


Z

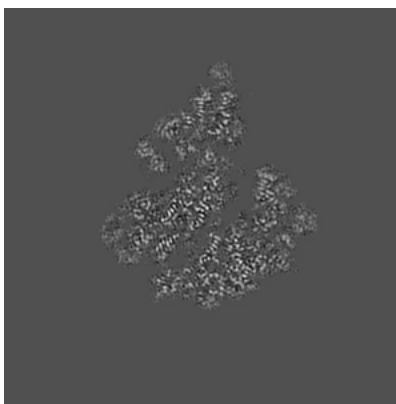
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

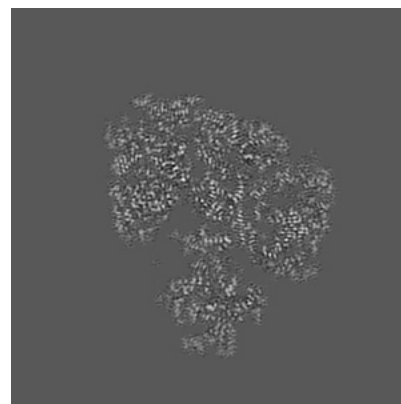
6.2.1 Primary map



X Index: 180



Y Index: 180

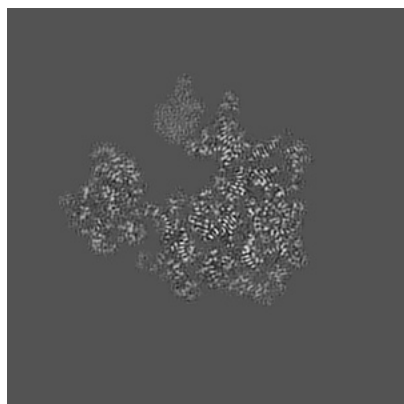


Z Index: 180

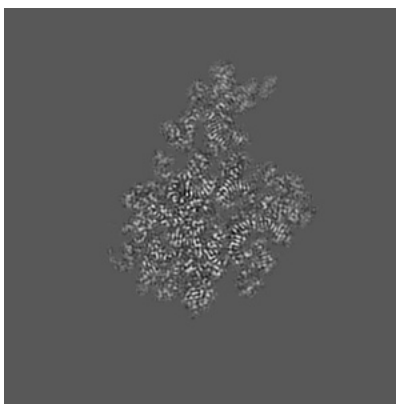
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

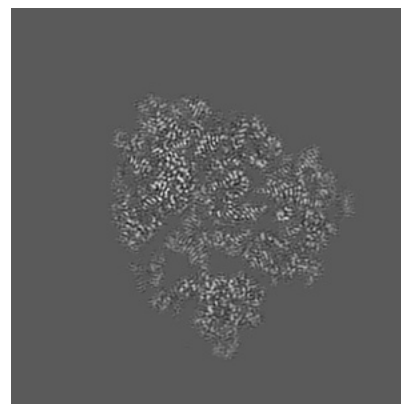
6.3.1 Primary map



X Index: 184



Y Index: 191

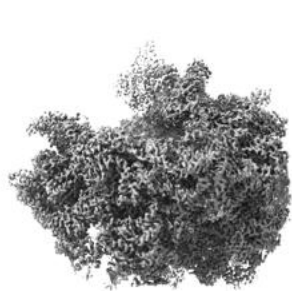


Z Index: 187

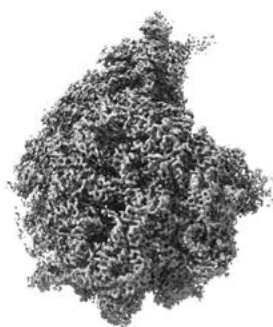
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

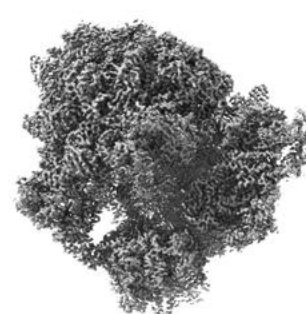
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.105. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

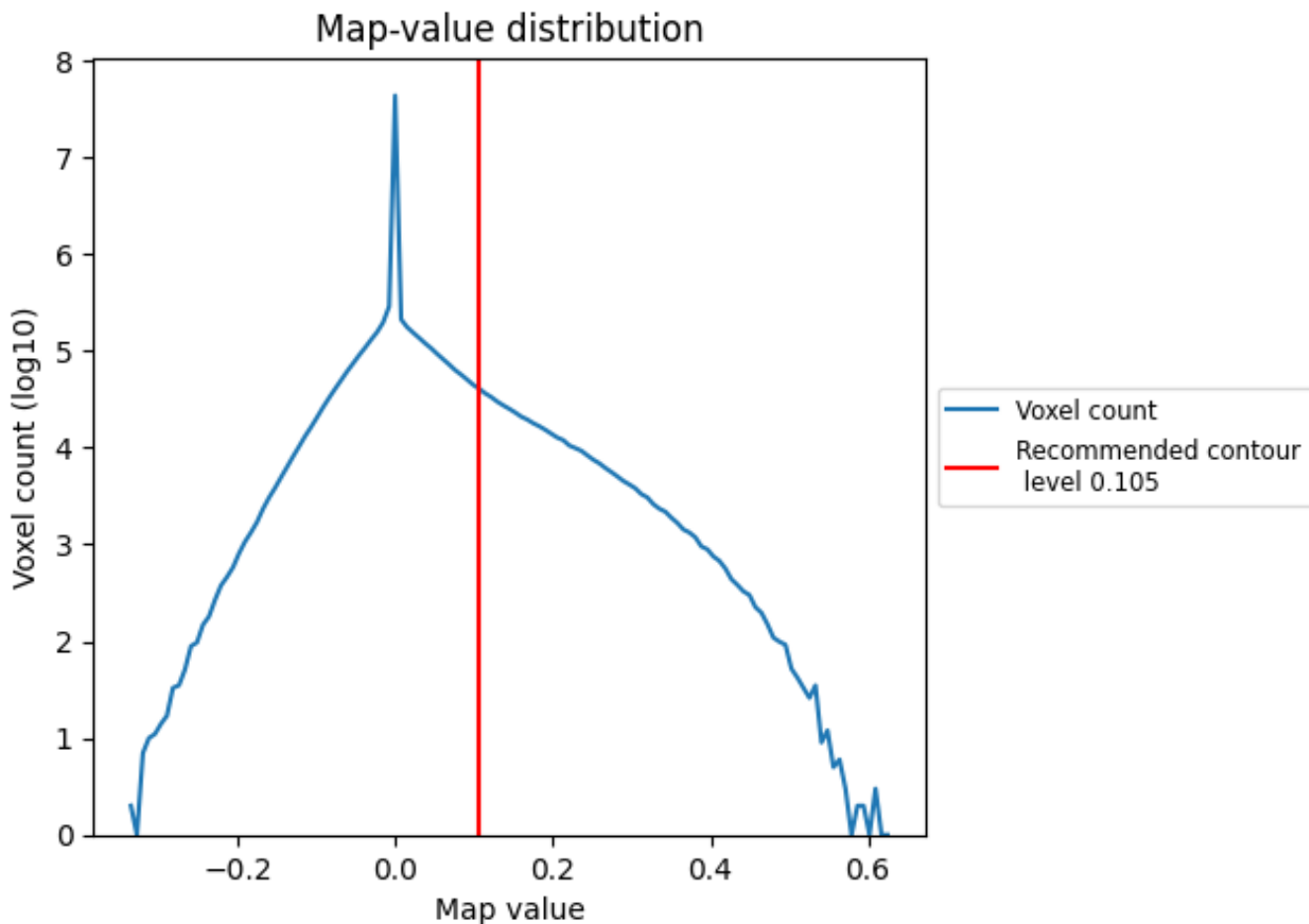
6.5 Mask visualisation

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

7 Map analysis [i](#)

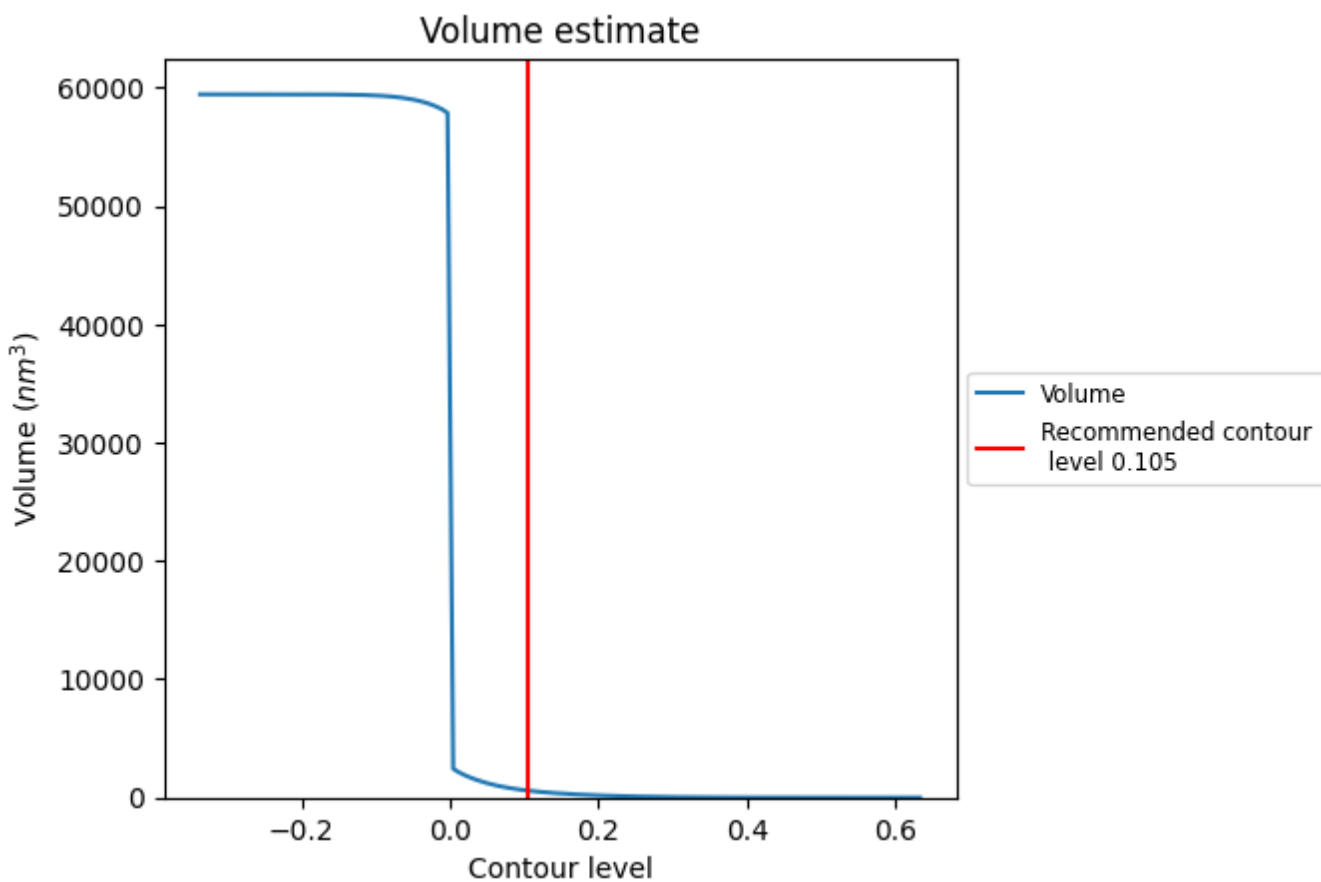
This section contains the results of statistical analysis of the map.

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.

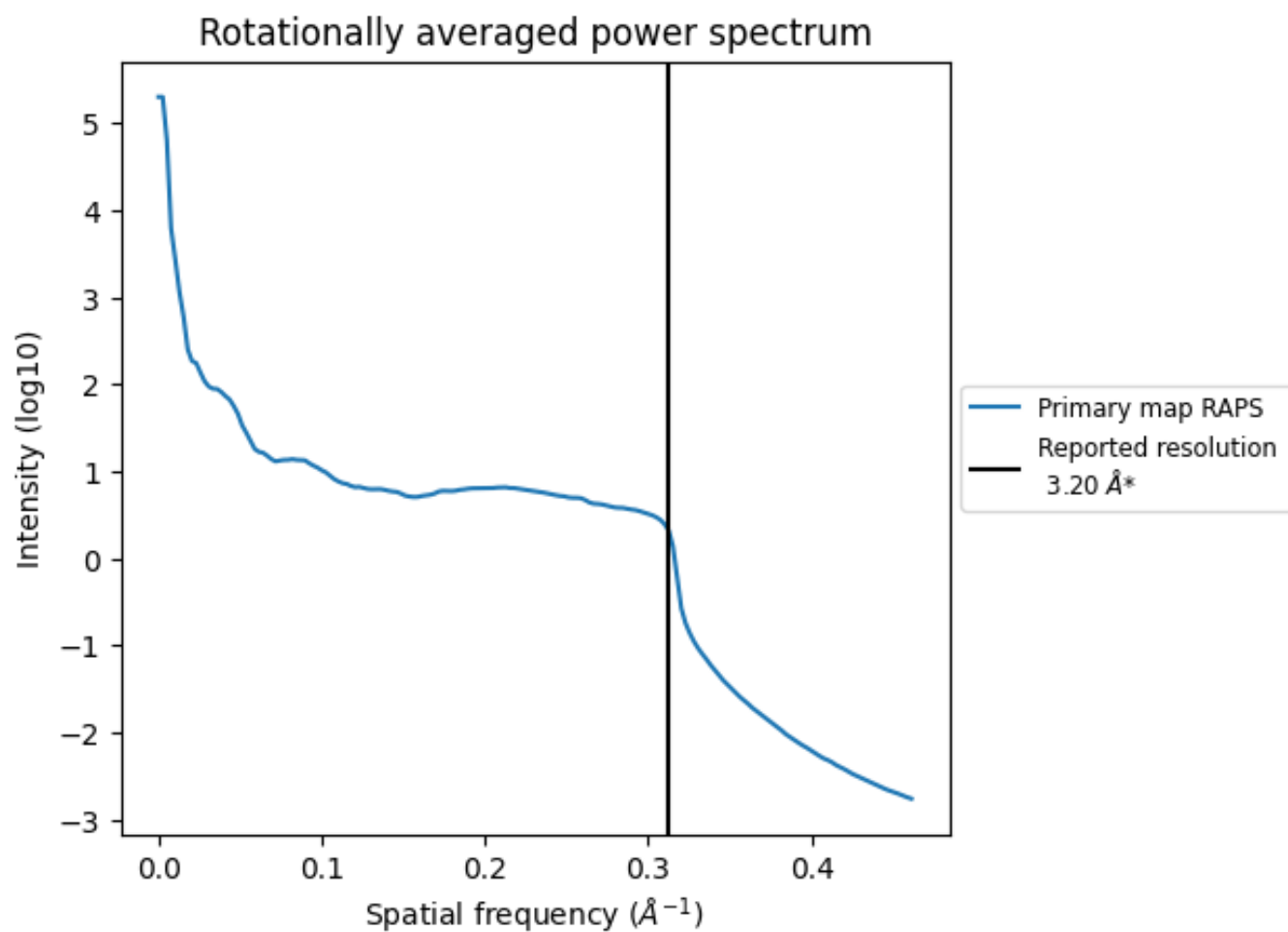
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 587 nm³; this corresponds to an approximate mass of 530 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.312\AA^{-1}

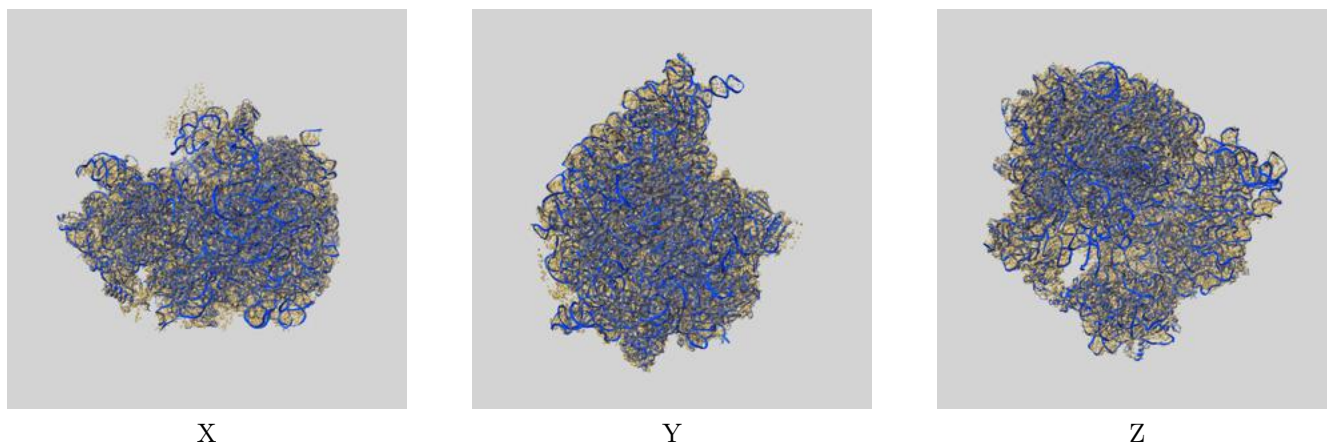
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

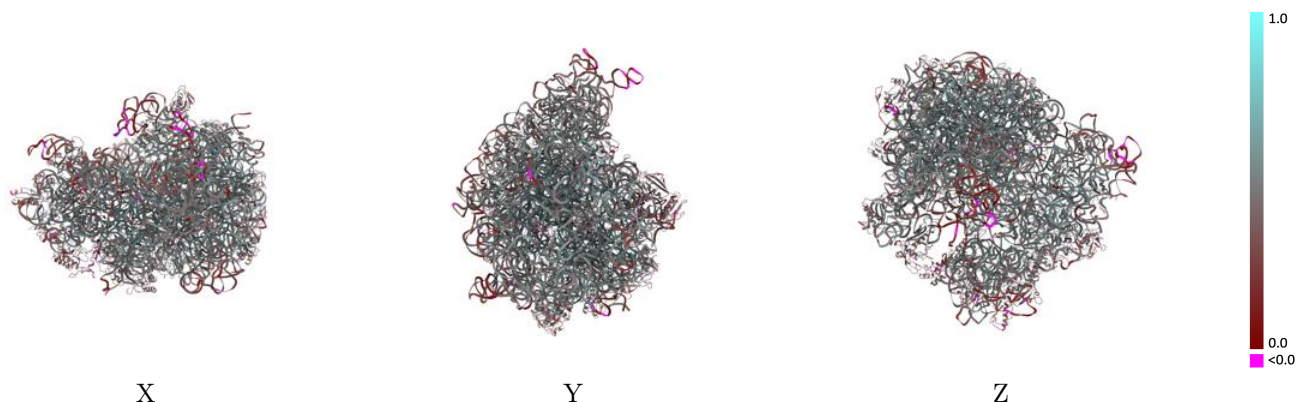
This section contains information regarding the fit between EMDB map EMD-3898 and PDB model 6ENF. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



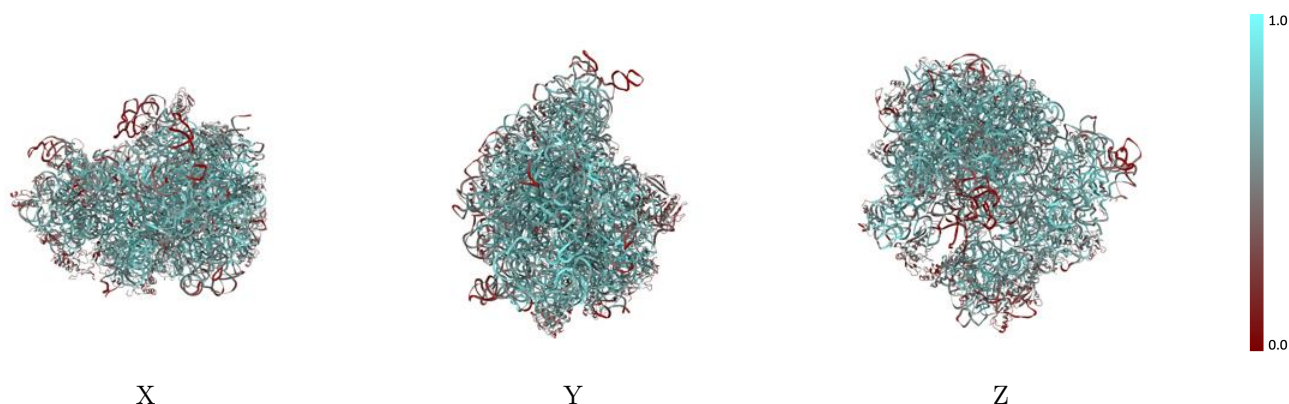
The images above show the 3D surface view of the map at the recommended contour level 0.105 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



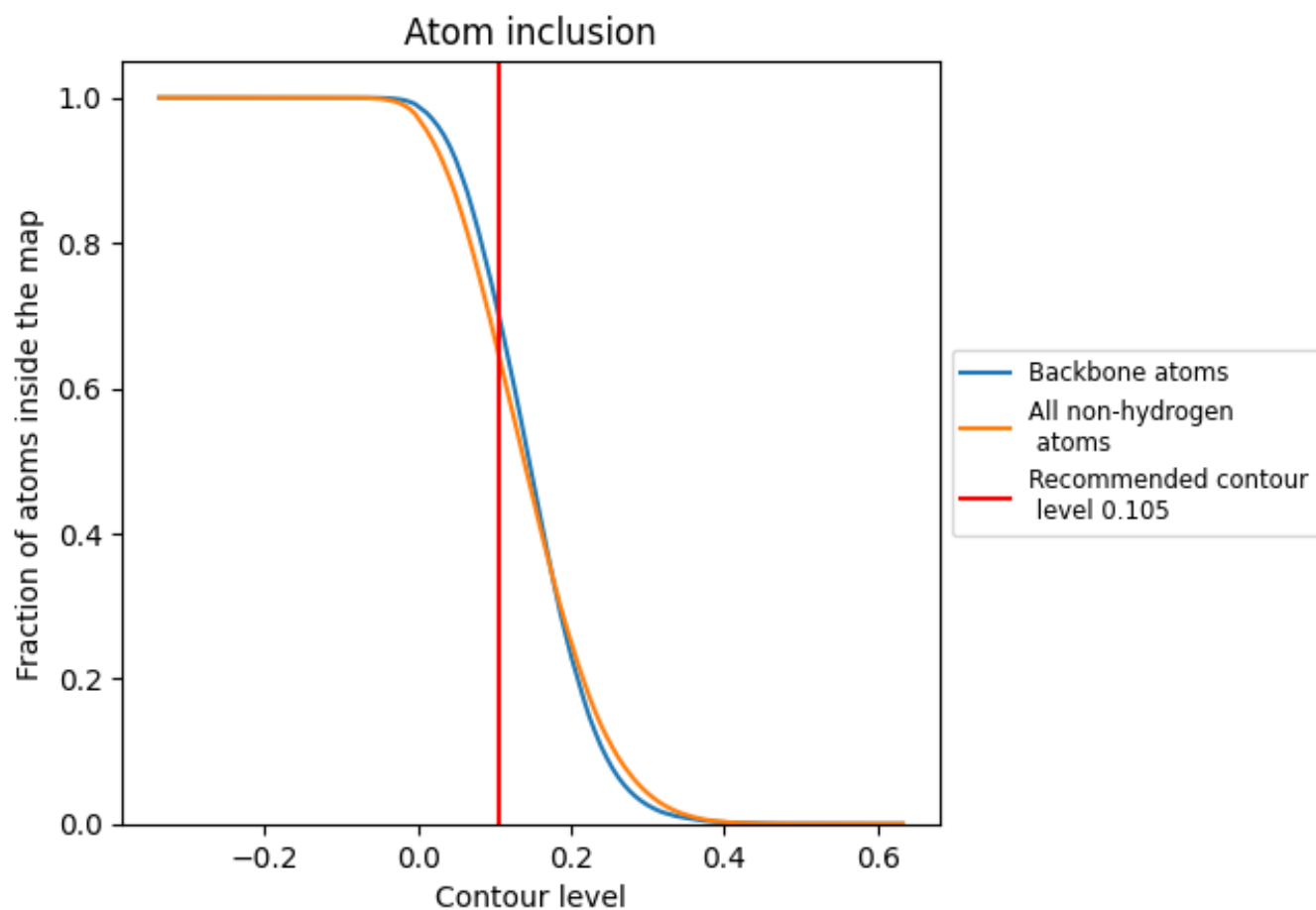
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.105).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 65% 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 (0.105) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6493	 0.4590
0	 0.5724	 0.4500
1	 0.4713	 0.4070
2	 0.6789	 0.4850
3	 0.6456	 0.4800
4	 0.6096	 0.4760
6	 0.2133	 0.2540
A	 0.7226	 0.4870
B	 0.6699	 0.4600
C	 0.6275	 0.4730
D	 0.6092	 0.4770
E	 0.4868	 0.4110
F	 0.4341	 0.3740
G	 0.3616	 0.3540
J	 0.6000	 0.4710
K	 0.5882	 0.4610
L	 0.5827	 0.4440
M	 0.5787	 0.4610
N	 0.6323	 0.4710
O	 0.5388	 0.4170
P	 0.5574	 0.4450
Q	 0.6751	 0.4990
R	 0.5144	 0.4290
S	 0.5478	 0.4450
T	 0.4945	 0.4010
U	 0.4055	 0.3690
V	 0.5041	 0.4170
W	 0.6580	 0.4950
X	 0.5574	 0.4420
Y	 0.3984	 0.3730
Z	 0.5652	 0.4430
a	 0.6956	 0.4690
b	 0.3893	 0.3310
c	 0.5330	 0.4190
d	 0.4667	 0.3720



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Chain	Atom inclusion	Q-score
e	 0.5648	 0.4300
f	 0.4171	 0.3440
g	 0.4056	 0.3600
h	 0.5635	 0.4550
i	 0.4668	 0.3640
j	 0.3916	 0.3480
k	 0.4947	 0.4000
l	 0.5353	 0.4310
m	 0.4501	 0.3710
n	 0.5091	 0.4180
o	 0.5377	 0.4340
p	 0.5439	 0.3940
q	 0.4620	 0.3990
r	 0.5567	 0.4170
s	 0.4638	 0.3820
t	 0.5123	 0.4080
u	 0.2710	 0.2270
v	 0.6984	 0.4580
x	 0.4708	 0.4090