



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 05:56 PM EST

PDB ID : 6O9J
EMDB ID : EMD-0661
Title : 70S Elongation Competent Ribosome
Authors : Frank, J.; Gonzalez Jr., R.L.; Kaledhonkar, S.; Fu, Z.; Caban, K.; Li, W.;
Chen, B.; Sun, M.
Deposited on : 2019-03-14
Resolution : 3.90 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

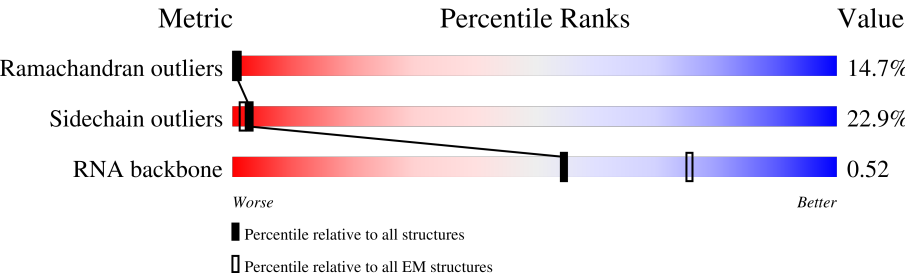
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	117	
2	B	2841	
3	V	94	
4	C	267	
5	D	209	
6	E	201	
7	F	178	
8	G	176	






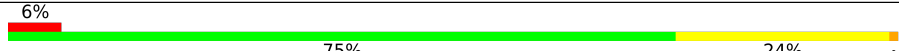
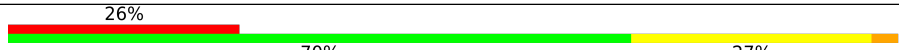

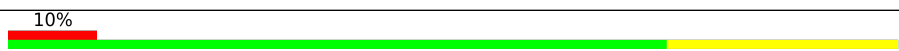

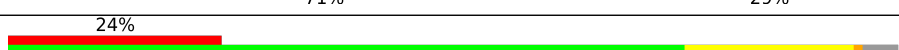
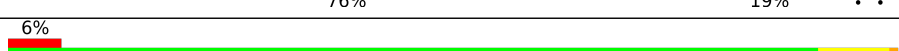
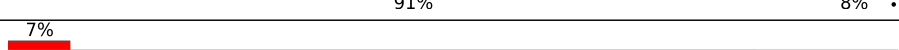
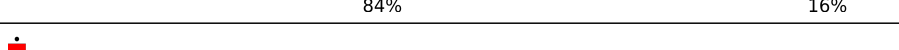
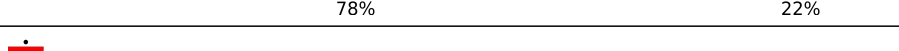
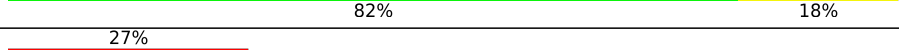




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Mol	Chain	Length	Quality of chain
9	H	149	
10	J	140	
11	K	121	
12	L	144	
13	M	136	
14	N	127	
15	O	117	
16	P	114	
17	Q	117	
18	R	103	
19	S	110	
20	T	99	
21	U	102	
22	W	84	
23	X	63	
24	Y	58	
25	Z	70	
26	1	56	
27	2	54	
28	3	46	
29	4	64	
30	5	38	
31	6	141	
32	a	1530	
33	c	206	

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Mol	Chain	Length	Quality of chain
34	d	205	
35	e	150	
36	f	100	
37	g	150	
38	h	129	
39	i	127	
40	j	98	
41	k	117	
42	l	123	
43	m	114	
44	n	100	
45	o	88	
46	p	82	
47	q	80	
48	r	55	
49	s	79	
50	t	85	
51	7	218	
52	u	51	
53	v	76	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 142682 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 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	117	Total	C	N	O	P	0	0
			2507	1116	459	815	117		

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2841	Total	C	N	O	P	0	0
			60995	27210	11229	19715	2841		

- Molecule 3 is a protein called 50S ribosomal protein L25.

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

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	267	Total	C	N	O	S	0	0
			2053	1271	416	359	7		

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	140	Total	C	N	O	S	0	0
			1112	704	210	194	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	121	Total	C	N	O	S	0	0
			930	582	179	164	5		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	99	Total	C	N	O	S	0	0
			777	491	145	139	2		

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	84	Total	C	N	O	S	
			634	391	129	113	1	0

- Molecule 23 is a protein called 50S ribosomal protein L29.

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

- Molecule 24 is a protein called 50S ribosomal protein L30.

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

- Molecule 25 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Z	70	Total	C	N	O	S	
			549	339	104	100	6	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	1	56	Total	C	N	O	S	
			444	269	94	80	1	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	2	54	Total	C	N	O		
			441	284	81	76	0	0

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1530	Total	C	N	O	P	0	0
			32831	14642	6024	10635	1530		

- Molecule 33 is a protein called 30S ribosomal protein S3.

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

- Molecule 34 is a protein called 30S ribosomal protein S4.

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

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

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

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	150	Total	C	N	O	S	0	0
			1174	730	226	214	4		

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

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

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 42 is a protein called 30S ribosomal protein S12.

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

- Molecule 43 is a protein called 30S ribosomal protein S13.

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

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

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

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 49 is a protein called 30S ribosomal protein S19.

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

- Molecule 50 is a protein called 30S ribosomal protein S20.

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

- Molecule 51 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	7	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 52 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	51	Total	C	N	O	S	0	0
			425	265	86	73	1		


- Molecule 53 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

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.

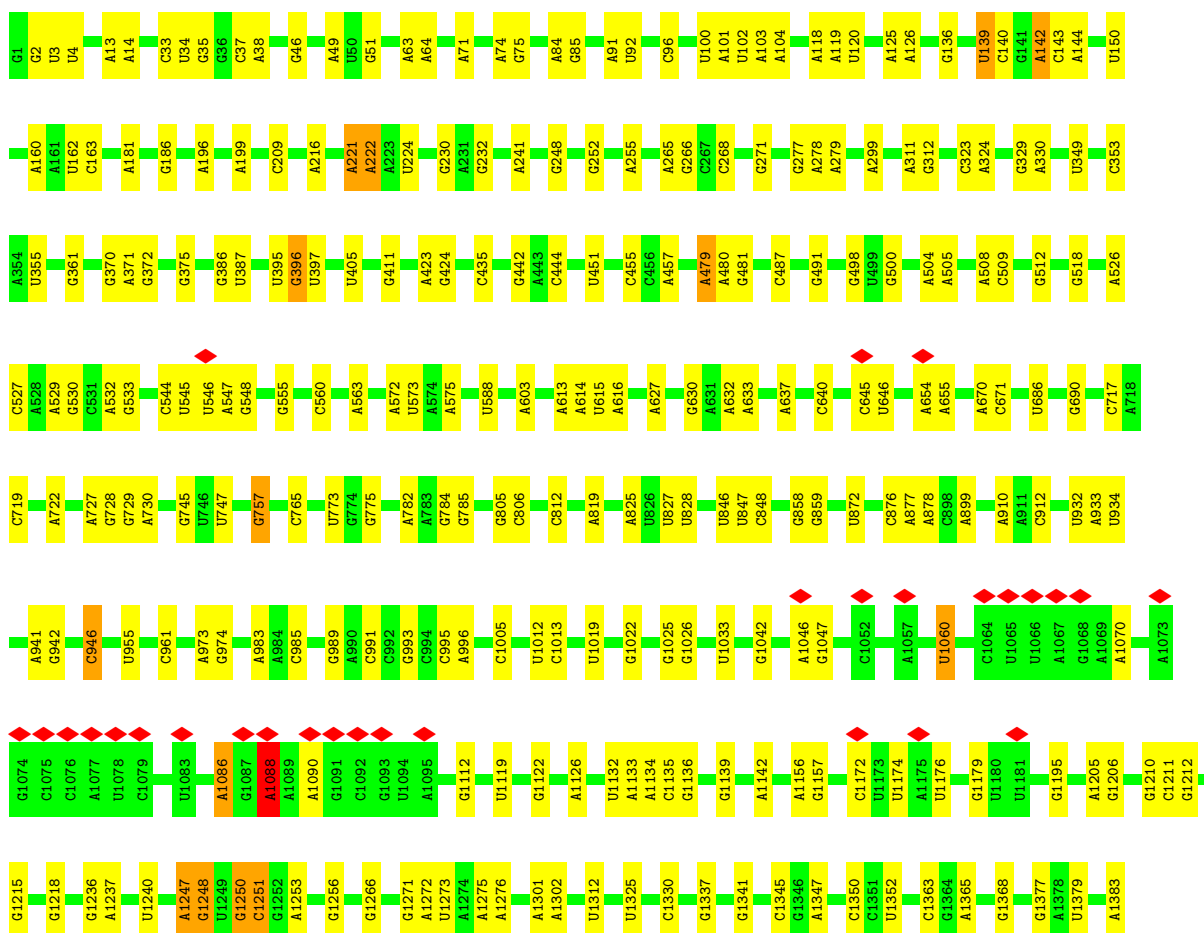
• Molecule 1: 5S rRNA

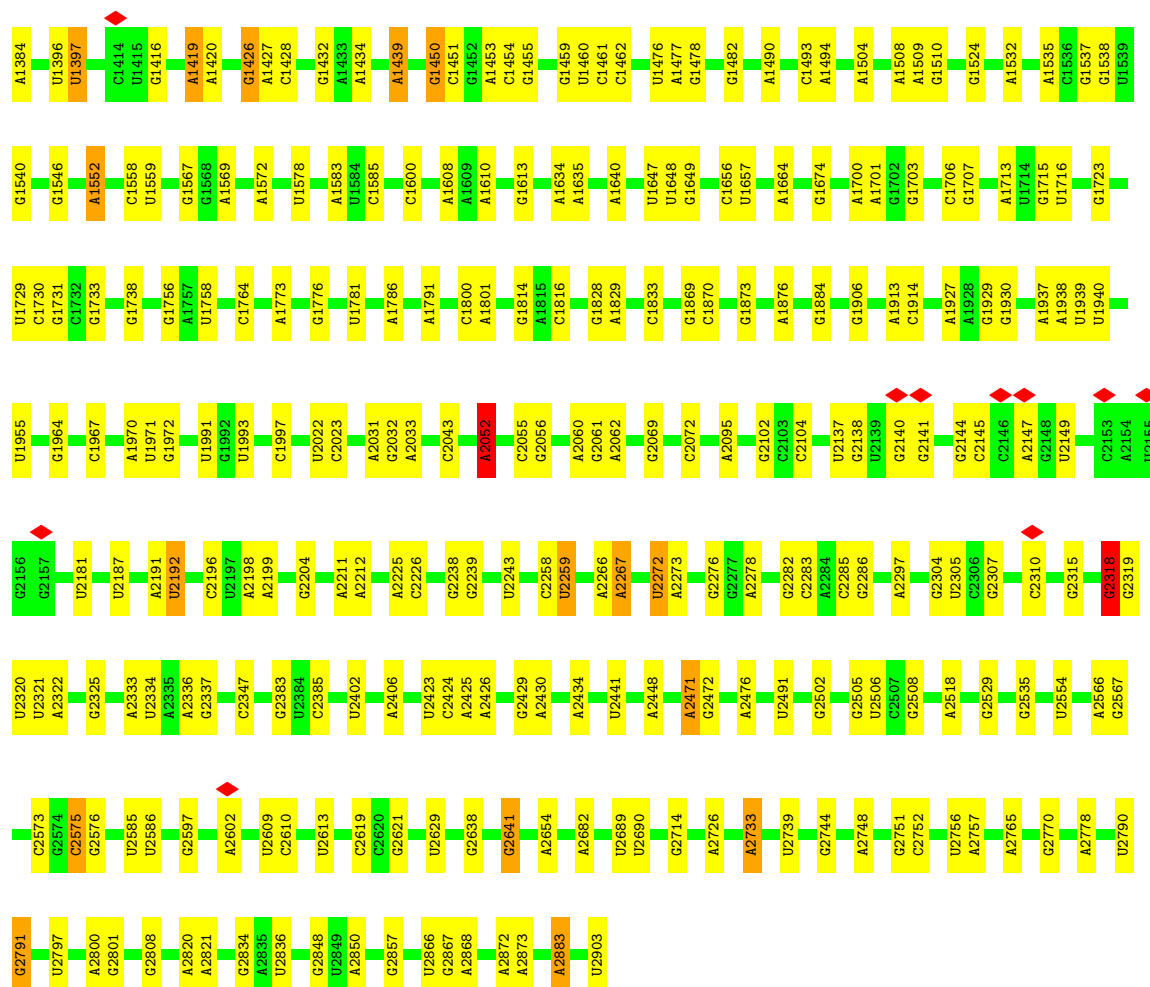
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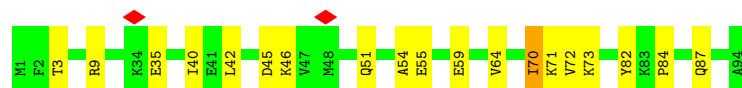
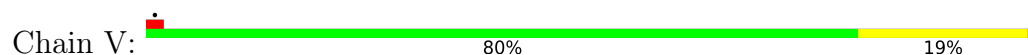
• Molecule 2: 23S rRNA

Chain B: 

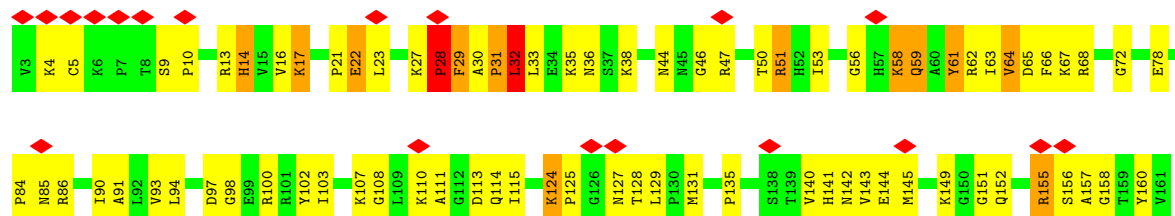


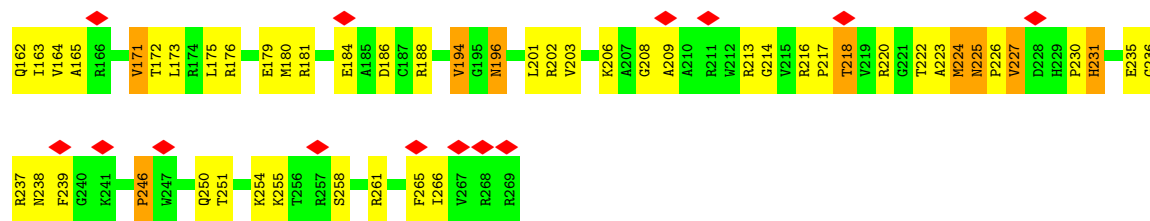


• Molecule 3: 50S ribosomal protein L25

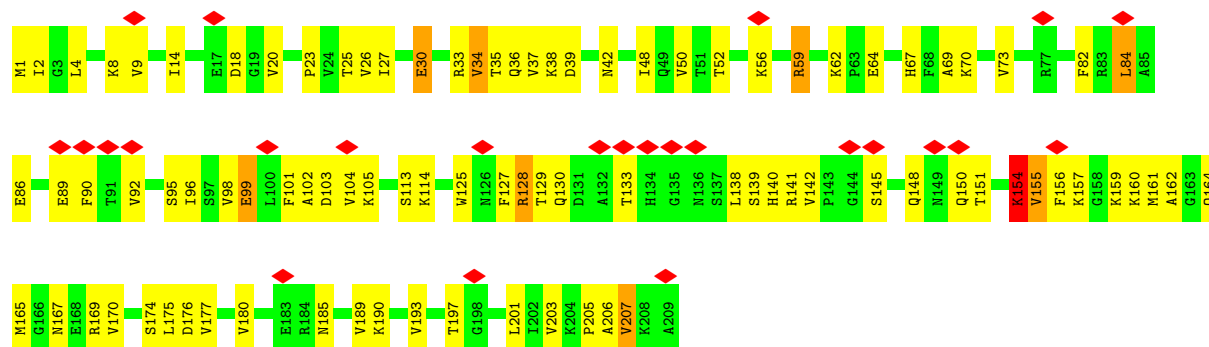


• Molecule 4: 50S ribosomal protein L2

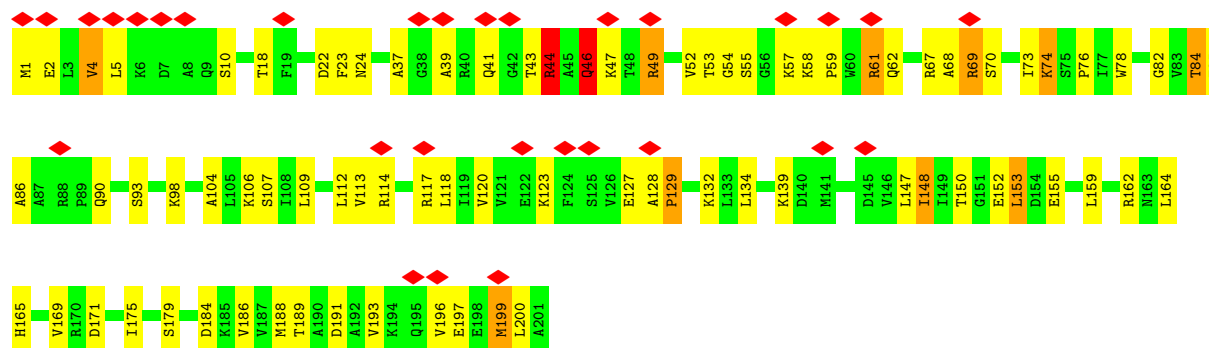




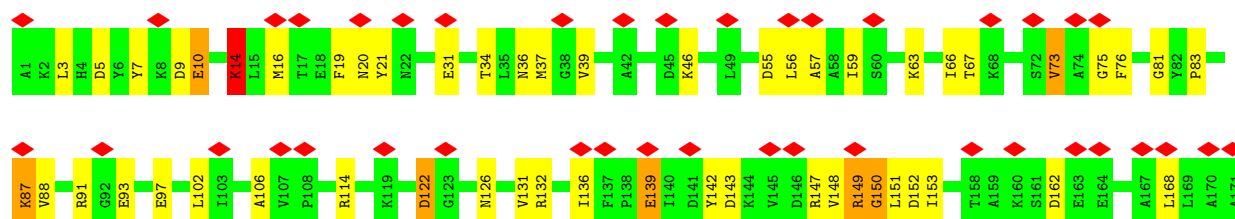
• Molecule 5: 50S ribosomal protein L3

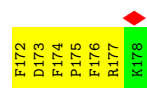


• Molecule 6: 50S ribosomal protein L4

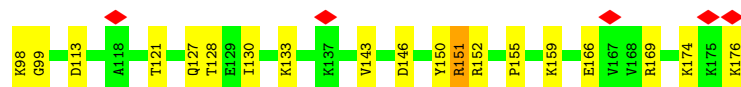
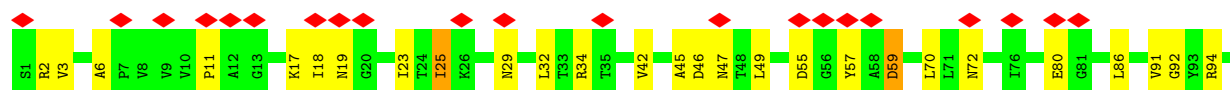
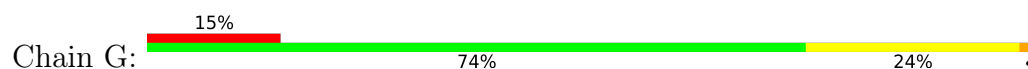


• Molecule 7: 50S ribosomal protein L5

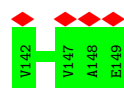
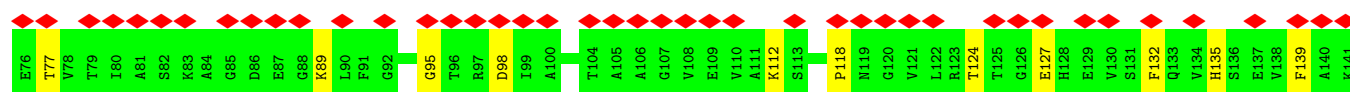
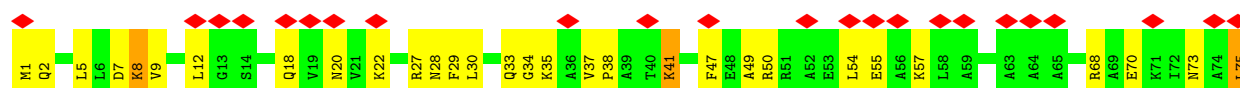
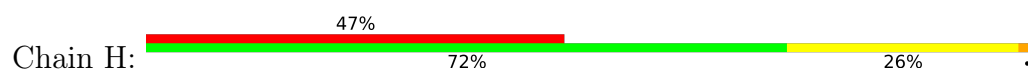




• Molecule 8: 50S ribosomal protein L6



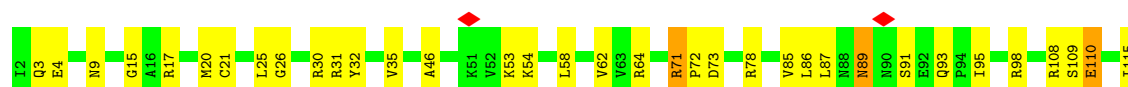
• Molecule 9: 50S ribosomal protein L9



• Molecule 10: 50S ribosomal protein L13

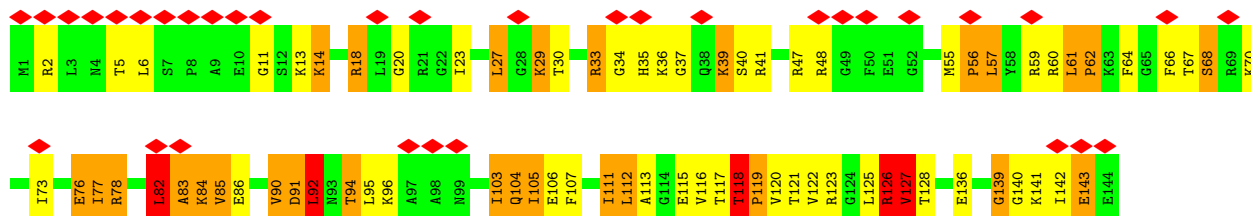


• Molecule 11: 50S ribosomal protein L14

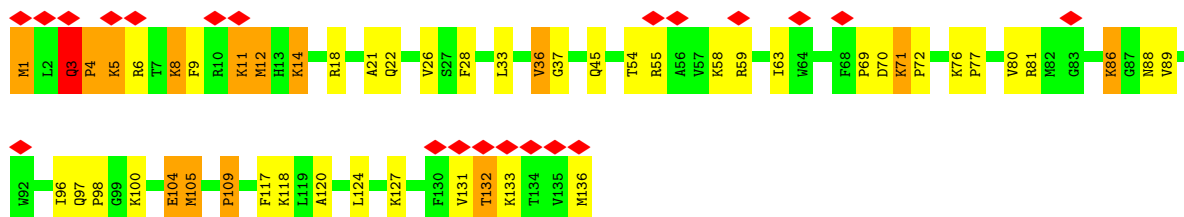




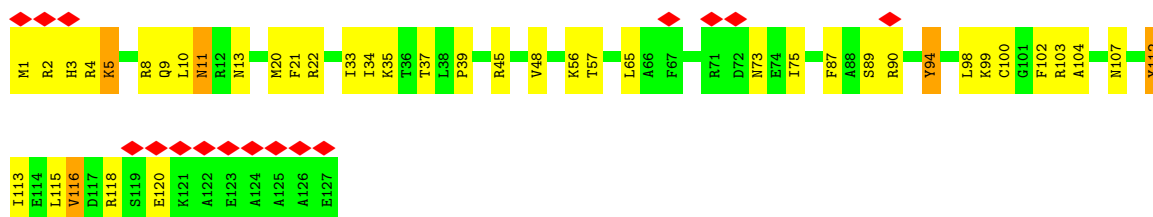
- Molecule 12: 50S ribosomal protein L15



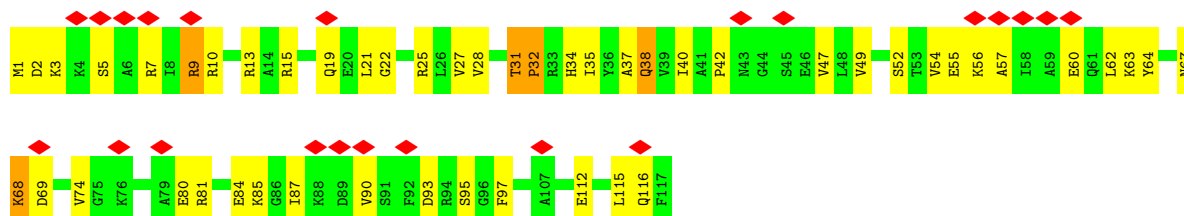
- Molecule 13: 50S ribosomal protein L16



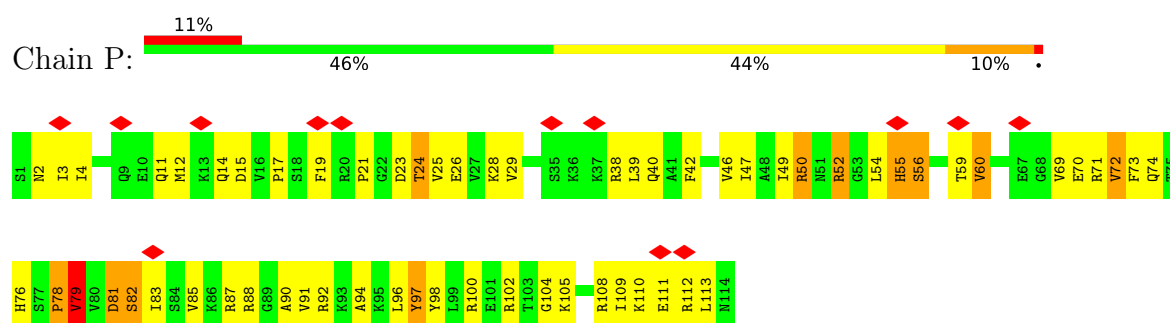
- Molecule 14: 50S ribosomal protein L17



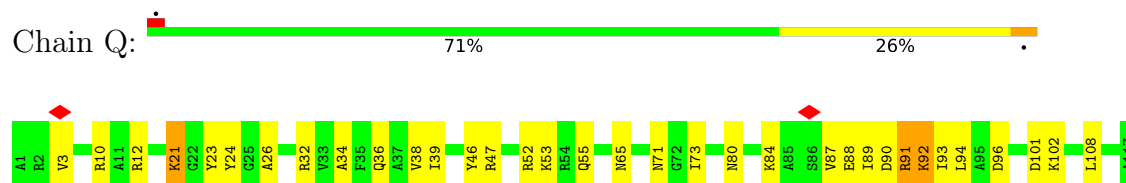
- Molecule 15: 50S ribosomal protein L18



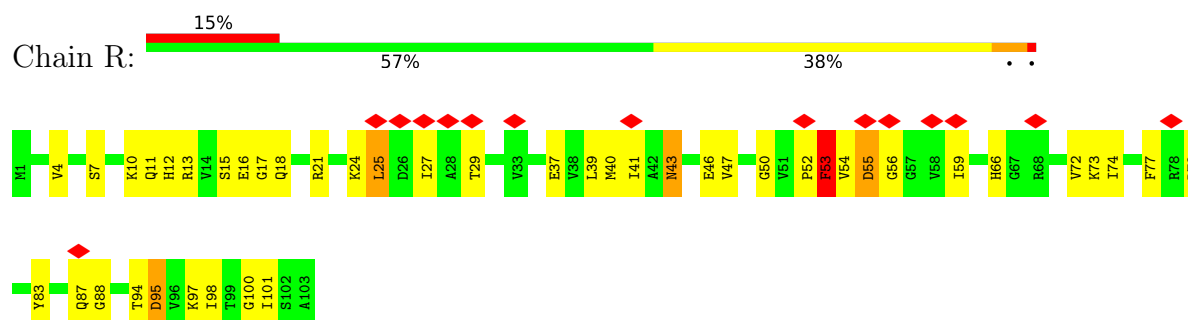
- Molecule 16: 50S ribosomal protein L19



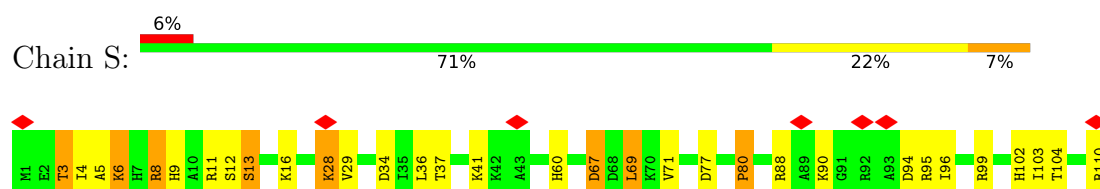
- Molecule 17: 50S ribosomal protein L20



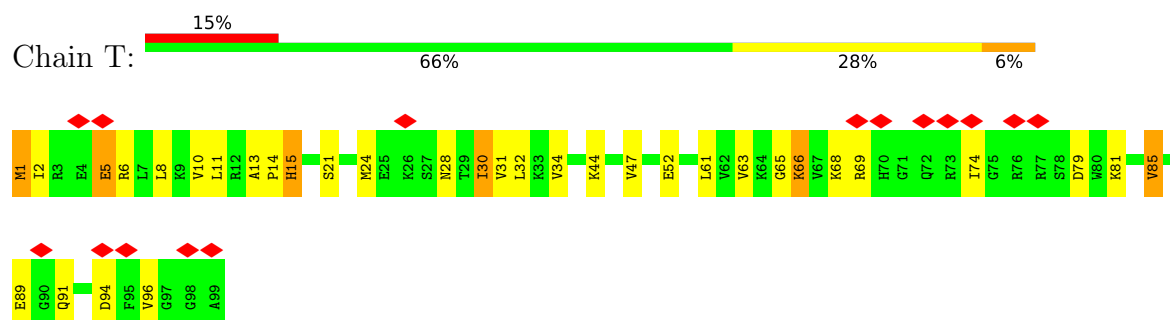
- Molecule 18: 50S ribosomal protein L21



- Molecule 19: 50S ribosomal protein L22

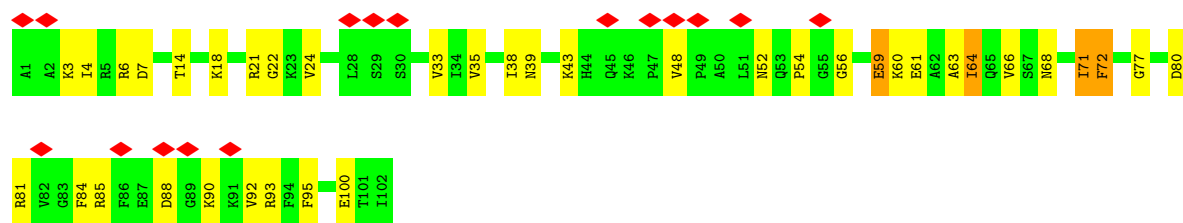


- Molecule 20: 50S ribosomal protein L23

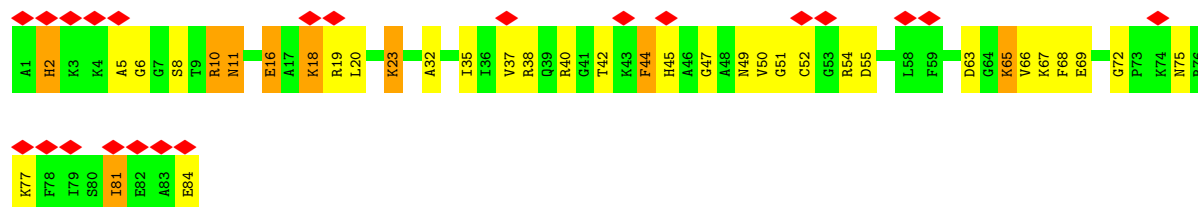


- Molecule 21: 50S ribosomal protein L24

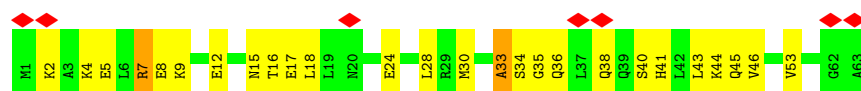




- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L29



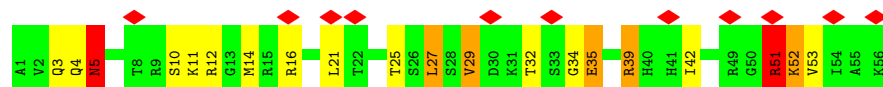
- Molecule 24: 50S ribosomal protein L30



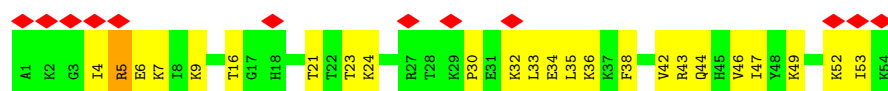
- Molecule 25: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L33



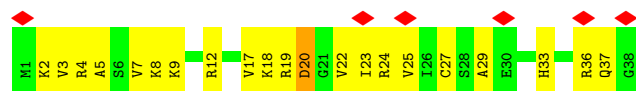
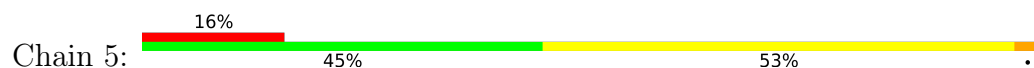
- Molecule 28: 50S ribosomal protein L34



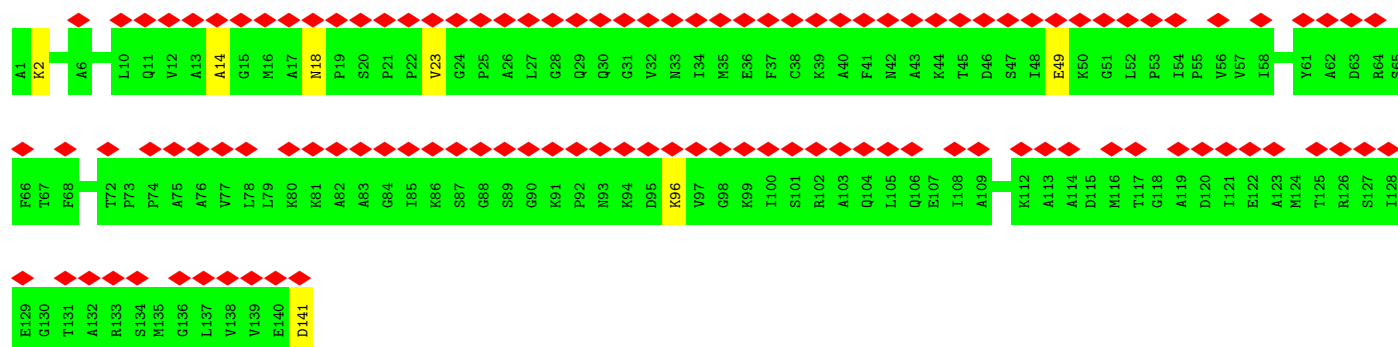
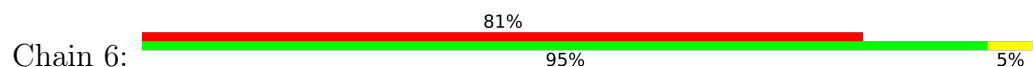
- Molecule 29: 50S ribosomal protein L35



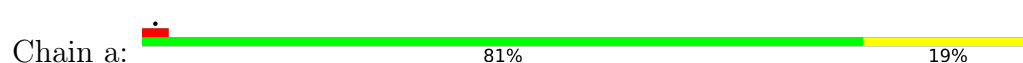
- Molecule 30: 50S ribosomal protein L36

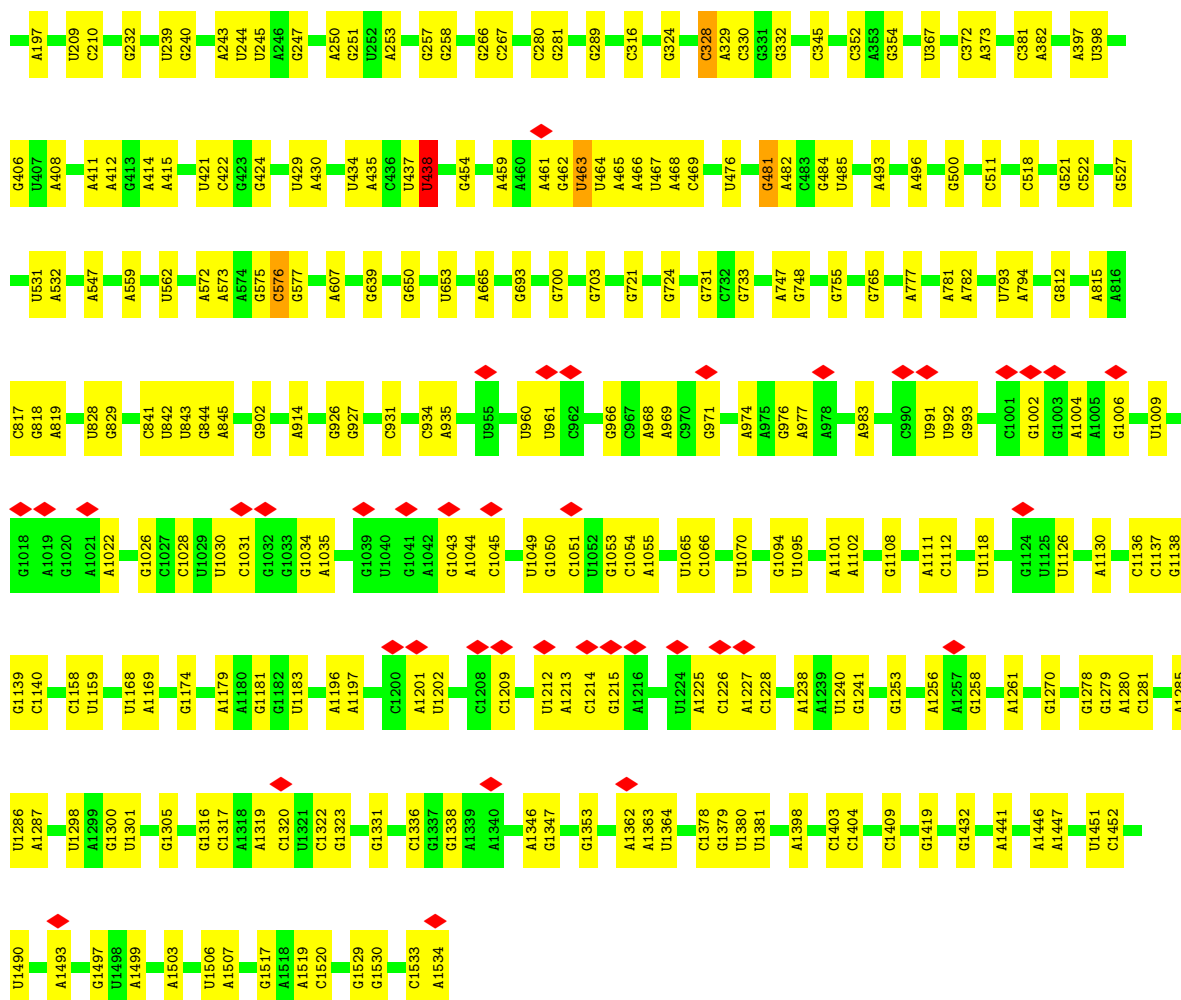


- Molecule 31: 50S ribosomal protein L11

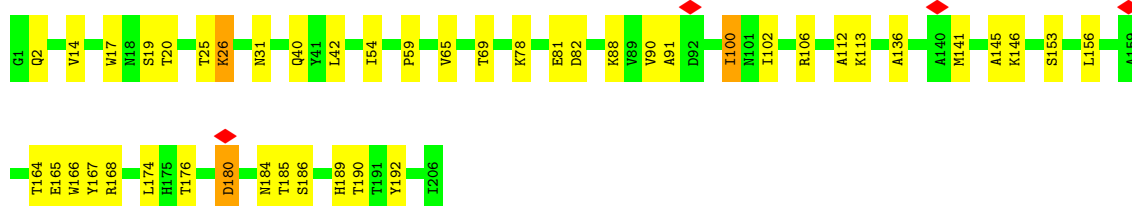
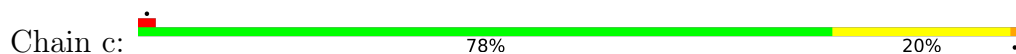


- Molecule 32: 16S rRNA

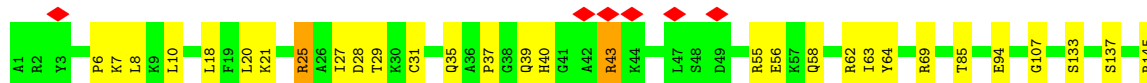
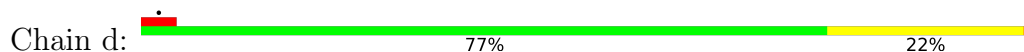


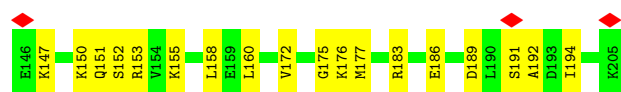


• Molecule 33: 30S ribosomal protein S3

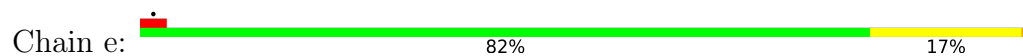


• Molecule 34: 30S ribosomal protein S4

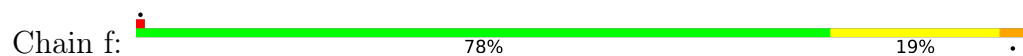




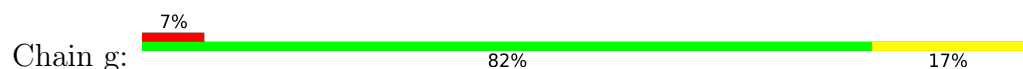
- Molecule 35: 30S ribosomal protein S5



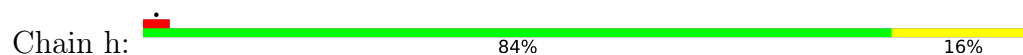
- Molecule 36: 30S ribosomal protein S6



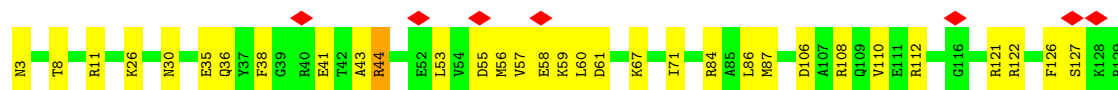
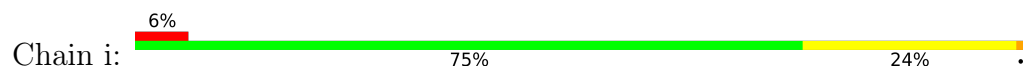
- Molecule 37: 30S ribosomal protein S7



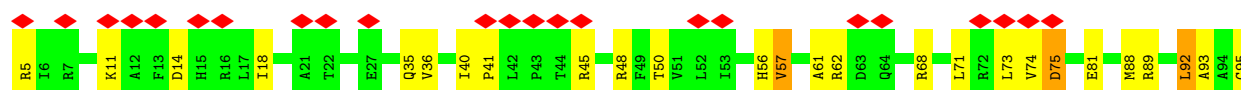
- Molecule 38: 30S ribosomal protein S8

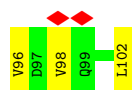


- Molecule 39: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S10

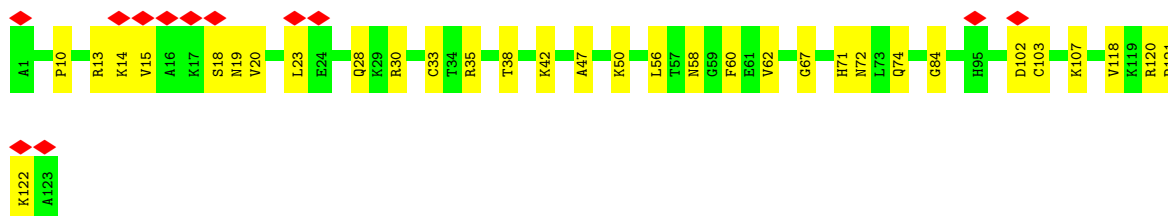




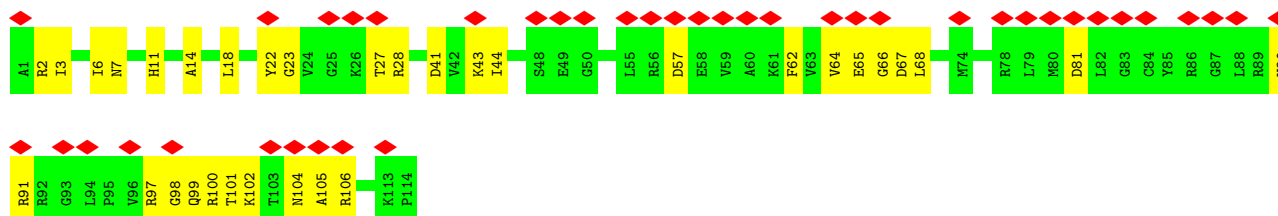
- Molecule 41: 30S ribosomal protein S11



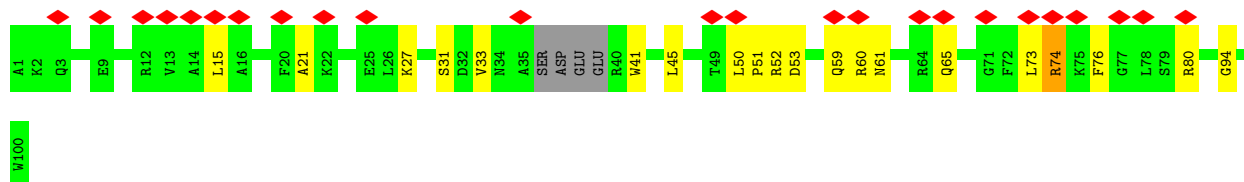
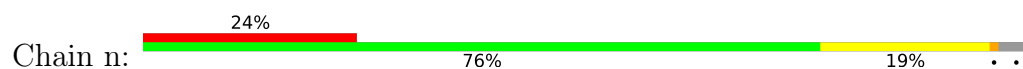
- Molecule 42: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S13

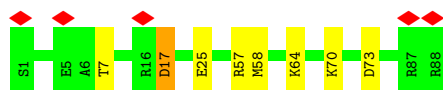


- Molecule 44: 30S ribosomal protein S14

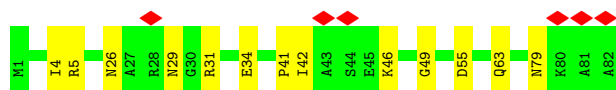
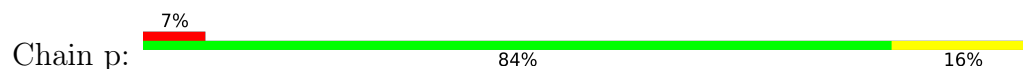


- Molecule 45: 30S ribosomal protein S15

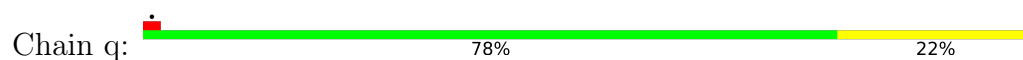




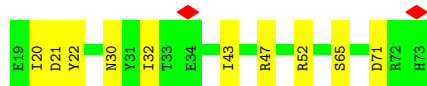
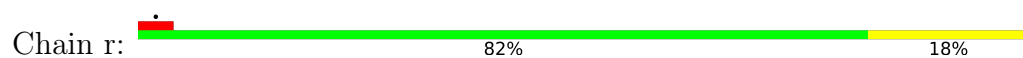
- Molecule 46: 30S ribosomal protein S16



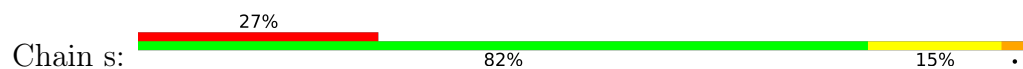
- Molecule 47: 30S ribosomal protein S17



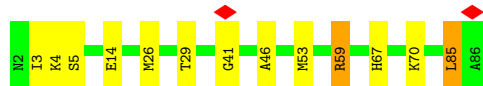
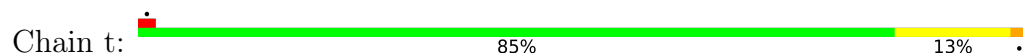
- Molecule 48: 30S ribosomal protein S18



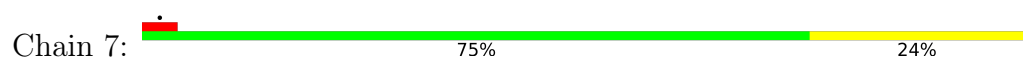
- Molecule 49: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S20

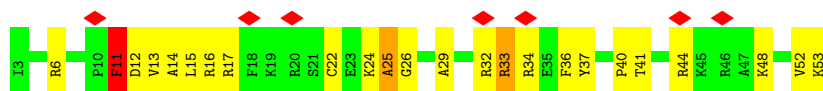


- Molecule 51: 30S ribosomal protein S2

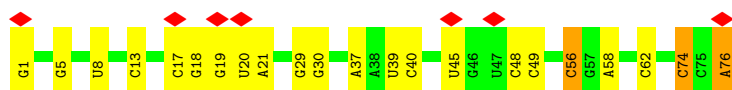




- Molecule 52: 30S ribosomal protein S21



- Molecule 53: P-tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46042	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8	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	0.302	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.66, 1.66, 1.66	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	A	0.27	0/2803	0.74	0/4371
2	B	0.33	15/68314 (0.0%)	0.79	63/106569 (0.1%)
3	V	0.30	0/766	0.53	0/1025
4	C	0.40	0/2092	0.88	7/2813 (0.2%)
5	D	0.40	0/1586	0.80	2/2134 (0.1%)
6	E	0.45	1/1571 (0.1%)	0.88	6/2113 (0.3%)
7	F	0.33	0/1444	0.87	5/1937 (0.3%)
8	G	0.31	0/1343	0.70	0/1816
9	H	0.27	0/1122	0.58	0/1515
10	J	0.41	1/1135 (0.1%)	0.72	3/1529 (0.2%)
11	K	0.35	0/939	0.99	2/1258 (0.2%)
12	L	0.69	0/1062	1.60	31/1413 (2.2%)
13	M	0.48	0/1093	1.03	7/1460 (0.5%)
14	N	0.37	0/1021	0.92	7/1364 (0.5%)
15	O	0.30	0/910	0.67	0/1219
16	P	0.55	0/929	1.40	16/1242 (1.3%)
17	Q	0.41	0/960	0.86	3/1278 (0.2%)
18	R	1.06	6/829 (0.7%)	1.42	13/1107 (1.2%)
19	S	0.28	0/864	0.68	1/1156 (0.1%)
20	T	0.39	0/784	0.78	4/1048 (0.4%)
21	U	0.33	0/787	0.74	0/1051
22	W	0.36	0/642	0.96	5/848 (0.6%)
23	X	0.29	0/510	0.80	1/677 (0.1%)
24	Y	0.31	0/453	0.63	0/605
25	Z	0.48	0/559	1.04	5/745 (0.7%)
26	1	0.53	1/450 (0.2%)	1.15	7/599 (1.2%)
27	2	0.36	0/448	0.71	0/594
28	3	0.33	0/380	0.64	0/498
29	4	0.47	0/513	0.96	1/676 (0.1%)
30	5	0.40	0/303	0.73	0/397
31	6	0.26	0/1046	0.58	0/1410
32	a	0.27	1/36762 (0.0%)	0.75	7/57350 (0.0%)
33	c	0.23	0/1651	0.45	0/2225
34	d	0.23	0/1665	0.46	0/2227

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	e	0.23	0/1118	0.45	0/1504
36	f	0.25	0/835	0.48	0/1128
37	g	0.23	0/1187	0.45	0/1591
38	h	0.23	0/989	0.45	0/1326
39	i	0.24	0/1034	0.45	0/1375
40	j	0.23	0/796	0.49	0/1077
41	k	0.24	0/893	0.47	0/1205
42	l	0.22	0/969	0.47	0/1300
43	m	0.21	0/892	0.48	0/1193
44	n	0.25	0/785	0.46	0/1043
45	o	0.23	0/724	0.45	0/966
46	p	0.26	0/659	0.44	0/884
47	q	0.24	0/657	0.46	0/881
48	r	0.23	0/462	0.46	0/621
49	s	0.26	0/652	0.46	0/877
50	t	0.24	0/671	0.42	0/888
51	7	0.25	0/1735	0.47	0/2338
52	u	1.01	4/430 (0.9%)	0.74	2/570 (0.4%)
53	v	0.75	1/1813 (0.1%)	1.23	11/2823 (0.4%)
All	All	0.34	30/155037 (0.0%)	0.78	209/231859 (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	61
4	C	0	3
9	H	0	1
10	J	0	2
12	L	0	1
16	P	0	1
17	Q	0	1
18	R	0	1
32	a	0	16
52	u	0	1
All	All	0	88

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	53	PHE	CB-CG	17.86	1.81	1.51
2	B	1086	A	C5-C6	-17.67	1.25	1.41
52	u	15	LEU	C-N	-15.07	0.99	1.34
18	R	54	VAL	N-CA	-11.65	1.23	1.46
18	R	54	VAL	CA-CB	11.10	1.78	1.54
2	B	1088	A	C6-N1	-10.41	1.28	1.35
2	B	2196	C	O3'-P	10.19	1.73	1.61
53	v	1	G	OP3-P	-9.39	1.49	1.61
52	u	25	ALA	C-N	-9.35	1.16	1.33
2	B	2052	A	C4'-C3'	-8.30	1.44	1.53
6	E	46	GLN	CB-CG	8.02	1.74	1.52
2	B	1060	U	C2-N3	7.71	1.43	1.37
18	R	53	PHE	CA-CB	7.53	1.70	1.53
2	B	2191	A	O3'-P	-7.45	1.52	1.61
2	B	1086	A	N7-C5	-7.39	1.34	1.39
18	R	54	VAL	CA-C	7.22	1.71	1.52
2	B	1248	G	C4'-C3'	7.09	1.60	1.53
32	a	463	U	O3'-P	-6.73	1.53	1.61
52	u	29	ALA	C-N	6.63	1.49	1.34
2	B	442	G	C5-C6	6.08	1.48	1.42
2	B	37	C	N1-C2	6.01	1.46	1.40
10	J	75	TYR	CD1-CE1	-5.53	1.31	1.39
18	R	53	PHE	CG-CD2	5.51	1.47	1.38
2	B	38	A	C5'-C4'	5.46	1.57	1.51
52	u	11	PHE	C-N	-5.38	1.21	1.34
2	B	1250	G	C4'-C3'	-5.25	1.47	1.52
2	B	442	G	C6-N1	-5.16	1.35	1.39
2	B	1426	G	O3'-P	5.13	1.67	1.61
2	B	2267	A	C5-C6	-5.09	1.36	1.41
26	1	52	LYS	N-CA	5.04	1.56	1.46

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2791	G	O5'-P-OP1	-28.70	76.26	110.70
2	B	2791	G	O5'-P-OP2	18.18	132.52	110.70
18	R	53	PHE	CA-C-N	-17.33	79.08	117.20
18	R	54	VAL	CB-CA-C	15.12	140.13	111.40
2	B	2790	U	OP1-P-O3'	14.27	136.59	105.20
18	R	54	VAL	CG1-CB-CG2	-14.14	88.27	110.90
14	N	118	ARG	NE-CZ-NH1	13.68	127.14	120.30
18	R	54	VAL	N-CA-C	-13.34	74.98	111.00
12	L	118	THR	C-N-CD	-12.92	92.17	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2052	A	C5'-C4'-C3'	-11.99	96.82	116.00
13	M	3	GLN	C-N-CD	-11.32	95.69	120.60
18	R	54	VAL	N-CA-CB	-10.09	89.31	111.50
2	B	139	U	N1-C1'-C2'	-10.08	100.89	114.00
16	P	72	VAL	N-CA-C	9.71	137.23	111.00
2	B	2272	U	C5-C4-O4	-9.62	120.13	125.90
13	M	5	LYS	N-CA-C	-9.26	85.99	111.00
17	Q	3	VAL	CB-CA-C	-8.86	94.56	111.40
26	1	52	LYS	CB-CA-C	-8.79	92.81	110.40
18	R	53	PHE	N-CA-CB	8.76	126.37	110.60
2	B	2641	G	N9-C1'-C2'	-8.65	102.49	112.00
12	L	6	LEU	N-CA-C	8.62	134.26	111.00
12	L	105	ILE	N-CA-C	8.51	133.98	111.00
12	L	85	VAL	N-CA-C	-8.43	88.25	111.00
32	a	765	G	N9-C1'-C2'	-8.22	102.96	112.00
6	E	84	THR	N-CA-C	8.22	133.18	111.00
6	E	44	ARG	NE-CZ-NH2	-8.21	116.20	120.30
16	P	71	ARG	N-CA-C	8.14	132.99	111.00
16	P	40	GLN	N-CA-C	-8.12	89.08	111.00
2	B	1088	A	N1-C6-N6	-8.06	113.76	118.60
2	B	773	U	C5'-C4'-C3'	-7.92	103.33	116.00
2	B	1350	C	C5'-C4'-C3'	-7.91	103.34	116.00
26	1	52	LYS	N-CA-CB	7.83	124.69	110.60
2	B	37	C	C4'-C3'-O3'	7.80	128.59	113.00
12	L	112	LEU	N-CA-C	-7.77	90.01	111.00
13	M	132	THR	N-CA-C	7.72	131.84	111.00
16	P	79	VAL	N-CA-C	7.70	131.80	111.00
6	E	73	ILE	N-CA-C	7.67	131.70	111.00
13	M	1	MET	CG-SD-CE	7.67	112.46	100.20
2	B	2733	A	N9-C1'-C2'	-7.64	103.60	112.00
18	R	53	PHE	CA-C-O	7.58	136.02	120.10
12	L	68	SER	N-CA-C	7.47	131.18	111.00
6	E	74	LYS	N-CA-C	-7.46	90.85	111.00
2	B	1060	U	C5-C4-O4	-7.44	121.43	125.90
18	R	46	GLU	N-CA-C	7.35	130.84	111.00
2	B	1552	A	N9-C1'-C2'	-7.32	103.95	112.00
2	B	825	A	C5'-C4'-C3'	-7.30	104.32	116.00
2	B	38	A	C5'-C4'-C3'	-7.26	104.38	116.00
17	Q	52	ARG	NE-CZ-NH2	-7.26	116.67	120.30
26	1	27	LEU	CB-CG-CD1	-7.17	98.81	111.00
12	L	77	ILE	N-CA-C	-7.16	91.68	111.00
16	P	28	LYS	N-CA-C	-7.13	91.76	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	150	GLY	N-CA-C	7.12	130.89	113.10
11	K	91	SER	N-CA-C	-7.08	91.88	111.00
29	4	44	ARG	NE-CZ-NH2	-7.08	116.76	120.30
12	L	126	ARG	N-CA-C	7.05	130.05	111.00
18	R	50	GLY	N-CA-C	-7.03	95.53	113.10
25	Z	68	GLY	N-CA-C	-7.01	95.57	113.10
12	L	76	GLU	N-CA-C	-6.94	92.26	111.00
22	W	11	ASN	N-CA-C	6.92	129.68	111.00
12	L	61	LEU	C-N-CD	-6.91	105.40	120.60
2	B	1086	A	C4-C5-C6	6.81	120.40	117.00
2	B	2052	A	O4'-C4'-C3'	6.80	111.54	106.10
2	B	1086	A	C6-C5-N7	-6.80	127.54	132.30
26	1	52	LYS	CA-CB-CG	6.79	128.34	113.40
2	B	2259	U	C5'-C4'-C3'	-6.77	105.17	116.00
12	L	14	LYS	N-CA-C	-6.76	92.75	111.00
53	v	74	C	C2-N1-C1'	6.72	126.19	118.80
2	B	1439	A	N9-C1'-C2'	-6.69	104.64	112.00
53	v	76	A	C8-N9-C4	6.62	108.45	105.80
12	L	78	ARG	N-CA-C	6.58	128.78	111.00
12	L	18	ARG	N-CA-C	6.54	128.65	111.00
14	N	118	ARG	CD-NE-CZ	6.54	132.75	123.60
53	v	49	C	N1-C2-O2	-6.52	114.99	118.90
23	X	33	ALA	N-CA-C	6.49	128.53	111.00
16	P	14	GLN	N-CA-C	-6.48	93.50	111.00
4	C	32	LEU	N-CA-C	6.45	128.42	111.00
26	1	51	ARG	C-N-CA	6.45	137.82	121.70
2	B	479	A	C4'-C3'-O3'	-6.43	95.91	109.40
22	W	10	ARG	N-CA-C	6.41	128.31	111.00
32	a	438	U	N1-C1'-C2'	-6.36	105.00	112.00
16	P	29	VAL	N-CA-C	-6.33	93.89	111.00
19	S	41	LYS	N-CA-C	-6.33	93.90	111.00
12	L	92	LEU	N-CA-C	6.33	128.09	111.00
12	L	125	LEU	N-CA-C	-6.31	93.95	111.00
12	L	139	GLY	N-CA-C	6.31	128.88	113.10
14	N	5	LYS	N-CA-C	6.31	128.04	111.00
16	P	70	GLU	N-CA-C	6.31	128.03	111.00
12	L	20	GLY	N-CA-C	6.30	128.85	113.10
12	L	67	THR	N-CA-C	6.29	128.00	111.00
14	N	118	ARG	NH1-CZ-NH2	-6.28	112.49	119.40
5	D	154	LYS	N-CA-C	-6.27	94.08	111.00
2	B	1088	A	C5-C6-N6	6.25	128.70	123.70
2	B	2318	G	N9-C1'-C2'	-6.25	105.12	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	46	GLN	CA-CB-CG	6.21	127.05	113.40
32	a	232	G	C5'-C4'-C3'	-6.20	106.08	116.00
12	L	103	ILE	N-CA-C	6.19	127.71	111.00
12	L	86	GLU	N-CA-CB	-6.14	99.55	110.60
4	C	238	ASN	N-CA-C	6.11	127.50	111.00
16	P	78	PRO	N-CA-C	6.09	127.94	112.10
53	v	13	C	C6-N1-C2	6.09	122.74	120.30
53	v	29	G	N3-C4-C5	6.09	131.65	128.60
2	B	745	G	C5'-C4'-C3'	-6.09	106.25	116.00
6	E	44	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	B	2052	A	C1'-O4'-C4'	-6.07	105.04	109.90
12	L	39	LYS	N-CA-C	-6.07	94.61	111.00
26	1	52	LYS	N-CA-C	-6.07	94.62	111.00
32	a	66	A	N9-C1'-C2'	-6.02	105.37	112.00
12	L	5	THR	C-N-CA	6.02	136.76	121.70
2	B	1250	G	C4'-C3'-C2'	6.01	108.61	102.60
2	B	268	C	C5'-C4'-C3'	-6.00	106.41	116.00
10	J	80	HIS	N-CA-C	5.95	127.07	111.00
16	P	81	ASP	N-CA-C	-5.95	94.93	111.00
4	C	28	PRO	CA-C-N	-5.95	104.12	117.20
2	B	1397	U	C5'-C4'-C3'	-5.94	106.50	116.00
2	B	2619	C	C5'-C4'-C3'	-5.93	106.51	116.00
5	D	145	SER	N-CA-CB	-5.92	101.62	110.50
2	B	1657	U	N1-C1'-C2'	-5.91	105.50	112.00
25	Z	42	PRO	N-CA-C	5.91	127.46	112.10
13	M	6	ARG	N-CA-C	-5.91	95.06	111.00
14	N	2	ARG	N-CA-C	-5.89	95.09	111.00
2	B	690	G	C5'-C4'-C3'	-5.89	106.58	116.00
18	R	53	PHE	O-C-N	5.88	132.10	122.70
16	P	82	SER	N-CA-C	5.85	126.78	111.00
2	B	38	A	N9-C1'-C2'	5.84	121.60	114.00
20	T	1	MET	N-CA-C	-5.81	95.31	111.00
13	M	8	LYS	N-CA-C	-5.79	95.36	111.00
25	Z	43	PHE	N-CA-C	-5.79	95.37	111.00
16	P	54	LEU	N-CA-C	5.79	126.63	111.00
53	v	40	C	N1-C2-O2	5.79	122.37	118.90
2	B	2790	U	O3'-P-O5'	-5.79	93.01	104.00
16	P	109	ILE	N-CA-C	-5.79	95.38	111.00
53	v	56	C	C6-N1-C2	-5.78	117.99	120.30
52	u	15	LEU	C-N-CA	5.77	136.13	121.70
22	W	11	ASN	N-CA-CB	-5.77	100.22	110.60
12	L	82	LEU	CA-CB-CG	-5.76	102.05	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	442	G	C5-C6-O6	5.76	132.06	128.60
7	F	14	LYS	N-CA-C	-5.76	95.45	111.00
2	B	2575	C	N1-C1'-C2'	-5.74	105.69	112.00
4	C	28	PRO	N-CA-C	5.73	127.01	112.10
10	J	115	GLY	N-CA-C	-5.73	98.78	113.10
14	N	4	ARG	N-CA-C	5.72	126.45	111.00
2	B	2267	A	C5-C6-N6	-5.72	119.12	123.70
14	N	100	CYS	N-CA-C	-5.72	95.55	111.00
18	R	88	GLY	N-CA-C	-5.70	98.86	113.10
12	L	111	ILE	N-CA-C	-5.69	95.64	111.00
7	F	106	ALA	N-CA-C	5.68	126.33	111.00
11	K	89	ASN	N-CA-C	5.66	126.28	111.00
26	1	5	ASN	N-CA-C	5.63	126.21	111.00
2	B	2267	A	O4'-C1'-N9	-5.63	103.70	108.20
10	J	4	PHE	N-CA-C	-5.62	95.82	111.00
20	T	2	ILE	CG1-CB-CG2	5.60	123.72	111.40
2	B	2267	A	C4-N9-C1'	5.59	136.36	126.30
20	T	2	ILE	N-CA-C	-5.58	95.94	111.00
25	Z	26	SER	N-CA-C	5.57	126.03	111.00
2	B	2272	U	N1-C1'-C2'	-5.56	105.89	112.00
12	L	83	ALA	N-CA-C	-5.55	96.03	111.00
16	P	50	ARG	N-CA-C	-5.52	96.09	111.00
2	B	150	U	C5'-C4'-C3'	-5.50	107.20	116.00
2	B	2267	A	C8-N9-C1'	-5.49	117.82	127.70
7	F	20	ASN	N-CA-C	5.49	125.81	111.00
22	W	10	ARG	C-N-CA	5.48	135.41	121.70
2	B	2272	U	N3-C4-O4	-5.48	115.56	119.40
16	P	104	GLY	N-CA-C	5.45	126.73	113.10
2	B	1363	C	C5'-C4'-C3'	-5.45	107.28	116.00
4	C	202	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	B	139	U	O4'-C1'-N1	5.44	112.55	108.20
2	B	2052	A	C4'-C3'-C2'	-5.44	97.16	102.60
52	u	11	PHE	CA-C-N	-5.44	105.24	117.20
2	B	848	C	C5'-C4'-C3'	-5.43	107.31	116.00
32	a	328	C	C2'-C3'-O3'	5.43	122.38	113.70
2	B	1250	G	C5'-C4'-C3'	-5.41	107.34	116.00
2	B	2052	A	N9-C1'-C2'	-5.39	106.07	112.00
16	P	71	ARG	C-N-CA	5.39	135.18	121.70
2	B	2191	A	P-O3'-C3'	5.39	126.16	119.70
12	L	62	PRO	CA-N-CD	-5.38	103.97	111.50
4	C	28	PRO	C-N-CA	5.37	135.11	121.70
2	B	2575	C	C5'-C4'-C3'	5.36	124.57	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1060	U	N1-C2-O2	-5.35	119.05	122.80
12	L	77	ILE	C-N-CA	-5.35	108.33	121.70
53	v	74	C	C6-N1-C1'	-5.34	114.39	120.80
12	L	94	THR	N-CA-C	5.34	125.41	111.00
2	B	2192	U	C5'-C4'-C3'	-5.32	107.50	116.00
2	B	375	G	C5'-C4'-C3'	-5.29	107.53	116.00
12	L	119	PRO	CA-N-CD	-5.29	104.10	111.50
32	a	1118	U	C5'-C4'-C3'	-5.29	107.54	116.00
2	B	1251	C	C5'-C4'-C3'	5.24	124.38	116.00
22	W	16	GLU	N-CA-C	5.24	125.13	111.00
20	T	2	ILE	CB-CA-C	5.23	122.06	111.60
18	R	56	GLY	N-CA-C	-5.23	100.03	113.10
2	B	2471	A	C5'-C4'-C3'	-5.22	107.65	116.00
2	B	560	C	C5'-C4'-C3'	-5.20	107.69	116.00
2	B	1600	C	C5'-C4'-C3'	-5.19	107.70	116.00
53	v	30	G	N3-C4-C5	-5.19	126.00	128.60
2	B	1664	A	C5'-C4'-C3'	-5.18	107.72	116.00
2	B	1060	U	N3-C2-O2	5.16	125.81	122.20
53	v	76	A	N9-C4-C5	-5.15	103.74	105.80
53	v	62	C	N1-C2-O2	-5.15	115.81	118.90
18	R	43	ASN	N-CA-C	-5.13	97.15	111.00
17	Q	52	ARG	NE-CZ-NH1	5.12	122.86	120.30
25	Z	20	ASN	N-CA-C	5.08	124.71	111.00
12	L	127	VAL	N-CA-C	5.06	124.67	111.00
4	C	31	PRO	N-CA-C	5.06	125.25	112.10
2	B	1086	A	C2-N3-C4	-5.05	108.08	110.60
7	F	73	VAL	N-CA-C	5.04	124.62	111.00
2	B	1656	C	N1-C1'-C2'	-5.02	106.47	112.00
2	B	2576	G	O5'-P-OP1	-5.02	101.18	105.70
13	M	4	PRO	N-CA-C	-5.02	99.06	112.10
32	a	576	C	C5'-C4'-O4'	5.01	115.11	109.10
12	L	123	ARG	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (88) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1060	U	Sidechain
2	B	1086	A	Sidechain
2	B	1088	A	Sidechain
2	B	1119	U	Sidechain
2	B	1215	G	Sidechain

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Mol	Chain	Res	Type	Group
2	B	1240	U	Sidechain
2	B	1247	A	Sidechain
2	B	1347	A	Sidechain
2	B	136	G	Sidechain
2	B	1377	G	Sidechain
2	B	139	U	Sidechain
2	B	1419	A	Sidechain
2	B	142	A	Sidechain
2	B	1426	G	Sidechain
2	B	143	C	Sidechain
2	B	1432	G	Sidechain
2	B	1439	A	Sidechain
2	B	1450	G	Sidechain
2	B	1462	C	Sidechain
2	B	1546	G	Sidechain
2	B	1572	A	Sidechain
2	B	1814	G	Sidechain
2	B	1828	G	Sidechain
2	B	1869	G	Sidechain
2	B	1964	G	Sidechain
2	B	2052	A	Sidechain
2	B	2138	G	Sidechain
2	B	221	A	Sidechain
2	B	222	A	Sidechain
2	B	2267	A	Sidechain
2	B	2272	U	Sidechain
2	B	2285	C	Sidechain
2	B	2318	G	Sidechain
2	B	232	G	Sidechain
2	B	2471	A	Sidechain
2	B	2508	G	Sidechain
2	B	2575	C	Sidechain
2	B	2638	G	Sidechain
2	B	2641	G	Sidechain
2	B	2733	A	Sidechain
2	B	2770	G	Sidechain
2	B	2834	G	Sidechain
2	B	2848	G	Sidechain
2	B	2857	G	Sidechain
2	B	2868	A	Sidechain
2	B	2883	A	Sidechain
2	B	299	A	Sidechain

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Mol	Chain	Res	Type	Group
2	B	361	G	Sidechain
2	B	370	G	Sidechain
2	B	396	G	Sidechain
2	B	487	C	Sidechain
2	B	500	G	Sidechain
2	B	51	G	Sidechain
2	B	526	A	Sidechain
2	B	630	G	Sidechain
2	B	633	A	Sidechain
2	B	727	A	Sidechain
2	B	729	G	Sidechain
2	B	757	G	Sidechain
2	B	942	G	Sidechain
2	B	946	C	Sidechain
4	C	160	TYR	Sidechain
4	C	29	PHE	Sidechain
4	C	61	TYR	Sidechain
9	H	49	ALA	Peptide
10	J	75	TYR	Sidechain
10	J	80	HIS	Sidechain
12	L	66	PHE	Sidechain
16	P	97	TYR	Sidechain
17	Q	46	TYR	Sidechain
18	R	53	PHE	Mainchain
32	a	1006	G	Sidechain
32	a	1028	C	Sidechain
32	a	1319	A	Sidechain
32	a	1331	G	Sidechain
32	a	1441	A	Sidechain
32	a	187	G	Sidechain
32	a	281	G	Sidechain
32	a	437	U	Sidechain
32	a	438	U	Sidechain
32	a	454	G	Sidechain
32	a	481	G	Sidechain
32	a	496	A	Sidechain
32	a	521	G	Sidechain
32	a	575	G	Sidechain
32	a	58	C	Sidechain
32	a	703	G	Sidechain
52	u	11	PHE	Mainchain

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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	V	92/94 (98%)	62 (67%)	22 (24%)	8 (9%)	1	13
4	C	265/267 (99%)	103 (39%)	82 (31%)	80 (30%)	0	0
5	D	207/209 (99%)	90 (44%)	69 (33%)	48 (23%)	0	1
6	E	199/201 (99%)	98 (49%)	60 (30%)	41 (21%)	0	2
7	F	176/178 (99%)	95 (54%)	48 (27%)	33 (19%)	0	2
8	G	174/176 (99%)	118 (68%)	39 (22%)	17 (10%)	0	10
9	H	147/149 (99%)	88 (60%)	46 (31%)	13 (9%)	1	13
10	J	138/140 (99%)	68 (49%)	41 (30%)	29 (21%)	0	2
11	K	119/121 (98%)	71 (60%)	32 (27%)	16 (13%)	0	4
12	L	142/144 (99%)	60 (42%)	40 (28%)	42 (30%)	0	0
13	M	134/136 (98%)	69 (52%)	37 (28%)	28 (21%)	0	2
14	N	125/127 (98%)	73 (58%)	35 (28%)	17 (14%)	0	4
15	O	115/117 (98%)	64 (56%)	26 (23%)	25 (22%)	0	1
16	P	112/114 (98%)	39 (35%)	36 (32%)	37 (33%)	0	0
17	Q	115/117 (98%)	81 (70%)	23 (20%)	11 (10%)	0	11
18	R	101/103 (98%)	43 (43%)	32 (32%)	26 (26%)	0	1
19	S	108/110 (98%)	63 (58%)	27 (25%)	18 (17%)	0	3
20	T	97/99 (98%)	42 (43%)	40 (41%)	15 (16%)	0	3
21	U	100/102 (98%)	33 (33%)	46 (46%)	21 (21%)	0	2
22	W	82/84 (98%)	29 (35%)	26 (32%)	27 (33%)	0	0
23	X	61/63 (97%)	28 (46%)	21 (34%)	12 (20%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	Y	56/58 (97%)	29 (52%)	17 (30%)	10 (18%)	0	2
25	Z	68/70 (97%)	29 (43%)	26 (38%)	13 (19%)	0	2
26	1	54/56 (96%)	30 (56%)	15 (28%)	9 (17%)	0	3
27	2	52/54 (96%)	19 (36%)	23 (44%)	10 (19%)	0	2
28	3	44/46 (96%)	23 (52%)	14 (32%)	7 (16%)	0	3
29	4	62/64 (97%)	30 (48%)	25 (40%)	7 (11%)	0	7
30	5	36/38 (95%)	18 (50%)	9 (25%)	9 (25%)	0	1
31	6	139/141 (99%)	124 (89%)	11 (8%)	4 (3%)	4	33
33	c	204/206 (99%)	135 (66%)	49 (24%)	20 (10%)	0	10
34	d	203/205 (99%)	130 (64%)	55 (27%)	18 (9%)	1	13
35	e	148/150 (99%)	107 (72%)	34 (23%)	7 (5%)	2	24
36	f	98/100 (98%)	69 (70%)	23 (24%)	6 (6%)	1	20
37	g	148/150 (99%)	102 (69%)	38 (26%)	8 (5%)	2	22
38	h	127/129 (98%)	105 (83%)	19 (15%)	3 (2%)	6	37
39	i	125/127 (98%)	87 (70%)	27 (22%)	11 (9%)	1	13
40	j	96/98 (98%)	63 (66%)	21 (22%)	12 (12%)	0	5
41	k	115/117 (98%)	75 (65%)	27 (24%)	13 (11%)	0	7
42	l	121/123 (98%)	74 (61%)	30 (25%)	17 (14%)	0	4
43	m	112/114 (98%)	87 (78%)	14 (12%)	11 (10%)	0	10
44	n	92/100 (92%)	59 (64%)	24 (26%)	9 (10%)	0	10
45	o	86/88 (98%)	66 (77%)	18 (21%)	2 (2%)	6	38
46	p	80/82 (98%)	59 (74%)	17 (21%)	4 (5%)	2	23
47	q	78/80 (98%)	48 (62%)	26 (33%)	4 (5%)	2	23
48	r	53/55 (96%)	27 (51%)	19 (36%)	7 (13%)	0	4
49	s	77/79 (98%)	57 (74%)	14 (18%)	6 (8%)	1	15
50	t	83/85 (98%)	69 (83%)	8 (10%)	6 (7%)	1	17
51	7	216/218 (99%)	145 (67%)	53 (24%)	18 (8%)	1	14
52	u	49/51 (96%)	22 (45%)	12 (24%)	15 (31%)	0	0
All	All	5631/5735 (98%)	3305 (59%)	1496 (27%)	830 (15%)	0	4

All (830) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	21	PRO
4	C	22	GLU
4	C	28	PRO
4	C	29	PHE
4	C	31	PRO
4	C	32	LEU
4	C	47	ARG
4	C	63	ILE
4	C	64	VAL
4	C	67	LYS
4	C	68	ARG
4	C	97	ASP
4	C	103	ILE
4	C	111	ALA
4	C	114	GLN
4	C	124	LYS
4	C	125	PRO
4	C	135	PRO
4	C	141	HIS
4	C	149	LYS
4	C	156	SER
4	C	176	ARG
4	C	209	ALA
4	C	226	PRO
4	C	227	VAL
4	C	239	PHE
4	C	246	PRO
4	C	258	SER
4	C	266	ILE
5	D	9	VAL
5	D	14	ILE
5	D	18	ASP
5	D	23	PRO
5	D	27	ILE
5	D	30	GLU
5	D	33	ARG
5	D	42	ASN
5	D	59	ARG
5	D	84	LEU
5	D	92	VAL
5	D	102	ALA
5	D	114	LYS
5	D	128	ARG

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Mol	Chain	Res	Type
5	D	130	GLN
5	D	139	SER
5	D	141	ARG
5	D	154	LYS
5	D	170	VAL
6	E	4	VAL
6	E	37	ALA
6	E	44	ARG
6	E	46	GLN
6	E	49	ARG
6	E	59	PRO
6	E	84	THR
6	E	86	ALA
6	E	117	ARG
6	E	129	PRO
6	E	147	LEU
6	E	148	ILE
6	E	165	HIS
6	E	196	VAL
7	F	66	ILE
7	F	73	VAL
7	F	76	PHE
7	F	131	VAL
7	F	139	GLU
7	F	149	ARG
7	F	173	ASP
8	G	6	ALA
8	G	19	ASN
8	G	91	VAL
9	H	29	PHE
9	H	38	PRO
10	J	43	GLU
10	J	44	TYR
10	J	64	VAL
10	J	74	TYR
10	J	100	VAL
10	J	101	ILE
10	J	119	PHE
11	K	35	VAL
11	K	46	ALA
11	K	53	LYS
11	K	71	ARG

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Mol	Chain	Res	Type
11	K	72	PRO
11	K	85	VAL
11	K	89	ASN
11	K	110	GLU
11	K	120	PRO
12	L	40	SER
12	L	56	PRO
12	L	62	PRO
12	L	68	SER
12	L	73	ILE
12	L	85	VAL
12	L	90	VAL
12	L	117	THR
12	L	118	THR
12	L	119	PRO
12	L	120	VAL
12	L	126	ARG
12	L	127	VAL
12	L	141	LYS
13	M	4	PRO
13	M	14	LYS
13	M	69	PRO
13	M	77	PRO
13	M	80	VAL
13	M	98	PRO
13	M	109	PRO
14	N	37	THR
14	N	89	SER
14	N	94	TYR
14	N	107	ASN
14	N	113	ILE
14	N	116	VAL
15	O	37	ALA
15	O	42	PRO
15	O	54	VAL
16	P	17	PRO
16	P	23	ASP
16	P	24	THR
16	P	52	ARG
16	P	55	HIS
16	P	60	VAL
16	P	72	VAL

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Mol	Chain	Res	Type
16	P	76	HIS
16	P	85	VAL
16	P	90	ALA
16	P	94	ALA
17	Q	34	ALA
17	Q	91	ARG
18	R	11	GLN
18	R	15	SER
18	R	17	GLY
18	R	24	LYS
18	R	47	VAL
18	R	59	ILE
18	R	74	ILE
18	R	95	ASP
18	R	101	ILE
19	S	3	THR
19	S	6	LYS
19	S	67	ASP
19	S	96	ILE
19	S	103	ILE
20	T	5	GLU
20	T	34	VAL
21	U	24	VAL
21	U	54	PRO
21	U	63	ALA
21	U	71	ILE
21	U	92	VAL
22	W	11	ASN
22	W	16	GLU
22	W	18	LYS
22	W	32	ALA
22	W	44	PHE
22	W	66	VAL
22	W	75	ASN
22	W	81	ILE
23	X	7	ARG
23	X	9	LYS
23	X	33	ALA
24	Y	9	THR
24	Y	51	SER
25	Z	7	PRO
25	Z	8	LYS

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Mol	Chain	Res	Type
25	Z	40	CYS
25	Z	58	ASP
25	Z	60	PHE
26	1	10	SER
26	1	29	VAL
26	1	35	GLU
27	2	46	VAL
28	3	4	THR
28	3	44	VAL
29	4	15	LYS
29	4	23	HIS
29	4	31	ILE
29	4	57	VAL
29	4	60	CYS
30	5	5	ALA
30	5	22	VAL
30	5	24	ARG
30	5	29	ALA
31	6	18	ASN
33	c	2	GLN
33	c	91	ALA
33	c	153	SER
34	d	18	LEU
34	d	31	CYS
34	d	191	SER
36	f	92	THR
39	i	8	THR
39	i	43	ALA
40	j	57	VAL
41	k	56	LYS
41	k	126	ARG
42	l	10	PRO
42	l	23	LEU
43	m	6	ILE
43	m	14	ALA
44	n	52	ARG
51	7	19	THR
51	7	22	TRP
51	7	163	ILE
51	7	186	VAL
52	u	14	ALA
52	u	22	CYS

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Mol	Chain	Res	Type
3	V	45	ASP
3	V	64	VAL
3	V	71	LYS
4	C	53	ILE
4	C	72	GLY
4	C	90	ILE
4	C	98	GLY
4	C	107	LYS
4	C	140	VAL
4	C	143	VAL
4	C	157	ALA
4	C	163	ILE
4	C	194	VAL
4	C	196	ASN
4	C	208	GLY
4	C	255	LYS
5	D	2	ILE
5	D	34	VAL
5	D	104	VAL
5	D	129	THR
5	D	155	VAL
5	D	162	ALA
5	D	180	VAL
5	D	206	ALA
5	D	207	VAL
6	E	23	PHE
6	E	52	VAL
6	E	61	ARG
6	E	62	GLN
6	E	82	GLY
6	E	90	GLN
6	E	104	ALA
6	E	120	VAL
6	E	128	ALA
6	E	171	ASP
6	E	186	VAL
7	F	3	LEU
7	F	7	TYR
7	F	19	PHE
7	F	31	GLU
7	F	46	LYS
7	F	57	ALA

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Mol	Chain	Res	Type
7	F	67	THR
7	F	75	GLY
7	F	122	ASP
7	F	136	ILE
7	F	148	VAL
7	F	150	GLY
7	F	153	ILE
7	F	162	ASP
7	F	176	PHE
8	G	25	ILE
8	G	151	ARG
8	G	159	LYS
8	G	166	GLU
9	H	8	LYS
9	H	41	LYS
10	J	4	PHE
10	J	6	ALA
10	J	50	THR
10	J	73	VAL
10	J	81	ILE
10	J	83	GLY
10	J	130	HIS
10	J	137	PRO
11	K	25	LEU
11	K	73	ASP
12	L	29	LYS
12	L	34	GLY
12	L	48	ARG
12	L	57	LEU
12	L	77	ILE
12	L	95	LEU
12	L	128	THR
12	L	140	GLY
13	M	11	LYS
13	M	36	VAL
13	M	58	LYS
13	M	86	LYS
13	M	104	GLU
14	N	5	LYS
14	N	8	ARG
14	N	11	ASN
14	N	90	ARG

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Mol	Chain	Res	Type
14	N	112	TYR
15	O	9	ARG
15	O	21	LEU
15	O	28	VAL
15	O	32	PRO
15	O	47	VAL
15	O	49	VAL
15	O	63	LYS
15	O	95	SER
15	O	115	LEU
16	P	49	ILE
16	P	78	PRO
16	P	82	SER
16	P	83	ILE
16	P	91	VAL
16	P	97	TYR
16	P	102	ARG
16	P	112	ARG
18	R	25	LEU
18	R	87	GLN
18	R	97	LYS
18	R	100	GLY
19	S	5	ALA
19	S	8	ARG
19	S	29	VAL
20	T	14	PRO
20	T	30	ILE
20	T	32	LEU
20	T	63	VAL
20	T	65	GLY
20	T	81	LYS
20	T	85	VAL
21	U	21	ARG
21	U	22	GLY
21	U	64	ILE
21	U	77	GLY
22	W	2	HIS
22	W	23	LYS
22	W	37	VAL
22	W	42	THR
22	W	47	GLY
22	W	49	ASN

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Mol	Chain	Res	Type
22	W	50	VAL
22	W	52	CYS
22	W	63	ASP
22	W	65	LYS
22	W	67	LYS
22	W	68	PHE
22	W	72	GLY
23	X	16	THR
23	X	30	MET
23	X	40	SER
23	X	46	VAL
25	Z	4	ASP
25	Z	9	TYR
25	Z	26	SER
25	Z	30	HIS
25	Z	32	LEU
25	Z	39	LYS
26	1	39	ARG
26	1	51	ARG
27	2	5	ARG
27	2	35	LEU
28	3	43	THR
29	4	16	THR
30	5	3	VAL
30	5	17	VAL
33	c	19	SER
33	c	25	THR
33	c	54	ILE
33	c	81	GLU
33	c	100	ILE
33	c	180	ASP
34	d	25	ARG
34	d	107	GLY
34	d	152	SER
34	d	172	VAL
34	d	192	ALA
35	e	20	VAL
35	e	128	GLY
36	f	62	MET
36	f	64	VAL
36	f	65	GLU
37	g	84	TYR

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Mol	Chain	Res	Type
37	g	129	ASN
39	i	57	VAL
39	i	71	ILE
39	i	108	ARG
40	j	75	ASP
40	j	92	LEU
41	k	50	GLY
41	k	53	GLY
41	k	125	LYS
42	l	19	ASN
42	l	72	ASN
42	l	84	GLY
43	m	3	ILE
43	m	66	GLY
43	m	104	ASN
44	n	51	PRO
44	n	61	ASN
45	o	73	ASP
46	p	79	ASN
47	q	6	THR
47	q	34	GLY
48	r	32	ILE
49	s	5	LYS
50	t	85	LEU
51	7	18	GLN
52	u	32	ARG
52	u	34	ARG
3	V	54	ALA
4	C	4	LYS
4	C	51	ARG
4	C	56	GLY
4	C	58	LYS
4	C	59	GLN
4	C	65	ASP
4	C	91	ALA
4	C	93	VAL
4	C	142	ASN
4	C	151	GLY
4	C	164	VAL
4	C	165	ALA
4	C	173	LEU
4	C	214	GLY

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Mol	Chain	Res	Type
5	D	69	ALA
5	D	99	GLU
5	D	140	HIS
5	D	156	PHE
5	D	169	ARG
5	D	174	SER
5	D	185	ASN
5	D	190	LYS
5	D	193	VAL
5	D	205	PRO
6	E	54	GLY
6	E	68	ALA
6	E	69	ARG
6	E	93	SER
6	E	127	GLU
6	E	191	ASP
7	F	10	GLU
7	F	14	LYS
7	F	81	GLY
7	F	83	PRO
7	F	87	LYS
7	F	114	ARG
8	G	45	ALA
8	G	127	GLN
9	H	20	ASN
9	H	37	VAL
9	H	127	GLU
10	J	46	PRO
10	J	121	LYS
10	J	127	GLY
10	J	138	GLN
11	K	3	GLN
11	K	121	GLU
12	L	27	LEU
12	L	64	PHE
12	L	82	LEU
12	L	84	LYS
12	L	91	ASP
12	L	94	THR
12	L	143	GLU
13	M	12	MET
13	M	72	PRO

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Mol	Chain	Res	Type
13	M	81	ARG
13	M	97	GLN
13	M	105	MET
13	M	120	ALA
13	M	131	VAL
14	N	104	ALA
14	N	115	LEU
15	O	7	ARG
15	O	38	GLN
15	O	57	ALA
15	O	68	LYS
16	P	12	MET
16	P	25	VAL
16	P	39	LEU
16	P	56	SER
16	P	81	ASP
16	P	105	LYS
17	Q	23	TYR
17	Q	26	ALA
17	Q	73	ILE
17	Q	88	GLU
17	Q	92	LYS
18	R	7	SER
18	R	10	LYS
18	R	29	THR
18	R	37	GLU
18	R	41	ILE
18	R	72	VAL
18	R	73	LYS
18	R	98	ILE
19	S	11	ARG
19	S	12	SER
19	S	104	THR
20	T	13	ALA
20	T	15	HIS
20	T	74	ILE
20	T	96	VAL
21	U	14	THR
21	U	35	VAL
21	U	39	ASN
21	U	59	GLU
21	U	60	LYS

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Mol	Chain	Res	Type
21	U	72	PHE
22	W	5	ALA
22	W	77	LYS
23	X	4	LYS
23	X	28	LEU
24	Y	2	LYS
24	Y	10	ARG
24	Y	12	ALA
24	Y	14	GLY
24	Y	16	LEU
24	Y	57	GLU
27	2	16	THR
27	2	43	ARG
27	2	47	ILE
29	4	26	ALA
31	6	23	VAL
33	c	59	PRO
33	c	78	LYS
33	c	136	ALA
34	d	27	ILE
34	d	28	ASP
34	d	43	ARG
34	d	151	GLN
34	d	177	MET
35	e	43	GLY
36	f	94	HIS
37	g	89	GLU
39	i	44	ARG
39	i	55	ASP
39	i	127	SER
40	j	62	ARG
40	j	93	ALA
41	k	70	ALA
41	k	77	GLY
41	k	91	GLY
42	l	13	ARG
42	l	60	PHE
42	l	122	LYS
43	m	7	ASN
43	m	22	TYR
43	m	65	GLU
43	m	98	GLY

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Mol	Chain	Res	Type
44	n	21	ALA
44	n	74	ARG
44	n	80	ARG
47	q	5	ARG
48	r	21	ASP
48	r	71	ASP
50	t	59	ARG
51	7	20	ARG
51	7	76	SER
52	u	6	ARG
52	u	24	LYS
52	u	25	ALA
52	u	40	PRO
4	C	61	TYR
4	C	66	PHE
4	C	224	MET
4	C	230	PRO
4	C	231	HIS
4	C	251	THR
4	C	265	PHE
5	D	73	VAL
5	D	125	TRP
5	D	201	LEU
6	E	39	ALA
6	E	53	THR
6	E	112	LEU
6	E	123	LYS
6	E	153	LEU
7	F	175	PRO
8	G	11	PRO
8	G	155	PRO
9	H	12	LEU
9	H	118	PRO
10	J	11	VAL
10	J	85	LYS
12	L	23	ILE
12	L	30	THR
12	L	33	ARG
12	L	35	HIS
12	L	136	GLU
13	M	3	GLN
13	M	21	ALA

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Mol	Chain	Res	Type
13	M	59	ARG
13	M	70	ASP
13	M	71	LYS
13	M	127	LYS
14	N	20	MET
15	O	19	GLN
15	O	55	GLU
15	O	80	GLU
16	P	26	GLU
16	P	79	VAL
16	P	96	LEU
16	P	98	TYR
17	Q	21	LYS
17	Q	24	TYR
18	R	21	ARG
18	R	55	ASP
19	S	13	SER
19	S	34	ASP
19	S	71	VAL
19	S	80	PRO
20	T	61	LEU
20	T	66	LYS
21	U	7	ASP
21	U	18	LYS
22	W	6	GLY
22	W	38	ARG
23	X	24	GLU
23	X	43	LEU
25	Z	42	PRO
26	1	53	VAL
27	2	21	THR
28	3	36	ALA
30	5	7	VAL
30	5	20	ASP
31	6	49	GLU
33	c	65	VAL
33	c	186	SER
34	d	29	THR
35	e	25	LYS
35	e	34	ALA
36	f	54	LEU
37	g	18	GLY

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Mol	Chain	Res	Type
37	g	57	GLU
37	g	75	LYS
37	g	86	VAL
38	h	46	GLU
39	i	67	LYS
40	j	56	HIS
40	j	61	ALA
40	j	74	VAL
41	k	57	SER
41	k	108	ASN
42	l	14	LYS
42	l	15	VAL
42	l	47	ALA
42	l	56	LEU
42	l	67	GLY
42	l	120	ARG
44	n	31	SER
44	n	94	GLY
46	p	42	ILE
47	q	69	THR
48	r	22	TYR
48	r	47	ARG
49	s	27	LYS
49	s	36	ARG
49	s	65	MET
51	7	11	ALA
51	7	41	ASN
51	7	88	GLN
51	7	200	PRO
52	u	26	GLY
52	u	33	ARG
52	u	36	PHE
52	u	37	TYR
52	u	41	THR
3	V	55	GLU
4	C	50	THR
4	C	85	ASN
4	C	115	ILE
4	C	218	THR
4	C	225	ASN
4	C	236	GLY
5	D	52	THR

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Mol	Chain	Res	Type
5	D	95	SER
5	D	101	PHE
5	D	189	VAL
7	F	34	THR
7	F	36	ASN
7	F	88	VAL
8	G	42	VAL
9	H	75	LEU
10	J	72	LYS
10	J	97	PRO
10	J	132	HIS
12	L	83	ALA
12	L	92	LEU
12	L	104	GLN
12	L	113	ALA
14	N	56	LYS
14	N	102	PHE
15	O	52	SER
15	O	90	VAL
16	P	3	ILE
16	P	19	PHE
16	P	59	THR
16	P	92	ARG
16	P	110	LYS
17	Q	93	ILE
18	R	77	PHE
19	S	28	LYS
19	S	69	LEU
19	S	99	ARG
21	U	56	GLY
21	U	84	PHE
23	X	35	GLY
24	Y	17	PRO
24	Y	53	MET
25	Z	66	ILE
26	1	5	ASN
28	3	8	SER
31	6	14	ALA
33	c	14	VAL
33	c	145	ALA
33	c	167	TYR
35	e	146	MET

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Mol	Chain	Res	Type
39	i	122	ARG
40	j	36	VAL
41	k	127	ARG
42	l	42	LYS
42	l	121	PRO
43	m	105	ALA
45	o	17	ASP
48	r	20	ILE
49	s	8	PRO
50	t	5	SER
50	t	46	ALA
51	7	24	PRO
51	7	27	LYS
51	7	87	ASP
51	7	94	ARG
4	C	14	HIS
4	C	17	LYS
4	C	30	ALA
4	C	155	ARG
4	C	223	ALA
5	D	175	LEU
6	E	24	ASN
6	E	199	MET
8	G	32	LEU
8	G	59	ASP
10	J	84	ILE
12	L	37	GLY
18	R	4	VAL
27	2	38	PHE
28	3	6	GLN
33	c	26	LYS
33	c	112	ALA
34	d	6	PRO
35	e	107	GLY
37	g	6	ILE
40	j	95	GLY
41	k	106	ILE
44	n	33	VAL
49	s	39	ILE
51	7	205	ALA
52	u	13	VAL
3	V	72	VAL

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Mol	Chain	Res	Type
3	V	84	PRO
4	C	16	VAL
6	E	113	VAL
8	G	99	GLY
13	M	26	VAL
13	M	89	VAL
14	N	39	PRO
16	P	21	PRO
16	P	69	VAL
17	Q	89	ILE
28	3	9	VAL
33	c	90	VAL
34	d	63	ILE
34	d	175	GLY
41	k	119	GLY
46	p	41	PRO
51	7	157	PRO
4	C	158	GLY
10	J	18	VAL
10	J	22	GLY
10	J	103	ILE
11	K	26	GLY
12	L	139	GLY
12	L	142	ILE
15	O	27	VAL
15	O	31	THR
22	W	35	ILE
27	2	30	PRO
30	5	25	VAL
46	p	49	GLY
50	t	3	ILE
4	C	46	GLY
4	C	108	GLY
4	C	171	VAL
4	C	217	PRO
5	D	98	VAL
7	F	39	VAL
9	H	34	GLY
9	H	95	GLY
10	J	66	GLY
11	K	115	ILE
13	M	37	GLY

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Mol	Chain	Res	Type
15	O	87	ILE
21	U	4	ILE
34	d	37	PRO
38	h	71	VAL
40	j	41	PRO
40	j	96	VAL
42	l	62	VAL
43	m	23	GLY
50	t	41	GLY
52	u	52	VAL
5	D	203	VAL
6	E	76	PRO
6	E	175	ILE
8	G	130	ILE
9	H	9	VAL
12	L	11	GLY
18	R	27	ILE
22	W	51	GLY
26	1	34	GLY
27	2	42	VAL
38	h	77	VAL
39	i	110	VAL
48	r	43	ILE
51	7	150	ILE
3	V	70	ILE
8	G	92	GLY
11	K	15	GLY
15	O	22	GLY
16	P	4	ILE
21	U	48	VAL
26	1	42	ILE

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	V	78/78 (100%)	66 (85%)	12 (15%)	2	17
4	C	213/213 (100%)	145 (68%)	68 (32%)	0	2
5	D	164/164 (100%)	112 (68%)	52 (32%)	0	2
6	E	165/165 (100%)	115 (70%)	50 (30%)	0	2
7	F	149/149 (100%)	119 (80%)	30 (20%)	1	8
8	G	137/137 (100%)	105 (77%)	32 (23%)	1	5
9	H	114/114 (100%)	84 (74%)	30 (26%)	0	4
10	J	114/114 (100%)	84 (74%)	30 (26%)	0	4
11	K	102/102 (100%)	78 (76%)	24 (24%)	1	5
12	L	103/103 (100%)	62 (60%)	41 (40%)	0	0
13	M	109/109 (100%)	77 (71%)	32 (29%)	0	2
14	N	103/103 (100%)	78 (76%)	25 (24%)	0	5
15	O	87/87 (100%)	57 (66%)	30 (34%)	0	1
16	P	99/99 (100%)	77 (78%)	22 (22%)	1	6
17	Q	89/89 (100%)	66 (74%)	23 (26%)	0	4
18	R	84/84 (100%)	68 (81%)	16 (19%)	1	10
19	S	93/93 (100%)	72 (77%)	21 (23%)	1	6
20	T	83/83 (100%)	60 (72%)	23 (28%)	0	3
21	U	83/83 (100%)	62 (75%)	21 (25%)	0	4
22	W	62/62 (100%)	46 (74%)	16 (26%)	0	4
23	X	55/55 (100%)	40 (73%)	15 (27%)	0	3
24	Y	48/48 (100%)	36 (75%)	12 (25%)	0	4
25	Z	62/62 (100%)	43 (69%)	19 (31%)	0	2
26	1	47/47 (100%)	31 (66%)	16 (34%)	0	1
27	2	48/48 (100%)	33 (69%)	15 (31%)	0	2
28	3	38/38 (100%)	27 (71%)	11 (29%)	0	2
29	4	51/51 (100%)	33 (65%)	18 (35%)	0	1
30	5	34/34 (100%)	21 (62%)	13 (38%)	0	0
31	6	109/109 (100%)	106 (97%)	3 (3%)	43	66
33	c	170/170 (100%)	142 (84%)	28 (16%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	d	172/172 (100%)	140 (81%)	32 (19%)	1	11
35	e	113/113 (100%)	92 (81%)	21 (19%)	1	11
36	f	87/87 (100%)	68 (78%)	19 (22%)	1	6
37	g	123/123 (100%)	102 (83%)	21 (17%)	2	14
38	h	104/104 (100%)	87 (84%)	17 (16%)	2	16
39	i	105/105 (100%)	83 (79%)	22 (21%)	1	7
40	j	86/86 (100%)	66 (77%)	20 (23%)	1	5
41	k	90/90 (100%)	70 (78%)	20 (22%)	1	6
42	l	103/103 (100%)	88 (85%)	15 (15%)	3	19
43	m	92/92 (100%)	70 (76%)	22 (24%)	0	5
44	n	79/83 (95%)	67 (85%)	12 (15%)	3	17
45	o	76/76 (100%)	69 (91%)	7 (9%)	9	34
46	p	65/65 (100%)	56 (86%)	9 (14%)	3	21
47	q	74/74 (100%)	60 (81%)	14 (19%)	1	10
48	r	48/48 (100%)	45 (94%)	3 (6%)	18	47
49	s	70/70 (100%)	60 (86%)	10 (14%)	3	20
50	t	65/65 (100%)	56 (86%)	9 (14%)	3	21
51	7	180/180 (100%)	142 (79%)	38 (21%)	1	7
52	u	44/44 (100%)	36 (82%)	8 (18%)	1	11
All	All	4669/4673 (100%)	3602 (77%)	1067 (23%)	3	6

All (1067) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	V	3	THR
3	V	9	ARG
3	V	35	GLU
3	V	40	ILE
3	V	42	LEU
3	V	46	LYS
3	V	51	GLN
3	V	59	GLU
3	V	70	ILE
3	V	73	LYS
3	V	82	TYR

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Mol	Chain	Res	Type
3	V	87	GLN
4	C	5	CYS
4	C	9	SER
4	C	10	PRO
4	C	13	ARG
4	C	14	HIS
4	C	17	LYS
4	C	22	GLU
4	C	23	LEU
4	C	27	LYS
4	C	28	PRO
4	C	32	LEU
4	C	33	LEU
4	C	35	LYS
4	C	36	ASN
4	C	38	LYS
4	C	44	ASN
4	C	51	ARG
4	C	58	LYS
4	C	59	GLN
4	C	62	ARG
4	C	64	VAL
4	C	78	GLU
4	C	84	PRO
4	C	86	ARG
4	C	94	LEU
4	C	100	ARG
4	C	102	TYR
4	C	110	LYS
4	C	113	ASP
4	C	124	LYS
4	C	127	ASN
4	C	128	THR
4	C	129	LEU
4	C	131	MET
4	C	144	GLU
4	C	145	MET
4	C	152	GLN
4	C	155	ARG
4	C	162	GLN
4	C	171	VAL
4	C	172	THR

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Mol	Chain	Res	Type
4	C	175	LEU
4	C	179	GLU
4	C	180	MET
4	C	181	ARG
4	C	184	GLU
4	C	186	ASP
4	C	188	ARG
4	C	194	VAL
4	C	196	ASN
4	C	201	LEU
4	C	203	VAL
4	C	206	LYS
4	C	213	ARG
4	C	216	ARG
4	C	218	THR
4	C	220	ARG
4	C	222	THR
4	C	224	MET
4	C	225	ASN
4	C	227	VAL
4	C	231	HIS
4	C	235	GLU
4	C	237	ARG
4	C	246	PRO
4	C	250	GLN
4	C	254	LYS
4	C	261	ARG
5	D	1	MET
5	D	4	LEU
5	D	8	LYS
5	D	20	VAL
5	D	25	THR
5	D	26	VAL
5	D	30	GLU
5	D	34	VAL
5	D	35	THR
5	D	36	GLN
5	D	37	VAL
5	D	38	LYS
5	D	39	ASP
5	D	48	ILE
5	D	50	VAL

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Mol	Chain	Res	Type
5	D	56	LYS
5	D	59	ARG
5	D	62	LYS
5	D	64	GLU
5	D	67	HIS
5	D	70	LYS
5	D	82	PHE
5	D	84	LEU
5	D	86	GLU
5	D	89	GLU
5	D	90	PHE
5	D	96	ILE
5	D	99	GLU
5	D	103	ASP
5	D	105	LYS
5	D	113	SER
5	D	127	PHE
5	D	128	ARG
5	D	133	THR
5	D	138	LEU
5	D	142	VAL
5	D	148	GLN
5	D	150	GLN
5	D	151	THR
5	D	154	LYS
5	D	155	VAL
5	D	157	LYS
5	D	159	LYS
5	D	160	LYS
5	D	161	MET
5	D	164	GLN
5	D	165	MET
5	D	167	ASN
5	D	176	ASP
5	D	177	VAL
5	D	197	THR
5	D	207	VAL
6	E	1	MET
6	E	2	GLU
6	E	4	VAL
6	E	5	LEU
6	E	10	SER

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Mol	Chain	Res	Type
6	E	18	THR
6	E	22	ASP
6	E	41	GLN
6	E	43	THR
6	E	44	ARG
6	E	46	GLN
6	E	47	LYS
6	E	49	ARG
6	E	55	SER
6	E	57	LYS
6	E	58	LYS
6	E	61	ARG
6	E	67	ARG
6	E	69	ARG
6	E	70	SER
6	E	74	LYS
6	E	78	TRP
6	E	85	PHE
6	E	98	LYS
6	E	106	LYS
6	E	107	SER
6	E	109	LEU
6	E	114	ARG
6	E	118	LEU
6	E	129	PRO
6	E	132	LYS
6	E	134	LEU
6	E	139	LYS
6	E	148	ILE
6	E	150	THR
6	E	152	GLU
6	E	153	LEU
6	E	155	GLU
6	E	159	LEU
6	E	162	ARG
6	E	164	LEU
6	E	169	VAL
6	E	179	SER
6	E	184	ASP
6	E	188	MET
6	E	189	THR
6	E	193	VAL

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Mol	Chain	Res	Type
6	E	197	GLU
6	E	199	MET
6	E	200	LEU
7	F	5	ASP
7	F	9	ASP
7	F	10	GLU
7	F	14	LYS
7	F	16	MET
7	F	21	TYR
7	F	37	MET
7	F	55	ASP
7	F	56	LEU
7	F	59	ILE
7	F	63	LYS
7	F	87	LYS
7	F	91	ARG
7	F	93	GLU
7	F	97	GLU
7	F	102	LEU
7	F	122	ASP
7	F	126	ASN
7	F	132	ARG
7	F	139	GLU
7	F	142	TYR
7	F	143	ASP
7	F	147	ARG
7	F	149	ARG
7	F	151	LEU
7	F	152	ASP
7	F	168	LEU
7	F	172	PHE
7	F	174	PHE
7	F	177	ARG
8	G	2	ARG
8	G	3	VAL
8	G	17	LYS
8	G	18	ILE
8	G	23	ILE
8	G	25	ILE
8	G	29	ASN
8	G	34	ARG
8	G	46	ASP

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Mol	Chain	Res	Type
8	G	47	ASN
8	G	49	LEU
8	G	55	ASP
8	G	57	TYR
8	G	59	ASP
8	G	70	LEU
8	G	72	ASN
8	G	80	GLU
8	G	86	LEU
8	G	94	ARG
8	G	98	LYS
8	G	113	ASP
8	G	121	THR
8	G	128	THR
8	G	133	LYS
8	G	143	VAL
8	G	146	ASP
8	G	150	TYR
8	G	151	ARG
8	G	152	ARG
8	G	169	ARG
8	G	174	LYS
8	G	176	LYS
9	H	1	MET
9	H	2	GLN
9	H	5	LEU
9	H	7	ASP
9	H	8	LYS
9	H	18	GLN
9	H	22	LYS
9	H	27	ARG
9	H	28	ASN
9	H	30	LEU
9	H	33	GLN
9	H	35	LYS
9	H	41	LYS
9	H	47	PHE
9	H	50	ARG
9	H	54	LEU
9	H	55	GLU
9	H	57	LYS
9	H	68	ARG

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Mol	Chain	Res	Type
9	H	70	GLU
9	H	73	ASN
9	H	75	LEU
9	H	77	THR
9	H	89	LYS
9	H	98	ASP
9	H	112	LYS
9	H	124	THR
9	H	132	PHE
9	H	135	HIS
9	H	139	PHE
10	J	3	THR
10	J	12	LYS
10	J	15	TRP
10	J	21	THR
10	J	23	LYS
10	J	24	THR
10	J	25	LEU
10	J	28	LEU
10	J	31	GLU
10	J	34	ARG
10	J	35	ARG
10	J	37	ARG
10	J	39	LYS
10	J	49	ASP
10	J	58	ASN
10	J	61	LYS
10	J	69	ARG
10	J	70	THR
10	J	75	TYR
10	J	90	GLU
10	J	96	ARG
10	J	98	GLU
10	J	102	GLU
10	J	114	LEU
10	J	116	ARG
10	J	118	MET
10	J	119	PHE
10	J	122	LEU
10	J	136	GLN
10	J	139	VAL
11	K	4	GLU

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Mol	Chain	Res	Type
11	K	9	ASN
11	K	17	ARG
11	K	20	MET
11	K	21	CYS
11	K	30	ARG
11	K	31	ARG
11	K	32	TYR
11	K	54	LYS
11	K	58	LEU
11	K	62	VAL
11	K	64	ARG
11	K	71	ARG
11	K	78	ARG
11	K	86	LEU
11	K	87	LEU
11	K	93	GLN
11	K	95	ILE
11	K	98	ARG
11	K	108	ARG
11	K	109	SER
11	K	110	GLU
11	K	116	ILE
11	K	120	PRO
12	L	2	ARG
12	L	13	LYS
12	L	14	LYS
12	L	18	ARG
12	L	27	LEU
12	L	29	LYS
12	L	33	ARG
12	L	36	LYS
12	L	39	LYS
12	L	41	ARG
12	L	47	ARG
12	L	55	MET
12	L	56	PRO
12	L	57	LEU
12	L	59	ARG
12	L	60	ARG
12	L	61	LEU
12	L	70	LYS
12	L	76	GLU

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Mol	Chain	Res	Type
12	L	78	ARG
12	L	82	LEU
12	L	84	LYS
12	L	90	VAL
12	L	91	ASP
12	L	92	LEU
12	L	96	LYS
12	L	103	ILE
12	L	104	GLN
12	L	105	ILE
12	L	106	GLU
12	L	107	PHE
12	L	111	ILE
12	L	112	LEU
12	L	115	GLU
12	L	116	VAL
12	L	118	THR
12	L	121	THR
12	L	122	VAL
12	L	126	ARG
12	L	127	VAL
12	L	143	GLU
13	M	1	MET
13	M	3	GLN
13	M	5	LYS
13	M	8	LYS
13	M	9	PHE
13	M	11	LYS
13	M	12	MET
13	M	14	LYS
13	M	18	ARG
13	M	22	GLN
13	M	28	PHE
13	M	33	LEU
13	M	36	VAL
13	M	45	GLN
13	M	54	THR
13	M	55	ARG
13	M	63	ILE
13	M	71	LYS
13	M	76	LYS
13	M	86	LYS

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Mol	Chain	Res	Type
13	M	88	ASN
13	M	96	ILE
13	M	100	LYS
13	M	104	GLU
13	M	105	MET
13	M	109	PRO
13	M	117	PHE
13	M	118	LYS
13	M	124	LEU
13	M	132	THR
13	M	133	LYS
13	M	136	MET
14	N	1	MET
14	N	3	HIS
14	N	9	GLN
14	N	10	LEU
14	N	11	ASN
14	N	13	ASN
14	N	21	PHE
14	N	22	ARG
14	N	33	ILE
14	N	34	ILE
14	N	35	LYS
14	N	45	ARG
14	N	48	VAL
14	N	57	THR
14	N	65	LEU
14	N	73	ASN
14	N	75	ILE
14	N	87	PHE
14	N	94	TYR
14	N	98	LEU
14	N	99	LYS
14	N	103	ARG
14	N	112	TYR
14	N	116	VAL
14	N	120	GLU
15	O	1	MET
15	O	2	ASP
15	O	3	LYS
15	O	5	SER
15	O	9	ARG

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Mol	Chain	Res	Type
15	O	10	ARG
15	O	13	ARG
15	O	15	ARG
15	O	25	ARG
15	O	31	THR
15	O	32	PRO
15	O	34	HIS
15	O	35	ILE
15	O	38	GLN
15	O	40	ILE
15	O	56	LYS
15	O	60	GLU
15	O	62	LEU
15	O	64	TYR
15	O	67	ASN
15	O	68	LYS
15	O	69	ASP
15	O	74	VAL
15	O	81	ARG
15	O	84	GLU
15	O	85	LYS
15	O	93	ASP
15	O	97	PHE
15	O	112	GLU
15	O	116	GLN
16	P	2	ASN
16	P	11	GLN
16	P	15	ASP
16	P	24	THR
16	P	38	ARG
16	P	42	PHE
16	P	46	VAL
16	P	47	ILE
16	P	50	ARG
16	P	52	ARG
16	P	55	HIS
16	P	56	SER
16	P	60	VAL
16	P	73	PHE
16	P	74	GLN
16	P	79	VAL
16	P	87	ARG

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Mol	Chain	Res	Type
16	P	88	ARG
16	P	100	ARG
16	P	108	ARG
16	P	111	GLU
16	P	113	LEU
17	Q	10	ARG
17	Q	12	ARG
17	Q	21	LYS
17	Q	32	ARG
17	Q	36	GLN
17	Q	38	VAL
17	Q	39	ILE
17	Q	47	ARG
17	Q	53	LYS
17	Q	55	GLN
17	Q	65	ASN
17	Q	71	ASN
17	Q	80	ASN
17	Q	84	LYS
17	Q	87	VAL
17	Q	90	ASP
17	Q	91	ARG
17	Q	92	LYS
17	Q	94	LEU
17	Q	96	ASP
17	Q	101	ASP
17	Q	102	LYS
17	Q	108	LEU
18	R	12	HIS
18	R	13	ARG
18	R	16	GLU
18	R	18	GLN
18	R	25	LEU
18	R	39	LEU
18	R	40	MET
18	R	43	ASN
18	R	52	PRO
18	R	53	PHE
18	R	55	ASP
18	R	66	HIS
18	R	79	ARG
18	R	83	TYR

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Mol	Chain	Res	Type
18	R	94	THR
18	R	95	ASP
19	S	3	THR
19	S	4	ILE
19	S	6	LYS
19	S	8	ARG
19	S	9	HIS
19	S	13	SER
19	S	16	LYS
19	S	28	LYS
19	S	36	LEU
19	S	37	THR
19	S	60	HIS
19	S	67	ASP
19	S	69	LEU
19	S	77	ASP
19	S	80	PRO
19	S	88	ARG
19	S	90	LYS
19	S	94	ASP
19	S	95	ARG
19	S	102	HIS
19	S	110	ARG
20	T	1	MET
20	T	5	GLU
20	T	6	ARG
20	T	8	LEU
20	T	10	VAL
20	T	11	LEU
20	T	15	HIS
20	T	21	SER
20	T	24	MET
20	T	28	ASN
20	T	30	ILE
20	T	31	VAL
20	T	44	LYS
20	T	47	VAL
20	T	52	GLU
20	T	66	LYS
20	T	68	LYS
20	T	69	ARG
20	T	79	ASP

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Mol	Chain	Res	Type
20	T	85	VAL
20	T	89	GLU
20	T	91	GLN
20	T	94	ASP
21	U	3	LYS
21	U	6	ARG
21	U	33	VAL
21	U	38	ILE
21	U	43	LYS
21	U	52	ASN
21	U	59	GLU
21	U	61	GLU
21	U	64	ILE
21	U	66	VAL
21	U	68	ASN
21	U	71	ILE
21	U	72	PHE
21	U	80	ASP
21	U	81	ARG
21	U	85	ARG
21	U	88	ASP
21	U	90	LYS
21	U	93	ARG
21	U	95	PHE
21	U	100	GLU
22	W	2	HIS
22	W	8	SER
22	W	10	ARG
22	W	18	LYS
22	W	19	ARG
22	W	20	LEU
22	W	23	LYS
22	W	40	ARG
22	W	44	PHE
22	W	45	HIS
22	W	54	ARG
22	W	55	ASP
22	W	65	LYS
22	W	69	GLU
22	W	81	ILE
22	W	84	GLU
23	X	2	LYS

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Mol	Chain	Res	Type
23	X	5	GLU
23	X	7	ARG
23	X	8	GLU
23	X	12	GLU
23	X	15	ASN
23	X	17	GLU
23	X	18	LEU
23	X	34	SER
23	X	36	GLN
23	X	38	GLN
23	X	41	HIS
23	X	44	LYS
23	X	45	GLN
23	X	53	VAL
24	Y	6	ILE
24	Y	7	THR
24	Y	8	GLN
24	Y	9	THR
24	Y	10	ARG
24	Y	15	ARG
24	Y	16	LEU
24	Y	19	HIS
24	Y	20	LYS
24	Y	31	ILE
24	Y	37	ARG
24	Y	39	ASP
25	Z	4	ASP
25	Z	6	HIS
25	Z	8	LYS
25	Z	13	THR
25	Z	15	SER
25	Z	18	CYS
25	Z	24	ILE
25	Z	25	ARG
25	Z	30	HIS
25	Z	32	LEU
25	Z	33	ASN
25	Z	35	ASP
25	Z	40	CYS
25	Z	49	ARG
25	Z	58	ASP
25	Z	63	ARG

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Mol	Chain	Res	Type
25	Z	65	ASN
25	Z	66	ILE
25	Z	70	LYS
26	1	3	GLN
26	1	4	GLN
26	1	5	ASN
26	1	11	LYS
26	1	12	ARG
26	1	14	MET
26	1	16	ARG
26	1	21	LEU
26	1	25	THR
26	1	27	LEU
26	1	29	VAL
26	1	32	THR
26	1	35	GLU
26	1	39	ARG
26	1	51	ARG
26	1	52	LYS
27	2	4	ILE
27	2	5	ARG
27	2	6	GLU
27	2	7	LYS
27	2	9	LYS
27	2	23	THR
27	2	24	LYS
27	2	32	LYS
27	2	33	LEU
27	2	34	GLU
27	2	36	LYS
27	2	44	GLN
27	2	49	LYS
27	2	52	LYS
27	2	53	ILE
28	3	12	ARG
28	3	18	PHE
28	3	19	ARG
28	3	21	ARG
28	3	25	LYS
28	3	26	ASN
28	3	29	GLN
28	3	33	ARG

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Mol	Chain	Res	Type
28	3	41	ARG
28	3	45	SER
28	3	46	LYS
29	4	3	ILE
29	4	4	LYS
29	4	6	VAL
29	4	11	LYS
29	4	12	ARG
29	4	18	LYS
29	4	21	PHE
29	4	25	HIS
29	4	28	LEU
29	4	29	ARG
29	4	30	HIS
29	4	32	LEU
29	4	35	LYS
29	4	37	THR
29	4	41	ARG
29	4	44	ARG
29	4	46	LYS
29	4	51	LYS
30	5	2	LYS
30	5	4	ARG
30	5	8	LYS
30	5	9	LYS
30	5	12	ARG
30	5	18	LYS
30	5	19	ARG
30	5	20	ASP
30	5	23	ILE
30	5	27	CYS
30	5	33	HIS
30	5	36	ARG
30	5	37	GLN
31	6	2	LYS
31	6	96	LYS
31	6	141	ASP
33	c	17	TRP
33	c	20	THR
33	c	26	LYS
33	c	31	ASN
33	c	40	GLN

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Mol	Chain	Res	Type
33	c	42	LEU
33	c	69	THR
33	c	82	ASP
33	c	88	LYS
33	c	100	ILE
33	c	102	ILE
33	c	106	ARG
33	c	113	LYS
33	c	141	MET
33	c	146	LYS
33	c	156	LEU
33	c	164	THR
33	c	165	GLU
33	c	166	TRP
33	c	168	ARG
33	c	174	LEU
33	c	176	THR
33	c	180	ASP
33	c	184	ASN
33	c	185	THR
33	c	189	HIS
33	c	190	THR
33	c	192	TYR
34	d	7	LYS
34	d	8	LEU
34	d	10	LEU
34	d	20	LEU
34	d	21	LYS
34	d	25	ARG
34	d	35	GLN
34	d	39	GLN
34	d	40	HIS
34	d	43	ARG
34	d	55	ARG
34	d	56	GLU
34	d	58	GLN
34	d	62	ARG
34	d	64	TYR
34	d	69	ARG
34	d	85	THR
34	d	94	GLU
34	d	133	SER

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Mol	Chain	Res	Type
34	d	137	SER
34	d	145	ARG
34	d	147	LYS
34	d	150	LYS
34	d	153	ARG
34	d	155	LYS
34	d	158	LEU
34	d	160	LEU
34	d	176	LYS
34	d	183	ARG
34	d	186	GLU
34	d	189	ASP
34	d	194	ILE
35	e	11	GLN
35	e	12	GLU
35	e	23	THR
35	e	25	LYS
35	e	32	PHE
35	e	44	ARG
35	e	45	VAL
35	e	55	VAL
35	e	68	ARG
35	e	72	ASN
35	e	81	GLN
35	e	92	ARG
35	e	102	THR
35	e	110	MET
35	e	122	VAL
35	e	123	LEU
35	e	125	LYS
35	e	139	THR
35	e	143	LEU
35	e	151	MET
35	e	158	LYS
36	f	24	ARG
36	f	37	HIS
36	f	38	ARG
36	f	39	LEU
36	f	46	GLN
36	f	53	LYS
36	f	54	LEU
36	f	55	HIS

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Mol	Chain	Res	Type
36	f	61	LEU
36	f	65	GLU
36	f	69	GLU
36	f	71	ILE
36	f	75	GLU
36	f	76	THR
36	f	78	PHE
36	f	86	ARG
36	f	87	SER
36	f	88	MET
36	f	92	THR
37	g	3	ARG
37	g	10	LYS
37	g	11	ILE
37	g	14	ASP
37	g	16	LYS
37	g	19	SER
37	g	21	LEU
37	g	22	LEU
37	g	29	LEU
37	g	46	LEU
37	g	52	ARG
37	g	55	LYS
37	g	72	VAL
37	g	78	ARG
37	g	84	TYR
37	g	89	GLU
37	g	94	ARG
37	g	112	ASP
37	g	114	SER
37	g	139	ASP
37	g	143	MET
38	h	4	ASP
38	h	17	GLN
38	h	26	MET
38	h	30	LYS
38	h	37	ASN
38	h	48	PHE
38	h	55	LYS
38	h	61	THR
38	h	64	TYR
38	h	76	ARG

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Mol	Chain	Res	Type
38	h	82	LEU
38	h	83	ARG
38	h	93	LYS
38	h	107	LYS
38	h	111	THR
38	h	113	ARG
38	h	120	LEU
39	i	3	ASN
39	i	11	ARG
39	i	26	LYS
39	i	30	ASN
39	i	35	GLU
39	i	36	GLN
39	i	38	PHE
39	i	41	GLU
39	i	44	ARG
39	i	53	LEU
39	i	56	MET
39	i	58	GLU
39	i	59	LYS
39	i	60	LEU
39	i	61	ASP
39	i	84	ARG
39	i	86	LEU
39	i	87	MET
39	i	106	ASP
39	i	112	ARG
39	i	121	ARG
39	i	126	PHE
40	j	5	ARG
40	j	11	LYS
40	j	14	ASP
40	j	18	ILE
40	j	35	GLN
40	j	40	ILE
40	j	45	ARG
40	j	48	ARG
40	j	50	THR
40	j	57	VAL
40	j	68	ARG
40	j	71	LEU
40	j	73	LEU

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Mol	Chain	Res	Type
40	j	75	ASP
40	j	81	GLU
40	j	88	MET
40	j	89	ARG
40	j	92	LEU
40	j	98	VAL
40	j	102	LEU
41	k	12	ARG
41	k	33	ILE
41	k	35	ASP
41	k	36	ARG
41	k	37	GLN
41	k	52	ARG
41	k	56	LYS
41	k	58	THR
41	k	71	ASP
41	k	73	VAL
41	k	83	VAL
41	k	84	MET
41	k	85	VAL
41	k	92	ARG
41	k	99	LEU
41	k	107	THR
41	k	108	ASN
41	k	117	HIS
41	k	121	ARG
41	k	126	ARG
42	l	18	SER
42	l	20	VAL
42	l	28	GLN
42	l	30	ARG
42	l	33	CYS
42	l	35	ARG
42	l	38	THR
42	l	50	LYS
42	l	58	ASN
42	l	71	HIS
42	l	74	GLN
42	l	102	ASP
42	l	103	CYS
42	l	107	LYS
42	l	118	VAL

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Mol	Chain	Res	Type
43	m	2	ARG
43	m	11	HIS
43	m	18	LEU
43	m	27	THR
43	m	28	ARG
43	m	41	ASP
43	m	43	LYS
43	m	44	ILE
43	m	57	ASP
43	m	62	PHE
43	m	64	VAL
43	m	67	ASP
43	m	68	LEU
43	m	81	ASP
43	m	90	HIS
43	m	91	ARG
43	m	97	ARG
43	m	99	GLN
43	m	100	ARG
43	m	101	THR
43	m	102	LYS
43	m	106	ARG
44	n	15	LEU
44	n	27	LYS
44	n	41	TRP
44	n	45	LEU
44	n	50	LEU
44	n	53	ASP
44	n	59	GLN
44	n	60	ARG
44	n	65	GLN
44	n	73	LEU
44	n	74	ARG
44	n	76	PHE
45	o	7	THR
45	o	17	ASP
45	o	25	GLU
45	o	57	ARG
45	o	58	MET
45	o	64	LYS
45	o	70	LYS
46	p	4	ILE

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Mol	Chain	Res	Type
46	p	5	ARG
46	p	26	ASN
46	p	29	ASN
46	p	31	ARG
46	p	34	GLU
46	p	46	LYS
46	p	55	ASP
46	p	63	GLN
47	q	4	ILE
47	q	10	ARG
47	q	15	LYS
47	q	25	GLU
47	q	26	ARG
47	q	39	ARG
47	q	45	VAL
47	q	52	CYS
47	q	60	ILE
47	q	67	SER
47	q	74	LEU
47	q	76	ARG
47	q	78	VAL
47	q	80	LYS
48	r	30	ASN
48	r	52	ARG
48	r	65	SER
49	s	5	LYS
49	s	12	LEU
49	s	14	LEU
49	s	20	LYS
49	s	28	LYS
49	s	36	ARG
49	s	40	PHE
49	s	47	THR
49	s	72	GLU
49	s	73	PHE
50	t	4	LYS
50	t	14	GLU
50	t	26	MET
50	t	29	THR
50	t	53	MET
50	t	59	ARG
50	t	67	HIS

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Mol	Chain	Res	Type
50	t	70	LYS
50	t	85	LEU
51	7	9	LEU
51	7	15	PHE
51	7	22	TRP
51	7	23	ASN
51	7	26	MET
51	7	31	PHE
51	7	36	LYS
51	7	38	HIS
51	7	40	ILE
51	7	46	VAL
51	7	48	MET
51	7	56	LEU
51	7	57	ASN
51	7	62	ARG
51	7	67	LEU
51	7	73	ARG
51	7	81	ASP
51	7	90	PHE
51	7	94	ARG
51	7	95	TRP
51	7	101	THR
51	7	116	LEU
51	7	119	GLN
51	7	121	GLN
51	7	122	ASP
51	7	125	PHE
51	7	127	LYS
51	7	128	LEU
51	7	145	ASN
51	7	158	ASP
51	7	162	VAL
51	7	188	THR
51	7	196	ASP
51	7	202	ASN
51	7	206	ILE
51	7	209	VAL
51	7	212	TYR
51	7	222	GLU
52	u	11	PHE
52	u	12	ASP

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Mol	Chain	Res	Type
52	u	16	ARG
52	u	17	ARG
52	u	33	ARG
52	u	44	ARG
52	u	48	LYS
52	u	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
3	V	49	ASN
3	V	51	GLN
3	V	80	HIS
3	V	88	HIS
4	C	20	ASN
4	C	36	ASN
4	C	43	ASN
4	C	52	HIS
4	C	89	ASN
4	C	127	ASN
4	C	133	ASN
4	C	162	GLN
4	C	225	ASN
4	C	250	GLN
5	D	32	ASN
5	D	58	ASN
5	D	130	GLN
5	D	134	HIS
5	D	149	ASN
5	D	164	GLN
5	D	167	ASN
5	D	173	GLN
5	D	185	ASN
6	E	29	HIS
6	E	46	GLN
6	E	92	HIS
6	E	97	ASN
6	E	136	GLN
6	E	156	ASN
6	E	195	GLN
7	F	26	GLN
7	F	36	ASN

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Mol	Chain	Res	Type
7	F	80	GLN
7	F	126	ASN
8	G	19	ASN
8	G	21	GLN
8	G	29	ASN
8	G	142	GLN
9	H	2	GLN
9	H	11	ASN
9	H	43	ASN
9	H	73	ASN
10	J	40	HIS
10	J	77	HIS
10	J	80	HIS
10	J	131	ASN
10	J	135	GLN
10	J	136	GLN
11	K	5	GLN
11	K	9	ASN
11	K	82	ASN
11	K	88	ASN
12	L	38	GLN
12	L	99	ASN
13	M	3	GLN
13	M	17	ASN
14	N	9	GLN
14	N	13	ASN
14	N	73	ASN
14	N	81	ASN
15	O	38	GLN
15	O	67	ASN
15	O	98	GLN
15	O	104	GLN
16	P	2	ASN
16	P	11	GLN
16	P	40	GLN
17	Q	43	GLN
17	Q	51	GLN
17	Q	55	GLN
17	Q	58	GLN
17	Q	80	ASN
18	R	18	GLN
18	R	87	GLN

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Mol	Chain	Res	Type
19	S	9	HIS
19	S	57	ASN
20	T	28	ASN
21	U	39	ASN
21	U	65	GLN
21	U	68	ASN
22	W	2	HIS
22	W	49	ASN
22	W	56	HIS
23	X	31	GLN
23	X	36	GLN
23	X	38	GLN
23	X	45	GLN
23	X	58	ASN
24	Y	8	GLN
24	Y	19	HIS
25	Z	30	HIS
25	Z	41	HIS
25	Z	65	ASN
26	1	3	GLN
27	2	25	ASN
29	4	23	HIS
30	5	13	ASN
30	5	35	GLN
31	6	11	GLN
31	6	29	GLN
31	6	30	GLN
31	6	33	ASN
31	6	93	ASN
33	c	2	GLN
33	c	5	HIS
33	c	24	ASN
33	c	40	GLN
33	c	68	HIS
33	c	122	GLN
33	c	139	ASN
33	c	184	ASN
34	d	35	GLN
34	d	84	ASN
34	d	99	ASN
34	d	135	GLN
34	d	151	GLN

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Mol	Chain	Res	Type
34	d	195	ASN
35	e	69	ASN
35	e	72	ASN
35	e	96	GLN
35	e	121	ASN
35	e	131	ASN
36	f	14	GLN
36	f	17	GLN
36	f	46	GLN
36	f	58	HIS
37	g	67	ASN
37	g	85	GLN
37	g	121	ASN
38	h	3	GLN
38	h	17	GLN
39	i	4	GLN
39	i	24	ASN
39	i	30	ASN
39	i	31	GLN
39	i	36	GLN
39	i	49	GLN
39	i	109	GLN
40	j	15	HIS
40	j	20	GLN
40	j	35	GLN
40	j	99	GLN
41	k	28	ASN
41	k	37	GLN
42	l	58	ASN
42	l	72	ASN
43	m	13	HIS
43	m	90	HIS
44	n	42	ASN
44	n	59	GLN
44	n	65	GLN
45	o	34	GLN
46	p	9	HIS
46	p	18	GLN
46	p	29	ASN
46	p	63	GLN
48	r	53	GLN
49	s	42	ASN

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Mol	Chain	Res	Type
49	s	51	HIS
49	s	55	GLN
49	s	68	HIS
50	t	12	GLN
50	t	20	ASN
50	t	60	GLN
50	t	69	ASN
51	7	17	HIS
51	7	23	ASN
51	7	35	ASN
51	7	88	GLN
51	7	108	GLN
51	7	119	GLN
51	7	121	GLN
51	7	145	ASN
51	7	167	HIS
51	7	202	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	116/117 (99%)	23 (19%)	0
2	B	2837/2841 (99%)	450 (15%)	18 (0%)
32	a	1529/1530 (99%)	277 (18%)	0
53	v	75/76 (98%)	15 (20%)	0
All	All	4557/4564 (99%)	765 (16%)	18 (0%)

All (765) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	C
1	A	12	C
1	A	13	G
1	A	14	U
1	A	15	A
1	A	16	G
1	A	25	U
1	A	26	C
1	A	28	C
1	A	29	A
1	A	30	C

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Mol	Chain	Res	Type
1	A	35	C
1	A	42	C
1	A	44	G
1	A	45	A
1	A	56	G
1	A	66	A
1	A	67	G
1	A	84	G
1	A	90	C
1	A	99	A
1	A	108	A
1	A	109	A
2	B	2	G
2	B	3	U
2	B	4	U
2	B	13	A
2	B	14	A
2	B	33	C
2	B	34	U
2	B	35	G
2	B	46	G
2	B	49	A
2	B	63	A
2	B	64	A
2	B	71	A
2	B	74	A
2	B	75	G
2	B	84	A
2	B	85	G
2	B	91	A
2	B	92	U
2	B	96	C
2	B	100	U
2	B	101	A
2	B	102	U
2	B	103	A
2	B	104	A
2	B	118	A
2	B	119	A
2	B	120	U
2	B	125	A
2	B	126	A

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Mol	Chain	Res	Type
2	B	140	C
2	B	142	A
2	B	144	A
2	B	160	A
2	B	162	U
2	B	163	C
2	B	181	A
2	B	186	G
2	B	196	A
2	B	199	A
2	B	209	C
2	B	216	A
2	B	221	A
2	B	222	A
2	B	224	U
2	B	230	G
2	B	241	A
2	B	248	G
2	B	252	G
2	B	255	A
2	B	265	A
2	B	266	G
2	B	271	G
2	B	277	G
2	B	278	A
2	B	279	A
2	B	311	A
2	B	312	G
2	B	323	C
2	B	324	A
2	B	329	G
2	B	330	A
2	B	349	U
2	B	353	C
2	B	355	U
2	B	371	A
2	B	372	G
2	B	386	G
2	B	387	U
2	B	395	U
2	B	396	G
2	B	397	U

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Mol	Chain	Res	Type
2	B	405	U
2	B	411	G
2	B	423	A
2	B	424	G
2	B	435	C
2	B	444	C
2	B	451	U
2	B	455	C
2	B	457	A
2	B	479	A
2	B	480	A
2	B	481	G
2	B	491	G
2	B	498	G
2	B	504	A
2	B	505	A
2	B	508	A
2	B	509	C
2	B	512	G
2	B	518	G
2	B	527	C
2	B	530	G
2	B	532	A
2	B	533	G
2	B	544	C
2	B	545	U
2	B	546	U
2	B	547	A
2	B	548	G
2	B	555	G
2	B	563	A
2	B	572	A
2	B	573	U
2	B	575	A
2	B	588	U
2	B	603	A
2	B	613	A
2	B	614	A
2	B	615	U
2	B	616	A
2	B	627	A
2	B	632	A

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Mol	Chain	Res	Type
2	B	637	A
2	B	640	C
2	B	645	C
2	B	646	U
2	B	654	A
2	B	655	A
2	B	671	C
2	B	686	U
2	B	717	C
2	B	719	C
2	B	722	A
2	B	728	G
2	B	730	A
2	B	747	U
2	B	757	G
2	B	765	C
2	B	775	G
2	B	782	A
2	B	784	G
2	B	785	G
2	B	805	G
2	B	806	C
2	B	812	C
2	B	819	A
2	B	827	U
2	B	828	U
2	B	846	U
2	B	847	U
2	B	859	G
2	B	872	U
2	B	876	C
2	B	877	A
2	B	878	A
2	B	899	A
2	B	910	A
2	B	912	C
2	B	932	U
2	B	933	A
2	B	934	U
2	B	941	A
2	B	946	C
2	B	955	U

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Mol	Chain	Res	Type
2	B	961	C
2	B	973	A
2	B	974	G
2	B	983	A
2	B	985	C
2	B	989	G
2	B	991	C
2	B	993	G
2	B	995	C
2	B	996	A
2	B	1005	C
2	B	1012	U
2	B	1013	C
2	B	1019	U
2	B	1022	G
2	B	1025	G
2	B	1026	G
2	B	1033	U
2	B	1042	G
2	B	1046	A
2	B	1047	G
2	B	1070	A
2	B	1088	A
2	B	1090	A
2	B	1112	G
2	B	1122	G
2	B	1126	A
2	B	1132	U
2	B	1133	A
2	B	1134	A
2	B	1135	C
2	B	1136	G
2	B	1139	G
2	B	1142	A
2	B	1156	A
2	B	1157	G
2	B	1172	C
2	B	1174	U
2	B	1176	U
2	B	1179	G
2	B	1195	G
2	B	1205	A

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Mol	Chain	Res	Type
2	B	1206	G
2	B	1211	C
2	B	1212	G
2	B	1218	G
2	B	1237	A
2	B	1247	A
2	B	1248	G
2	B	1251	C
2	B	1253	A
2	B	1256	G
2	B	1266	G
2	B	1271	G
2	B	1272	A
2	B	1273	U
2	B	1275	A
2	B	1276	A
2	B	1301	A
2	B	1302	A
2	B	1312	U
2	B	1325	U
2	B	1330	C
2	B	1337	G
2	B	1341	G
2	B	1345	C
2	B	1352	U
2	B	1365	A
2	B	1368	G
2	B	1379	U
2	B	1383	A
2	B	1384	A
2	B	1396	U
2	B	1397	U
2	B	1416	G
2	B	1419	A
2	B	1420	A
2	B	1427	A
2	B	1428	C
2	B	1434	A
2	B	1450	G
2	B	1451	C
2	B	1453	A
2	B	1454	C

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Mol	Chain	Res	Type
2	B	1455	G
2	B	1459	G
2	B	1460	U
2	B	1461	C
2	B	1476	U
2	B	1477	A
2	B	1478	G
2	B	1482	G
2	B	1490	A
2	B	1493	C
2	B	1494	A
2	B	1504	A
2	B	1508	A
2	B	1509	A
2	B	1510	G
2	B	1524	G
2	B	1532	A
2	B	1535	A
2	B	1537	G
2	B	1538	G
2	B	1540	G
2	B	1552	A
2	B	1558	C
2	B	1559	U
2	B	1567	G
2	B	1569	A
2	B	1578	U
2	B	1583	A
2	B	1585	C
2	B	1608	A
2	B	1610	A
2	B	1613	G
2	B	1634	A
2	B	1635	A
2	B	1640	A
2	B	1647	U
2	B	1648	U
2	B	1649	G
2	B	1674	G
2	B	1700	A
2	B	1701	A
2	B	1703	G

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Mol	Chain	Res	Type
2	B	1706	C
2	B	1707	G
2	B	1713	A
2	B	1715	G
2	B	1716	U
2	B	1723	G
2	B	1729	U
2	B	1730	C
2	B	1731	G
2	B	1733	G
2	B	1738	G
2	B	1756	G
2	B	1758	U
2	B	1764	C
2	B	1773	A
2	B	1776	G
2	B	1781	U
2	B	1786	A
2	B	1791	A
2	B	1800	C
2	B	1801	A
2	B	1816	C
2	B	1829	A
2	B	1833	C
2	B	1870	C
2	B	1873	G
2	B	1876	A
2	B	1884	G
2	B	1906	G
2	B	1914	C
2	B	1927	A
2	B	1929	G
2	B	1930	G
2	B	1937	A
2	B	1938	A
2	B	1939	U
2	B	1940	U
2	B	1955	U
2	B	1967	C
2	B	1970	A
2	B	1971	U
2	B	1972	G

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Mol	Chain	Res	Type
2	B	1991	U
2	B	1993	U
2	B	1997	C
2	B	2022	U
2	B	2023	C
2	B	2031	A
2	B	2032	G
2	B	2033	A
2	B	2043	C
2	B	2052	A
2	B	2055	C
2	B	2056	G
2	B	2060	A
2	B	2061	G
2	B	2062	A
2	B	2069	G
2	B	2072	C
2	B	2095	A
2	B	2102	G
2	B	2104	C
2	B	2137	U
2	B	2140	G
2	B	2141	G
2	B	2144	G
2	B	2145	C
2	B	2147	A
2	B	2149	U
2	B	2181	U
2	B	2187	U
2	B	2192	U
2	B	2199	A
2	B	2204	G
2	B	2211	A
2	B	2212	A
2	B	2225	A
2	B	2226	C
2	B	2238	G
2	B	2239	G
2	B	2243	U
2	B	2259	U
2	B	2266	A
2	B	2273	A

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Mol	Chain	Res	Type
2	B	2276	G
2	B	2278	A
2	B	2283	C
2	B	2286	G
2	B	2297	A
2	B	2304	G
2	B	2305	U
2	B	2307	G
2	B	2310	C
2	B	2315	G
2	B	2318	G
2	B	2319	G
2	B	2320	U
2	B	2321	U
2	B	2322	A
2	B	2325	G
2	B	2333	A
2	B	2334	U
2	B	2336	A
2	B	2337	G
2	B	2347	C
2	B	2383	G
2	B	2385	C
2	B	2402	U
2	B	2406	A
2	B	2423	U
2	B	2424	C
2	B	2426	A
2	B	2429	G
2	B	2430	A
2	B	2434	A
2	B	2441	U
2	B	2448	A
2	B	2472	G
2	B	2476	A
2	B	2491	U
2	B	2502	G
2	B	2505	G
2	B	2506	U
2	B	2518	A
2	B	2529	G
2	B	2535	G

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Mol	Chain	Res	Type
2	B	2554	U
2	B	2566	A
2	B	2567	G
2	B	2573	C
2	B	2585	U
2	B	2586	U
2	B	2597	G
2	B	2602	A
2	B	2609	U
2	B	2610	C
2	B	2613	U
2	B	2621	G
2	B	2629	U
2	B	2654	A
2	B	2682	A
2	B	2689	U
2	B	2690	U
2	B	2714	G
2	B	2726	A
2	B	2739	U
2	B	2744	G
2	B	2748	A
2	B	2751	G
2	B	2752	C
2	B	2757	A
2	B	2765	A
2	B	2778	A
2	B	2791	G
2	B	2797	U
2	B	2800	A
2	B	2801	G
2	B	2808	G
2	B	2820	A
2	B	2821	A
2	B	2836	U
2	B	2850	A
2	B	2866	U
2	B	2867	G
2	B	2872	A
2	B	2873	A
2	B	2883	A
2	B	2903	U

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Mol	Chain	Res	Type
32	a	7	A
32	a	9	G
32	a	14	U
32	a	31	G
32	a	32	A
32	a	39	G
32	a	47	C
32	a	48	C
32	a	51	A
32	a	52	C
32	a	55	A
32	a	61	G
32	a	66	A
32	a	72	A
32	a	76	G
32	a	78	A
32	a	79	G
32	a	83	C
32	a	85	U
32	a	86	G
32	a	87	C
32	a	88	U
32	a	89	U
32	a	95	C
32	a	108	G
32	a	121	U
32	a	122	G
32	a	131	A
32	a	151	A
32	a	164	G
32	a	182	A
32	a	183	C
32	a	197	A
32	a	209	U
32	a	210	C
32	a	239	U
32	a	240	G
32	a	243	A
32	a	244	U
32	a	245	U
32	a	247	G
32	a	250	A

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Mol	Chain	Res	Type
32	a	251	G
32	a	253	A
32	a	257	G
32	a	258	G
32	a	266	G
32	a	267	C
32	a	280	C
32	a	289	G
32	a	316	C
32	a	324	G
32	a	328	C
32	a	329	A
32	a	330	C
32	a	332	G
32	a	345	C
32	a	352	C
32	a	354	G
32	a	367	U
32	a	372	C
32	a	373	A
32	a	381	C
32	a	382	A
32	a	397	A
32	a	398	U
32	a	406	G
32	a	408	A
32	a	411	A
32	a	412	A
32	a	414	A
32	a	415	A
32	a	421	U
32	a	422	C
32	a	424	G
32	a	429	U
32	a	430	A
32	a	434	U
32	a	435	A
32	a	438	U
32	a	459	A
32	a	461	A
32	a	462	G
32	a	463	U

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Mol	Chain	Res	Type
32	a	464	U
32	a	465	A
32	a	466	A
32	a	467	U
32	a	468	A
32	a	469	C
32	a	476	U
32	a	481	G
32	a	482	A
32	a	484	G
32	a	485	U
32	a	493	A
32	a	500	G
32	a	511	C
32	a	518	C
32	a	522	C
32	a	527	G
32	a	531	U
32	a	532	A
32	a	547	A
32	a	559	A
32	a	562	U
32	a	572	A
32	a	573	A
32	a	576	C
32	a	577	G
32	a	607	A
32	a	639	G
32	a	650	G
32	a	653	U
32	a	665	A
32	a	693	G
32	a	700	G
32	a	721	G
32	a	724	G
32	a	731	G
32	a	733	G
32	a	747	A
32	a	748	G
32	a	755	G
32	a	777	A
32	a	781	A

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Mol	Chain	Res	Type
32	a	782	A
32	a	793	U
32	a	794	A
32	a	812	G
32	a	815	A
32	a	817	C
32	a	818	G
32	a	819	A
32	a	828	U
32	a	829	G
32	a	841	C
32	a	842	U
32	a	843	U
32	a	844	G
32	a	845	A
32	a	902	G
32	a	914	A
32	a	926	G
32	a	927	G
32	a	931	C
32	a	934	C
32	a	935	A
32	a	960	U
32	a	961	U
32	a	966	G
32	a	968	A
32	a	969	A
32	a	971	G
32	a	974	A
32	a	976	G
32	a	977	A
32	a	983	A
32	a	991	U
32	a	992	U
32	a	993	G
32	a	1002	G
32	a	1004	A
32	a	1009	U
32	a	1022	A
32	a	1026	G
32	a	1030	U
32	a	1031	C

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Mol	Chain	Res	Type
32	a	1034	G
32	a	1035	A
32	a	1043	G
32	a	1044	A
32	a	1045	C
32	a	1049	U
32	a	1050	G
32	a	1051	C
32	a	1053	G
32	a	1054	C
32	a	1055	A
32	a	1065	U
32	a	1066	C
32	a	1070	U
32	a	1094	G
32	a	1095	U
32	a	1101	A
32	a	1102	A
32	a	1108	G
32	a	1111	A
32	a	1112	C
32	a	1126	U
32	a	1130	A
32	a	1136	C
32	a	1137	C
32	a	1138	G
32	a	1139	G
32	a	1140	C
32	a	1158	C
32	a	1159	U
32	a	1168	U
32	a	1169	A
32	a	1174	G
32	a	1179	A
32	a	1181	G
32	a	1183	U
32	a	1196	A
32	a	1197	A
32	a	1201	A
32	a	1202	U
32	a	1209	C
32	a	1212	U

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Mol	Chain	Res	Type
32	a	1213	A
32	a	1214	C
32	a	1215	G
32	a	1225	A
32	a	1226	C
32	a	1227	A
32	a	1228	C
32	a	1238	A
32	a	1240	U
32	a	1241	G
32	a	1253	G
32	a	1256	A
32	a	1258	G
32	a	1261	A
32	a	1270	G
32	a	1278	G
32	a	1279	G
32	a	1280	A
32	a	1281	C
32	a	1285	A
32	a	1286	U
32	a	1287	A
32	a	1298	U
32	a	1300	G
32	a	1301	U
32	a	1305	G
32	a	1316	G
32	a	1317	C
32	a	1320	C
32	a	1322	C
32	a	1323	G
32	a	1336	C
32	a	1338	G
32	a	1346	A
32	a	1347	G
32	a	1353	G
32	a	1362	A
32	a	1363	A
32	a	1364	U
32	a	1378	C
32	a	1379	G
32	a	1380	U

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Mol	Chain	Res	Type
32	a	1381	U
32	a	1398	A
32	a	1403	C
32	a	1404	C
32	a	1409	C
32	a	1419	G
32	a	1432	G
32	a	1446	A
32	a	1447	A
32	a	1451	U
32	a	1452	C
32	a	1490	U
32	a	1493	A
32	a	1497	G
32	a	1499	A
32	a	1503	A
32	a	1506	U
32	a	1507	A
32	a	1517	G
32	a	1519	A
32	a	1520	C
32	a	1529	G
32	a	1530	G
32	a	1533	C
32	a	1534	A
53	v	5	G
53	v	8	U
53	v	17	C
53	v	18	G
53	v	19	G
53	v	20	U
53	v	21	A
53	v	37	A
53	v	39	U
53	v	45	U
53	v	48	C
53	v	56	C
53	v	58	A
53	v	74	C
53	v	76	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	63	A
2	B	102	U
2	B	162	U
2	B	529	A
2	B	670	A
2	B	858	G
2	B	1205	A
2	B	1210	G
2	B	1236	G
2	B	1250	G
2	B	1301	A
2	B	1913	A
2	B	2198	A
2	B	2258	C
2	B	2282	G
2	B	2336	A
2	B	2425	A
2	B	2756	U

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	3
52	u	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2157:G	O3'	2179:C	P	42.86
1	B	2110:G	O3'	2133:G	P	29.82
1	B	878:A	O3'	898:C	P	11.30
1	u	25:ALA	C	26:GLY	N	1.16
1	u	15:LEU	C	16:ARG	N	0.99

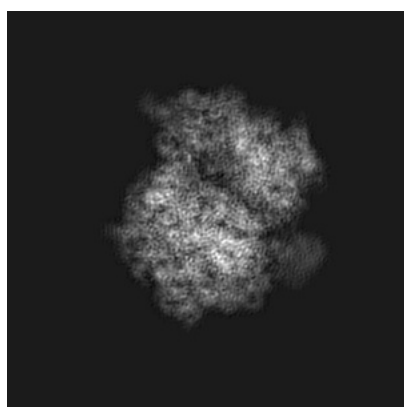
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0661. These allow visual inspection of the internal detail of the map and identification of artifacts.

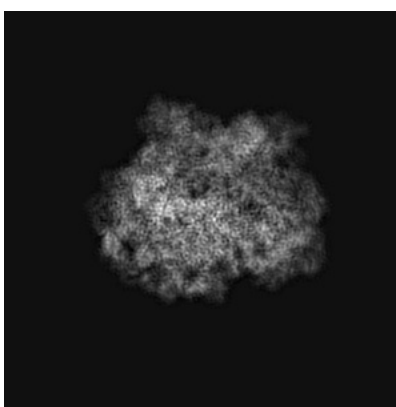
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

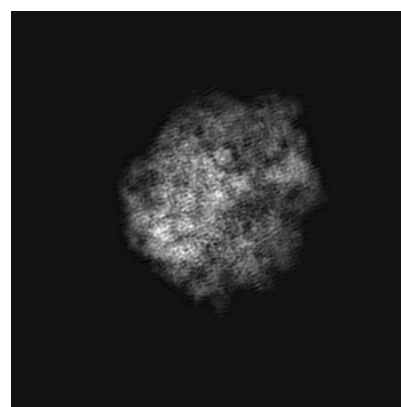
6.1.1 Primary map



X



Y

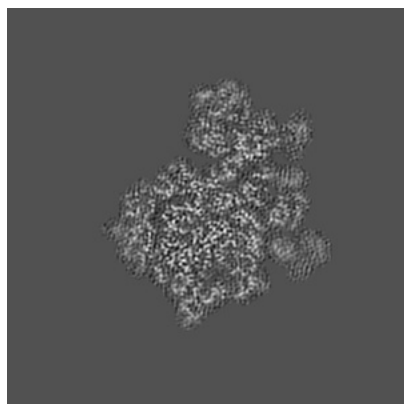


Z

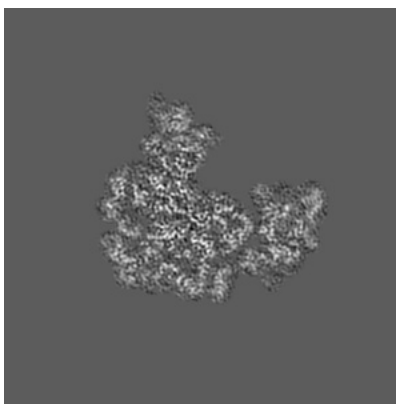
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

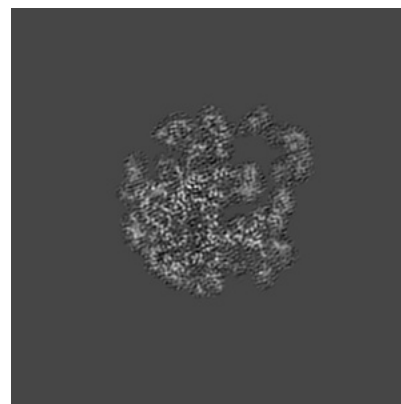
6.2.1 Primary map



X Index: 128



Y Index: 128

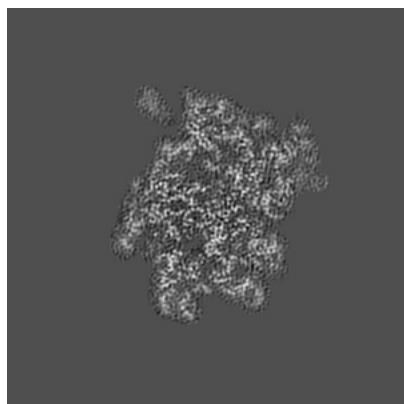


Z Index: 128

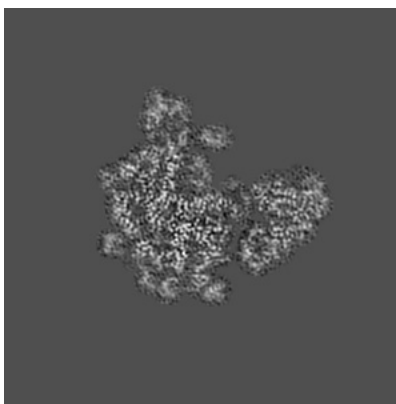
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

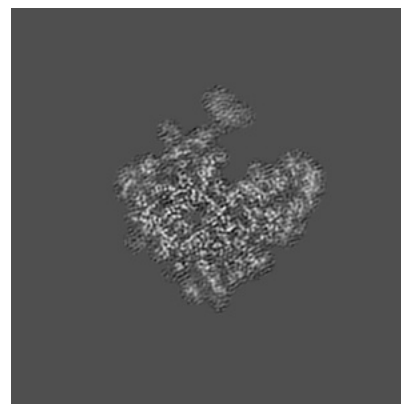
6.3.1 Primary map



X Index: 116



Y Index: 137

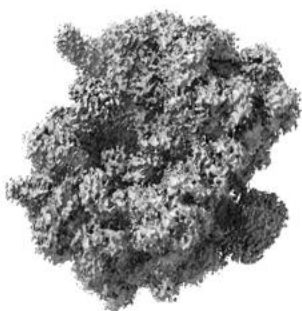


Z Index: 108

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

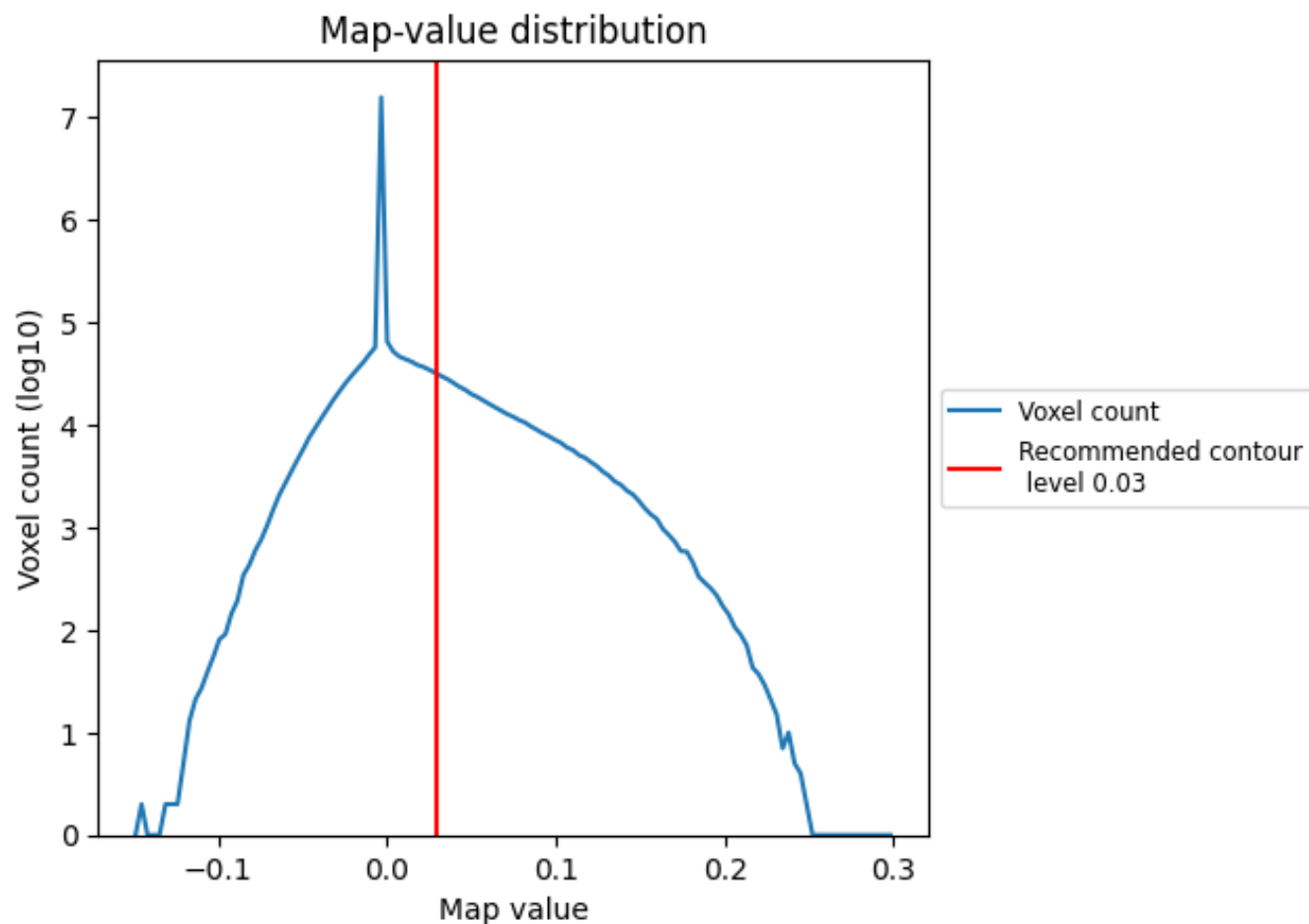
6.5 Mask visualisation

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

7 Map analysis [i](#)

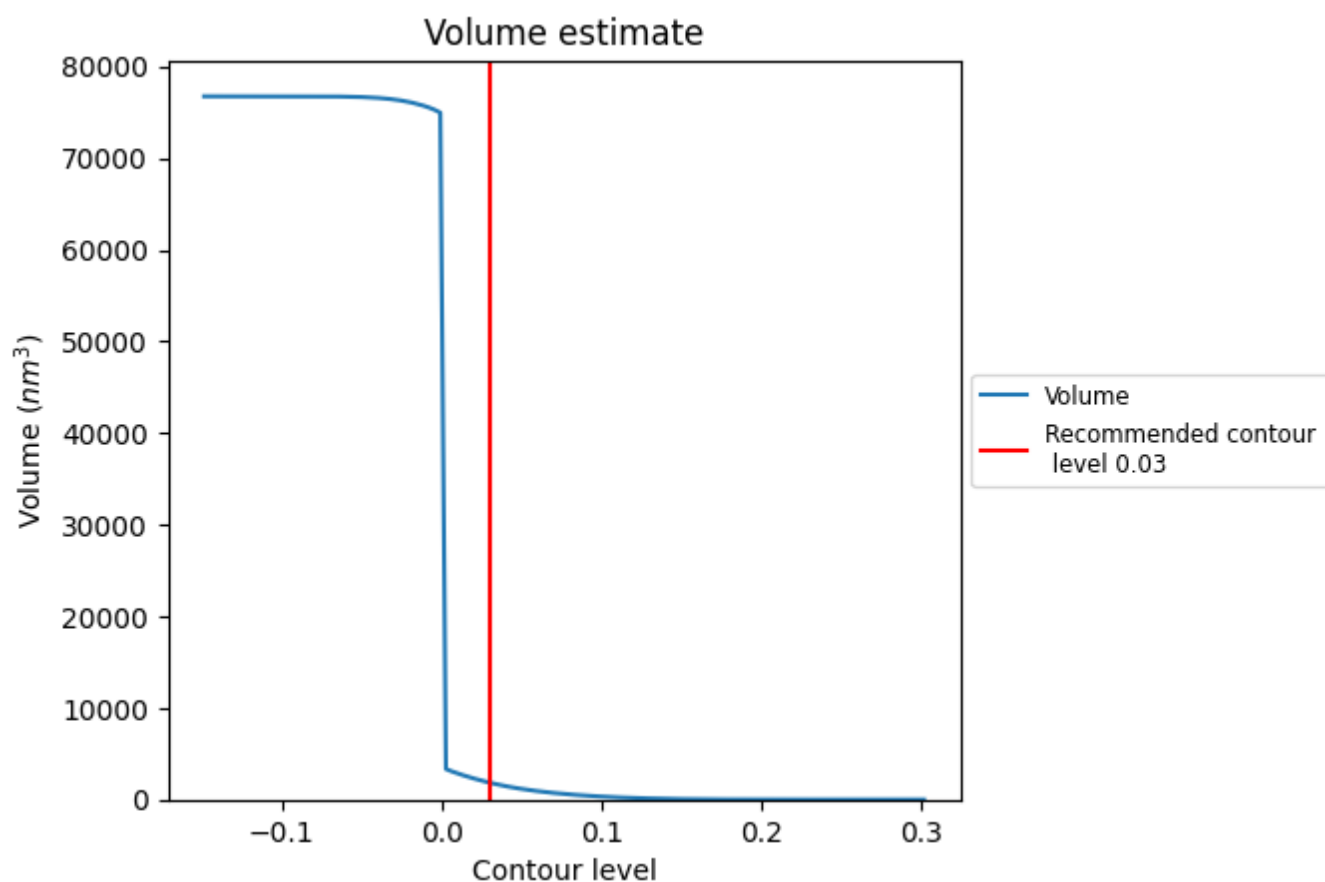
This section contains the results of statistical analysis of the map.

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.

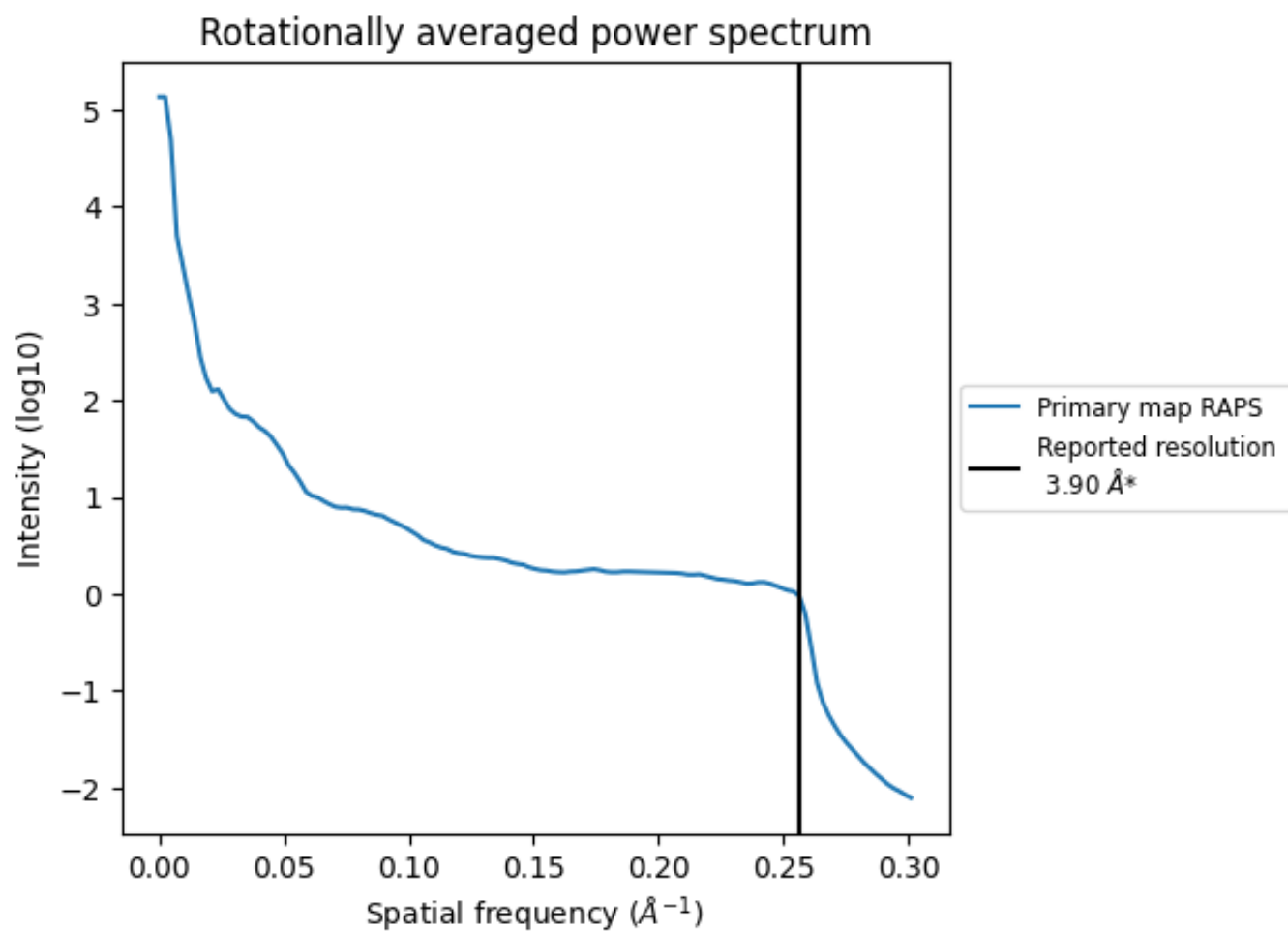
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1845 nm³; this corresponds to an approximate mass of 1667 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 ⓘ

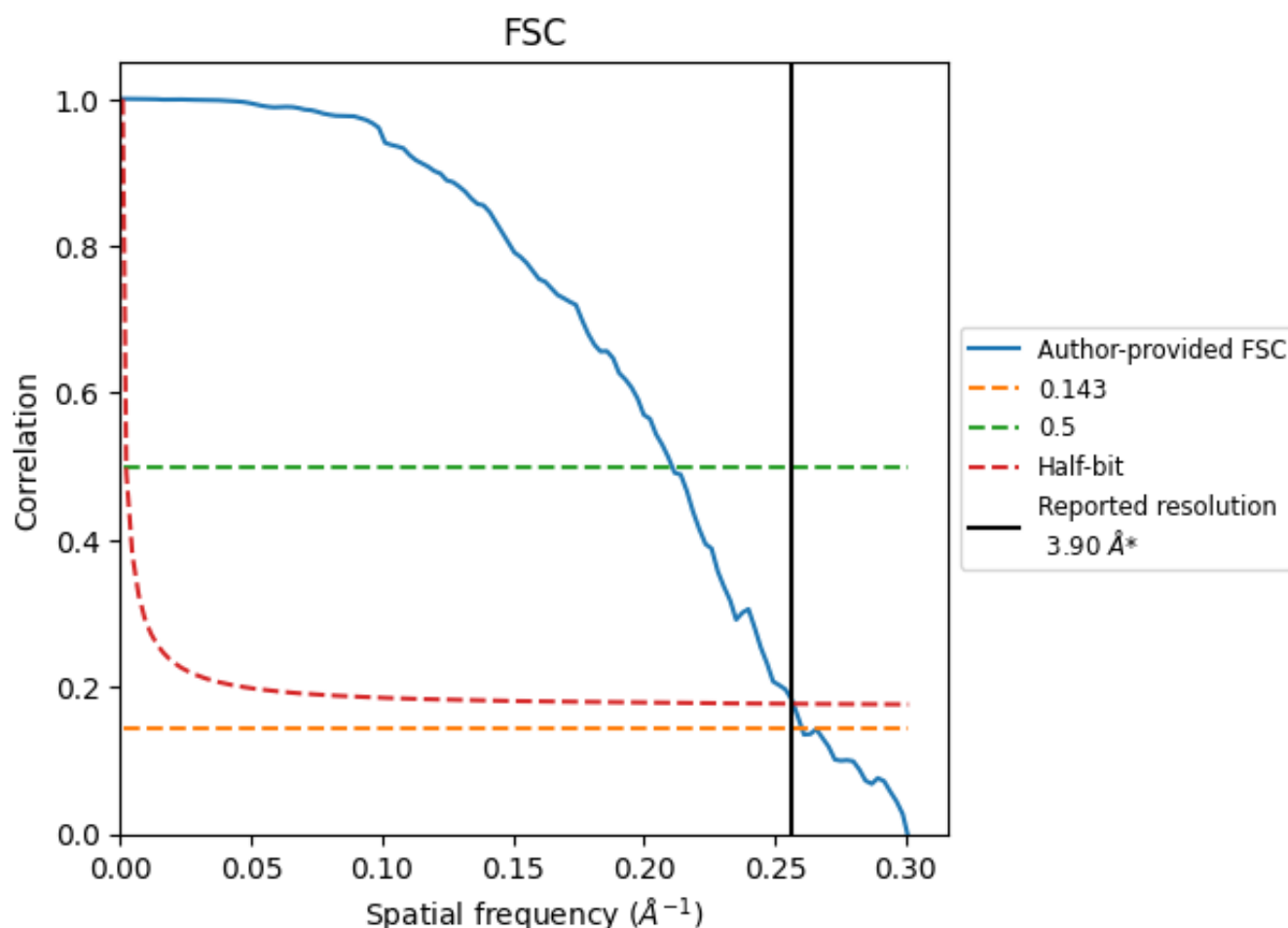


*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

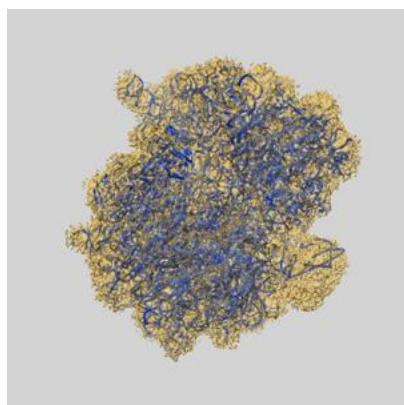
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.84	4.74	3.89
Unmasked-calculated*	-	-	-

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

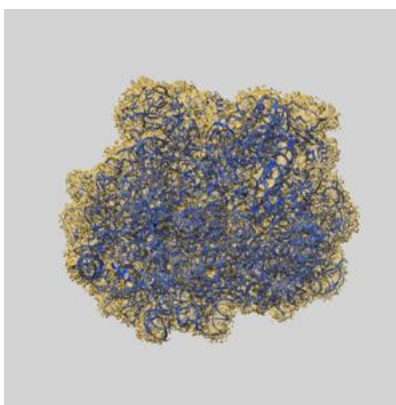
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0661 and PDB model 6O9J. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

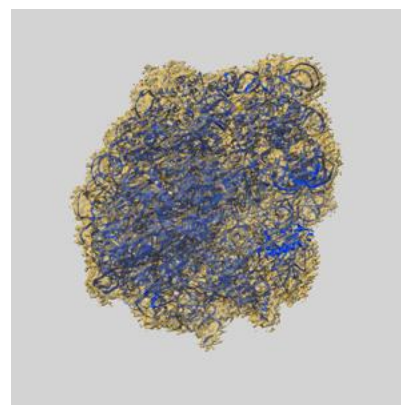
9.1 Map-model overlay [i](#)



X



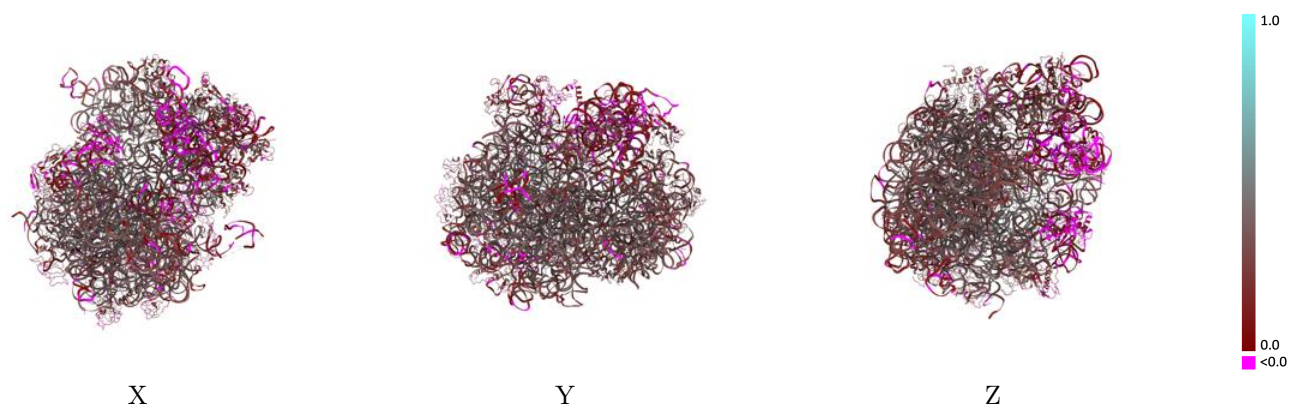
Y



Z

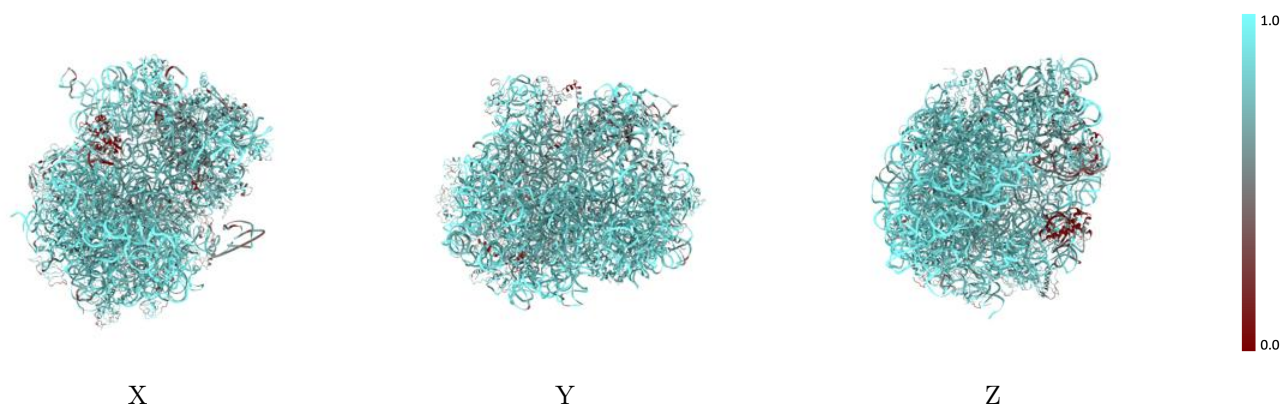
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



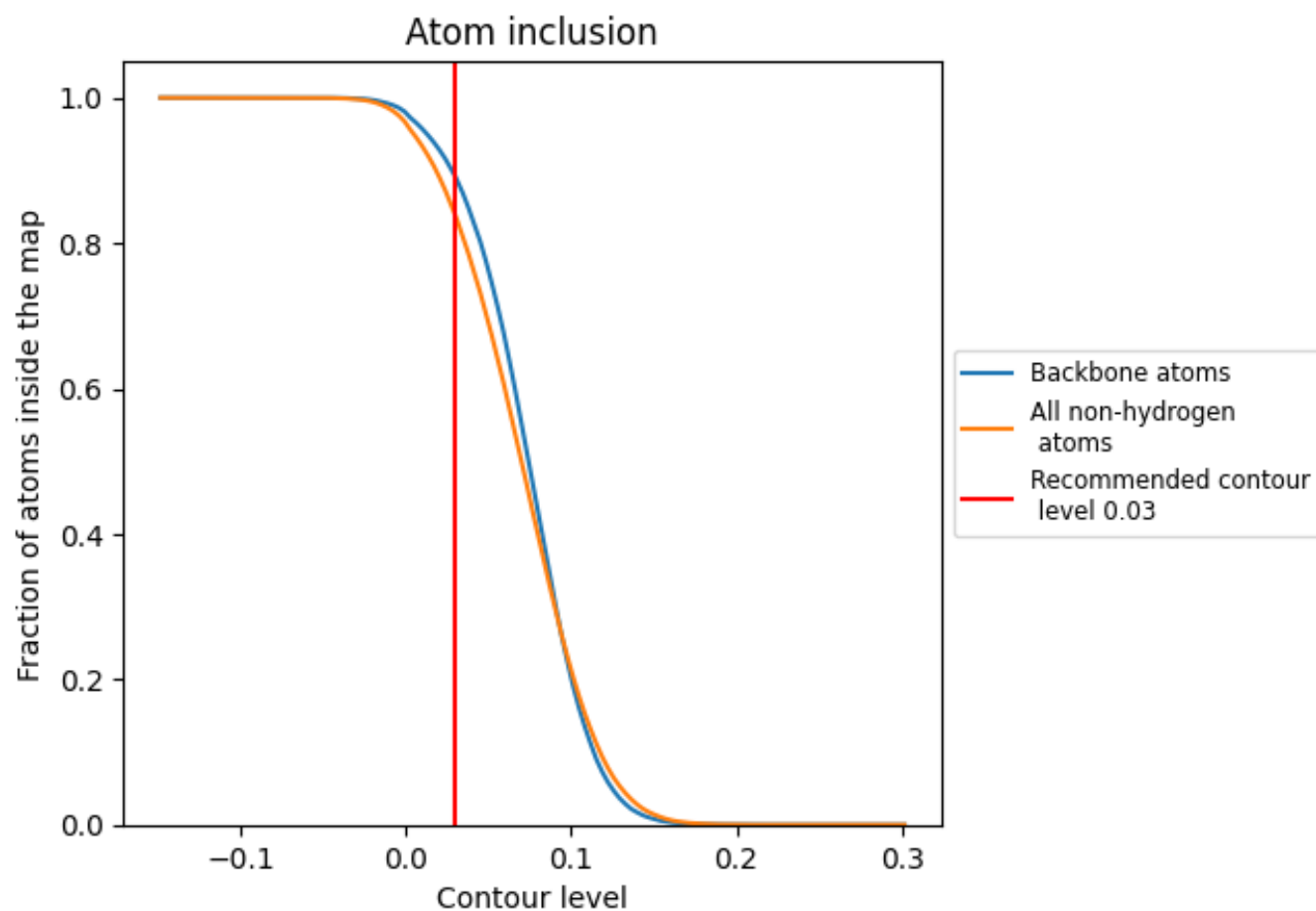
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8372	 0.2750
1	 0.6168	 0.1870
2	 0.6051	 0.1960
3	 0.7014	 0.2750
4	 0.6293	 0.2290
5	 0.6849	 0.1590
6	 0.1849	 -0.0110
7	 0.7624	 0.2650
A	 0.9230	 0.2570
B	 0.9145	 0.3270
C	 0.7014	 0.2810
D	 0.7055	 0.2420
E	 0.6862	 0.2150
F	 0.6059	 0.0750
G	 0.6746	 0.1580
H	 0.4672	 0.0970
J	 0.7267	 0.2500
K	 0.7492	 0.3210
L	 0.6162	 0.1750
M	 0.6708	 0.2220
N	 0.7031	 0.2540
O	 0.6969	 0.1820
P	 0.6678	 0.2140
Q	 0.7786	 0.2960
R	 0.6813	 0.2040
S	 0.7321	 0.2860
T	 0.6807	 0.2240
U	 0.6701	 0.1620
V	 0.7778	 0.2670
W	 0.5922	 0.1690
X	 0.7002	 0.1870
Y	 0.7002	 0.2310
Z	 0.6877	 0.2420
a	 0.8790	 0.2530
c	 0.7896	 0.3010



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Chain	Atom inclusion	Q-score
d	 0.7893	 0.2820
e	 0.7932	 0.3240
f	 0.7965	 0.3000
g	 0.7405	 0.2420
h	 0.8052	 0.3350
i	 0.8192	 0.2830
j	 0.6216	 0.0450
k	 0.7761	 0.2970
l	 0.7394	 0.3080
m	 0.5476	 0.0590
n	 0.6528	 0.0540
o	 0.7768	 0.2970
p	 0.7735	 0.3010
q	 0.7563	 0.2920
r	 0.7890	 0.3150
s	 0.6071	 0.0470
t	 0.7862	 0.2700
u	 0.6921	 0.2530
v	 0.7813	 0.2140