



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 10:29 PM UTC

PDB ID : 6O9K / pdb_00006o9k
EMDB ID : EMD-0662
Title : 70S initiation complex
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 : 4.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

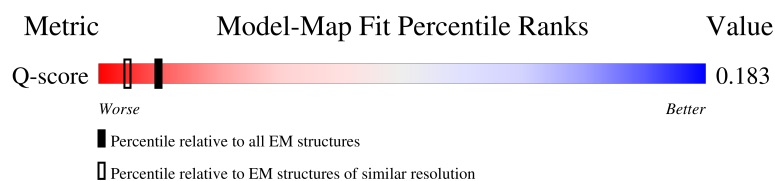
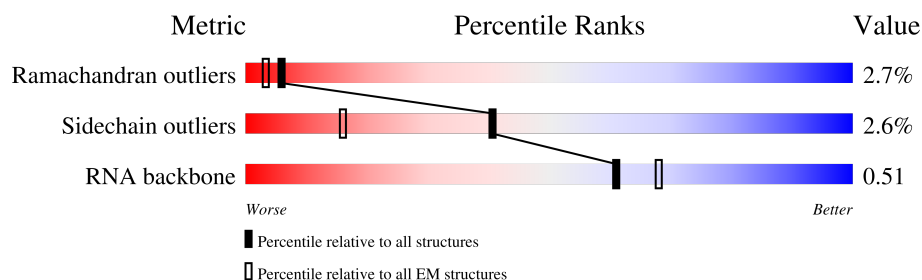
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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

Mol	Chain	Length	Quality of chain
1	a	1539	
2	b	218	
3	c	206	
4	d	205	

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Mol	Chain	Length	Quality of chain
5	e	150	
6	f	100	
7	g	151	
8	h	129	
9	i	127	
10	j	98	
11	k	117	
12	l	123	
13	m	114	
14	n	61	
15	o	88	
16	p	82	
17	q	80	
18	r	54	
19	s	79	
20	t	85	
21	u	51	
22	x	6	
23	y	77	
24	z	509	
25	A	2854	
26	E	201	
27	F	177	
28	G	117	
29	H	176	

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Mol	Chain	Length	Quality of chain
30	I	141	
31	J	142	
32	K	122	
33	L	143	
34	M	136	
35	N	120	
36	O	116	
37	P	114	
38	Q	117	
39	R	103	
40	S	110	
41	T	93	
42	U	102	
43	V	94	
44	X	118	
45	Y	38	
46	0	79	
47	1	77	
48	2	63	
49	3	58	
50	4	209	
51	5	56	
52	6	50	
53	7	46	
54	8	64	

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Mol	Chain	Length	Quality of chain
55	9	271	38% 91% 7%

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 146597 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	150	Total	C	N	O	S	0	0
			1106	687	211	202	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	61	Total	C	N	O	S	0	0
			500	310	108	80	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	54	Total	C	N	O	0	0
			445	282	83	80		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	51	Total	C	N	O	S	0	0
			426	265	86	74	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	x	6	Total	C	N	O	P	0	0
			126	58	24	39	5		

- Molecule 23 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	y	77	Total	C	N	O	P	0	0
			1639	732	297	534	76		

- Molecule 24 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	z	509	Total	C	N	O	S	0	0
			3847	2409	675	748	15		

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2854	Total	C	N	O	P	0	0
			61262	27334	11279	19799	2850		

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 28 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	117	Total	C	N	O	S	0	0
			885	559	157	164	5		

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

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

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	U	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	X	118	Total	C	N	O	P	0	0
			2526	1126	464	819	117		

- Molecule 45 is a protein called 50S ribosomal protein L36.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	0	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	4	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	6	50	Total	C	N	O	S	0	0
			410	263	75	72			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	7	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	8	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

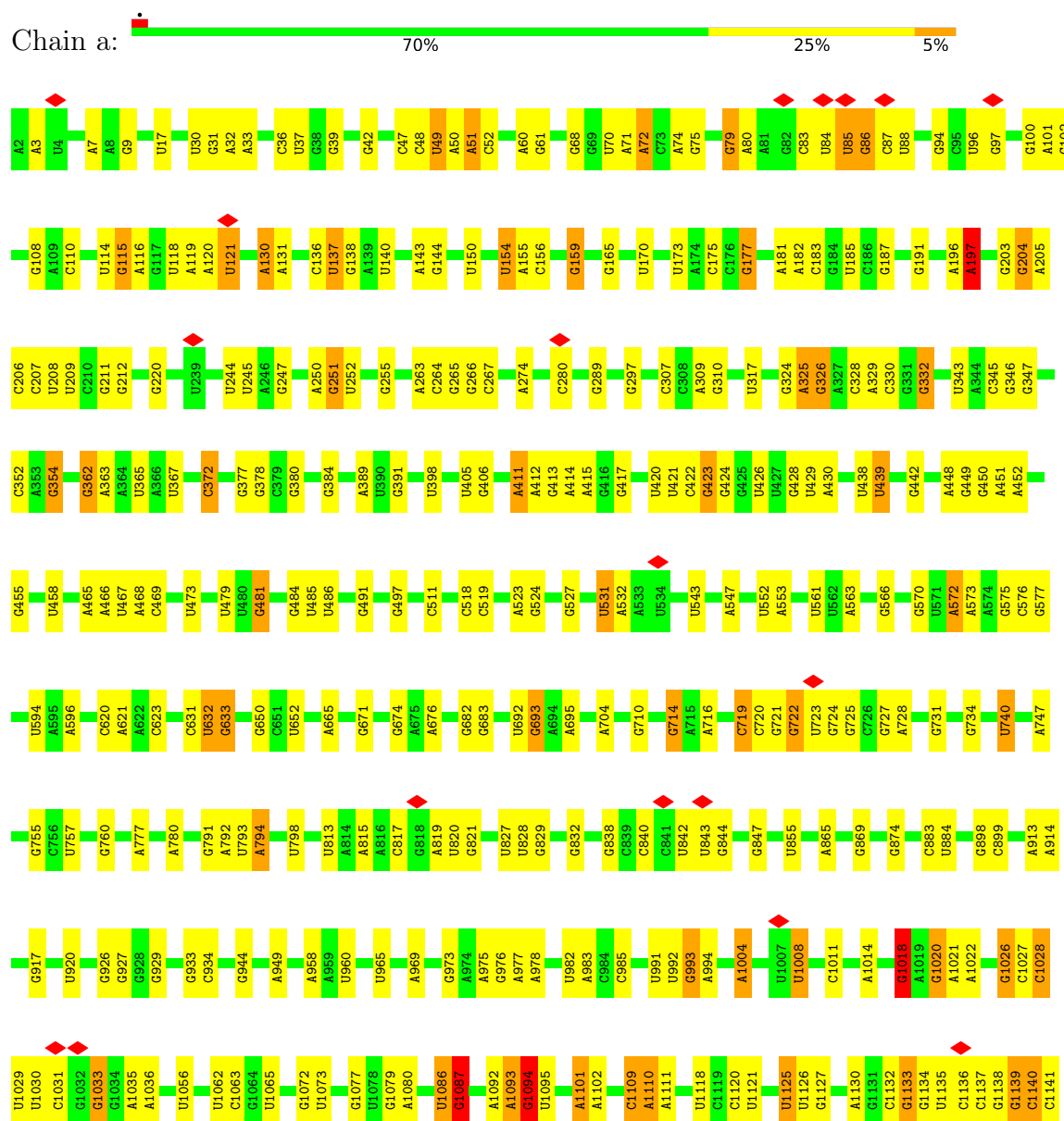
- Molecule 55 is a protein called 50S ribosomal protein L2.

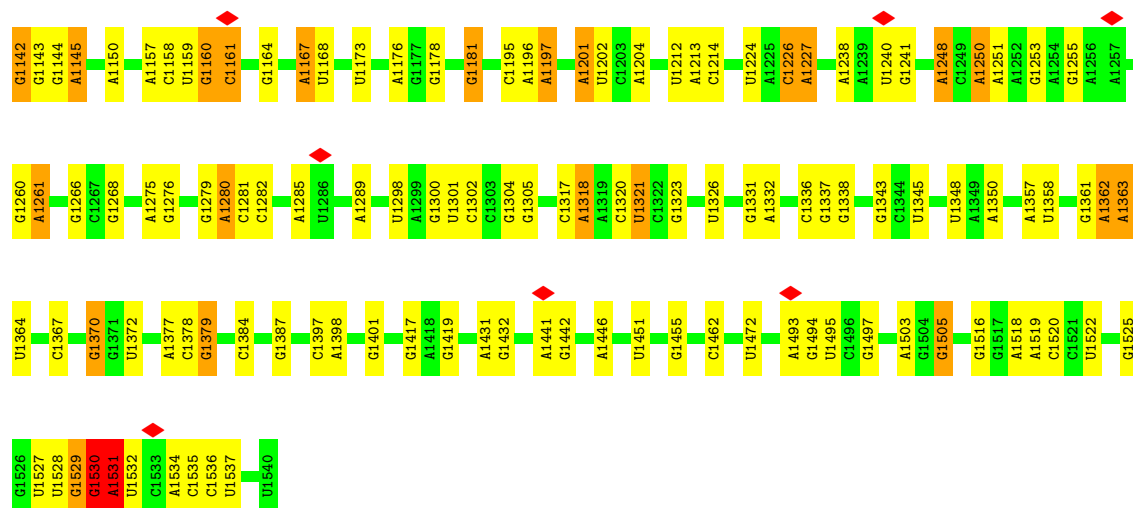
Mol	Chain	Residues	Atoms					AltConf	Trace
55	9	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

3 Residue-property plots

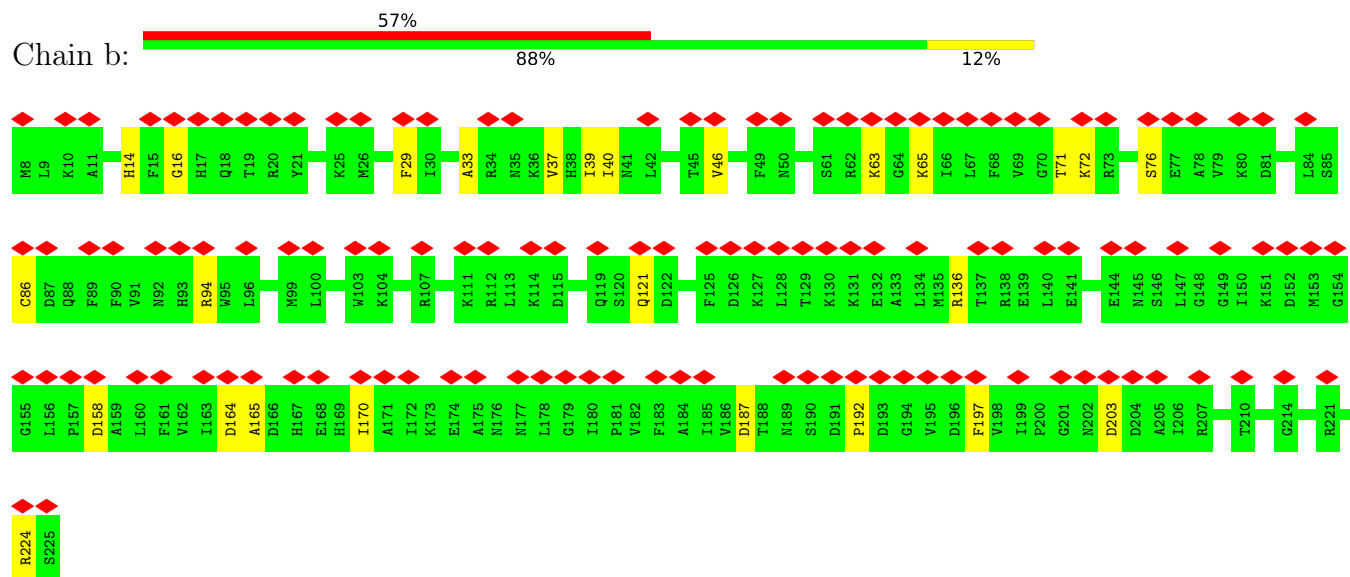
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

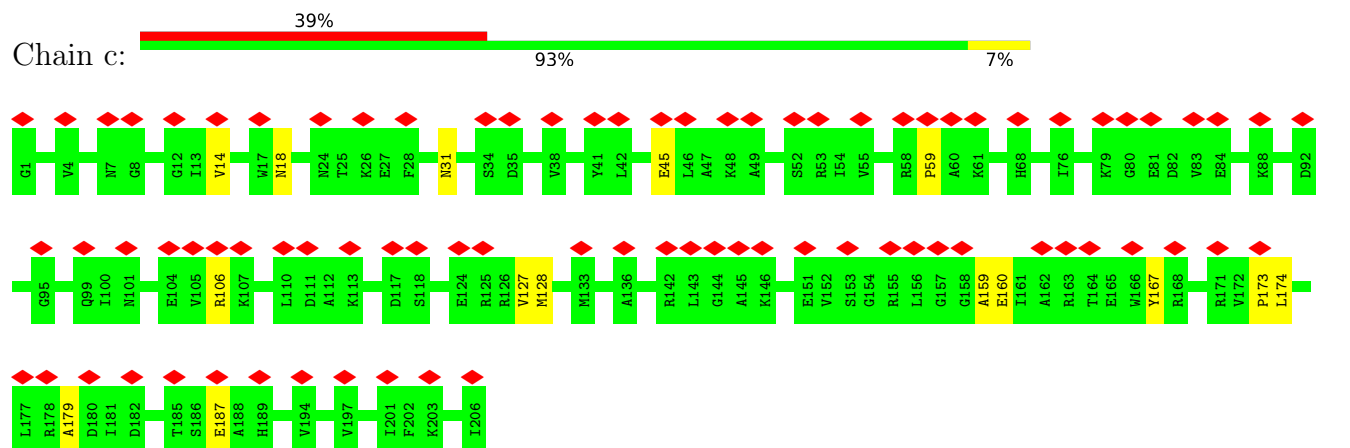




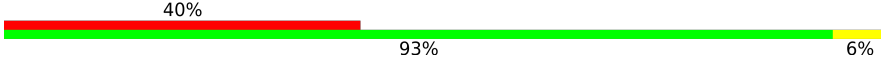
• Molecule 2: 30S ribosomal protein S2

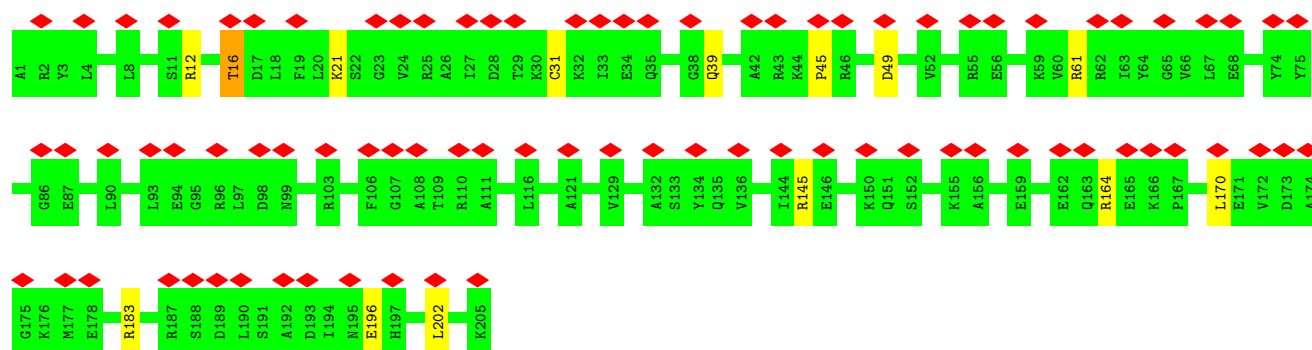


• Molecule 3: 30S ribosomal protein S3

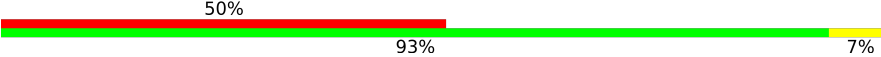


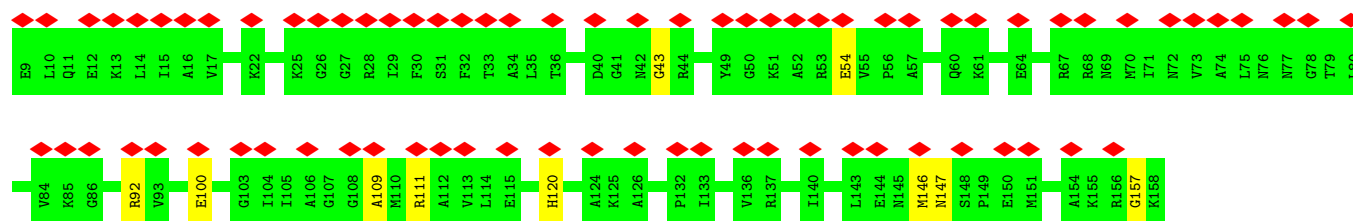
• Molecule 4: 30S ribosomal protein S4

Chain d: 



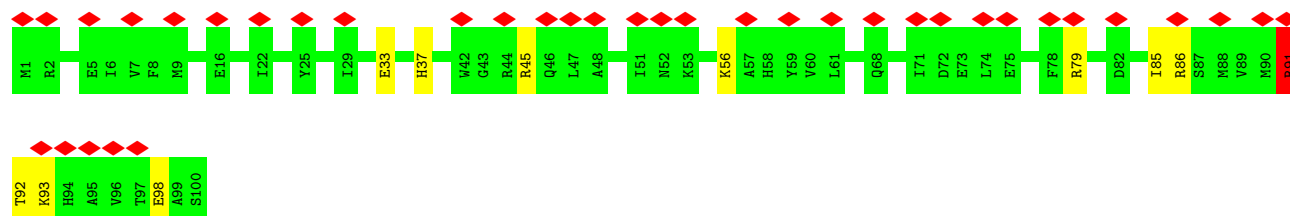
• Molecule 5: 30S ribosomal protein S5

Chain e: 

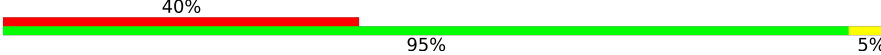


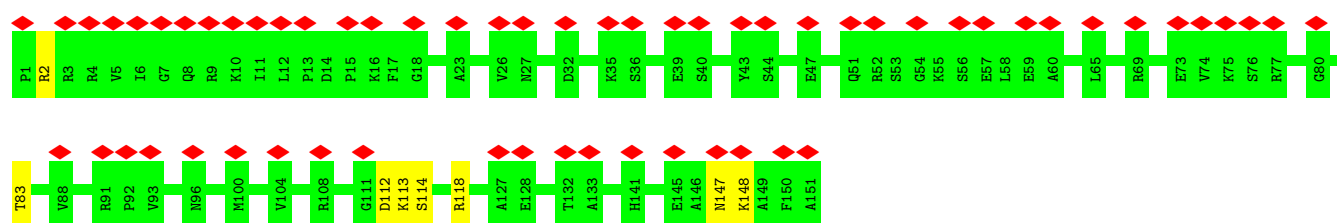
• Molecule 6: 30S ribosomal protein S6

Chain f: 

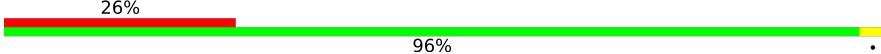


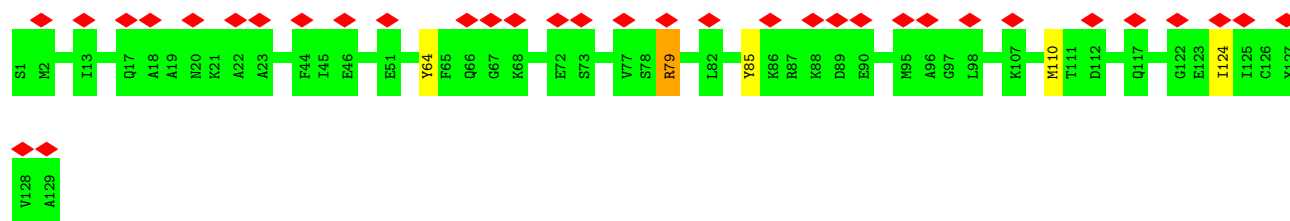
• Molecule 7: 30S ribosomal protein S7

Chain g: 

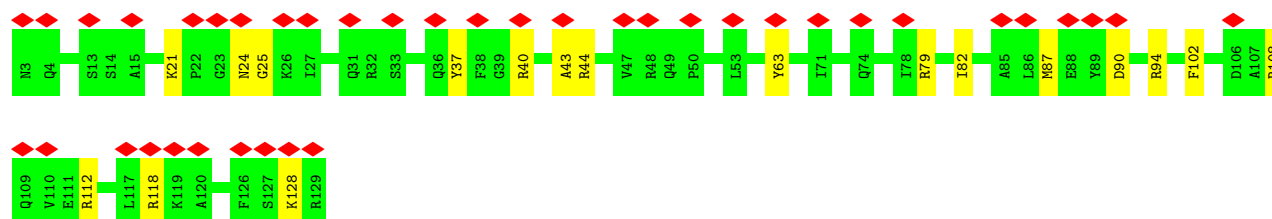
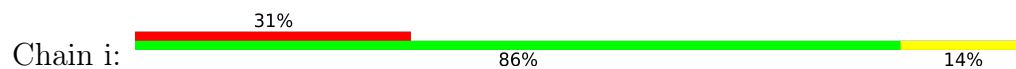


• Molecule 8: 30S ribosomal protein S8

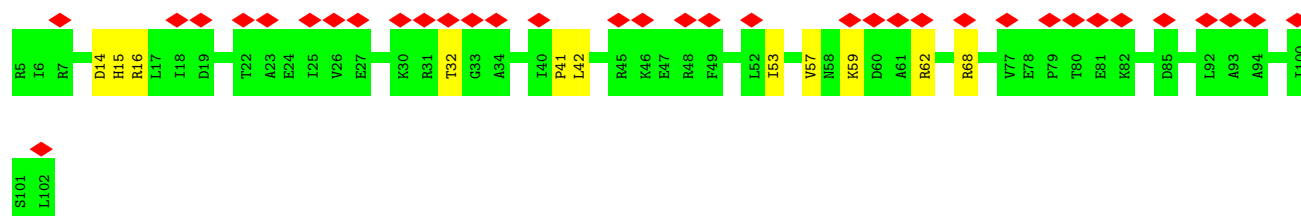
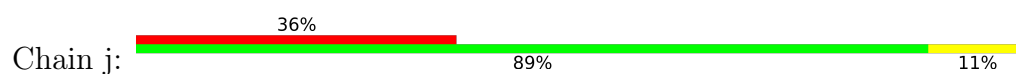
Chain h: 



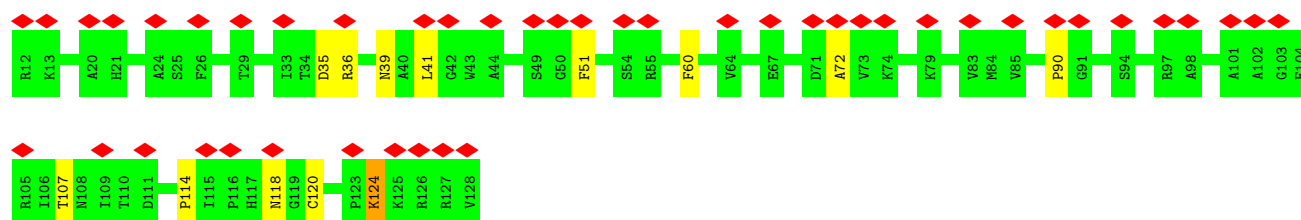
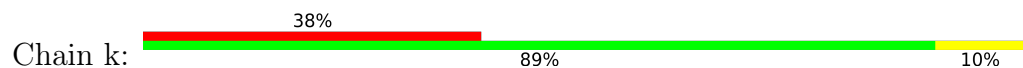
• Molecule 9: 30S ribosomal protein S9



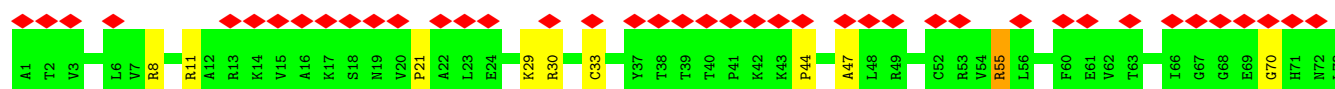
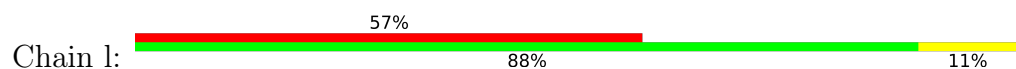
• Molecule 10: 30S ribosomal protein S10

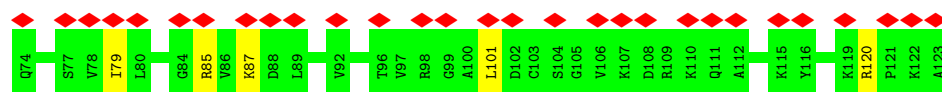


• Molecule 11: 30S ribosomal protein S11

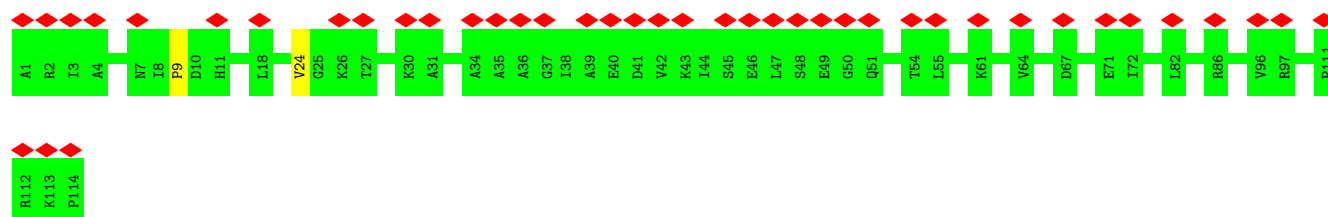


• Molecule 12: 30S ribosomal protein S12

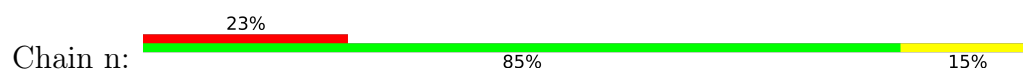




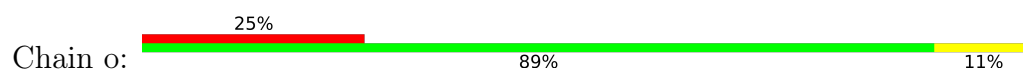
• Molecule 13: 30S ribosomal protein S13



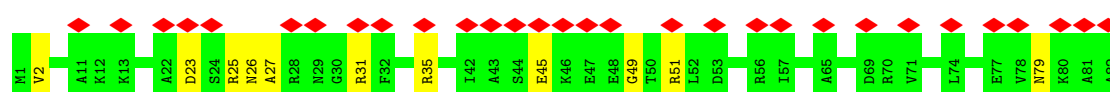
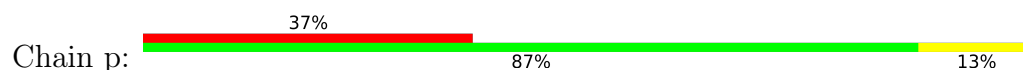
• Molecule 14: 30S ribosomal protein S14



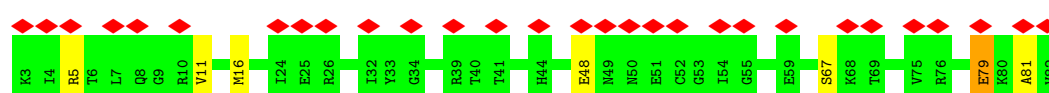
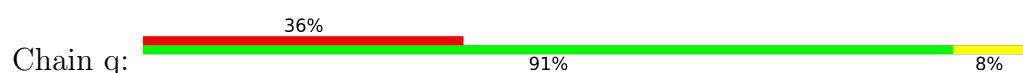
• Molecule 15: 30S ribosomal protein S15



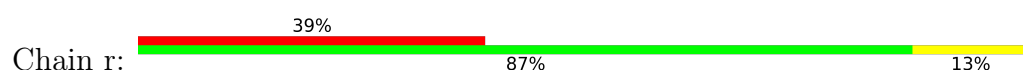
• Molecule 16: 30S ribosomal protein S16

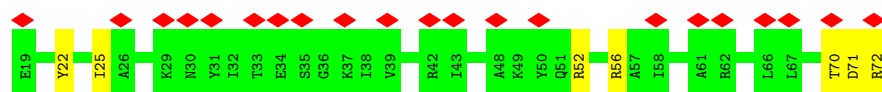


• Molecule 17: 30S ribosomal protein S17

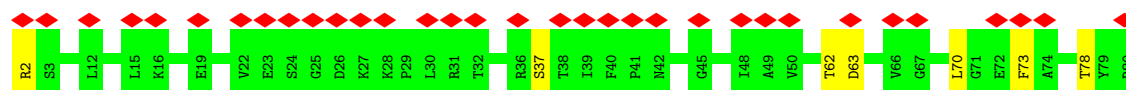
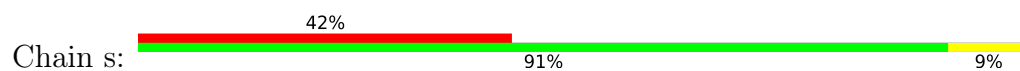


• Molecule 18: 30S ribosomal protein S18

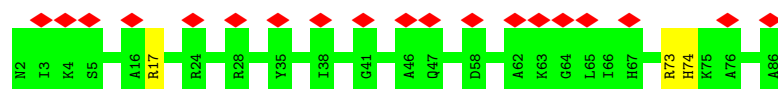




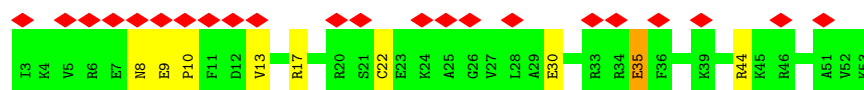
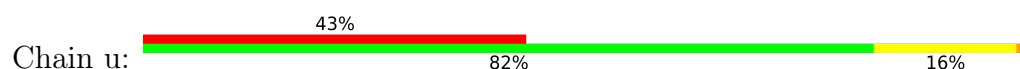
- Molecule 19: 30S ribosomal protein S19



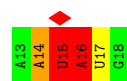
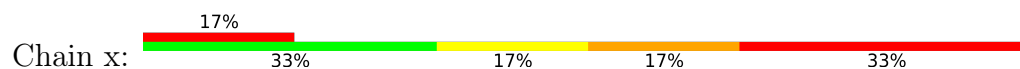
- Molecule 20: 30S ribosomal protein S20



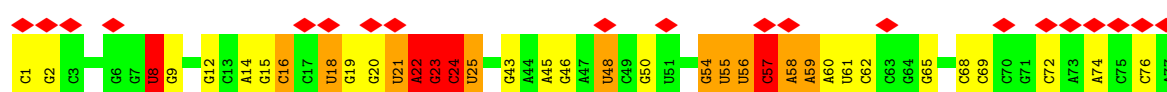
- Molecule 21: 30S ribosomal protein S21



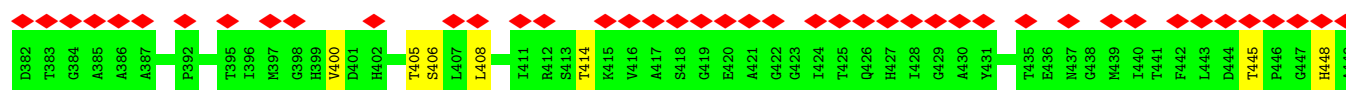
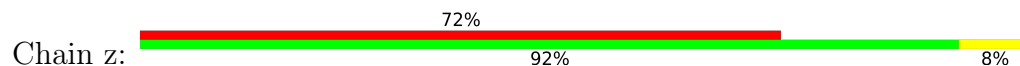
- Molecule 22: mRNA

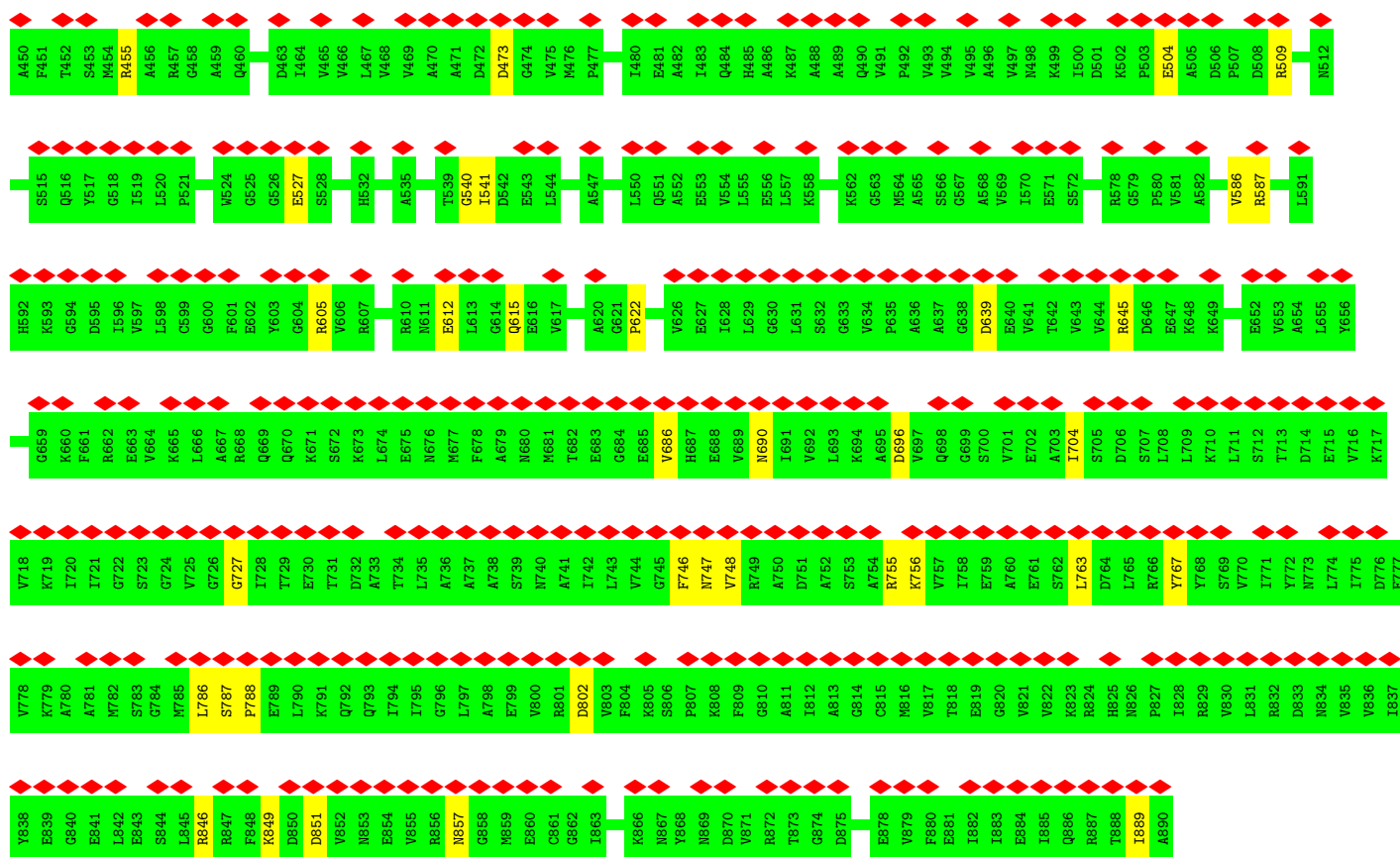


- Molecule 23: tRNA



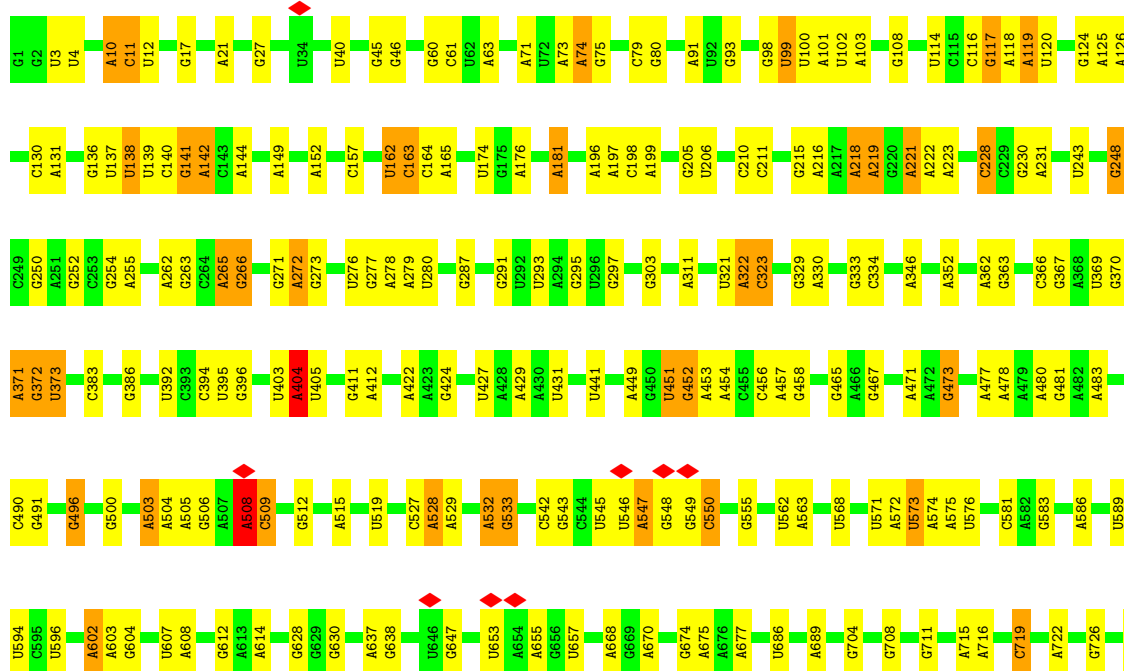
- Molecule 24: Translation initiation factor IF-2

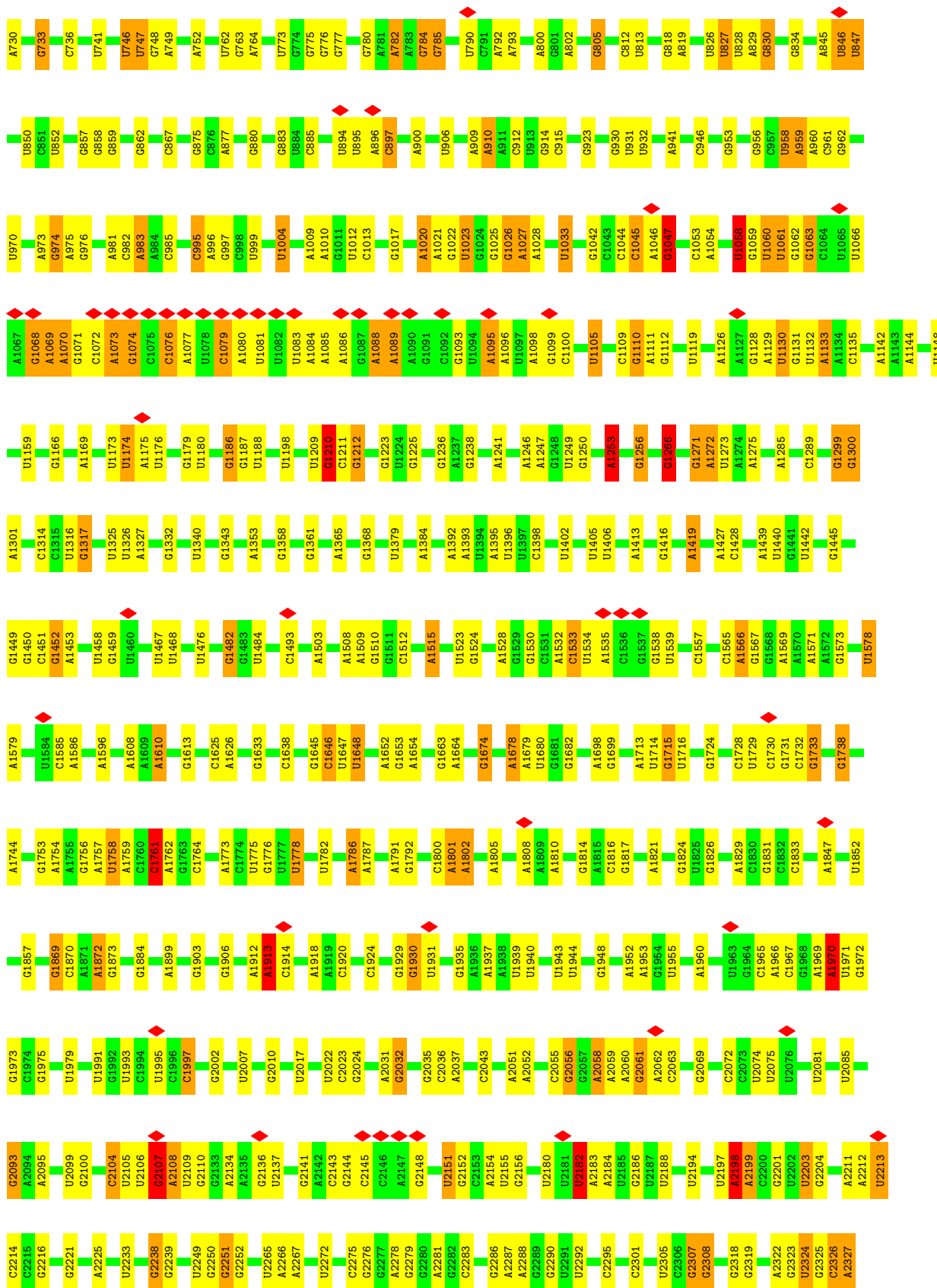


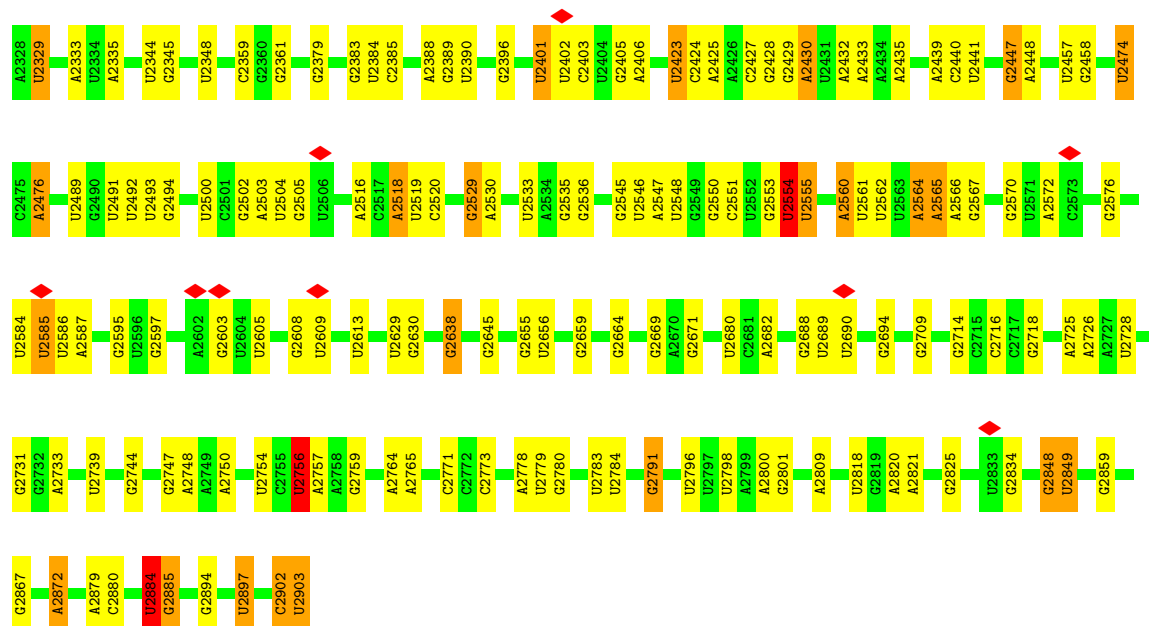


• Molecule 25: 23S rRNA

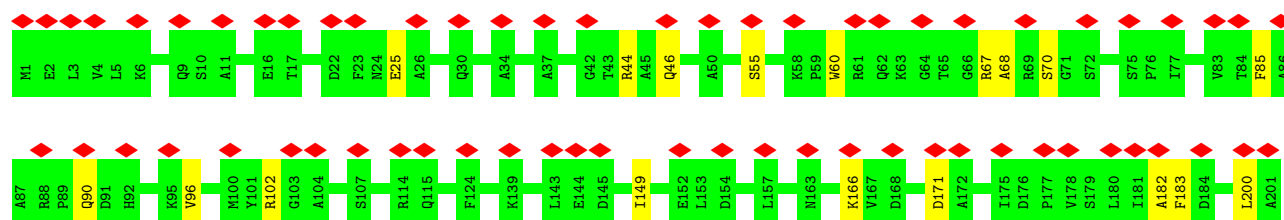
Chain A: 69% 25% 5%



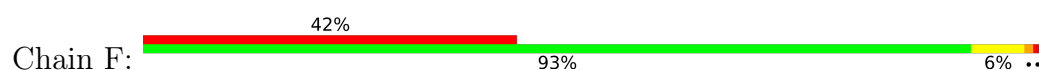




• Molecule 26: 50S ribosomal protein L4



• Molecule 27: 50S ribosomal protein L5

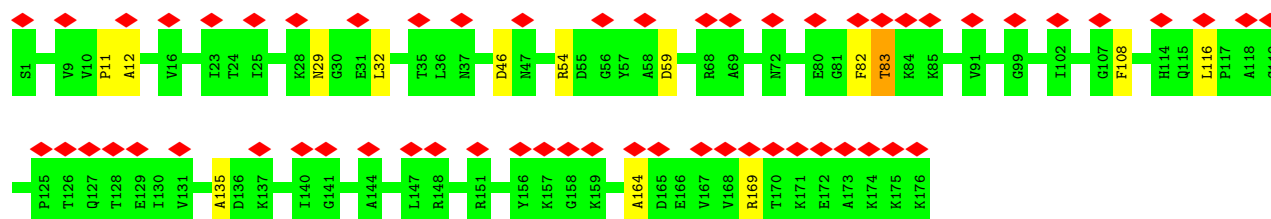


• Molecule 28: 50S ribosomal protein L10

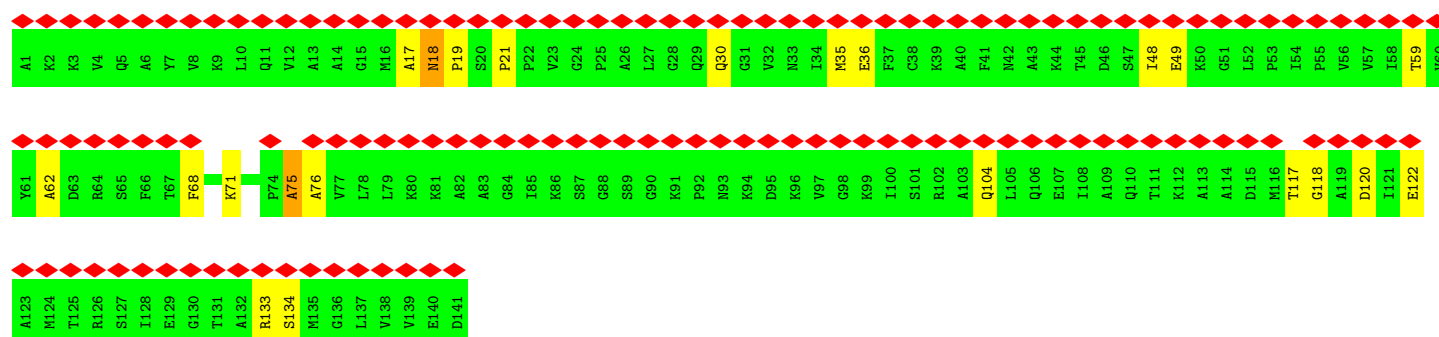
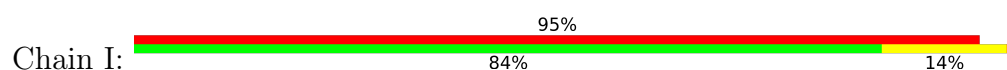




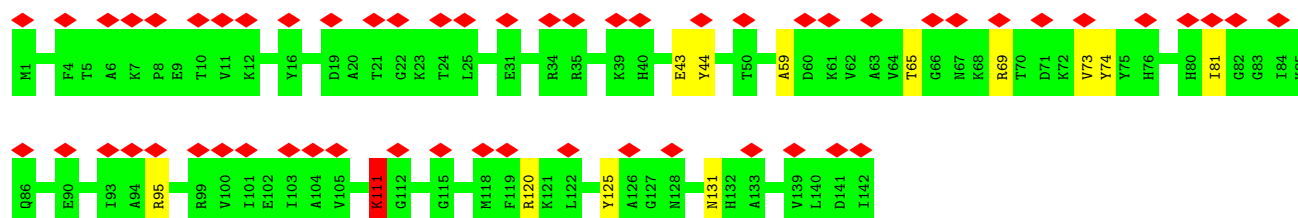
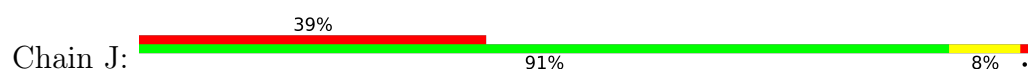
• Molecule 29: 50S ribosomal protein L6



• Molecule 30: 50S ribosomal protein L11

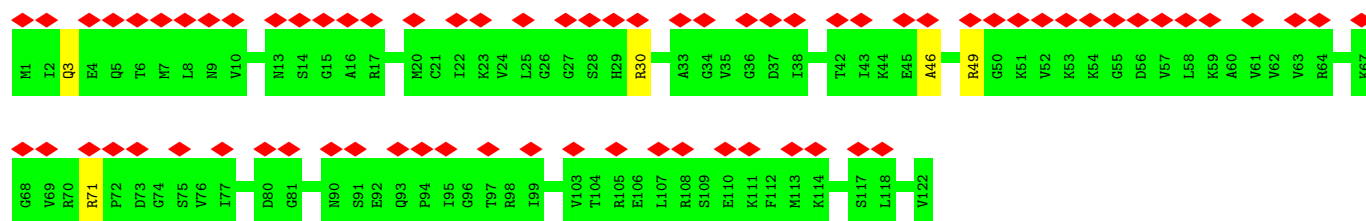


• Molecule 31: 50S ribosomal protein L13

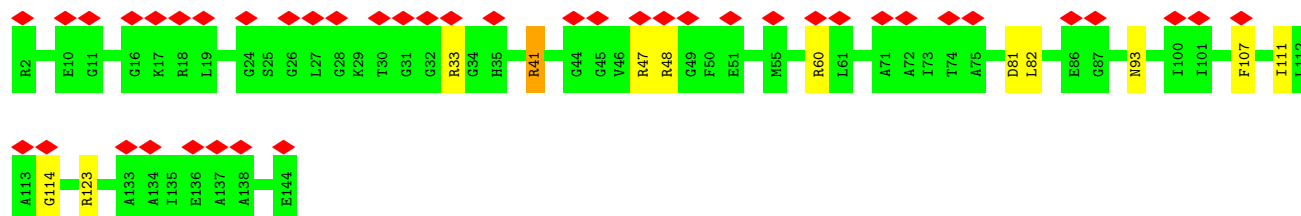
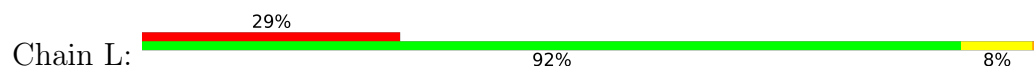


• Molecule 32: 50S ribosomal protein L14

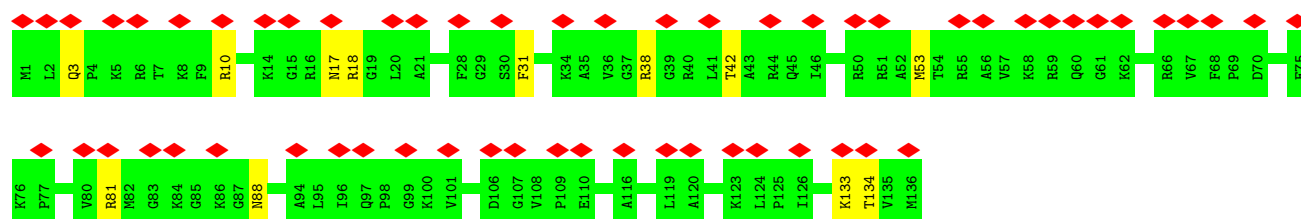
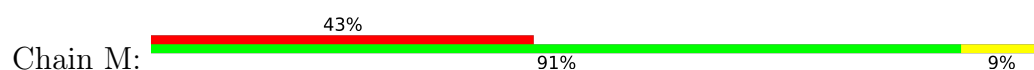




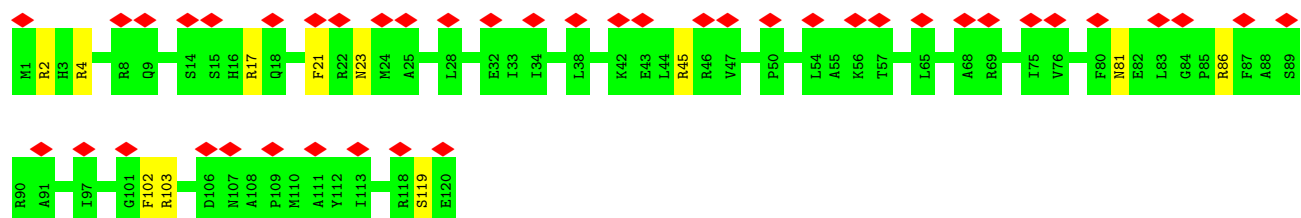
• Molecule 33: 50S ribosomal protein L15



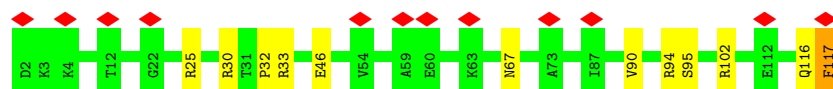
• Molecule 34: 50S ribosomal protein L16



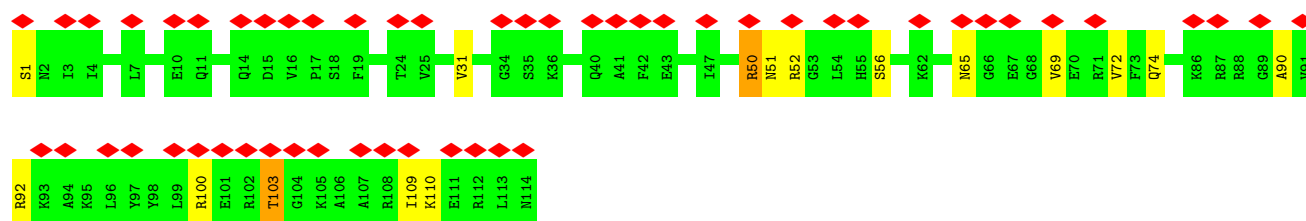
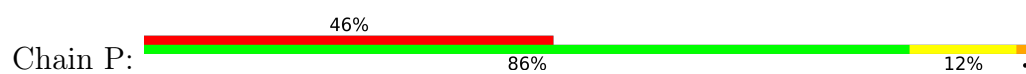
• Molecule 35: 50S ribosomal protein L17



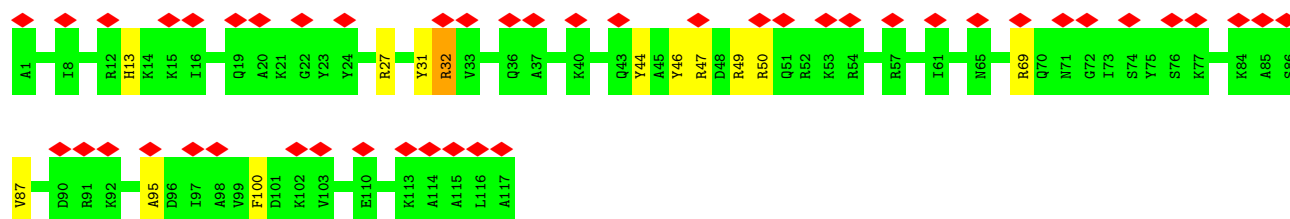
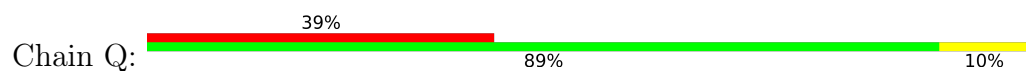
• Molecule 36: 50S ribosomal protein L18



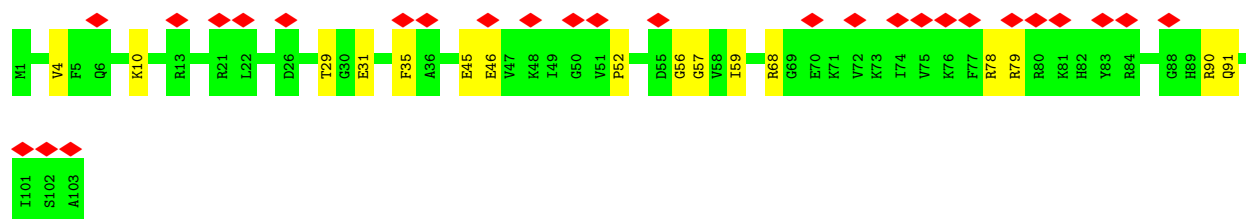
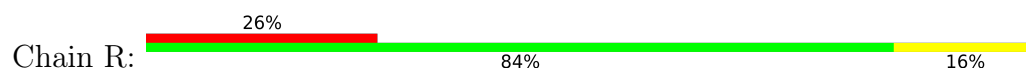
• Molecule 37: 50S ribosomal protein L19



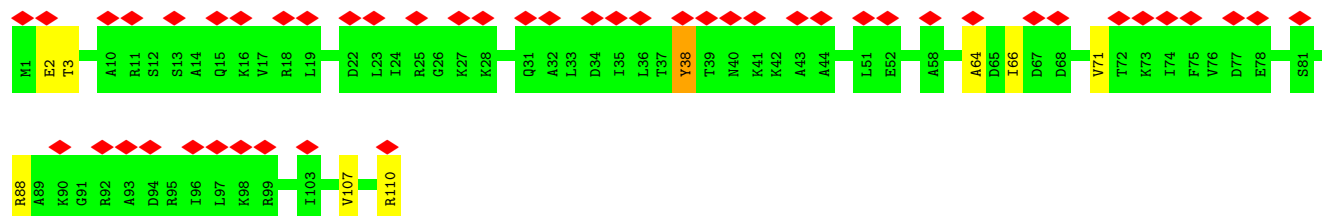
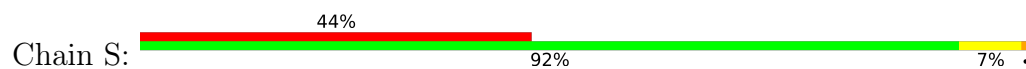
- Molecule 38: 50S ribosomal protein L20



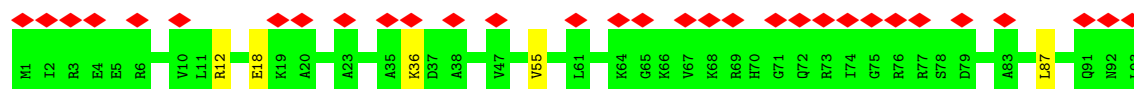
- Molecule 39: 50S ribosomal protein L21



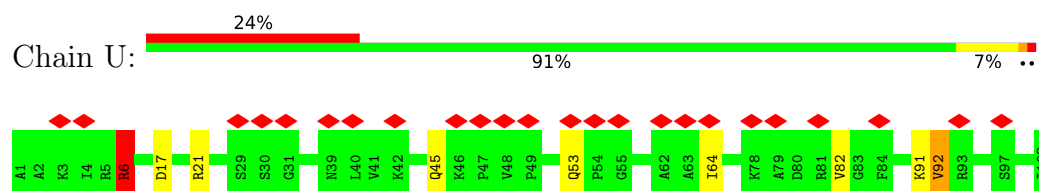
- Molecule 40: 50S ribosomal protein L22



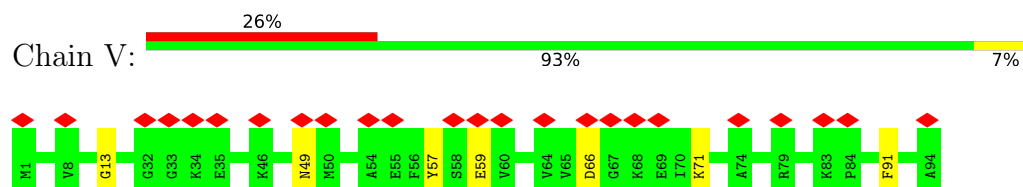
- Molecule 41: 50S ribosomal protein L23



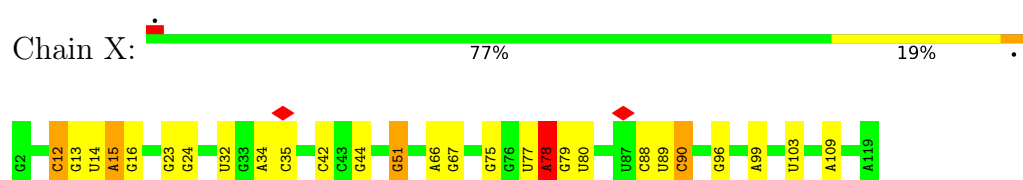
- Molecule 42: 50S ribosomal protein L24



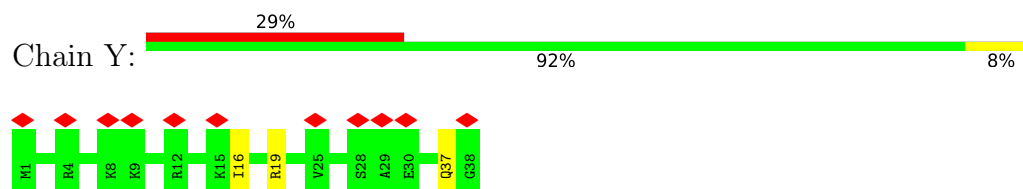
- Molecule 43: 50S ribosomal protein L25



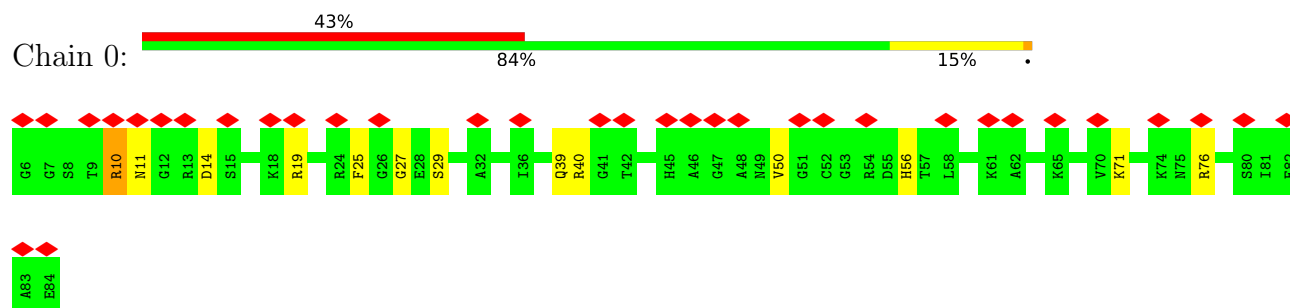
- Molecule 44: 5S rRNA



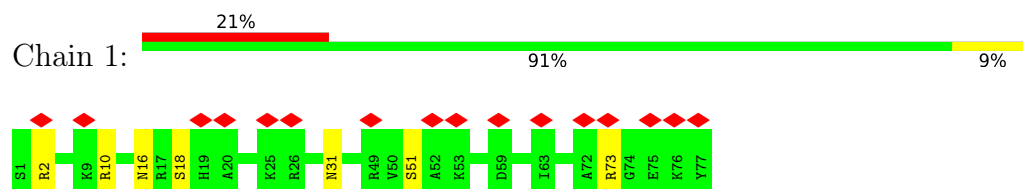
- Molecule 45: 50S ribosomal protein L36



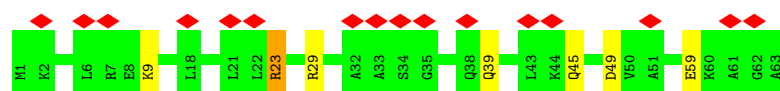
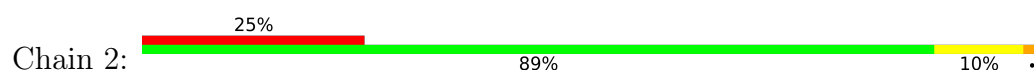
- Molecule 46: 50S ribosomal protein L27



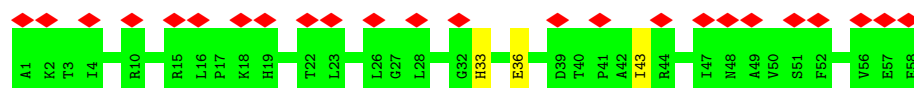
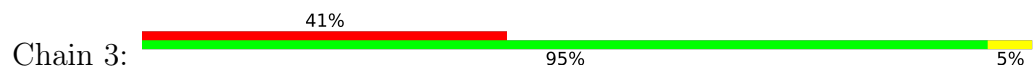
- Molecule 47: 50S ribosomal protein L28



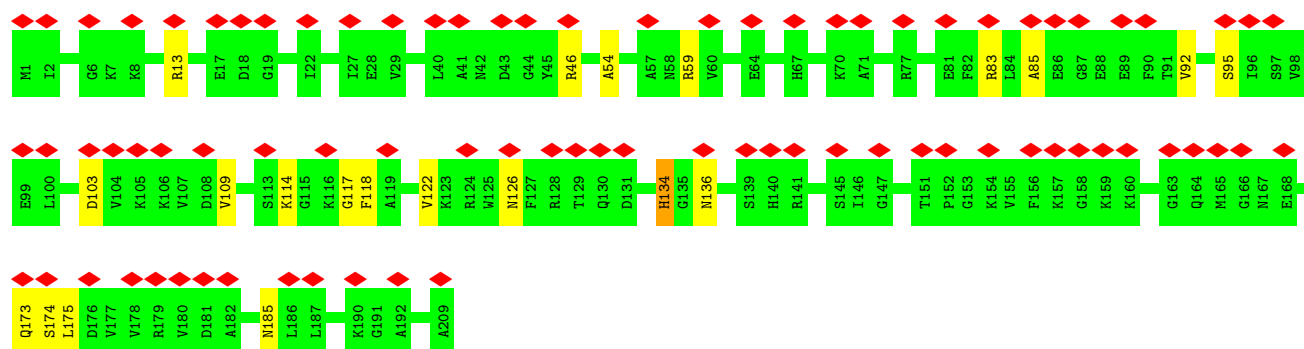
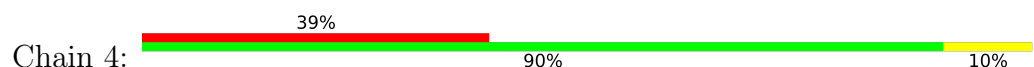
- Molecule 48: 50S ribosomal protein L29



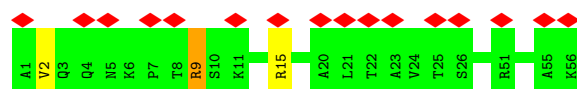
- Molecule 49: 50S ribosomal protein L30



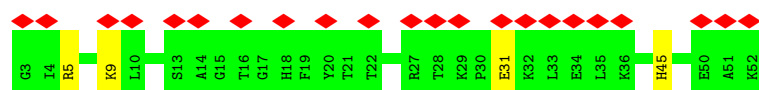
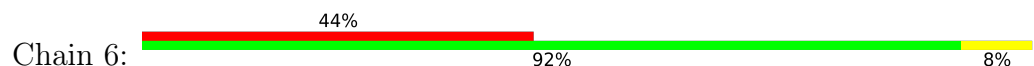
- Molecule 50: 50S ribosomal protein L3



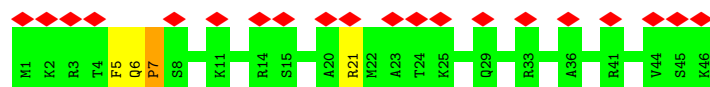
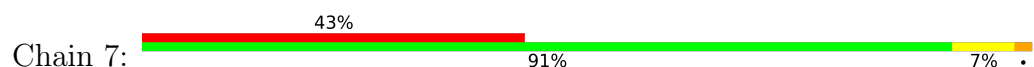
- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33

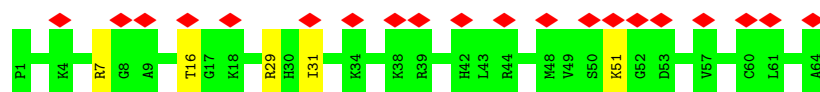


- Molecule 53: 50S ribosomal protein L34



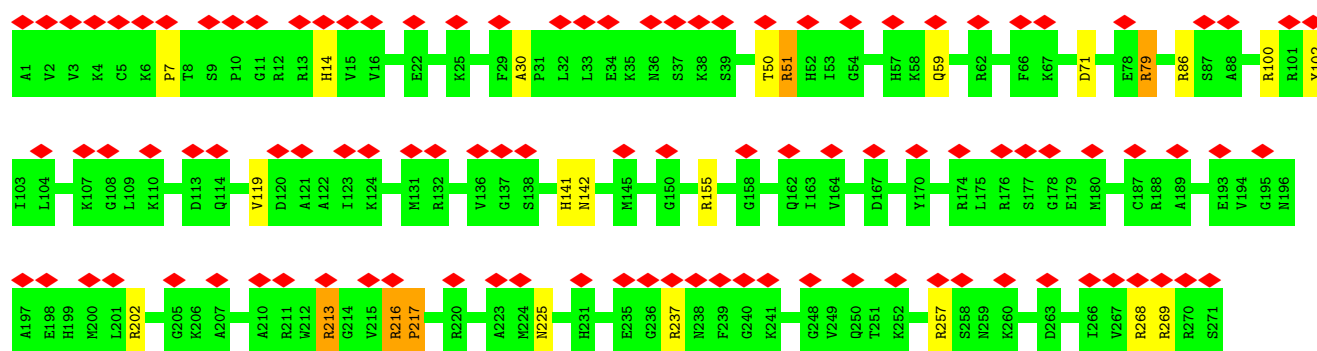
- Molecule 54: 50S ribosomal protein L35

Chain 8: 



- Molecule 55: 50S ribosomal protein L2

Chain 9: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34096	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 ($e^-/\text{\AA}^2$)	35	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	0.167	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.04	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	0.95	1/36963 (0.0%)	1.15	94/57662 (0.2%)
2	b	0.86	0/1736	1.55	13/2338 (0.6%)
3	c	0.85	0/1652	1.42	6/2225 (0.3%)
4	d	0.86	0/1665	1.40	6/2227 (0.3%)
5	e	0.87	0/1119	1.42	5/1504 (0.3%)
6	f	0.88	0/836	1.52	3/1128 (0.3%)
7	g	0.85	0/1196	1.47	2/1602 (0.1%)
8	h	0.85	0/989	1.35	2/1326 (0.2%)
9	i	0.88	0/1034	1.47	7/1375 (0.5%)
10	j	0.90	0/797	1.55	5/1077 (0.5%)
11	k	0.87	0/893	1.50	5/1205 (0.4%)
12	l	0.86	0/969	1.39	2/1300 (0.2%)
13	m	0.87	0/893	1.52	0/1193
14	n	0.88	0/510	1.50	4/679 (0.6%)
15	o	0.92	0/722	1.49	5/964 (0.5%)
16	p	0.89	0/659	1.52	5/884 (0.6%)
17	q	0.86	0/658	1.41	1/881 (0.1%)
18	r	0.86	0/451	1.48	1/606 (0.2%)
19	s	0.85	0/653	1.60	7/877 (0.8%)
20	t	0.89	0/671	1.42	1/888 (0.1%)
21	u	0.91	0/431	1.56	3/570 (0.5%)
22	x	1.19	0/141	1.99	5/218 (2.3%)
23	y	1.01	0/1831	1.32	21/2853 (0.7%)
24	z	0.83	0/3895	1.45	15/5264 (0.3%)
25	A	0.96	1/68614 (0.0%)	1.15	216/107040 (0.2%)
26	E	0.84	0/1571	1.44	8/2113 (0.4%)
27	F	0.84	0/1435	1.45	9/1926 (0.5%)
28	G	0.87	0/896	1.60	3/1203 (0.2%)
29	H	0.85	0/1343	1.44	7/1816 (0.4%)
30	I	0.85	0/1046	1.58	8/1410 (0.6%)
31	J	0.88	0/1152	1.52	4/1551 (0.3%)
32	K	0.86	0/948	1.36	0/1268
33	L	0.86	0/1054	1.47	8/1403 (0.6%)
34	M	0.86	0/1093	1.46	6/1460 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	N	0.86	0/974	1.57	7/1301 (0.5%)
36	O	0.89	0/902	1.43	2/1209 (0.2%)
37	P	0.86	0/929	1.53	5/1242 (0.4%)
38	Q	0.88	0/960	1.48	6/1278 (0.5%)
39	R	0.87	0/829	1.58	11/1107 (1.0%)
40	S	0.87	0/864	1.56	6/1156 (0.5%)
41	T	0.89	0/745	1.40	0/994
42	U	0.83	0/788	1.49	5/1051 (0.5%)
43	V	0.85	0/766	1.41	2/1025 (0.2%)
44	X	0.97	0/2825	1.14	6/4406 (0.1%)
45	Y	0.94	0/303	1.48	0/397
46	0	0.91	0/603	1.60	3/797 (0.4%)
47	1	0.91	0/635	1.52	4/848 (0.5%)
48	2	0.87	0/510	1.38	1/677 (0.1%)
49	3	0.90	0/453	1.55	0/605
50	4	0.86	0/1586	1.49	5/2134 (0.2%)
51	5	0.89	0/450	1.56	1/599 (0.2%)
52	6	0.87	0/417	1.37	1/554 (0.2%)
53	7	0.93	0/380	1.63	0/498
54	8	0.88	0/513	1.52	4/676 (0.6%)
55	9	0.85	0/2122	1.47	9/2852 (0.3%)
All	All	0.93	2/159070 (0.0%)	1.25	565/237442 (0.2%)

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
1	a	0	228
2	b	0	2
3	c	0	1
4	d	0	5
5	e	0	2
6	f	0	3
7	g	0	2
8	h	0	3
9	i	0	7
10	j	0	3
11	k	0	2
12	l	0	6
14	n	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
15	o	0	1
16	p	0	2
18	r	0	4
19	s	0	1
20	t	0	2
21	u	0	2
22	x	0	2
23	y	0	18
24	z	0	7
25	A	0	434
26	E	0	1
27	F	0	3
28	G	0	3
29	H	0	1
30	I	0	5
31	J	0	5
32	K	0	2
33	L	0	2
34	M	0	3
35	N	0	4
36	O	0	3
37	P	0	6
38	Q	0	7
39	R	0	2
40	S	0	3
42	U	0	2
43	V	0	2
44	X	0	12
45	Y	0	1
46	0	0	3
47	1	0	3
48	2	0	2
50	4	0	3
51	5	0	1
52	6	0	1
53	7	0	2
54	8	0	2
55	9	0	12
All	All	0	834

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	426	U	O3'-P	-5.27	1.53	1.61
25	A	996	A	O3'-P	-5.16	1.53	1.61

All (565) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	x	14	A	P-O3'-C3'	12.72	139.28	120.20
23	y	8	U	P-O3'-C3'	12.61	139.11	120.20
25	A	1728	C	P-O3'-C3'	11.30	137.15	120.20
1	a	96	U	P-O3'-C3'	10.91	136.56	120.20
25	A	1061	U	P-O3'-C3'	10.85	136.47	120.20
23	y	58	A	P-O3'-C3'	10.77	136.35	120.20
25	A	1069	A	P-O3'-C3'	10.50	135.95	120.20
22	x	16	A	P-O5'-C5'	10.15	136.13	120.90
25	A	1566	A	P-O3'-C3'	9.89	135.04	120.20
25	A	372	G	P-O3'-C3'	9.83	134.94	120.20
25	A	2182	U	P-O5'-C5'	9.64	135.36	120.90
31	J	73	VAL	N-CA-C	9.62	120.43	110.72
44	X	12	C	P-O3'-C3'	9.26	134.09	120.20
25	A	846	U	P-O3'-C3'	9.21	134.01	120.20
1	a	1337	G	P-O3'-C3'	9.07	133.80	120.20
23	y	57	C	P-O3'-C3'	9.01	133.71	120.20
25	A	99	U	P-O3'-C3'	8.93	133.59	120.20
25	A	2585	U	P-O3'-C3'	8.77	133.36	120.20
25	A	2902	C	P-O3'-C3'	8.73	133.30	120.20
23	y	1	C	P-O3'-C3'	8.53	132.99	120.20
24	z	540	GLY	CA-C-N	8.48	136.97	121.70
24	z	540	GLY	C-N-CA	8.48	136.97	121.70
42	U	82	VAL	CA-C-N	8.36	127.34	121.65
42	U	82	VAL	C-N-CA	8.36	127.34	121.65
25	A	958	U	P-O3'-C3'	8.23	132.55	120.20
25	A	352	A	C5'-C4'-C3'	-8.13	103.80	116.00
25	A	995	C	P-O5'-C5'	8.13	133.10	120.90
1	a	1201	A	P-O3'-C3'	8.10	132.35	120.20
25	A	2585	U	C2'-C3'-O3'	8.07	121.60	109.50
11	k	35	ASP	CA-C-N	8.06	132.15	120.38
11	k	35	ASP	C-N-CA	8.06	132.15	120.38
25	A	1095	A	P-O3'-C3'	8.04	132.27	120.20
25	A	503	A	P-O3'-C3'	8.01	132.22	120.20
35	N	102	PHE	CA-CB-CG	-8.00	105.80	113.80
25	A	137	U	P-O3'-C3'	-8.00	108.21	120.20
25	A	2198	A	P-O3'-C3'	7.99	132.19	120.20
25	A	119	A	C2'-C3'-O3'	7.99	121.48	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1069	A	C2'-C3'-O3'	7.94	121.41	109.50
25	A	404	A	P-O3'-C3'	7.86	131.99	120.20
25	A	2199	A	C5'-C4'-C3'	-7.85	104.23	116.00
1	a	723	U	P-O3'-C3'	-7.79	108.51	120.20
38	Q	100	PHE	CA-CB-CG	-7.78	106.02	113.80
38	Q	32	ARG	NE-CZ-NH2	7.69	126.12	119.20
25	A	746	U	P-O3'-C3'	7.65	131.67	120.20
23	y	23	G	C2'-C3'-O3'	7.64	120.96	109.50
26	E	55	SER	N-CA-C	7.57	120.08	110.24
1	a	458	U	C5'-C4'-C3'	-7.54	104.69	116.00
10	j	59	LYS	CA-C-N	7.54	130.38	120.28
10	j	59	LYS	C-N-CA	7.54	130.38	120.28
25	A	119	A	P-O3'-C3'	7.54	131.50	120.20
23	y	15	G	P-O3'-C3'	7.49	131.44	120.20
22	x	15	U	P-O3'-C3'	-7.48	108.98	120.20
55	9	14	HIS	CA-CB-CG	-7.43	106.37	113.80
2	b	187	ASP	CA-C-N	7.41	130.20	120.28
2	b	187	ASP	C-N-CA	7.41	130.20	120.28
23	y	22	A	O4'-C1'-C2'	-7.41	98.39	105.80
25	A	2401	U	P-O3'-C3'	7.39	131.29	120.20
25	A	547	A	O4'-C1'-C2'	-7.36	100.24	107.60
35	N	81	ASN	CA-CB-CG	-7.35	105.25	112.60
25	A	1076	C	P-O3'-C3'	7.31	131.16	120.20
25	A	894	U	P-O5'-C5'	7.31	131.86	120.90
1	a	1280	A	C5'-C4'-C3'	-7.30	104.25	115.20
25	A	1061	U	C2'-C3'-O3'	7.30	120.44	109.50
25	A	1678	A	P-O3'-C3'	7.29	131.13	120.20
33	L	60	ARG	NE-CZ-NH2	7.28	125.75	119.20
19	s	63	ASP	N-CA-C	7.27	118.85	111.07
25	A	163	C	P-O3'-C3'	7.24	131.07	120.20
23	y	21	U	P-O3'-C3'	7.24	131.06	120.20
4	d	21	LYS	CA-C-N	7.21	129.94	120.28
4	d	21	LYS	C-N-CA	7.21	129.94	120.28
25	A	1045	C	P-O3'-C3'	7.19	130.99	120.20
25	A	2251	G	P-O3'-C3'	7.19	130.99	120.20
1	a	1361	G	C5'-C4'-C3'	-7.18	105.24	116.00
25	A	547	A	C4'-C3'-C2'	-7.16	95.44	102.60
22	x	15	U	C5'-C4'-C3'	-7.15	105.28	116.00
34	M	133	LYS	N-CA-C	7.12	118.69	111.07
25	A	1169	A	C5'-C4'-C3'	-7.11	105.34	116.00
1	a	85	U	P-O3'-C3'	7.06	130.79	120.20
6	f	92	THR	N-CA-C	7.06	118.62	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1301	U	P-O5'-C5'	-6.99	110.42	120.90
28	G	7	ASP	N-CA-C	6.97	118.95	111.36
25	A	1093	G	P-O5'-C5'	6.95	131.33	120.90
37	P	51	ASN	CA-C-N	6.90	134.73	121.54
37	P	51	ASN	C-N-CA	6.90	134.73	121.54
1	a	1248	A	C2'-C3'-O3'	6.88	119.82	109.50
25	A	1538	G	P-O5'-C5'	6.88	131.22	120.90
25	A	322	A	P-O3'-C3'	6.85	130.48	120.20
1	a	1109	C	P-O3'-C3'	6.83	130.45	120.20
30	I	35	MET	N-CA-C	6.82	119.55	111.71
25	A	827	U	C4'-C3'-C2'	-6.79	95.81	102.60
25	A	1111	A	P-O3'-C3'	6.77	130.36	120.20
55	9	51	ARG	NE-CZ-NH1	-6.76	114.74	121.50
2	b	197	PHE	CA-CB-CG	-6.75	107.05	113.80
23	y	8	U	C5'-C4'-C3'	6.74	126.11	116.00
25	A	218	A	P-O3'-C3'	6.74	130.30	120.20
52	6	45	HIS	CA-CB-CG	-6.74	107.06	113.80
25	A	2560	A	P-O3'-C3'	6.72	130.28	120.20
10	j	14	ASP	CA-C-N	6.71	129.94	120.28
10	j	14	ASP	C-N-CA	6.71	129.94	120.28
23	y	24	C	C2'-C3'-O3'	6.70	119.55	109.50
39	R	45	GLU	CA-C-N	6.69	130.38	120.87
39	R	45	GLU	C-N-CA	6.69	130.38	120.87
25	A	1413	A	C5'-C4'-C3'	-6.68	105.98	116.00
2	b	63	LYS	CA-C-N	6.60	126.37	120.10
2	b	63	LYS	C-N-CA	6.60	126.37	120.10
25	A	1452	G	P-O5'-C5'	6.60	130.79	120.90
25	A	163	C	C2'-C3'-O3'	6.57	119.36	109.50
19	s	62	THR	CA-C-N	6.55	128.96	120.44
19	s	62	THR	C-N-CA	6.55	128.96	120.44
23	y	54	G	C5'-C4'-C3'	-6.55	106.17	116.00
23	y	16	C	P-O5'-C5'	6.55	130.72	120.90
23	y	8	U	C4'-C3'-C2'	-6.54	96.06	102.60
25	A	452	G	P-O3'-C3'	6.54	130.02	120.20
25	A	1761	C	P-O3'-C3'	6.54	130.01	120.20
25	A	2107	G	C2'-C3'-O3'	6.54	119.30	109.50
1	a	130	A	P-O3'-C3'	6.53	130.00	120.20
44	X	78	A	P-O3'-C3'	6.53	129.99	120.20
5	e	147	ASN	CA-CB-CG	-6.52	106.08	112.60
2	b	29	PHE	CA-CB-CG	-6.52	107.28	113.80
1	a	1101	A	P-O3'-C3'	6.50	129.95	120.20
25	A	1004	U	P-O3'-C3'	-6.48	110.48	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	86	G	P-O3'-C3'	6.47	129.91	120.20
25	A	1960	A	C5'-C4'-C3'	-6.46	106.30	116.00
26	E	85	PHE	CA-CB-CG	-6.42	107.38	113.80
25	A	1074	G	C5'-C4'-C3'	-6.42	106.37	116.00
25	A	1060	U	C2'-C3'-O3'	6.41	119.12	109.50
1	a	1535	C	P-O3'-C3'	6.41	129.81	120.20
25	A	1512	C	C5'-C4'-C3'	-6.40	106.41	116.00
16	p	26	ASN	CA-CB-CG	-6.39	106.21	112.60
29	H	135	ALA	N-CA-C	6.39	118.25	111.28
55	9	51	ARG	NE-CZ-NH2	6.39	124.95	119.20
25	A	2326	C	P-O3'-C3'	6.38	129.77	120.20
25	A	2554	U	P-O3'-C3'	6.37	129.75	120.20
1	a	1462	C	C5'-C4'-C3'	-6.37	106.45	116.00
51	5	15	ARG	NE-CZ-NH2	6.37	124.93	119.20
40	S	66	ILE	CA-C-N	6.36	128.81	120.28
40	S	66	ILE	C-N-CA	6.36	128.81	120.28
25	A	1913	A	O4'-C1'-N9	6.34	118.01	108.50
25	A	1975	G	C5'-C4'-C3'	-6.33	106.50	116.00
3	c	18	ASN	CA-CB-CG	-6.29	106.31	112.60
37	P	51	ASN	N-CA-C	6.29	119.37	110.50
1	a	372	C	P-O3'-C3'	6.28	129.62	120.20
25	A	1072	C	P-O3'-C3'	-6.28	110.78	120.20
25	A	1068	G	C2'-C3'-O3'	6.27	118.91	109.50
44	X	12	C	P-O5'-C5'	6.27	130.30	120.90
25	A	528	A	P-O3'-C3'	6.25	129.57	120.20
6	f	37	HIS	CA-CB-CG	-6.24	107.56	113.80
25	A	74	A	C5'-C4'-C3'	-6.24	105.84	115.20
25	A	1247	A	C5'-C4'-C3'	-6.23	105.85	115.20
1	a	1110	A	P-O3'-C3'	6.23	129.54	120.20
25	A	2423	U	C2'-C3'-O3'	6.23	118.84	109.50
9	i	25	GLY	N-CA-C	6.22	118.64	111.36
9	i	102	PHE	CA-CB-CG	-6.22	107.58	113.80
27	F	121	PHE	CA-C-N	6.21	132.79	122.54
27	F	121	PHE	C-N-CA	6.21	132.79	122.54
33	L	33	ARG	NE-CZ-NH2	6.21	124.79	119.20
27	F	84	ILE	N-CA-C	6.20	116.98	110.72
25	A	1913	A	O4'-C1'-C2'	-6.18	101.42	107.60
1	a	1101	A	C2'-C3'-O3'	6.16	118.74	109.50
25	A	1299	G	P-O3'-C3'	6.16	129.44	120.20
50	4	117	GLY	CA-C-N	6.15	133.29	121.54
50	4	117	GLY	C-N-CA	6.15	133.29	121.54
1	a	719	C	P-O3'-C3'	6.15	129.42	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1969	A	O3'-P-O5'	-6.13	94.80	104.00
25	A	877	A	O3'-P-O5'	-6.13	94.81	104.00
25	A	2002	G	C5'-C4'-C3'	-6.13	106.81	116.00
25	A	830	G	C5'-C4'-O4'	6.12	118.29	109.10
16	p	23	ASP	CA-C-N	6.12	128.47	120.28
16	p	23	ASP	C-N-CA	6.12	128.47	120.28
9	i	44	ARG	N-CA-C	6.11	117.61	111.07
42	U	91	LYS	N-CA-C	6.11	117.63	110.97
1	a	485	U	P-O5'-C5'	-6.11	111.74	120.90
25	A	2324	U	C2'-C3'-O3'	6.10	118.65	109.50
47	l	31	ASN	CA-CB-CG	-6.09	106.51	112.60
1	a	1028	C	C5'-C4'-C3'	-6.08	106.87	116.00
25	A	543	G	C5'-C4'-C3'	-6.07	106.90	116.00
1	a	137	U	C5'-C4'-C3'	-6.06	106.91	116.00
42	U	17	ASP	CA-CB-CG	-6.05	106.55	112.60
1	a	442	G	C5'-C4'-C3'	-6.04	106.93	116.00
23	y	22	A	C5'-C4'-C3'	6.04	124.27	115.20
25	A	1317	G	C5'-C4'-C3'	-6.04	106.94	116.00
25	A	2095	A	C5'-C4'-C3'	-6.04	106.95	116.00
21	u	22	CYS	CA-C-N	6.03	128.96	120.28
21	u	22	CYS	C-N-CA	6.03	128.96	120.28
25	A	2329	U	C5'-C4'-C3'	6.02	125.03	116.00
25	A	1058	U	C2'-C3'-O3'	6.01	118.51	109.50
25	A	657	U	P-O5'-C5'	6.00	129.91	120.90
25	A	323	C	C2'-C3'-O3'	6.00	118.51	109.50
25	A	1210	G	C1'-O4'-C4'	-5.99	103.91	109.90
27	F	70	ARG	NE-CZ-NH2	5.99	124.59	119.20
25	A	1105	U	C5'-C4'-C3'	5.99	124.98	116.00
19	s	70	LEU	CA-C-N	5.98	127.62	120.14
19	s	70	LEU	C-N-CA	5.98	127.62	120.14
25	A	404	A	C2'-C3'-O3'	5.98	118.47	109.50
25	A	2554	U	C2'-C3'-O3'	5.97	118.46	109.50
43	V	91	PHE	CA-CB-CG	-5.97	107.83	113.80
1	a	1181	G	C2'-C3'-O3'	5.96	118.45	109.50
26	E	183	PHE	CA-CB-CG	-5.96	107.84	113.80
33	L	82	LEU	CA-C-N	5.96	128.27	120.28
33	L	82	LEU	C-N-CA	5.96	128.27	120.28
25	A	2656	U	P-O5'-C5'	-5.96	111.96	120.90
1	a	354	G	C5'-C4'-C3'	-5.95	107.07	116.00
34	M	88	ASN	CA-CB-CG	-5.95	106.65	112.60
40	S	88	ARG	NE-CZ-NH2	5.95	124.56	119.20
25	A	677	A	C5'-C4'-C3'	-5.94	107.08	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	542	C	C4'-C3'-O3'	-5.94	104.09	113.00
16	p	31	ARG	N-CA-C	5.93	118.66	110.35
25	A	785	G	C5'-C4'-C3'	-5.93	107.11	116.00
25	A	1852	U	P-O3'-C3'	-5.93	111.31	120.20
15	o	14	PHE	CA-CB-CG	-5.92	107.88	113.80
1	a	115	G	C4'-C3'-O3'	5.92	118.28	109.40
1	a	1167	A	C1'-O4'-C4'	-5.92	103.98	109.90
4	d	49	ASP	CA-CB-CG	-5.91	106.69	112.60
25	A	2716	C	O4'-C1'-N1	5.90	117.35	108.50
39	R	46	GLU	N-CA-C	5.90	119.02	110.28
25	A	2773	C	P-O5'-C5'	5.89	129.74	120.90
25	A	2800	A	C5'-C4'-C3'	-5.89	106.36	115.20
25	A	1451	C	P-O5'-C5'	5.89	129.73	120.90
46	0	39	GLN	N-CA-C	5.89	117.37	111.07
1	a	121	U	P-O3'-C3'	-5.88	111.38	120.20
25	A	1452	G	P-O3'-C3'	5.88	129.02	120.20
21	u	30	GLU	N-CA-C	5.87	117.35	111.07
15	o	47	LYS	CA-C-N	5.87	131.65	122.26
15	o	47	LYS	C-N-CA	5.87	131.65	122.26
1	a	652	U	C2'-C3'-O3'	5.86	118.28	109.50
25	A	2184	A	C5'-C4'-C3'	-5.85	107.23	116.00
25	A	784	G	P-O3'-C3'	5.84	128.97	120.20
1	a	384	G	C5'-C4'-C3'	-5.84	107.24	116.00
25	A	1578	U	C5'-C4'-C3'	-5.84	107.24	116.00
5	e	100	GLU	N-CA-C	5.83	117.31	111.07
25	A	80	G	C5'-C4'-C3'	-5.83	107.25	116.00
1	a	949	A	C5'-C4'-C3'	-5.83	107.25	116.00
34	M	10	ARG	NE-CZ-NH2	5.83	124.44	119.20
39	R	57	GLY	N-CA-C	5.83	118.18	111.36
24	z	846	ARG	NE-CZ-NH1	-5.82	115.68	121.50
25	A	2669	G	C5'-C4'-C3'	-5.82	107.27	116.00
48	2	49	ASP	CA-CB-CG	-5.80	106.80	112.60
11	k	51	PHE	CA-CB-CG	-5.80	108.00	113.80
1	a	72	A	P-O5'-C5'	-5.80	112.20	120.90
26	E	44	ARG	NE-CZ-NH2	5.79	124.41	119.20
11	k	118	ASN	CA-CB-CG	-5.79	106.81	112.60
1	a	1086	U	C4'-C3'-C2'	-5.78	96.82	102.60
1	a	1125	U	C2'-C3'-O3'	5.78	118.17	109.50
24	z	690	ASN	CA-CB-CG	-5.78	106.83	112.60
35	N	17	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	a	177	G	C5'-C4'-C3'	-5.77	107.35	116.00
1	a	1094	G	C2'-C3'-O3'	5.77	118.15	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	156	C	C5'-C4'-C3'	-5.76	107.36	116.00
23	y	55	U	C2'-C3'-O3'	5.76	118.14	109.50
25	A	2201	G	P-O5'-C5'	-5.75	112.28	120.90
1	a	79	G	P-O5'-C5'	5.74	129.52	120.90
55	9	79	ARG	NE-CZ-NH1	-5.74	115.76	121.50
25	A	1020	A	C2'-C3'-O3'	5.74	118.11	109.50
25	A	2476	A	C5'-C4'-C3'	-5.74	107.39	116.00
1	a	1087	G	C5'-C4'-C3'	-5.73	107.40	116.00
25	A	1060	U	P-O3'-C3'	5.73	128.80	120.20
30	I	117	THR	N-CA-CB	5.73	118.64	110.16
25	A	2275	C	P-O3'-C3'	-5.73	111.61	120.20
3	c	174	LEU	N-CA-C	5.72	117.52	111.28
25	A	2884	U	C2'-C3'-O3'	5.72	118.08	109.50
25	A	1119	U	C5'-C4'-C3'	-5.72	107.42	116.00
55	9	216	ARG	CA-C-N	5.72	126.99	119.84
55	9	216	ARG	C-N-CA	5.72	126.99	119.84
17	q	81	ALA	N-CA-C	5.71	117.18	111.07
25	A	404	A	O4'-C1'-N9	5.70	116.75	108.20
46	0	76	ARG	NE-CZ-NH2	5.70	124.33	119.20
25	A	1821	A	C5'-C4'-C3'	-5.69	107.46	116.00
25	A	404	A	C1'-O4'-C4'	-5.69	104.01	109.70
47	l	73	ARG	NE-CZ-NH1	-5.69	115.81	121.50
25	A	131	A	C5'-C4'-C3'	-5.68	107.47	116.00
25	A	1758	U	C2'-C3'-O3'	5.68	118.02	109.50
1	a	208	U	P-O5'-C5'	5.67	129.41	120.90
36	O	94	ARG	NE-CZ-NH1	-5.67	115.83	121.50
25	A	1249	U	O3'-P-O5'	-5.67	95.50	104.00
25	A	997	G	C5'-C4'-C3'	-5.67	107.50	116.00
24	z	747	ASN	CA-CB-CG	-5.67	106.93	112.60
25	A	708	G	C5'-C4'-C3'	-5.67	107.50	116.00
23	y	8	U	O4'-C1'-C2'	-5.66	101.94	107.60
44	X	23	G	P-O3'-C3'	5.66	128.69	120.20
38	Q	69	ARG	NE-CZ-NH2	5.66	124.30	119.20
25	A	2756	U	C4'-C3'-O3'	5.66	117.89	109.40
5	e	109	ALA	CA-C-N	5.66	127.79	120.44
5	e	109	ALA	C-N-CA	5.66	127.79	120.44
25	A	2212	A	C5'-C4'-C3'	5.65	123.68	115.20
25	A	877	A	P-O5'-C5'	-5.65	112.42	120.90
23	y	59	A	C2'-C3'-O3'	5.65	117.97	109.50
1	a	1036	A	C5'-C4'-C3'	-5.64	107.54	116.00
25	A	829	A	P-O3'-C3'	5.64	128.66	120.20
29	H	108	PHE	CA-CB-CG	-5.64	108.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1072	G	C5'-C4'-C3'	-5.63	107.55	116.00
25	A	974	G	P-O3'-C3'	5.63	128.65	120.20
25	A	1970	A	P-O3'-C3'	-5.63	111.75	120.20
25	A	157	C	P-O5'-C5'	5.62	129.34	120.90
1	a	1157	A	C5'-C4'-C3'	-5.61	106.78	115.20
25	A	223	A	C5'-C4'-C3'	-5.61	107.58	116.00
25	A	996	A	P-O3'-C3'	5.61	128.62	120.20
37	P	50	ARG	N-CA-C	5.61	117.39	111.28
25	A	2194	U	C5'-C4'-C3'	-5.61	107.59	116.00
25	A	11	C	P-O3'-C3'	5.60	128.60	120.20
25	A	2379	G	C5'-C4'-C3'	-5.60	107.60	116.00
25	A	1076	C	C2'-C3'-O3'	5.60	122.10	113.70
14	n	42	TRP	CA-C-N	5.59	132.23	121.54
14	n	42	TRP	C-N-CA	5.59	132.23	121.54
38	Q	13	HIS	CA-CB-CG	-5.59	108.21	113.80
47	1	73	ARG	NE-CZ-NH2	5.59	124.23	119.20
25	A	574	A	P-O5'-C5'	5.58	129.26	120.90
1	a	1377	A	C5'-C4'-C3'	-5.57	107.65	116.00
1	a	1343	G	C5'-C4'-C3'	-5.57	107.65	116.00
25	A	1869	G	C5'-C4'-C3'	-5.57	107.65	116.00
1	a	1021	A	O3'-P-O5'	-5.55	95.68	104.00
25	A	722	A	C5'-C4'-C3'	-5.55	107.68	116.00
25	A	1061	U	O4'-C1'-N1	5.55	116.52	108.20
30	I	62	ALA	N-CA-C	5.54	117.32	111.28
25	A	1452	G	C2'-C3'-O3'	5.54	117.81	109.50
25	A	547	A	O4'-C1'-N9	5.54	116.80	108.50
25	A	152	A	C5'-C4'-C3'	-5.53	107.70	116.00
25	A	2731	G	C4'-C3'-C2'	5.53	108.13	102.60
50	4	134	HIS	N-CA-CB	5.53	119.84	110.49
25	A	995	C	P-O3'-C3'	-5.53	111.91	120.20
1	a	780	A	O3'-P-O5'	-5.53	95.71	104.00
29	H	59	ASP	CA-CB-CG	-5.53	107.08	112.60
1	a	325	A	P-O3'-C3'	5.52	128.48	120.20
16	p	2	VAL	N-CA-C	5.52	116.70	109.58
30	I	30	GLN	N-CA-C	5.52	118.28	110.50
1	a	1397	C	P-O3'-C3'	5.51	128.47	120.20
2	b	158	ASP	CA-CB-CG	-5.51	107.09	112.60
40	S	38	TYR	CA-CB-CG	-5.51	103.97	113.90
47	1	16	ASN	CA-CB-CG	-5.51	107.09	112.60
25	A	1899	A	C5'-C4'-C3'	5.51	124.26	116.00
25	A	458	G	C2'-C3'-O3'	5.51	117.76	109.50
39	R	35	PHE	CA-CB-CG	-5.50	108.30	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1145	A	C2'-C3'-O3'	5.50	121.95	113.70
31	J	131	ASN	CA-CB-CG	-5.49	107.11	112.60
25	A	2564	A	P-O5'-C5'	-5.49	112.67	120.90
19	s	73	PHE	CA-CB-CG	-5.48	108.32	113.80
25	A	1419	A	P-O5'-C5'	5.48	129.12	120.90
1	a	143	A	C5'-C4'-C3'	-5.47	107.79	116.00
24	z	406	SER	N-CA-C	5.47	117.95	111.33
24	z	445	THR	O-C-N	-5.47	118.02	121.85
24	z	802	ASP	N-CA-C	5.47	117.31	110.91
1	a	114	U	C4'-C3'-C2'	5.46	108.06	102.60
25	A	830	G	C4'-C3'-C2'	-5.46	97.14	102.60
20	t	74	HIS	CA-CB-CG	-5.45	108.35	113.80
25	A	1061	U	C1'-O4'-C4'	-5.45	104.25	109.70
25	A	2276	G	C5'-C4'-C3'	-5.45	107.82	116.00
3	c	128	MET	CA-C-N	5.44	127.58	120.28
3	c	128	MET	C-N-CA	5.44	127.58	120.28
25	A	291	G	C5'-C4'-C3'	-5.44	107.84	116.00
25	A	2403	C	O4'-C1'-N1	5.43	116.65	108.50
10	j	53	ILE	N-CA-C	5.43	115.63	110.53
25	A	1534	U	P-O5'-C5'	5.42	129.04	120.90
30	I	36	GLU	N-CA-C	5.42	119.16	112.54
4	d	16	THR	N-CA-CB	5.42	119.66	110.49
25	A	1017	G	C5'-C4'-C3'	-5.42	107.87	116.00
25	A	1533	C	O3'-P-O5'	-5.42	95.87	104.00
18	r	25	ILE	N-CA-C	5.41	118.64	111.17
40	S	2	GLU	CA-C-N	5.41	131.88	121.54
40	S	2	GLU	C-N-CA	5.41	131.88	121.54
55	9	79	ARG	NE-CZ-NH2	5.41	124.07	119.20
27	F	91	ARG	NE-CZ-NH2	5.40	124.06	119.20
14	n	56	SER	N-CA-C	5.39	116.49	109.64
25	A	2655	G	C2'-C3'-O3'	5.39	117.59	109.50
1	a	1204	A	P-O5'-C5'	-5.39	112.81	120.90
25	A	958	U	C2'-C3'-O3'	5.39	121.78	113.70
25	A	1920	C	P-O5'-C5'	5.39	128.98	120.90
35	N	21	PHE	CA-CB-CG	-5.39	108.41	113.80
1	a	1018	G	C5'-C4'-C3'	-5.39	107.92	116.00
1	a	1397	C	C2'-C3'-O3'	5.38	117.57	109.50
1	a	1150	A	C5'-C4'-C3'	5.38	124.07	116.00
38	Q	47	ARG	NE-CZ-NH1	-5.38	116.12	121.50
55	9	30	ALA	N-CA-C	5.37	120.06	112.75
1	a	191	G	C5'-C4'-C3'	-5.37	107.94	116.00
34	M	42	THR	N-CA-CB	5.37	118.04	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	372	G	C4'-C3'-C2'	-5.37	97.23	102.60
33	L	41	ARG	NE-CZ-NH1	-5.37	116.13	121.50
25	A	2848	G	P-O3'-C3'	5.37	128.25	120.20
1	a	676	A	C5'-C4'-C3'	-5.36	107.96	116.00
25	A	503	A	C4'-C3'-O3'	5.36	117.43	109.40
25	A	1358	G	O3'-P-O5'	-5.36	95.97	104.00
6	f	56	LYS	N-CA-C	5.35	119.39	112.86
25	A	1786	A	C1'-O4'-C4'	-5.35	104.35	109.70
11	k	124	LYS	N-CA-C	5.35	116.92	111.14
25	A	1110	G	P-O5'-C5'	5.34	128.91	120.90
15	o	42	PHE	CA-CB-CG	-5.34	108.46	113.80
25	A	162	U	C2'-C3'-O3'	5.34	117.51	109.50
27	F	73	VAL	N-CA-C	5.34	116.58	109.37
7	g	148	LYS	N-CA-C	5.33	117.17	111.36
1	a	175	C	C5'-C4'-C3'	-5.33	108.00	116.00
1	a	1201	A	C2'-C3'-O3'	5.33	117.50	109.50
42	U	6	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	a	1531	A	P-O3'-C3'	5.32	128.19	120.20
25	A	1913	A	C1'-O4'-C4'	-5.32	104.58	109.90
25	A	10	A	C5'-C4'-C3'	-5.32	108.02	116.00
12	l	55	ARG	NE-CZ-NH1	-5.31	116.19	121.50
26	E	182	ALA	N-CA-C	5.31	116.92	111.03
1	a	473	U	C5'-C4'-C3'	-5.30	108.04	116.00
1	a	570	G	C5'-C4'-C3'	-5.30	108.05	116.00
14	n	54	ASP	CA-CB-CG	-5.30	107.30	112.60
1	a	115	G	C5'-C4'-C3'	-5.30	107.25	115.20
25	A	1648	U	C5'-C4'-C3'	-5.30	108.05	116.00
23	y	16	C	P-O3'-C3'	-5.29	112.26	120.20
25	A	198	C	P-O5'-C5'	5.29	128.84	120.90
1	a	1455	G	C5'-C4'-C3'	-5.29	108.07	116.00
25	A	784	G	C2'-C3'-O3'	5.29	121.63	113.70
8	h	79	ARG	CA-C-N	5.28	124.73	119.24
8	h	79	ARG	C-N-CA	5.28	124.73	119.24
1	a	1227	A	C5'-C4'-C3'	-5.28	108.08	116.00
29	H	82	PHE	CA-C-N	5.28	131.63	121.54
29	H	82	PHE	C-N-CA	5.28	131.63	121.54
35	N	23	ASN	CA-CB-CG	-5.28	107.32	112.60
24	z	756	LYS	N-CA-CB	-5.28	102.36	110.12
23	y	8	U	C2'-C3'-O3'	5.27	121.61	113.70
43	V	49	ASN	CA-CB-CG	-5.27	107.33	112.60
37	P	65	ASN	CA-CB-CG	-5.27	107.33	112.60
4	d	202	LEU	N-CA-C	5.26	117.76	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	y	56	U	C5'-C4'-C3'	-5.26	108.11	116.00
25	A	1174	U	C1'-O4'-C4'	-5.26	104.44	109.70
1	a	1350	A	C5'-C4'-C3'	-5.26	108.12	116.00
9	i	24	ASN	CA-C-N	5.26	124.97	119.92
9	i	24	ASN	C-N-CA	5.26	124.97	119.92
25	A	2423	U	P-O3'-C3'	5.26	128.09	120.20
15	o	13	GLU	N-CA-C	5.25	116.86	111.03
46	0	11	ASN	N-CA-C	5.25	117.85	110.23
1	a	405	U	C5'-C4'-C3'	-5.25	108.12	116.00
54	8	16	THR	CA-C-N	5.25	125.92	119.99
54	8	16	THR	C-N-CA	5.25	125.92	119.99
1	a	51	A	C2'-C3'-O3'	5.25	117.37	109.50
25	A	2186	G	P-O5'-C5'	5.24	128.75	120.90
25	A	2295	C	C5'-C4'-C3'	-5.24	108.15	116.00
3	c	45	GLU	N-CA-C	5.23	117.06	111.36
25	A	2664	G	P-O3'-C3'	-5.23	112.36	120.20
25	A	1063	G	C5'-C4'-C3'	-5.22	108.17	116.00
1	a	362	G	C5'-C4'-C3'	5.22	123.83	116.00
2	b	165	ALA	CA-C-N	5.22	127.28	120.28
2	b	165	ALA	C-N-CA	5.22	127.28	120.28
31	J	111	LYS	N-CA-C	5.22	121.91	110.80
34	M	31	PHE	CA-CB-CG	-5.21	108.59	113.80
1	a	411	A	P-O5'-C5'	5.21	128.72	120.90
19	s	37	SER	N-CA-C	5.21	118.02	110.42
25	A	1073	A	P-O5'-C5'	5.21	128.71	120.90
25	A	280	U	P-O3'-C3'	-5.19	112.41	120.20
1	a	309	A	P-O5'-C5'	-5.19	113.11	120.90
23	y	8	U	O4'-C4'-C3'	-5.19	98.81	104.00
25	A	252	G	C5'-C4'-C3'	-5.19	108.21	116.00
25	A	1930	G	C2'-C3'-O3'	5.18	117.28	109.50
25	A	1997	C	O4'-C1'-N1	5.18	116.28	108.50
1	a	140	U	C5'-C4'-C3'	-5.18	108.23	116.00
25	A	1732	C	C4'-C3'-C2'	-5.18	97.42	102.60
1	a	1020	G	C4'-C3'-O3'	-5.18	105.23	113.00
25	A	1266	G	C2'-C3'-O3'	5.18	117.27	109.50
25	A	895	U	C5'-C4'-C3'	-5.18	108.24	116.00
39	R	29	THR	N-CA-C	5.18	116.92	111.28
25	A	1054	A	C5'-C4'-C3'	-5.17	108.24	116.00
25	A	1047	G	O4'-C1'-N9	5.17	115.96	108.20
39	R	68	ARG	NE-CZ-NH2	5.17	123.85	119.20
54	8	51	LYS	CA-C-N	5.17	125.69	120.00
54	8	51	LYS	C-N-CA	5.17	125.69	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	98	G	C4'-C3'-C2'	-5.16	97.44	102.60
26	E	70	SER	N-CA-C	5.16	117.37	110.35
1	a	450	G	P-O3'-C3'	-5.16	112.47	120.20
25	A	2897	U	C5'-C4'-C3'	-5.16	108.27	116.00
25	A	334	C	P-O5'-C5'	5.15	128.63	120.90
25	A	210	C	C5'-C4'-C3'	-5.15	108.28	116.00
25	A	847	U	C5'-C4'-C3'	-5.15	108.27	116.00
25	A	1253	A	P-O3'-C3'	-5.14	112.48	120.20
50	4	114	LYS	CA-C-N	5.14	125.56	120.31
50	4	114	LYS	C-N-CA	5.14	125.56	120.31
1	a	716	A	C5'-C4'-C3'	-5.14	108.29	116.00
1	a	531	U	C2'-C3'-O3'	5.13	117.20	109.50
1	a	1195	C	P-O3'-C3'	5.13	127.90	120.20
25	A	394	C	O3'-P-O5'	-5.13	96.31	104.00
27	F	91	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	a	1248	A	C1'-O4'-C4'	-5.13	104.57	109.70
2	b	203	ASP	CA-C-N	5.12	129.28	120.72
2	b	203	ASP	C-N-CA	5.12	129.28	120.72
25	A	1484	U	C5'-C4'-C3'	-5.12	108.32	116.00
1	a	1520	C	C5'-C4'-C3'	-5.12	108.32	116.00
24	z	846	ARG	NE-CZ-NH2	5.12	123.81	119.20
25	A	1026	G	C5'-C4'-C3'	-5.12	108.32	116.00
25	A	1173	U	C5'-C4'-C3'	-5.12	108.33	116.00
1	a	740	U	P-O3'-C3'	-5.11	112.54	120.20
25	A	547	A	C1'-O4'-C4'	-5.11	104.79	109.90
1	a	1026	G	O3'-P-O5'	-5.11	96.34	104.00
12	l	55	ARG	NE-CZ-NH2	5.11	123.80	119.20
24	z	405	THR	CA-C-N	5.11	127.38	120.38
24	z	405	THR	C-N-CA	5.11	127.38	120.38
25	A	2796	U	P-O5'-C5'	5.11	128.56	120.90
7	g	112	ASP	N-CA-C	5.10	116.69	110.41
35	N	4	ARG	CA-C-N	5.10	128.02	120.82
35	N	4	ARG	C-N-CA	5.10	128.02	120.82
25	A	930	G	P-O3'-C3'	5.10	127.85	120.20
25	A	1130	U	P-O3'-C3'	-5.10	112.56	120.20
25	A	1715	G	C2'-C3'-O3'	5.09	117.14	109.50
25	A	1756	G	C5'-C4'-C3'	-5.09	108.36	116.00
33	L	93	ASN	CA-CB-CG	-5.09	107.51	112.60
4	d	39	GLN	N-CA-C	5.09	116.83	111.28
25	A	130	C	C5'-C4'-C3'	-5.09	108.37	116.00
39	R	59	ILE	CA-C-N	5.09	129.54	122.77
39	R	59	ILE	C-N-CA	5.09	129.54	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	E	166	LYS	N-CA-C	5.09	116.91	111.36
24	z	615	GLN	N-CA-C	5.08	116.51	111.07
2	b	164	ASP	CA-C-N	5.08	127.09	120.28
2	b	164	ASP	C-N-CA	5.08	127.09	120.28
3	c	179	ALA	N-CA-C	5.08	117.58	109.96
9	i	82	ILE	N-CA-C	5.08	115.85	110.72
25	A	857	G	C5'-C4'-C3'	-5.08	108.39	116.00
25	A	1180	U	C5'-C4'-C3'	-5.08	108.39	116.00
22	x	15	U	O3'-P-O5'	5.07	111.61	104.00
39	R	56	GLY	CA-C-N	5.07	124.79	119.92
39	R	56	GLY	C-N-CA	5.07	124.79	119.92
55	9	142	ASN	N-CA-C	5.07	117.45	110.35
28	G	98	GLU	CA-C-N	5.07	127.49	120.29
28	G	98	GLU	C-N-CA	5.07	127.49	120.29
25	A	508	A	C1'-O4'-C4'	-5.07	104.63	109.70
25	A	1646	C	C2'-C3'-O3'	5.07	117.10	109.50
36	O	117	PHE	CA-CB-CG	5.07	118.87	113.80
26	E	200	LEU	N-CA-C	5.07	117.70	111.82
29	H	116	LEU	CA-C-N	5.06	125.06	119.89
29	H	116	LEU	C-N-CA	5.06	125.06	119.89
1	a	1530	G	O4'-C1'-N9	5.06	115.79	108.20
24	z	587	ARG	NE-CZ-NH2	5.06	123.75	119.20
30	I	75	ALA	N-CA-C	5.06	121.58	110.80
31	J	59	ALA	N-CA-C	5.06	116.88	111.36
25	A	1970	A	C2'-C3'-O3'	5.06	117.09	109.50
25	A	1733	G	P-O5'-C5'	5.06	128.48	120.90
25	A	1778	U	C4'-C3'-C2'	5.06	107.66	102.60
27	F	137	PHE	CA-CB-CG	-5.05	108.75	113.80
1	a	68	G	C5'-C4'-C3'	-5.05	108.42	116.00
25	A	2199	A	O5'-C5'-C4'	5.05	119.08	111.50
1	a	714	G	P-O3'-C3'	-5.05	112.63	120.20
25	A	1912	A	P-O5'-C5'	5.05	128.47	120.90
30	I	76	ALA	CA-C-N	5.05	127.38	120.46
30	I	76	ALA	C-N-CA	5.05	127.38	120.46
1	a	1361	G	C5'-C4'-O4'	5.05	117.37	109.80
25	A	383	C	C4'-C3'-C2'	5.05	107.65	102.60
24	z	455	ARG	NE-CZ-NH2	5.04	123.74	119.20
25	A	733	G	C5'-C4'-C3'	-5.04	108.44	116.00
44	X	34	A	P-O3'-C3'	5.04	127.76	120.20
5	e	120	HIS	CA-CB-CG	-5.04	108.76	113.80
25	A	496	G	C5'-C4'-C3'	-5.04	108.44	116.00
1	a	428	G	P-O3'-C3'	5.04	127.76	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2638	G	C2'-C3'-O3'	5.04	117.06	109.50
27	F	79	ARG	NE-CZ-NH2	5.04	123.73	119.20
25	A	2756	U	P-O3'-C3'	5.03	127.75	120.20
1	a	36	C	P-O3'-C3'	-5.03	112.66	120.20
33	L	114	GLY	CA-C-N	5.03	127.85	120.71
33	L	114	GLY	C-N-CA	5.03	127.85	120.71
44	X	77	U	P-O3'-C3'	-5.03	112.66	120.20
25	A	1913	A	C4'-C3'-C2'	-5.02	97.58	102.60
1	a	154	U	C5'-C4'-C3'	-5.02	108.47	116.00
9	i	21	LYS	O-C-N	-5.02	117.64	121.55
25	A	141	G	C2'-C3'-O3'	5.02	117.03	109.50
25	A	197	A	C4'-C3'-C2'	-5.02	97.58	102.60
34	M	17	ASN	CA-CB-CG	-5.02	107.58	112.60
25	A	1451	C	P-O3'-C3'	5.01	127.72	120.20
1	a	692	U	C4'-C3'-C2'	-5.01	97.59	102.60
25	A	549	G	P-O3'-C3'	5.01	127.72	120.20
25	A	2213	U	O4'-C1'-N1	5.01	115.72	108.20
25	A	508	A	O4'-C1'-N9	5.01	115.71	108.20
38	Q	32	ARG	NE-CZ-NH1	-5.01	116.49	121.50
1	a	415	A	C5'-C4'-C3'	5.01	123.51	116.00
25	A	1724	G	O3'-P-O5'	-5.01	96.49	104.00
1	a	197	A	C2'-C3'-O3'	5.00	117.01	109.50
25	A	711	G	C5'-C4'-C3'	-5.00	108.49	116.00
1	a	1140	C	C2'-C3'-O3'	5.00	117.00	109.50

There are no chirality outliers.

All (834) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	0	10	ARG	Sidechain
46	0	25	PHE	Peptide
46	0	27	GLY	Peptide
47	1	10	ARG	Sidechain
47	1	2	ARG	Sidechain
47	1	51	SER	Peptide
48	2	23	ARG	Sidechain
48	2	29	ARG	Sidechain
50	4	13	ARG	Sidechain
50	4	185	ASN	Peptide
50	4	83	ARG	Sidechain
51	5	9	ARG	Sidechain
52	6	5	ARG	Sidechain

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Mol	Chain	Res	Type	Group
53	7	21	ARG	Sidechain
53	7	6	GLN	Peptide
54	8	29	ARG	Sidechain
54	8	7	ARG	Sidechain
55	9	100	ARG	Sidechain
55	9	102	TYR	Sidechain
55	9	155	ARG	Sidechain
55	9	202	ARG	Sidechain
55	9	213	ARG	Sidechain
55	9	216	ARG	Sidechain
55	9	225	ASN	Peptide
55	9	237	ARG	Sidechain
55	9	257	ARG	Sidechain
55	9	268	ARG	Sidechain
55	9	51	ARG	Sidechain
55	9	79	ARG	Sidechain
25	A	1004	U	Sidechain
25	A	1010	A	Sidechain
25	A	1023	U	Sidechain
25	A	1025	G	Sidechain
25	A	1027	A	Sidechain
25	A	1028	A	Sidechain
25	A	1033	U	Sidechain
25	A	1042	G	Sidechain
25	A	1047	G	Sidechain
25	A	1053	C	Sidechain
25	A	1058	U	Sidechain
25	A	1063	G	Sidechain
25	A	1070	A	Sidechain
25	A	1073	A	Sidechain
25	A	1074	G	Sidechain
25	A	1079	C	Sidechain
25	A	108	G	Sidechain
25	A	1081	U	Sidechain
25	A	1086	A	Sidechain
25	A	1088	A	Sidechain
25	A	1089	A	Sidechain
25	A	1098	A	Sidechain
25	A	1099	G	Sidechain
25	A	1105	U	Sidechain
25	A	1110	G	Sidechain
25	A	1126	A	Sidechain

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Mol	Chain	Res	Type	Group
25	A	1131	G	Sidechain
25	A	1133	A	Sidechain
25	A	114	U	Sidechain
25	A	1148	U	Sidechain
25	A	1159	U	Sidechain
25	A	116	C	Sidechain
25	A	1166	G	Sidechain
25	A	117	G	Sidechain
25	A	1179	G	Sidechain
25	A	1186	G	Sidechain
25	A	1187	G	Sidechain
25	A	1188	U	Sidechain
25	A	1198	U	Sidechain
25	A	1209	U	Sidechain
25	A	1210	G	Sidechain
25	A	1212	G	Sidechain
25	A	1223	G	Sidechain
25	A	1225	G	Sidechain
25	A	1236	G	Sidechain
25	A	124	G	Sidechain
25	A	1241	A	Sidechain
25	A	1246	A	Sidechain
25	A	1253	A	Sidechain
25	A	1256	G	Sidechain
25	A	1266	G	Sidechain
25	A	1271	G	Sidechain
25	A	1272	A	Sidechain
25	A	1275	A	Sidechain
25	A	1289	C	Sidechain
25	A	1299	G	Sidechain
25	A	1300	G	Sidechain
25	A	1314	C	Sidechain
25	A	1316	U	Sidechain
25	A	1317	G	Sidechain
25	A	1325	U	Sidechain
25	A	1326	U	Sidechain
25	A	1327	A	Sidechain
25	A	1332	G	Sidechain
25	A	1340	U	Sidechain
25	A	1343	G	Sidechain
25	A	1353	A	Sidechain
25	A	1361	G	Sidechain

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Mol	Chain	Res	Type	Group
25	A	1379	U	Sidechain
25	A	138	U	Sidechain
25	A	1392	A	Sidechain
25	A	1393	A	Sidechain
25	A	1395	A	Sidechain
25	A	1398	C	Sidechain
25	A	1402	U	Sidechain
25	A	1405	U	Sidechain
25	A	142	A	Sidechain
25	A	1427	A	Sidechain
25	A	1439	A	Sidechain
25	A	144	A	Sidechain
25	A	1440	U	Sidechain
25	A	1442	U	Sidechain
25	A	1445	G	Sidechain
25	A	1449	G	Sidechain
25	A	1450	G	Sidechain
25	A	1467	U	Sidechain
25	A	1468	U	Sidechain
25	A	1476	U	Sidechain
25	A	1482	G	Sidechain
25	A	1503	A	Sidechain
25	A	1515	A	Sidechain
25	A	1528	A	Sidechain
25	A	1530	G	Sidechain
25	A	1532	A	Sidechain
25	A	1539	U	Sidechain
25	A	1557	C	Sidechain
25	A	1565	C	Sidechain
25	A	1571	A	Sidechain
25	A	1573	G	Sidechain
25	A	1579	A	Sidechain
25	A	1586	A	Sidechain
25	A	1596	A	Sidechain
25	A	1610	A	Sidechain
25	A	1613	G	Sidechain
25	A	1625	C	Sidechain
25	A	1626	A	Sidechain
25	A	1633	G	Sidechain
25	A	1638	C	Sidechain
25	A	1645	G	Sidechain
25	A	165	A	Sidechain

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Mol	Chain	Res	Type	Group
25	A	1652	A	Sidechain
25	A	1653	G	Sidechain
25	A	1654	A	Sidechain
25	A	1663	G	Sidechain
25	A	1664	A	Sidechain
25	A	1674	G	Sidechain
25	A	1680	U	Sidechain
25	A	1682	G	Sidechain
25	A	1698	A	Sidechain
25	A	1699	G	Sidechain
25	A	17	G	Sidechain
25	A	1713	A	Sidechain
25	A	1716	U	Sidechain
25	A	1731	G	Sidechain
25	A	1738	G	Sidechain
25	A	174	U	Sidechain
25	A	1753	G	Sidechain
25	A	1754	A	Sidechain
25	A	1757	A	Sidechain
25	A	176	A	Sidechain
25	A	1761	C	Sidechain
25	A	1775	U	Sidechain
25	A	1776	G	Sidechain
25	A	1778	U	Sidechain
25	A	1782	U	Sidechain
25	A	1791	A	Sidechain
25	A	1792	G	Sidechain
25	A	1801	A	Sidechain
25	A	1802	A	Sidechain
25	A	1805	A	Sidechain
25	A	181	A	Sidechain
25	A	1814	G	Sidechain
25	A	1817	G	Sidechain
25	A	1824	G	Sidechain
25	A	1826	G	Sidechain
25	A	1831	G	Sidechain
25	A	1857	G	Sidechain
25	A	1869	G	Sidechain
25	A	1872	A	Sidechain
25	A	1884	G	Sidechain
25	A	1903	G	Sidechain
25	A	1913	A	Sidechain

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Mol	Chain	Res	Type	Group
25	A	1918	A	Sidechain
25	A	1924	C	Sidechain
25	A	1931	U	Sidechain
25	A	1935	G	Sidechain
25	A	1939	U	Sidechain
25	A	1940	U	Sidechain
25	A	1943	U	Sidechain
25	A	1944	U	Sidechain
25	A	1948	G	Sidechain
25	A	1970	A	Sidechain
25	A	1973	G	Sidechain
25	A	1979	U	Sidechain
25	A	1995	U	Sidechain
25	A	2007	U	Sidechain
25	A	2010	G	Sidechain
25	A	2017	U	Sidechain
25	A	2024	G	Sidechain
25	A	2032	G	Sidechain
25	A	2035	G	Sidechain
25	A	2036	C	Sidechain
25	A	2037	A	Sidechain
25	A	205	G	Sidechain
25	A	2056	G	Sidechain
25	A	2058	A	Sidechain
25	A	206	U	Sidechain
25	A	2061	G	Sidechain
25	A	2063	C	Sidechain
25	A	2074	U	Sidechain
25	A	2075	U	Sidechain
25	A	2081	U	Sidechain
25	A	2085	U	Sidechain
25	A	2093	G	Sidechain
25	A	2099	U	Sidechain
25	A	21	A	Sidechain
25	A	2100	G	Sidechain
25	A	2104	C	Sidechain
25	A	2107	G	Sidechain
25	A	2108	A	Sidechain
25	A	211	C	Sidechain
25	A	2141	G	Sidechain
25	A	2143	C	Sidechain
25	A	2151	U	Sidechain

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Mol	Chain	Res	Type	Group
25	A	2154	A	Sidechain
25	A	2182	U	Sidechain
25	A	2188	U	Sidechain
25	A	219	A	Sidechain
25	A	2197	U	Sidechain
25	A	2198	A	Sidechain
25	A	2203	U	Sidechain
25	A	221	A	Sidechain
25	A	2213	U	Sidechain
25	A	2216	G	Sidechain
25	A	2221	G	Sidechain
25	A	2233	U	Sidechain
25	A	2238	G	Sidechain
25	A	2249	U	Sidechain
25	A	2265	U	Sidechain
25	A	2266	A	Sidechain
25	A	2267	A	Sidechain
25	A	2272	U	Sidechain
25	A	2279	G	Sidechain
25	A	228	C	Sidechain
25	A	2281	A	Sidechain
25	A	2288	A	Sidechain
25	A	2290	G	Sidechain
25	A	2292	U	Sidechain
25	A	2301	C	Sidechain
25	A	2307	G	Sidechain
25	A	2308	G	Sidechain
25	A	231	A	Sidechain
25	A	2318	G	Sidechain
25	A	2319	G	Sidechain
25	A	2323	G	Sidechain
25	A	2327	A	Sidechain
25	A	2329	U	Sidechain
25	A	2335	A	Sidechain
25	A	2344	U	Sidechain
25	A	2348	U	Sidechain
25	A	2389	G	Sidechain
25	A	2396	G	Sidechain
25	A	2405	G	Sidechain
25	A	2427	C	Sidechain
25	A	243	U	Sidechain
25	A	2430	A	Sidechain

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Mol	Chain	Res	Type	Group
25	A	2447	G	Sidechain
25	A	2457	U	Sidechain
25	A	2458	G	Sidechain
25	A	2474	U	Sidechain
25	A	248	G	Sidechain
25	A	2489	U	Sidechain
25	A	2492	U	Sidechain
25	A	2493	U	Sidechain
25	A	250	G	Sidechain
25	A	2500	U	Sidechain
25	A	2504	U	Sidechain
25	A	2516	A	Sidechain
25	A	2518	A	Sidechain
25	A	2519	U	Sidechain
25	A	2529	G	Sidechain
25	A	2530	A	Sidechain
25	A	2536	G	Sidechain
25	A	254	G	Sidechain
25	A	2545	G	Sidechain
25	A	2546	U	Sidechain
25	A	2547	A	Sidechain
25	A	2548	U	Sidechain
25	A	2550	G	Sidechain
25	A	2551	C	Sidechain
25	A	2554	U	Sidechain
25	A	2555	U	Sidechain
25	A	2562	U	Sidechain
25	A	2564	A	Sidechain
25	A	2565	A	Sidechain
25	A	2570	G	Sidechain
25	A	2576	G	Sidechain
25	A	2587	A	Sidechain
25	A	2595	G	Sidechain
25	A	2597	G	Sidechain
25	A	2605	U	Sidechain
25	A	2608	G	Sidechain
25	A	262	A	Sidechain
25	A	263	G	Sidechain
25	A	2638	G	Sidechain
25	A	2645	G	Sidechain
25	A	265	A	Sidechain
25	A	2659	G	Sidechain

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Mol	Chain	Res	Type	Group
25	A	266	G	Sidechain
25	A	2680	U	Sidechain
25	A	2682	A	Sidechain
25	A	2688	G	Sidechain
25	A	2694	G	Sidechain
25	A	27	G	Sidechain
25	A	2709	G	Sidechain
25	A	271	G	Sidechain
25	A	2718	G	Sidechain
25	A	272	A	Sidechain
25	A	2728	U	Sidechain
25	A	2739	U	Sidechain
25	A	2747	G	Sidechain
25	A	2750	A	Sidechain
25	A	2754	U	Sidechain
25	A	2756	U	Sidechain
25	A	2759	G	Sidechain
25	A	2764	A	Sidechain
25	A	277	G	Sidechain
25	A	2771	C	Sidechain
25	A	2779	U	Sidechain
25	A	278	A	Sidechain
25	A	2780	G	Sidechain
25	A	2783	U	Sidechain
25	A	2784	U	Sidechain
25	A	279	A	Sidechain
25	A	2791	G	Sidechain
25	A	2825	G	Sidechain
25	A	2834	G	Sidechain
25	A	2848	G	Sidechain
25	A	2849	U	Sidechain
25	A	2859	G	Sidechain
25	A	287	G	Sidechain
25	A	2872	A	Sidechain
25	A	2879	A	Sidechain
25	A	2884	U	Sidechain
25	A	2885	G	Sidechain
25	A	2897	U	Sidechain
25	A	2903	U	Sidechain
25	A	293	U	Sidechain
25	A	295	G	Sidechain
25	A	297	G	Sidechain

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Mol	Chain	Res	Type	Group
25	A	3	U	Sidechain
25	A	333	G	Sidechain
25	A	346	A	Sidechain
25	A	363	G	Sidechain
25	A	366	C	Sidechain
25	A	370	G	Sidechain
25	A	371	A	Sidechain
25	A	373	U	Sidechain
25	A	392	U	Sidechain
25	A	395	U	Sidechain
25	A	4	U	Sidechain
25	A	40	U	Sidechain
25	A	403	U	Sidechain
25	A	404	A	Sidechain
25	A	422	A	Sidechain
25	A	427	U	Sidechain
25	A	429	A	Sidechain
25	A	431	U	Sidechain
25	A	441	U	Sidechain
25	A	449	A	Sidechain
25	A	45	G	Sidechain
25	A	451	U	Sidechain
25	A	454	A	Sidechain
25	A	465	G	Sidechain
25	A	471	A	Sidechain
25	A	473	G	Sidechain
25	A	477	A	Sidechain
25	A	478	A	Sidechain
25	A	483	A	Sidechain
25	A	496	G	Sidechain
25	A	500	G	Sidechain
25	A	506	G	Sidechain
25	A	508	A	Sidechain
25	A	509	C	Sidechain
25	A	512	G	Sidechain
25	A	515	A	Sidechain
25	A	519	U	Sidechain
25	A	532	A	Sidechain
25	A	533	G	Sidechain
25	A	545	U	Sidechain
25	A	550	C	Sidechain
25	A	555	G	Sidechain

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Mol	Chain	Res	Type	Group
25	A	562	U	Sidechain
25	A	568	U	Sidechain
25	A	571	U	Sidechain
25	A	573	U	Sidechain
25	A	576	U	Sidechain
25	A	581	C	Sidechain
25	A	583	G	Sidechain
25	A	589	U	Sidechain
25	A	594	U	Sidechain
25	A	596	U	Sidechain
25	A	60	G	Sidechain
25	A	602	A	Sidechain
25	A	607	U	Sidechain
25	A	608	A	Sidechain
25	A	612	G	Sidechain
25	A	630	G	Sidechain
25	A	668	A	Sidechain
25	A	670	A	Sidechain
25	A	674	G	Sidechain
25	A	675	A	Sidechain
25	A	689	A	Sidechain
25	A	704	G	Sidechain
25	A	715	A	Sidechain
25	A	719	C	Sidechain
25	A	726	G	Sidechain
25	A	729	G	Sidechain
25	A	733	G	Sidechain
25	A	736	C	Sidechain
25	A	741	U	Sidechain
25	A	747	U	Sidechain
25	A	763	G	Sidechain
25	A	773	U	Sidechain
25	A	777	G	Sidechain
25	A	780	G	Sidechain
25	A	782	A	Sidechain
25	A	79	C	Sidechain
25	A	790	U	Sidechain
25	A	793	A	Sidechain
25	A	800	A	Sidechain
25	A	802	A	Sidechain
25	A	805	G	Sidechain
25	A	813	U	Sidechain

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Mol	Chain	Res	Type	Group
25	A	818	G	Sidechain
25	A	826	U	Sidechain
25	A	830	G	Sidechain
25	A	834	G	Sidechain
25	A	850	U	Sidechain
25	A	852	U	Sidechain
25	A	858	G	Sidechain
25	A	862	G	Sidechain
25	A	867	C	Sidechain
25	A	875	G	Sidechain
25	A	880	G	Sidechain
25	A	897	C	Sidechain
25	A	900	A	Sidechain
25	A	906	U	Sidechain
25	A	909	A	Sidechain
25	A	91	A	Sidechain
25	A	910	A	Sidechain
25	A	912	C	Sidechain
25	A	915	C	Sidechain
25	A	923	G	Sidechain
25	A	93	G	Sidechain
25	A	953	G	Sidechain
25	A	956	G	Sidechain
25	A	959	A	Sidechain
25	A	960	A	Sidechain
25	A	970	U	Sidechain
25	A	973	A	Sidechain
25	A	976	G	Sidechain
25	A	983	A	Sidechain
25	A	999	U	Sidechain
26	E	67	ARG	Sidechain
27	F	137	PHE	Peptide
27	F	149	ARG	Sidechain
27	F	91	ARG	Sidechain
28	G	42	ARG	Sidechain
28	G	53	ARG	Sidechain
28	G	61	ARG	Sidechain
29	H	54	ARG	Sidechain
30	I	120	ASP	Peptide
30	I	133	ARG	Sidechain
30	I	18	ASN	Peptide
30	I	19	PRO	Peptide

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Mol	Chain	Res	Type	Group
30	I	71	LYS	Peptide
31	J	120	ARG	Sidechain
31	J	125	TYR	Sidechain
31	J	44	TYR	Sidechain
31	J	69	ARG	Sidechain
31	J	95	ARG	Sidechain
32	K	30	ARG	Sidechain
32	K	49	ARG	Sidechain
33	L	123	ARG	Sidechain
33	L	48	ARG	Sidechain
34	M	18	ARG	Sidechain
34	M	38	ARG	Sidechain
34	M	81	ARG	Sidechain
35	N	103	ARG	Sidechain
35	N	2	ARG	Sidechain
35	N	45	ARG	Sidechain
35	N	86	ARG	Sidechain
36	O	102	ARG	Sidechain
36	O	25	ARG	Sidechain
36	O	30	ARG	Sidechain
37	P	1	SER	Peptide
37	P	100	ARG	Sidechain
37	P	31	VAL	Peptide
37	P	50	ARG	Peptide
37	P	90	ALA	Peptide
37	P	92	ARG	Sidechain
38	Q	27	ARG	Sidechain
38	Q	31	TYR	Sidechain
38	Q	32	ARG	Sidechain
38	Q	44	TYR	Sidechain
38	Q	46	TYR	Sidechain
38	Q	49	ARG	Sidechain
38	Q	50	ARG	Sidechain
39	R	78	ARG	Sidechain
39	R	90	ARG	Sidechain
40	S	107	VAL	Peptide
40	S	110	ARG	Sidechain
40	S	38	TYR	Sidechain
42	U	21	ARG	Sidechain
42	U	53	GLN	Peptide
43	V	13	GLY	Peptide
43	V	57	TYR	Sidechain

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Mol	Chain	Res	Type	Group
44	X	103	U	Sidechain
44	X	15	A	Sidechain
44	X	16	G	Sidechain
44	X	32	U	Sidechain
44	X	51	G	Sidechain
44	X	66	A	Sidechain
44	X	67	G	Sidechain
44	X	75	G	Sidechain
44	X	78	A	Sidechain
44	X	80	U	Sidechain
44	X	90	C	Sidechain
44	X	96	G	Sidechain
45	Y	19	ARG	Sidechain
1	a	100	G	Sidechain
1	a	1004	A	Sidechain
1	a	1008	U	Sidechain
1	a	101	A	Sidechain
1	a	1011	C	Sidechain
1	a	1014	A	Sidechain
1	a	1018	G	Sidechain
1	a	102	G	Sidechain
1	a	1020	G	Sidechain
1	a	1033	G	Sidechain
1	a	1035	A	Sidechain
1	a	1056	U	Sidechain
1	a	1062	U	Sidechain
1	a	1063	C	Sidechain
1	a	1077	G	Sidechain
1	a	1079	G	Sidechain
1	a	108	G	Sidechain
1	a	1087	G	Sidechain
1	a	1092	A	Sidechain
1	a	1093	A	Sidechain
1	a	1094	G	Sidechain
1	a	110	C	Sidechain
1	a	1118	U	Sidechain
1	a	1120	C	Sidechain
1	a	1121	U	Sidechain
1	a	1126	U	Sidechain
1	a	1127	G	Sidechain
1	a	1130	A	Sidechain
1	a	1133	G	Sidechain

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Mol	Chain	Res	Type	Group
1	a	1138	G	Sidechain
1	a	1139	G	Sidechain
1	a	1142	G	Sidechain
1	a	1143	G	Sidechain
1	a	1144	G	Sidechain
1	a	115	G	Sidechain
1	a	1158	C	Sidechain
1	a	1160	G	Sidechain
1	a	1161	C	Sidechain
1	a	1164	G	Sidechain
1	a	1173	U	Sidechain
1	a	1176	A	Sidechain
1	a	1178	G	Sidechain
1	a	1181	G	Sidechain
1	a	119	A	Sidechain
1	a	1197	A	Sidechain
1	a	1214	C	Sidechain
1	a	1224	U	Sidechain
1	a	1226	C	Sidechain
1	a	1227	A	Sidechain
1	a	1250	A	Sidechain
1	a	1255	G	Sidechain
1	a	1260	G	Sidechain
1	a	1261	A	Sidechain
1	a	1266	G	Sidechain
1	a	1268	G	Sidechain
1	a	1276	G	Sidechain
1	a	1285	A	Sidechain
1	a	1289	A	Sidechain
1	a	1298	U	Sidechain
1	a	1318	A	Sidechain
1	a	1320	C	Sidechain
1	a	1321	U	Sidechain
1	a	1323	G	Sidechain
1	a	1326	U	Sidechain
1	a	1331	G	Sidechain
1	a	1332	A	Sidechain
1	a	1338	G	Sidechain
1	a	1345	U	Sidechain
1	a	1348	U	Sidechain
1	a	1357	A	Sidechain
1	a	1358	U	Sidechain

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Mol	Chain	Res	Type	Group
1	a	1362	A	Sidechain
1	a	1363	A	Sidechain
1	a	1367	C	Sidechain
1	a	137	U	Sidechain
1	a	1370	G	Sidechain
1	a	1372	U	Sidechain
1	a	1379	G	Sidechain
1	a	138	G	Sidechain
1	a	1384	C	Sidechain
1	a	1387	G	Sidechain
1	a	1401	G	Sidechain
1	a	1417	G	Sidechain
1	a	1431	A	Sidechain
1	a	1432	G	Sidechain
1	a	1451	U	Sidechain
1	a	1472	U	Sidechain
1	a	1494	G	Sidechain
1	a	1495	U	Sidechain
1	a	150	U	Sidechain
1	a	1505	G	Sidechain
1	a	1516	G	Sidechain
1	a	1518	A	Sidechain
1	a	1519	A	Sidechain
1	a	1522	U	Sidechain
1	a	1525	G	Sidechain
1	a	1527	U	Sidechain
1	a	1528	U	Sidechain
1	a	1529	G	Sidechain
1	a	1530	G	Sidechain
1	a	1531	A	Sidechain
1	a	154	U	Sidechain
1	a	159	G	Sidechain
1	a	165	G	Sidechain
1	a	17	U	Sidechain
1	a	170	U	Sidechain
1	a	173	U	Sidechain
1	a	177	G	Sidechain
1	a	181	A	Sidechain
1	a	185	U	Sidechain
1	a	187	G	Sidechain
1	a	196	A	Sidechain
1	a	197	A	Sidechain

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Mol	Chain	Res	Type	Group
1	a	203	G	Sidechain
1	a	204	G	Sidechain
1	a	205	A	Sidechain
1	a	206	C	Sidechain
1	a	220	G	Sidechain
1	a	244	U	Sidechain
1	a	250	A	Sidechain
1	a	251	G	Sidechain
1	a	252	U	Sidechain
1	a	255	G	Sidechain
1	a	263	A	Sidechain
1	a	264	C	Sidechain
1	a	265	G	Sidechain
1	a	274	A	Sidechain
1	a	297	G	Sidechain
1	a	30	U	Sidechain
1	a	310	G	Sidechain
1	a	317	U	Sidechain
1	a	324	G	Sidechain
1	a	325	A	Sidechain
1	a	326	G	Sidechain
1	a	33	A	Sidechain
1	a	332	G	Sidechain
1	a	343	U	Sidechain
1	a	346	G	Sidechain
1	a	362	G	Sidechain
1	a	363	A	Sidechain
1	a	365	U	Sidechain
1	a	37	U	Sidechain
1	a	377	G	Sidechain
1	a	378	G	Sidechain
1	a	380	G	Sidechain
1	a	389	A	Sidechain
1	a	391	G	Sidechain
1	a	398	U	Sidechain
1	a	417	G	Sidechain
1	a	42	G	Sidechain
1	a	420	U	Sidechain
1	a	423	G	Sidechain
1	a	439	U	Sidechain
1	a	448	A	Sidechain
1	a	449	G	Sidechain

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Mol	Chain	Res	Type	Group
1	a	452	A	Sidechain
1	a	455	G	Sidechain
1	a	481	G	Sidechain
1	a	484	G	Sidechain
1	a	49	U	Sidechain
1	a	491	G	Sidechain
1	a	519	C	Sidechain
1	a	523	A	Sidechain
1	a	543	U	Sidechain
1	a	552	U	Sidechain
1	a	553	A	Sidechain
1	a	561	U	Sidechain
1	a	566	G	Sidechain
1	a	572	A	Sidechain
1	a	575	G	Sidechain
1	a	594	U	Sidechain
1	a	621	A	Sidechain
1	a	623	C	Sidechain
1	a	632	U	Sidechain
1	a	633	G	Sidechain
1	a	671	G	Sidechain
1	a	674	G	Sidechain
1	a	682	G	Sidechain
1	a	683	G	Sidechain
1	a	693	G	Sidechain
1	a	695	A	Sidechain
1	a	704	A	Sidechain
1	a	710	G	Sidechain
1	a	714	G	Sidechain
1	a	721	G	Sidechain
1	a	722	G	Sidechain
1	a	725	G	Sidechain
1	a	727	G	Sidechain
1	a	728	A	Sidechain
1	a	740	U	Sidechain
1	a	75	G	Sidechain
1	a	757	U	Sidechain
1	a	760	G	Sidechain
1	a	79	G	Sidechain
1	a	791	G	Sidechain
1	a	792	A	Sidechain
1	a	794	A	Sidechain

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Mol	Chain	Res	Type	Group
1	a	798	U	Sidechain
1	a	80	A	Sidechain
1	a	813	U	Sidechain
1	a	827	U	Sidechain
1	a	838	G	Sidechain
1	a	84	U	Sidechain
1	a	847	G	Sidechain
1	a	855	U	Sidechain
1	a	865	A	Sidechain
1	a	869	G	Sidechain
1	a	874	G	Sidechain
1	a	883	C	Sidechain
1	a	884	U	Sidechain
1	a	898	G	Sidechain
1	a	899	C	Sidechain
1	a	917	G	Sidechain
1	a	920	U	Sidechain
1	a	929	G	Sidechain
1	a	933	G	Sidechain
1	a	94	G	Sidechain
1	a	944	G	Sidechain
1	a	958	A	Sidechain
1	a	965	U	Sidechain
1	a	973	G	Sidechain
1	a	978	A	Sidechain
1	a	982	U	Sidechain
1	a	985	C	Sidechain
1	a	991	U	Sidechain
1	a	992	U	Sidechain
1	a	993	G	Sidechain
1	a	994	A	Sidechain
2	b	136	ARG	Sidechain
2	b	94	ARG	Sidechain
3	c	167	TYR	Sidechain
4	d	12	ARG	Sidechain
4	d	145	ARG	Sidechain
4	d	164	ARG	Sidechain
4	d	183	ARG	Sidechain
4	d	61	ARG	Sidechain
5	e	111	ARG	Sidechain
5	e	92	ARG	Sidechain
6	f	79	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	f	86	ARG	Sidechain
6	f	91	ARG	Sidechain
7	g	118	ARG	Sidechain
7	g	2	ARG	Sidechain
8	h	64	TYR	Sidechain
8	h	79	ARG	Sidechain
8	h	85	TYR	Sidechain
9	i	112	ARG	Sidechain
9	i	118	ARG	Sidechain
9	i	37	TYR	Sidechain
9	i	43	ALA	Peptide
9	i	63	TYR	Sidechain
9	i	79	ARG	Sidechain
9	i	94	ARG	Sidechain
10	j	16	ARG	Sidechain
10	j	62	ARG	Sidechain
10	j	68	ARG	Sidechain
11	k	124	LYS	Peptide
11	k	36	ARG	Sidechain
12	l	11	ARG	Sidechain
12	l	120	ARG	Sidechain
12	l	30	ARG	Sidechain
12	l	55	ARG	Sidechain
12	l	8	ARG	Sidechain
12	l	85	ARG	Sidechain
14	n	59	ARG	Sidechain
15	o	53	ARG	Sidechain
16	p	25	ARG	Sidechain
16	p	51	ARG	Sidechain
18	r	22	TYR	Sidechain
18	r	52	ARG	Sidechain
18	r	56	ARG	Sidechain
18	r	72	ARG	Sidechain
19	s	2	ARG	Sidechain
20	t	17	ARG	Sidechain
20	t	73	ARG	Sidechain
21	u	17	ARG	Sidechain
21	u	44	ARG	Sidechain
22	x	15	U	Sidechain
22	x	16	A	Sidechain
23	y	12	G	Sidechain
23	y	14	A	Sidechain

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Mol	Chain	Res	Type	Group
23	y	18	U	Sidechain
23	y	19	G	Sidechain
23	y	22	A	Sidechain
23	y	23	G	Sidechain
23	y	24	C	Sidechain
23	y	25	U	Sidechain
23	y	45	A	Sidechain
23	y	46	G	Sidechain
23	y	48	U	Sidechain
23	y	50	G	Sidechain
23	y	54	G	Sidechain
23	y	57	C	Sidechain
23	y	65	G	Sidechain
23	y	68	C	Sidechain
23	y	69	C	Sidechain
23	y	8	U	Sidechain
24	z	509	ARG	Sidechain
24	z	527	GLU	Peptide
24	z	605	ARG	Sidechain
24	z	639	ASP	Peptide
24	z	755	ARG	Sidechain
24	z	767	TYR	Peptide
24	z	787	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33012	0	16618	0	0
2	b	1705	0	1732	0	0
3	c	1625	0	1699	0	0
4	d	1643	0	1710	0	0
5	e	1106	0	1148	0	0
6	f	818	0	808	0	0
7	g	1182	0	1240	0	0
8	h	979	0	1034	0	0
9	i	1022	0	1070	0	0
10	j	787	0	828	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	k	877	0	887	0	0
12	l	955	0	1019	0	0
13	m	884	0	944	0	0
14	n	500	0	526	0	0
15	o	714	0	737	0	0
16	p	649	0	666	0	0
17	q	649	0	691	0	0
18	r	445	0	471	0	0
19	s	638	0	665	0	0
20	t	665	0	714	0	0
21	u	426	0	449	0	0
22	x	126	0	66	0	0
23	y	1639	0	837	0	0
24	z	3847	0	3909	0	0
25	A	61262	0	30823	0	0
26	E	1552	0	1619	0	0
27	F	1411	0	1447	0	0
28	G	885	0	913	0	0
29	H	1323	0	1374	0	0
30	I	1032	0	1088	0	0
31	J	1129	0	1162	0	0
32	K	939	0	1012	0	0
33	L	1045	0	1117	0	0
34	M	1074	0	1157	0	0
35	N	961	0	1000	0	0
36	O	892	0	923	0	0
37	P	917	0	965	0	0
38	Q	947	0	1022	0	0
39	R	816	0	839	0	0
40	S	857	0	922	0	0
41	T	739	0	807	0	0
42	U	780	0	834	0	0
43	V	753	0	780	0	0
44	X	2526	0	1282	0	0
45	Y	302	0	343	0	0
46	0	596	0	610	0	0
47	1	625	0	655	0	0
48	2	509	0	543	0	0
49	3	449	0	491	0	0
50	4	1565	0	1616	0	0
51	5	444	0	461	0	0
52	6	410	0	440	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	7	377	0	418	0	0
54	8	504	0	574	0	0
55	9	2083	0	2157	0	0
All	All	146597	0	99862	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	216/218 (99%)	191 (88%)	16 (7%)	9 (4%)	2	21
3	c	204/206 (99%)	190 (93%)	9 (4%)	5 (2%)	4	29
4	d	203/205 (99%)	184 (91%)	16 (8%)	3 (2%)	8	38
5	e	148/150 (99%)	135 (91%)	9 (6%)	4 (3%)	4	28
6	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2	21
7	g	149/151 (99%)	134 (90%)	11 (7%)	4 (3%)	4	28
8	h	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
9	i	125/127 (98%)	111 (89%)	10 (8%)	4 (3%)	3	25
10	j	96/98 (98%)	85 (88%)	8 (8%)	3 (3%)	3	25
11	k	115/117 (98%)	98 (85%)	13 (11%)	4 (4%)	3	23
12	l	121/123 (98%)	100 (83%)	15 (12%)	6 (5%)	1	18
13	m	112/114 (98%)	106 (95%)	5 (4%)	1 (1%)	14	48
14	n	59/61 (97%)	52 (88%)	4 (7%)	3 (5%)	1	18
15	o	86/88 (98%)	77 (90%)	6 (7%)	3 (4%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	p	80/82 (98%)	71 (89%)	6 (8%)	3 (4%)	2	22
17	q	78/80 (98%)	64 (82%)	10 (13%)	4 (5%)	1	18
18	r	52/54 (96%)	48 (92%)	2 (4%)	2 (4%)	2	22
19	s	77/79 (98%)	69 (90%)	8 (10%)	0	100	100
20	t	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
21	u	49/51 (96%)	35 (71%)	10 (20%)	4 (8%)	0	11
24	z	507/509 (100%)	464 (92%)	30 (6%)	13 (3%)	4	29
26	E	199/201 (99%)	182 (92%)	14 (7%)	3 (2%)	8	38
27	F	175/177 (99%)	157 (90%)	13 (7%)	5 (3%)	3	26
28	G	115/117 (98%)	100 (87%)	10 (9%)	5 (4%)	2	20
29	H	174/176 (99%)	157 (90%)	11 (6%)	6 (3%)	3	24
30	I	139/141 (99%)	117 (84%)	15 (11%)	7 (5%)	1	18
31	J	140/142 (99%)	127 (91%)	10 (7%)	3 (2%)	5	32
32	K	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	7	36
33	L	141/143 (99%)	119 (84%)	19 (14%)	3 (2%)	5	32
34	M	134/136 (98%)	123 (92%)	10 (8%)	1 (1%)	18	54
35	N	118/120 (98%)	105 (89%)	12 (10%)	1 (1%)	16	52
36	O	114/116 (98%)	108 (95%)	5 (4%)	1 (1%)	14	48
37	P	112/114 (98%)	102 (91%)	5 (4%)	5 (4%)	2	20
38	Q	115/117 (98%)	107 (93%)	7 (6%)	1 (1%)	14	48
39	R	101/103 (98%)	85 (84%)	14 (14%)	2 (2%)	6	33
40	S	108/110 (98%)	100 (93%)	6 (6%)	2 (2%)	6	34
41	T	91/93 (98%)	77 (85%)	13 (14%)	1 (1%)	11	44
42	U	100/102 (98%)	88 (88%)	10 (10%)	2 (2%)	6	33
43	V	92/94 (98%)	88 (96%)	2 (2%)	2 (2%)	5	31
45	Y	36/38 (95%)	30 (83%)	4 (11%)	2 (6%)	1	17
46	0	77/79 (98%)	59 (77%)	13 (17%)	5 (6%)	1	15
47	1	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	9	41
48	2	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	7	37
49	3	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
50	4	207/209 (99%)	177 (86%)	18 (9%)	12 (6%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	5	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
52	6	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
53	7	44/46 (96%)	38 (86%)	4 (9%)	2 (4%)	2	20
54	8	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	7	37
55	9	269/271 (99%)	243 (90%)	19 (7%)	7 (3%)	4	29
All	All	6062/6162 (98%)	5429 (90%)	471 (8%)	162 (3%)	6	28

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	14	HIS
2	b	37	VAL
4	d	31	CYS
6	f	91	ARG
7	g	113	LYS
7	g	114	SER
7	g	147	ASN
14	n	43	ASN
21	u	35	GLU
24	z	541	ILE
28	G	106	PHE
30	I	21	PRO
37	P	52	ARG
41	T	55	VAL
42	U	92	VAL
46	0	56	HIS
47	1	18	SER
50	4	54	ALA
50	4	118	PHE
50	4	174	SER
53	7	7	PRO
2	b	72	LYS
2	b	76	SER
4	d	16	THR
6	f	33	GLU
6	f	85	ILE
9	i	90	ASP
9	i	128	LYS
10	j	57	VAL
12	l	47	ALA

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Mol	Chain	Res	Type
14	n	62	ASN
16	p	49	GLY
17	q	16	MET
17	q	79	GLU
24	z	400	VAL
24	z	473	ASP
26	E	68	ALA
27	F	11	VAL
27	F	111	ARG
28	G	108	VAL
34	M	134	THR
36	O	90	VAL
40	S	3	THR
45	Y	37	GLN
46	0	10	ARG
50	4	46	ARG
50	4	134	HIS
53	7	5	PHE
55	9	71	ASP
55	9	119	VAL
55	9	217	PRO
2	b	86	CYS
3	c	14	VAL
3	c	173	PRO
4	d	45	PRO
5	e	43	GLY
5	e	54	GLU
7	g	83	THR
12	l	33	CYS
13	m	9	PRO
15	o	45	HIS
16	p	27	ALA
21	u	8	ASN
24	z	448	HIS
24	z	763	LEU
24	z	788	PRO
26	E	96	VAL
27	F	138	PRO
28	G	81	LEU
28	G	88	HIS
29	H	12	ALA
29	H	83	THR

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Mol	Chain	Res	Type
30	I	17	ALA
30	I	75	ALA
30	I	118	GLY
31	J	65	THR
31	J	74	TYR
33	L	111	ILE
38	Q	95	ALA
39	R	31	GLU
46	0	29	SER
46	0	40	ARG
50	4	85	ALA
50	4	95	SER
50	4	122	VAL
50	4	136	ASN
55	9	141	HIS
2	b	224	ARG
3	c	59	PRO
6	f	98	GLU
9	i	108	ARG
11	k	72	ALA
11	k	90	PRO
12	l	21	PRO
18	r	70	THR
21	u	10	PRO
24	z	746	PHE
28	G	58	THR
29	H	32	LEU
29	H	164	ALA
30	I	18	ASN
30	I	104	GLN
31	J	111	LYS
33	L	81	ASP
35	N	119	SER
37	P	103	THR
40	S	64	ALA
42	U	6	ARG
43	V	66	ASP
48	2	9	LYS
55	9	50	THR
55	9	59	GLN
2	b	33	ALA
2	b	192	PRO

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Mol	Chain	Res	Type
5	e	146	MET
5	e	157	GLY
9	i	87	MET
10	j	42	LEU
11	k	114	PRO
11	k	120	CYS
12	l	101	LEU
14	n	70	PRO
15	o	87	ARG
16	p	79	ASN
17	q	5	ARG
17	q	11	VAL
24	z	622	PRO
24	z	849	LYS
24	z	857	ASN
27	F	149	ARG
32	K	46	ALA
33	L	41	ARG
37	P	56	SER
45	Y	16	ILE
46	0	14	ASP
50	4	92	VAL
50	4	103	ASP
50	4	109	VAL
54	8	31	ILE
3	c	159	ALA
10	j	41	PRO
12	l	44	PRO
12	l	70	GLY
15	o	16	ARG
18	r	71	ASP
24	z	686	VAL
26	E	46	GLN
29	H	46	ASP
32	K	71	ARG
43	V	71	LYS
24	z	748	VAL
27	F	135	ILE
55	9	7	PRO
2	b	16	GLY
3	c	127	VAL
30	I	48	ILE

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Mol	Chain	Res	Type
37	P	69	VAL
37	P	109	ILE
39	R	52	PRO
21	u	13	VAL
29	H	11	PRO
24	z	727	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/180 (100%)	173 (96%)	7 (4%)	28	51
3	c	170/170 (100%)	166 (98%)	4 (2%)	43	63
4	d	172/172 (100%)	170 (99%)	2 (1%)	63	73
5	e	113/113 (100%)	113 (100%)	0	100	100
6	f	87/87 (100%)	84 (97%)	3 (3%)	32	55
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	102 (98%)	2 (2%)	50	67
9	i	105/105 (100%)	104 (99%)	1 (1%)	68	76
10	j	86/86 (100%)	84 (98%)	2 (2%)	44	64
11	k	90/90 (100%)	86 (96%)	4 (4%)	25	48
12	l	103/103 (100%)	100 (97%)	3 (3%)	37	58
13	m	92/92 (100%)	91 (99%)	1 (1%)	65	74
14	n	52/52 (100%)	50 (96%)	2 (4%)	29	51
15	o	76/76 (100%)	74 (97%)	2 (3%)	40	61
16	p	65/65 (100%)	63 (97%)	2 (3%)	35	56
17	q	74/74 (100%)	71 (96%)	3 (4%)	27	49
18	r	47/47 (100%)	47 (100%)	0	100	100
19	s	70/70 (100%)	69 (99%)	1 (1%)	59	71
20	t	65/65 (100%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	u	44/44 (100%)	42 (96%)	2 (4%)	24	47
24	z	409/409 (100%)	398 (97%)	11 (3%)	39	60
26	E	165/165 (100%)	159 (96%)	6 (4%)	31	53
27	F	148/148 (100%)	146 (99%)	2 (1%)	59	71
28	G	88/88 (100%)	84 (96%)	4 (4%)	24	47
29	H	137/137 (100%)	134 (98%)	3 (2%)	45	65
30	I	109/109 (100%)	104 (95%)	5 (5%)	24	47
31	J	116/116 (100%)	113 (97%)	3 (3%)	40	61
32	K	103/103 (100%)	102 (99%)	1 (1%)	68	76
33	L	102/102 (100%)	100 (98%)	2 (2%)	48	66
34	M	109/109 (100%)	107 (98%)	2 (2%)	51	68
35	N	100/100 (100%)	100 (100%)	0	100	100
36	O	86/86 (100%)	79 (92%)	7 (8%)	11	34
37	P	99/99 (100%)	95 (96%)	4 (4%)	28	50
38	Q	89/89 (100%)	88 (99%)	1 (1%)	65	74
39	R	84/84 (100%)	80 (95%)	4 (5%)	23	46
40	S	93/93 (100%)	92 (99%)	1 (1%)	65	74
41	T	80/80 (100%)	76 (95%)	4 (5%)	22	45
42	U	83/83 (100%)	79 (95%)	4 (5%)	23	46
43	V	78/78 (100%)	77 (99%)	1 (1%)	61	72
45	Y	34/34 (100%)	34 (100%)	0	100	100
46	0	59/59 (100%)	56 (95%)	3 (5%)	21	45
47	1	67/67 (100%)	67 (100%)	0	100	100
48	2	55/55 (100%)	51 (93%)	4 (7%)	13	37
49	3	48/48 (100%)	45 (94%)	3 (6%)	16	41
50	4	164/164 (100%)	160 (98%)	4 (2%)	43	63
51	5	47/47 (100%)	45 (96%)	2 (4%)	26	48
52	6	45/45 (100%)	43 (96%)	2 (4%)	25	48
53	7	38/38 (100%)	37 (97%)	1 (3%)	40	61
54	8	51/51 (100%)	51 (100%)	0	100	100
55	9	216/216 (100%)	212 (98%)	4 (2%)	50	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5021/5021 (100%)	4892 (97%)	129 (3%)	41 61

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	39	ILE
2	b	40	ILE
2	b	46	VAL
2	b	65	LYS
2	b	71	THR
2	b	121	GLN
2	b	170	ILE
3	c	31	ASN
3	c	106	ARG
3	c	160	GLU
3	c	187	GLU
4	d	170	LEU
4	d	196	GLU
6	f	45	ARG
6	f	91	ARG
6	f	93	LYS
8	h	110	MET
8	h	124	ILE
9	i	40	ARG
10	j	15	HIS
10	j	32	THR
11	k	39	ASN
11	k	41	LEU
11	k	60	PHE
11	k	107	THR
12	l	29	LYS
12	l	79	ILE
12	l	87	LYS
13	m	24	VAL
14	n	82	ILE
14	n	101	TRP
15	o	50	HIS
15	o	56	LEU
16	p	35	ARG
16	p	45	GLU
17	q	48	GLU
17	q	67	SER

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Mol	Chain	Res	Type
17	q	79	GLU
19	s	78	THR
21	u	9	GLU
21	u	35	GLU
24	z	408	LEU
24	z	414	THR
24	z	504	GLU
24	z	586	VAL
24	z	612	GLU
24	z	645	ARG
24	z	696	ASP
24	z	704	ILE
24	z	786	LEU
24	z	851	ASP
24	z	889	ILE
26	E	25	GLU
26	E	60	TRP
26	E	90	GLN
26	E	102	ARG
26	E	149	ILE
26	E	171	ASP
27	F	35	LEU
27	F	137	PHE
28	G	52	MET
28	G	62	ARG
28	G	96	PHE
28	G	108	VAL
29	H	29	ASN
29	H	83	THR
29	H	169	ARG
30	I	49	GLU
30	I	59	THR
30	I	68	PHE
30	I	122	GLU
30	I	134	SER
31	J	43	GLU
31	J	81	ILE
31	J	111	LYS
32	K	3	GLN
33	L	47	ARG
33	L	107	PHE
34	M	3	GLN

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Mol	Chain	Res	Type
34	M	53	MET
36	O	32	PRO
36	O	33	ARG
36	O	46	GLU
36	O	67	ASN
36	O	95	SER
36	O	116	GLN
36	O	117	PHE
37	P	72	VAL
37	P	74	GLN
37	P	103	THR
37	P	110	LYS
38	Q	87	VAL
39	R	4	VAL
39	R	10	LYS
39	R	79	ARG
39	R	91	GLN
40	S	71	VAL
41	T	12	ARG
41	T	18	GLU
41	T	36	LYS
41	T	87	LEU
42	U	6	ARG
42	U	45	GLN
42	U	64	ILE
42	U	92	VAL
43	V	59	GLU
46	0	19	ARG
46	0	50	VAL
46	0	71	LYS
48	2	23	ARG
48	2	39	GLN
48	2	45	GLN
48	2	59	GLU
49	3	33	HIS
49	3	36	GLU
49	3	43	ILE
50	4	59	ARG
50	4	126	ASN
50	4	173	GLN
50	4	175	LEU
51	5	2	VAL

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Mol	Chain	Res	Type
51	5	9	ARG
52	6	9	LYS
52	6	31	GLU
53	7	7	PRO
55	9	86	ARG
55	9	213	ARG
55	9	217	PRO
55	9	269	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1538/1539 (99%)	230 (14%)	0
22	x	5/6 (83%)	4 (80%)	0
23	y	76/77 (98%)	24 (31%)	0
25	A	2850/2854 (99%)	418 (14%)	74 (2%)
44	X	117/118 (99%)	15 (12%)	3 (2%)
All	All	4586/4594 (99%)	691 (15%)	77 (1%)

All (691) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	3	A
1	a	7	A
1	a	9	G
1	a	31	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	49	U
1	a	50	A
1	a	51	A
1	a	52	C
1	a	60	A
1	a	61	G
1	a	70	U
1	a	71	A

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Mol	Chain	Res	Type
1	a	72	A
1	a	74	A
1	a	83	C
1	a	85	U
1	a	86	G
1	a	87	C
1	a	88	U
1	a	97	G
1	a	116	A
1	a	118	U
1	a	120	A
1	a	121	U
1	a	130	A
1	a	131	A
1	a	136	C
1	a	144	G
1	a	155	A
1	a	159	G
1	a	182	A
1	a	183	C
1	a	197	A
1	a	204	G
1	a	207	C
1	a	209	U
1	a	211	G
1	a	212	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	280	C
1	a	289	G
1	a	307	C
1	a	326	G
1	a	328	C
1	a	329	A
1	a	330	C
1	a	332	G
1	a	345	C
1	a	347	G
1	a	352	C

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Mol	Chain	Res	Type
1	a	354	G
1	a	367	U
1	a	372	C
1	a	406	G
1	a	411	A
1	a	412	A
1	a	413	G
1	a	414	A
1	a	421	U
1	a	422	C
1	a	423	G
1	a	424	G
1	a	429	U
1	a	430	A
1	a	438	U
1	a	439	U
1	a	451	A
1	a	465	A
1	a	466	A
1	a	467	U
1	a	468	A
1	a	469	C
1	a	479	U
1	a	481	G
1	a	486	U
1	a	497	G
1	a	511	C
1	a	518	C
1	a	524	G
1	a	527	G
1	a	531	U
1	a	532	A
1	a	547	A
1	a	563	A
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	596	A
1	a	620	C
1	a	631	C
1	a	632	U

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Mol	Chain	Res	Type
1	a	633	G
1	a	650	G
1	a	665	A
1	a	693	G
1	a	719	C
1	a	720	C
1	a	722	G
1	a	724	G
1	a	731	G
1	a	734	G
1	a	747	A
1	a	755	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	815	A
1	a	817	C
1	a	819	A
1	a	820	U
1	a	821	G
1	a	828	U
1	a	829	G
1	a	832	G
1	a	840	C
1	a	842	U
1	a	843	U
1	a	844	G
1	a	913	A
1	a	914	A
1	a	926	G
1	a	927	G
1	a	934	C
1	a	960	U
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	983	A
1	a	993	G
1	a	1004	A
1	a	1008	U
1	a	1018	G

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Mol	Chain	Res	Type
1	a	1022	A
1	a	1026	G
1	a	1027	C
1	a	1028	C
1	a	1029	U
1	a	1030	U
1	a	1031	C
1	a	1033	G
1	a	1065	U
1	a	1073	U
1	a	1080	A
1	a	1086	U
1	a	1087	G
1	a	1093	A
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1102	A
1	a	1109	C
1	a	1110	A
1	a	1111	A
1	a	1125	U
1	a	1132	C
1	a	1133	G
1	a	1134	G
1	a	1135	U
1	a	1136	C
1	a	1137	C
1	a	1139	G
1	a	1140	C
1	a	1141	C
1	a	1142	G
1	a	1145	A
1	a	1159	U
1	a	1160	G
1	a	1161	C
1	a	1167	A
1	a	1168	U
1	a	1196	A
1	a	1197	A
1	a	1201	A
1	a	1202	U

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Mol	Chain	Res	Type
1	a	1212	U
1	a	1213	A
1	a	1226	C
1	a	1238	A
1	a	1240	U
1	a	1241	G
1	a	1248	A
1	a	1250	A
1	a	1251	A
1	a	1253	G
1	a	1261	A
1	a	1275	A
1	a	1279	G
1	a	1280	A
1	a	1281	C
1	a	1282	C
1	a	1300	G
1	a	1302	C
1	a	1304	G
1	a	1305	G
1	a	1317	C
1	a	1318	A
1	a	1321	U
1	a	1336	C
1	a	1362	A
1	a	1363	A
1	a	1364	U
1	a	1370	G
1	a	1378	C
1	a	1379	G
1	a	1398	A
1	a	1419	G
1	a	1441	A
1	a	1442	G
1	a	1446	A
1	a	1493	A
1	a	1497	G
1	a	1503	A
1	a	1505	G
1	a	1529	G
1	a	1530	G
1	a	1531	A

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Mol	Chain	Res	Type
1	a	1532	U
1	a	1534	A
1	a	1536	C
1	a	1537	U
22	x	14	A
22	x	15	U
22	x	16	A
22	x	17	U
23	y	2	G
23	y	8	U
23	y	9	G
23	y	16	C
23	y	18	U
23	y	20	G
23	y	21	U
23	y	22	A
23	y	23	G
23	y	24	C
23	y	25	U
23	y	43	G
23	y	48	U
23	y	55	U
23	y	56	U
23	y	57	C
23	y	58	A
23	y	59	A
23	y	60	A
23	y	61	U
23	y	62	C
23	y	72	C
23	y	74	A
23	y	76	C
25	A	10	A
25	A	12	U
25	A	46	G
25	A	61	C
25	A	63	A
25	A	71	A
25	A	73	A
25	A	74	A
25	A	75	G
25	A	100	U

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Mol	Chain	Res	Type
25	A	101	A
25	A	102	U
25	A	103	A
25	A	118	A
25	A	119	A
25	A	120	U
25	A	125	A
25	A	126	A
25	A	136	G
25	A	138	U
25	A	139	U
25	A	140	C
25	A	141	G
25	A	142	A
25	A	149	A
25	A	162	U
25	A	163	C
25	A	164	C
25	A	181	A
25	A	196	A
25	A	199	A
25	A	215	G
25	A	216	A
25	A	219	A
25	A	221	A
25	A	222	A
25	A	228	C
25	A	230	G
25	A	248	G
25	A	255	A
25	A	265	A
25	A	266	G
25	A	272	A
25	A	273	G
25	A	276	U
25	A	303	G
25	A	311	A
25	A	321	U
25	A	322	A
25	A	323	C
25	A	329	G
25	A	330	A

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Mol	Chain	Res	Type
25	A	362	A
25	A	367	G
25	A	369	U
25	A	371	A
25	A	372	G
25	A	373	U
25	A	386	G
25	A	396	G
25	A	404	A
25	A	405	U
25	A	411	G
25	A	412	A
25	A	424	G
25	A	451	U
25	A	452	G
25	A	453	A
25	A	456	C
25	A	457	A
25	A	467	G
25	A	473	G
25	A	480	A
25	A	481	G
25	A	490	C
25	A	491	G
25	A	504	A
25	A	505	A
25	A	508	A
25	A	509	C
25	A	527	C
25	A	528	A
25	A	529	A
25	A	532	A
25	A	533	G
25	A	546	U
25	A	547	A
25	A	548	G
25	A	550	C
25	A	563	A
25	A	572	A
25	A	573	U
25	A	575	A
25	A	586	A

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Mol	Chain	Res	Type
25	A	603	A
25	A	604	G
25	A	614	A
25	A	628	G
25	A	637	A
25	A	638	G
25	A	647	G
25	A	653	U
25	A	655	A
25	A	686	U
25	A	716	A
25	A	730	A
25	A	747	U
25	A	748	G
25	A	749	A
25	A	752	A
25	A	762	U
25	A	764	A
25	A	775	G
25	A	776	G
25	A	782	A
25	A	784	G
25	A	785	G
25	A	792	A
25	A	805	G
25	A	812	C
25	A	819	A
25	A	827	U
25	A	828	U
25	A	845	A
25	A	846	U
25	A	847	U
25	A	859	G
25	A	883	G
25	A	885	C
25	A	896	A
25	A	897	C
25	A	910	A
25	A	914	G
25	A	931	U
25	A	932	U
25	A	941	A

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Mol	Chain	Res	Type
25	A	946	C
25	A	958	U
25	A	959	A
25	A	961	C
25	A	962	G
25	A	974	G
25	A	975	A
25	A	981	A
25	A	982	C
25	A	983	A
25	A	985	C
25	A	995	C
25	A	1009	A
25	A	1012	U
25	A	1013	C
25	A	1021	A
25	A	1022	G
25	A	1023	U
25	A	1026	G
25	A	1027	A
25	A	1033	U
25	A	1045	C
25	A	1046	A
25	A	1047	G
25	A	1058	U
25	A	1059	G
25	A	1060	U
25	A	1061	U
25	A	1062	G
25	A	1066	U
25	A	1068	G
25	A	1069	A
25	A	1070	A
25	A	1071	G
25	A	1076	C
25	A	1077	A
25	A	1079	C
25	A	1080	A
25	A	1083	U
25	A	1084	A
25	A	1085	A
25	A	1088	A

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Mol	Chain	Res	Type
25	A	1089	A
25	A	1096	A
25	A	1100	C
25	A	1112	G
25	A	1128	G
25	A	1129	A
25	A	1130	U
25	A	1132	U
25	A	1133	A
25	A	1135	C
25	A	1142	A
25	A	1144	A
25	A	1174	U
25	A	1175	A
25	A	1176	U
25	A	1186	G
25	A	1210	G
25	A	1211	C
25	A	1212	G
25	A	1238	G
25	A	1250	G
25	A	1253	A
25	A	1256	G
25	A	1266	G
25	A	1271	G
25	A	1272	A
25	A	1273	U
25	A	1285	A
25	A	1300	G
25	A	1301	A
25	A	1365	A
25	A	1368	G
25	A	1384	A
25	A	1396	U
25	A	1416	G
25	A	1419	A
25	A	1428	C
25	A	1453	A
25	A	1458	U
25	A	1459	G
25	A	1482	G
25	A	1493	C

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Mol	Chain	Res	Type
25	A	1508	A
25	A	1509	A
25	A	1510	G
25	A	1515	A
25	A	1523	U
25	A	1524	G
25	A	1533	C
25	A	1535	A
25	A	1566	A
25	A	1567	G
25	A	1569	A
25	A	1578	U
25	A	1585	C
25	A	1608	A
25	A	1610	A
25	A	1647	U
25	A	1648	U
25	A	1674	G
25	A	1679	A
25	A	1714	U
25	A	1715	G
25	A	1729	U
25	A	1730	C
25	A	1733	G
25	A	1738	G
25	A	1744	A
25	A	1758	U
25	A	1759	A
25	A	1761	C
25	A	1762	A
25	A	1764	C
25	A	1773	A
25	A	1786	A
25	A	1787	A
25	A	1800	C
25	A	1801	A
25	A	1802	A
25	A	1808	A
25	A	1810	A
25	A	1816	C
25	A	1829	A
25	A	1833	C

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Mol	Chain	Res	Type
25	A	1847	A
25	A	1870	C
25	A	1872	A
25	A	1873	G
25	A	1906	G
25	A	1913	A
25	A	1914	C
25	A	1929	G
25	A	1930	G
25	A	1937	A
25	A	1952	A
25	A	1953	A
25	A	1955	U
25	A	1965	C
25	A	1966	A
25	A	1967	C
25	A	1970	A
25	A	1971	U
25	A	1972	G
25	A	1991	U
25	A	1993	U
25	A	1997	C
25	A	2022	U
25	A	2023	C
25	A	2031	A
25	A	2032	G
25	A	2043	C
25	A	2052	A
25	A	2055	C
25	A	2056	G
25	A	2058	A
25	A	2059	A
25	A	2060	A
25	A	2061	G
25	A	2069	G
25	A	2072	C
25	A	2093	G
25	A	2104	C
25	A	2105	U
25	A	2106	U
25	A	2107	G
25	A	2108	A

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Mol	Chain	Res	Type
25	A	2109	U
25	A	2110	G
25	A	2134	A
25	A	2136	G
25	A	2137	U
25	A	2144	G
25	A	2145	C
25	A	2148	G
25	A	2151	U
25	A	2152	G
25	A	2155	U
25	A	2156	G
25	A	2180	U
25	A	2182	U
25	A	2183	A
25	A	2198	A
25	A	2199	A
25	A	2203	U
25	A	2204	G
25	A	2211	A
25	A	2214	C
25	A	2225	A
25	A	2238	G
25	A	2239	G
25	A	2250	G
25	A	2252	G
25	A	2278	A
25	A	2283	C
25	A	2286	G
25	A	2287	A
25	A	2305	U
25	A	2307	G
25	A	2308	G
25	A	2322	A
25	A	2325	G
25	A	2327	A
25	A	2333	A
25	A	2345	G
25	A	2359	C
25	A	2361	G
25	A	2383	G
25	A	2384	U

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Mol	Chain	Res	Type
25	A	2385	C
25	A	2388	A
25	A	2390	U
25	A	2402	U
25	A	2406	A
25	A	2423	U
25	A	2424	C
25	A	2425	A
25	A	2428	G
25	A	2429	G
25	A	2430	A
25	A	2433	A
25	A	2435	A
25	A	2440	C
25	A	2441	U
25	A	2447	G
25	A	2448	A
25	A	2474	U
25	A	2476	A
25	A	2491	U
25	A	2494	G
25	A	2502	G
25	A	2503	A
25	A	2505	G
25	A	2518	A
25	A	2520	C
25	A	2529	G
25	A	2533	U
25	A	2535	G
25	A	2553	G
25	A	2554	U
25	A	2555	U
25	A	2561	U
25	A	2565	A
25	A	2566	A
25	A	2567	G
25	A	2572	A
25	A	2584	U
25	A	2585	U
25	A	2586	U
25	A	2603	G
25	A	2609	U

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Mol	Chain	Res	Type
25	A	2613	U
25	A	2629	U
25	A	2630	G
25	A	2671	G
25	A	2689	U
25	A	2690	U
25	A	2714	G
25	A	2725	A
25	A	2726	A
25	A	2733	A
25	A	2744	G
25	A	2748	A
25	A	2757	A
25	A	2765	A
25	A	2778	A
25	A	2791	G
25	A	2798	U
25	A	2801	G
25	A	2809	A
25	A	2818	U
25	A	2820	A
25	A	2821	A
25	A	2849	U
25	A	2867	G
25	A	2872	A
25	A	2880	C
25	A	2884	U
25	A	2885	G
25	A	2894	G
25	A	2903	U
44	X	12	C
44	X	13	G
44	X	14	U
44	X	15	A
44	X	24	G
44	X	35	C
44	X	42	C
44	X	44	G
44	X	51	G
44	X	79	G
44	X	88	C
44	X	89	U

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Mol	Chain	Res	Type
44	X	90	C
44	X	99	A
44	X	109	A

All (77) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	11	C
25	A	99	U
25	A	117	G
25	A	119	A
25	A	141	G
25	A	162	U
25	A	218	A
25	A	228	C
25	A	303	G
25	A	322	A
25	A	329	G
25	A	404	A
25	A	452	G
25	A	503	A
25	A	527	C
25	A	602	A
25	A	603	A
25	A	637	A
25	A	719	C
25	A	746	U
25	A	747	U
25	A	784	G
25	A	845	A
25	A	846	U
25	A	958	U
25	A	1020	A
25	A	1044	C
25	A	1060	U
25	A	1061	U
25	A	1068	G
25	A	1069	A
25	A	1076	C
25	A	1095	A
25	A	1109	C
25	A	1128	G

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Mol	Chain	Res	Type
25	A	1174	U
25	A	1300	G
25	A	1406	U
25	A	1452	G
25	A	1566	A
25	A	1646	C
25	A	1678	A
25	A	1744	A
25	A	1758	U
25	A	1761	C
25	A	1786	A
25	A	1913	A
25	A	1952	A
25	A	1971	U
25	A	1997	C
25	A	2051	A
25	A	2058	A
25	A	2062	A
25	A	2105	U
25	A	2107	G
25	A	2109	U
25	A	2144	G
25	A	2251	G
25	A	2286	G
25	A	2324	U
25	A	2326	C
25	A	2401	U
25	A	2423	U
25	A	2429	G
25	A	2432	A
25	A	2439	A
25	A	2502	G
25	A	2554	U
25	A	2560	A
25	A	2585	U
25	A	2756	U
25	A	2798	U
25	A	2820	A
25	A	2902	C
44	X	12	C
44	X	13	G
44	X	78	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

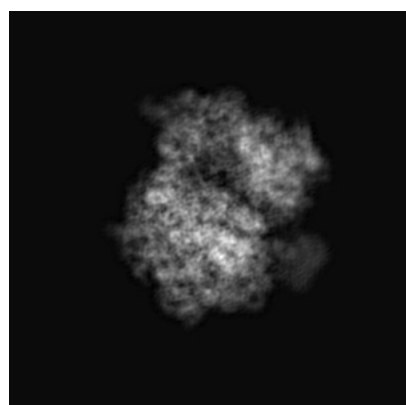
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0662. These allow visual inspection of the internal detail of the map and identification of artifacts.

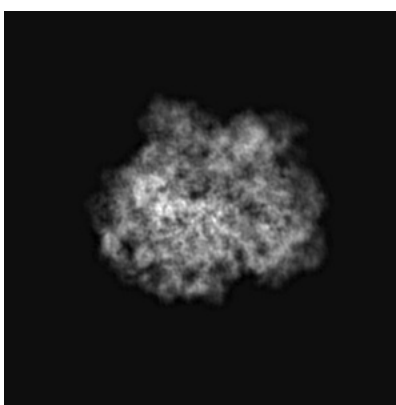
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

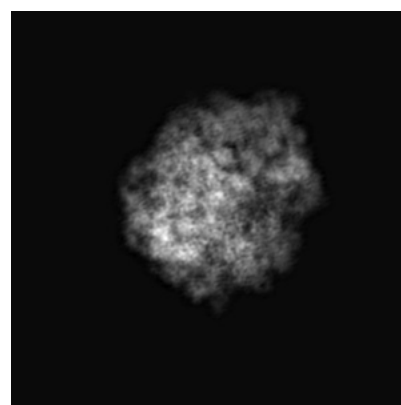
6.1.1 Primary map



X



Y

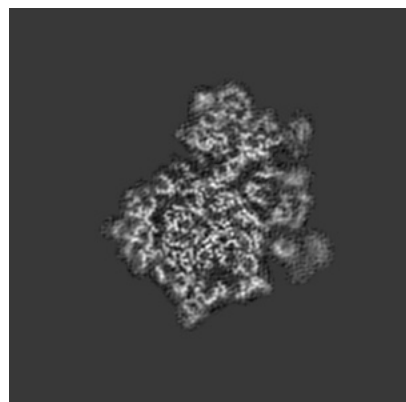


Z

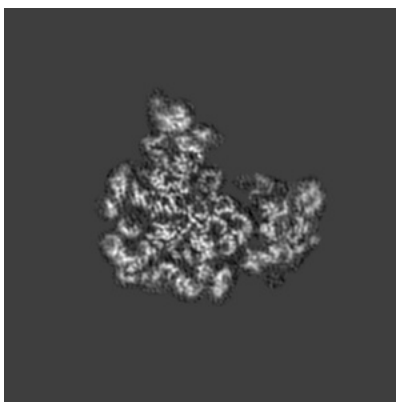
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

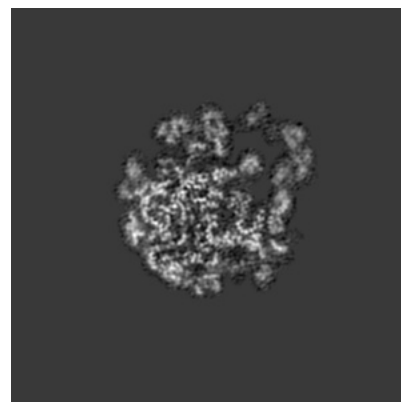
6.2.1 Primary map



X Index: 128



Y Index: 128

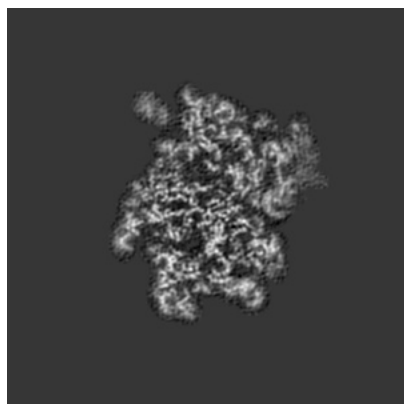


Z Index: 128

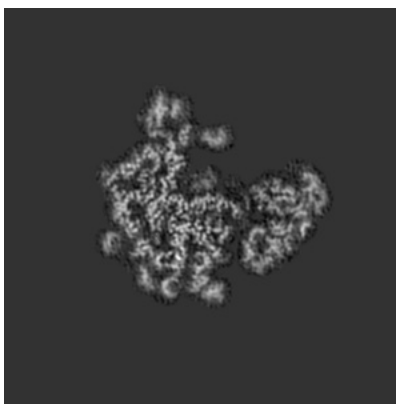
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

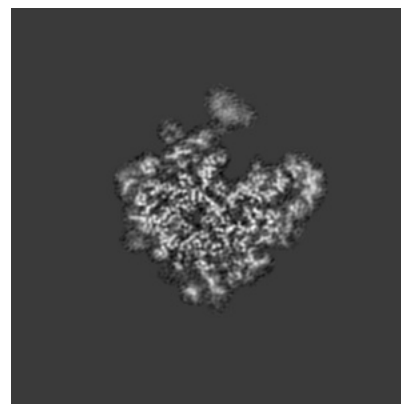
6.3.1 Primary map



X Index: 116



Y Index: 137

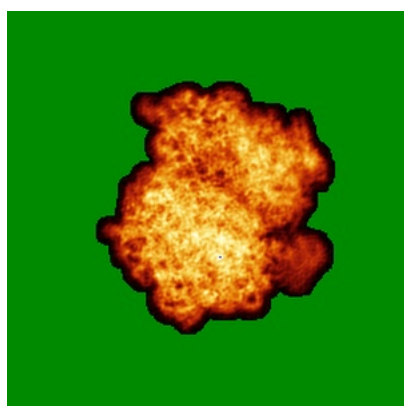


Z Index: 108

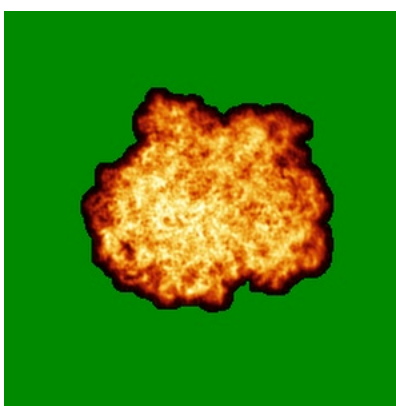
The images above show the largest variance slices of the map in three orthogonal directions.

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

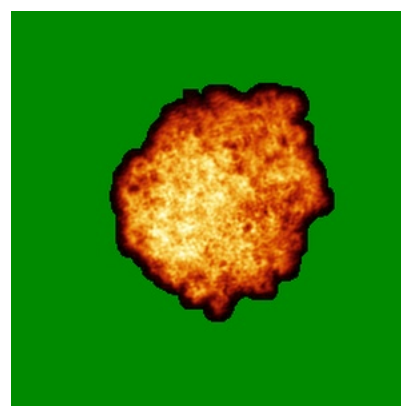
6.4.1 Primary map



X



Y

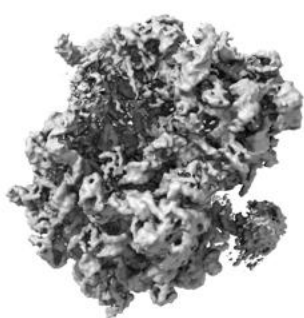


Z

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

6.5 Orthogonal surface views [i](#)

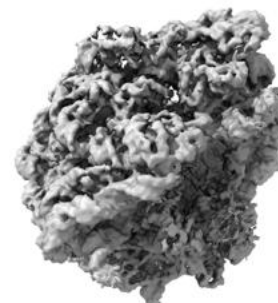
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

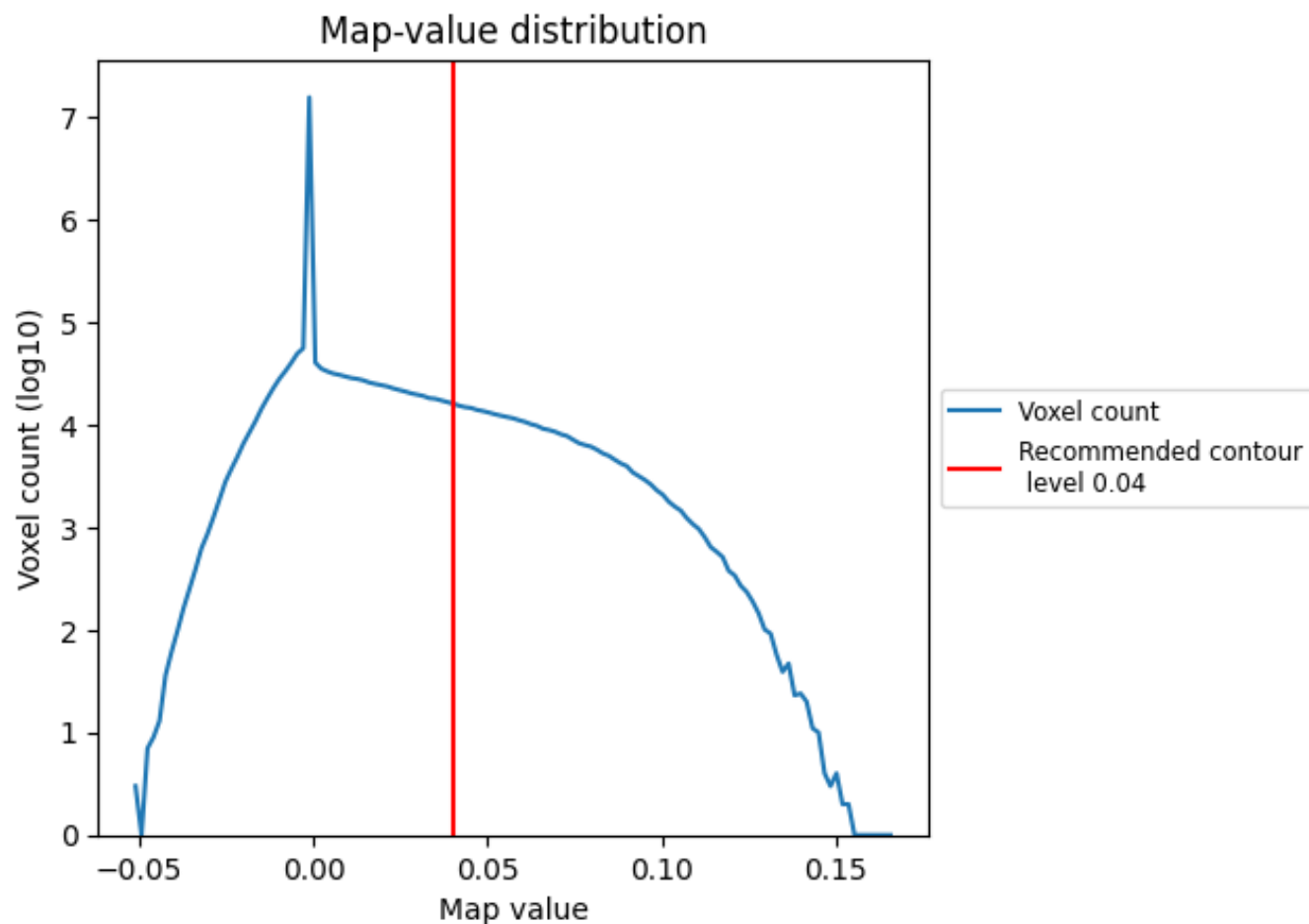
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

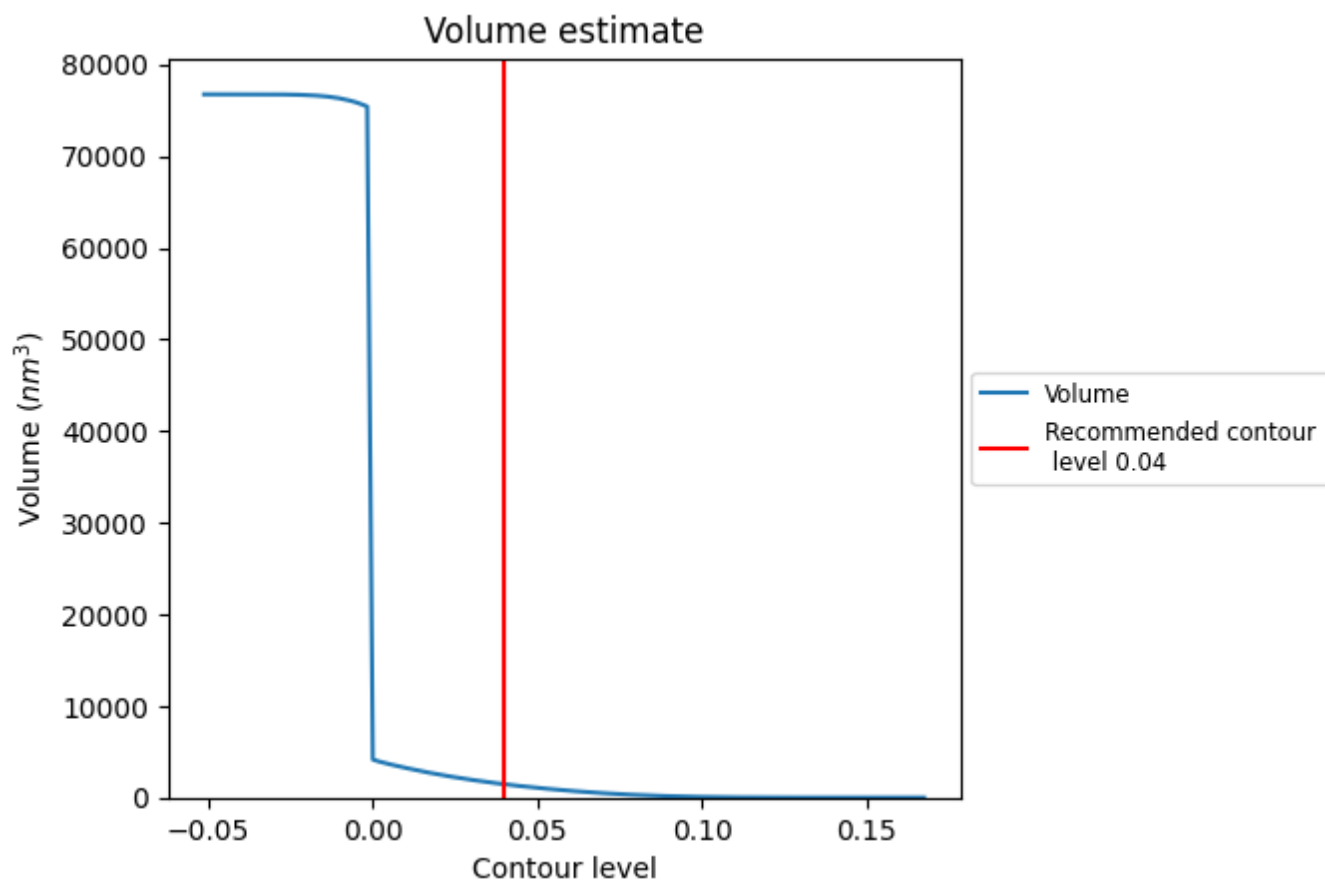
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

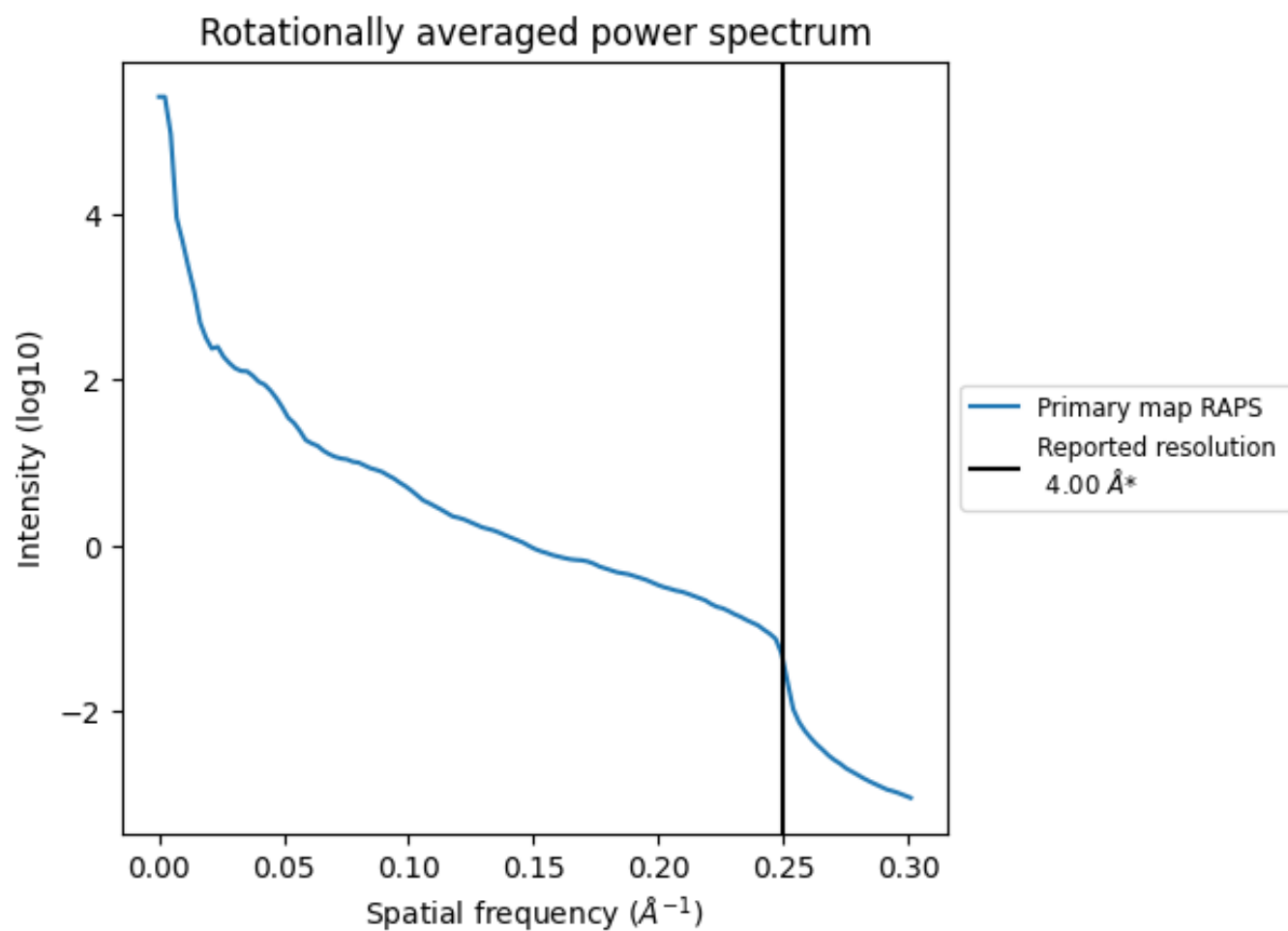
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1458 nm³; this corresponds to an approximate mass of 1317 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

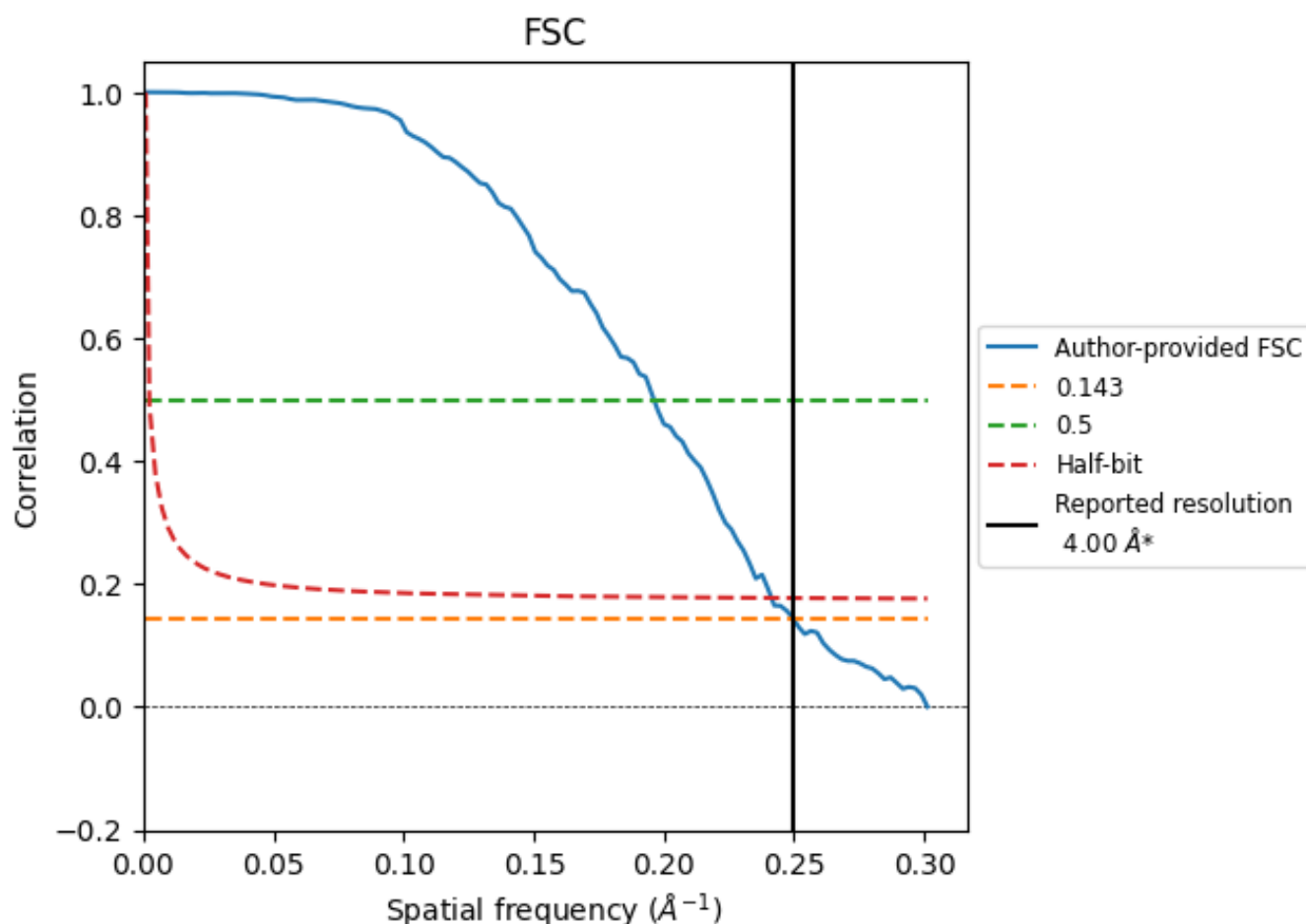


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

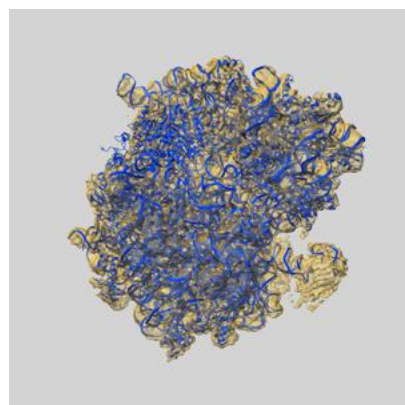
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.00	5.10	4.14
Unmasked-calculated*	-	-	-

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

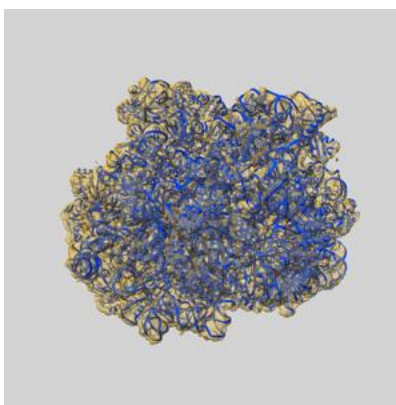
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0662 and PDB model 6O9K. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

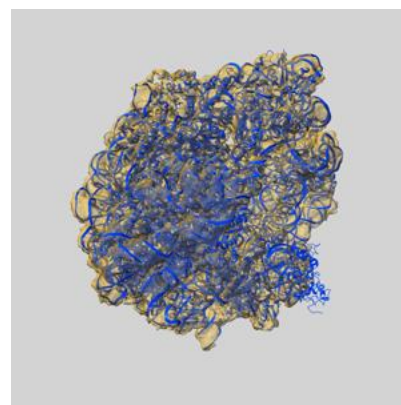
9.1 Map-model overlay [i](#)



X



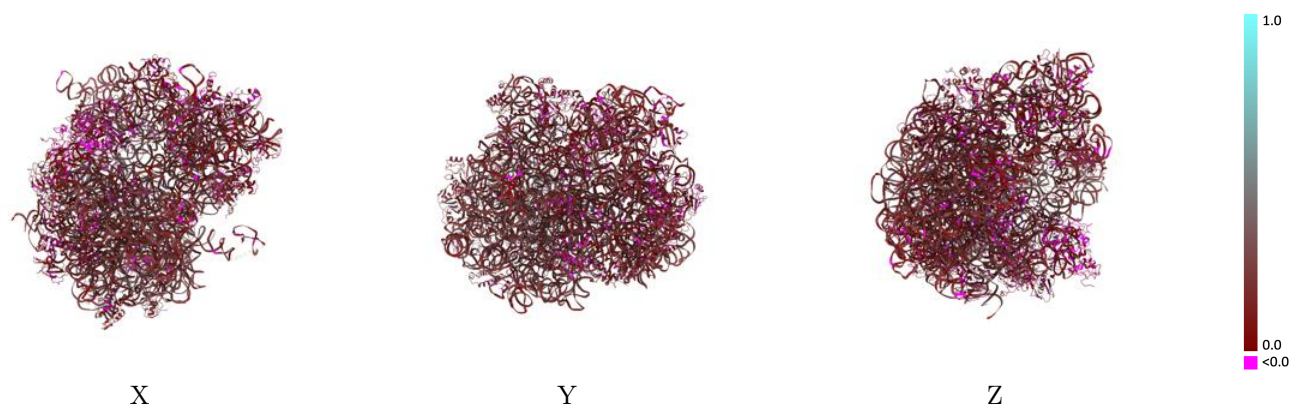
Y



Z

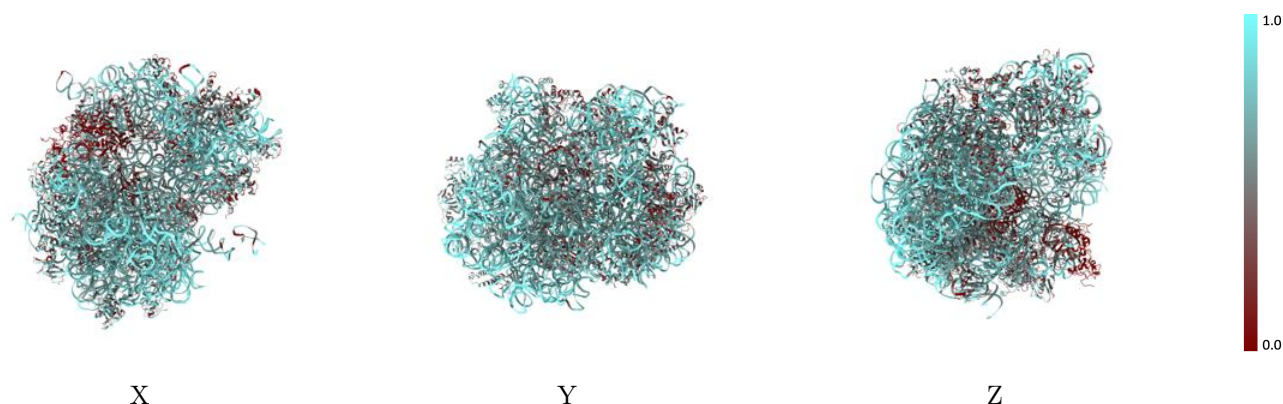
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



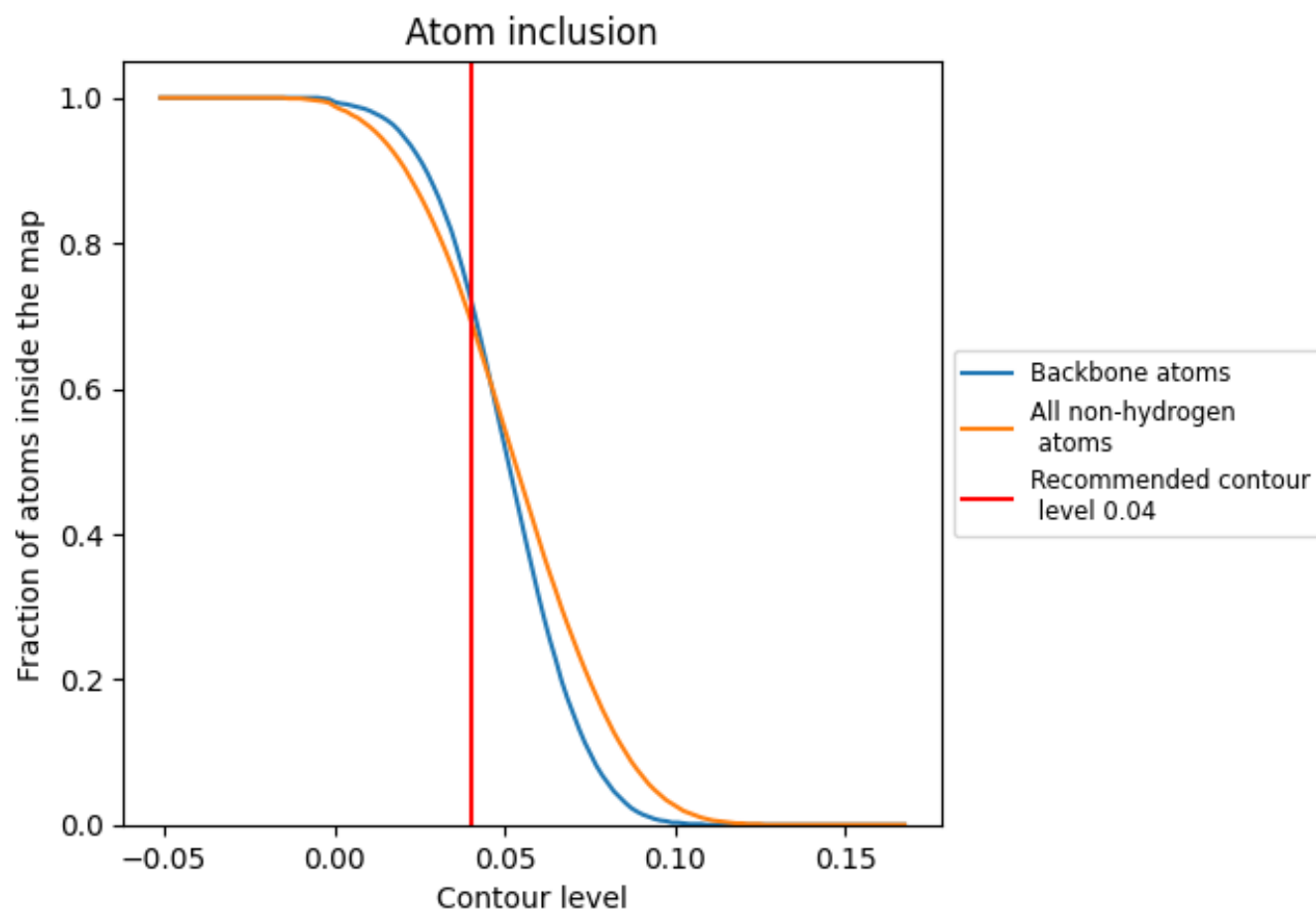
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 69% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6940	 0.1830
0	 0.4600	 0.1120
1	 0.5810	 0.2200
2	 0.6360	 0.1570
3	 0.4850	 0.1680
4	 0.4880	 0.1370
5	 0.5610	 0.1510
6	 0.4550	 0.1540
7	 0.4840	 0.1790
8	 0.5030	 0.1880
9	 0.5030	 0.2120
A	 0.8020	 0.2150
E	 0.5530	 0.1700
F	 0.4890	 0.1420
G	 0.0680	 0.0320
H	 0.5430	 0.1560
I	 0.0550	 0.0500
J	 0.4980	 0.1210
K	 0.3710	 0.1510
L	 0.5560	 0.1860
M	 0.4660	 0.1610
N	 0.5320	 0.1430
O	 0.6910	 0.1820
P	 0.4480	 0.1500
Q	 0.5250	 0.1160
R	 0.5680	 0.1430
S	 0.4620	 0.1290
T	 0.4980	 0.1390
U	 0.6110	 0.1440
V	 0.5540	 0.1470
X	 0.8700	 0.2010
Y	 0.5200	 0.1650
a	 0.8070	 0.1830
b	 0.3780	 0.1420
c	 0.5070	 0.1320



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Chain	Atom inclusion	Q-score
d	 0.4840	 0.1120
e	 0.4600	 0.1240
f	 0.5160	 0.1080
g	 0.4630	 0.1590
h	 0.5320	 0.1610
i	 0.5570	 0.1330
j	 0.5330	 0.1540
k	 0.5240	 0.1570
l	 0.3700	 0.1410
m	 0.5190	 0.1440
n	 0.5800	 0.1620
o	 0.5770	 0.1620
p	 0.5060	 0.1430
q	 0.4960	 0.1740
r	 0.4580	 0.1460
s	 0.5050	 0.1250
t	 0.5600	 0.1070
u	 0.4450	 0.1480
x	 0.6910	 0.2210
y	 0.5880	 0.1580
z	 0.2600	 0.1170