



Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 01:52 pm GMT

PDB ID : 7NSP
EMDB ID : EMD-12574
Title : Structure of ErmDL-Erythromycin-stalled 70S E. coli ribosomal complex with A and P-tRNA
Authors : Beckert, B.; Wilson, D.N.
Deposited on : 2021-03-08
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

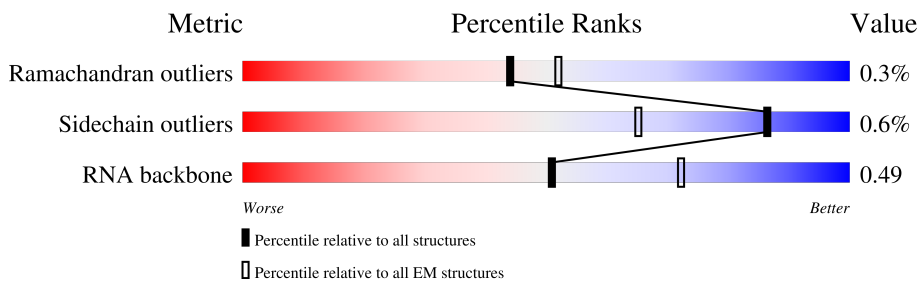
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	2903	
2	B	120	
3	C	271	
4	D	209	
5	E	201	
6	F	177	
7	G	174	
8	H	149	

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Mol	Chain	Length	Quality of chain
9	J	142	32% 100%
10	K	122	40% 100%
11	L	144	49% 99%
12	M	136	37% 98%
13	N	118	14% 100%
14	O	116	60% 99%
15	P	114	42% 98%
16	Q	117	24% 100%
17	R	103	42% 98%
18	S	110	30% 100%
19	T	89	46% 100%
20	U	102	61% 97%
21	V	94	55% 100%
22	W	75	27% 100%
23	X	77	40% 100%
24	Y	63	59% 100%
25	Z	58	34% 100%
26	0	55	42% 100%
27	1	50	100% 96%
28	2	46	13% 100%
29	3	64	28% 94% 6%
30	4	38	32% 97%
31	5	65	95% 97%
32	6	6	50% 50%
33	7	7	29% 71% 14% 14%

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Mol	Chain	Length	Quality of chain
34	8	87	43% 67% 28% 6%
35	a	1540	13% 72% 25%
36	b	224	96% 99%
37	c	206	58% 99%
38	d	205	87% 97%
39	e	157	43% 97%
40	f	99	64% 100%
41	g	151	82% 99%
42	h	129	48% 100%
43	i	127	64% 98%
44	j	98	71% 98%
45	k	117	58% 100%
46	l	123	46% 98%
47	m	114	67% 99%
48	n	100	47% 98%
49	o	88	51% 99%
50	p	82	56% 99%
51	q	80	59% 99%
52	r	66	56% 100%
53	s	83	58% 100%
54	t	86	56% 100%
55	u	70	99% 99%
56	v	77	92% 52% 43% 5%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 146148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2903	62320	27801	11467	20149	2903	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2570	1144	468	838	120	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	174	1304	820	239	243	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	118	945	585	194	161	5	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	89	Total	C	N	O	S	0	0
			709	449	133	125	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
27	1	50	Total	C	N	O	0	0
			409	263	75	71		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

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

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	65	Total	C	N	O	S	0	0
			514	317	98	93	6		

- Molecule 32 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	6	Total	C	N	O	P	0	0
			123	55	17	45	6		

- Molecule 33 is a protein called ermDL.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	7	Total	C	N	O	S	0	0
			58	35	12	9	2		

- Molecule 34 is a RNA chain called P-tRNA (leu).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	87	Total	C	N	O	P	0	0
			1861	829	333	612	87		

- Molecule 35 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
35	a	1540	33037	14735	6057	10705	1540	0	0

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	b	224	1753	1109	315	321	8	0	0

- Molecule 37 is a protein called 30S ribosomal protein S3.

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

- Molecule 38 is a protein called 30S ribosomal protein S4.

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

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	e	157	1156	719	218	213	6	0	0

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	f	99	811	512	147	146	6	0	0

- Molecule 41 is a protein called 30S ribosomal protein S7.

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

- Molecule 42 is a protein called 30S ribosomal protein S8.

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

- Molecule 43 is a protein called 30S ribosomal protein S9.

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

- Molecule 44 is a protein called 30S ribosomal protein S10.

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

- Molecule 45 is a protein called 30S ribosomal protein S11.

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

- Molecule 46 is a protein called 30S ribosomal protein S12.

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

- Molecule 47 is a protein called 30S ribosomal protein S13.

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

- Molecule 48 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	n	100	805	499	164	139	3	0	0

- Molecule 49 is a protein called 30S ribosomal protein S15.

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

- Molecule 50 is a protein called 30S ribosomal protein S16.

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

- Molecule 51 is a protein called 30S ribosomal protein S17.

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

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	r	66	Total	C	N	O	S	0	0
			545	344	102	98	1		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	t	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

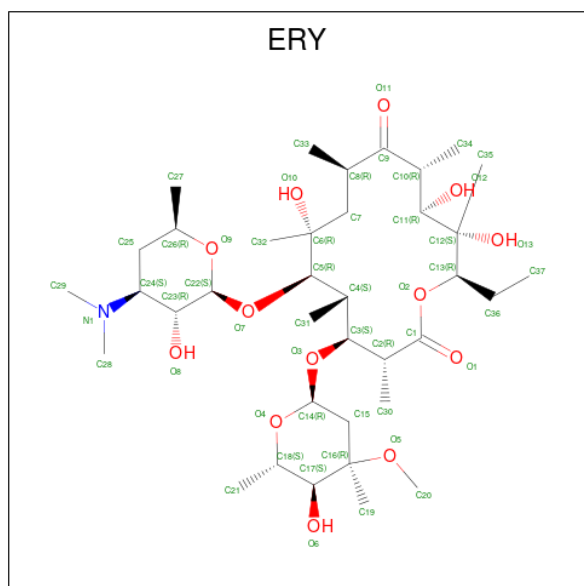
- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	u	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 56 is a RNA chain called A-tRNA (Arg).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	v	77	1643	733	297	536	77	0	0

- Molecule 57 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$) (labeled as "Ligand of Interest" by depositor).

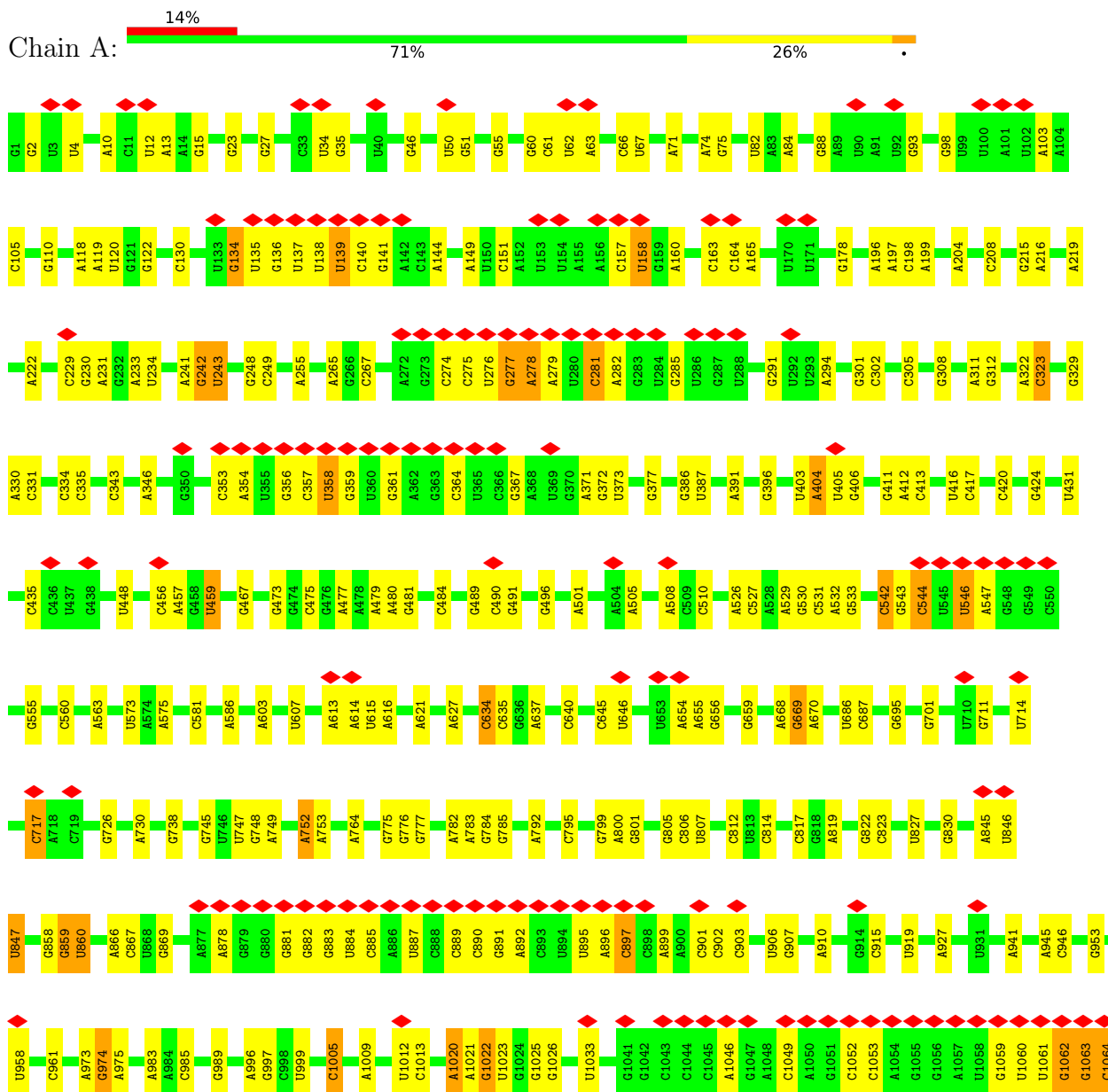


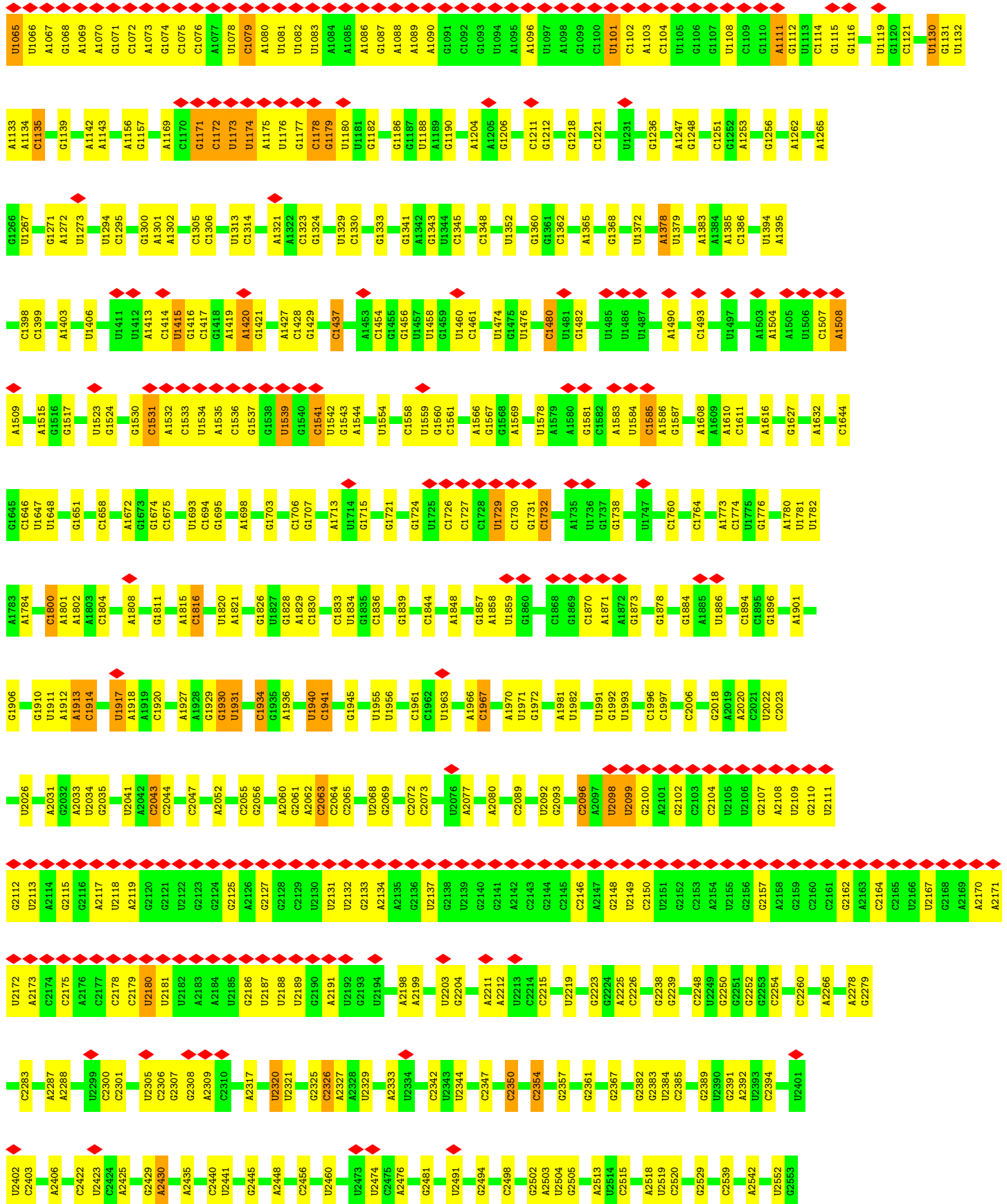
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
57	7	1	51	37	1	13	0

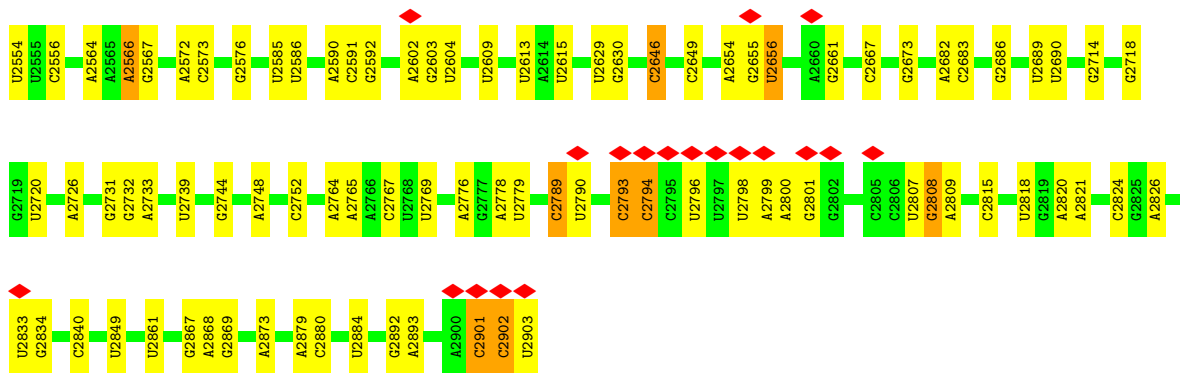
3 Residue-property plots

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

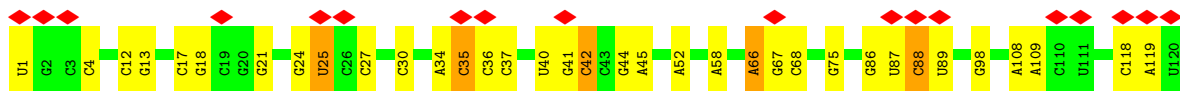
- Molecule 1: 23S rRNA



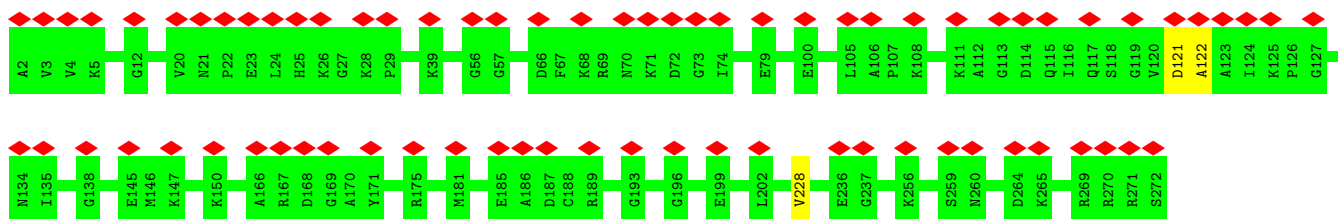




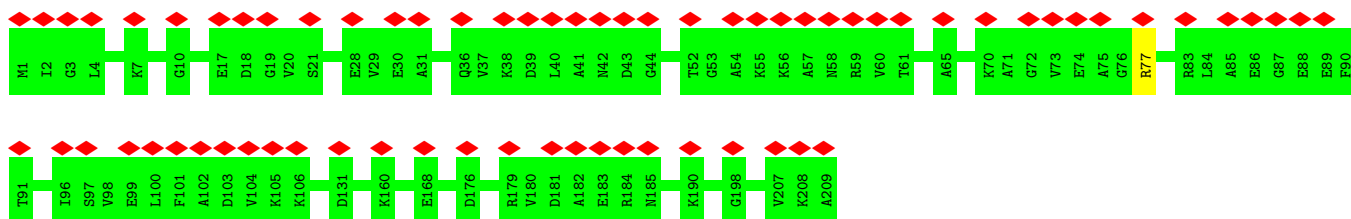
• Molecule 2: 5S rRNA



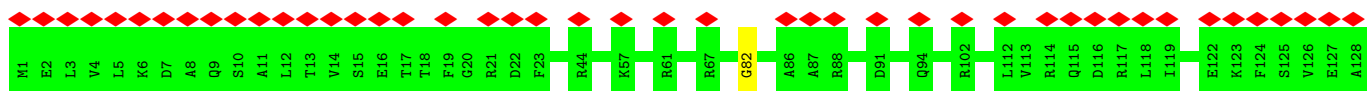
• Molecule 3: 50S ribosomal protein L2

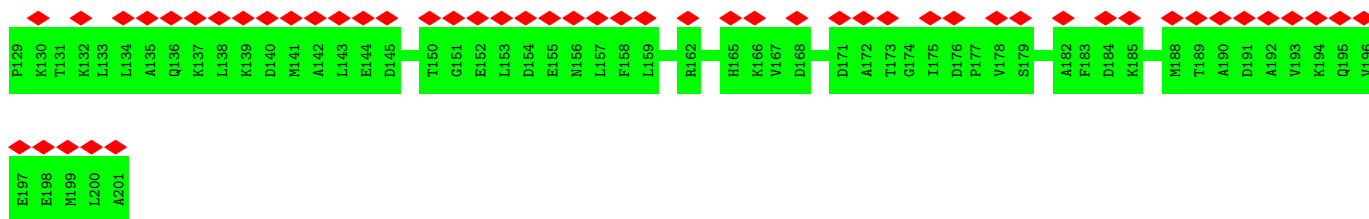


• Molecule 4: 50S ribosomal protein L3

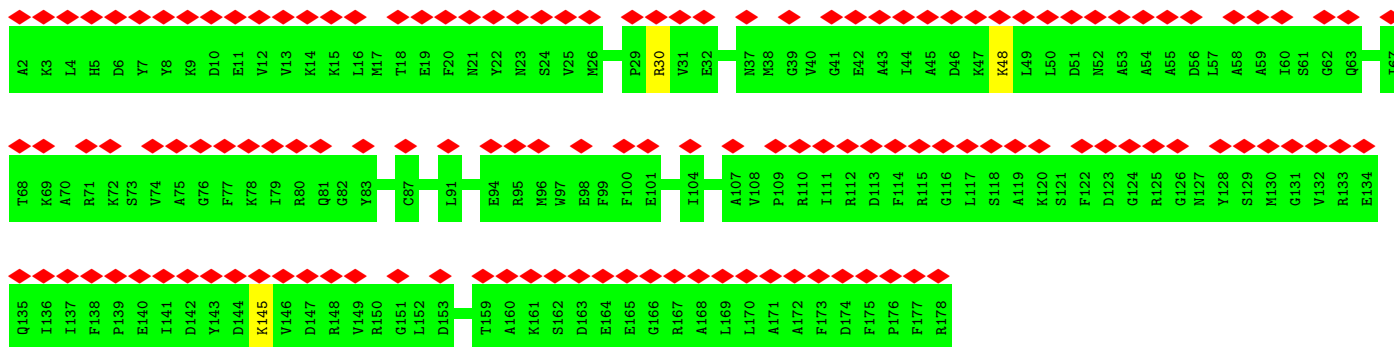
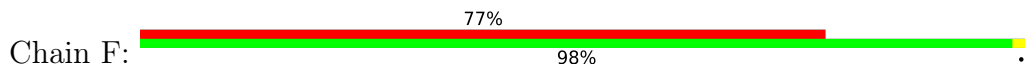


• Molecule 5: 50S ribosomal protein L4

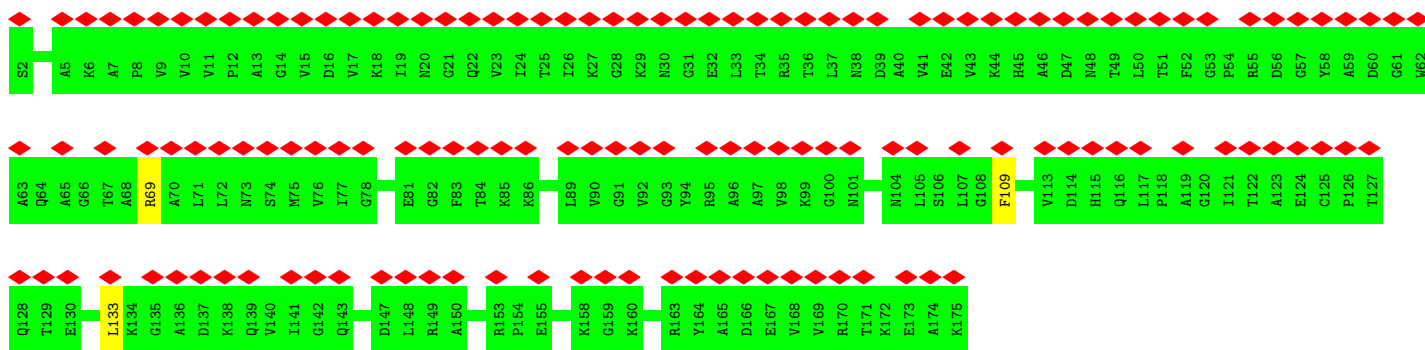
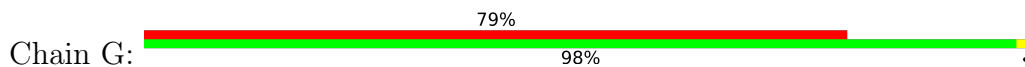




• Molecule 6: 50S ribosomal protein L5

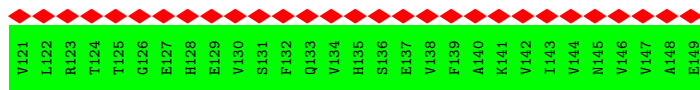


• Molecule 7: 50S ribosomal protein L6

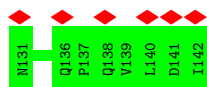
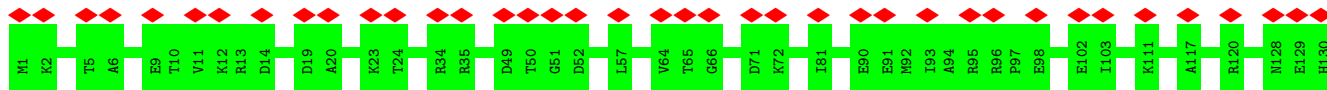


• Molecule 8: 50S ribosomal protein L9

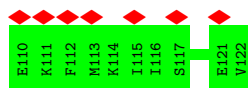
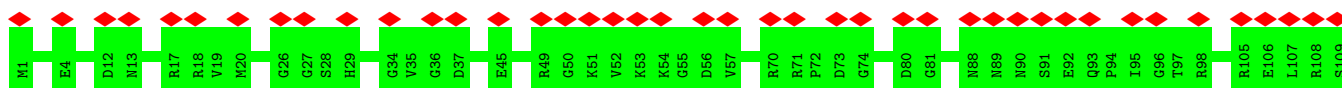
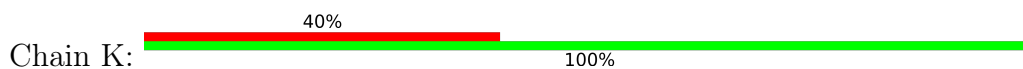




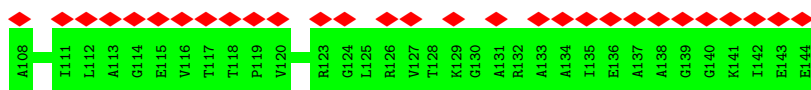
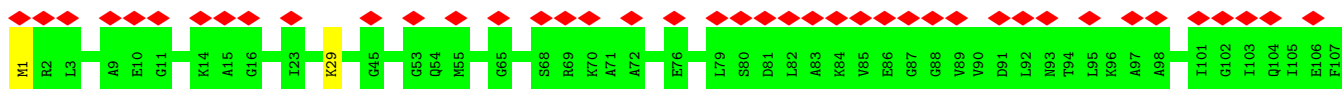
- Molecule 9: 50S ribosomal protein L13



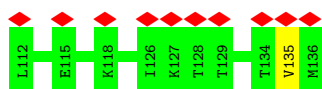
- Molecule 10: 50S ribosomal protein L14



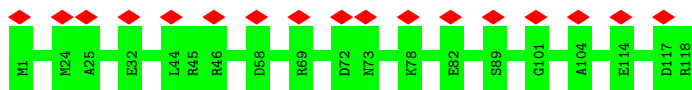
- Molecule 11: 50S ribosomal protein L15



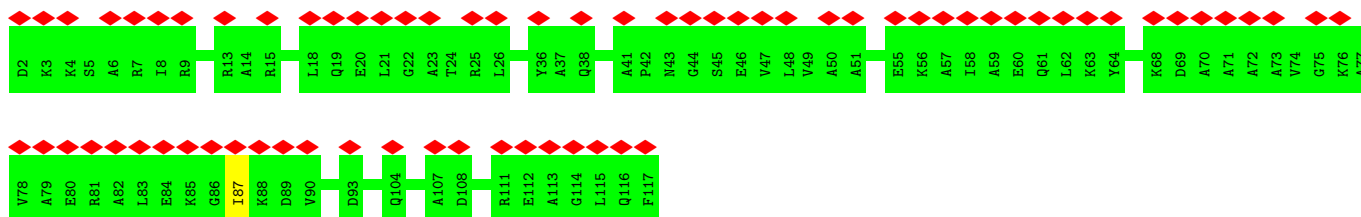
- Molecule 12: 50S ribosomal protein L16



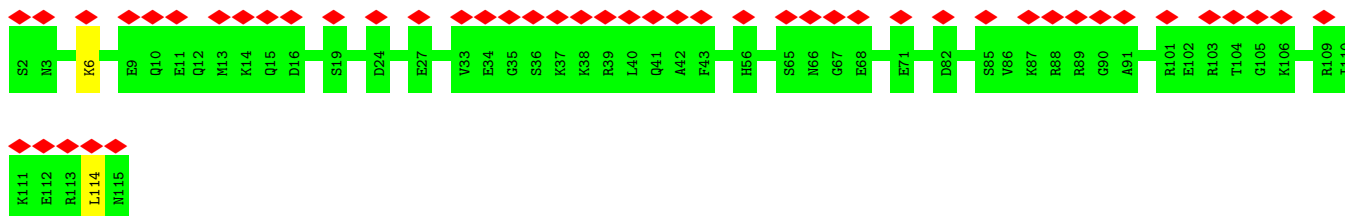
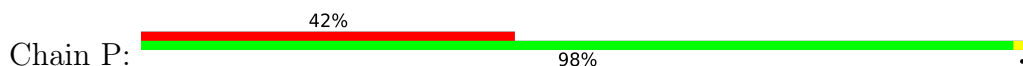
- Molecule 13: 50S ribosomal protein L17



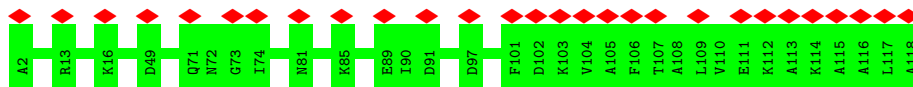
- Molecule 14: 50S ribosomal protein L18



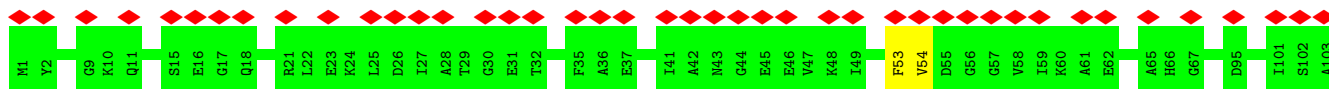
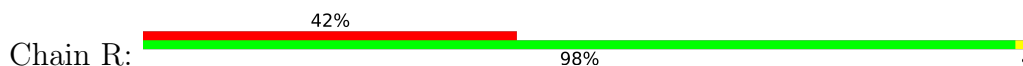
- Molecule 15: 50S ribosomal protein L19



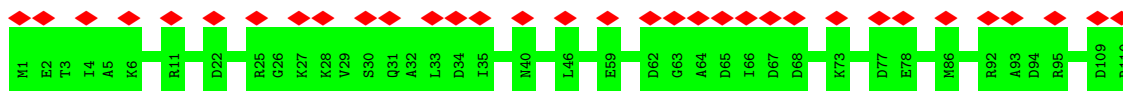
- Molecule 16: 50S ribosomal protein L20



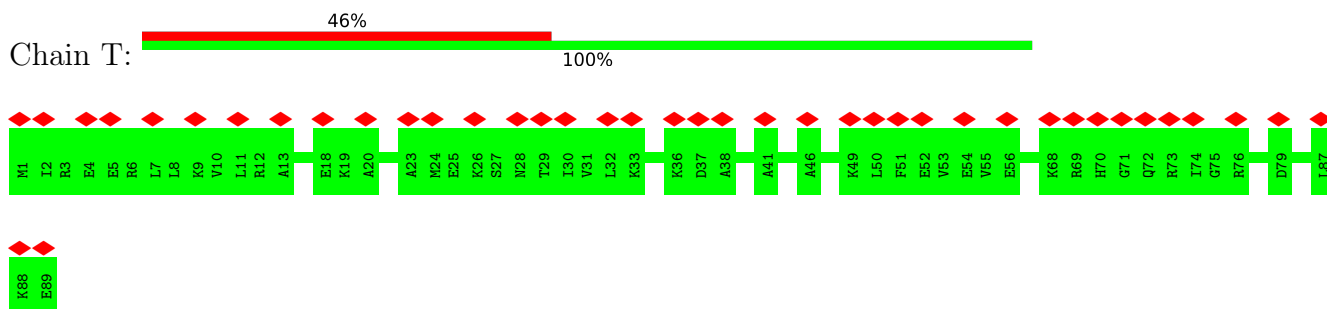
- Molecule 17: 50S ribosomal protein L21



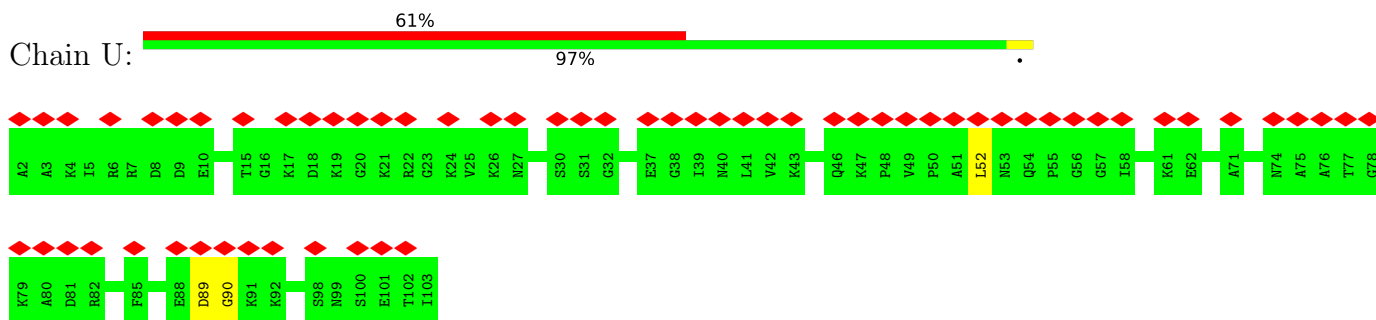
- Molecule 18: 50S ribosomal protein L22



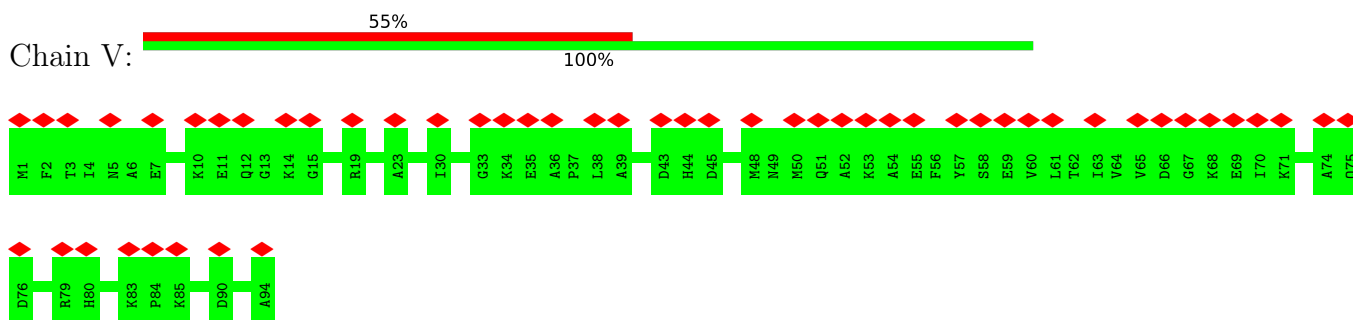
- Molecule 19: 50S ribosomal protein L23



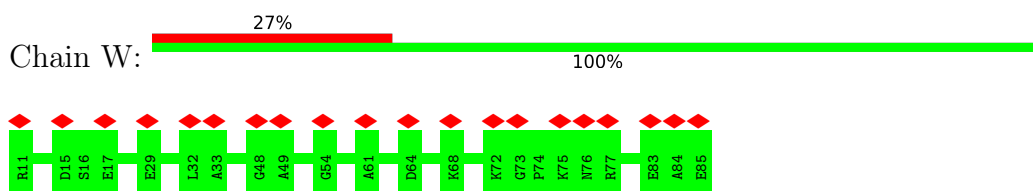
- Molecule 20: 50S ribosomal protein L24



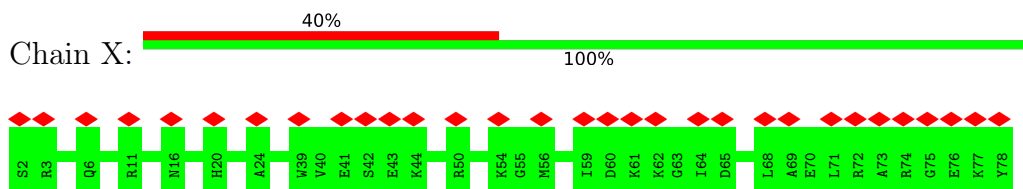
- Molecule 21: 50S ribosomal protein L25



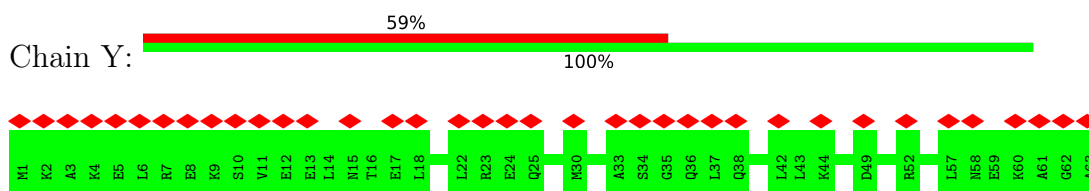
- Molecule 22: 50S ribosomal protein L27



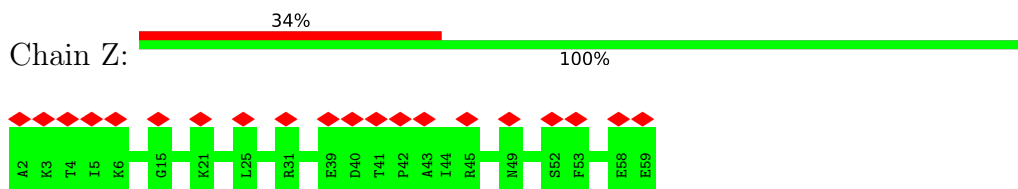
- Molecule 23: 50S ribosomal protein L28



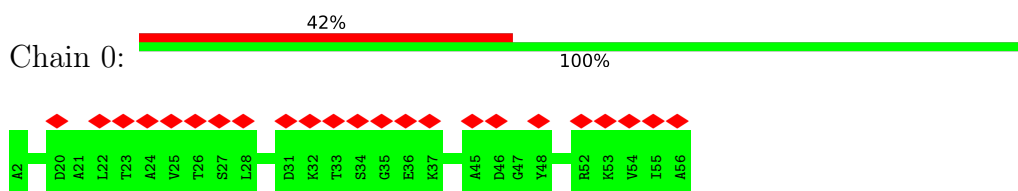
- Molecule 24: 50S ribosomal protein L29



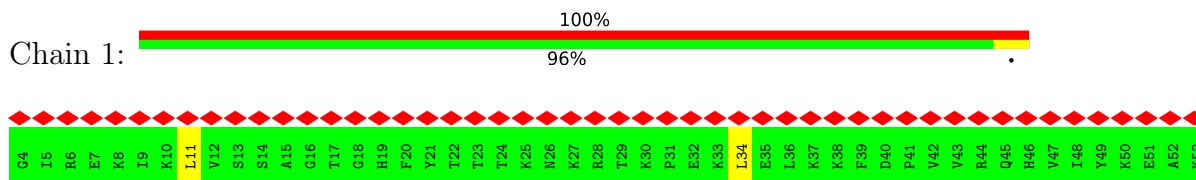
- Molecule 25: 50S ribosomal protein L30



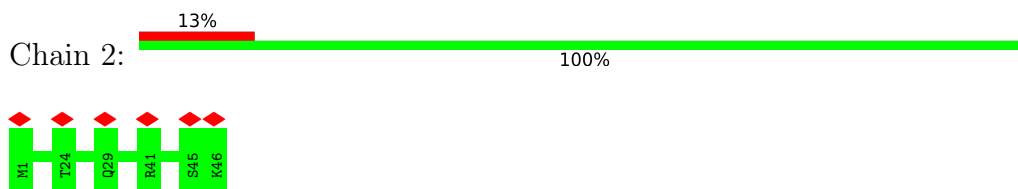
- Molecule 26: 50S ribosomal protein L32



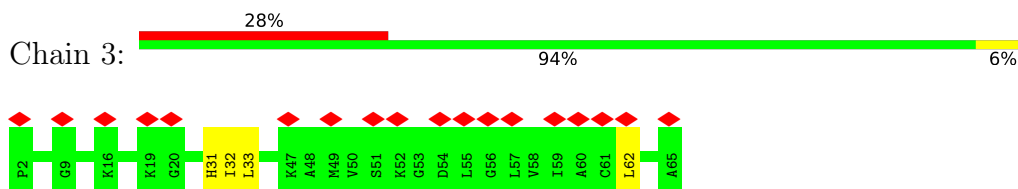
- Molecule 27: 50S ribosomal protein L33



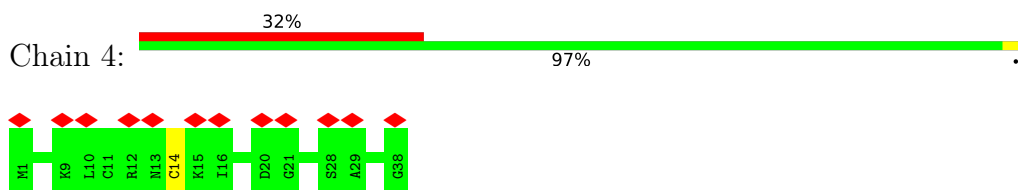
- Molecule 28: 50S ribosomal protein L34



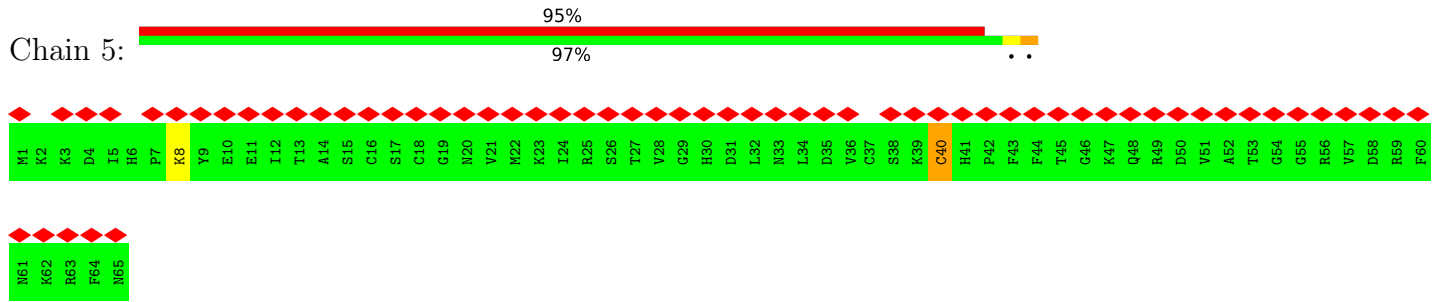
- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



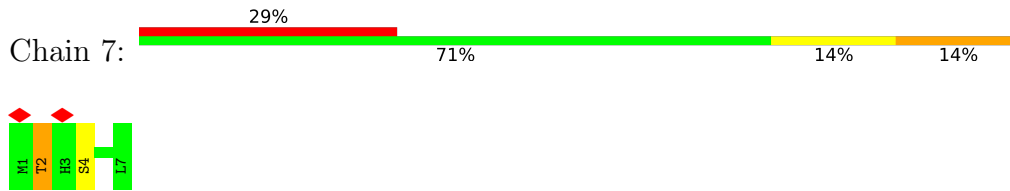
• Molecule 31: 50S ribosomal protein L31



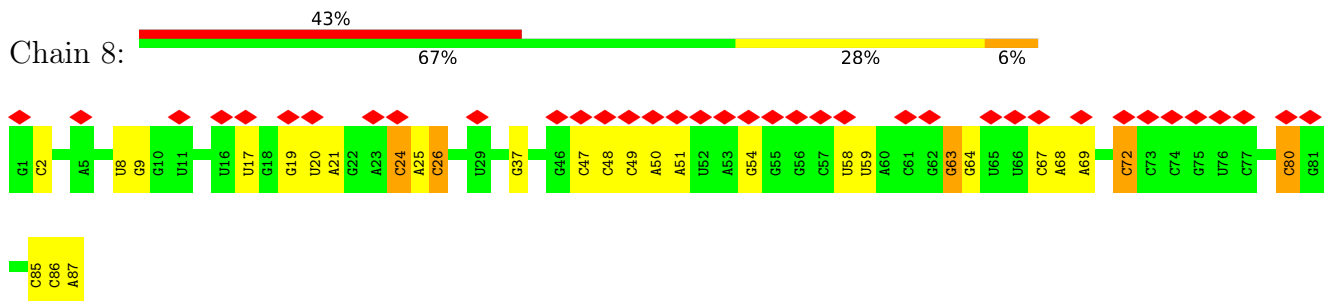
• Molecule 32: mRNA



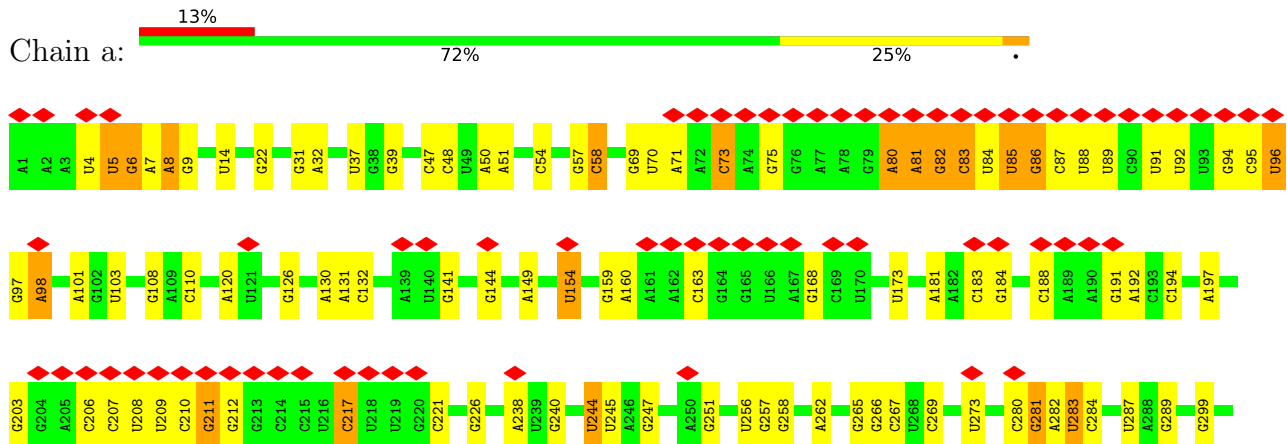
• Molecule 33: ermDL

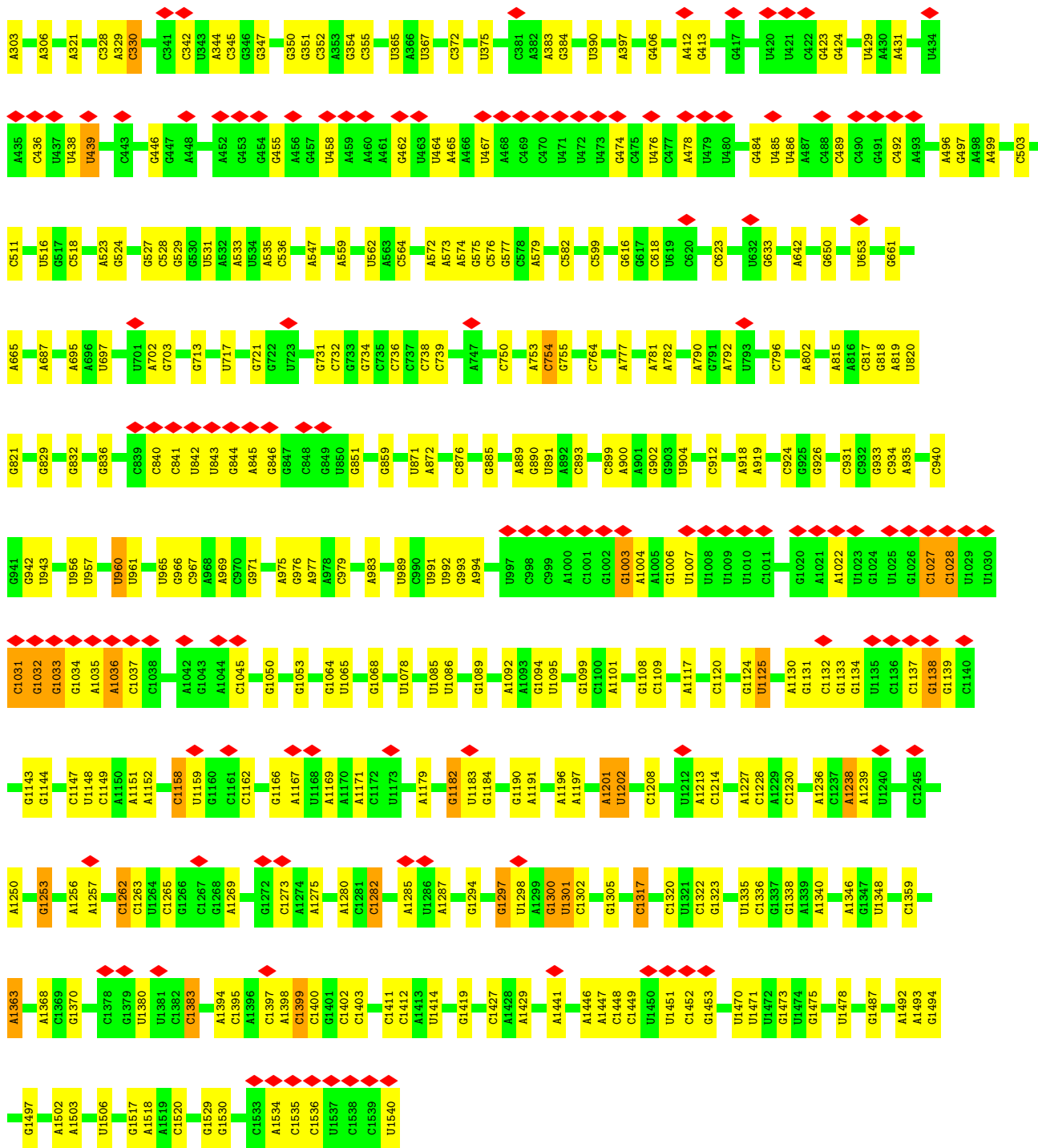


• Molecule 34: P-tRNA (leu)

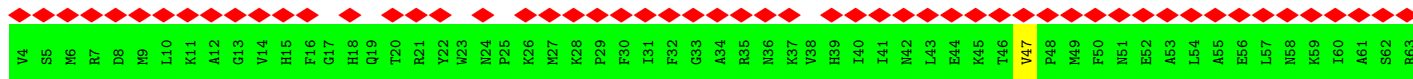


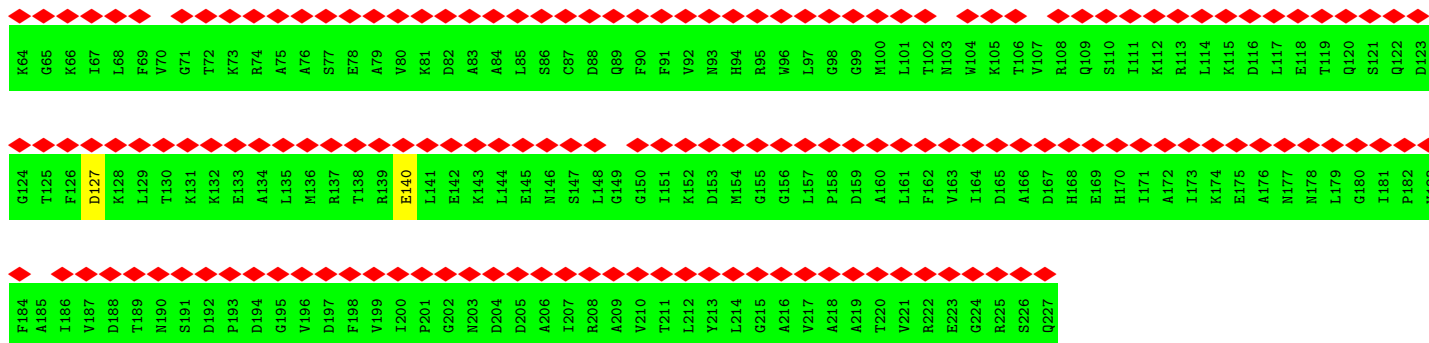
• Molecule 35: 16S rRNA



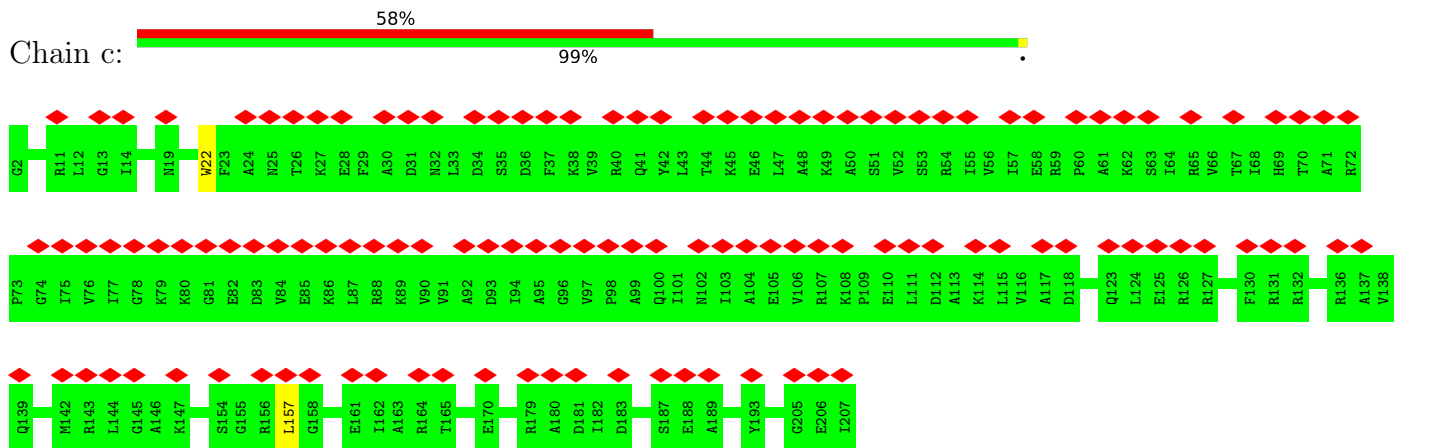


• Molecule 36: 30S ribosomal protein S2

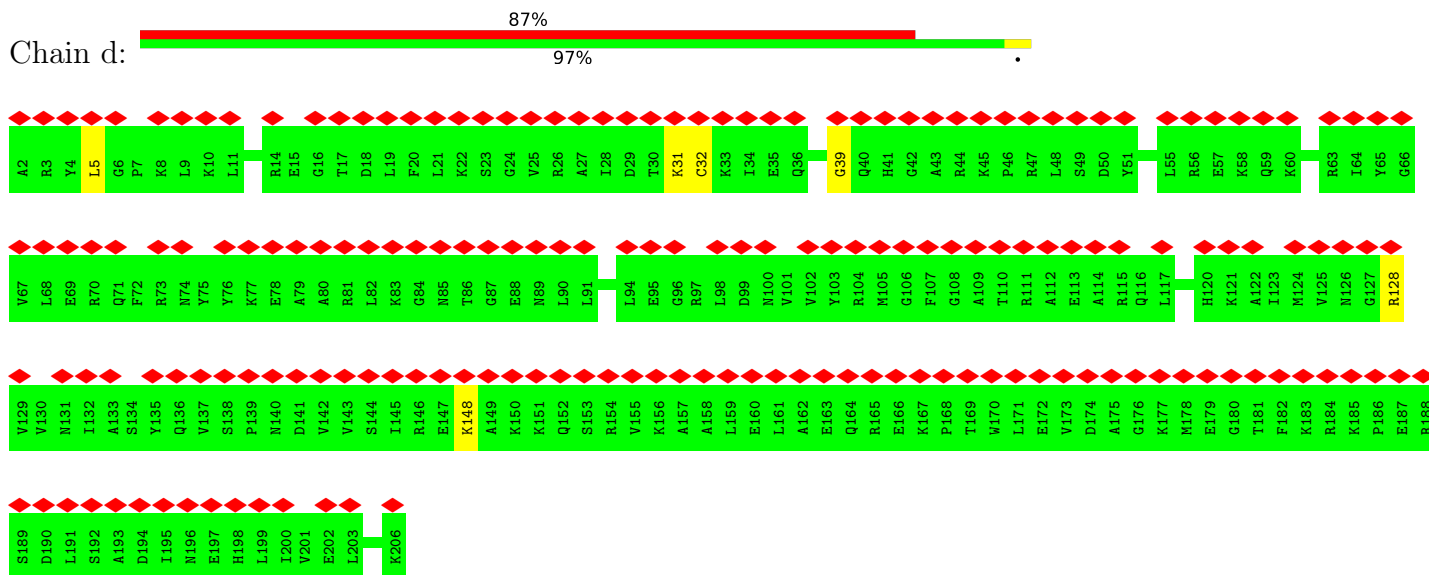




• Molecule 37: 30S ribosomal protein S3

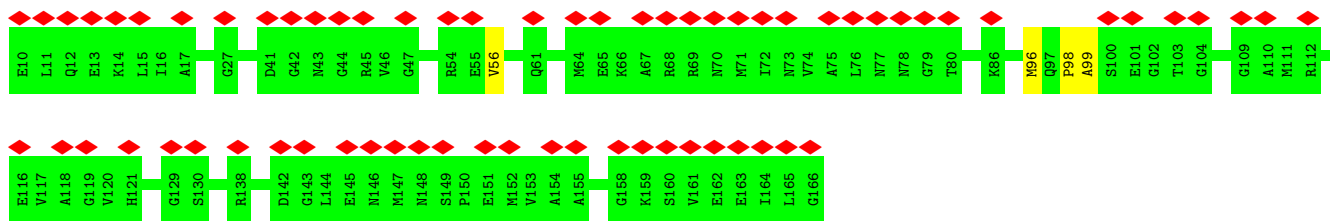


• Molecule 38: 30S ribosomal protein S4

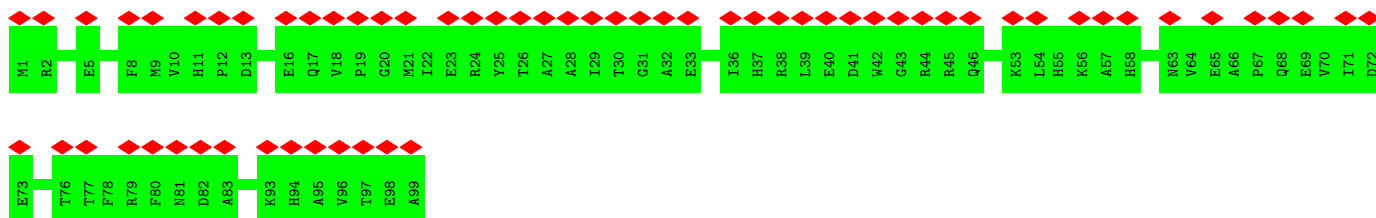


• Molecule 39: 30S ribosomal protein S5

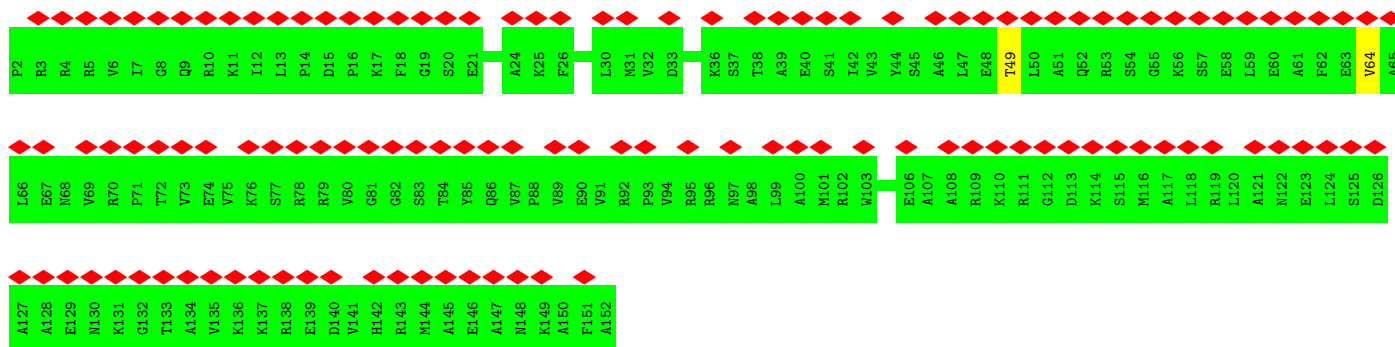
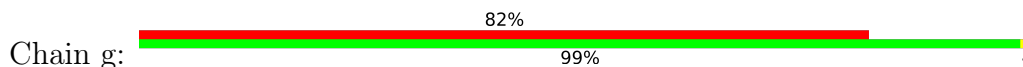




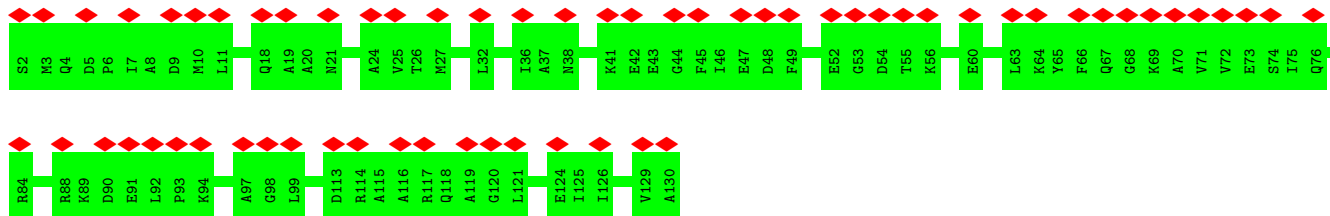
- Molecule 40: 30S ribosomal protein S6



- Molecule 41: 30S ribosomal protein S7

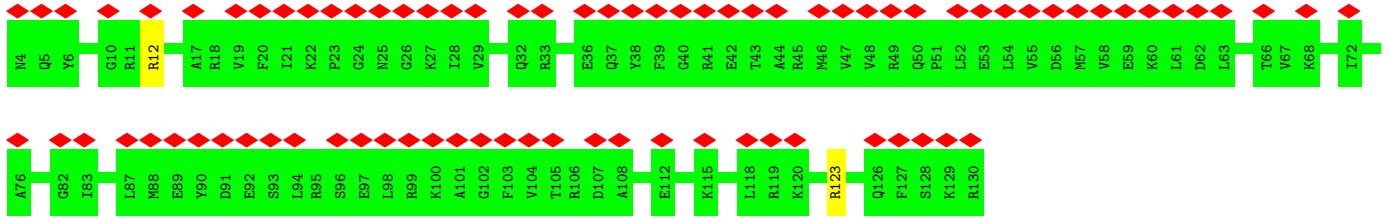


- Molecule 42: 30S ribosomal protein S8

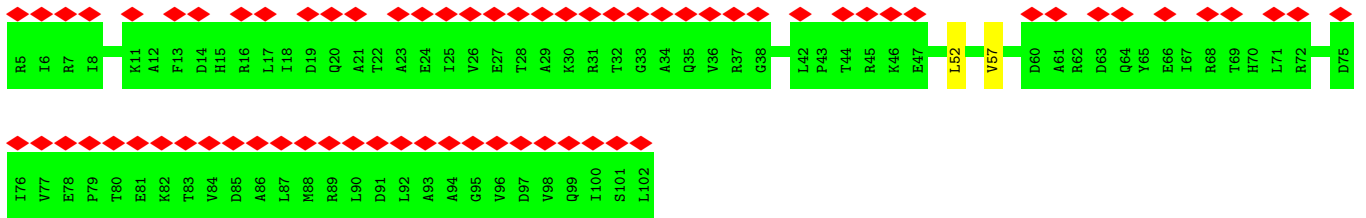


- Molecule 43: 30S ribosomal protein S9

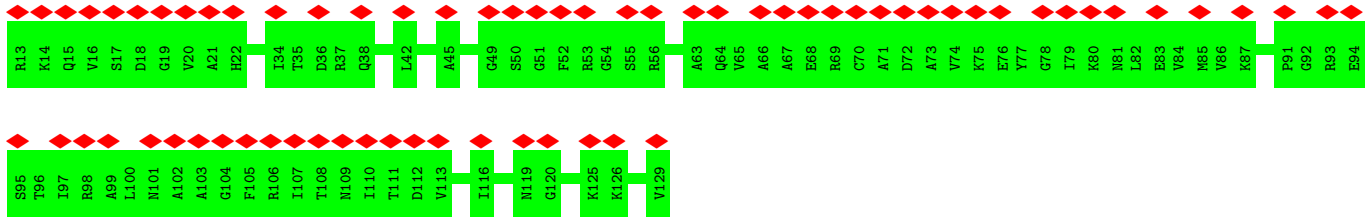




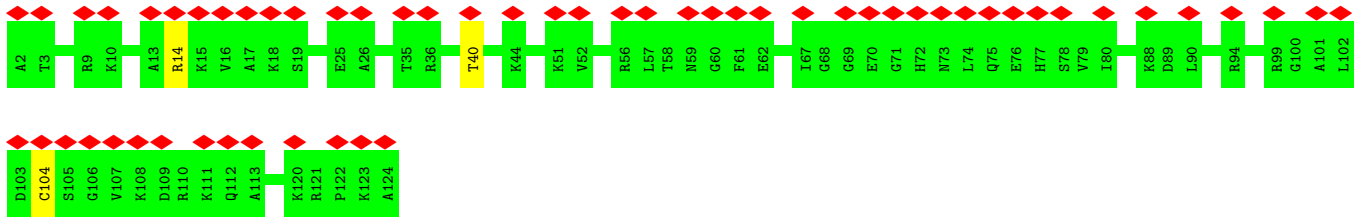
• Molecule 44: 30S ribosomal protein S10



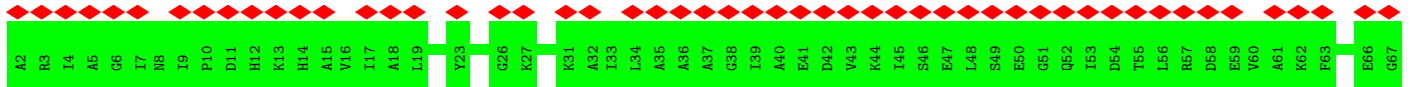
• Molecule 45: 30S ribosomal protein S11

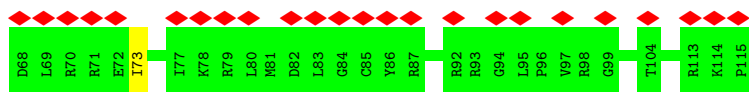


• Molecule 46: 30S ribosomal protein S12

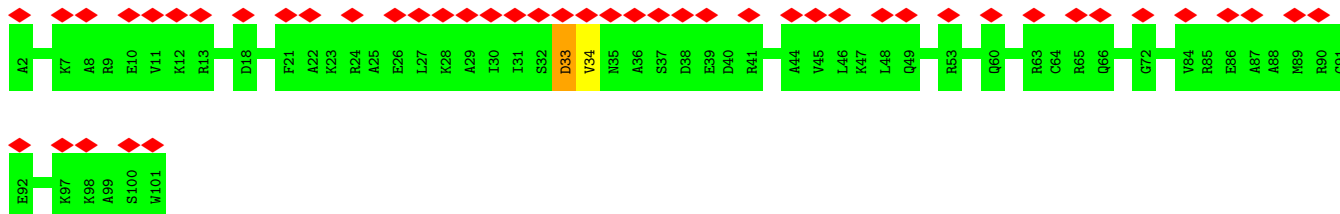


• Molecule 47: 30S ribosomal protein S13

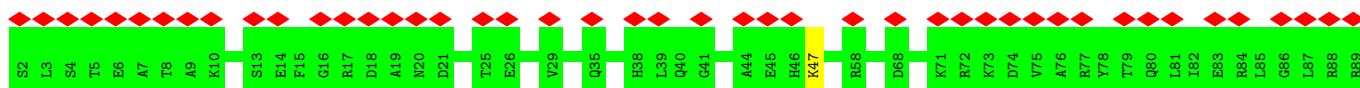




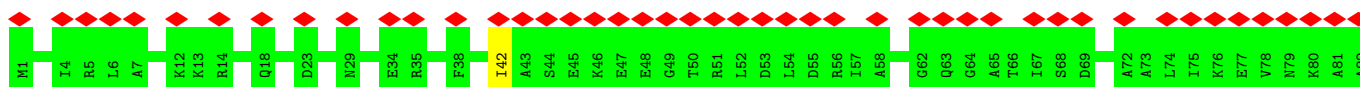
- Molecule 48: 30S ribosomal protein S14



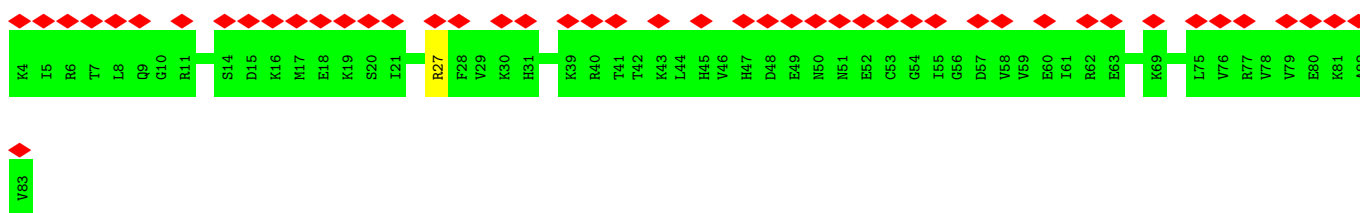
- Molecule 49: 30S ribosomal protein S15



- Molecule 50: 30S ribosomal protein S16



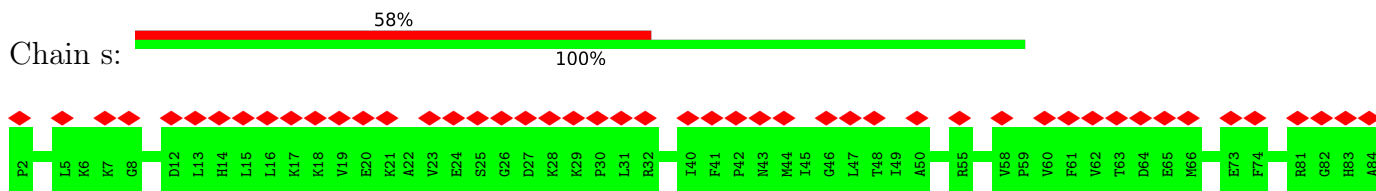
- Molecule 51: 30S ribosomal protein S17



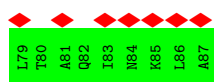
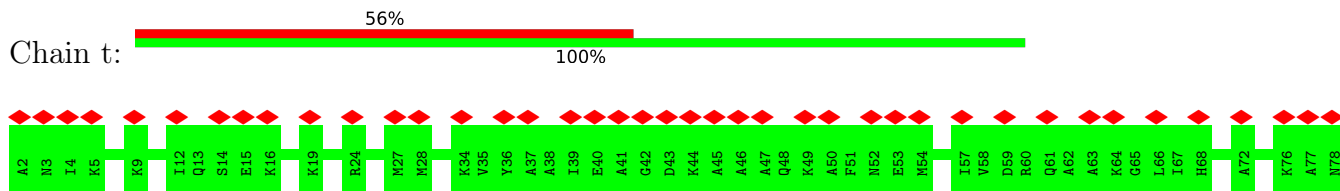
- Molecule 52: 30S ribosomal protein S18



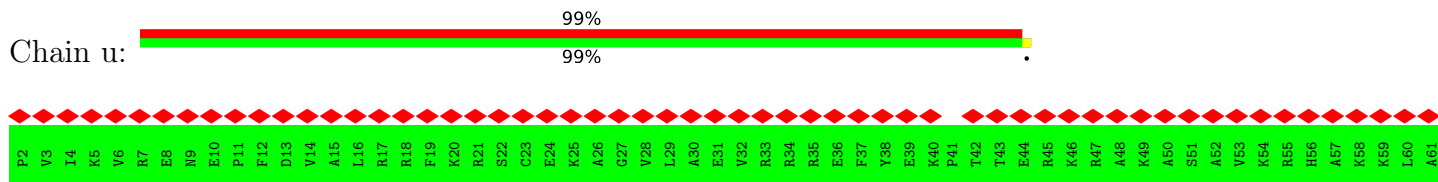
- Molecule 53: 30S ribosomal protein S19



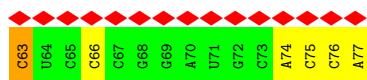
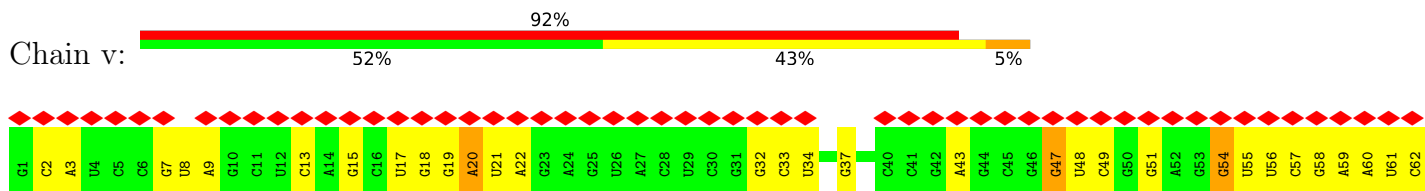
• Molecule 54: 30S ribosomal protein S20



• Molecule 55: 30S ribosomal protein S21



• Molecule 56: A-tRNA (Arg)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27397	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.318	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	398.88, 398.88, 398.88	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ERY

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	0.85	2/69799 (0.0%)	1.17	474/108892 (0.4%)
2	B	0.68	1/2873 (0.0%)	1.20	28/4478 (0.6%)
3	C	0.45	0/2121	0.58	0/2852
4	D	0.43	0/1586	0.58	0/2134
5	E	0.38	0/1571	0.56	0/2113
6	F	0.35	0/1434	0.61	0/1926
7	G	0.34	0/1324	0.58	1/1794 (0.1%)
8	H	0.33	0/1122	0.66	0/1515
9	J	0.41	0/1152	0.54	0/1551
10	K	0.41	0/947	0.62	0/1268
11	L	0.38	0/1062	0.62	1/1413 (0.1%)
12	M	0.42	0/1093	0.61	1/1460 (0.1%)
13	N	0.37	0/958	0.60	0/1281
14	O	0.36	0/902	0.57	0/1209
15	P	0.42	0/929	0.58	1/1242 (0.1%)
16	Q	0.47	0/960	0.48	0/1278
17	R	0.42	0/829	0.61	0/1107
18	S	0.38	0/864	0.56	0/1156
19	T	0.36	0/715	0.56	0/955
20	U	0.37	0/787	0.62	1/1051 (0.1%)
21	V	0.37	0/766	0.54	0/1025
22	W	0.39	0/582	0.50	0/769
23	X	0.40	0/635	0.53	0/848
24	Y	0.34	0/510	0.58	0/677
25	Z	0.32	0/453	0.56	0/605
26	0	0.39	0/440	0.54	0/588
27	1	0.34	0/416	0.65	1/554 (0.2%)
28	2	0.40	0/380	0.56	0/498
29	3	0.38	0/513	0.67	1/676 (0.1%)
30	4	0.44	0/303	0.62	0/397
31	5	0.32	0/523	0.68	1/698 (0.1%)
32	6	0.87	0/135	1.41	2/207 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	7	1.11	0/58	1.59	2/75 (2.7%)
34	8	0.62	0/2080	1.19	15/3242 (0.5%)
35	a	1.01	2/36991 (0.0%)	1.23	268/57705 (0.5%)
36	b	0.37	0/1784	0.62	1/2403 (0.0%)
37	c	0.46	0/1651	0.60	1/2225 (0.0%)
38	d	0.40	0/1665	0.64	1/2227 (0.0%)
39	e	0.52	0/1169	0.67	0/1573
40	f	0.43	0/829	0.62	0/1120
41	g	0.36	0/1195	0.60	0/1602
42	h	0.47	0/989	0.62	0/1326
43	i	0.44	0/1034	0.67	0/1375
44	j	0.44	0/796	0.67	0/1077
45	k	0.43	0/893	0.58	0/1205
46	l	0.46	0/969	0.66	1/1300 (0.1%)
47	m	0.42	0/892	0.64	0/1193
48	n	0.44	0/817	0.55	0/1088
49	o	0.42	0/722	0.62	0/964
50	p	0.43	0/659	0.66	0/884
51	q	0.48	0/657	0.69	0/881
52	r	0.43	0/554	0.57	0/743
53	s	0.42	0/680	0.60	0/915
54	t	0.38	0/676	0.50	0/895
55	u	0.37	0/598	0.54	0/792
56	v	0.50	0/1836	1.22	20/2860 (0.7%)
All	All	0.79	5/158878 (0.0%)	1.07	821/237887 (0.3%)

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
3	C	0	1
5	E	0	1
6	F	0	1
8	H	0	3
14	O	0	1
17	R	0	1
20	U	0	1
27	1	0	1
29	3	0	1
38	d	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	e	0	1
41	g	0	1
48	n	0	2
50	p	0	1
All	All	0	18

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.75	1.48	1.61
1	A	2604	U	N3-C4	-6.44	1.32	1.38
35	a	523	A	N9-C4	-5.81	1.34	1.37
1	A	1800	C	N1-C6	-5.17	1.34	1.37
35	a	574	A	N9-C4	-5.06	1.34	1.37

All (821) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2590	A	N1-C6-N6	-17.89	107.87	118.60
35	a	330	C	N1-C2-O2	12.04	126.12	118.90
1	A	2604	U	N3-C2-O2	-11.88	113.89	122.20
1	A	12	U	N1-C2-O2	11.52	130.86	122.80
1	A	2590	A	C5-C6-N6	11.48	132.88	123.70
1	A	12	U	C2-N1-C1'	11.38	131.35	117.70
1	A	12	U	N3-C2-O2	-11.22	114.35	122.20
1	A	2320	U	N3-C2-O2	-11.05	114.46	122.20
1	A	2604	U	C2-N1-C1'	10.98	130.87	117.70
1	A	2063	C	C6-N1-C2	-10.51	116.10	120.30
1	A	2320	U	C2-N1-C1'	10.26	130.01	117.70
1	A	2320	U	N1-C2-O2	10.24	129.97	122.80
1	A	867	C	N1-C2-O2	9.51	124.61	118.90
1	A	2604	U	N1-C2-O2	9.46	129.42	122.80
1	A	1914	C	N1-C2-O2	9.36	124.52	118.90
1	A	2063	C	C5-C6-N1	9.19	125.60	121.00
1	A	2179	C	N1-C2-O2	9.11	124.36	118.90
1	A	2604	U	C5-C4-O4	9.10	131.36	125.90
1	A	2604	U	N3-C4-O4	-9.10	113.03	119.40
1	A	2226	C	N1-C2-O2	9.09	124.36	118.90
1	A	2063	C	C2-N1-C1'	9.07	128.78	118.80
34	8	2	C	N1-C2-O2	8.87	124.22	118.90
1	A	2063	C	N1-C2-O2	8.72	124.14	118.90
35	a	330	C	C2-N1-C1'	8.71	128.38	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	36	C	N1-C2-O2	8.70	124.12	118.90
1	A	2180	U	N3-C2-O2	-8.61	116.17	122.20
35	a	1086	U	N1-C2-O2	8.57	128.80	122.80
2	B	35	C	N1-C2-O2	8.53	124.02	118.90
1	A	2180	U	N1-C2-O2	8.52	128.76	122.80
1	A	1082	U	C5-C6-N1	8.50	126.95	122.70
1	A	1313	U	C2-N1-C1'	8.44	127.83	117.70
35	a	330	C	N3-C2-O2	-8.44	115.99	121.90
35	a	1086	U	N3-C2-O2	-8.42	116.30	122.20
35	a	1301	U	C2-N1-C1'	8.41	127.79	117.70
1	A	1917	U	N3-C2-O2	-8.29	116.39	122.20
1	A	2342	C	N3-C2-O2	-8.29	116.10	121.90
1	A	1507	C	C6-N1-C2	-8.28	116.99	120.30
1	A	1914	C	C2-N1-C1'	8.27	127.89	118.80
35	a	516	U	N3-C2-O2	-8.27	116.41	122.20
1	A	2098	U	C2-N1-C1'	8.27	127.62	117.70
35	a	582	C	N1-C2-O2	8.26	123.85	118.90
1	A	2604	U	C6-N1-C1'	-8.23	109.68	121.20
1	A	1348	C	N1-C2-O2	8.20	123.82	118.90
1	A	1065	U	C2-N1-C1'	8.19	127.53	117.70
35	a	1027	C	C2-N1-C1'	8.17	127.78	118.80
35	a	439	U	N3-C2-O2	-8.16	116.49	122.20
35	a	1158	C	C2-N1-C1'	8.14	127.76	118.80
1	A	364	C	N1-C2-O2	8.13	123.78	118.90
35	a	967	C	C6-N1-C2	-8.10	117.06	120.30
1	A	2326	C	C6-N1-C2	-8.05	117.08	120.30
35	a	96	U	N1-C2-O2	8.01	128.40	122.80
1	A	1731	G	N3-C4-N9	-7.98	121.21	126.00
35	a	991	U	C2-N1-C1'	7.96	127.26	117.70
35	a	96	U	C2-N1-C1'	7.93	127.22	117.70
1	A	1517	G	N3-C2-N2	-7.93	114.35	119.90
35	a	95	C	N1-C2-O2	7.88	123.63	118.90
1	A	1102	C	N1-C2-O2	7.88	123.62	118.90
1	A	1517	G	C6-N1-C2	-7.86	120.39	125.10
35	a	269	C	C2-N1-C1'	7.85	127.44	118.80
1	A	1914	C	N3-C2-O2	-7.85	116.41	121.90
1	A	1172	C	N1-C2-O2	7.85	123.61	118.90
35	a	1032	G	N3-C4-C5	-7.80	124.70	128.60
35	a	103	U	N3-C2-O2	-7.75	116.77	122.20
35	a	439	U	N1-C2-O2	7.75	128.22	122.80
1	A	2656	U	C5-C6-N1	7.74	126.57	122.70
1	A	2793	C	C2-N1-C1'	7.73	127.30	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1993	U	N3-C2-O2	-7.72	116.80	122.20
1	A	867	C	N3-C2-O2	-7.70	116.51	121.90
1	A	1313	U	N3-C2-O2	-7.69	116.81	122.20
2	B	30	C	C6-N1-C2	-7.68	117.23	120.30
1	A	847	U	N3-C2-O2	-7.67	116.83	122.20
1	A	2098	U	N1-C2-O2	7.64	128.15	122.80
1	A	2226	C	N3-C2-O2	-7.61	116.57	121.90
1	A	1917	U	C2-N1-C1'	7.61	126.83	117.70
1	A	2098	U	N3-C2-O2	-7.61	116.87	122.20
1	A	2179	C	N3-C2-O2	-7.59	116.58	121.90
2	B	35	C	C6-N1-C2	-7.54	117.28	120.30
1	A	2238	G	N3-C4-C5	-7.54	124.83	128.60
1	A	2096	C	C2-N1-C1'	7.50	127.05	118.80
1	A	1539	U	C2-N1-C1'	7.48	126.68	117.70
35	a	439	U	C2-N1-C1'	7.46	126.65	117.70
1	A	2109	U	C5-C6-N1	7.46	126.43	122.70
1	A	1178	C	C5-C6-N1	7.43	124.72	121.00
1	A	1178	C	C6-N1-C2	-7.43	117.33	120.30
1	A	1517	G	N9-C4-C5	7.42	108.37	105.40
35	a	217	C	N1-C2-O2	7.40	123.34	118.90
35	a	96	U	N3-C2-O2	-7.37	117.04	122.20
1	A	2683	C	N1-C2-O2	7.36	123.31	118.90
1	A	806	C	C6-N1-C2	-7.33	117.37	120.30
35	a	1027	C	N1-C2-O2	7.33	123.30	118.90
31	5	40	CYS	C-N-CA	7.32	139.99	121.70
1	A	2354	C	C6-N1-C2	-7.30	117.38	120.30
35	a	1427	C	C6-N1-C2	-7.30	117.38	120.30
1	A	510	C	C2-N1-C1'	7.27	126.80	118.80
1	A	1313	U	N1-C2-O2	7.27	127.89	122.80
1	A	1774	C	C6-N1-C2	-7.27	117.39	120.30
35	a	188	C	N1-C2-O2	7.25	123.25	118.90
56	v	56	U	C2-N1-C1'	7.25	126.40	117.70
35	a	58	C	C6-N1-C2	-7.24	117.41	120.30
1	A	2901	C	N3-C2-O2	-7.23	116.84	121.90
35	a	5	U	N1-C2-O2	7.22	127.86	122.80
1	A	1956	U	N3-C2-O2	-7.22	117.15	122.20
1	A	2321	U	N3-C2-O2	-7.21	117.15	122.20
35	a	207	C	C6-N1-C2	-7.21	117.42	120.30
35	a	1518	A	O4'-C1'-N9	7.21	113.97	108.20
1	A	542	C	C2-N1-C1'	7.21	126.73	118.80
1	A	12	U	C6-N1-C1'	-7.20	111.12	121.20
1	A	1956	U	N1-C2-O2	7.18	127.82	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	669	G	C4-N9-C1'	7.17	135.81	126.50
1	A	2752	C	N1-C2-O2	7.16	123.19	118.90
34	8	2	C	C2-N1-C1'	7.15	126.66	118.80
1	A	2179	C	C6-N1-C2	-7.13	117.45	120.30
1	A	2591	C	C5-C6-N1	7.12	124.56	121.00
2	B	25	U	N1-C2-O2	7.12	127.78	122.80
35	a	413	G	C4-N9-C1'	-7.11	117.26	126.50
34	8	2	C	N3-C2-O2	-7.11	116.93	121.90
1	A	1062	G	P-O3'-C3'	7.10	128.22	119.70
34	8	2	C	C6-N1-C2	-7.08	117.47	120.30
1	A	1049	C	N1-C2-O2	7.08	123.15	118.90
35	a	330	C	C6-N1-C1'	-7.07	112.31	120.80
35	a	413	G	C8-N9-C1'	7.07	136.19	127.00
1	A	2063	C	N3-C2-O2	-7.06	116.96	121.90
1	A	1993	U	N1-C2-O2	7.04	127.73	122.80
35	a	1230	C	C6-N1-C2	-7.03	117.49	120.30
1	A	752	A	P-O3'-C3'	7.02	128.12	119.70
1	A	277	G	N3-C4-C5	-7.02	125.09	128.60
35	a	207	C	C5-C6-N1	7.02	124.51	121.00
35	a	764	C	C6-N1-C2	-7.02	117.49	120.30
1	A	1135	C	N1-C2-O2	7.01	123.11	118.90
35	a	582	C	N3-C2-O2	-7.01	116.99	121.90
1	A	1917	U	N1-C2-O2	7.00	127.70	122.80
1	A	889	C	C6-N1-C2	-7.00	117.50	120.30
1	A	2793	C	N1-C2-O2	7.00	123.10	118.90
1	A	1517	G	N1-C2-N3	6.98	128.09	123.90
1	A	1804	C	C6-N1-C2	-6.97	117.51	120.30
35	a	991	U	N1-C2-O2	6.97	127.68	122.80
2	B	42	C	N1-C2-O2	6.96	123.07	118.90
1	A	357	C	N3-C2-O2	-6.95	117.03	121.90
35	a	1125	U	N3-C2-O2	-6.95	117.34	122.20
35	a	438	U	P-O3'-C3'	6.93	128.02	119.70
1	A	2456	C	C5-C6-N1	6.92	124.46	121.00
35	a	623	C	C5-C6-N1	6.92	124.46	121.00
35	a	1032	G	N3-C4-N9	6.90	130.14	126.00
35	a	413	G	N1-C6-O6	-6.89	115.76	119.90
1	A	847	U	N1-C2-O2	6.89	127.62	122.80
1	A	1914	C	C6-N1-C2	-6.89	117.55	120.30
12	M	70	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	2585	U	C2-N1-C1'	6.86	125.94	117.70
1	A	459	U	N1-C2-O2	6.86	127.60	122.80
1	A	2604	U	O4'-C1'-N1	6.85	113.68	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1173	U	P-O3'-C3'	6.81	127.88	119.70
35	a	1282	C	C2-N1-C1'	6.81	126.29	118.80
35	a	1162	C	N1-C2-O2	6.80	122.98	118.90
35	a	1109	C	C6-N1-C2	-6.80	117.58	120.30
35	a	95	C	N3-C2-O2	-6.79	117.14	121.90
1	A	1507	C	C5-C6-N1	6.79	124.40	121.00
1	A	1934	C	N1-C2-O2	6.79	122.97	118.90
1	A	277	G	N3-C4-N9	6.79	130.07	126.00
1	A	2354	C	C5-C6-N1	6.79	124.39	121.00
1	A	2354	C	C2-N1-C1'	6.77	126.25	118.80
35	a	764	C	C5-C6-N1	6.77	124.38	121.00
1	A	1130	U	P-O3'-C3'	6.77	127.82	119.70
1	A	985	C	N1-C2-O2	6.76	122.96	118.90
2	B	35	C	N3-C2-O2	-6.76	117.17	121.90
35	a	529	G	C5-C6-O6	-6.76	124.55	128.60
35	a	98	A	C8-N9-C4	-6.75	103.10	105.80
35	a	960	U	P-O3'-C3'	6.75	127.80	119.70
35	a	754	C	C2-N1-C1'	6.75	126.22	118.80
35	a	221	C	N1-C2-O2	6.75	122.95	118.90
1	A	847	U	C2-N1-C1'	6.74	125.79	117.70
1	A	2072	C	C6-N1-C2	-6.74	117.60	120.30
1	A	198	C	C5-C6-N1	6.74	124.37	121.00
1	A	544	C	C2-N1-C1'	6.73	126.20	118.80
1	A	1022	G	P-O3'-C3'	6.73	127.78	119.70
1	A	1378	A	P-O3'-C3'	6.73	127.77	119.70
1	A	2796	U	C5-C6-N1	6.72	126.06	122.70
1	A	915	C	C2-N1-C1'	6.72	126.19	118.80
35	a	221	C	C6-N1-C2	-6.71	117.61	120.30
35	a	58	C	C2-N1-C1'	6.71	126.18	118.80
1	A	807	U	N3-C2-O2	-6.68	117.53	122.20
1	A	1174	U	C2-N1-C1'	6.67	125.71	117.70
1	A	2667	C	N1-C2-O2	6.66	122.90	118.90
2	B	36	C	N3-C2-O2	-6.64	117.25	121.90
35	a	750	C	C6-N1-C2	-6.64	117.64	120.30
1	A	1967	C	N1-C2-O2	6.63	122.88	118.90
1	A	2109	U	C2-N1-C1'	6.62	125.65	117.70
1	A	2180	U	C2-N1-C1'	6.61	125.63	117.70
1	A	1372	U	N3-C2-O2	-6.61	117.58	122.20
1	A	2238	G	N3-C4-N9	6.59	129.96	126.00
15	P	114	LEU	CA-CB-CG	6.59	130.47	115.30
1	A	2456	C	C6-N1-C2	-6.59	117.66	120.30
35	a	1032	G	C4-N9-C1'	6.58	135.06	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1064	C	P-O3'-C3'	6.58	127.59	119.70
1	A	1267	U	N1-C2-O2	6.57	127.40	122.80
1	A	2686	G	N3-C4-N9	6.57	129.94	126.00
35	a	1301	U	N3-C2-O2	-6.57	117.60	122.20
1	A	1314	C	C6-N1-C2	-6.57	117.67	120.30
35	a	503	C	C6-N1-C2	-6.57	117.67	120.30
1	A	2667	C	N3-C2-O2	-6.56	117.31	121.90
56	v	54	G	C4-N9-C1'	6.56	135.03	126.50
1	A	353	C	N1-C2-O2	6.54	122.83	118.90
32	6	25	C	C6-N1-C2	-6.54	117.69	120.30
1	A	1065	U	N1-C2-O2	6.54	127.38	122.80
1	A	2300	C	C2-N1-C1'	6.53	125.98	118.80
1	A	417	C	C2-N1-C1'	6.53	125.98	118.80
1	A	510	C	N1-C2-O2	6.53	122.82	118.90
1	A	2460	U	N3-C2-O2	-6.53	117.63	122.20
1	A	1930	G	P-O3'-C3'	6.53	127.53	119.70
1	A	867	C	C2-N1-C1'	6.52	125.97	118.80
1	A	2646	C	C6-N1-C2	-6.52	117.69	120.30
35	a	110	C	N1-C2-O2	6.50	122.80	118.90
35	a	956	U	N3-C2-O2	-6.50	117.65	122.20
1	A	1130	U	OP1-P-O3'	6.49	119.48	105.20
35	a	582	C	C6-N1-C2	-6.48	117.71	120.30
1	A	242	G	P-O3'-C3'	6.48	127.48	119.70
1	A	1294	U	N3-C2-O2	-6.47	117.67	122.20
35	a	1120	C	N1-C2-O2	6.46	122.78	118.90
1	A	1062	G	OP1-P-O3'	6.46	119.41	105.20
1	A	783	A	C5-N7-C8	-6.45	100.68	103.90
1	A	2430	A	C2-N3-C4	6.44	113.82	110.60
1	A	2460	U	N1-C2-O2	6.44	127.31	122.80
1	A	2585	U	N1-C2-O2	6.44	127.31	122.80
1	A	1539	U	C5-C6-N1	6.43	125.92	122.70
35	a	979	C	N1-C2-O2	6.43	122.76	118.90
35	a	1138	G	C4-N9-C1'	6.43	134.86	126.50
1	A	67	U	N3-C4-O4	6.42	123.90	119.40
1	A	2043	C	C2-N1-C1'	6.42	125.86	118.80
1	A	1020	A	P-O3'-C3'	6.40	127.38	119.70
1	A	198	C	C6-N1-C2	-6.40	117.74	120.30
35	a	5	U	C2-N1-C1'	6.39	125.37	117.70
35	a	1201	A	P-O3'-C3'	6.39	127.37	119.70
35	a	103	U	N1-C2-O2	6.39	127.28	122.80
35	a	1399	C	P-O3'-C3'	6.38	127.36	119.70
35	a	1003	G	N1-C6-O6	-6.38	116.07	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2072	C	C5-C6-N1	6.37	124.18	121.00
35	a	1301	U	N1-C2-O2	6.37	127.26	122.80
56	v	63	C	C2-N1-C1'	6.37	125.81	118.80
1	A	2096	C	N1-C2-O2	6.37	122.72	118.90
56	v	57	C	N1-C2-O2	6.35	122.71	118.90
1	A	2226	C	C2-N1-C1'	6.35	125.78	118.80
1	A	2321	U	C2-N1-C1'	6.35	125.32	117.70
35	a	110	C	N3-C2-O2	-6.35	117.46	121.90
35	a	191	G	C6-C5-N7	-6.35	126.59	130.40
35	a	1109	C	N1-C2-O2	6.35	122.71	118.90
1	A	1941	C	N1-C2-O2	6.34	122.71	118.90
1	A	130	C	C6-N1-C2	-6.34	117.76	120.30
1	A	1420	A	P-O3'-C3'	6.34	127.31	119.70
35	a	355	C	N1-C2-O2	6.34	122.70	118.90
35	a	528	C	N1-C2-O2	6.33	122.70	118.90
1	A	2646	C	C5-C6-N1	6.33	124.17	121.00
35	a	98	A	N7-C8-N9	6.33	116.97	113.80
34	8	85	C	C5-C6-N1	6.33	124.17	121.00
35	a	924	C	C6-N1-C2	-6.33	117.77	120.30
1	A	1934	C	C2-N1-C1'	6.32	125.76	118.80
35	a	5	U	O4'-C1'-N1	6.32	113.26	108.20
1	A	1102	C	N3-C2-O2	-6.32	117.48	121.90
1	A	2226	C	C6-N1-C2	-6.31	117.78	120.30
35	a	1427	C	C5-C6-N1	6.31	124.15	121.00
1	A	12	U	C5-C6-N1	6.30	125.85	122.70
35	a	979	C	N3-C2-O2	-6.29	117.49	121.90
1	A	634	C	C6-N1-C2	-6.28	117.79	120.30
35	a	1300	G	P-O3'-C3'	6.27	127.22	119.70
1	A	67	U	C5-C4-O4	-6.27	122.14	125.90
35	a	516	U	C2-N1-C1'	6.27	125.22	117.70
1	A	2350	C	N1-C2-O2	6.27	122.66	118.90
1	A	1940	U	P-O3'-C3'	6.26	127.22	119.70
1	A	640	C	C6-N1-C2	-6.26	117.80	120.30
1	A	919	U	N3-C2-O2	-6.26	117.82	122.20
35	a	1109	C	N3-C2-O2	-6.25	117.52	121.90
1	A	1398	C	C2-N1-C1'	6.25	125.67	118.80
35	a	269	C	C6-N1-C2	-6.25	117.80	120.30
1	A	1111	A	P-O3'-C3'	6.25	127.20	119.70
1	A	2320	U	C6-N1-C1'	-6.24	112.46	121.20
1	A	2394	C	N1-C2-O2	6.24	122.64	118.90
35	a	1158	C	C6-N1-C1'	-6.24	113.31	120.80
1	A	669	G	C8-N9-C1'	-6.24	118.89	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	859	G	P-O3'-C3'	6.24	127.18	119.70
1	A	1913	A	P-O3'-C3'	6.22	127.16	119.70
2	B	42	C	N3-C2-O2	-6.21	117.55	121.90
35	a	283	U	N3-C2-O2	-6.21	117.85	122.20
34	8	2	C	C5-C6-N1	6.21	124.11	121.00
35	a	1383	C	N1-C2-O2	6.21	122.62	118.90
1	A	1894	C	N1-C2-O2	6.20	122.62	118.90
1	A	139	U	C2-N1-C1'	6.19	125.13	117.70
35	a	1190	G	P-O3'-C3'	6.19	127.13	119.70
1	A	2566	A	P-O3'-C3'	6.18	127.12	119.70
2	B	35	C	C5-C6-N1	6.18	124.09	121.00
1	A	2808	G	P-O3'-C3'	6.18	127.11	119.70
35	a	1086	U	C2-N1-C1'	6.18	125.11	117.70
1	A	1101	U	N3-C2-O2	-6.17	117.88	122.20
1	A	1135	C	C2-N1-C1'	6.17	125.59	118.80
1	A	1108	U	C2-N1-C1'	6.17	125.10	117.70
1	A	234	U	N3-C2-O2	-6.17	117.88	122.20
56	v	47	G	P-O3'-C3'	6.16	127.10	119.70
1	A	2179	C	C2-N1-C1'	6.16	125.58	118.80
35	a	188	C	N3-C2-O2	-6.16	117.59	121.90
35	a	623	C	C6-N1-C2	-6.16	117.84	120.30
2	B	36	C	C2-N1-C1'	6.16	125.57	118.80
1	A	2321	U	N1-C2-O2	6.15	127.11	122.80
1	A	2109	U	N1-C2-O2	6.15	127.10	122.80
1	A	2793	C	C5-C6-N1	6.14	124.07	121.00
1	A	357	C	N1-C2-O2	6.14	122.58	118.90
1	A	635	C	C6-N1-C2	-6.14	117.85	120.30
1	A	1539	U	C5-C4-O4	-6.13	122.22	125.90
1	A	277	G	C4-N9-C1'	6.12	134.46	126.50
1	A	2539	C	N1-C2-O2	6.12	122.57	118.90
1	A	2044	C	C6-N1-C2	-6.11	117.85	120.30
35	a	191	G	C4-C5-N7	6.11	113.25	110.80
1	A	1836	C	C6-N1-C2	-6.11	117.86	120.30
35	a	365	U	C2-N1-C1'	6.11	125.03	117.70
34	8	26	C	C6-N1-C2	-6.11	117.86	120.30
35	a	88	U	O4'-C1'-N1	6.10	113.08	108.20
1	A	2656	U	C2-N1-C1'	6.10	125.02	117.70
29	3	62	LEU	CA-CB-CG	6.10	129.33	115.30
1	A	2342	C	N1-C2-O2	6.10	122.56	118.90
1	A	2026	U	C5-C6-N1	6.10	125.75	122.70
1	A	1658	C	C5-C6-N1	6.09	124.04	121.00
1	A	353	C	N3-C2-O2	-6.08	117.64	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2342	C	C6-N1-C2	-6.08	117.87	120.30
1	A	897	C	C2-N1-C1'	6.07	125.48	118.80
1	A	2043	C	N1-C2-O2	6.07	122.54	118.90
1	A	860	U	C5-C6-N1	6.06	125.73	122.70
1	A	897	C	C5-C6-N1	6.06	124.03	121.00
1	A	1049	C	N3-C2-O2	-6.06	117.66	121.90
1	A	1531	C	N1-C2-O2	6.06	122.54	118.90
1	A	2150	C	C6-N1-C2	-6.05	117.88	120.30
1	A	157	C	C5-C6-N1	6.05	124.03	121.00
35	a	188	C	C2-N1-C1'	6.05	125.46	118.80
1	A	459	U	N3-C2-O2	-6.05	117.97	122.20
35	a	1147	C	C6-N1-C2	-6.05	117.88	120.30
1	A	919	U	N1-C2-O2	6.04	127.03	122.80
35	a	1162	C	N3-C2-O2	-6.04	117.68	121.90
1	A	1508	A	P-O3'-C3'	6.03	126.93	119.70
1	A	2065	C	C6-N1-C2	-6.03	117.89	120.30
1	A	2089	C	C6-N1-C2	-6.02	117.89	120.30
1	A	581	C	C5-C6-N1	6.02	124.01	121.00
56	v	56	U	N1-C2-O2	6.02	127.02	122.80
1	A	1005	C	C5-C6-N1	6.02	124.01	121.00
1	A	1585	C	N1-C2-O2	6.01	122.51	118.90
1	A	2047	C	C6-N1-C2	-6.01	117.89	120.30
35	a	8	A	C8-N9-C4	6.01	108.21	105.80
35	a	697	U	N1-C2-O2	6.01	127.01	122.80
35	a	1138	G	N3-C4-N9	6.01	129.61	126.00
1	A	1911	U	N3-C2-O2	-6.01	118.00	122.20
1	A	1053	C	N1-C2-O2	6.00	122.50	118.90
33	7	2	THR	N-CA-C	6.00	127.20	111.00
35	a	697	U	N3-C2-O2	-5.99	118.01	122.20
1	A	105	C	C5-C6-N1	5.99	123.99	121.00
1	A	2884	U	C2-N1-C1'	5.99	124.88	117.70
1	A	1348	C	N3-C2-O2	-5.98	117.71	121.90
1	A	974	G	O4'-C1'-N9	5.98	112.98	108.20
1	A	1082	U	C6-N1-C2	-5.98	117.41	121.00
35	a	269	C	C5-C6-N1	5.98	123.99	121.00
1	A	1859	U	N3-C2-O2	-5.97	118.02	122.20
1	A	1541	C	P-O3'-C3'	5.97	126.86	119.70
1	A	12	U	C6-N1-C2	-5.97	117.42	121.00
1	A	1931	U	C2-N1-C1'	5.97	124.86	117.70
35	a	221	C	N3-C2-O2	-5.97	117.72	121.90
1	A	2789	C	C2-N1-C1'	5.96	125.35	118.80
1	A	2238	G	C2-N3-C4	5.96	114.88	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2350	C	N3-C2-O2	-5.96	117.73	121.90
35	a	1032	G	C2-N3-C4	5.95	114.88	111.90
34	8	72	C	N1-C2-O2	5.95	122.47	118.90
1	A	1378	A	OP1-P-O3'	5.95	118.29	105.20
56	v	20	A	O4'-C1'-N9	-5.95	103.44	108.20
35	a	1297	G	P-O3'-C3'	5.95	126.84	119.70
1	A	1064	C	C2-N1-C1'	5.95	125.34	118.80
1	A	208	C	C5-C6-N1	5.94	123.97	121.00
1	A	1343	G	C4-N9-C1'	5.94	134.22	126.50
35	a	1411	C	C6-N1-C2	-5.93	117.93	120.30
35	a	528	C	C2-N1-C1'	5.93	125.33	118.80
1	A	234	U	N1-C2-O2	5.93	126.95	122.80
1	A	2006	C	C6-N1-C2	-5.93	117.93	120.30
35	a	439	U	C5-C6-N1	5.92	125.66	122.70
1	A	2576	G	C4-N9-C1'	5.92	134.19	126.50
1	A	2306	C	C6-N1-C2	-5.92	117.93	120.30
2	B	25	U	N3-C2-O2	-5.92	118.06	122.20
1	A	2686	G	N3-C4-C5	-5.91	125.64	128.60
1	A	860	U	N1-C2-O2	5.91	126.94	122.80
35	a	1414	U	N3-C2-O2	-5.91	118.06	122.20
1	A	1053	C	C6-N1-C2	-5.91	117.94	120.30
1	A	151	C	C5-C6-N1	5.90	123.95	121.00
35	a	126	G	N3-C4-C5	-5.90	125.65	128.60
35	a	383	A	P-O3'-C3'	5.90	126.78	119.70
35	a	899	C	C6-N1-C2	-5.90	117.94	120.30
1	A	1063	G	N3-C4-N9	5.89	129.54	126.00
1	A	1174	U	N1-C2-O2	5.89	126.92	122.80
1	A	281	C	P-O3'-C3'	5.89	126.77	119.70
35	a	1147	C	N1-C2-O2	5.89	122.43	118.90
35	a	1297	G	OP2-P-O3'	5.88	118.15	105.20
1	A	105	C	C6-N1-C2	-5.88	117.95	120.30
1	A	2794	C	C5-C6-N1	5.88	123.94	121.00
1	A	274	C	N1-C2-O2	5.87	122.42	118.90
56	v	63	C	C6-N1-C2	-5.87	117.95	120.30
1	A	2592	G	N3-C4-N9	5.87	129.52	126.00
1	A	1961	C	N1-C2-O2	5.87	122.42	118.90
1	A	2552	U	N3-C2-O2	-5.86	118.10	122.20
35	a	5	U	N3-C2-O2	-5.86	118.10	122.20
1	A	2072	C	C2-N1-C1'	5.86	125.25	118.80
1	A	1221	C	C2-N1-C1'	5.86	125.24	118.80
35	a	1182	G	P-O3'-C3'	5.86	126.73	119.70
35	a	1120	C	N3-C2-O2	-5.85	117.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	1301	U	C5-C6-N1	5.85	125.62	122.70
1	A	2901	C	N1-C2-O2	5.84	122.41	118.90
35	a	1027	C	C6-N1-C1'	-5.84	113.79	120.80
1	A	1859	U	N1-C2-O2	5.84	126.89	122.80
1	A	560	C	C6-N1-C2	-5.84	117.97	120.30
1	A	607	U	N3-C2-O2	-5.84	118.11	122.20
1	A	2043	C	C5-C6-N1	5.84	123.92	121.00
35	a	211	G	N3-C4-N9	5.83	129.50	126.00
35	a	1007	U	N3-C2-O2	-5.83	118.12	122.20
1	A	243	U	N1-C2-O2	5.83	126.88	122.80
56	v	66	C	N1-C2-O2	5.82	122.39	118.90
20	U	52	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	2590	A	N9-C4-C5	5.82	108.13	105.80
1	A	2591	C	C6-N1-C2	-5.82	117.97	120.30
1	A	2320	U	C6-N1-C2	-5.79	117.52	121.00
1	A	139	U	N1-C2-O2	5.79	126.86	122.80
35	a	940	C	C5-C6-N1	5.79	123.90	121.00
1	A	546	U	P-O3'-C3'	5.79	126.65	119.70
1	A	2044	C	C5-C6-N1	5.78	123.89	121.00
35	a	1003	G	N9-C4-C5	5.78	107.71	105.40
56	v	54	G	OP1-P-O3'	5.78	117.92	105.20
1	A	1294	U	N1-C2-O2	5.78	126.84	122.80
1	A	1295	C	C6-N1-C2	-5.78	117.99	120.30
35	a	191	G	N9-C4-C5	-5.77	103.09	105.40
35	a	82	G	C4-N9-C1'	5.76	133.99	126.50
1	A	1314	C	C2-N1-C1'	5.76	125.13	118.80
1	A	1993	U	C2-N1-C1'	5.76	124.61	117.70
1	A	1171	G	P-O3'-C3'	5.75	126.61	119.70
1	A	2794	C	C6-N1-C2	-5.75	118.00	120.30
35	a	211	G	C4-N9-C1'	5.75	133.98	126.50
1	A	640	C	C5-C6-N1	5.75	123.88	121.00
35	a	582	C	C5-C6-N1	5.75	123.87	121.00
1	A	157	C	C6-N1-C2	-5.75	118.00	120.30
1	A	1267	U	C2-N1-C1'	5.74	124.59	117.70
1	A	2793	C	C6-N1-C2	-5.74	118.00	120.30
1	A	1830	C	C5-C6-N1	5.74	123.87	121.00
1	A	2585	U	N3-C2-O2	-5.74	118.19	122.20
35	a	904	U	C5-C6-N1	5.74	125.57	122.70
35	a	1003	G	C5-C6-O6	5.73	132.04	128.60
1	A	484	C	C5-C6-N1	5.72	123.86	121.00
56	v	56	U	N3-C2-O2	-5.72	118.19	122.20
35	a	516	U	N1-C2-O2	5.72	126.80	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	C	C5-C6-N1	5.72	123.86	121.00
1	A	208	C	C6-N1-C2	-5.72	118.01	120.30
1	A	1830	C	C6-N1-C2	-5.71	118.02	120.30
1	A	323	C	N1-C2-O2	5.71	122.33	118.90
1	A	2649	C	C5-C6-N1	5.71	123.85	121.00
1	A	305	C	C5-C6-N1	5.71	123.85	121.00
1	A	1731	G	C8-N9-C1'	5.71	134.42	127.00
35	a	221	C	C2-N1-C1'	5.71	125.08	118.80
35	a	283	U	N1-C2-O2	5.70	126.79	122.80
35	a	413	G	C6-C5-N7	5.69	133.82	130.40
1	A	795	C	C5-C6-N1	5.69	123.84	121.00
1	A	1101	U	N1-C2-O2	5.69	126.78	122.80
1	A	1172	C	N3-C2-O2	-5.69	117.92	121.90
34	8	85	C	C6-N1-C2	-5.69	118.03	120.30
1	A	1941	C	N3-C2-O2	-5.68	117.92	121.90
35	a	623	C	N1-C2-O2	5.68	122.31	118.90
1	A	1267	U	N3-C2-O2	-5.68	118.22	122.20
35	a	88	U	N3-C2-O2	-5.68	118.22	122.20
46	l	40	THR	C-N-CA	5.68	135.90	121.70
1	A	1531	C	N3-C2-O2	-5.67	117.93	121.90
1	A	1731	G	N9-C4-C5	5.67	107.67	105.40
1	A	2552	U	C2-N1-C1'	5.67	124.50	117.70
1	A	151	C	C6-N1-C2	-5.67	118.03	120.30
1	A	2686	G	C4-N9-C1'	5.66	133.86	126.50
35	a	1125	U	N1-C2-O2	5.66	126.76	122.80
1	A	2326	C	C5-C6-N1	5.66	123.83	121.00
1	A	1005	C	C6-N1-C2	-5.65	118.04	120.30
1	A	2592	G	C4-N9-C1'	5.65	133.84	126.50
35	a	86	G	C8-N9-C4	-5.64	104.14	106.40
35	a	1031	C	C6-N1-C2	-5.64	118.04	120.30
1	A	2248	C	C5-C6-N1	5.64	123.82	121.00
35	a	154	U	C2-N1-C1'	5.63	124.46	117.70
1	A	1857	G	O4'-C1'-N9	5.62	112.70	108.20
35	a	1230	C	C5-C6-N1	5.62	123.81	121.00
1	A	274	C	N3-C2-O2	-5.62	117.96	121.90
35	a	1138	G	N3-C4-C5	-5.62	125.79	128.60
35	a	732	C	N3-C2-O2	-5.62	117.97	121.90
35	a	1190	G	N3-C4-N9	-5.62	122.63	126.00
1	A	1065	U	C6-N1-C1'	-5.61	113.34	121.20
1	A	1816	C	N1-C2-O2	5.61	122.27	118.90
1	A	1178	C	O5'-P-OP1	-5.61	100.65	105.70
35	a	244	U	O4'-C1'-N1	-5.61	103.71	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	1149	C	C6-N1-C2	-5.61	118.06	120.30
1	A	66	C	C5-C6-N1	5.60	123.80	121.00
1	A	1064	C	N1-C2-O2	5.60	122.26	118.90
1	A	1760	C	C6-N1-C2	-5.60	118.06	120.30
2	B	68	C	C6-N1-C2	-5.60	118.06	120.30
1	A	1539	U	N3-C4-O4	5.60	123.32	119.40
35	a	1348	U	N1-C2-O2	5.60	126.72	122.80
35	a	287	U	N1-C2-O2	5.59	126.71	122.80
1	A	1157	G	C6-C5-N7	-5.59	127.05	130.40
35	a	191	G	C4-N9-C1'	5.59	133.76	126.50
35	a	924	C	C5-C6-N1	5.59	123.79	121.00
35	a	73	C	N1-C2-O2	5.58	122.25	118.90
1	A	2109	U	N3-C2-O2	-5.58	118.30	122.20
35	a	1412	C	C6-N1-C2	-5.58	118.07	120.30
35	a	1449	C	N1-C2-O2	5.58	122.25	118.90
1	A	2667	C	C6-N1-C2	-5.57	118.07	120.30
1	A	2539	C	N3-C2-O2	-5.56	118.01	121.90
2	B	66	A	P-O3'-C3'	5.56	126.37	119.70
35	a	991	U	C6-N1-C1'	-5.56	113.42	121.20
1	A	2794	C	C2-N1-C1'	5.56	124.91	118.80
35	a	126	G	N3-C4-N9	5.55	129.33	126.00
1	A	157	C	C2-N1-C1'	5.55	124.91	118.80
1	A	2096	C	C6-N1-C2	-5.55	118.08	120.30
35	a	54	C	N3-C2-O2	-5.55	118.01	121.90
1	A	1931	U	N1-C2-O2	5.54	126.68	122.80
35	a	1282	C	C6-N1-C2	-5.54	118.08	120.30
1	A	2474	U	N3-C2-O2	-5.54	118.32	122.20
35	a	355	C	N3-C2-O2	-5.54	118.02	121.90
1	A	1886	U	N3-C2-O2	-5.53	118.33	122.20
1	A	2840	C	C2-N3-C4	5.53	122.67	119.90
35	a	991	U	C5-C6-N1	5.53	125.47	122.70
1	A	2301	C	C6-N1-C2	-5.53	118.09	120.30
1	A	1894	C	N3-C2-O2	-5.53	118.03	121.90
1	A	2064	C	C6-N1-C2	-5.53	118.09	120.30
56	v	66	C	C6-N1-C2	-5.52	118.09	120.30
1	A	752	A	OP2-P-O3'	5.52	117.35	105.20
35	a	191	G	C8-N9-C1'	-5.52	119.82	127.00
1	A	1480	C	N1-C2-O2	5.52	122.21	118.90
1	A	2096	C	C5-C6-N1	5.52	123.76	121.00
1	A	1135	C	N3-C2-O2	-5.52	118.04	121.90
35	a	4	U	P-O3'-C3'	5.52	126.32	119.70
35	a	891	U	N1-C2-O2	5.51	126.66	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	C	C2-N1-C1'	5.51	124.86	118.80
35	a	739	C	C6-N1-C2	-5.51	118.10	120.30
35	a	750	C	N3-C2-O2	-5.51	118.04	121.90
35	a	1028	C	C5-C6-N1	5.51	123.75	121.00
35	a	1208	C	C6-N1-C2	-5.51	118.10	120.30
1	A	634	C	C5-C6-N1	5.50	123.75	121.00
1	A	1941	C	C2-N1-C1'	5.50	124.85	118.80
1	A	2592	G	C8-N9-C1'	-5.50	119.85	127.00
1	A	2099	U	C2-N1-C1'	5.50	124.30	117.70
35	a	912	C	C5-C6-N1	5.50	123.75	121.00
35	a	1411	C	C5-C6-N1	5.50	123.75	121.00
1	A	420	C	C6-N1-C2	-5.49	118.10	120.30
1	A	1644	C	N3-C2-O2	-5.49	118.06	121.90
35	a	455	G	N7-C8-N9	5.49	115.85	113.10
35	a	85	U	N3-C2-O2	-5.49	118.36	122.20
1	A	358	U	C5-C6-N1	5.49	125.44	122.70
1	A	1108	U	N1-C2-O2	5.49	126.64	122.80
1	A	2073	C	N3-C2-O2	-5.49	118.06	121.90
1	A	1348	C	C2-N1-C1'	5.48	124.83	118.80
1	A	2394	C	C5-C6-N1	5.48	123.74	121.00
2	B	36	C	C6-N1-C2	-5.48	118.11	120.30
35	a	69	G	C4-N9-C1'	5.48	133.62	126.50
35	a	96	U	C6-N1-C1'	-5.48	113.53	121.20
1	A	1913	A	OP2-P-O3'	5.48	117.25	105.20
1	A	1221	C	N1-C2-O2	5.48	122.19	118.90
1	A	807	U	N1-C2-O2	5.47	126.63	122.80
1	A	1323	C	N1-C2-O2	5.47	122.18	118.90
1	A	484	C	C6-N1-C2	-5.46	118.11	120.30
2	B	17	C	C6-N1-C2	-5.46	118.11	120.30
35	a	81	A	N7-C8-N9	5.46	116.53	113.80
1	A	542	C	C5-C6-N1	5.46	123.73	121.00
1	A	1830	C	N1-C2-O2	5.46	122.17	118.90
1	A	889	C	C5-C6-N1	5.46	123.73	121.00
1	A	915	C	C6-N1-C2	-5.45	118.12	120.30
35	a	1028	C	N1-C2-O2	5.45	122.17	118.90
1	A	1945	G	N3-C4-N9	5.44	129.27	126.00
1	A	2752	C	N3-C2-O2	-5.44	118.09	121.90
2	B	27	C	N1-C2-O2	5.44	122.16	118.90
35	a	840	C	C5-C6-N1	5.44	123.72	121.00
1	A	1517	G	C4-C5-N7	-5.43	108.63	110.80
1	A	1911	U	C2-N1-C1'	5.43	124.22	117.70
35	a	623	C	C2-N1-C1'	5.43	124.78	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	1238	A	C2-N3-C4	5.43	113.32	110.60
1	A	2815	C	C6-N1-C2	-5.42	118.13	120.30
35	a	413	G	O4'-C1'-N9	5.42	112.54	108.20
35	a	1003	G	C4-C5-N7	-5.42	108.63	110.80
1	A	1417	C	C2-N1-C1'	5.41	124.75	118.80
11	L	29	LYS	C-N-CA	5.41	135.24	121.70
1	A	2300	C	C5-C6-N1	5.41	123.70	121.00
2	B	68	C	C5-C6-N1	5.41	123.70	121.00
35	a	1138	G	C8-N9-C1'	-5.41	119.97	127.00
35	a	1197	A	O5'-P-OP2	-5.41	100.83	105.70
2	B	30	C	C5-C6-N1	5.40	123.70	121.00
1	A	2789	C	C5-C6-N1	5.40	123.70	121.00
2	B	25	U	C2-N1-C1'	5.40	124.18	117.70
34	8	80	C	C5-C6-N1	5.40	123.70	121.00
35	a	1497	G	C8-N9-C1'	-5.39	119.99	127.00
1	A	404	A	P-O3'-C3'	5.39	126.17	119.70
35	a	1208	C	C2-N1-C1'	5.38	124.72	118.80
36	b	127	ASP	CB-CG-OD1	5.38	123.14	118.30
35	a	58	C	C5-C6-N1	5.38	123.69	121.00
35	a	957	U	N3-C2-O2	-5.38	118.43	122.20
35	a	967	C	C5-C6-N1	5.38	123.69	121.00
1	A	783	A	N7-C8-N9	5.38	116.49	113.80
1	A	475	C	C6-N1-C2	-5.38	118.15	120.30
1	A	2248	C	C2-N1-C1'	5.38	124.71	118.80
35	a	796	C	C6-N1-C2	-5.38	118.15	120.30
1	A	1064	C	C6-N1-C2	-5.37	118.15	120.30
1	A	2683	C	N3-C2-O2	-5.37	118.14	121.90
1	A	1517	G	C8-N9-C4	-5.37	104.25	106.40
2	B	66	A	OP1-P-O3'	5.36	116.99	105.20
35	a	438	U	O4'-C1'-N1	5.36	112.49	108.20
35	a	489	C	C5-C6-N1	5.36	123.68	121.00
1	A	364	C	N3-C2-O2	-5.36	118.15	121.90
56	v	54	G	C8-N9-C1'	-5.35	120.04	127.00
1	A	1658	C	C6-N1-C2	-5.35	118.16	120.30
35	a	217	C	C2-N1-C1'	5.35	124.68	118.80
35	a	350	G	N3-C4-C5	5.34	131.27	128.60
1	A	2884	U	N1-C2-O2	5.34	126.54	122.80
1	A	1362	C	C5-C6-N1	5.34	123.67	121.00
35	a	1027	C	C5-C6-N1	5.34	123.67	121.00
1	A	1174	U	N3-C2-O2	-5.34	118.46	122.20
1	A	823	C	C6-N1-C2	-5.33	118.17	120.30
1	A	1102	C	C2-N1-C1'	5.33	124.67	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	273	U	N3-C2-O2	-5.33	118.47	122.20
35	a	1202	U	N1-C2-O2	5.33	126.53	122.80
56	v	54	G	N3-C4-N9	5.33	129.20	126.00
1	A	158	U	C2-N1-C1'	5.32	124.08	117.70
35	a	1265	C	C6-N1-C2	-5.32	118.17	120.30
1	A	323	C	C2-N1-C1'	5.31	124.64	118.80
35	a	95	C	C2-N1-C1'	5.31	124.64	118.80
1	A	1415	U	N1-C2-O2	5.31	126.51	122.80
35	a	287	U	N3-C2-O2	-5.30	118.49	122.20
1	A	2300	C	C6-N1-C2	-5.30	118.18	120.30
35	a	991	U	N3-C2-O2	-5.30	118.49	122.20
35	a	1032	G	C8-N9-C1'	-5.30	120.11	127.00
35	a	1262	C	N1-C2-O2	5.30	122.08	118.90
35	a	891	U	N3-C2-O2	-5.29	118.49	122.20
35	a	1033	G	P-O3'-C3'	5.29	126.05	119.70
35	a	1132	C	N1-C2-O2	5.29	122.07	118.90
35	a	70	U	P-O3'-C3'	5.29	126.05	119.70
35	a	899	C	C5-C6-N1	5.29	123.64	121.00
1	A	2098	U	C6-N1-C1'	-5.29	113.80	121.20
1	A	1079	C	N1-C2-O2	5.28	122.07	118.90
35	a	194	C	C6-N1-C2	-5.28	118.19	120.30
35	a	1301	U	C6-N1-C1'	-5.28	113.81	121.20
1	A	1934	C	N3-C2-O2	-5.28	118.20	121.90
35	a	85	U	N1-C2-O2	5.28	126.49	122.80
1	A	783	A	C4-C5-N7	5.27	113.34	110.70
1	A	867	C	C6-N1-C2	-5.27	118.19	120.30
35	a	256	U	C5-C6-N1	5.27	125.34	122.70
35	a	764	C	N1-C2-O2	5.27	122.06	118.90
1	A	1917	U	N3-C4-C5	5.27	117.76	114.60
35	a	439	U	C6-N1-C2	-5.27	117.84	121.00
35	a	1359	C	C5-C6-N1	5.27	123.64	121.00
1	A	1934	C	C6-N1-C2	-5.27	118.19	120.30
35	a	536	C	C6-N1-C2	-5.27	118.19	120.30
37	c	157	LEU	CA-CB-CG	5.27	127.41	115.30
1	A	373	U	N1-C2-O2	5.26	126.48	122.80
35	a	54	C	N1-C2-O2	5.26	122.06	118.90
1	A	2789	C	C6-N1-C2	-5.26	118.19	120.30
35	a	599	C	C5-C6-N1	5.26	123.63	121.00
35	a	1148	U	N3-C2-O2	-5.26	118.52	122.20
1	A	1474	U	N1-C2-O2	5.26	126.48	122.80
1	A	889	C	C6-N1-C1'	5.26	127.11	120.80
1	A	1172	C	C2-N1-C1'	5.26	124.58	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	C	C6-N1-C2	-5.26	118.20	120.30
35	a	188	C	C6-N1-C2	-5.25	118.20	120.30
35	a	1045	C	C6-N1-C2	-5.25	118.20	120.30
2	B	88	C	OP1-P-O3'	5.25	116.76	105.20
1	A	669	G	N3-C4-C5	-5.25	125.98	128.60
1	A	1611	C	C2-N1-C1'	5.25	124.57	118.80
2	B	35	C	C2-N1-C1'	5.25	124.57	118.80
35	a	269	C	N1-C2-O2	5.25	122.05	118.90
56	v	66	C	N3-C2-O2	-5.25	118.23	121.90
1	A	1727	C	N3-C2-O2	-5.24	118.23	121.90
35	a	1383	C	C2-N1-C1'	5.24	124.56	118.80
1	A	1914	C	C5-C6-N1	5.24	123.62	121.00
35	a	1109	C	C2-N1-C1'	5.24	124.56	118.80
1	A	2065	C	C5-C6-N1	5.23	123.62	121.00
1	A	2329	U	C5-C6-N1	5.23	125.32	122.70
35	a	893	C	N1-C2-O2	5.23	122.04	118.90
1	A	1930	G	OP2-P-O3'	5.23	116.70	105.20
1	A	542	C	N1-C2-O2	5.23	122.04	118.90
35	a	1317	C	N1-C2-O2	5.22	122.03	118.90
35	a	492	C	N1-C2-O2	5.22	122.03	118.90
1	A	122	G	C6-C5-N7	-5.22	127.27	130.40
56	v	32	G	N3-C4-N9	5.22	129.13	126.00
1	A	544	C	N1-C2-O2	5.21	122.03	118.90
1	A	1914	C	C6-N1-C1'	-5.21	114.55	120.80
1	A	2793	C	C6-N1-C1'	-5.21	114.55	120.80
1	A	2840	C	N1-C2-O2	5.21	122.03	118.90
1	A	814	C	C6-N1-C2	-5.21	118.22	120.30
1	A	1844	C	N3-C2-O2	-5.21	118.25	121.90
1	A	2576	G	C8-N9-C1'	-5.21	120.23	127.00
35	a	194	C	C5-C6-N1	5.21	123.60	121.00
1	A	1005	C	C2-N1-C1'	5.20	124.52	118.80
1	A	1049	C	C6-N1-C2	-5.20	118.22	120.30
1	A	1173	U	OP1-P-O3'	5.20	116.64	105.20
56	v	33	C	C6-N1-C2	-5.20	118.22	120.30
1	A	356	G	N3-C4-N9	5.19	129.12	126.00
56	v	57	C	N3-C2-O2	-5.19	118.27	121.90
35	a	206	C	N1-C2-O2	5.19	122.01	118.90
1	A	2215	C	N1-C2-O2	5.19	122.01	118.90
1	A	2769	U	N3-C2-O2	-5.18	118.57	122.20
1	A	1157	G	C4-N9-C1'	5.18	133.24	126.50
1	A	2649	C	C6-N1-C2	-5.18	118.23	120.30
1	A	2902	C	N1-C2-O2	5.18	122.01	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	269	C	C6-N1-C1'	-5.18	114.58	120.80
1	A	669	G	N3-C4-N9	5.18	129.11	126.00
2	B	25	U	C5-C6-N1	5.18	125.29	122.70
1	A	278	A	C2-N3-C4	5.17	113.19	110.60
35	a	738	C	C6-N1-C2	-5.17	118.23	120.30
1	A	1415	U	N3-C2-O2	-5.17	118.58	122.20
35	a	1363	A	C2-N3-C4	5.17	113.19	110.60
1	A	2767	C	C6-N1-C2	-5.17	118.23	120.30
35	a	208	U	N1-C2-O2	5.17	126.42	122.80
35	a	957	U	C6-N1-C2	-5.17	117.90	121.00
35	a	413	G	N3-C4-N9	-5.16	122.90	126.00
1	A	1314	C	C5-C6-N1	5.16	123.58	121.00
1	A	1732	C	N1-C2-N3	5.16	122.81	119.20
35	a	464	U	C5-C6-N1	5.16	125.28	122.70
1	A	2089	C	C5-C6-N1	5.16	123.58	121.00
1	A	2099	U	N3-C2-O2	-5.15	118.59	122.20
1	A	1065	U	N3-C2-O2	-5.15	118.59	122.20
35	a	943	U	N3-C2-O2	-5.15	118.59	122.20
1	A	1053	C	C5-C6-N1	5.15	123.57	121.00
35	a	436	C	N3-C2-O2	-5.15	118.30	121.90
1	A	1362	C	C6-N1-C2	-5.14	118.24	120.30
56	v	54	G	N7-C8-N9	5.14	115.67	113.10
1	A	2326	C	P-O3'-C3'	5.14	125.87	119.70
1	A	1157	G	C4-C5-N7	5.14	112.86	110.80
1	A	2592	G	N3-C4-C5	-5.14	126.03	128.60
35	a	82	G	C8-N9-C1'	-5.13	120.33	127.00
1	A	2794	C	N1-C2-O2	5.13	121.98	118.90
32	6	25	C	C5-C6-N1	5.13	123.57	121.00
35	a	792	A	O4'-C1'-N9	5.13	112.31	108.20
35	a	582	C	C2-N1-C1'	5.13	124.44	118.80
1	A	1644	C	N1-C2-O2	5.13	121.98	118.90
1	A	1065	U	C5-C6-N1	5.13	125.26	122.70
1	A	1940	U	OP2-P-O3'	5.13	116.48	105.20
2	B	17	C	N1-C2-O2	5.13	121.98	118.90
35	a	80	A	P-O3'-C3'	5.12	125.85	119.70
1	A	1086	A	N1-C6-N6	-5.12	115.53	118.60
1	A	312	G	C6-C5-N7	-5.12	127.33	130.40
1	A	1774	C	C5-C6-N1	5.12	123.56	121.00
34	8	63	G	P-O3'-C3'	5.12	125.85	119.70
1	A	1945	G	C4-N9-C1'	5.12	133.16	126.50
35	a	1414	U	N1-C2-O2	5.12	126.38	122.80
1	A	1295	C	C2-N1-C1'	5.12	124.43	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1157	G	C8-N9-C1'	-5.12	120.35	127.00
1	A	1830	C	C2-N1-C1'	5.12	124.43	118.80
2	B	68	C	N1-C2-O2	5.11	121.97	118.90
1	A	158	U	C5-C6-N1	5.11	125.25	122.70
1	A	510	C	C6-N1-C2	-5.11	118.25	120.30
35	a	1253	G	C4-N9-C1'	5.11	133.14	126.50
1	A	2474	U	N1-C2-O2	5.11	126.38	122.80
1	A	1052	C	C6-N1-C2	-5.11	118.26	120.30
1	A	1539	U	C6-N1-C1'	-5.11	114.05	121.20
1	A	2720	U	N3-C2-O2	-5.10	118.63	122.20
35	a	83	C	N3-C2-O2	-5.10	118.33	121.90
35	a	6	G	C4-C5-N7	5.10	112.84	110.80
35	a	211	G	C8-N9-C1'	-5.10	120.37	127.00
35	a	840	C	C6-N1-C2	-5.10	118.26	120.30
56	v	57	C	C2-N1-C1'	5.10	124.41	118.80
1	A	2515	C	C6-N1-C2	-5.10	118.26	120.30
35	a	191	G	N3-C4-N9	5.10	129.06	126.00
1	A	243	U	N3-C2-O2	-5.10	118.63	122.20
1	A	2840	C	C5-C6-N1	5.10	123.55	121.00
35	a	1068	G	C6-C5-N7	-5.10	127.34	130.40
1	A	2215	C	N3-C2-O2	-5.10	118.33	121.90
35	a	1497	G	C4-N9-C1'	5.10	133.12	126.50
1	A	416	U	C5-C6-N1	5.09	125.25	122.70
1	A	542	C	C6-N1-C1'	-5.09	114.69	120.80
1	A	817	C	C6-N1-C2	-5.09	118.26	120.30
34	8	80	C	C6-N1-C2	-5.09	118.27	120.30
35	a	281	G	O5'-P-OP2	-5.09	101.12	105.70
1	A	1064	C	N3-C2-O2	-5.08	118.34	121.90
1	A	417	C	C6-N1-C2	-5.08	118.27	120.30
35	a	754	C	N1-C2-O2	5.08	121.95	118.90
1	A	2260	C	C6-N1-C2	-5.08	118.27	120.30
1	A	2683	C	C2-N1-C1'	5.08	124.38	118.80
1	A	1313	U	C6-N1-C1'	-5.07	114.10	121.20
1	A	1179	G	P-O3'-C3'	5.07	125.78	119.70
1	A	1323	C	C2-N1-C1'	5.07	124.38	118.80
1	A	1804	C	N3-C2-O2	-5.07	118.35	121.90
33	7	4	SER	CB-CA-C	-5.07	100.47	110.10
2	B	37	C	N1-C2-O2	5.07	121.94	118.90
35	a	1033	G	C4-N9-C1'	5.07	133.09	126.50
1	A	1917	U	C6-N1-C1'	-5.07	114.11	121.20
35	a	284	C	C6-N1-C2	-5.07	118.27	120.30
35	a	738	C	C5-C6-N1	5.06	123.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	523	A	C2-N3-C4	-5.06	108.07	110.60
35	a	1449	C	N3-C2-O2	-5.06	118.36	121.90
34	8	26	C	C2-N1-C1'	5.06	124.36	118.80
35	a	1348	U	N3-C2-O2	-5.06	118.66	122.20
1	A	2394	C	C6-N1-C2	-5.06	118.28	120.30
2	B	37	C	N3-C2-O2	-5.05	118.36	121.90
1	A	134	G	P-O3'-C3'	5.05	125.76	119.70
1	A	1729	U	N1-C2-O2	5.05	126.33	122.80
35	a	1036	A	C4-N9-C1'	5.05	135.39	126.30
1	A	1188	U	N1-C2-O2	5.05	126.33	122.80
35	a	88	U	C6-N1-C2	-5.05	117.97	121.00
35	a	283	U	C2-N1-C1'	5.05	123.76	117.70
1	A	1343	G	C8-N9-C1'	-5.04	120.44	127.00
1	A	1727	C	N1-C2-O2	5.04	121.93	118.90
1	A	2789	C	N1-C2-O2	5.04	121.93	118.90
38	d	5	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	1437	C	C5-C6-N1	5.04	123.52	121.00
1	A	2254	C	N1-C2-O2	5.04	121.92	118.90
35	a	1078	U	N1-C2-O2	5.04	126.33	122.80
1	A	717	C	N1-C2-O2	5.04	121.92	118.90
7	G	133	LEU	CA-CB-CG	5.04	126.89	115.30
1	A	356	G	C4-C5-N7	5.04	112.81	110.80
1	A	510	C	N3-C2-O2	-5.03	118.38	121.90
1	A	1731	G	N3-C4-C5	5.03	131.12	128.60
35	a	912	C	C6-N1-C2	-5.03	118.29	120.30
35	a	1263	C	N1-C2-O2	5.03	121.92	118.90
1	A	897	C	C6-N1-C2	-5.03	118.29	120.30
1	A	999	U	N3-C2-O2	-5.02	118.68	122.20
35	a	257	G	P-O3'-C3'	5.02	125.73	119.70
35	a	431	A	N1-C6-N6	-5.02	115.59	118.60
35	a	1068	G	N3-C4-N9	5.02	129.01	126.00
1	A	1920	C	C5-C6-N1	5.01	123.51	121.00
35	a	983	A	C4-N9-C1'	5.01	135.32	126.30
1	A	1480	C	N3-C2-O2	-5.01	118.39	121.90
34	8	24	C	C2-N1-C1'	5.01	124.31	118.80
1	A	2073	C	N1-C2-O2	5.01	121.91	118.90
1	A	1121	C	C6-N1-C2	-5.01	118.30	120.30
34	8	85	C	C2-N1-C1'	5.01	124.31	118.80
27	1	11	LEU	CA-CB-CG	5.00	126.81	115.30
35	a	979	C	C2-N1-C1'	5.00	124.30	118.80
35	a	1109	C	C5-C6-N1	5.00	123.50	121.00

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	1	34	LEU	Peptide
29	3	31	HIS	Peptide
3	C	121	ASP	Peptide
5	E	82	GLY	Peptide
6	F	145	LYS	Peptide
8	H	3	VAL	Peptide
8	H	39	ALA	Peptide
8	H	8	LYS	Peptide
14	O	87	ILE	Peptide
17	R	53	PHE	Peptide
20	U	89	ASP	Peptide
38	d	31	LYS	Peptide
38	d	39	GLY	Peptide
39	e	99	ALA	Peptide
41	g	64	VAL	Peptide
48	n	33	ASP	Peptide
48	n	34	VAL	Peptide
50	p	42	ILE	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/271 (99%)	249 (93%)	19 (7%)	1 (0%)	34	72
4	D	207/209 (99%)	189 (91%)	18 (9%)	0	100	100
5	E	199/201 (99%)	187 (94%)	12 (6%)	0	100	100
6	F	175/177 (99%)	157 (90%)	18 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	172/174 (99%)	157 (91%)	14 (8%)	1 (1%)	25	64
8	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	5	33
9	J	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
10	K	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
11	L	142/144 (99%)	128 (90%)	14 (10%)	0	100	100
12	M	134/136 (98%)	126 (94%)	7 (5%)	1 (1%)	22	61
13	N	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
14	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
15	P	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
16	Q	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
17	R	101/103 (98%)	91 (90%)	9 (9%)	1 (1%)	15	54
18	S	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
19	T	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
20	U	100/102 (98%)	90 (90%)	9 (9%)	1 (1%)	15	54
21	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
22	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
23	X	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
24	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
25	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
26	0	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
27	1	48/50 (96%)	38 (79%)	10 (21%)	0	100	100
28	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
29	3	62/64 (97%)	51 (82%)	9 (14%)	2 (3%)	4	29
30	4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
31	5	63/65 (97%)	54 (86%)	9 (14%)	0	100	100
33	7	5/7 (71%)	4 (80%)	0	1 (20%)	0	1
36	b	222/224 (99%)	201 (90%)	21 (10%)	0	100	100
37	c	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
38	d	203/205 (99%)	176 (87%)	26 (13%)	1 (0%)	29	68
39	e	155/157 (99%)	143 (92%)	11 (7%)	1 (1%)	25	64
40	f	97/99 (98%)	89 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	g	149/151 (99%)	134 (90%)	15 (10%)	0	100	100
42	h	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
43	i	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
44	j	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	15	54
45	k	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
46	l	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
47	m	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
48	n	98/100 (98%)	87 (89%)	10 (10%)	1 (1%)	15	54
49	o	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	13	50
50	p	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
51	q	78/80 (98%)	69 (88%)	9 (12%)	0	100	100
52	r	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
53	s	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
54	t	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
55	u	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
All	All	5591/5691 (98%)	5120 (92%)	454 (8%)	17 (0%)	44	75

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	3	32	ILE
33	7	2	THR
8	H	40	THR
20	U	90	GLY
29	3	33	LEU
39	e	98	PRO
8	H	2	GLN
44	j	57	VAL
48	n	33	ASP
49	o	47	LYS
3	C	122	ALA
7	G	109	PHE
8	H	8	LYS
8	H	9	VAL
38	d	32	CYS
12	M	69	PRO
17	R	54	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	216/216 (100%)	215 (100%)	1 (0%)	88	94
4	D	164/164 (100%)	163 (99%)	1 (1%)	86	94
5	E	165/165 (100%)	165 (100%)	0	100	100
6	F	148/148 (100%)	146 (99%)	2 (1%)	67	85
7	G	135/135 (100%)	134 (99%)	1 (1%)	84	93
8	H	114/114 (100%)	114 (100%)	0	100	100
9	J	116/116 (100%)	116 (100%)	0	100	100
10	K	103/103 (100%)	103 (100%)	0	100	100
11	L	103/103 (100%)	102 (99%)	1 (1%)	76	88
12	M	109/109 (100%)	108 (99%)	1 (1%)	78	90
13	N	98/98 (100%)	98 (100%)	0	100	100
14	O	86/86 (100%)	86 (100%)	0	100	100
15	P	99/99 (100%)	98 (99%)	1 (1%)	76	88
16	Q	89/89 (100%)	89 (100%)	0	100	100
17	R	84/84 (100%)	84 (100%)	0	100	100
18	S	93/93 (100%)	93 (100%)	0	100	100
19	T	77/77 (100%)	77 (100%)	0	100	100
20	U	83/83 (100%)	83 (100%)	0	100	100
21	V	78/78 (100%)	78 (100%)	0	100	100
22	W	57/57 (100%)	57 (100%)	0	100	100
23	X	67/67 (100%)	67 (100%)	0	100	100
24	Y	55/55 (100%)	55 (100%)	0	100	100
25	Z	48/48 (100%)	48 (100%)	0	100	100
26	0	46/46 (100%)	46 (100%)	0	100	100
27	1	45/45 (100%)	45 (100%)	0	100	100
28	2	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	3	51/51 (100%)	51 (100%)	0	100	100
30	4	34/34 (100%)	33 (97%)	1 (3%)	42	71
31	5	58/58 (100%)	56 (97%)	2 (3%)	37	68
33	7	7/7 (100%)	7 (100%)	0	100	100
36	b	186/186 (100%)	184 (99%)	2 (1%)	73	88
37	c	170/170 (100%)	169 (99%)	1 (1%)	86	94
38	d	172/172 (100%)	170 (99%)	2 (1%)	71	87
39	e	119/119 (100%)	117 (98%)	2 (2%)	60	82
40	f	86/86 (100%)	86 (100%)	0	100	100
41	g	124/124 (100%)	123 (99%)	1 (1%)	81	91
42	h	104/104 (100%)	104 (100%)	0	100	100
43	i	105/105 (100%)	103 (98%)	2 (2%)	57	80
44	j	86/86 (100%)	85 (99%)	1 (1%)	71	87
45	k	90/90 (100%)	90 (100%)	0	100	100
46	l	103/103 (100%)	101 (98%)	2 (2%)	57	80
47	m	92/92 (100%)	91 (99%)	1 (1%)	73	88
48	n	83/83 (100%)	83 (100%)	0	100	100
49	o	76/76 (100%)	76 (100%)	0	100	100
50	p	65/65 (100%)	65 (100%)	0	100	100
51	q	74/74 (100%)	73 (99%)	1 (1%)	67	85
52	r	57/57 (100%)	57 (100%)	0	100	100
53	s	72/72 (100%)	72 (100%)	0	100	100
54	t	65/65 (100%)	65 (100%)	0	100	100
55	u	60/60 (100%)	59 (98%)	1 (2%)	60	82
All	All	4655/4655 (100%)	4628 (99%)	27 (1%)	86	94

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	228	VAL
4	D	77	ARG
6	F	30	ARG
6	F	48	LYS
7	G	69	ARG

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Mol	Chain	Res	Type
11	L	1	MET
12	M	135	VAL
15	P	6	LYS
30	4	14	CYS
31	5	8	LYS
31	5	40	CYS
36	b	47	VAL
36	b	140	GLU
37	c	22	TRP
38	d	128	ARG
38	d	148	LYS
39	e	56	VAL
39	e	96	MET
41	g	49	THR
43	i	12	ARG
43	i	123	ARG
44	j	52	LEU
46	l	14	ARG
46	l	104	CYS
47	m	73	ILE
51	q	27	ARG
55	u	69	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	37	ASN
3	C	45	ASN
3	C	86	ASN
3	C	142	HIS
4	D	32	ASN
4	D	36	GLN
4	D	49	GLN
4	D	130	GLN
5	E	41	GLN
5	E	94	GLN
7	G	22	GLN
8	H	2	GLN
8	H	11	ASN
8	H	18	GLN
8	H	43	ASN
9	J	40	HIS

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Mol	Chain	Res	Type
13	N	3	HIS
13	N	31	HIS
13	N	107	ASN
15	P	77	HIS
18	S	7	HIS
18	S	40	ASN
18	S	60	HIS
18	S	61	ASN
19	T	48	GLN
20	U	69	ASN
24	Y	15	ASN
24	Y	20	ASN
24	Y	58	ASN
26	0	19	HIS
36	b	58	ASN
36	b	177	ASN
38	d	85	ASN
38	d	116	GLN
39	e	43	ASN
40	f	55	HIS
41	g	52	GLN
42	h	4	GLN
42	h	18	GLN
42	h	21	ASN
42	h	118	GLN
43	i	50	GLN
44	j	64	GLN
46	l	5	ASN
47	m	8	ASN
47	m	100	GLN
48	n	4	GLN
50	p	29	ASN
51	q	45	HIS
52	r	52	GLN
52	r	54	GLN
52	r	74	HIS
53	s	52	HIS
53	s	57	HIS
53	s	69	HIS
55	u	64	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2902/2903 (99%)	677 (23%)	45 (1%)
2	B	119/120 (99%)	27 (22%)	3 (2%)
32	6	5/6 (83%)	2 (40%)	1 (20%)
34	8	86/87 (98%)	26 (30%)	1 (1%)
35	a	1539/1540 (99%)	337 (21%)	0
56	v	76/77 (98%)	32 (42%)	0
All	All	4727/4733 (99%)	1101 (23%)	50 (1%)

All (1101) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	10	A
1	A	13	A
1	A	15	G
1	A	23	G
1	A	27	G
1	A	34	U
1	A	35	G
1	A	46	G
1	A	50	U
1	A	51	G
1	A	55	G
1	A	60	G
1	A	61	C
1	A	62	U
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	82	U
1	A	84	A
1	A	88	G
1	A	93	G
1	A	98	G
1	A	103	A
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	135	U
1	A	136	G
1	A	137	U

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Mol	Chain	Res	Type
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	144	A
1	A	149	A
1	A	158	U
1	A	160	A
1	A	163	C
1	A	164	C
1	A	165	A
1	A	178	G
1	A	196	A
1	A	197	A
1	A	199	A
1	A	204	A
1	A	215	G
1	A	216	A
1	A	219	A
1	A	222	A
1	A	229	C
1	A	230	G
1	A	231	A
1	A	233	A
1	A	241	A
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	265	A
1	A	267	C
1	A	275	C
1	A	276	U
1	A	278	A
1	A	279	A
1	A	282	A
1	A	285	G
1	A	291	G
1	A	294	A
1	A	301	G
1	A	302	C

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Mol	Chain	Res	Type
1	A	308	G
1	A	311	A
1	A	322	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	331	C
1	A	334	C
1	A	335	C
1	A	343	C
1	A	346	A
1	A	354	A
1	A	358	U
1	A	359	G
1	A	361	G
1	A	367	G
1	A	371	A
1	A	372	G
1	A	377	G
1	A	386	G
1	A	387	U
1	A	391	A
1	A	396	G
1	A	403	U
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	413	C
1	A	424	G
1	A	431	U
1	A	435	C
1	A	448	U
1	A	456	C
1	A	457	A
1	A	459	U
1	A	467	G
1	A	473	G
1	A	477	A
1	A	480	A
1	A	481	G
1	A	489	G

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Mol	Chain	Res	Type
1	A	491	G
1	A	496	G
1	A	501	A
1	A	505	A
1	A	508	A
1	A	526	A
1	A	527	C
1	A	529	A
1	A	530	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	542	C
1	A	543	G
1	A	544	C
1	A	547	A
1	A	555	G
1	A	563	A
1	A	573	U
1	A	575	A
1	A	586	A
1	A	603	A
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	621	A
1	A	627	A
1	A	634	C
1	A	637	A
1	A	645	C
1	A	646	U
1	A	654	A
1	A	655	A
1	A	656	G
1	A	659	G
1	A	668	A
1	A	669	G
1	A	670	A
1	A	686	U
1	A	687	C
1	A	695	G

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Mol	Chain	Res	Type
1	A	701	G
1	A	711	G
1	A	714	U
1	A	717	C
1	A	726	G
1	A	730	A
1	A	738	G
1	A	745	G
1	A	747	U
1	A	748	G
1	A	749	A
1	A	752	A
1	A	753	A
1	A	764	A
1	A	775	G
1	A	776	G
1	A	777	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	792	A
1	A	799	G
1	A	800	A
1	A	801	G
1	A	805	G
1	A	812	C
1	A	819	A
1	A	822	G
1	A	827	U
1	A	830	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	858	G
1	A	859	G
1	A	860	U
1	A	866	A
1	A	869	G
1	A	878	A
1	A	881	G
1	A	882	G
1	A	883	G

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Mol	Chain	Res	Type
1	A	884	U
1	A	885	C
1	A	887	U
1	A	890	C
1	A	891	G
1	A	892	A
1	A	895	U
1	A	896	A
1	A	897	C
1	A	899	A
1	A	901	C
1	A	902	C
1	A	903	C
1	A	906	U
1	A	907	G
1	A	910	A
1	A	927	A
1	A	941	A
1	A	945	A
1	A	946	C
1	A	953	G
1	A	958	U
1	A	961	C
1	A	973	A
1	A	974	G
1	A	975	A
1	A	983	A
1	A	989	G
1	A	996	A
1	A	997	G
1	A	1005	C
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1021	A
1	A	1023	U
1	A	1025	G
1	A	1026	G
1	A	1033	U
1	A	1046	A
1	A	1059	G
1	A	1060	U

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Mol	Chain	Res	Type
1	A	1061	U
1	A	1062	G
1	A	1063	G
1	A	1065	U
1	A	1066	U
1	A	1067	A
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1073	A
1	A	1075	C
1	A	1076	C
1	A	1078	U
1	A	1079	C
1	A	1080	A
1	A	1081	U
1	A	1083	U
1	A	1087	G
1	A	1088	A
1	A	1089	A
1	A	1090	A
1	A	1096	A
1	A	1101	U
1	A	1103	A
1	A	1104	C
1	A	1111	A
1	A	1112	G
1	A	1114	C
1	A	1115	G
1	A	1116	G
1	A	1119	U
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1134	A
1	A	1135	C
1	A	1139	G
1	A	1142	A
1	A	1143	A
1	A	1156	A

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Mol	Chain	Res	Type
1	A	1169	A
1	A	1172	C
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1180	U
1	A	1186	G
1	A	1204	A
1	A	1206	G
1	A	1211	C
1	A	1212	G
1	A	1218	G
1	A	1236	G
1	A	1247	A
1	A	1248	G
1	A	1251	C
1	A	1253	A
1	A	1256	G
1	A	1262	A
1	A	1265	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1300	G
1	A	1301	A
1	A	1302	A
1	A	1305	C
1	A	1306	C
1	A	1321	A
1	A	1324	G
1	A	1329	U
1	A	1330	C
1	A	1333	G
1	A	1341	G
1	A	1345	C
1	A	1352	U
1	A	1360	G
1	A	1365	A
1	A	1368	G

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Mol	Chain	Res	Type
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1385	A
1	A	1386	C
1	A	1394	U
1	A	1395	A
1	A	1403	A
1	A	1406	U
1	A	1413	A
1	A	1414	C
1	A	1415	U
1	A	1416	G
1	A	1419	A
1	A	1420	A
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1429	G
1	A	1437	C
1	A	1454	C
1	A	1456	G
1	A	1458	U
1	A	1460	U
1	A	1461	C
1	A	1476	U
1	A	1480	C
1	A	1482	G
1	A	1490	A
1	A	1493	C
1	A	1504	A
1	A	1508	A
1	A	1509	A
1	A	1515	A
1	A	1523	U
1	A	1524	G
1	A	1530	G
1	A	1531	C
1	A	1532	A
1	A	1533	C
1	A	1534	U
1	A	1535	A

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Mol	Chain	Res	Type
1	A	1536	C
1	A	1537	G
1	A	1539	U
1	A	1542	U
1	A	1543	G
1	A	1544	A
1	A	1554	U
1	A	1558	C
1	A	1559	U
1	A	1560	G
1	A	1561	C
1	A	1566	A
1	A	1567	G
1	A	1569	A
1	A	1578	U
1	A	1581	G
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1586	A
1	A	1587	G
1	A	1608	A
1	A	1610	A
1	A	1616	A
1	A	1627	G
1	A	1632	A
1	A	1646	C
1	A	1647	U
1	A	1648	U
1	A	1651	G
1	A	1672	A
1	A	1674	G
1	A	1675	C
1	A	1693	U
1	A	1694	C
1	A	1695	G
1	A	1698	A
1	A	1703	G
1	A	1706	C
1	A	1707	G
1	A	1713	A
1	A	1715	G

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Mol	Chain	Res	Type
1	A	1721	G
1	A	1724	G
1	A	1726	C
1	A	1729	U
1	A	1730	C
1	A	1732	C
1	A	1738	G
1	A	1764	C
1	A	1773	A
1	A	1776	G
1	A	1780	A
1	A	1781	U
1	A	1782	U
1	A	1784	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1811	G
1	A	1815	A
1	A	1816	C
1	A	1820	U
1	A	1821	A
1	A	1826	G
1	A	1828	G
1	A	1829	A
1	A	1833	C
1	A	1834	U
1	A	1839	G
1	A	1848	A
1	A	1858	A
1	A	1870	C
1	A	1871	A
1	A	1873	G
1	A	1878	G
1	A	1884	G
1	A	1896	G
1	A	1901	A
1	A	1906	G
1	A	1910	G
1	A	1912	A
1	A	1913	A

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Mol	Chain	Res	Type
1	A	1914	C
1	A	1917	U
1	A	1918	A
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1934	C
1	A	1936	A
1	A	1940	U
1	A	1941	C
1	A	1955	U
1	A	1963	U
1	A	1966	A
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1981	A
1	A	1982	U
1	A	1991	U
1	A	1992	G
1	A	1996	C
1	A	1997	C
1	A	2018	G
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2031	A
1	A	2033	A
1	A	2034	U
1	A	2035	G
1	A	2041	U
1	A	2043	C
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	C
1	A	2068	U

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Mol	Chain	Res	Type
1	A	2069	G
1	A	2077	A
1	A	2080	A
1	A	2092	U
1	A	2093	G
1	A	2096	C
1	A	2098	U
1	A	2099	U
1	A	2100	G
1	A	2102	G
1	A	2104	C
1	A	2107	G
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2115	G
1	A	2117	A
1	A	2118	U
1	A	2119	A
1	A	2125	G
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2137	U
1	A	2146	C
1	A	2148	G
1	A	2149	U
1	A	2157	G
1	A	2162	G
1	A	2164	C
1	A	2167	U
1	A	2170	A
1	A	2171	A
1	A	2172	U
1	A	2173	A
1	A	2175	C
1	A	2178	C
1	A	2180	U

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Mol	Chain	Res	Type
1	A	2181	U
1	A	2186	G
1	A	2187	U
1	A	2188	U
1	A	2189	U
1	A	2191	A
1	A	2198	A
1	A	2199	A
1	A	2203	U
1	A	2204	G
1	A	2211	A
1	A	2212	A
1	A	2219	U
1	A	2223	G
1	A	2225	A
1	A	2239	G
1	A	2250	G
1	A	2252	G
1	A	2266	A
1	A	2278	A
1	A	2279	G
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2305	U
1	A	2307	G
1	A	2308	G
1	A	2309	A
1	A	2317	A
1	A	2320	U
1	A	2325	G
1	A	2327	A
1	A	2333	A
1	A	2344	U
1	A	2347	C
1	A	2350	C
1	A	2354	C
1	A	2357	G
1	A	2361	G
1	A	2367	G
1	A	2382	G
1	A	2383	G

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Mol	Chain	Res	Type
1	A	2384	U
1	A	2385	C
1	A	2389	G
1	A	2392	A
1	A	2402	U
1	A	2403	C
1	A	2406	A
1	A	2422	C
1	A	2423	U
1	A	2425	A
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2440	C
1	A	2441	U
1	A	2445	G
1	A	2448	A
1	A	2476	A
1	A	2481	G
1	A	2491	U
1	A	2494	G
1	A	2498	C
1	A	2502	G
1	A	2503	A
1	A	2504	U
1	A	2505	G
1	A	2513	A
1	A	2518	A
1	A	2519	U
1	A	2520	C
1	A	2529	G
1	A	2542	A
1	A	2554	U
1	A	2556	C
1	A	2564	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2586	U
1	A	2602	A
1	A	2603	G
1	A	2609	U

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Mol	Chain	Res	Type
1	A	2613	U
1	A	2615	U
1	A	2629	U
1	A	2630	G
1	A	2646	C
1	A	2654	A
1	A	2655	G
1	A	2656	U
1	A	2661	G
1	A	2673	G
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2718	G
1	A	2726	A
1	A	2731	G
1	A	2732	G
1	A	2733	A
1	A	2739	U
1	A	2744	G
1	A	2748	A
1	A	2764	A
1	A	2765	A
1	A	2776	A
1	A	2778	A
1	A	2779	U
1	A	2789	C
1	A	2790	U
1	A	2793	C
1	A	2794	C
1	A	2798	U
1	A	2799	A
1	A	2800	A
1	A	2801	G
1	A	2807	U
1	A	2808	G
1	A	2809	A
1	A	2818	U
1	A	2820	A
1	A	2821	A
1	A	2824	C

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Mol	Chain	Res	Type
1	A	2826	A
1	A	2833	U
1	A	2834	G
1	A	2849	U
1	A	2861	U
1	A	2867	G
1	A	2868	A
1	A	2869	G
1	A	2873	A
1	A	2879	A
1	A	2880	C
1	A	2892	G
1	A	2893	A
1	A	2902	C
1	A	2903	U
2	B	4	C
2	B	12	C
2	B	13	G
2	B	18	G
2	B	21	G
2	B	24	G
2	B	25	U
2	B	34	A
2	B	35	C
2	B	40	U
2	B	41	G
2	B	42	C
2	B	44	G
2	B	45	A
2	B	52	A
2	B	58	A
2	B	66	A
2	B	67	G
2	B	75	G
2	B	87	U
2	B	88	C
2	B	89	U
2	B	98	G
2	B	108	A
2	B	109	A
2	B	118	C
2	B	119	A

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Mol	Chain	Res	Type
32	6	27	U
32	6	28	C
34	8	8	U
34	8	9	G
34	8	17	U
34	8	19	G
34	8	20	U
34	8	21	A
34	8	24	C
34	8	25	A
34	8	26	C
34	8	37	G
34	8	47	C
34	8	48	C
34	8	49	C
34	8	50	A
34	8	51	A
34	8	54	G
34	8	58	U
34	8	59	U
34	8	64	G
34	8	67	C
34	8	68	A
34	8	69	A
34	8	72	C
34	8	80	C
34	8	86	C
34	8	87	A
35	a	5	U
35	a	6	G
35	a	7	A
35	a	8	A
35	a	9	G
35	a	14	U
35	a	22	G
35	a	31	G
35	a	32	A
35	a	37	U
35	a	39	G
35	a	47	C
35	a	48	C
35	a	50	A

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Mol	Chain	Res	Type
35	a	51	A
35	a	57	G
35	a	58	C
35	a	71	A
35	a	73	C
35	a	75	G
35	a	80	A
35	a	81	A
35	a	82	G
35	a	83	C
35	a	84	U
35	a	85	U
35	a	86	G
35	a	87	C
35	a	89	U
35	a	91	U
35	a	92	U
35	a	94	G
35	a	96	U
35	a	97	G
35	a	98	A
35	a	101	A
35	a	108	G
35	a	120	A
35	a	130	A
35	a	131	A
35	a	132	C
35	a	141	G
35	a	144	G
35	a	149	A
35	a	154	U
35	a	159	G
35	a	160	A
35	a	163	C
35	a	168	G
35	a	173	U
35	a	181	A
35	a	183	C
35	a	184	G
35	a	192	A
35	a	197	A
35	a	203	G

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Mol	Chain	Res	Type
35	a	209	U
35	a	210	C
35	a	211	G
35	a	212	G
35	a	217	C
35	a	226	G
35	a	238	A
35	a	240	G
35	a	244	U
35	a	245	U
35	a	247	G
35	a	251	G
35	a	258	G
35	a	262	A
35	a	265	G
35	a	266	G
35	a	267	C
35	a	280	C
35	a	281	G
35	a	282	A
35	a	283	U
35	a	289	G
35	a	299	G
35	a	303	A
35	a	306	A
35	a	321	A
35	a	328	C
35	a	329	A
35	a	330	C
35	a	342	C
35	a	344	A
35	a	345	C
35	a	347	G
35	a	351	G
35	a	352	C
35	a	354	G
35	a	367	U
35	a	372	C
35	a	375	U
35	a	384	G
35	a	390	U
35	a	397	A

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Mol	Chain	Res	Type
35	a	406	G
35	a	412	A
35	a	423	G
35	a	424	G
35	a	429	U
35	a	439	U
35	a	446	G
35	a	458	U
35	a	462	G
35	a	465	A
35	a	467	U
35	a	474	G
35	a	476	U
35	a	478	A
35	a	484	G
35	a	485	U
35	a	486	U
35	a	496	A
35	a	497	G
35	a	499	A
35	a	511	C
35	a	518	C
35	a	524	G
35	a	527	G
35	a	531	U
35	a	533	A
35	a	535	A
35	a	547	A
35	a	559	A
35	a	562	U
35	a	564	C
35	a	572	A
35	a	573	A
35	a	575	G
35	a	576	C
35	a	577	G
35	a	579	A
35	a	616	G
35	a	618	C
35	a	633	G
35	a	642	A
35	a	650	G

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Mol	Chain	Res	Type
35	a	653	U
35	a	661	G
35	a	665	A
35	a	687	A
35	a	695	A
35	a	702	A
35	a	703	G
35	a	713	G
35	a	717	U
35	a	721	G
35	a	731	G
35	a	734	G
35	a	736	C
35	a	753	A
35	a	754	C
35	a	755	G
35	a	777	A
35	a	781	A
35	a	782	A
35	a	790	A
35	a	802	A
35	a	815	A
35	a	817	C
35	a	818	G
35	a	819	A
35	a	820	U
35	a	821	G
35	a	829	G
35	a	832	G
35	a	836	G
35	a	841	C
35	a	842	U
35	a	843	U
35	a	844	G
35	a	845	A
35	a	846	G
35	a	851	G
35	a	859	G
35	a	871	U
35	a	872	A
35	a	876	C
35	a	885	G

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Mol	Chain	Res	Type
35	a	889	A
35	a	890	G
35	a	900	A
35	a	902	G
35	a	918	A
35	a	919	A
35	a	926	G
35	a	931	C
35	a	933	G
35	a	934	C
35	a	935	A
35	a	942	G
35	a	960	U
35	a	961	U
35	a	965	U
35	a	966	G
35	a	969	A
35	a	971	G
35	a	975	A
35	a	976	G
35	a	977	A
35	a	989	U
35	a	992	U
35	a	993	G
35	a	994	A
35	a	1003	G
35	a	1004	A
35	a	1006	G
35	a	1022	A
35	a	1027	C
35	a	1028	C
35	a	1031	C
35	a	1032	G
35	a	1033	G
35	a	1034	G
35	a	1035	A
35	a	1036	A
35	a	1037	C
35	a	1050	G
35	a	1053	G
35	a	1064	G
35	a	1065	U

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Mol	Chain	Res	Type
35	a	1085	U
35	a	1089	G
35	a	1092	A
35	a	1094	G
35	a	1095	U
35	a	1099	G
35	a	1101	A
35	a	1108	G
35	a	1117	A
35	a	1124	G
35	a	1125	U
35	a	1130	A
35	a	1131	G
35	a	1133	G
35	a	1134	G
35	a	1137	C
35	a	1138	G
35	a	1139	G
35	a	1143	G
35	a	1144	G
35	a	1151	A
35	a	1152	A
35	a	1158	C
35	a	1159	U
35	a	1166	G
35	a	1167	A
35	a	1169	A
35	a	1171	A
35	a	1179	A
35	a	1182	G
35	a	1183	U
35	a	1184	G
35	a	1191	A
35	a	1196	A
35	a	1201	A
35	a	1202	U
35	a	1213	A
35	a	1214	C
35	a	1227	A
35	a	1228	C
35	a	1236	A
35	a	1238	A

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Mol	Chain	Res	Type
35	a	1239	A
35	a	1250	A
35	a	1253	G
35	a	1256	A
35	a	1257	A
35	a	1262	C
35	a	1269	A
35	a	1273	C
35	a	1275	A
35	a	1280	A
35	a	1282	C
35	a	1285	A
35	a	1287	A
35	a	1294	G
35	a	1297	G
35	a	1298	U
35	a	1300	G
35	a	1301	U
35	a	1302	C
35	a	1305	G
35	a	1317	C
35	a	1320	C
35	a	1322	C
35	a	1323	G
35	a	1335	U
35	a	1336	C
35	a	1338	G
35	a	1340	A
35	a	1346	A
35	a	1363	A
35	a	1368	A
35	a	1370	G
35	a	1380	U
35	a	1383	C
35	a	1394	A
35	a	1395	C
35	a	1397	C
35	a	1398	A
35	a	1399	C
35	a	1400	C
35	a	1402	C
35	a	1403	C

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Mol	Chain	Res	Type
35	a	1419	G
35	a	1429	A
35	a	1441	A
35	a	1446	A
35	a	1447	A
35	a	1448	C
35	a	1451	U
35	a	1452	C
35	a	1453	G
35	a	1470	U
35	a	1471	U
35	a	1473	G
35	a	1475	G
35	a	1478	U
35	a	1487	G
35	a	1492	A
35	a	1493	A
35	a	1494	G
35	a	1502	A
35	a	1503	A
35	a	1506	U
35	a	1517	G
35	a	1520	C
35	a	1529	G
35	a	1530	G
35	a	1534	A
35	a	1535	C
35	a	1536	C
35	a	1540	U
56	v	2	C
56	v	3	A
56	v	7	G
56	v	8	U
56	v	9	A
56	v	13	C
56	v	15	G
56	v	17	U
56	v	18	G
56	v	19	G
56	v	20	A
56	v	21	U
56	v	22	A

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Mol	Chain	Res	Type
56	v	34	U
56	v	37	G
56	v	43	A
56	v	47	G
56	v	48	U
56	v	49	C
56	v	51	G
56	v	54	G
56	v	55	U
56	v	58	G
56	v	59	A
56	v	60	A
56	v	61	U
56	v	62	C
56	v	63	C
56	v	74	A
56	v	75	C
56	v	76	C
56	v	77	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	134	G
1	A	242	G
1	A	277	G
1	A	281	C
1	A	358	U
1	A	404	A
1	A	479	A
1	A	490	C
1	A	546	U
1	A	655	A
1	A	752	A
1	A	827	U
1	A	858	G
1	A	859	G
1	A	890	C
1	A	1020	A
1	A	1022	G
1	A	1062	G

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Mol	Chain	Res	Type
1	A	1064	C
1	A	1074	G
1	A	1111	A
1	A	1130	U
1	A	1171	G
1	A	1173	U
1	A	1179	G
1	A	1182	G
1	A	1190	G
1	A	1300	G
1	A	1378	A
1	A	1399	C
1	A	1420	A
1	A	1508	A
1	A	1530	G
1	A	1541	C
1	A	1729	U
1	A	1913	A
1	A	1930	G
1	A	1940	U
1	A	2326	C
1	A	2391	G
1	A	2566	A
1	A	2655	G
1	A	2808	G
1	A	2901	C
2	B	66	A
2	B	86	G
2	B	88	C
32	6	27	U
34	8	63	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	ERY	7	101	-	53,53,53	1.60	5 (9%)	82,82,82	1.76	19 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	ERY	7	101	-	-	14/72/107/107	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	7	101	ERY	C10-C9	-7.52	1.41	1.52
57	7	101	ERY	C2-C1	-5.71	1.39	1.51
57	7	101	ERY	C8-C9	-2.95	1.42	1.52
57	7	101	ERY	O7-C22	2.29	1.48	1.41
57	7	101	ERY	O3-C14	2.13	1.47	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	7	101	ERY	O5-C16-C17	5.99	112.68	103.81
57	7	101	ERY	O7-C5-C6	4.42	111.84	106.39
57	7	101	ERY	C6-C5-C4	-4.05	108.31	114.05
57	7	101	ERY	C32-C6-C5	3.38	116.06	110.12
57	7	101	ERY	C36-C13-C12	-3.16	109.20	115.20
57	7	101	ERY	C13-O2-C1	-2.89	113.05	118.18
57	7	101	ERY	O2-C13-C36	2.75	112.64	107.40
57	7	101	ERY	C8-C9-C10	2.72	123.83	119.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	7	101	ERY	C27-C26-C25	-2.57	109.37	113.40
57	7	101	ERY	C31-C4-C3	-2.41	107.08	111.40
57	7	101	ERY	C22-O9-C26	2.29	116.54	112.91
57	7	101	ERY	C14-O3-C3	-2.23	110.15	114.66
57	7	101	ERY	C7-C6-C5	-2.21	106.16	110.48
57	7	101	ERY	C19-C16-C15	-2.20	106.56	110.49
57	7	101	ERY	C32-C6-C7	-2.08	107.58	111.09
57	7	101	ERY	C16-C17-C18	-2.06	107.97	111.14
57	7	101	ERY	O3-C14-O4	2.03	116.44	109.86
57	7	101	ERY	C35-C12-C11	-2.01	109.53	113.05
57	7	101	ERY	C2-C3-C4	-2.00	107.25	113.05

There are no chirality outliers.

All (14) torsion outliers are listed below:

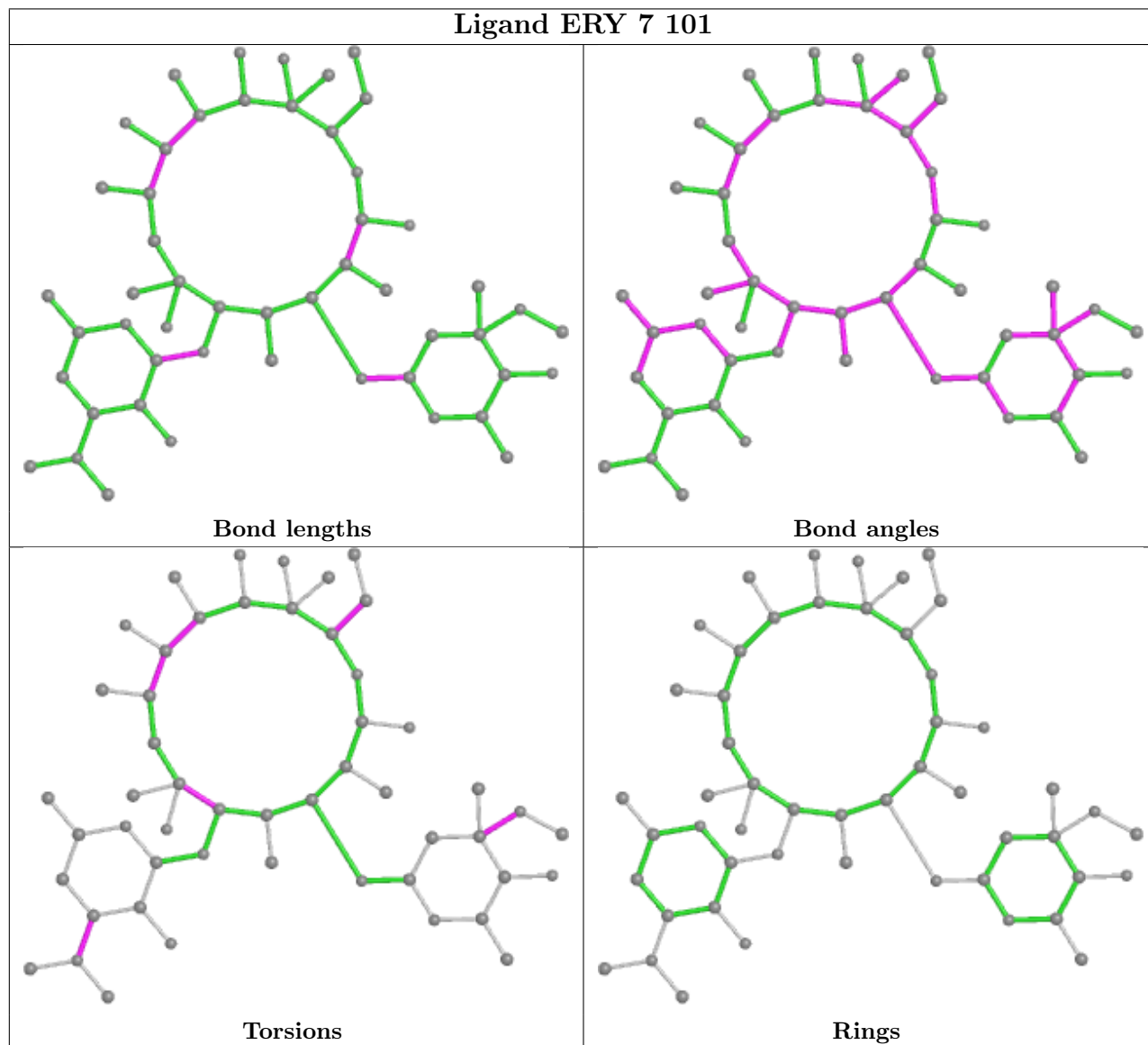
Mol	Chain	Res	Type	Atoms
57	7	101	ERY	C12-C13-C36-C37
57	7	101	ERY	C25-C24-N1-C28
57	7	101	ERY	C19-C16-O5-C20
57	7	101	ERY	O2-C13-C36-C37
57	7	101	ERY	C4-C5-C6-O10
57	7	101	ERY	C15-C16-O5-C20
57	7	101	ERY	C17-C16-O5-C20
57	7	101	ERY	C33-C8-C9-O11
57	7	101	ERY	C23-C24-N1-C29
57	7	101	ERY	C4-C5-C6-C32
57	7	101	ERY	C33-C8-C9-C10
57	7	101	ERY	C34-C10-C9-C8
57	7	101	ERY	C7-C8-C9-O11
57	7	101	ERY	C25-C24-N1-C29

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

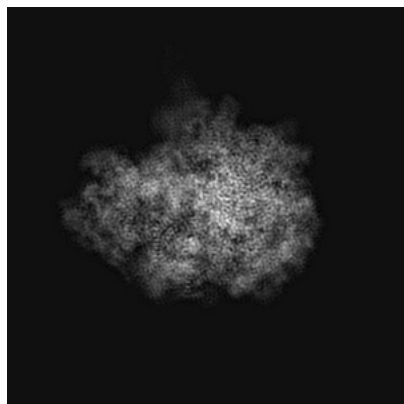
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12574. These allow visual inspection of the internal detail of the map and identification of artifacts.

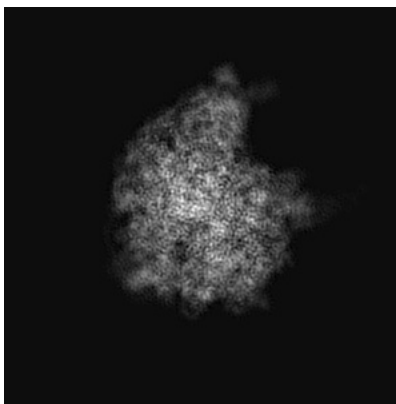
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

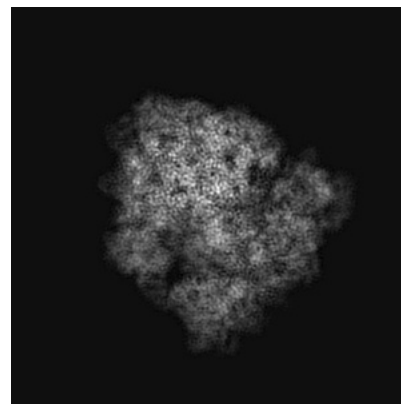
6.1.1 Primary map



X

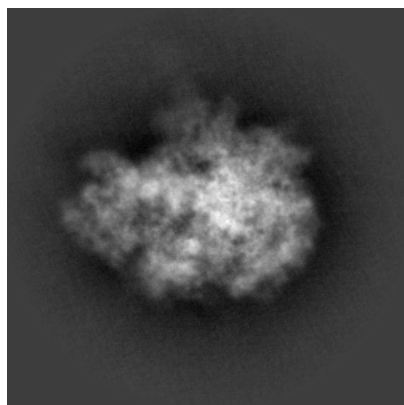


Y

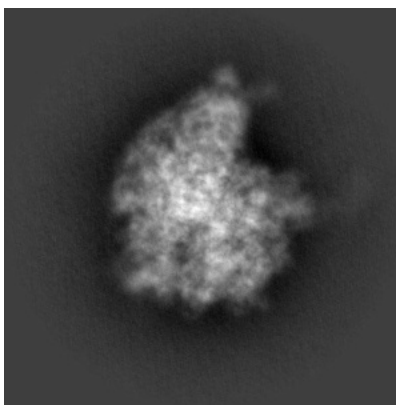


Z

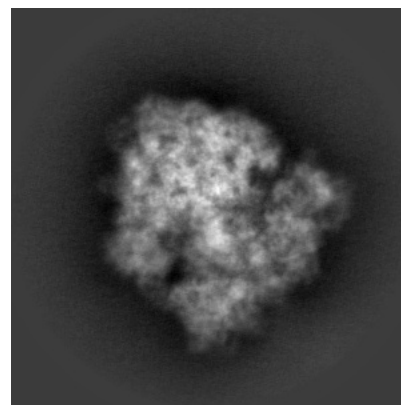
6.1.2 Raw map



X



Y

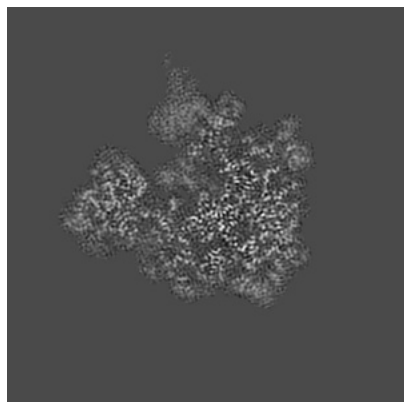


Z

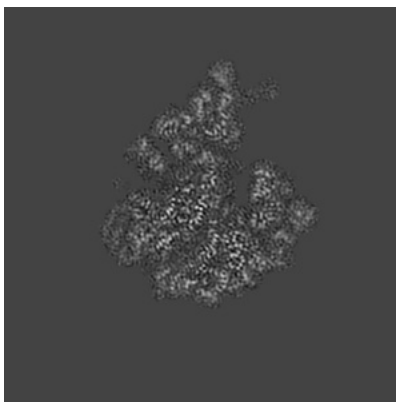
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

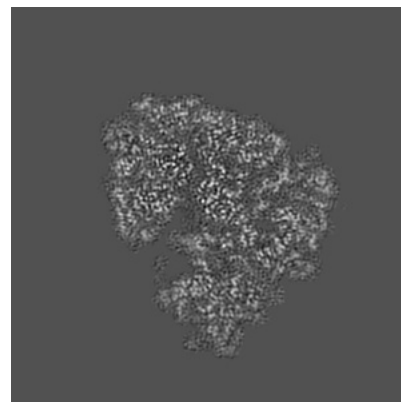
6.2.1 Primary map



X Index: 180

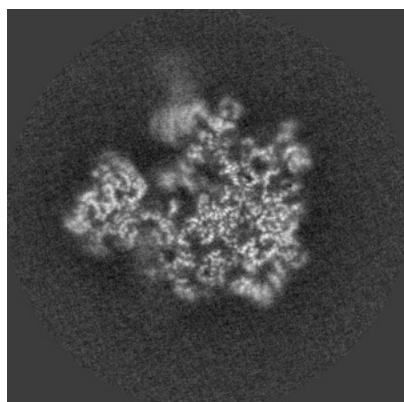


Y Index: 180

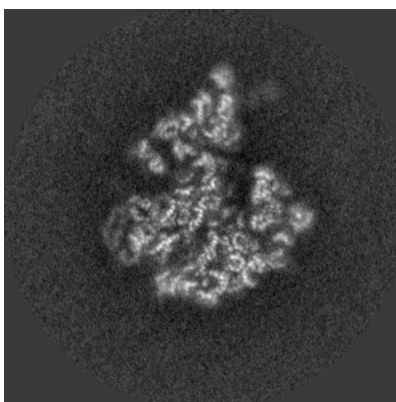


Z Index: 180

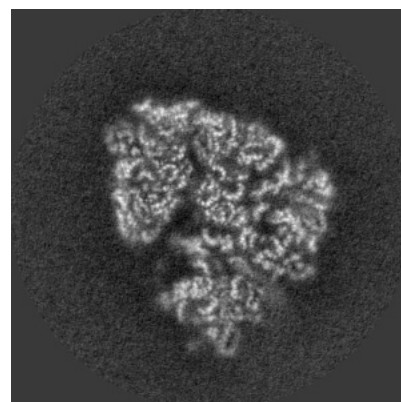
6.2.2 Raw map



X Index: 180



Y Index: 180

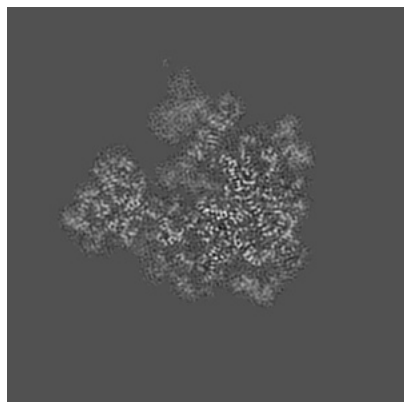


Z Index: 180

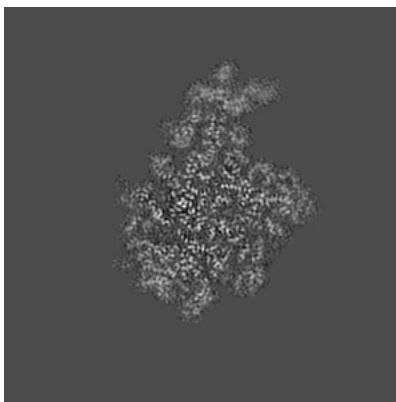
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

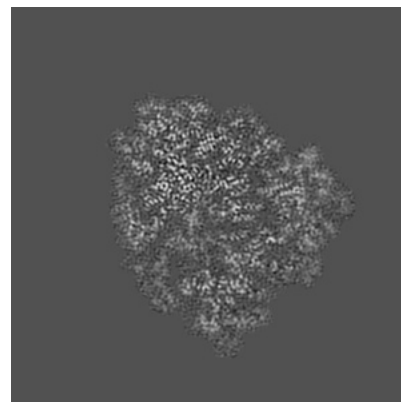
6.3.1 Primary map



X Index: 178

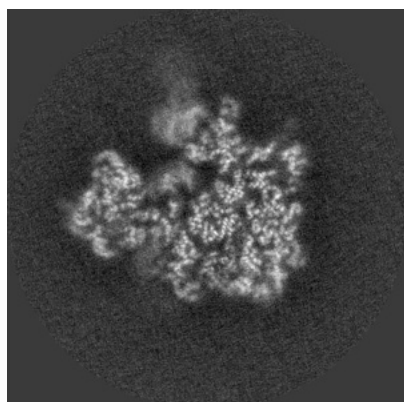


Y Index: 194

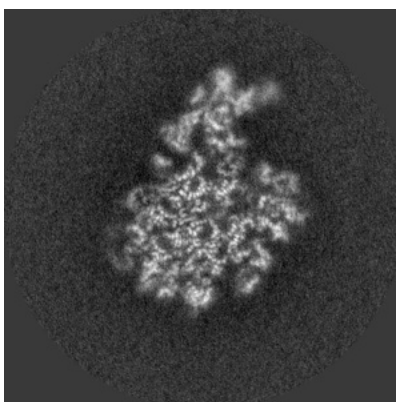


Z Index: 187

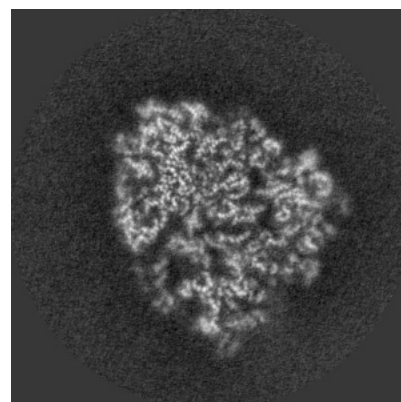
6.3.2 Raw map



X Index: 184



Y Index: 189

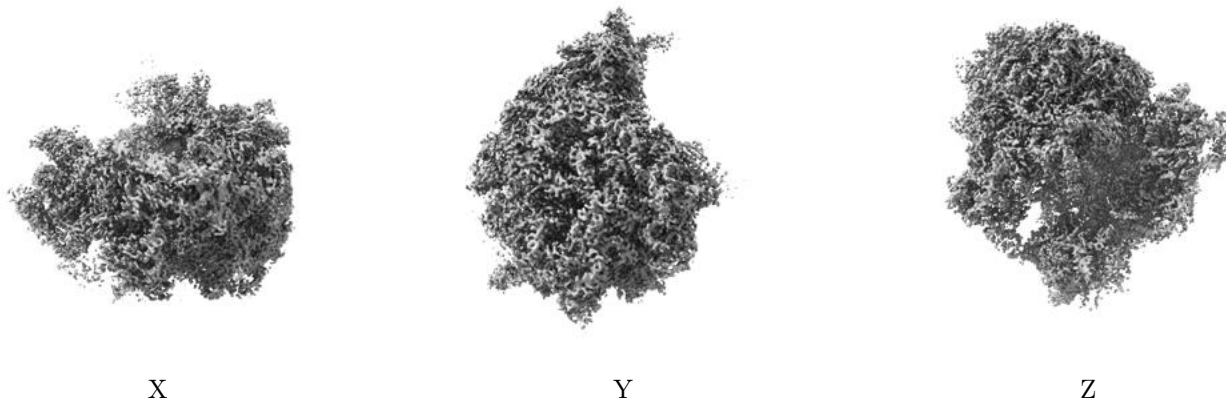


Z Index: 186

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

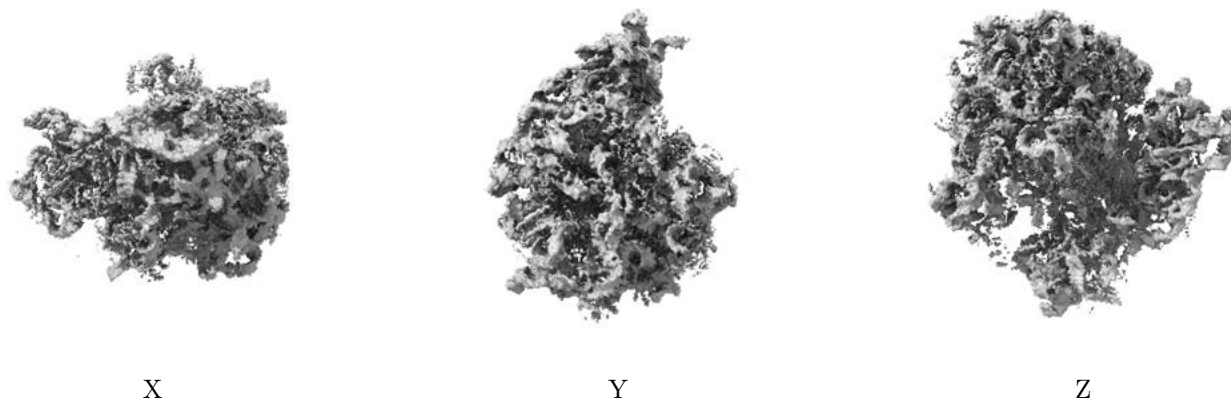
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

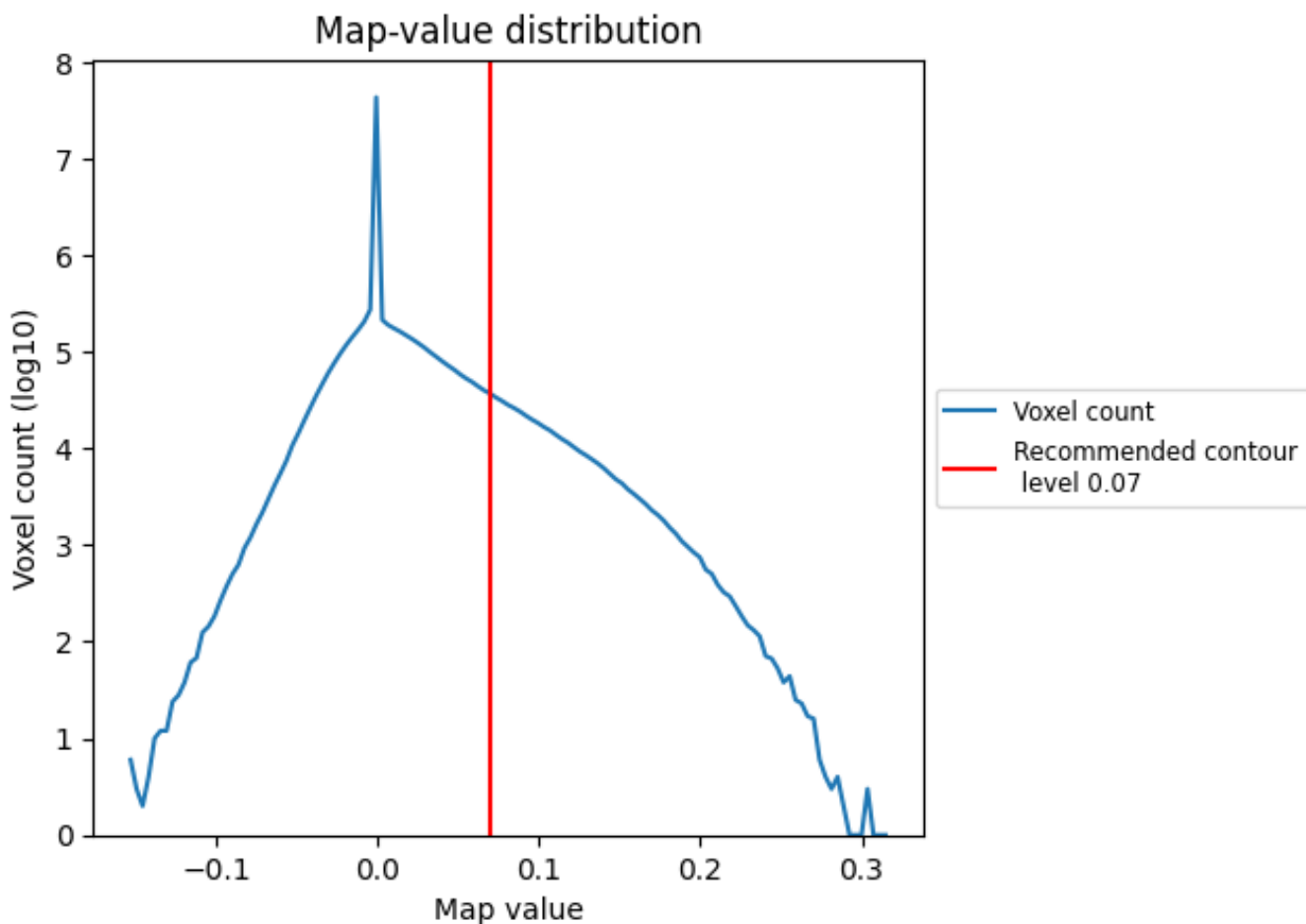
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

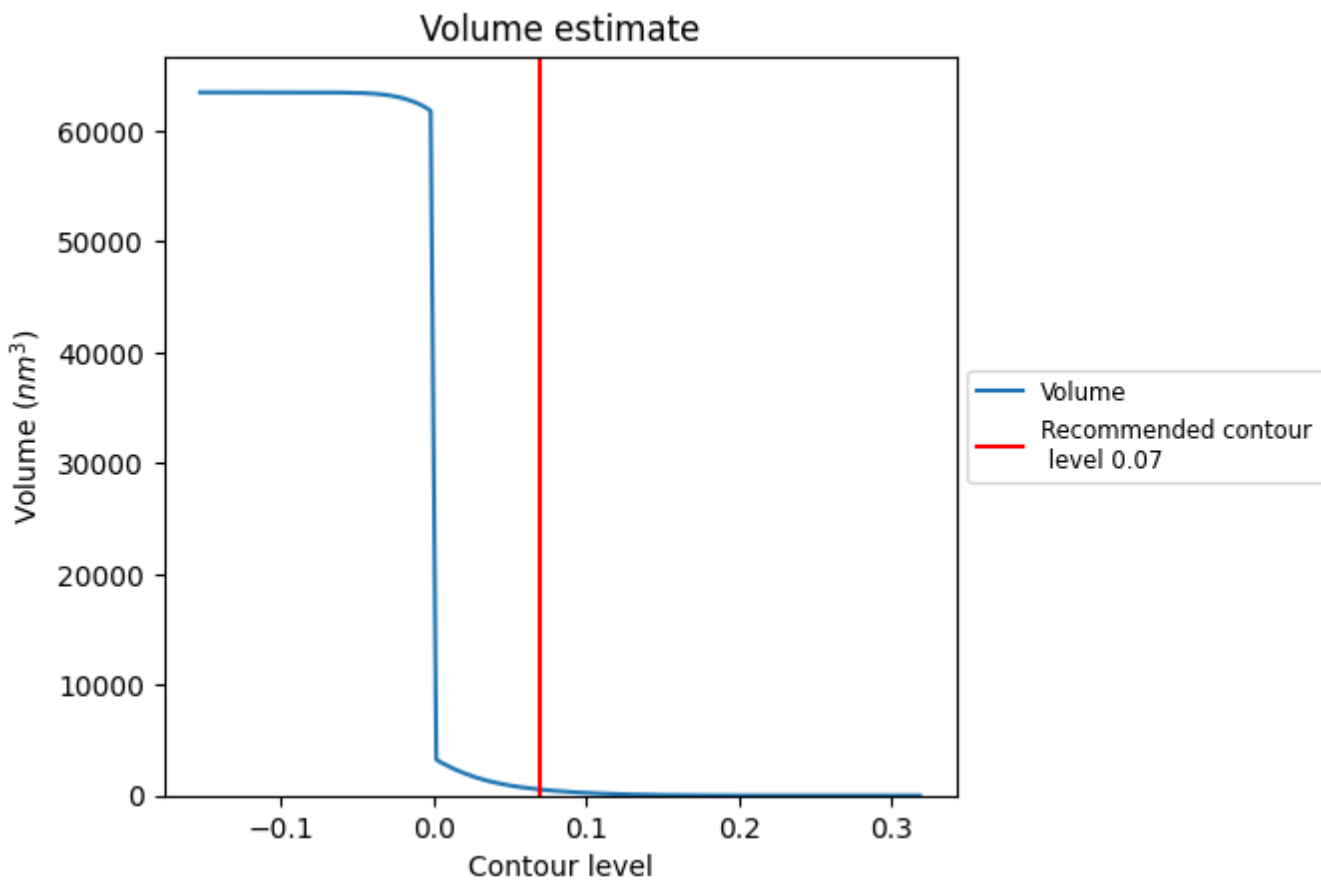
This section contains the results of statistical analysis of the map.

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.

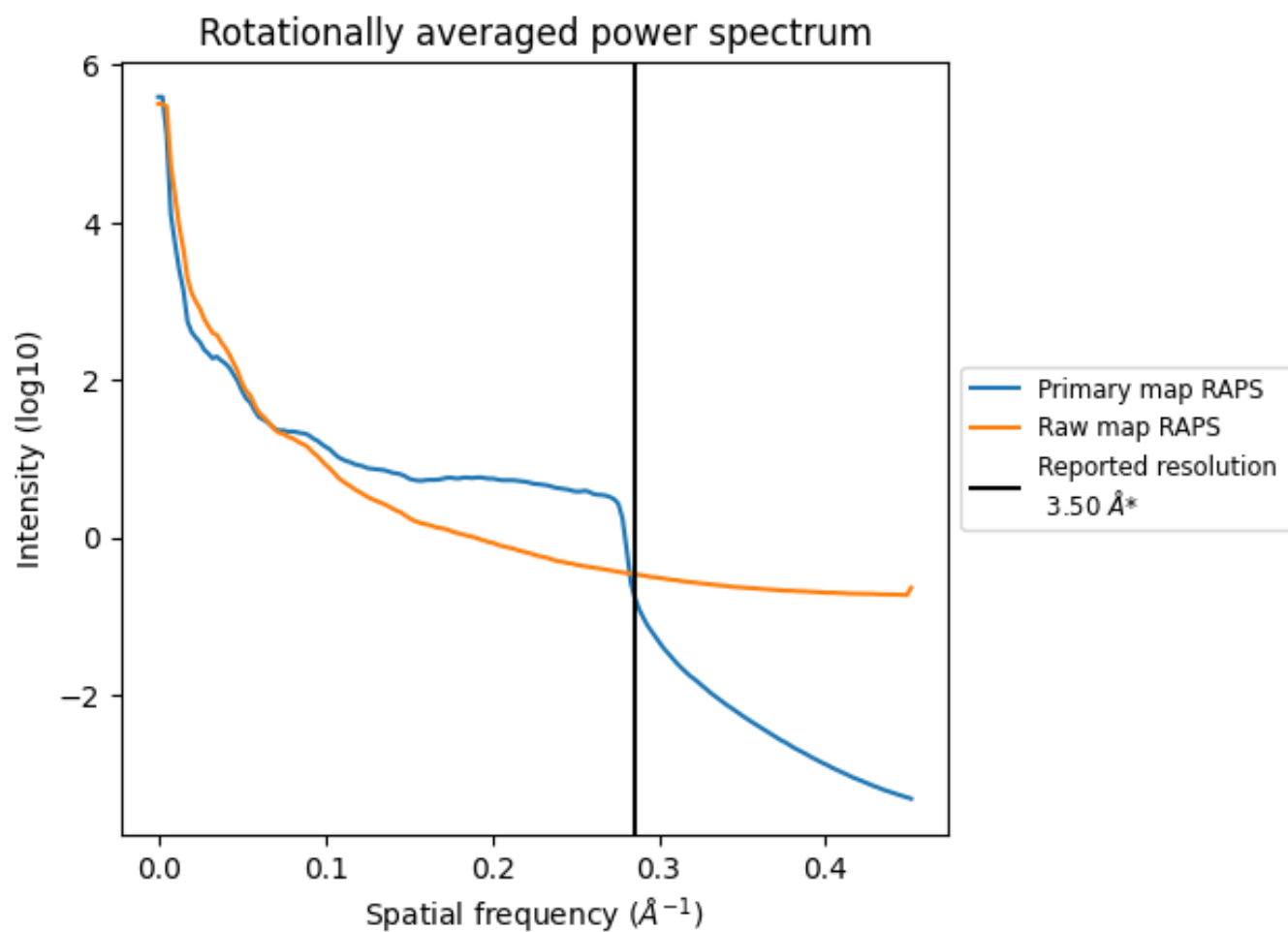
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 543 nm³; this corresponds to an approximate mass of 490 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

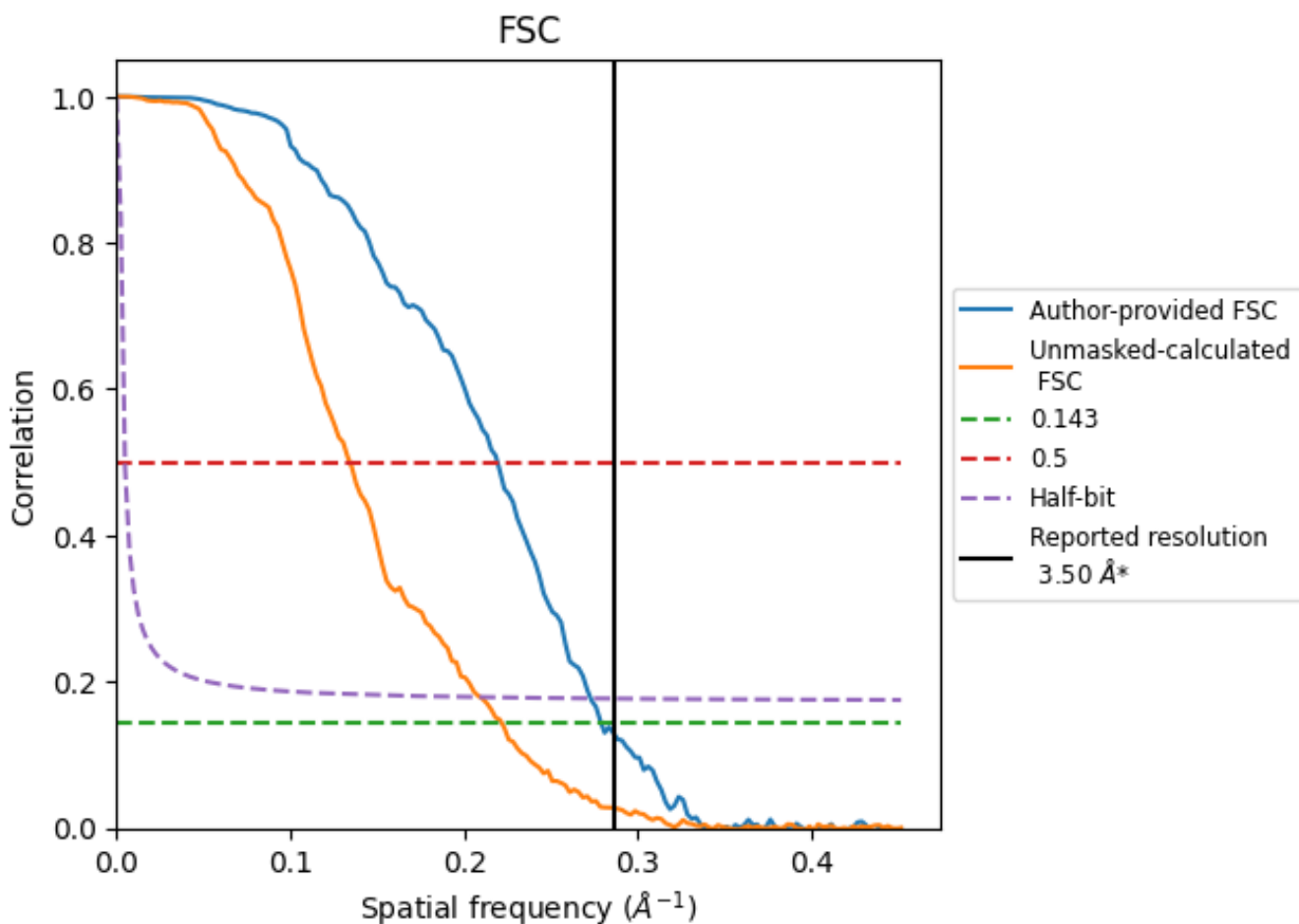


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

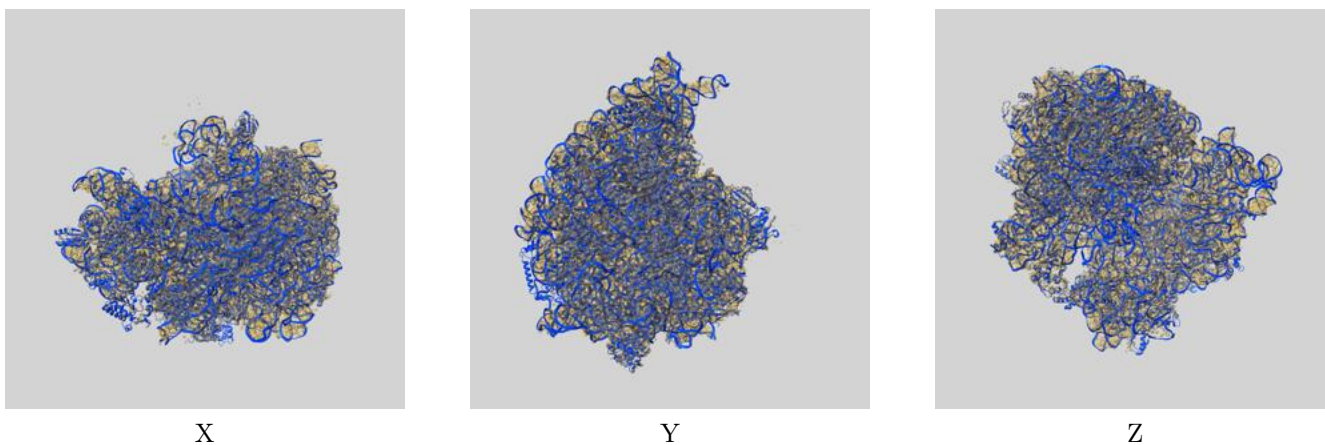
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.59	4.56	3.67
Unmasked-calculated*	4.51	7.45	4.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

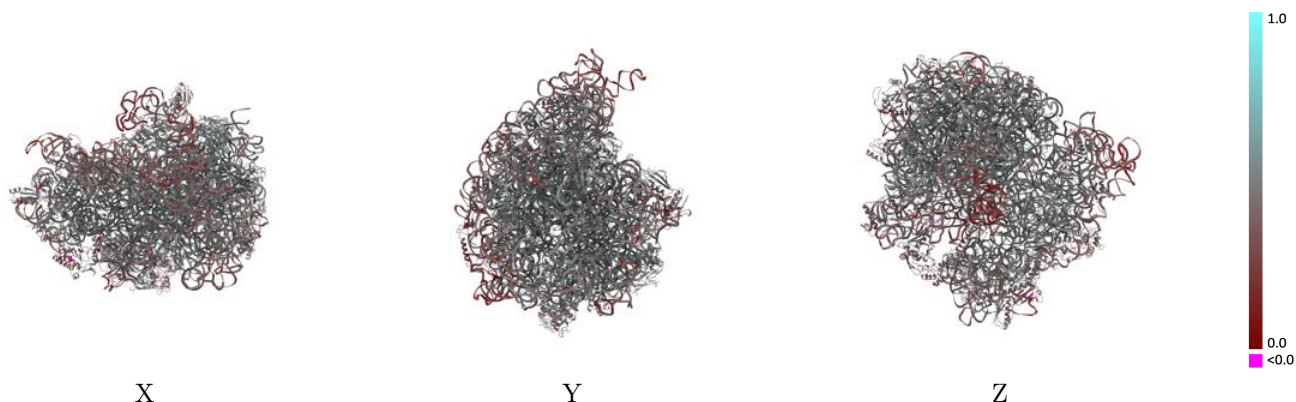
This section contains information regarding the fit between EMDB map EMD-12574 and PDB model 7NSP. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



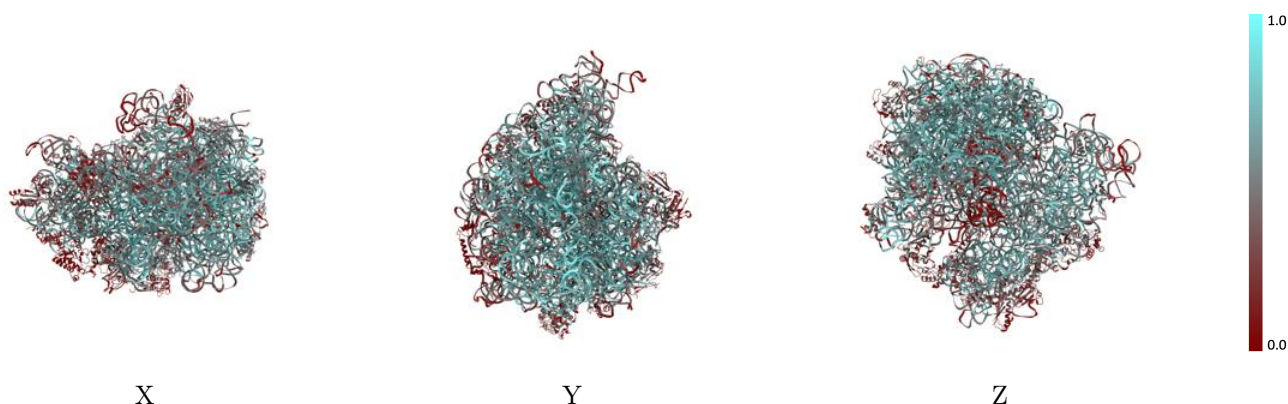
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



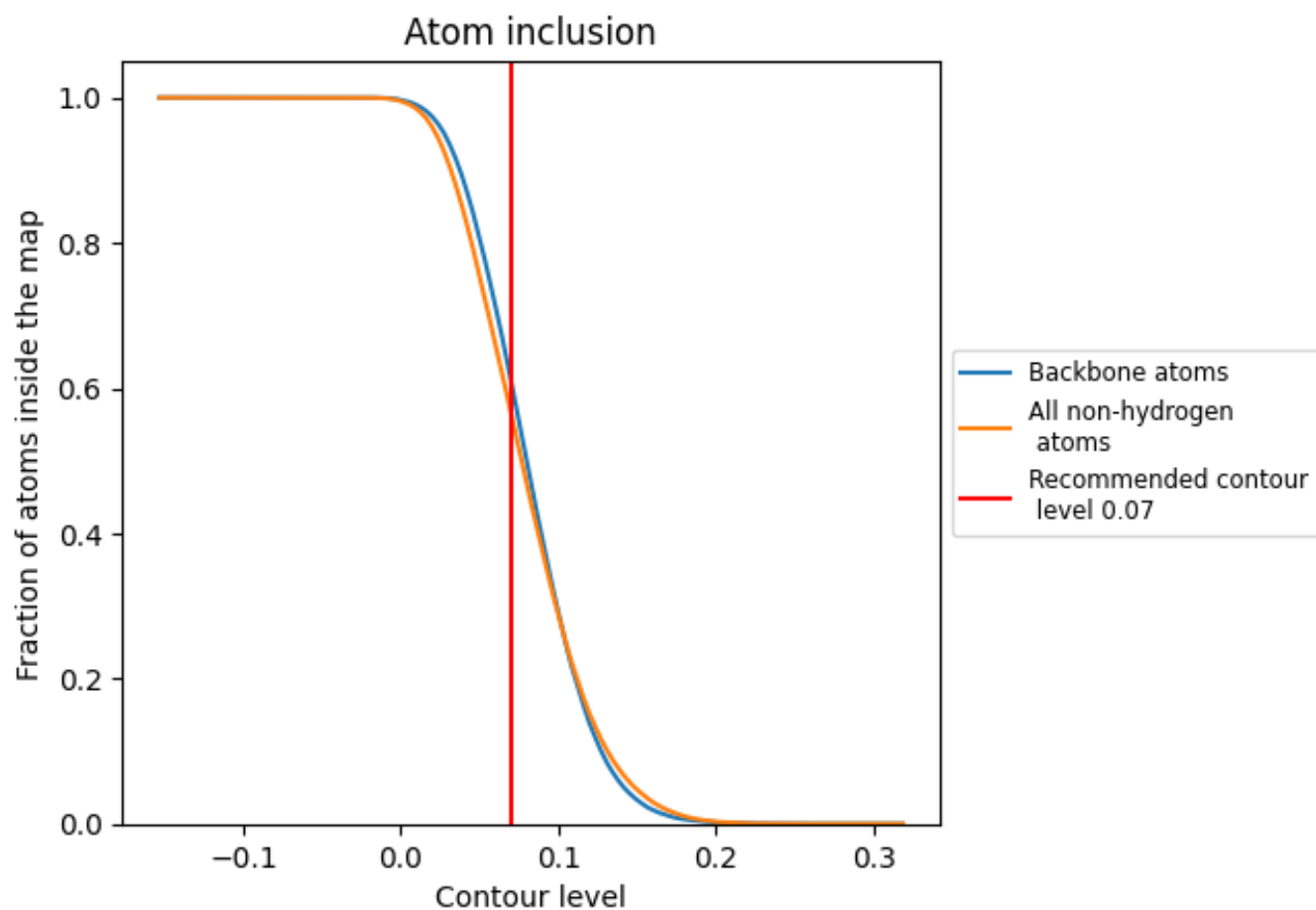
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 56% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5645	 0.4480
0	 0.4880	 0.4810
1	 0.0648	 0.4140
2	 0.6141	 0.5250
3	 0.5336	 0.5130
4	 0.4760	 0.5040
5	 0.1372	 0.3730
6	 0.6748	 0.4740
7	 0.3832	 0.4550
8	 0.4444	 0.4000
A	 0.6696	 0.4520
B	 0.6074	 0.4120
C	 0.5441	 0.5170
D	 0.4792	 0.4870
E	 0.4000	 0.4700
F	 0.2739	 0.4040
G	 0.2277	 0.4160
H	 0.0274	 0.3200
J	 0.5009	 0.4960
K	 0.4337	 0.4880
L	 0.4375	 0.4770
M	 0.4693	 0.4980
N	 0.5524	 0.4920
O	 0.3465	 0.4240
P	 0.4448	 0.4880
Q	 0.5837	 0.5040
R	 0.4467	 0.4800
S	 0.4904	 0.4950
T	 0.4228	 0.4670
U	 0.3416	 0.4570
V	 0.3875	 0.4570
W	 0.5081	 0.5160
X	 0.4493	 0.4830
Y	 0.3521	 0.4150
Z	 0.4691	 0.4690



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Chain	Atom inclusion	Q-score
a	 0.6418	 0.4420
b	 0.1028	 0.4020
c	 0.3669	 0.4540
d	 0.2258	 0.4190
e	 0.4312	 0.4780
f	 0.3456	 0.4420
g	 0.2142	 0.4110
h	 0.4313	 0.4740
i	 0.3289	 0.4270
j	 0.2812	 0.4400
k	 0.3681	 0.4610
l	 0.4093	 0.4880
m	 0.3408	 0.4280
n	 0.4199	 0.4630
o	 0.4058	 0.4520
p	 0.3652	 0.4480
q	 0.3544	 0.4520
r	 0.3607	 0.4780
s	 0.3663	 0.4580
t	 0.3969	 0.4400
u	 0.0518	 0.4060
v	 0.1990	 0.3210