



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 05:39 am GMT

PDB ID : 6H4N
EMDB ID : EMD-0137
Title : Structure of a hibernating 100S ribosome reveals an inactive conformation of the ribosomal protein S1 - 70S Hibernating E. coli Ribosome
Authors : Beckert, B.; Turk, M.; Czech, A.; Berninghausen, O.; Beckmann, R.; Ignatova, Z.; Plitzko, J.; Wilson, N.D.
Deposited on : 2018-07-22
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

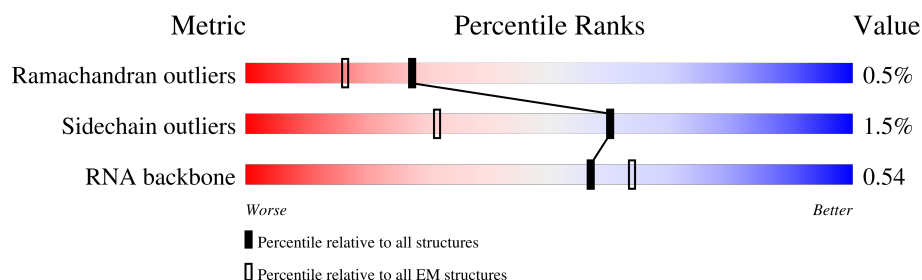
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	a	1534	
2	b	218	
3	c	206	
4	d	205	
5	e	157	
6	f	100	
7	g	161	
8	h	129	

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Mol	Chain	Length	Quality of chain
9	i	127	<div> <div>31%</div> <div>96%</div> <div>..</div> </div>
10	j	98	<div> <div>48%</div> <div>99%</div> <div>.</div> </div>
11	k	116	<div> <div>26%</div> <div>97%</div> <div>..</div> </div>
12	l	123	<div> <div>26%</div> <div>98%</div> <div>.</div> </div>
13	m	114	<div> <div>39%</div> <div>98%</div> <div>.</div> </div>
14	n	101	<div> <div>30%</div> <div>98%</div> <div>.</div> </div>
15	o	88	<div> <div>23%</div> <div>98%</div> <div>.</div> </div>
16	p	82	<div> <div>23%</div> <div>98%</div> <div>.</div> </div>
17	q	80	<div> <div>40%</div> <div>99%</div> <div>.</div> </div>
18	r	65	<div> <div>20%</div> <div>100%</div> <div></div> </div>
19	s	79	<div> <div>32%</div> <div>100%</div> <div></div> </div>
20	t	85	<div> <div>22%</div> <div>98%</div> <div>..</div> </div>
21	u	65	<div> <div>74%</div> <div>91%</div> <div>9%</div> </div>
22	A	2903	<div> <div>11%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
23	B	120	<div> <div>7%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
24	C	271	<div> <div>11%</div> <div>99%</div> <div>.</div> </div>
25	D	209	<div> <div>16%</div> <div>98%</div> <div>.</div> </div>
26	E	201	<div> <div>38%</div> <div>99%</div> <div>.</div> </div>
27	F	177	<div> <div>44%</div> <div>99%</div> <div>.</div> </div>
28	G	176	<div> <div>47%</div> <div>98%</div> <div>.</div> </div>
29	H	149	<div> <div>89%</div> <div>98%</div> <div>.</div> </div>
30	J	142	<div> <div>19%</div> <div>99%</div> <div>.</div> </div>
31	K	122	<div> <div>22%</div> <div>99%</div> <div>.</div> </div>
32	L	143	<div> <div>19%</div> <div>99%</div> <div>.</div> </div>
33	M	136	<div> <div>14%</div> <div>96%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
34	N	120	
35	O	116	
36	P	114	
37	Q	117	
38	R	103	
39	S	110	
40	T	93	
41	U	102	
42	V	94	
43	W	75	
44	X	77	
45	Y	63	
46	Z	58	
47	0	56	
48	1	50	
49	2	46	
50	3	64	
51	4	38	
52	6	66	
53	w	77	
54	v	55	
55	y	557	
56	x	95	
57	I	5	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 147282 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1534	Total	C	N	O	P	0	0
			32916	14680	6039	10663	1534		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	161	Total	C	N	O	S	0	0
			1266	791	243	228	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	154	ALA	ARG	conflict	UNP P02359
g	161	ALA	PHE	conflict	UNP P02359

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	2900	Total	C	N	O	P	0	0
			62261	27774	11460	20127	2900		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 1036415628
A	1847	G	A	conflict	GB 1036415628
A	2069	A	G	conflict	GB 1036415628

- Molecule 23 is a RNA chain called 5S ribosomal RNA.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	-	expression tag	GB 1393501787

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

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

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

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

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	77	Total	C	N	O	P	0	0
			1642	732	296	537	77		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	29	U	G	conflict	GB 1063812051
w	41	A	C	conflict	GB 1063812051

- Molecule 54 is a protein called Ribosome modulation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	55	Total	C	N	O	S	0	0
			453	275	96	77	5		

- Molecule 55 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	351	Total	C	N	O	S	0	0
			2180	1339	397	441	3		

- Molecule 56 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	95	Total	C	N	O	S	0	0
			754	474	133	145	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	57	ASP	ASN	conflict	UNP P0AFX0
x	61	LEU	ILE	conflict	UNP P0AFX0

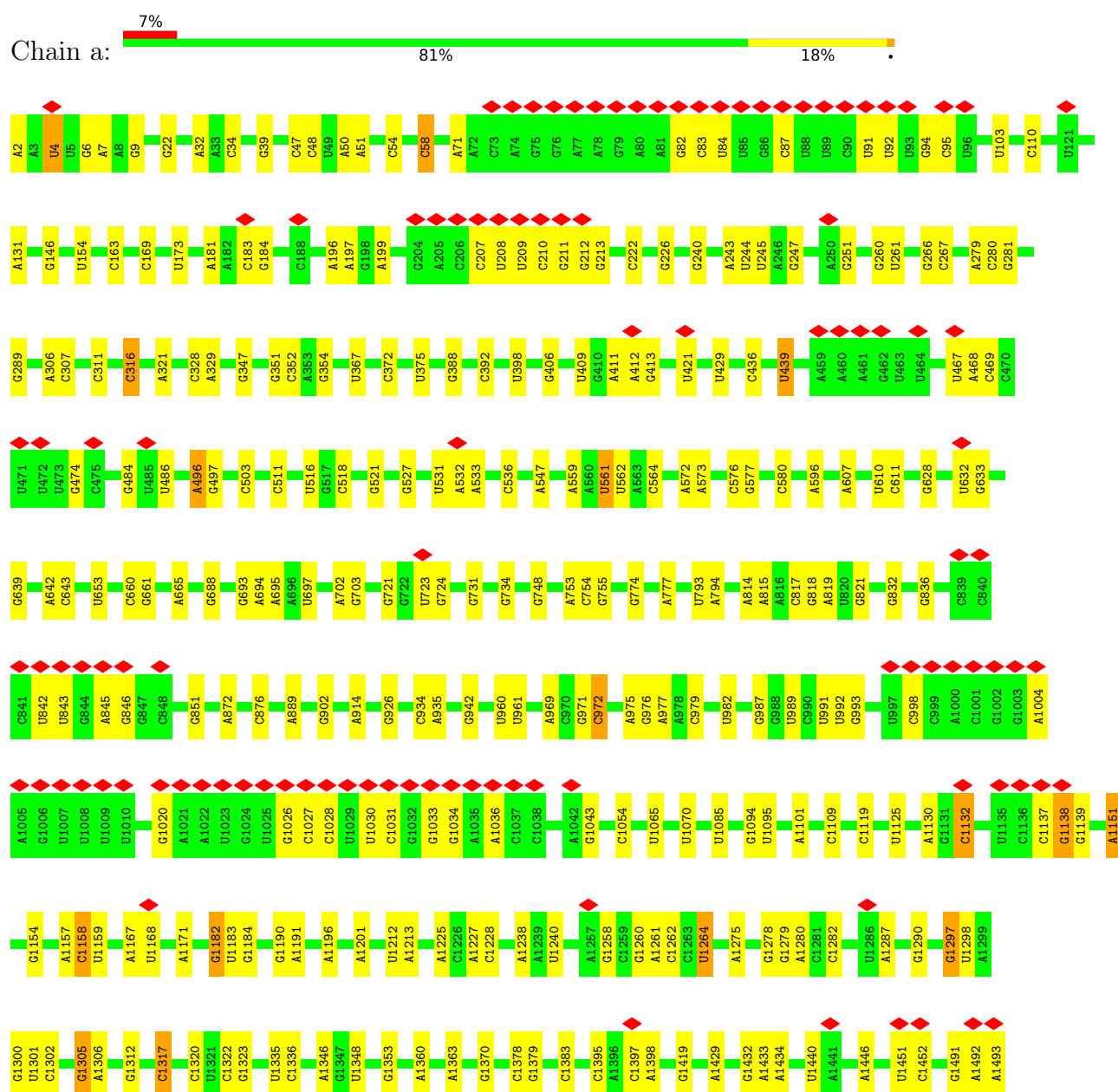
- Molecule 57 is a RNA chain called RNA (5'-R(P*CP*UP*CP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	I	5	100	45	13	37	5	0	0

3 Residue-property plots

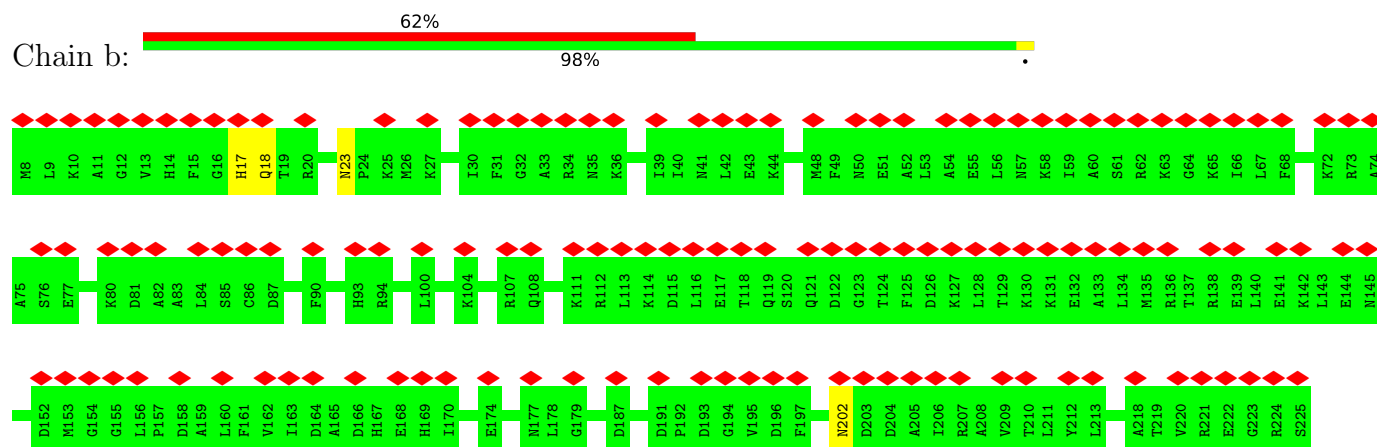
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S ribosomal RNA

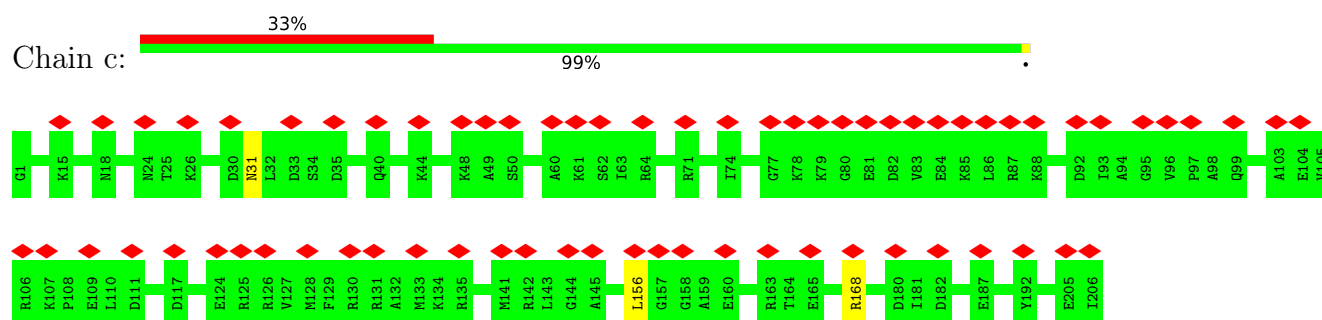




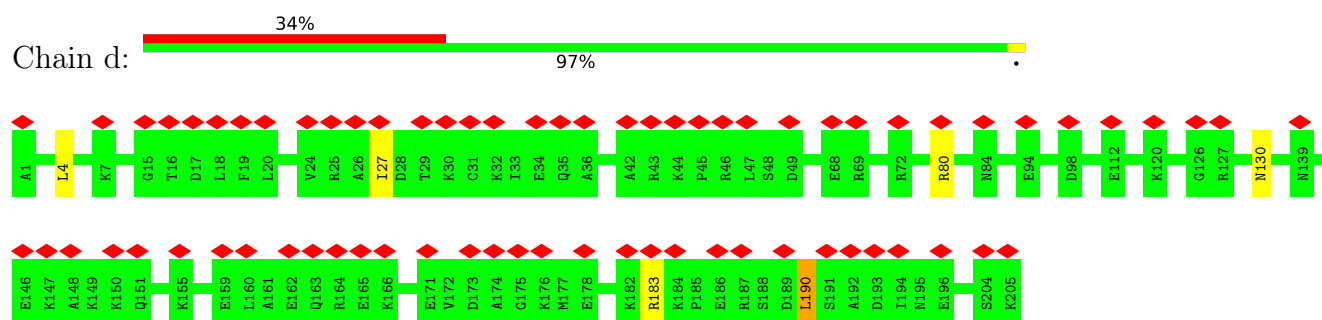
• Molecule 2: 30S ribosomal protein S2



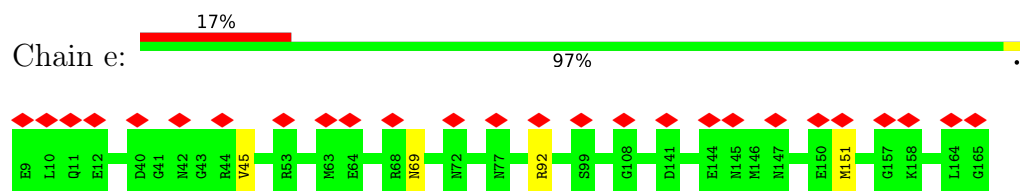
• Molecule 3: 30S ribosomal protein S3



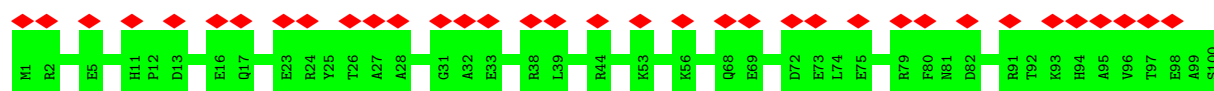
• Molecule 4: 30S ribosomal protein S4



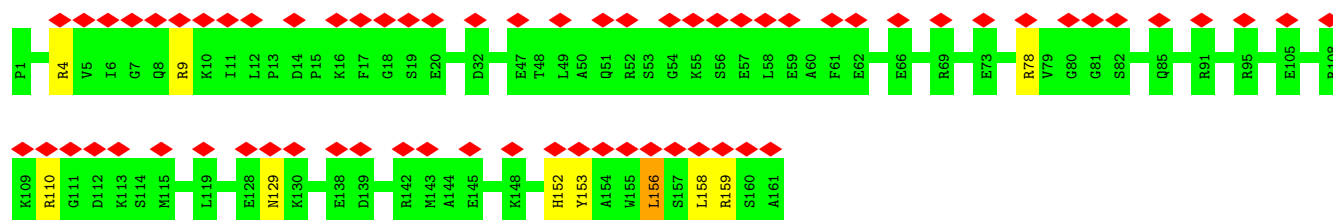
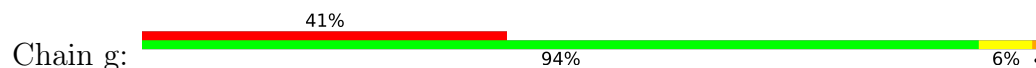
• Molecule 5: 30S ribosomal protein S5



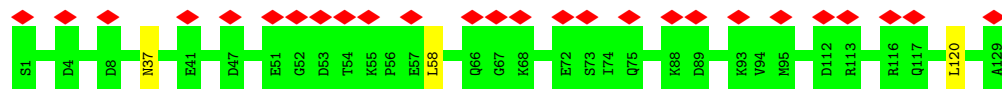
• Molecule 6: 30S ribosomal protein S6



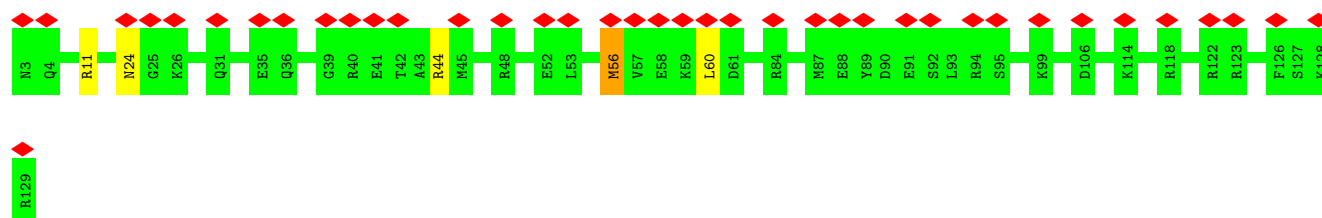
• Molecule 7: 30S ribosomal protein S7



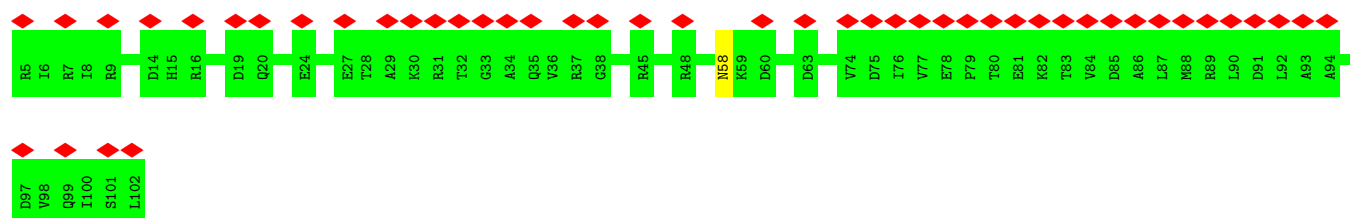
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10



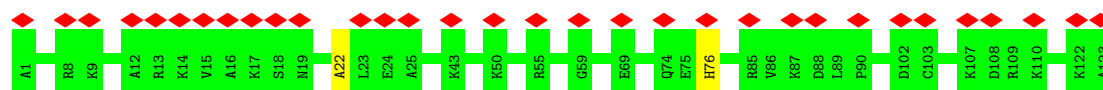
• Molecule 11: 30S ribosomal protein S11





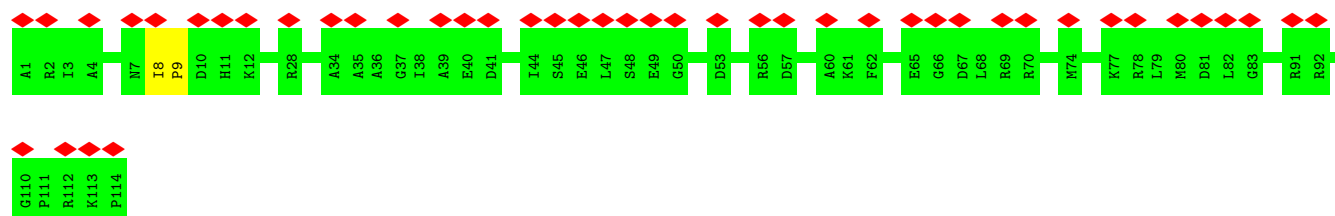
- Molecule 12: 30S ribosomal protein S12

Chain l: 26% 98%



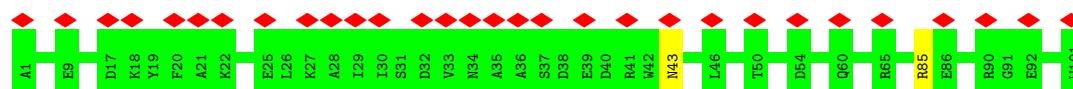
- Molecule 13: 30S ribosomal protein S13

Chain m: 39% 98%



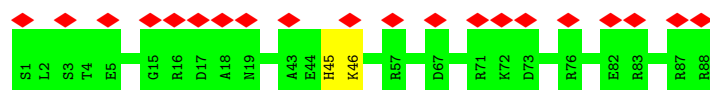
- Molecule 14: 30S ribosomal protein S14

Chain n: 30% 98%



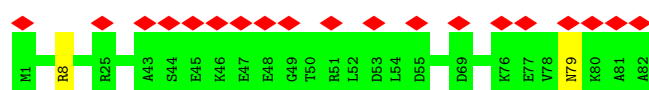
- Molecule 15: 30S ribosomal protein S15

Chain o: 23% 98%



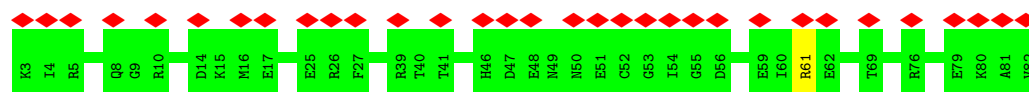
- Molecule 16: 30S ribosomal protein S16

Chain p: 23% 98%

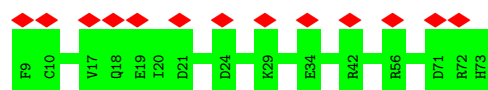


- Molecule 17: 30S ribosomal protein S17

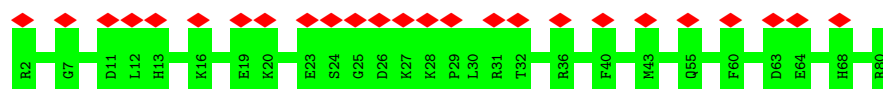
Chain q: 40% 99%



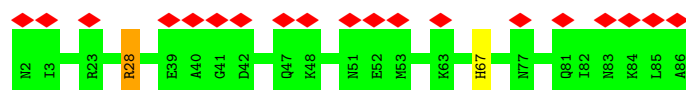
- Molecule 18: 30S ribosomal protein S18



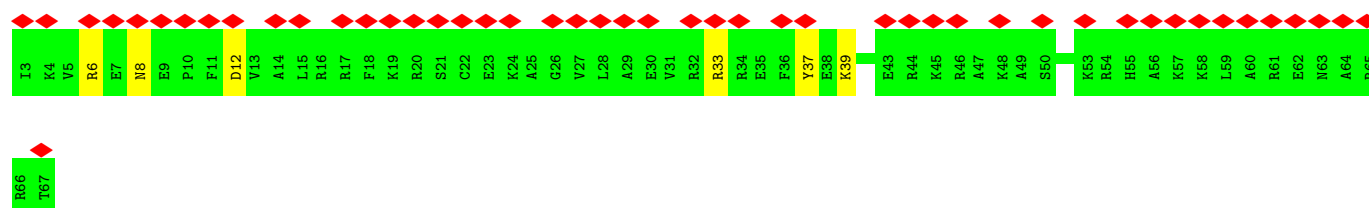
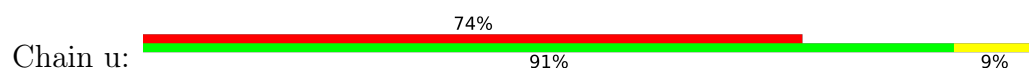
- Molecule 19: 30S ribosomal protein S19



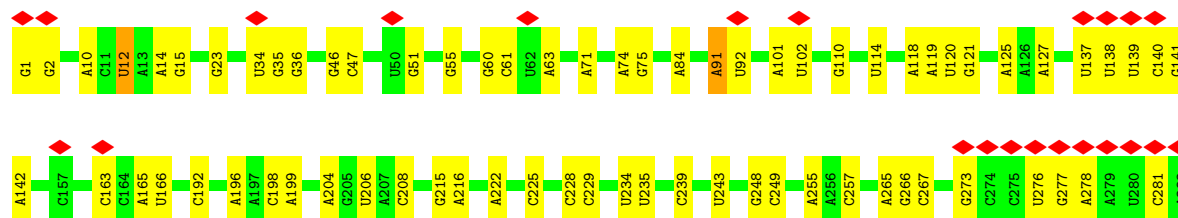
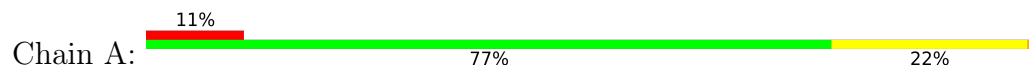
- Molecule 20: 30S ribosomal protein S20

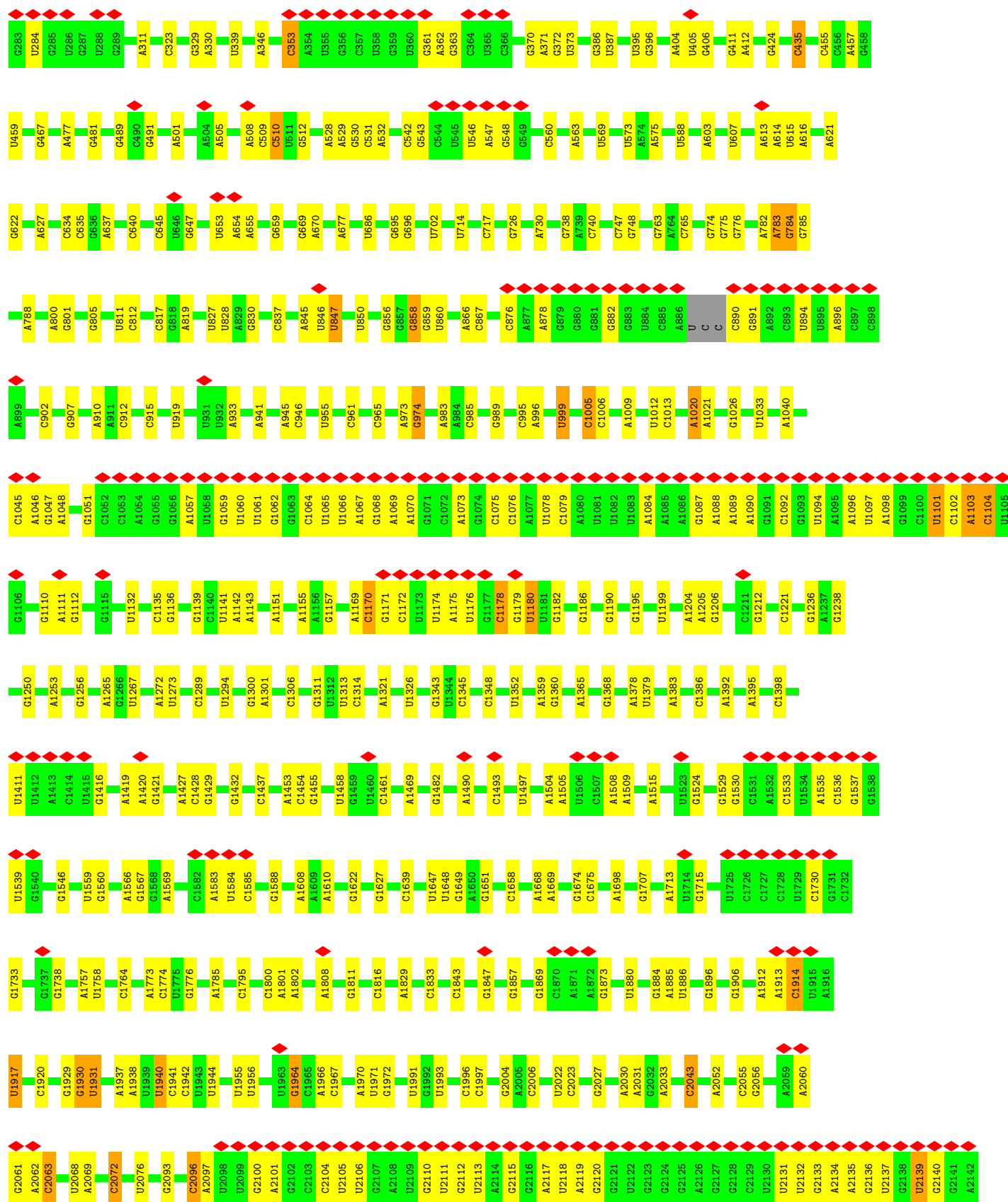


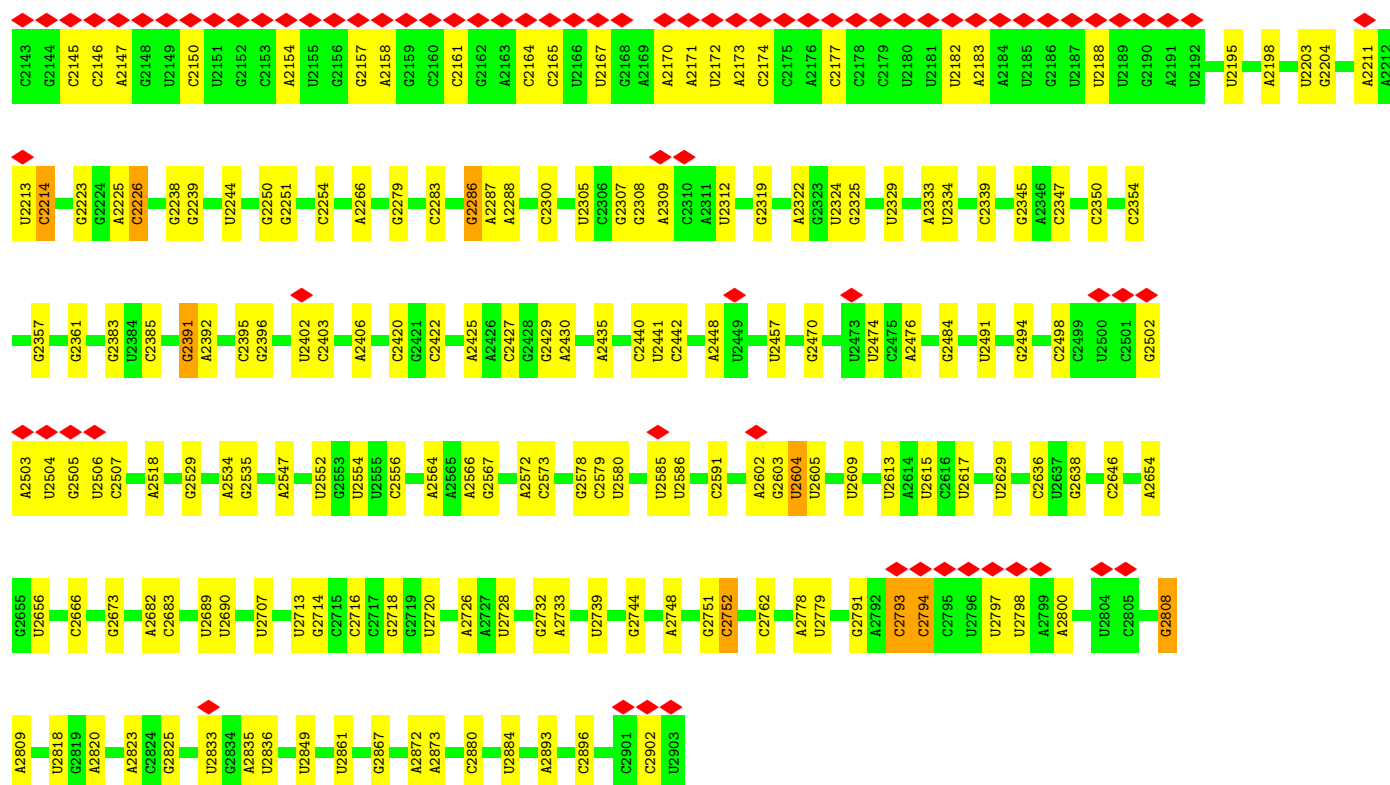
- Molecule 21: 30S ribosomal protein S21



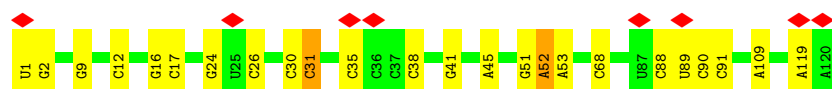
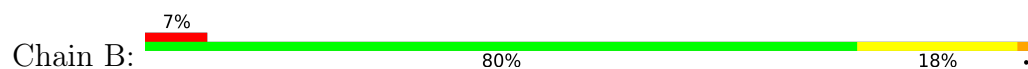
- Molecule 22: 23S ribosomal RNA



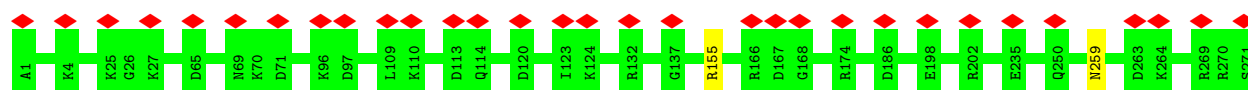




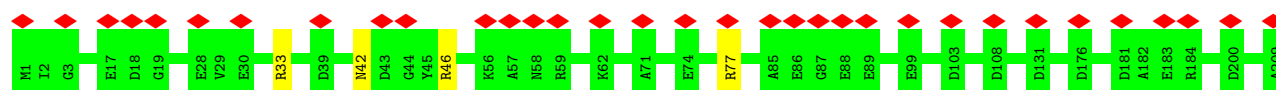
• Molecule 23: 5S ribosomal RNA



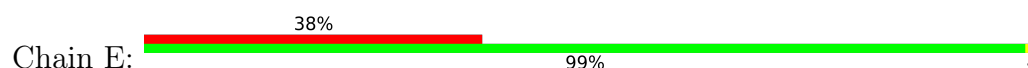
• Molecule 24: 50S ribosomal protein L2

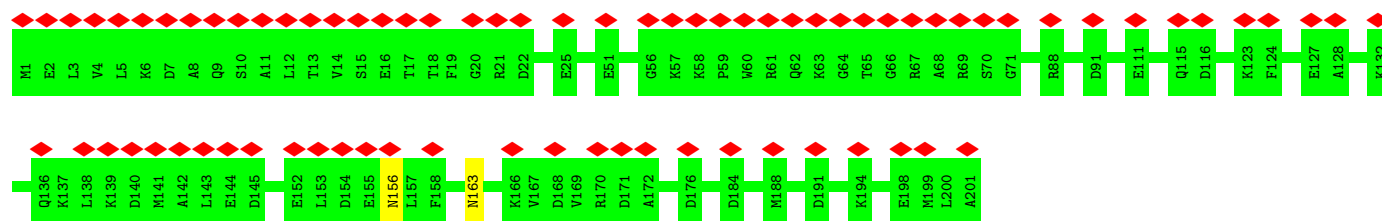


• Molecule 25: 50S ribosomal protein L3



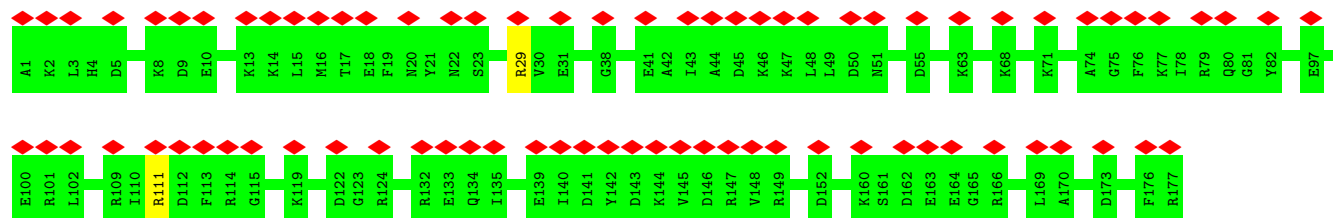
• Molecule 26: 50S ribosomal protein L4





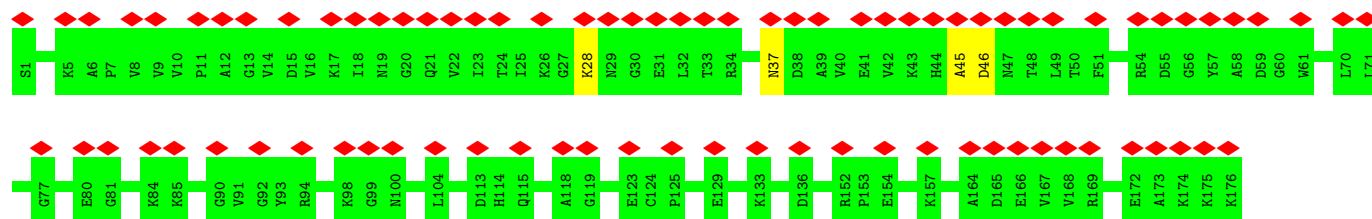
• Molecule 27: 50S ribosomal protein L5

Chain F: .



• Molecule 28: 50S ribosomal protein L6

Chain G: .



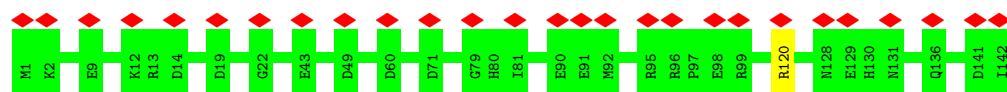
• Molecule 29: 50S ribosomal protein L9

Chain H: .

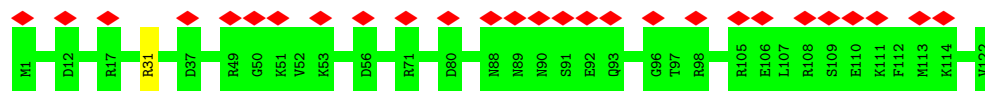


• Molecule 30: 50S ribosomal protein L13

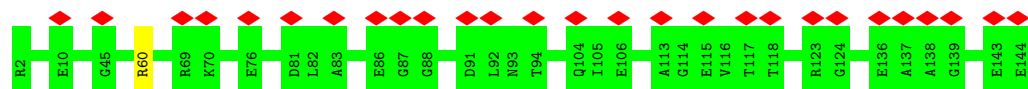
Chain J: .



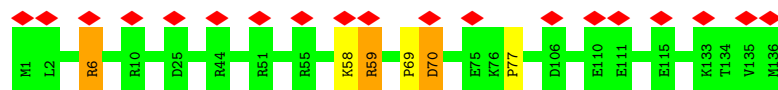
- Molecule 31: 50S ribosomal protein L14



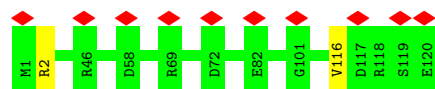
- Molecule 32: 50S ribosomal protein L15



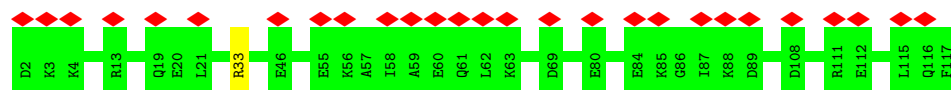
- Molecule 33: 50S ribosomal protein L16



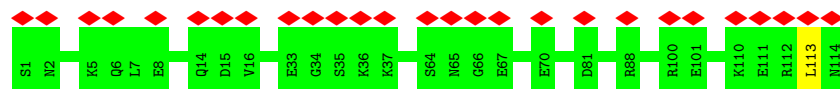
- Molecule 34: 50S ribosomal protein L17



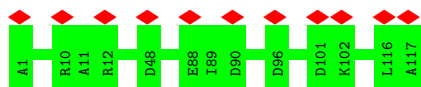
- Molecule 35: 50S ribosomal protein L18



- Molecule 36: 50S ribosomal protein L19



- Molecule 37: 50S ribosomal protein L20



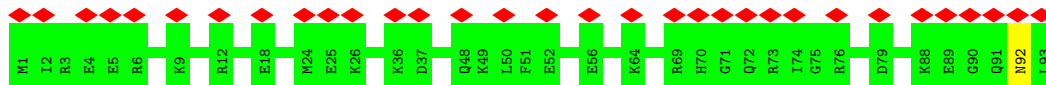
- Molecule 38: 50S ribosomal protein L21



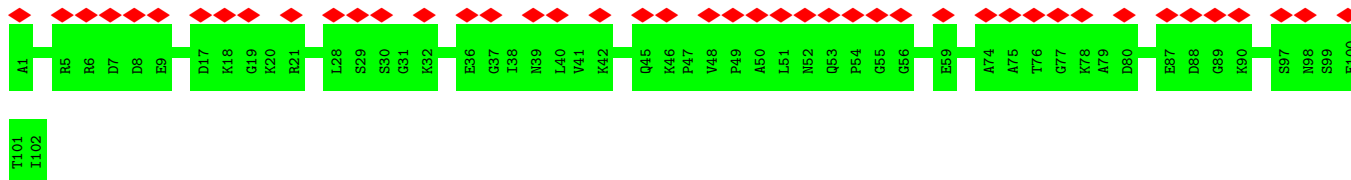
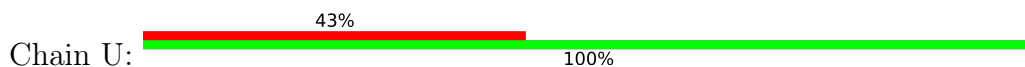
- Molecule 39: 50S ribosomal protein L22



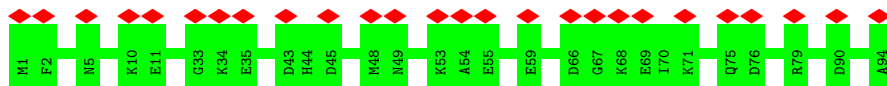
- Molecule 40: 50S ribosomal protein L23



- Molecule 41: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L25

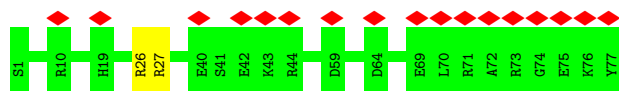


- Molecule 43: 50S ribosomal protein L27

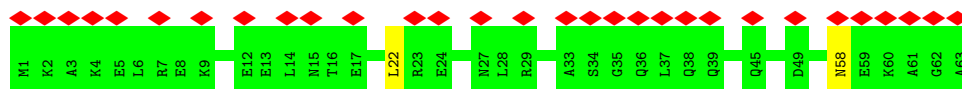




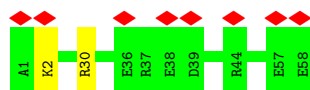
- Molecule 44: 50S ribosomal protein L28



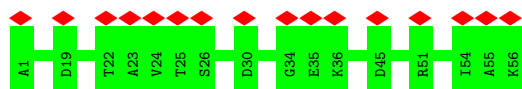
- Molecule 45: 50S ribosomal protein L29



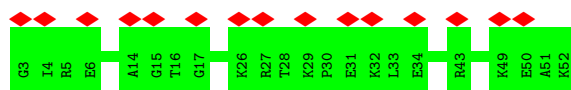
- Molecule 46: 50S ribosomal protein L30



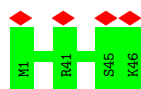
- Molecule 47: 50S ribosomal protein L32



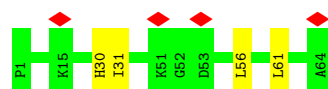
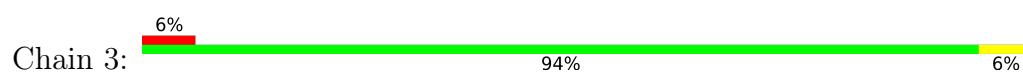
- Molecule 48: 50S ribosomal protein L33



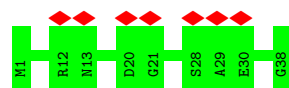
- Molecule 49: 50S ribosomal protein L34



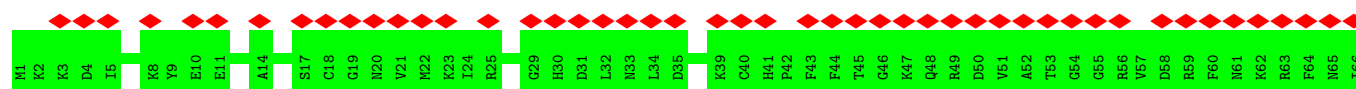
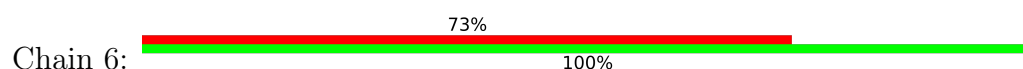
- Molecule 50: 50S ribosomal protein L35



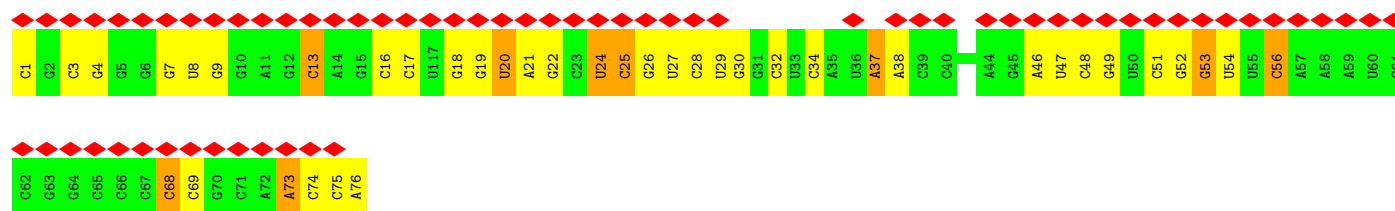
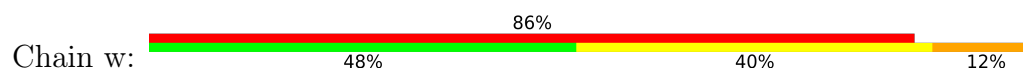
- Molecule 51: 50S ribosomal protein L36



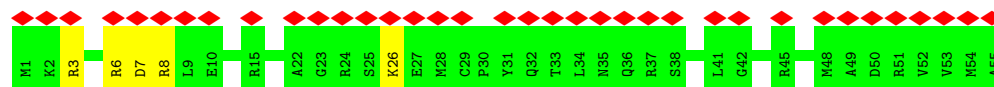
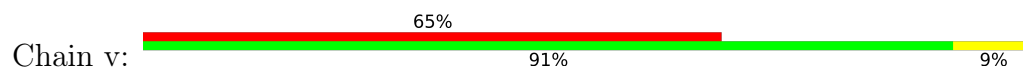
- Molecule 52: 50S ribosomal protein L31



- Molecule 53: tRNA

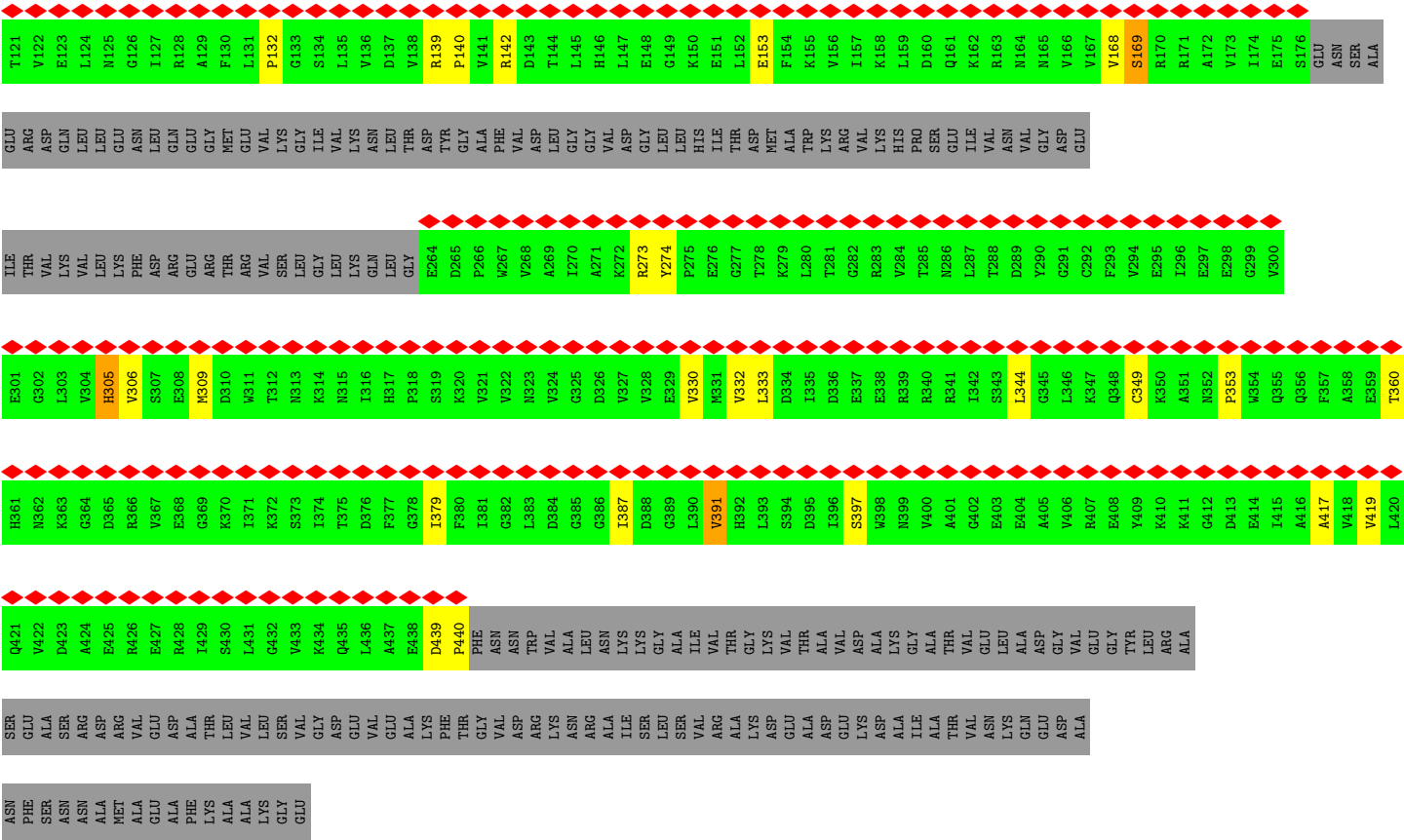


- Molecule 54: Ribosome modulation factor

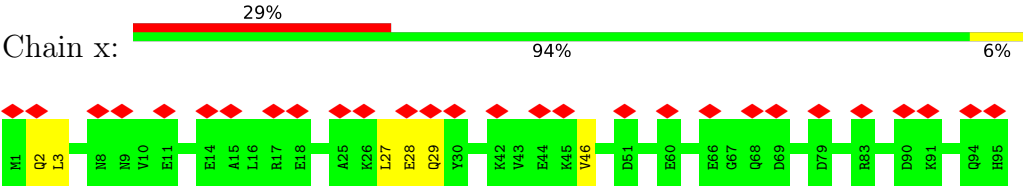


- Molecule 55: 30S ribosomal protein S1

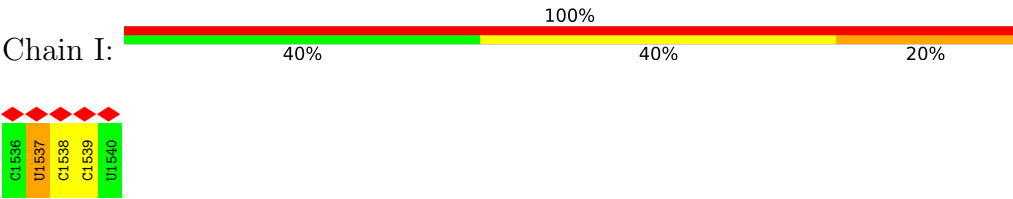




● Molecule 56: Ribosome hibernation promoting factor



● Molecule 57: RNA (5'-R(P*CP*UP*CP*CP*U)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	188304	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 ($e^-/\text{\AA}^2$)	2.5	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	0.439	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	398.912, 398.912, 398.912	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	0.76	1/36857 (0.0%)	1.04	93/57496 (0.2%)
2	b	0.36	0/1735	0.62	0/2338
3	c	0.40	0/1651	0.59	1/2225 (0.0%)
4	d	0.38	0/1665	0.64	2/2227 (0.1%)
5	e	0.41	0/1154	0.66	0/1554
6	f	0.39	0/835	0.64	0/1128
7	g	0.36	0/1284	0.66	1/1724 (0.1%)
8	h	0.38	0/989	0.60	1/1326 (0.1%)
9	i	0.40	0/1034	0.65	0/1375
10	j	0.38	0/796	0.63	0/1077
11	k	0.39	0/885	0.67	0/1195
12	l	0.41	0/969	0.63	0/1300
13	m	0.34	0/892	0.63	0/1193
14	n	0.37	0/811	0.55	0/1081
15	o	0.35	0/722	0.61	0/964
16	p	0.42	0/659	0.60	0/884
17	q	0.37	0/657	0.63	0/881
18	r	0.40	0/511	0.55	0/689
19	s	0.40	0/652	0.63	0/877
20	t	0.33	0/671	0.58	1/888 (0.1%)
21	u	0.45	0/500	0.85	1/668 (0.1%)
22	A	0.81	2/69733 (0.0%)	1.07	266/108786 (0.2%)
23	B	0.72	1/2876 (0.0%)	1.09	10/4483 (0.2%)
24	C	0.46	0/2121	0.61	0/2852
25	D	0.42	0/1586	0.58	0/2134
26	E	0.38	0/1571	0.53	0/2113
27	F	0.37	0/1434	0.60	0/1926
28	G	0.35	0/1343	0.56	0/1816
29	H	0.32	0/1122	0.58	0/1515
30	J	0.42	0/1152	0.57	0/1551
31	K	0.41	0/947	0.62	0/1268
32	L	0.42	0/1054	0.65	0/1403
33	M	0.41	0/1093	0.62	2/1460 (0.1%)
34	N	0.39	0/973	0.63	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	O	0.37	0/902	0.54	0/1209
36	P	0.42	0/929	0.62	1/1242 (0.1%)
37	Q	0.46	0/960	0.53	0/1278
38	R	0.43	0/829	0.62	0/1107
39	S	0.42	0/864	0.59	0/1156
40	T	0.37	0/744	0.60	0/994
41	U	0.37	0/787	0.61	0/1051
42	V	0.40	0/766	0.59	0/1025
43	W	0.42	0/582	0.52	0/769
44	X	0.42	0/635	0.56	0/848
45	Y	0.34	0/510	0.63	1/677 (0.1%)
46	Z	0.36	0/453	0.58	0/605
47	0	0.38	0/450	0.59	0/599
48	1	0.38	0/416	0.58	0/554
49	2	0.40	0/380	0.57	0/498
50	3	0.41	0/513	0.68	2/676 (0.3%)
51	4	0.44	0/303	0.59	0/397
52	6	0.33	0/531	0.58	0/709
53	w	0.54	1/1833 (0.1%)	1.28	26/2851 (0.9%)
54	v	0.36	0/460	0.65	0/611
55	y	0.50	1/2196 (0.0%)	0.98	13/3006 (0.4%)
56	x	1.05	1/764 (0.1%)	1.20	6/1028 (0.6%)
57	I	0.77	0/109	1.49	1/166 (0.6%)
All	All	0.70	7/159850 (0.0%)	0.97	428/238754 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
4	d	0	2
7	g	0	4
9	i	0	1
11	k	0	4
12	l	0	2
13	m	0	1
15	o	0	1
20	t	0	1
21	u	0	3
28	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	M	0	1
34	N	0	1
35	O	0	1
50	3	0	1
54	v	0	2
55	y	0	6
All	All	0	33

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	x	2	GLN	C-N	-27.49	0.70	1.34
23	B	1	U	OP3-P	-10.69	1.48	1.61
22	A	1	G	OP3-P	-10.66	1.48	1.61
53	w	1	C	OP3-P	-10.51	1.48	1.61
1	a	2	A	OP3-P	-10.49	1.48	1.61
55	y	169	SER	N-CA	7.46	1.61	1.46
22	A	528	A	N9-C4	-5.80	1.34	1.37

All (428) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	x	3	LEU	O-C-N	-23.60	84.94	122.70
56	x	3	LEU	CA-C-N	16.62	153.77	117.20
1	a	516	U	N3-C2-O2	-10.93	114.55	122.20
1	a	961	U	N3-C2-O2	-10.54	114.82	122.20
22	A	2580	U	N3-C2-O2	-10.52	114.84	122.20
55	y	169	SER	N-CA-C	9.97	137.92	111.00
22	A	1917	U	N3-C2-O2	-9.77	115.36	122.20
22	A	1092	C	N1-C2-O2	9.60	124.66	118.90
22	A	955	U	N3-C2-O2	-9.47	115.57	122.20
22	A	2604	U	N3-C2-O2	-9.30	115.69	122.20
22	A	1914	C	C2-N1-C1'	9.25	128.98	118.80
22	A	1914	C	N1-C2-O2	9.14	124.38	118.90
56	x	3	LEU	C-N-CA	9.07	144.38	121.70
22	A	1005	C	C2-N1-C1'	8.98	128.68	118.80
22	A	890	C	N1-C2-O2	8.90	124.24	118.90
22	A	2580	U	N1-C2-O2	8.87	129.01	122.80
22	A	1313	U	C2-N1-C1'	8.82	128.29	117.70
1	a	58	C	C6-N1-C2	-8.80	116.78	120.30
21	u	12	ASP	CB-CG-OD1	8.78	126.21	118.30
55	y	88	LYS	C-N-CA	8.76	143.60	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	2457	U	N3-C2-O2	-8.74	116.08	122.20
22	A	890	C	C2-N1-C1'	8.70	128.37	118.80
53	w	68	C	C2-N1-C1'	8.66	128.33	118.80
22	A	1313	U	N1-C2-O2	8.55	128.78	122.80
22	A	1092	C	N3-C2-O2	-8.51	115.94	121.90
53	w	25	C	N1-C2-O2	8.42	123.95	118.90
22	A	2063	C	C6-N1-C2	-8.38	116.95	120.30
1	a	516	U	N1-C2-O2	8.36	128.65	122.80
22	A	1774	C	N3-C2-O2	-8.13	116.21	121.90
22	A	1917	U	N1-C2-O2	8.11	128.48	122.80
22	A	2457	U	C2-N1-C1'	8.10	127.42	117.70
22	A	1917	U	C2-N1-C1'	8.06	127.38	117.70
22	A	510	C	N1-C2-O2	8.06	123.73	118.90
22	A	1313	U	N3-C2-O2	-8.05	116.56	122.20
22	A	2604	U	N1-C2-O2	8.01	128.41	122.80
22	A	12	U	C2-N1-C1'	8.00	127.30	117.70
22	A	1956	U	N3-C2-O2	-7.92	116.66	122.20
53	w	56	C	C2-N1-C1'	7.91	127.50	118.80
1	a	169	C	N1-C2-O2	7.88	123.63	118.90
22	A	890	C	C6-N1-C2	-7.83	117.17	120.30
22	A	837	C	N1-C2-O2	7.77	123.56	118.90
22	A	234	U	N3-C2-O2	-7.68	116.83	122.20
22	A	955	U	N1-C2-O2	7.61	128.13	122.80
22	A	2457	U	N1-C2-O2	7.58	128.11	122.80
22	A	955	U	C2-N1-C1'	7.58	126.79	117.70
53	w	56	C	C5-C6-N1	7.57	124.79	121.00
22	A	1348	C	N1-C2-O2	7.55	123.43	118.90
22	A	2605	U	C2-N1-C1'	7.55	126.76	117.70
4	d	4	LEU	CA-CB-CG	7.51	132.58	115.30
55	y	305	HIS	N-CA-C	7.46	131.16	111.00
1	a	516	U	C2-N1-C1'	7.45	126.64	117.70
22	A	2096	C	C2-N1-C1'	7.44	126.98	118.80
22	A	2605	U	N3-C2-O2	-7.44	116.99	122.20
22	A	890	C	C5-C6-N1	7.43	124.72	121.00
23	B	31	C	C2-N1-C1'	7.41	126.95	118.80
1	a	307	C	N1-C2-O2	7.41	123.35	118.90
22	A	2617	U	N3-C2-O2	-7.40	117.02	122.20
22	A	512	G	O4'-C1'-N9	7.40	114.12	108.20
22	A	2604	U	C2-N1-C1'	7.38	126.56	117.70
22	A	2139	U	N3-C2-O2	-7.37	117.04	122.20
22	A	2226	C	N1-C2-O2	7.32	123.29	118.90
53	w	25	C	N3-C2-O2	-7.30	116.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1956	U	N1-C2-O2	7.29	127.90	122.80
53	w	56	C	C6-N1-C2	-7.23	117.41	120.30
22	A	542	C	C2-N1-C1'	7.22	126.74	118.80
22	A	2580	U	C2-N1-C1'	7.18	126.32	117.70
22	A	1914	C	N3-C2-O2	-7.18	116.87	121.90
1	a	58	C	C5-C6-N1	7.18	124.59	121.00
1	a	1158	C	C2-N1-C1'	7.17	126.69	118.80
1	a	979	C	N1-C2-O2	7.12	123.17	118.90
22	A	1005	C	C6-N1-C2	-7.11	117.46	120.30
53	w	56	C	N1-C2-O2	7.09	123.15	118.90
22	A	2072	C	C2-N1-C1'	7.06	126.57	118.80
1	a	611	C	N1-C2-O2	7.06	123.14	118.90
1	a	1125	U	N1-C2-O2	7.06	127.74	122.80
22	A	510	C	C2-N1-C1'	7.04	126.55	118.80
22	A	837	C	N3-C2-O2	-7.04	116.97	121.90
55	y	440	PRO	N-CA-CB	7.01	111.71	103.30
22	A	137	U	N3-C2-O2	-7.00	117.30	122.20
22	A	1170	C	N1-C2-O2	6.99	123.09	118.90
22	A	2072	C	C5-C6-N1	6.98	124.49	121.00
1	a	1125	U	N3-C2-O2	-6.97	117.32	122.20
22	A	1178	C	N1-C2-O2	6.96	123.08	118.90
1	a	979	C	N3-C2-O2	-6.96	117.03	121.90
36	P	113	LEU	CA-CB-CG	6.95	131.28	115.30
22	A	1170	C	C2-N1-C1'	6.94	126.44	118.80
1	a	961	U	N1-C2-N3	6.91	119.04	114.90
22	A	1314	C	C2-N1-C1'	6.88	126.37	118.80
55	y	104	ASP	N-CA-C	-6.88	92.43	111.00
22	A	2104	C	N1-C2-O2	6.87	123.02	118.90
22	A	1005	C	C5-C6-N1	6.86	124.43	121.00
1	a	1301	U	C2-N1-C1'	6.85	125.92	117.70
1	a	307	C	N3-C2-O2	-6.83	117.12	121.90
22	A	2312	U	C5-C6-N1	6.82	126.11	122.70
22	A	2063	C	C2-N1-C1'	6.81	126.29	118.80
22	A	1092	C	C2-N1-C1'	6.80	126.28	118.80
22	A	974	G	C4-N9-C1'	6.74	135.27	126.50
1	a	169	C	N3-C2-O2	-6.71	117.20	121.90
1	a	1297	G	P-O3'-C3'	6.71	127.75	119.70
7	g	156	LEU	CA-CB-CG	6.70	130.71	115.30
23	B	31	C	C6-N1-C2	-6.70	117.62	120.30
1	a	1305	G	P-O3'-C3'	6.68	127.72	119.70
22	A	837	C	C6-N1-C2	-6.67	117.63	120.30
22	A	2043	C	C2-N1-C1'	6.67	126.14	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1294	U	N3-C2-O2	-6.66	117.54	122.20
22	A	1020	A	P-O3'-C3'	6.65	127.68	119.70
22	A	1880	U	N3-C2-O2	-6.63	117.56	122.20
22	A	1940	U	P-O3'-C3'	6.62	127.64	119.70
22	A	2096	C	C6-N1-C2	-6.62	117.65	120.30
22	A	137	U	N1-C2-O2	6.61	127.43	122.80
1	a	1432	G	P-O3'-C3'	6.60	127.62	119.70
53	w	20	U	P-O3'-C3'	6.59	127.61	119.70
22	A	912	C	C2-N1-C1'	6.58	126.04	118.80
22	A	1930	G	P-O3'-C3'	6.58	127.60	119.70
1	a	92	U	C2-N1-C1'	6.56	125.57	117.70
22	A	867	C	N1-C2-O2	6.54	122.82	118.90
22	A	2063	C	N1-C2-O2	6.47	122.78	118.90
22	A	1178	C	N3-C2-O2	-6.47	117.37	121.90
22	A	1005	C	N1-C2-O2	6.45	122.77	118.90
1	a	961	U	C2-N3-C4	-6.43	123.14	127.00
53	w	51	C	C2-N1-C1'	6.42	125.87	118.80
1	a	1262	C	N1-C2-O2	6.42	122.75	118.90
22	A	1774	C	N1-C2-O2	6.42	122.75	118.90
22	A	2063	C	N3-C2-O2	-6.40	117.42	121.90
1	a	92	U	N1-C2-O2	6.40	127.28	122.80
22	A	1914	C	C6-N1-C1'	-6.40	113.12	120.80
3	c	156	LEU	CA-CB-CG	6.40	130.01	115.30
23	B	30	C	C6-N1-C2	-6.40	117.74	120.30
22	A	114	U	C2-N1-C1'	6.39	125.37	117.70
22	A	257	C	N1-C2-O2	6.39	122.73	118.90
1	a	1348	U	N1-C2-O2	6.37	127.26	122.80
22	A	1931	U	N1-C2-O2	6.37	127.26	122.80
22	A	91	A	P-O3'-C3'	6.36	127.33	119.70
22	A	635	C	C6-N1-C2	-6.35	117.76	120.30
22	A	12	U	N3-C2-O2	-6.34	117.76	122.20
22	A	2300	C	C2-N1-C1'	6.33	125.77	118.80
22	A	890	C	N3-C2-O2	-6.33	117.47	121.90
22	A	2442	C	N1-C2-O2	6.32	122.69	118.90
22	A	1508	A	O4'-C1'-N9	6.32	113.26	108.20
50	3	61	LEU	CA-CB-CG	6.32	129.83	115.30
22	A	1313	U	C6-N1-C1'	-6.32	112.35	121.20
22	A	2139	U	N1-C2-O2	6.30	127.21	122.80
53	w	73	A	O5'-P-OP1	6.29	118.25	110.70
22	A	1092	C	C6-N1-C2	-6.29	117.78	120.30
22	A	2808	G	P-O3'-C3'	6.28	127.24	119.70
22	A	435	C	N1-C2-O2	6.28	122.67	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	169	C	C6-N1-C2	-6.26	117.80	120.30
22	A	2793	C	C2-N1-C1'	6.25	125.67	118.80
22	A	2354	C	C6-N1-C2	-6.24	117.80	120.30
22	A	1920	C	C6-N1-C2	-6.24	117.80	120.30
22	A	1267	U	N1-C2-O2	6.24	127.16	122.80
22	A	2617	U	N1-C2-O2	6.24	127.17	122.80
22	A	2072	C	C6-N1-C2	-6.22	117.81	120.30
22	A	1314	C	C6-N1-C2	-6.22	117.81	120.30
1	a	1317	C	N1-C2-O2	6.21	122.62	118.90
53	w	68	C	C6-N1-C2	-6.20	117.82	120.30
22	A	783	A	C5-N7-C8	-6.19	100.80	103.90
22	A	234	U	N1-C2-O2	6.18	127.12	122.80
22	A	2226	C	N3-C2-O2	-6.18	117.58	121.90
22	A	847	U	N3-C2-O2	-6.17	117.88	122.20
56	x	2	GLN	O-C-N	6.14	132.52	122.70
22	A	965	C	C6-N1-C2	-6.13	117.85	120.30
22	A	1102	C	N3-C2-O2	-6.13	117.61	121.90
22	A	2214	C	N1-C2-O2	6.11	122.57	118.90
1	a	610	U	N1-C2-O2	6.11	127.08	122.80
1	a	58	C	C2-N1-C1'	6.10	125.51	118.80
22	A	1267	U	N3-C2-O2	-6.10	117.93	122.20
53	w	25	C	C6-N1-C2	-6.10	117.86	120.30
22	A	1180	U	C2-N1-C1'	6.10	125.02	117.70
56	x	2	GLN	C-N-CA	-6.09	106.48	121.70
1	a	998	C	N3-C2-O2	-6.07	117.65	121.90
22	A	2072	C	N1-C2-O2	6.07	122.54	118.90
22	A	1993	U	N1-C2-O2	6.05	127.04	122.80
1	a	316	C	C2-N1-C1'	6.05	125.46	118.80
22	A	858	G	P-O3'-C3'	6.05	126.96	119.70
22	A	902	C	C2-N1-C1'	6.04	125.45	118.80
22	A	1993	U	N3-C2-O2	-6.04	117.97	122.20
1	a	754	C	C2-N1-C1'	6.03	125.44	118.80
1	a	610	U	N3-C2-O2	-6.03	117.98	122.20
1	a	1138	G	C4-N9-C1'	6.02	134.33	126.50
22	A	2104	C	N3-C2-O2	-6.02	117.68	121.90
53	w	53	G	P-O3'-C3'	6.02	126.93	119.70
22	A	1914	C	C6-N1-C2	-6.01	117.89	120.30
22	A	2605	U	N1-C2-O2	5.99	126.99	122.80
53	w	3	C	C2-N1-C1'	5.99	125.39	118.80
22	A	1348	C	N3-C2-O2	-5.98	117.71	121.90
55	y	353	PRO	N-CA-CB	5.98	110.47	103.30
22	A	1880	U	N1-C2-O2	5.97	126.98	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	17	C	C2-N1-C1'	5.96	125.36	118.80
55	y	140	PRO	N-CA-CB	5.96	110.45	103.30
22	A	2214	C	N3-C2-O2	-5.95	117.73	121.90
1	a	536	C	C2-N1-C1'	5.95	125.34	118.80
22	A	1079	C	N1-C2-O2	5.94	122.47	118.90
22	A	208	C	C6-N1-C2	-5.94	117.92	120.30
22	A	1221	C	C2-N1-C1'	5.93	125.33	118.80
22	A	783	A	N7-C8-N9	5.92	116.76	113.80
22	A	1005	C	C6-N1-C1'	-5.92	113.70	120.80
22	A	2636	C	C2-N1-C1'	5.92	125.31	118.80
23	B	52	A	P-O3'-C3'	5.91	126.80	119.70
55	y	330	VAL	N-CA-C	5.90	126.92	111.00
1	a	1138	G	N3-C4-C5	-5.89	125.65	128.60
22	A	339	U	N3-C2-O2	-5.88	118.08	122.20
22	A	1102	C	N1-C2-O2	5.88	122.43	118.90
53	w	68	C	C6-N1-C1'	-5.88	113.75	120.80
1	a	611	C	N3-C2-O2	-5.86	117.80	121.90
22	A	2683	C	C6-N1-C2	-5.85	117.96	120.30
55	y	132	PRO	N-CA-CB	5.85	110.32	103.30
22	A	2139	U	C2-N1-C1'	5.85	124.72	117.70
22	A	607	U	N3-C2-O2	-5.84	118.11	122.20
45	Y	22	LEU	CA-CB-CG	5.84	128.73	115.30
22	A	1348	C	C2-N1-C1'	5.83	125.22	118.80
22	A	206	U	N1-C2-O2	5.83	126.88	122.80
22	A	2195	U	N3-C2-O2	-5.83	118.12	122.20
55	y	168	VAL	C-N-CA	5.83	136.26	121.70
1	a	1158	C	N1-C2-O2	5.82	122.39	118.90
22	A	2656	U	N1-C2-O2	5.82	126.87	122.80
1	a	1190	G	P-O3'-C3'	5.82	126.68	119.70
22	A	1314	C	C5-C6-N1	5.82	123.91	121.00
22	A	2739	U	N3-C2-O2	-5.82	118.13	122.20
22	A	640	C	C5-C6-N1	5.81	123.91	121.00
53	w	37	A	O5'-P-OP1	5.81	117.67	110.70
1	a	311	C	C6-N1-C2	-5.80	117.98	120.30
1	a	561	U	P-O3'-C3'	5.80	126.66	119.70
22	A	1993	U	C2-N1-C1'	5.79	124.65	117.70
22	A	2244	U	N3-C4-O4	5.78	123.45	119.40
1	a	103	U	N3-C2-O2	-5.78	118.16	122.20
22	A	1103	A	OP1-P-O3'	5.78	117.91	105.20
1	a	1182	G	P-O3'-C3'	5.77	126.63	119.70
22	A	2457	U	C6-N1-C1'	-5.77	113.12	121.20
22	A	459	U	N3-C2-O2	-5.77	118.16	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1343	G	C4-N9-C1'	5.76	133.99	126.50
22	A	1920	C	C5-C6-N1	5.75	123.88	121.00
1	a	1109	C	N3-C2-O2	-5.74	117.88	121.90
1	a	169	C	C2-N1-C1'	5.73	125.10	118.80
22	A	2063	C	C5-C6-N1	5.72	123.86	121.00
22	A	12	U	N1-C2-O2	5.71	126.80	122.80
22	A	974	G	N7-C8-N9	5.71	115.96	113.10
1	a	503	C	C6-N1-C2	-5.71	118.02	120.30
1	a	1348	U	N3-C2-O2	-5.71	118.21	122.20
22	A	2329	U	C5-C6-N1	5.70	125.55	122.70
55	y	344	LEU	CA-CB-CG	5.70	128.42	115.30
22	A	2474	U	C2-N1-C1'	5.68	124.51	117.70
22	A	1157	G	C6-C5-N7	-5.67	127.00	130.40
22	A	2552	U	N3-C2-O2	-5.67	118.23	122.20
22	A	634	C	C6-N1-C2	-5.67	118.03	120.30
22	A	2104	C	C6-N1-C2	-5.66	118.04	120.30
23	B	17	C	C6-N1-C2	-5.66	118.04	120.30
1	a	660	C	C2-N1-C1'	5.65	125.01	118.80
22	A	542	C	C6-N1-C2	-5.64	118.04	120.30
22	A	459	U	N1-C2-O2	5.63	126.74	122.80
1	a	697	U	N3-C2-O2	-5.62	118.27	122.20
1	a	1301	U	N1-C2-O2	5.62	126.73	122.80
22	A	2339	C	C2-N1-C1'	5.61	124.97	118.80
53	w	68	C	N1-C2-O2	5.61	122.27	118.90
22	A	999	U	N3-C2-O2	-5.61	118.28	122.20
22	A	847	U	N1-C2-O2	5.60	126.72	122.80
22	A	2683	C	N1-C2-O2	5.60	122.26	118.90
1	a	998	C	N1-C2-O2	5.60	122.26	118.90
22	A	860	U	N1-C2-O2	5.60	126.72	122.80
22	A	1289	C	C2-N1-C1'	5.60	124.96	118.80
33	M	70	ASP	CB-CG-OD1	5.60	123.34	118.30
22	A	1306	C	C2-N1-C1'	5.59	124.95	118.80
22	A	1931	U	C2-N1-C1'	5.58	124.40	117.70
1	a	1109	C	N1-C2-O2	5.58	122.25	118.90
22	A	192	C	C6-N1-C2	-5.58	118.07	120.30
22	A	1101	U	N3-C2-O2	-5.58	118.30	122.20
22	A	2794	C	C2-N1-C1'	5.58	124.93	118.80
22	A	965	C	C2-N1-C1'	5.57	124.93	118.80
22	A	1914	C	C5-C6-N1	5.57	123.79	121.00
22	A	860	U	N3-C2-O2	-5.57	118.30	122.20
22	A	257	C	N3-C2-O2	-5.57	118.00	121.90
22	A	2474	U	N1-C2-O2	5.57	126.70	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	974	G	C4-C5-N7	5.56	113.02	110.80
1	a	436	C	C2-N1-C1'	5.56	124.91	118.80
22	A	1931	U	N3-C2-O2	-5.56	118.31	122.20
22	A	2244	U	C5-C4-O4	-5.55	122.57	125.90
1	a	1262	C	N3-C2-O2	-5.54	118.02	121.90
56	x	2	GLN	CA-C-N	-5.54	105.00	117.20
1	a	643	C	C6-N1-C2	-5.54	118.08	120.30
22	A	1101	U	N1-C2-O2	5.53	126.67	122.80
1	a	439	U	N3-C2-O2	-5.53	118.33	122.20
22	A	198	C	C5-C6-N1	5.53	123.76	121.00
22	A	915	C	C2-N1-C1'	5.52	124.88	118.80
22	A	2161	C	N3-C2-O2	-5.52	118.03	121.90
22	A	1795	C	C6-N1-C2	-5.52	118.09	120.30
22	A	850	U	N3-C2-O2	-5.50	118.35	122.20
53	w	3	C	N1-C2-O2	5.50	122.20	118.90
22	A	510	C	C5-C6-N1	5.50	123.75	121.00
22	A	1294	U	N1-C2-O2	5.50	126.65	122.80
53	w	13	C	C2-N1-C1'	5.50	124.85	118.80
1	a	611	C	C6-N1-C2	-5.50	118.10	120.30
1	a	1317	C	N3-C2-O2	-5.49	118.06	121.90
4	d	190	LEU	CA-CB-CG	5.49	127.93	115.30
22	A	1843	C	C5-C6-N1	5.48	123.74	121.00
22	A	1940	U	OP2-P-O3'	5.48	117.25	105.20
1	a	1383	C	N1-C2-O2	5.47	122.19	118.90
23	B	31	C	C5-C6-N1	5.47	123.74	121.00
20	t	67	HIS	C-N-CA	5.46	135.36	121.70
22	A	2720	U	N3-C2-O2	-5.46	118.38	122.20
22	A	2656	U	N3-C2-O2	-5.45	118.39	122.20
53	w	32	C	N1-C2-O2	5.45	122.17	118.90
22	A	783	A	C8-N9-C4	-5.45	103.62	105.80
22	A	2666	C	N1-C2-O2	5.44	122.16	118.90
1	a	979	C	C6-N1-C2	-5.44	118.12	120.30
1	a	972	C	C6-N1-C2	-5.42	118.13	120.30
22	A	890	C	C2-N3-C4	5.42	122.61	119.90
22	A	1931	U	C5-C6-N1	5.41	125.41	122.70
22	A	784	G	P-O3'-C3'	5.41	126.19	119.70
22	A	2391	G	P-O3'-C3'	5.40	126.18	119.70
22	A	560	C	C6-N1-C2	-5.40	118.14	120.30
22	A	1104	C	C6-N1-C2	-5.40	118.14	120.30
22	A	974	G	C8-N9-C1'	-5.39	119.99	127.00
22	A	1170	C	N3-C2-O2	-5.39	118.13	121.90
22	A	2474	U	N3-C2-O2	-5.39	118.43	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	2552	U	C2-N1-C1'	5.39	124.17	117.70
1	a	516	U	C6-N1-C2	-5.38	117.77	121.00
23	B	30	C	C5-C6-N1	5.38	123.69	121.00
22	A	2076	U	C2-N1-C1'	5.38	124.16	117.70
1	a	611	C	C2-N1-C1'	5.38	124.72	118.80
1	a	110	C	N1-C2-O2	5.37	122.12	118.90
22	A	2043	C	C5-C6-N1	5.37	123.69	121.00
23	B	26	C	N1-C2-O2	5.37	122.12	118.90
1	a	1151	A	O4'-C1'-N9	5.37	112.49	108.20
22	A	2579	C	C6-N1-C2	-5.37	118.15	120.30
22	A	890	C	C6-N1-C1'	-5.36	114.37	120.80
1	a	4	U	C2-N1-C1'	5.36	124.13	117.70
1	a	92	U	N3-C2-O2	-5.34	118.47	122.20
22	A	12	U	C5-C6-N1	5.33	125.37	122.70
22	A	1221	C	N1-C2-O2	5.33	122.09	118.90
22	A	882	G	N3-C4-N9	5.32	129.19	126.00
22	A	1157	G	C4-N9-C1'	5.31	133.40	126.50
22	A	1348	C	C6-N1-C2	-5.31	118.18	120.30
22	A	47	C	C6-N1-C2	-5.30	118.18	120.30
22	A	1795	C	C5-C6-N1	5.30	123.65	121.00
22	A	206	U	N3-C2-O2	-5.29	118.49	122.20
22	A	1585	C	N1-C2-O2	5.29	122.07	118.90
1	a	1264	U	N3-C2-O2	-5.29	118.50	122.20
1	a	1190	G	OP2-P-O3'	5.29	116.83	105.20
22	A	702	U	C2-N1-C1'	5.28	124.04	117.70
22	A	1343	G	C8-N9-C1'	-5.28	120.13	127.00
22	A	1658	C	C6-N1-C2	-5.28	118.19	120.30
1	a	697	U	N1-C2-O2	5.28	126.50	122.80
22	A	2096	C	C5-C6-N1	5.28	123.64	121.00
1	a	469	C	N1-C2-O2	5.28	122.07	118.90
1	a	516	U	C5-C4-O4	5.27	129.06	125.90
22	A	208	C	C5-C6-N1	5.27	123.63	121.00
22	A	2226	C	C2-N1-C1'	5.26	124.59	118.80
1	a	1301	U	N3-C2-O2	-5.26	118.52	122.20
1	a	409	U	N3-C2-O2	-5.26	118.52	122.20
22	A	2106	U	C2-N1-C1'	5.25	124.00	117.70
23	B	12	C	C2-N1-C1'	5.25	124.57	118.80
22	A	12	U	C6-N1-C2	-5.23	117.86	121.00
22	A	2286	G	P-O3'-C3'	5.23	125.98	119.70
22	A	2591	C	C6-N1-C2	-5.23	118.21	120.30
1	a	4	U	N1-C2-O2	5.22	126.45	122.80
1	a	34	C	C5-C6-N1	5.22	123.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1178	C	C6-N1-C2	-5.22	118.21	120.30
8	h	58	LEU	CA-CB-CG	5.21	127.30	115.30
1	a	1109	C	C6-N1-C2	-5.20	118.22	120.30
22	A	353	C	C2-N1-C1'	5.20	124.52	118.80
22	A	1886	U	N1-C2-O2	5.20	126.44	122.80
22	A	2556	C	N1-C2-O2	5.20	122.02	118.90
22	A	353	C	C6-N1-C2	-5.20	118.22	120.30
1	a	1264	U	N1-C2-O2	5.20	126.44	122.80
22	A	817	C	C6-N1-C2	-5.20	118.22	120.30
22	A	435	C	N3-C2-O2	-5.19	118.27	121.90
22	A	640	C	C6-N1-C2	-5.19	118.22	120.30
57	I	1537	U	P-O3'-C3'	5.18	125.92	119.70
22	A	1157	G	C4-C5-N7	5.18	112.87	110.80
22	A	2752	C	N1-C2-O2	5.18	122.00	118.90
1	a	54	C	N1-C2-O2	5.17	122.00	118.90
22	A	965	C	C5-C6-N1	5.17	123.59	121.00
22	A	1076	C	C6-N1-C2	-5.17	118.23	120.30
53	w	68	C	C5-C6-N1	5.16	123.58	121.00
22	A	974	G	C6-C5-N7	-5.16	127.31	130.40
22	A	1326	U	N1-C2-O2	5.16	126.41	122.80
1	a	1138	G	N3-C4-N9	5.15	129.09	126.00
1	a	1158	C	C6-N1-C1'	-5.15	114.62	120.80
55	y	169	SER	N-CA-CB	-5.15	102.78	110.50
53	w	34	C	C5-C6-N1	5.14	123.57	121.00
1	a	1132	C	N1-C2-O2	5.14	121.99	118.90
22	A	370	G	O4'-C1'-N9	-5.14	104.09	108.20
22	A	1398	C	C2-N1-C1'	5.14	124.46	118.80
22	A	1157	G	C8-N9-C1'	-5.14	120.32	127.00
22	A	2896	C	C5-C6-N1	5.14	123.57	121.00
33	M	6	ARG	CA-CB-CG	5.13	124.69	113.40
22	A	1348	C	C5-C6-N1	5.13	123.57	121.00
22	A	2656	U	C5-C6-N1	5.13	125.27	122.70
22	A	192	C	C5-C6-N1	5.13	123.56	121.00
1	a	516	U	O4'-C1'-N1	5.12	112.30	108.20
22	A	1157	G	N3-C4-N9	5.12	129.07	126.00
22	A	243	U	N1-C2-O2	5.12	126.38	122.80
22	A	510	C	N3-C2-O2	-5.11	118.32	121.90
22	A	2442	C	N3-C2-O2	-5.10	118.33	121.90
50	3	56	LEU	CA-CB-CG	5.10	127.03	115.30
53	w	29	U	C2-N1-C1'	5.09	123.81	117.70
22	A	2825	G	C4-N9-C1'	5.09	133.12	126.50
22	A	955	U	O4'-C1'-N1	5.09	112.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	542	C	C5-C6-N1	5.08	123.54	121.00
22	A	1669	A	C4-N9-C1'	5.08	135.45	126.30
53	w	51	C	N1-C2-O2	5.08	121.95	118.90
1	a	580	C	C5-C6-N1	5.08	123.54	121.00
53	w	29	U	N1-C2-O2	5.08	126.36	122.80
22	A	2113	U	N1-C2-O2	5.08	126.35	122.80
22	A	1843	C	C6-N1-C2	-5.07	118.27	120.30
53	w	24	U	C2-N1-C1'	5.07	123.78	117.70
22	A	1964	G	O4'-C1'-N9	-5.07	104.15	108.20
22	A	2339	C	C6-N1-C2	-5.07	118.27	120.30
22	A	2395	C	C6-N1-C2	-5.07	118.27	120.30
1	a	979	C	C2-N1-C1'	5.05	124.35	118.80
55	y	332	VAL	N-CA-C	5.05	124.63	111.00
1	a	1119	C	C5-C6-N1	5.04	123.52	121.00
1	a	496	A	O4'-C1'-N9	5.04	112.23	108.20
22	A	955	U	C6-N1-C1'	-5.03	114.15	121.20
1	a	1125	U	C2-N1-C1'	5.03	123.74	117.70
22	A	1199	U	C5-C6-N1	5.03	125.22	122.70
22	A	2006	C	C5-C6-N1	5.03	123.52	121.00
1	a	1317	C	C2-N1-C1'	5.03	124.33	118.80
22	A	235	U	N3-C2-O2	-5.02	118.69	122.20
22	A	1774	C	C6-N1-C2	-5.02	118.29	120.30
22	A	867	C	N3-C2-O2	-5.02	118.39	121.90
22	A	2254	C	N1-C2-O2	5.02	121.91	118.90
22	A	1170	C	C6-N1-C2	-5.01	118.30	120.30
1	a	1440	U	C2-N1-C1'	5.01	123.71	117.70
22	A	243	U	N3-C2-O2	-5.01	118.69	122.20
1	a	1520	C	C2-N1-C1'	5.01	124.31	118.80
1	a	439	U	N1-C2-O2	5.00	126.30	122.80
22	A	2312	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	3	30	HIS	Peptide
28	G	45	ALA	Peptide
33	M	58	LYS	Peptide
34	N	116	VAL	Peptide
35	O	33	ARG	Peptide
2	b	17	HIS	Peptide
4	d	190	LEU	Peptide

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Mol	Chain	Res	Type	Group
4	d	27	ILE	Peptide
7	g	110	ARG	Peptide
7	g	152	HIS	Peptide
7	g	158	LEU	Peptide
7	g	4	ARG	Peptide
9	i	56	MET	Peptide
11	k	117	HIS	Peptide
11	k	12	ARG	Peptide
11	k	125	LYS	Peptide
11	k	72	ALA	Peptide
12	l	22	ALA	Peptide
12	l	76	HIS	Peptide
13	m	8	ILE	Peptide
15	o	45	HIS	Peptide
20	t	28	ARG	Peptide
21	u	39	LYS	Peptide
21	u	6	ARG	Peptide
21	u	8	ASN	Peptide
54	v	26	LYS	Peptide
54	v	6	ARG	Peptide
55	y	274	TYR	Peptide
55	y	391	VAL	Peptide
55	y	417	ALA	Peptide
55	y	419	VAL	Peptide
55	y	81	GLU	Peptide
55	y	82	THR	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	216/218 (99%)	182 (84%)	33 (15%)	1 (0%)	25	61
3	c	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
4	d	203/205 (99%)	181 (89%)	22 (11%)	0	100	100
5	e	155/157 (99%)	142 (92%)	13 (8%)	0	100	100
6	f	98/100 (98%)	86 (88%)	12 (12%)	0	100	100
7	g	159/161 (99%)	137 (86%)	21 (13%)	1 (1%)	22	57
8	h	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
9	i	125/127 (98%)	102 (82%)	23 (18%)	0	100	100
10	j	96/98 (98%)	82 (85%)	13 (14%)	1 (1%)	13	46
11	k	114/116 (98%)	97 (85%)	17 (15%)	0	100	100
12	l	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
13	m	112/114 (98%)	96 (86%)	15 (13%)	1 (1%)	14	49
14	n	99/101 (98%)	85 (86%)	14 (14%)	0	100	100
15	o	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	11	41
16	p	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
17	q	78/80 (98%)	66 (85%)	12 (15%)	0	100	100
18	r	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
19	s	77/79 (98%)	71 (92%)	6 (8%)	0	100	100
20	t	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
21	u	63/65 (97%)	46 (73%)	16 (25%)	1 (2%)	8	34
24	C	269/271 (99%)	244 (91%)	25 (9%)	0	100	100
25	D	207/209 (99%)	192 (93%)	15 (7%)	0	100	100
26	E	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
27	F	175/177 (99%)	163 (93%)	12 (7%)	0	100	100
28	G	174/176 (99%)	160 (92%)	13 (8%)	1 (1%)	22	57
29	H	147/149 (99%)	127 (86%)	20 (14%)	0	100	100
30	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
31	K	120/122 (98%)	103 (86%)	17 (14%)	0	100	100
32	L	141/143 (99%)	126 (89%)	15 (11%)	0	100	100
33	M	134/136 (98%)	126 (94%)	4 (3%)	4 (3%)	3	20
34	N	118/120 (98%)	108 (92%)	10 (8%)	0	100	100
35	O	114/116 (98%)	103 (90%)	11 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	P	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
37	Q	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
38	R	101/103 (98%)	89 (88%)	12 (12%)	0	100	100
39	S	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
40	T	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
41	U	100/102 (98%)	86 (86%)	14 (14%)	0	100	100
42	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
43	W	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
44	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
45	Y	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
46	Z	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
47	0	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
48	1	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
49	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
50	3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	8	34
51	4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
52	6	64/66 (97%)	56 (88%)	8 (12%)	0	100	100
54	v	53/55 (96%)	43 (81%)	9 (17%)	1 (2%)	6	31
55	y	347/557 (62%)	253 (73%)	75 (22%)	19 (6%)	1	8
56	x	93/95 (98%)	85 (91%)	7 (8%)	1 (1%)	12	44
All	All	6082/6394 (95%)	5435 (89%)	614 (10%)	33 (0%)	27	61

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	18	GLN
21	u	37	TYR
55	y	139	ARG
55	y	153	GLU
55	y	169	SER
55	y	306	VAL
55	y	379	ILE
55	y	387	ILE
15	o	46	LYS
55	y	104	ASP

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Mol	Chain	Res	Type
55	y	108	VAL
55	y	309	MET
55	y	333	LEU
55	y	360	THR
55	y	397	SER
7	g	153	TYR
54	v	7	ASP
55	y	76	GLU
55	y	142	ARG
55	y	349	CYS
28	G	46	ASP
33	M	70	ASP
50	3	31	ILE
55	y	82	THR
33	M	59	ARG
33	M	77	PRO
55	y	70	VAL
55	y	439	ASP
10	j	58	ASN
33	M	69	PRO
55	y	391	VAL
13	m	9	PRO
56	x	46	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/180 (100%)	178 (99%)	2 (1%)	70	87
3	c	170/170 (100%)	168 (99%)	2 (1%)	67	86
4	d	172/172 (100%)	169 (98%)	3 (2%)	56	81
5	e	114/119 (96%)	110 (96%)	4 (4%)	31	65
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	132/132 (100%)	127 (96%)	5 (4%)	28	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	h	104/104 (100%)	102 (98%)	2 (2%)	52	79
9	i	105/105 (100%)	100 (95%)	5 (5%)	21	55
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	88 (99%)	1 (1%)	70	87
12	l	103/103 (100%)	103 (100%)	0	100	100
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	77 (98%)	2 (2%)	42	73
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	63 (97%)	2 (3%)	35	68
17	q	74/74 (100%)	73 (99%)	1 (1%)	62	83
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	64 (98%)	1 (2%)	60	83
21	u	44/55 (80%)	43 (98%)	1 (2%)	45	75
24	C	216/216 (100%)	214 (99%)	2 (1%)	75	89
25	D	164/164 (100%)	160 (98%)	4 (2%)	44	74
26	E	165/165 (100%)	163 (99%)	2 (1%)	67	86
27	F	148/148 (100%)	146 (99%)	2 (1%)	62	83
28	G	137/137 (100%)	135 (98%)	2 (2%)	60	83
29	H	114/114 (100%)	111 (97%)	3 (3%)	41	72
30	J	116/116 (100%)	115 (99%)	1 (1%)	75	89
31	K	103/103 (100%)	102 (99%)	1 (1%)	73	88
32	L	102/102 (100%)	101 (99%)	1 (1%)	73	88
33	M	109/109 (100%)	107 (98%)	2 (2%)	54	80
34	N	100/100 (100%)	99 (99%)	1 (1%)	73	88
35	O	86/86 (100%)	86 (100%)	0	100	100
36	P	99/99 (100%)	99 (100%)	0	100	100
37	Q	89/89 (100%)	89 (100%)	0	100	100
38	R	84/84 (100%)	82 (98%)	2 (2%)	44	74
39	S	93/93 (100%)	91 (98%)	2 (2%)	47	76
40	T	80/80 (100%)	79 (99%)	1 (1%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	U	83/83 (100%)	83 (100%)	0	100	100
42	V	78/78 (100%)	78 (100%)	0	100	100
43	W	57/57 (100%)	54 (95%)	3 (5%)	19	51
44	X	67/67 (100%)	65 (97%)	2 (3%)	36	69
45	Y	55/55 (100%)	54 (98%)	1 (2%)	54	80
46	Z	48/48 (100%)	46 (96%)	2 (4%)	25	59
47	0	47/47 (100%)	47 (100%)	0	100	100
48	1	45/45 (100%)	45 (100%)	0	100	100
49	2	38/38 (100%)	38 (100%)	0	100	100
50	3	51/51 (100%)	51 (100%)	0	100	100
51	4	34/34 (100%)	34 (100%)	0	100	100
52	6	59/59 (100%)	59 (100%)	0	100	100
54	v	44/44 (100%)	42 (96%)	2 (4%)	23	57
55	y	137/461 (30%)	134 (98%)	3 (2%)	47	76
56	x	80/81 (99%)	77 (96%)	3 (4%)	28	62
All	All	4883/5236 (93%)	4810 (98%)	73 (2%)	60	83

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	23	ASN
2	b	202	ASN
3	c	31	ASN
3	c	168	ARG
4	d	80	ARG
4	d	130	ASN
4	d	183	ARG
5	e	45	VAL
5	e	69	ASN
5	e	92	ARG
5	e	151	MET
7	g	9	ARG
7	g	78	ARG
7	g	129	ASN
7	g	156	LEU
7	g	159	ARG
8	h	37	ASN

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Mol	Chain	Res	Type
8	h	120	LEU
9	i	11	ARG
9	i	24	ASN
9	i	44	ARG
9	i	56	MET
9	i	60	LEU
11	k	12	ARG
14	n	43	ASN
14	n	85	ARG
16	p	8	ARG
16	p	79	ASN
17	q	61	ARG
20	t	28	ARG
21	u	33	ARG
24	C	155	ARG
24	C	259	ASN
25	D	33	ARG
25	D	42	ASN
25	D	46	ARG
25	D	77	ARG
26	E	156	ASN
26	E	163	ASN
27	F	29	ARG
27	F	111	ARG
28	G	28	LYS
28	G	37	ASN
29	H	11	ASN
29	H	73	ASN
29	H	145	ASN
30	J	120	ARG
31	K	31	ARG
32	L	60	ARG
33	M	6	ARG
33	M	59	ARG
34	N	2	ARG
38	R	48	LYS
38	R	80	ARG
39	S	82	MET
39	S	110	ARG
40	T	92	ASN
43	W	10	ARG
43	W	46	ASN

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Mol	Chain	Res	Type
43	W	72	ASN
44	X	26	ARG
44	X	27	ARG
45	Y	58	ASN
46	Z	2	LYS
46	Z	30	ARG
54	v	3	ARG
54	v	8	ARG
55	y	54	LYS
55	y	273	ARG
55	y	305	HIS
56	x	27	LEU
56	x	28	GLU
56	x	29	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	18	GLN
2	b	23	ASN
2	b	202	ASN
3	c	31	ASN
3	c	139	ASN
3	c	189	HIS
4	d	99	ASN
4	d	115	GLN
5	e	69	ASN
6	f	3	HIS
6	f	55	HIS
7	g	51	GLN
7	g	129	ASN
8	h	37	ASN
9	i	4	GLN
9	i	24	ASN
9	i	31	GLN
9	i	36	GLN
9	i	125	GLN
12	l	28	GLN
14	n	43	ASN
15	o	45	HIS
16	p	18	GLN
16	p	63	GLN

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Mol	Chain	Res	Type
16	p	79	ASN
17	q	8	GLN
17	q	30	HIS
19	s	68	HIS
20	t	20	ASN
20	t	47	GLN
20	t	51	ASN
24	C	85	ASN
24	C	238	ASN
24	C	259	ASN
25	D	42	ASN
25	D	150	GLN
25	D	164	GLN
26	E	156	ASN
26	E	163	ASN
28	G	110	HIS
29	H	11	ASN
29	H	73	ASN
29	H	135	HIS
29	H	145	ASN
30	J	40	HIS
30	J	58	ASN
31	K	29	HIS
35	O	38	GLN
36	P	11	GLN
36	P	40	GLN
37	Q	36	GLN
37	Q	43	GLN
38	R	18	GLN
38	R	89	HIS
38	R	91	GLN
39	S	61	ASN
40	T	92	ASN
41	U	68	ASN
42	V	49	ASN
43	W	8	ASN
43	W	46	ASN
43	W	72	ASN
47	0	5	ASN
47	0	41	HIS
49	2	26	ASN
50	3	42	HIS

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Mol	Chain	Res	Type
51	4	35	GLN
54	v	18	GLN
56	x	2	GLN
56	x	36	GLN
56	x	55	HIS
56	x	88	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1533/1534 (99%)	260 (16%)	0
22	A	2898/2903 (99%)	569 (19%)	13 (0%)
23	B	119/120 (99%)	18 (15%)	1 (0%)
53	w	75/77 (97%)	34 (45%)	0
57	I	4/5 (80%)	2 (50%)	2 (50%)
All	All	4629/4639 (99%)	883 (19%)	16 (0%)

All (883) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	6	G
1	a	7	A
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	50	A
1	a	51	A
1	a	58	C
1	a	71	A
1	a	82	G
1	a	83	C
1	a	84	U
1	a	87	C
1	a	91	U
1	a	94	G
1	a	95	C
1	a	131	A

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Mol	Chain	Res	Type
1	a	146	G
1	a	154	U
1	a	163	C
1	a	173	U
1	a	181	A
1	a	183	C
1	a	184	G
1	a	196	A
1	a	197	A
1	a	199	A
1	a	207	C
1	a	208	U
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	213	G
1	a	222	C
1	a	226	G
1	a	240	G
1	a	243	A
1	a	244	U
1	a	245	U
1	a	247	G
1	a	251	G
1	a	260	G
1	a	261	U
1	a	266	G
1	a	267	C
1	a	279	A
1	a	280	C
1	a	281	G
1	a	289	G
1	a	306	A
1	a	316	C
1	a	321	A
1	a	328	C
1	a	329	A
1	a	347	G
1	a	351	G
1	a	352	C
1	a	354	G

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Mol	Chain	Res	Type
1	a	367	U
1	a	372	C
1	a	375	U
1	a	388	G
1	a	392	C
1	a	398	U
1	a	406	G
1	a	411	A
1	a	412	A
1	a	413	G
1	a	421	U
1	a	429	U
1	a	439	U
1	a	467	U
1	a	468	A
1	a	474	G
1	a	484	G
1	a	486	U
1	a	496	A
1	a	497	G
1	a	511	C
1	a	518	C
1	a	521	G
1	a	527	G
1	a	531	U
1	a	532	A
1	a	533	A
1	a	547	A
1	a	559	A
1	a	561	U
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	596	A
1	a	607	A
1	a	628	G
1	a	632	U
1	a	633	G
1	a	639	G

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Mol	Chain	Res	Type
1	a	642	A
1	a	653	U
1	a	661	G
1	a	665	A
1	a	688	G
1	a	693	G
1	a	694	A
1	a	695	A
1	a	702	A
1	a	703	G
1	a	721	G
1	a	723	U
1	a	724	G
1	a	731	G
1	a	734	G
1	a	748	G
1	a	753	A
1	a	755	G
1	a	774	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	814	A
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	821	G
1	a	832	G
1	a	836	G
1	a	842	U
1	a	843	U
1	a	845	A
1	a	846	G
1	a	851	G
1	a	872	A
1	a	876	C
1	a	889	A
1	a	902	G
1	a	914	A
1	a	926	G
1	a	934	C

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Mol	Chain	Res	Type
1	a	935	A
1	a	942	G
1	a	960	U
1	a	969	A
1	a	971	G
1	a	972	C
1	a	975	A
1	a	976	G
1	a	977	A
1	a	982	U
1	a	987	G
1	a	989	U
1	a	991	U
1	a	992	U
1	a	993	G
1	a	1004	A
1	a	1020	G
1	a	1026	G
1	a	1027	C
1	a	1028	C
1	a	1030	U
1	a	1031	C
1	a	1033	G
1	a	1034	G
1	a	1036	A
1	a	1043	G
1	a	1054	C
1	a	1065	U
1	a	1070	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1130	A
1	a	1132	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1151	A
1	a	1154	G
1	a	1157	A
1	a	1158	C

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Mol	Chain	Res	Type
1	a	1159	U
1	a	1167	A
1	a	1168	U
1	a	1171	A
1	a	1182	G
1	a	1183	U
1	a	1184	G
1	a	1191	A
1	a	1196	A
1	a	1201	A
1	a	1212	U
1	a	1213	A
1	a	1225	A
1	a	1227	A
1	a	1228	C
1	a	1238	A
1	a	1240	U
1	a	1258	G
1	a	1260	G
1	a	1261	A
1	a	1264	U
1	a	1275	A
1	a	1278	G
1	a	1279	G
1	a	1280	A
1	a	1282	C
1	a	1287	A
1	a	1290	G
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1302	C
1	a	1305	G
1	a	1306	A
1	a	1312	G
1	a	1317	C
1	a	1320	C
1	a	1322	C
1	a	1323	G
1	a	1335	U
1	a	1336	C
1	a	1346	A

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Mol	Chain	Res	Type
1	a	1353	G
1	a	1360	A
1	a	1363	A
1	a	1370	G
1	a	1378	C
1	a	1379	G
1	a	1395	C
1	a	1397	C
1	a	1398	A
1	a	1419	G
1	a	1429	A
1	a	1433	A
1	a	1434	A
1	a	1446	A
1	a	1451	U
1	a	1452	C
1	a	1491	G
1	a	1492	A
1	a	1493	A
1	a	1494	G
1	a	1499	A
1	a	1502	A
1	a	1503	A
1	a	1506	U
1	a	1517	G
1	a	1527	U
1	a	1529	G
1	a	1530	G
1	a	1531	A
22	A	2	G
22	A	10	A
22	A	12	U
22	A	14	A
22	A	15	G
22	A	23	G
22	A	34	U
22	A	35	G
22	A	36	G
22	A	46	G
22	A	51	G
22	A	55	G
22	A	60	G

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Mol	Chain	Res	Type
22	A	61	C
22	A	63	A
22	A	71	A
22	A	74	A
22	A	75	G
22	A	84	A
22	A	91	A
22	A	92	U
22	A	101	A
22	A	102	U
22	A	110	G
22	A	118	A
22	A	119	A
22	A	120	U
22	A	121	G
22	A	125	A
22	A	127	A
22	A	138	U
22	A	139	U
22	A	140	C
22	A	141	G
22	A	142	A
22	A	163	C
22	A	165	A
22	A	166	U
22	A	196	A
22	A	199	A
22	A	204	A
22	A	215	G
22	A	216	A
22	A	222	A
22	A	225	C
22	A	228	C
22	A	229	C
22	A	239	C
22	A	248	G
22	A	249	C
22	A	255	A
22	A	265	A
22	A	266	G
22	A	267	C
22	A	273	G

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Mol	Chain	Res	Type
22	A	276	U
22	A	277	G
22	A	278	A
22	A	281	C
22	A	284	U
22	A	311	A
22	A	323	C
22	A	329	G
22	A	330	A
22	A	346	A
22	A	353	C
22	A	361	G
22	A	362	A
22	A	363	G
22	A	371	A
22	A	372	G
22	A	373	U
22	A	386	G
22	A	387	U
22	A	395	U
22	A	396	G
22	A	404	A
22	A	405	U
22	A	406	G
22	A	411	G
22	A	412	A
22	A	424	G
22	A	435	C
22	A	455	C
22	A	457	A
22	A	467	G
22	A	477	A
22	A	481	G
22	A	489	G
22	A	491	G
22	A	501	A
22	A	505	A
22	A	508	A
22	A	509	C
22	A	510	C
22	A	529	A
22	A	530	G

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Mol	Chain	Res	Type
22	A	531	C
22	A	532	A
22	A	543	G
22	A	546	U
22	A	547	A
22	A	548	G
22	A	563	A
22	A	569	U
22	A	573	U
22	A	575	A
22	A	588	U
22	A	603	A
22	A	613	A
22	A	614	A
22	A	615	U
22	A	616	A
22	A	621	A
22	A	622	G
22	A	627	A
22	A	637	A
22	A	645	C
22	A	647	G
22	A	653	U
22	A	654	A
22	A	655	A
22	A	659	G
22	A	669	G
22	A	670	A
22	A	677	A
22	A	686	U
22	A	695	G
22	A	696	G
22	A	714	U
22	A	717	C
22	A	726	G
22	A	730	A
22	A	738	G
22	A	740	C
22	A	747	C
22	A	748	G
22	A	763	G
22	A	765	C

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Mol	Chain	Res	Type
22	A	774	G
22	A	775	G
22	A	776	G
22	A	782	A
22	A	783	A
22	A	784	G
22	A	785	G
22	A	788	A
22	A	800	A
22	A	801	G
22	A	805	G
22	A	811	U
22	A	812	C
22	A	819	A
22	A	827	U
22	A	828	U
22	A	830	G
22	A	845	A
22	A	846	U
22	A	847	U
22	A	856	G
22	A	858	G
22	A	859	G
22	A	866	A
22	A	876	C
22	A	878	A
22	A	891	G
22	A	894	U
22	A	896	A
22	A	907	G
22	A	910	A
22	A	919	U
22	A	933	A
22	A	941	A
22	A	945	A
22	A	946	C
22	A	961	C
22	A	973	A
22	A	974	G
22	A	983	A
22	A	985	C
22	A	989	G

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Mol	Chain	Res	Type
22	A	995	C
22	A	996	A
22	A	999	U
22	A	1005	C
22	A	1006	C
22	A	1009	A
22	A	1012	U
22	A	1013	C
22	A	1021	A
22	A	1026	G
22	A	1033	U
22	A	1040	A
22	A	1045	C
22	A	1046	A
22	A	1047	G
22	A	1048	A
22	A	1051	G
22	A	1057	A
22	A	1059	G
22	A	1060	U
22	A	1061	U
22	A	1062	G
22	A	1064	C
22	A	1065	U
22	A	1066	U
22	A	1067	A
22	A	1068	G
22	A	1069	A
22	A	1070	A
22	A	1073	A
22	A	1075	C
22	A	1078	U
22	A	1084	A
22	A	1087	G
22	A	1088	A
22	A	1089	A
22	A	1090	A
22	A	1094	U
22	A	1096	A
22	A	1097	U
22	A	1098	A
22	A	1101	U

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Mol	Chain	Res	Type
22	A	1103	A
22	A	1104	C
22	A	1110	G
22	A	1111	A
22	A	1112	G
22	A	1132	U
22	A	1135	C
22	A	1136	G
22	A	1139	G
22	A	1141	U
22	A	1142	A
22	A	1143	A
22	A	1151	A
22	A	1155	A
22	A	1169	A
22	A	1170	C
22	A	1171	G
22	A	1172	C
22	A	1174	U
22	A	1175	A
22	A	1176	U
22	A	1178	C
22	A	1179	G
22	A	1180	U
22	A	1186	G
22	A	1195	G
22	A	1204	A
22	A	1205	A
22	A	1206	G
22	A	1212	G
22	A	1236	G
22	A	1238	G
22	A	1250	G
22	A	1253	A
22	A	1256	G
22	A	1265	A
22	A	1272	A
22	A	1273	U
22	A	1300	G
22	A	1301	A
22	A	1311	G
22	A	1321	A

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Mol	Chain	Res	Type
22	A	1345	C
22	A	1352	U
22	A	1359	A
22	A	1360	G
22	A	1365	A
22	A	1368	G
22	A	1378	A
22	A	1379	U
22	A	1383	A
22	A	1386	C
22	A	1392	A
22	A	1395	A
22	A	1411	U
22	A	1416	G
22	A	1419	A
22	A	1420	A
22	A	1421	G
22	A	1427	A
22	A	1428	C
22	A	1429	G
22	A	1437	C
22	A	1453	A
22	A	1454	C
22	A	1455	G
22	A	1458	U
22	A	1461	C
22	A	1469	A
22	A	1482	G
22	A	1490	A
22	A	1493	C
22	A	1497	U
22	A	1504	A
22	A	1505	A
22	A	1509	A
22	A	1515	A
22	A	1524	G
22	A	1529	G
22	A	1530	G
22	A	1533	C
22	A	1535	A
22	A	1536	C
22	A	1537	G

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Mol	Chain	Res	Type
22	A	1539	U
22	A	1546	G
22	A	1559	U
22	A	1560	G
22	A	1566	A
22	A	1567	G
22	A	1569	A
22	A	1583	A
22	A	1584	U
22	A	1588	G
22	A	1608	A
22	A	1610	A
22	A	1622	G
22	A	1627	G
22	A	1639	C
22	A	1647	U
22	A	1648	U
22	A	1649	G
22	A	1651	G
22	A	1668	A
22	A	1674	G
22	A	1675	C
22	A	1698	A
22	A	1707	G
22	A	1713	A
22	A	1715	G
22	A	1730	C
22	A	1733	G
22	A	1738	G
22	A	1757	A
22	A	1758	U
22	A	1764	C
22	A	1773	A
22	A	1776	G
22	A	1785	A
22	A	1800	C
22	A	1801	A
22	A	1802	A
22	A	1808	A
22	A	1811	G
22	A	1816	C
22	A	1829	A

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Mol	Chain	Res	Type
22	A	1833	C
22	A	1847	G
22	A	1857	G
22	A	1869	G
22	A	1873	G
22	A	1884	G
22	A	1885	A
22	A	1896	G
22	A	1906	G
22	A	1912	A
22	A	1913	A
22	A	1914	C
22	A	1917	U
22	A	1929	G
22	A	1930	G
22	A	1931	U
22	A	1937	A
22	A	1938	A
22	A	1940	U
22	A	1941	C
22	A	1942	C
22	A	1944	U
22	A	1955	U
22	A	1964	G
22	A	1966	A
22	A	1967	C
22	A	1970	A
22	A	1971	U
22	A	1972	G
22	A	1991	U
22	A	1996	C
22	A	1997	C
22	A	2004	G
22	A	2022	U
22	A	2023	C
22	A	2027	G
22	A	2030	A
22	A	2031	A
22	A	2033	A
22	A	2043	C
22	A	2052	A
22	A	2055	C

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Mol	Chain	Res	Type
22	A	2056	G
22	A	2060	A
22	A	2061	G
22	A	2062	A
22	A	2063	C
22	A	2068	U
22	A	2069	A
22	A	2072	C
22	A	2093	G
22	A	2096	C
22	A	2097	A
22	A	2100	G
22	A	2101	A
22	A	2105	U
22	A	2110	G
22	A	2111	U
22	A	2112	G
22	A	2115	G
22	A	2117	A
22	A	2118	U
22	A	2119	A
22	A	2120	G
22	A	2131	U
22	A	2132	U
22	A	2133	G
22	A	2134	A
22	A	2135	A
22	A	2136	G
22	A	2137	U
22	A	2139	U
22	A	2140	G
22	A	2145	C
22	A	2146	C
22	A	2147	A
22	A	2150	C
22	A	2154	A
22	A	2157	G
22	A	2158	A
22	A	2164	C
22	A	2165	C
22	A	2167	U
22	A	2170	A

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Mol	Chain	Res	Type
22	A	2171	A
22	A	2172	U
22	A	2173	A
22	A	2174	C
22	A	2177	C
22	A	2182	U
22	A	2183	A
22	A	2188	U
22	A	2198	A
22	A	2203	U
22	A	2204	G
22	A	2211	A
22	A	2213	U
22	A	2214	C
22	A	2223	G
22	A	2225	A
22	A	2226	C
22	A	2238	G
22	A	2239	G
22	A	2250	G
22	A	2251	G
22	A	2266	A
22	A	2279	G
22	A	2283	C
22	A	2287	A
22	A	2288	A
22	A	2305	U
22	A	2307	G
22	A	2308	G
22	A	2309	A
22	A	2319	G
22	A	2322	A
22	A	2325	G
22	A	2333	A
22	A	2334	U
22	A	2345	G
22	A	2347	C
22	A	2350	C
22	A	2357	G
22	A	2361	G
22	A	2383	G
22	A	2385	C

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Mol	Chain	Res	Type
22	A	2392	A
22	A	2396	G
22	A	2402	U
22	A	2403	C
22	A	2406	A
22	A	2420	C
22	A	2422	C
22	A	2425	A
22	A	2427	C
22	A	2429	G
22	A	2430	A
22	A	2435	A
22	A	2440	C
22	A	2441	U
22	A	2448	A
22	A	2470	G
22	A	2476	A
22	A	2484	G
22	A	2491	U
22	A	2494	G
22	A	2498	C
22	A	2502	G
22	A	2503	A
22	A	2504	U
22	A	2505	G
22	A	2506	U
22	A	2507	C
22	A	2518	A
22	A	2529	G
22	A	2534	A
22	A	2535	G
22	A	2547	A
22	A	2554	U
22	A	2564	A
22	A	2566	A
22	A	2567	G
22	A	2572	A
22	A	2573	C
22	A	2578	G
22	A	2585	U
22	A	2586	U
22	A	2602	A

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Mol	Chain	Res	Type
22	A	2603	G
22	A	2604	U
22	A	2609	U
22	A	2613	U
22	A	2615	U
22	A	2629	U
22	A	2638	G
22	A	2646	C
22	A	2654	A
22	A	2673	G
22	A	2682	A
22	A	2689	U
22	A	2690	U
22	A	2707	U
22	A	2713	U
22	A	2714	G
22	A	2716	C
22	A	2718	G
22	A	2726	A
22	A	2728	U
22	A	2732	G
22	A	2733	A
22	A	2744	G
22	A	2748	A
22	A	2751	G
22	A	2752	C
22	A	2762	C
22	A	2778	A
22	A	2779	U
22	A	2791	G
22	A	2793	C
22	A	2794	C
22	A	2797	U
22	A	2798	U
22	A	2800	A
22	A	2808	G
22	A	2809	A
22	A	2818	U
22	A	2820	A
22	A	2823	A
22	A	2833	U
22	A	2835	A

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Mol	Chain	Res	Type
22	A	2836	U
22	A	2849	U
22	A	2861	U
22	A	2867	G
22	A	2872	A
22	A	2873	A
22	A	2880	C
22	A	2884	U
22	A	2893	A
22	A	2902	C
23	B	2	G
23	B	9	G
23	B	16	G
23	B	24	G
23	B	31	C
23	B	35	C
23	B	38	C
23	B	41	G
23	B	45	A
23	B	51	G
23	B	53	A
23	B	68	C
23	B	88	C
23	B	89	U
23	B	90	C
23	B	91	C
23	B	109	A
23	B	119	A
53	w	4	G
53	w	7	G
53	w	8	U
53	w	9	G
53	w	13	C
53	w	16	C
53	w	17	C
53	w	18	G
53	w	19	G
53	w	20	U
53	w	21	A
53	w	22	G
53	w	24	U
53	w	25	C

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Mol	Chain	Res	Type
53	w	26	G
53	w	27	U
53	w	28	C
53	w	30	G
53	w	37	A
53	w	38	A
53	w	46	A
53	w	47	U
53	w	48	C
53	w	49	G
53	w	52	G
53	w	53	G
53	w	54	U
53	w	56	C
53	w	68	C
53	w	69	C
53	w	73	A
53	w	74	C
53	w	75	C
53	w	76	A
57	I	1538	C
57	I	1539	C

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	A	91	A
22	A	784	G
22	A	858	G
22	A	1020	A
22	A	1182	G
22	A	1190	G
22	A	1432	G
22	A	1930	G
22	A	1940	U
22	A	2286	G
22	A	2324	U
22	A	2391	G
22	A	2808	G
23	B	52	A
57	I	1537	U
57	I	1538	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
53	w	1
56	x	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	17:C	O3'	117:U	P	3.73
1	x	2:GLN	C	3:LEU	N	0.70

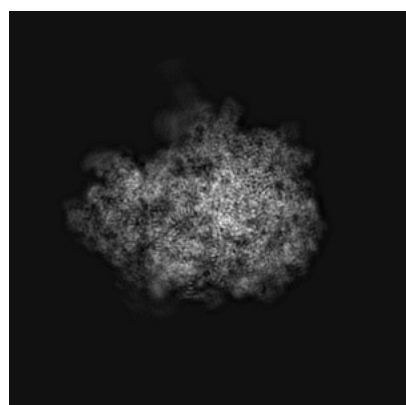
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0137. These allow visual inspection of the internal detail of the map and identification of artifacts.

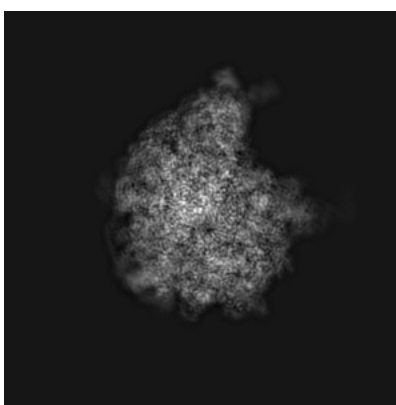
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

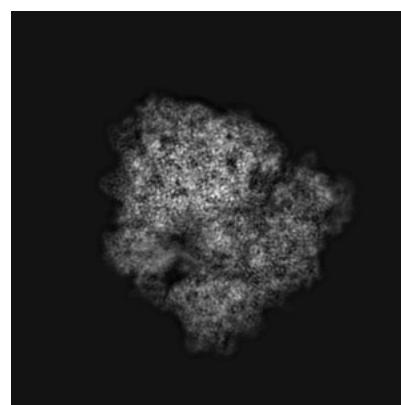
6.1.1 Primary map



X



Y

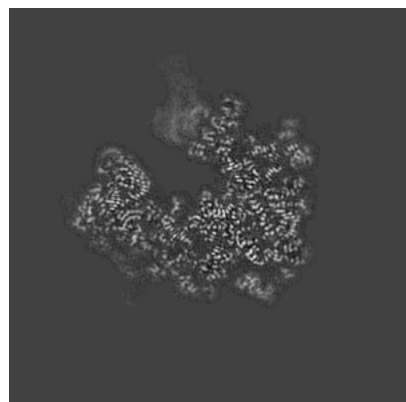


Z

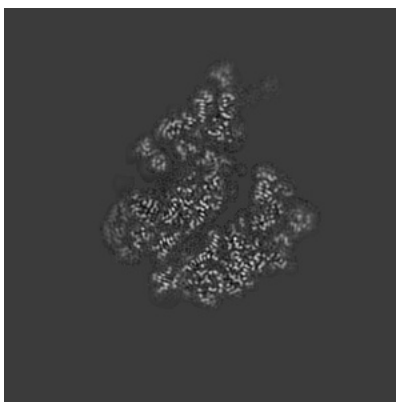
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

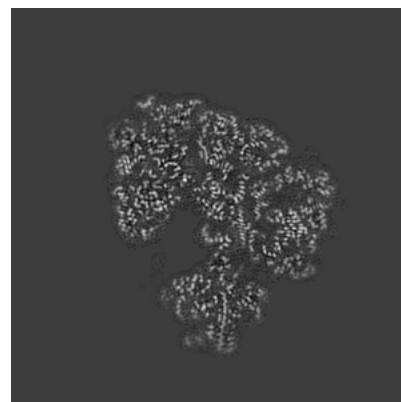
6.2.1 Primary map



X Index: 184



Y Index: 184

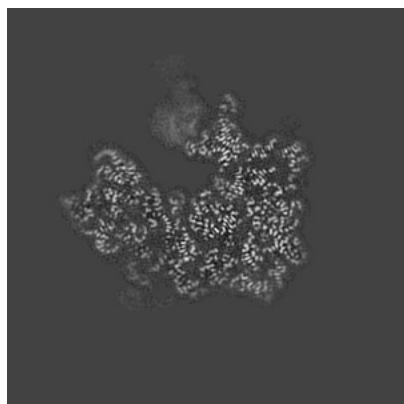


Z Index: 184

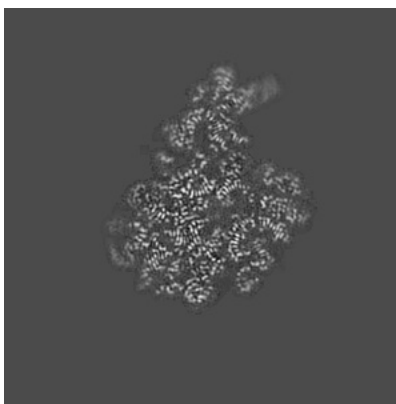
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

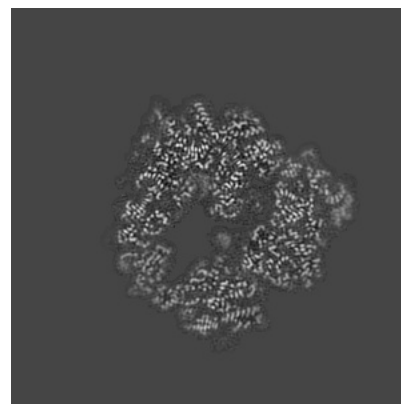
6.3.1 Primary map



X Index: 189



Y Index: 194

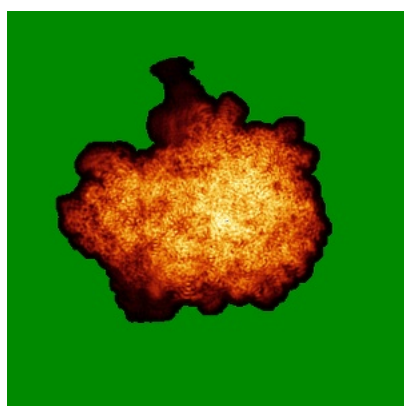


Z Index: 198

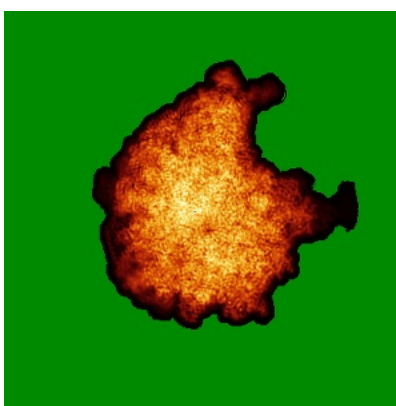
The images above show the largest variance slices of the map in three orthogonal directions.

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

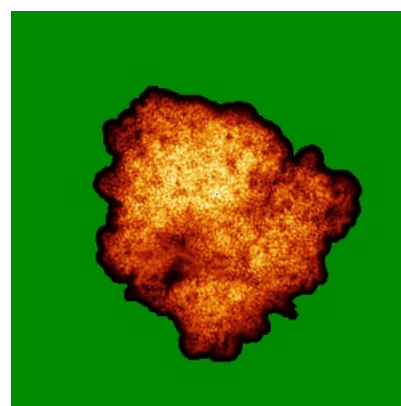
6.4.1 Primary map



X



Y

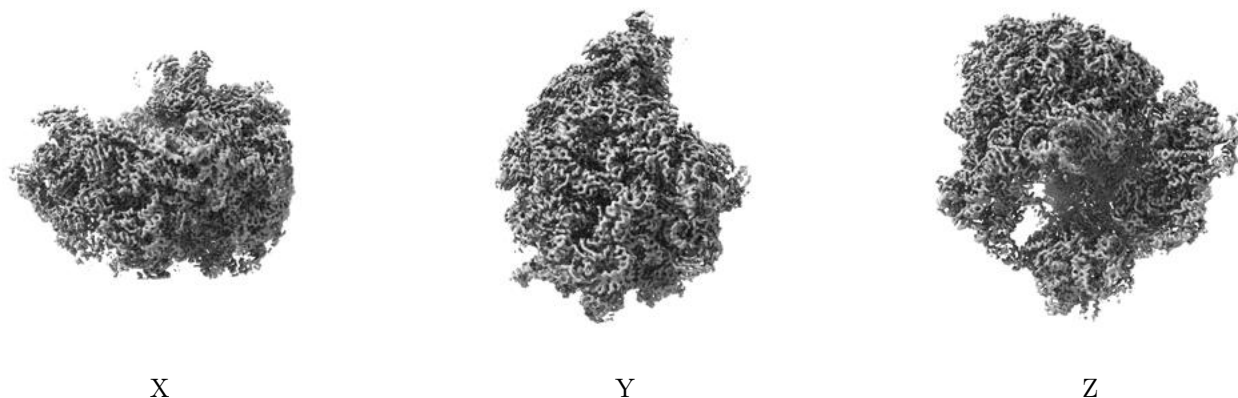


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

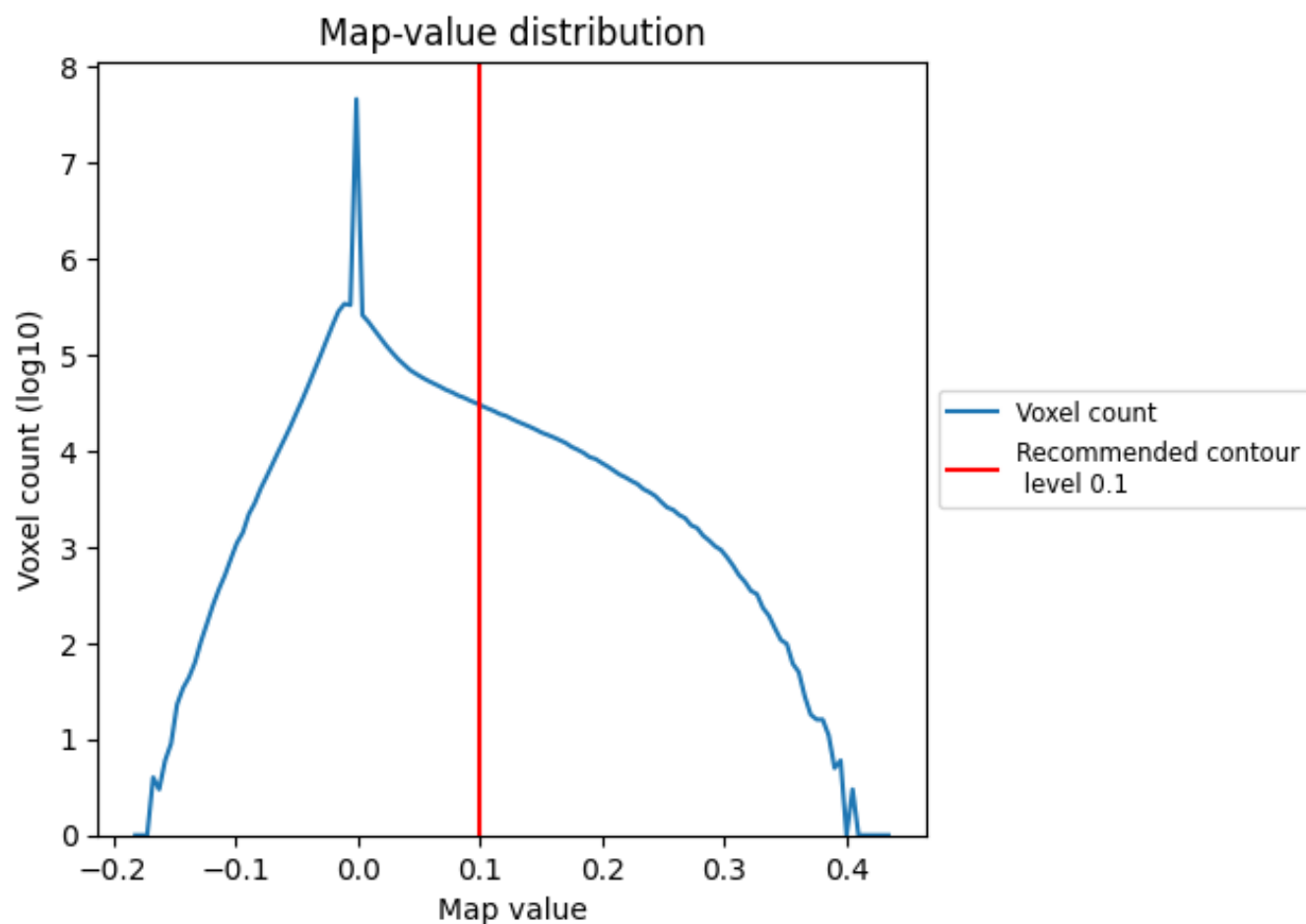
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

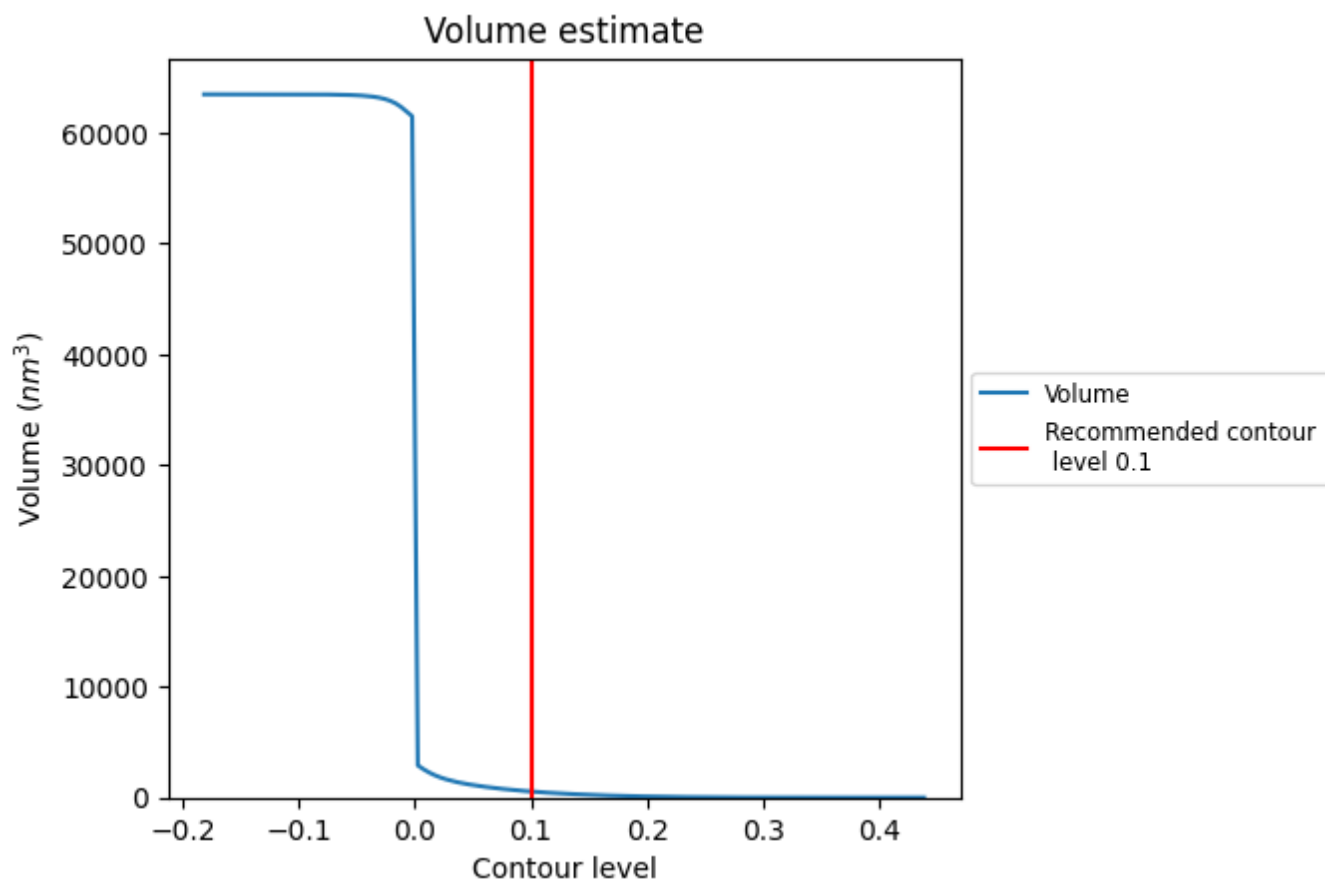
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

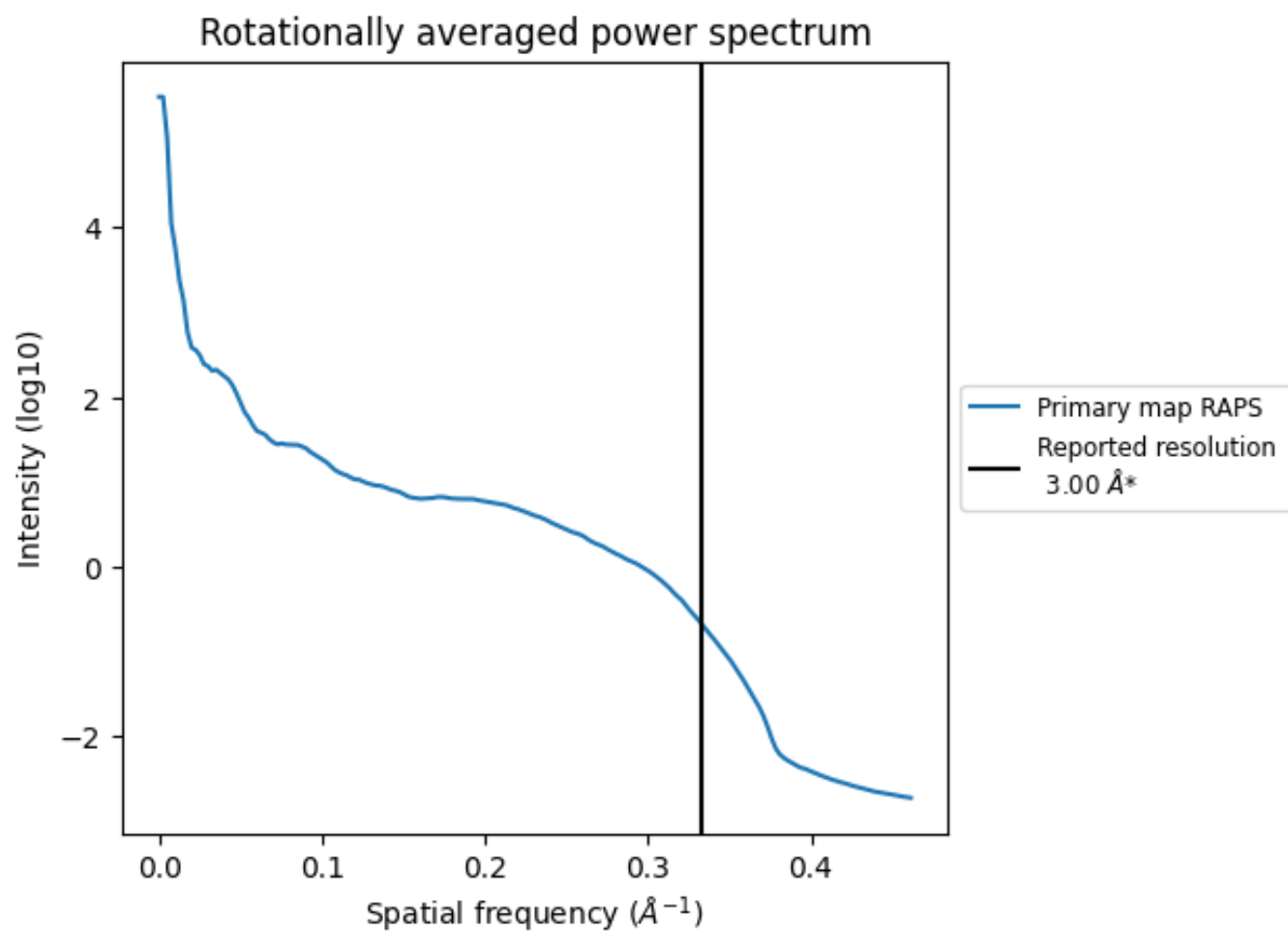
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 547 nm³; this corresponds to an approximate mass of 494 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

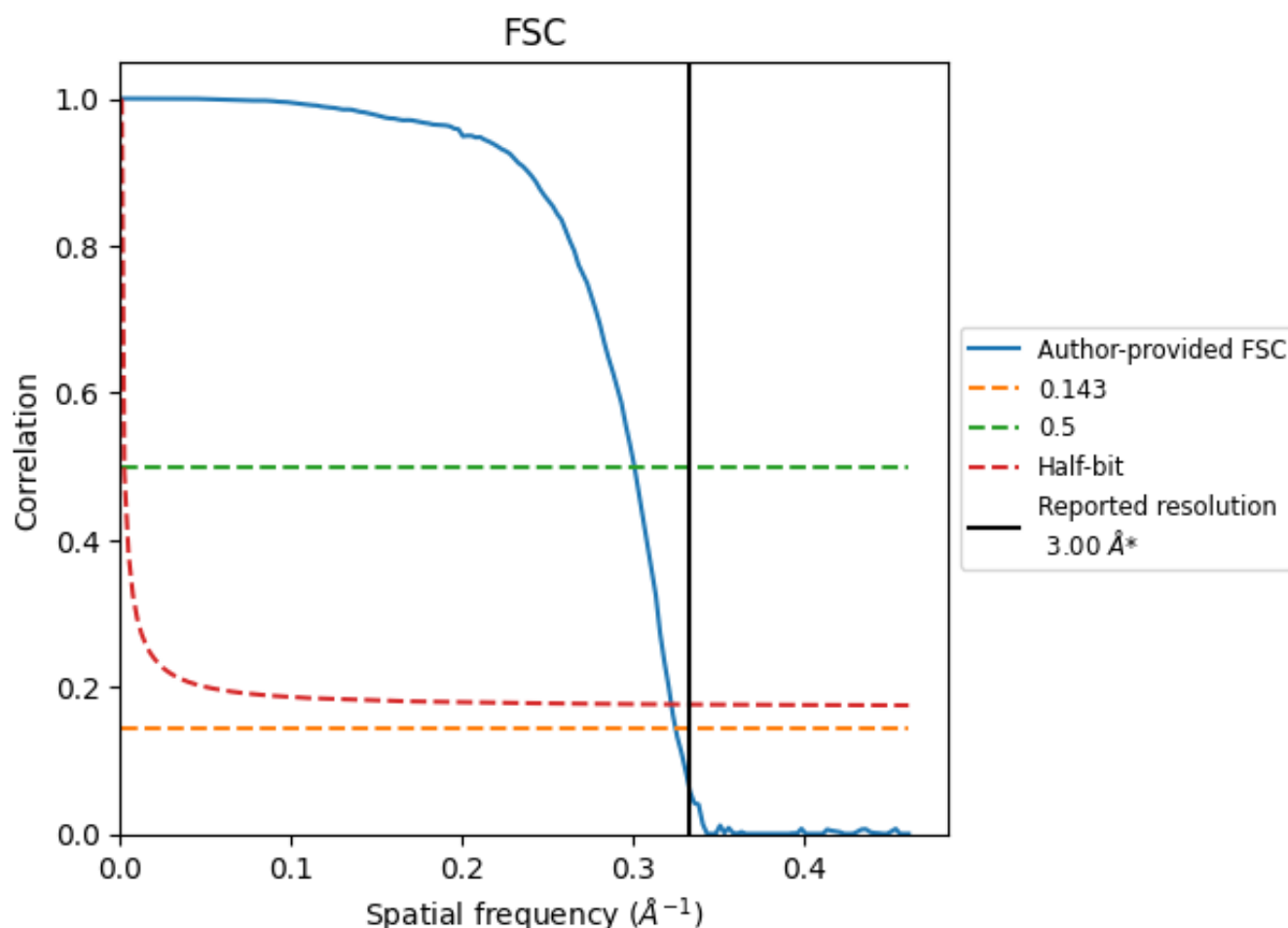


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

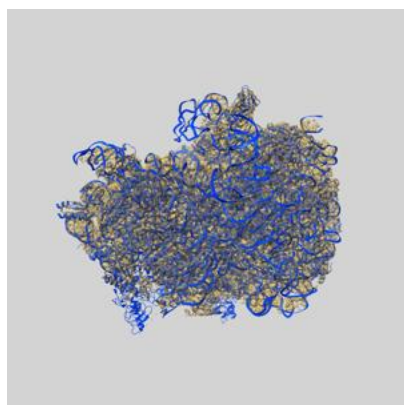
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.08	3.32	3.10
Unmasked-calculated*	-	-	-

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

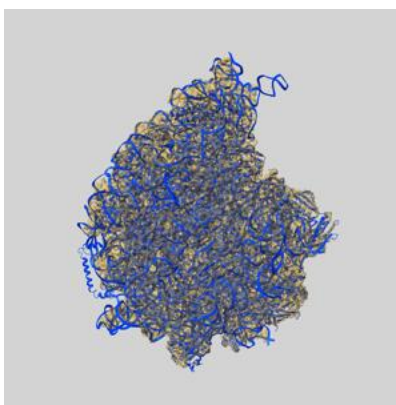
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0137 and PDB model 6H4N. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

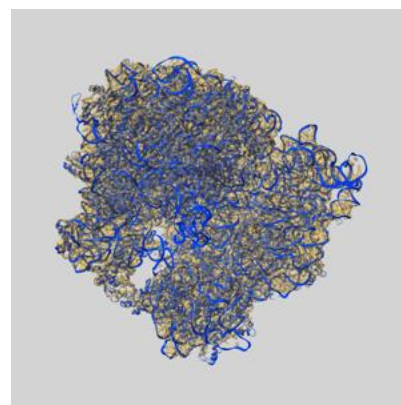
9.1 Map-model overlay [i](#)



X



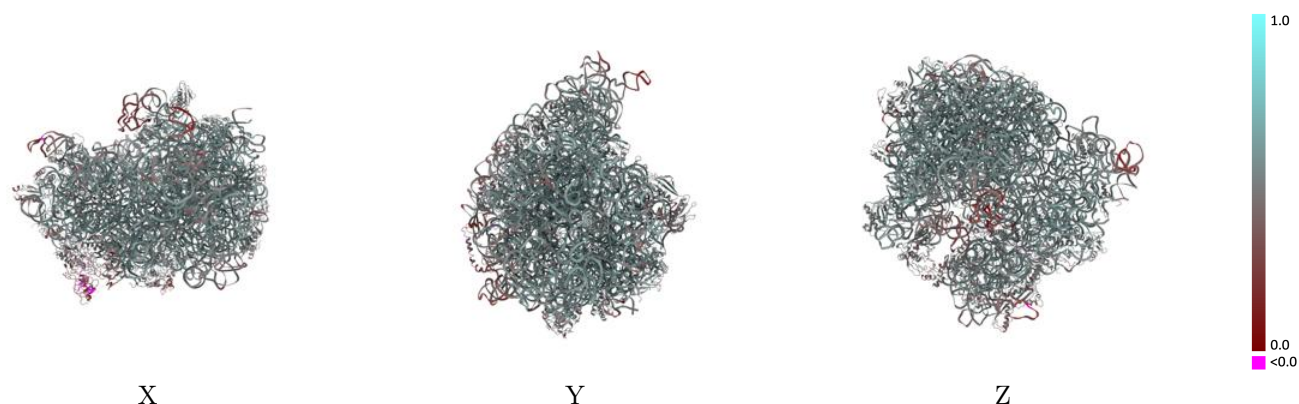
Y



Z

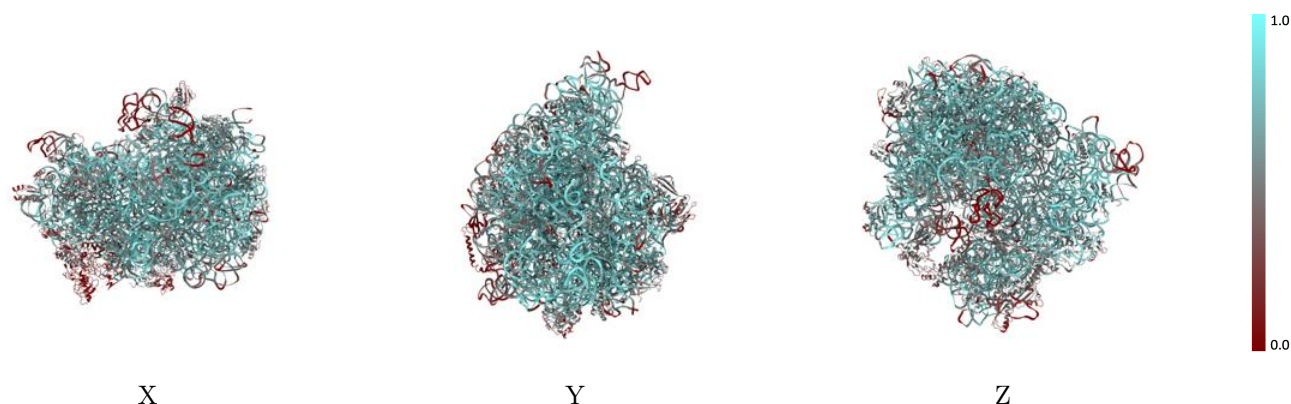
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



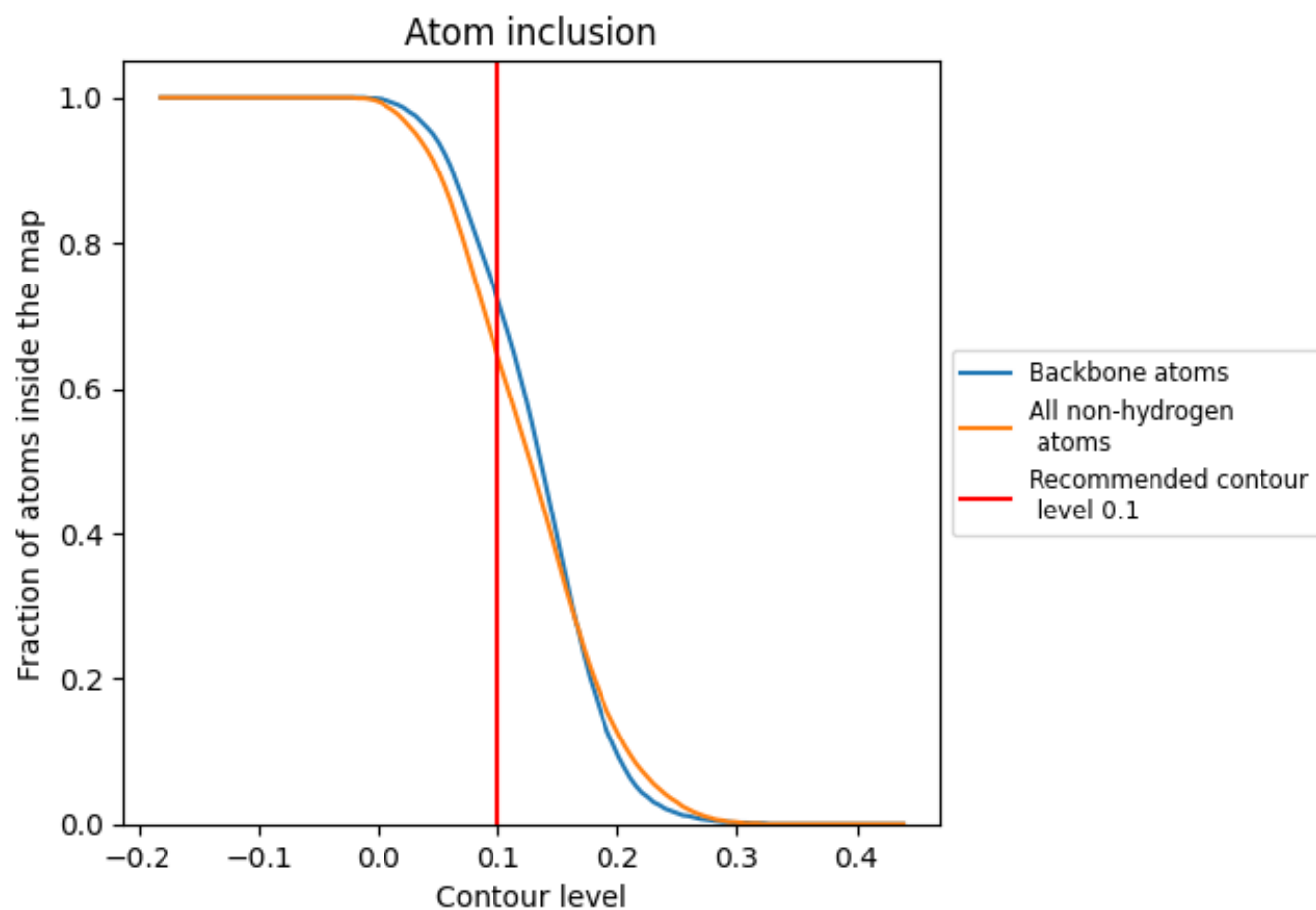
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 64% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6450	 0.5230
0	 0.5750	 0.5230
1	 0.5410	 0.5190
2	 0.6650	 0.5640
3	 0.6560	 0.5590
4	 0.5410	 0.5290
6	 0.2840	 0.4060
A	 0.7290	 0.5420
B	 0.7210	 0.5370
C	 0.6180	 0.5530
D	 0.5810	 0.5450
E	 0.4410	 0.4960
F	 0.4200	 0.4670
G	 0.3880	 0.4800
H	 0.0880	 0.3740
I	 0.0900	 0.4400
J	 0.5800	 0.5360
K	 0.5310	 0.5270
L	 0.5620	 0.5140
M	 0.5720	 0.5380
N	 0.6170	 0.5400
O	 0.5480	 0.5020
P	 0.5460	 0.5290
Q	 0.6490	 0.5450
R	 0.5410	 0.5150
S	 0.5350	 0.5190
T	 0.4830	 0.5070
U	 0.4210	 0.4860
V	 0.5260	 0.5110
W	 0.6280	 0.5570
X	 0.5620	 0.5380
Y	 0.4180	 0.4440
Z	 0.5680	 0.5360
a	 0.7440	 0.5430
b	 0.3470	 0.4460



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Chain	Atom inclusion	Q-score
c	 0.5040	 0.4930
d	 0.4790	 0.4900
e	 0.5560	 0.5140
f	 0.4810	 0.4620
g	 0.4300	 0.4610
h	 0.5410	 0.5210
i	 0.5000	 0.4820
j	 0.4180	 0.4640
k	 0.5100	 0.5010
l	 0.5400	 0.5230
m	 0.4430	 0.4640
n	 0.5250	 0.4920
o	 0.5380	 0.4940
p	 0.5490	 0.5030
q	 0.4450	 0.4920
r	 0.5790	 0.5260
s	 0.4830	 0.4860
t	 0.4950	 0.4880
u	 0.2710	 0.3150
v	 0.3320	 0.4630
w	 0.2500	 0.4010
x	 0.4890	 0.4810
y	 0.0060	 0.2690