



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:25 pm GMT

PDB ID : 6ENJ
EMDB ID : EMD-3899
Title : Polyproline-stalled ribosome in the presence of A+P site tRNA and elongation-factor P (EF-P)
Authors : Huter, P.; Wilson, D.N.
Deposited on : 2017-10-05
Resolution : 3.70 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:

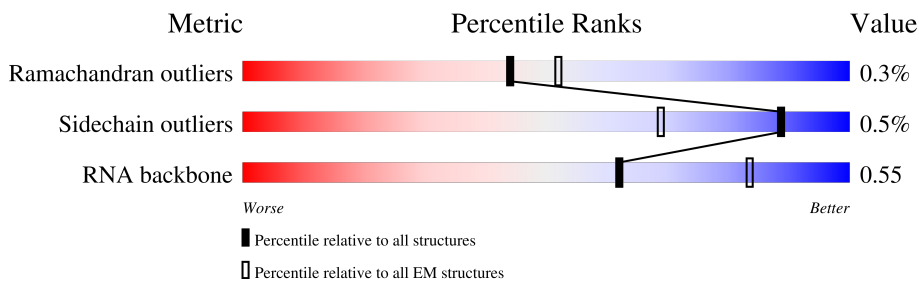
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 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	<div style="display: flex; align-items: center;"> <div style="width: 14%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: right; margin-right: 5px;">..</p>
2	B	120	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="text-align: right; margin-right: 5px;">.</p>
3	C	271	<div style="display: flex; align-items: center;"> <div style="width: 21%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 99%; height: 10px; background-color: green; margin-right: 5px;"></div> </div> <p style="text-align: right; margin-right: 5px;">.</p>
4	D	209	<div style="display: flex; align-items: center;"> <div style="width: 29%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 99%; height: 10px; background-color: green; margin-right: 5px;"></div> </div> <p style="text-align: right; margin-right: 5px;">.</p>
5	E	201	<div style="display: flex; align-items: center;"> <div style="width: 51%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 10px; background-color: green; margin-right: 5px;"></div> </div> <p style="text-align: right; margin-right: 5px;">.</p>
6	F	177	<div style="display: flex; align-items: center;"> <div style="width: 56%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 99%; height: 10px; background-color: green; margin-right: 5px;"></div> </div> <p style="text-align: right; margin-right: 5px;">.</p>
7	G	176	<div style="display: flex; align-items: center;"> <div style="width: 70%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 98%; height: 10px; background-color: green; margin-right: 5px;"></div> </div> <p style="text-align: right; margin-right: 5px;">.</p>
8	J	142	<div style="display: flex; align-items: center;"> <div style="width: 28%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 10px; background-color: green; margin-right: 5px;"></div> </div> <p style="text-align: right; margin-right: 5px;">.</p>

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Mol	Chain	Length	Quality of chain
9	K	122	33% 99%
10	L	143	41% 99%
11	M	136	32% 96%
12	N	120	18% 99%
13	O	116	46% 100%
14	P	114	41% 99%
15	Q	117	27% 100%
16	R	103	51% 97%
17	S	110	35% 99%
18	T	93	45% 100%
19	U	102	60% 97%
20	V	94	53% 100%
21	W	84	31% 99%
22	X	77	40% 99%
23	Y	63	62% 100%
24	Z	58	41% 100%
25	0	56	30% 100%
26	1	50	74% 100%
27	2	46	20% 100%
28	3	64	20% 95% 5%
29	4	38	37% 100%
30	6	66	86% 100%
31	a	1539	18% 80% 20%
32	b	218	67% 97%
33	c	206	49% 100%

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Mol	Chain	Length	Quality of chain
34	d	205	86% 98%
35	e	157	36% 99%
36	f	100	55% 98%
37	g	151	55% 100%
38	h	129	32% 100%
39	i	127	56% 98%
40	j	98	60% 99%
41	k	116	50% 99%
42	l	123	49% 98%
43	m	114	66% 97%
44	n	101	45% 100%
45	o	88	43% 100%
46	p	82	62% 99%
47	q	80	64% 96%
48	r	65	34% 100%
49	s	79	43% 100%
50	t	85	65% 100%
51	u	65	78% 100%
52	w	188	68% 97%
53	v	9	56% 44%
54	9	77	68% 58% 32% 9%
54	x	77	31% 74% 25%
55	7	224	99% 100%

2 Entry composition i

There are 56 unique types of molecules in this entry. The entry contains 147111 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 Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2871	61641	27498	11350	19922	2871	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 802133627
A	1847	G	A	conflict	GB 802133627
A	2069	A	G	conflict	GB 802133627
A	2104	U	C	conflict	GB 802133627

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

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

There is a discrepancy between the modelled and reference sequences:

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

- 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	176	1323	832	243	246	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L13.

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

- Molecule 9 is a protein called 50S ribosomal protein L14.

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

- Molecule 10 is a protein called 50S ribosomal protein L15.

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

- Molecule 11 is a protein called 50S ribosomal protein L16.

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

- Molecule 12 is a protein called 50S ribosomal protein L17.

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

- Molecule 13 is a protein called 50S ribosomal protein L18.

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

- Molecule 14 is a protein called 50S ribosomal protein L19.

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

- Molecule 15 is a protein called 50S ribosomal protein L20.

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

- Molecule 16 is a protein called 50S ribosomal protein L21.

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

- Molecule 17 is a protein called 50S ribosomal protein L22.

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

- Molecule 18 is a protein called 50S ribosomal protein L23.

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

- Molecule 19 is a protein called 50S ribosomal protein L24.

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

- Molecule 20 is a protein called 50S ribosomal protein L25.

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

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	84	637	394	129	113	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	6	GLY	ALA	conflict	UNP P0A7L8
W	7	LEU	GLY	conflict	UNP P0A7L8

- Molecule 22 is a protein called 50S ribosomal protein L28.

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

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

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

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

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

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace	
26	1	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 32 is a protein called 30S ribosomal protein S2.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 51 is a protein called 30S ribosomal protein S21.

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

- Molecule 52 is a protein called Elongation factor P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	w	188	1461	928	242	286	5	0	0

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	v	9	189	84	33	63	9	0	0

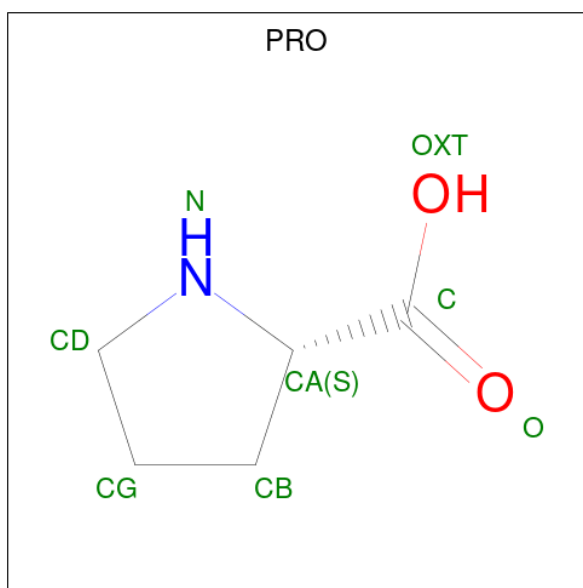
- Molecule 54 is a RNA chain called Proline tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	x	77	1646	733	295	541	77	0	0
54	9	77	1646	733	295	541	77	0	0

- Molecule 55 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	7	224	1663	1039	303	315	6	0	0

- Molecule 56 is PROLINE (three-letter code: PRO) (formula: C₅H₉NO₂).

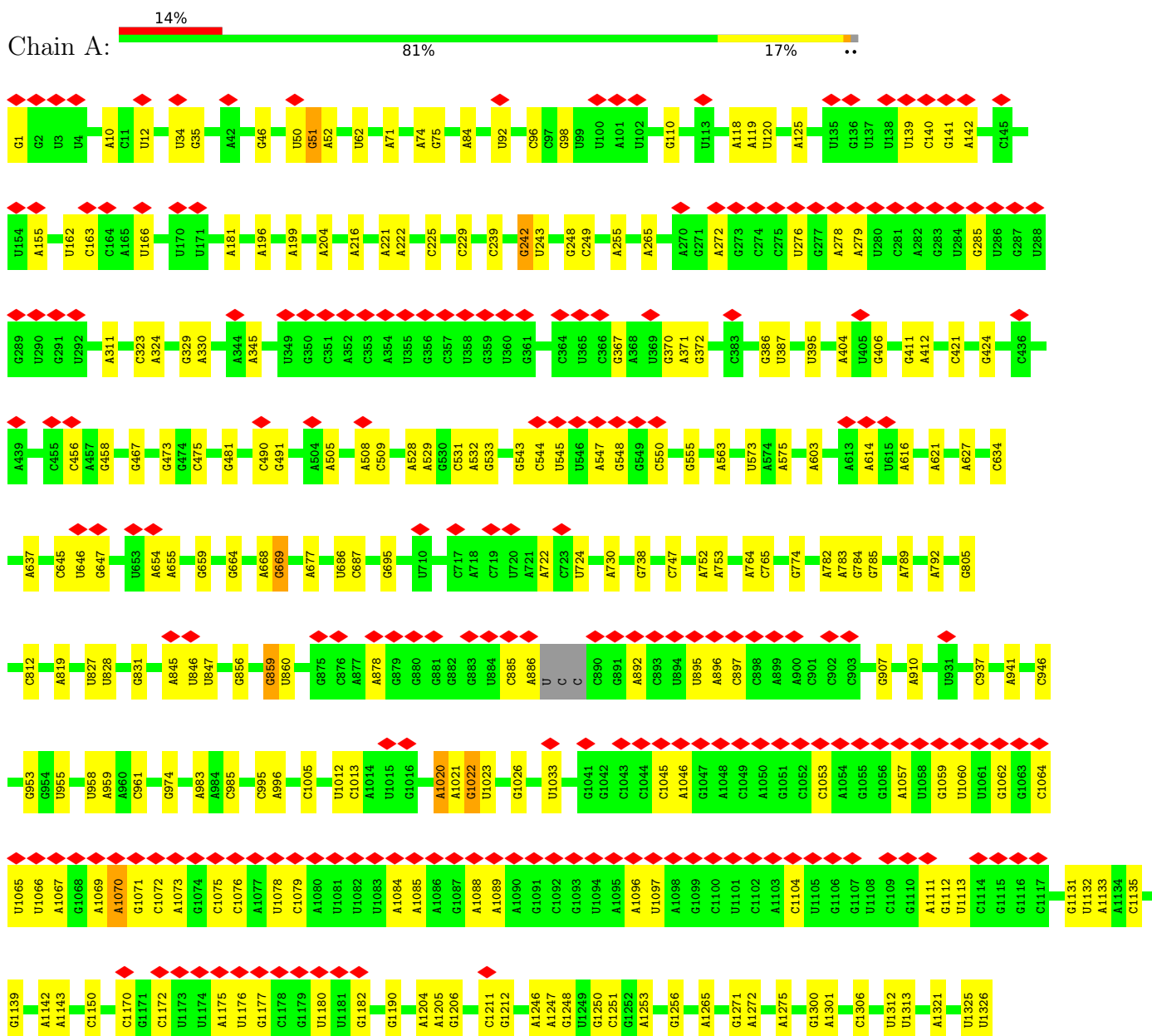


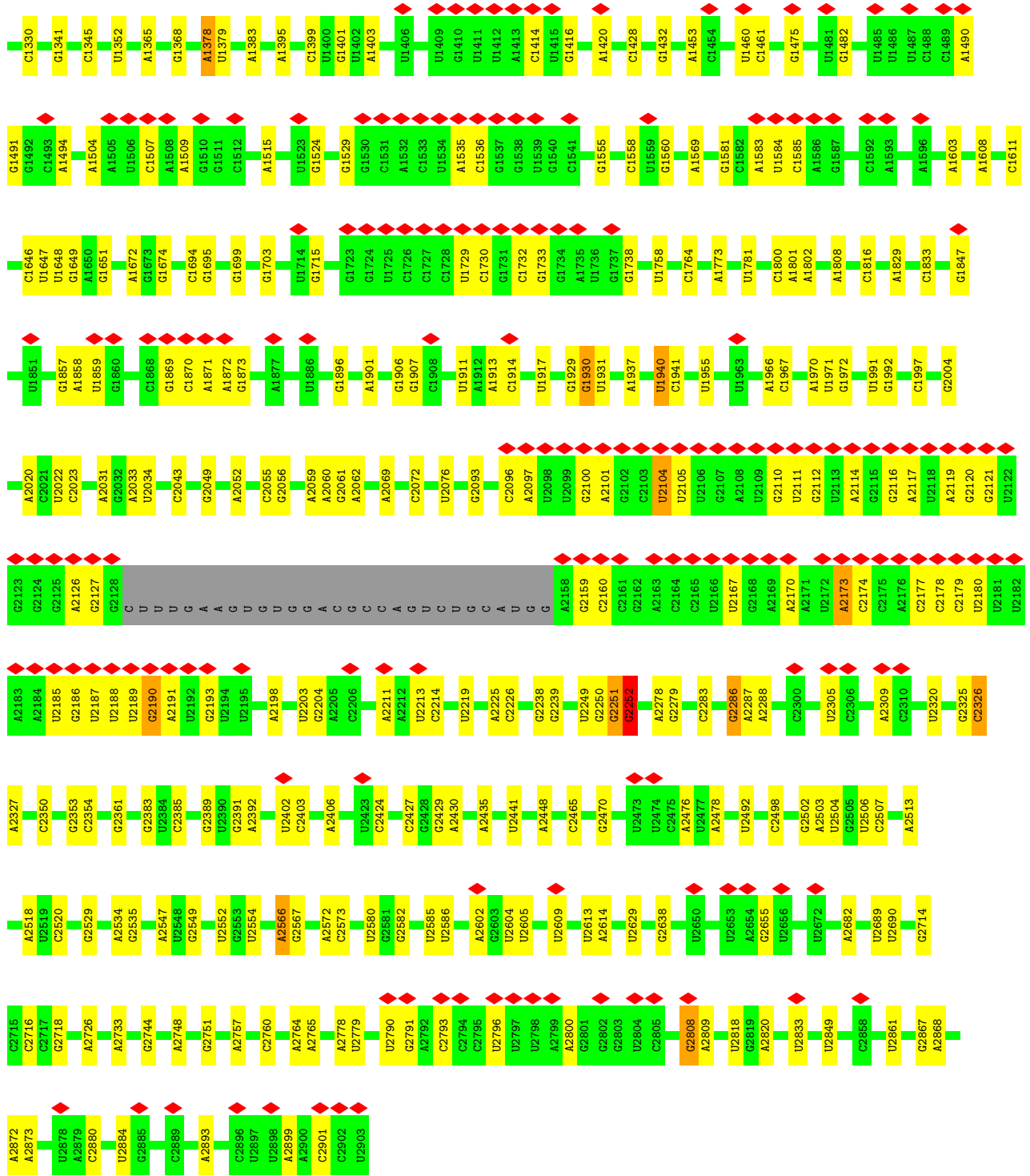
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
56	9	1	7	5	1	1	0

3 Residue-property plots

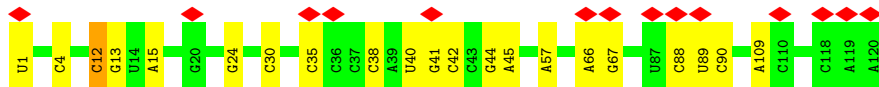
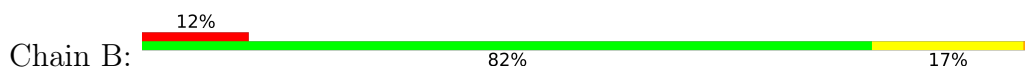
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 Ribosomal RNA

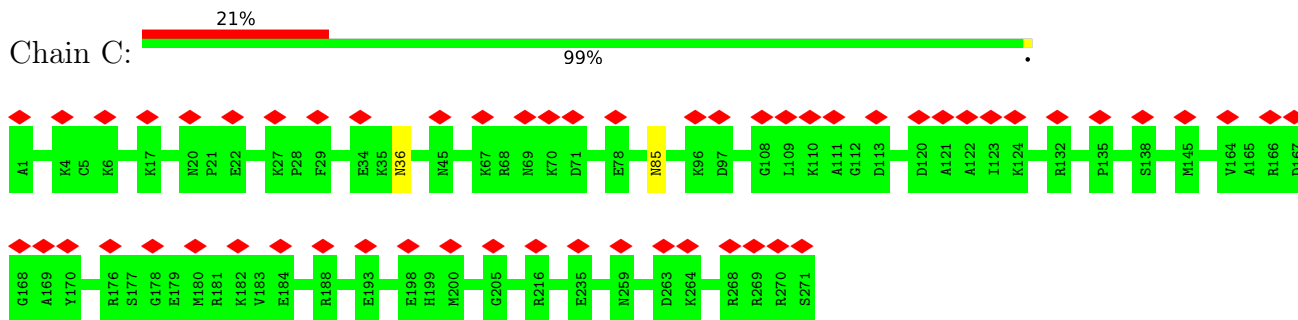




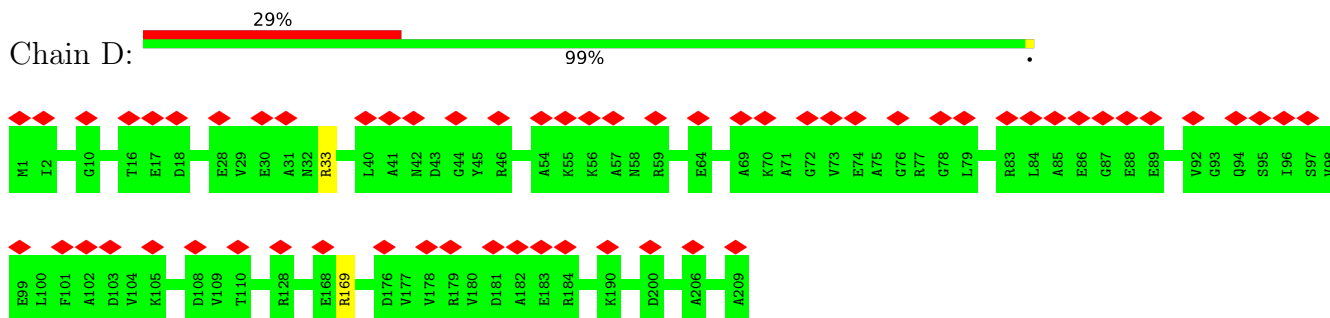
• Molecule 2: 5S Ribosomal RNA



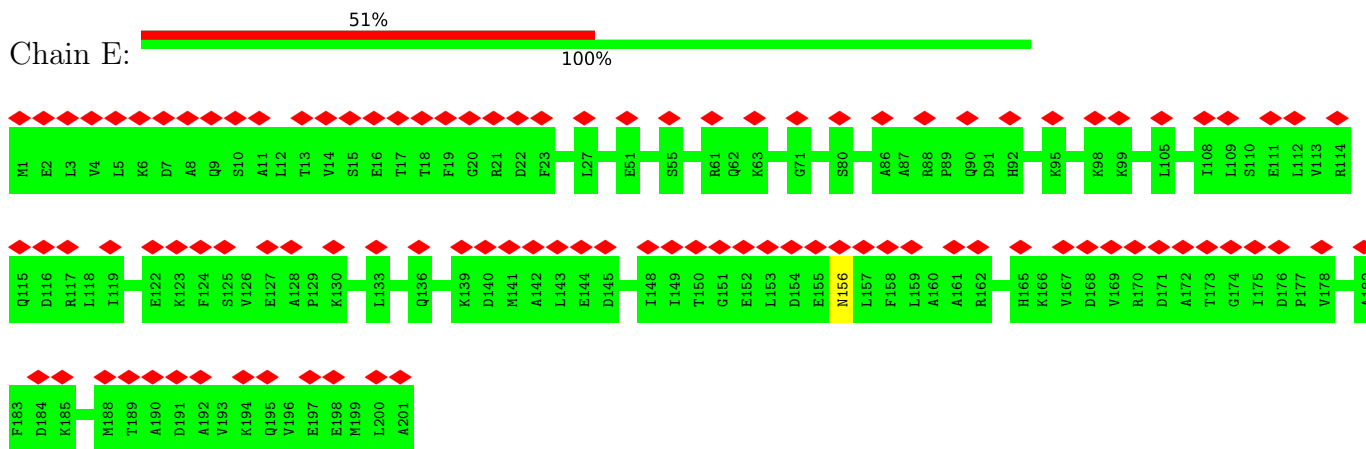
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3

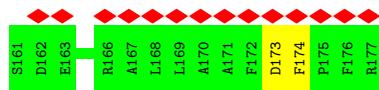


- Molecule 5: 50S ribosomal protein L4



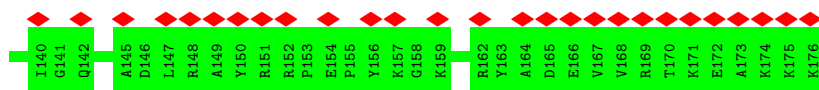
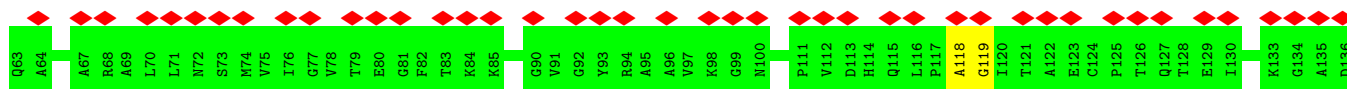
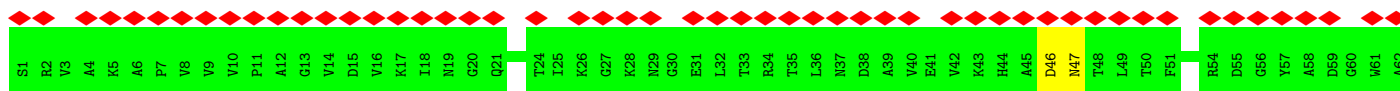
- Molecule 6: 50S ribosomal protein L5





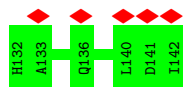
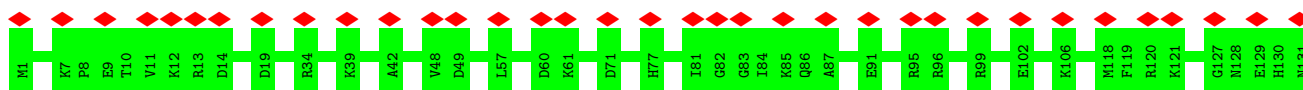
- Molecule 7: 50S ribosomal protein L6

Chain G: 70%
98%



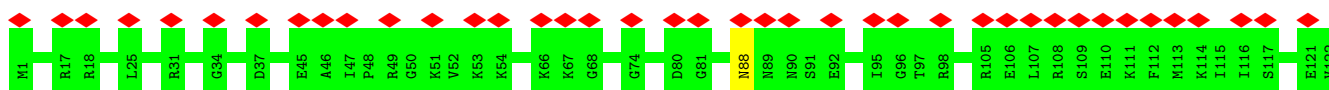
- Molecule 8: 50S ribosomal protein L13

Chain J: 28%
100%



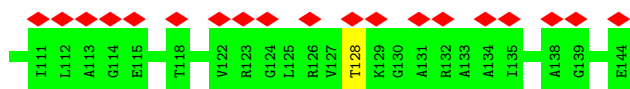
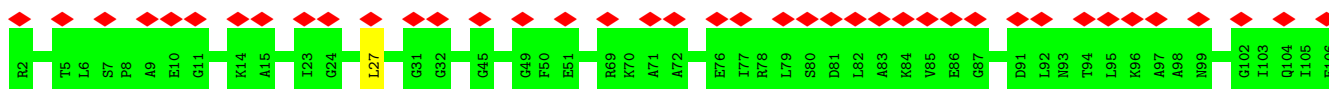
- Molecule 9: 50S ribosomal protein L14

Chain K: 33%
99%

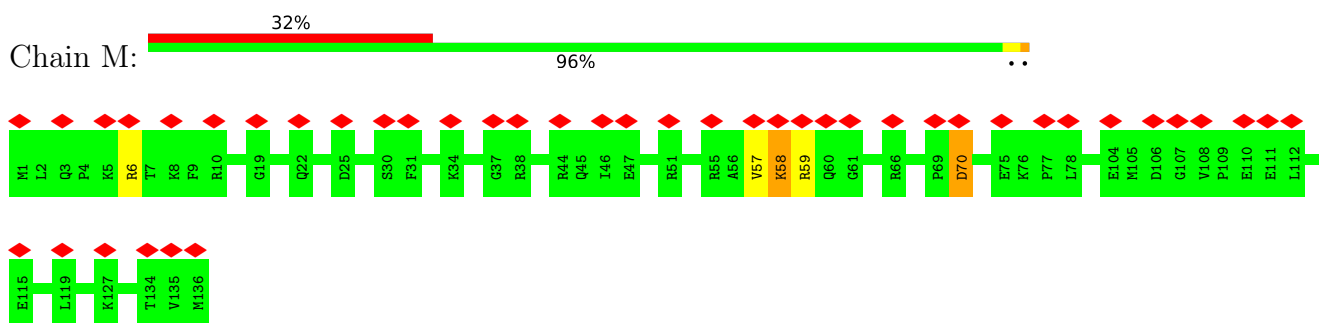


- Molecule 10: 50S ribosomal protein L15

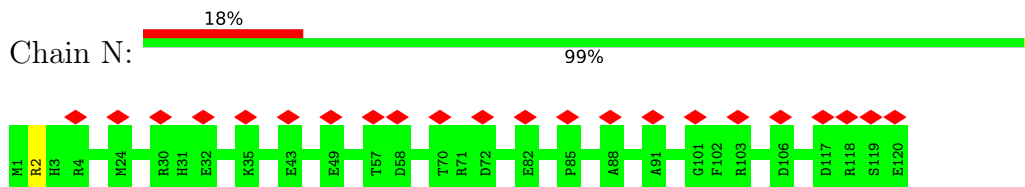
Chain L: 41%
99%



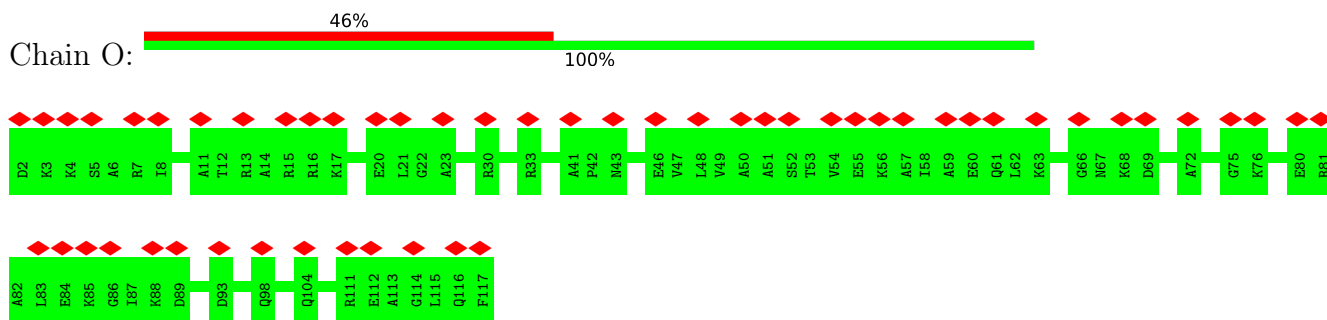
- Molecule 11: 50S ribosomal protein L16



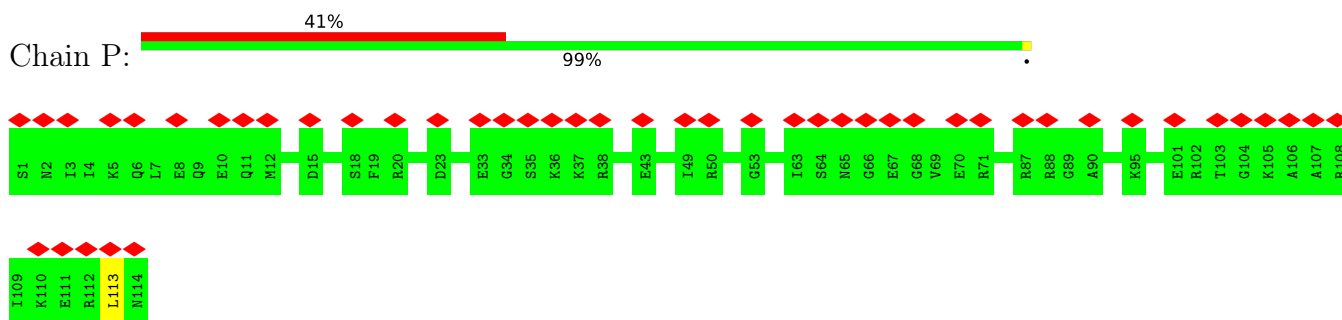
- Molecule 12: 50S ribosomal protein L17



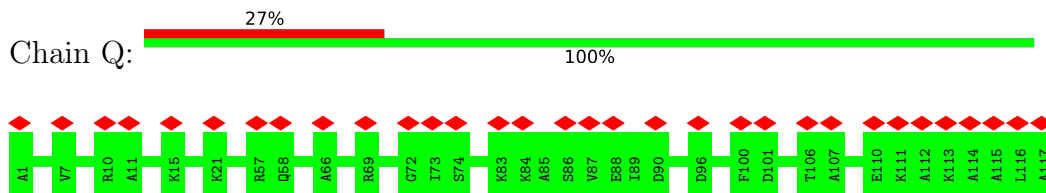
- Molecule 13: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L19

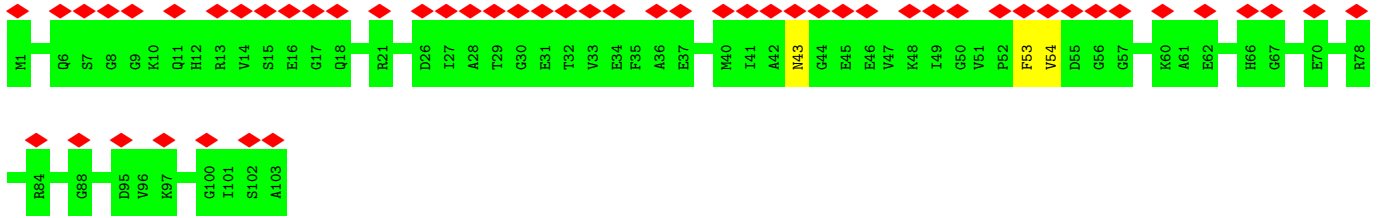


- Molecule 15: 50S ribosomal protein L20

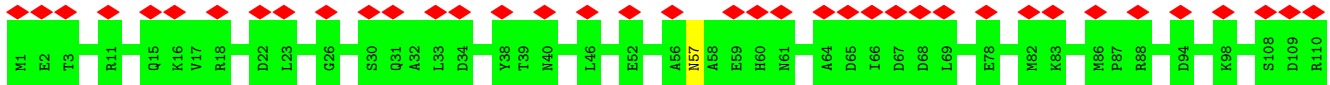


- Molecule 16: 50S ribosomal protein L21

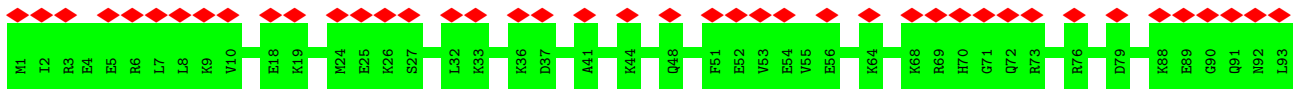




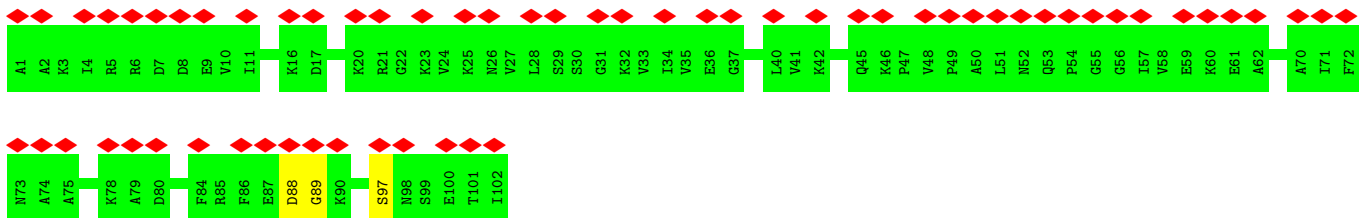
- Molecule 17: 50S ribosomal protein L22



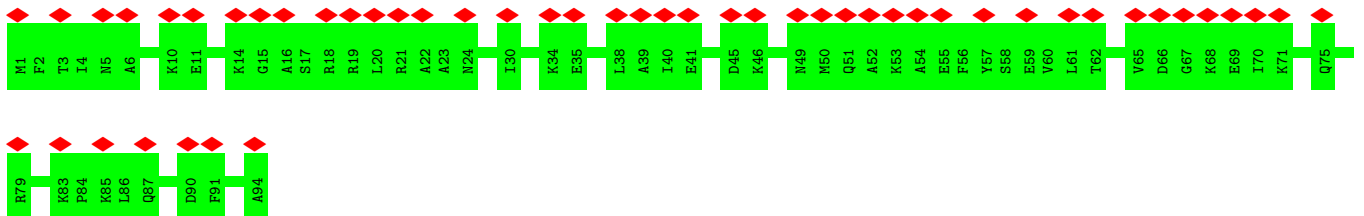
- Molecule 18: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L24

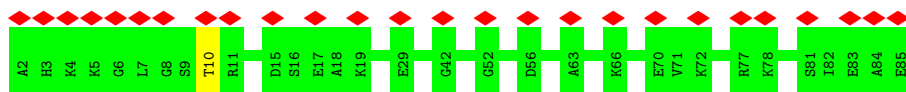


- Molecule 20: 50S ribosomal protein L25

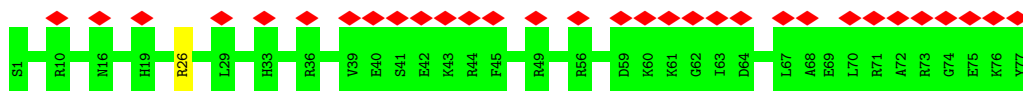
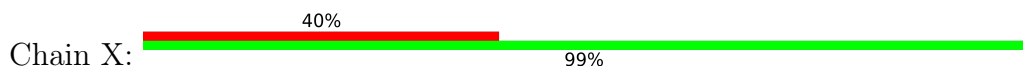


- Molecule 21: 50S ribosomal protein L27

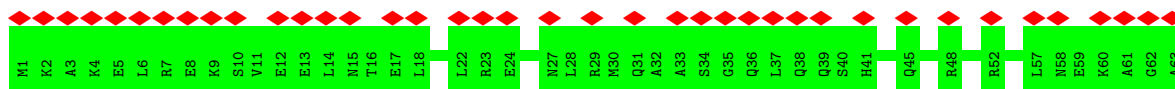




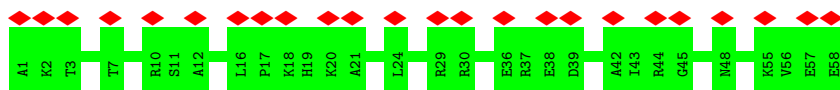
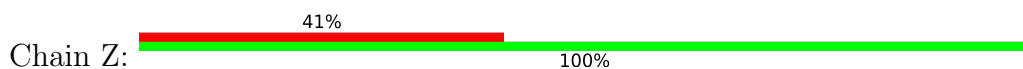
- Molecule 22: 50S ribosomal protein L28



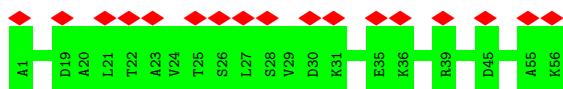
- Molecule 23: 50S ribosomal protein L29



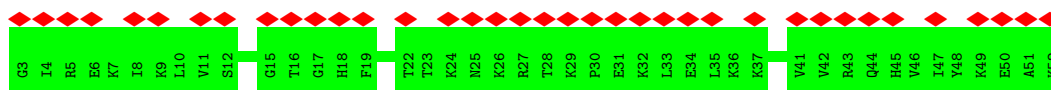
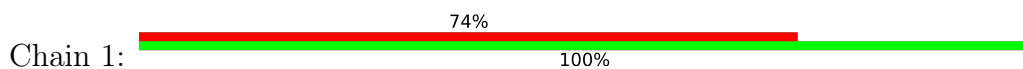
- Molecule 24: 50S ribosomal protein L30



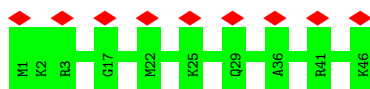
- Molecule 25: 50S ribosomal protein L32



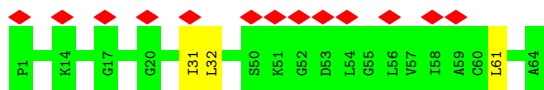
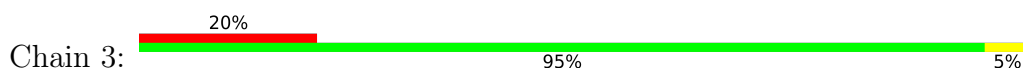
- Molecule 26: 50S ribosomal protein L33



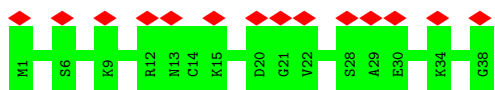
- Molecule 27: 50S ribosomal protein L34



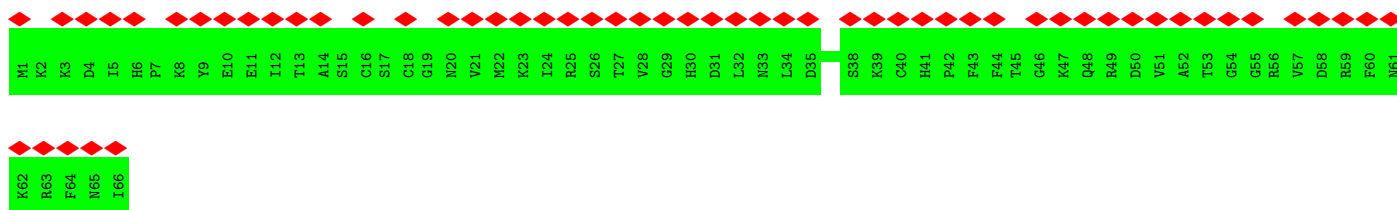
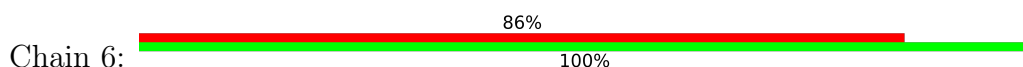
- Molecule 28: 50S ribosomal protein L35



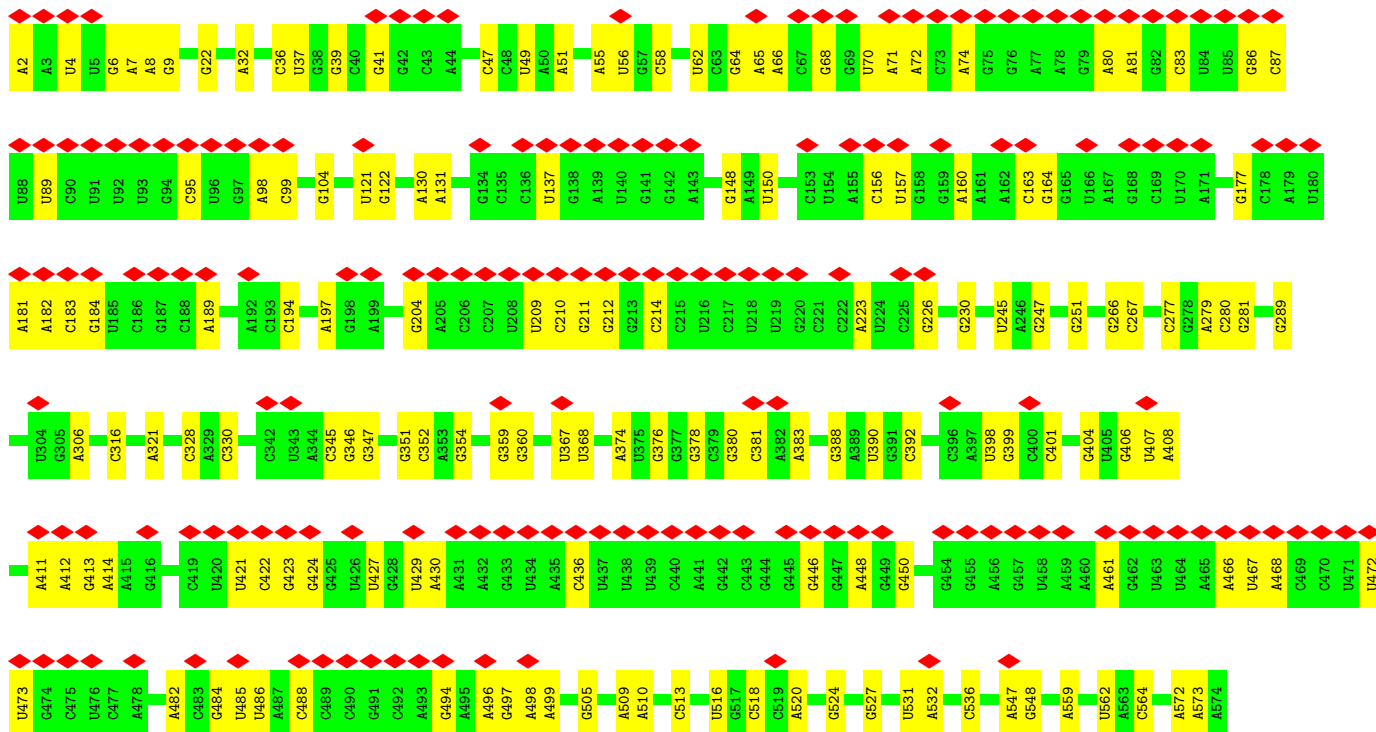
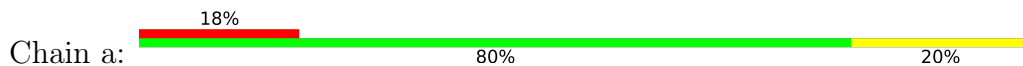
• Molecule 29: 50S ribosomal protein L36

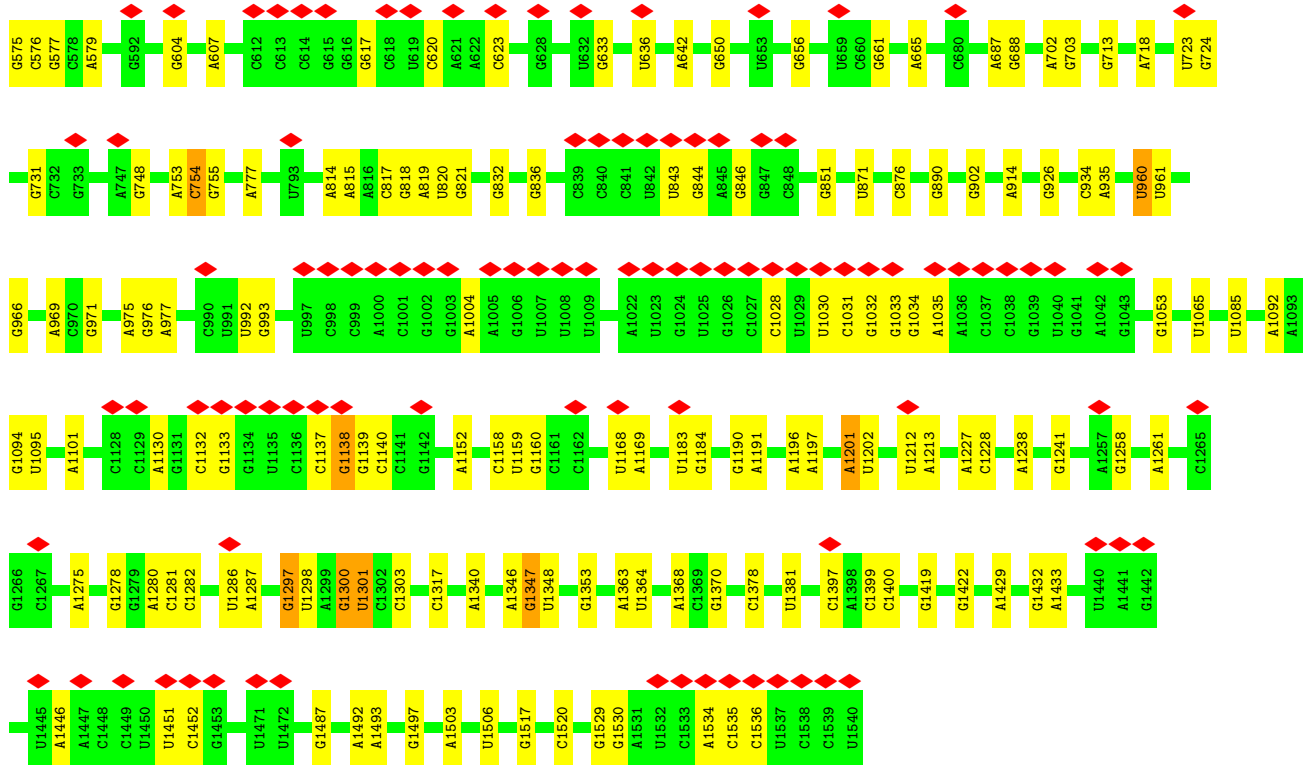


• Molecule 30: 50S ribosomal protein L31

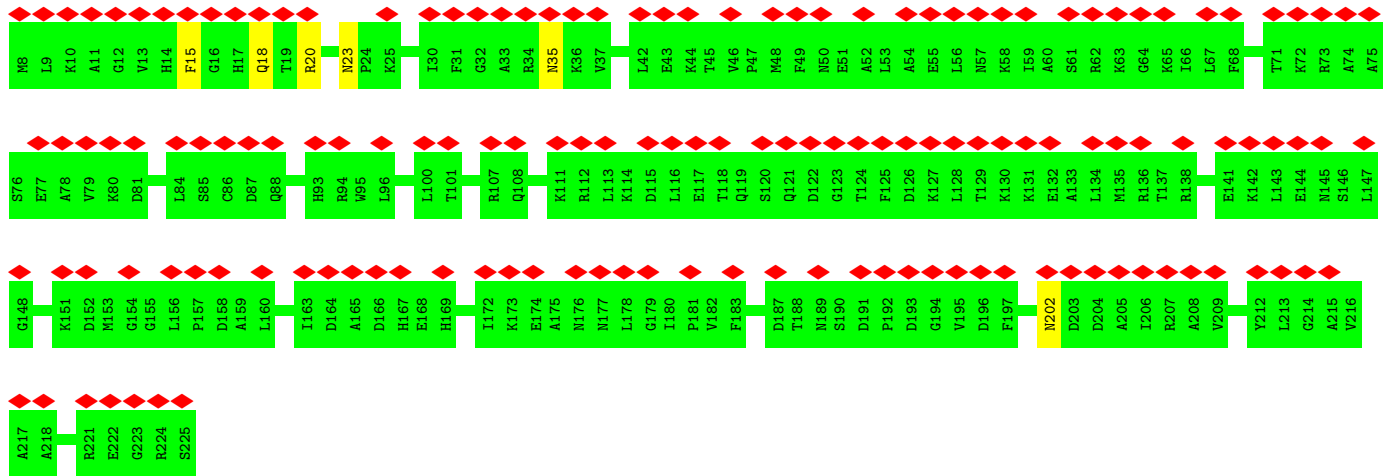


• Molecule 31: 16S ribosomal RNA

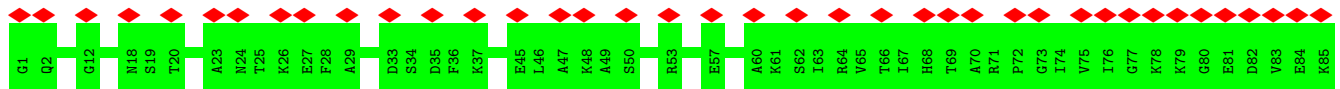


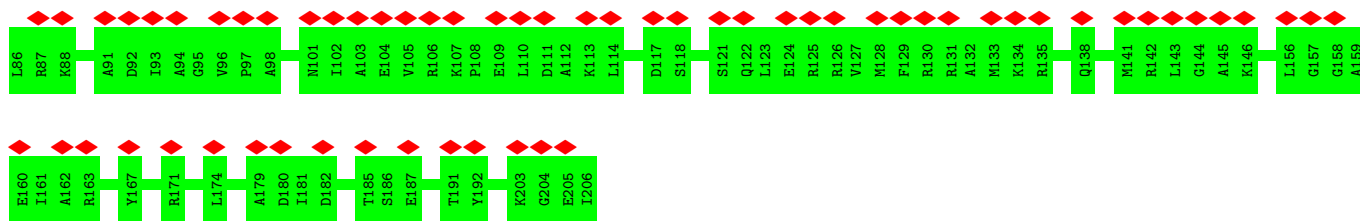


• Molecule 32: 30S ribosomal protein S2

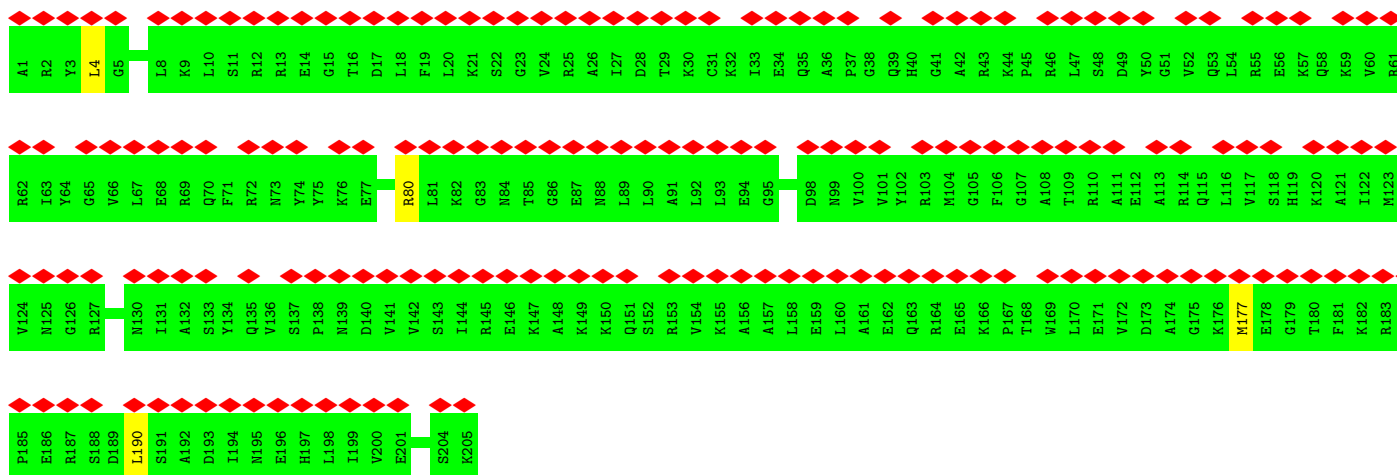
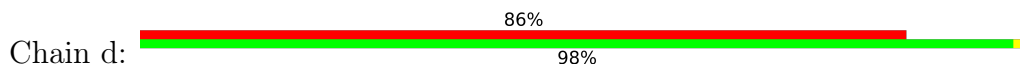


• Molecule 33: 30S ribosomal protein S3

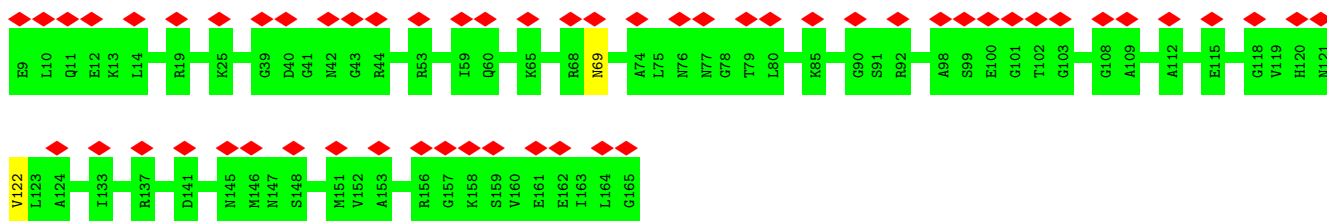




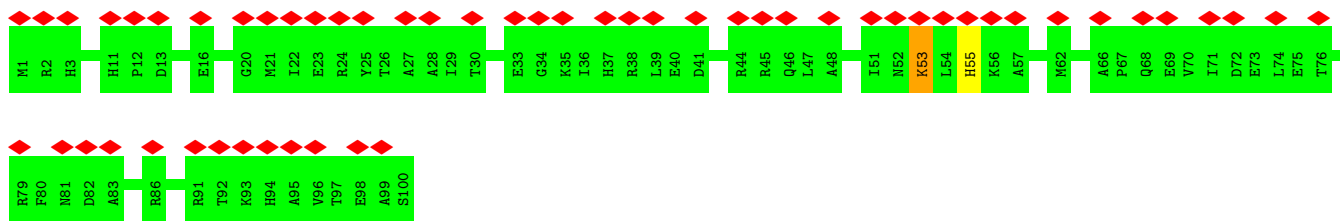
- Molecule 34: 30S ribosomal protein S4



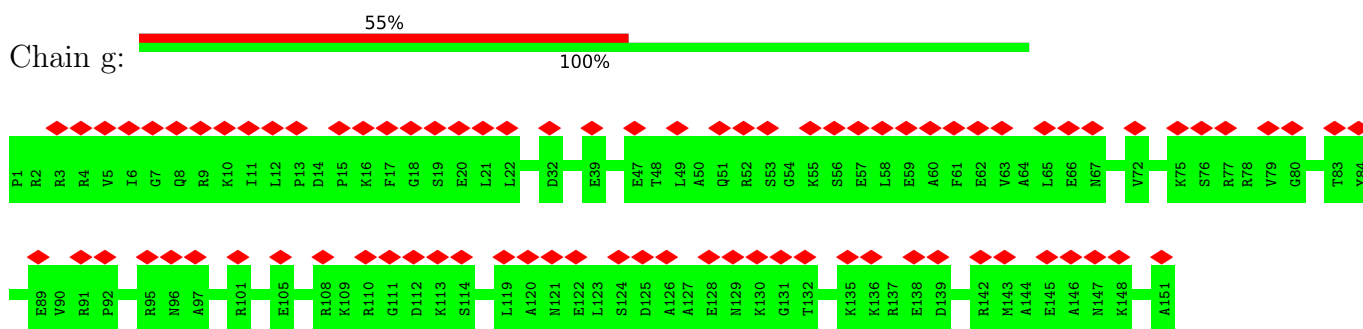
- Molecule 35: 30S ribosomal protein S5



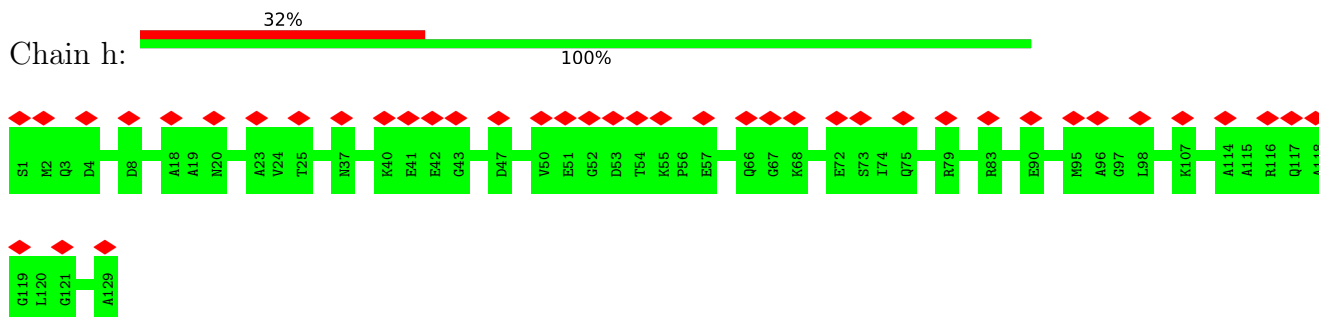
- Molecule 36: 30S ribosomal protein S6



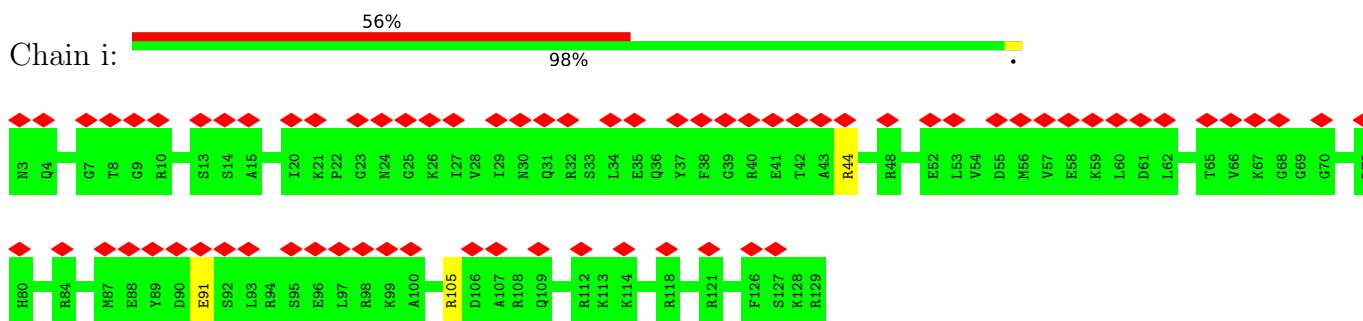
- Molecule 37: 30S ribosomal protein S7



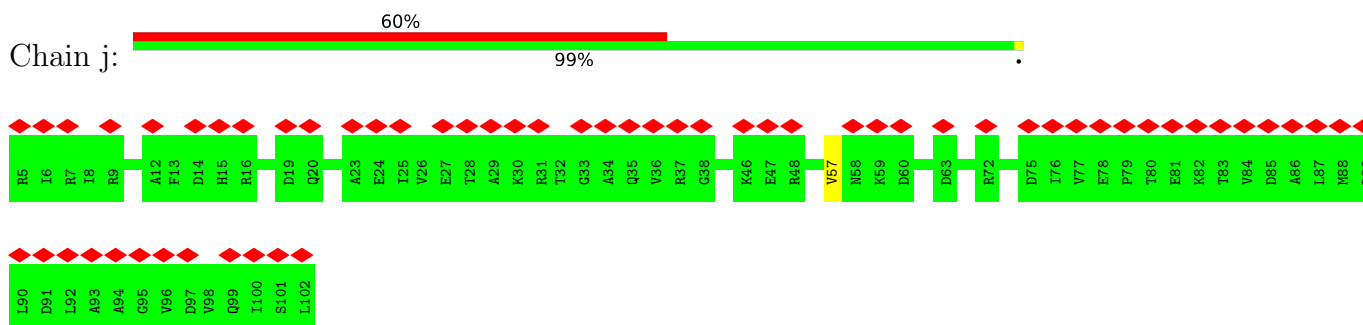
- Molecule 38: 30S ribosomal protein S8



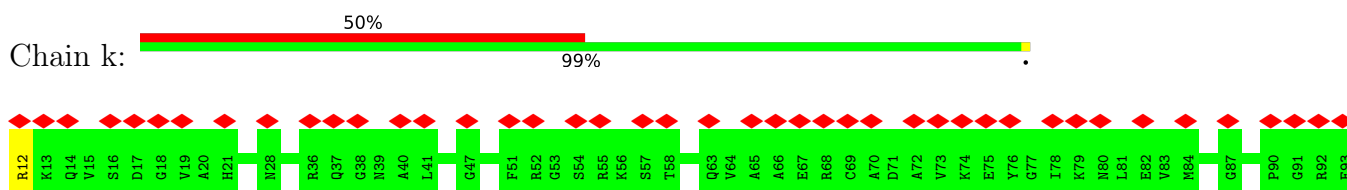
- Molecule 39: 30S ribosomal protein S9

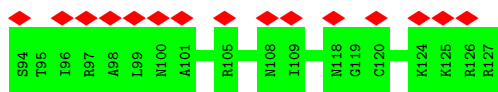


- Molecule 40: 30S ribosomal protein S10

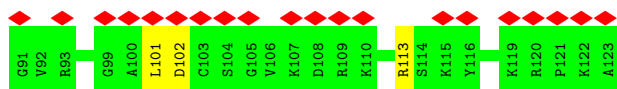


- Molecule 41: 30S ribosomal protein S11

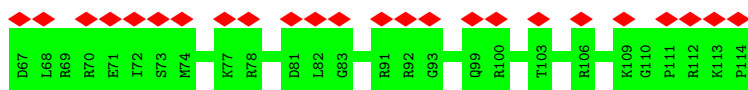
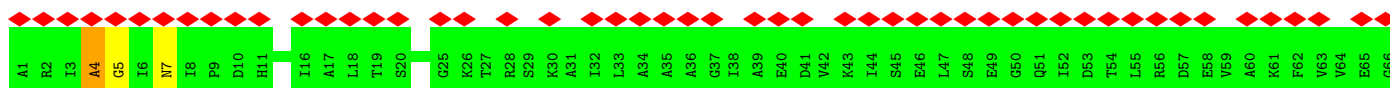




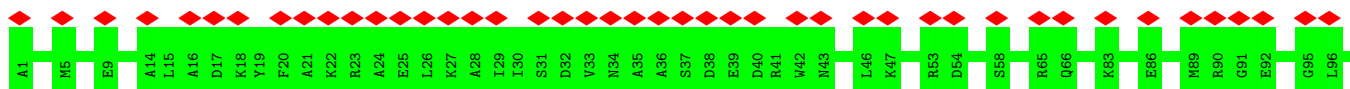
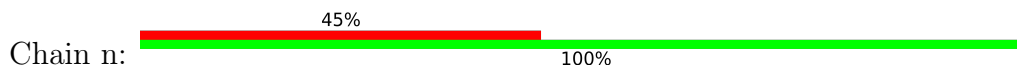
- Molecule 42: 30S ribosomal protein S12



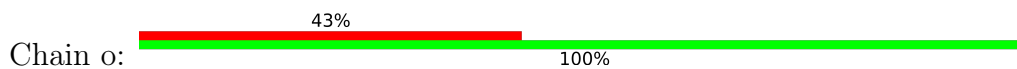
- Molecule 43: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S14

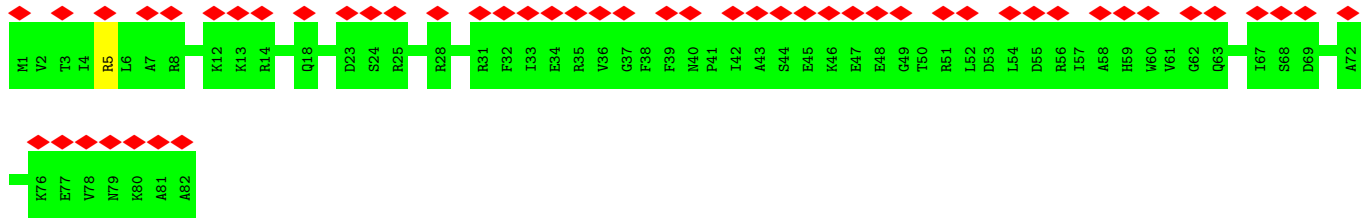


- Molecule 45: 30S ribosomal protein S15

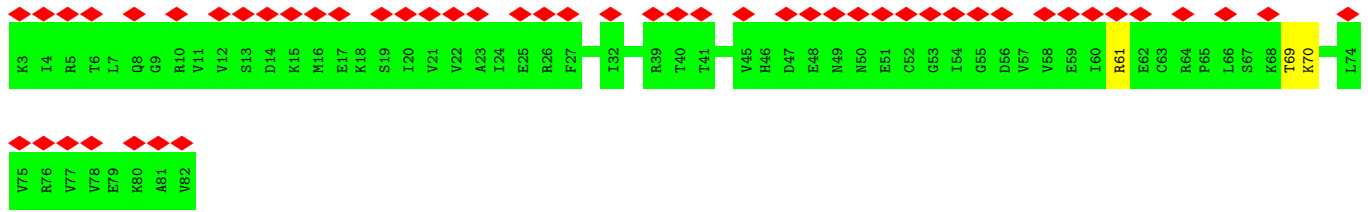


- Molecule 46: 30S ribosomal protein S16

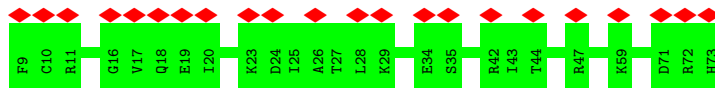




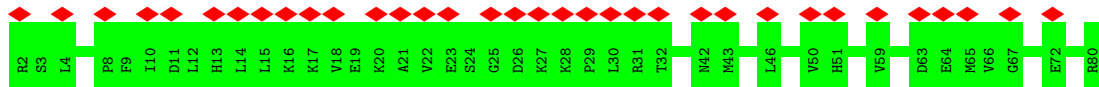
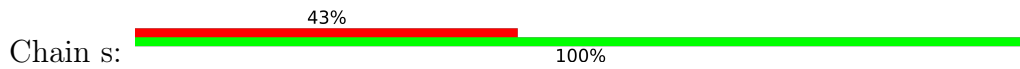
• Molecule 47: 30S ribosomal protein S17



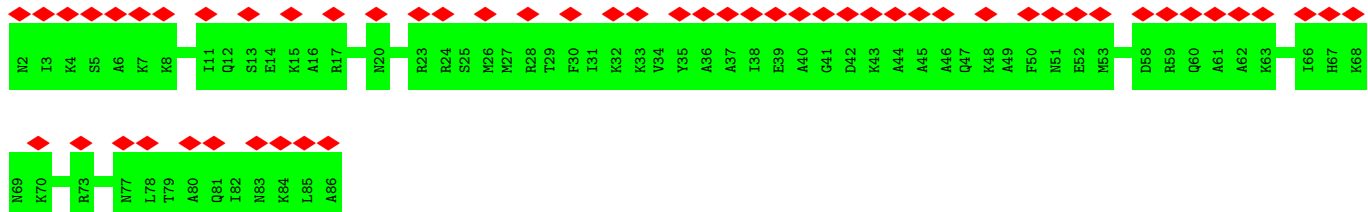
• Molecule 48: 30S ribosomal protein S18



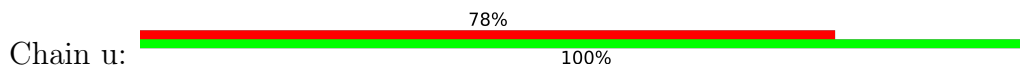
• Molecule 49: 30S ribosomal protein S19

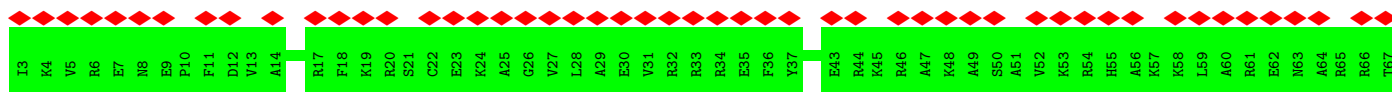


• Molecule 50: 30S ribosomal protein S20

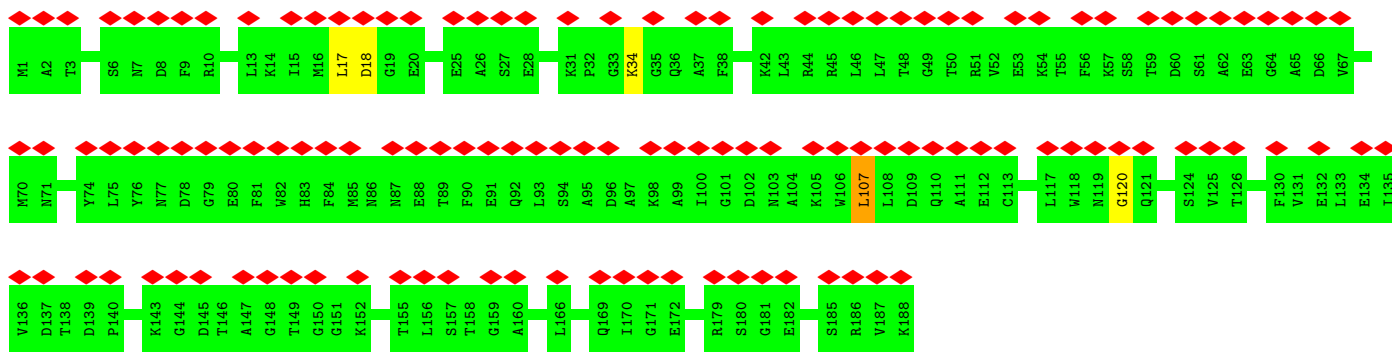


• Molecule 51: 30S ribosomal protein S21

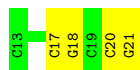




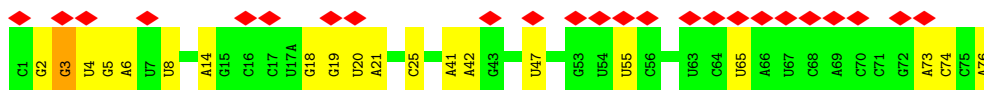
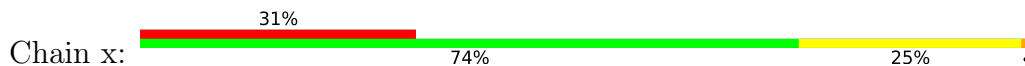
• Molecule 52: Elongation factor P



• Molecule 53: mRNA



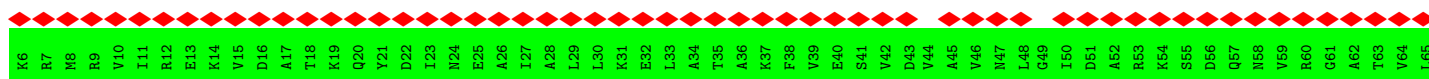
• Molecule 54: Proline tRNA



• Molecule 54: Proline tRNA



• Molecule 55: 50S ribosomal protein L1



P66	H67	G68	T69	G70	R71	S72	V73	R74	V75	A76	V77	F78	T79	Q80	G81	A82	N83	A84	E85	A86	A87	K88	A89	A90	G91	A92	E93	L94	V95	G96	M97	E98	D99	L100	A101	D102	Q103	I104	K105	K106	G107	E108	M109	M110	F111	D112	V113	V114	I115	A116	S117	P118	D119	A120	M121	R122	V123	V124	G125
Q126	L127	G128	Q129	V130	L131	G132	P133	R134	G135	L136	M137	P138	N139	P140	K141	V142	G143	T144	V145	T146	P147	N148	V149	A150	E151	A152	V153	K154	N155	A156	K157	A158	G159	Q160	V161	R162	Y163	R164	N165	D166	K167	N168	G169	I170	I171	H172	T173	T174	I175	G176	K177	V178	D179	F180	D181	A182	D183	K184	L185
K186	E187	N188	L189	E190	A191	L192	L193	V194	A195	L196	K197	K198	A199	K200	P201	T202	Q203	A204	K205	G206	V207	Y208	I209	K210	K211	V212	S213	I214	S215	T216	T217	M218	G219	A220	G221	V222	A223	V224	D225	Q226	A227	G228	L229																

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21655	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.443	Depositor
Minimum map value	-0.298	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0963	Depositor
Map size (\AA)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.084, 1.084, 1.084	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.21	3/69039 (0.0%)	0.81	49/107701 (0.0%)
2	B	0.27	1/2876 (0.0%)	0.82	2/4483 (0.0%)
3	C	0.25	0/2121	0.51	0/2852
4	D	0.26	0/1586	0.51	0/2134
5	E	0.25	0/1571	0.45	0/2113
6	F	0.28	0/1434	0.53	0/1926
7	G	0.25	0/1343	0.47	0/1816
8	J	0.25	0/1152	0.46	0/1551
9	K	0.26	0/947	0.54	0/1268
10	L	0.26	0/1054	0.58	0/1403
11	M	0.27	0/1093	0.54	1/1460 (0.1%)
12	N	0.26	0/973	0.52	0/1301
13	O	0.24	0/902	0.46	0/1209
14	P	0.25	0/929	0.50	1/1242 (0.1%)
15	Q	0.25	0/960	0.42	0/1278
16	R	0.26	0/829	0.51	0/1107
17	S	0.24	0/864	0.50	0/1156
18	T	0.24	0/744	0.50	0/994
19	U	0.27	0/787	0.53	0/1051
20	V	0.25	0/766	0.49	0/1025
21	W	0.57	1/645 (0.2%)	0.56	0/852
22	X	0.23	0/635	0.46	0/848
23	Y	0.22	0/510	0.44	0/677
24	Z	0.23	0/453	0.48	0/605
25	0	0.23	0/450	0.46	0/599
26	1	0.25	0/416	0.52	0/554
27	2	0.23	0/380	0.47	0/498
28	3	0.28	0/513	0.63	1/676 (0.1%)
29	4	0.25	0/303	0.54	0/397
30	6	0.25	0/531	0.49	0/709
31	a	0.20	1/36967 (0.0%)	0.80	23/57666 (0.0%)
32	b	0.27	0/1735	0.51	0/2338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.25	0/1651	0.50	0/2225
34	d	0.26	0/1665	0.59	2/2227 (0.1%)
35	e	0.28	0/1154	0.56	0/1554
36	f	0.27	0/835	0.57	0/1128
37	g	0.26	0/1195	0.54	0/1602
38	h	0.26	0/989	0.53	0/1326
39	i	0.28	0/1034	0.58	0/1375
40	j	0.26	0/796	0.60	0/1077
41	k	0.27	0/885	0.53	0/1195
42	l	0.28	0/969	0.58	0/1300
43	m	0.24	0/892	0.55	0/1193
44	n	0.23	0/811	0.49	0/1081
45	o	0.23	0/722	0.49	0/964
46	p	0.27	0/659	0.54	0/884
47	q	0.26	0/657	0.56	0/881
48	r	0.23	0/511	0.47	0/689
49	s	0.26	0/652	0.50	0/877
50	t	0.25	0/671	0.45	0/888
51	u	0.30	0/500	0.62	0/668
52	w	0.29	0/1470	0.69	2/1992 (0.1%)
53	v	0.31	0/209	1.14	3/323 (0.9%)
54	9	0.77	1/1839 (0.1%)	1.31	17/2866 (0.6%)
54	x	0.22	0/1838	0.82	4/2862 (0.1%)
55	7	0.25	0/1672	0.48	0/2244
All	All	0.24	7/159784 (0.0%)	0.75	105/238910 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
6	F	0	2
7	G	0	2
9	K	0	1
11	M	0	2
16	R	0	1
19	U	0	2
32	b	0	2
36	f	0	1
40	j	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	l	0	1
43	m	0	1
47	q	0	1
52	w	0	2
All	All	0	20

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2252	G	O3'-P	-11.54	1.47	1.61
1	A	1	G	OP3-P	-10.64	1.48	1.61
31	a	2	A	OP3-P	-10.62	1.48	1.61
54	9	76	A	C3'-O3'	-10.58	1.27	1.42
2	B	1	U	OP3-P	-10.53	1.48	1.61
21	W	10	THR	C-N	-10.03	1.10	1.34
1	A	2252	G	C3'-O3'	-5.72	1.34	1.42

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1158	C	N1-C2-O2	8.85	124.21	118.90
31	a	1158	C	C2-N1-C1'	8.72	128.39	118.80
1	A	1313	U	C2-N1-C1'	8.45	127.84	117.70
54	9	74	C	N1-C2-O2	8.27	123.86	118.90
1	A	1313	U	N1-C2-O2	7.99	128.39	122.80
1	A	955	U	C2-N1-C1'	7.50	126.70	117.70
1	A	1313	U	N3-C2-O2	-7.46	116.98	122.20
1	A	1070	A	OP2-P-O3'	7.18	121.00	105.20
52	w	107	LEU	CA-CB-CG	7.07	131.56	115.30
31	a	1158	C	N3-C2-O2	-7.07	116.95	121.90
54	9	74	C	C2-N1-C1'	6.82	126.31	118.80
53	v	20	C	C6-N1-C2	-6.78	117.59	120.30
1	A	2252	G	C2'-C3'-O3'	-6.78	94.59	109.50
1	A	1070	A	P-O3'-C3'	6.77	127.83	119.70
1	A	1022	G	P-O3'-C3'	6.75	127.79	119.70
54	9	3	G	P-O3'-C3'	6.67	127.71	119.70
1	A	1020	A	P-O3'-C3'	6.66	127.69	119.70
1	A	1917	U	C2-N1-C1'	6.64	125.67	117.70
1	A	1378	A	P-O3'-C3'	6.64	127.67	119.70
31	a	1297	G	P-O3'-C3'	6.63	127.65	119.70
1	A	242	G	P-O3'-C3'	6.61	127.64	119.70
31	a	754	C	C2-N1-C1'	6.58	126.04	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	9	74	C	N3-C2-O2	-6.56	117.31	121.90
1	A	2251	G	C2'-C3'-O3'	6.56	124.19	113.70
31	a	1201	A	P-O3'-C3'	6.51	127.51	119.70
31	a	1138	G	C4-N9-C1'	6.46	134.90	126.50
1	A	955	U	N3-C2-O2	-6.38	117.74	122.20
1	A	669	G	C4-N9-C1'	6.37	134.78	126.50
54	9	2	G	P-O3'-C3'	6.31	127.27	119.70
31	a	1347	G	P-O3'-C3'	6.29	127.25	119.70
31	a	1138	G	N3-C4-C5	-6.24	125.48	128.60
1	A	51	G	P-O3'-C3'	6.23	127.18	119.70
1	A	2251	G	N9-C1'-C2'	6.19	122.05	114.00
31	a	1138	G	N3-C4-N9	6.14	129.69	126.00
31	a	1399	C	P-O3'-C3'	6.14	127.07	119.70
1	A	955	U	N1-C2-O2	6.14	127.10	122.80
52	w	17	LEU	CA-CB-CG	5.99	129.08	115.30
34	d	4	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	1930	G	P-O3'-C3'	5.96	126.85	119.70
31	a	1158	C	C6-N1-C2	-5.95	117.92	120.30
31	a	1158	C	C6-N1-C1'	-5.95	113.66	120.80
1	A	2104	U	C2-N1-C1'	5.93	124.82	117.70
1	A	1378	A	OP1-P-O3'	5.92	118.23	105.20
1	A	2190	G	P-O3'-C3'	5.92	126.80	119.70
28	3	61	LEU	CA-CB-CG	5.88	128.84	115.30
1	A	1940	U	P-O3'-C3'	5.87	126.74	119.70
1	A	1911	U	C2-N1-C1'	5.84	124.71	117.70
53	v	20	C	N1-C2-O2	5.84	122.41	118.90
54	x	3	G	P-O3'-C3'	5.80	126.66	119.70
14	P	113	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	2104	U	N1-C2-O2	5.79	126.85	122.80
31	a	960	U	P-O3'-C3'	5.77	126.62	119.70
1	A	859	G	P-O3'-C3'	5.75	126.60	119.70
2	B	12	C	C2-N1-C1'	5.75	125.12	118.80
1	A	1917	U	N3-C2-O2	-5.74	118.18	122.20
31	a	1190	G	P-O3'-C3'	5.73	126.58	119.70
1	A	51	G	OP2-P-O3'	5.72	117.80	105.20
11	M	70	ASP	CB-CG-OD1	5.72	123.45	118.30
54	x	55	U	C2-N1-C1'	5.70	124.54	117.70
31	a	1300	G	P-O3'-C3'	5.69	126.53	119.70
31	a	1432	G	P-O3'-C3'	5.69	126.53	119.70
54	9	25	C	C5-C6-N1	5.67	123.83	121.00
1	A	2566	A	P-O3'-C3'	5.66	126.49	119.70
54	9	70	C	N1-C2-O2	5.65	122.29	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	754	C	N1-C2-O2	5.64	122.28	118.90
2	B	12	C	N1-C2-O2	5.58	122.25	118.90
1	A	2605	U	C2-N1-C1'	5.56	124.37	117.70
1	A	1917	U	N1-C2-O2	5.55	126.69	122.80
1	A	1313	U	C6-N1-C1'	-5.51	113.48	121.20
54	9	17	C	C6-N1-C2	-5.51	118.09	120.30
1	A	2076	U	C2-N1-C1'	5.50	124.30	117.70
1	A	2173	A	C4-N9-C1'	5.50	136.19	126.30
34	d	190	LEU	CA-CB-CG	5.49	127.93	115.30
53	v	20	C	N3-C2-O2	-5.46	118.07	121.90
1	A	669	G	N3-C4-N9	5.46	129.28	126.00
54	9	76	A	C2'-C3'-O3'	-5.42	97.58	109.50
1	A	2104	U	N3-C2-O2	-5.40	118.42	122.20
1	A	669	G	N3-C4-C5	-5.40	125.90	128.60
31	a	1138	G	C8-N9-C1'	-5.40	119.98	127.00
31	a	1301	U	N1-C2-O2	5.37	126.56	122.80
54	9	25	C	C6-N1-C2	-5.37	118.15	120.30
54	9	19	G	C4-N9-C1'	-5.36	119.53	126.50
1	A	2173	A	C2-N3-C4	5.36	113.28	110.60
1	A	669	G	C8-N9-C1'	-5.34	120.06	127.00
1	A	2252	G	C3'-C2'-C1'	-5.33	97.23	101.50
54	9	55	U	N3-C2-O2	-5.33	118.47	122.20
54	9	62	C	N1-C2-O2	5.28	122.07	118.90
1	A	475	C	C6-N1-C2	-5.27	118.19	120.30
1	A	2326	C	P-O3'-C3'	5.27	126.03	119.70
1	A	62	U	C2-N1-C1'	5.26	124.01	117.70
1	A	2808	G	P-O3'-C3'	5.21	125.96	119.70
31	a	1301	U	C2-N1-C1'	5.21	123.96	117.70
1	A	2604	U	C2-N1-C1'	5.21	123.95	117.70
1	A	2580	U	N3-C2-O2	-5.21	118.56	122.20
31	a	516	U	C2-N1-C1'	5.20	123.94	117.70
54	9	55	U	C2-N1-C1'	5.20	123.94	117.70
54	x	2	G	P-O3'-C3'	5.16	125.89	119.70
1	A	2552	U	C2-N1-C1'	5.15	123.88	117.70
1	A	2286	G	P-O3'-C3'	5.14	125.87	119.70
54	9	70	C	C5-C6-N1	5.10	123.55	121.00
1	A	2884	U	C2-N1-C1'	5.09	123.81	117.70
54	x	41	A	P-O3'-C3'	5.06	125.77	119.70
54	9	19	G	O4'-C1'-N9	-5.04	104.17	108.20
31	a	1301	U	N3-C2-O2	-5.03	118.68	122.20
54	9	3	G	OP1-P-O3'	5.00	116.20	105.20

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2252	G	Sidechain
6	F	173	ASP	Peptide
6	F	174	PHE	Peptide
7	G	118	ALA	Peptide
7	G	46	ASP	Peptide
9	K	88	ASN	Peptide
11	M	57	VAL	Peptide
11	M	58	LYS	Peptide
16	R	53	PHE	Peptide
19	U	88	ASP	Peptide
19	U	97	SER	Peptide
32	b	15	PHE	Peptide
32	b	18	GLN	Peptide
36	f	53	LYS	Peptide
40	j	57	VAL	Peptide
42	l	101	LEU	Peptide
43	m	4	ALA	Peptide
47	q	69	THR	Peptide
52	w	120	GLY	Peptide
52	w	18	ASP	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%)	251 (93%)	18 (7%)	0	100	100
4	D	207/209 (99%)	196 (95%)	11 (5%)	0	100	100
5	E	199/201 (99%)	188 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
7	G	174/176 (99%)	163 (94%)	9 (5%)	2 (1%)	14	50
8	J	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
9	K	120/122 (98%)	104 (87%)	16 (13%)	0	100	100
10	L	141/143 (99%)	126 (89%)	14 (10%)	1 (1%)	22	59
11	M	134/136 (98%)	126 (94%)	5 (4%)	3 (2%)	6	37
12	N	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
13	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
14	P	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
15	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
16	R	101/103 (98%)	91 (90%)	9 (9%)	1 (1%)	15	51
17	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
18	T	91/93 (98%)	81 (89%)	10 (11%)	0	100	100
19	U	100/102 (98%)	86 (86%)	13 (13%)	1 (1%)	15	51
20	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
21	W	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
22	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
23	Y	61/63 (97%)	61 (100%)	0	0	100	100
24	Z	56/58 (97%)	56 (100%)	0	0	100	100
25	0	54/56 (96%)	54 (100%)	0	0	100	100
26	1	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
27	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
28	3	62/64 (97%)	56 (90%)	4 (6%)	2 (3%)	4	31
29	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
30	6	64/66 (97%)	55 (86%)	9 (14%)	0	100	100
32	b	216/218 (99%)	197 (91%)	19 (9%)	0	100	100
33	c	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
34	d	203/205 (99%)	178 (88%)	25 (12%)	0	100	100
35	e	155/157 (99%)	139 (90%)	15 (10%)	1 (1%)	25	62
36	f	98/100 (98%)	81 (83%)	15 (15%)	2 (2%)	7	39
37	g	149/151 (99%)	134 (90%)	15 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	h	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
39	i	125/127 (98%)	105 (84%)	19 (15%)	1 (1%)	19	56
40	j	96/98 (98%)	81 (84%)	15 (16%)	0	100	100
41	k	114/116 (98%)	101 (89%)	13 (11%)	0	100	100
42	l	121/123 (98%)	94 (78%)	26 (22%)	1 (1%)	19	56
43	m	112/114 (98%)	101 (90%)	9 (8%)	2 (2%)	8	41
44	n	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
45	o	86/88 (98%)	79 (92%)	7 (8%)	0	100	100
46	p	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
47	q	78/80 (98%)	66 (85%)	11 (14%)	1 (1%)	12	47
48	r	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
49	s	77/79 (98%)	71 (92%)	6 (8%)	0	100	100
50	t	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
51	u	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
52	w	185/188 (98%)	161 (87%)	24 (13%)	0	100	100
55	7	210/224 (94%)	189 (90%)	21 (10%)	0	100	100
All	All	5836/5949 (98%)	5327 (91%)	491 (8%)	18 (0%)	44	74

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	3	31	ILE
7	G	47	ASN
11	M	59	ARG
28	3	32	LEU
36	f	55	HIS
47	q	70	LYS
11	M	58	LYS
42	l	102	ASP
43	m	4	ALA
19	U	89	GLY
36	f	53	LYS
43	m	5	GLY
10	L	128	THR
11	M	70	ASP
39	i	91	GLU

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Mol	Chain	Res	Type
35	e	122	VAL
7	G	119	GLY
16	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%)	214 (99%)	2 (1%)	78	88
4	D	164/164 (100%)	162 (99%)	2 (1%)	71	84
5	E	165/165 (100%)	164 (99%)	1 (1%)	86	93
6	F	148/148 (100%)	148 (100%)	0	100	100
7	G	137/137 (100%)	137 (100%)	0	100	100
8	J	116/116 (100%)	116 (100%)	0	100	100
9	K	103/103 (100%)	103 (100%)	0	100	100
10	L	102/102 (100%)	101 (99%)	1 (1%)	76	86
11	M	109/109 (100%)	108 (99%)	1 (1%)	78	88
12	N	100/100 (100%)	99 (99%)	1 (1%)	76	86
13	O	86/86 (100%)	86 (100%)	0	100	100
14	P	99/99 (100%)	99 (100%)	0	100	100
15	Q	89/89 (100%)	89 (100%)	0	100	100
16	R	84/84 (100%)	83 (99%)	1 (1%)	71	84
17	S	93/93 (100%)	92 (99%)	1 (1%)	73	85
18	T	80/80 (100%)	80 (100%)	0	100	100
19	U	83/83 (100%)	83 (100%)	0	100	100
20	V	78/78 (100%)	78 (100%)	0	100	100
21	W	63/63 (100%)	63 (100%)	0	100	100
22	X	67/67 (100%)	66 (98%)	1 (2%)	65	81
23	Y	55/55 (100%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Z	48/48 (100%)	48 (100%)	0	100	100
25	0	47/47 (100%)	47 (100%)	0	100	100
26	1	45/45 (100%)	45 (100%)	0	100	100
27	2	38/38 (100%)	38 (100%)	0	100	100
28	3	51/51 (100%)	51 (100%)	0	100	100
29	4	34/34 (100%)	34 (100%)	0	100	100
30	6	59/59 (100%)	59 (100%)	0	100	100
32	b	180/180 (100%)	176 (98%)	4 (2%)	52	72
33	c	170/170 (100%)	170 (100%)	0	100	100
34	d	172/172 (100%)	170 (99%)	2 (1%)	71	84
35	e	114/119 (96%)	113 (99%)	1 (1%)	78	88
36	f	87/87 (100%)	87 (100%)	0	100	100
37	g	124/124 (100%)	124 (100%)	0	100	100
38	h	104/104 (100%)	104 (100%)	0	100	100
39	i	105/105 (100%)	103 (98%)	2 (2%)	57	76
40	j	86/86 (100%)	86 (100%)	0	100	100
41	k	89/89 (100%)	88 (99%)	1 (1%)	73	85
42	l	103/103 (100%)	102 (99%)	1 (1%)	76	86
43	m	92/92 (100%)	91 (99%)	1 (1%)	73	85
44	n	79/83 (95%)	79 (100%)	0	100	100
45	o	76/76 (100%)	76 (100%)	0	100	100
46	p	65/65 (100%)	64 (98%)	1 (2%)	65	81
47	q	74/74 (100%)	73 (99%)	1 (1%)	67	82
48	r	48/56 (86%)	48 (100%)	0	100	100
49	s	70/70 (100%)	70 (100%)	0	100	100
50	t	65/65 (100%)	65 (100%)	0	100	100
51	u	44/55 (80%)	44 (100%)	0	100	100
52	w	154/154 (100%)	153 (99%)	1 (1%)	86	93
55	7	173/173 (100%)	173 (100%)	0	100	100
All	All	4833/4861 (99%)	4807 (100%)	26 (0%)	89	94

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	36	ASN
3	C	85	ASN
4	D	33	ARG
4	D	169	ARG
5	E	156	ASN
10	L	27	LEU
11	M	6	ARG
12	N	2	ARG
16	R	43	ASN
17	S	57	ASN
22	X	26	ARG
32	b	20	ARG
32	b	23	ASN
32	b	35	ASN
32	b	202	ASN
34	d	80	ARG
34	d	177	MET
35	e	69	ASN
39	i	44	ARG
39	i	105	ARG
41	k	12	ARG
42	l	113	ARG
43	m	7	ASN
46	p	5	ARG
47	q	61	ARG
52	w	107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	36	ASN
3	C	85	ASN
3	C	114	GLN
3	C	225	ASN
5	E	156	ASN
7	G	63	GLN
7	G	138	GLN
8	J	40	HIS
9	K	3	GLN
13	O	38	GLN
14	P	11	GLN
14	P	55	HIS
15	Q	43	GLN

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Mol	Chain	Res	Type
16	R	6	GLN
16	R	18	GLN
16	R	43	ASN
16	R	91	GLN
17	S	7	HIS
17	S	9	HIS
17	S	57	ASN
21	W	12	ASN
23	Y	58	ASN
24	Z	19	HIS
30	6	41	HIS
32	b	23	ASN
32	b	35	ASN
32	b	202	ASN
35	e	69	ASN
36	f	55	HIS
38	h	15	ASN
39	i	36	GLN
40	j	58	ASN
46	p	26	ASN
46	p	63	GLN
47	q	30	HIS
49	s	68	HIS
50	t	60	GLN
52	w	119	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2868/2903 (98%)	504 (17%)	23 (0%)
2	B	119/120 (99%)	20 (16%)	1 (0%)
31	a	1538/1539 (99%)	304 (19%)	0
53	v	8/9 (88%)	3 (37%)	0
54	9	76/77 (98%)	27 (35%)	4 (5%)
54	x	75/77 (97%)	17 (22%)	0
All	All	4684/4725 (99%)	875 (18%)	28 (0%)

All (875) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A

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Mol	Chain	Res	Type
1	A	12	U
1	A	34	U
1	A	35	G
1	A	46	G
1	A	50	U
1	A	51	G
1	A	52	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	92	U
1	A	96	C
1	A	98	G
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	A
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	155	A
1	A	162	U
1	A	163	C
1	A	166	U
1	A	181	A
1	A	196	A
1	A	199	A
1	A	204	A
1	A	216	A
1	A	221	A
1	A	222	A
1	A	225	C
1	A	229	C
1	A	239	C
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A

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Mol	Chain	Res	Type
1	A	265	A
1	A	272	A
1	A	276	U
1	A	278	A
1	A	279	A
1	A	285	G
1	A	311	A
1	A	323	C
1	A	324	A
1	A	329	G
1	A	330	A
1	A	345	A
1	A	367	G
1	A	370	G
1	A	371	A
1	A	372	G
1	A	386	G
1	A	387	U
1	A	395	U
1	A	404	A
1	A	406	G
1	A	411	G
1	A	412	A
1	A	421	C
1	A	424	G
1	A	456	C
1	A	458	G
1	A	467	G
1	A	473	G
1	A	481	G
1	A	491	G
1	A	505	A
1	A	508	A
1	A	509	C
1	A	528	A
1	A	529	A
1	A	531	C
1	A	532	A
1	A	533	G
1	A	543	G
1	A	544	C
1	A	545	U

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Mol	Chain	Res	Type
1	A	547	A
1	A	548	G
1	A	550	C
1	A	555	G
1	A	563	A
1	A	573	U
1	A	575	A
1	A	603	A
1	A	614	A
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	647	G
1	A	654	A
1	A	655	A
1	A	659	G
1	A	664	G
1	A	668	A
1	A	669	G
1	A	677	A
1	A	686	U
1	A	687	C
1	A	695	G
1	A	722	A
1	A	724	U
1	A	730	A
1	A	738	G
1	A	747	C
1	A	752	A
1	A	753	A
1	A	764	A
1	A	765	C
1	A	774	G
1	A	782	A
1	A	783	A
1	A	784	G
1	A	785	G
1	A	789	A

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Mol	Chain	Res	Type
1	A	792	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	831	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	856	G
1	A	859	G
1	A	860	U
1	A	878	A
1	A	885	C
1	A	886	A
1	A	892	A
1	A	895	U
1	A	896	A
1	A	897	C
1	A	907	G
1	A	910	A
1	A	937	C
1	A	941	A
1	A	946	C
1	A	953	G
1	A	958	U
1	A	959	A
1	A	961	C
1	A	974	G
1	A	983	A
1	A	985	C
1	A	995	C
1	A	996	A
1	A	1005	C
1	A	1012	U
1	A	1013	C
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1026	G
1	A	1033	U

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Mol	Chain	Res	Type
1	A	1045	C
1	A	1046	A
1	A	1053	C
1	A	1057	A
1	A	1059	G
1	A	1060	U
1	A	1062	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1067	A
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	1084	A
1	A	1085	A
1	A	1088	A
1	A	1089	A
1	A	1096	A
1	A	1097	U
1	A	1104	C
1	A	1111	A
1	A	1112	G
1	A	1113	U
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1139	G
1	A	1142	A
1	A	1143	A
1	A	1150	C
1	A	1170	C
1	A	1172	C
1	A	1175	A
1	A	1176	U

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Mol	Chain	Res	Type
1	A	1177	G
1	A	1180	U
1	A	1204	A
1	A	1205	A
1	A	1206	G
1	A	1211	C
1	A	1212	G
1	A	1246	A
1	A	1247	A
1	A	1248	G
1	A	1250	G
1	A	1251	C
1	A	1253	A
1	A	1256	G
1	A	1265	A
1	A	1271	G
1	A	1272	A
1	A	1275	A
1	A	1300	G
1	A	1301	A
1	A	1306	C
1	A	1312	U
1	A	1321	A
1	A	1325	U
1	A	1326	U
1	A	1330	C
1	A	1341	G
1	A	1345	C
1	A	1352	U
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1395	A
1	A	1401	G
1	A	1403	A
1	A	1414	C
1	A	1416	G
1	A	1420	A
1	A	1428	C
1	A	1453	A

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Mol	Chain	Res	Type
1	A	1460	U
1	A	1461	C
1	A	1475	G
1	A	1482	G
1	A	1490	A
1	A	1491	G
1	A	1494	A
1	A	1504	A
1	A	1507	C
1	A	1509	A
1	A	1515	A
1	A	1524	G
1	A	1529	G
1	A	1535	A
1	A	1536	C
1	A	1555	G
1	A	1558	C
1	A	1560	G
1	A	1569	A
1	A	1581	G
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1603	A
1	A	1608	A
1	A	1611	C
1	A	1646	C
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1651	G
1	A	1672	A
1	A	1674	G
1	A	1694	C
1	A	1695	G
1	A	1699	G
1	A	1703	G
1	A	1715	G
1	A	1729	U
1	A	1730	C
1	A	1732	C
1	A	1733	G

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Mol	Chain	Res	Type
1	A	1738	G
1	A	1758	U
1	A	1764	C
1	A	1773	A
1	A	1781	U
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1816	C
1	A	1829	A
1	A	1833	C
1	A	1847	G
1	A	1857	G
1	A	1858	A
1	A	1859	U
1	A	1869	G
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1896	G
1	A	1901	A
1	A	1906	G
1	A	1907	G
1	A	1913	A
1	A	1914	C
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1937	A
1	A	1940	U
1	A	1941	C
1	A	1955	U
1	A	1966	A
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1991	U
1	A	1992	G
1	A	1997	C

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Mol	Chain	Res	Type
1	A	2004	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	2043	C
1	A	2049	G
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	A
1	A	2072	C
1	A	2093	G
1	A	2096	C
1	A	2097	A
1	A	2100	G
1	A	2101	A
1	A	2104	U
1	A	2105	U
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2114	A
1	A	2116	G
1	A	2117	A
1	A	2119	A
1	A	2120	G
1	A	2121	G
1	A	2126	A
1	A	2127	G
1	A	2159	G
1	A	2160	C
1	A	2167	U
1	A	2170	A
1	A	2173	A
1	A	2174	C

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Mol	Chain	Res	Type
1	A	2177	C
1	A	2178	C
1	A	2179	C
1	A	2180	U
1	A	2185	U
1	A	2186	G
1	A	2187	U
1	A	2188	U
1	A	2189	U
1	A	2190	G
1	A	2191	A
1	A	2193	G
1	A	2198	A
1	A	2203	U
1	A	2204	G
1	A	2211	A
1	A	2213	U
1	A	2214	C
1	A	2219	U
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2239	G
1	A	2249	U
1	A	2250	G
1	A	2251	G
1	A	2252	G
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	2309	A
1	A	2320	U
1	A	2325	G
1	A	2327	A
1	A	2350	C
1	A	2353	G
1	A	2354	C
1	A	2361	G
1	A	2383	G

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Mol	Chain	Res	Type
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	2424	C
1	A	2427	C
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2441	U
1	A	2448	A
1	A	2465	C
1	A	2470	G
1	A	2476	A
1	A	2478	A
1	A	2492	U
1	A	2498	C
1	A	2502	G
1	A	2503	A
1	A	2504	U
1	A	2506	U
1	A	2507	C
1	A	2513	A
1	A	2518	A
1	A	2520	C
1	A	2529	G
1	A	2534	A
1	A	2535	G
1	A	2547	A
1	A	2549	G
1	A	2554	U
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2582	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2609	U
1	A	2613	U

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Mol	Chain	Res	Type
1	A	2614	A
1	A	2629	U
1	A	2638	G
1	A	2655	G
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2716	C
1	A	2718	G
1	A	2726	A
1	A	2733	A
1	A	2744	G
1	A	2748	A
1	A	2751	G
1	A	2757	A
1	A	2760	C
1	A	2764	A
1	A	2765	A
1	A	2778	A
1	A	2779	U
1	A	2790	U
1	A	2791	G
1	A	2793	C
1	A	2796	U
1	A	2800	A
1	A	2808	G
1	A	2809	A
1	A	2818	U
1	A	2820	A
1	A	2833	U
1	A	2849	U
1	A	2861	U
1	A	2867	G
1	A	2868	A
1	A	2872	A
1	A	2873	A
1	A	2880	C
1	A	2893	A
1	A	2899	A
1	A	2901	C
2	B	4	C

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Mol	Chain	Res	Type
2	B	12	C
2	B	13	G
2	B	15	A
2	B	24	G
2	B	30	C
2	B	35	C
2	B	38	C
2	B	40	U
2	B	41	G
2	B	42	C
2	B	44	G
2	B	45	A
2	B	57	A
2	B	66	A
2	B	67	G
2	B	88	C
2	B	89	U
2	B	90	C
2	B	109	A
31	a	4	U
31	a	6	G
31	a	7	A
31	a	8	A
31	a	9	G
31	a	22	G
31	a	32	A
31	a	36	C
31	a	37	U
31	a	39	G
31	a	41	G
31	a	47	C
31	a	49	U
31	a	51	A
31	a	55	A
31	a	56	U
31	a	58	C
31	a	62	U
31	a	64	G
31	a	65	A
31	a	66	A
31	a	68	G
31	a	70	U

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Mol	Chain	Res	Type
31	a	71	A
31	a	72	A
31	a	74	A
31	a	80	A
31	a	81	A
31	a	83	C
31	a	86	G
31	a	87	C
31	a	89	U
31	a	95	C
31	a	98	A
31	a	99	C
31	a	104	G
31	a	121	U
31	a	122	G
31	a	130	A
31	a	131	A
31	a	137	U
31	a	148	G
31	a	150	U
31	a	156	C
31	a	157	U
31	a	160	A
31	a	163	C
31	a	164	G
31	a	177	G
31	a	181	A
31	a	182	A
31	a	183	C
31	a	184	G
31	a	189	A
31	a	194	C
31	a	197	A
31	a	204	G
31	a	209	U
31	a	210	C
31	a	211	G
31	a	212	G
31	a	214	C
31	a	223	A
31	a	226	G
31	a	230	G

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Mol	Chain	Res	Type
31	a	245	U
31	a	247	G
31	a	251	G
31	a	266	G
31	a	267	C
31	a	277	C
31	a	279	A
31	a	280	C
31	a	281	G
31	a	289	G
31	a	306	A
31	a	316	C
31	a	321	A
31	a	328	C
31	a	330	C
31	a	345	C
31	a	346	G
31	a	347	G
31	a	351	G
31	a	352	C
31	a	354	G
31	a	359	G
31	a	360	G
31	a	367	U
31	a	368	U
31	a	374	A
31	a	376	G
31	a	378	G
31	a	380	G
31	a	381	C
31	a	383	A
31	a	388	G
31	a	390	U
31	a	392	C
31	a	398	U
31	a	399	G
31	a	401	C
31	a	404	G
31	a	406	G
31	a	407	U
31	a	408	A
31	a	411	A

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Mol	Chain	Res	Type
31	a	412	A
31	a	413	G
31	a	414	A
31	a	421	U
31	a	422	C
31	a	423	G
31	a	424	G
31	a	427	U
31	a	429	U
31	a	430	A
31	a	436	C
31	a	446	G
31	a	448	A
31	a	450	G
31	a	461	A
31	a	466	A
31	a	467	U
31	a	468	A
31	a	472	U
31	a	473	U
31	a	482	A
31	a	484	G
31	a	485	U
31	a	486	U
31	a	488	C
31	a	494	G
31	a	496	A
31	a	497	G
31	a	498	A
31	a	499	A
31	a	505	G
31	a	509	A
31	a	510	A
31	a	513	C
31	a	518	C
31	a	520	A
31	a	524	G
31	a	527	G
31	a	531	U
31	a	532	A
31	a	536	C
31	a	547	A

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Mol	Chain	Res	Type
31	a	548	G
31	a	559	A
31	a	562	U
31	a	564	C
31	a	572	A
31	a	573	A
31	a	575	G
31	a	576	C
31	a	577	G
31	a	579	A
31	a	604	G
31	a	607	A
31	a	617	G
31	a	620	C
31	a	623	C
31	a	633	G
31	a	636	U
31	a	642	A
31	a	650	G
31	a	656	G
31	a	661	G
31	a	665	A
31	a	687	A
31	a	688	G
31	a	702	A
31	a	703	G
31	a	713	G
31	a	718	A
31	a	723	U
31	a	724	G
31	a	731	G
31	a	748	G
31	a	753	A
31	a	754	C
31	a	755	G
31	a	777	A
31	a	814	A
31	a	815	A
31	a	817	C
31	a	818	G
31	a	819	A
31	a	820	U

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Mol	Chain	Res	Type
31	a	821	G
31	a	832	G
31	a	836	G
31	a	843	U
31	a	844	G
31	a	846	G
31	a	851	G
31	a	871	U
31	a	876	C
31	a	890	G
31	a	902	G
31	a	914	A
31	a	926	G
31	a	934	C
31	a	935	A
31	a	960	U
31	a	961	U
31	a	966	G
31	a	969	A
31	a	971	G
31	a	975	A
31	a	976	G
31	a	977	A
31	a	992	U
31	a	993	G
31	a	1004	A
31	a	1028	C
31	a	1030	U
31	a	1031	C
31	a	1032	G
31	a	1033	G
31	a	1034	G
31	a	1035	A
31	a	1053	G
31	a	1065	U
31	a	1085	U
31	a	1092	A
31	a	1094	G
31	a	1095	U
31	a	1101	A
31	a	1130	A
31	a	1132	C

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Mol	Chain	Res	Type
31	a	1133	G
31	a	1137	C
31	a	1138	G
31	a	1139	G
31	a	1140	C
31	a	1152	A
31	a	1159	U
31	a	1160	G
31	a	1168	U
31	a	1169	A
31	a	1183	U
31	a	1184	G
31	a	1191	A
31	a	1196	A
31	a	1197	A
31	a	1201	A
31	a	1202	U
31	a	1212	U
31	a	1213	A
31	a	1227	A
31	a	1228	C
31	a	1238	A
31	a	1241	G
31	a	1258	G
31	a	1261	A
31	a	1275	A
31	a	1278	G
31	a	1280	A
31	a	1281	C
31	a	1282	C
31	a	1286	U
31	a	1287	A
31	a	1297	G
31	a	1298	U
31	a	1300	G
31	a	1301	U
31	a	1303	C
31	a	1317	C
31	a	1340	A
31	a	1346	A
31	a	1347	G
31	a	1348	U

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Mol	Chain	Res	Type
31	a	1353	G
31	a	1363	A
31	a	1364	U
31	a	1368	A
31	a	1370	G
31	a	1378	C
31	a	1381	U
31	a	1397	C
31	a	1400	C
31	a	1419	G
31	a	1422	G
31	a	1429	A
31	a	1433	A
31	a	1446	A
31	a	1451	U
31	a	1452	C
31	a	1487	G
31	a	1492	A
31	a	1493	A
31	a	1497	G
31	a	1503	A
31	a	1506	U
31	a	1517	G
31	a	1520	C
31	a	1529	G
31	a	1530	G
31	a	1534	A
31	a	1535	C
31	a	1536	C
53	v	17	C
53	v	18	G
53	v	21	G
54	x	3	G
54	x	4	U
54	x	5	G
54	x	6	A
54	x	8	U
54	x	14	A
54	x	18	G
54	x	19	G
54	x	20	U
54	x	21	A

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Mol	Chain	Res	Type
54	x	25	C
54	x	42	A
54	x	47	U
54	x	65	U
54	x	73	A
54	x	74	C
54	x	76	A
54	9	3	G
54	9	4	U
54	9	5	G
54	9	6	A
54	9	8	U
54	9	16	C
54	9	17	C
54	9	18	G
54	9	19	G
54	9	20	U
54	9	21	A
54	9	22	G
54	9	28	U
54	9	35	G
54	9	40	G
54	9	42	A
54	9	47	U
54	9	48	C
54	9	54	U
54	9	56	C
54	9	61	C
54	9	62	C
54	9	69	A
54	9	72	G
54	9	74	C
54	9	75	C
54	9	76	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	242	G
1	A	490	C
1	A	859	G

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Mol	Chain	Res	Type
1	A	1020	A
1	A	1022	G
1	A	1070	A
1	A	1111	A
1	A	1182	G
1	A	1190	G
1	A	1300	G
1	A	1378	A
1	A	1399	C
1	A	1432	G
1	A	1930	G
1	A	1940	U
1	A	2190	G
1	A	2251	G
1	A	2286	G
1	A	2326	C
1	A	2391	G
1	A	2566	A
1	A	2808	G
2	B	66	A
54	9	2	G
54	9	3	G
54	9	19	G
54	9	41	A

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
52	KEO	w	34	52	16,18,19	1.50	2 (12%)	14,21,23	1.25	1 (7%)

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
52	KEO	w	34	52	-	11/19/20/22	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	w	34	KEO	C05-NZ	5.39	1.45	1.33
52	w	34	KEO	O02-C05	-2.14	1.18	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	w	34	KEO	C06-C05-NZ	2.97	120.08	115.97

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	w	34	KEO	O-C-CA-CB
52	w	34	KEO	N-CA-CB-CG
52	w	34	KEO	C-CA-CB-CG
52	w	34	KEO	C06-C07-C08-C09
52	w	34	KEO	N02-C07-C08-C09
52	w	34	KEO	C06-C05-NZ-CE
52	w	34	KEO	O02-C05-NZ-CE
52	w	34	KEO	CA-CB-CG-O01
52	w	34	KEO	C05-C06-C07-C08
52	w	34	KEO	C05-C06-C07-N02
52	w	34	KEO	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
56	PRO	9	101	54	5,7,8	0.64	0	7,8,10	1.57	1 (14%)

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
56	PRO	9	101	54	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
56	9	101	PRO	O-C-CA	-3.33	116.04	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
55	7	6
54	x	1
21	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	66:PRO	C	67:HIS	N	6.78
1	7	138:PRO	C	139:ASN	N	6.13
1	7	201:PRO	C	202:THR	N	4.61
1	7	133:PRO	C	134:ARG	N	3.99
1	7	140:PRO	C	141:LYS	N	3.47
1	7	118:PRO	C	119:ASP	N	3.31
1	x	40:G	O3'	41:A	P	2.28
1	W	10:THR	C	11:ARG	N	1.11

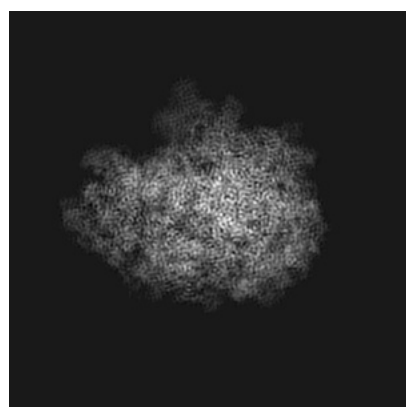
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3899. These allow visual inspection of the internal detail of the map and identification of artifacts.

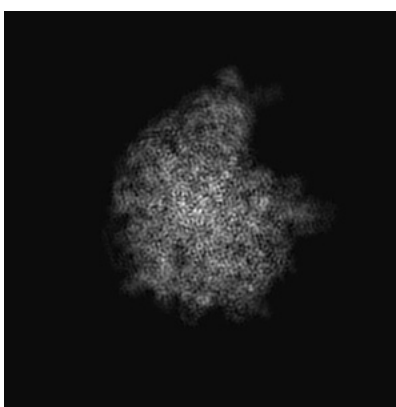
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

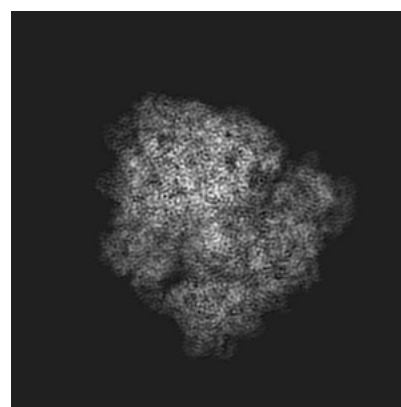
6.1.1 Primary map



X



Y

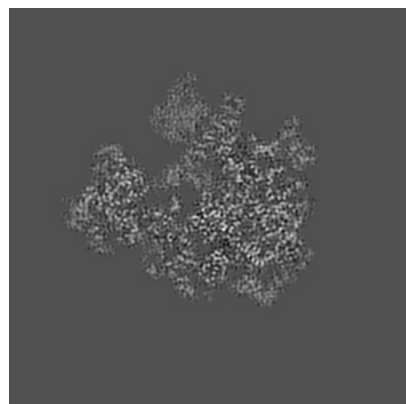


Z

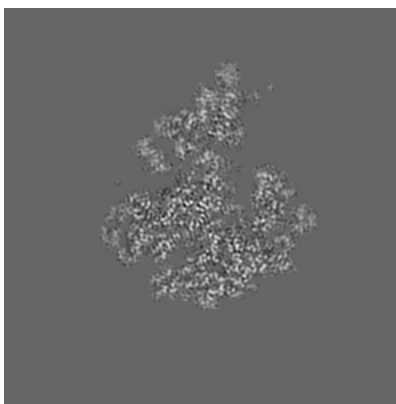
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

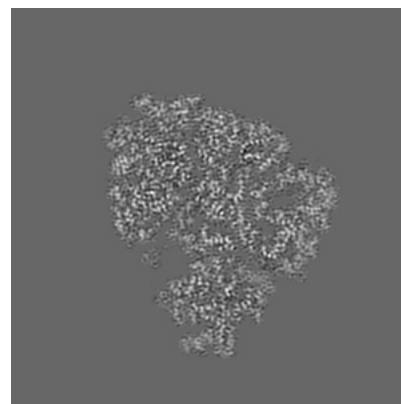
6.2.1 Primary map



X Index: 180



Y Index: 180

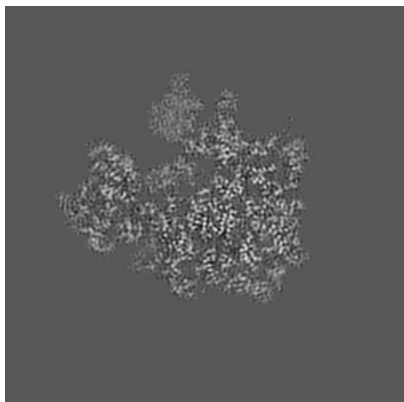


Z Index: 180

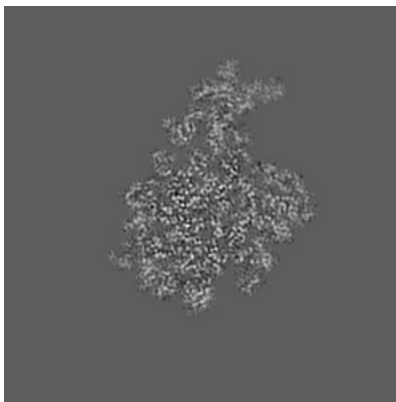
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

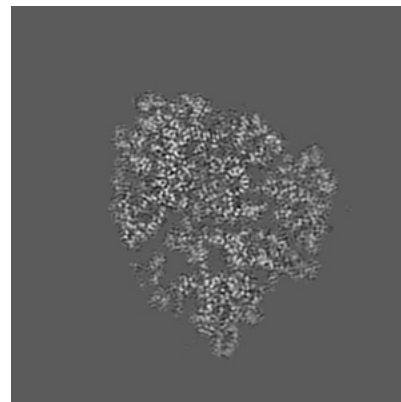
6.3.1 Primary map



X Index: 184



Y Index: 192

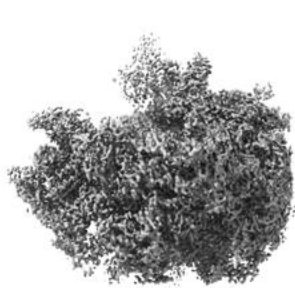


Z Index: 186

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0963. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

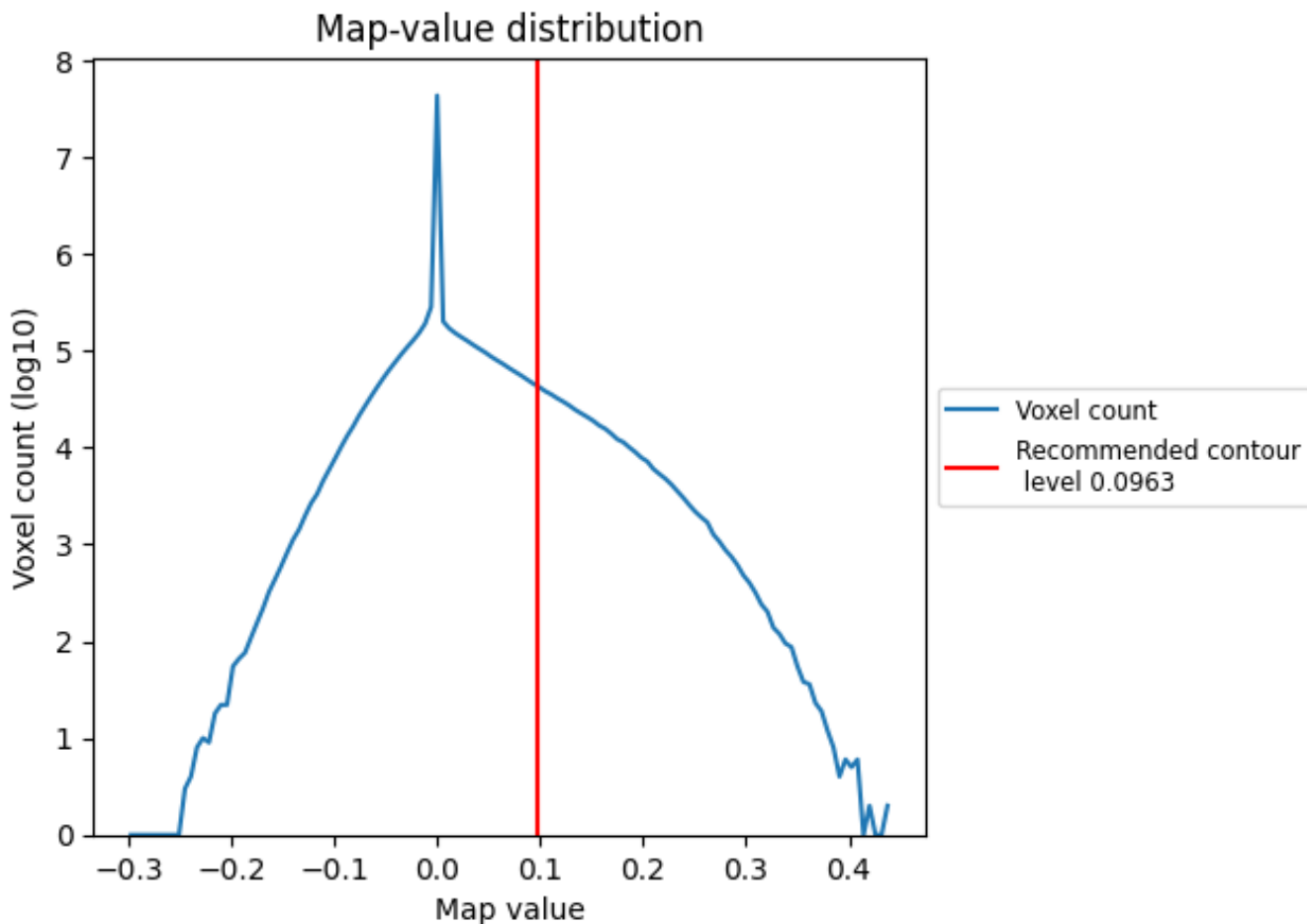
6.5 Mask visualisation

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

7 Map analysis [i](#)

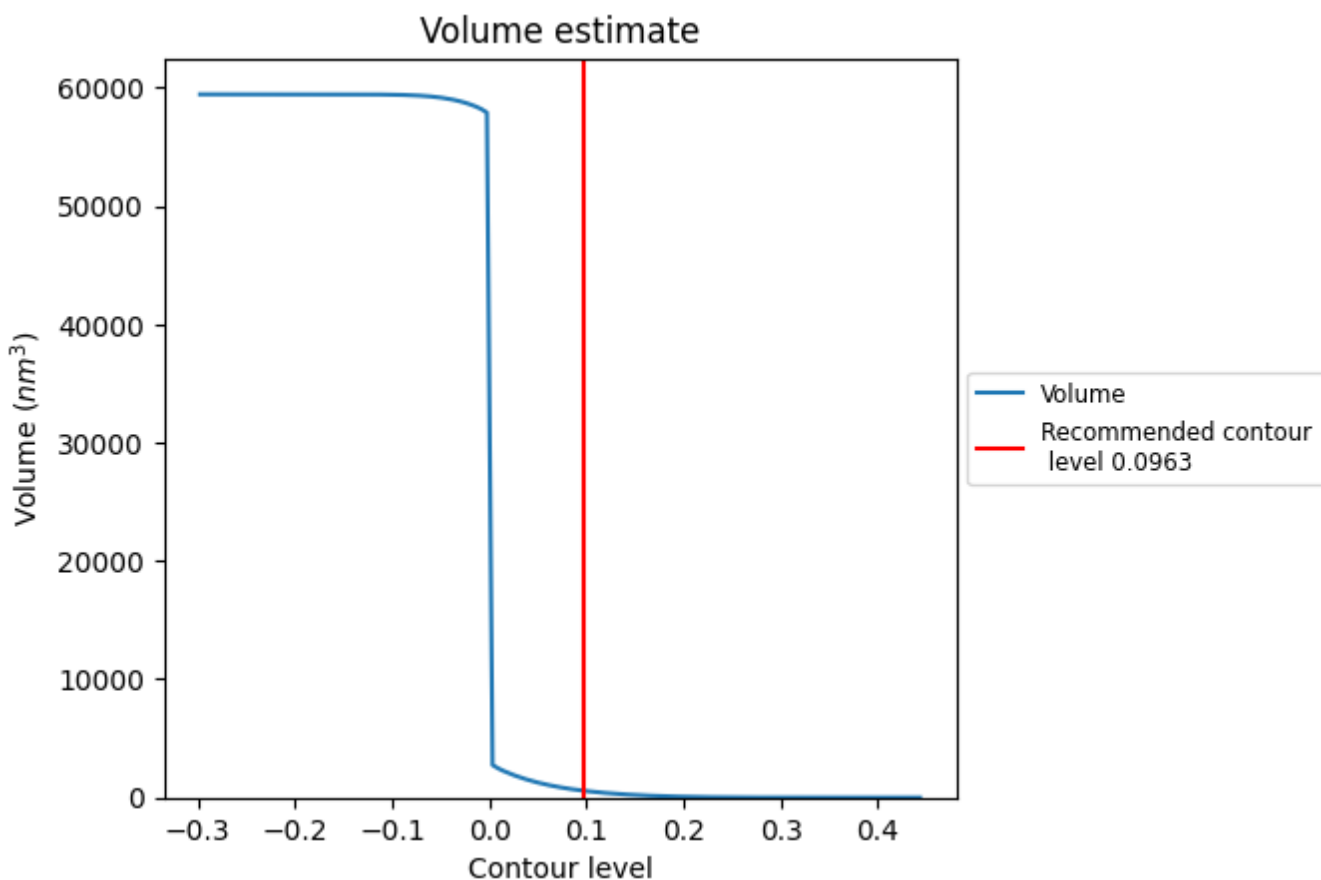
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

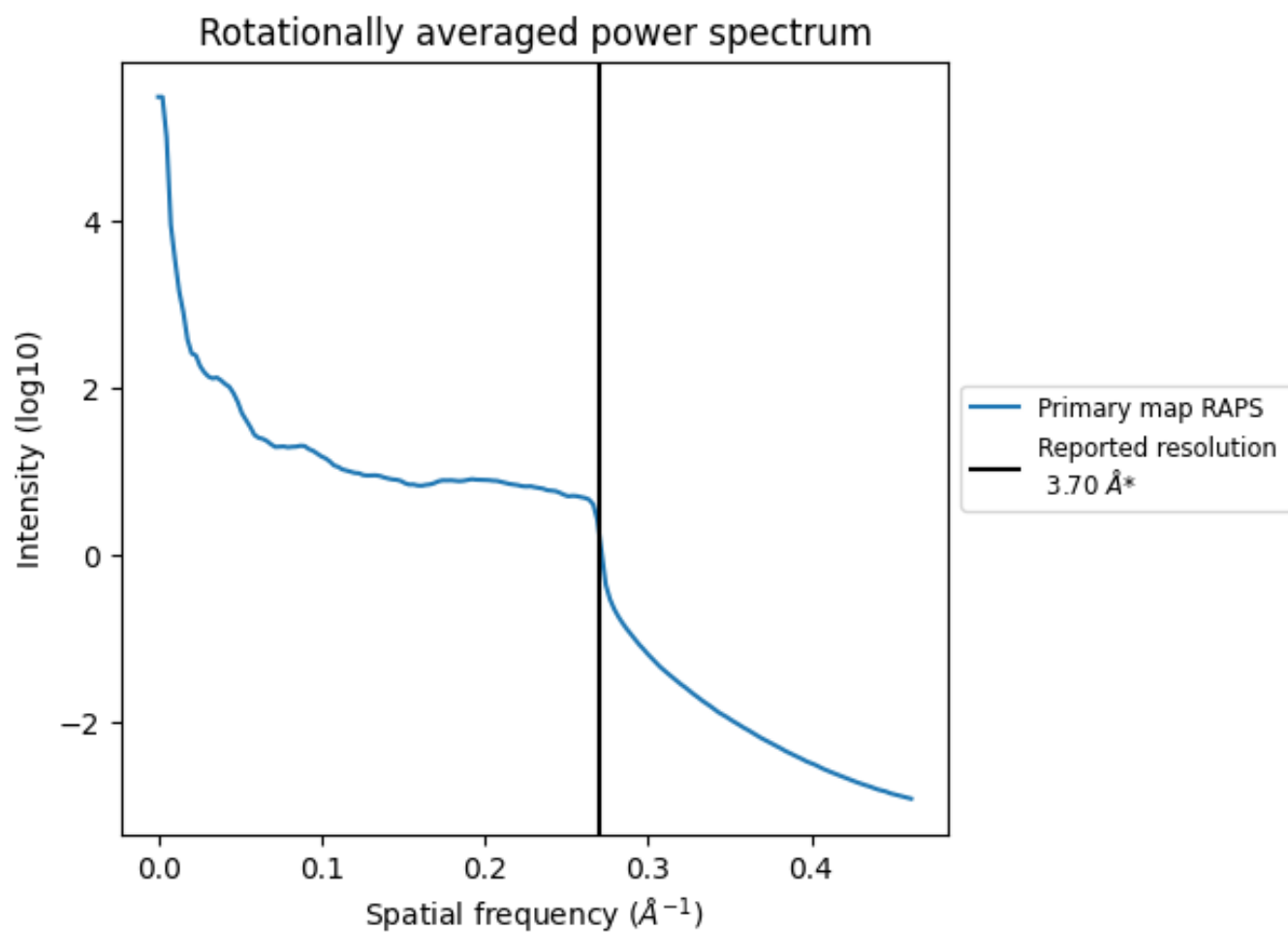
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 584 nm³; this corresponds to an approximate mass of 528 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 0.270\AA^{-1}

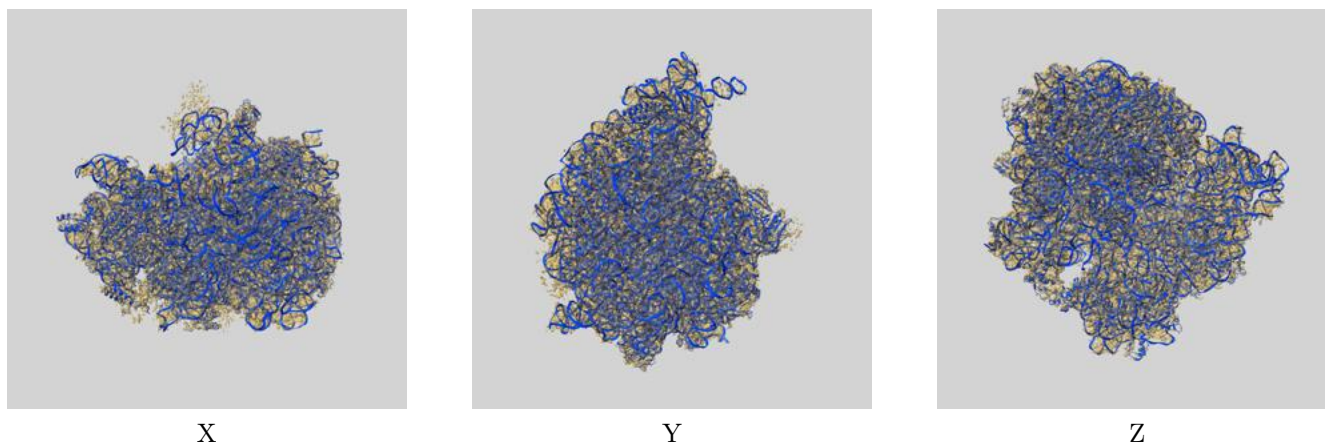
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

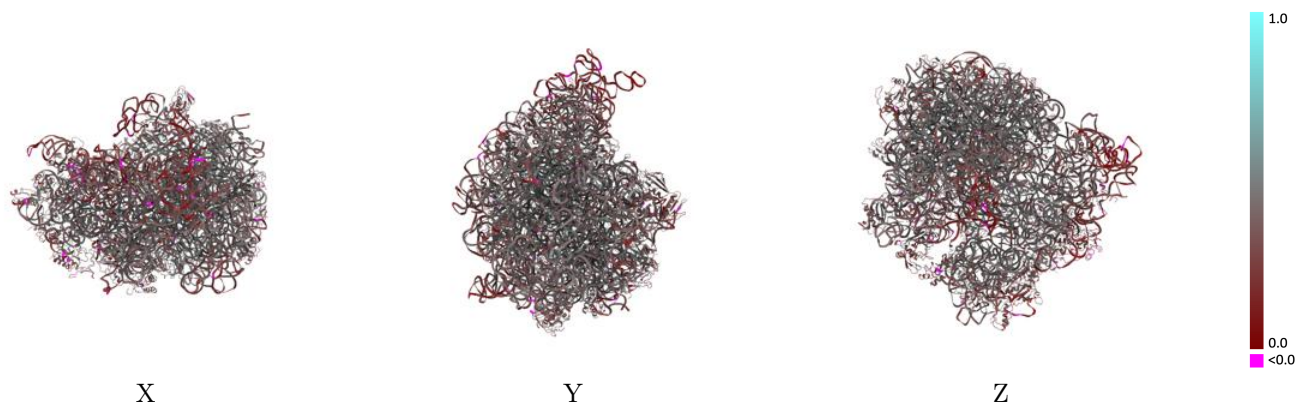
This section contains information regarding the fit between EMDB map EMD-3899 and PDB model 6ENJ. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



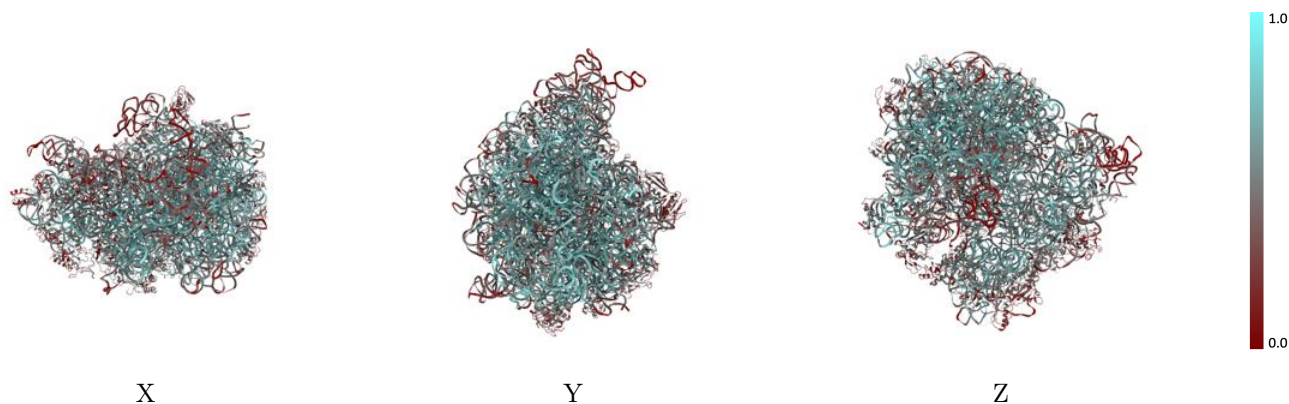
The images above show the 3D surface view of the map at the recommended contour level 0.0963 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



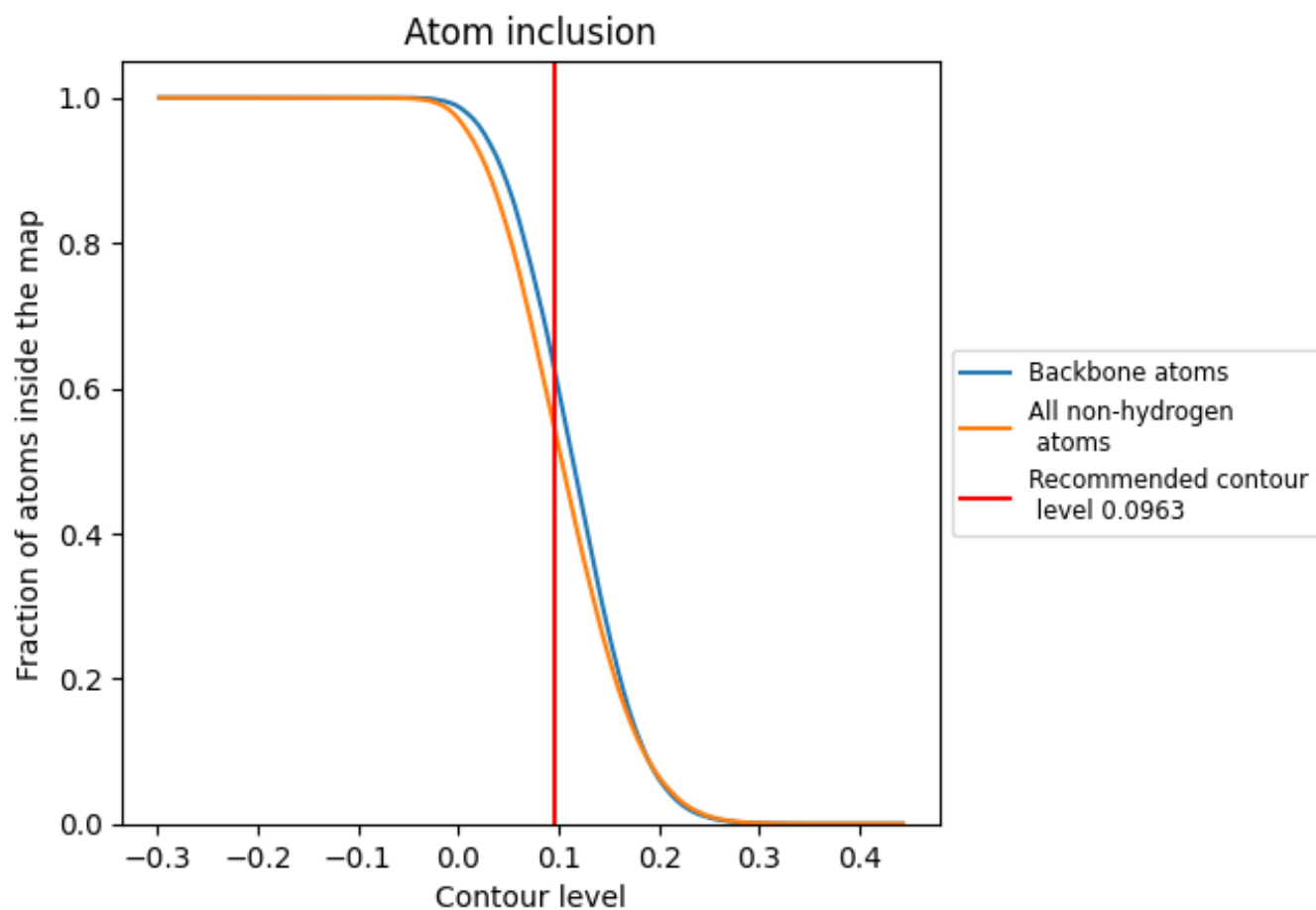
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0963).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 54% 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 (0.0963) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5429	 0.3850
0	 0.4650	 0.4000
1	 0.3292	 0.3700
2	 0.6028	 0.4330
3	 0.5356	 0.4250
4	 0.4623	 0.3920
6	 0.1957	 0.2460
7	 0.0488	 0.1530
9	 0.3073	 0.2590
A	 0.6331	 0.4120
B	 0.5995	 0.3980
C	 0.5511	 0.4370
D	 0.4941	 0.4280
E	 0.3980	 0.3700
F	 0.3765	 0.3340
G	 0.2930	 0.3220
J	 0.5064	 0.4040
K	 0.4666	 0.4040
L	 0.4596	 0.3990
M	 0.4866	 0.4220
N	 0.5380	 0.4050
O	 0.4380	 0.3740
P	 0.4583	 0.4050
Q	 0.5275	 0.4210
R	 0.3864	 0.3780
S	 0.4629	 0.4090
T	 0.4072	 0.3750
U	 0.3559	 0.3410
V	 0.3889	 0.3820
W	 0.4960	 0.4170
X	 0.4592	 0.3960
Y	 0.3561	 0.3190
Z	 0.4737	 0.4020
a	 0.5835	 0.3820
b	 0.3158	 0.3070



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Chain	Atom inclusion	Q-score
c	█ 0.4278	█ 0.3800
d	█ 0.1987	█ 0.2200
e	█ 0.4593	█ 0.3680
f	█ 0.3781	█ 0.3300
g	█ 0.3671	█ 0.3500
h	█ 0.4833	█ 0.3900
i	█ 0.3871	█ 0.3500
j	█ 0.3574	█ 0.3240
k	█ 0.4012	█ 0.3700
l	█ 0.3974	█ 0.3500
m	█ 0.3643	█ 0.3390
n	█ 0.4245	█ 0.3680
o	█ 0.4333	█ 0.3740
p	█ 0.3142	█ 0.2770
q	█ 0.3528	█ 0.3080
r	█ 0.4619	█ 0.3750
s	█ 0.4251	█ 0.3750
t	█ 0.3538	█ 0.3000
u	█ 0.2479	█ 0.2700
v	█ 0.6508	█ 0.4300
w	█ 0.3046	█ 0.3380
x	█ 0.4763	█ 0.3570