



Full wwPDB EM Validation Report ⓘ

Dec 28, 2024 – 10:39 AM EST

PDB ID : 6WOO
EMDB ID : EMD-21859
Title : CryoEM structure of yeast 80S ribosome with Met-tRNAⁱMet, eIF5B, and GDP
Authors : Wang, J.; Wang, J.; Puglisi, J.; Fernandez, I.S.
Deposited on : 2020-04-25
Resolution : 2.90 Å(reported)
Based on initial model : 4V8Y

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:

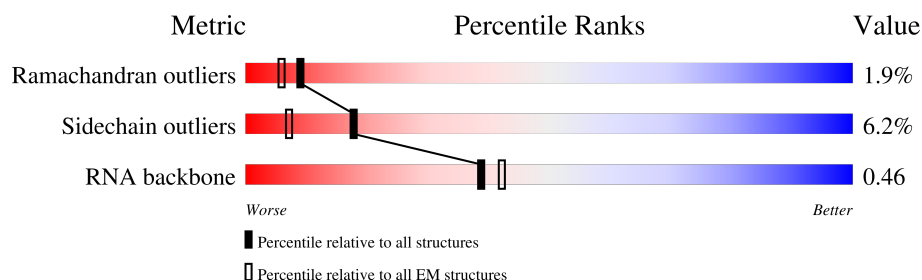
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	5	3271	
2	7	121	
3	8	157	
4	A	249	
5	B	384	
6	C	359	
7	D	295	
8	E	175	

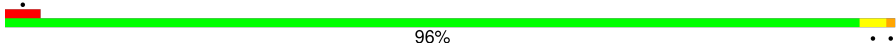

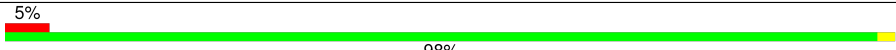
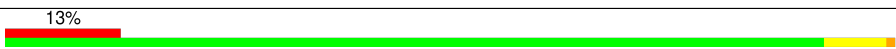
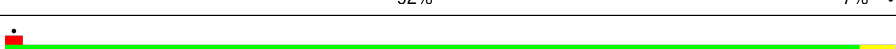

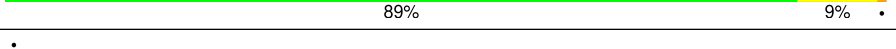
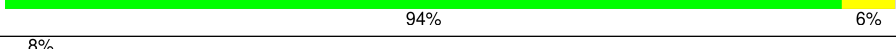
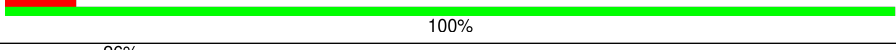



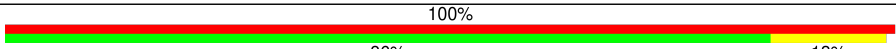
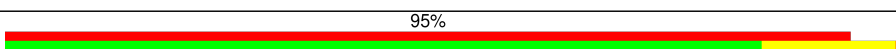
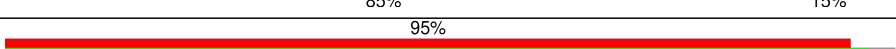
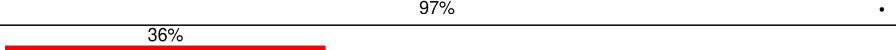
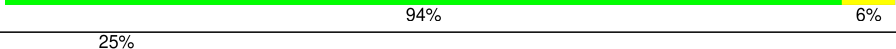
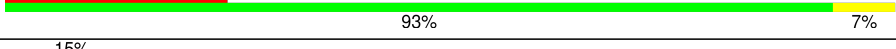
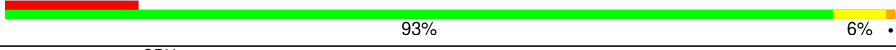
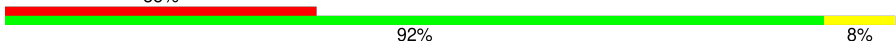
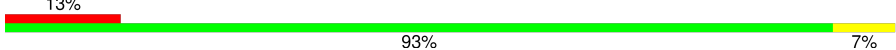


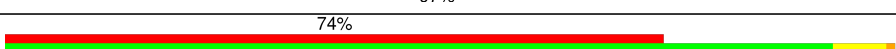
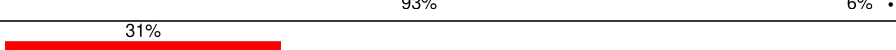
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Mol	Chain	Length	Quality of chain
9	F	222	8% 94% 5%
10	G	233	22% 96% .
11	H	191	9% 93% 7%
12	I	216	8% 94% 6%
13	J	168	40% 94% 6%
14	L	198	16% 93% 7%
15	M	136	10% 94% 6%
16	N	202	. 97% .
17	O	197	8% 98% ..
18	P	180	10% 96% .
19	Q	184	. 98% .
20	R	188	23% 94% 6%
21	S	169	6% 94% 5% .
22	T	158	15% 91% 9%
23	U	100	32% 96% .
24	V	132	14% 92% 8%
25	W	62	10% 97% .
26	X	121	9% 95% 5%
27	Y	125	8% 95% 5%
28	Z	134	23% 92% 8%
29	a	147	. 94% 5% .
30	b	57	16% 95% 5%
31	c	97	24% 94% 6%
32	d	106	12% 97% .
33	e	122	. 92% 7% ..

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Mol	Chain	Length	Quality of chain
34	f	105	
35	g	121	
36	h	116	
37	i	98	
38	j	85	
39	k	76	
40	l	49	
41	m	51	
42	n	23	
43	o	101	
44	p	87	
45	q	217	
46	r	195	
47	K	152	
48	AA	206	
49	BB	214	
50	CC	217	
51	DD	223	
52	EE	257	
53	FF	206	
54	GG	226	
55	HH	184	
56	II	199	
57	JJ	182	
58	KK	96	

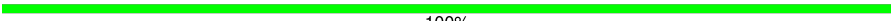
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Mol	Chain	Length	Quality of chain
59	LL	145	<div> <div>25%</div> <div>97%</div> </div>
60	MM	124	<div> <div>99%</div> <div>93%</div> <div>7%</div> </div>
61	NN	150	<div> <div>33%</div> <div>94%</div> <div>5%</div> </div>
62	OO	127	<div> <div>13%</div> <div>90%</div> <div>10%</div> </div>
63	PP	103	<div> <div>33%</div> <div>92%</div> <div>8%</div> </div>
64	QQ	141	<div> <div>15%</div> <div>91%</div> <div>9%</div> </div>
65	RR	123	<div> <div>53%</div> <div>91%</div> <div>9%</div> </div>
66	SS	136	<div> <div>23%</div> <div>93%</div> <div>7%</div> </div>
67	TT	143	<div> <div>17%</div> <div>92%</div> <div>7%</div> </div>
68	UU	106	<div> <div>44%</div> <div>98%</div> </div>
69	VV	87	<div> <div>25%</div> <div>92%</div> <div>8%</div> </div>
70	WW	129	<div> <div>10%</div> <div>93%</div> <div>7%</div> </div>
71	XX	144	<div> <div>10%</div> <div>91%</div> <div>9%</div> </div>
72	YY	134	<div> <div>26%</div> <div>97%</div> </div>
73	ZZ	70	<div> <div>36%</div> <div>96%</div> </div>
74	aa	97	<div> <div>13%</div> <div>90%</div> <div>10%</div> </div>
75	bb	81	<div> <div>44%</div> <div>90%</div> <div>10%</div> </div>
76	cc	63	<div> <div>21%</div> <div>94%</div> <div>6%</div> </div>
77	dd	53	<div> <div>9%</div> <div>91%</div> <div>9%</div> </div>
78	ee	53	<div> <div>25%</div> <div>94%</div> <div>6%</div> </div>
79	ff	57	<div> <div>70%</div> <div>72%</div> <div>5%</div> <div>23%</div> </div>
80	gg	318	<div> <div>60%</div> <div>92%</div> <div>8%</div> </div>
81	2	1796	<div> <div>15%</div> <div>68%</div> <div>31%</div> </div>
82	1	600	<div> <div>29%</div> <div>87%</div> <div>12%</div> </div>
83	3	76	<div> <div>14%</div> <div>78%</div> <div>22%</div> </div>

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Mol	Chain	Length	Quality of chain
84	4	6	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	U6A	3	101	-	X	-	-

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 211119 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	3271	Total	C	N	O	P	0	0
			69936	31236	12597	22832	3271		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 3 is a RNA chain called 5.8S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	157	Total	C	N	O	P	0	0
			3333	1491	584	1101	157		

- Molecule 4 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	249	Total	C	N	O	S	0	0
			1893	1178	384	330	1		

- Molecule 5 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	384	Total	C	N	O	S	0	0
			3065	1946	582	529	8		

- Molecule 6 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	359	Total	C	N	O	S	0	0
			2735	1723	520	489	3		

- Molecule 7 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	295	Total	C	N	O	S	0	0
			2370	1498	413	457	2		

- Molecule 8 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 9 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 10 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	233	Total	C	N	O	S	0	0
			1809	1154	324	328	3		

- Molecule 11 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	191	Total	C	N	O	S	0	0
			1524	966	274	280	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	191	GLU	-	insertion	UNP P51401

- Molecule 12 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	216	Total	C	N	O	S	0	0
			1750	1109	331	303	7		

- Molecule 13 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	168	Total	C	N	O	S	0	0
			1344	841	251	248	4		

- Molecule 14 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	198	Total	C	N	O	S	0	0
			1584	988	323	273			

- Molecule 15 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	136	Total	C	N	O	S	0	0
			1054	675	199	178	2		

- Molecule 16 is a protein called eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	202	Total	C	N	O	S	0	0
			1711	1071	359	280	1		

- Molecule 17 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 18 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	180	Total	C	N	O	S	0	0
			1427	887	284	256			

- Molecule 19 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	184	Total	C	N	O	S	0	0
			1437	906	289	240	2		

- Molecule 20 is a protein called eL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 21 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	169	Total	C	N	O	S	0	0
			1422	916	262	241	3		

- Molecule 22 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	158	Total	C	N	O	S	0	0
			1268	799	245	220	4		

- Molecule 23 is a protein called eL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 24 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	132	Total	C	N	O	S	0	0
			978	614	184	173	7		

- Molecule 25 is a protein called eL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	W	62	Total	C	N	O	0	0
			513	331	101	81		

- Molecule 26 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	121	Total	C	N	O	S	0	0
			968	623	170	173	2		

- Molecule 27 is a protein called uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Y	125	Total	C	N	O	0	0
			988	622	191	175		

- Molecule 28 is a protein called eL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Z	134	Total	C	N	O	0	0
			1087	707	201	179		

- Molecule 29 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	147	Total	C	N	O	S	0	0
			1168	746	230	189	3		

- Molecule 30 is a protein called eL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	b	57	Total	C	N	O	0	0
			457	286	99	72		

- Molecule 31 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 32 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	106	Total	C	N	O	S	0	0
			865	550	165	149	1		

- Molecule 33 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	122	Total	C	N	O	S	0	0
			988	626	200	161	1		

- Molecule 34 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	105	Total	C	N	O	S	0	0
			842	534	164	143	1		

- Molecule 35 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	121	Total	C	N	O	S	0	0
			954	592	194	164	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	122	LYS	-	insertion	UNP P87262

- Molecule 36 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	116	Total	C	N	O	S	0	0
			950	603	182	164	1		

- Molecule 37 is a protein called eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	98	Total	C	N	O	S	0	0
			764	477	155	130	2		

- Molecule 38 is a protein called eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	85	Total	C	N	O	S	0	0
			673	410	147	111	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	84	LYS	-	insertion	UNP P49166
j	85	ALA	-	insertion	UNP P49166
j	86	GLN	-	insertion	UNP P49166

- Molecule 39 is a protein called eL38.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	76	Total	C	N	O	0	0
			607	388	114	105		

- Molecule 40 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	49	Total	C	N	O	S	0	0
			428	266	96	64	2		

- Molecule 41 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	51	Total	C	N	O	S	0	0
			409	253	85	66	5		

- Molecule 42 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	23	Total	C	N	O	S	0	0
			218	133	60	24	1		

- Molecule 43 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	101	Total	C	N	O	S	0	0
			814	511	165	133	5		

- Molecule 44 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	87	Total	C	N	O	S	0	0
			668	413	134	115	6		

- Molecule 45 is a protein called uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	217	Total	C	N	O	S	0	0
			1718	1097	299	312	10		

- Molecule 46 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	195	Total	C	N	O	S	0	0
			1512	968	261	279	4		

- Molecule 47 is a protein called L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	K	147	Total	C	N	O	S	0	0
			735	441	147	147			

- Molecule 48 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AA	206	Total	C	N	O	S	0	0
			1615	1037	286	290	2		

- Molecule 49 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BB	214	Total	C	N	O	S	0	0
			1716	1086	314	312	4		

- Molecule 50 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	CC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 51 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	DD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 52 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	EE	257	Total	C	N	O	S	0	0
			2047	1303	385	356	3		

- Molecule 53 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	FF	201	Total	C	N	O	S	0	0
			1588	996	295	294	3		

- Molecule 54 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	GG	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 55 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	HH	184	Total	C	N	O	S	0	0
			1481	951	265	265			

- Molecule 56 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	II	187	Total	C	N	O	S	0	0
			1480	919	296	263	2		

- Molecule 57 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	JJ	182	Total	C	N	O	S	0	0
			1477	933	288	255	1		

- Molecule 58 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	KK	96	Total	C	N	O	S	0	0
			818	530	133	153	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
KK	89	ALA	GLY	conflict	UNP Q08745

- Molecule 59 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LL	145	Total	C	N	O	S	0	0
			1166	746	220	197	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LL	146	THR	-	insertion	UNP P0CX47

- Molecule 60 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	MM	124	Total	C	N	O	S	0	0
			934	587	165	180	2		

- Molecule 61 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	NN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 62 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	OO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 63 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	PP	103	Total	C	N	O	S	0	0
			814	520	149	138	7		

- Molecule 64 is a protein called uS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	QQ	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 65 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	RR	123	Total	C	N	O	S	0	0
			989	619	186	182	2		

- Molecule 66 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SS	136	Total	C	N	O	S	0	0
			1121	700	223	196	2		

- Molecule 67 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	TT	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 68 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	UU	106	Total	C	N	O	S	0	0
			847	535	154	157	1		

- Molecule 69 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	VV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 70 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	WW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 71 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	XX	144	Total	C	N	O	S	0	0
			1123	710	220	190	3		

- Molecule 72 is a protein called eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	YY	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 73 is a protein called eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	ZZ	70	Total	C	N	O	0	0
			563	360	104	99		

- Molecule 74 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	aa	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 75 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	bb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 76 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	cc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 77 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	dd	53	Total	C	N	O	S	0	0
			443	275	92	72	4		

- Molecule 78 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	ee	53	Total	C	N	O	S	0	0
			426	268	88	69	1		

- Molecule 79 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	ff	44	Total	C	N	O	S	0	0
			344	216	68	56	4		

- Molecule 80 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	gg	318	Total	C	N	O	S	0	0
			2444	1546	419	471	8		

- Molecule 81 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	2	1780	Total	C	N	O	P	0	0
			37790	16890	6651	12469	1780		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	677	A	G	conflict	GB 1329886537
2	678	U	A	conflict	GB 1329886537

- Molecule 82 is a protein called eIF5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	1	600	Total	C	N	O	S	0	0
			4704	2989	801	893	21		

- Molecule 83 is a RNA chain called Met-tRNA-iMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	3	76	Total	C	N	O	P	0	0
			1630	726	302	526	76		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	17	G	-	insertion	GB 176433

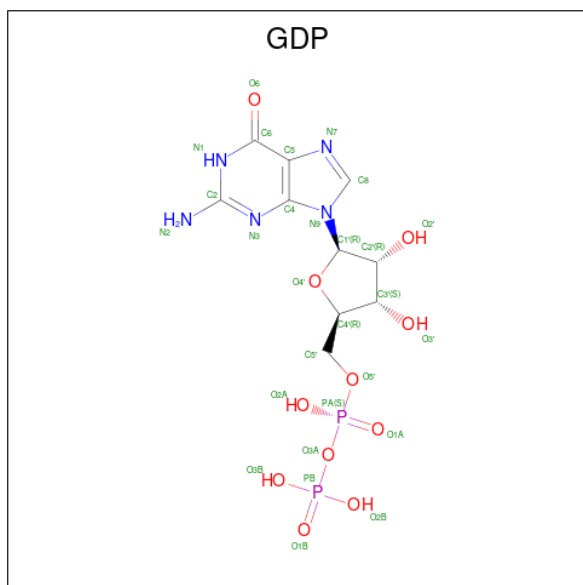
- Molecule 84 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	4	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

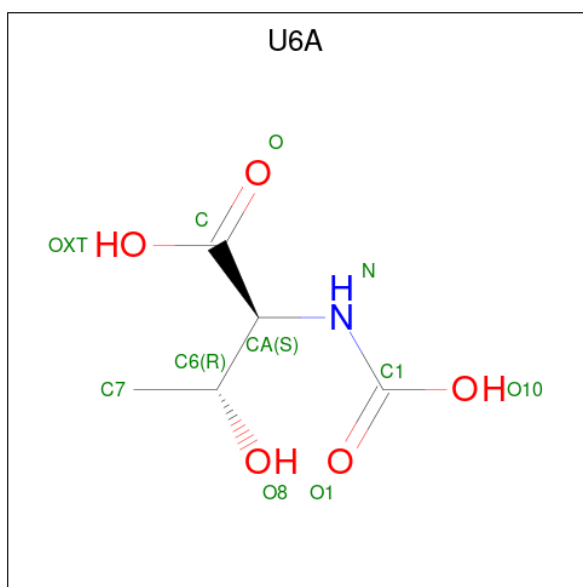
Mol	Chain	Residues	Atoms		AltConf
85	j	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	
85	o	1	Total	Zn	0
			1	1	
85	aa	1	Total	Zn	0
			1	1	
85	bb	1	Total	Zn	0
			1	1	
85	ff	1	Total	Zn	0
			1	1	

- Molecule 86 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



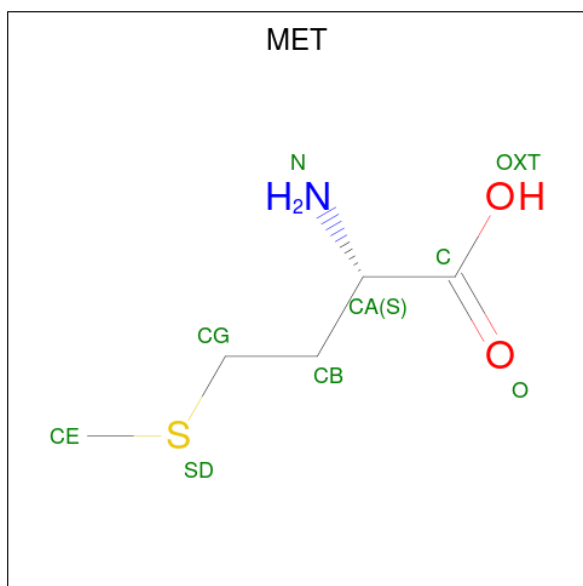
Mol	Chain	Residues	Atoms					AltConf
86	1	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 87 is N-carboxy-L-threonine (three-letter code: U6A) (formula: $C_5H_9NO_5$).



Mol	Chain	Residues	Atoms				AltConf
87	3	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 88 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).

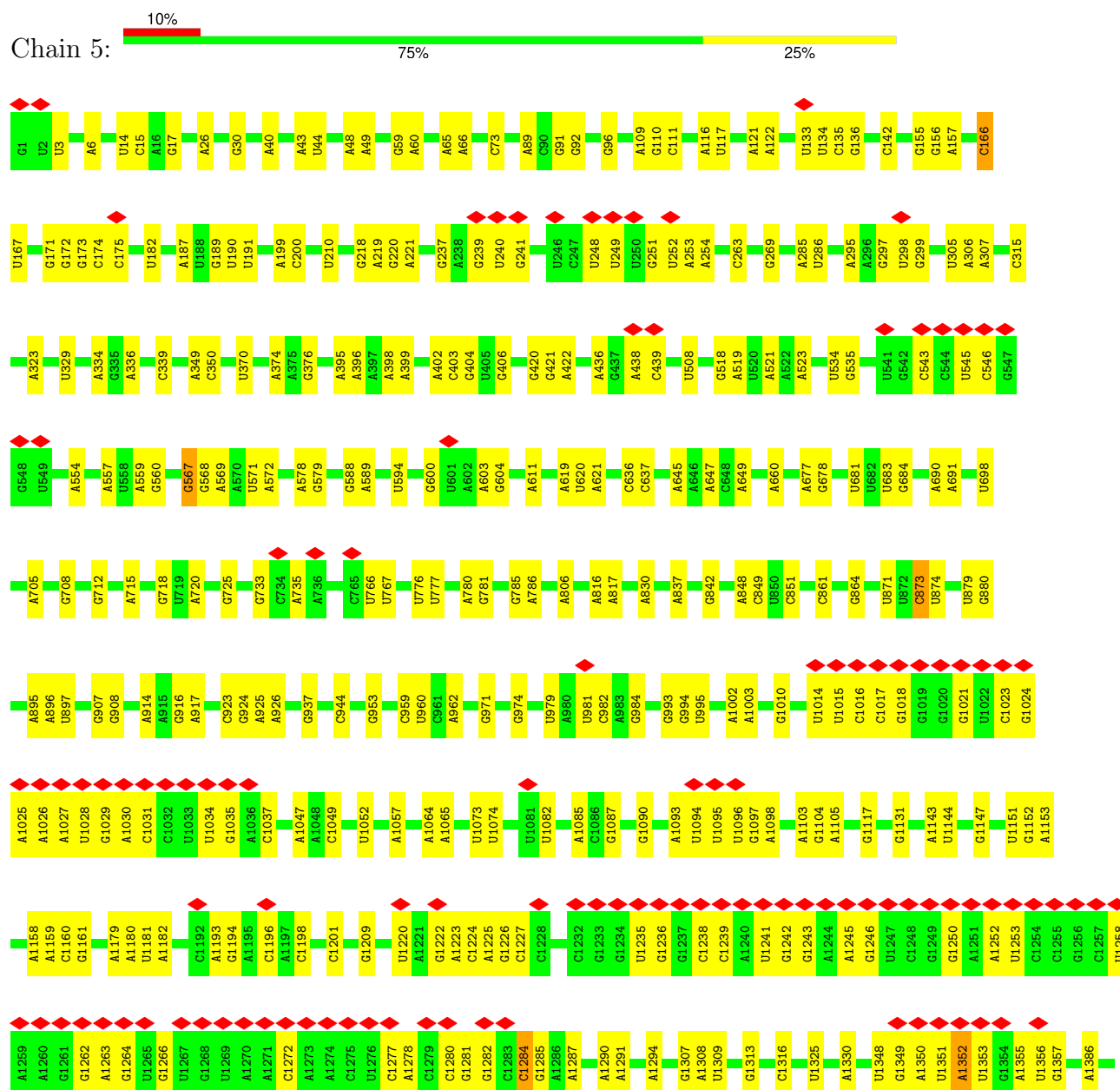


Mol	Chain	Residues	Atoms					AltConf
88	3	1	Total	C	N	O	S	0
			8	5	1	1	1	

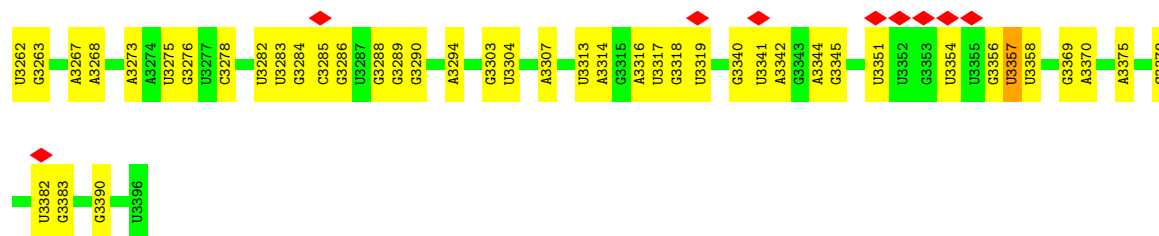
3 Residue-property plots

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.

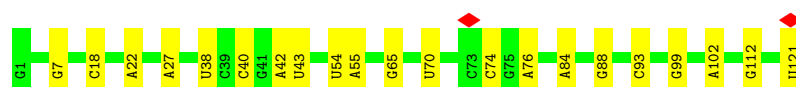
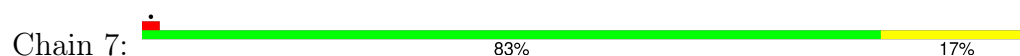
• Molecule 1: 25S ribosomal RNA



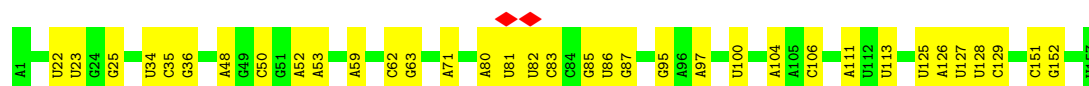
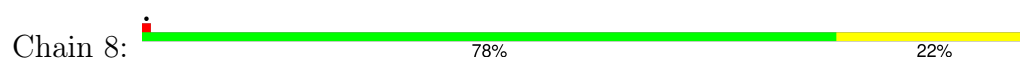




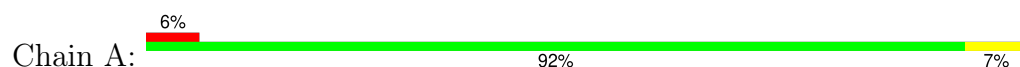
• Molecule 2: 5S ribosomal RNA



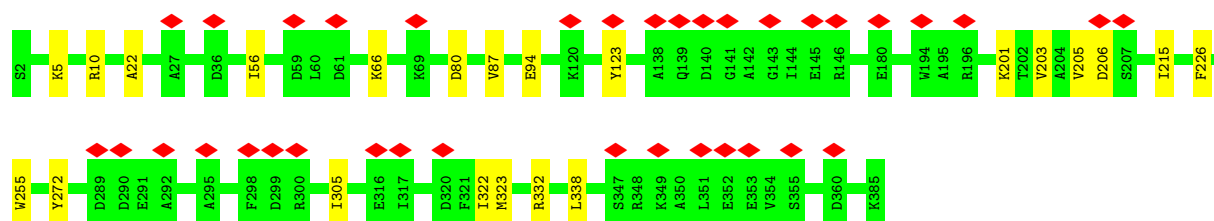
• Molecule 3: 5.8S ribosomal rRNA



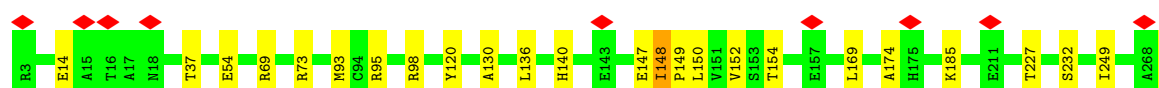
• Molecule 4: uL2

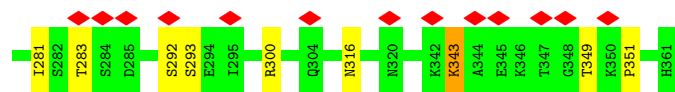


• Molecule 5: uL3

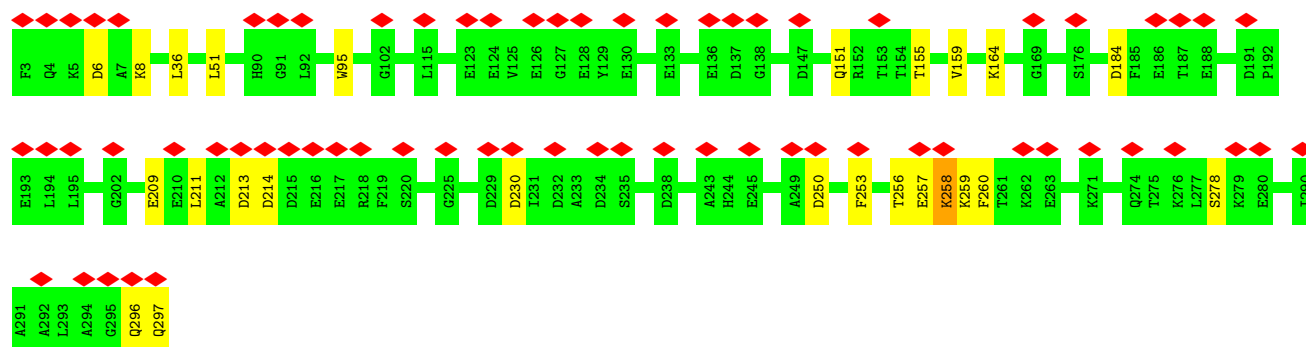


• Molecule 6: uL4

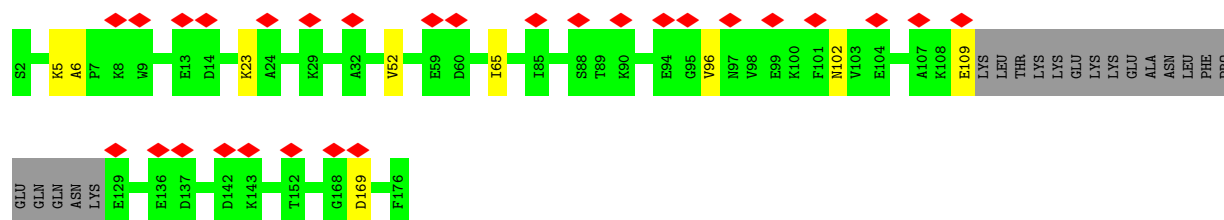
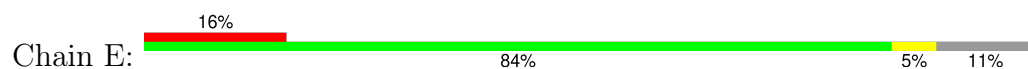




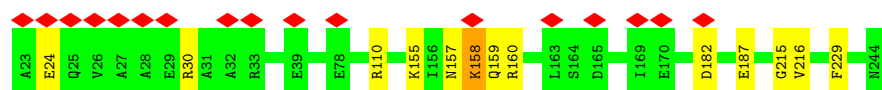
• Molecule 7: uL18



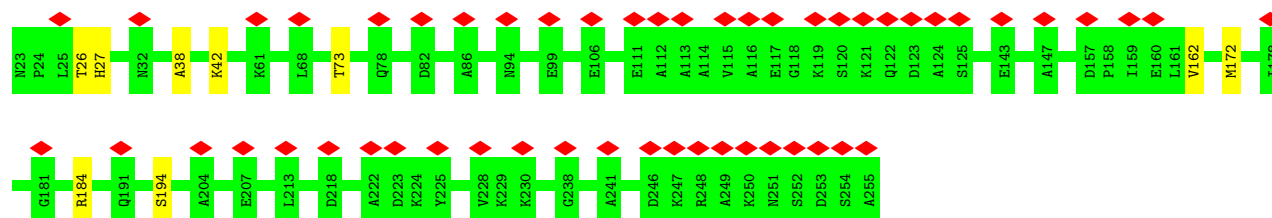
• Molecule 8: eL6



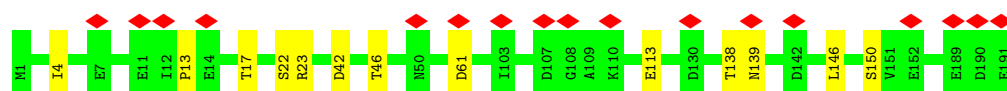
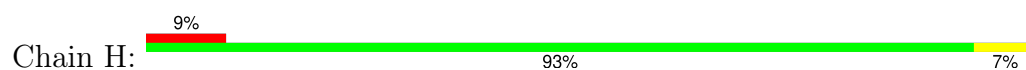
• Molecule 9: uL30



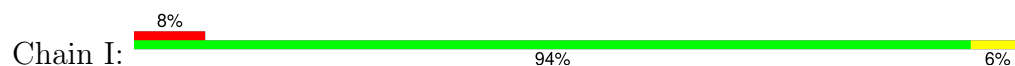
• Molecule 10: eL8



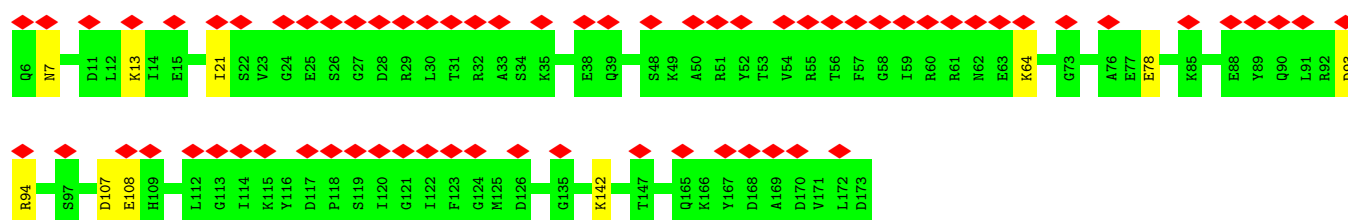
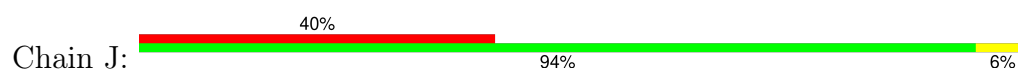
• Molecule 11: uL6



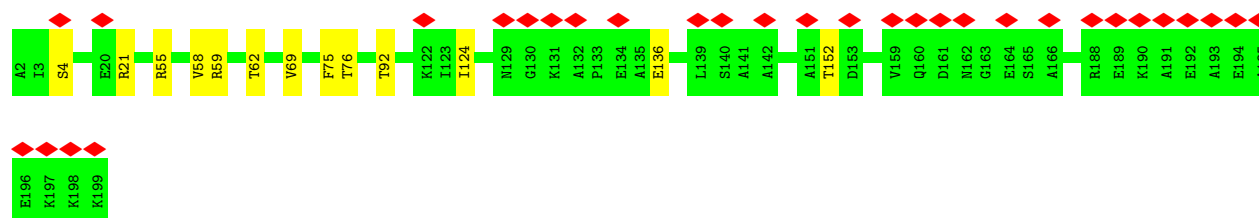
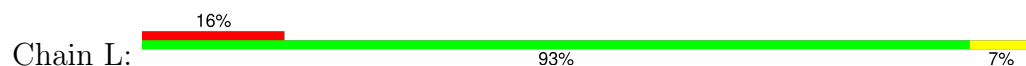
• Molecule 12: uL16



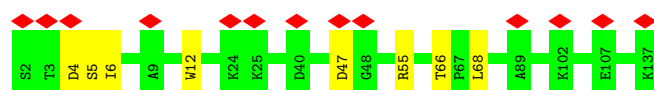
• Molecule 13: uL5



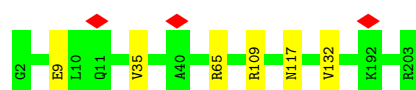
• Molecule 14: eL13



• Molecule 15: eL14

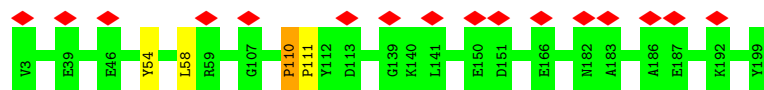


• Molecule 16: eL15



- Molecule 17: uL13

Chain O:  8% 98%



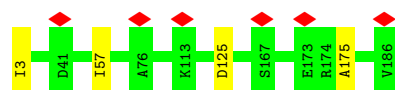
- Molecule 18: uL22

Chain P:  10% 96%



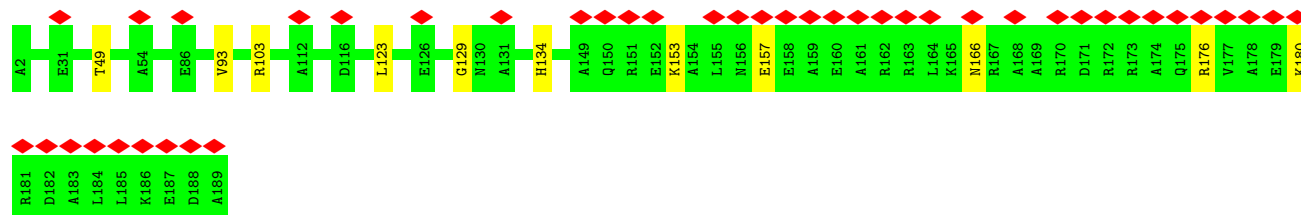
- Molecule 19: eL18

Chain Q:  98%



- Molecule 20: eL19

Chain R:  23% 94% 6%

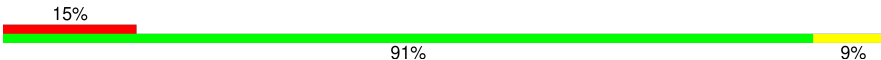


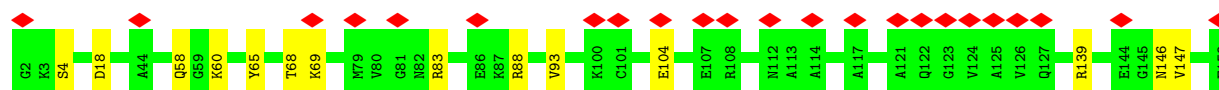
- Molecule 21: eL20

Chain S:  6% 94% 5%

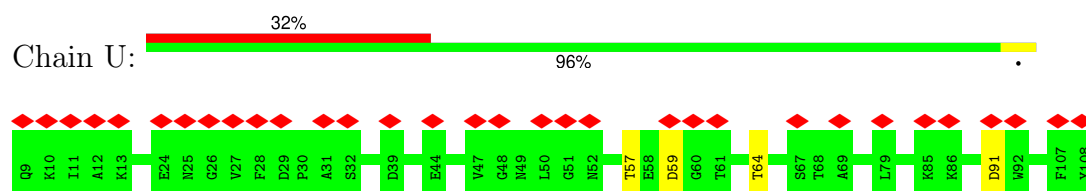


- Molecule 22: eL21

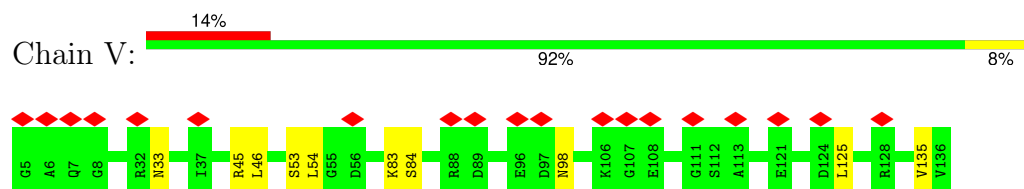
Chain T:  15% 91% 9%



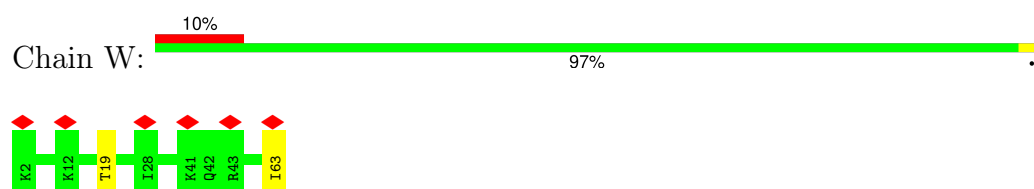
- Molecule 23: eL22



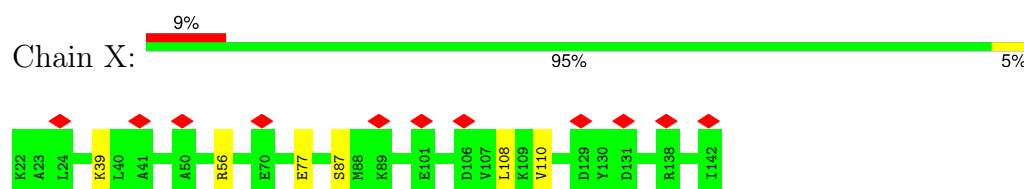
- Molecule 24: uL14



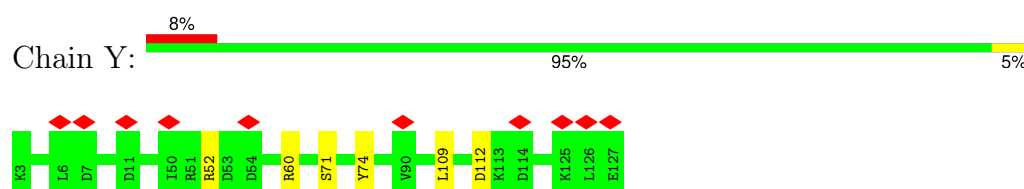
- Molecule 25: eL24



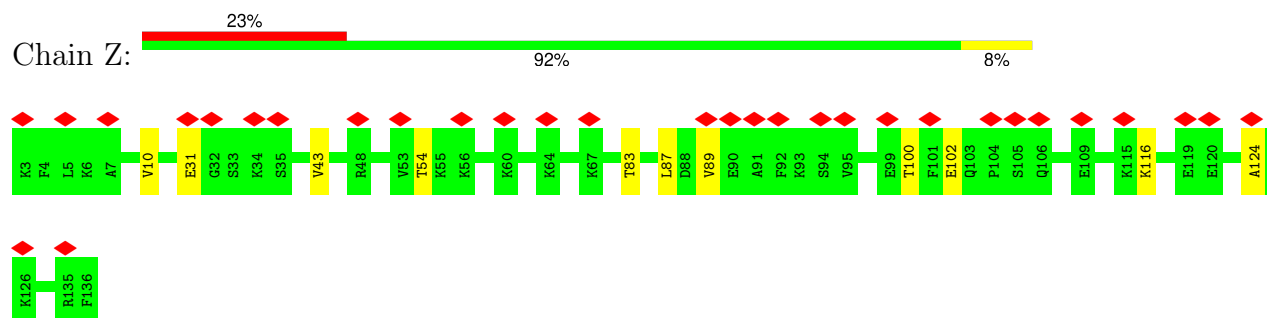
- Molecule 26: uL23



- Molecule 27: uL24

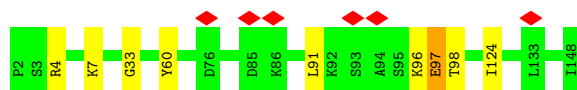


- Molecule 28: eL27

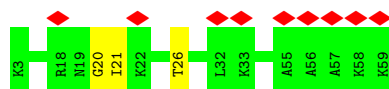


- Molecule 29: uL15

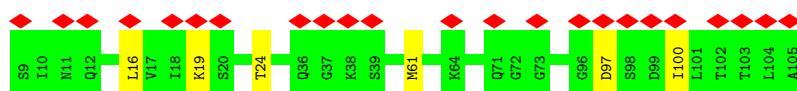




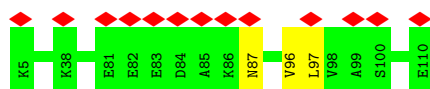
- Molecule 30: eL29



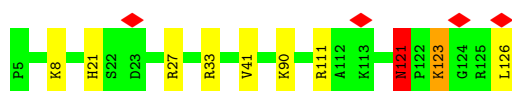
- Molecule 31: eL30



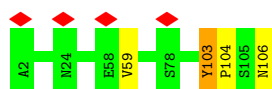
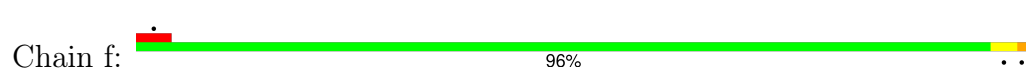
- Molecule 32: eL31



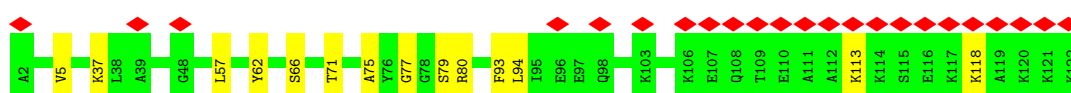
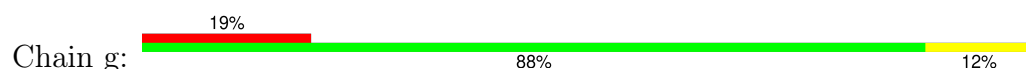
- Molecule 33: eL32



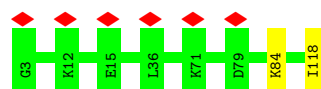
- Molecule 34: eL33



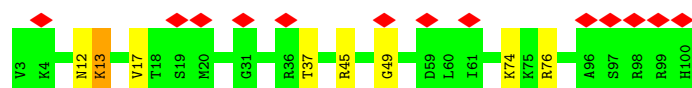
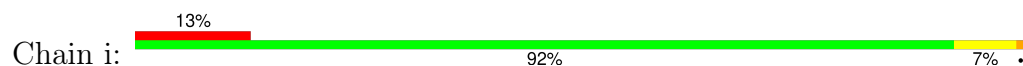
- Molecule 35: eL34



- Molecule 36: uL29



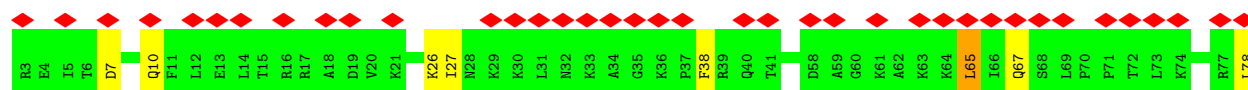
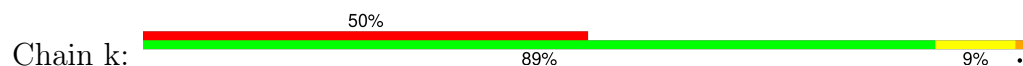
- Molecule 37: eL36



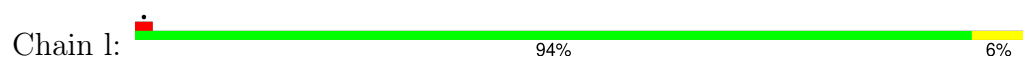
- Molecule 38: eL37



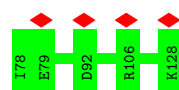
- Molecule 39: eL38



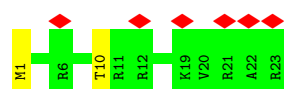
- Molecule 40: eL39



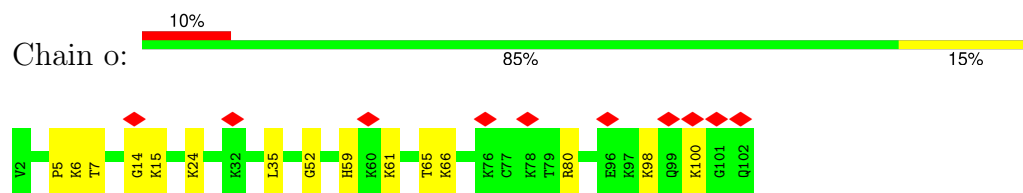
- Molecule 41: eL40



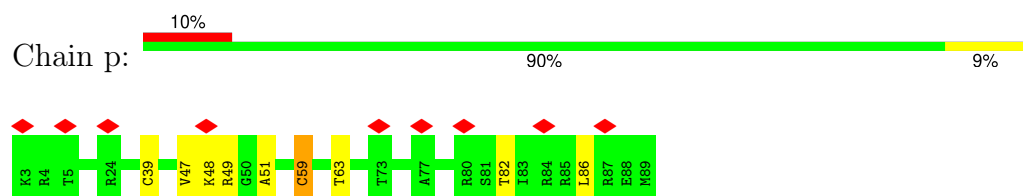
- Molecule 42: eL41



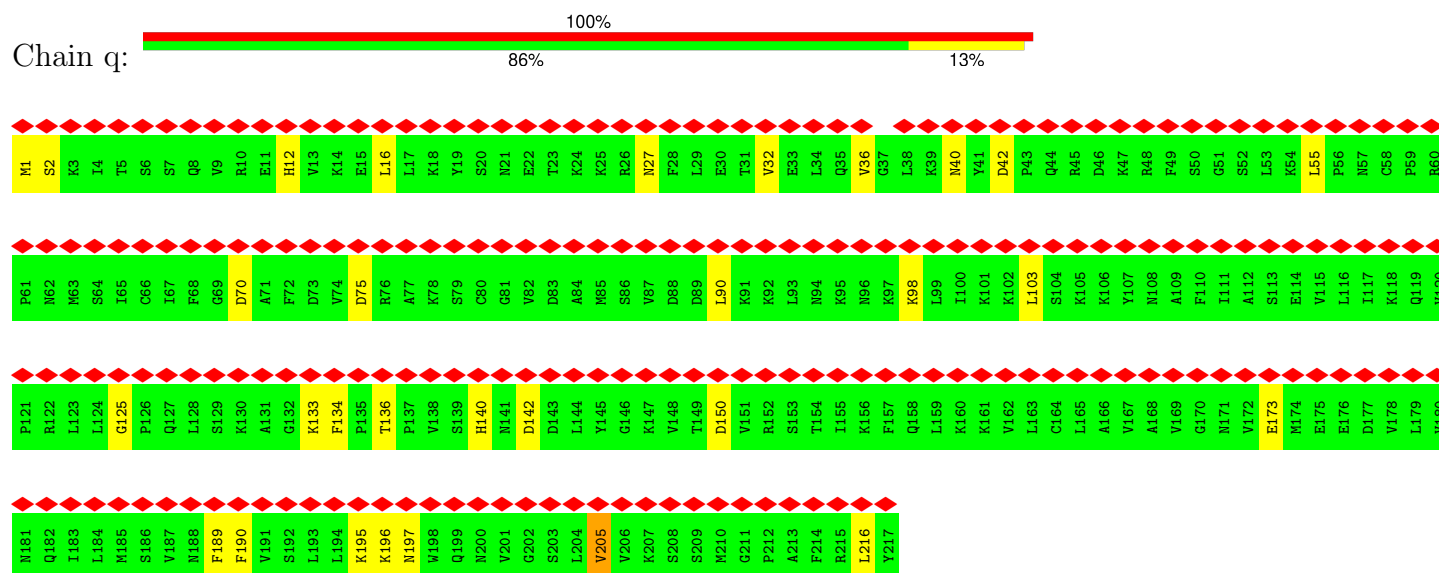
- Molecule 43: eL42



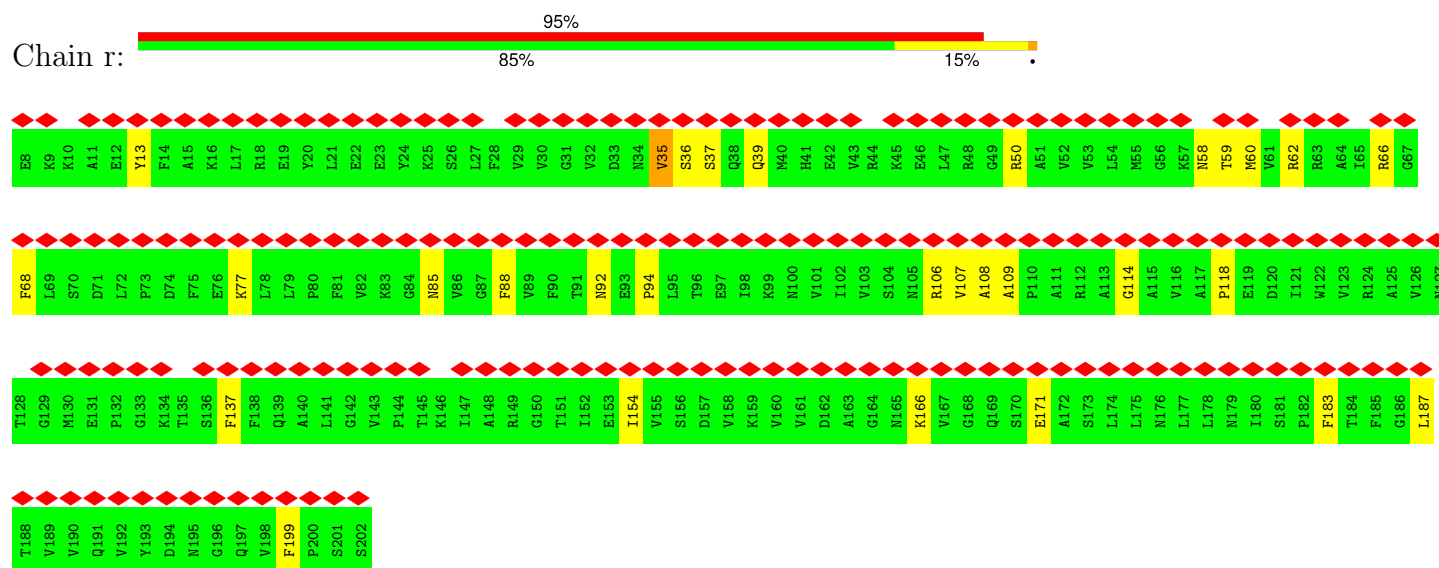
- Molecule 44: eL43



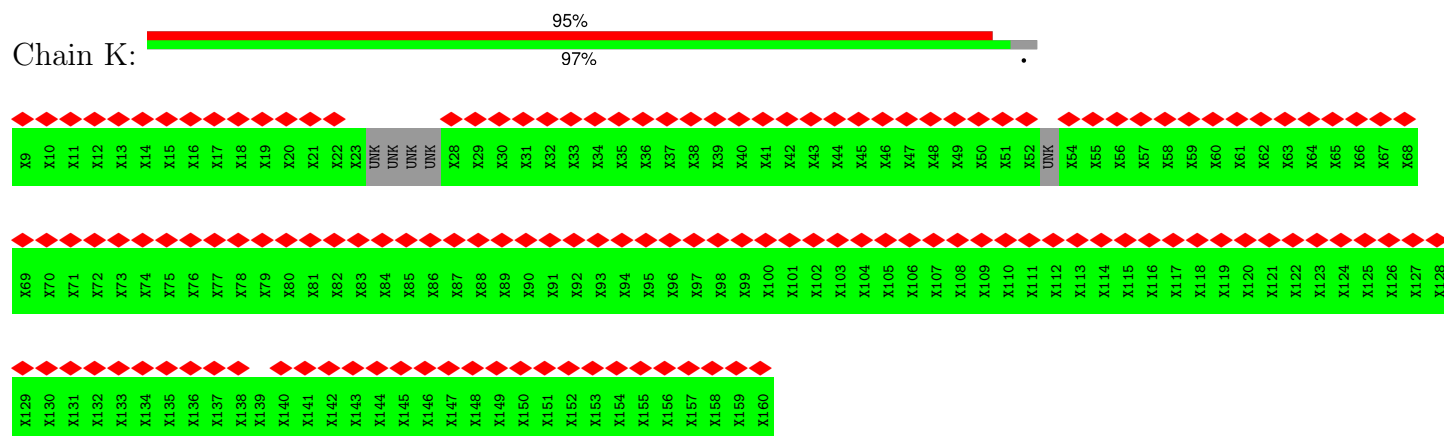
- Molecule 45: uL1



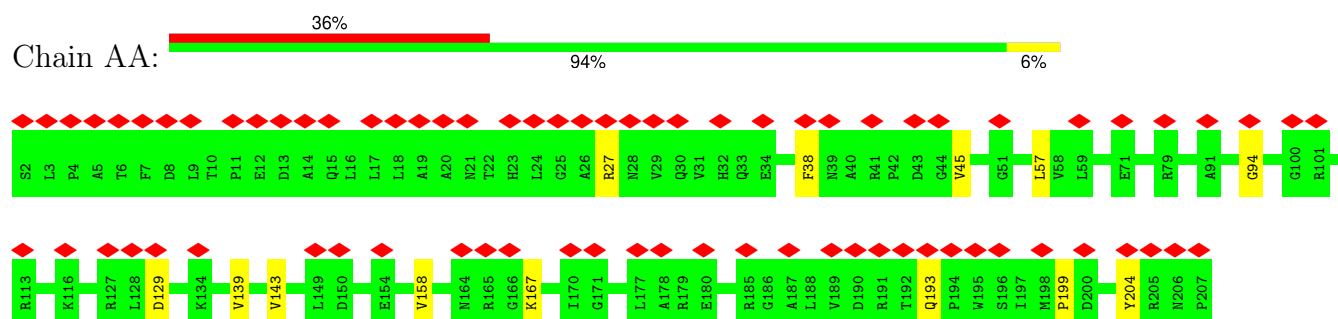
- Molecule 46: uL10



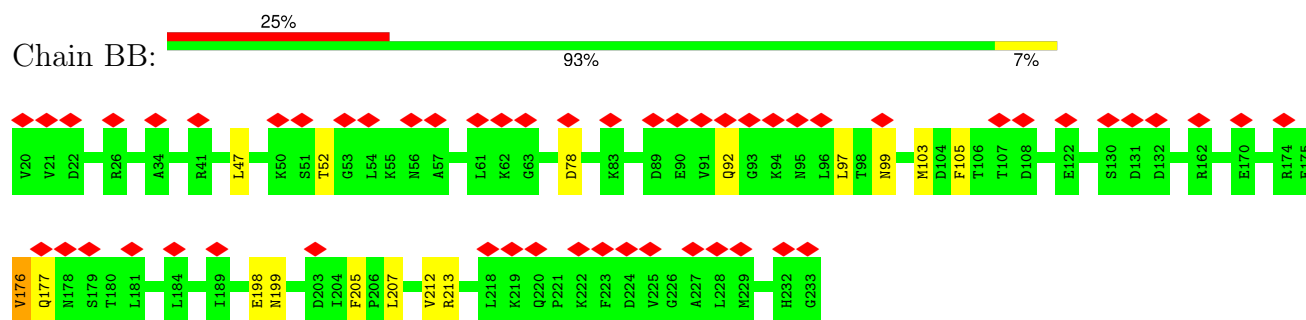
- Molecule 47: L10



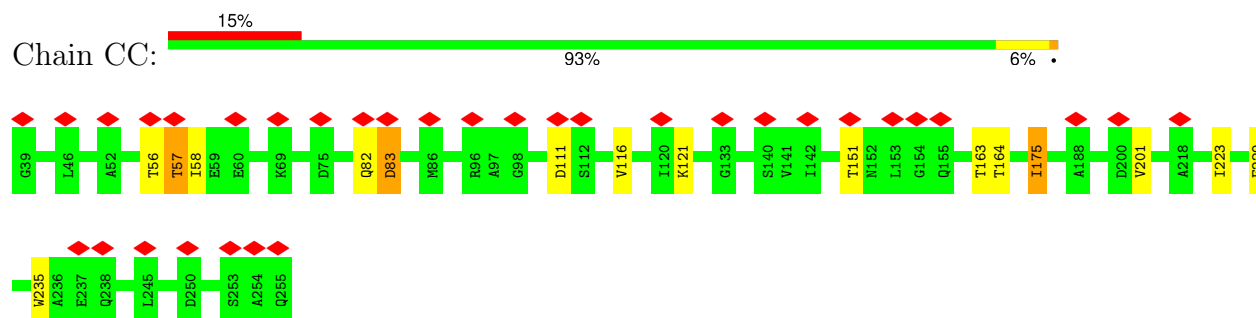
- Molecule 48: uS2



- Molecule 49: eS1

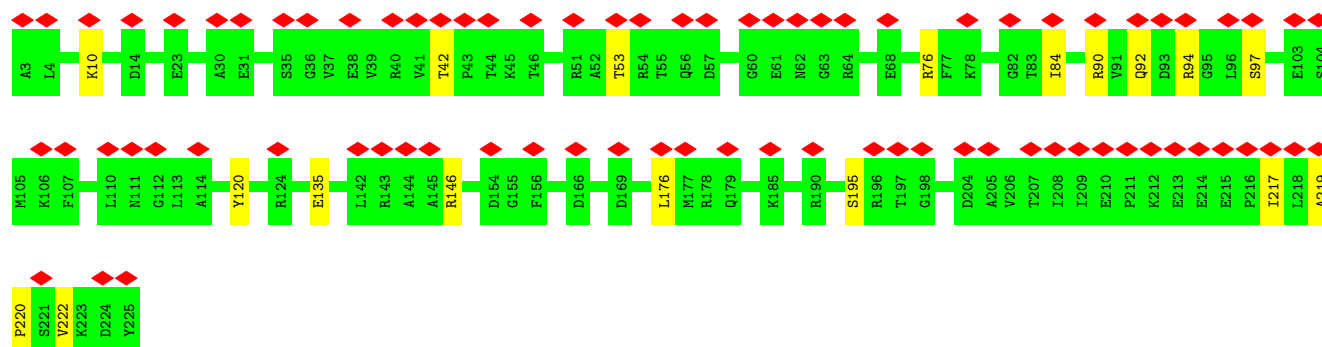


- Molecule 50: uS5

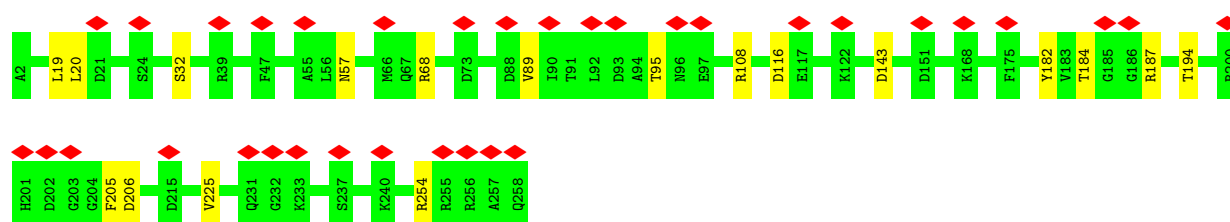


- Molecule 51: uS3

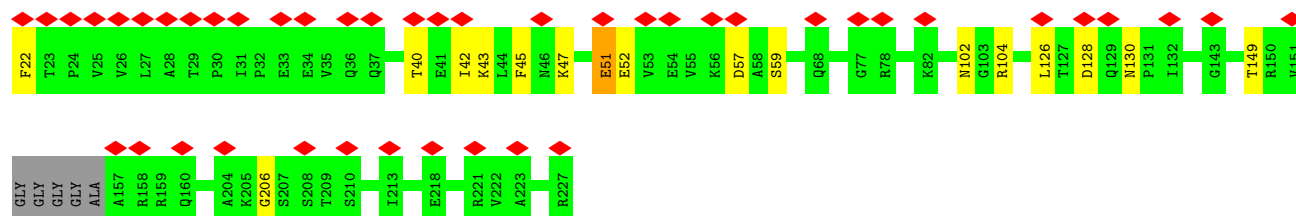




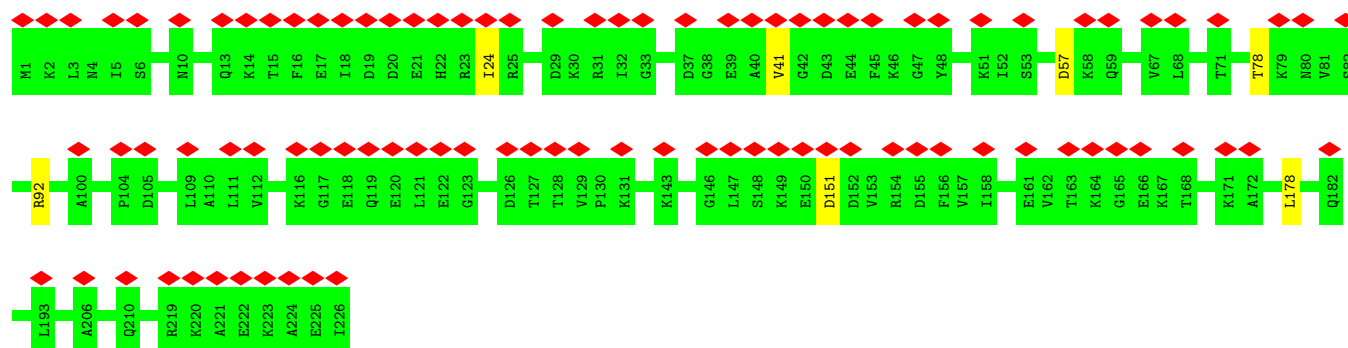
- Molecule 52: eS4



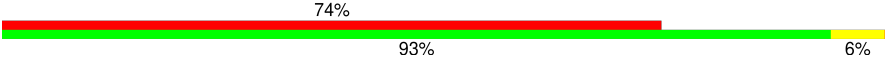
- Molecule 53: uS7

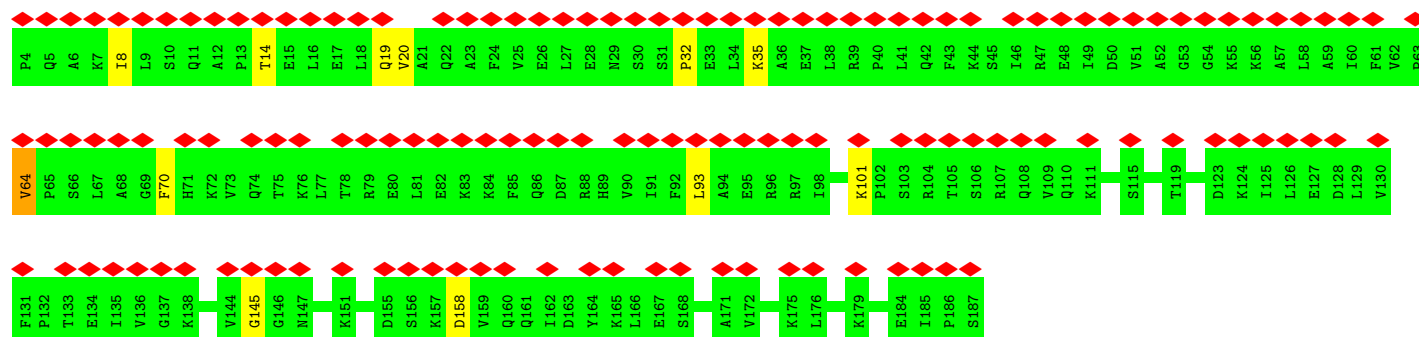


- Molecule 54: eS6




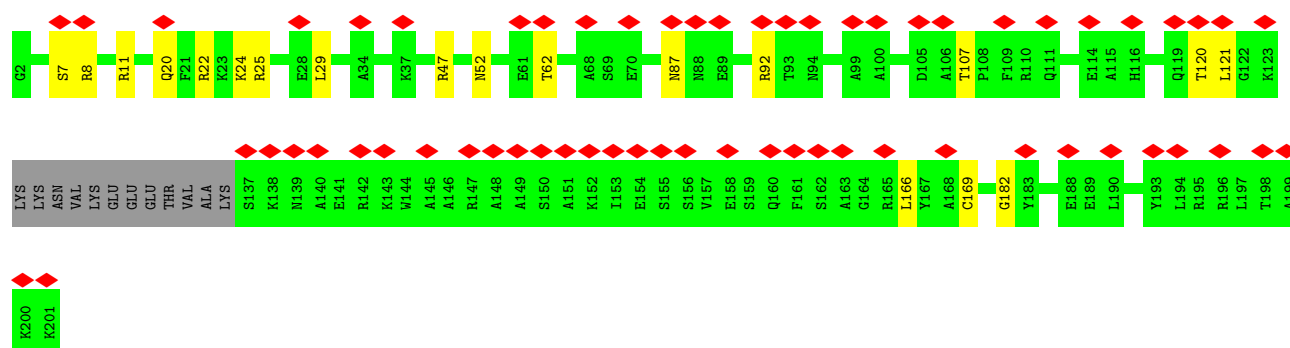
- Molecule 55: eS7

Chain HH: 



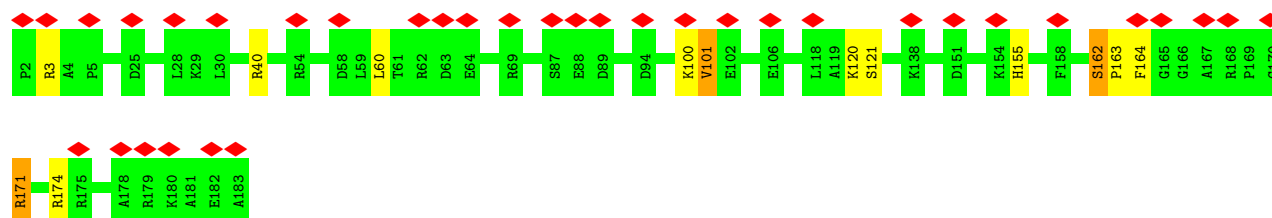
• Molecule 56: eS8

Chain II: 




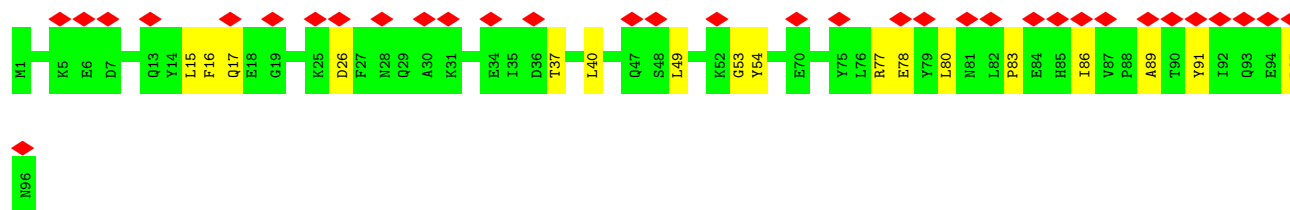
• Molecule 57: uS4

Chain JJ: 

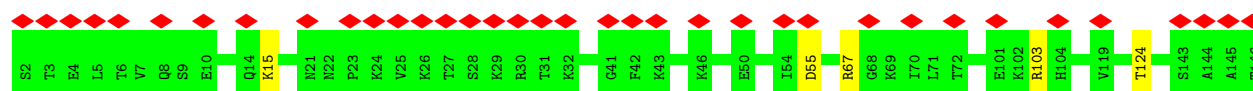


• Molecule 58: eS10

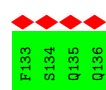
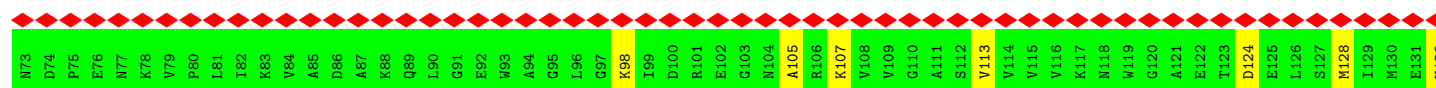
Chain KK: 



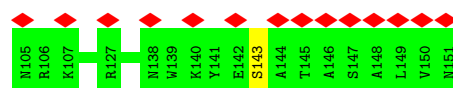
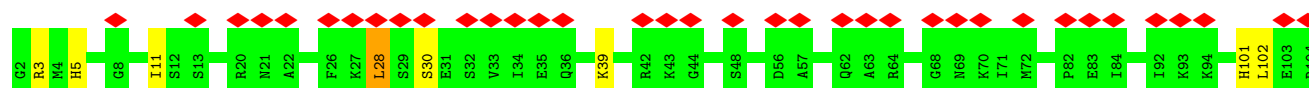
• Molecule 59: uS17



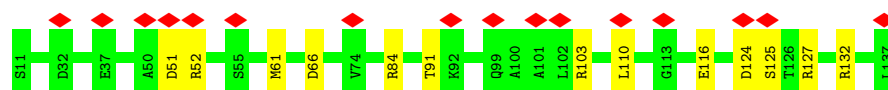
• Molecule 60: eS12



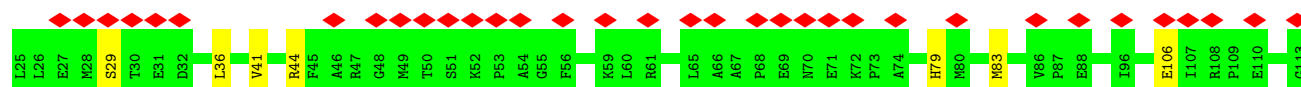
• Molecule 61: uS15



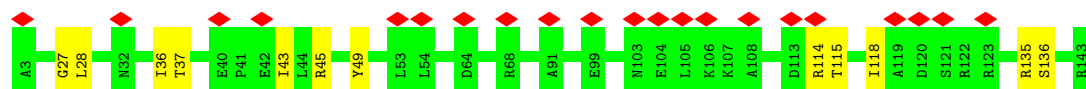
• Molecule 62: uS11



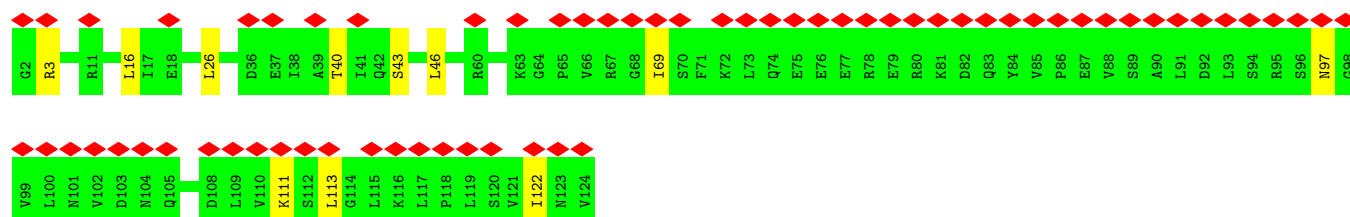
• Molecule 63: uS19



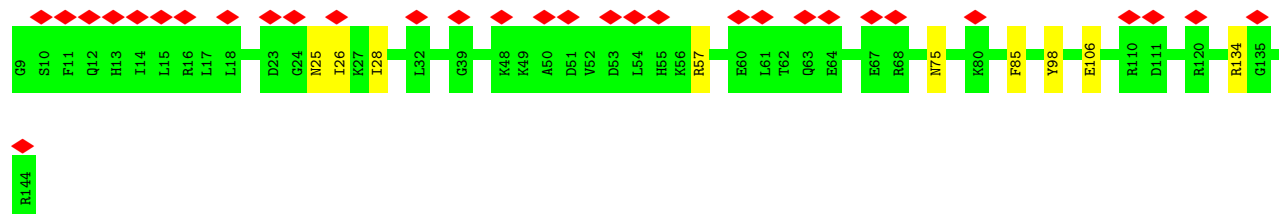
• Molecule 64: uS19



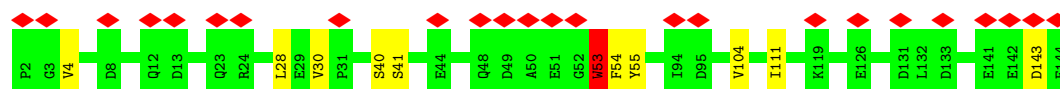
• Molecule 65: eS17



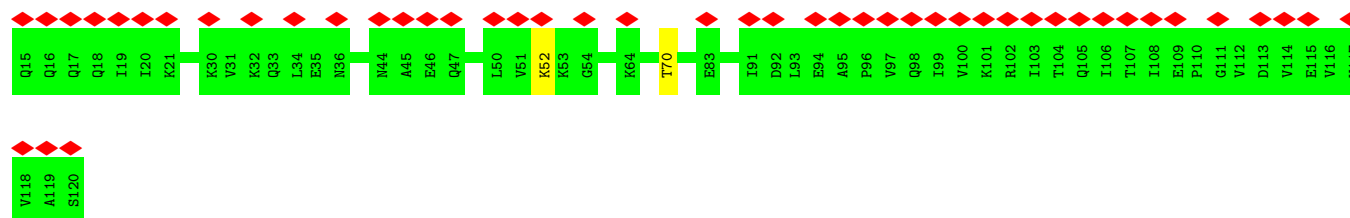
• Molecule 66: uS13



• Molecule 67: eS19



• Molecule 68: uS10

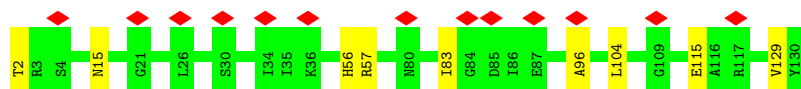


• Molecule 69: eS21

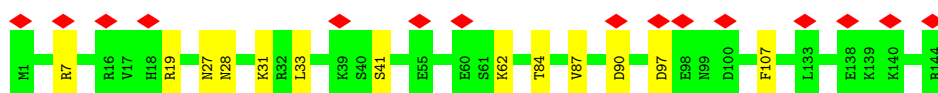




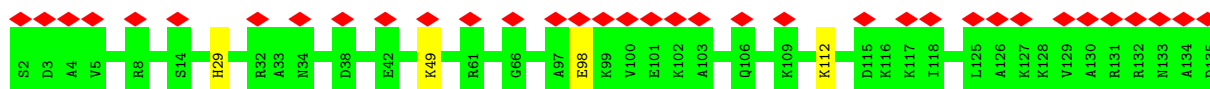
- Molecule 70: uS8



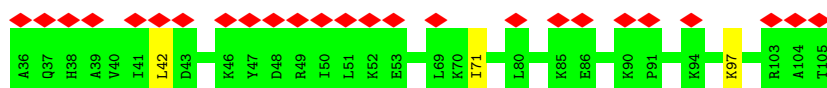
- Molecule 71: uS12



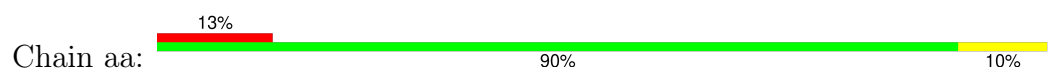
- Molecule 72: eS24



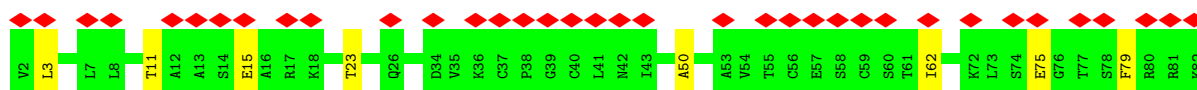
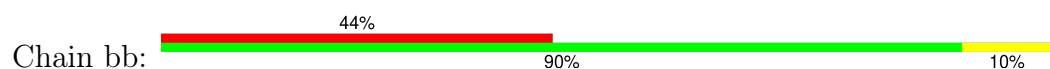
- Molecule 73: eS25



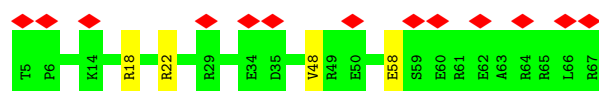
- Molecule 74: eS26



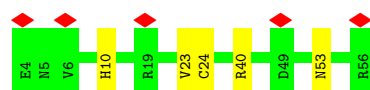
- Molecule 75: eS27



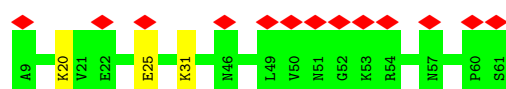
- Molecule 76: eS28



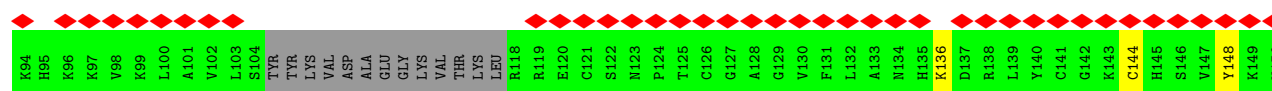
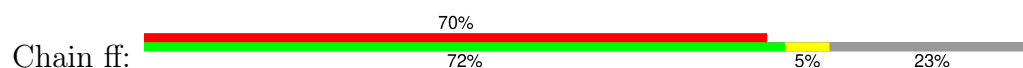
• Molecule 77: uS14



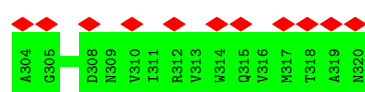
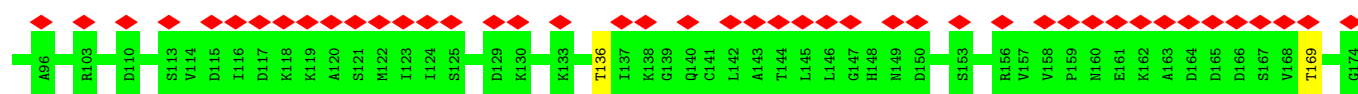
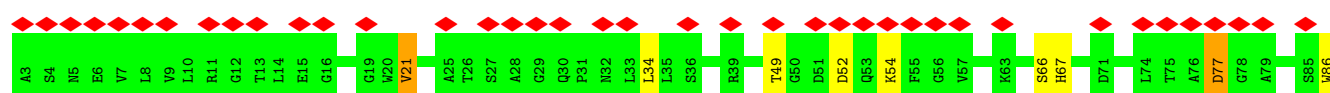
• Molecule 78: eS30



• Molecule 79: eS31

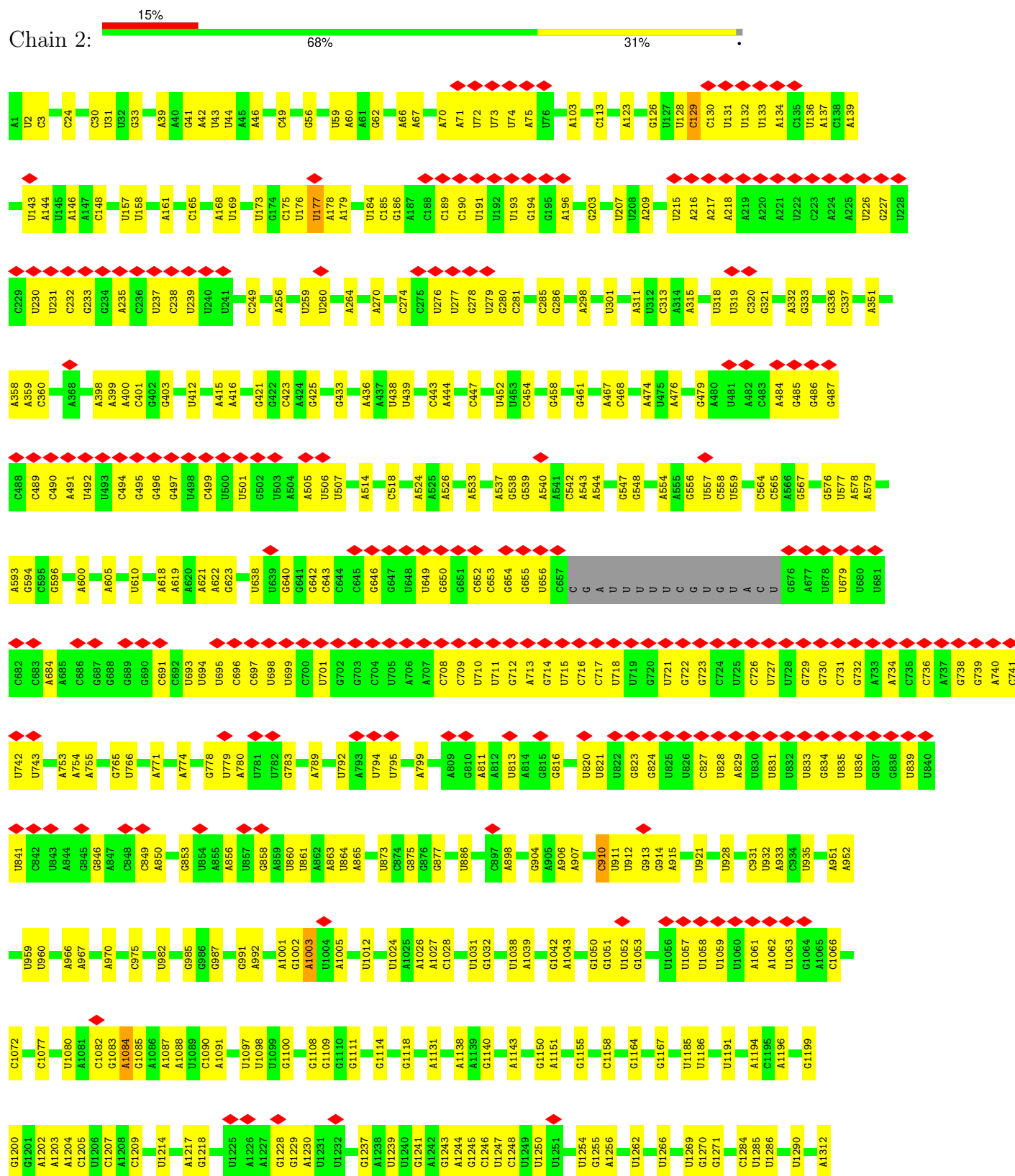


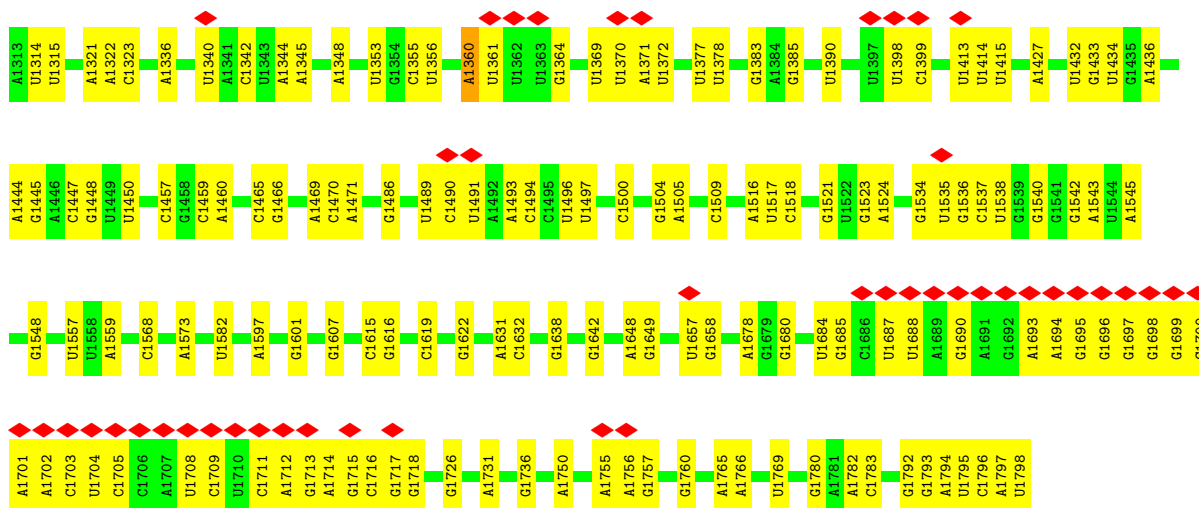
• Molecule 80: RACK1



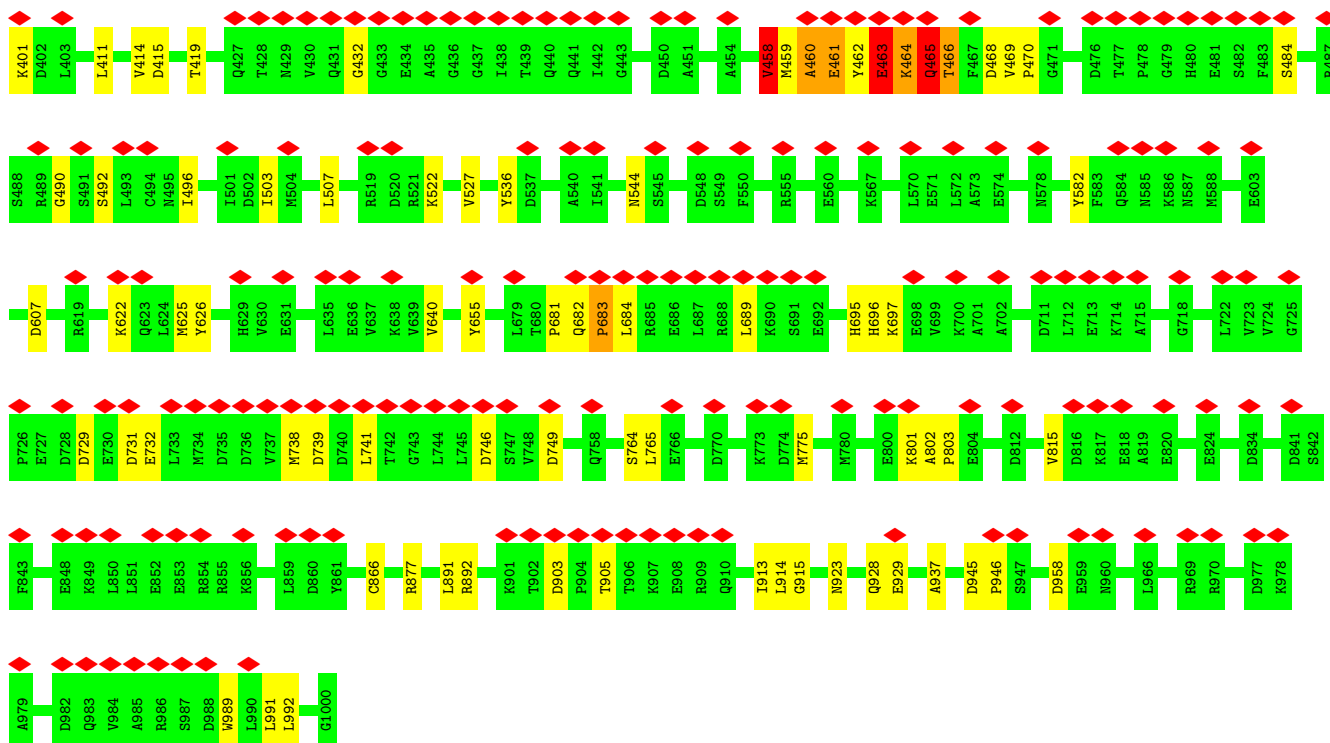
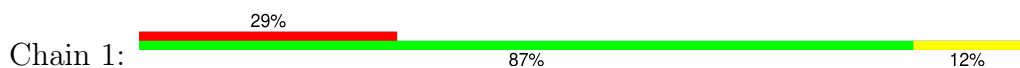
● Molecule 81: 18S ribosomal RNA

Chain 2:

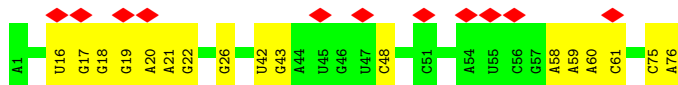
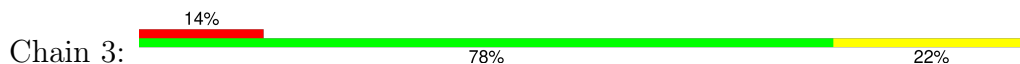




• Molecule 82: eIF5B



• Molecule 83: Met-tRNA-iMet



• Molecule 84: mRNA

Chain 4:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.258	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.042	Depositor
Map size (Å)	424.8, 424.8, 424.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.416, 1.416, 1.416	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: U6A, GDP, ZN

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	5	0.27	0/78264	0.70	10/121981 (0.0%)
2	7	0.24	0/2883	0.68	0/4491
3	8	0.26	0/3724	0.69	0/5798
4	A	0.66	0/1927	0.84	0/2589
5	B	0.65	0/3136	0.83	0/4217
6	C	0.66	0/2787	0.84	1/3773 (0.0%)
7	D	0.67	0/2420	0.80	0/3264
8	E	0.67	0/1260	0.80	0/1694
9	F	0.65	0/1821	0.81	0/2451
10	G	0.67	0/1841	0.79	0/2486
11	H	0.67	0/1545	0.82	0/2081
12	I	0.65	0/1787	0.81	0/2397
13	J	0.68	0/1365	0.82	0/1831
14	L	0.65	0/1609	0.86	0/2158
15	M	0.67	0/1069	0.83	0/1439
16	N	0.62	0/1748	0.82	0/2343
17	O	0.65	0/1585	0.80	0/2128
18	P	0.66	0/1450	0.84	0/1947
19	Q	0.65	0/1461	0.82	0/1960
20	R	0.67	0/1538	0.84	0/2050
21	S	0.63	0/1457	0.81	0/1958
22	T	0.66	0/1292	0.82	0/1732
23	U	0.68	0/812	0.80	0/1099
24	V	0.67	0/993	0.83	0/1335
25	W	0.65	0/525	0.81	0/697
26	X	0.65	0/983	0.78	0/1325
27	Y	0.67	0/999	0.82	0/1334
28	Z	0.66	0/1113	0.82	0/1490
29	a	0.63	0/1199	0.82	0/1605
30	b	0.64	0/468	0.82	0/622
31	c	0.70	0/751	0.79	0/1008
32	d	0.66	0/879	0.80	0/1179

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.66	0/1009	0.85	1/1349 (0.1%)
34	f	0.64	0/860	0.82	0/1157
35	g	0.67	0/964	0.86	0/1282
36	h	0.66	0/959	0.82	0/1276
37	i	0.68	0/770	0.86	0/1021
38	j	0.65	0/688	0.88	0/912
39	k	0.69	1/613 (0.2%)	0.87	0/819
40	l	0.63	0/435	0.80	0/577
41	m	0.64	0/415	0.82	0/551
42	n	0.64	0/219	0.95	0/281
43	o	0.63	0/826	0.84	0/1090
44	p	0.70	0/675	0.86	0/898
45	q	0.71	0/1744	0.84	0/2339
46	r	0.71	0/1538	0.86	0/2079
48	AA	0.66	0/1656	0.81	0/2266
49	BB	0.68	0/1742	0.81	0/2346
50	CC	0.68	0/1665	0.81	1/2263 (0.0%)
51	DD	0.69	0/1759	0.83	0/2368
52	EE	0.66	0/2088	0.82	0/2811
53	FF	0.68	0/1607	0.82	0/2172
54	GG	0.67	0/1844	0.83	0/2464
55	HH	0.68	0/1506	0.83	0/2028
56	II	0.67	0/1505	0.87	0/2010
57	JJ	0.67	0/1502	0.83	0/2013
58	KK	0.66	0/838	0.79	0/1133
59	LL	0.66	0/1192	0.82	0/1608
60	MM	0.74	0/942	0.85	0/1274
61	NN	0.68	0/1215	0.81	0/1638
62	OO	0.69	0/952	0.87	0/1279
63	PP	0.67	0/831	0.81	0/1117
64	QQ	0.67	0/1125	0.83	0/1510
65	RR	0.69	0/998	0.84	0/1337
66	SS	0.67	0/1140	0.84	0/1532
67	TT	0.68	0/1130	0.82	0/1517
68	UU	0.69	0/857	0.82	0/1158
69	VV	0.69	0/693	0.84	0/935
70	WW	0.67	0/1038	0.84	0/1395
71	XX	0.66	0/1141	0.82	0/1520
72	YY	0.68	0/1087	0.83	0/1449
73	ZZ	0.69	0/571	0.82	0/768
74	aa	0.66	0/782	0.87	0/1047
75	bb	0.70	0/620	0.83	0/838
76	cc	0.68	0/499	0.87	0/670

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
77	dd	0.66	0/453	0.85	0/602
78	ee	0.65	0/433	0.81	0/576
79	ff	0.69	0/349	0.88	0/463
80	gg	0.68	0/2495	0.81	0/3392
81	2	0.25	0/42249	0.69	6/65802 (0.0%)
82	1	0.96	30/4776 (0.6%)	0.93	12/6454 (0.2%)
83	3	0.21	0/1823	0.67	0/2842
84	4	0.23	0/147	0.61	0/227
All	All	0.49	31/225656 (0.0%)	0.75	31/330917 (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
4	A	0	1
6	C	0	2
7	D	0	1
9	F	0	2
11	H	0	1
13	J	0	1
17	O	0	1
21	S	0	1
30	b	0	1
33	e	0	1
34	f	0	1
37	i	0	1
39	k	0	1
44	p	0	2
46	r	0	3
49	BB	0	1
50	CC	0	1
51	DD	0	1
52	EE	0	1
53	FF	0	2
54	GG	0	1
55	HH	0	1
56	II	0	3
57	JJ	0	1
58	KK	0	1
59	LL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
64	QQ	0	2
66	SS	0	1
67	TT	0	1
71	XX	0	2
72	YY	0	1
82	1	0	7
All	All	0	48

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	463	GLU	CD-OE1	-13.34	1.10	1.25
82	1	458	VAL	CA-C	-10.00	1.26	1.52
82	1	461	GLU	C-O	-9.97	1.04	1.23
82	1	459	MET	CA-CB	-9.84	1.32	1.53
82	1	462	TYR	CB-CG	-9.81	1.36	1.51
82	1	458	VAL	C-O	-9.32	1.05	1.23
82	1	459	MET	C-O	-9.01	1.06	1.23
82	1	463	GLU	CG-CD	-8.90	1.38	1.51
82	1	462	TYR	CE1-CZ	-8.75	1.27	1.38
82	1	462	TYR	CZ-OH	-8.60	1.23	1.37
82	1	463	GLU	C-O	-8.00	1.08	1.23
82	1	459	MET	CG-SD	-7.77	1.60	1.81
82	1	463	GLU	CD-OE2	-7.74	1.17	1.25
82	1	461	GLU	CD-OE2	-7.48	1.17	1.25
82	1	460	ALA	C-O	-7.09	1.09	1.23
82	1	460	ALA	CA-C	-6.53	1.35	1.52
82	1	464	LYS	CA-CB	-6.46	1.39	1.53
82	1	462	TYR	C-O	-6.43	1.11	1.23
82	1	465	GLN	N-CA	-6.16	1.34	1.46
82	1	462	TYR	CA-C	-6.16	1.36	1.52
82	1	462	TYR	CD1-CE1	-6.10	1.30	1.39
82	1	459	MET	N-CA	-5.80	1.34	1.46
82	1	464	LYS	CA-C	-5.51	1.38	1.52
82	1	463	GLU	CB-CG	-5.49	1.41	1.52
82	1	464	LYS	N-CA	-5.27	1.35	1.46
82	1	462	TYR	CD2-CE2	-5.22	1.31	1.39
82	1	461	GLU	CA-C	-5.21	1.39	1.52
82	1	461	GLU	CD-OE1	-5.19	1.20	1.25
82	1	461	GLU	C-N	-5.14	1.22	1.34
82	1	458	VAL	CB-CG1	-5.11	1.42	1.52
39	k	78	LEU	C-O	5.03	1.32	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	1	458	VAL	CG1-CB-CG2	-9.46	95.76	110.90
82	1	464	LYS	N-CA-C	9.16	135.74	111.00
82	1	463	GLU	CB-CA-C	-9.05	92.30	110.40
82	1	461	GLU	N-CA-CB	-8.50	95.31	110.60
1	5	1607	U	C2'-C3'-O3'	8.22	127.58	109.50
1	5	2662	G	C2'-C3'-O3'	7.57	126.16	109.50
1	5	567	G	C2'-C3'-O3'	7.38	125.74	109.50
1	5	3239	G	C2'-C3'-O3'	6.74	124.49	113.70
81	2	1084	A	C2'-C3'-O3'	6.67	124.37	113.70
82	1	463	GLU	CB-CG-CD	-6.57	96.46	114.20
82	1	464	LYS	CD-CE-NZ	-6.52	96.70	111.70
82	1	461	GLU	N-CA-C	6.52	128.60	111.00
1	5	1352	A	C2'-C3'-O3'	6.26	123.72	113.70
82	1	465	GLN	N-CA-CB	-6.15	99.53	110.60
82	1	460	ALA	C-N-CA	6.13	137.03	121.70
1	5	1284	C	C2'-C3'-O3'	6.04	123.36	113.70
1	5	3357	U	C2'-C3'-O3'	5.81	123.00	113.70
82	1	462	TYR	CB-CA-C	-5.74	98.93	110.40
82	1	462	TYR	CA-C-O	-5.73	108.06	120.10
1	5	166	C	C2'-C3'-O3'	5.59	122.65	113.70
81	2	1360	A	C2'-C3'-O3'	5.55	122.58	113.70
1	5	873	C	C4'-C3'-O3'	5.50	123.99	113.00
6	C	343	LYS	CB-CA-C	5.49	121.38	110.40
81	2	910	C	C2'-C3'-O3'	5.34	122.24	113.70
82	1	461	GLU	OE1-CD-OE2	-5.30	116.94	123.30
81	2	129	C	C2'-C3'-O3'	5.21	122.05	113.70
81	2	1003	A	N9-C1'-C2'	5.19	120.75	114.00
81	2	177	U	C2'-C3'-O3'	5.10	121.86	113.70
50	CC	83	ASP	CB-CA-C	5.10	120.60	110.40
1	5	91	G	C2'-C3'-O3'	5.08	121.83	113.70
33	e	121	ASN	CB-CA-C	5.08	120.56	110.40

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
82	1	458	VAL	Mainchain
82	1	463	GLU	Mainchain
82	1	683	PRO	Peptide
82	1	802	ALA	Peptide
82	1	903	ASP	Peptide

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Mol	Chain	Res	Type	Group
82	1	914	LEU	Peptide
82	1	915	GLY	Peptide
4	A	196	TRP	Peptide
49	BB	177	GLN	Peptide
6	C	148	ILE	Peptide
6	C	349	THR	Peptide
50	CC	82	GLN	Peptide
7	D	258	LYS	Peptide
51	DD	219	ALA	Peptide
52	EE	19	LEU	Peptide
9	F	157	ASN	Peptide
9	F	215	GLY	Peptide
53	FF	45	PHE	Peptide
53	FF	51	GLU	Peptide
54	GG	57	ASP	Peptide
11	H	22	SER	Peptide
55	HH	64	VAL	Peptide
56	II	107	THR	Peptide
56	II	182	GLY	Peptide
56	II	8	ARG	Peptide
13	J	93	ASP	Peptide
57	JJ	163	PRO	Peptide
58	KK	53	GLY	Peptide
59	LL	15	LYS	Peptide
17	O	110	PRO	Peptide
64	QQ	114	ARG	Peptide
64	QQ	115	THR	Peptide
21	S	22	PRO	Peptide
66	SS	25	ASN	Peptide
67	TT	53	TRP	Peptide
71	XX	62	LYS	Peptide
71	XX	87	VAL	Peptide
72	YY	29	HIS	Peptide
30	b	20	GLY	Peptide
33	e	121	ASN	Peptide
34	f	103	TYR	Peptide
37	i	12	ASN	Peptide
39	k	65	LEU	Peptide
44	p	47	VAL	Peptide
44	p	59	CYS	Peptide
46	r	108	ALA	Peptide
46	r	109	ALA	Peptide

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Mol	Chain	Res	Type	Group
46	r	36	SER	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	
4	A	247/249 (99%)	223 (90%)	17 (7%)	7 (3%)	4	16
5	B	382/384 (100%)	325 (85%)	54 (14%)	3 (1%)	16	45
6	C	357/359 (99%)	287 (80%)	54 (15%)	16 (4%)	2	8
7	D	293/295 (99%)	266 (91%)	24 (8%)	3 (1%)	13	40
8	E	152/175 (87%)	142 (93%)	8 (5%)	2 (1%)	10	33
9	F	220/222 (99%)	194 (88%)	22 (10%)	4 (2%)	7	25
10	G	231/233 (99%)	210 (91%)	19 (8%)	2 (1%)	14	43
11	H	189/191 (99%)	165 (87%)	21 (11%)	3 (2%)	8	28
12	I	214/216 (99%)	191 (89%)	18 (8%)	5 (2%)	5	20
13	J	166/168 (99%)	149 (90%)	16 (10%)	1 (1%)	22	52
14	L	196/198 (99%)	173 (88%)	19 (10%)	4 (2%)	6	23
15	M	134/136 (98%)	118 (88%)	14 (10%)	2 (2%)	8	29
16	N	200/202 (99%)	183 (92%)	16 (8%)	1 (0%)	25	56
17	O	195/197 (99%)	184 (94%)	9 (5%)	2 (1%)	13	40
18	P	178/180 (99%)	158 (89%)	18 (10%)	2 (1%)	12	37
19	Q	182/184 (99%)	169 (93%)	12 (7%)	1 (0%)	25	56
20	R	186/188 (99%)	174 (94%)	11 (6%)	1 (0%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	S	167/169 (99%)	152 (91%)	12 (7%)	3 (2%)	7	25
22	T	156/158 (99%)	141 (90%)	13 (8%)	2 (1%)	10	33
23	U	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
24	V	130/132 (98%)	115 (88%)	13 (10%)	2 (2%)	8	29
25	W	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
26	X	119/121 (98%)	108 (91%)	10 (8%)	1 (1%)	16	45
27	Y	123/125 (98%)	111 (90%)	12 (10%)	0	100	100
28	Z	132/134 (98%)	114 (86%)	16 (12%)	2 (2%)	8	29
29	a	145/147 (99%)	122 (84%)	19 (13%)	4 (3%)	4	16
30	b	55/57 (96%)	46 (84%)	7 (13%)	2 (4%)	3	12
31	c	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
32	d	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
33	e	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	7	27
34	f	103/105 (98%)	92 (89%)	9 (9%)	2 (2%)	6	24
35	g	119/121 (98%)	106 (89%)	10 (8%)	3 (2%)	4	18
36	h	114/116 (98%)	108 (95%)	5 (4%)	1 (1%)	14	43
37	i	94/98 (96%)	79 (84%)	13 (14%)	2 (2%)	5	22
38	j	83/85 (98%)	75 (90%)	8 (10%)	0	100	100
39	k	74/76 (97%)	64 (86%)	10 (14%)	0	100	100
40	l	47/49 (96%)	39 (83%)	7 (15%)	1 (2%)	5	22
41	m	49/51 (96%)	46 (94%)	3 (6%)	0	100	100
42	n	21/23 (91%)	19 (90%)	2 (10%)	0	100	100
43	o	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	2
44	p	85/87 (98%)	70 (82%)	12 (14%)	3 (4%)	3	12
45	q	213/217 (98%)	163 (76%)	45 (21%)	5 (2%)	5	20
46	r	191/195 (98%)	144 (75%)	41 (22%)	6 (3%)	3	14
48	AA	204/206 (99%)	166 (81%)	31 (15%)	7 (3%)	3	13
49	BB	212/214 (99%)	187 (88%)	23 (11%)	2 (1%)	14	43
50	CC	215/217 (99%)	188 (87%)	21 (10%)	6 (3%)	4	16
51	DD	221/223 (99%)	189 (86%)	26 (12%)	6 (3%)	4	17
52	EE	255/257 (99%)	217 (85%)	33 (13%)	5 (2%)	6	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	FF	197/206 (96%)	155 (79%)	36 (18%)	6 (3%)	3	15
54	GG	224/226 (99%)	201 (90%)	22 (10%)	1 (0%)	30	60
55	HH	182/184 (99%)	157 (86%)	22 (12%)	3 (2%)	8	28
56	II	183/199 (92%)	153 (84%)	25 (14%)	5 (3%)	4	17
57	JJ	180/182 (99%)	156 (87%)	17 (9%)	7 (4%)	2	10
58	KK	94/96 (98%)	81 (86%)	10 (11%)	3 (3%)	3	13
59	LL	143/145 (99%)	127 (89%)	15 (10%)	1 (1%)	19	49
60	MM	122/124 (98%)	85 (70%)	34 (28%)	3 (2%)	4	18
61	NN	148/150 (99%)	137 (93%)	7 (5%)	4 (3%)	4	17
62	OO	125/127 (98%)	106 (85%)	16 (13%)	3 (2%)	5	19
63	PP	101/103 (98%)	88 (87%)	12 (12%)	1 (1%)	13	40
64	QQ	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9	31
65	RR	119/123 (97%)	99 (83%)	19 (16%)	1 (1%)	16	45
66	SS	134/136 (98%)	116 (87%)	17 (13%)	1 (1%)	19	49
67	TT	141/143 (99%)	128 (91%)	10 (7%)	3 (2%)	5	22
68	UU	104/106 (98%)	94 (90%)	10 (10%)	0	100	100
69	VV	85/87 (98%)	71 (84%)	14 (16%)	0	100	100
70	WW	127/129 (98%)	114 (90%)	10 (8%)	3 (2%)	5	19
71	XX	142/144 (99%)	125 (88%)	14 (10%)	3 (2%)	5	22
72	YY	132/134 (98%)	119 (90%)	12 (9%)	1 (1%)	16	45
73	ZZ	68/70 (97%)	59 (87%)	8 (12%)	1 (2%)	8	29
74	aa	95/97 (98%)	76 (80%)	14 (15%)	5 (5%)	1	5
75	bb	79/81 (98%)	63 (80%)	15 (19%)	1 (1%)	10	33
76	cc	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
77	dd	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
78	ee	51/53 (96%)	44 (86%)	7 (14%)	0	100	100
79	ff	40/57 (70%)	20 (50%)	19 (48%)	1 (2%)	4	18
80	gg	312/318 (98%)	265 (85%)	43 (14%)	4 (1%)	10	33
82	1	598/600 (100%)	476 (80%)	94 (16%)	28 (5%)	2	7
All	All	11802/12025 (98%)	10238 (87%)	1339 (11%)	225 (2%)	9	24

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	181	LYS
4	A	196	TRP
6	C	54	GLU
6	C	148	ILE
6	C	316	ASN
7	D	259	LYS
9	F	158	LYS
11	H	23	ARG
14	L	4	SER
14	L	76	THR
15	M	5	SER
15	M	6	ILE
17	O	110	PRO
17	O	111	PRO
21	S	13	ARG
22	T	18	ASP
30	b	21	ILE
33	e	121	ASN
34	f	103	TYR
37	i	13	LYS
48	AA	158	VAL
51	DD	217	ILE
53	FF	52	GLU
54	GG	151	ASP
56	II	11	ARG
60	MM	113	VAL
62	OO	51	ASP
66	SS	26	ILE
70	WW	96	ALA
73	ZZ	71	ILE
74	aa	86	VAL
82	1	463	GLU
82	1	465	GLN
82	1	684	LEU
82	1	695	HIS
82	1	696	HIS
82	1	923	ASN
4	A	144	ASN
5	B	5	LYS
5	B	22	ALA
6	C	73	ARG
6	C	130	ALA
6	C	140	HIS

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Mol	Chain	Res	Type
9	F	159	GLN
10	G	38	ALA
12	I	111	LEU
12	I	114	GLY
12	I	144	ASN
13	J	94	ARG
21	S	24	LEU
24	V	84	SER
28	Z	124	ALA
29	a	124	ILE
30	b	26	THR
35	g	57	LEU
40	l	33	ASN
43	o	6	LYS
43	o	14	GLY
44	p	39	CYS
44	p	48	LYS
45	q	27	ASN
45	q	40	ASN
45	q	125	GLY
46	r	35	VAL
48	AA	94	GLY
50	CC	57	THR
51	DD	53	THR
52	EE	20	LEU
52	EE	187	ARG
55	HH	145	GLY
56	II	52	ASN
57	JJ	100	LYS
57	JJ	171	ARG
58	KK	83	PRO
62	OO	52	ARG
62	OO	103	ARG
67	TT	53	TRP
67	TT	54	PHE
67	TT	55	TYR
70	WW	56	HIS
71	XX	97	ASP
74	aa	12	LYS
80	gg	77	ASP
82	1	461	GLU
82	1	626	TYR

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Mol	Chain	Res	Type
82	1	640	VAL
82	1	729	ASP
4	A	123	ARG
4	A	180	LEU
4	A	182	ALA
6	C	147	GLU
6	C	149	PRO
6	C	185	LYS
6	C	269	SER
6	C	293	SER
6	C	351	PRO
18	P	4	TYR
19	Q	175	ALA
20	R	129	GLY
29	a	96	LYS
29	a	97	GLU
33	e	123	LYS
34	f	104	PRO
35	g	75	ALA
46	r	94	PRO
48	AA	27	ARG
48	AA	204	TYR
49	BB	176	VAL
50	CC	56	THR
51	DD	97	SER
53	FF	47	LYS
53	FF	102	ASN
56	II	120	THR
57	JJ	121	SER
58	KK	26	ASP
59	LL	55	ASP
60	MM	105	ALA
63	PP	29	SER
72	YY	49	LYS
74	aa	7	SER
79	ff	144	CYS
80	gg	54	LYS
82	1	432	GLY
82	1	466	THR
82	1	496	ILE
82	1	689	LEU
82	1	803	PRO

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Mol	Chain	Res	Type
82	1	945	ASP
5	B	272	TYR
6	C	14	GLU
6	C	292	SER
7	D	260	PHE
8	E	5	LYS
9	F	24	GLU
12	I	112	GLN
18	P	158	ALA
22	T	69	LYS
24	V	53	SER
36	h	84	LYS
43	o	15	LYS
43	o	66	LYS
46	r	118	PRO
48	AA	167	LYS
50	CC	111	ASP
50	CC	175	ILE
51	DD	92	GLN
51	DD	220	PRO
52	EE	205	PHE
53	FF	130	ASN
53	FF	206	GLY
55	HH	64	VAL
56	II	22	ARG
56	II	24	LYS
57	JJ	162	SER
57	JJ	164	PHE
58	KK	89	ALA
60	MM	124	ASP
61	NN	143	SER
70	WW	57	ARG
71	XX	90	ASP
74	aa	61	GLU
80	gg	21	VAL
82	1	460	ALA
82	1	484	SER
82	1	682	GLN
82	1	905	THR
4	A	197	PRO
6	C	174	ALA
6	C	232	SER

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Mol	Chain	Res	Type
7	D	214	ASP
8	E	6	ALA
12	I	19	LYS
14	L	62	THR
14	L	75	PHE
21	S	18	SER
26	X	56	ARG
28	Z	87	LEU
43	o	52	GLY
43	o	65	THR
45	q	2	SER
46	r	58	ASN
50	CC	151	THR
51	DD	94	ARG
53	FF	59	SER
57	JJ	101	VAL
57	JJ	120	LYS
61	NN	3	ARG
61	NN	28	LEU
61	NN	30	SER
74	aa	80	HIS
75	bb	50	ALA
80	gg	269	GLN
82	1	683	PRO
82	1	731	ASP
82	1	937	ALA
82	1	946	PRO
9	F	216	VAL
10	G	42	LYS
11	H	13	PRO
29	a	33	GLY
43	o	7	THR
44	p	51	ALA
46	r	114	GLY
48	AA	193	GLN
48	AA	199	PRO
49	BB	207	LEU
52	EE	32	SER
52	EE	68	ARG
55	HH	32	PRO
64	QQ	136	SER
65	RR	26	LEU

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Mol	Chain	Res	Type
71	XX	41	SER
82	1	490	GLY
16	N	35	VAL
35	g	77	GLY
37	i	49	GLY
46	r	107	VAL
45	q	205	VAL
50	CC	201	VAL
82	1	414	VAL
82	1	470	PRO
11	H	4	ILE
43	o	5	PRO
64	QQ	27	GLY
82	1	681	PRO

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	
4	A	191/191 (100%)	178 (93%)	13 (7%)	13	38
5	B	320/320 (100%)	301 (94%)	19 (6%)	16	45
6	C	286/286 (100%)	269 (94%)	17 (6%)	16	45
7	D	244/244 (100%)	222 (91%)	22 (9%)	8	25
8	E	134/152 (88%)	127 (95%)	7 (5%)	19	50
9	F	186/186 (100%)	178 (96%)	8 (4%)	25	57
10	G	189/191 (99%)	182 (96%)	7 (4%)	29	64
11	H	172/172 (100%)	163 (95%)	9 (5%)	19	50
12	I	184/185 (100%)	175 (95%)	9 (5%)	21	53
13	J	146/146 (100%)	138 (94%)	8 (6%)	18	48
14	L	158/158 (100%)	149 (94%)	9 (6%)	17	47
15	M	108/108 (100%)	102 (94%)	6 (6%)	17	47
16	N	174/174 (100%)	169 (97%)	5 (3%)	37	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	O	160/160 (100%)	158 (99%)	2 (1%)	65	88
18	P	145/145 (100%)	139 (96%)	6 (4%)	26	60
19	Q	150/150 (100%)	147 (98%)	3 (2%)	50	79
20	R	153/153 (100%)	143 (94%)	10 (6%)	14	40
21	S	154/154 (100%)	147 (96%)	7 (4%)	23	56
22	T	135/135 (100%)	123 (91%)	12 (9%)	8	26
23	U	87/87 (100%)	83 (95%)	4 (5%)	23	55
24	V	101/101 (100%)	93 (92%)	8 (8%)	10	30
25	W	54/54 (100%)	52 (96%)	2 (4%)	29	64
26	X	105/105 (100%)	100 (95%)	5 (5%)	21	54
27	Y	109/109 (100%)	103 (94%)	6 (6%)	18	48
28	Z	115/115 (100%)	106 (92%)	9 (8%)	10	31
29	a	118/118 (100%)	112 (95%)	6 (5%)	20	51
30	b	46/46 (100%)	46 (100%)	0	100	100
31	c	81/81 (100%)	75 (93%)	6 (7%)	11	34
32	d	93/93 (100%)	90 (97%)	3 (3%)	34	69
33	e	106/106 (100%)	97 (92%)	9 (8%)	8	27
34	f	89/89 (100%)	87 (98%)	2 (2%)	47	78
35	g	103/103 (100%)	92 (89%)	11 (11%)	5	17
36	h	103/103 (100%)	102 (99%)	1 (1%)	73	91
37	i	80/80 (100%)	74 (92%)	6 (8%)	11	33
38	j	69/69 (100%)	66 (96%)	3 (4%)	25	57
39	k	68/68 (100%)	61 (90%)	7 (10%)	6	19
40	l	44/44 (100%)	42 (96%)	2 (4%)	23	56
41	m	46/46 (100%)	46 (100%)	0	100	100
42	n	21/21 (100%)	19 (90%)	2 (10%)	7	22
43	o	87/87 (100%)	80 (92%)	7 (8%)	10	30
44	p	69/69 (100%)	64 (93%)	5 (7%)	12	35
45	q	198/198 (100%)	172 (87%)	26 (13%)	3	10
46	r	165/165 (100%)	143 (87%)	22 (13%)	3	10
48	AA	173/173 (100%)	167 (96%)	6 (4%)	31	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BB	192/192 (100%)	178 (93%)	14 (7%)	11	34
50	CC	176/176 (100%)	165 (94%)	11 (6%)	15	42
51	DD	182/182 (100%)	171 (94%)	11 (6%)	16	44
52	EE	219/219 (100%)	207 (94%)	12 (6%)	18	48
53	FF	173/173 (100%)	163 (94%)	10 (6%)	17	46
54	GG	193/193 (100%)	188 (97%)	5 (3%)	41	74
55	HH	165/165 (100%)	156 (94%)	9 (6%)	18	48
56	II	149/160 (93%)	138 (93%)	11 (7%)	11	34
57	JJ	156/156 (100%)	148 (95%)	8 (5%)	20	51
58	KK	89/89 (100%)	76 (85%)	13 (15%)	2	8
59	LL	130/130 (100%)	127 (98%)	3 (2%)	45	77
60	MM	100/100 (100%)	94 (94%)	6 (6%)	16	44
61	NN	127/127 (100%)	121 (95%)	6 (5%)	22	55
62	OO	96/96 (100%)	86 (90%)	10 (10%)	5	18
63	PP	86/86 (100%)	79 (92%)	7 (8%)	9	29
64	QQ	117/117 (100%)	109 (93%)	8 (7%)	13	38
65	RR	112/112 (100%)	102 (91%)	10 (9%)	8	26
66	SS	120/120 (100%)	113 (94%)	7 (6%)	17	46
67	TT	115/115 (100%)	106 (92%)	9 (8%)	10	31
68	UU	99/99 (100%)	97 (98%)	2 (2%)	50	79
69	VV	74/74 (100%)	67 (90%)	7 (10%)	7	22
70	WW	110/110 (100%)	104 (94%)	6 (6%)	18	48
71	XX	119/119 (100%)	111 (93%)	8 (7%)	13	39
72	YY	112/112 (100%)	110 (98%)	2 (2%)	54	82
73	ZZ	61/61 (100%)	59 (97%)	2 (3%)	33	68
74	aa	83/83 (100%)	78 (94%)	5 (6%)	16	44
75	bb	70/70 (100%)	63 (90%)	7 (10%)	6	20
76	cc	56/56 (100%)	52 (93%)	4 (7%)	12	36
77	dd	47/47 (100%)	42 (89%)	5 (11%)	5	18
78	ee	46/46 (100%)	43 (94%)	3 (6%)	14	40
79	ff	38/49 (78%)	36 (95%)	2 (5%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
80	gg	261/261 (100%)	237 (91%)	24 (9%)	7	24
82	1	524/524 (100%)	479 (91%)	45 (9%)	8	27
All	All	10116/10159 (100%)	9487 (94%)	629 (6%)	18	43

All (629) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	7	ASN
4	A	18	SER
4	A	73	GLU
4	A	84	THR
4	A	86	GLN
4	A	102	LEU
4	A	134	VAL
4	A	148	VAL
4	A	181	LYS
4	A	195	SER
4	A	207	VAL
4	A	218	HIS
4	A	245	LEU
5	B	10	ARG
5	B	56	ILE
5	B	66	LYS
5	B	80	ASP
5	B	87	VAL
5	B	94	GLU
5	B	123	TYR
5	B	201	LYS
5	B	203	VAL
5	B	205	VAL
5	B	206	ASP
5	B	215	ILE
5	B	226	PHE
5	B	255	TRP
5	B	305	ILE
5	B	322	ILE
5	B	323	MET
5	B	332	ARG
5	B	338	LEU
6	C	37	THR
6	C	69	ARG

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Mol	Chain	Res	Type
6	C	93	MET
6	C	95	ARG
6	C	98	ARG
6	C	120	TYR
6	C	136	LEU
6	C	150	LEU
6	C	152	VAL
6	C	154	THR
6	C	169	LEU
6	C	227	THR
6	C	249	ILE
6	C	281	ILE
6	C	283	THR
6	C	300	ARG
6	C	343	LYS
7	D	6	ASP
7	D	8	LYS
7	D	36	LEU
7	D	51	LEU
7	D	95	TRP
7	D	151	GLN
7	D	155	THR
7	D	159	VAL
7	D	164	LYS
7	D	184	ASP
7	D	209	GLU
7	D	211	LEU
7	D	213	ASP
7	D	230	ASP
7	D	250	ASP
7	D	253	PHE
7	D	256	THR
7	D	257	GLU
7	D	258	LYS
7	D	278	SER
7	D	296	GLN
7	D	297	GLN
8	E	23	LYS
8	E	52	VAL
8	E	65	ILE
8	E	96	VAL
8	E	102	ASN

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Mol	Chain	Res	Type
8	E	109	GLU
8	E	169	ASP
9	F	30	ARG
9	F	110	ARG
9	F	155	LYS
9	F	158	LYS
9	F	160	ARG
9	F	182	ASP
9	F	187	GLU
9	F	229	PHE
10	G	26	THR
10	G	27	HIS
10	G	73	THR
10	G	162	VAL
10	G	172	MET
10	G	184	ARG
10	G	194	SER
11	H	17	THR
11	H	42	ASP
11	H	46	THR
11	H	61	ASP
11	H	113	GLU
11	H	138	THR
11	H	139	ASN
11	H	146	LEU
11	H	150	SER
12	I	35	ASP
12	I	48	LEU
12	I	73	ASN
12	I	91	VAL
12	I	112	GLN
12	I	129	VAL
12	I	145	LYS
12	I	180	GLU
12	I	182	LEU
13	J	7	ASN
13	J	13	LYS
13	J	21	ILE
13	J	64	LYS
13	J	78	GLU
13	J	107	ASP
13	J	108	GLU

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Mol	Chain	Res	Type
13	J	142	LYS
14	L	21	ARG
14	L	55	ARG
14	L	58	VAL
14	L	59	ARG
14	L	69	VAL
14	L	92	THR
14	L	124	ILE
14	L	136	GLU
14	L	152	THR
15	M	4	ASP
15	M	12	TRP
15	M	47	ASP
15	M	55	ARG
15	M	66	THR
15	M	68	LEU
16	N	9	GLU
16	N	65	ARG
16	N	109	ARG
16	N	117	ASN
16	N	132	VAL
17	O	54	TYR
17	O	58	LEU
18	P	24	VAL
18	P	41	LEU
18	P	69	ARG
18	P	79	THR
18	P	127	ARG
18	P	150	VAL
19	Q	3	ILE
19	Q	57	ILE
19	Q	125	ASP
20	R	49	THR
20	R	93	VAL
20	R	103	ARG
20	R	123	LEU
20	R	134	HIS
20	R	153	LYS
20	R	157	GLU
20	R	166	ASN
20	R	176	ARG
20	R	180	LYS

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Mol	Chain	Res	Type
21	S	13	ARG
21	S	45	LEU
21	S	57	GLU
21	S	96	ASP
21	S	109	ASP
21	S	171	PHE
21	S	172	TYR
22	T	4	SER
22	T	58	GLN
22	T	60	LYS
22	T	65	TYR
22	T	68	THR
22	T	83	ARG
22	T	88	ARG
22	T	93	VAL
22	T	104	GLU
22	T	139	ARG
22	T	146	ASN
22	T	147	VAL
23	U	57	THR
23	U	59	ASP
23	U	64	THR
23	U	91	ASP
24	V	33	ASN
24	V	45	ARG
24	V	46	LEU
24	V	54	LEU
24	V	83	LYS
24	V	98	ASN
24	V	125	LEU
24	V	135	VAL
25	W	19	THR
25	W	63	ILE
26	X	39	LYS
26	X	77	GLU
26	X	87	SER
26	X	108	LEU
26	X	110	VAL
27	Y	52	ARG
27	Y	60	ARG
27	Y	71	SER
27	Y	74	TYR

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Mol	Chain	Res	Type
27	Y	109	LEU
27	Y	112	ASP
28	Z	10	VAL
28	Z	31	GLU
28	Z	43	VAL
28	Z	54	THR
28	Z	83	THR
28	Z	89	VAL
28	Z	100	THR
28	Z	102	GLU
28	Z	116	LYS
29	a	4	ARG
29	a	7	LYS
29	a	60	TYR
29	a	91	LEU
29	a	97	GLU
29	a	98	THR
31	c	16	LEU
31	c	19	LYS
31	c	24	THR
31	c	61	MET
31	c	97	ASP
31	c	100	ILE
32	d	87	ASN
32	d	96	VAL
32	d	97	LEU
33	e	8	LYS
33	e	21	HIS
33	e	27	ARG
33	e	33	ARG
33	e	41	VAL
33	e	90	LYS
33	e	111	ARG
33	e	123	LYS
33	e	126	LEU
34	f	59	VAL
34	f	106	ASN
35	g	5	VAL
35	g	37	LYS
35	g	62	TYR
35	g	66	SER
35	g	71	THR

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Mol	Chain	Res	Type
35	g	79	SER
35	g	80	ARG
35	g	93	PHE
35	g	94	LEU
35	g	113	LYS
35	g	118	LYS
36	h	118	ILE
37	i	13	LYS
37	i	17	VAL
37	i	37	THR
37	i	45	ARG
37	i	74	LYS
37	i	76	ARG
38	j	28	HIS
38	j	58	THR
38	j	84	LYS
39	k	7	ASP
39	k	10	GLN
39	k	26	LYS
39	k	27	ILE
39	k	38	PHE
39	k	65	LEU
39	k	67	GLN
40	l	21	ARG
40	l	23	LEU
42	n	1	MET
42	n	10	THR
43	o	24	LYS
43	o	35	LEU
43	o	59	HIS
43	o	61	LYS
43	o	80	ARG
43	o	98	LYS
43	o	100	LYS
44	p	49	ARG
44	p	59	CYS
44	p	63	THR
44	p	82	THR
44	p	86	LEU
45	q	1	MET
45	q	12	HIS
45	q	16	LEU

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Mol	Chain	Res	Type
45	q	32	VAL
45	q	36	VAL
45	q	42	ASP
45	q	55	LEU
45	q	70	ASP
45	q	75	ASP
45	q	90	LEU
45	q	98	LYS
45	q	103	LEU
45	q	133	LYS
45	q	134	PHE
45	q	136	THR
45	q	140	HIS
45	q	142	ASP
45	q	150	ASP
45	q	173	GLU
45	q	189	PHE
45	q	190	PHE
45	q	195	LYS
45	q	196	LYS
45	q	197	ASN
45	q	205	VAL
45	q	216	LEU
46	r	13	TYR
46	r	35	VAL
46	r	37	SER
46	r	39	GLN
46	r	50	ARG
46	r	59	THR
46	r	60	MET
46	r	62	ARG
46	r	66	ARG
46	r	68	PHE
46	r	77	LYS
46	r	85	ASN
46	r	88	PHE
46	r	92	ASN
46	r	106	ARG
46	r	137	PHE
46	r	154	ILE
46	r	166	LYS
46	r	171	GLU

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Mol	Chain	Res	Type
46	r	183	PHE
46	r	187	LEU
46	r	199	PHE
48	AA	38	PHE
48	AA	45	VAL
48	AA	57	LEU
48	AA	129	ASP
48	AA	139	VAL
48	AA	143	VAL
49	BB	47	LEU
49	BB	52	THR
49	BB	78	ASP
49	BB	92	GLN
49	BB	97	LEU
49	BB	99	ASN
49	BB	103	MET
49	BB	105	PHE
49	BB	176	VAL
49	BB	198	GLU
49	BB	199	ASN
49	BB	205	PHE
49	BB	212	VAL
49	BB	213	ARG
50	CC	57	THR
50	CC	58	ILE
50	CC	83	ASP
50	CC	116	VAL
50	CC	121	LYS
50	CC	163	THR
50	CC	164	THR
50	CC	175	ILE
50	CC	223	ILE
50	CC	229	PHE
50	CC	235	TRP
51	DD	10	LYS
51	DD	42	THR
51	DD	76	ARG
51	DD	84	ILE
51	DD	90	ARG
51	DD	120	TYR
51	DD	135	GLU
51	DD	146	ARG

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Mol	Chain	Res	Type
51	DD	176	LEU
51	DD	195	SER
51	DD	222	VAL
52	EE	57	ASN
52	EE	89	VAL
52	EE	95	THR
52	EE	108	ARG
52	EE	116	ASP
52	EE	143	ASP
52	EE	182	TYR
52	EE	184	THR
52	EE	194	THR
52	EE	206	ASP
52	EE	225	VAL
52	EE	254	ARG
53	FF	22	PHE
53	FF	40	THR
53	FF	42	ILE
53	FF	43	LYS
53	FF	51	GLU
53	FF	57	ASP
53	FF	104	ARG
53	FF	126	LEU
53	FF	128	ASP
53	FF	149	THR
54	GG	24	ILE
54	GG	41	VAL
54	GG	78	THR
54	GG	92	ARG
54	GG	178	LEU
55	HH	8	ILE
55	HH	14	THR
55	HH	19	GLN
55	HH	20	VAL
55	HH	35	LYS
55	HH	70	PHE
55	HH	93	LEU
55	HH	101	LYS
55	HH	158	ASP
56	II	7	SER
56	II	20	GLN
56	II	25	ARG

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Mol	Chain	Res	Type
56	II	29	LEU
56	II	47	ARG
56	II	62	THR
56	II	87	ASN
56	II	92	ARG
56	II	121	LEU
56	II	166	LEU
56	II	169	CYS
57	JJ	3	ARG
57	JJ	40	ARG
57	JJ	60	LEU
57	JJ	101	VAL
57	JJ	155	HIS
57	JJ	162	SER
57	JJ	171	ARG
57	JJ	174	ARG
58	KK	15	LEU
58	KK	16	PHE
58	KK	17	GLN
58	KK	37	THR
58	KK	40	LEU
58	KK	49	LEU
58	KK	54	TYR
58	KK	77	ARG
58	KK	78	GLU
58	KK	80	LEU
58	KK	86	ILE
58	KK	91	TYR
58	KK	95	ARG
59	LL	67	ARG
59	LL	103	ARG
59	LL	124	THR
60	MM	38	LEU
60	MM	55	LEU
60	MM	98	LYS
60	MM	107	LYS
60	MM	128	MET
60	MM	132	HIS
61	NN	5	HIS
61	NN	11	ILE
61	NN	28	LEU
61	NN	39	LYS

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Mol	Chain	Res	Type
61	NN	101	HIS
61	NN	102	LEU
62	OO	61	MET
62	OO	66	ASP
62	OO	84	ARG
62	OO	91	THR
62	OO	110	LEU
62	OO	116	GLU
62	OO	124	ASP
62	OO	125	SER
62	OO	127	ARG
62	OO	132	ARG
63	PP	36	LEU
63	PP	41	VAL
63	PP	44	ARG
63	PP	79	HIS
63	PP	83	MET
63	PP	106	GLU
63	PP	127	ARG
64	QQ	28	LEU
64	QQ	36	ILE
64	QQ	37	THR
64	QQ	43	ILE
64	QQ	45	ARG
64	QQ	49	TYR
64	QQ	118	ILE
64	QQ	135	ARG
65	RR	3	ARG
65	RR	16	LEU
65	RR	40	THR
65	RR	43	SER
65	RR	46	LEU
65	RR	69	ILE
65	RR	97	ASN
65	RR	111	LYS
65	RR	113	LEU
65	RR	122	ILE
66	SS	28	ILE
66	SS	57	ARG
66	SS	75	ASN
66	SS	85	PHE
66	SS	98	TYR

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Mol	Chain	Res	Type
66	SS	106	GLU
66	SS	134	ARG
67	TT	4	VAL
67	TT	28	LEU
67	TT	30	VAL
67	TT	40	SER
67	TT	41	SER
67	TT	53	TRP
67	TT	104	VAL
67	TT	111	ILE
67	TT	143	ASP
68	UU	52	LYS
68	UU	70	THR
69	VV	34	ILE
69	VV	40	ASP
69	VV	44	ARG
69	VV	52	THR
69	VV	62	ARG
69	VV	74	GLN
69	VV	76	ASP
70	WW	2	THR
70	WW	15	ASN
70	WW	83	ILE
70	WW	104	LEU
70	WW	115	GLU
70	WW	129	VAL
71	XX	7	ARG
71	XX	19	ARG
71	XX	27	ASN
71	XX	28	ASN
71	XX	31	LYS
71	XX	33	LEU
71	XX	84	THR
71	XX	107	PHE
72	YY	98	GLU
72	YY	112	LYS
73	ZZ	42	LEU
73	ZZ	97	LYS
74	aa	21	VAL
74	aa	39	MET
74	aa	52	ASP
74	aa	82	ARG

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Mol	Chain	Res	Type
74	aa	87	ARG
75	bb	3	LEU
75	bb	11	THR
75	bb	15	GLU
75	bb	23	THR
75	bb	62	ILE
75	bb	75	GLU
75	bb	79	PHE
76	cc	18	ARG
76	cc	22	ARG
76	cc	48	VAL
76	cc	58	GLU
77	dd	10	HIS
77	dd	23	VAL
77	dd	24	CYS
77	dd	40	ARG
77	dd	53	ASN
78	ee	20	LYS
78	ee	25	GLU
78	ee	31	LYS
79	ff	136	LYS
79	ff	148	TYR
80	gg	21	VAL
80	gg	34	LEU
80	gg	49	THR
80	gg	52	ASP
80	gg	66	SER
80	gg	67	HIS
80	gg	77	ASP
80	gg	86	TRP
80	gg	136	THR
80	gg	169	THR
80	gg	178	MET
80	gg	190	GLU
80	gg	192	ASP
80	gg	194	ILE
80	gg	198	SER
80	gg	208	ASP
80	gg	224	TRP
80	gg	226	LEU
80	gg	230	LYS
80	gg	235	LEU

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Mol	Chain	Res	Type
80	gg	267	ASP
80	gg	271	LEU
80	gg	284	LYS
80	gg	300	GLN
82	1	401	LYS
82	1	411	LEU
82	1	415	ASP
82	1	419	THR
82	1	458	VAL
82	1	464	LYS
82	1	465	GLN
82	1	466	THR
82	1	468	ASP
82	1	469	VAL
82	1	492	SER
82	1	503	ILE
82	1	507	LEU
82	1	522	LYS
82	1	527	VAL
82	1	536	TYR
82	1	544	ASN
82	1	582	TYR
82	1	607	ASP
82	1	622	LYS
82	1	625	MET
82	1	655	TYR
82	1	697	LYS
82	1	732	GLU
82	1	738	MET
82	1	739	ASP
82	1	741	LEU
82	1	746	ASP
82	1	749	ASP
82	1	764	SER
82	1	765	LEU
82	1	775	MET
82	1	801	LYS
82	1	815	VAL
82	1	866	CYS
82	1	877	ARG
82	1	891	LEU
82	1	892	ARG

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Mol	Chain	Res	Type
82	1	913	ILE
82	1	928	GLN
82	1	929	GLU
82	1	958	ASP
82	1	989	TRP
82	1	991	LEU
82	1	992	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	7	ASN
4	A	86	GLN
4	A	132	ASN
4	A	233	GLN
5	B	173	GLN
5	B	313	HIS
6	C	36	HIS
6	C	48	GLN
6	C	59	GLN
7	D	4	GLN
7	D	17	GLN
7	D	39	GLN
7	D	40	HIS
8	E	97	ASN
8	E	167	ASN
10	G	58	GLN
10	G	154	ASN
10	G	251	ASN
11	H	139	ASN
11	H	156	GLN
11	H	163	GLN
12	I	12	GLN
12	I	59	GLN
12	I	133	GLN
13	J	150	ASN
14	L	28	GLN
15	M	59	ASN
16	N	15	GLN
17	O	26	GLN
17	O	50	ASN
18	P	50	GLN

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Mol	Chain	Res	Type
18	P	118	GLN
18	P	121	GLN
21	S	8	GLN
21	S	62	ASN
21	S	63	GLN
21	S	138	GLN
21	S	142	GLN
22	T	26	HIS
22	T	103	GLN
22	T	122	GLN
22	T	131	GLN
22	T	134	GLN
22	T	146	ASN
23	U	25	ASN
24	V	33	ASN
26	X	91	ASN
26	X	137	ASN
27	Y	100	HIS
29	a	25	HIS
29	a	44	ASN
29	a	74	ASN
30	b	6	ASN
30	b	10	HIS
30	b	12	GLN
32	d	57	GLN
32	d	87	ASN
33	e	31	ASN
34	f	26	ASN
34	f	77	ASN
34	f	106	ASN
36	h	62	GLN
36	h	68	GLN
37	i	35	ASN
38	j	79	GLN
39	k	28	ASN
40	l	19	GLN
40	l	50	ASN
45	q	35	GLN
46	r	58	ASN
46	r	191	GLN
48	AA	83	GLN
48	AA	92	HIS

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Mol	Chain	Res	Type
48	AA	131	GLN
49	BB	56	ASN
49	BB	99	ASN
49	BB	199	ASN
50	CC	113	ASN
50	CC	152	ASN
51	DD	162	GLN
52	EE	8	HIS
52	EE	17	HIS
52	EE	50	ASN
52	EE	209	HIS
53	FF	65	GLN
53	FF	88	GLN
54	GG	56	ASN
54	GG	59	GLN
54	GG	185	GLN
55	HH	5	GLN
56	II	32	GLN
56	II	84	HIS
56	II	94	ASN
57	JJ	112	GLN
58	KK	62	GLN
59	LL	37	ASN
60	MM	132	HIS
62	OO	29	HIS
63	PP	98	ASN
64	QQ	94	GLN
64	QQ	139	GLN
65	RR	97	ASN
66	SS	89	GLN
66	SS	136	GLN
69	VV	3	ASN
70	WW	16	ASN
70	WW	42	GLN
70	WW	70	ASN
72	YY	34	ASN
72	YY	110	GLN
73	ZZ	95	HIS
78	ee	46	ASN
80	gg	186	GLN
82	1	427	GLN
82	1	440	GLN

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Mol	Chain	Res	Type
82	1	465	GLN
82	1	543	ASN
82	1	544	ASN
82	1	569	GLN
82	1	575	GLN
82	1	585	ASN
82	1	928	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3250/3271 (99%)	786 (24%)	76 (2%)
2	7	120/121 (99%)	21 (17%)	0
3	8	156/157 (99%)	34 (21%)	2 (1%)
81	2	1767/1796 (98%)	554 (31%)	32 (1%)
83	3	75/76 (98%)	17 (22%)	0
84	4	5/6 (83%)	0	0
All	All	5373/5427 (99%)	1412 (26%)	110 (2%)

All (1412) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	3	U
1	5	6	A
1	5	14	U
1	5	15	C
1	5	17	G
1	5	26	A
1	5	30	G
1	5	40	A
1	5	43	A
1	5	44	U
1	5	48	A
1	5	49	A
1	5	59	G
1	5	60	A
1	5	65	A
1	5	66	A
1	5	73	C
1	5	89	A
1	5	92	G

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Mol	Chain	Res	Type
1	5	96	G
1	5	109	A
1	5	110	G
1	5	111	C
1	5	116	A
1	5	117	U
1	5	121	A
1	5	122	A
1	5	134	U
1	5	135	C
1	5	136	G
1	5	142	C
1	5	155	G
1	5	156	G
1	5	157	A
1	5	167	U
1	5	171	G
1	5	172	G
1	5	174	C
1	5	175	C
1	5	182	U
1	5	187	A
1	5	189	G
1	5	190	U
1	5	191	U
1	5	199	A
1	5	200	C
1	5	210	U
1	5	218	G
1	5	219	A
1	5	220	G
1	5	221	A
1	5	237	G
1	5	239	G
1	5	240	U
1	5	241	G
1	5	248	U
1	5	249	U
1	5	251	G
1	5	252	U
1	5	253	A
1	5	254	A

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Mol	Chain	Res	Type
1	5	263	C
1	5	269	G
1	5	285	A
1	5	286	U
1	5	295	A
1	5	298	U
1	5	299	G
1	5	305	U
1	5	306	A
1	5	307	A
1	5	315	C
1	5	323	A
1	5	329	U
1	5	334	A
1	5	336	A
1	5	339	C
1	5	349	A
1	5	350	C
1	5	370	U
1	5	374	A
1	5	376	G
1	5	395	A
1	5	396	A
1	5	398	A
1	5	399	A
1	5	402	A
1	5	403	C
1	5	404	G
1	5	420	G
1	5	421	G
1	5	422	A
1	5	436	A
1	5	438	A
1	5	439	C
1	5	508	U
1	5	519	A
1	5	521	A
1	5	523	A
1	5	534	U
1	5	535	G
1	5	543	C
1	5	545	U

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Mol	Chain	Res	Type
1	5	546	C
1	5	554	A
1	5	557	A
1	5	559	A
1	5	560	G
1	5	568	G
1	5	569	A
1	5	571	U
1	5	572	A
1	5	578	A
1	5	579	G
1	5	589	A
1	5	600	G
1	5	603	A
1	5	604	G
1	5	611	A
1	5	619	A
1	5	620	U
1	5	621	A
1	5	636	C
1	5	637	C
1	5	645	A
1	5	647	A
1	5	649	A
1	5	660	A
1	5	677	A
1	5	678	G
1	5	681	U
1	5	683	U
1	5	684	G
1	5	690	A
1	5	691	A
1	5	698	U
1	5	705	A
1	5	708	G
1	5	712	G
1	5	715	A
1	5	720	A
1	5	725	G
1	5	733	G
1	5	735	A
1	5	767	U

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Mol	Chain	Res	Type
1	5	776	U
1	5	777	U
1	5	780	A
1	5	781	G
1	5	785	G
1	5	786	A
1	5	806	A
1	5	817	A
1	5	830	A
1	5	837	A
1	5	842	G
1	5	848	A
1	5	849	C
1	5	851	C
1	5	861	C
1	5	864	G
1	5	871	U
1	5	874	U
1	5	879	U
1	5	880	G
1	5	895	A
1	5	896	A
1	5	897	U
1	5	907	G
1	5	908	G
1	5	914	A
1	5	916	G
1	5	917	A
1	5	923	C
1	5	924	G
1	5	925	A
1	5	926	A
1	5	937	G
1	5	944	C
1	5	953	G
1	5	959	C
1	5	960	U
1	5	962	A
1	5	971	G
1	5	974	G
1	5	979	U
1	5	981	U

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Mol	Chain	Res	Type
1	5	982	C
1	5	984	G
1	5	993	G
1	5	994	G
1	5	995	U
1	5	1002	A
1	5	1003	A
1	5	1010	G
1	5	1014	U
1	5	1015	U
1	5	1016	C
1	5	1017	C
1	5	1018	G
1	5	1021	G
1	5	1023	C
1	5	1024	G
1	5	1025	A
1	5	1026	A
1	5	1027	A
1	5	1028	U
1	5	1029	G
1	5	1030	A
1	5	1031	C
1	5	1034	U
1	5	1035	G
1	5	1037	C
1	5	1047	A
1	5	1049	C
1	5	1052	U
1	5	1057	A
1	5	1064	A
1	5	1065	A
1	5	1074	U
1	5	1082	U
1	5	1085	A
1	5	1087	G
1	5	1090	G
1	5	1093	A
1	5	1094	U
1	5	1095	U
1	5	1096	U
1	5	1098	A

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Mol	Chain	Res	Type
1	5	1103	A
1	5	1104	G
1	5	1105	A
1	5	1117	G
1	5	1131	G
1	5	1143	A
1	5	1144	U
1	5	1147	G
1	5	1151	U
1	5	1152	G
1	5	1153	A
1	5	1158	A
1	5	1159	A
1	5	1161	G
1	5	1179	A
1	5	1180	A
1	5	1181	U
1	5	1182	A
1	5	1193	A
1	5	1194	G
1	5	1196	C
1	5	1198	C
1	5	1201	C
1	5	1209	G
1	5	1220	U
1	5	1222	G
1	5	1223	A
1	5	1224	C
1	5	1225	A
1	5	1226	G
1	5	1227	C
1	5	1235	U
1	5	1236	G
1	5	1239	C
1	5	1241	U
1	5	1242	G
1	5	1243	G
1	5	1245	A
1	5	1246	G
1	5	1250	G
1	5	1252	A
1	5	1253	U

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Mol	Chain	Res	Type
1	5	1258	U
1	5	1262	G
1	5	1263	A
1	5	1264	G
1	5	1266	G
1	5	1272	C
1	5	1277	C
1	5	1278	A
1	5	1280	C
1	5	1281	G
1	5	1282	G
1	5	1285	G
1	5	1287	A
1	5	1290	A
1	5	1291	A
1	5	1294	A
1	5	1307	G
1	5	1308	A
1	5	1309	U
1	5	1313	G
1	5	1316	C
1	5	1325	U
1	5	1330	A
1	5	1348	U
1	5	1350	A
1	5	1351	U
1	5	1352	A
1	5	1353	U
1	5	1355	A
1	5	1356	U
1	5	1357	G
1	5	1386	A
1	5	1392	G
1	5	1399	A
1	5	1408	G
1	5	1418	A
1	5	1419	A
1	5	1421	G
1	5	1434	G
1	5	1437	C
1	5	1443	G
1	5	1446	A

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Mol	Chain	Res	Type
1	5	1450	G
1	5	1453	A
1	5	1454	A
1	5	1475	A
1	5	1481	A
1	5	1482	A
1	5	1483	G
1	5	1485	G
1	5	1495	U
1	5	1508	C
1	5	1523	U
1	5	1527	C
1	5	1533	U
1	5	1536	G
1	5	1538	G
1	5	1547	G
1	5	1549	U
1	5	1554	U
1	5	1555	U
1	5	1557	A
1	5	1560	G
1	5	1561	G
1	5	1562	C
1	5	1564	U
1	5	1565	G
1	5	1567	U
1	5	1568	U
1	5	1569	U
1	5	1570	U
1	5	1571	A
1	5	1573	G
1	5	1575	A
1	5	1578	C
1	5	1579	C
1	5	1580	A
1	5	1581	C
1	5	1582	C
1	5	1583	A
1	5	1589	A
1	5	1593	A
1	5	1604	G
1	5	1605	A

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Mol	Chain	Res	Type
1	5	1607	U
1	5	1608	C
1	5	1612	A
1	5	1620	U
1	5	1628	C
1	5	1629	U
1	5	1630	U
1	5	1632	A
1	5	1639	C
1	5	1642	A
1	5	1643	A
1	5	1645	U
1	5	1646	G
1	5	1657	C
1	5	1659	U
1	5	1662	G
1	5	1683	A
1	5	1688	U
1	5	1689	U
1	5	1694	U
1	5	1696	A
1	5	1705	U
1	5	1715	A
1	5	1716	U
1	5	1717	U
1	5	1724	U
1	5	1728	G
1	5	1729	A
1	5	1730	G
1	5	1750	A
1	5	1751	G
1	5	1759	C
1	5	1760	A
1	5	1762	C
1	5	1764	U
1	5	1765	U
1	5	1766	G
1	5	1775	G
1	5	1780	G
1	5	1788	C
1	5	1797	A
1	5	1808	G

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Mol	Chain	Res	Type
1	5	1814	A
1	5	1815	U
1	5	1816	A
1	5	1817	G
1	5	1818	U
1	5	1820	U
1	5	1821	U
1	5	1823	A
1	5	1833	G
1	5	1837	U
1	5	1842	A
1	5	1846	C
1	5	1849	C
1	5	1850	A
1	5	1866	C
1	5	1871	U
1	5	1878	G
1	5	1879	A
1	5	1880	U
1	5	1881	A
1	5	1884	A
1	5	1886	A
1	5	1893	A
1	5	1896	A
1	5	1906	G
1	5	1935	G
1	5	1953	G
1	5	1958	U
1	5	1960	A
1	5	1965	C
1	5	1968	G
1	5	1972	A
1	5	1973	G
1	5	1975	C
1	5	2054	G
1	5	2057	G
1	5	2059	C
1	5	2065	U
1	5	2070	G
1	5	2073	C
1	5	2074	U
1	5	2075	C

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Mol	Chain	Res	Type
1	5	2078	G
1	5	2083	U
1	5	2086	U
1	5	2089	A
1	5	2090	A
1	5	2091	U
1	5	2092	U
1	5	2093	A
1	5	2100	A
1	5	2101	C
1	5	2102	U
1	5	2110	G
1	5	2111	G
1	5	2112	U
1	5	2113	A
1	5	2116	G
1	5	2121	G
1	5	2122	G
1	5	2131	A
1	5	2140	U
1	5	2144	A
1	5	2145	A
1	5	2158	A
1	5	2160	G
1	5	2166	A
1	5	2169	G
1	5	2171	G
1	5	2188	A
1	5	2205	U
1	5	2208	A
1	5	2210	G
1	5	2211	U
1	5	2223	A
1	5	2229	A
1	5	2231	C
1	5	2232	A
1	5	2235	C
1	5	2239	G
1	5	2244	A
1	5	2249	G
1	5	2250	G
1	5	2253	G

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Mol	Chain	Res	Type
1	5	2257	C
1	5	2258	U
1	5	2259	A
1	5	2260	U
1	5	2261	G
1	5	2262	A
1	5	2266	U
1	5	2267	C
1	5	2268	U
1	5	2270	A
1	5	2272	G
1	5	2273	G
1	5	2274	U
1	5	2281	A
1	5	2283	G
1	5	2286	U
1	5	2307	G
1	5	2308	C
1	5	2310	U
1	5	2313	A
1	5	2315	G
1	5	2327	U
1	5	2334	U
1	5	2335	G
1	5	2336	U
1	5	2372	A
1	5	2373	A
1	5	2374	C
1	5	2375	G
1	5	2385	G
1	5	2388	U
1	5	2393	G
1	5	2397	A
1	5	2398	A
1	5	2401	A
1	5	2402	A
1	5	2403	G
1	5	2404	A
1	5	2411	U
1	5	2418	G
1	5	2419	A
1	5	2434	U

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Mol	Chain	Res	Type
1	5	2435	G
1	5	2441	A
1	5	2442	G
1	5	2443	A
1	5	2444	C
1	5	2446	U
1	5	2447	A
1	5	2448	G
1	5	2449	A
1	5	2450	G
1	5	2451	G
1	5	2452	G
1	5	2453	U
1	5	2454	G
1	5	2457	G
1	5	2458	A
1	5	2459	A
1	5	2461	A
1	5	2467	G
1	5	2468	A
1	5	2469	G
1	5	2474	G
1	5	2475	G
1	5	2477	G
1	5	2478	C
1	5	2486	A
1	5	2487	U
1	5	2489	C
1	5	2491	A
1	5	2494	A
1	5	2495	C
1	5	2499	U
1	5	2500	A
1	5	2501	U
1	5	2502	A
1	5	2503	G
1	5	2504	U
1	5	2505	U
1	5	2506	U
1	5	2508	U
1	5	2509	U
1	5	2513	U

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Mol	Chain	Res	Type
1	5	2514	U
1	5	2519	A
1	5	2522	G
1	5	2523	A
1	5	2524	A
1	5	2525	G
1	5	2531	C
1	5	2534	G
1	5	2536	A
1	5	2537	U
1	5	2538	U
1	5	2539	C
1	5	2540	A
1	5	2541	U
1	5	2542	U
1	5	2543	U
1	5	2544	U
1	5	2545	C
1	5	2547	A
1	5	2550	U
1	5	2551	U
1	5	2552	C
1	5	2554	A
1	5	2560	C
1	5	2561	A
1	5	2562	A
1	5	2568	C
1	5	2569	A
1	5	2570	U
1	5	2571	U
1	5	2572	C
1	5	2573	G
1	5	2575	G
1	5	2580	A
1	5	2581	U
1	5	2585	G
1	5	2586	G
1	5	2593	A
1	5	2594	C
1	5	2606	G
1	5	2607	G
1	5	2614	G

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Mol	Chain	Res	Type
1	5	2619	G
1	5	2620	G
1	5	2626	A
1	5	2627	C
1	5	2652	U
1	5	2655	U
1	5	2656	A
1	5	2657	A
1	5	2663	G
1	5	2674	A
1	5	2677	G
1	5	2689	A
1	5	2690	G
1	5	2691	A
1	5	2694	A
1	5	2696	A
1	5	2704	A
1	5	2714	G
1	5	2715	A
1	5	2719	U
1	5	2720	G
1	5	2728	G
1	5	2737	C
1	5	2747	A
1	5	2752	U
1	5	2753	G
1	5	2762	A
1	5	2771	U
1	5	2777	G
1	5	2787	G
1	5	2790	A
1	5	2791	G
1	5	2794	G
1	5	2796	G
1	5	2799	A
1	5	2800	G
1	5	2801	A
1	5	2802	A
1	5	2810	C
1	5	2814	G
1	5	2817	A
1	5	2818	U

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Mol	Chain	Res	Type
1	5	2843	U
1	5	2845	A
1	5	2847	A
1	5	2853	A
1	5	2856	G
1	5	2861	U
1	5	2863	G
1	5	2871	G
1	5	2872	A
1	5	2873	U
1	5	2875	U
1	5	2887	A
1	5	2899	C
1	5	2907	G
1	5	2911	A
1	5	2914	G
1	5	2916	U
1	5	2923	U
1	5	2933	A
1	5	2935	U
1	5	2936	A
1	5	2938	G
1	5	2941	A
1	5	2942	C
1	5	2943	G
1	5	2947	G
1	5	2954	U
1	5	2955	U
1	5	2972	G
1	5	2983	C
1	5	2996	U
1	5	2997	G
1	5	3004	C
1	5	3006	A
1	5	3011	A
1	5	3012	A
1	5	3021	A
1	5	3042	U
1	5	3059	G
1	5	3069	G
1	5	3078	U
1	5	3079	U

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Mol	Chain	Res	Type
1	5	3080	G
1	5	3086	A
1	5	3092	C
1	5	3094	A
1	5	3109	G
1	5	3115	C
1	5	3117	C
1	5	3122	A
1	5	3123	A
1	5	3125	U
1	5	3130	A
1	5	3131	U
1	5	3142	A
1	5	3154	C
1	5	3156	U
1	5	3157	U
1	5	3158	G
1	5	3159	C
1	5	3173	G
1	5	3174	A
1	5	3175	U
1	5	3176	G
1	5	3179	U
1	5	3181	C
1	5	3182	G
1	5	3187	A
1	5	3194	C
1	5	3195	U
1	5	3196	U
1	5	3200	G
1	5	3202	G
1	5	3204	C
1	5	3207	U
1	5	3210	A
1	5	3213	A
1	5	3215	A
1	5	3216	G
1	5	3217	C
1	5	3218	A
1	5	3219	G
1	5	3224	G
1	5	3227	A

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Mol	Chain	Res	Type
1	5	3229	G
1	5	3236	U
1	5	3238	G
1	5	3239	G
1	5	3240	C
1	5	3243	A
1	5	3244	A
1	5	3245	A
1	5	3248	C
1	5	3249	C
1	5	3252	G
1	5	3253	G
1	5	3256	G
1	5	3259	U
1	5	3260	G
1	5	3262	U
1	5	3263	G
1	5	3268	A
1	5	3273	A
1	5	3275	U
1	5	3276	G
1	5	3278	C
1	5	3282	U
1	5	3283	U
1	5	3284	G
1	5	3285	C
1	5	3286	G
1	5	3288	G
1	5	3290	G
1	5	3294	A
1	5	3304	U
1	5	3307	A
1	5	3313	U
1	5	3314	A
1	5	3316	A
1	5	3317	U
1	5	3318	G
1	5	3319	U
1	5	3341	U
1	5	3342	A
1	5	3344	A
1	5	3345	G

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Mol	Chain	Res	Type
1	5	3351	U
1	5	3354	U
1	5	3356	G
1	5	3358	U
1	5	3369	G
1	5	3370	A
1	5	3375	A
1	5	3378	C
1	5	3382	U
1	5	3383	G
1	5	3390	G
2	7	7	G
2	7	18	C
2	7	22	A
2	7	27	A
2	7	38	U
2	7	40	C
2	7	42	A
2	7	43	U
2	7	54	U
2	7	55	A
2	7	65	G
2	7	70	U
2	7	74	C
2	7	76	A
2	7	84	A
2	7	88	G
2	7	93	C
2	7	99	G
2	7	102	A
2	7	112	G
2	7	121	U
3	8	23	U
3	8	25	G
3	8	34	U
3	8	35	C
3	8	36	G
3	8	48	A
3	8	50	C
3	8	52	A
3	8	53	A
3	8	59	A

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Mol	Chain	Res	Type
3	8	62	C
3	8	63	G
3	8	71	A
3	8	80	A
3	8	81	U
3	8	82	U
3	8	83	C
3	8	85	G
3	8	86	U
3	8	87	G
3	8	95	G
3	8	97	A
3	8	100	U
3	8	104	A
3	8	106	C
3	8	111	A
3	8	113	U
3	8	125	U
3	8	126	A
3	8	127	U
3	8	128	U
3	8	129	C
3	8	151	C
3	8	152	G
81	2	2	U
81	2	3	C
81	2	24	C
81	2	30	C
81	2	31	U
81	2	33	G
81	2	39	A
81	2	41	G
81	2	42	A
81	2	43	U
81	2	44	U
81	2	46	A
81	2	49	C
81	2	56	G
81	2	59	U
81	2	60	A
81	2	62	G
81	2	66	A

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Mol	Chain	Res	Type
81	2	67	A
81	2	70	A
81	2	71	A
81	2	72	U
81	2	73	U
81	2	74	U
81	2	75	A
81	2	103	A
81	2	113	C
81	2	123	A
81	2	126	G
81	2	128	U
81	2	129	C
81	2	130	C
81	2	131	U
81	2	132	U
81	2	133	U
81	2	134	A
81	2	136	U
81	2	137	A
81	2	139	A
81	2	143	U
81	2	144	A
81	2	146	A
81	2	148	C
81	2	157	U
81	2	158	U
81	2	161	A
81	2	165	C
81	2	168	A
81	2	169	U
81	2	173	U
81	2	175	C
81	2	176	U
81	2	177	U
81	2	178	A
81	2	179	A
81	2	184	U
81	2	185	C
81	2	186	G
81	2	189	C
81	2	190	C

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Mol	Chain	Res	Type
81	2	191	U
81	2	193	U
81	2	194	G
81	2	196	A
81	2	203	G
81	2	207	U
81	2	209	A
81	2	215	U
81	2	216	A
81	2	217	A
81	2	218	A
81	2	226	U
81	2	227	G
81	2	230	U
81	2	231	U
81	2	232	C
81	2	233	G
81	2	235	A
81	2	237	U
81	2	238	C
81	2	239	U
81	2	249	C
81	2	256	A
81	2	259	U
81	2	260	U
81	2	264	A
81	2	270	A
81	2	274	C
81	2	276	U
81	2	277	U
81	2	278	G
81	2	279	U
81	2	280	G
81	2	281	C
81	2	286	G
81	2	298	A
81	2	301	U
81	2	311	A
81	2	313	C
81	2	315	A
81	2	319	U
81	2	320	C

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Mol	Chain	Res	Type
81	2	321	G
81	2	332	A
81	2	333	G
81	2	336	G
81	2	337	C
81	2	351	A
81	2	358	A
81	2	359	A
81	2	360	C
81	2	398	A
81	2	399	A
81	2	400	A
81	2	401	C
81	2	403	G
81	2	412	U
81	2	415	A
81	2	416	A
81	2	421	G
81	2	423	C
81	2	425	G
81	2	433	G
81	2	436	A
81	2	438	U
81	2	439	U
81	2	443	C
81	2	444	A
81	2	447	C
81	2	452	U
81	2	454	C
81	2	458	G
81	2	461	G
81	2	467	A
81	2	468	C
81	2	474	A
81	2	476	A
81	2	479	G
81	2	484	A
81	2	485	G
81	2	486	G
81	2	487	G
81	2	489	C
81	2	490	C

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Mol	Chain	Res	Type
81	2	491	A
81	2	492	U
81	2	494	C
81	2	495	G
81	2	496	G
81	2	497	G
81	2	499	C
81	2	501	U
81	2	505	A
81	2	506	U
81	2	507	U
81	2	514	A
81	2	518	C
81	2	524	A
81	2	526	A
81	2	533	A
81	2	537	A
81	2	539	G
81	2	540	A
81	2	542	C
81	2	543	A
81	2	544	A
81	2	547	G
81	2	548	G
81	2	554	A
81	2	556	G
81	2	557	U
81	2	558	C
81	2	559	U
81	2	564	C
81	2	565	C
81	2	567	G
81	2	576	G
81	2	577	U
81	2	578	A
81	2	579	A
81	2	593	A
81	2	594	G
81	2	596	G
81	2	600	A
81	2	605	A
81	2	610	U

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Mol	Chain	Res	Type
81	2	618	A
81	2	619	A
81	2	621	A
81	2	622	A
81	2	623	G
81	2	638	U
81	2	640	G
81	2	642	G
81	2	643	C
81	2	646	G
81	2	649	U
81	2	650	G
81	2	652	C
81	2	653	C
81	2	654	G
81	2	655	G
81	2	656	U
81	2	679	U
81	2	684	A
81	2	691	C
81	2	693	U
81	2	694	U
81	2	695	U
81	2	696	C
81	2	697	C
81	2	698	U
81	2	699	U
81	2	701	U
81	2	708	C
81	2	709	C
81	2	710	U
81	2	711	U
81	2	712	G
81	2	713	A
81	2	714	G
81	2	715	U
81	2	716	C
81	2	717	C
81	2	718	U
81	2	721	U
81	2	722	G
81	2	723	G

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Mol	Chain	Res	Type
81	2	726	C
81	2	727	U
81	2	729	G
81	2	730	G
81	2	731	C
81	2	732	G
81	2	734	A
81	2	736	C
81	2	738	G
81	2	739	G
81	2	740	A
81	2	741	C
81	2	742	U
81	2	743	U
81	2	753	A
81	2	754	A
81	2	755	A
81	2	765	G
81	2	766	U
81	2	771	A
81	2	774	A
81	2	778	G
81	2	779	U
81	2	780	A
81	2	783	G
81	2	789	A
81	2	792	U
81	2	794	U
81	2	795	U
81	2	799	A
81	2	811	A
81	2	813	U
81	2	816	G
81	2	820	U
81	2	821	U
81	2	823	G
81	2	824	G
81	2	827	C
81	2	828	U
81	2	829	A
81	2	831	U
81	2	833	U

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Mol	Chain	Res	Type
81	2	834	G
81	2	835	U
81	2	836	U
81	2	839	U
81	2	841	U
81	2	846	G
81	2	849	C
81	2	850	A
81	2	853	G
81	2	856	A
81	2	858	G
81	2	860	U
81	2	861	U
81	2	863	A
81	2	864	U
81	2	865	A
81	2	873	U
81	2	875	G
81	2	877	G
81	2	886	U
81	2	898	A
81	2	904	G
81	2	906	A
81	2	907	A
81	2	911	U
81	2	912	U
81	2	913	G
81	2	914	G
81	2	915	A
81	2	921	U
81	2	928	U
81	2	931	C
81	2	932	U
81	2	933	A
81	2	935	U
81	2	951	A
81	2	952	A
81	2	959	U
81	2	960	U
81	2	966	A
81	2	967	A
81	2	970	A

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Mol	Chain	Res	Type
81	2	975	C
81	2	982	U
81	2	985	G
81	2	987	G
81	2	991	G
81	2	992	A
81	2	1001	A
81	2	1002	G
81	2	1003	A
81	2	1005	A
81	2	1012	U
81	2	1024	U
81	2	1026	A
81	2	1027	A
81	2	1028	C
81	2	1031	U
81	2	1032	G
81	2	1038	U
81	2	1039	A
81	2	1042	G
81	2	1043	A
81	2	1050	G
81	2	1051	G
81	2	1052	U
81	2	1053	G
81	2	1057	U
81	2	1058	U
81	2	1059	U
81	2	1061	A
81	2	1062	A
81	2	1063	U
81	2	1066	C
81	2	1072	C
81	2	1077	C
81	2	1080	U
81	2	1082	C
81	2	1083	G
81	2	1085	G
81	2	1087	A
81	2	1088	A
81	2	1090	C
81	2	1091	A

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Mol	Chain	Res	Type
81	2	1097	U
81	2	1098	U
81	2	1100	G
81	2	1109	G
81	2	1111	G
81	2	1114	G
81	2	1118	G
81	2	1131	A
81	2	1138	A
81	2	1140	G
81	2	1143	A
81	2	1150	G
81	2	1151	A
81	2	1155	G
81	2	1158	C
81	2	1164	G
81	2	1167	G
81	2	1185	U
81	2	1186	U
81	2	1191	U
81	2	1194	A
81	2	1196	A
81	2	1199	G
81	2	1200	G
81	2	1202	A
81	2	1203	A
81	2	1204	A
81	2	1205	C
81	2	1207	C
81	2	1209	C
81	2	1214	U
81	2	1217	A
81	2	1218	G
81	2	1228	G
81	2	1229	G
81	2	1230	A
81	2	1237	G
81	2	1239	U
81	2	1241	G
81	2	1243	G
81	2	1244	A
81	2	1245	G

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Mol	Chain	Res	Type
81	2	1246	C
81	2	1247	U
81	2	1248	C
81	2	1250	U
81	2	1254	U
81	2	1255	G
81	2	1256	A
81	2	1262	U
81	2	1266	U
81	2	1269	U
81	2	1270	G
81	2	1271	G
81	2	1284	C
81	2	1285	U
81	2	1286	U
81	2	1290	U
81	2	1312	A
81	2	1314	U
81	2	1315	U
81	2	1321	A
81	2	1322	A
81	2	1323	C
81	2	1336	A
81	2	1340	U
81	2	1342	C
81	2	1344	A
81	2	1345	A
81	2	1348	A
81	2	1353	U
81	2	1355	C
81	2	1356	U
81	2	1361	U
81	2	1364	G
81	2	1369	U
81	2	1370	U
81	2	1371	A
81	2	1372	U
81	2	1377	U
81	2	1378	U
81	2	1383	G
81	2	1385	G
81	2	1390	U

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Mol	Chain	Res	Type
81	2	1398	U
81	2	1399	C
81	2	1413	U
81	2	1415	U
81	2	1427	A
81	2	1432	U
81	2	1433	G
81	2	1434	U
81	2	1436	A
81	2	1444	A
81	2	1445	G
81	2	1448	G
81	2	1450	U
81	2	1459	C
81	2	1460	A
81	2	1465	C
81	2	1466	G
81	2	1469	A
81	2	1470	C
81	2	1471	A
81	2	1486	G
81	2	1489	U
81	2	1490	C
81	2	1491	U
81	2	1494	C
81	2	1496	U
81	2	1497	U
81	2	1500	C
81	2	1504	G
81	2	1505	A
81	2	1509	C
81	2	1516	A
81	2	1517	U
81	2	1518	C
81	2	1521	G
81	2	1523	G
81	2	1524	A
81	2	1534	G
81	2	1535	U
81	2	1536	G
81	2	1537	C
81	2	1538	U

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Mol	Chain	Res	Type
81	2	1540	G
81	2	1543	A
81	2	1545	A
81	2	1548	G
81	2	1557	U
81	2	1559	A
81	2	1568	C
81	2	1573	A
81	2	1582	U
81	2	1597	A
81	2	1601	G
81	2	1607	G
81	2	1616	G
81	2	1619	C
81	2	1622	G
81	2	1631	A
81	2	1632	C
81	2	1638	G
81	2	1642	G
81	2	1648	A
81	2	1649	G
81	2	1657	U
81	2	1658	G
81	2	1678	A
81	2	1680	G
81	2	1684	U
81	2	1685	G
81	2	1687	U
81	2	1688	U
81	2	1690	G
81	2	1693	A
81	2	1694	A
81	2	1695	G
81	2	1696	G
81	2	1697	G
81	2	1698	G
81	2	1699	G
81	2	1700	C
81	2	1701	A
81	2	1702	A
81	2	1703	C
81	2	1704	U

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Mol	Chain	Res	Type
81	2	1705	C
81	2	1708	U
81	2	1709	C
81	2	1711	C
81	2	1712	A
81	2	1713	G
81	2	1714	A
81	2	1715	G
81	2	1716	C
81	2	1717	G
81	2	1718	G
81	2	1726	G
81	2	1731	A
81	2	1736	G
81	2	1750	A
81	2	1755	A
81	2	1756	A
81	2	1757	G
81	2	1760	G
81	2	1765	A
81	2	1766	A
81	2	1769	U
81	2	1780	G
81	2	1782	A
81	2	1783	C
81	2	1792	G
81	2	1793	G
81	2	1794	A
81	2	1795	U
81	2	1796	C
81	2	1797	A
81	2	1798	U
83	3	16	U
83	3	17	G
83	3	18	G
83	3	19	G
83	3	20	A
83	3	21	A
83	3	22	G
83	3	26	G
83	3	42	U
83	3	43	G

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Mol	Chain	Res	Type
83	3	48	C
83	3	58	A
83	3	59	A
83	3	60	A
83	3	61	C
83	3	75	C
83	3	76	A

All (110) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	133	U
1	5	166	C
1	5	173	G
1	5	249	U
1	5	297	G
1	5	298	U
1	5	406	G
1	5	518	G
1	5	567	G
1	5	588	G
1	5	594	U
1	5	718	G
1	5	766	U
1	5	816	A
1	5	873	C
1	5	896	A
1	5	916	G
1	5	993	G
1	5	1016	C
1	5	1064	A
1	5	1073	U
1	5	1097	G
1	5	1160	C
1	5	1181	U
1	5	1222	G
1	5	1223	A
1	5	1238	C
1	5	1241	U
1	5	1284	C
1	5	1307	G
1	5	1349	G

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Mol	Chain	Res	Type
1	5	1352	A
1	5	1355	A
1	5	1560	G
1	5	1568	U
1	5	1607	U
1	5	1729	A
1	5	1816	A
1	5	1841	A
1	5	2064	U
1	5	2072	U
1	5	2110	G
1	5	2112	U
1	5	2116	G
1	5	2248	C
1	5	2453	U
1	5	2467	G
1	5	2477	G
1	5	2486	A
1	5	2500	A
1	5	2505	U
1	5	2561	A
1	5	2570	U
1	5	2571	U
1	5	2585	G
1	5	2662	G
1	5	2911	A
1	5	2941	A
1	5	2996	U
1	5	3057	U
1	5	3078	U
1	5	3093	C
1	5	3121	U
1	5	3194	C
1	5	3217	C
1	5	3228	C
1	5	3239	G
1	5	3242	G
1	5	3259	U
1	5	3267	A
1	5	3284	G
1	5	3289	G
1	5	3303	G

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Mol	Chain	Res	Type
1	5	3317	U
1	5	3340	G
1	5	3357	U
3	8	22	U
3	8	125	U
81	2	67	A
81	2	71	A
81	2	129	C
81	2	177	U
81	2	217	A
81	2	277	U
81	2	279	U
81	2	280	G
81	2	285	C
81	2	318	U
81	2	399	A
81	2	538	G
81	2	564	C
81	2	695	U
81	2	721	U
81	2	829	A
81	2	863	A
81	2	910	C
81	2	1084	A
81	2	1108	G
81	2	1244	A
81	2	1344	A
81	2	1360	A
81	2	1371	A
81	2	1414	U
81	2	1444	A
81	2	1447	C
81	2	1457	C
81	2	1493	A
81	2	1542	G
81	2	1615	C
81	2	1755	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
87	U6A	3	101	83	9,9,10	1.69	2 (22%)	10,11,13	2.60	1 (10%)
88	MET	3	102	83	6,7,8	0.48	0	2,7,9	1.44	0
86	GDP	1	1101	-	25,30,30	0.96	1 (4%)	30,47,47	1.24	2 (6%)

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
87	U6A	3	101	83	-	10/11/11/12	-
88	MET	3	102	83	-	1/5/6/8	-
86	GDP	1	1101	-	-	3/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	3	101	U6A	O1-C1	3.32	1.36	1.22
87	3	101	U6A	CA-N	2.80	1.49	1.45
86	1	1101	GDP	C6-N1	-2.30	1.34	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	3	101	U6A	O1-C1-N	7.63	145.02	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	1	1101	GDP	C8-N7-C5	3.33	108.22	102.55
86	1	1101	GDP	C5-C6-N1	2.16	118.18	114.07

There are no chirality outliers.

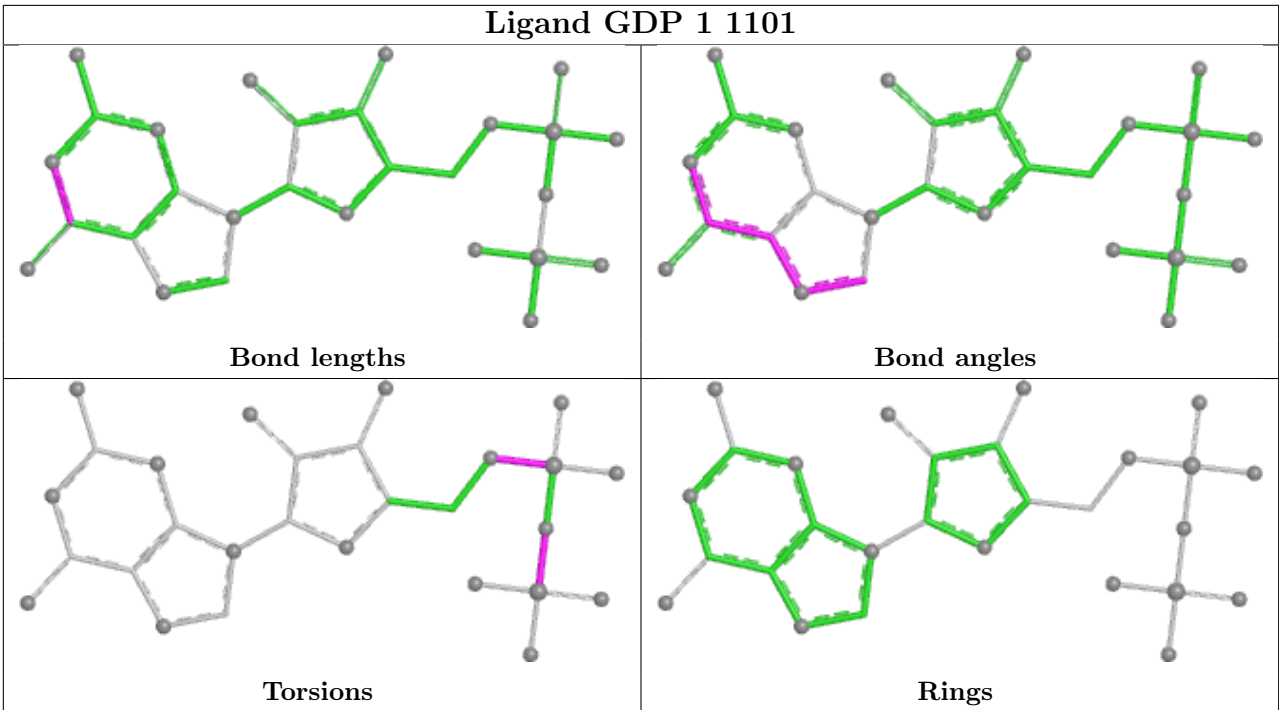
All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	1	1101	GDP	PA-O3A-PB-O2B
86	1	1101	GDP	C5'-O5'-PA-O1A
87	3	101	U6A	O1-C1-N-CA
87	3	101	U6A	C7-C6-CA-C
87	3	101	U6A	O8-C6-CA-C
87	3	101	U6A	C7-C6-CA-N
87	3	101	U6A	O8-C6-CA-N
87	3	101	U6A	OXT-C-CA-N
87	3	101	U6A	C-CA-N-C1
87	3	101	U6A	O-C-CA-N
88	3	102	MET	CB-CG-SD-CE
87	3	101	U6A	OXT-C-CA-C6
87	3	101	U6A	O-C-CA-C6
86	1	1101	GDP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	18
81	2	11
80	gg	2
45	q	1
37	i	1
65	RR	1
46	r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1980:C	O3'	2051:G	P	18.54
1	5	2083:U	O3'	2084:G	P	11.15
1	5	1954:G	O3'	1955:U	P	7.40
1	5	439:C	O3'	495:G	P	7.21
1	2	856:A	O3'	857:U	P	7.17

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1015:U	O3'	1016:C	P	7.16
1	q	215:ARG	C	216:LEU	N	7.12
1	5	2084:G	O3'	2085:C	P	6.55
1	2	134:A	O3'	135:C	P	6.49
1	2	1039:A	O3'	1040:G	P	6.18
1	2	861:U	O3'	862:A	P	6.08
1	5	2081:G	O3'	2082:A	P	6.07
1	5	547:G	O3'	548:G	P	5.67
1	gg	163:ALA	C	164:ASP	N	5.57
1	2	1014:G	O3'	1015:U	P	5.51
1	5	1576:G	O3'	1577:G	P	5.41
1	5	17:G	O3'	18:G	P	4.72
1	5	2506:U	O3'	2507:C	P	4.70
1	i	34:SER	C	35:ASN	N	4.56
1	5	2093:A	O3'	2094:C	P	4.48
1	5	2439:A	O3'	2440:G	P	4.43
1	2	239:U	O3'	240:U	P	4.17
1	RR	99:VAL	C	100:LEU	N	4.13
1	r	115:ALA	C	116:VAL	N	3.89
1	2	1091:A	O3'	1092:A	P	3.88
1	5	2531:C	O3'	2532:U	P	3.87
1	5	2532:U	O3'	2533:G	P	3.77
1	5	1228:C	O3'	1229:G	P	3.64
1	5	1955:U	O3'	1956:A	P	3.51
1	2	240:U	O3'	241:U	P	3.35
1	2	643:C	O3'	644:C	P	3.35
1	2	811:A	O3'	812:A	P	3.34
1	gg	185:ASN	C	186:GLN	N	3.33
1	5	2748:A	O3'	2749:G	P	3.23
1	5	2548:C	O3'	2549:G	P	3.22

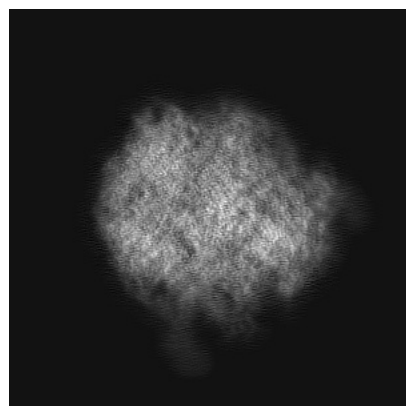
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21859. These allow visual inspection of the internal detail of the map and identification of artifacts.

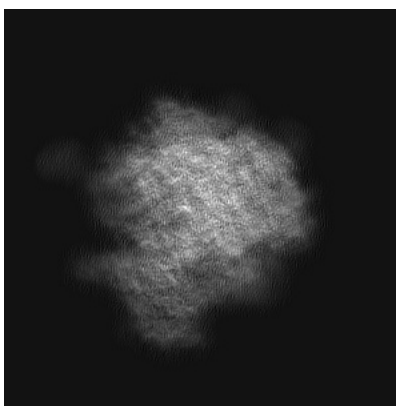
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

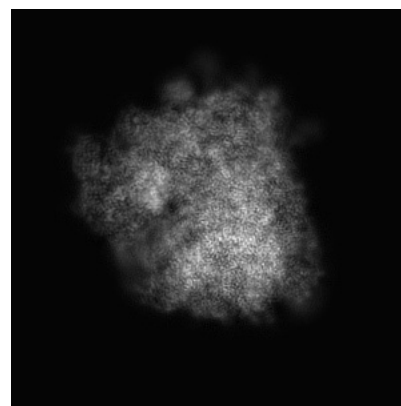
6.1.1 Primary map



X

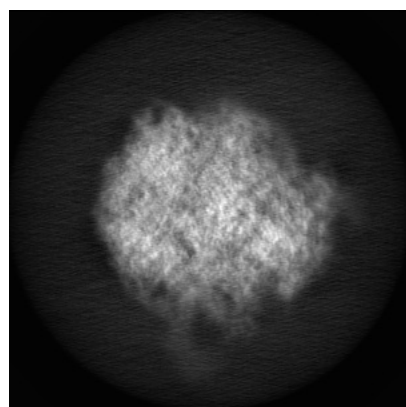


Y

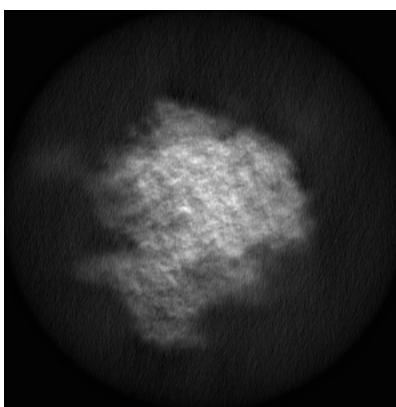


Z

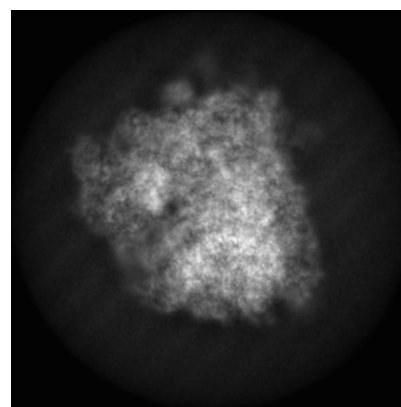
6.1.2 Raw map



X



Y

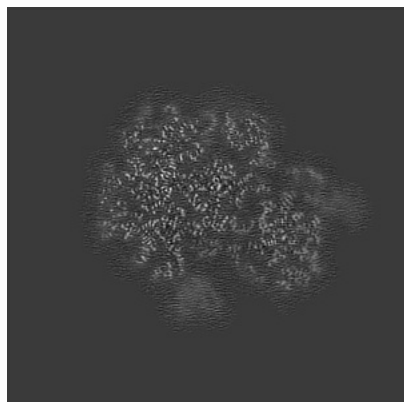


Z

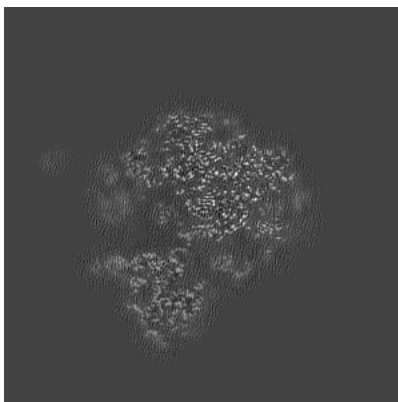
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

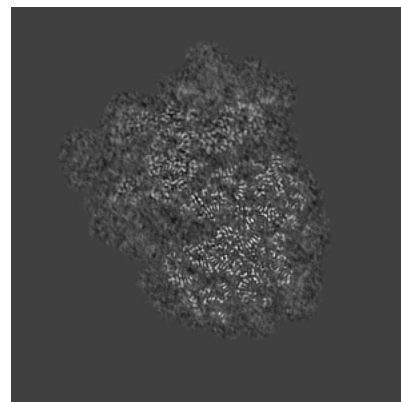
6.2.1 Primary map



X Index: 150

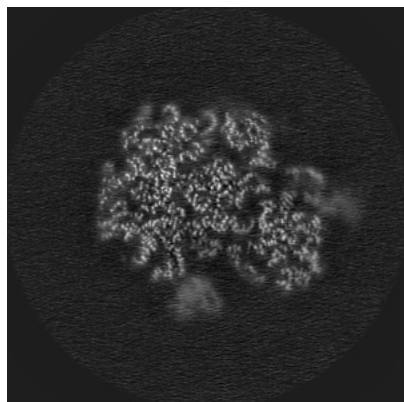


Y Index: 150

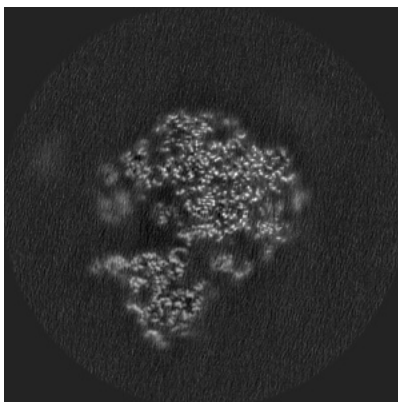


Z Index: 150

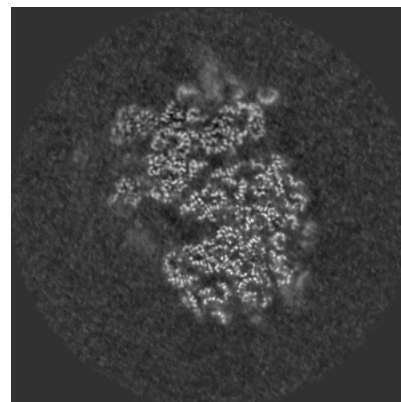
6.2.2 Raw map



X Index: 150



Y Index: 150

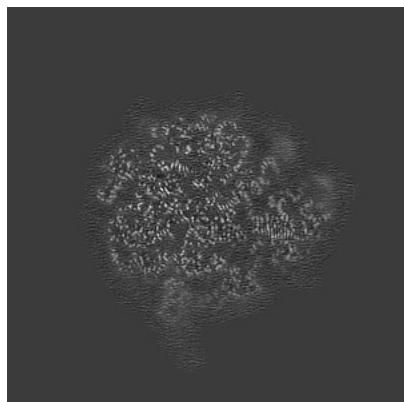


Z Index: 150

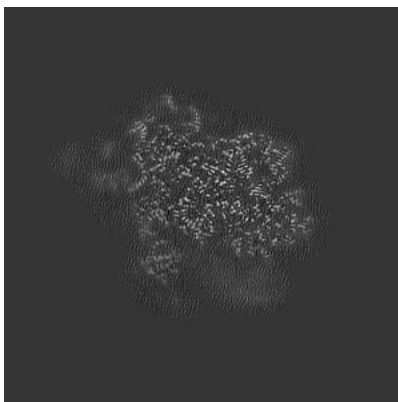
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

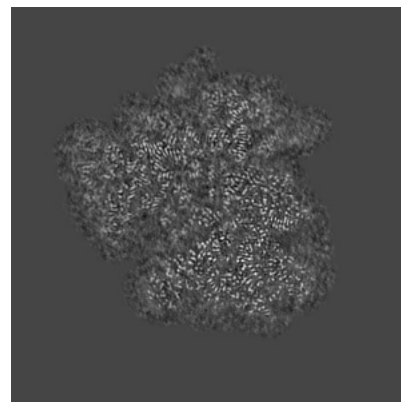
6.3.1 Primary map



X Index: 172

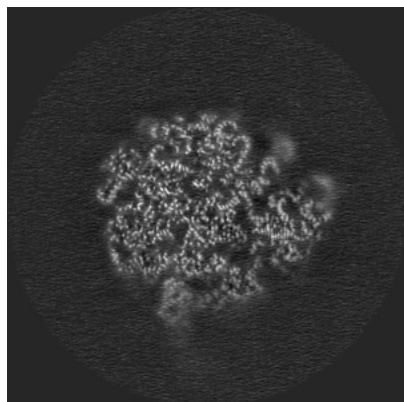


Y Index: 117

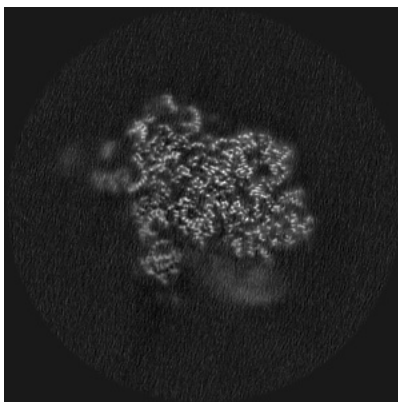


Z Index: 132

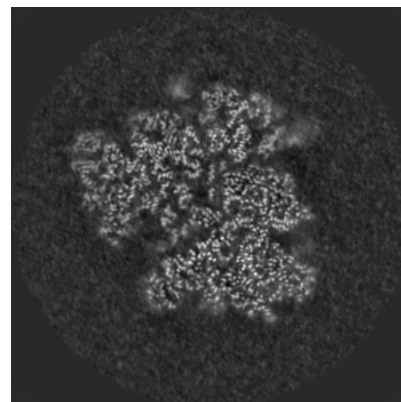
6.3.2 Raw map



X Index: 172



Y Index: 117

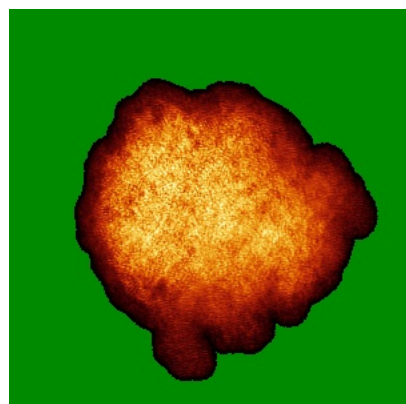


Z Index: 132

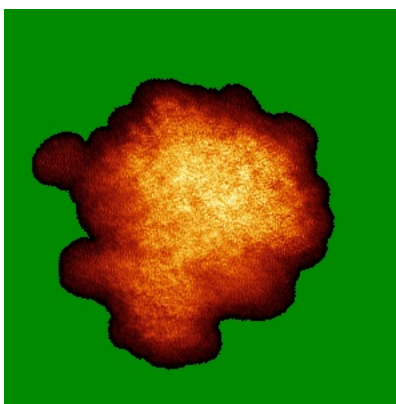
The images above show the largest variance slices of the map in three orthogonal directions.

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

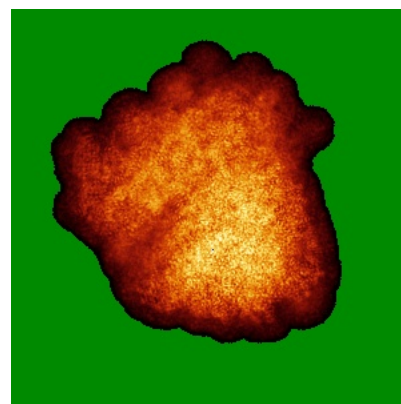
6.4.1 Primary map



X

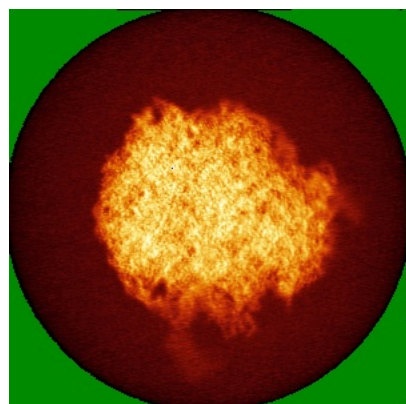


Y

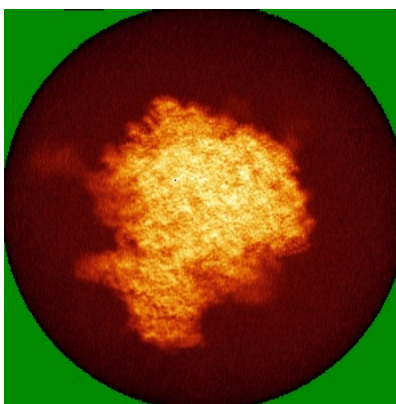


Z

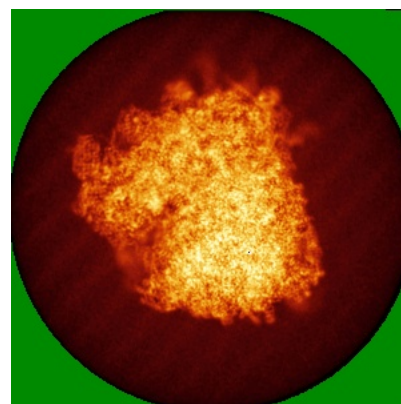
6.4.2 Raw map



X



Y

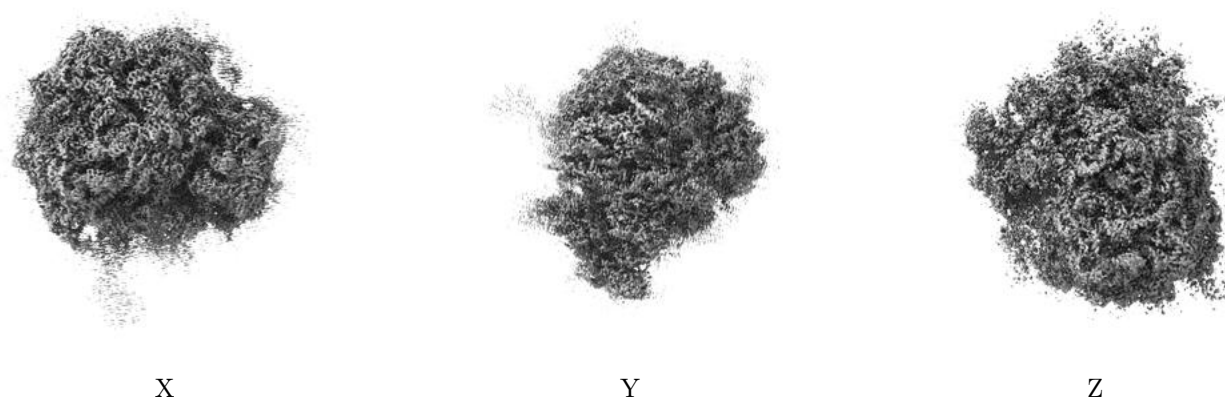


Z

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

6.5.2 Raw map



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

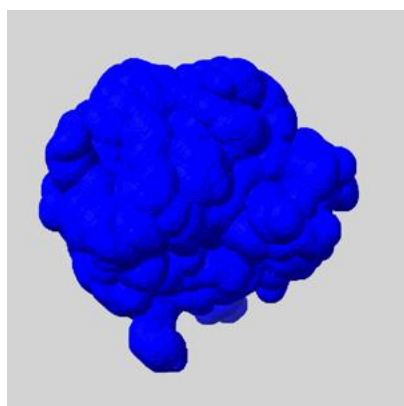
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

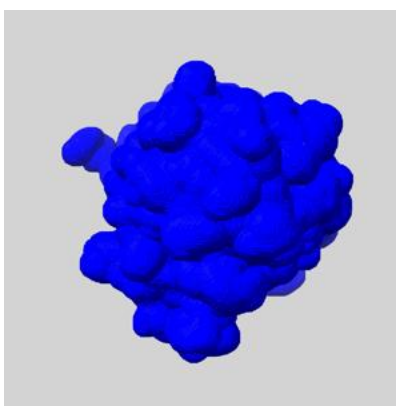
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

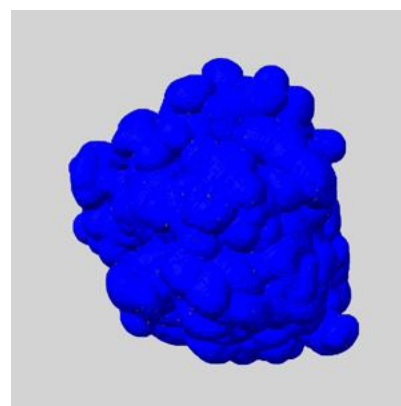
6.6.1 emd_21859_msk_1.map [i](#)



X



Y

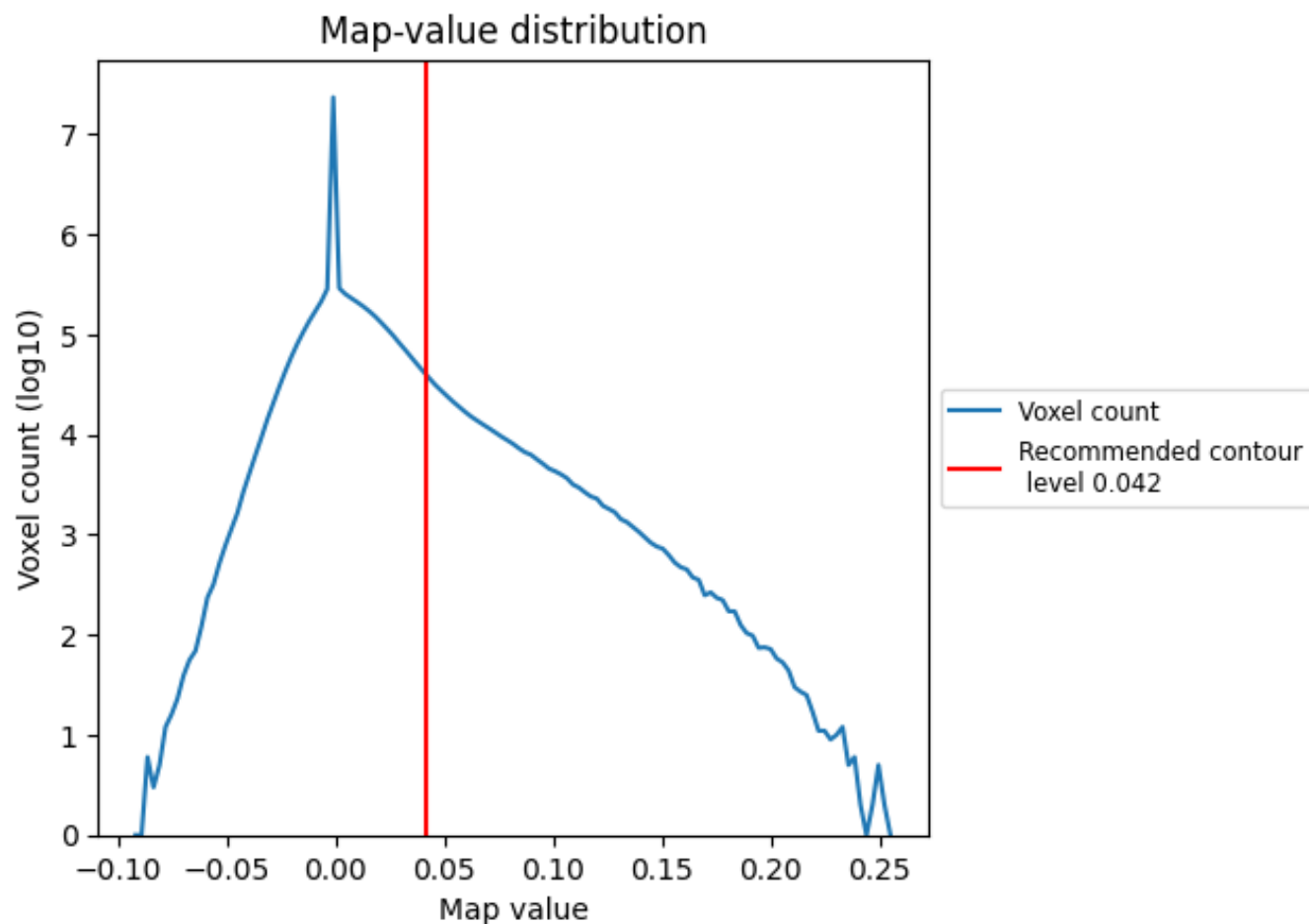


Z

7 Map analysis [i](#)

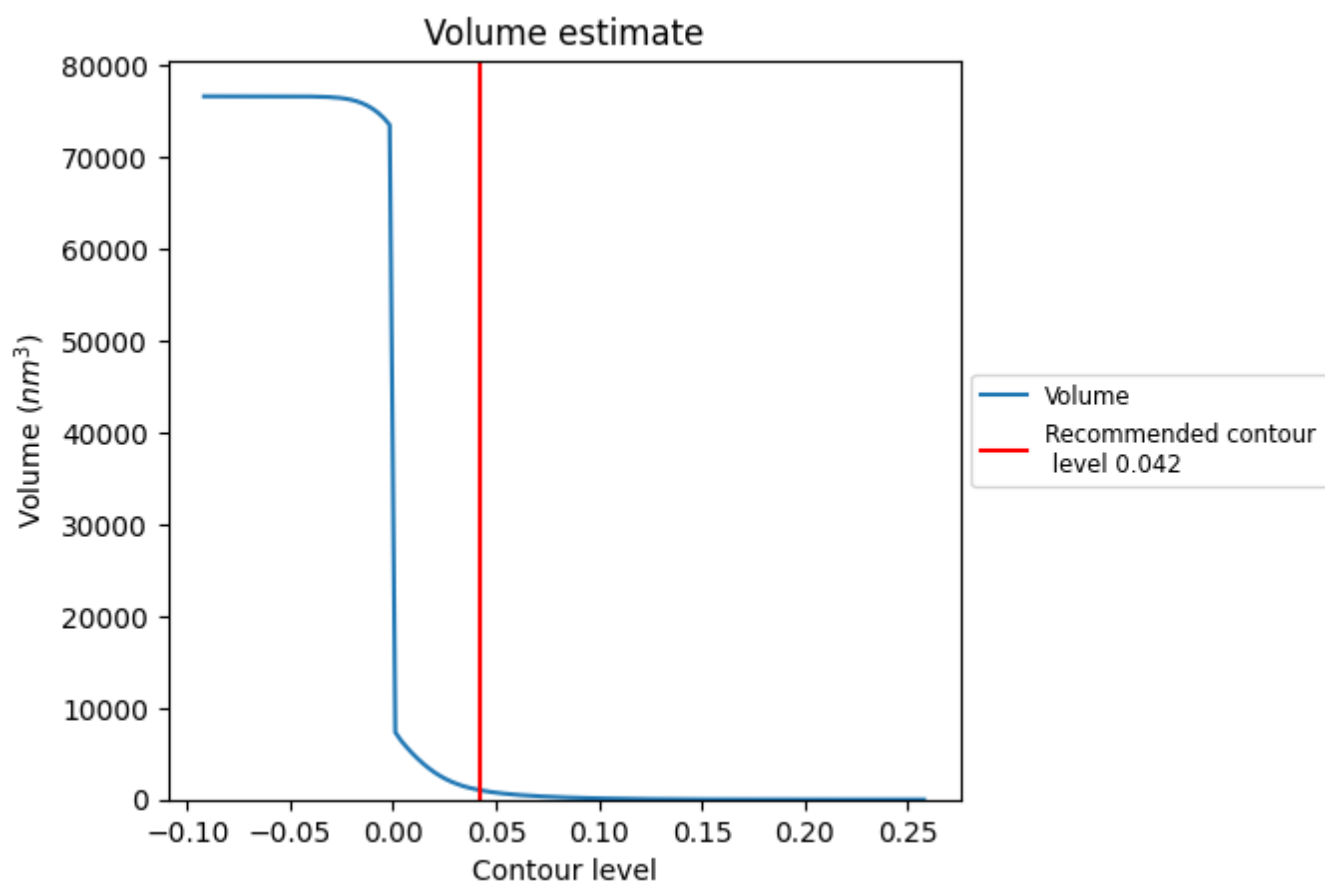
This section contains the results of statistical analysis of the map.

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.

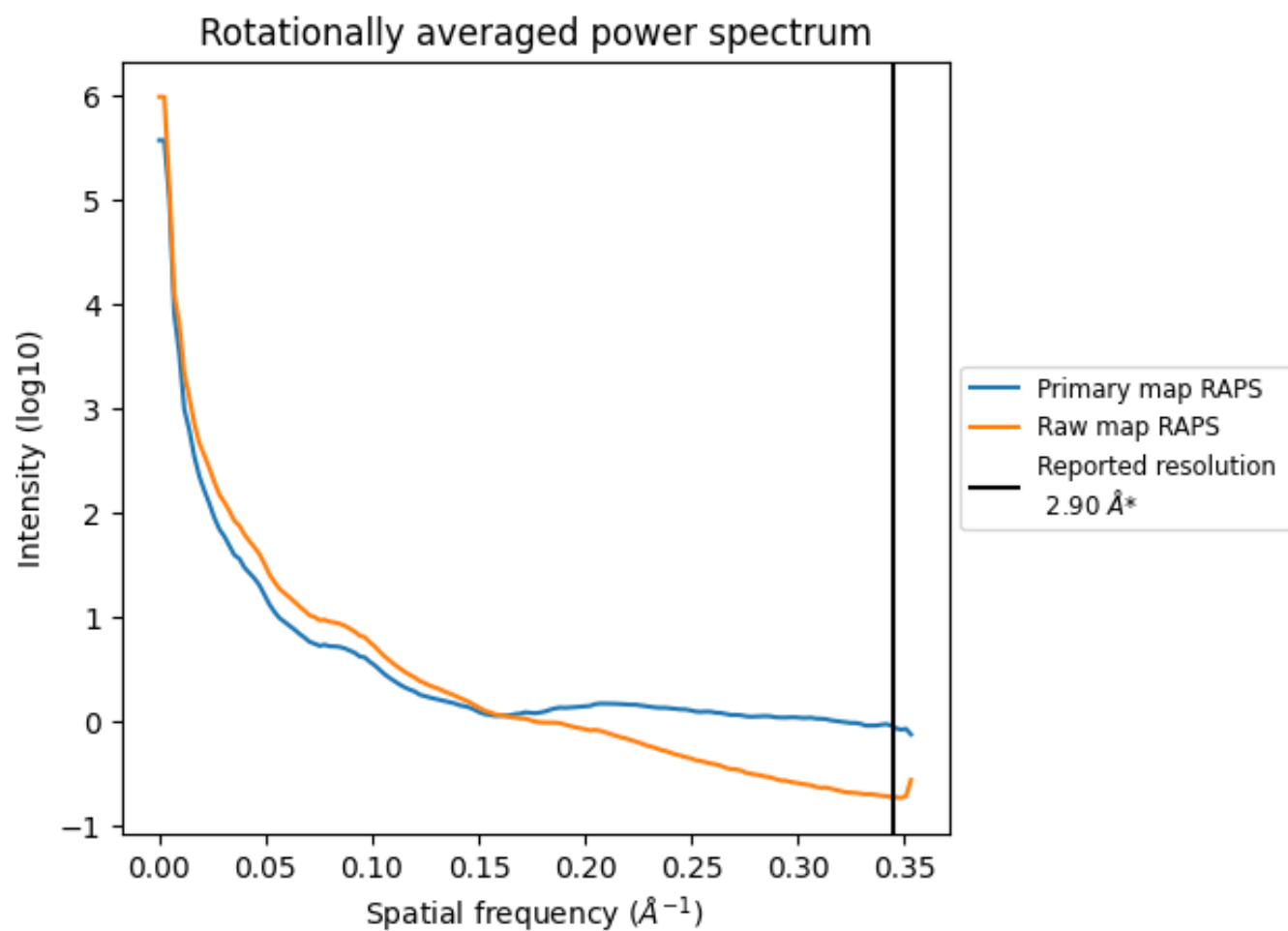
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1033 nm³; this corresponds to an approximate mass of 933 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 ⓘ

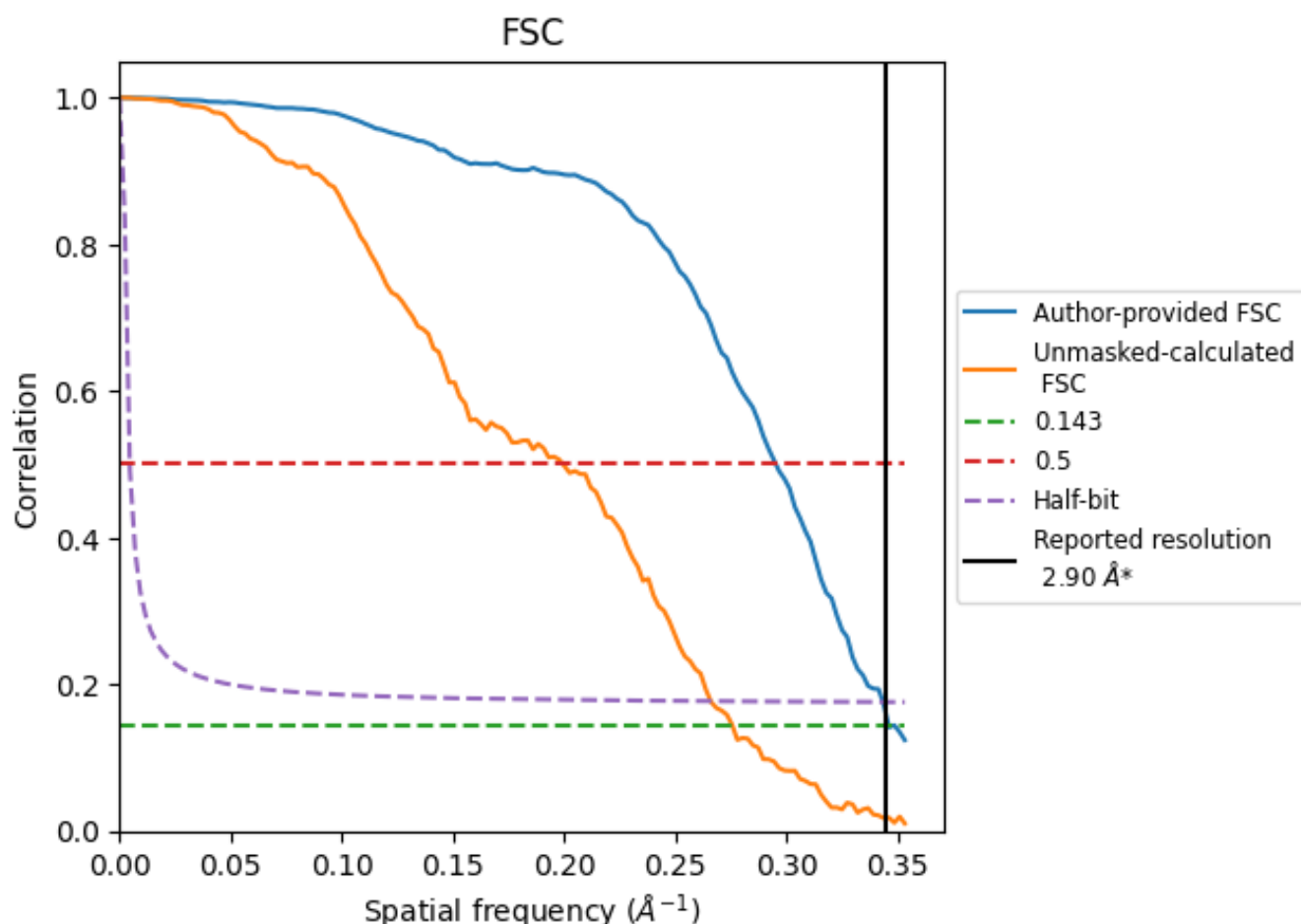


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

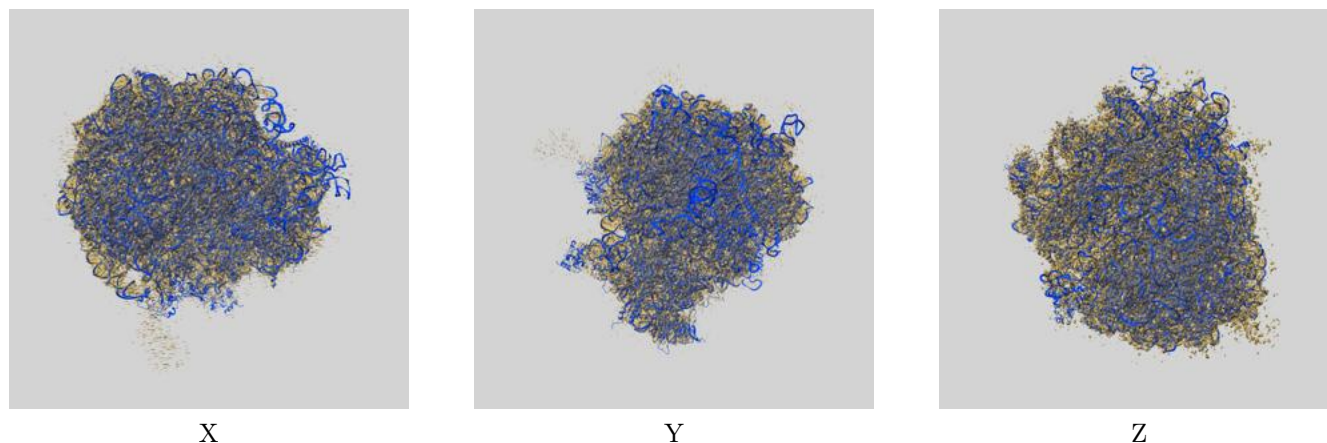
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.89	3.39	2.91
Unmasked-calculated*	3.63	5.02	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.63 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

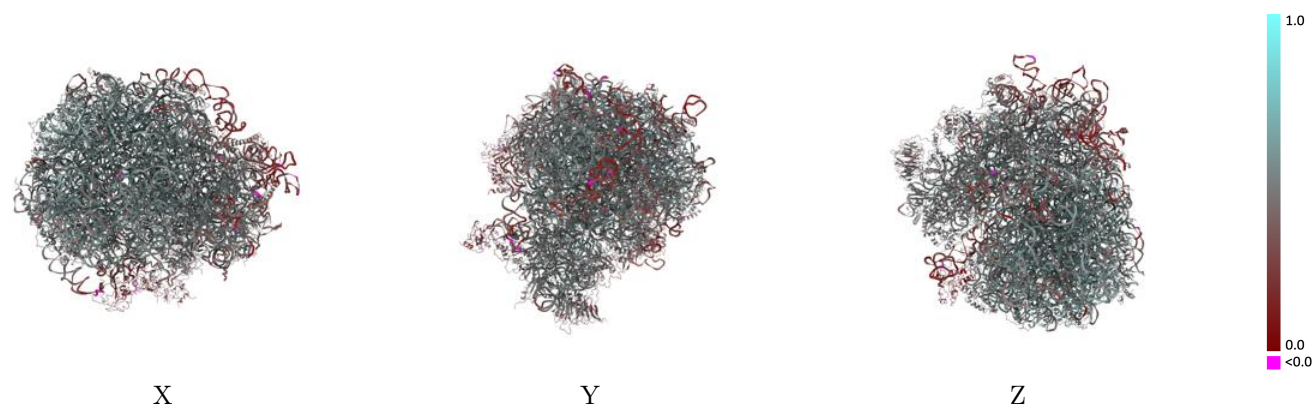
This section contains information regarding the fit between EMDB map EMD-21859 and PDB model 6WOO. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



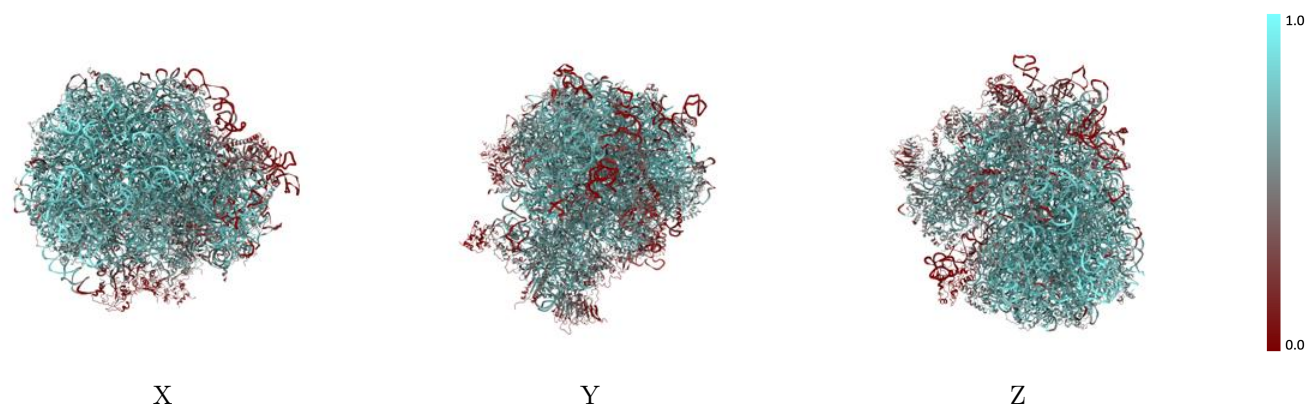
The images above show the 3D surface view of the map at the recommended contour level 0.042 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



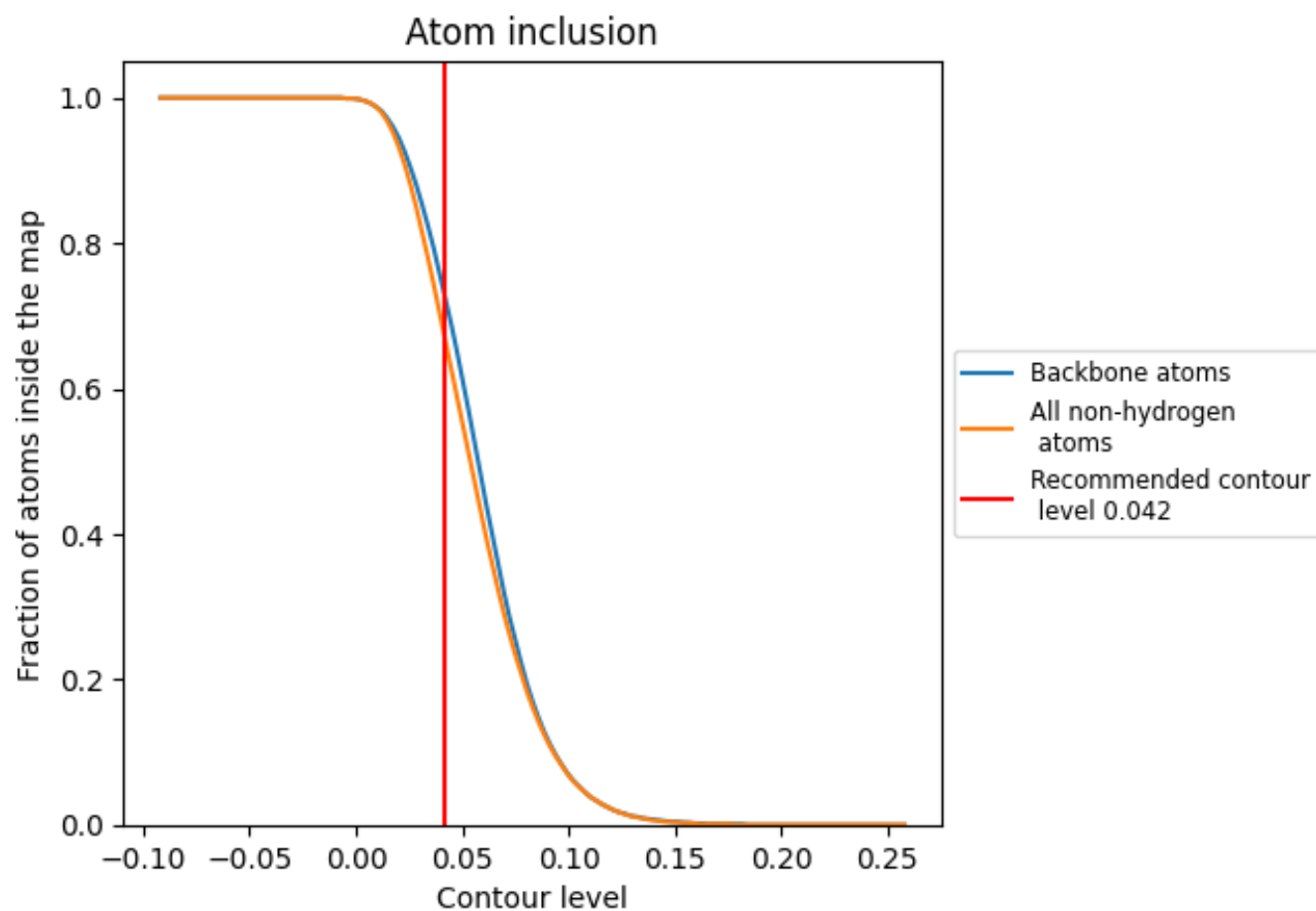
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.042).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 67% 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 (0.042) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.4870
1	 0.5100	 0.4650
2	 0.7060	 0.4640
3	 0.6180	 0.4540
4	 0.8170	 0.5400
5	 0.7780	 0.5030
7	 0.8310	 0.5330
8	 0.8590	 0.5460
A	 0.7070	 0.5420
AA	 0.4640	 0.4490
B	 0.6680	 0.5200
BB	 0.5380	 0.4660
C	 0.7030	 0.5290
CC	 0.5750	 0.4890
D	 0.5690	 0.4800
DD	 0.4780	 0.4570
E	 0.6100	 0.4800
EE	 0.6250	 0.5100
F	 0.6770	 0.5210
FF	 0.5530	 0.4630
G	 0.5660	 0.4780
GG	 0.4580	 0.4370
H	 0.6370	 0.5020
HH	 0.2820	 0.4220
I	 0.6610	 0.5220
II	 0.5190	 0.4780
J	 0.4790	 0.4670
JJ	 0.6030	 0.4770
K	 0.0530	 0.2380
KK	 0.4480	 0.4130
L	 0.6680	 0.5220
LL	 0.5460	 0.4990
M	 0.6290	 0.5010
MM	 0.0540	 0.2660
N	 0.7630	 0.5580



















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Chain	Atom inclusion	Q-score
NN	0.5070	0.4820
O	0.6800	0.5310
OO	0.6100	0.4860
P	0.6890	0.5270
PP	0.5440	0.4390
Q	0.7210	0.5410
QQ	0.5830	0.4990
R	0.5730	0.4900
RR	0.4140	0.4480
S	0.6740	0.5260
SS	0.5680	0.4960
T	0.6450	0.5250
TT	0.5740	0.4920
U	0.4850	0.4440
UU	0.4310	0.4500
V	0.6590	0.5440
VV	0.5060	0.4740
W	0.6400	0.5310
WW	0.6100	0.5140
X	0.6390	0.5150
XX	0.6380	0.5260
Y	0.6740	0.5300
YY	0.5110	0.4650
Z	0.5630	0.4800
ZZ	0.5010	0.4620
a	0.7640	0.5600
aa	0.6530	0.4900
b	0.6290	0.5090
bb	0.4340	0.4650
c	0.5530	0.4570
cc	0.5430	0.4810
d	0.6260	0.5090
dd	0.6700	0.5000
e	0.7180	0.5390
ee	0.5340	0.4690
f	0.7230	0.5520
ff	0.1370	0.3230
g	0.5840	0.4980
gg	0.3410	0.4240
h	0.6540	0.5170
i	0.6220	0.4850
j	0.7760	0.5620

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Chain	Atom inclusion	Q-score
k	 0.4500	 0.4400
l	 0.7300	 0.5520
m	 0.6770	 0.5280
n	 0.6400	 0.5120
o	 0.6680	 0.5240
p	 0.6440	 0.5060
q	 0.0230	 0.2450
r	 0.0940	 0.2690