



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 04:36 am GMT

PDB ID : 6GQB
EMDB ID : EMD-0048
Title : Cryo-EM reconstruction of yeast 80S ribosome in complex with mRNA, tRNA and eEF2 (GDP+AlF₄/sordarin)
Authors : Pellegrino, S.; Yusupov, M.; Yusupova, G.; Hashem, Y.
Deposited on : 2018-06-07
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

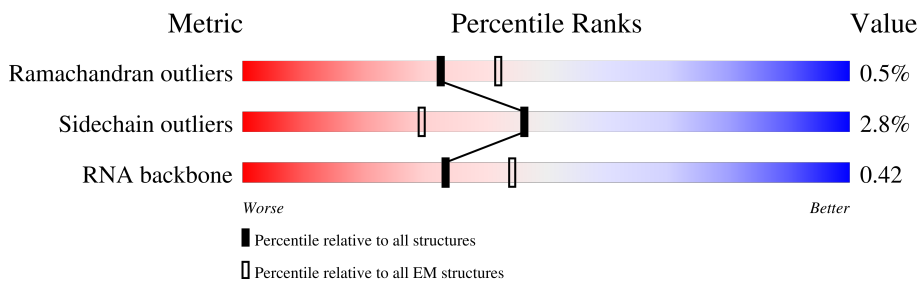
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	1	3396	
2	3	121	
3	4	158	
4	P0	189	
5	P2	94	
6	A	252	
7	B	386	
8	C	361	

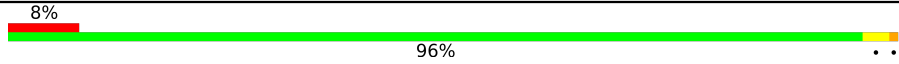
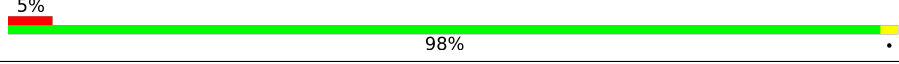
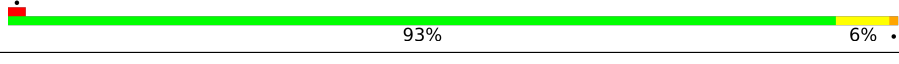
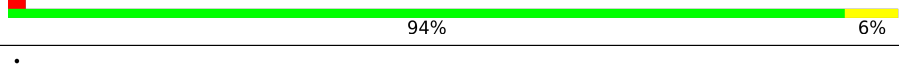
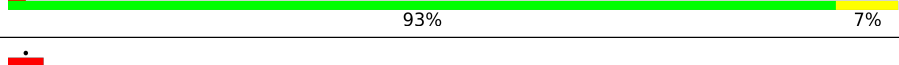
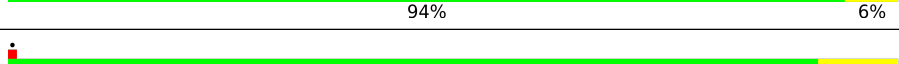
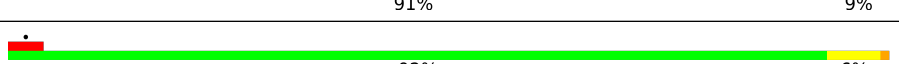
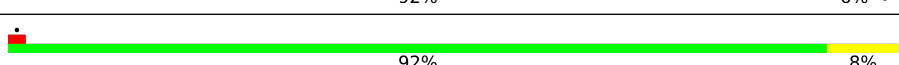
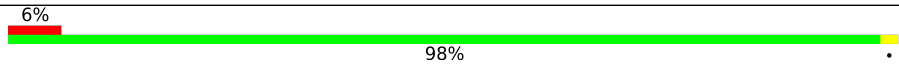
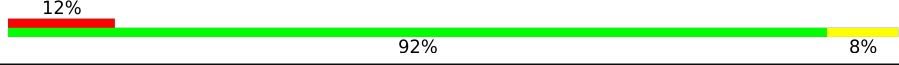
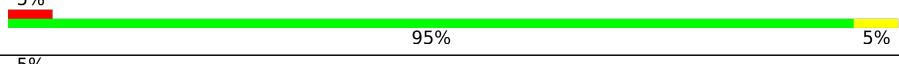
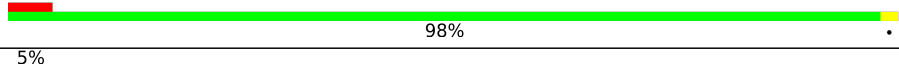
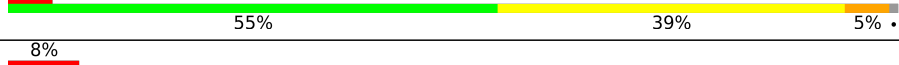
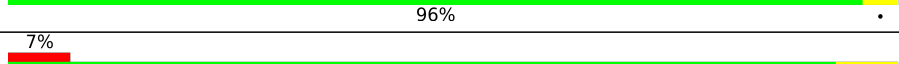
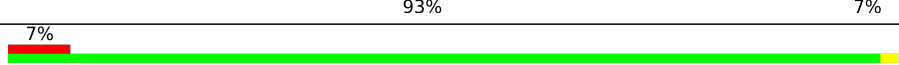
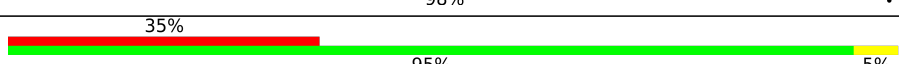
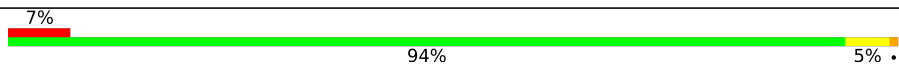
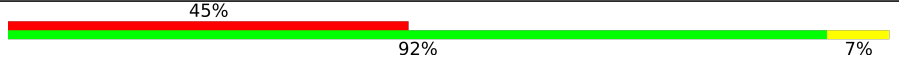
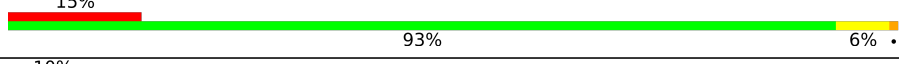
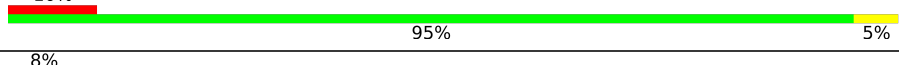
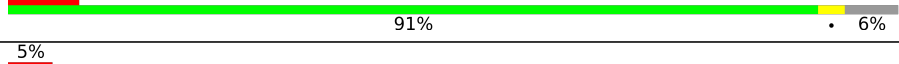
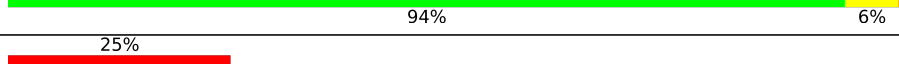
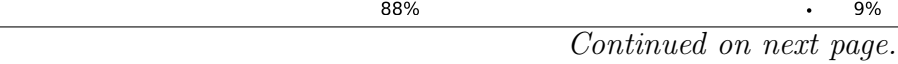


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Mol	Chain	Length	Quality of chain
9	D	296	7% 96%
10	E	175	84% 5% 11%
11	F	222	97%
12	G	233	97%
13	H	191	92% 8%
14	I	220	5% 92%
15	J	169	5% 95%
16	L	193	95% 5%
17	M	136	99%
18	N	203	95% 5%
19	O	197	91% 9%
20	P	183	7% 97%
21	Q	185	98%
22	R	188	6% 96%
23	S	172	94% 5%
24	T	159	99%
25	U	100	98%
26	V	136	13% 96%
27	W	64	14% 97%
28	X	121	5% 98%
29	Y	126	98%
30	Z	135	96%
31	a	148	95% 5%
32	b	58	7% 98%
33	c	97	96%

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Mol	Chain	Length	Quality of chain
34	d	109	
35	e	127	
36	f	106	
37	g	112	
38	h	119	
39	i	99	
40	j	87	
41	k	77	
42	l	50	
43	m	52	
44	n	25	
45	o	105	
46	p	91	
47	2	1797	
48	q	206	
49	r	214	
50	s	217	
51	t	223	
52	u	260	
53	v	206	
54	w	223	
55	x	184	
56	y	199	
57	z	185	
58	AA	105	

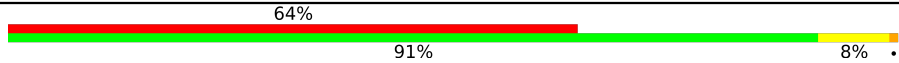
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Mol	Chain	Length	Quality of chain
59	AB	153	19% 98%
60	AC	124	93% 98%
61	AD	150	91% 8%
62	AE	127	99%
63	AF	124	26% 94% 6%
64	AG	141	31% 93% 7%
65	AH	125	30% 89% 7%
66	AI	145	25% 94% 6%
67	AJ	143	24% 98%
68	AK	107	42% 96%
69	AL	87	13% 95% 5%
70	AM	129	95% 5%
71	AN	144	8% 94% 6%
72	AO	134	8% 98%
73	AP	70	69% 99%
74	AQ	97	8% 98%
75	AR	81	95% 5%
76	AS	63	59% 98%
77	AT	53	13% 96%
78	AU	60	25% 93% 7%
79	AV	318	45% 97%
80	AW	37	70% 100%
81	AX	76	54% 43%
82	AY	7	43% 57%
83	BA	204	45% 97%

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Mol	Chain	Length	Quality of chain
84	AZ	840	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '64%', a green segment in the middle labeled '91%', and a yellow segment on the right labeled '8%'. A small black dot is located at the end of the yellow segment.</p>

2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 212143 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 *Saccharomyces cerevisiae* S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	3223	68931	30790	12416	22502	3223	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	3	121	2579	1152	461	845	121	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	158	3353	1500	586	1109	158	0	0

- Molecule 4 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	P0	189	1473	942	257	270	4	0	0

- Molecule 5 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	P2	94	723	448	138	135	2	0	0

- Molecule 6 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	252	1914	1191	388	334	1	0	0

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	386	3075	1950	584	533	8	0	0

- Molecule 8 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	C	361	2748	1729	522	494	3	0	0

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	D	296	2375	1501	414	458	2	0	0

- Molecule 10 is a protein called 60S ribosomal protein L6-A.

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

- Molecule 11 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 12 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	233	1804	1151	323	327	3	0	0

- Molecule 13 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	H	191	1518	963	274	277	4	0	0

- Molecule 14 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	211	Total	C	N	O	S	0	0
			1705	1083	322	294	6		

- Molecule 15 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 16 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	193	Total	C	N	O	S	0	0
			1543	962	315	266			

- Molecule 17 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 18 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 19 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 20 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	183	Total	C	N	O	S	0	0
			1420	882	281	257			

- Molecule 21 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q	185	1441	908	290	241	2	0	0

- Molecule 22 is a protein called 60S ribosomal protein L19-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	S	172	1445	930	267	244	4	0	0

- Molecule 24 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	T	159	1276	805	246	221	4	0	0

- Molecule 25 is a protein called 60S ribosomal protein L22-A.

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

- Molecule 26 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	V	136	1003	628	189	179	7	0	0

- Molecule 27 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	W	64	528	340	103	84	1	0	0

- Molecule 28 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	X	121	964	620	169	173	2	0	0

- Molecule 29 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Y	126	993	625	192	176		0	0

- Molecule 30 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Z	135	1092	710	202	180		0	0

- Molecule 31 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	a	148	1173	749	231	190	3	0	0

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	b	58	462	289	100	73		0	0

- Molecule 33 is a protein called 60S ribosomal protein L30.

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

- Molecule 34 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	d	109	883	559	167	156	1	0	0

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 36 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 37 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 38 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 39 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 40 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 41 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 42 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 43 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 44 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 45 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 46 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	1776	Total	C	N	O	P	0	0
			37845	16918	6702	12449	1776		

- Molecule 48 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 49 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 50 is a protein called 40S ribosomal protein S2.

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

- Molecule 51 is a protein called 40S ribosomal protein S3.

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

- Molecule 52 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 54 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	223	Total	C	N	O	S	0	0
			1790	1123	346	318	3		

- Molecule 55 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 56 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	y	188	1489	925	298	264	2	0	0

- Molecule 57 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	z	185	1494	943	289	261	1	0	0

- Molecule 58 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	AA	96	772	499	126	145	2	0	0

- Molecule 59 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	AB	153	1220	780	231	206	3	0	0

- Molecule 60 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	AC	124	890	560	156	172	2	0	0

- Molecule 61 is a protein called 40S ribosomal protein S13.

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

- Molecule 62 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	AE	127	891	545	182	163	1	0	0

- Molecule 63 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	AF	124	977	622	182	166	7	0	0

- Molecule 64 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 65 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	AH	120	926	577	177	170	2	0	0

- Molecule 66 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	AI	145	1192	743	237	210	2	0	0

- Molecule 67 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 68 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	AK	107	855	539	156	159	1	0	0

- Molecule 69 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 70 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 71 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	AN	144	1121	708	220	191	2	0	0

- Molecule 72 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 74 is a protein called 40S ribosomal protein S26-B.

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

- Molecule 75 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 76 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 77 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AT	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 78 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AU	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AV	318	Total	C	N	O	S	0	0
			2437	1541	418	470	8		

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AW	37	Total	C	N	O	S	0	0
			287	177	57	49	4		

- Molecule 81 is a RNA chain called Transfer RNA - Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	AX	76	Total	C	N	O	P	0	0
			1626	725	293	532	76		

- Molecule 82 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	AY	7	Total	C	N	O	P	0	0
			144	65	21	51	7		

- Molecule 83 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	BA	204	Total	C	N	O	S	0	0
			1609	1031	279	290	9		

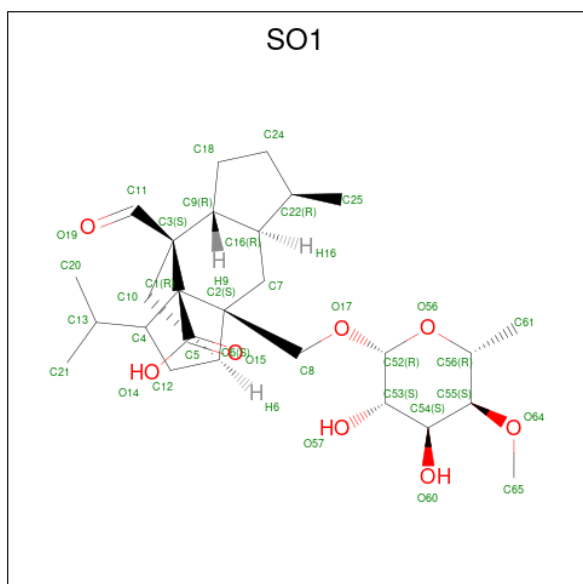
- Molecule 84 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	AZ	840	6551	4161	1124	1237	29	0	0

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

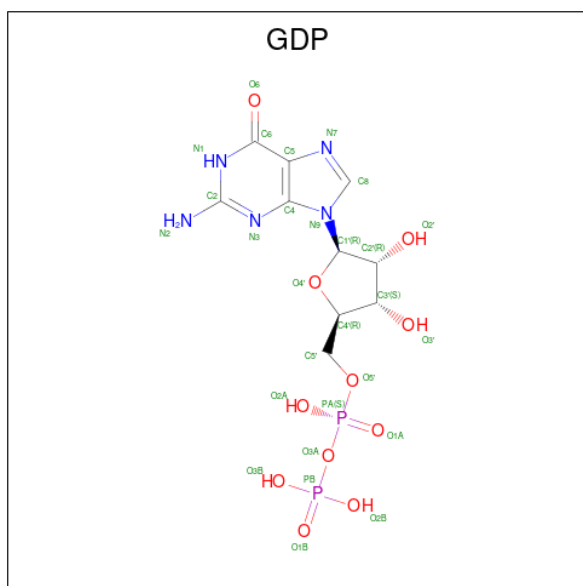
Mol	Chain	Residues	Atoms		AltConf
85	j	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	
85	o	1	Total	Zn	0
			1	1	
85	p	1	Total	Zn	0
			1	1	
85	AQ	1	Total	Zn	0
			1	1	
85	AR	1	Total	Zn	0
			1	1	
85	AT	1	Total	Zn	0
			1	1	
85	AW	1	Total	Zn	0
			1	1	

- Molecule 86 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.B.ETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (three-letter code: SO1) (formula: C₂₇H₄₂O₈).



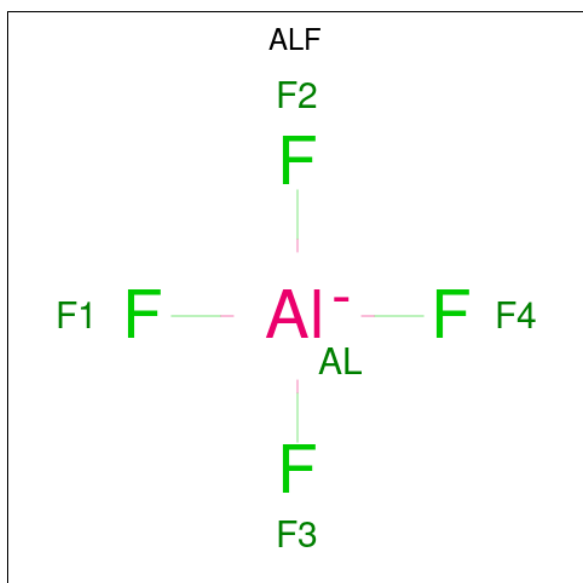
Mol	Chain	Residues	Atoms			AltConf
86	AZ	1	Total	C	O	0
			35	27	8	

- Molecule 87 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 88 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).

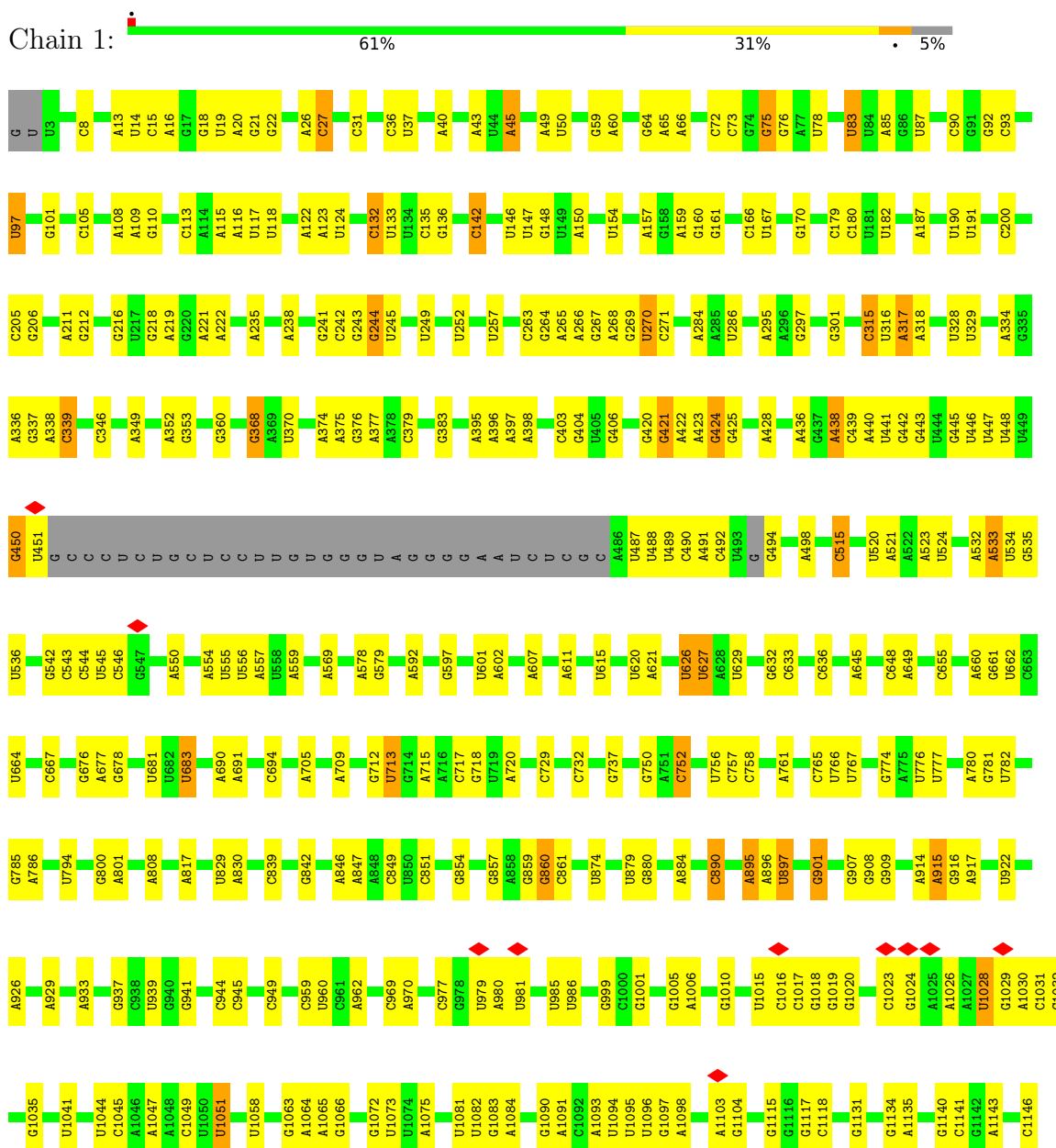


Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
88	AZ	1	5	1	4	0

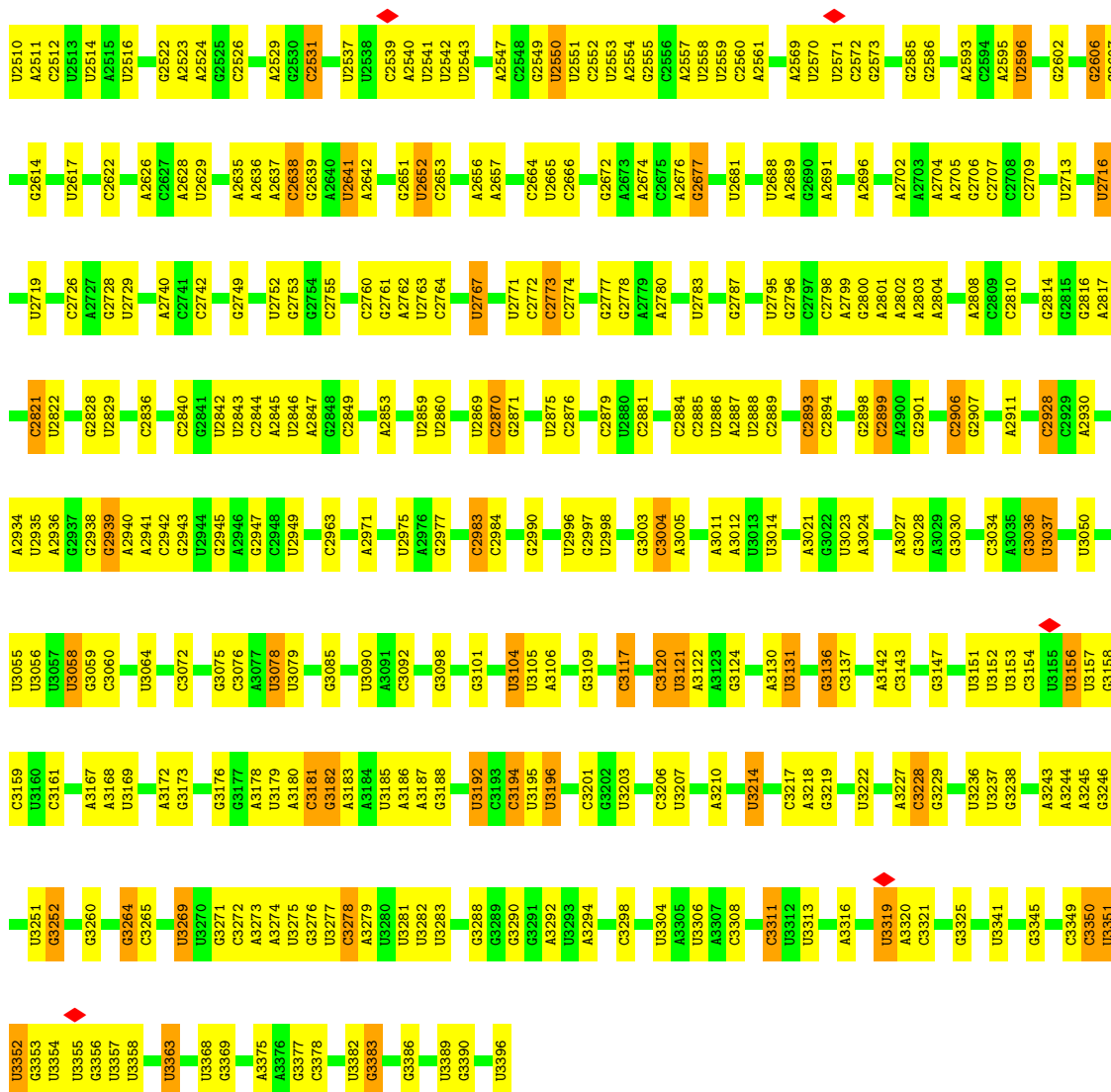
3 Residue-property plots

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

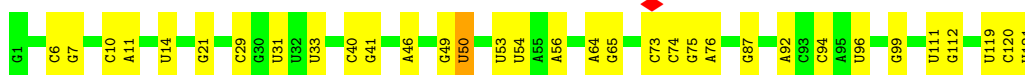
- Molecule 1: *Saccharomyces cerevisiae* S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA



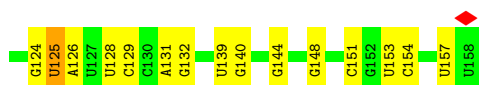
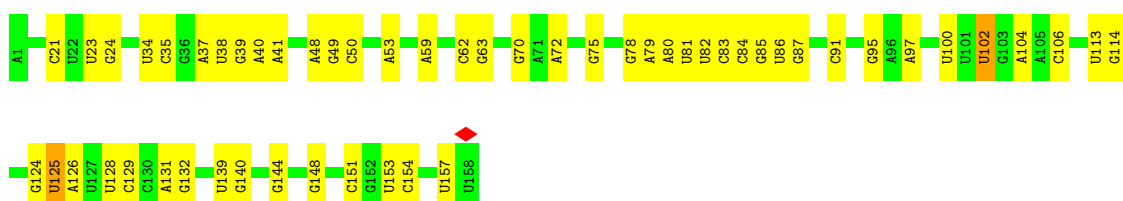
A2443	G2450	U2334	G2206	U	A1858	A1741	U1626	G1532	C1411	G1300	G1299	U1151
C2444	G2451	G2335	U2209	U	G1863	U1742	U1629	U1533	G1417	A1301	G1230	G1152
A2445	G2452	U2337	G2210	A	A1864	A1749	U1630	G1536	A1418	A1302	A1231	A1153
U2446	G2453	C2338	C2094	C	A1865	A1750	C1631	A1546	A1419	A1303	C1233	C1154
A2447	G2454	C2339	C2101	C	A1866	G1751	A1632	U1626	U4295	A1304	G1234	A1155
G2450	G2455	U2349	U2102	C	C1870	C1756	C1633	C1851	U4295	U1305	U1235	A1156
G2451	G2456	C2231	U2103	C	U1871	G1759	A1637	C1856	G1434	G1306	G1236	A1159
U2452	G2457	C2235	U2109	C	U1872	C1759	C1638	C1556	G1434	G1307	G1237	G1160
G2454	G2458	A2236	G2110	C	U1873	A1760	A1639	A1557	A1435	A1308	C1238	C1161
U2455	G2459	A2244	G2111	C	G1878	C1762	G1640	A1559	C4437	U1309	U1240	A1165
A2456	U2460	C2362	G2114	C	A1879	U1763	U1641	G1560	A1446	C1312	U1241	A1168
G2457	U2461	C2366	G2115	C	U1880	U1764	A1642	G1561	A1447	G1313	G1242	U1171
U2458	U2462	U2369	G2116	C	U1885	U1765	C1643	C1562	U1448	U1314	G1243	A1244
A2459	G2463	G2372	G2117	C	A1886	G1766	U1645	C1563	A1449	U1315	A1245	A1245
U2460	G2464	C2374	A2117	C	U1889	U1767	A1656	U1564	G1450	C1316	U1246	G1174
A2461	G2465	A2372	G2118	C	A1893	U1768	A1657	A1566	U1455	C1320	U1247	G1178
G2463	G2466	U2258	G2122	C	A1896	G1769	G1658	U1567	U1455	A1326	C1248	A1179
G2466	G2467	U2269	A2131	C	A1896	C1779	C1671	U1568	G1466	C1327	G1249	A1180
G2467	A2468	A2270	U2137	G	A1901	G1780	U1672	U1569	U1471	A1330	A1251	U1181
A2468	G2469	A2271	C1781	C	G1906	C1781	U1672	U1570	U1471	U1331	A1252	A1182
G2469	G2470	G2272	U2133	C	U1907	U1782	G1677	U1571	A1477	A1332	U1253	U1254
U2471	G2471	C2273	G2134	C	C1907	U1783	U1678	U1572	C4478	C1333	C1255	G1196
U2472	G2472	G2276	U2137	C	G1788	C1788	G1678	U1573	U1481	U1347	G1266	C1189
C2473	G2473	C2277	U2138	C	U1795	U1795	A1683	C1574	A1481	U1348	C1267	A1190
G2474	G2474	A2280	A2139	C	U1796	U1796	U1684	U1577	A1482	A1190	U1268	U1191
G2475	G2475	A2281	U2139	C	A1797	A1797	C1685	G1578	G1483	G1349	A1269	G1192
C2476	G2476	C2284	C1926	C	C1926	U1926	U1688	C1579	G1488	A1350	G1261	A1193
C2477	G2477	C2287	G1927	C	G1927	G1927	A1689	A1580	A1489	U1351	G1262	C1196
C2478	G2478	C2287	U1928	C	U1928	C1928	C1690	C1581	A1490	U1352	A1263	A1197
C2479	G2479	A2291	A1930	C	A1930	A1930	U1703	C1582	A1491	G1354	G1264	C1198
A2480	G2480	A2295	U1931	C	U1931	G1907	A1704	A1583	G1492	A1355	U1265	C1201
A2486	G2481	A2295	G1934	C	G1934	G1908	U1705	U1584	U1493	U1356	G1266	A1202
U2487	G2482	A2295	G1935	C	G1935	U1814	C1706	C1585	C1496	G1357	U1267	A1203
A2488	G2483	U2298	U1948	C	U1948	U1815	A1707	A1589	C1499	U1361	A1273	G1206
C2489	G2484	U2298	G1948	C	G1948	A1816	A1708	A1593	C1499	G1370	A1274	G1209
C2490	G2485	G3305	G1953	C	G1953	U1819	A1714	A1602	A1503	U1370	U1275	G1209
A2491	G2486	C2306	U1954	C	U1954	U1820	G1717	A1603	G1507	C1385	U1276	U1214
C2492	G2487	G2307	U1955	C	U1955	U1821	G1718	G1604	C1508	A1386	C1277	C1216
U2493	G2488	C2308	A	C	A	G1830	U1721	A1605	U1511	G1387	C1279	U1217
A2494	G2489	U2309	G	C	G	U1840	U1722	G1608	U1512	G1392	C1280	U1218
U2495	G2490	U2310	U	C	U	U1841	A1723	A1394	C1516	A1393	G1281	A1221
C2496	G2491	G2313	U	C	U	A1842	U1724	A1394	C1516	A1394	G1282	G1222
U2497	G2492	U2314	G	C	G	A1842	C1725	A1399	C1516	A1399	C1283	A1222
U2498	G2493	G2315	U	C	U	G1845	U1729	A1400	G1523	G1400	G1284	G1222
U2499	G2494	G2315	U	C	U	C1846	A1729	G1405	A1524	G1400	A1285	A1286
U2501	G2495	G2323	G	C	G	C1846	A1729	U1405	A1524	U1405	C1224	C1224
U2502	G2496	U2324	U	C	U	A1850	G1736	G1408	G1526	G1408	A1287	A1285
G2503	G2497	G2325	C	C	C	G1851	U1737	G1409	U1527	G1409	C1227	C1226
U2504	G2498	U2327	A	C	A	C1854	C1738	U1410	C1531	U1410	C1227	A1287
U2505	G2499	U2327	U	C	U	C1854	C1738	U1410	C1531	U1410	C1227	A1287
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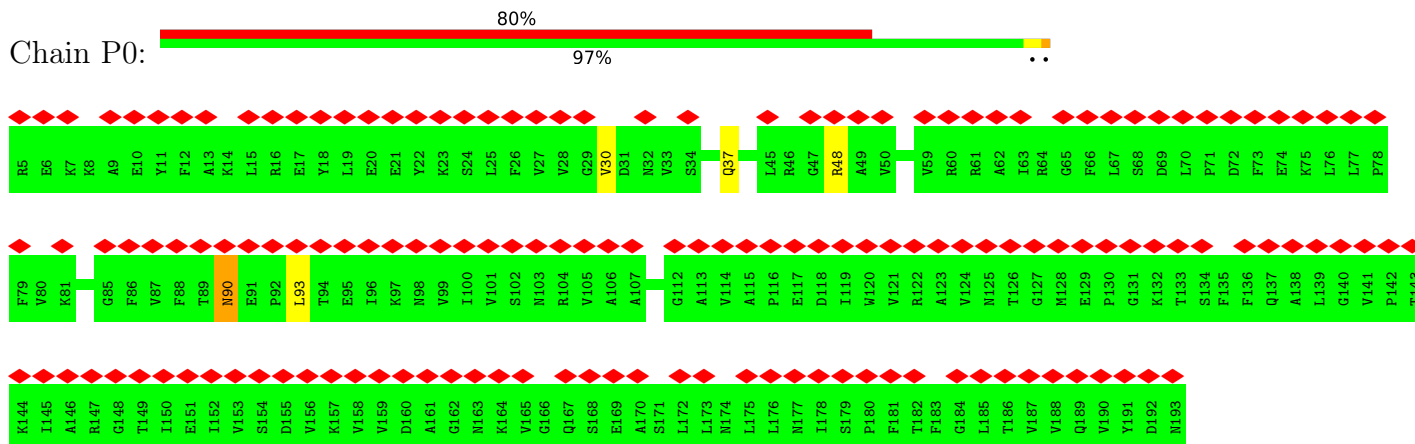
• Molecule 2: 5S ribosomal RNA



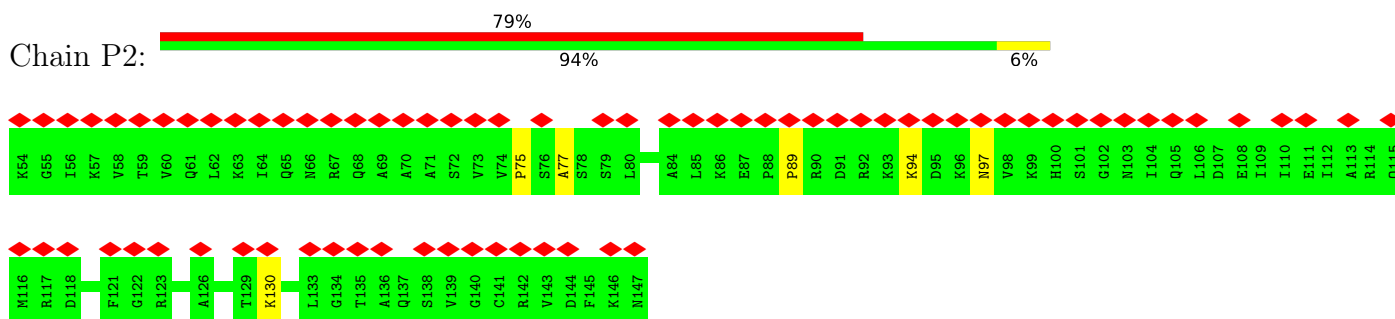
• Molecule 3: 5.8S ribosomal RNA



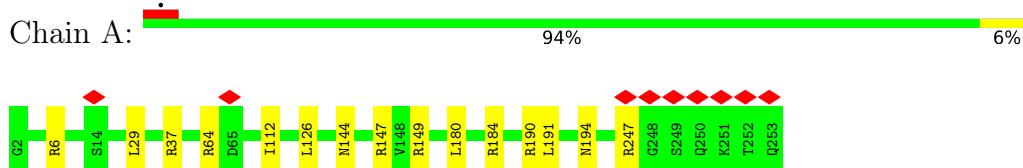
- Molecule 4: 60S acidic ribosomal protein P0



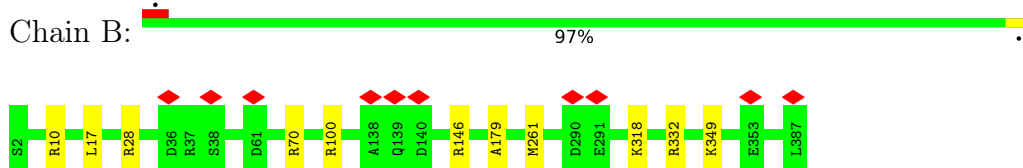
- Molecule 5: 60S ribosomal protein L12-A



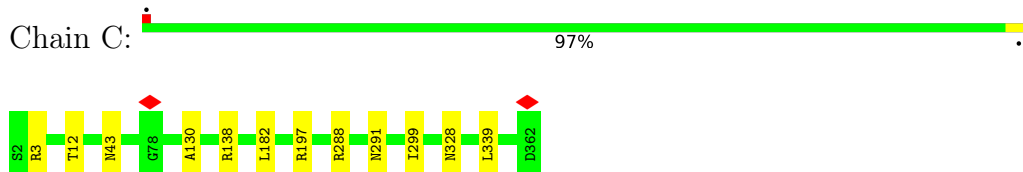
- Molecule 6: 60S ribosomal protein L2-A



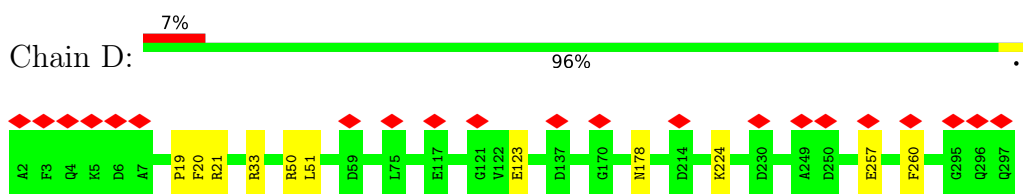
- Molecule 7: 60S ribosomal protein L3



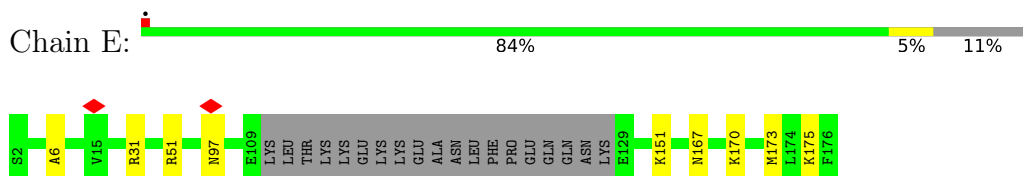
- Molecule 8: 60S ribosomal protein L4-A



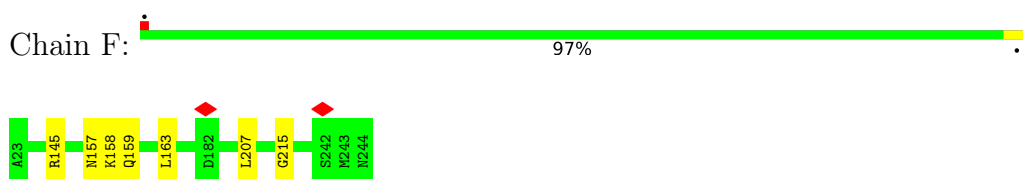
- Molecule 9: 60S ribosomal protein L5



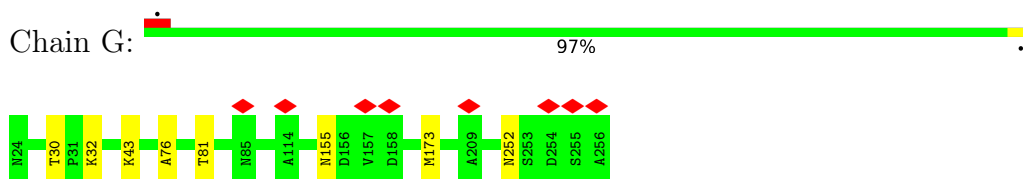
- Molecule 10: 60S ribosomal protein L6-A



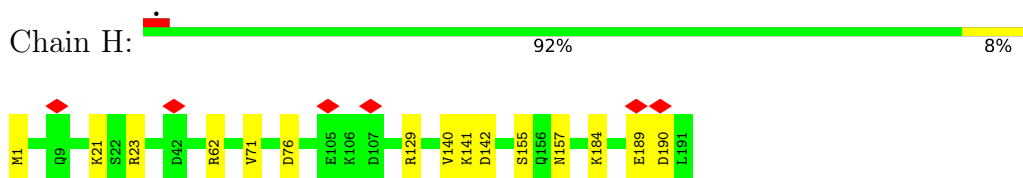
- Molecule 11: 60S ribosomal protein L7-A



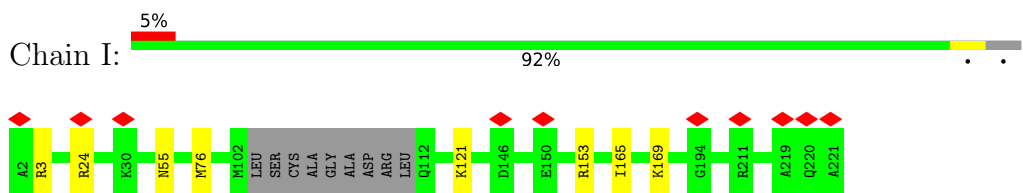
- Molecule 12: 60S ribosomal protein L8-A



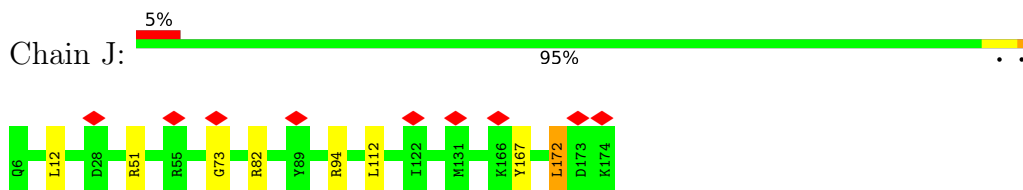
- Molecule 13: 60S ribosomal protein L9-A



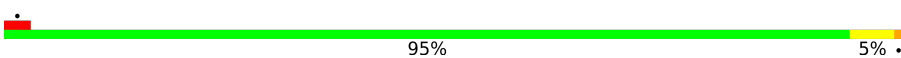
- Molecule 14: 60S ribosomal protein L10

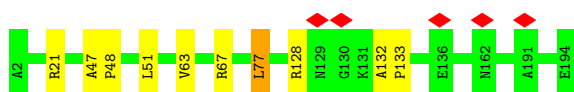


- Molecule 15: 60S ribosomal protein L11-B



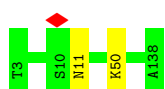
- Molecule 16: 60S ribosomal protein L13-A

Chain L:  95% 5%



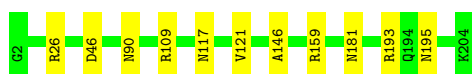
- Molecule 17: 60S ribosomal protein L14-A

Chain M:  99%



- Molecule 18: 60S ribosomal protein L15-A

Chain N:  95% 5%



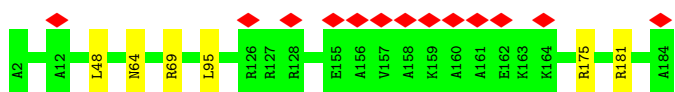
- Molecule 19: 60S ribosomal protein L16-A

Chain O:  91% 9%



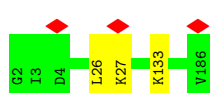
- Molecule 20: 60S ribosomal protein L17-A

Chain P:  7% 97%

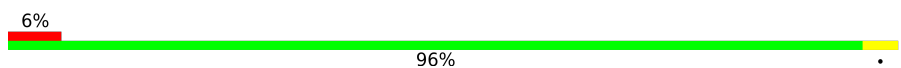


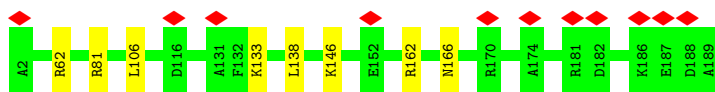
- Molecule 21: 60S ribosomal protein L18-A

Chain Q:  98%

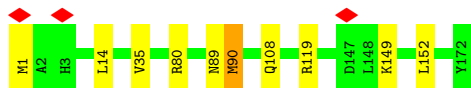


- Molecule 22: 60S ribosomal protein L19-A

Chain R:  6% 96%



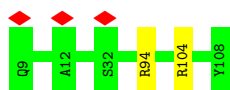
- Molecule 23: 60S ribosomal protein L20-A



- Molecule 24: 60S ribosomal protein L21-A



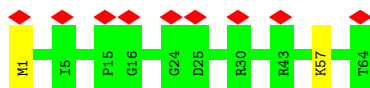
- Molecule 25: 60S ribosomal protein L22-A



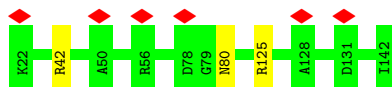
- Molecule 26: 60S ribosomal protein L23-A



- Molecule 27: 60S ribosomal protein L24-A

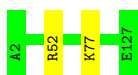


- Molecule 28: 60S ribosomal protein L25



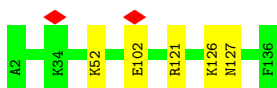
- Molecule 29: 60S ribosomal protein L26-A

Chain Y:  98%



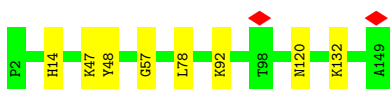
- Molecule 30: 60S ribosomal protein L27-A

Chain Z:  96%



- Molecule 31: 60S ribosomal protein L28

Chain a:  95%



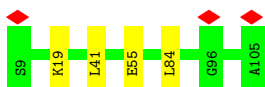
- Molecule 32: 60S ribosomal protein L29

Chain b:  98%



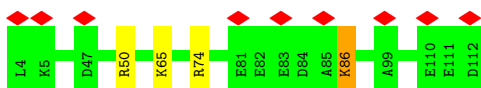
- Molecule 33: 60S ribosomal protein L30

Chain c:  96%



- Molecule 34: 60S ribosomal protein L31-A

Chain d:  96%

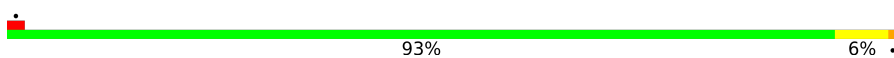


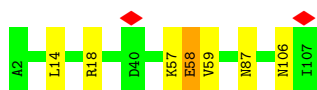
- Molecule 35: 60S ribosomal protein L32

Chain e:  98%



- Molecule 36: 60S ribosomal protein L33-A

Chain f:  93% 6%



- Molecule 37: 60S ribosomal protein L34-A

Chain g:  94% 6%

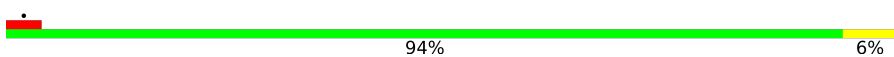


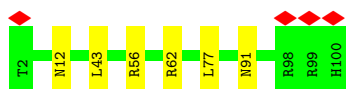
- Molecule 38: 60S ribosomal protein L35-A

Chain h:  93% 7%

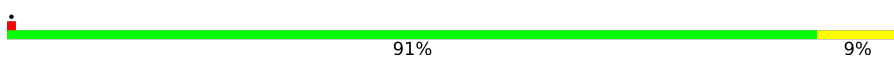


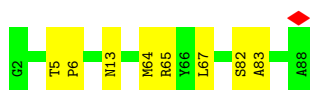
- Molecule 39: 60S ribosomal protein L36-A

Chain i:  94% 6%

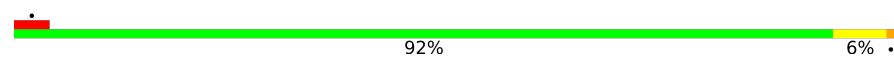


- Molecule 40: 60S ribosomal protein L37-A

Chain j:  91% 9%



- Molecule 41: 60S ribosomal protein L38

Chain k:  92% 6%

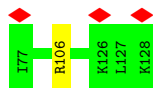


- Molecule 42: 60S ribosomal protein L39

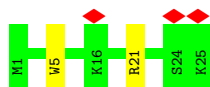
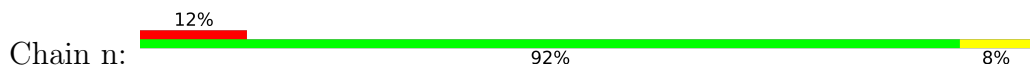
Chain l:  92% 8%



- Molecule 43: Ubiquitin-60S ribosomal protein L40



- Molecule 44: 60S ribosomal protein L41-B



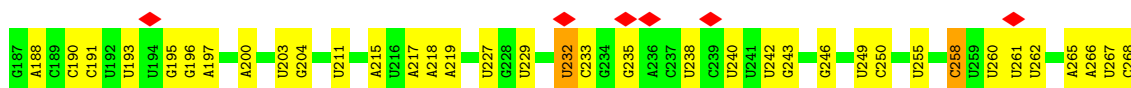
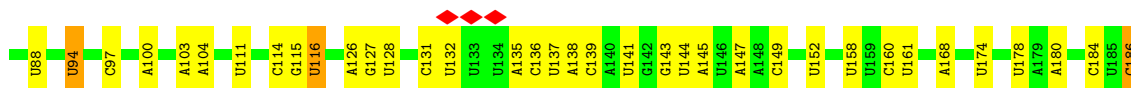
- Molecule 45: 60S ribosomal protein L42-A

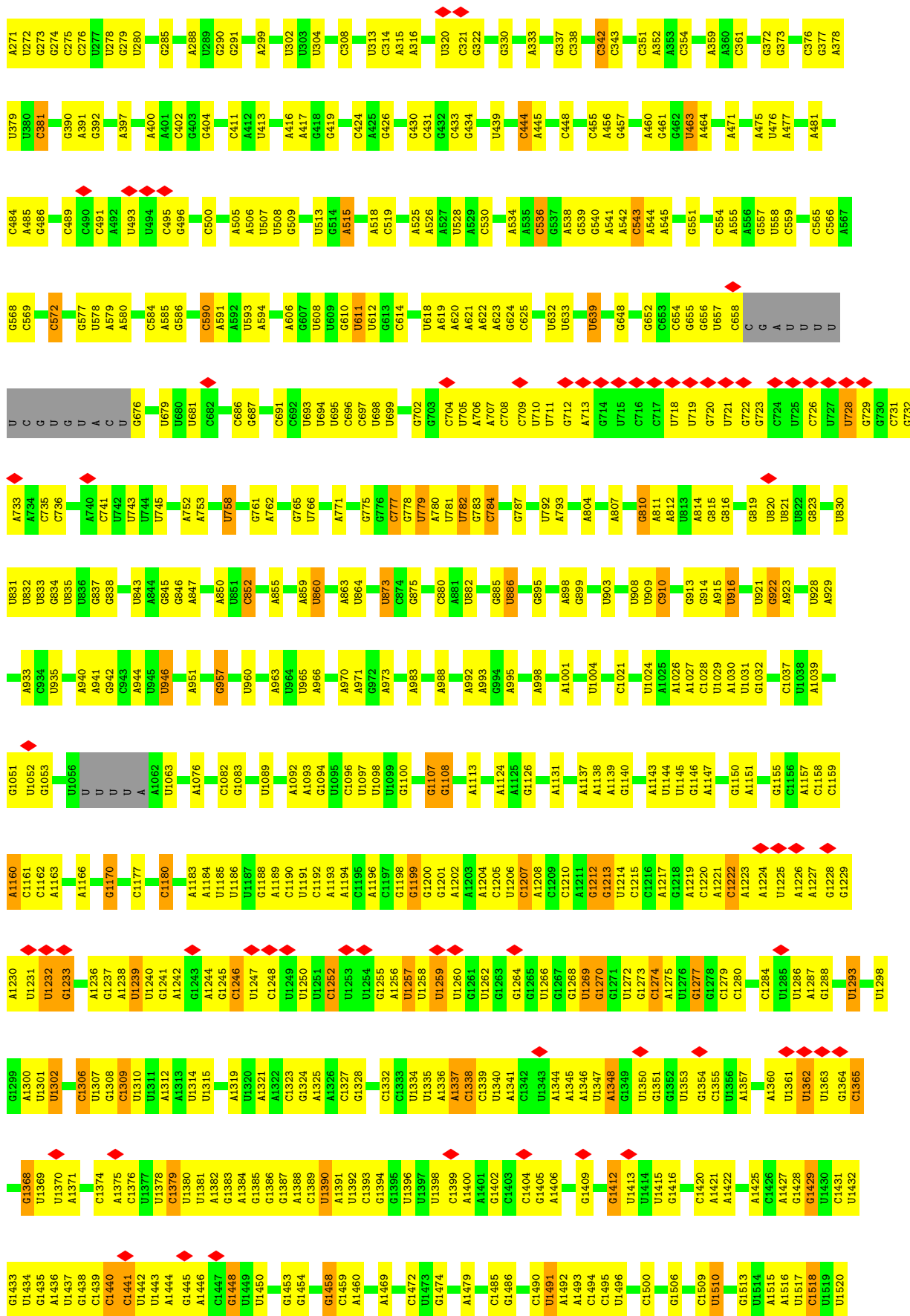


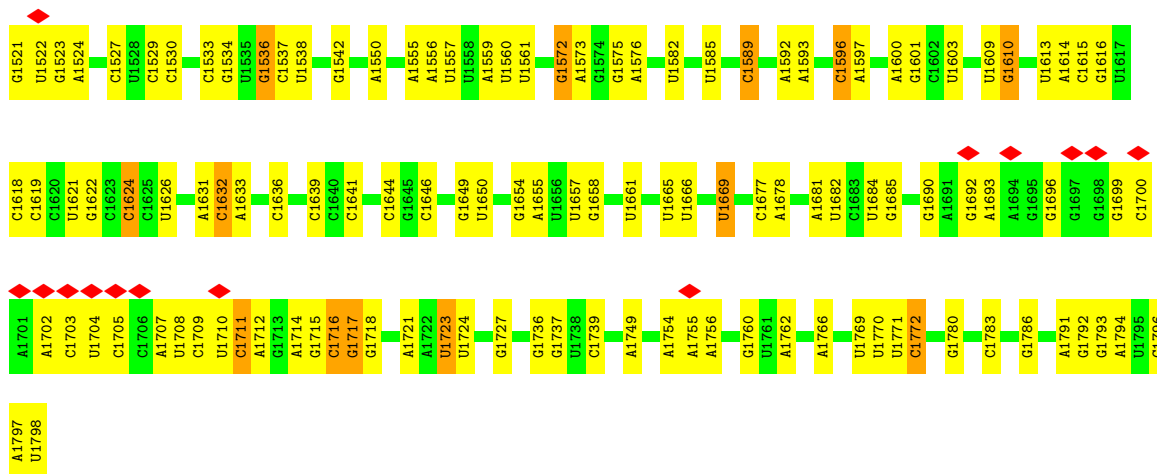
- Molecule 46: 60S ribosomal protein L43-A



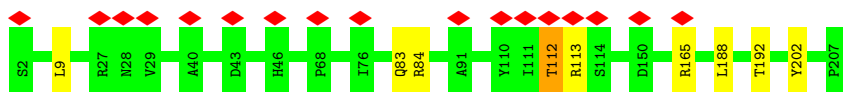
- Molecule 47: 18S ribosomal RNA



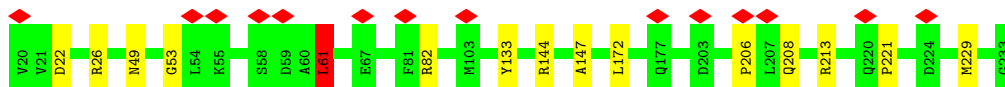
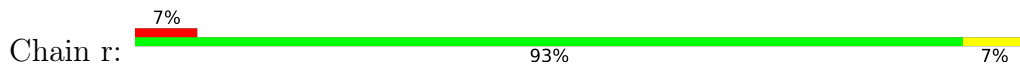




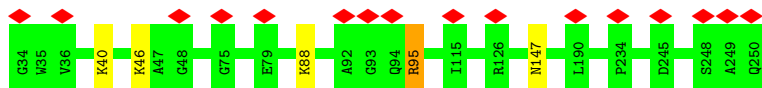
• Molecule 48: 40S ribosomal protein S0-A



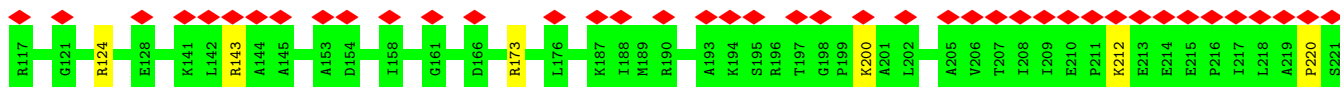
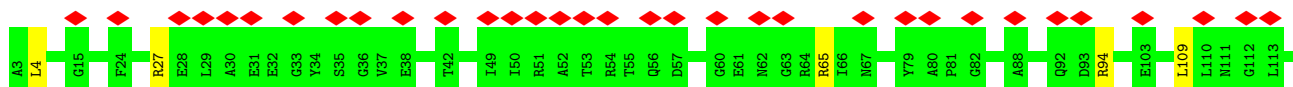
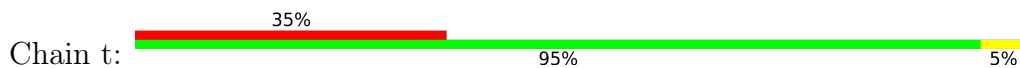
• Molecule 49: 40S ribosomal protein S1-A

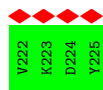


• Molecule 50: 40S ribosomal protein S2

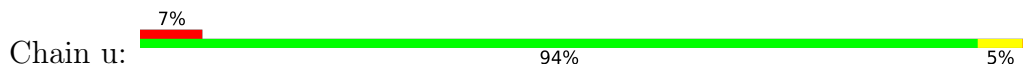


• Molecule 51: 40S ribosomal protein S3

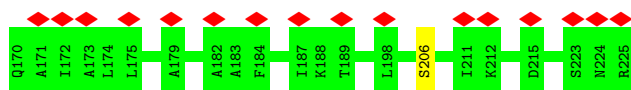
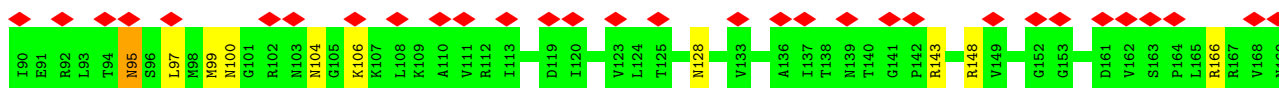
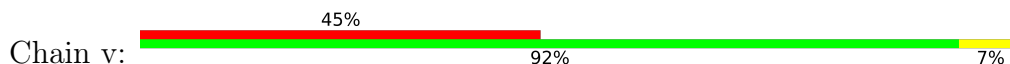




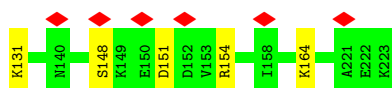
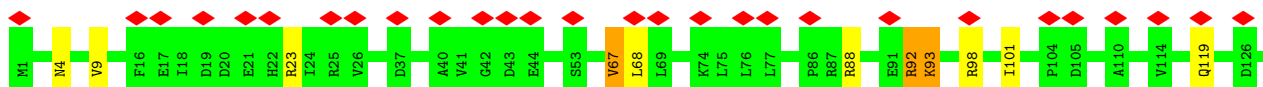
- Molecule 52: 40S ribosomal protein S4-A



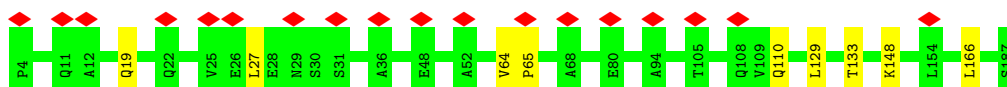
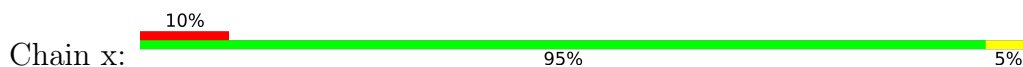
- Molecule 53: 40S ribosomal protein S5



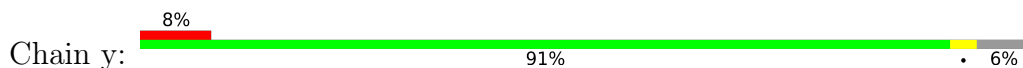
- Molecule 54: 40S ribosomal protein S6-A

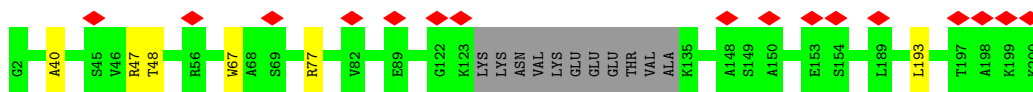


- Molecule 55: 40S ribosomal protein S7-A

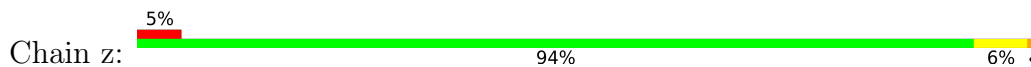


- Molecule 56: 40S ribosomal protein S8-A

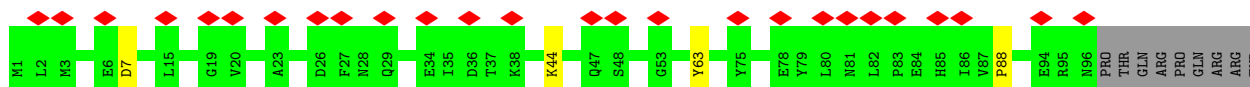
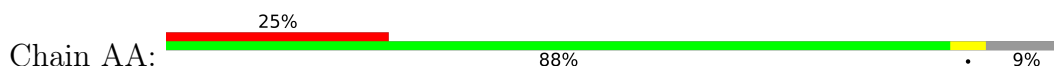




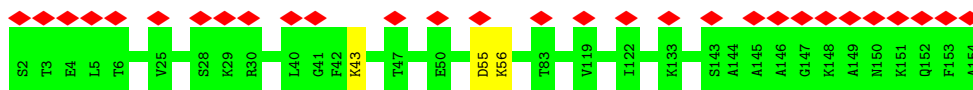
- Molecule 57: 40S ribosomal protein S9-A



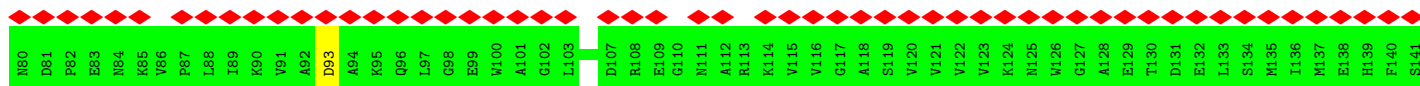
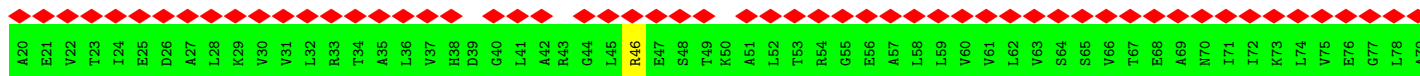
- Molecule 58: 40S ribosomal protein S10-A



- Molecule 59: 40S ribosomal protein S11-A



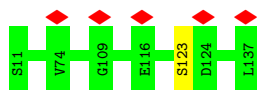
- Molecule 60: 40S ribosomal protein S12



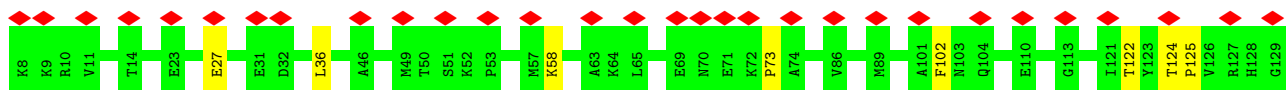
- Molecule 61: 40S ribosomal protein S13



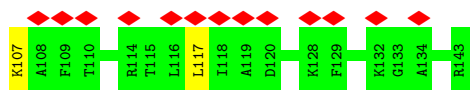
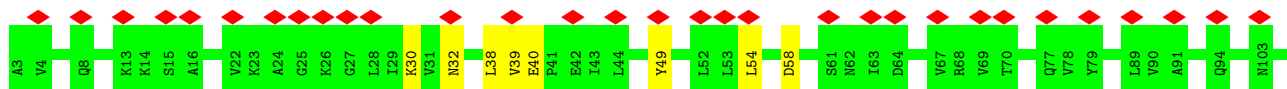
- Molecule 62: 40S ribosomal protein S14-B



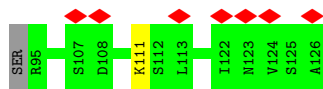
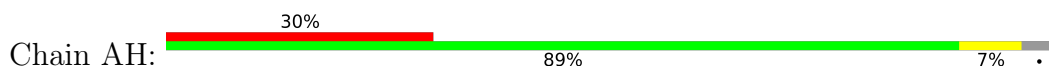
• Molecule 63: 40S ribosomal protein S15



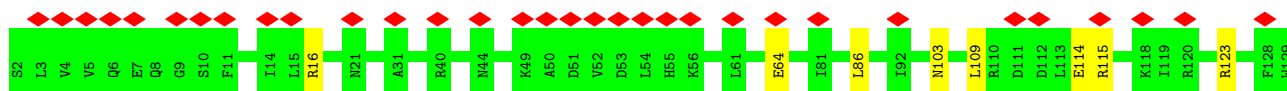
• Molecule 64: 40S ribosomal protein S16-A



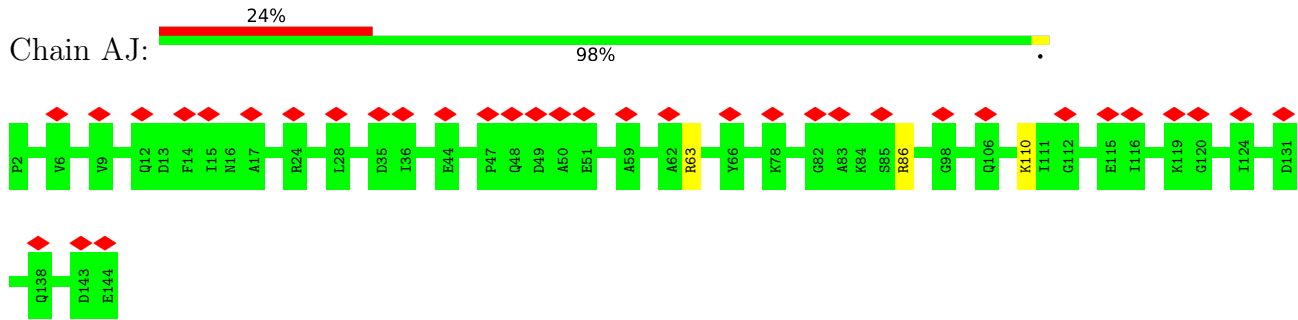
• Molecule 65: 40S ribosomal protein S17-B



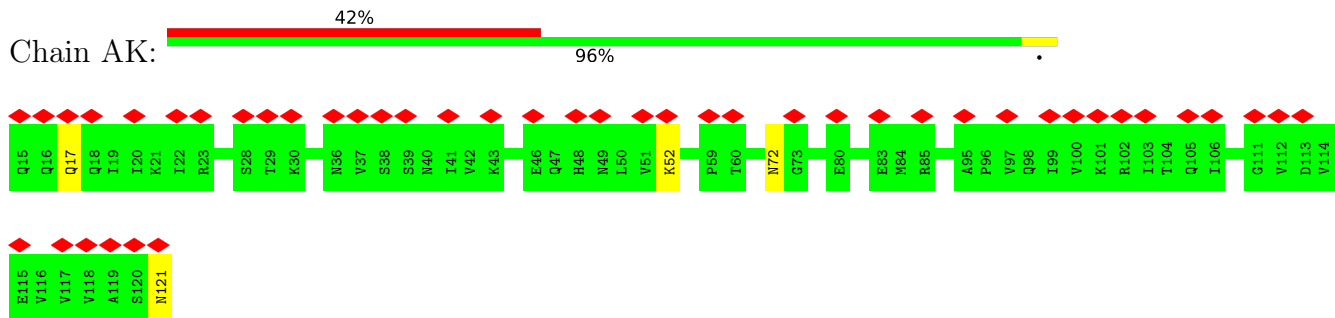
• Molecule 66: 40S ribosomal protein S18-A



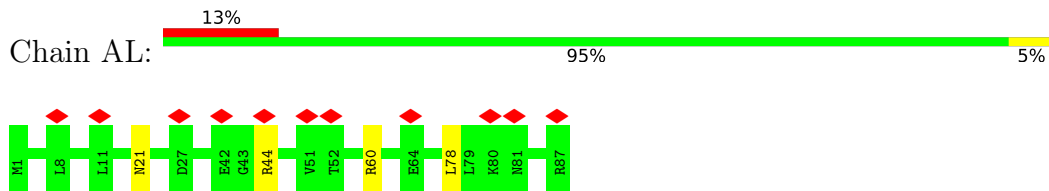
- Molecule 67: 40S ribosomal protein S19-A



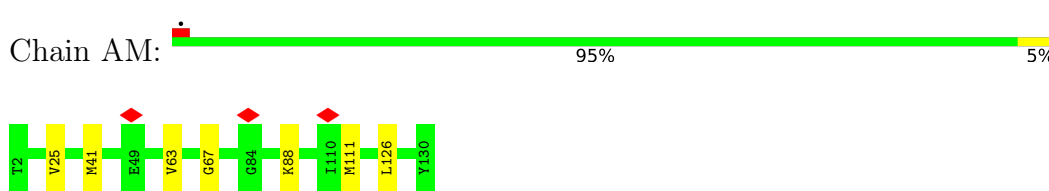
- Molecule 68: 40S ribosomal protein S20



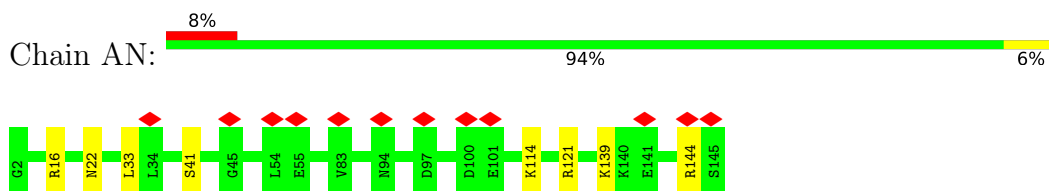
- Molecule 69: 40S ribosomal protein S21-A



- Molecule 70: 40S ribosomal protein S22-A

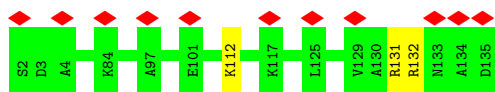


- Molecule 71: 40S ribosomal protein S23-A

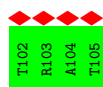
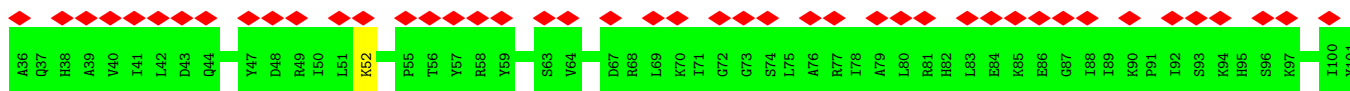


- Molecule 72: 40S ribosomal protein S24-A

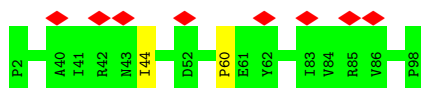




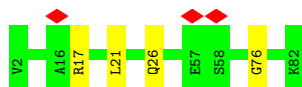
- Molecule 73: 40S ribosomal protein S25-A



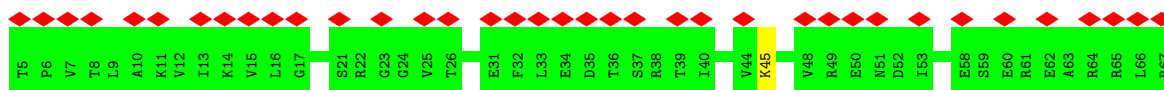
- Molecule 74: 40S ribosomal protein S26-B



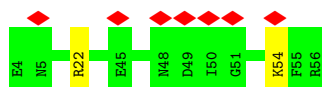
- Molecule 75: 40S ribosomal protein S27-A



- Molecule 76: 40S ribosomal protein S28-A

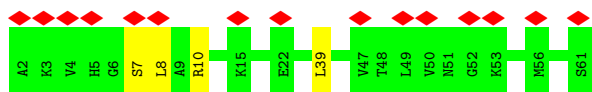


- Molecule 77: 40S ribosomal protein S29-A

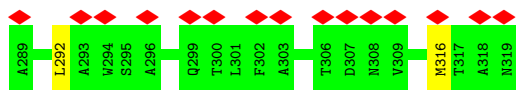
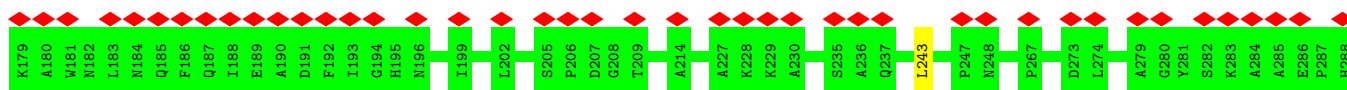
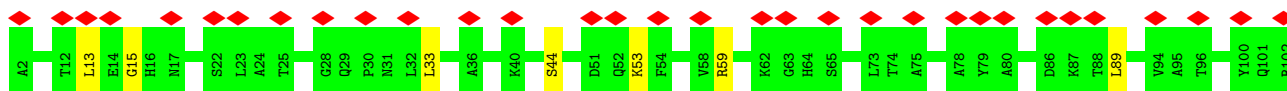


- Molecule 78: 40S ribosomal protein S30-A

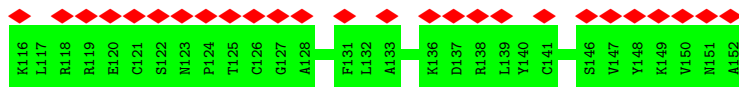
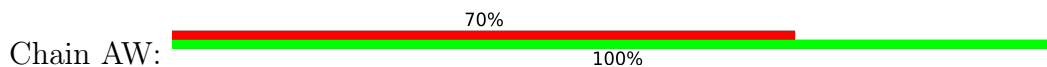




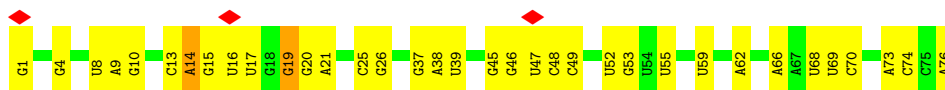
- Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein



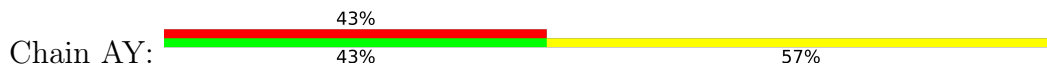
- Molecule 80: Ubiquitin-40S ribosomal protein S31



- Molecule 81: Transfer RNA - Phe

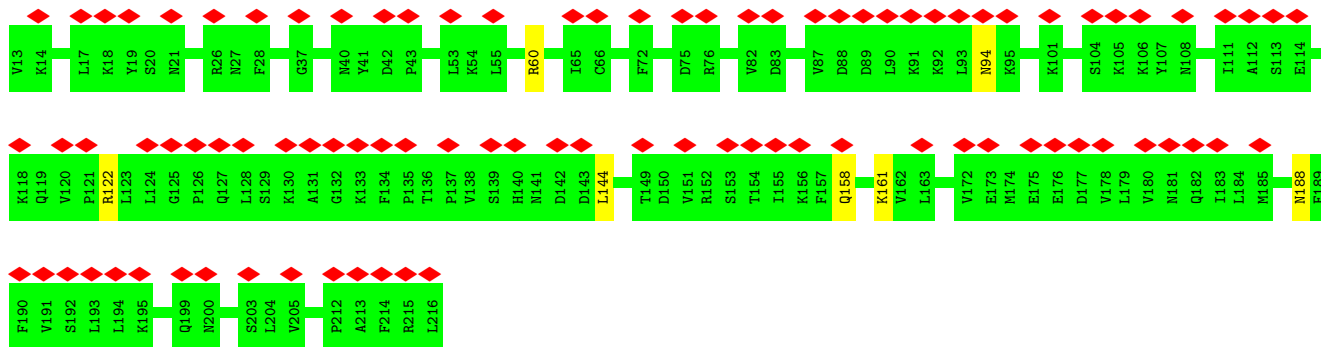


- Molecule 82: Messenger RNA

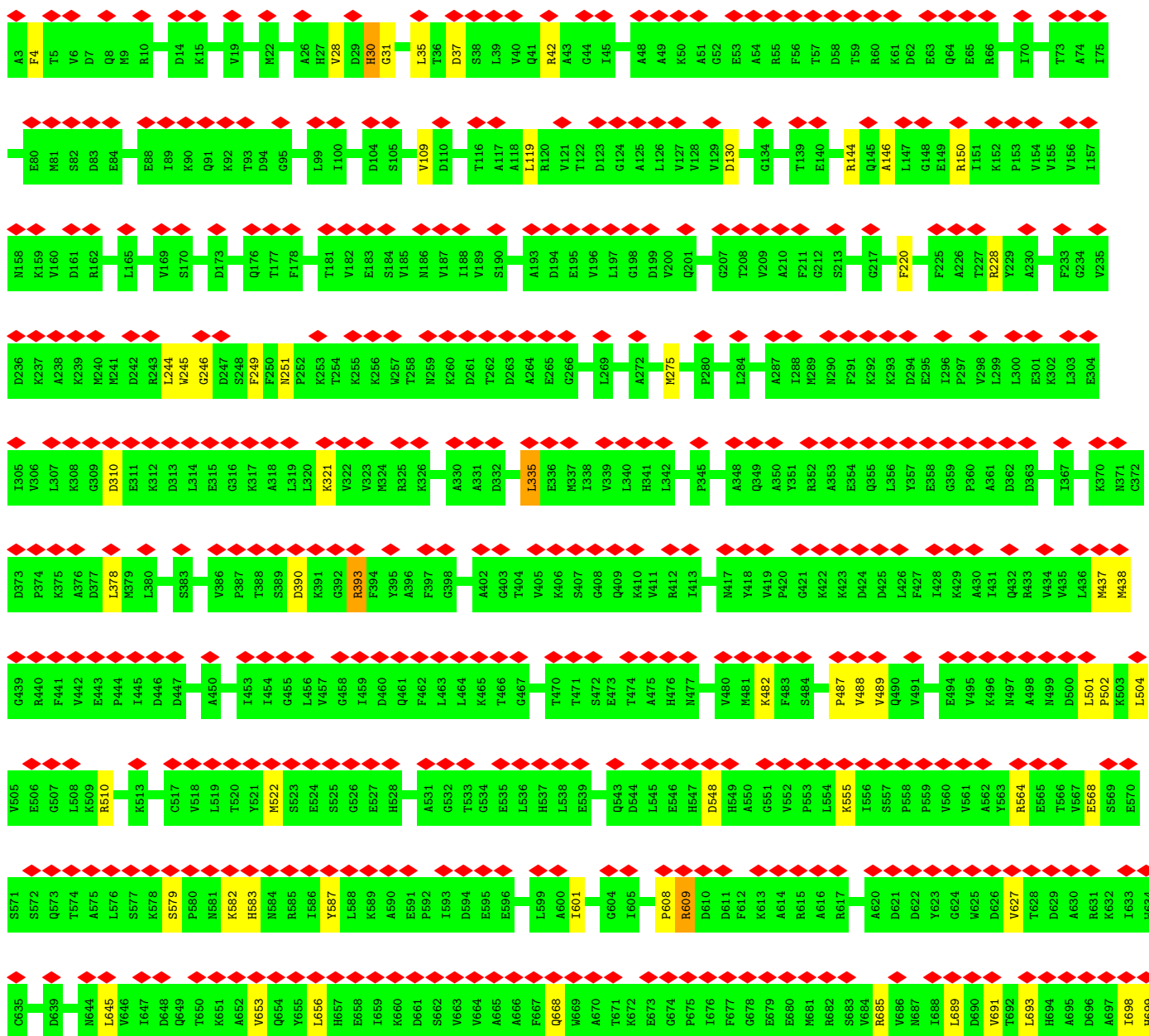
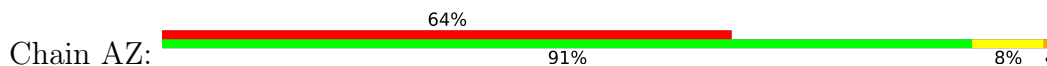


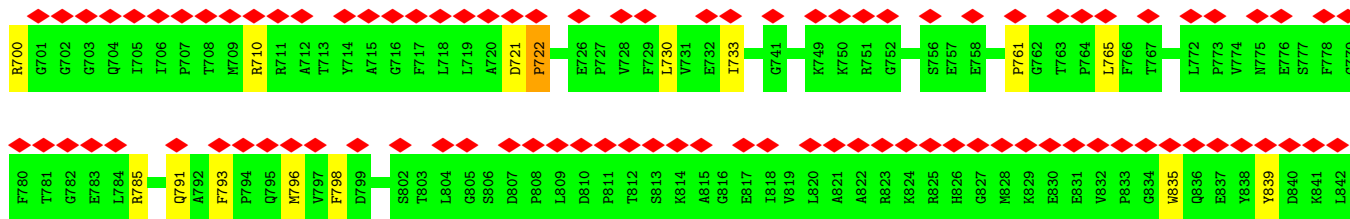
- Molecule 83: 60S ribosomal protein L1-A





• Molecule 84: Elongation factor 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77200	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.358	Depositor
Minimum map value	-0.193	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, SO1, ALF, DDE, 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	1	0.71	0/77157	1.22	611/120295 (0.5%)
2	3	0.58	0/2883	1.11	11/4491 (0.2%)
3	4	0.71	0/3746	1.18	19/5832 (0.3%)
4	P0	0.33	0/1498	0.72	2/2025 (0.1%)
5	P2	0.34	0/728	0.73	0/975
6	A	0.43	0/1948	0.69	3/2617 (0.1%)
7	B	0.41	0/3146	0.67	1/4228 (0.0%)
8	C	0.38	0/2800	0.69	1/3790 (0.0%)
9	D	0.38	0/2425	0.69	2/3271 (0.1%)
10	E	0.34	0/1260	0.62	0/1694
11	F	0.42	0/1821	0.72	2/2451 (0.1%)
12	G	0.37	0/1836	0.67	0/2481
13	H	0.39	0/1539	0.73	4/2073 (0.2%)
14	I	0.39	0/1741	0.64	0/2335
15	J	0.36	0/1374	0.78	2/1842 (0.1%)
16	L	0.39	0/1568	0.68	2/2106 (0.1%)
17	M	0.35	0/1068	0.62	0/1438
18	N	0.47	0/1757	0.72	0/2354
19	O	0.41	0/1585	0.76	3/2128 (0.1%)
20	P	0.42	0/1443	0.65	1/1944 (0.1%)
21	Q	0.37	0/1465	0.67	0/1965
22	R	0.35	0/1538	0.62	1/2050 (0.0%)
23	S	0.40	0/1481	0.68	2/1990 (0.1%)
24	T	0.39	0/1300	0.65	0/1743
25	U	0.37	0/812	0.66	0/1099
26	V	0.42	0/1018	0.72	1/1369 (0.1%)
27	W	0.39	0/540	0.58	0/717
28	X	0.42	0/979	0.65	0/1321
29	Y	0.37	0/1004	0.66	0/1341
30	Z	0.41	0/1118	0.66	0/1497
31	a	0.41	0/1204	0.74	1/1612 (0.1%)
32	b	0.32	0/473	0.60	1/629 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.39	0/751	0.71	1/1008 (0.1%)
34	d	0.42	0/897	0.72	1/1205 (0.1%)
35	e	0.39	0/1041	0.64	0/1394
36	f	0.44	0/868	0.69	1/1168 (0.1%)
37	g	0.46	0/890	0.68	0/1189
38	h	0.37	0/978	0.74	2/1301 (0.2%)
39	i	0.36	0/778	0.74	2/1034 (0.2%)
40	j	0.41	0/696	0.72	1/923 (0.1%)
41	k	0.35	0/618	0.81	2/826 (0.2%)
42	l	0.38	0/443	0.84	0/588
43	m	0.37	0/423	0.70	0/562
44	n	0.36	0/234	0.72	0/300
45	o	0.37	0/860	0.67	1/1136 (0.1%)
46	p	0.45	0/701	0.67	1/934 (0.1%)
47	2	0.58	2/42328 (0.0%)	1.25	408/65955 (0.6%)
48	q	0.35	0/1617	0.76	2/2215 (0.1%)
49	r	0.37	0/1735	0.77	4/2335 (0.2%)
50	s	0.35	0/1665	0.68	0/2263
51	t	0.32	0/1759	0.70	2/2368 (0.1%)
52	u	0.35	0/2109	0.79	1/2839 (0.0%)
53	v	0.32	0/1629	0.77	2/2202 (0.1%)
54	w	0.33	0/1814	0.77	0/2425
55	x	0.35	0/1506	0.75	3/2028 (0.1%)
56	y	0.35	0/1514	0.73	1/2021 (0.0%)
57	z	0.35	0/1519	0.75	4/2035 (0.2%)
58	AA	0.34	0/789	0.76	1/1067 (0.1%)
59	AB	0.39	0/1247	0.69	2/1681 (0.1%)
60	AC	0.30	0/898	0.71	1/1220 (0.1%)
61	AD	0.38	0/1215	0.76	0/1638
62	AE	0.33	0/901	0.61	0/1217
63	AF	0.34	0/998	0.70	1/1341 (0.1%)
64	AG	0.34	0/1125	0.74	2/1510 (0.1%)
65	AH	0.33	0/935	0.76	3/1254 (0.2%)
66	AI	0.32	0/1211	0.74	2/1628 (0.1%)
67	AJ	0.32	0/1130	0.68	0/1517
68	AK	0.32	0/865	0.69	0/1169
69	AL	0.40	0/693	0.84	1/935 (0.1%)
70	AM	0.38	0/1038	0.74	0/1395
71	AN	0.35	0/1139	0.72	0/1518
72	AO	0.33	0/1087	0.61	0/1449
73	AP	0.29	0/571	0.69	0/768
74	AQ	0.40	0/782	0.77	0/1047
75	AR	0.34	0/620	0.77	1/838 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	AS	0.34	0/499	0.76	0/670
77	AT	0.37	0/452	0.66	0/600
78	AU	0.32	0/483	0.67	1/643 (0.2%)
79	AV	0.33	0/2490	0.76	5/3389 (0.1%)
80	AW	0.34	0/292	0.67	0/390
81	AX	0.55	1/1818 (0.1%)	1.25	14/2831 (0.5%)
82	AY	0.44	0/159	1.01	1/244 (0.4%)
83	BA	0.31	0/1634	0.69	0/2195
84	AZ	0.43	0/6655	0.85	16/9009 (0.2%)
All	All	0.56	3/227354 (0.0%)	1.05	1160/333120 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	P0	0	1
5	P2	0	4
6	A	0	1
7	B	0	3
8	C	0	1
9	D	0	5
10	E	0	1
11	F	0	2
12	G	0	3
13	H	0	4
15	J	0	4
16	L	0	2
18	N	0	3
19	O	0	6
20	P	0	2
21	Q	0	1
23	S	0	4
26	V	0	1
30	Z	0	1
31	a	0	2
33	c	0	2
36	f	0	2
37	g	0	2
38	h	0	2
39	i	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	j	0	3
41	k	0	2
44	n	0	1
45	o	0	2
48	q	0	3
49	r	0	4
50	s	0	1
51	t	0	1
52	u	0	6
53	v	0	8
54	w	0	8
55	x	0	2
56	y	0	2
57	z	0	3
58	AA	0	2
61	AD	0	7
62	AE	0	1
63	AF	0	4
64	AG	0	6
66	AI	0	3
68	AK	0	1
70	AM	0	1
71	AN	0	2
72	AO	0	1
74	AQ	0	2
76	AS	0	1
78	AU	0	1
79	AV	0	2
83	BA	0	1
84	AZ	0	29
All	All	0	170

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	AX	1	G	OP3-P	-10.71	1.48	1.61
47	2	1221	A	N7-C5	-5.02	1.36	1.39
47	2	1221	A	C8-N7	-5.00	1.28	1.31

The worst 5 of 1160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	94	U	C2-N3-C4	21.63	139.98	127.00
1	1	1581	C	N1-C2-O2	12.01	126.11	118.90
47	2	1362	U	C2-N1-C1'	11.91	131.99	117.70
47	2	258	C	C2-N1-C1'	11.68	131.65	118.80
47	2	1374	C	N1-C2-O2	11.52	125.81	118.90

There are no chirality outliers.

5 of 170 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	P0	30	VAL	Peptide
5	P2	130	LYS	Peptide
5	P2	75	PRO	Peptide
5	P2	77	ALA	Peptide
5	P2	89	PRO	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	P0	187/189 (99%)	143 (76%)	44 (24%)	0	100	100
5	P2	92/94 (98%)	65 (71%)	27 (29%)	0	100	100
6	A	250/252 (99%)	216 (86%)	34 (14%)	0	100	100
7	B	384/386 (100%)	326 (85%)	58 (15%)	0	100	100
8	C	359/361 (99%)	298 (83%)	60 (17%)	1 (0%)	41	75
9	D	294/296 (99%)	256 (87%)	38 (13%)	0	100	100
10	E	152/175 (87%)	138 (91%)	14 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	F	220/222 (99%)	196 (89%)	23 (10%)	1 (0%)	29	67
12	G	231/233 (99%)	202 (87%)	29 (13%)	0	100	100
13	H	189/191 (99%)	162 (86%)	27 (14%)	0	100	100
14	I	207/220 (94%)	178 (86%)	29 (14%)	0	100	100
15	J	167/169 (99%)	140 (84%)	27 (16%)	0	100	100
16	L	191/193 (99%)	158 (83%)	29 (15%)	4 (2%)	7	39
17	M	134/136 (98%)	120 (90%)	14 (10%)	0	100	100
18	N	201/203 (99%)	174 (87%)	26 (13%)	1 (0%)	29	67
19	O	195/197 (99%)	174 (89%)	19 (10%)	2 (1%)	15	52
20	P	181/183 (99%)	163 (90%)	18 (10%)	0	100	100
21	Q	183/185 (99%)	167 (91%)	16 (9%)	0	100	100
22	R	186/188 (99%)	169 (91%)	17 (9%)	0	100	100
23	S	170/172 (99%)	147 (86%)	22 (13%)	1 (1%)	25	63
24	T	157/159 (99%)	132 (84%)	25 (16%)	0	100	100
25	U	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
26	V	134/136 (98%)	118 (88%)	16 (12%)	0	100	100
27	W	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
28	X	119/121 (98%)	108 (91%)	11 (9%)	0	100	100
29	Y	124/126 (98%)	114 (92%)	10 (8%)	0	100	100
30	Z	133/135 (98%)	115 (86%)	18 (14%)	0	100	100
31	a	146/148 (99%)	117 (80%)	27 (18%)	2 (1%)	11	46
32	b	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
33	c	95/97 (98%)	88 (93%)	7 (7%)	0	100	100
34	d	107/109 (98%)	96 (90%)	11 (10%)	0	100	100
35	e	125/127 (98%)	110 (88%)	14 (11%)	1 (1%)	19	57
36	f	104/106 (98%)	88 (85%)	14 (14%)	2 (2%)	8	41
37	g	110/112 (98%)	96 (87%)	14 (13%)	0	100	100
38	h	117/119 (98%)	102 (87%)	15 (13%)	0	100	100
39	i	97/99 (98%)	75 (77%)	22 (23%)	0	100	100
40	j	85/87 (98%)	66 (78%)	16 (19%)	3 (4%)	3	30
41	k	75/77 (97%)	58 (77%)	16 (21%)	1 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	l	48/50 (96%)	36 (75%)	10 (21%)	2 (4%)	3	26
43	m	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
44	n	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
45	o	103/105 (98%)	81 (79%)	22 (21%)	0	100	100
46	p	89/91 (98%)	80 (90%)	9 (10%)	0	100	100
48	q	204/206 (99%)	157 (77%)	45 (22%)	2 (1%)	15	52
49	r	212/214 (99%)	171 (81%)	39 (18%)	2 (1%)	17	54
50	s	215/217 (99%)	184 (86%)	30 (14%)	1 (0%)	29	67
51	t	221/223 (99%)	189 (86%)	31 (14%)	1 (0%)	29	67
52	u	258/260 (99%)	209 (81%)	46 (18%)	3 (1%)	13	49
53	v	204/206 (99%)	163 (80%)	40 (20%)	1 (0%)	29	67
54	w	221/223 (99%)	176 (80%)	42 (19%)	3 (1%)	11	46
55	x	182/184 (99%)	142 (78%)	39 (21%)	1 (0%)	29	67
56	y	184/199 (92%)	134 (73%)	50 (27%)	0	100	100
57	z	183/185 (99%)	157 (86%)	25 (14%)	1 (0%)	29	67
58	AA	94/105 (90%)	71 (76%)	23 (24%)	0	100	100
59	AB	151/153 (99%)	125 (83%)	25 (17%)	1 (1%)	22	60
60	AC	122/124 (98%)	100 (82%)	22 (18%)	0	100	100
61	AD	148/150 (99%)	122 (82%)	22 (15%)	4 (3%)	5	35
62	AE	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
63	AF	122/124 (98%)	88 (72%)	32 (26%)	2 (2%)	9	44
64	AG	139/141 (99%)	107 (77%)	31 (22%)	1 (1%)	22	60
65	AH	116/125 (93%)	98 (84%)	18 (16%)	0	100	100
66	AI	143/145 (99%)	109 (76%)	34 (24%)	0	100	100
67	AJ	141/143 (99%)	118 (84%)	23 (16%)	0	100	100
68	AK	105/107 (98%)	93 (89%)	12 (11%)	0	100	100
69	AL	85/87 (98%)	60 (71%)	24 (28%)	1 (1%)	13	49
70	AM	127/129 (98%)	109 (86%)	17 (13%)	1 (1%)	19	57
71	AN	142/144 (99%)	107 (75%)	34 (24%)	1 (1%)	22	60
72	AO	132/134 (98%)	116 (88%)	16 (12%)	0	100	100
73	AP	68/70 (97%)	53 (78%)	15 (22%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	AQ	95/97 (98%)	69 (73%)	26 (27%)	0	100	100
75	AR	79/81 (98%)	61 (77%)	17 (22%)	1 (1%)	12	48
76	AS	61/63 (97%)	48 (79%)	13 (21%)	0	100	100
77	AT	51/53 (96%)	42 (82%)	9 (18%)	0	100	100
78	AU	58/60 (97%)	47 (81%)	11 (19%)	0	100	100
79	AV	316/318 (99%)	256 (81%)	59 (19%)	1 (0%)	41	75
80	AW	35/37 (95%)	26 (74%)	9 (26%)	0	100	100
83	BA	202/204 (99%)	154 (76%)	48 (24%)	0	100	100
84	AZ	837/840 (100%)	626 (75%)	203 (24%)	8 (1%)	15	52
All	All	12208/12426 (98%)	10128 (83%)	2023 (17%)	57 (0%)	32	67

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	f	59	VAL
40	j	83	ALA
42	l	30	ARG
48	q	113	ARG
54	w	93	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	P0	160/160 (100%)	157 (98%)	3 (2%)	57	75
5	P2	81/81 (100%)	79 (98%)	2 (2%)	47	69
6	A	193/194 (100%)	182 (94%)	11 (6%)	20	50
7	B	320/322 (99%)	313 (98%)	7 (2%)	52	71
8	C	288/288 (100%)	279 (97%)	9 (3%)	40	64
9	D	244/244 (100%)	240 (98%)	4 (2%)	62	79
10	E	134/152 (88%)	126 (94%)	8 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	F	186/186 (100%)	184 (99%)	2 (1%)	73	84
12	G	187/191 (98%)	182 (97%)	5 (3%)	44	67
13	H	171/171 (100%)	164 (96%)	7 (4%)	30	58
14	I	177/186 (95%)	169 (96%)	8 (4%)	27	56
15	J	147/147 (100%)	144 (98%)	3 (2%)	55	74
16	L	154/154 (100%)	151 (98%)	3 (2%)	57	75
17	M	107/107 (100%)	105 (98%)	2 (2%)	57	75
18	N	175/175 (100%)	168 (96%)	7 (4%)	31	58
19	O	160/160 (100%)	154 (96%)	6 (4%)	33	59
20	P	140/145 (97%)	137 (98%)	3 (2%)	53	73
21	Q	150/150 (100%)	148 (99%)	2 (1%)	69	82
22	R	153/153 (100%)	146 (95%)	7 (5%)	27	55
23	S	156/156 (100%)	152 (97%)	4 (3%)	46	68
24	T	136/136 (100%)	134 (98%)	2 (2%)	65	80
25	U	87/87 (100%)	85 (98%)	2 (2%)	50	71
26	V	104/104 (100%)	100 (96%)	4 (4%)	33	59
27	W	56/56 (100%)	54 (96%)	2 (4%)	35	61
28	X	104/105 (99%)	101 (97%)	3 (3%)	42	65
29	Y	109/109 (100%)	107 (98%)	2 (2%)	59	77
30	Z	115/115 (100%)	111 (96%)	4 (4%)	36	62
31	a	118/118 (100%)	115 (98%)	3 (2%)	47	69
32	b	46/46 (100%)	46 (100%)	0	100	100
33	c	81/81 (100%)	80 (99%)	1 (1%)	71	83
34	d	94/96 (98%)	90 (96%)	4 (4%)	29	57
35	e	109/109 (100%)	107 (98%)	2 (2%)	59	77
36	f	90/90 (100%)	87 (97%)	3 (3%)	38	63
37	g	95/95 (100%)	90 (95%)	5 (5%)	22	52
38	h	104/104 (100%)	100 (96%)	4 (4%)	33	59
39	i	81/81 (100%)	78 (96%)	3 (4%)	34	60
40	j	70/70 (100%)	69 (99%)	1 (1%)	67	81
41	k	68/68 (100%)	66 (97%)	2 (3%)	42	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	l	45/45 (100%)	43 (96%)	2 (4%)	28	56
43	m	47/47 (100%)	46 (98%)	1 (2%)	53	73
44	n	23/23 (100%)	22 (96%)	1 (4%)	29	57
45	o	90/90 (100%)	88 (98%)	2 (2%)	52	71
46	p	71/71 (100%)	70 (99%)	1 (1%)	67	81
48	q	164/173 (95%)	161 (98%)	3 (2%)	59	77
49	r	191/191 (100%)	183 (96%)	8 (4%)	30	57
50	s	176/176 (100%)	172 (98%)	4 (2%)	50	71
51	t	182/182 (100%)	175 (96%)	7 (4%)	33	59
52	u	221/221 (100%)	214 (97%)	7 (3%)	39	63
53	v	173/173 (100%)	167 (96%)	6 (4%)	36	62
54	w	189/191 (99%)	181 (96%)	8 (4%)	30	57
55	x	165/165 (100%)	162 (98%)	3 (2%)	59	77
56	y	150/160 (94%)	147 (98%)	3 (2%)	55	74
57	z	158/158 (100%)	153 (97%)	5 (3%)	39	63
58	AA	77/98 (79%)	76 (99%)	1 (1%)	69	82
59	AB	133/134 (99%)	133 (100%)	0	100	100
60	AC	88/100 (88%)	87 (99%)	1 (1%)	73	84
61	AD	127/127 (100%)	122 (96%)	5 (4%)	32	59
62	AE	81/96 (84%)	81 (100%)	0	100	100
63	AF	101/104 (97%)	100 (99%)	1 (1%)	76	86
64	AG	117/117 (100%)	116 (99%)	1 (1%)	78	87
65	AH	94/113 (83%)	88 (94%)	6 (6%)	17	47
66	AI	128/128 (100%)	124 (97%)	4 (3%)	40	64
67	AJ	115/115 (100%)	112 (97%)	3 (3%)	46	68
68	AK	100/100 (100%)	97 (97%)	3 (3%)	41	64
69	AL	74/74 (100%)	72 (97%)	2 (3%)	44	67
70	AM	110/110 (100%)	105 (96%)	5 (4%)	27	56
71	AN	119/119 (100%)	114 (96%)	5 (4%)	30	57
72	AO	112/112 (100%)	110 (98%)	2 (2%)	59	77
73	AP	61/61 (100%)	60 (98%)	1 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	AQ	83/83 (100%)	83 (100%)	0	100	100
75	AR	70/70 (100%)	68 (97%)	2 (3%)	42	65
76	AS	56/56 (100%)	56 (100%)	0	100	100
77	AT	47/47 (100%)	45 (96%)	2 (4%)	29	57
78	AU	51/51 (100%)	49 (96%)	2 (4%)	32	59
79	AV	259/261 (99%)	255 (98%)	4 (2%)	65	80
80	AW	31/31 (100%)	31 (100%)	0	100	100
83	BA	185/185 (100%)	179 (97%)	6 (3%)	39	63
84	AZ	711/712 (100%)	685 (96%)	26 (4%)	34	60
All	All	10325/10462 (99%)	10032 (97%)	293 (3%)	46	66

5 of 293 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
67	AJ	86	ARG
84	AZ	685	ARG
70	AM	25	VAL
79	AV	316	MET
22	R	162	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
31	a	120	ASN
72	AO	113	ASN
45	o	82	GLN
71	AN	63	GLN
84	AZ	365	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3220/3396 (94%)	983 (30%)	24 (0%)
2	3	120/121 (99%)	29 (24%)	0
3	4	157/158 (99%)	49 (31%)	0
47	2	1774/1797 (98%)	695 (39%)	22 (1%)
81	AX	75/76 (98%)	29 (38%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
82	AY	6/7 (85%)	3 (50%)	1 (16%)
All	All	5352/5555 (96%)	1788 (33%)	47 (0%)

5 of 1788 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	14	U
1	1	16	A
1	1	18	G
1	1	19	U
1	1	20	A

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	2	505	A
47	2	1207	C
47	2	590	C
47	2	1107	G
47	2	1368	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	DDE	AZ	699	84	14,20,21	1.98	3 (21%)	14,28,30	3.40	7 (50%)

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
84	DDE	AZ	699	84	-	5/20/21/23	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	AZ	699	DDE	CBI-NAD	5.91	1.47	1.32
84	AZ	699	DDE	CAT-CE1	2.61	1.54	1.50
84	AZ	699	DDE	OAG-CBI	-2.59	1.18	1.23

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	AZ	699	DDE	CBW-CBI-NAD	9.82	127.80	115.28
84	AZ	699	DDE	OAG-CBI-NAD	-4.30	115.52	123.00
84	AZ	699	DDE	CAC-NCB-CAB	3.36	117.28	108.10
84	AZ	699	DDE	OAG-CBI-CBW	-3.02	116.67	120.49
84	AZ	699	DDE	CAU-CBW-CBI	-2.89	105.48	111.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	AZ	699	DDE	CA-CB-CG-ND1
84	AZ	699	DDE	CA-CB-CG-CD2
84	AZ	699	DDE	CAT-CAU-CBW-CBI
84	AZ	699	DDE	CAT-CAU-CBW-NCB
84	AZ	699	DDE	CE1-CAT-CAU-CBW

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 8 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	GDP	AZ	902	-	24,30,30	3.60	12 (50%)	30,47,47	1.62	6 (20%)
86	SO1	AZ	901	-	35,39,39	0.15	0	39,64,64	0.82	2 (5%)
88	ALF	AZ	903	-	0,4,4	-	-	-	-	-

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	GDP	AZ	902	-	-	0/12/32/32	0/3/3/3
86	SO1	AZ	901	-	-	16/21/104/104	0/7/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AZ	902	GDP	C3'-C4'	-7.83	1.33	1.53
87	AZ	902	GDP	O4'-C4'	6.95	1.60	1.45
87	AZ	902	GDP	O4'-C1'	-6.23	1.32	1.41
87	AZ	902	GDP	C2-N2	5.69	1.47	1.34
87	AZ	902	GDP	C2-N3	5.42	1.46	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	AZ	902	GDP	PA-O3A-PB	-4.83	116.24	132.83
86	AZ	901	SO1	C18-C9-C16	-3.92	98.02	103.64
87	AZ	902	GDP	C5-C6-N1	3.31	119.81	113.95
87	AZ	902	GDP	C8-N7-C5	2.96	108.63	102.99
87	AZ	902	GDP	C2-N1-C6	-2.75	120.03	125.10

There are no chirality outliers.

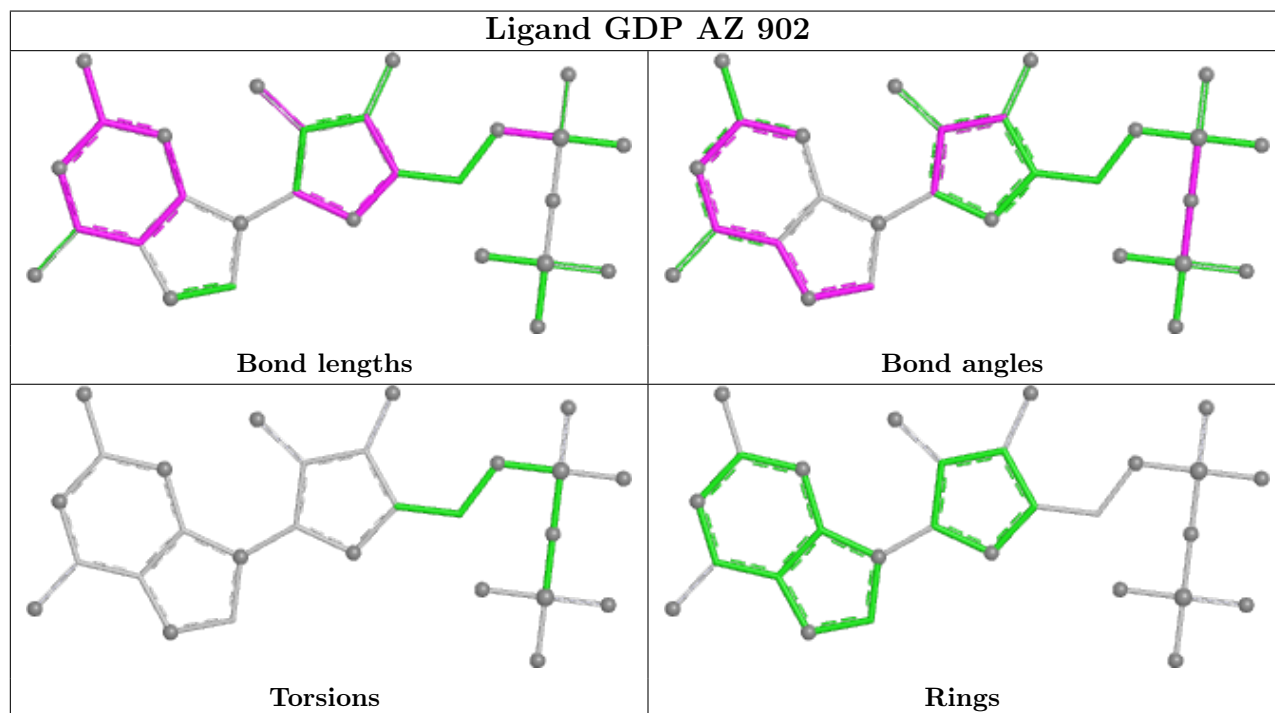
5 of 16 torsion outliers are listed below:

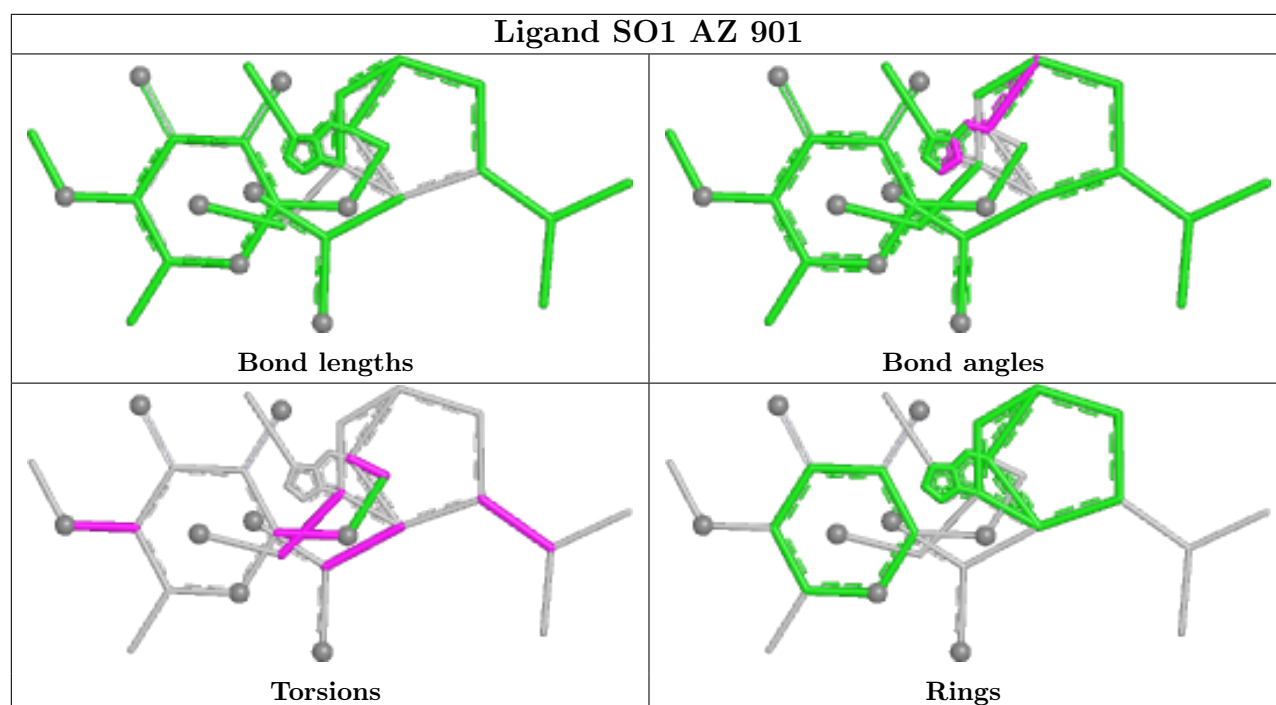
Mol	Chain	Res	Type	Atoms
86	AZ	901	SO1	C4-C1-C5-O14
86	AZ	901	SO1	C2-C1-C5-O14
86	AZ	901	SO1	C2-C1-C5-O15
86	AZ	901	SO1	O19-C11-C3-C1
86	AZ	901	SO1	C56-C55-O64-C65

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

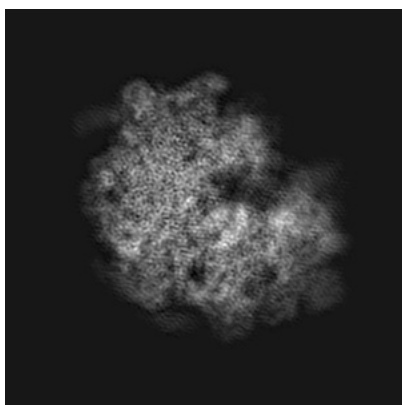
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0048. These allow visual inspection of the internal detail of the map and identification of artifacts.

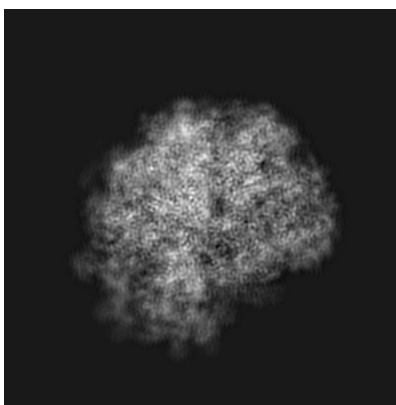
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

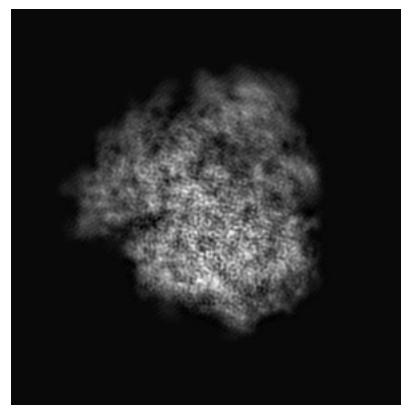
6.1.1 Primary map



X



Y

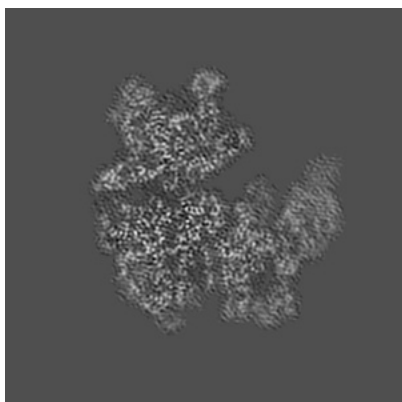


Z

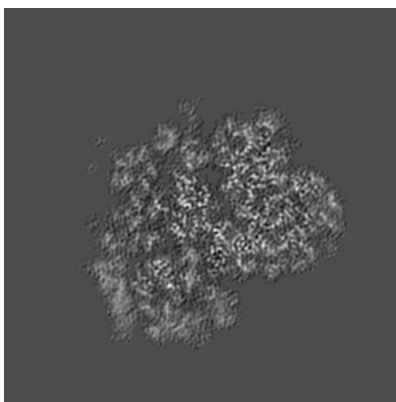
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

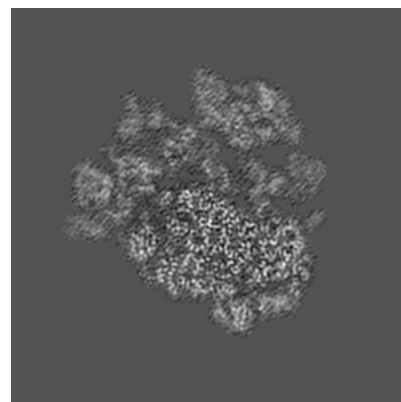
6.2.1 Primary map



X Index: 180



Y Index: 180

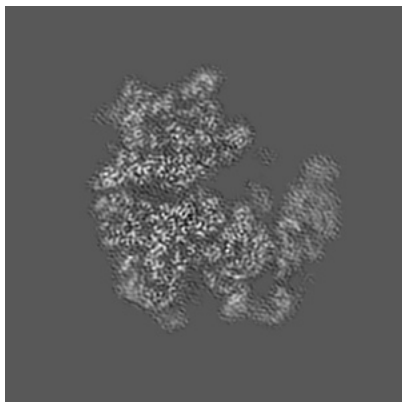


Z Index: 180

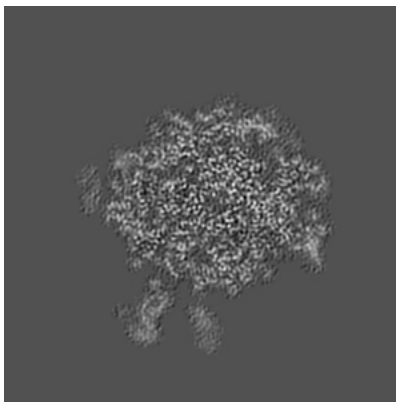
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

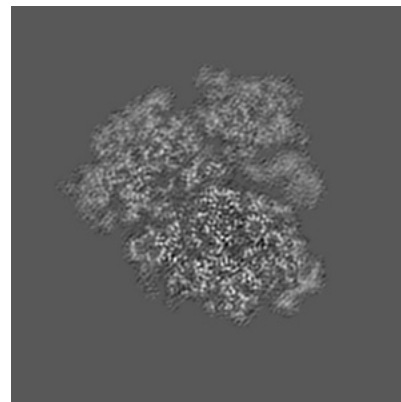
6.3.1 Primary map



X Index: 184



Y Index: 157

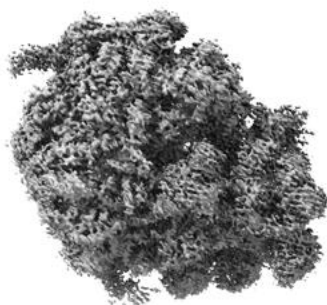


Z Index: 166

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

6.4 Orthogonal surface views [i](#)

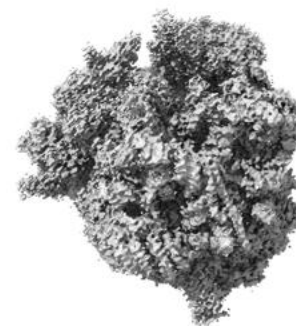
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

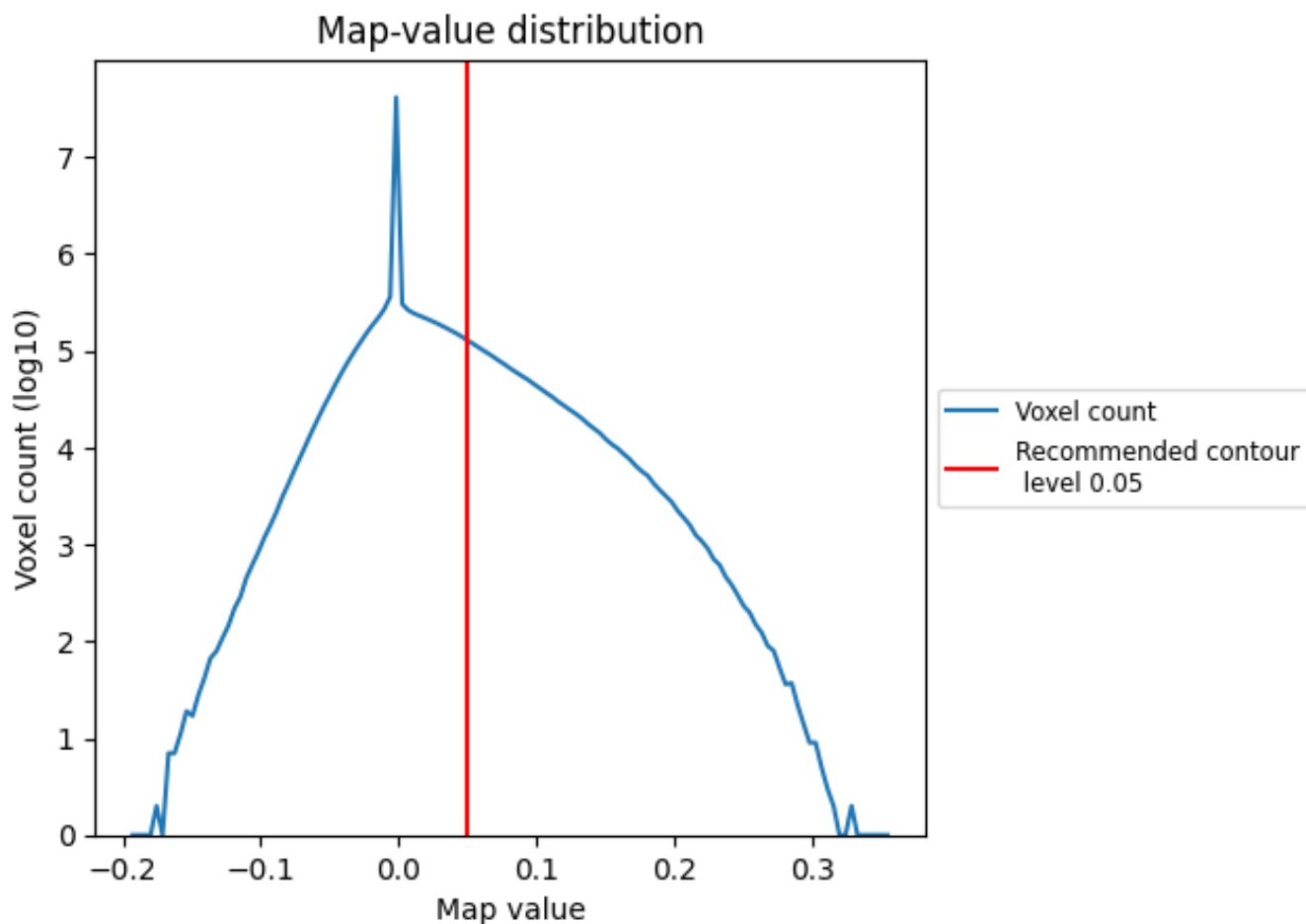
6.5 Mask visualisation

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

7 Map analysis [i](#)

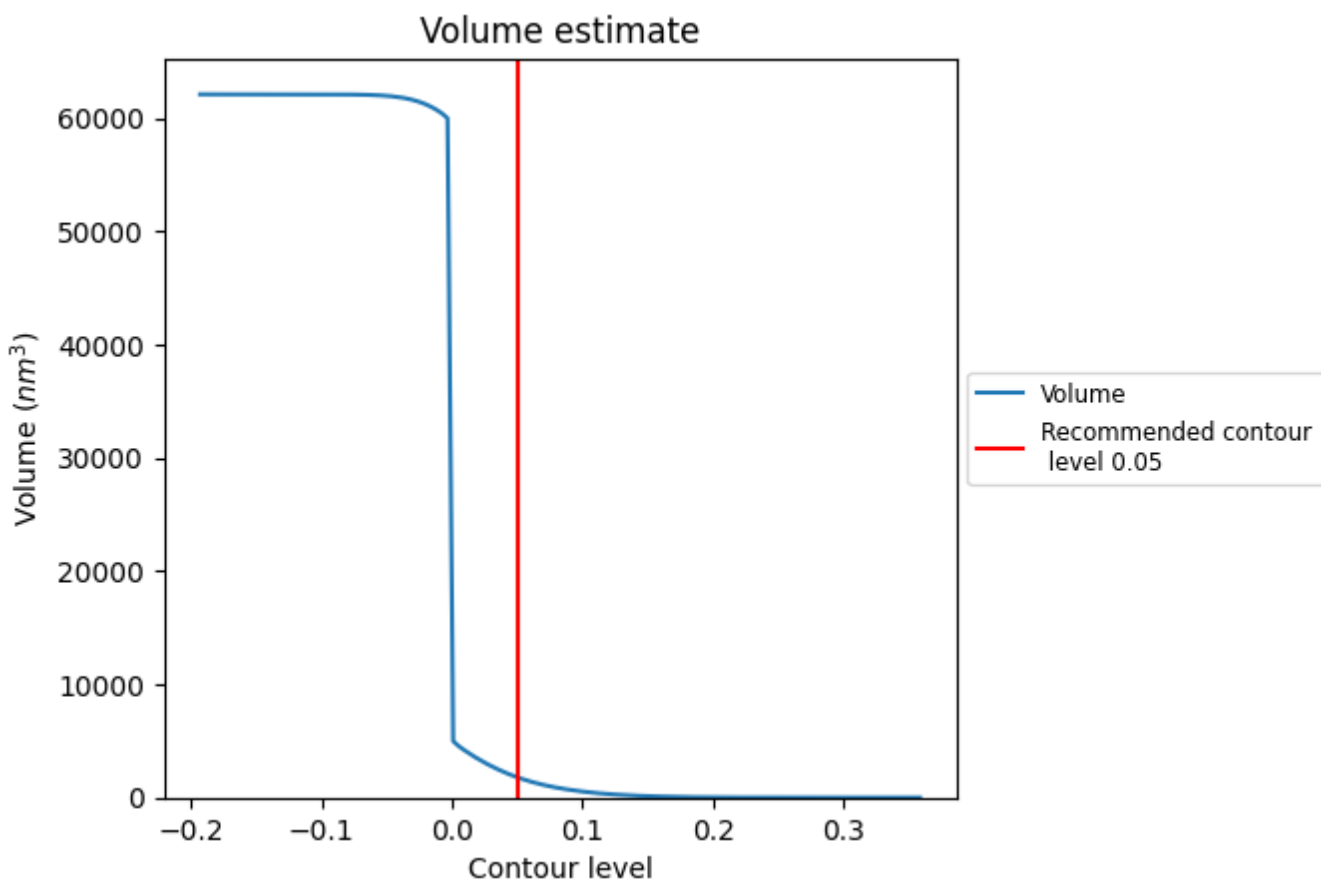
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

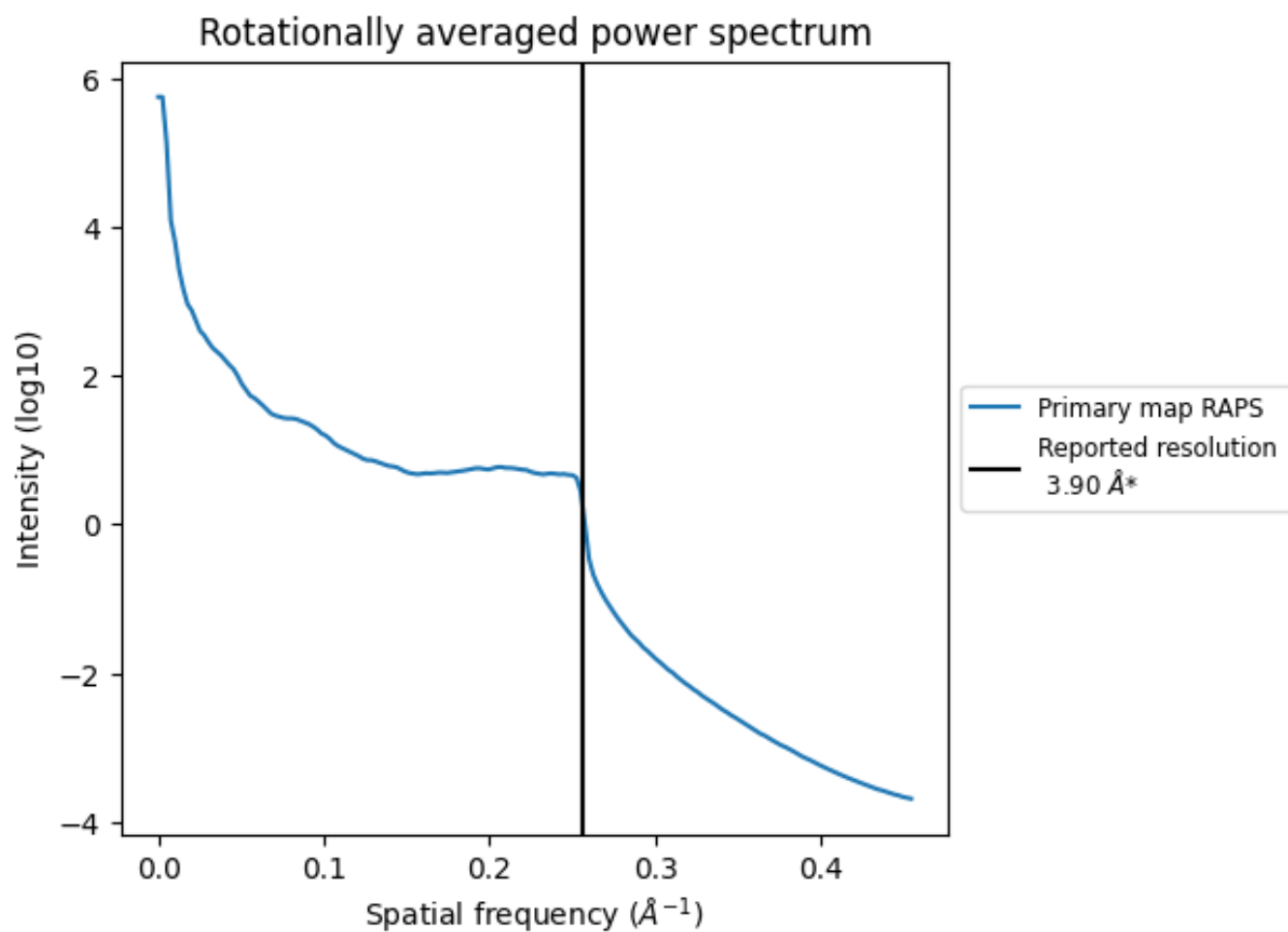
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1789 nm³; this corresponds to an approximate mass of 1616 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.256\AA^{-1}

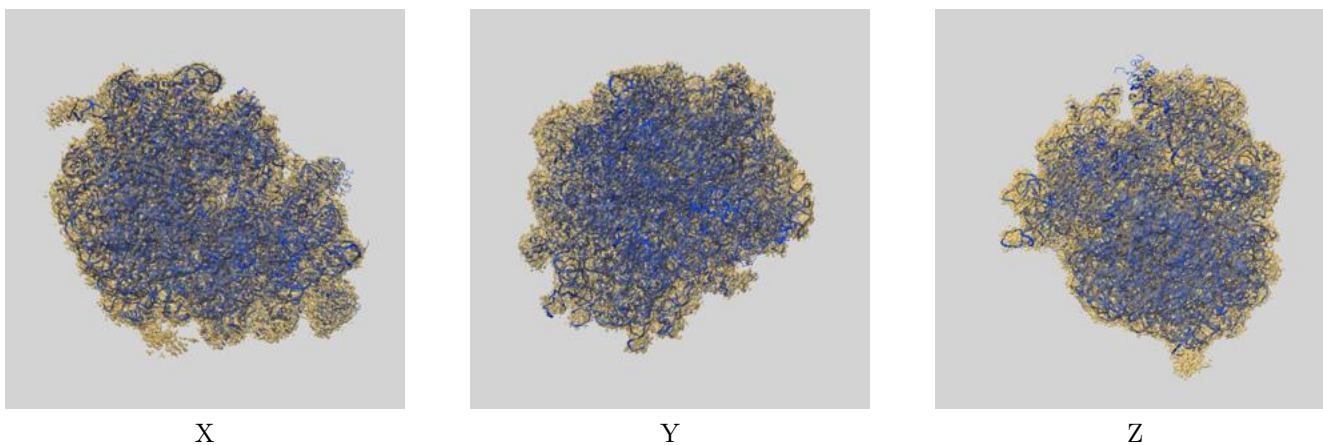
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

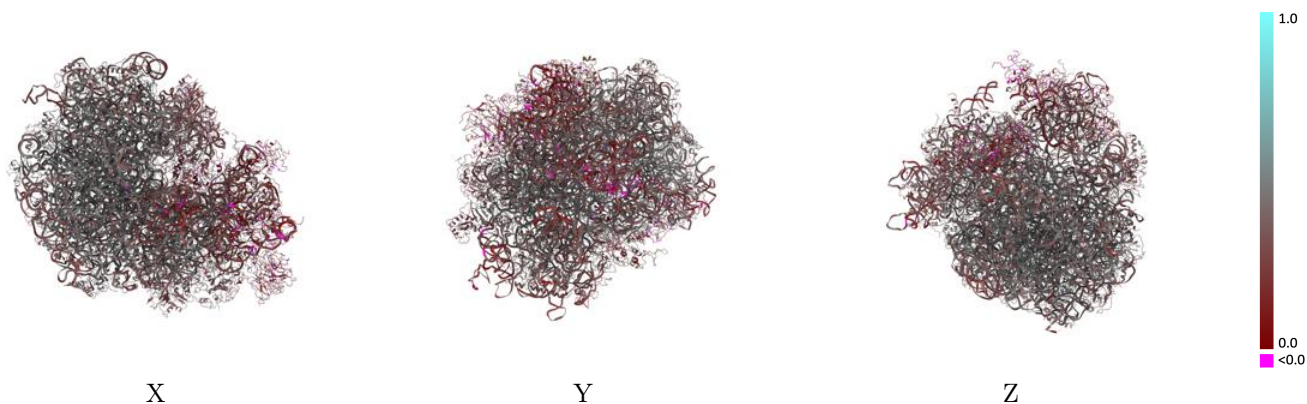
This section contains information regarding the fit between EMDB map EMD-0048 and PDB model 6GQB. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



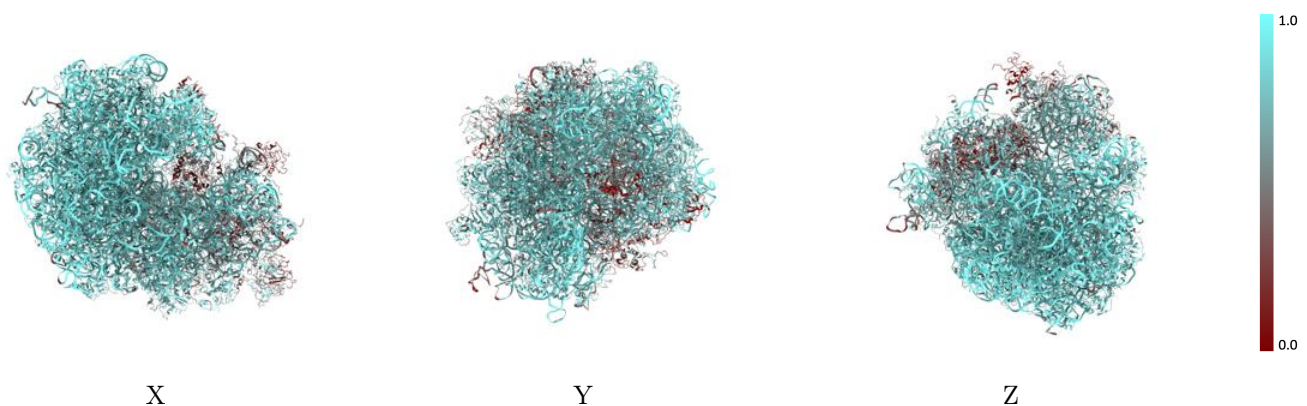
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



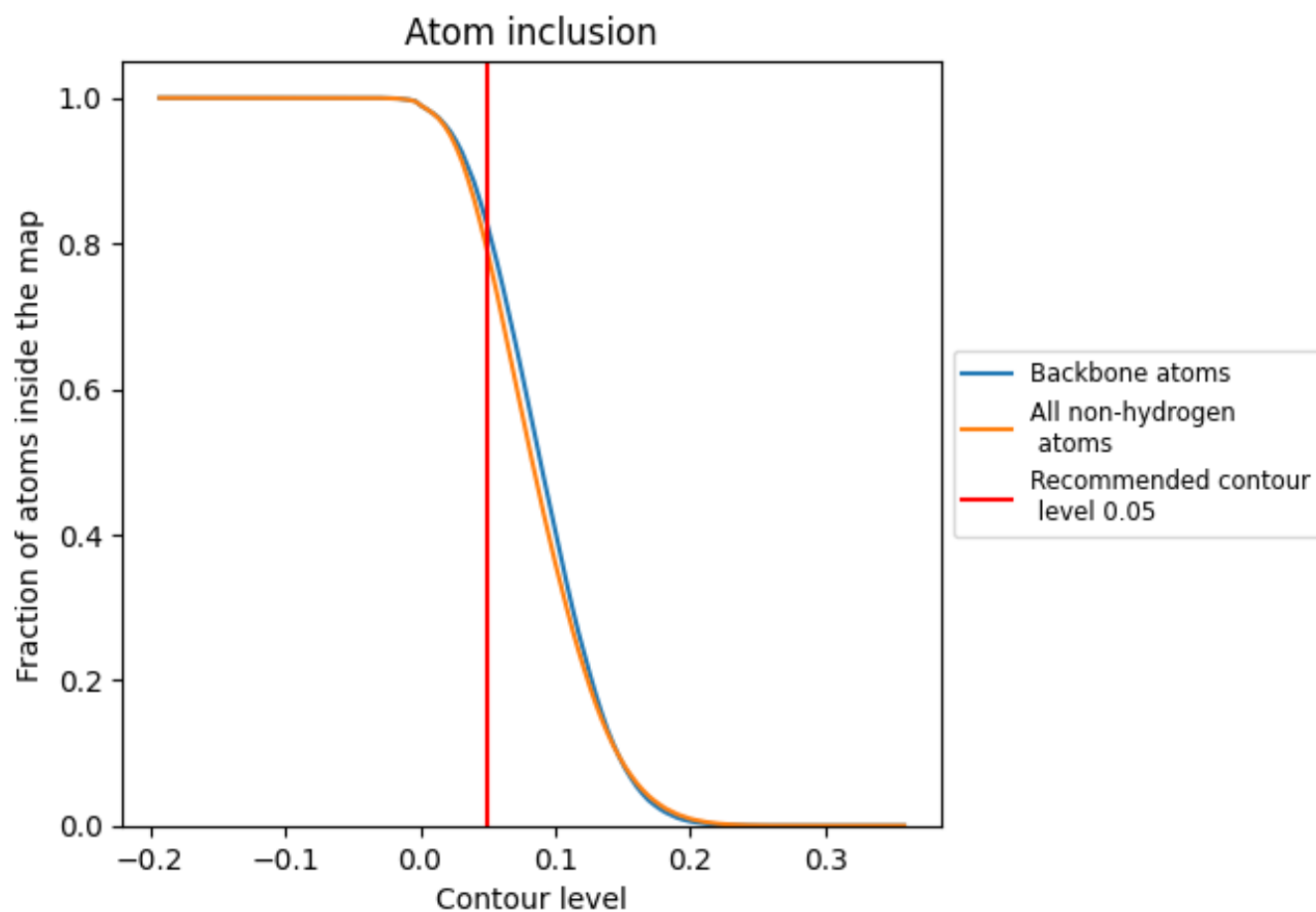
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 79% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7871	 0.3860
1	 0.9088	 0.4170
2	 0.8326	 0.3500
3	 0.9372	 0.4000
4	 0.9275	 0.4290
A	 0.7648	 0.4780
AA	 0.6332	 0.2540
AB	 0.6341	 0.4200
AC	 0.0932	 0.1320
AD	 0.7524	 0.4160
AE	 0.7796	 0.4120
AF	 0.6207	 0.2940
AG	 0.5357	 0.2490
AH	 0.5533	 0.2950
AI	 0.6005	 0.3030
AJ	 0.5828	 0.2620
AK	 0.4631	 0.2710
AL	 0.7274	 0.3860
AM	 0.7315	 0.4320
AN	 0.6856	 0.4300
AO	 0.7233	 0.3440
AP	 0.3309	 0.1820
AQ	 0.7095	 0.4060
AR	 0.7342	 0.3640
AS	 0.3732	 0.2350
AT	 0.6792	 0.3240
AU	 0.6187	 0.3780
AV	 0.4669	 0.2250
AW	 0.3607	 0.1930
AX	 0.7153	 0.2840
AY	 0.4167	 0.3360
AZ	 0.3199	 0.2650
B	 0.8007	 0.4530
BA	 0.4440	 0.2740
C	 0.8246	 0.4530



















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Chain	Atom inclusion	Q-score
D	 0.7686	 0.3740
E	 0.8219	 0.4200
F	 0.7997	 0.4400
G	 0.8030	 0.4100
H	 0.7638	 0.4180
I	 0.7730	 0.4390
J	 0.7186	 0.3720
L	 0.8319	 0.4450
M	 0.8129	 0.4070
N	 0.8332	 0.4670
O	 0.7853	 0.4410
P	 0.8045	 0.4670
P0	 0.1988	 0.2200
P2	 0.2059	 0.2190
Q	 0.8258	 0.4670
R	 0.7697	 0.4340
S	 0.7789	 0.4420
T	 0.7960	 0.4520
U	 0.7852	 0.4150
V	 0.6925	 0.4590
W	 0.7344	 0.4460
X	 0.7834	 0.4410
Y	 0.8447	 0.4590
Z	 0.8179	 0.4320
a	 0.8327	 0.4580
b	 0.7588	 0.4310
c	 0.8030	 0.4260
d	 0.7643	 0.4500
e	 0.7918	 0.4720
f	 0.8210	 0.4850
g	 0.7814	 0.4600
h	 0.8197	 0.4320
i	 0.7866	 0.4100
j	 0.8765	 0.5050
k	 0.7145	 0.4030
l	 0.8096	 0.4560
m	 0.7698	 0.4340
n	 0.6604	 0.4620
o	 0.7563	 0.4480
p	 0.7627	 0.4760
q	 0.6973	 0.3590
r	 0.7242	 0.3790

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Chain	Atom inclusion	Q-score
s	 0.6940	 0.3960
t	 0.5009	 0.2560
u	 0.7080	 0.3760
v	 0.4449	 0.2560
w	 0.6622	 0.3180
x	 0.7218	 0.3530
y	 0.7208	 0.3890
z	 0.7413	 0.3760