



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 09:23 PM UTC

PDB ID : 6GQ1 / pdb_00006gq1
EMDB ID : EMD-0047
Title : Cryo-EM reconstruction of yeast 80S ribosome in complex with mRNA, tRNA and eEF2 (GMPPCP/sordarin)
Authors : Pellegrino, S.; Demeshkina, N.; Mancera-Martinez, E.; Melnikov, S.; Simonetti, A.; Myasnikov, A.; Yusupov, M.; Yusupova, G.; Hashem, Y.
Deposited on : 2018-06-07
Resolution : 4.40 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:

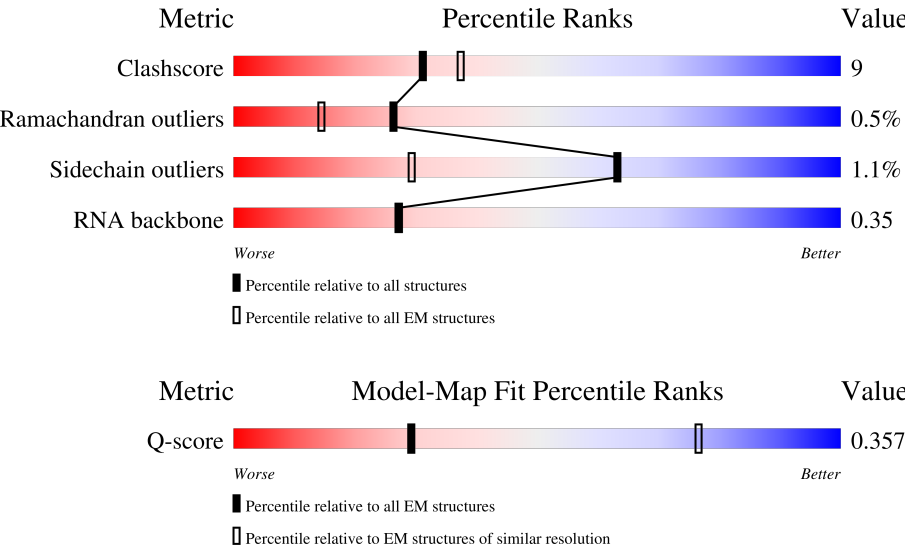
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	

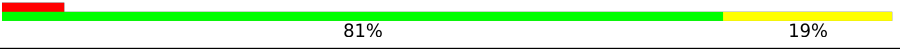
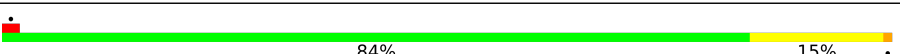
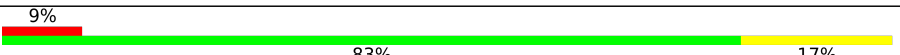
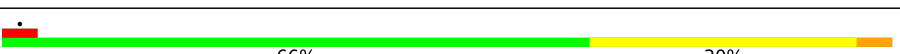
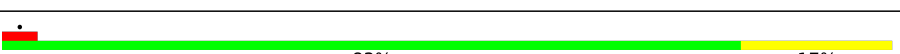
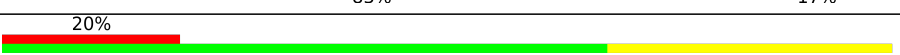
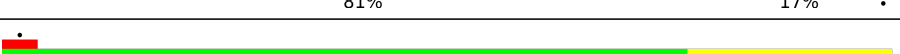
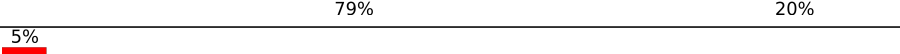
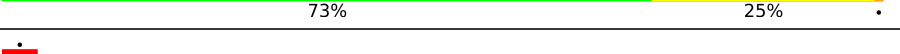
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Mol	Chain	Length	Quality of chain
4	P0	189	
5	P2	94	
6	A	252	
7	B	386	
8	C	361	
9	D	296	
10	E	175	
11	F	222	
12	G	233	
13	H	191	
14	I	220	
15	J	169	
16	L	193	
17	M	136	
18	N	203	
19	O	197	
20	P	183	
21	Q	185	
22	R	188	
23	S	172	
24	T	159	
25	U	100	
26	V	136	
27	W	63	
28	X	121	

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Mol	Chain	Length	Quality of chain
29	Y	126	
30	Z	135	
31	a	148	
32	b	58	
33	c	97	
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	

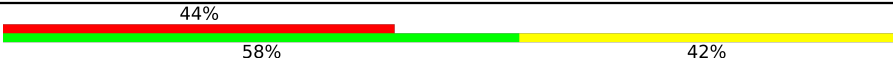
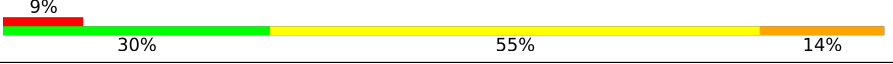
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Mol	Chain	Length	Quality of chain
54	w	223	
55	x	184	
56	y	199	
57	z	185	
58	AA	105	
59	AB	153	
60	AC	124	
61	AD	150	
62	AE	127	
63	AF	124	
64	AG	141	
65	AH	125	
66	AI	145	
67	AJ	143	
68	AK	107	
69	AL	87	
70	AM	129	
71	AN	144	
72	AO	134	
73	AP	70	
74	AQ	97	
75	AR	81	
76	AS	63	
77	AT	53	
78	AU	60	

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Mol	Chain	Length	Quality of chain
79	AV	318	
80	AW	37	
81	AX	76	
82	AY	8	
83	AZ	840	

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 210540 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
1	1	3223	Total	C	N	O	P	0	0
			68931	30790	12416	22502	3223		

- Molecule 2 is a RNA chain called 5.8S ribosomal RNA.

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

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
21	Q	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			227	139	60	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
56	y	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	8	Total	C	N	O	P	0	0
			164	74	23	59	8		

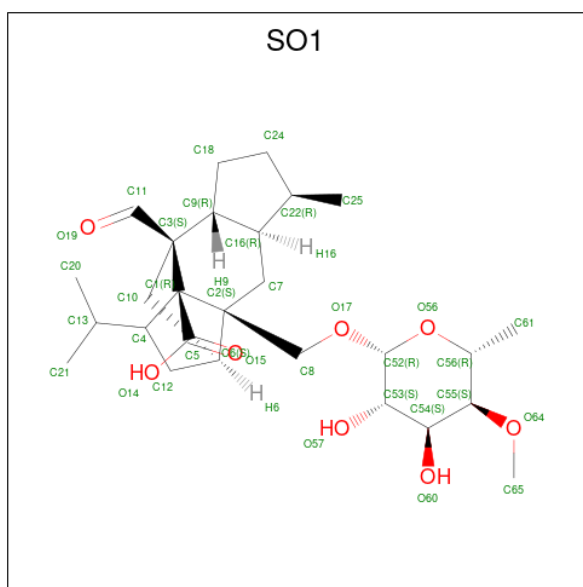
- Molecule 83 is a protein called Elongation factor 2.

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

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

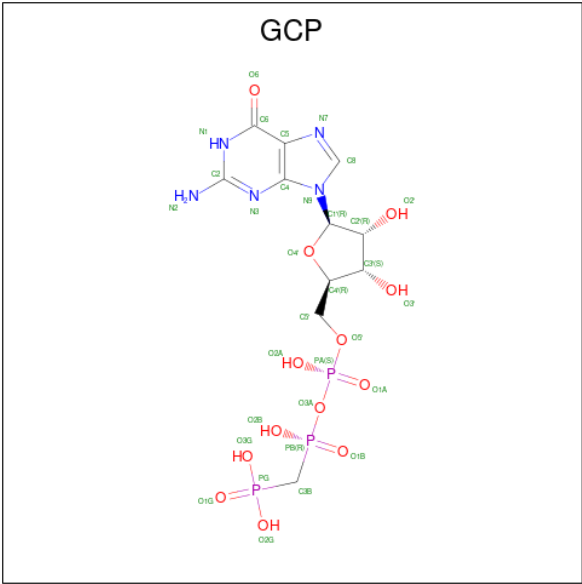
- Molecule 85 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.BETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (CCD ID: SO1) (formula: $C_{27}H_{42}O_8$).



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

- Molecule 86 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD

ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

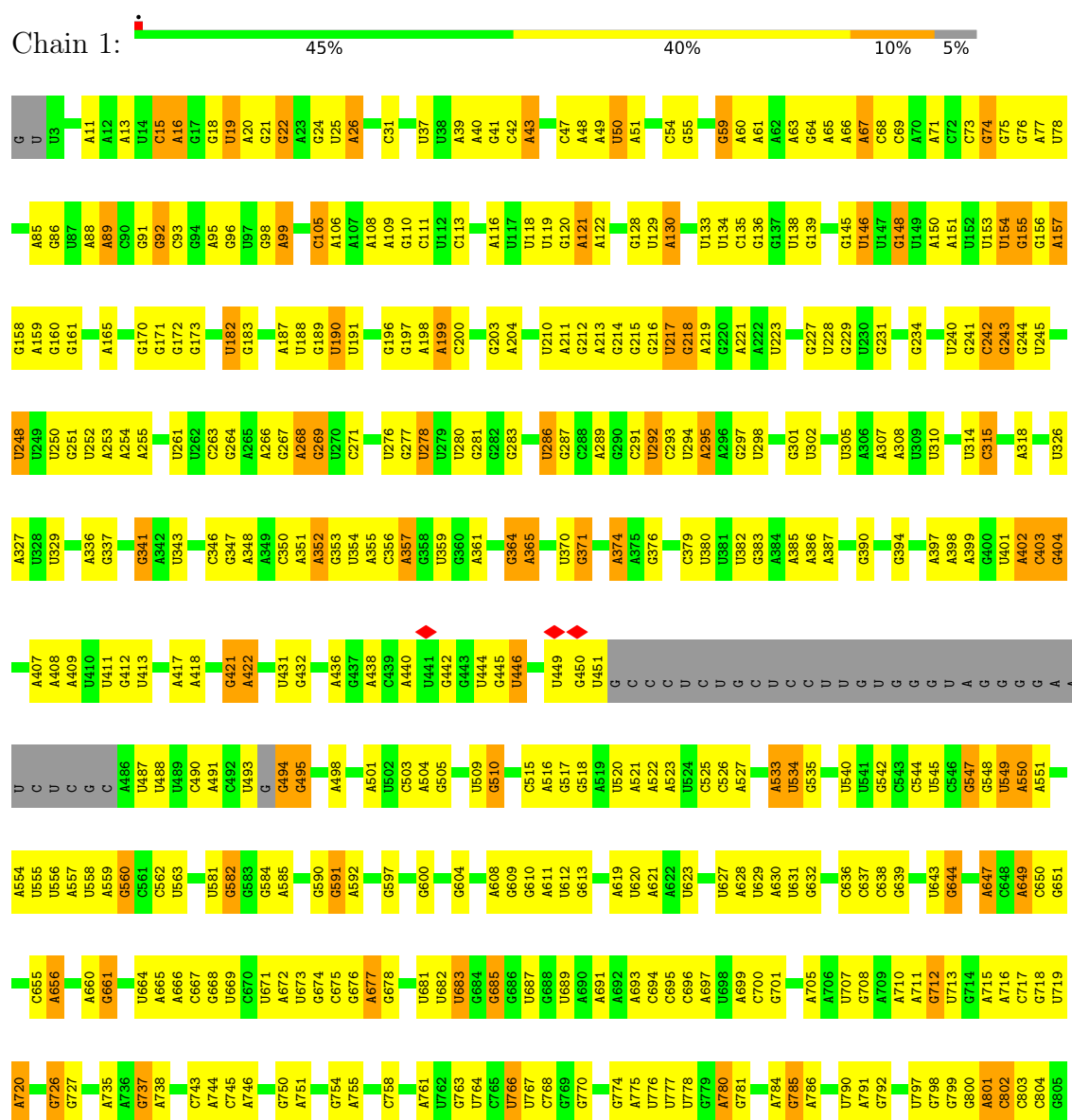


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
86	AZ	1	32	11	5	13	3	0

3 Residue-property plots

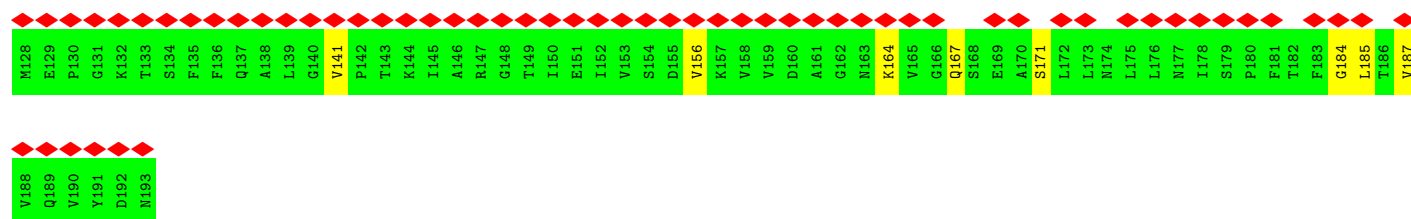
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

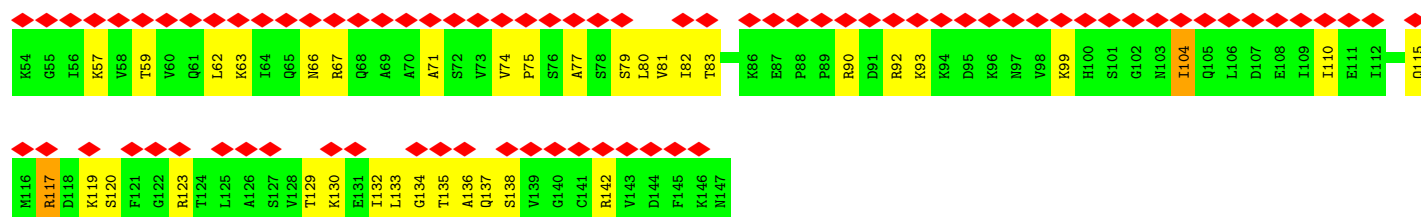
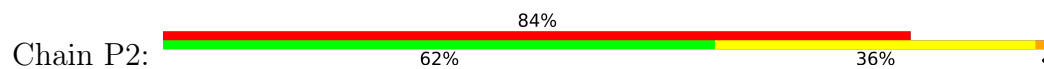


A1839	U1840	A1841	C1842	C1843	C1844	G1845	C1846	C1847	C1848	C1849	C1850	G1851	U1855	A1859	C1860	G1863	A1864	A1865	A1866	A1867	G1868	U1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	A1884	U1885	A1886	A1887	U1888	G1889	A1893	A1896	A1900	C1904	C1905	C1906	C1907	A1908	U1912	A1915				
G1770	C1771	U1772	C1773	C1774	G1775	U1778	C1779	G1780	U1694	C1781	U1782	U1783	C1784	U1785	C1786	A1787	C1788	G1789	C1790	C1793	G1794	U1795	G1796	A1797	A1798	C1872	U1873	A1874	C1805	A1806	C1807	G1808	A1881	C1882	A1883	A1884	U1815	A1816	U1817	U1818	U1819	U1820	U1821	C1822	A1823	C1827	A1828	U1831	C1832	C1906	C1907	A1908	U1912	A1915
G1671	U1672	A1683	U1687	U1688	U1689	G1604	A1605	U1606	U1695	C1706	A1707	C1710	C1711	G1712	A1713	U1714	A1715	U1716	U1717	G1718	G1719	A1720	U1721	A1722	U1723	U1724	G1727	U1728	A1729	U1730	A1731	G1736	U1737	C1738	U1739	U1740	U1741	U1742	G1748	A1749	U1750	G1751	C1756	A1757	U1760	C1761	C1762	U1763	U1764	U1765	G1769			
G1592	A1593	A1594	U1595	C1596	U1599	G1604	A1605	U1606	U1607	C1608	C1609	G1610	A1613	G1618	A1619	U1620	A1621	U1622	G1623	G1624	A1625	U1626	U1627	C1628	U1629	U1630	G1634	C1635	U1636	A1637	A1638	C1639	G1640	A1643	C1644	U1645	G1646	G1653	A1654	G1655	A1656	C1657	U1658	U1659	C1660	G1661	C1662	C1663	G1664	C1665	G1666	A1667	C1668	
G1510	U1511	U1512	C1516	C1517	G1521	U1522	U1523	A1524	G1525	U1526	A1529	U1530	U1533	A1534	A1535	G1541	C1551	C1552	U1553	U1554	U1555	C1556	A1557	A1558	U1559	C1560	U1561	C1562	C1563	U1564	G1565	A1566	U1567	U1568	U1569	U1570	A1571	U1572	G1573	C1574	G1577	C1578	C1579	A1580	C1581	C1582	A1583	U1584	A1587	A1588	A1589			
U1435	U1436	C1437	U1438	U1439	G1440	G1443	A1446	U1447	U1448	U1449	G1450	C1451	U1455	A1456	U1457	U1458	C1459	A1460	G1464	U1468	C1469	U1470	U1471	U1472	U1473	U1474	A1475	U1476	A1482	C1483	U1484	G1485	U1486	U1487	U1488	A1489	A1490	A1491	U1492	G1493	U1494	C1497	A1498	C1499	G1500	U1501	C1502	A1503	A1506	U1507	C1508	A1509		
U1347	U1348	G1349	A1350	U1351	A1352	U1353	G1354	A1355	U1356	G1357	G1362	A1363	U1368	A1369	G1370	G1371	C1372	A1373	G1374	G1382	G1383	U1384	C1385	A1386	C1387	U1388	G1389	A1390	C1391	C1392	A1393	A1394	A1399	G1400	U1405	G1408	C1411	G1417	A1418	A1419	C1420	G1421	G1422	C1423	C1424	U1425	U1430	G1431	G1434					
U1269	A1270	C1271	C1272	A1273	A1274	C1275	U1276	U1277	C1278	U1279	C1280	G1281	U1282	C1283	U1284	G1285	A1286	A1287	A1290	C1291	G1295	C1296	C1297	A1301	A1302	U1305	G1306	C1307	A1308	U1309	G1313	C1314	U1315	C1316	A1317	G1321	U1322	G1323	U1324	U1325	A1330	U1336	A1337	G1340	U1341	C1342	A1343	G1344						
C1198	G1126	G1127	U1128	A1129	C1045	A1046	A1047	A1053	A1054	A1055	A1062	G1063	A1064	A1065	G1066	C1069	U1070	U1071	G1072	A1076	A1079	A1080	C1086	G1087	U1094	U1095	U1096	G1097	A1098	A1099	U1100	G1101	A1102	A1103	G1104	A1105	G1106	U1110	G1115	G1116	G1117	U1119	G1192	A1193	G1194	C1195	U1121	U1125						
A967	G968	C969	A970	C975	U976	C977	U981	G984	U985	U990	G991	A992	G993	U994	U995	A998	G999	C1000	G1001	U1001	A1002	C1003	A1004	G1005	A1006	U982	A953	G954	G957	C958	U939	G940	G941	U942	U943	C944	G945	U946	G947	C948	C949	G950	A951	A952	C959	U960	G961	A962	G963	G964	A965	U966		
A806	A807	A808	A816	A817	U821	C822	C823	G826	A827	G908	G909	C911	G833	U834	G835	A836	A837	G838	A920	A921	G924	A925	C928	C929	U850	C851	U852	G853	U855	G856	G857	A858	G859	U942	U943	C944	G945	U946	G947	C948	C949	G950	A951	A952	C959	U960	G961	A962	G963	G964	A965	U966		

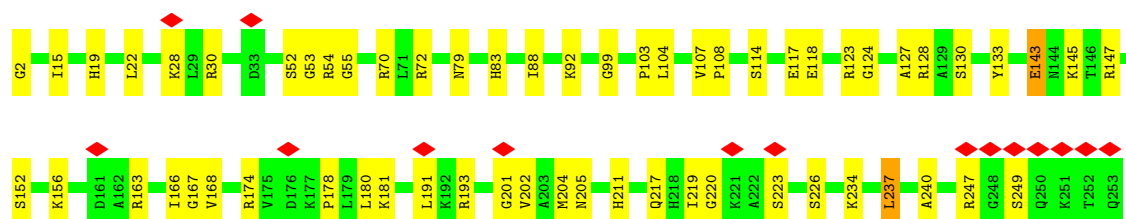
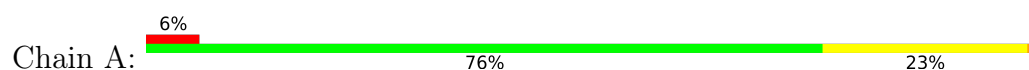




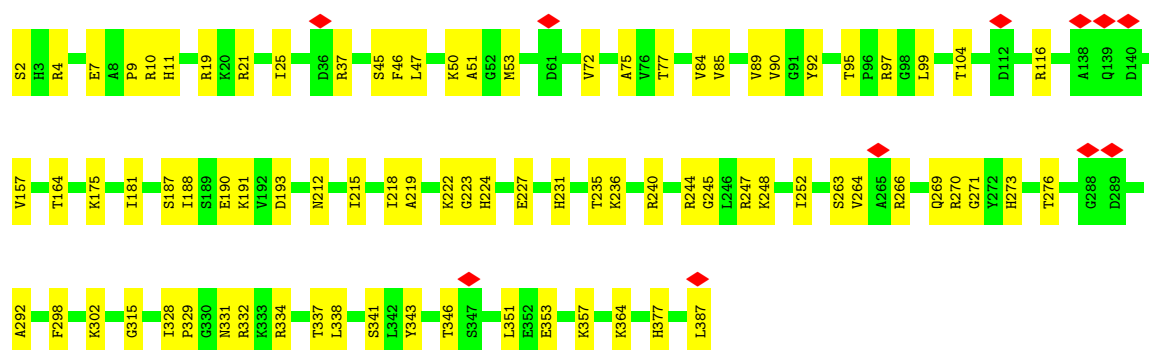
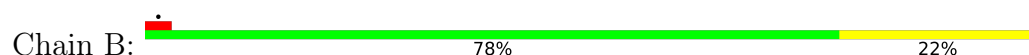
• Molecule 5: 60S ribosomal protein L12-A



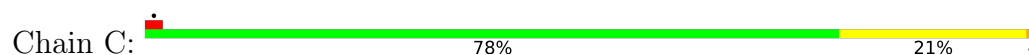
• Molecule 6: 60S ribosomal protein L2-A

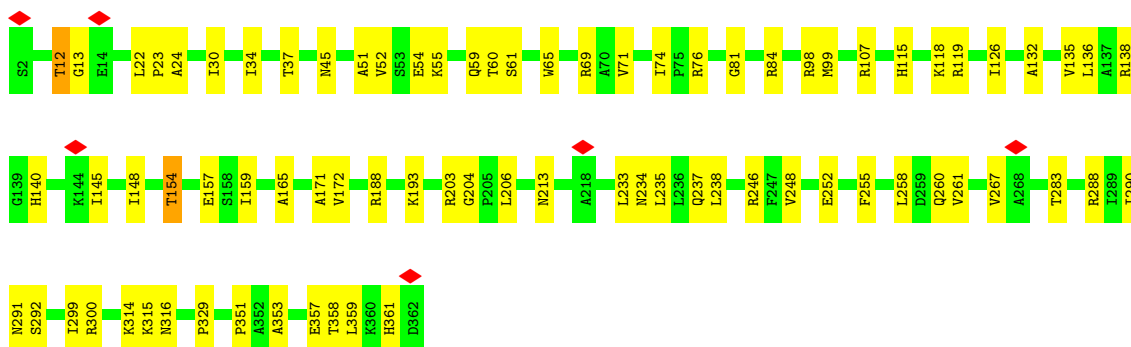


• Molecule 7: 60S ribosomal protein L3

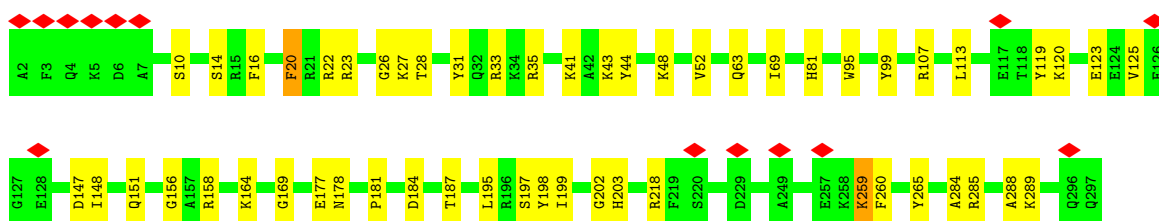
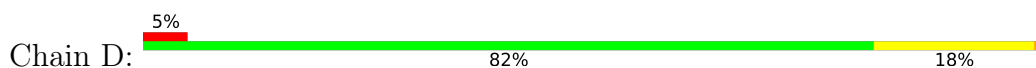


• Molecule 8: 60S ribosomal protein L4-A

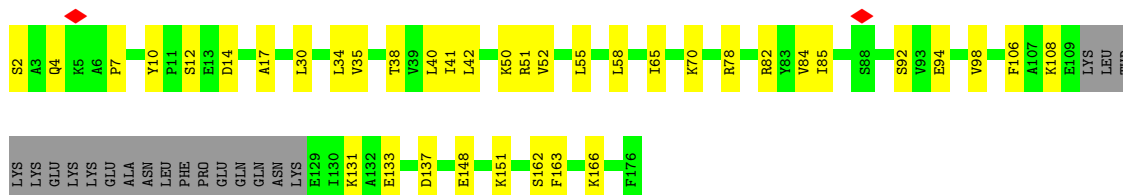




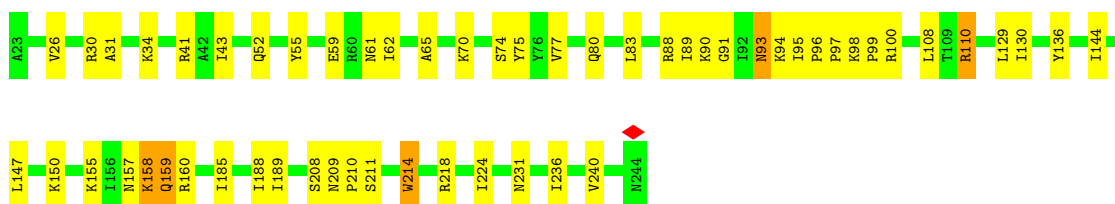
• Molecule 9: 60S ribosomal protein L5



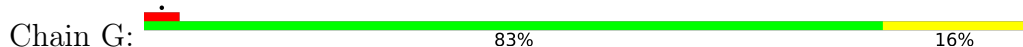
• Molecule 10: 60S ribosomal protein L6-A

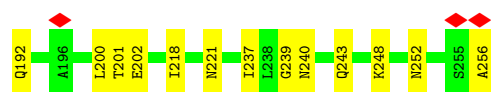


• Molecule 11: 60S ribosomal protein L7-A

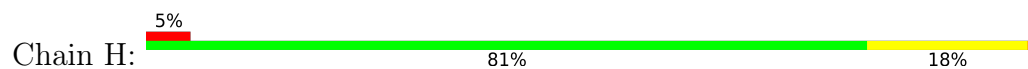


• Molecule 12: 60S ribosomal protein L8-A

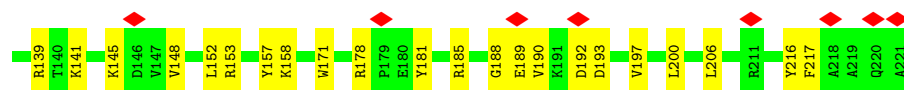
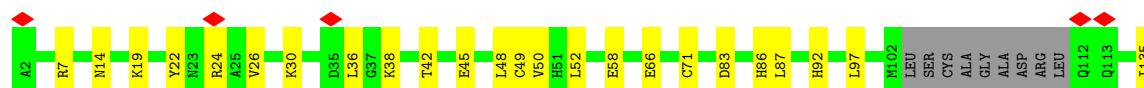
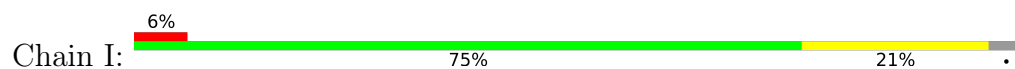




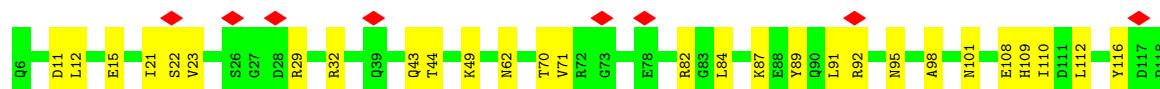
- Molecule 13: 60S ribosomal protein L9-A



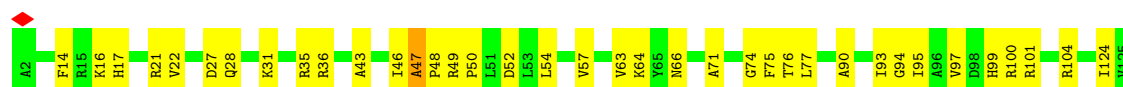
- Molecule 14: 60S ribosomal protein L10



- Molecule 15: 60S ribosomal protein L11-B

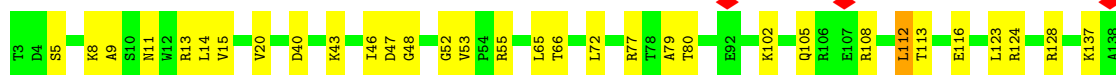


- Molecule 16: 60S ribosomal protein L13-A



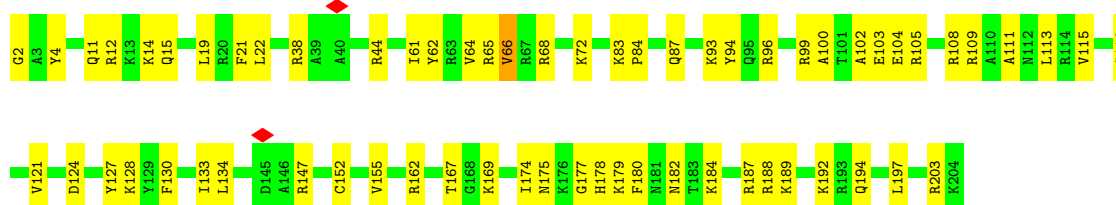
- Molecule 17: 60S ribosomal protein L14-A

Chain M:  76% 23%



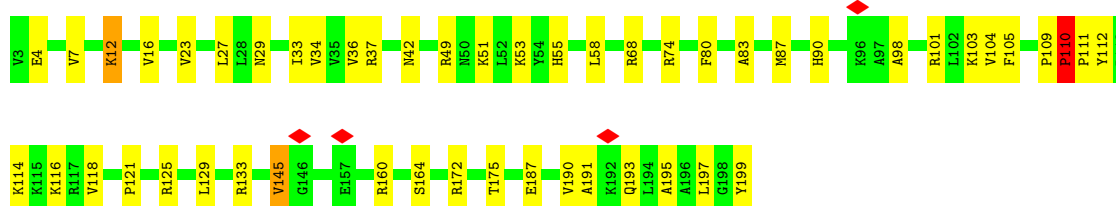
- Molecule 18: 60S ribosomal protein L15-A

Chain N:  68% 31%



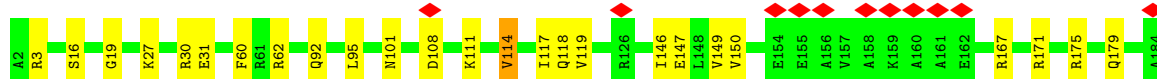
- Molecule 19: 60S ribosomal protein L16-A

Chain O:  74% 24%



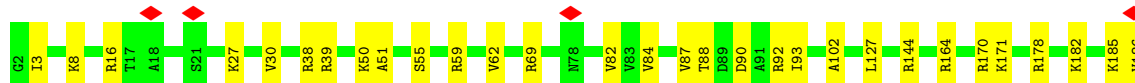
- Molecule 20: 60S ribosomal protein L17-A

Chain P:  6% 86% 13%



- Molecule 21: 60S ribosomal protein L18-A

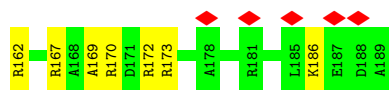
Chain Q:  84% 16%



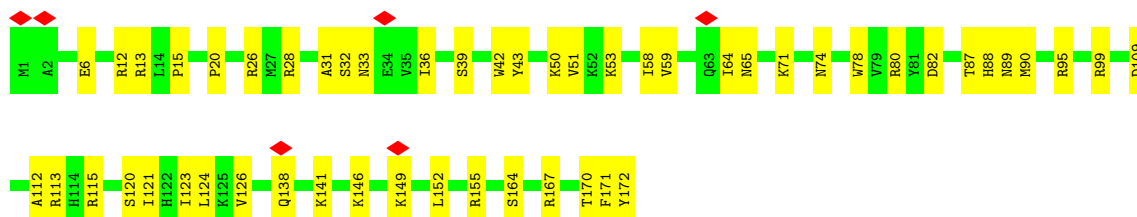
- Molecule 22: 60S ribosomal protein L19-A

Chain R:  81% 18%

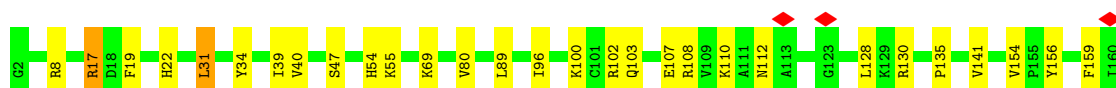
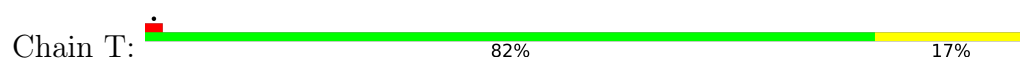




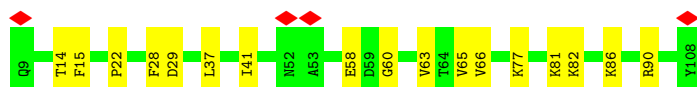
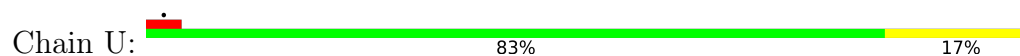
- Molecule 23: 60S ribosomal protein L20-A



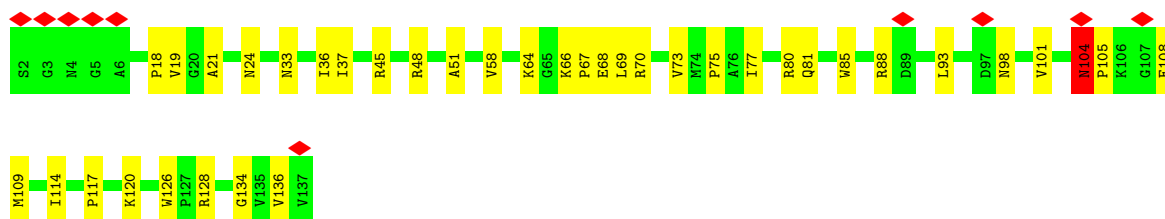
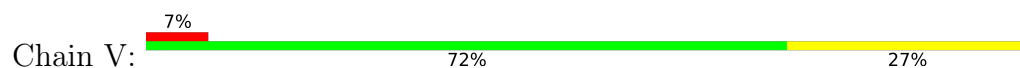
- Molecule 24: 60S ribosomal protein L21-A



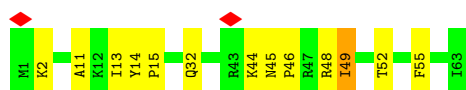
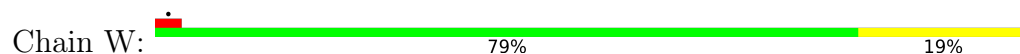
- Molecule 25: 60S ribosomal protein L22-A



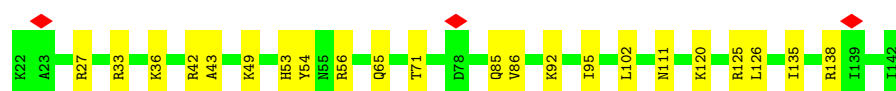
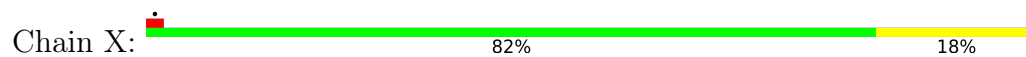
- Molecule 26: 60S ribosomal protein L23-A



- Molecule 27: 60S ribosomal protein L24-A



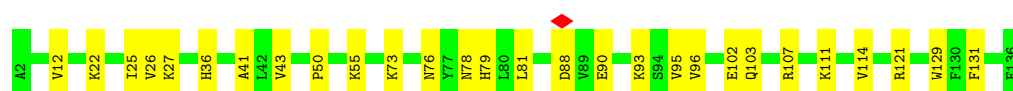
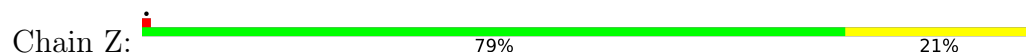
- Molecule 28: 60S ribosomal protein L25



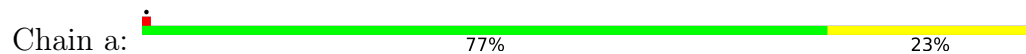
- Molecule 29: 60S ribosomal protein L26-A



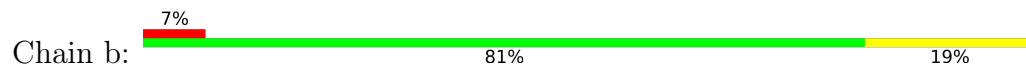
- Molecule 30: 60S ribosomal protein L27-A



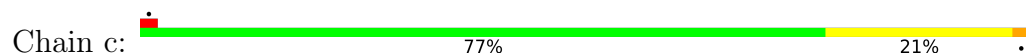
- Molecule 31: 60S ribosomal protein L28



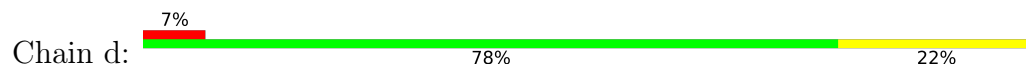
- Molecule 32: 60S ribosomal protein L29



- Molecule 33: 60S ribosomal protein L30

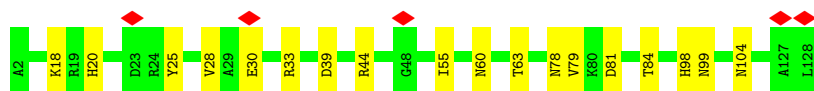
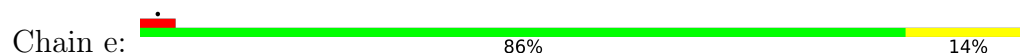


- Molecule 34: 60S ribosomal protein L31-A

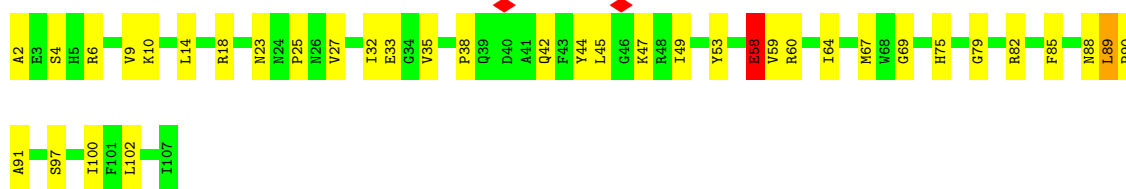




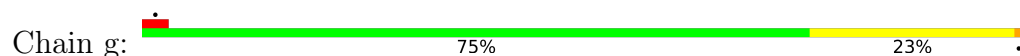
- Molecule 35: 60S ribosomal protein L32



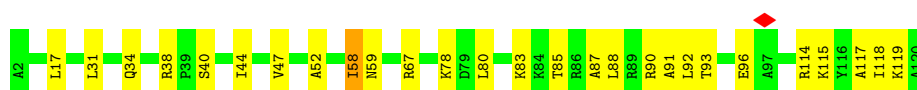
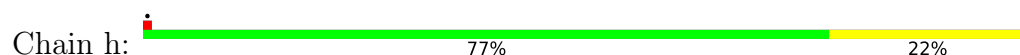
- Molecule 36: 60S ribosomal protein L33-A



- Molecule 37: 60S ribosomal protein L34-A



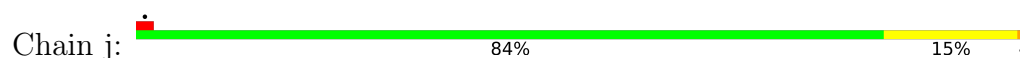
- Molecule 38: 60S ribosomal protein L35-A



- Molecule 39: 60S ribosomal protein L36-A

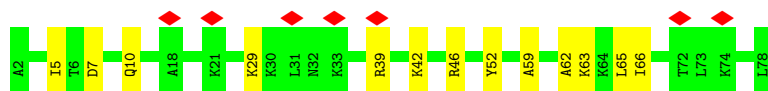
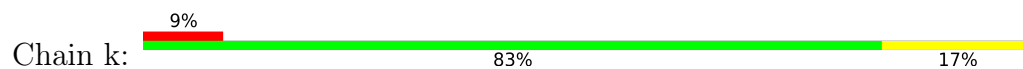


- Molecule 40: 60S ribosomal protein L37-A

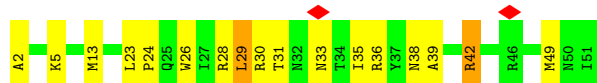




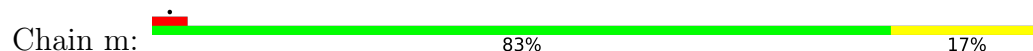
- Molecule 41: 60S ribosomal protein L38



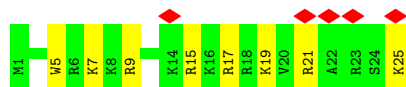
- Molecule 42: 60S ribosomal protein L39



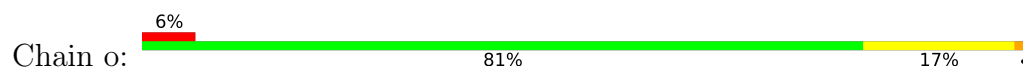
- Molecule 43: Ubiquitin-60S ribosomal protein L40



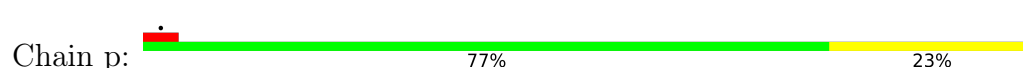
- Molecule 44: 60S ribosomal protein L41-B



- Molecule 45: 60S ribosomal protein L42-A

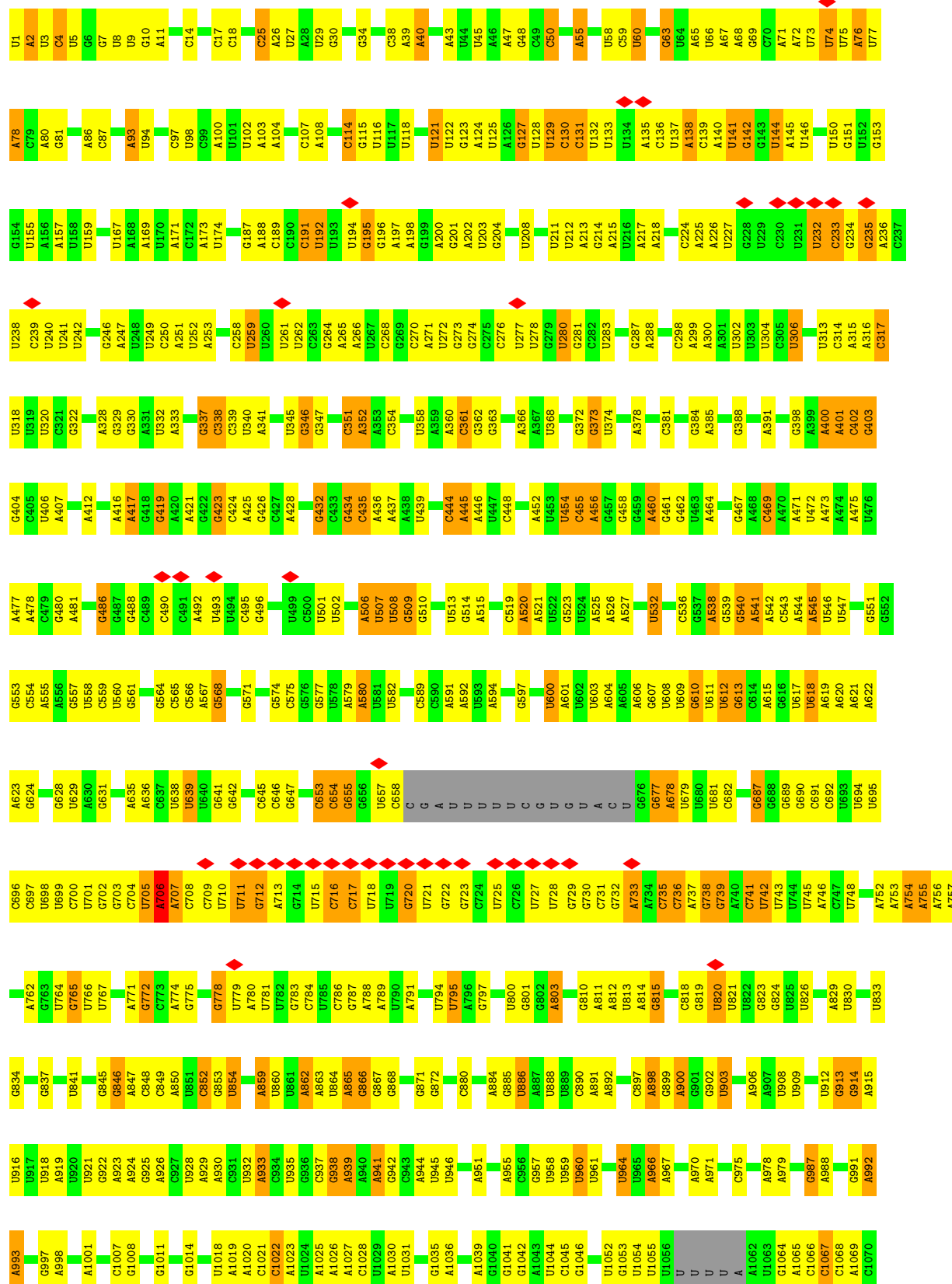


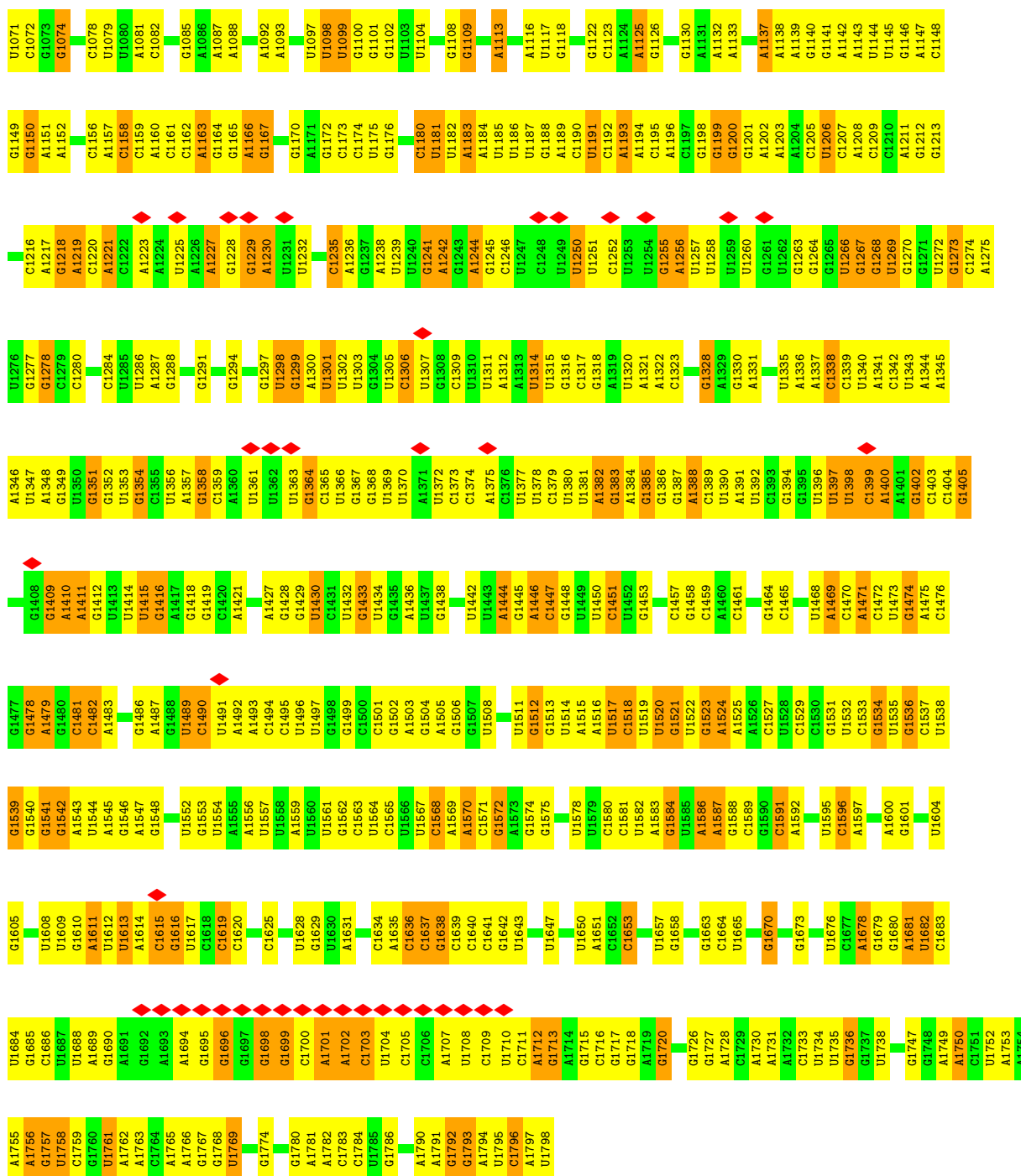
- Molecule 46: 60S ribosomal protein L43-A



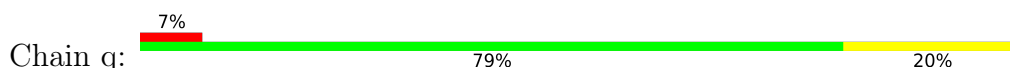
- Molecule 47: 18S ribosomal RNA

Chain 2:  39% 45% 15%



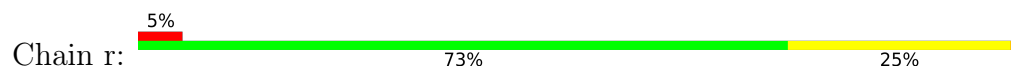


• Molecule 48: 40S ribosomal protein S0-A

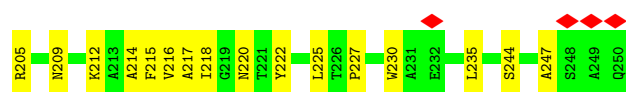
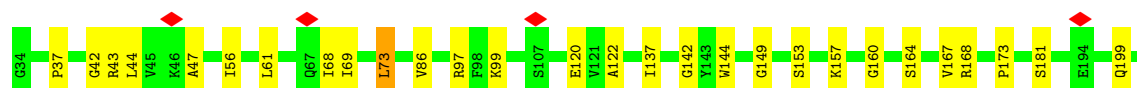
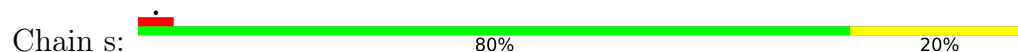




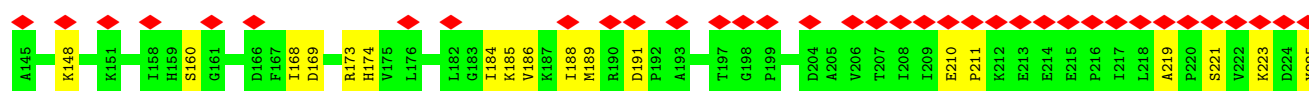
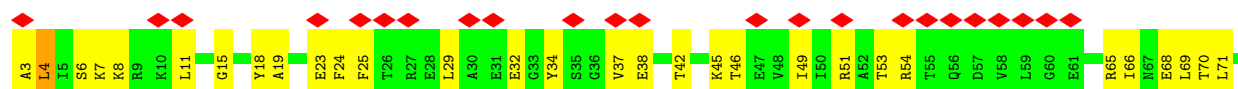
- Molecule 49: 40S ribosomal protein S1-A



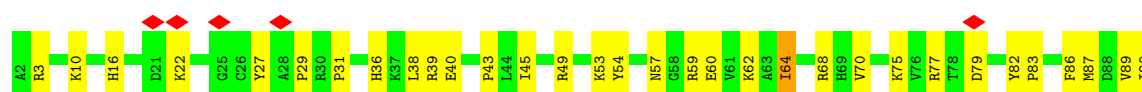
- Molecule 50: 40S ribosomal protein S2

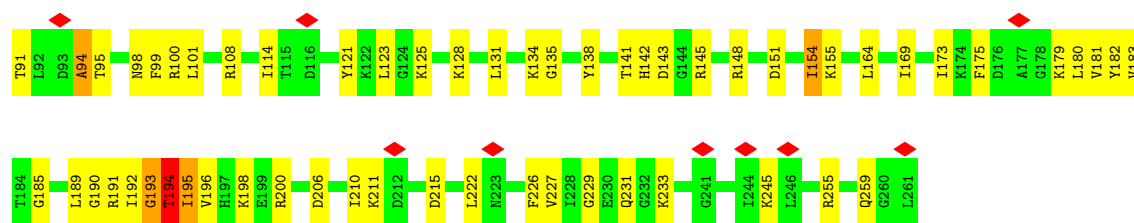


- Molecule 51: 40S ribosomal protein S3

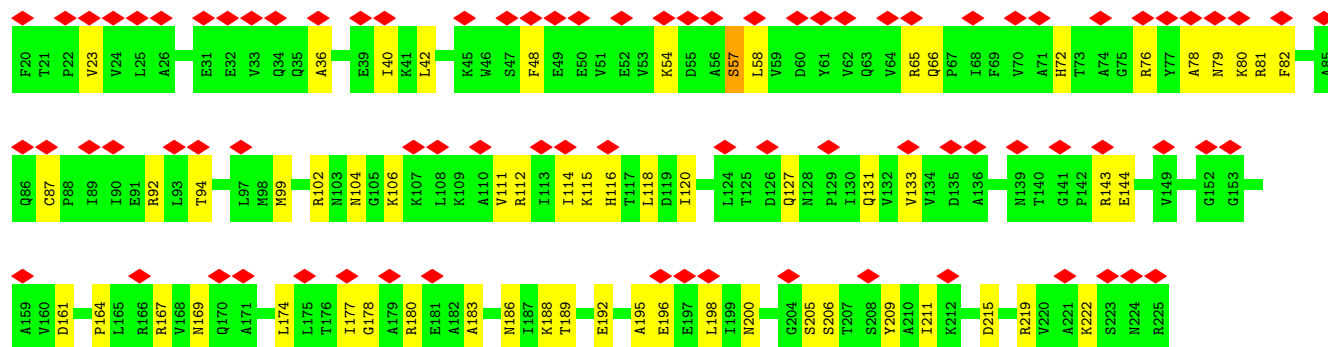
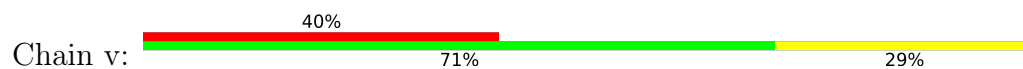


- Molecule 52: 40S ribosomal protein S4-A

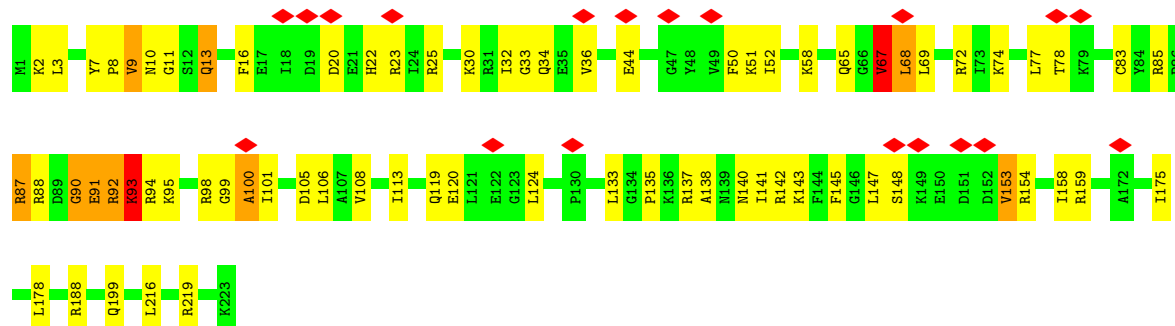




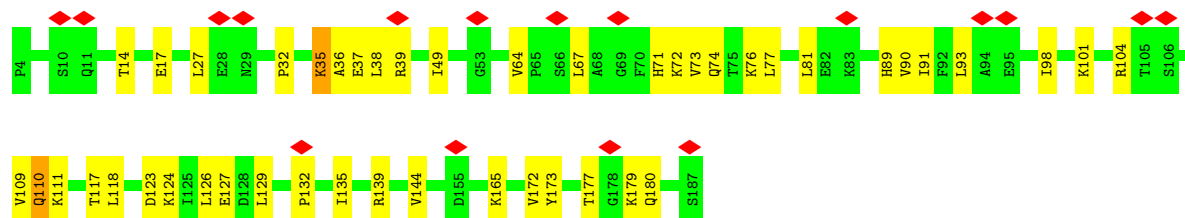
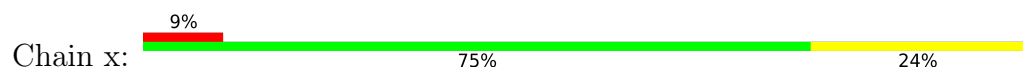
• Molecule 53: 40S ribosomal protein S5



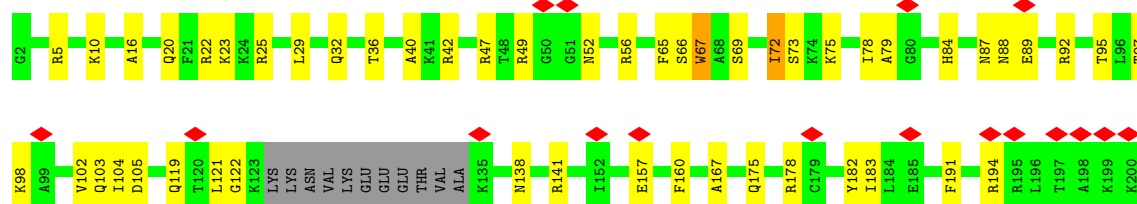
• Molecule 54: 40S ribosomal protein S6-A



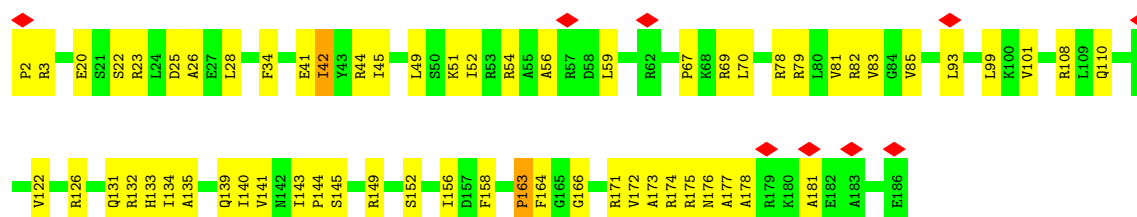
• Molecule 55: 40S ribosomal protein S7-A



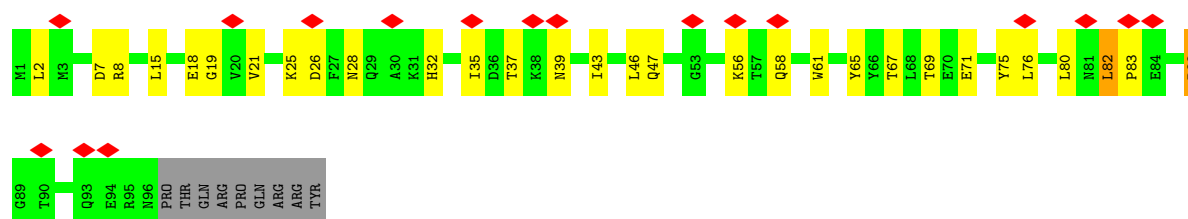
• Molecule 56: 40S ribosomal protein S8-A



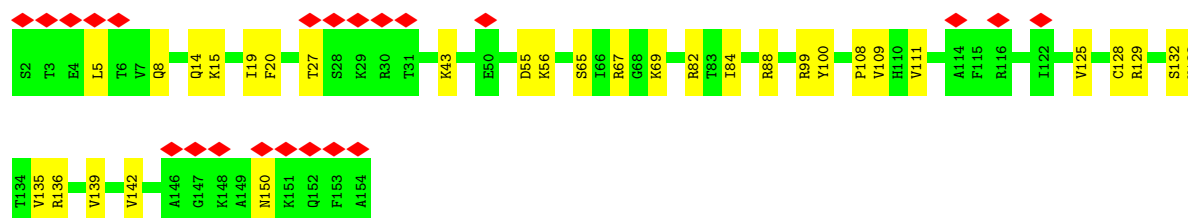
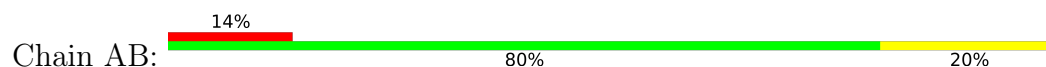
- Molecule 57: 40S ribosomal protein S9-A



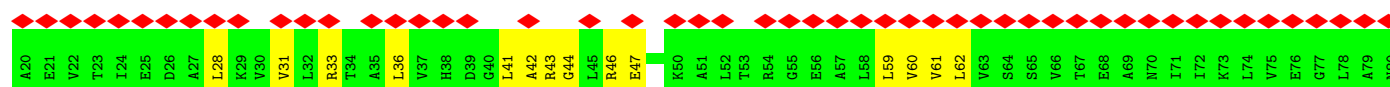
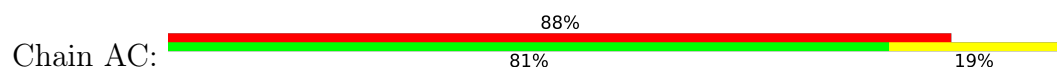
- Molecule 58: 40S ribosomal protein S10-A

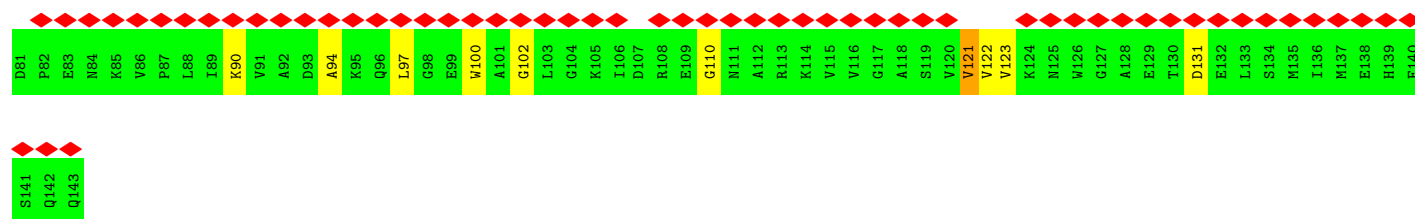


- Molecule 59: 40S ribosomal protein S11-A

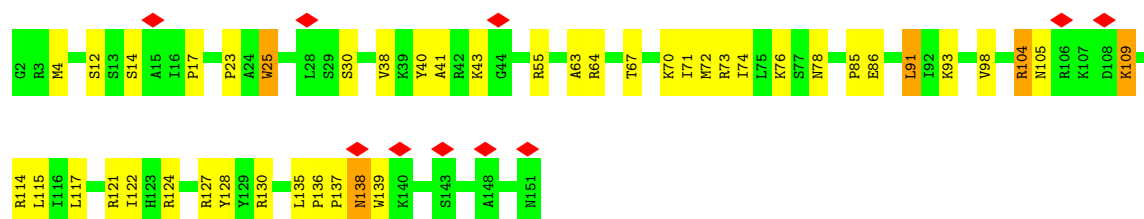
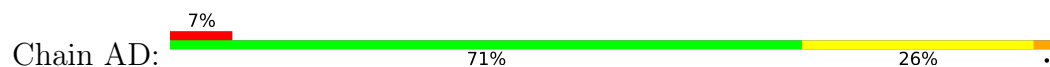


- Molecule 60: 40S ribosomal protein S12

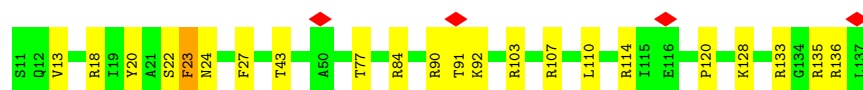
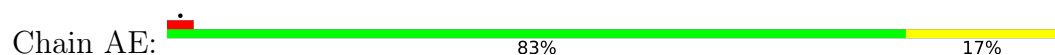




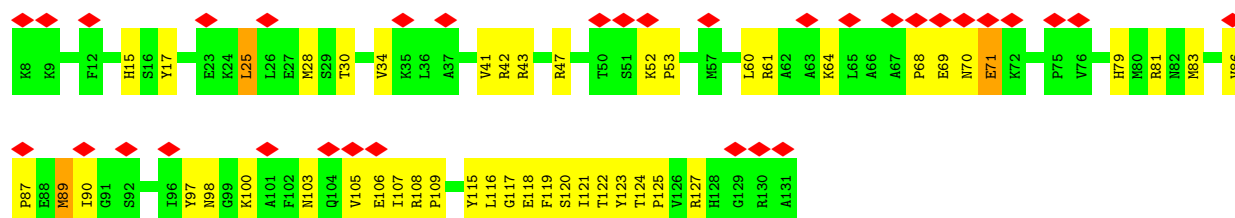
- Molecule 61: 40S ribosomal protein S13



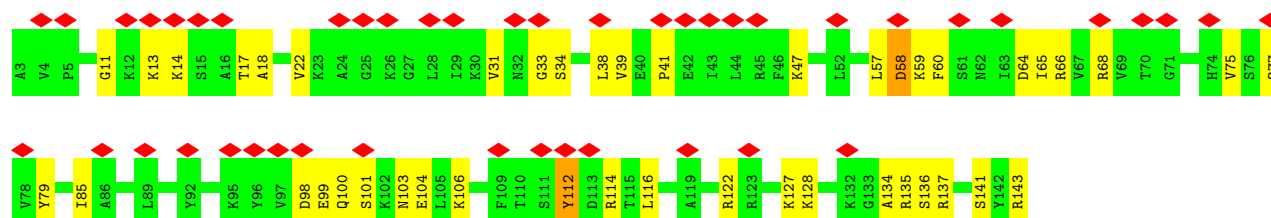
- Molecule 62: 40S ribosomal protein S14-B



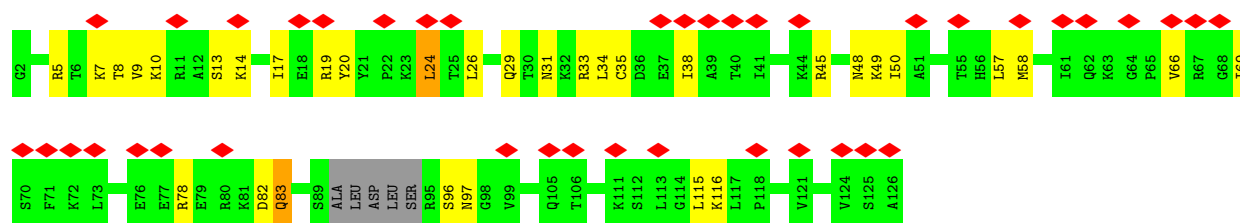
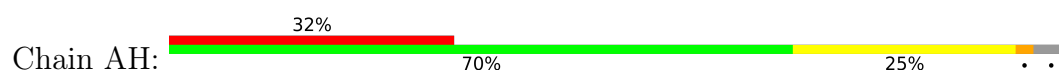
- Molecule 63: 40S ribosomal protein S15



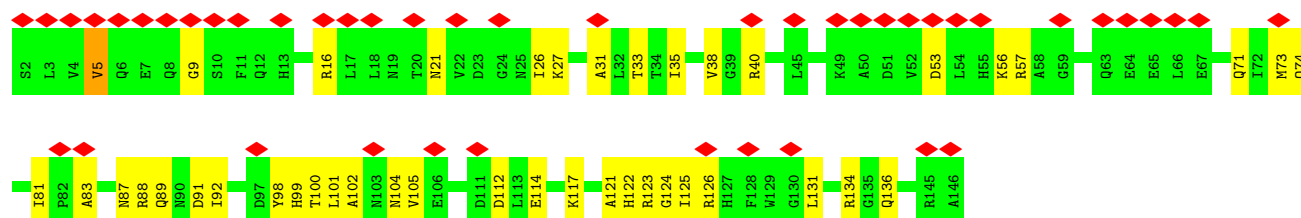
- Molecule 64: 40S ribosomal protein S16-A



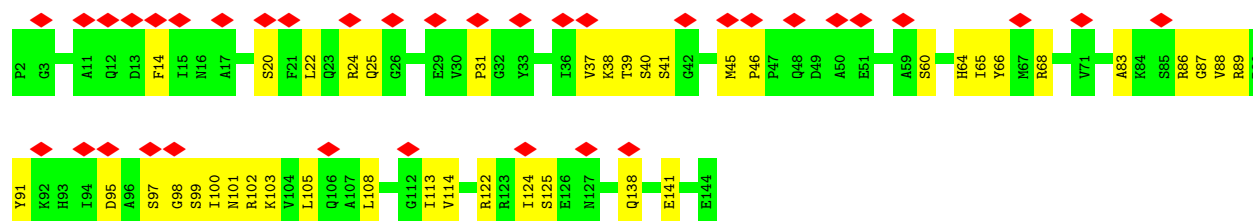
- Molecule 65: 40S ribosomal protein S17-B



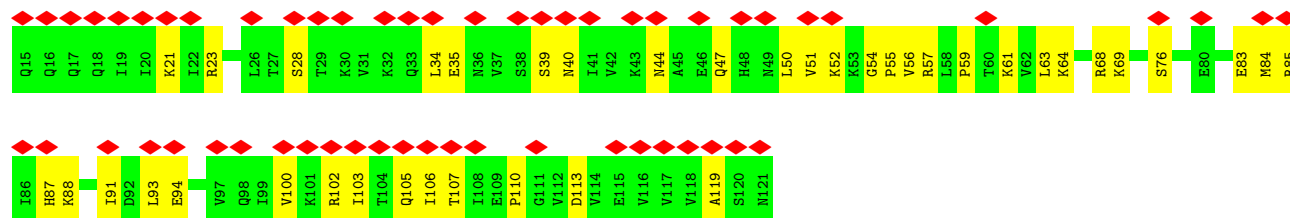
- Molecule 66: 40S ribosomal protein S18-A



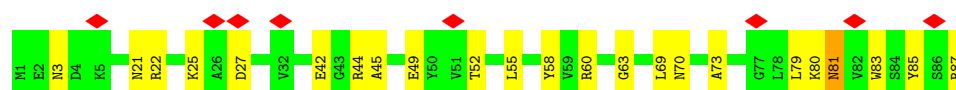
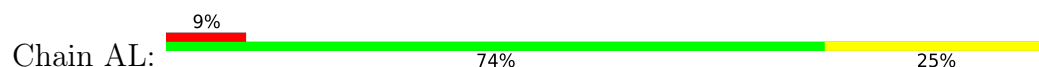
- Molecule 67: 40S ribosomal protein S19-A



- Molecule 68: 40S ribosomal protein S20



- Molecule 69: 40S ribosomal protein S21-A



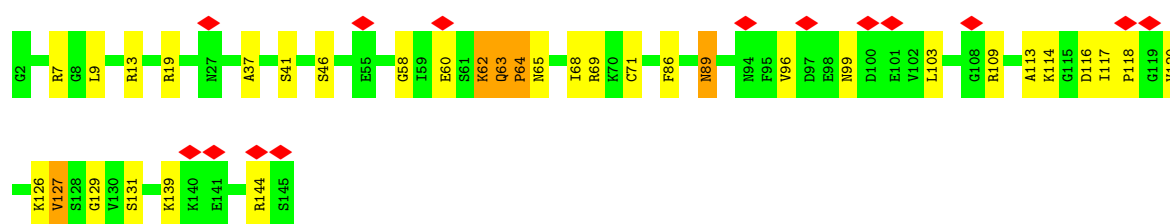
- Molecule 70: 40S ribosomal protein S22-A

Chain AM:  72% 26%



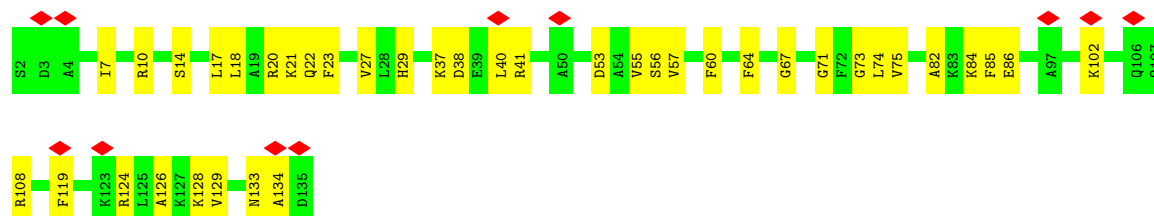
- Molecule 71: 40S ribosomal protein S23-A

Chain AN:  10% 76% 20%

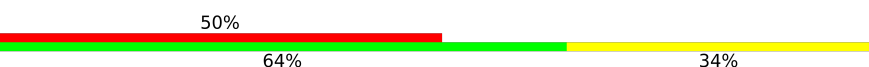


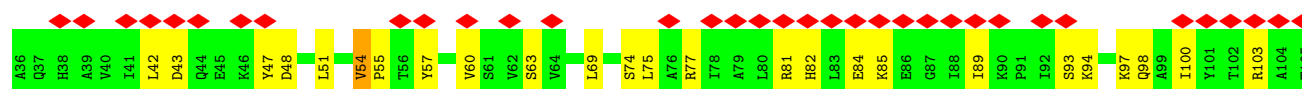
- Molecule 72: 40S ribosomal protein S24-A

Chain AO:  8% 71% 29%



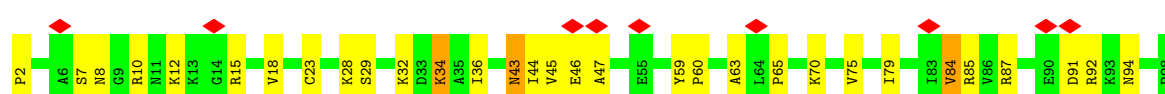
- Molecule 73: 40S ribosomal protein S25-A

Chain AP:  50% 64% 34%

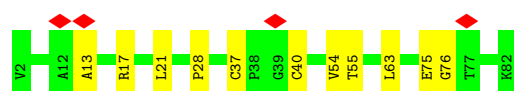
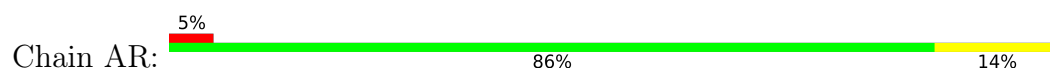


- Molecule 74: 40S ribosomal protein S26-B

Chain AQ:  9% 68% 29%



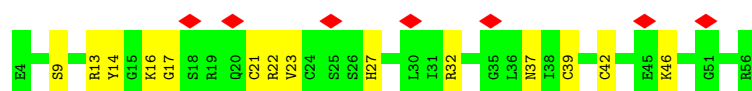
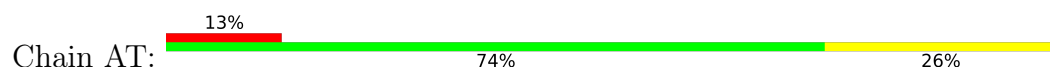
- Molecule 75: 40S ribosomal protein S27-A



- Molecule 76: 40S ribosomal protein S28-A



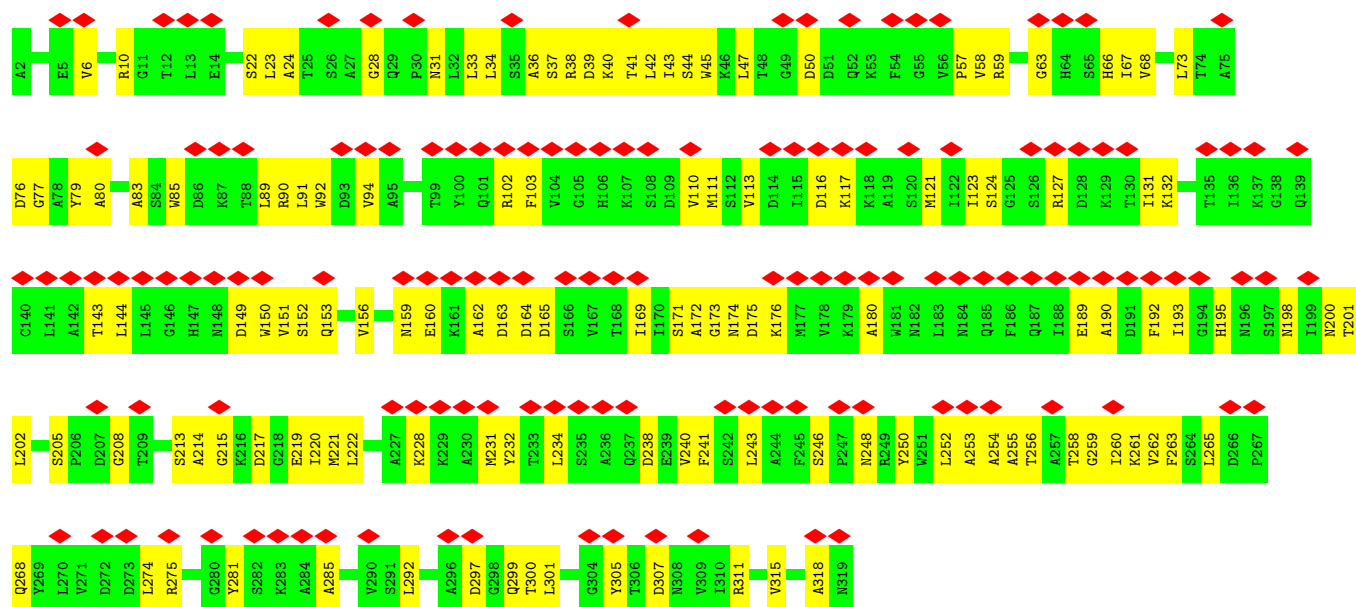
- Molecule 77: 40S ribosomal protein S29-A



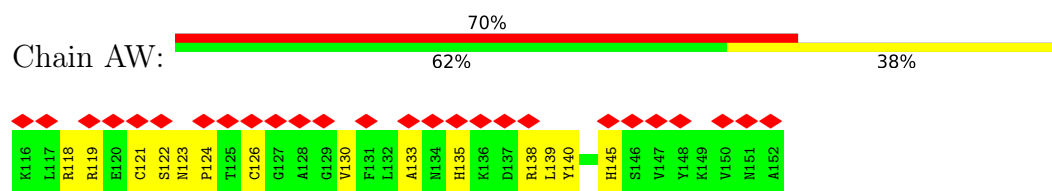
- Molecule 78: 40S ribosomal protein S30-A



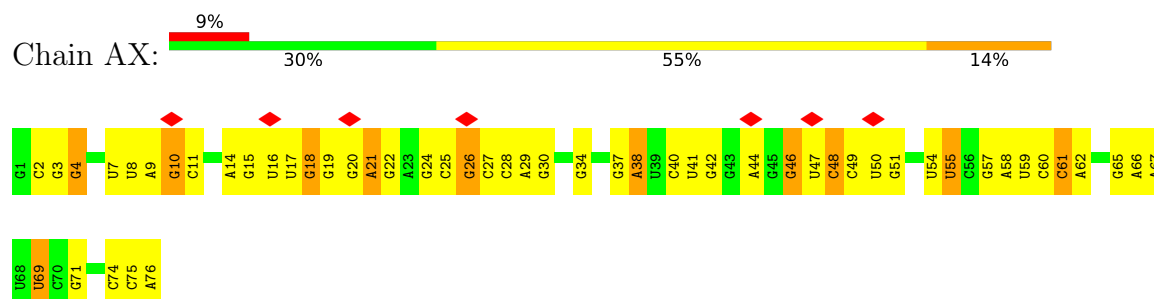
- Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein



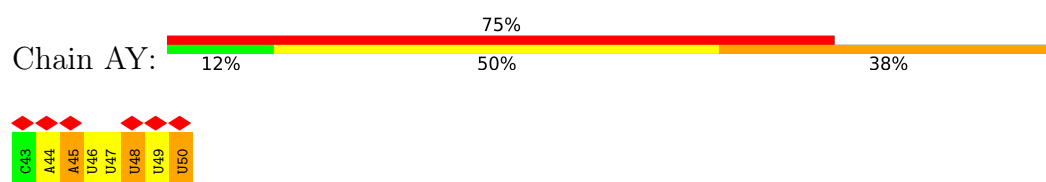
- Molecule 80: Ubiquitin-40S ribosomal protein S31



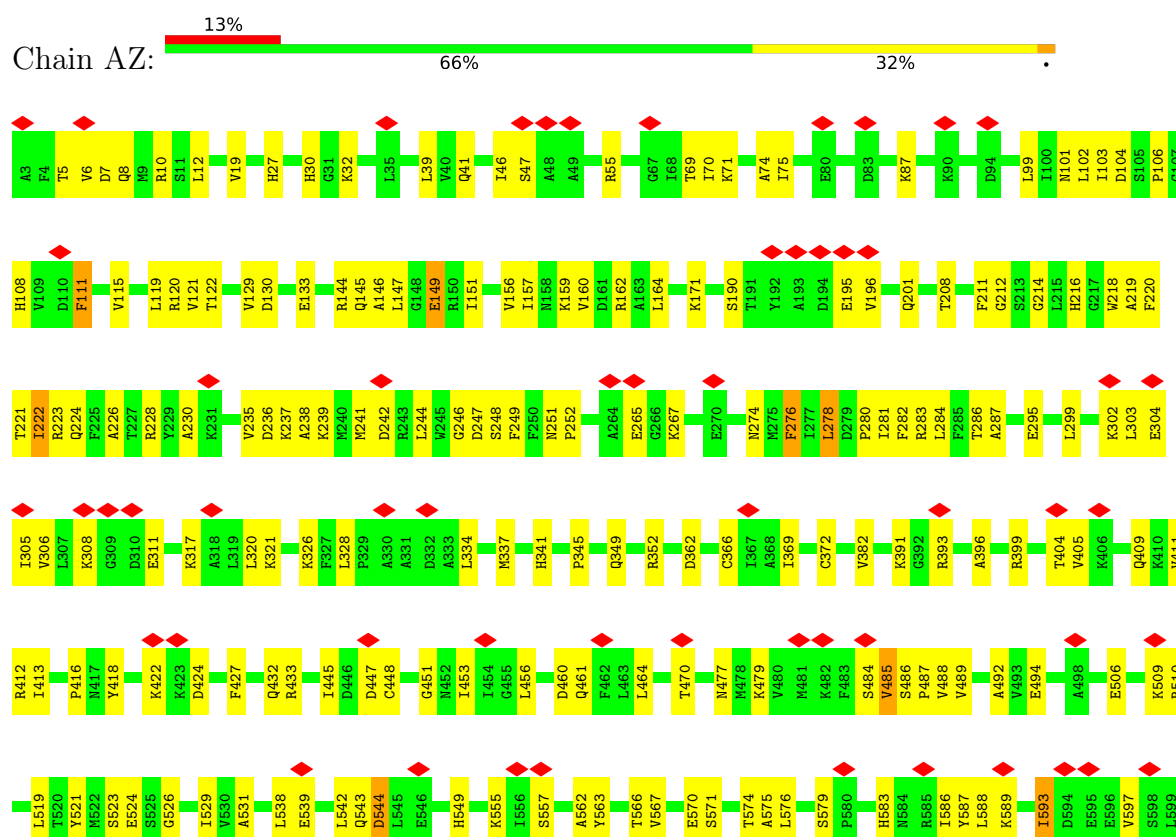
- Molecule 81: Transfer RNA - Phe

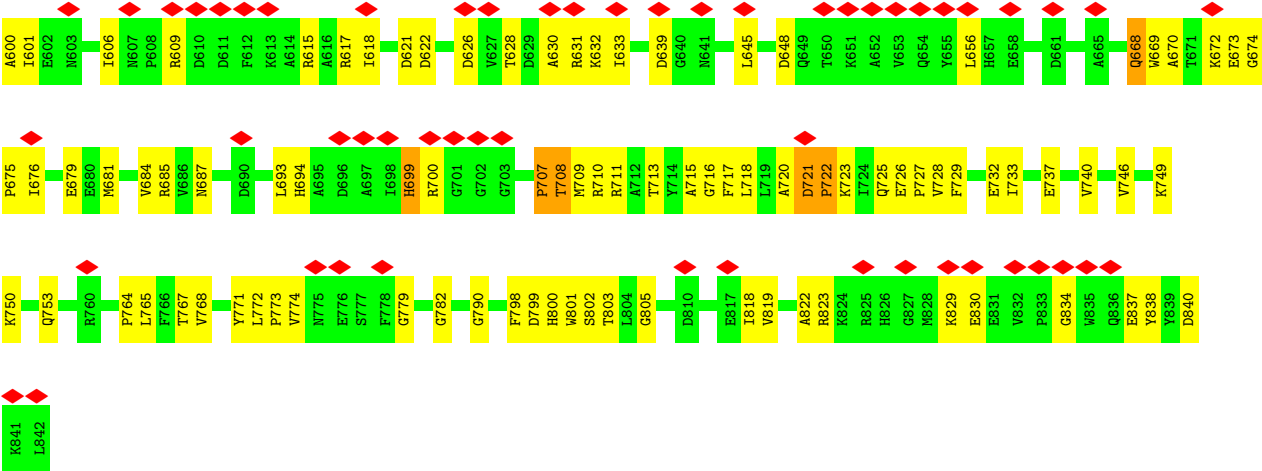


- Molecule 82: Messenger RNA



- Molecule 83: Elongation factor 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	189700	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	0.347	Depositor
Minimum map value	-0.197	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, DDE, ZN, SO1

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	0.30	0/77157	0.47	1/120295 (0.0%)
2	3	0.26	0/2883	0.42	0/4491
3	4	0.29	0/3746	0.46	0/5832
4	P0	0.25	0/1498	0.70	1/2025 (0.0%)
5	P2	0.27	0/728	0.80	0/975
6	A	0.37	0/1948	0.72	0/2617
7	B	0.32	0/3146	0.68	0/4228
8	C	0.30	0/2800	0.67	0/3790
9	D	0.27	0/2425	0.66	0/3271
10	E	0.23	0/1260	0.59	0/1694
11	F	0.31	0/1821	0.71	0/2451
12	G	0.28	0/1836	0.72	0/2481
13	H	0.27	0/1539	0.70	0/2073
14	I	0.31	0/1741	0.70	0/2335
15	J	0.27	0/1374	0.78	0/1842
16	L	0.31	0/1568	0.79	3/2106 (0.1%)
17	M	0.26	0/1068	0.61	0/1438
18	N	0.35	0/1757	0.79	0/2354
19	O	0.33	0/1585	0.73	1/2128 (0.0%)
20	P	0.29	0/1443	0.64	0/1944
21	Q	0.28	0/1465	0.66	0/1965
22	R	0.28	0/1538	0.65	0/2050
23	S	0.29	0/1481	0.66	0/1990
24	T	0.30	0/1300	0.73	2/1743 (0.1%)
25	U	0.25	0/812	0.65	2/1099 (0.2%)
26	V	0.31	0/1018	0.72	1/1369 (0.1%)
27	W	0.31	0/533	0.70	0/707
28	X	0.27	0/979	0.65	0/1321
29	Y	0.27	0/1004	0.66	0/1341
30	Z	0.28	0/1118	0.68	3/1497 (0.2%)
31	a	0.32	0/1204	0.70	0/1612
32	b	0.24	0/473	0.67	0/629

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.27	0/751	0.62	0/1008
34	d	0.31	0/897	0.65	0/1205
35	e	0.28	0/1041	0.67	0/1394
36	f	0.34	0/868	0.81	2/1168 (0.2%)
37	g	0.32	0/890	0.77	1/1189 (0.1%)
38	h	0.29	0/978	0.71	1/1301 (0.1%)
39	i	0.28	0/778	0.74	0/1034
40	j	0.36	0/696	0.85	1/923 (0.1%)
41	k	0.24	0/618	0.66	0/826
42	l	0.45	0/443	1.02	0/588
43	m	0.28	0/423	0.64	0/562
44	n	0.26	0/228	0.71	0/293
45	o	0.29	0/860	0.72	0/1136
46	p	0.32	0/701	0.76	0/934
47	2	0.26	0/42328	0.48	3/65955 (0.0%)
48	q	0.26	0/1617	0.70	0/2215
49	r	0.30	0/1735	0.83	4/2335 (0.2%)
50	s	0.27	0/1665	0.68	0/2263
51	t	0.29	0/1759	0.74	1/2368 (0.0%)
52	u	0.29	0/2109	0.83	8/2839 (0.3%)
53	v	0.29	0/1629	0.77	2/2202 (0.1%)
54	w	0.30	0/1814	0.90	7/2425 (0.3%)
55	x	0.31	0/1506	0.80	2/2028 (0.1%)
56	y	0.29	0/1514	0.79	5/2021 (0.2%)
57	z	0.28	0/1519	0.78	3/2035 (0.1%)
58	AA	0.31	0/789	0.78	1/1067 (0.1%)
59	AB	0.27	0/1247	0.72	1/1681 (0.1%)
60	AC	0.26	0/898	0.73	0/1220
61	AD	0.29	0/1215	0.80	2/1638 (0.1%)
62	AE	0.28	0/901	0.73	2/1217 (0.2%)
63	AF	0.34	0/998	0.91	4/1341 (0.3%)
64	AG	0.28	0/1125	0.81	0/1510
65	AH	0.27	0/935	0.72	1/1254 (0.1%)
66	AI	0.25	0/1211	0.70	0/1628
67	AJ	0.26	0/1130	0.70	0/1517
68	AK	0.28	0/865	0.70	0/1169
69	AL	0.34	0/693	0.87	2/935 (0.2%)
70	AM	0.33	0/1038	0.73	1/1395 (0.1%)
71	AN	0.33	0/1139	0.82	0/1518
72	AO	0.25	0/1087	0.67	0/1449
73	AP	0.31	0/571	0.76	0/768
74	AQ	0.34	0/782	0.98	4/1047 (0.4%)
75	AR	0.31	0/620	0.86	0/838

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
76	AS	0.25	0/499	0.70	0/670
77	AT	0.22	0/452	0.67	0/600
78	AU	0.24	0/483	0.65	0/643
79	AV	0.26	0/2490	0.70	4/3389 (0.1%)
80	AW	0.23	0/292	0.76	3/390 (0.8%)
81	AX	0.22	0/1818	0.48	0/2831
82	AY	0.32	0/181	0.64	0/278
83	AZ	0.31	0/6655	0.82	10/9009 (0.1%)
All	All	0.29	0/225729	0.59	89/330942 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	P0	0	2
5	P2	0	1
6	A	0	1
7	B	0	1
9	D	0	5
10	E	0	1
11	F	0	3
12	G	0	3
13	H	0	2
14	I	0	2
15	J	0	1
16	L	0	1
19	O	0	2
21	Q	0	1
24	T	0	2
26	V	0	2
27	W	0	1
31	a	0	1
34	d	0	2
35	e	0	2
36	f	0	1
37	g	0	3
38	h	0	1
39	i	0	3
40	j	0	1
42	l	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	o	0	3
48	q	0	4
49	r	0	4
51	t	0	1
52	u	0	5
53	v	0	2
54	w	0	11
55	x	0	2
56	y	0	1
57	z	0	2
59	AB	0	1
60	AC	0	1
61	AD	0	3
63	AF	0	2
64	AG	0	3
65	AH	0	2
66	AI	0	1
69	AL	0	2
71	AN	0	1
72	AO	0	1
73	AP	0	1
74	AQ	0	7
75	AR	0	2
79	AV	0	1
83	AZ	0	14
All	All	0	123

There are no bond length outliers.

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	z	164	PHE	N-CA-C	-8.78	100.04	111.02
63	AF	71	GLU	CA-C-N	8.65	132.41	120.39
63	AF	71	GLU	C-N-CA	8.65	132.41	120.39
63	AF	69	GLU	CA-C-N	7.75	136.35	121.54
63	AF	69	GLU	C-N-CA	7.75	136.35	121.54

There are no chirality outliers.

5 of 123 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	143	GLU	Peptide
7	B	25	ILE	Peptide
4	P0	39	HIS	Peptide
4	P0	41	VAL	Peptide
5	P2	117	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	68931	0	34637	848	0
2	3	2579	0	1304	32	0
3	4	3353	0	1695	32	0
4	P0	1473	0	1514	39	0
5	P2	723	0	774	31	0
6	A	1914	0	1981	47	0
7	B	3075	0	3142	57	0
8	C	2748	0	2859	57	0
9	D	2375	0	2325	34	0
10	E	1239	0	1326	24	0
11	F	1784	0	1862	38	0
12	G	1804	0	1877	26	0
13	H	1518	0	1587	28	0
14	I	1705	0	1736	30	0
15	J	1353	0	1383	29	0
16	L	1543	0	1608	41	0
17	M	1053	0	1149	25	0
18	N	1720	0	1779	51	0
19	O	1555	0	1659	30	0
20	P	1420	0	1437	17	0
21	Q	1441	0	1543	26	0
22	R	1521	0	1617	28	0
23	S	1445	0	1487	44	0
24	T	1276	0	1323	23	0
25	U	796	0	812	9	0
26	V	1003	0	1048	20	0
27	W	521	0	551	6	0
28	X	964	0	1025	19	0
29	Y	993	0	1081	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Z	1092	0	1155	20	0
31	a	1173	0	1215	31	0
32	b	462	0	491	8	0
33	c	743	0	797	13	0
34	d	883	0	918	19	0
35	e	1020	0	1090	11	0
36	f	850	0	880	24	0
37	g	880	0	941	20	0
38	h	969	0	1078	19	0
39	i	771	0	849	19	0
40	j	681	0	683	9	0
41	k	612	0	682	7	0
42	l	436	0	475	14	0
43	m	417	0	458	6	0
44	n	227	0	273	9	0
45	o	847	0	915	15	0
46	p	694	0	734	20	0
47	2	37845	0	19040	632	0
48	q	1577	0	1567	24	0
49	r	1709	0	1784	31	0
50	s	1635	0	1723	29	0
51	t	1734	0	1817	47	0
52	u	2068	0	2154	60	0
53	v	1609	0	1675	49	0
54	w	1790	0	1881	48	0
55	x	1481	0	1572	31	0
56	y	1489	0	1525	37	0
57	z	1494	0	1573	40	0
58	AA	772	0	727	20	0
59	AB	1220	0	1281	21	0
60	AC	890	0	887	14	0
61	AD	1192	0	1255	30	0
62	AE	891	0	883	15	0
63	AF	977	0	1002	42	0
64	AG	1105	0	1166	29	0
65	AH	926	0	930	23	0
66	AI	1192	0	1222	34	0
67	AJ	1112	0	1124	32	0
68	AK	855	0	917	27	0
69	AL	684	0	672	17	0
70	AM	1021	0	1060	26	0
71	AN	1121	0	1196	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	AO	1073	0	1132	26	0
73	AP	563	0	603	17	0
74	AQ	769	0	816	23	0
75	AR	610	0	632	5	0
76	AS	497	0	535	19	0
77	AT	442	0	431	18	0
78	AU	475	0	525	4	0
79	AV	2437	0	2386	77	0
80	AW	287	0	287	8	0
81	AX	1626	0	820	24	0
82	AY	164	0	84	10	0
83	AZ	6551	0	6613	194	0
84	AQ	1	0	0	0	0
84	AR	1	0	0	0	0
84	AT	1	0	0	0	0
84	AW	1	0	0	0	0
84	j	1	0	0	0	0
84	m	1	0	0	0	0
84	o	1	0	0	0	0
84	p	1	0	0	0	0
85	AZ	35	0	41	13	0
86	AZ	32	0	14	5	0
All	All	210540	0	157307	3106	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 3106 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:2:40:A:H62	47:2:467:G:N2	1.55	1.03
47:2:214:G:N2	47:2:251:A:H62	1.55	1.03
1:1:1636:U:H5'	1:1:1636:U:H6	1.24	1.02
1:1:1636:U:H5'	1:1:1636:U:C6	1.94	1.02
47:2:214:G:H21	47:2:251:A:N6	1.59	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	151 (81%)	36 (19%)	0	100	100
5	P2	92/94 (98%)	71 (77%)	21 (23%)	0	100	100
6	A	250/252 (99%)	212 (85%)	38 (15%)	0	100	100
7	B	384/386 (100%)	337 (88%)	47 (12%)	0	100	100
8	C	359/361 (99%)	307 (86%)	52 (14%)	0	100	100
9	D	294/296 (99%)	257 (87%)	35 (12%)	2 (1%)	18	55
10	E	152/175 (87%)	135 (89%)	17 (11%)	0	100	100
11	F	220/222 (99%)	184 (84%)	34 (16%)	2 (1%)	14	49
12	G	231/233 (99%)	199 (86%)	31 (13%)	1 (0%)	30	66
13	H	189/191 (99%)	159 (84%)	30 (16%)	0	100	100
14	I	207/220 (94%)	182 (88%)	24 (12%)	1 (0%)	24	62
15	J	167/169 (99%)	135 (81%)	31 (19%)	1 (1%)	21	58
16	L	191/193 (99%)	155 (81%)	34 (18%)	2 (1%)	12	47
17	M	134/136 (98%)	119 (89%)	15 (11%)	0	100	100
18	N	201/203 (99%)	171 (85%)	30 (15%)	0	100	100
19	O	195/197 (99%)	170 (87%)	22 (11%)	3 (2%)	8	38
20	P	181/183 (99%)	161 (89%)	20 (11%)	0	100	100
21	Q	183/185 (99%)	162 (88%)	21 (12%)	0	100	100
22	R	186/188 (99%)	173 (93%)	13 (7%)	0	100	100
23	S	170/172 (99%)	147 (86%)	23 (14%)	0	100	100
24	T	157/159 (99%)	137 (87%)	19 (12%)	1 (1%)	21	58
25	U	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
26	V	134/136 (98%)	114 (85%)	19 (14%)	1 (1%)	18	55
27	W	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
28	X	119/121 (98%)	103 (87%)	16 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Y	124/126 (98%)	112 (90%)	12 (10%)	0	100	100
30	Z	133/135 (98%)	111 (84%)	22 (16%)	0	100	100
31	a	146/148 (99%)	117 (80%)	28 (19%)	1 (1%)	18	55
32	b	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
33	c	95/97 (98%)	84 (88%)	11 (12%)	0	100	100
34	d	107/109 (98%)	91 (85%)	16 (15%)	0	100	100
35	e	125/127 (98%)	111 (89%)	12 (10%)	2 (2%)	7	36
36	f	104/106 (98%)	82 (79%)	20 (19%)	2 (2%)	6	32
37	g	110/112 (98%)	99 (90%)	9 (8%)	2 (2%)	6	33
38	h	117/119 (98%)	103 (88%)	14 (12%)	0	100	100
39	i	97/99 (98%)	78 (80%)	19 (20%)	0	100	100
40	j	85/87 (98%)	65 (76%)	19 (22%)	1 (1%)	10	42
41	k	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
42	l	48/50 (96%)	36 (75%)	11 (23%)	1 (2%)	5	29
43	m	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
44	n	23/25 (92%)	23 (100%)	0	0	100	100
45	o	103/105 (98%)	78 (76%)	25 (24%)	0	100	100
46	p	89/91 (98%)	78 (88%)	11 (12%)	0	100	100
48	q	204/206 (99%)	169 (83%)	33 (16%)	2 (1%)	12	47
49	r	212/214 (99%)	161 (76%)	49 (23%)	2 (1%)	14	49
50	s	215/217 (99%)	183 (85%)	32 (15%)	0	100	100
51	t	221/223 (99%)	182 (82%)	39 (18%)	0	100	100
52	u	258/260 (99%)	200 (78%)	56 (22%)	2 (1%)	16	52
53	v	204/206 (99%)	164 (80%)	40 (20%)	0	100	100
54	w	221/223 (99%)	157 (71%)	61 (28%)	3 (1%)	9	39
55	x	182/184 (99%)	150 (82%)	31 (17%)	1 (0%)	24	62
56	y	184/199 (92%)	141 (77%)	43 (23%)	0	100	100
57	z	183/185 (99%)	153 (84%)	30 (16%)	0	100	100
58	AA	94/105 (90%)	77 (82%)	16 (17%)	1 (1%)	11	45
59	AB	151/153 (99%)	125 (83%)	26 (17%)	0	100	100
60	AC	122/124 (98%)	98 (80%)	23 (19%)	1 (1%)	16	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	AD	148/150 (99%)	129 (87%)	15 (10%)	4 (3%)	4	25
62	AE	125/127 (98%)	105 (84%)	20 (16%)	0	100	100
63	AF	122/124 (98%)	85 (70%)	33 (27%)	4 (3%)	3	21
64	AG	139/141 (99%)	111 (80%)	26 (19%)	2 (1%)	9	39
65	AH	116/125 (93%)	97 (84%)	19 (16%)	0	100	100
66	AI	143/145 (99%)	122 (85%)	19 (13%)	2 (1%)	9	39
67	AJ	141/143 (99%)	124 (88%)	17 (12%)	0	100	100
68	AK	105/107 (98%)	91 (87%)	14 (13%)	0	100	100
69	AL	85/87 (98%)	64 (75%)	20 (24%)	1 (1%)	10	42
70	AM	127/129 (98%)	114 (90%)	12 (9%)	1 (1%)	16	52
71	AN	142/144 (99%)	114 (80%)	26 (18%)	2 (1%)	9	39
72	AO	132/134 (98%)	112 (85%)	20 (15%)	0	100	100
73	AP	68/70 (97%)	46 (68%)	21 (31%)	1 (2%)	8	38
74	AQ	95/97 (98%)	65 (68%)	30 (32%)	0	100	100
75	AR	79/81 (98%)	57 (72%)	21 (27%)	1 (1%)	9	41
76	AS	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
77	AT	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
78	AU	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
79	AV	316/318 (99%)	254 (80%)	61 (19%)	1 (0%)	36	71
80	AW	35/37 (95%)	26 (74%)	9 (26%)	0	100	100
83	AZ	837/840 (100%)	676 (81%)	157 (19%)	4 (0%)	24	62
All	All	12005/12221 (98%)	10010 (83%)	1937 (16%)	58 (0%)	26	62

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	O	111	PRO
48	q	113	ARG
49	r	207	LEU
54	w	10	ASN
54	w	68	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	P0	160/160 (100%)	160 (100%)	0	100	100
5	P2	81/81 (100%)	80 (99%)	1 (1%)	63	73
6	A	193/194 (100%)	192 (100%)	1 (0%)	81	81
7	B	321/322 (100%)	316 (98%)	5 (2%)	55	69
8	C	288/288 (100%)	285 (99%)	3 (1%)	68	76
9	D	244/244 (100%)	243 (100%)	1 (0%)	84	82
10	E	134/152 (88%)	134 (100%)	0	100	100
11	F	186/186 (100%)	183 (98%)	3 (2%)	55	69
12	G	187/191 (98%)	186 (100%)	1 (0%)	81	81
13	H	171/171 (100%)	170 (99%)	1 (1%)	78	80
14	I	177/186 (95%)	175 (99%)	2 (1%)	65	74
15	J	147/147 (100%)	147 (100%)	0	100	100
16	L	154/154 (100%)	154 (100%)	0	100	100
17	M	107/107 (100%)	104 (97%)	3 (3%)	38	59
18	N	175/175 (100%)	170 (97%)	5 (3%)	37	58
19	O	160/160 (100%)	154 (96%)	6 (4%)	29	50
20	P	140/145 (97%)	137 (98%)	3 (2%)	47	65
21	Q	150/150 (100%)	149 (99%)	1 (1%)	76	79
22	R	153/153 (100%)	150 (98%)	3 (2%)	48	66
23	S	156/156 (100%)	155 (99%)	1 (1%)	78	80
24	T	136/136 (100%)	133 (98%)	3 (2%)	45	64
25	U	87/87 (100%)	87 (100%)	0	100	100
26	V	104/104 (100%)	103 (99%)	1 (1%)	68	76
27	W	55/55 (100%)	52 (94%)	3 (6%)	19	42
28	X	104/105 (99%)	103 (99%)	1 (1%)	68	76
29	Y	109/109 (100%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	Z	115/115 (100%)	115 (100%)	0	100	100
31	a	118/118 (100%)	118 (100%)	0	100	100
32	b	46/46 (100%)	45 (98%)	1 (2%)	45	64
33	c	81/81 (100%)	78 (96%)	3 (4%)	30	51
34	d	94/96 (98%)	94 (100%)	0	100	100
35	e	109/109 (100%)	108 (99%)	1 (1%)	70	76
36	f	90/90 (100%)	89 (99%)	1 (1%)	65	74
37	g	95/95 (100%)	95 (100%)	0	100	100
38	h	104/104 (100%)	102 (98%)	2 (2%)	50	66
39	i	81/81 (100%)	81 (100%)	0	100	100
40	j	70/70 (100%)	70 (100%)	0	100	100
41	k	68/68 (100%)	67 (98%)	1 (2%)	57	70
42	l	45/45 (100%)	44 (98%)	1 (2%)	45	64
43	m	47/47 (100%)	46 (98%)	1 (2%)	47	65
44	n	22/23 (96%)	22 (100%)	0	100	100
45	o	90/90 (100%)	90 (100%)	0	100	100
46	p	71/71 (100%)	70 (99%)	1 (1%)	59	71
48	q	164/173 (95%)	163 (99%)	1 (1%)	78	80
49	r	191/191 (100%)	188 (98%)	3 (2%)	55	69
50	s	176/176 (100%)	174 (99%)	2 (1%)	65	74
51	t	182/182 (100%)	181 (100%)	1 (0%)	81	81
52	u	221/221 (100%)	219 (99%)	2 (1%)	70	76
53	v	173/173 (100%)	173 (100%)	0	100	100
54	w	189/191 (99%)	188 (100%)	1 (0%)	81	81
55	x	165/165 (100%)	164 (99%)	1 (1%)	78	80
56	y	150/160 (94%)	148 (99%)	2 (1%)	61	72
57	z	158/158 (100%)	157 (99%)	1 (1%)	78	80
58	AA	77/98 (79%)	76 (99%)	1 (1%)	61	72
59	AB	133/134 (99%)	131 (98%)	2 (2%)	57	70
60	AC	88/100 (88%)	85 (97%)	3 (3%)	32	54
61	AD	127/127 (100%)	124 (98%)	3 (2%)	43	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	AE	81/96 (84%)	79 (98%)	2 (2%)	42	62
63	AF	101/104 (97%)	100 (99%)	1 (1%)	68	76
64	AG	117/117 (100%)	116 (99%)	1 (1%)	70	76
65	AH	94/113 (83%)	94 (100%)	0	100	100
66	AI	128/128 (100%)	127 (99%)	1 (1%)	73	77
67	AJ	115/115 (100%)	115 (100%)	0	100	100
68	AK	100/100 (100%)	99 (99%)	1 (1%)	68	76
69	AL	74/74 (100%)	74 (100%)	0	100	100
70	AM	110/110 (100%)	107 (97%)	3 (3%)	39	59
71	AN	119/119 (100%)	114 (96%)	5 (4%)	26	48
72	AO	112/112 (100%)	111 (99%)	1 (1%)	70	76
73	AP	61/61 (100%)	60 (98%)	1 (2%)	55	69
74	AQ	83/83 (100%)	81 (98%)	2 (2%)	43	63
75	AR	70/70 (100%)	69 (99%)	1 (1%)	59	71
76	AS	56/56 (100%)	56 (100%)	0	100	100
77	AT	47/47 (100%)	47 (100%)	0	100	100
78	AU	51/51 (100%)	51 (100%)	0	100	100
79	AV	259/261 (99%)	258 (100%)	1 (0%)	84	82
80	AW	31/31 (100%)	30 (97%)	1 (3%)	34	55
83	AZ	711/712 (100%)	702 (99%)	9 (1%)	61	72
All	All	10139/10276 (99%)	10026 (99%)	113 (1%)	63	74

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	l	42	ARG
83	AZ	593	ILE
56	y	72	ILE
83	AZ	529	ILE
74	AQ	36	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
57	z	139	GLN
72	AO	113	ASN
59	AB	8	GLN
66	AI	44	ASN
79	AV	184	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3220/3396 (94%)	1049 (32%)	18 (0%)
2	3	120/121 (99%)	31 (25%)	0
3	4	157/158 (99%)	50 (31%)	2 (1%)
47	2	1774/1797 (98%)	665 (37%)	23 (1%)
81	AX	75/76 (98%)	33 (44%)	1 (1%)
82	AY	7/8 (87%)	5 (71%)	0
All	All	5353/5556 (96%)	1833 (34%)	44 (0%)

5 of 1833 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	11	A
1	1	15	C
1	1	16	A
1	1	18	G
1	1	19	U

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	2	865	A
47	2	1338	C
47	2	941	A
47	2	1273	G
47	2	1491	U

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

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
83	DDE	AZ	699	83	18,20,21	2.05	5 (27%)	17,28,30	1.43	3 (17%)

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
83	DDE	AZ	699	83	-	6/20/21/23	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	AZ	699	DDE	CBI-NAD	6.09	1.47	1.32
83	AZ	699	DDE	CAT-CE1	3.06	1.54	1.49
83	AZ	699	DDE	CG-ND1	-3.04	1.32	1.38
83	AZ	699	DDE	OAG-CBI	-2.22	1.19	1.23
83	AZ	699	DDE	CBW-NCB	-2.15	1.49	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	AZ	699	DDE	OAG-CBI-NAD	-2.78	118.14	123.04
83	AZ	699	DDE	CAC-NCB-CAB	2.58	117.80	107.99
83	AZ	699	DDE	CAU-CBW-CBI	-2.31	106.70	111.22

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	AZ	699	DDE	N-CA-CB-CG
83	AZ	699	DDE	C-CA-CB-CG
83	AZ	699	DDE	CAT-CAU-CBW-CBI
83	AZ	699	DDE	CAT-CAU-CBW-NCB
83	AZ	699	DDE	NAD-CBI-CBW-NCB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	AZ	699	DDE	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	$\# Z > 2$
85	SO1	AZ	901	-	34,39,39	0.19	0	38,64,64	0.90	2 (5%)
86	GCP	AZ	902	-	32,34,34	0.84	3 (9%)	49,54,54	0.96	5 (10%)

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
85	SO1	AZ	901	-	-	8/21/104/104	0/7/5/5
86	GCP	AZ	902	-	-	5/19/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	AZ	902	GCP	PB-O2B	-2.63	1.50	1.56
86	AZ	902	GCP	PG-O1G	2.25	1.54	1.50
86	AZ	902	GCP	PG-O3G	-2.22	1.50	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	AZ	901	SO1	C18-C9-C16	-4.39	97.73	103.72
86	AZ	902	GCP	O2B-PB-C3B	3.85	122.68	106.73
86	AZ	902	GCP	O3G-PG-C3B	2.58	112.66	106.40
86	AZ	902	GCP	O1G-PG-C3B	-2.44	106.06	111.37
85	AZ	901	SO1	C7-C2-C6	2.31	116.47	112.05

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

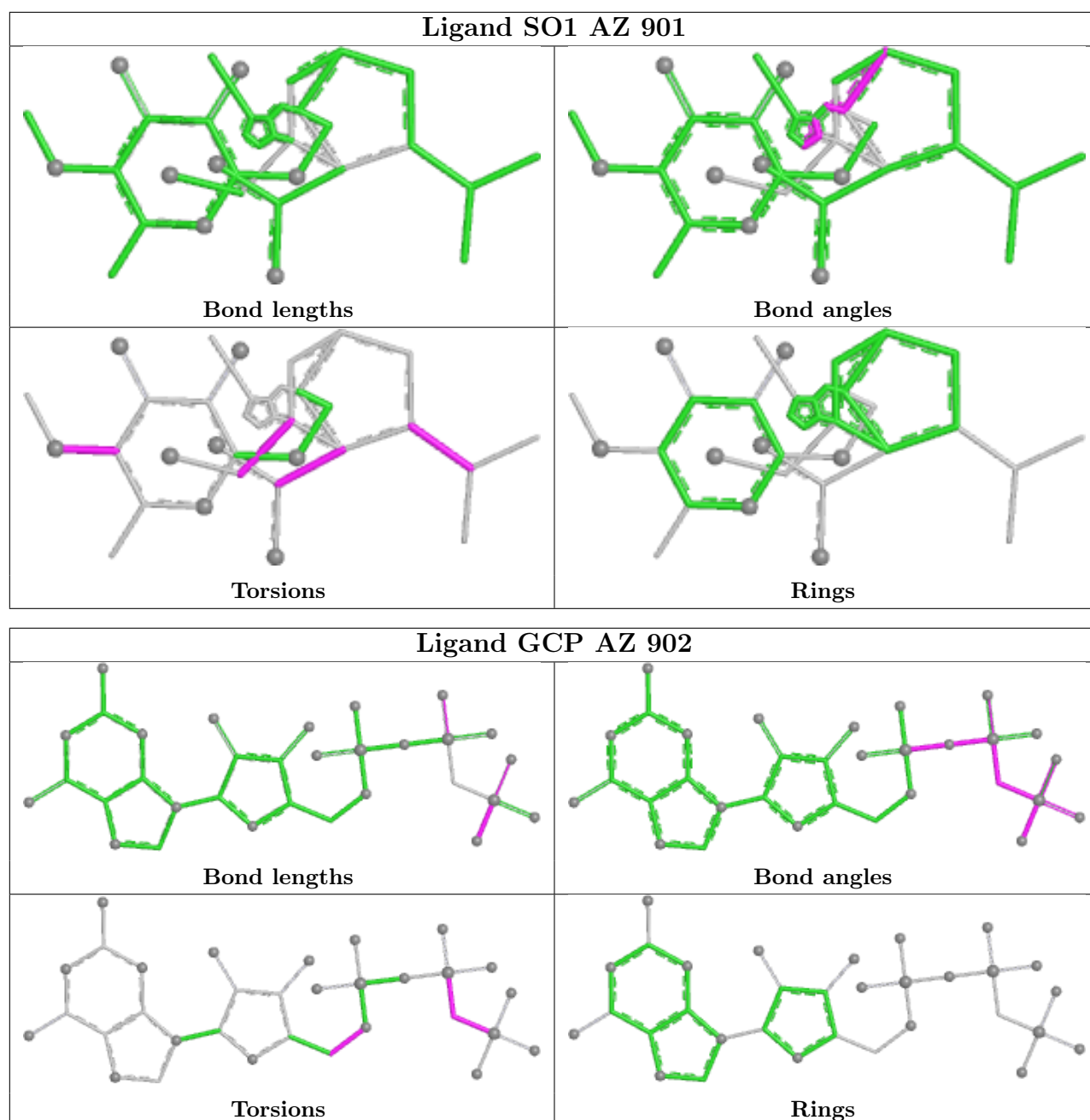
Mol	Chain	Res	Type	Atoms
86	AZ	902	GCP	PG-C3B-PB-O1B
86	AZ	902	GCP	PG-C3B-PB-O3A
85	AZ	901	SO1	C56-C55-O64-C65
85	AZ	901	SO1	C2-C1-C5-O14
85	AZ	901	SO1	C2-C1-C5-O15

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	AZ	901	SO1	13	0
86	AZ	902	GCP	5	0

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.

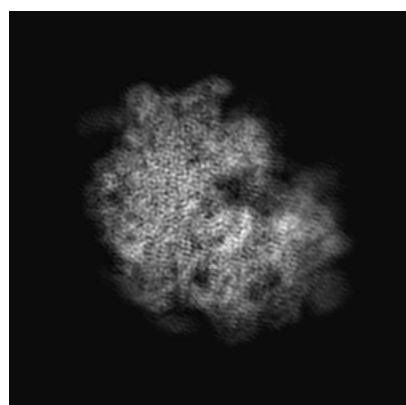
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0047. These allow visual inspection of the internal detail of the map and identification of artifacts.

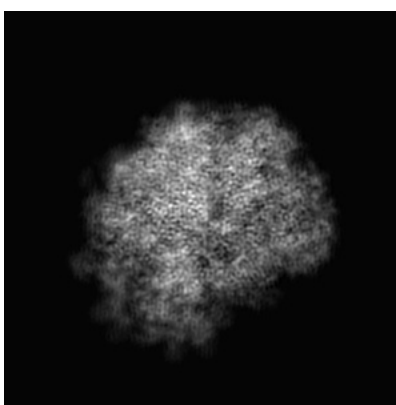
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

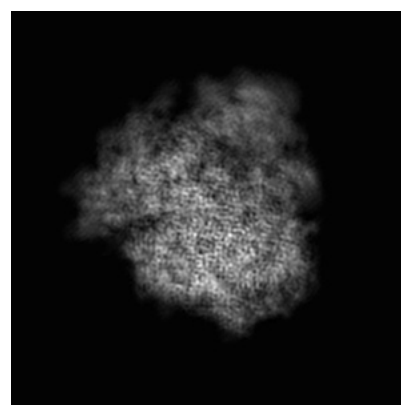
6.1.1 Primary map



X



Y

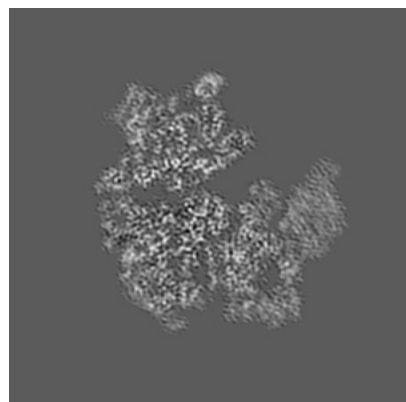


Z

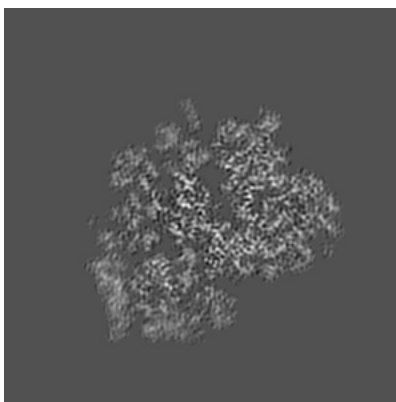
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

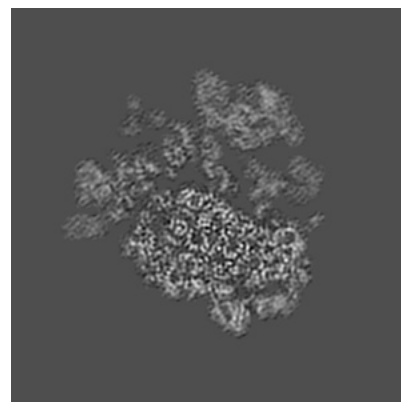
6.2.1 Primary map



X Index: 180



Y Index: 180

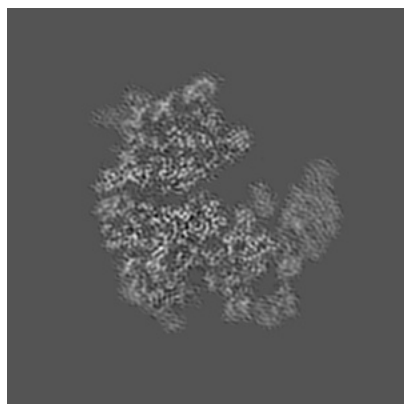


Z Index: 180

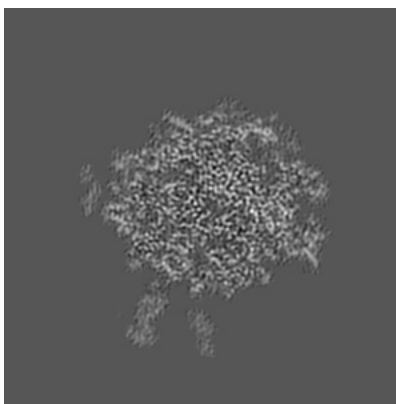
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

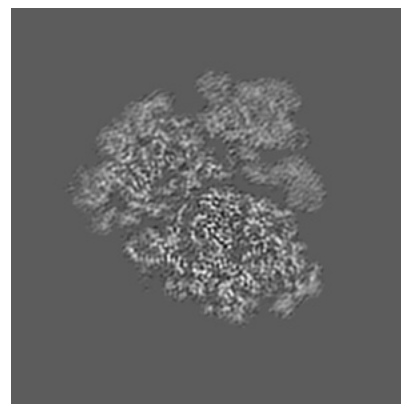
6.3.1 Primary map



X Index: 183



Y Index: 156

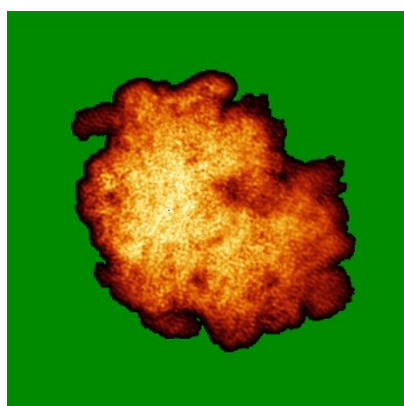


Z Index: 166

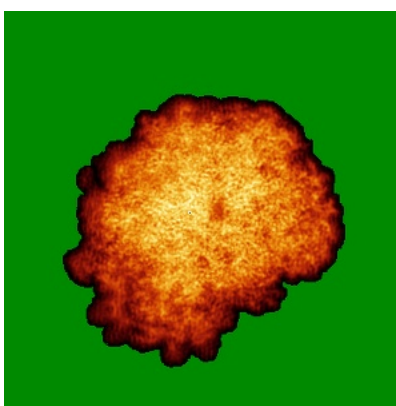
The images above show the largest variance slices of the map in three orthogonal directions.

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

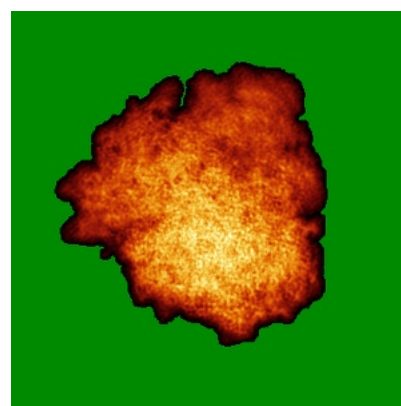
6.4.1 Primary map



X



Y



Z

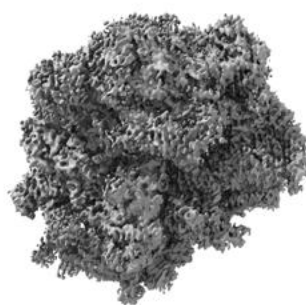
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

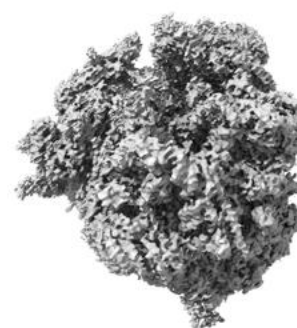
6.5.1 Primary map



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.

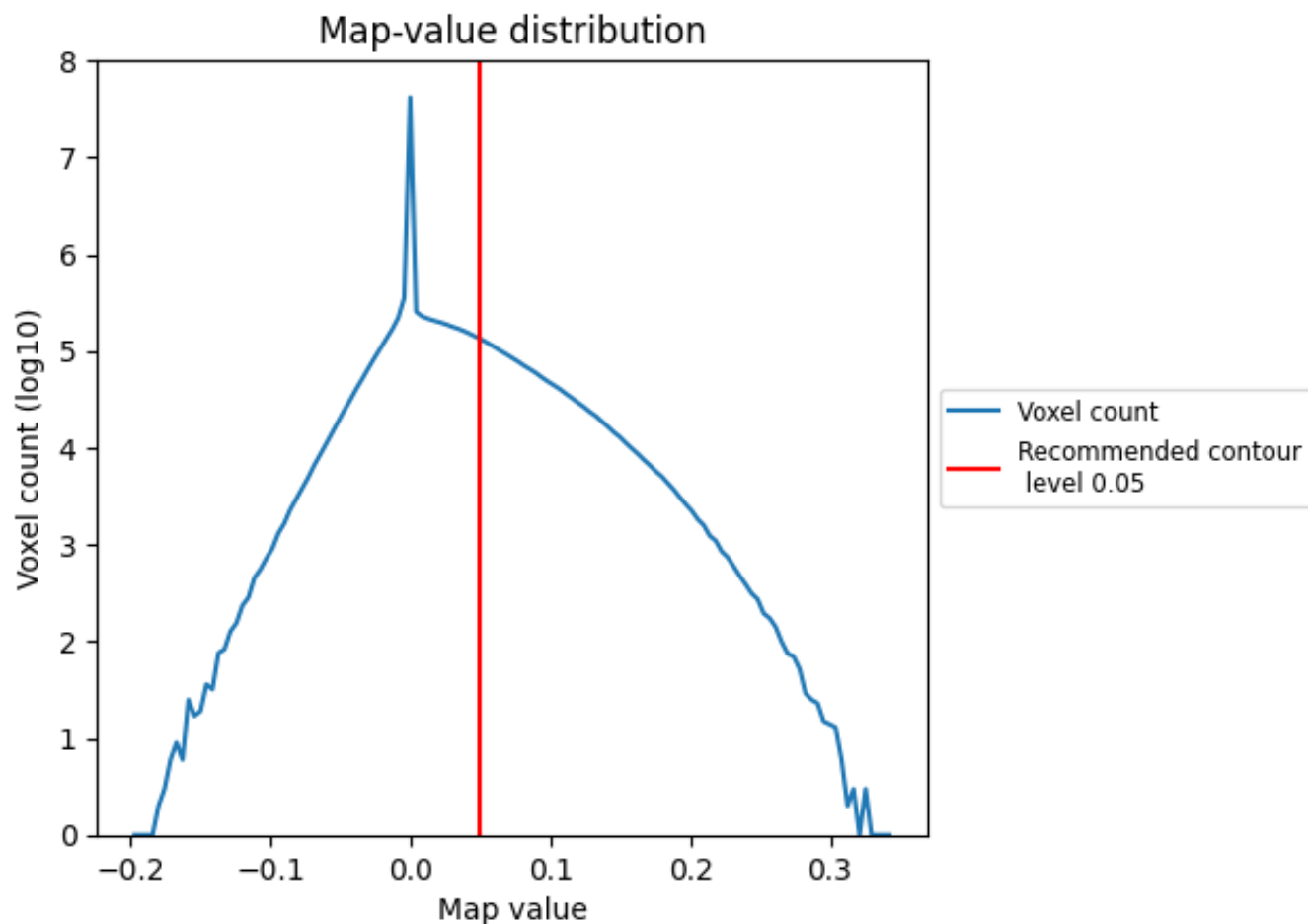
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

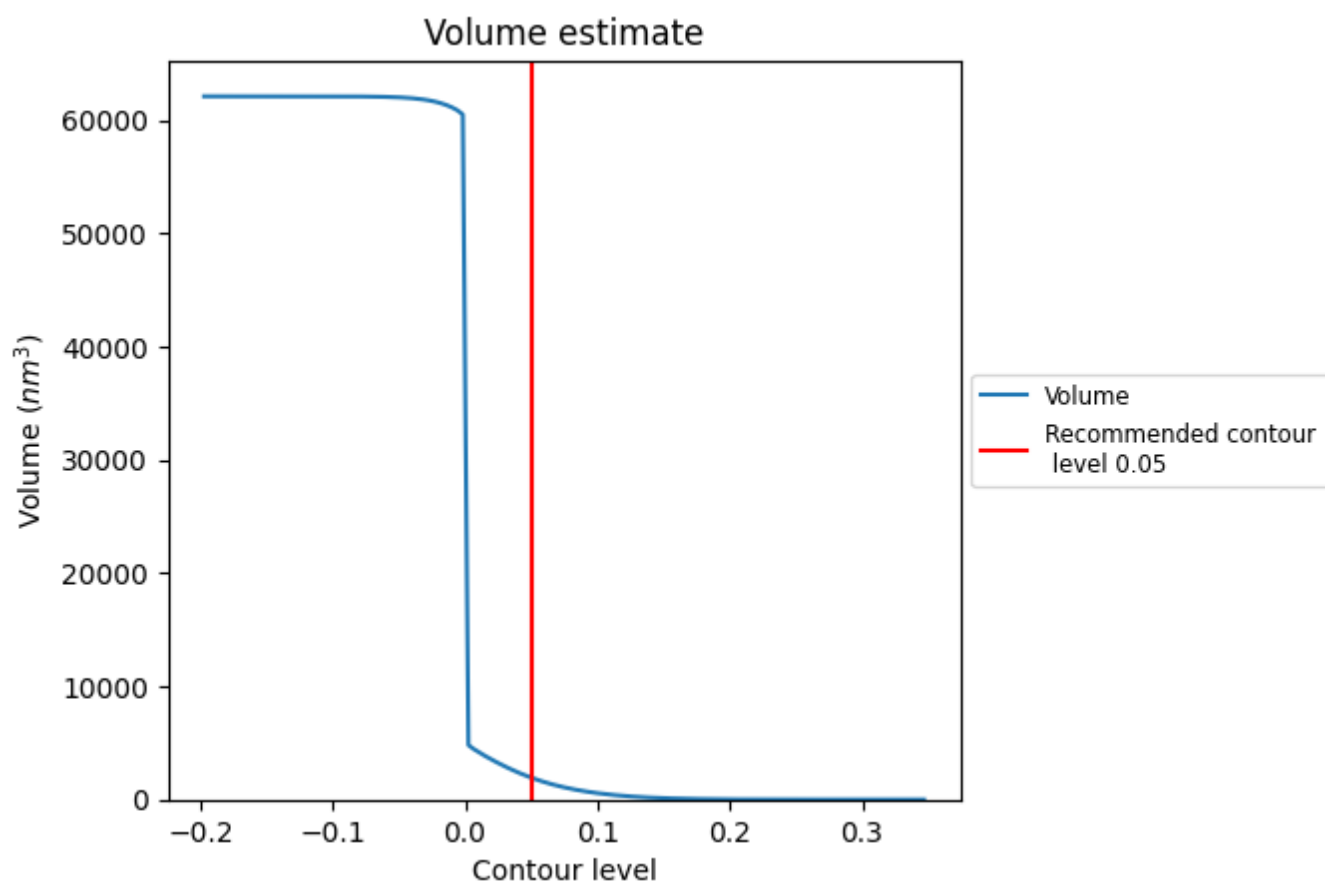
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

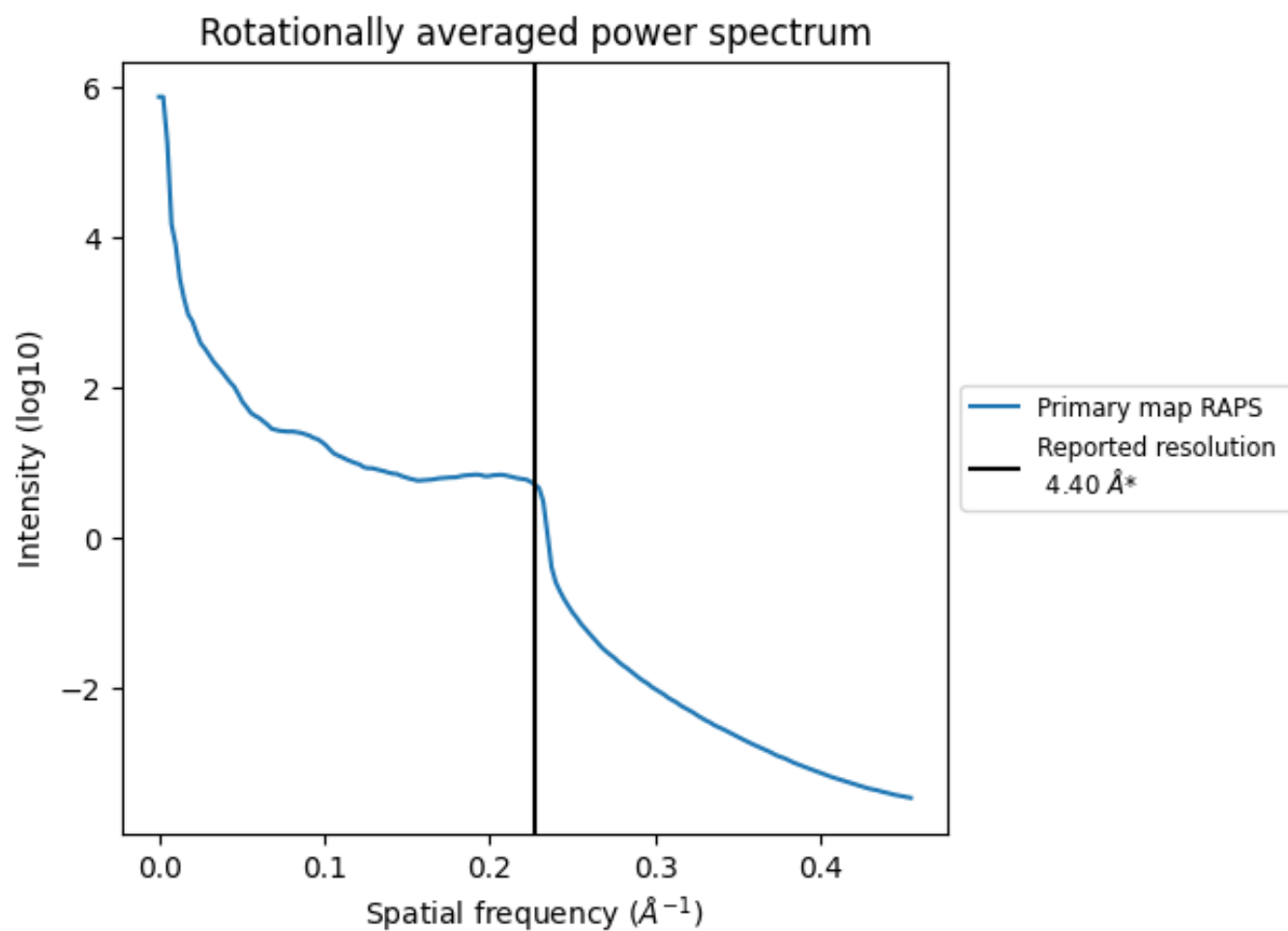
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1936 nm³; this corresponds to an approximate mass of 1749 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

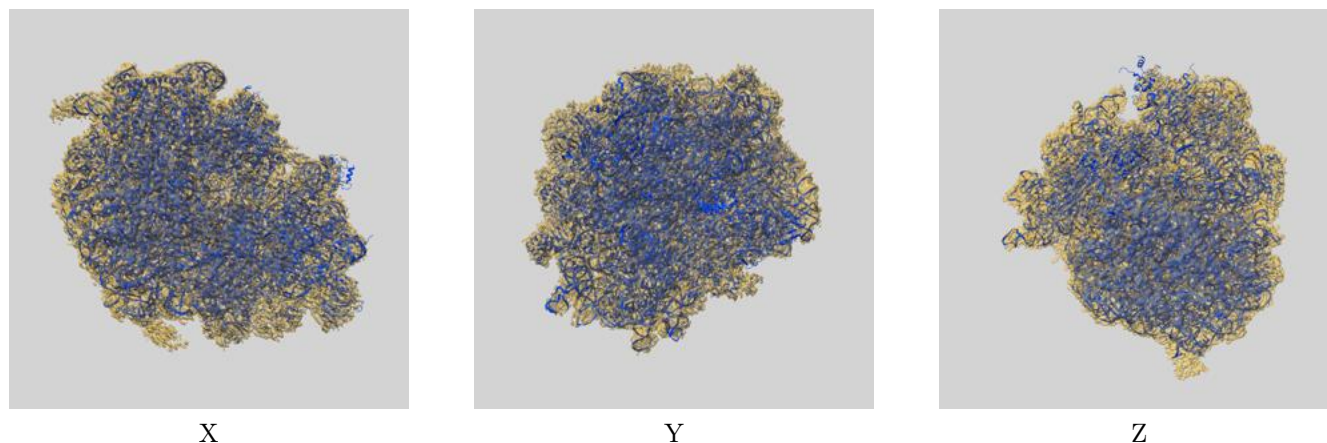
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

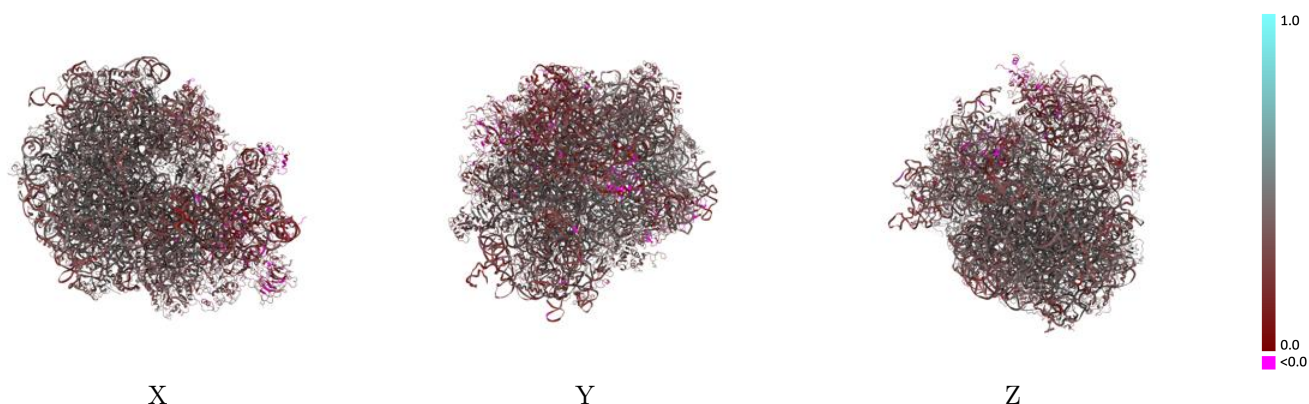
This section contains information regarding the fit between EMDB map EMD-0047 and PDB model 6GQ1. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



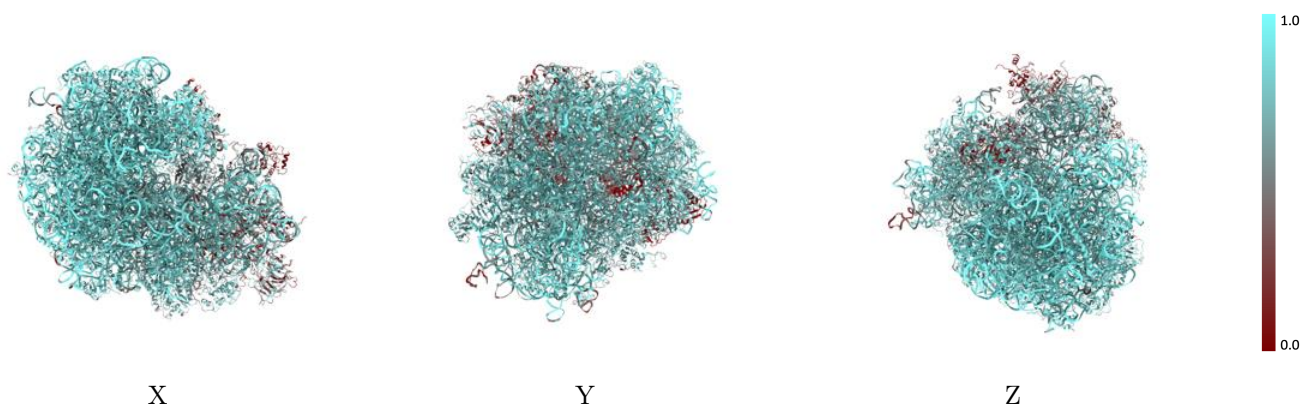
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



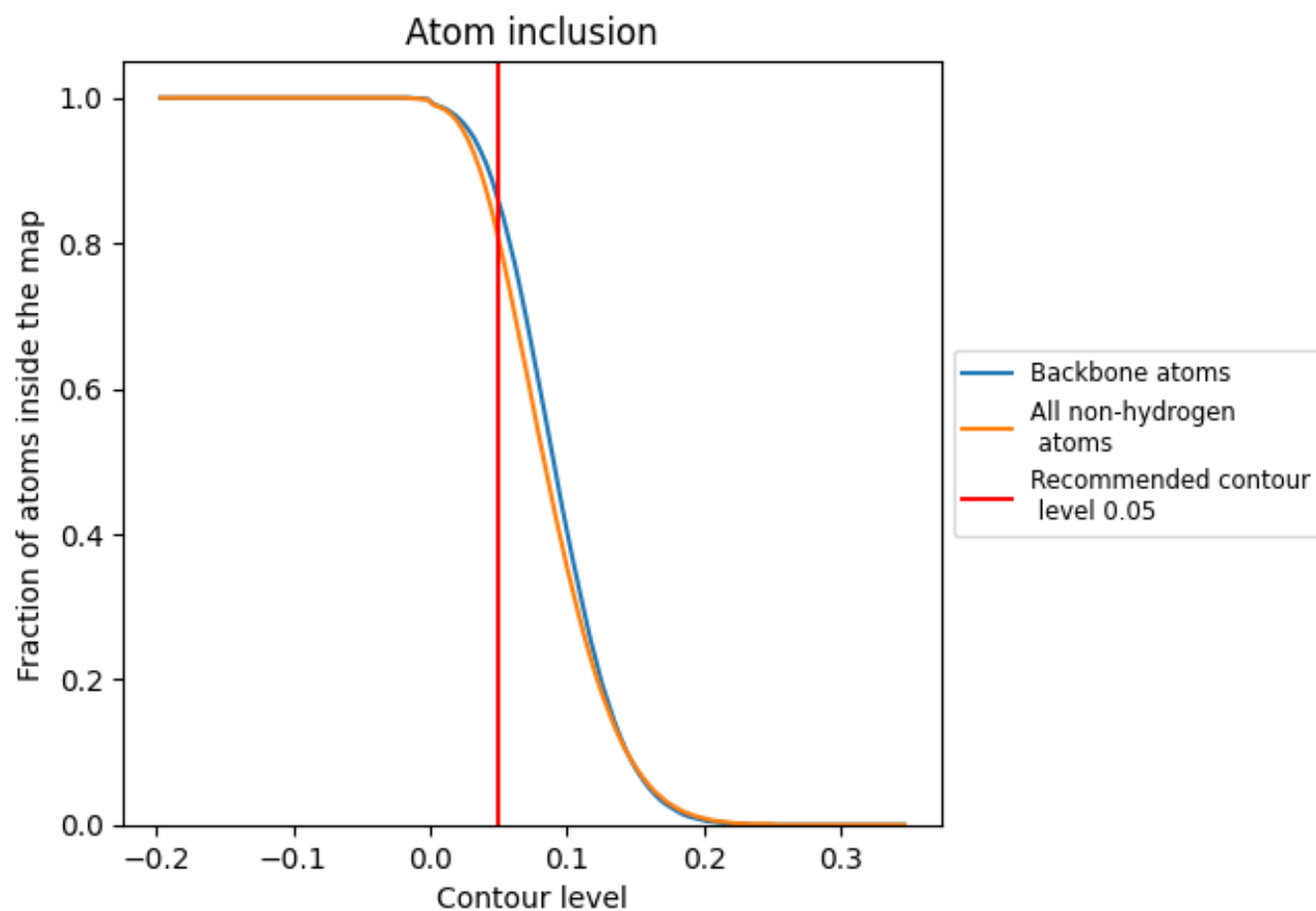
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 81% 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	 0.8060	 0.3570
1	 0.9110	 0.3810
2	 0.8440	 0.3240
3	 0.9360	 0.3530
4	 0.9340	 0.3930
A	 0.7740	 0.4380
AA	 0.6570	 0.2610
AB	 0.6780	 0.3880
AC	 0.1070	 0.1250
AD	 0.7700	 0.3720
AE	 0.7990	 0.3800
AF	 0.6000	 0.2770
AG	 0.5530	 0.2570
AH	 0.5300	 0.2530
AI	 0.5570	 0.2540
AJ	 0.5780	 0.2420
AK	 0.3580	 0.2170
AL	 0.7110	 0.3380
AM	 0.7650	 0.3910
AN	 0.6980	 0.3920
AO	 0.7460	 0.3370
AP	 0.3710	 0.1990
AQ	 0.7460	 0.3600
AR	 0.7480	 0.3620
AS	 0.4110	 0.2240
AT	 0.7030	 0.2720
AU	 0.6250	 0.3360
AV	 0.4710	 0.2100
AW	 0.3210	 0.1830
AX	 0.6670	 0.2570
AY	 0.2990	 0.3080
AZ	 0.6610	 0.3520
B	 0.8060	 0.4140
C	 0.8280	 0.4080
D	 0.7760	 0.3260



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Chain	Atom inclusion	Q-score
E	 0.8090	 0.3660
F	 0.8180	 0.3970
G	 0.7980	 0.3630
H	 0.7720	 0.3940
I	 0.7780	 0.4000
J	 0.7450	 0.3430
L	 0.8120	 0.3950
M	 0.8110	 0.3730
N	 0.8330	 0.4160
O	 0.8140	 0.3990
P	 0.8200	 0.4120
P0	 0.1920	 0.1770
P2	 0.1750	 0.1800
Q	 0.8150	 0.4190
R	 0.7980	 0.3970
S	 0.8030	 0.4050
T	 0.7980	 0.4070
U	 0.7560	 0.3640
V	 0.7370	 0.4370
W	 0.7860	 0.4210
X	 0.7830	 0.4060
Y	 0.8320	 0.4070
Z	 0.8170	 0.3910
a	 0.8350	 0.4160
b	 0.7630	 0.4150
c	 0.7970	 0.3830
d	 0.7530	 0.4080
e	 0.8160	 0.4230
f	 0.8030	 0.4150
g	 0.7860	 0.4240
h	 0.7840	 0.3870
i	 0.7950	 0.3630
j	 0.8550	 0.4370
k	 0.7460	 0.3910
l	 0.7900	 0.4110
m	 0.7770	 0.4180
n	 0.6300	 0.4360
o	 0.7720	 0.4100
p	 0.7630	 0.4320
q	 0.7250	 0.3320
r	 0.7530	 0.3650
s	 0.7290	 0.3740

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Chain	Atom inclusion	Q-score
t	 0.5030	 0.2530
u	 0.7380	 0.3500
v	 0.4740	 0.2470
w	 0.7180	 0.3120
x	 0.7030	 0.3170
y	 0.7330	 0.3570
z	 0.7560	 0.3450