



## wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 07:57 AM UTC

PDB ID : 7B7D / pdb\_00007b7d  
EMDB ID : EMD-12081  
Title : Yeast 80S ribosome bound to eEF3 and A/A- and P/P-tRNAs  
Authors : Ranjan, N.; Pochopien, A.A.; Wu, C.C.; Beckert, B.; Blanchet, S.; Green, R.;  
Rodnina, M.V.; Wilson, D.N.  
Deposited on : 2020-12-10  
Resolution : 3.30 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](mailto: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>.

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

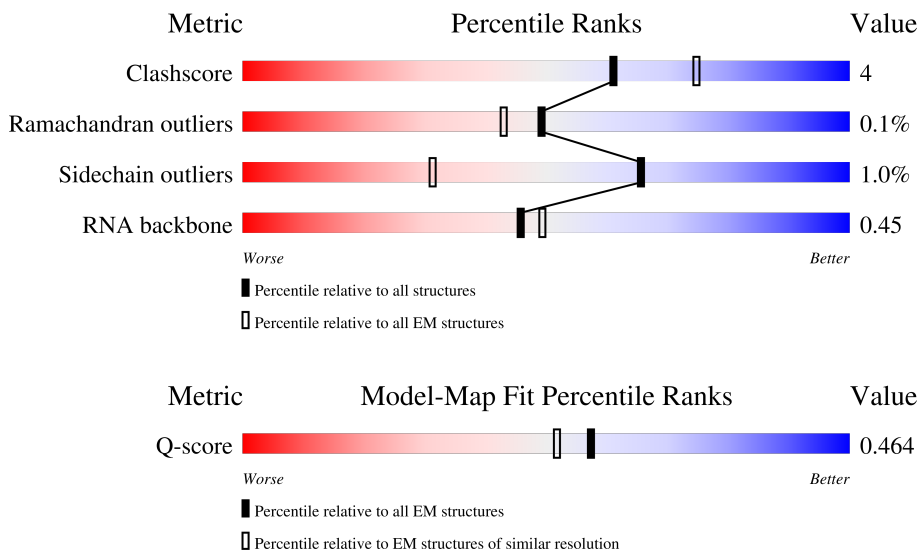
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.30 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	15087 ( 2.80 - 3.80 )

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  $\geq 3$ , 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	2	1771	
2	1	7	
3	P	206	

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Mol	Chain	Length	Quality of chain
4	Q	232	22% 80% 17%
5	E	117	29% 82% 17%
6	R	216	11% 84% 16%
7	A	222	25% 84% 16%
8	S	258	39% 83% 16%
9	B	206	17% 83% 17%
10	T	228	58% 81% 18%
11	U	184	46% 86% 13%
12	V	198	15% 75% 19% 6%
13	W	184	44% 88% 11%
14	C	92	29% 79% 20%
15	X	142	24% 83% 17%
16	D	121	88% 74% 24%
17	Y	150	15% 84% 15%
18	Z	127	7% 85% 13%
19	F	141	9% 77% 22%
20	G	125	25% 78% 18%
21	H	145	10% 79% 21%
22	I	143	9% 78% 22%
23	J	100	30% 79% 21%
24	a	87	17% 84% 16%
25	b	129	9% 87% 13%
26	c	144	22% 84% 16%
27	d	134	51% 77% 22%
28	K	82	32% 84% 15%

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Mol	Chain	Length	Quality of chain
29	e	97	9% 87% 13%
30	f	81	30% 83% 17%
31	M	53	6% 87% 13%
32	g	60	47% 83% 15%
33	N	73	70% 82% 16%
34	O	312	38% 79% 20%
35	L	63	22% 73% 25%
36	LA	3223	7% 67% 29% 5%
37	LB	121	70% 28%
38	LC	158	66% 32%
39	LD	251	81% 19%
40	LE	386	87% 13%
41	LF	361	83% 16%
42	LG	294	7% 83% 17%
43	LH	175	17% 79% 16% 5%
44	LI	222	86% 13%
45	LJ	233	12% 85% 15%
46	LK	191	6% 81% 19%
47	LL	218	13% 80% 20%
48	LM	169	5% 86% 14%
49	LN	193	9% 89% 11%
50	LO	136	79% 21%
51	LP	203	84% 16%
52	LQ	197	89% 11%
53	LR	183	8% 86% 14%

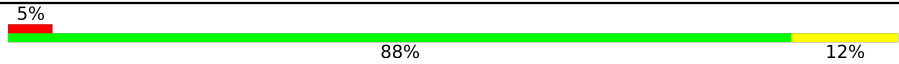

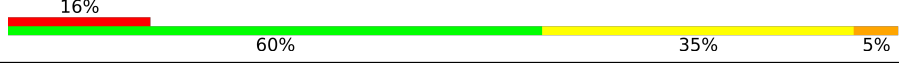
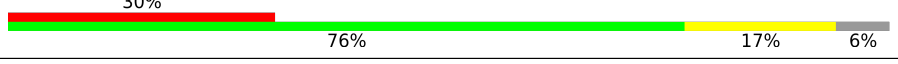
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Mol	Chain	Length	Quality of chain
54	Lm	185	88% 12% 14%
55	Ln	188	88% 12% 14%
56	Lo	171	84% 16% 6%
57	Lp	159	89% 11% 6%
58	Lq	100	92% 8% 16%
59	Lr	136	86% 14% 10%
60	LS	126	94% 6% 48%
61	LT	121	89% 11% 6%
62	LU	125	89% 11% 6%
63	LV	135	88% 11% 6%
64	LW	148	82% 18% 6%
65	LX	58	86% 14% 9%
66	LY	96	89% 11% 8%
67	LZ	109	83% 17% 12%
68	La	127	86% 14% 6%
69	Lb	106	87% 13% 6%
70	Lc	112	90% 8% 11%
71	Ld	119	87% 13% 6%
72	Le	99	92% 8% 7%
73	Lf	81	74% 26% 6%
74	Lg	77	88% 12% 12%
75	Lh	50	76% 24% 6%
76	Li	52	83% 17% 8%
77	Lj	25	84% 12% 12%
78	Lk	103	87% 13% 5%

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Mol	Chain	Length	Quality of chain
79	L1	91	
80	Sm	75	
80	Sn	75	
81	EF	1044	

## 2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 211144 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1771	37739	16872	6683	12413	1771	0	0

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	7	149	67	26	49	7	0	0

- Molecule 3 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	P	206	1603	1030	284	287	2	0	0

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	Q	226	1798	1139	330	325	4	0	0

- Molecule 5 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	117	916	583	171	155	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	R	216	1626	1042	287	295	2	0	0

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	A	222	1729	1098	312	313	6	0	0

- Molecule 8 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	S	258	2056	1308	387	358	3	0	0

- Molecule 9 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	206	1605	1005	299	298	3	0	0

- Molecule 10 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	T	228	1815	1138	351	323	3	0	0

- Molecule 11 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	U	184	1473	946	263	264	0	0

- Molecule 12 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	V	187	1476	916	295	263	2	0	0

- Molecule 13 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	W	184	1479	935	285	258	1	0	0

- Molecule 14 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	92	Total	C	N	O	S	0	0
			752	487	122	141	2		

- Molecule 15 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	142	Total	C	N	O	S	0	0
			1142	733	217	189	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	121	Total	C	N	O	S	0	0
			875	551	153	169	2		

- Molecule 17 is a protein called 40S ribosomal protein S13.

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

- Molecule 18 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	127	Total	C	N	O	S	0	0
			923	568	185	167	3		

- Molecule 19 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 20 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 21 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	145	Total	C	N	O	S	0	0
			1188	741	237	208	2		

- Molecule 22 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 23 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	100	Total	C	N	O	S	0	0
			797	506	144	146	1		

- Molecule 24 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	87	Total	C	N	O	S	0	0
			673	415	125	131	2		

- Molecule 25 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 26 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 27 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 28 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	K	82	651	416	123	112	0	0

- Molecule 29 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	e	97	765	473	160	127	5	0	0

- Molecule 30 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

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

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	60	472	298	97	76	1	0	0

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	N	73	556	352	105	95	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	97	ALA	LYS	conflict	UNP P05759

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	O	312	Total	C	N	O	S	0	0
			2383	1514	409	452	8		

- Molecule 35 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	63	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 36 is a RNA chain called 25S rRNA.

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

- Molecule 37 is a RNA chain called 5S rRNA.

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

- Molecule 38 is a RNA chain called 5.8S rRNA.

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

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LD	251	Total	C	N	O	S	0	0
			1899	1182	385	331	1		

- Molecule 40 is a protein called 60S ribosomal protein L3.

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

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LG	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

- Molecule 43 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	LH	167	Total	C	N	O	0	0
			1307	843	234	230		

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

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

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LK	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LL	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	LM	169	1346	843	252	247	4	0	0

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	LR	183	1416	879	284	253		0	0

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	Ln	188	1515	932	323	260	0	0

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	Lo	171	1437	925	266	243	3	0	0

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	Lp	159	1272	802	245	221	4	0	0

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

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

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	LS	126	836	525	165	145	1	0	0

- Molecule 61 is a protein called 60S ribosomal protein L25.

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

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
62	LU	125	984	620	191	173	0	0

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
63	LV	135	1080	701	199	180	0	0

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	LW	148	1169	747	231	188	3	0	0

- Molecule 65 is a protein called 60S ribosomal protein L29.

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

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	LY	96	737	476	123	137	1	0	0

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	LZ	109	876	556	167	152	1	0	0

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	La	127	1013	642	205	165	1	0	0

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	Le	99	766	478	154	132	2	0	0

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	Lf	81	645	393	141	106	5	0	0

- Molecule 74 is a protein called 60S ribosomal protein L38.

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

- Molecule 75 is a protein called 60S ribosomal protein L39.

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

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Li	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

- Molecule 77 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Lj	25	Total	C	N	O	S	0	0
			229	139	62	27	1		

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Lk	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 80 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sn	75	Total	C	N	O	P	0	0
			1606	716	297	518	75		
80	Sm	75	Total	C	N	O	P	0	0
			1605	716	297	517	75		

- Molecule 81 is a protein called Elongation factor 3A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
81	EF	977	Total	C	N	O	S	Se	0	0
			7479	4729	1294	1419	32	5		

There are 5 discrepancies between the modelled and reference sequences:

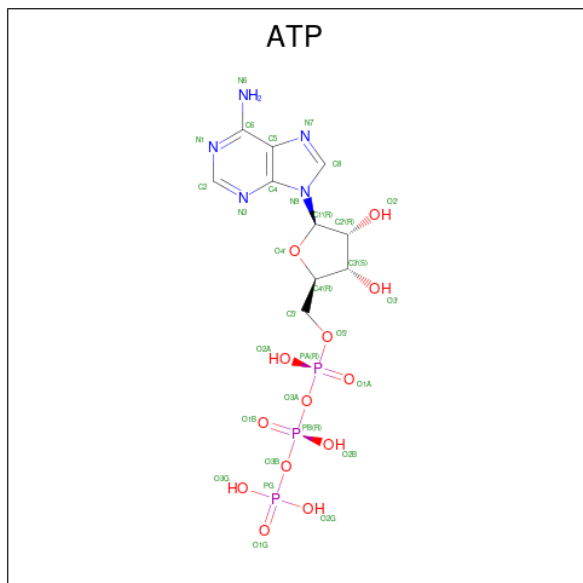
Chain	Residue	Modelled	Actual	Comment	Reference
EF	24	ASP	ASN	conflict	UNP P16521
EF	152	PHE	ILE	conflict	UNP P16521
EF	331	LEU	VAL	conflict	UNP P16521
EF	541	GLY	SER	conflict	UNP P16521

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
EF	542	SER	ALA	conflict	UNP P16521

- Molecule 82 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

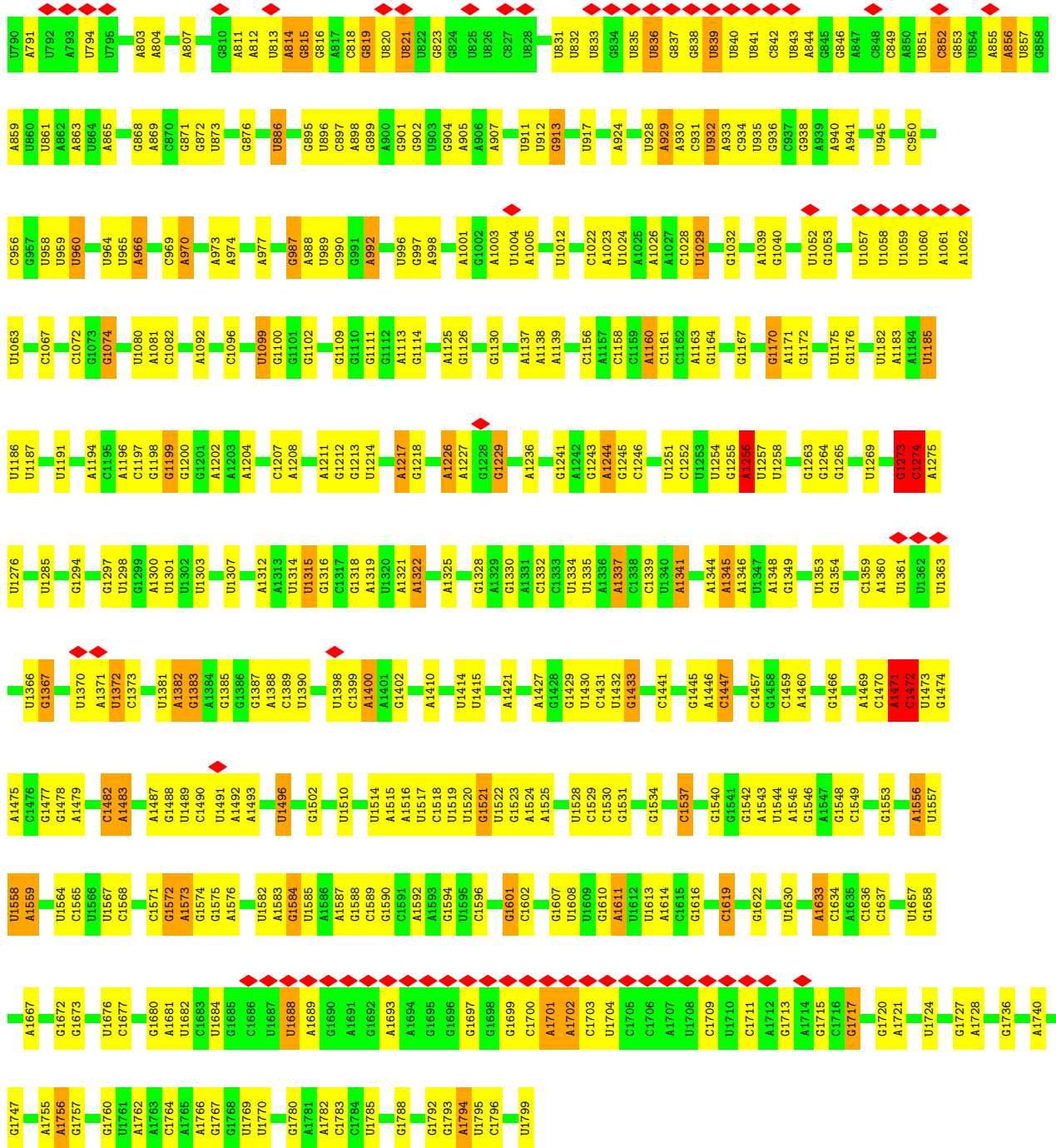


### 3 Residue-property plots [i](#)

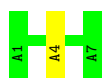
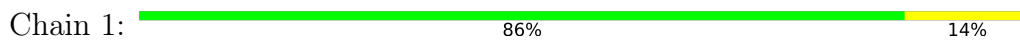
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 18S rRNA

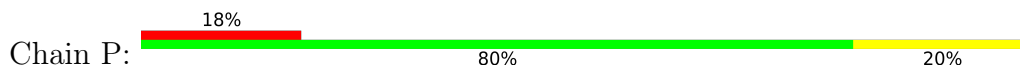


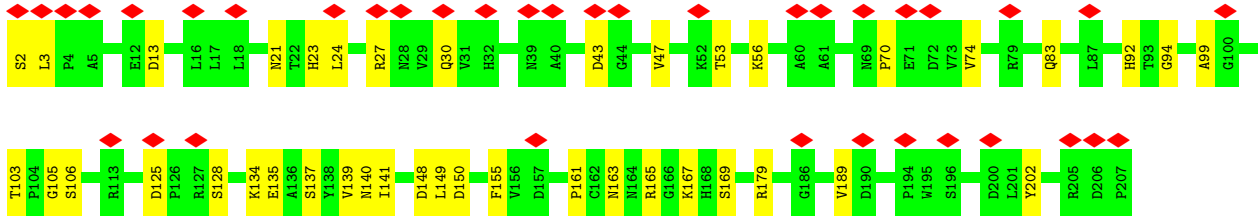


• Molecule 2: mRNA

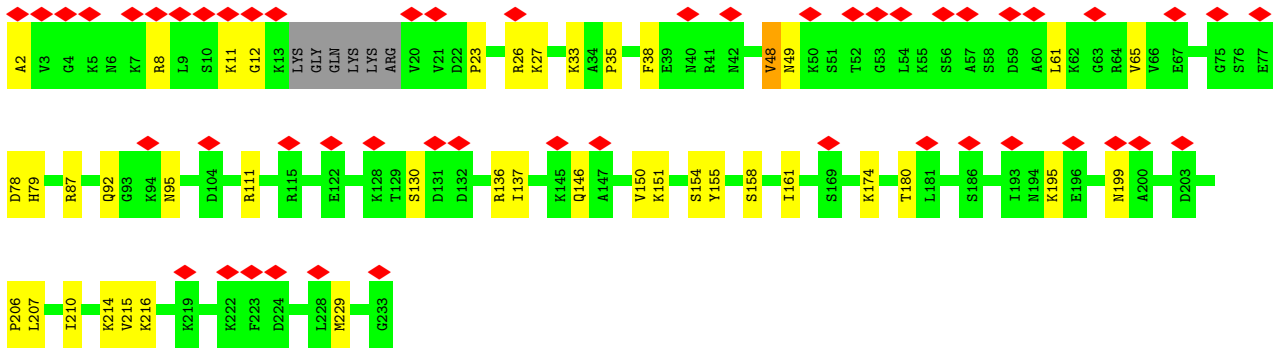
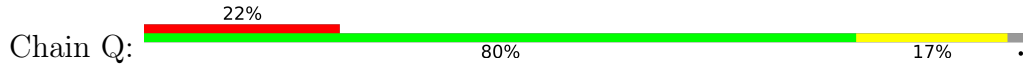


• Molecule 3: 40S ribosomal protein S0-A

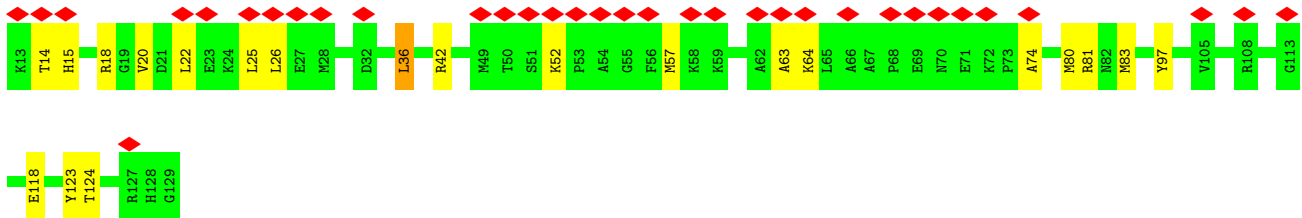
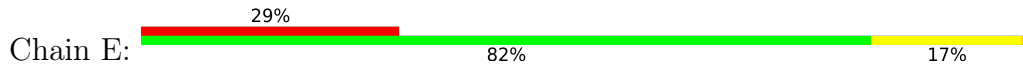




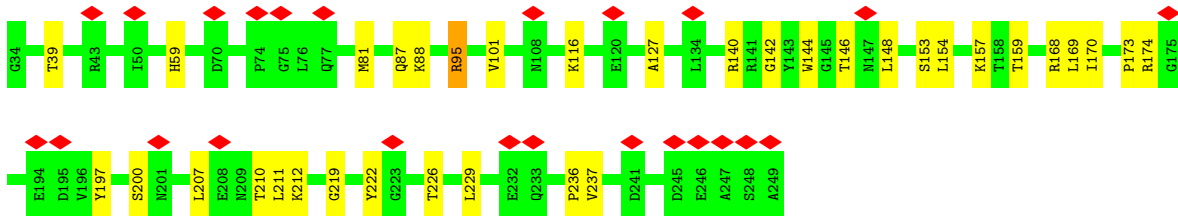
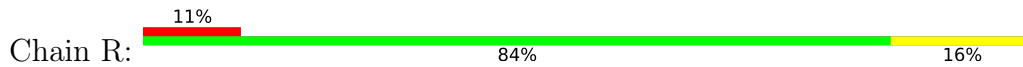
- Molecule 4: 40S ribosomal protein S1-A



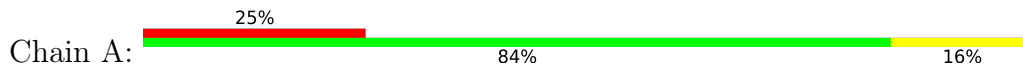
- Molecule 5: 40S ribosomal protein S15

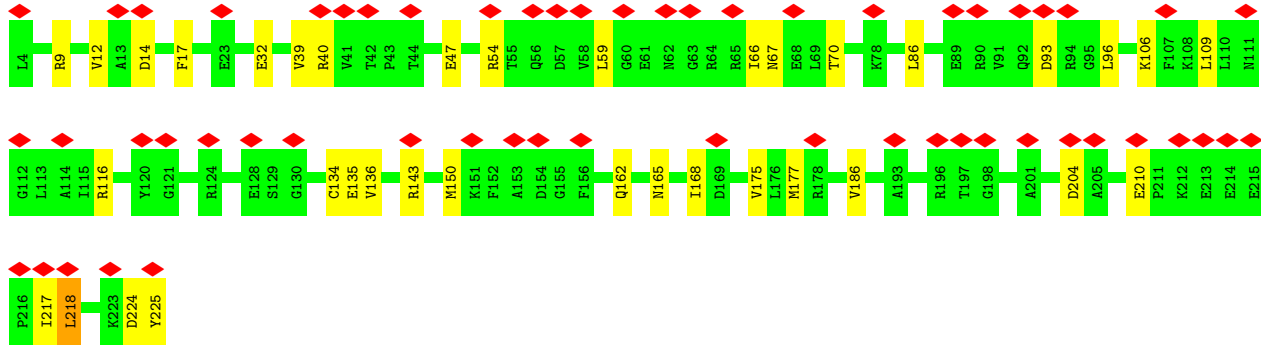


- Molecule 6: 40S ribosomal protein S2

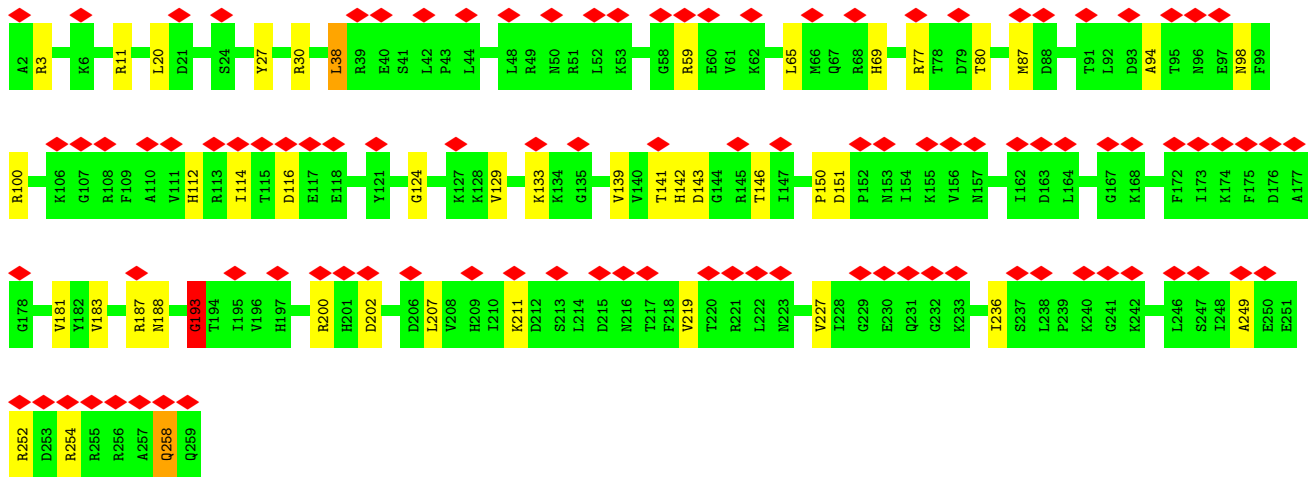
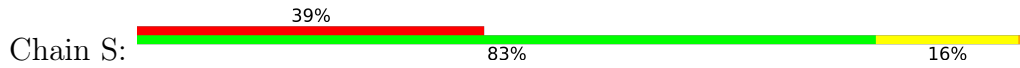


- Molecule 7: 40S ribosomal protein S3

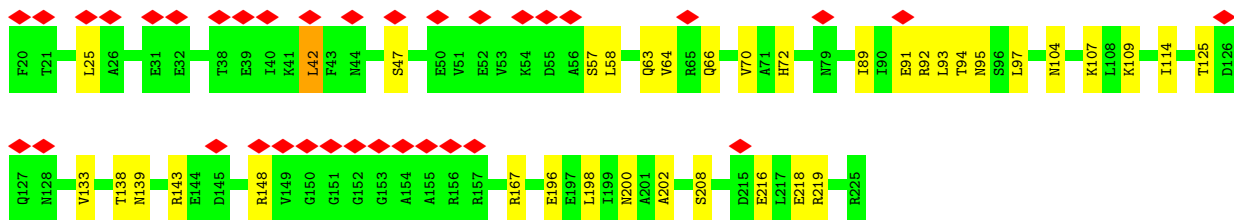
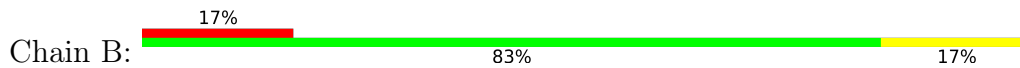




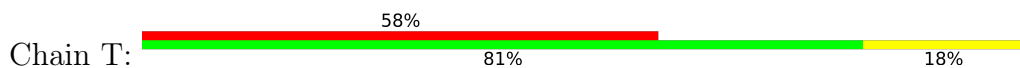
• Molecule 8: 40S ribosomal protein S4-A

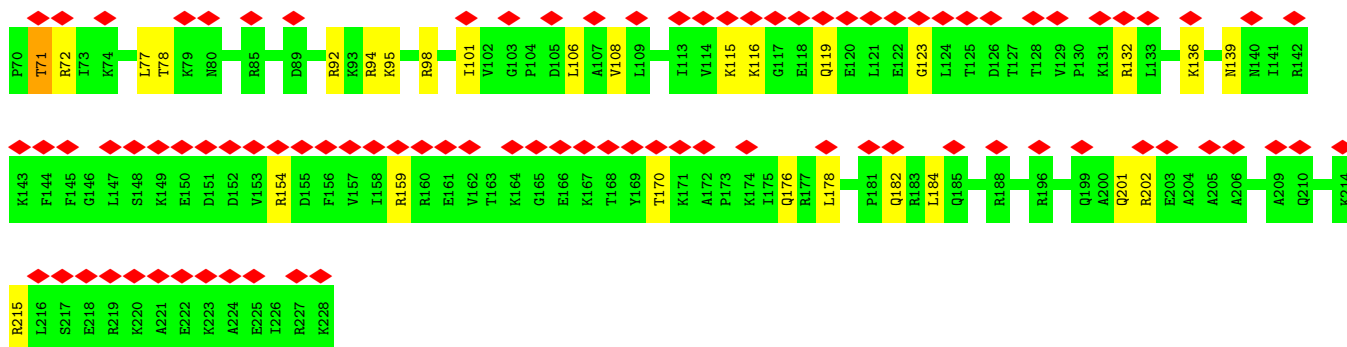


• Molecule 9: 40S ribosomal protein S5

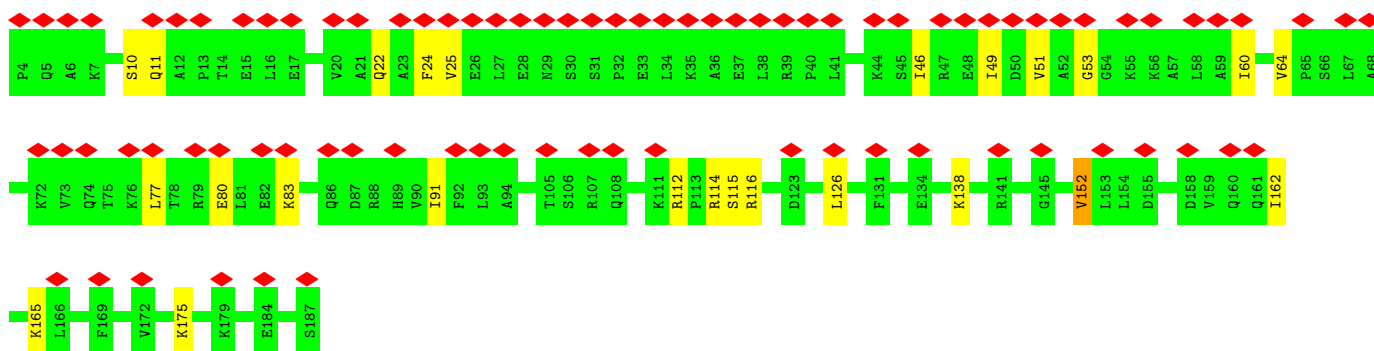
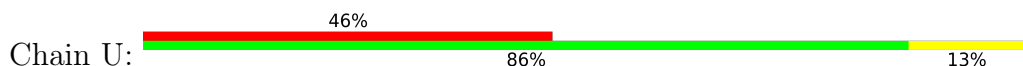


• Molecule 10: 40S ribosomal protein S6-A

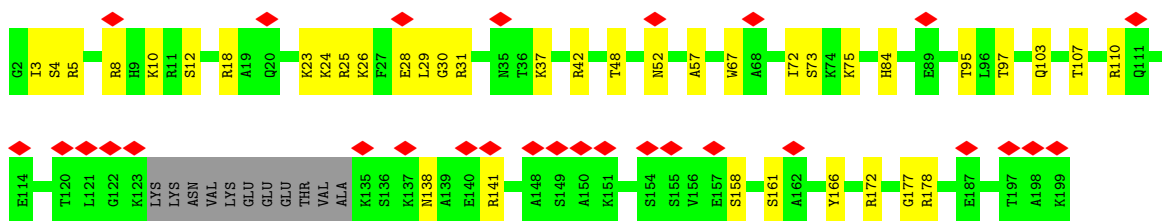
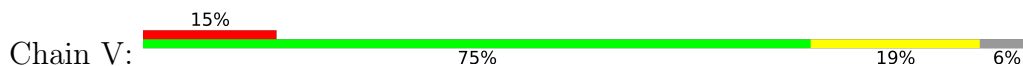




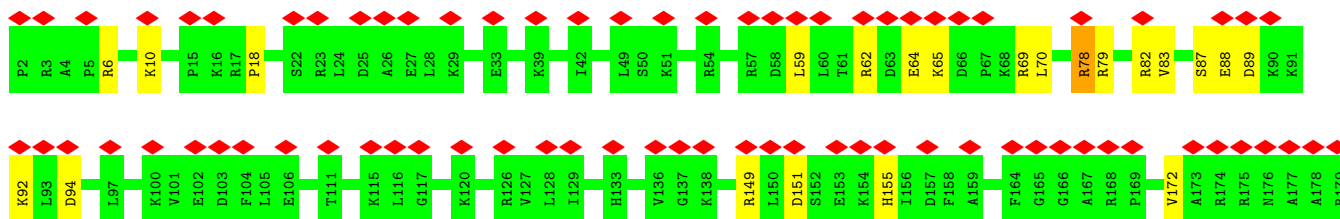
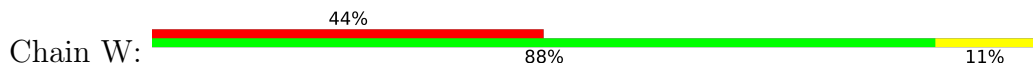
- Molecule 11: 40S ribosomal protein S7-A

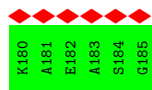


- Molecule 12: 40S ribosomal protein S8-A

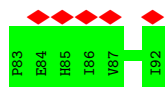
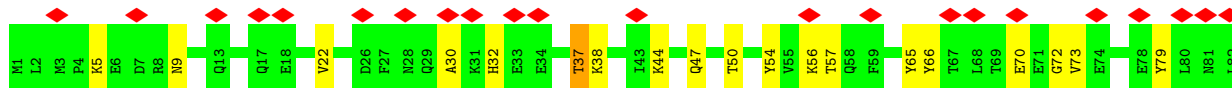
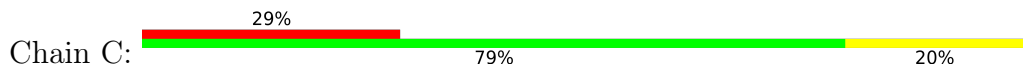


- Molecule 13: 40S ribosomal protein S9-A

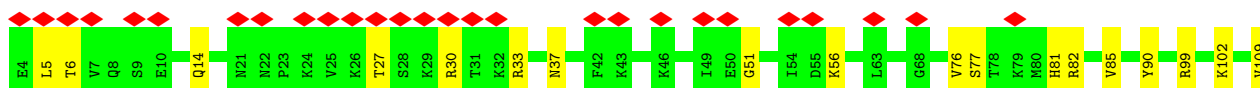
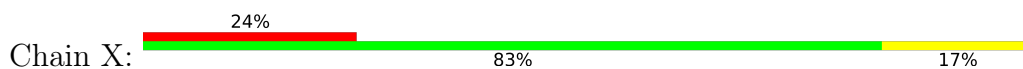




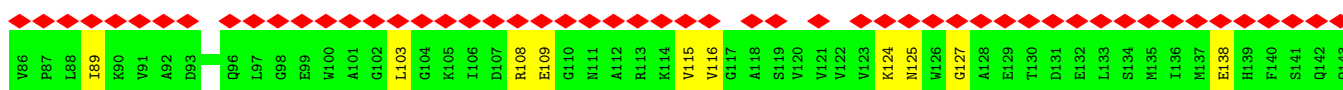
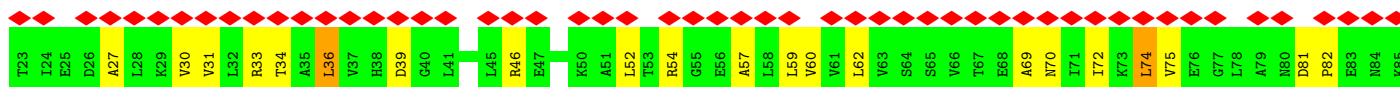
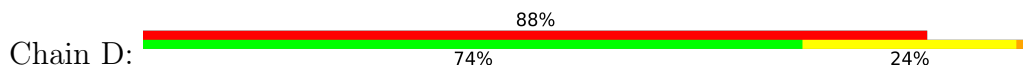
- Molecule 14: 40S ribosomal protein S10-A



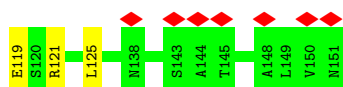
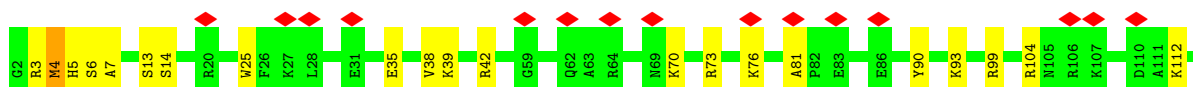
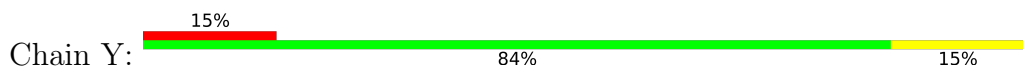
- Molecule 15: 40S ribosomal protein S11-A



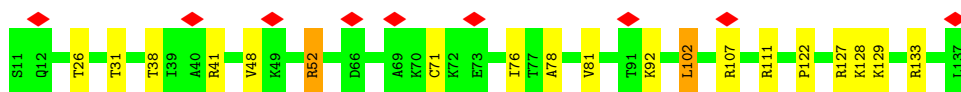
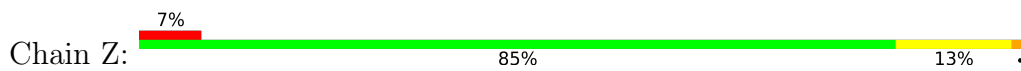
- Molecule 16: 40S ribosomal protein S12



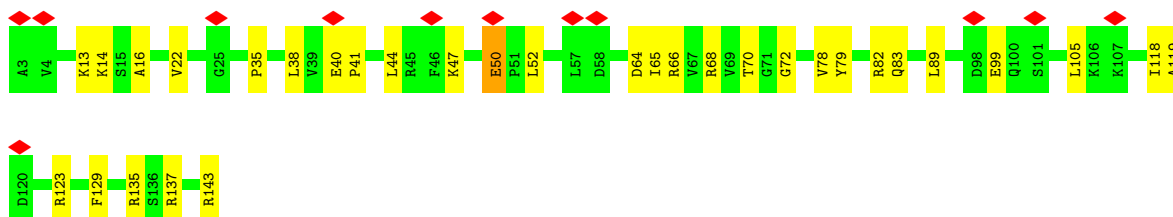
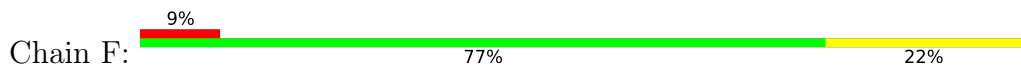
- Molecule 17: 40S ribosomal protein S13



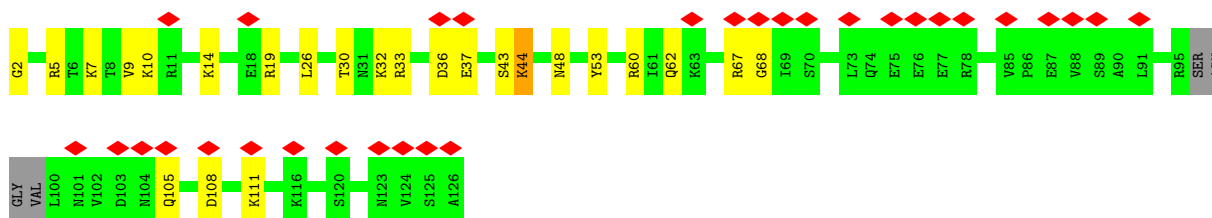
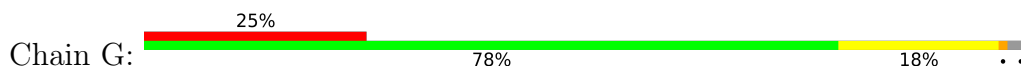
- Molecule 18: 40S ribosomal protein S14-B



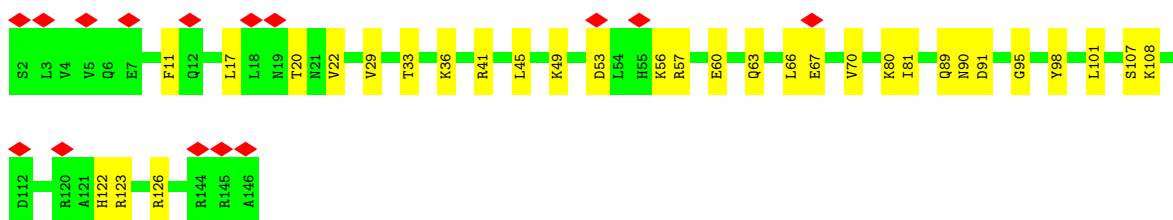
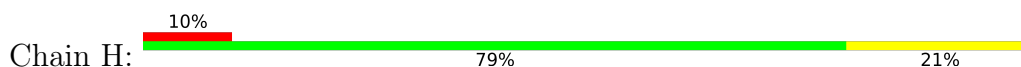
• Molecule 19: 40S ribosomal protein S16-A



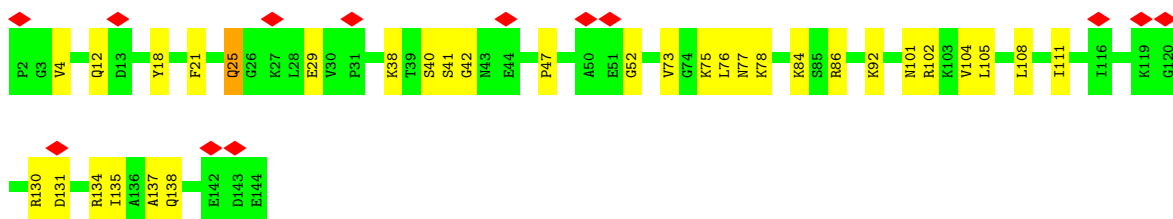
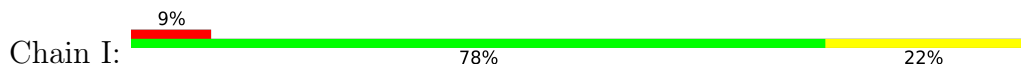
• Molecule 20: 40S ribosomal protein S17-B



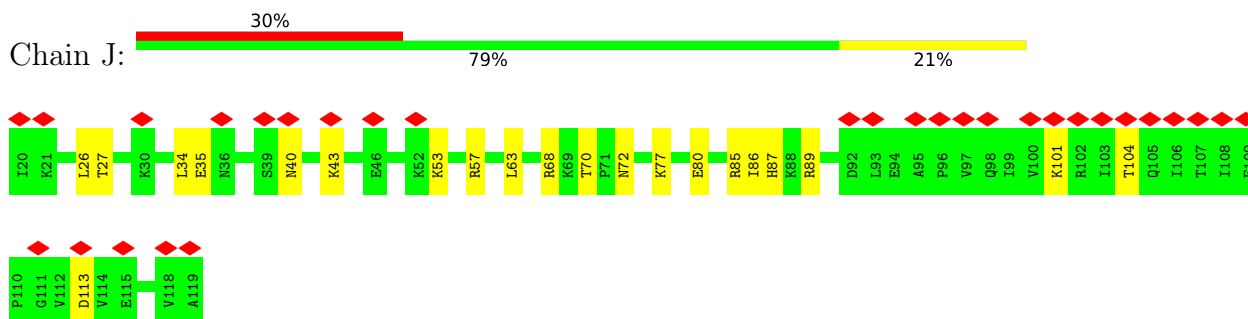
• Molecule 21: 40S ribosomal protein S18-A



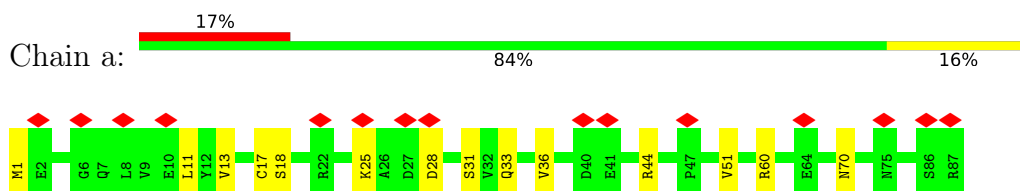
• Molecule 22: 40S ribosomal protein S19-A



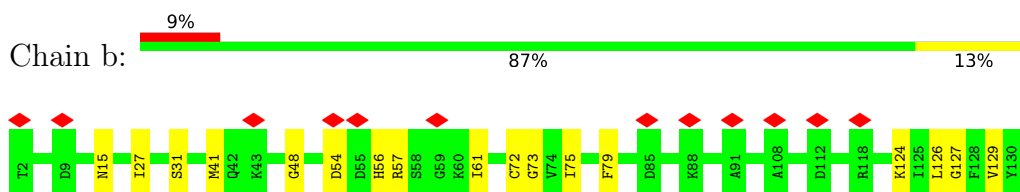
- Molecule 23: 40S ribosomal protein S20



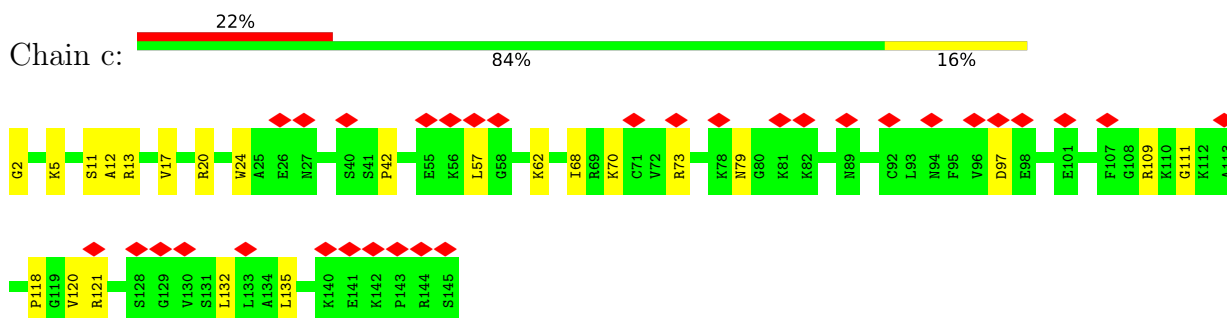
- Molecule 24: 40S ribosomal protein S21-A



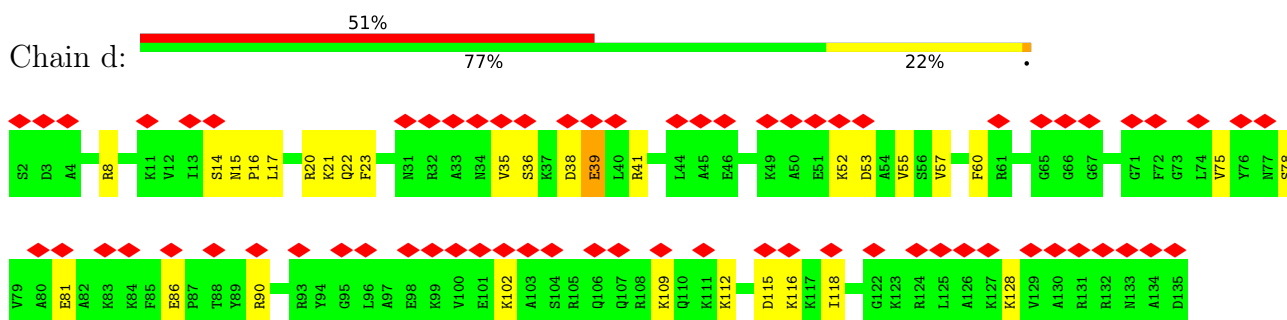
- Molecule 25: 40S ribosomal protein S22-A



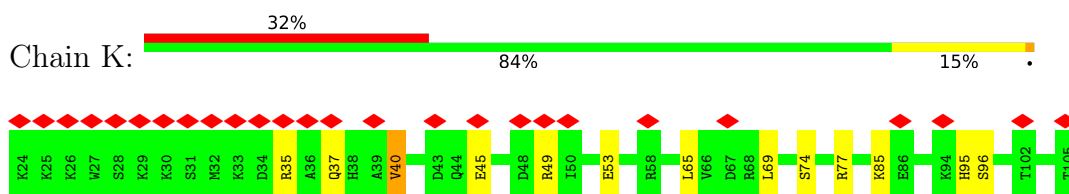
- Molecule 26: 40S ribosomal protein S23-A



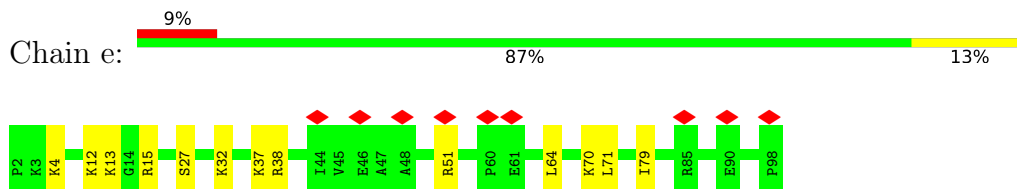
- Molecule 27: 40S ribosomal protein S24-A



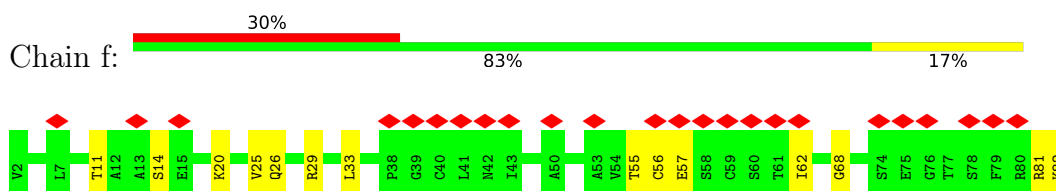
- Molecule 28: 40S ribosomal protein S25-A



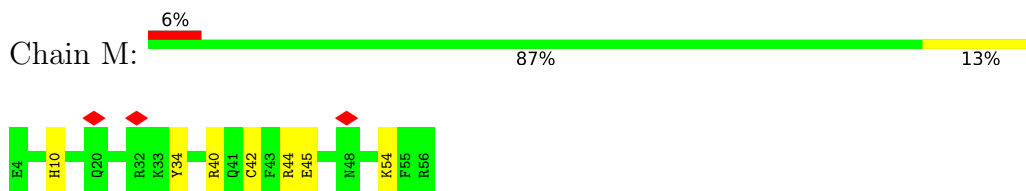
- Molecule 29: 40S ribosomal protein S26-B



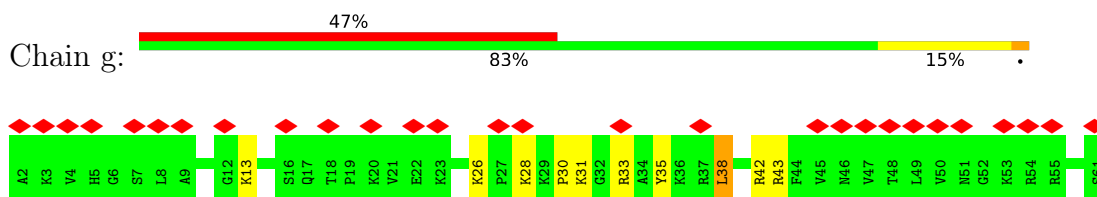
- Molecule 30: 40S ribosomal protein S27-A



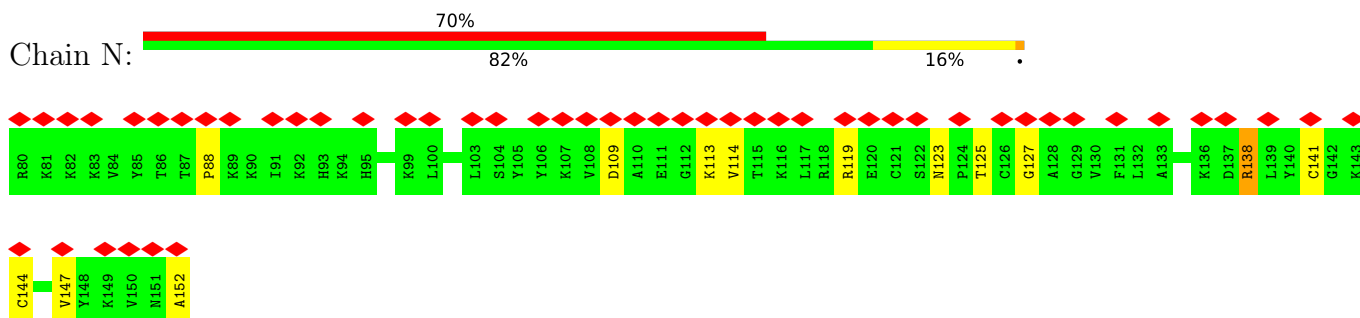
- Molecule 31: 40S ribosomal protein S29-A



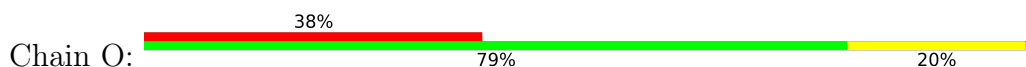
- Molecule 32: 40S ribosomal protein S30-A

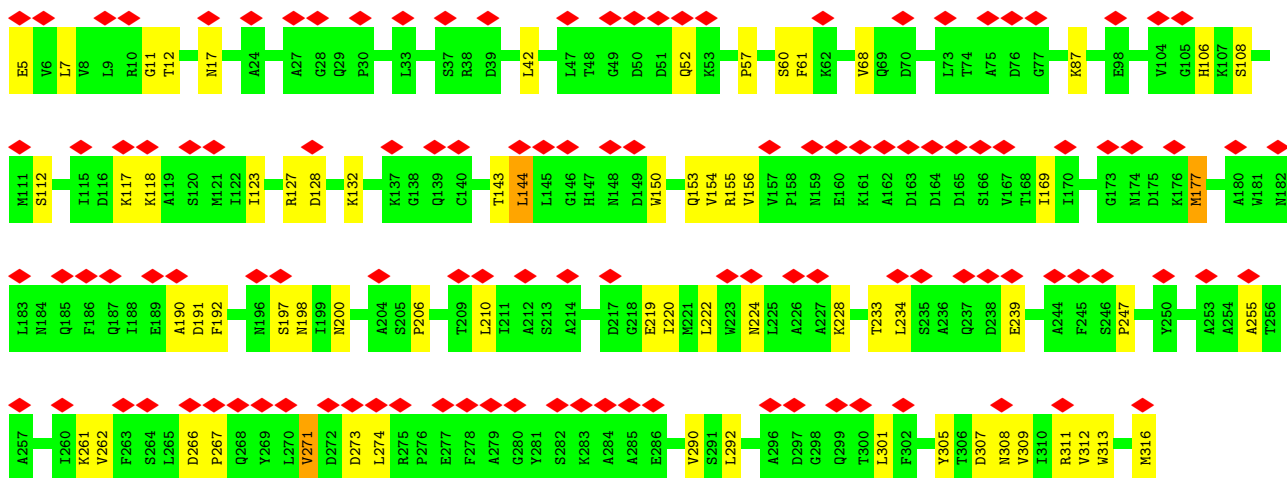


- Molecule 33: Ubiquitin-40S ribosomal protein S31



- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

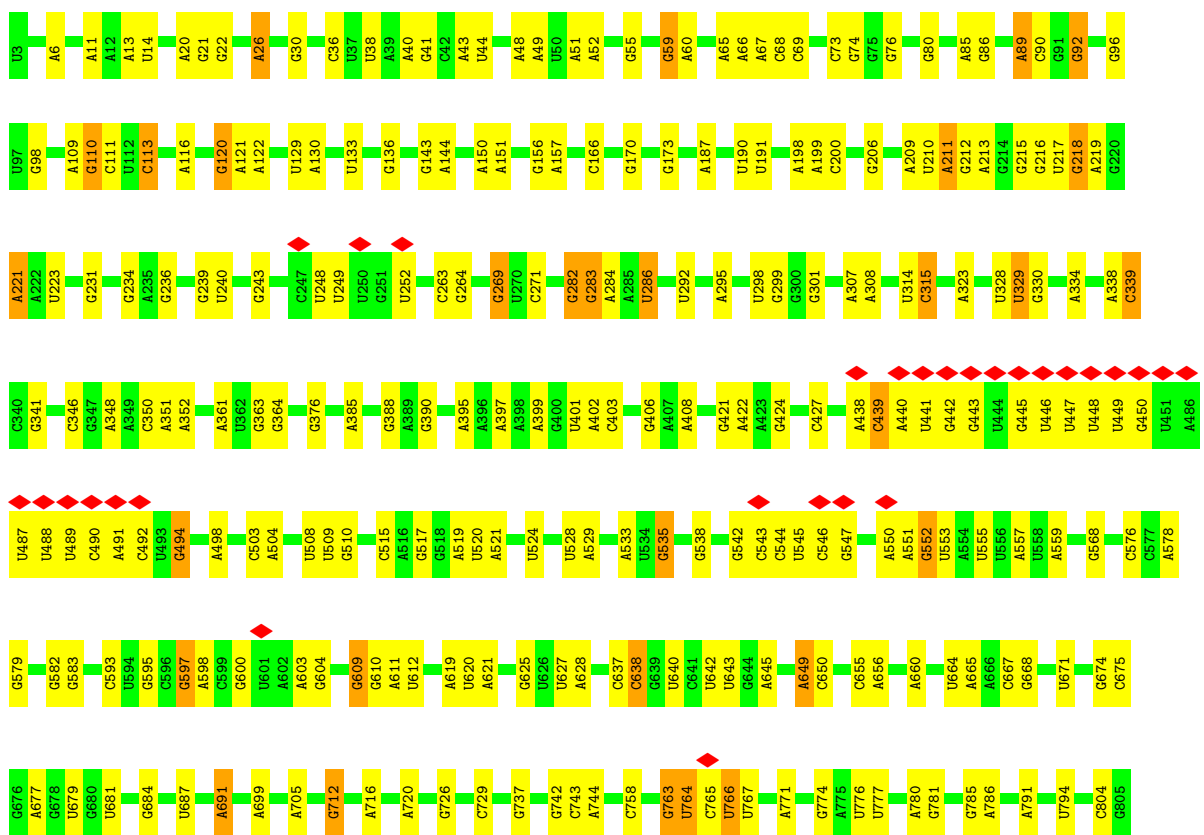




• Molecule 35: 40S ribosomal protein S28-A

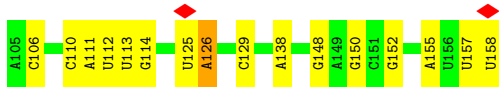


• Molecule 36: 25S rRNA

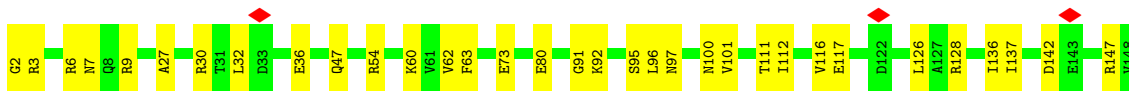
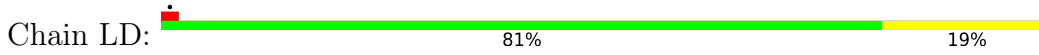




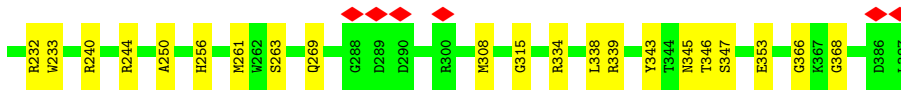
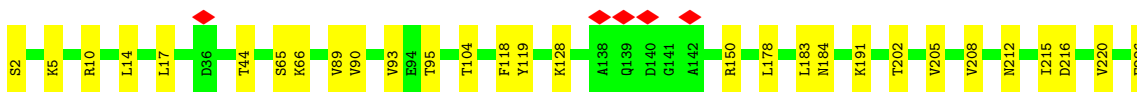
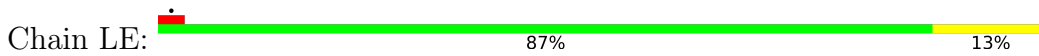




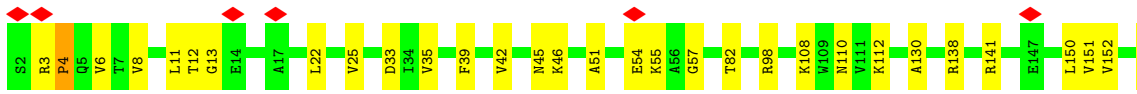
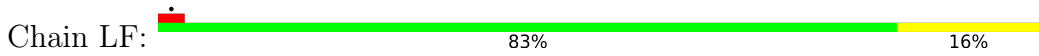
• Molecule 39: 60S ribosomal protein L2-A



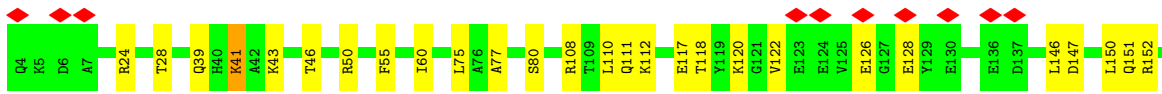
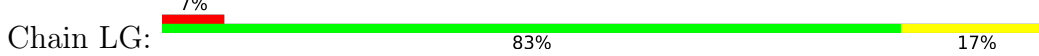
• Molecule 40: 60S ribosomal protein L3

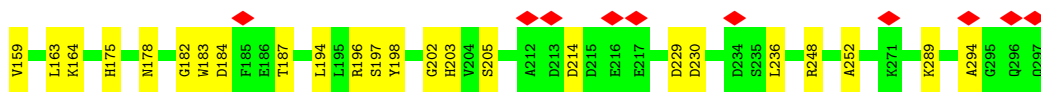


• Molecule 41: 60S ribosomal protein L4-A

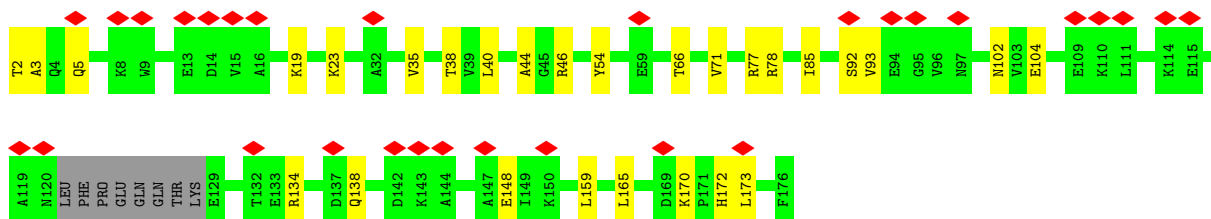
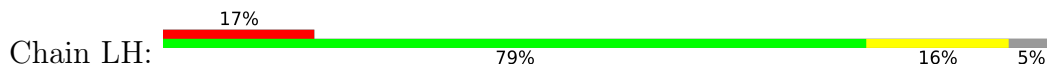


• Molecule 42: 60S ribosomal protein L5

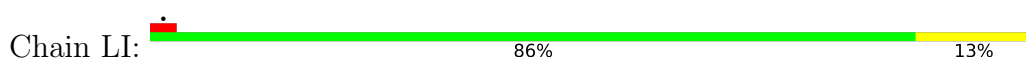




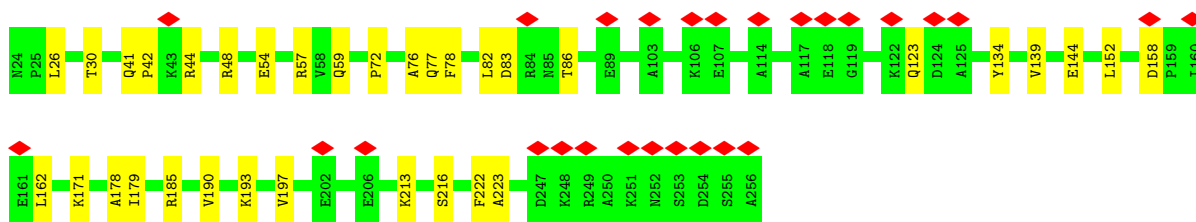
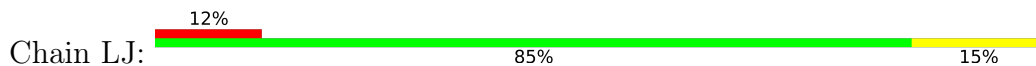
- Molecule 43: 60S ribosomal protein L6-B



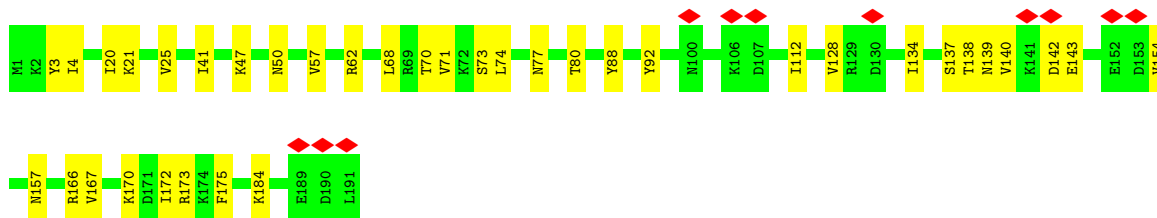
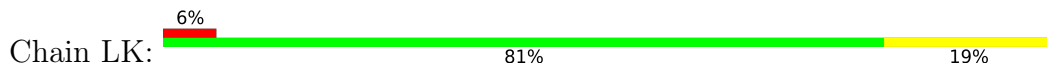
- Molecule 44: 60S ribosomal protein L7-A



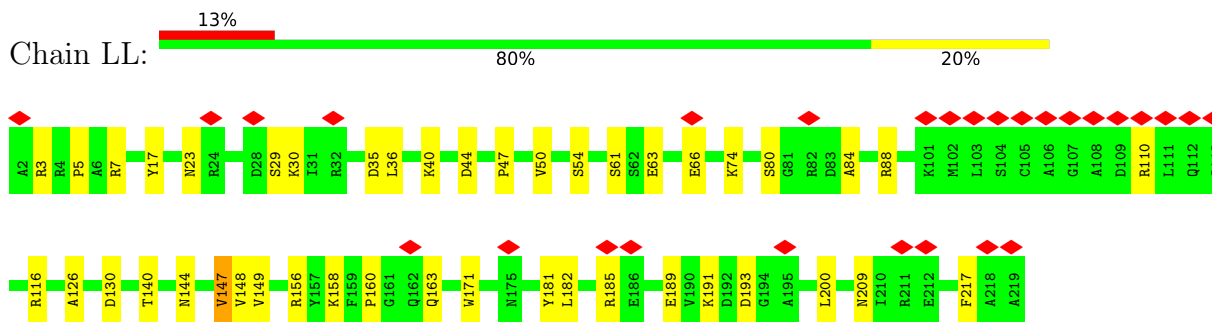
- Molecule 45: 60S ribosomal protein L8-A



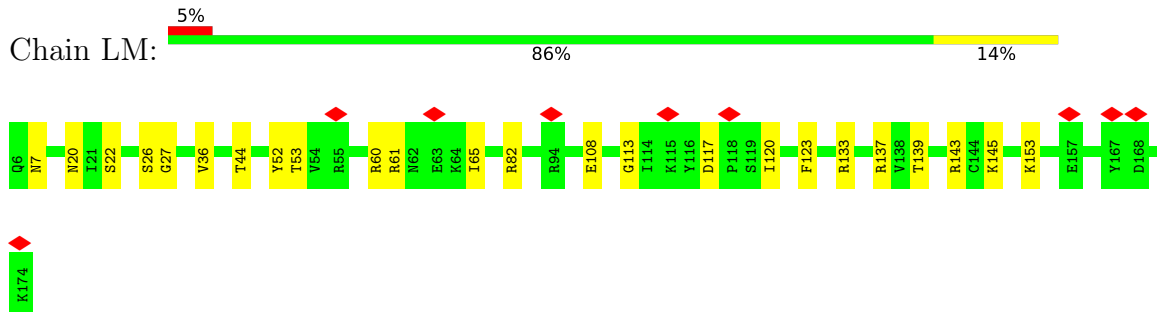
- Molecule 46: 60S ribosomal protein L9-A



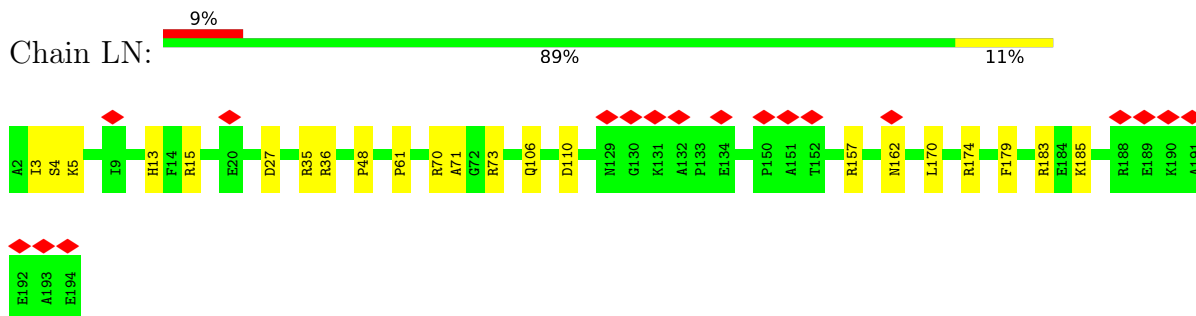
- Molecule 47: 60S ribosomal protein L10



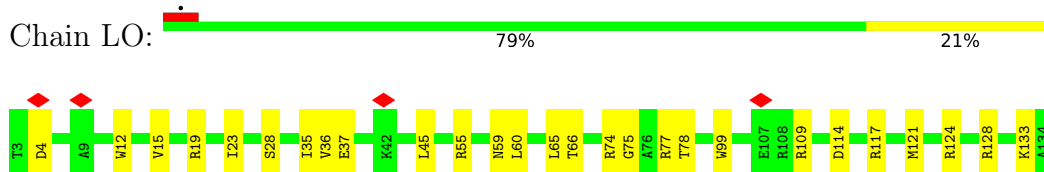
• Molecule 48: 60S ribosomal protein L11-B



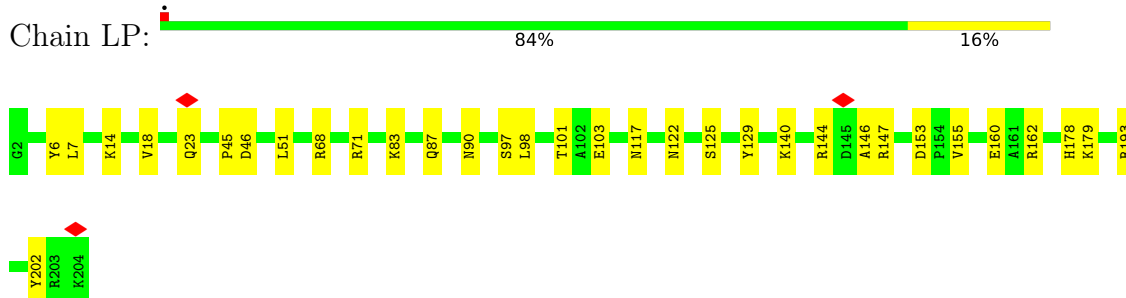
• Molecule 49: 60S ribosomal protein L13-A



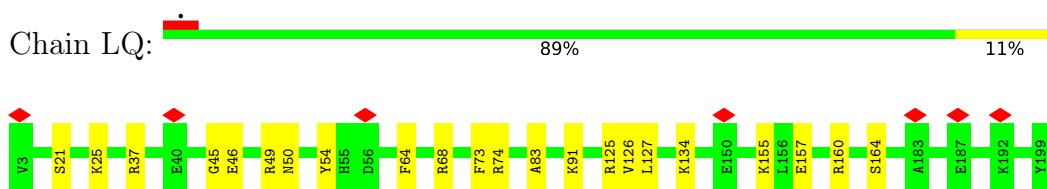
• Molecule 50: 60S ribosomal protein L14-A



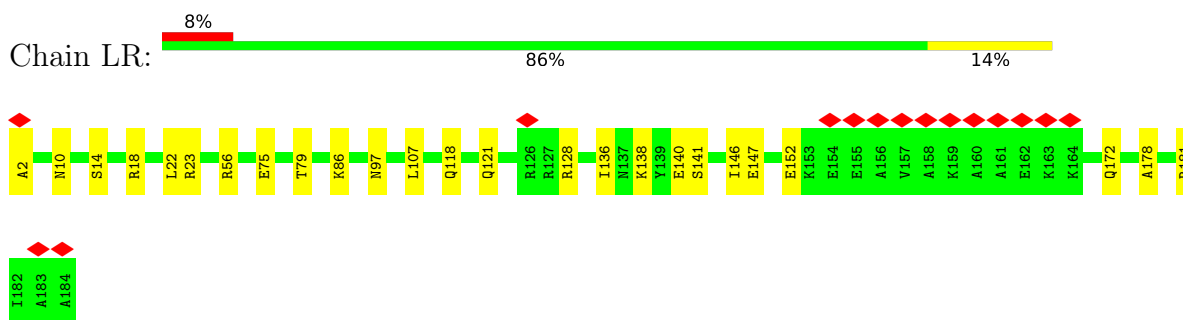
• Molecule 51: 60S ribosomal protein L15-A



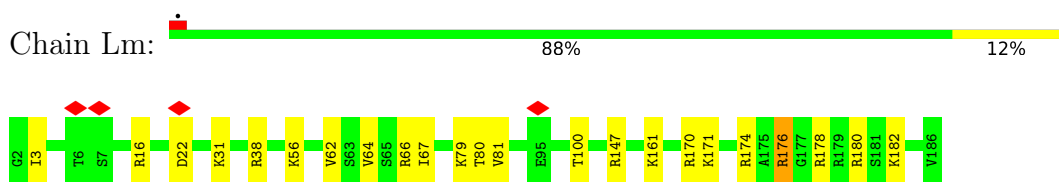
- Molecule 52: 60S ribosomal protein L16-A



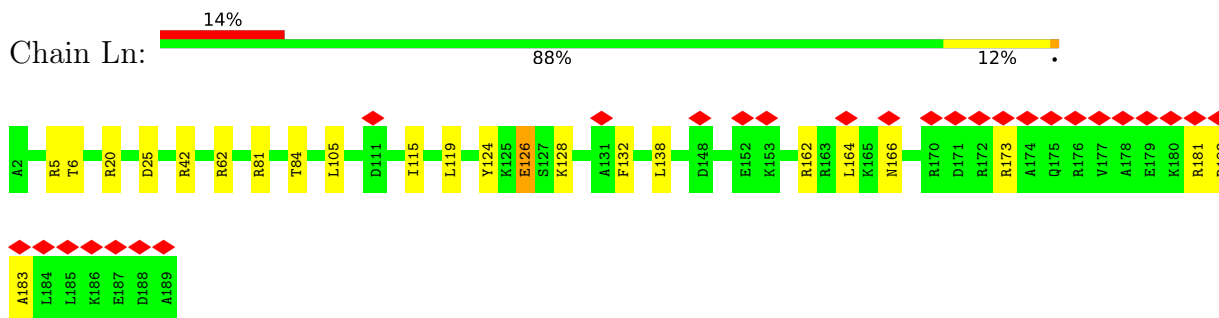
- Molecule 53: 60S ribosomal protein L17-A



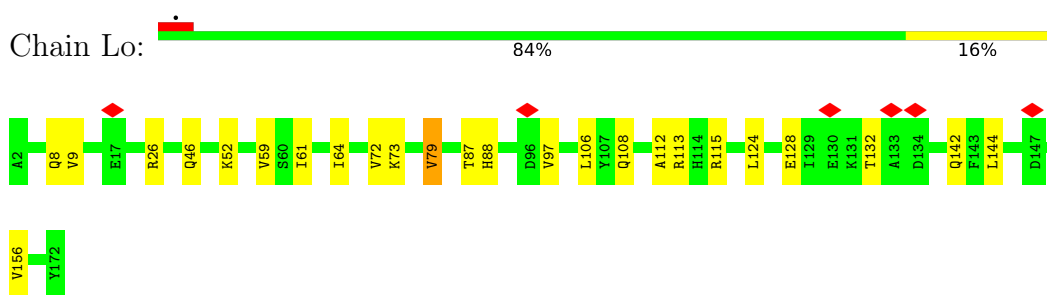
- Molecule 54: 60S ribosomal protein L18-A



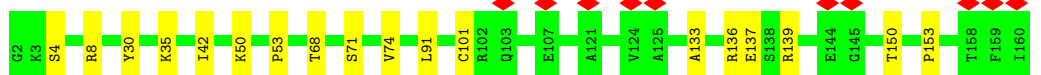
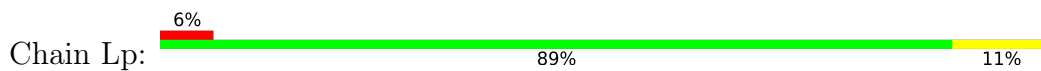
- Molecule 55: 60S ribosomal protein L19-A



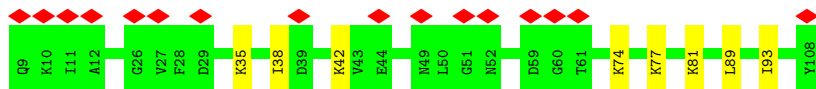
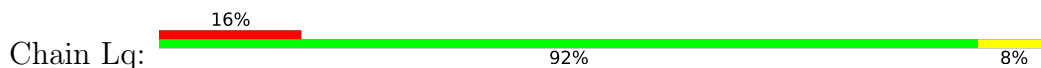
- Molecule 56: 60S ribosomal protein L20-A



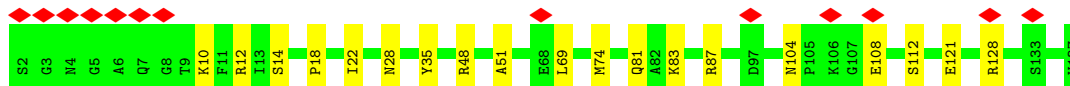
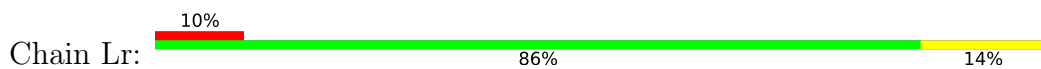
- Molecule 57: 60S ribosomal protein L21-A



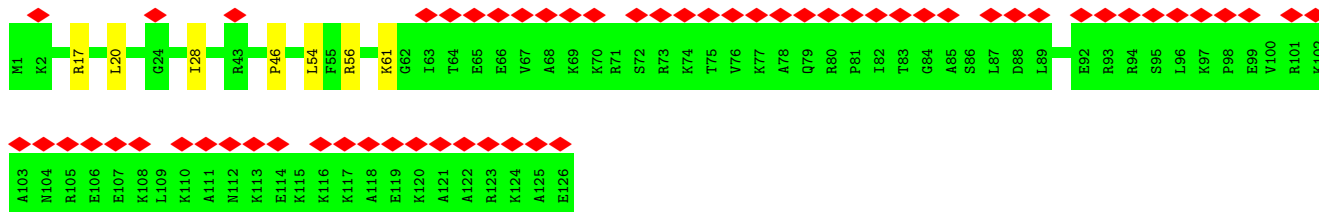
- Molecule 58: 60S ribosomal protein L22-A



- Molecule 59: 60S ribosomal protein L23-A



- Molecule 60: 60S ribosomal protein L24-A



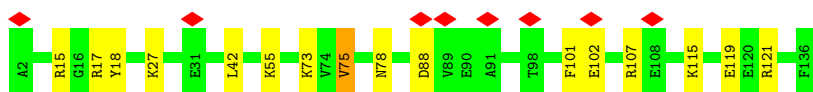
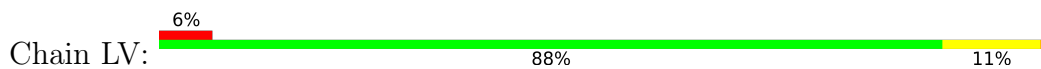
- Molecule 61: 60S ribosomal protein L25



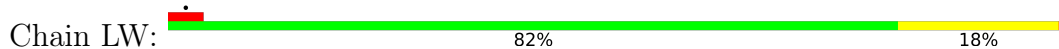
- Molecule 62: 60S ribosomal protein L26-A



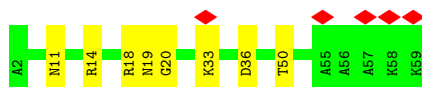
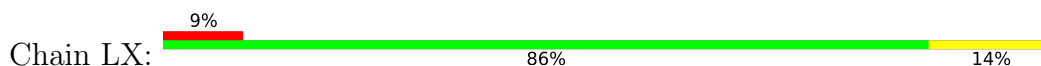
- Molecule 63: 60S ribosomal protein L27-A



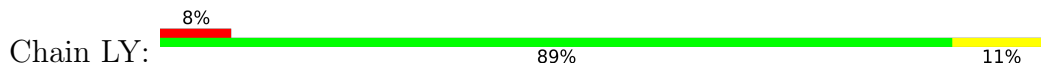
- Molecule 64: 60S ribosomal protein L28



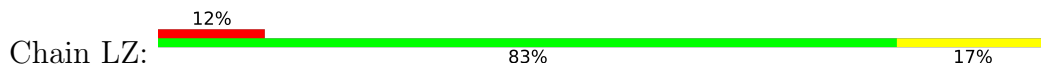
- Molecule 65: 60S ribosomal protein L29



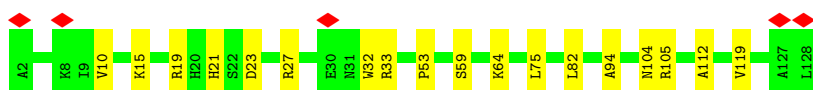
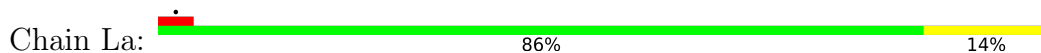
- Molecule 66: 60S ribosomal protein L30



- Molecule 67: 60S ribosomal protein L31-A

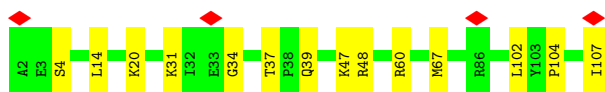


- Molecule 68: 60S ribosomal protein L32

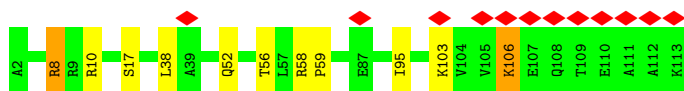
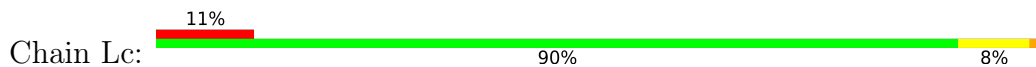


- Molecule 69: 60S ribosomal protein L33-A

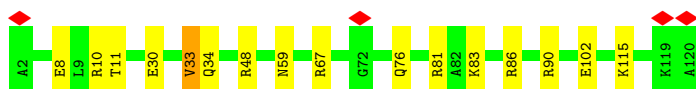
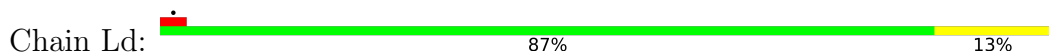




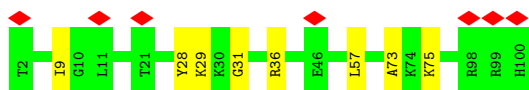
- Molecule 70: 60S ribosomal protein L34-A



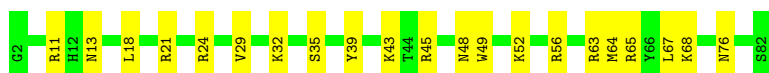
- Molecule 71: 60S ribosomal protein L35-A



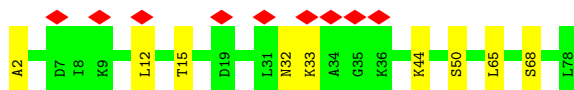
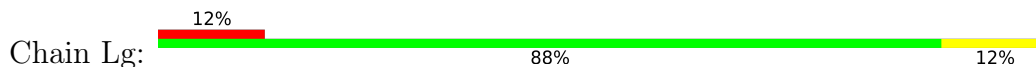
- Molecule 72: 60S ribosomal protein L36-A



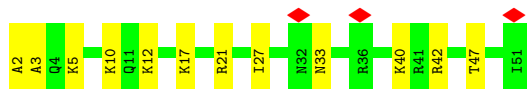
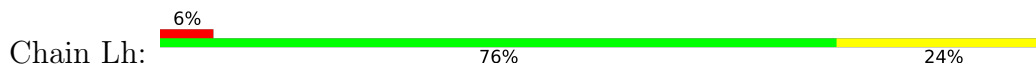
- Molecule 73: 60S ribosomal protein L37-A



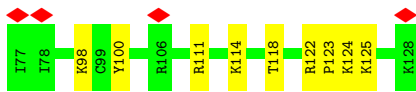
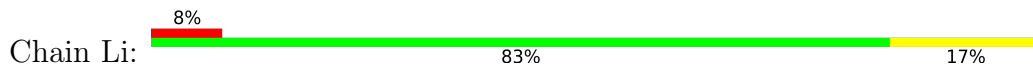
- Molecule 74: 60S ribosomal protein L38



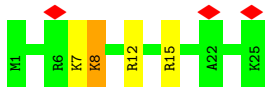
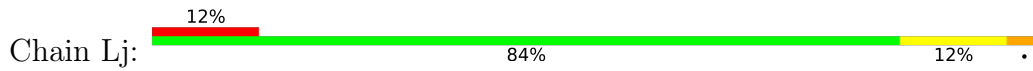
- Molecule 75: 60S ribosomal protein L39



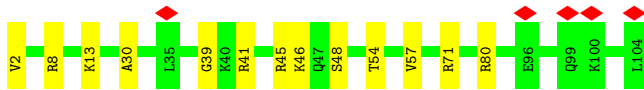
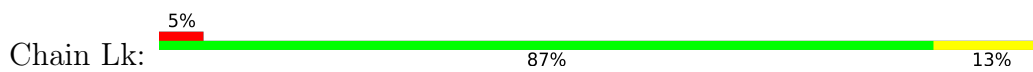
- Molecule 76: Ubiquitin-60S ribosomal protein L40



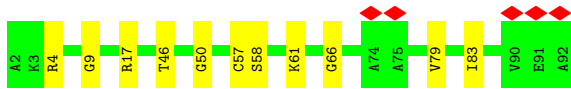
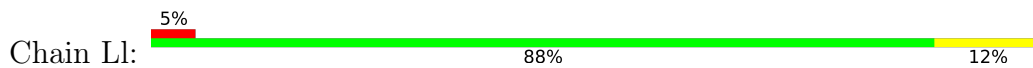
- Molecule 77: 60S ribosomal protein L41-B



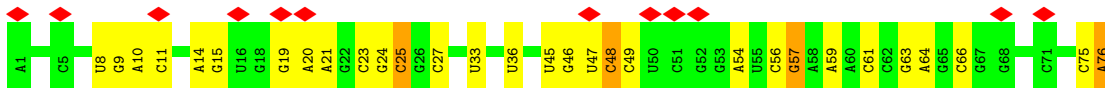
- Molecule 78: 60S ribosomal protein L42-A



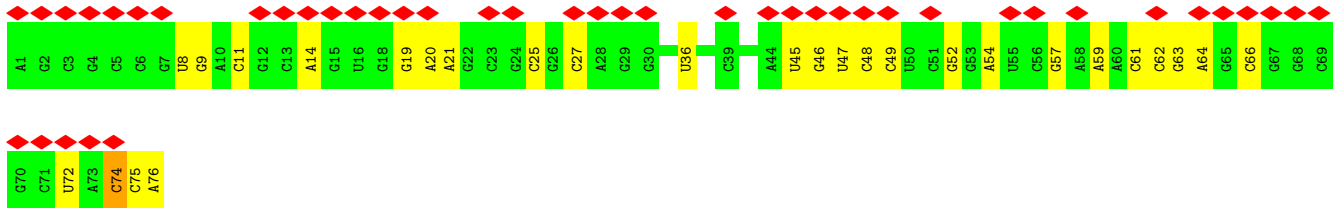
- Molecule 79: 60S ribosomal protein L43-A



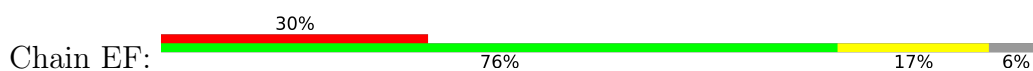
- Molecule 80: tRNA



- Molecule 80: tRNA



- Molecule 81: Elongation factor 3A





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	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 ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.391	Depositor
Minimum map value	-0.234	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.04	Depositor
Map size ( $\text{\AA}$ )	455.28, 455.28, 455.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.084, 1.084, 1.084	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	2	0.43	0/42211	0.70	25/65773 (0.0%)
2	1	0.35	0/166	0.42	0/256
3	P	0.42	0/1644	0.88	1/2249 (0.0%)
4	Q	0.44	0/1823	0.98	0/2447
5	E	0.51	0/936	1.04	2/1259 (0.2%)
6	R	0.46	0/1656	0.94	0/2251
7	A	0.45	0/1754	0.99	5/2361 (0.2%)
8	S	0.40	0/2097	0.95	2/2823 (0.1%)
9	B	0.45	0/1625	0.99	3/2197 (0.1%)
10	T	0.39	0/1839	0.96	0/2460
11	U	0.42	0/1498	0.95	0/2019
12	V	0.42	0/1501	0.89	0/2006
13	W	0.39	0/1504	0.94	0/2016
14	C	0.47	0/769	1.00	0/1039
15	X	0.41	0/1168	0.85	0/1575
16	D	0.47	0/883	1.16	3/1199 (0.3%)
17	Y	0.43	0/1215	0.92	2/1638 (0.1%)
18	Z	0.50	0/934	1.04	1/1257 (0.1%)
19	F	0.49	0/1125	1.00	1/1510 (0.1%)
20	G	0.43	0/957	0.90	0/1283
21	H	0.47	0/1207	1.00	0/1623
22	I	0.51	0/1130	1.02	2/1517 (0.1%)
23	J	0.49	0/807	0.98	0/1091
24	a	0.41	0/682	0.89	0/921
25	b	0.47	0/1038	0.95	1/1395 (0.1%)
26	c	0.47	0/1139	0.95	0/1518
27	d	0.38	0/1087	0.98	2/1449 (0.1%)
28	K	0.43	0/661	1.06	1/888 (0.1%)
29	e	0.46	0/778	0.98	0/1042
30	f	0.37	0/620	0.93	0/838
31	M	0.43	0/452	0.94	0/600
32	g	0.42	0/480	0.99	0/639

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	N	0.37	0/567	1.04	0/764
34	O	0.38	0/2436	0.93	3/3318 (0.1%)
35	L	0.50	0/493	1.18	2/663 (0.3%)
36	LA	0.52	0/77157	0.64	15/120295 (0.0%)
37	LB	0.48	0/2883	0.60	0/4491
38	LC	0.51	0/3746	0.61	0/5832
39	LD	0.61	0/1933	0.90	0/2598
40	LE	0.53	0/3146	0.85	0/4228
41	LF	0.52	0/2800	0.91	2/3790 (0.1%)
42	LG	0.51	0/2400	0.91	5/3239 (0.2%)
43	LH	0.44	0/1329	0.94	1/1794 (0.1%)
44	LI	0.52	0/1821	0.91	0/2451
45	LJ	0.50	0/1836	0.90	0/2481
46	LK	0.48	0/1529	0.95	2/2060 (0.1%)
47	LL	0.48	0/1801	0.93	0/2416
48	LM	0.51	0/1367	0.95	1/1834 (0.1%)
49	LN	0.52	0/1568	0.87	0/2106
50	LO	0.45	0/1068	0.87	0/1438
51	LP	0.59	0/1757	0.88	0/2354
52	LQ	0.51	0/1585	0.85	0/2128
53	LR	0.54	0/1439	0.84	0/1938
54	Lm	0.54	0/1465	0.93	0/1965
55	Ln	0.50	0/1532	0.92	2/2043 (0.1%)
56	Lo	0.51	0/1473	0.81	0/1980
57	Lp	0.54	0/1296	0.88	1/1739 (0.1%)
58	Lq	0.45	0/812	0.89	0/1099
59	Lr	0.52	0/1018	0.88	1/1369 (0.1%)
60	LS	0.41	0/850	0.82	0/1152
61	LT	0.52	0/979	0.86	0/1321
62	LU	0.45	0/995	0.84	0/1329
63	LV	0.47	0/1106	0.86	0/1485
64	LW	0.58	0/1200	0.88	0/1607
65	LX	0.46	0/473	0.84	0/629
66	LY	0.45	0/745	0.82	0/1001
67	LZ	0.52	0/890	0.85	0/1196
68	La	0.48	0/1034	0.78	0/1385
69	Lb	0.56	0/868	0.87	1/1168 (0.1%)
70	Lc	0.60	0/890	0.96	2/1189 (0.2%)
71	Ld	0.44	0/978	0.79	0/1301
72	Le	0.44	0/772	0.88	0/1026
73	Lf	0.67	0/660	1.04	1/875 (0.1%)
74	Lg	0.48	0/618	0.94	0/826
75	Lh	0.59	0/443	0.98	0/588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	Li	0.51	0/416	0.93	0/553
77	Lj	0.49	0/230	0.95	0/296
78	Lk	0.52	0/836	0.87	0/1104
79	Ll	0.56	0/701	0.83	0/934
80	Sm	0.34	0/1795	0.73	2/2797 (0.1%)
80	Sn	0.39	0/1796	0.72	0/2799
81	EF	0.33	0/7610	0.71	6/10311 (0.1%)
All	All	0.48	0/226528	0.77	98/332424 (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
8	S	0	1
9	B	0	2
11	U	0	1
16	D	0	1
19	F	0	1
25	b	0	1
33	N	0	1
36	LA	0	1
41	LF	0	3
44	LI	0	1
45	LJ	0	3
54	Lm	0	1
64	LW	0	2
65	LX	0	2
66	LY	0	1
67	LZ	0	1
71	Ld	0	1
81	EF	0	6
All	All	0	30

There are no bond length outliers.

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
27	d	39	GLU	CA-CB-CG	8.91	131.92	114.10
81	EF	415	PRO	N-CA-CB	7.58	110.39	103.34
80	Sm	74	C	O3'-P-O5'	7.39	115.08	104.00

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
81	EF	418	PRO	N-CA-CB	7.38	111.00	103.25
7	A	218	LEU	CA-CB-CG	7.22	141.58	116.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	B	125	THR	Peptide
9	B	42	LEU	Peptide
16	D	108	ARG	Peptide
8	S	193	GLY	Peptide
11	U	64	VAL	Peptide

## 5.2 Too-close contacts [i](#)

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	2	37739	0	18987	297	0
2	1	149	0	75	0	0
3	P	1603	0	1610	24	0
4	Q	1798	0	1890	28	0
5	E	916	0	941	15	0
6	R	1626	0	1715	23	0
7	A	1729	0	1812	18	0
8	S	2056	0	2140	30	0
9	B	1605	0	1669	21	0
10	T	1815	0	1894	32	0
11	U	1473	0	1555	14	0
12	V	1476	0	1501	27	0
13	W	1479	0	1556	19	0
14	C	752	0	719	11	0
15	X	1142	0	1209	15	0
16	D	875	0	878	19	0
17	Y	1192	0	1255	16	0
18	Z	923	0	948	13	0
19	F	1105	0	1166	24	0
20	G	948	0	990	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	H	1188	0	1218	21	0
22	I	1112	0	1124	24	0
23	J	797	0	863	18	0
24	a	673	0	662	11	0
25	b	1021	0	1060	10	0
26	c	1121	0	1196	16	0
27	d	1073	0	1132	19	0
28	K	651	0	682	7	0
29	e	765	0	814	11	0
30	f	610	0	633	10	0
31	M	442	0	432	7	0
32	g	472	0	521	10	0
33	N	556	0	552	10	0
34	O	2383	0	2332	37	0
35	L	491	0	524	10	0
36	LA	68931	0	34637	373	0
37	LB	2579	0	1304	22	0
38	LC	3353	0	1695	25	0
39	LD	1899	0	1957	34	0
40	LE	3075	0	3142	33	0
41	LF	2748	0	2859	44	0
42	LG	2351	0	2294	34	0
43	LH	1307	0	1377	19	0
44	LI	1784	0	1862	25	0
45	LJ	1804	0	1877	22	0
46	LK	1508	0	1572	22	0
47	LL	1764	0	1804	28	0
48	LM	1346	0	1370	19	0
49	LN	1543	0	1608	19	0
50	LO	1053	0	1149	20	0
51	LP	1720	0	1779	26	0
52	LQ	1555	0	1659	16	0
53	LR	1416	0	1433	14	0
54	Lm	1441	0	1543	19	0
55	Ln	1515	0	1606	21	0
56	Lo	1437	0	1475	22	0
57	Lp	1272	0	1312	13	0
58	Lq	796	0	812	4	0
59	Lr	1003	0	1048	12	0
60	LS	836	0	706	4	0
61	LT	964	0	1025	7	0
62	LU	984	0	1075	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	LV	1080	0	1122	11	0
64	LW	1169	0	1211	23	0
65	LX	462	0	491	5	0
66	LY	737	0	792	6	0
67	LZ	876	0	912	8	0
68	La	1013	0	1077	13	0
69	Lb	850	0	880	8	0
70	Lc	880	0	945	9	0
71	Ld	969	0	1078	11	0
72	Le	766	0	844	8	0
73	Lf	645	0	649	18	0
74	Lg	612	0	682	6	0
75	Lh	436	0	475	11	0
76	Li	410	0	446	7	0
77	Lj	229	0	273	3	0
78	Lk	824	0	892	12	0
79	Ll	694	0	738	9	0
80	Sm	1605	0	816	3	0
80	Sn	1606	0	816	10	0
81	EF	7479	0	7407	102	0
82	EF	62	0	24	5	0
All	All	211144	0	156805	1568	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 4.

The worst 5 of 1568 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)
36:LA:1896:A:H61	36:LA:2339:C:N4	1.57	1.01
36:LA:2471:U:H3	36:LA:2475:G:H1	1.01	0.97
1:2:1697:G:H1	1:2:1704:U:H3	1.05	0.96
36:LA:1896:A:N6	36:LA:2339:C:H42	1.63	0.94
1:2:821:U:H3	1:2:852:C:N4	1.64	0.94

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	
3	P	204/206 (99%)	182 (89%)	22 (11%)	0	100	100
4	Q	222/232 (96%)	196 (88%)	26 (12%)	0	100	100
5	E	115/117 (98%)	100 (87%)	15 (13%)	0	100	100
6	R	214/216 (99%)	188 (88%)	26 (12%)	0	100	100
7	A	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
8	S	256/258 (99%)	229 (90%)	27 (10%)	0	100	100
9	B	204/206 (99%)	188 (92%)	16 (8%)	0	100	100
10	T	226/228 (99%)	212 (94%)	14 (6%)	0	100	100
11	U	182/184 (99%)	162 (89%)	20 (11%)	0	100	100
12	V	183/198 (92%)	168 (92%)	15 (8%)	0	100	100
13	W	182/184 (99%)	165 (91%)	16 (9%)	1 (0%)	24	55
14	C	90/92 (98%)	79 (88%)	11 (12%)	0	100	100
15	X	140/142 (99%)	124 (89%)	16 (11%)	0	100	100
16	D	119/121 (98%)	90 (76%)	27 (23%)	2 (2%)	7	30
17	Y	148/150 (99%)	134 (90%)	14 (10%)	0	100	100
18	Z	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
19	F	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
20	G	117/125 (94%)	112 (96%)	5 (4%)	0	100	100
21	H	143/145 (99%)	130 (91%)	13 (9%)	0	100	100
22	I	141/143 (99%)	129 (92%)	10 (7%)	2 (1%)	9	33
23	J	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
24	a	85/87 (98%)	71 (84%)	14 (16%)	0	100	100
25	b	127/129 (98%)	113 (89%)	14 (11%)	0	100	100
26	c	142/144 (99%)	125 (88%)	17 (12%)	0	100	100
27	d	132/134 (98%)	124 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	K	80/82 (98%)	70 (88%)	10 (12%)	0	100	100
29	e	95/97 (98%)	86 (90%)	9 (10%)	0	100	100
30	f	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
31	M	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
32	g	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
33	N	71/73 (97%)	51 (72%)	20 (28%)	0	100	100
34	O	310/312 (99%)	269 (87%)	41 (13%)	0	100	100
35	L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
39	LD	249/251 (99%)	222 (89%)	27 (11%)	0	100	100
40	LE	384/386 (100%)	357 (93%)	27 (7%)	0	100	100
41	LF	359/361 (99%)	324 (90%)	33 (9%)	2 (1%)	21	52
42	LG	292/294 (99%)	266 (91%)	26 (9%)	0	100	100
43	LH	163/175 (93%)	146 (90%)	17 (10%)	0	100	100
44	LI	220/222 (99%)	206 (94%)	14 (6%)	0	100	100
45	LJ	231/233 (99%)	210 (91%)	21 (9%)	0	100	100
46	LK	189/191 (99%)	172 (91%)	17 (9%)	0	100	100
47	LL	216/218 (99%)	190 (88%)	26 (12%)	0	100	100
48	LM	167/169 (99%)	153 (92%)	14 (8%)	0	100	100
49	LN	191/193 (99%)	171 (90%)	19 (10%)	1 (0%)	24	55
50	LO	134/136 (98%)	120 (90%)	13 (10%)	1 (1%)	18	49
51	LP	201/203 (99%)	181 (90%)	19 (10%)	1 (0%)	24	55
52	LQ	195/197 (99%)	187 (96%)	8 (4%)	0	100	100
53	LR	181/183 (99%)	168 (93%)	13 (7%)	0	100	100
54	Lm	183/185 (99%)	168 (92%)	15 (8%)	0	100	100
55	Ln	186/188 (99%)	180 (97%)	6 (3%)	0	100	100
56	Lo	169/171 (99%)	155 (92%)	14 (8%)	0	100	100
57	Lp	157/159 (99%)	143 (91%)	14 (9%)	0	100	100
58	Lq	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
59	Lr	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
60	LS	124/126 (98%)	109 (88%)	15 (12%)	0	100	100
61	LT	119/121 (98%)	111 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	LU	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
63	LV	133/135 (98%)	117 (88%)	16 (12%)	0	100	100
64	LW	146/148 (99%)	127 (87%)	19 (13%)	0	100	100
65	LX	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
66	LY	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
67	LZ	107/109 (98%)	92 (86%)	15 (14%)	0	100	100
68	La	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
69	Lb	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
70	Lc	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
71	Ld	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
72	Le	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
73	Lf	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
74	Lg	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
75	Lh	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
76	Li	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
77	Lj	23/25 (92%)	23 (100%)	0	0	100	100
78	Lk	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
79	Ll	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
81	EF	975/1044 (93%)	857 (88%)	117 (12%)	1 (0%)	48	75
All	All	11953/12207 (98%)	10821 (90%)	1121 (9%)	11 (0%)	49	75

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
81	EF	418	PRO
16	D	109	GLU
22	I	25	GLN
22	I	29	GLU
41	LF	4	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	170/173 (98%)	170 (100%)	0	100	100
4	Q	200/205 (98%)	198 (99%)	2 (1%)	68	76
5	E	95/98 (97%)	93 (98%)	2 (2%)	47	67
6	R	175/175 (100%)	171 (98%)	4 (2%)	44	66
7	A	182/182 (100%)	179 (98%)	3 (2%)	55	72
8	S	220/220 (100%)	218 (99%)	2 (1%)	70	78
9	B	172/173 (99%)	171 (99%)	1 (1%)	78	81
10	T	189/195 (97%)	186 (98%)	3 (2%)	55	72
11	U	163/165 (99%)	161 (99%)	2 (1%)	63	75
12	V	148/159 (93%)	148 (100%)	0	100	100
13	W	156/157 (99%)	155 (99%)	1 (1%)	78	81
14	C	77/85 (91%)	76 (99%)	1 (1%)	61	74
15	X	126/127 (99%)	126 (100%)	0	100	100
16	D	88/98 (90%)	85 (97%)	3 (3%)	32	59
17	Y	127/127 (100%)	125 (98%)	2 (2%)	55	72
18	Z	90/96 (94%)	88 (98%)	2 (2%)	45	66
19	F	117/117 (100%)	116 (99%)	1 (1%)	70	78
20	G	101/113 (89%)	100 (99%)	1 (1%)	68	76
21	H	127/128 (99%)	126 (99%)	1 (1%)	73	79
22	I	115/115 (100%)	115 (100%)	0	100	100
23	J	93/93 (100%)	92 (99%)	1 (1%)	65	76
24	a	71/74 (96%)	70 (99%)	1 (1%)	59	73
25	b	110/110 (100%)	110 (100%)	0	100	100
26	c	119/119 (100%)	118 (99%)	1 (1%)	73	79
27	d	112/112 (100%)	110 (98%)	2 (2%)	51	70
28	K	67/73 (92%)	65 (97%)	2 (3%)	36	61
29	e	82/83 (99%)	81 (99%)	1 (1%)	63	75
30	f	70/70 (100%)	69 (99%)	1 (1%)	59	73
31	M	47/47 (100%)	47 (100%)	0	100	100
32	g	50/51 (98%)	49 (98%)	1 (2%)	48	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	N	56/63 (89%)	55 (98%)	1 (2%)	51	70
34	O	250/257 (97%)	245 (98%)	5 (2%)	48	68
35	L	55/56 (98%)	54 (98%)	1 (2%)	51	70
39	LD	190/193 (98%)	189 (100%)	1 (0%)	81	83
40	LE	321/322 (100%)	316 (98%)	5 (2%)	55	72
41	LF	288/288 (100%)	285 (99%)	3 (1%)	68	76
42	LG	241/243 (99%)	240 (100%)	1 (0%)	84	84
43	LH	139/154 (90%)	138 (99%)	1 (1%)	76	80
44	LI	186/186 (100%)	185 (100%)	1 (0%)	81	83
45	LJ	187/191 (98%)	185 (99%)	2 (1%)	65	76
46	LK	168/171 (98%)	167 (99%)	1 (1%)	78	81
47	LL	185/185 (100%)	182 (98%)	3 (2%)	55	72
48	LM	145/147 (99%)	145 (100%)	0	100	100
49	LN	154/154 (100%)	154 (100%)	0	100	100
50	LO	107/107 (100%)	105 (98%)	2 (2%)	50	68
51	LP	175/175 (100%)	174 (99%)	1 (1%)	78	81
52	LQ	160/160 (100%)	158 (99%)	2 (1%)	61	74
53	LR	138/145 (95%)	137 (99%)	1 (1%)	76	80
54	Lm	150/150 (100%)	147 (98%)	3 (2%)	48	68
55	Ln	152/153 (99%)	150 (99%)	2 (1%)	61	74
56	Lo	155/155 (100%)	154 (99%)	1 (1%)	78	81
57	Lp	135/136 (99%)	134 (99%)	1 (1%)	76	80
58	Lq	87/87 (100%)	86 (99%)	1 (1%)	65	76
59	Lr	104/104 (100%)	104 (100%)	0	100	100
60	LS	56/108 (52%)	56 (100%)	0	100	100
61	LT	104/105 (99%)	102 (98%)	2 (2%)	50	68
62	LU	108/108 (100%)	107 (99%)	1 (1%)	70	78
63	LV	112/115 (97%)	111 (99%)	1 (1%)	70	78
64	LW	117/118 (99%)	116 (99%)	1 (1%)	70	78
65	LX	46/46 (100%)	46 (100%)	0	100	100
66	LY	81/81 (100%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	LZ	92/96 (96%)	90 (98%)	2 (2%)	45	66
68	La	107/109 (98%)	106 (99%)	1 (1%)	70	78
69	Lb	90/90 (100%)	89 (99%)	1 (1%)	65	76
70	Lc	95/95 (100%)	94 (99%)	1 (1%)	65	76
71	Ld	104/104 (100%)	102 (98%)	2 (2%)	50	68
72	Le	80/81 (99%)	80 (100%)	0	100	100
73	Lf	67/67 (100%)	67 (100%)	0	100	100
74	Lg	68/68 (100%)	68 (100%)	0	100	100
75	Lh	45/45 (100%)	45 (100%)	0	100	100
76	Li	45/47 (96%)	45 (100%)	0	100	100
77	Lj	22/23 (96%)	20 (91%)	2 (9%)	9	31
78	Lk	87/88 (99%)	86 (99%)	1 (1%)	65	76
79	Ll	71/71 (100%)	71 (100%)	0	100	100
81	EF	789/885 (89%)	785 (100%)	4 (0%)	81	83
All	All	9973/10272 (97%)	9874 (99%)	99 (1%)	65	76

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	LG	110	LEU
53	LR	79	THR
44	LI	168	ILE
47	LL	191	LYS
55	Ln	6	THR

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

Mol	Chain	Res	Type
44	LI	37	ASN
81	EF	296	ASN
47	LL	51	HIS
81	EF	271	ASN
81	EF	611	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1768/1771 (99%)	534 (30%)	54 (3%)
2	1	6/7 (85%)	1 (16%)	0
36	LA	3220/3223 (99%)	751 (23%)	42 (1%)
37	LB	120/121 (99%)	15 (12%)	1 (0%)
38	LC	157/158 (99%)	32 (20%)	3 (1%)
80	Sm	74/75 (98%)	24 (32%)	0
80	Sn	74/75 (98%)	23 (31%)	0
All	All	5419/5430 (99%)	1380 (25%)	100 (1%)

5 of 1380 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	14	C
1	2	25	C
1	2	26	A

5 of 100 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	LA	637	C
36	LA	1582	C
38	LC	125	U
36	LA	849	C
36	LA	1097	G

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are 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
82	ATP	EF	1101	-	32,33,33	1.28	4 (12%)	48,52,52	1.91	13 (27%)
82	ATP	EF	1102	-	32,33,33	1.32	5 (15%)	48,52,52	1.86	8 (16%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	ATP	EF	1101	-	-	2/22/38/38	0/3/3/3
82	ATP	EF	1102	-	-	0/22/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	EF	1101	ATP	C5-C4	4.31	1.46	1.39
82	EF	1102	ATP	C5-C4	4.12	1.46	1.39
82	EF	1102	ATP	C5-N7	-2.73	1.34	1.39
82	EF	1101	ATP	C5-N7	-2.57	1.34	1.39
82	EF	1101	ATP	C5-C6	2.44	1.47	1.41

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	EF	1102	ATP	C5-C4-N3	-5.72	118.85	126.72
82	EF	1101	ATP	C5-C4-N3	-5.66	118.92	126.72
82	EF	1102	ATP	N3-C4-N9	4.80	135.32	127.17
82	EF	1101	ATP	N3-C4-N9	4.72	135.19	127.17
82	EF	1102	ATP	C4-C5-N7	-3.67	106.38	110.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

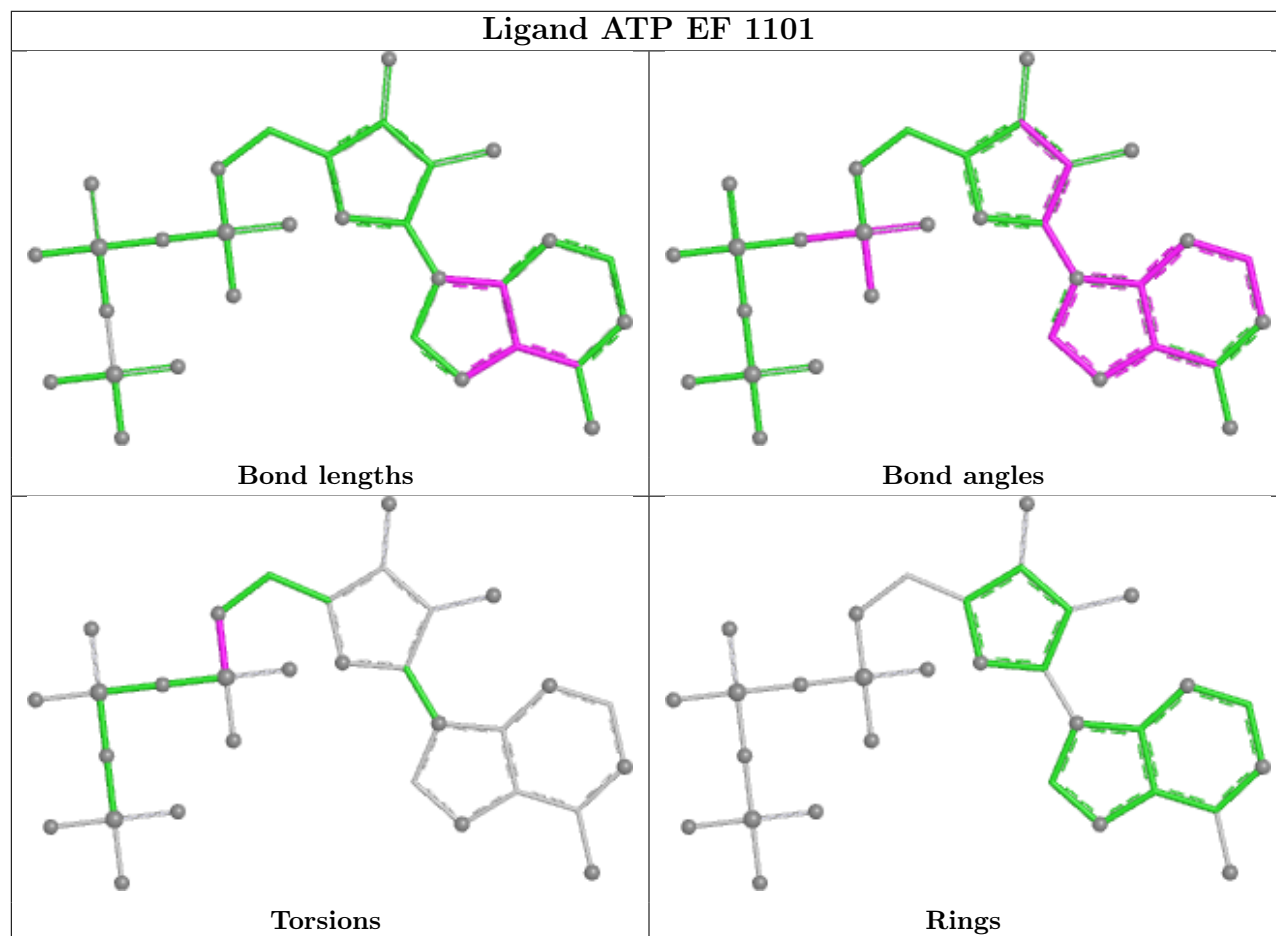
Mol	Chain	Res	Type	Atoms
82	EF	1101	ATP	C5'-O5'-PA-O2A
82	EF	1101	ATP	C5'-O5'-PA-O3A

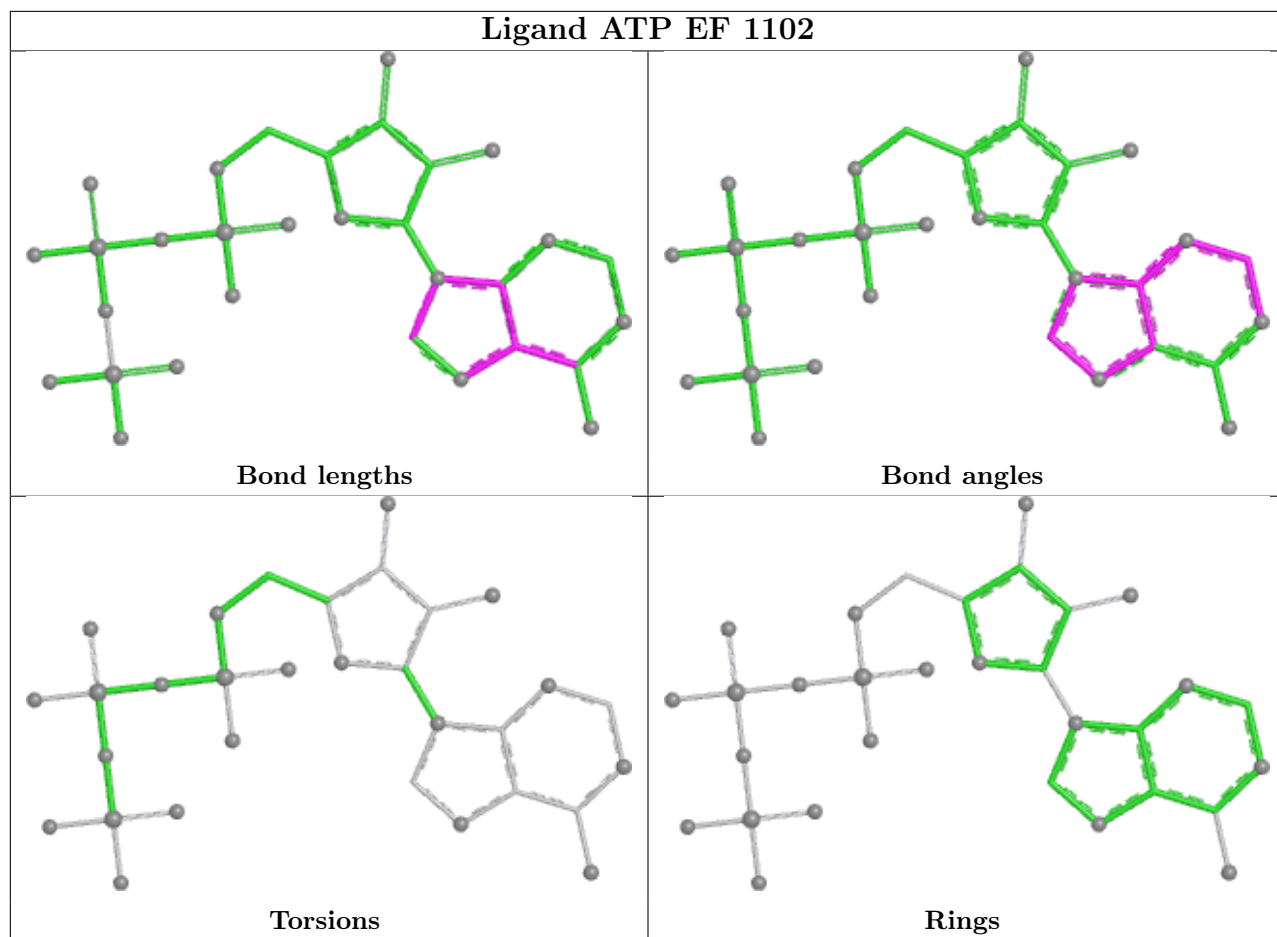
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	EF	1101	ATP	1	0
82	EF	1102	ATP	4	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
36	LA	2
1	2	2
6	R	1
45	LJ	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	LA	1955:U	O3'	2093:A	P	27.27
1	2	658:C	O3'	676:G	P	15.54

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	LA	451:U	O3'	486:A	P	11.17
1	2	714:G	O3'	726:C	P	10.44
1	R	60:SER	C	61:LEU	N	1.18

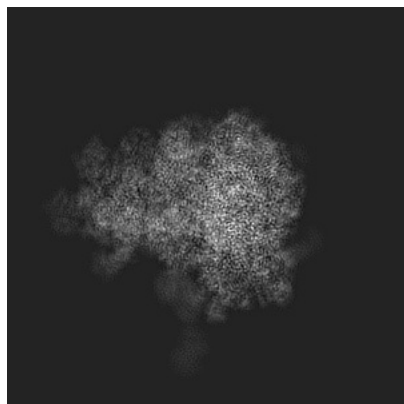
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12081. These allow visual inspection of the internal detail of the map and identification of artifacts.

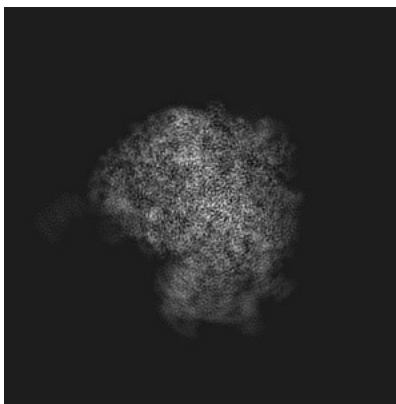
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

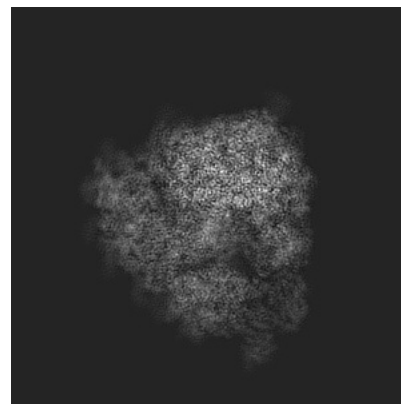
#### 6.1.1 Primary map



X

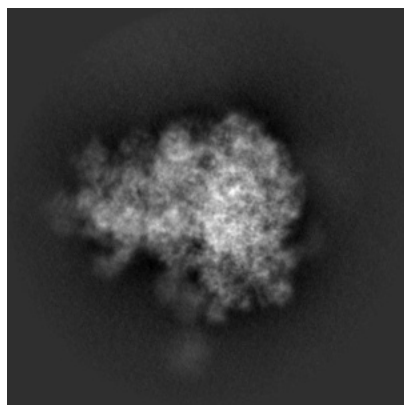


Y

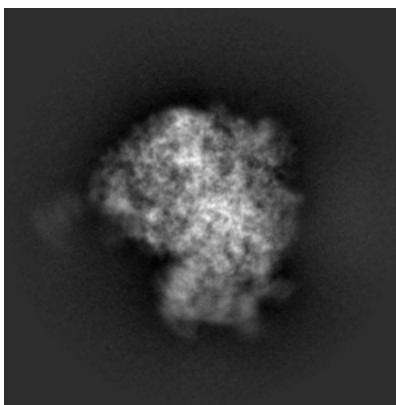


Z

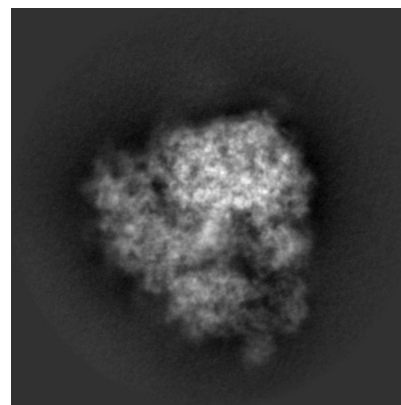
#### 6.1.2 Raw map



X



Y

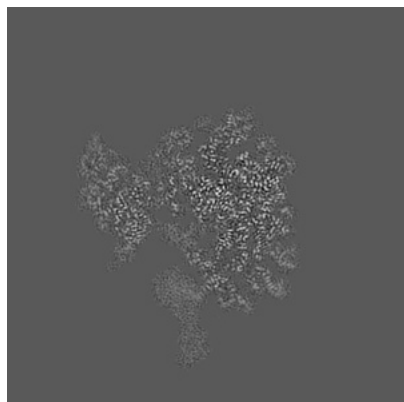


Z

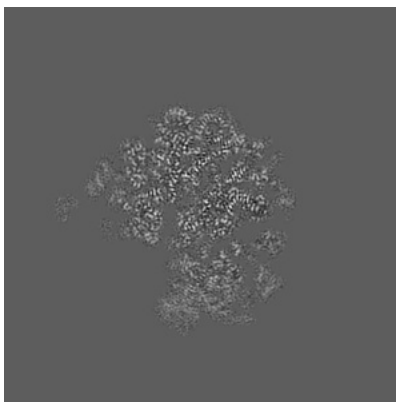
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

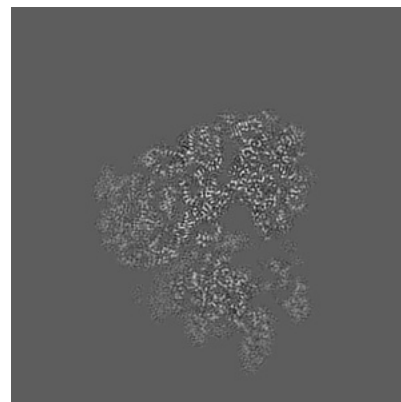
### 6.2.1 Primary map



X Index: 210

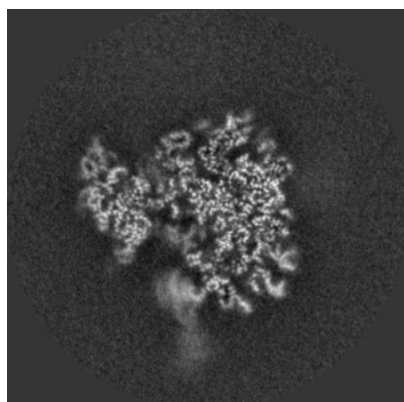


Y Index: 210

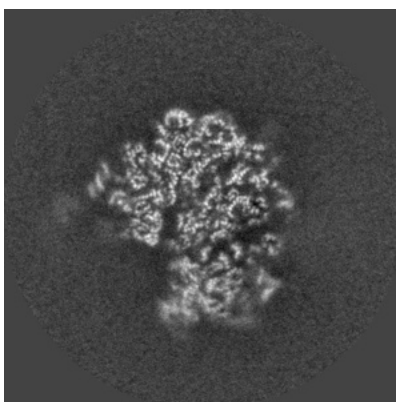


Z Index: 210

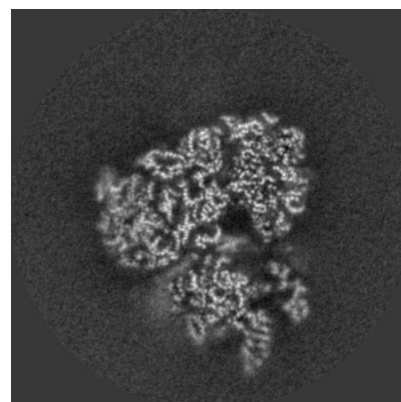
### 6.2.2 Raw map



X Index: 210



Y Index: 210

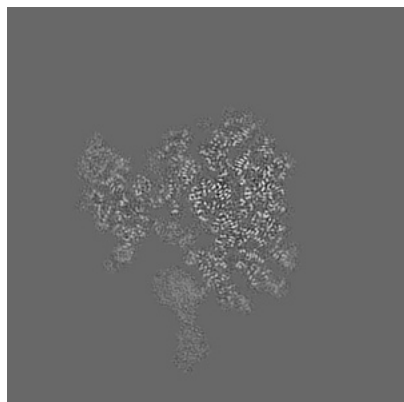


Z Index: 210

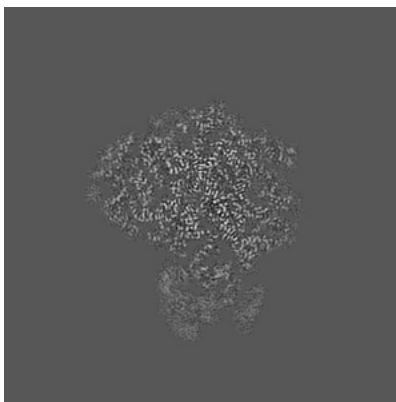
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

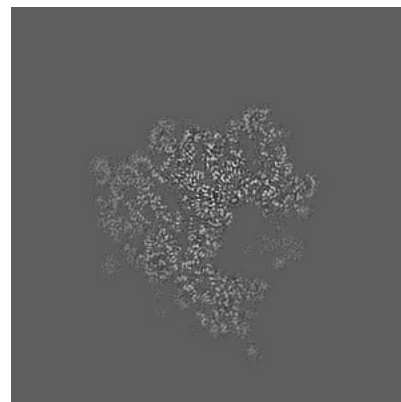
### 6.3.1 Primary map



X Index: 207

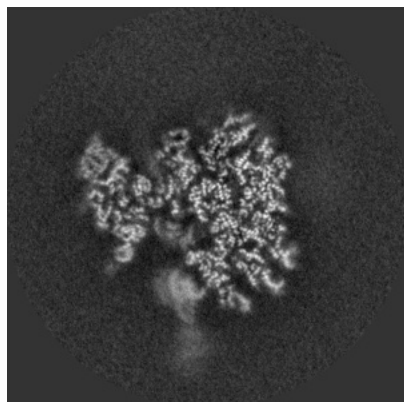


Y Index: 228

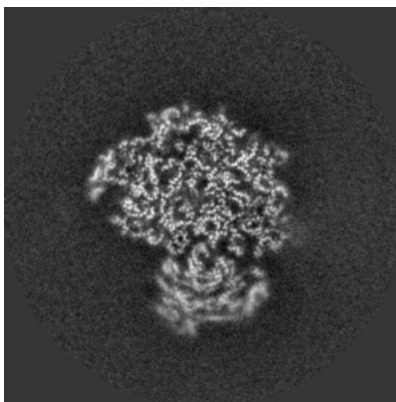


Z Index: 228

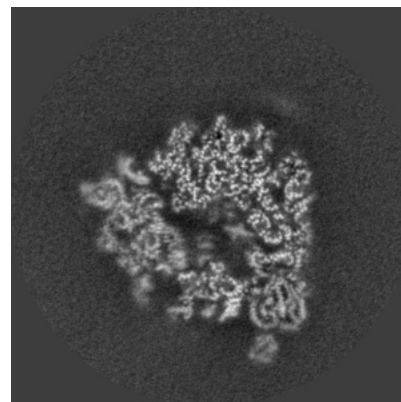
### 6.3.2 Raw map



X Index: 207



Y Index: 219

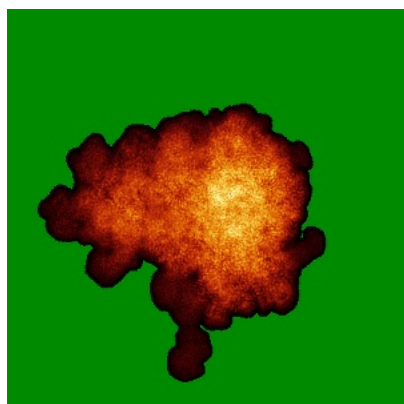


Z Index: 192

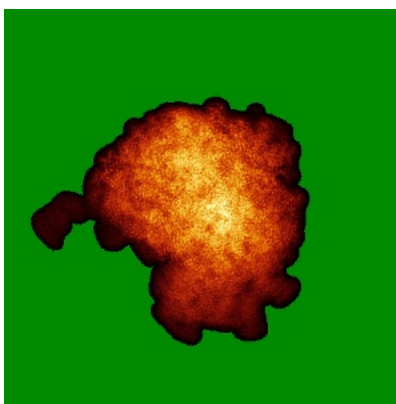
The images above show the largest variance slices of the map in three orthogonal directions.

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

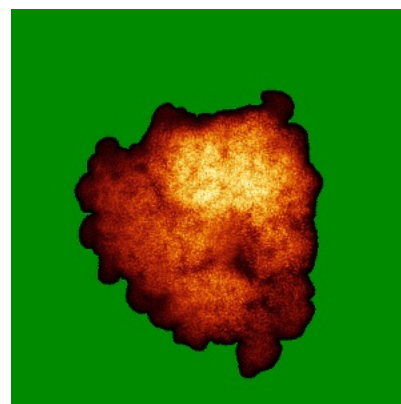
### 6.4.1 Primary map



X

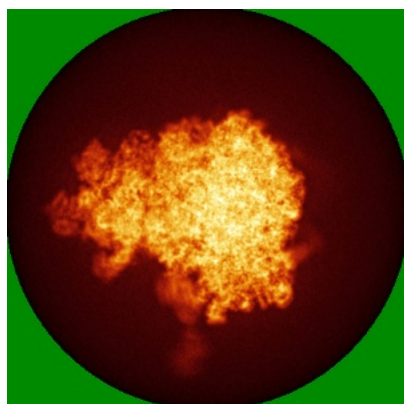


Y

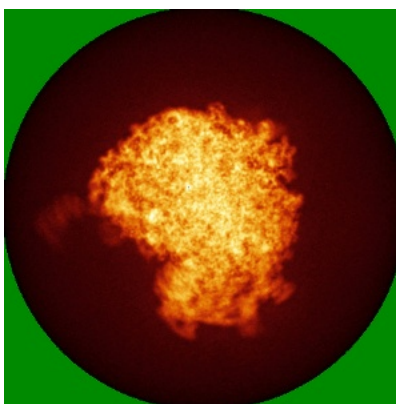


Z

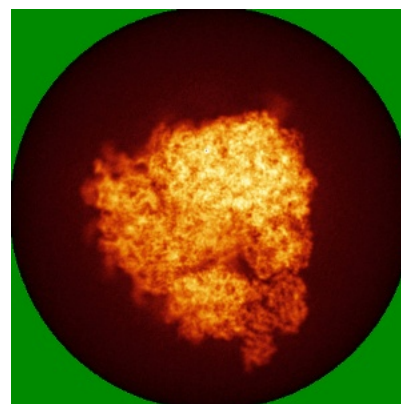
### 6.4.2 Raw map



X



Y

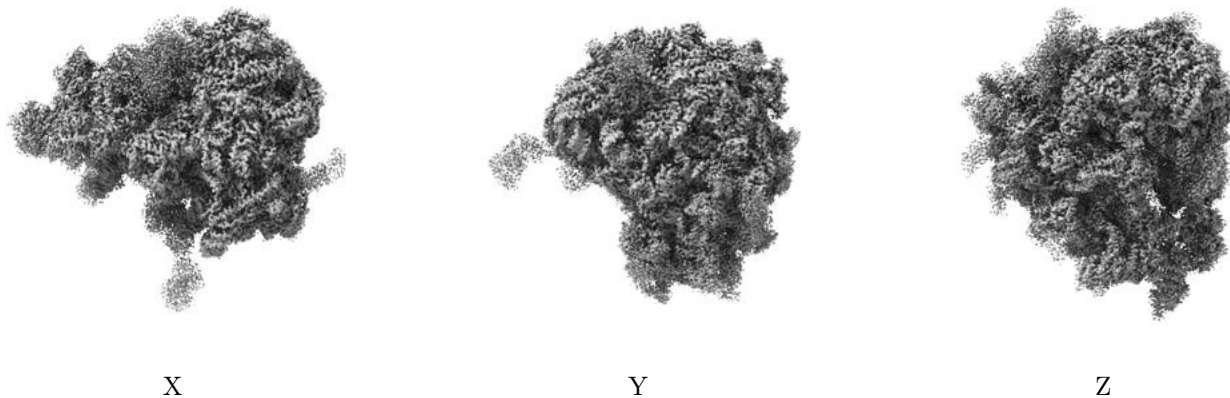


Z

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

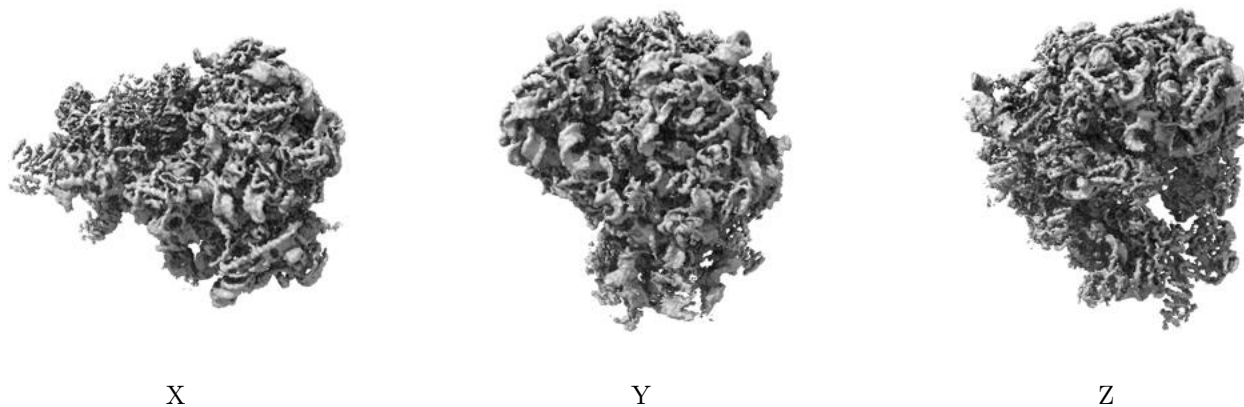
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

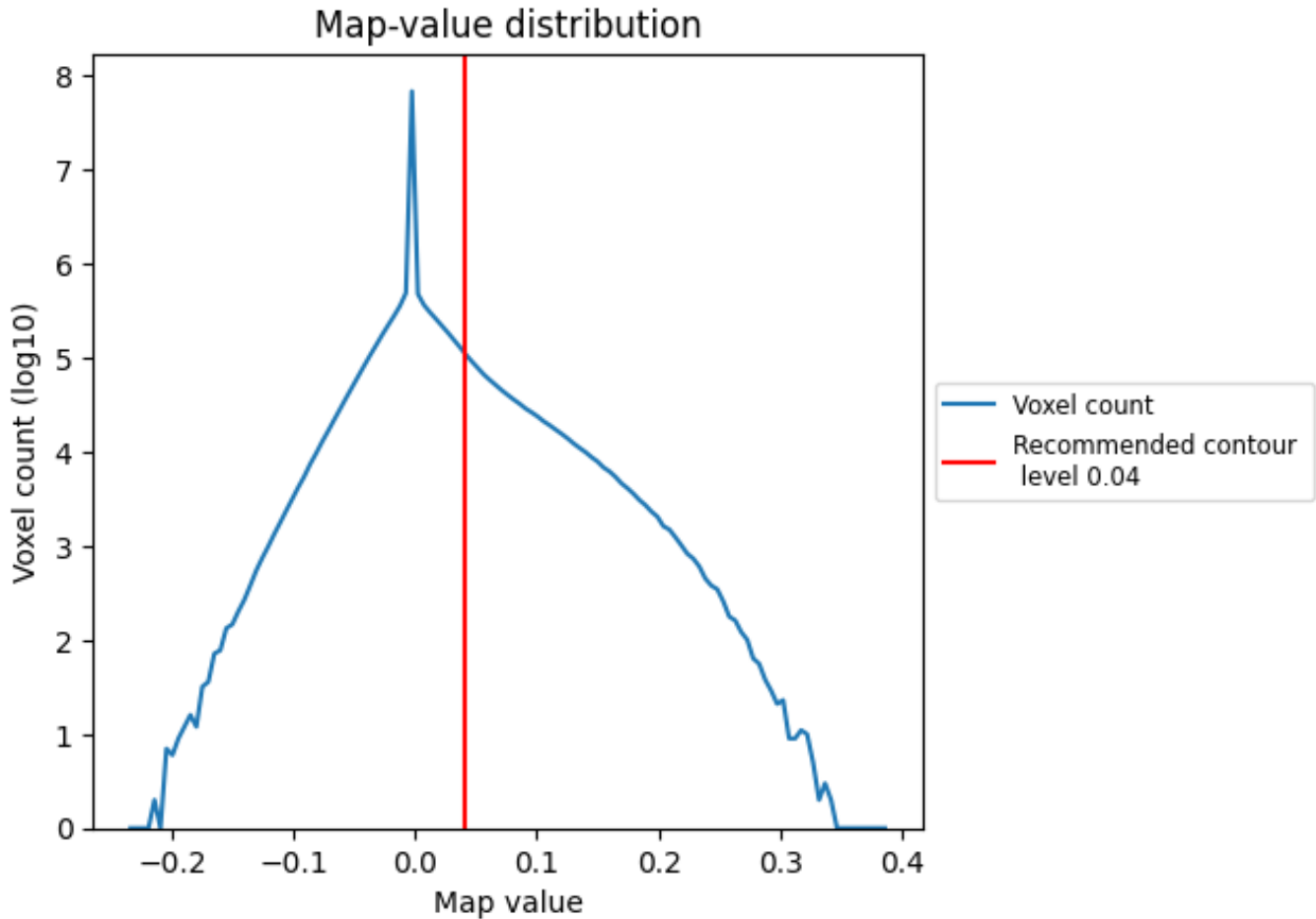
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

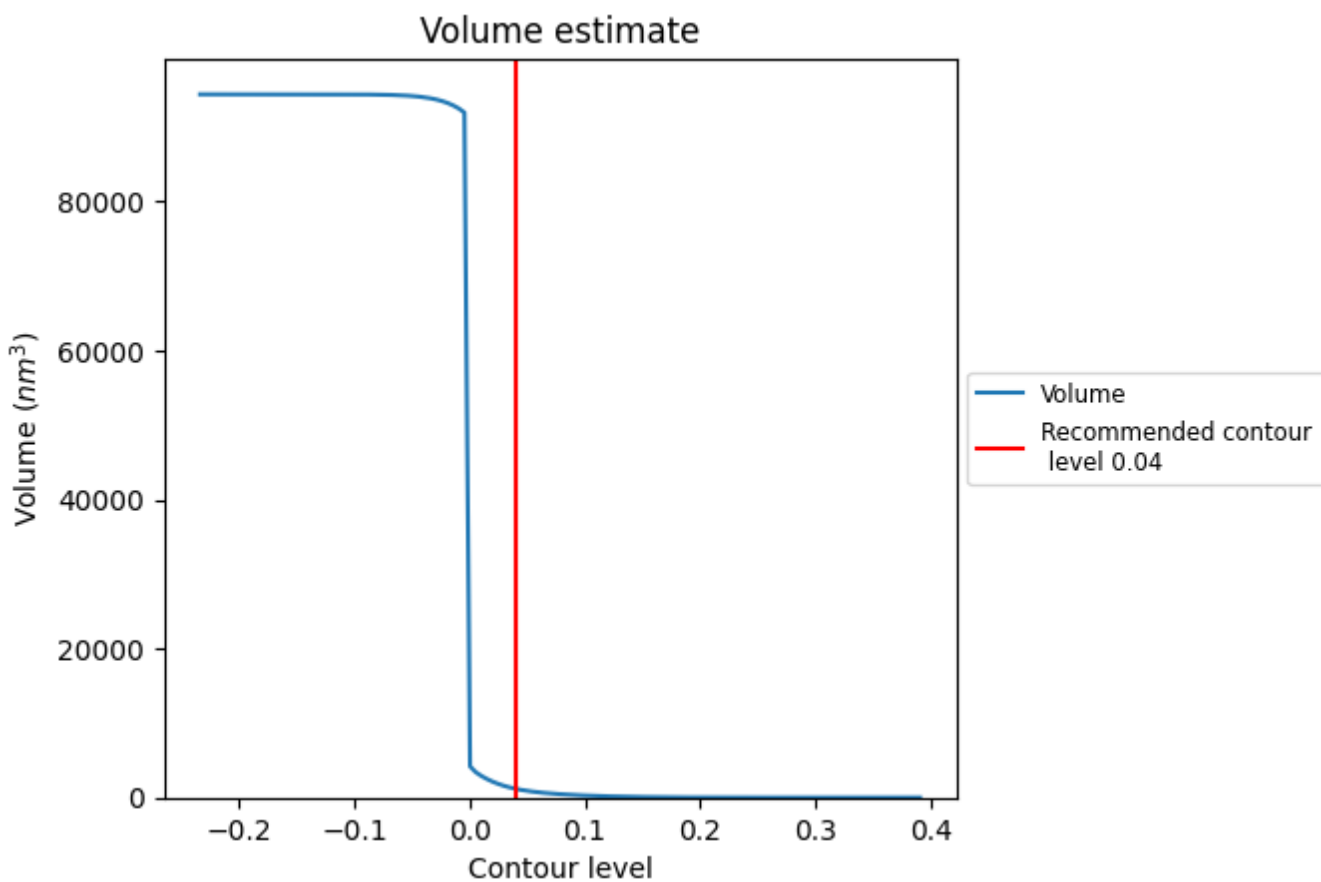
This section contains the results of statistical analysis of the map.

### 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.

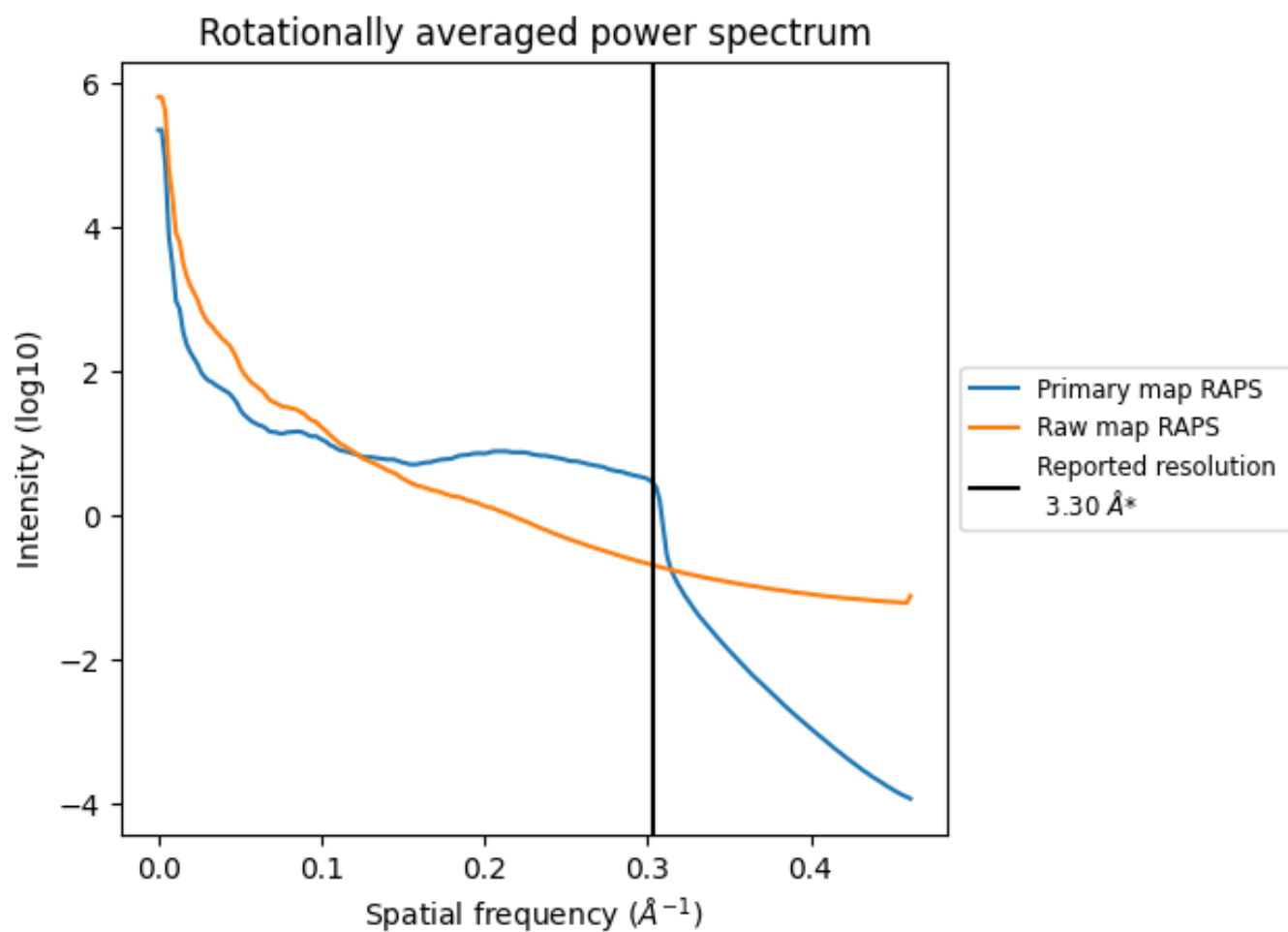
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1176  $\text{nm}^3$ ; this corresponds to an approximate mass of 1062 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

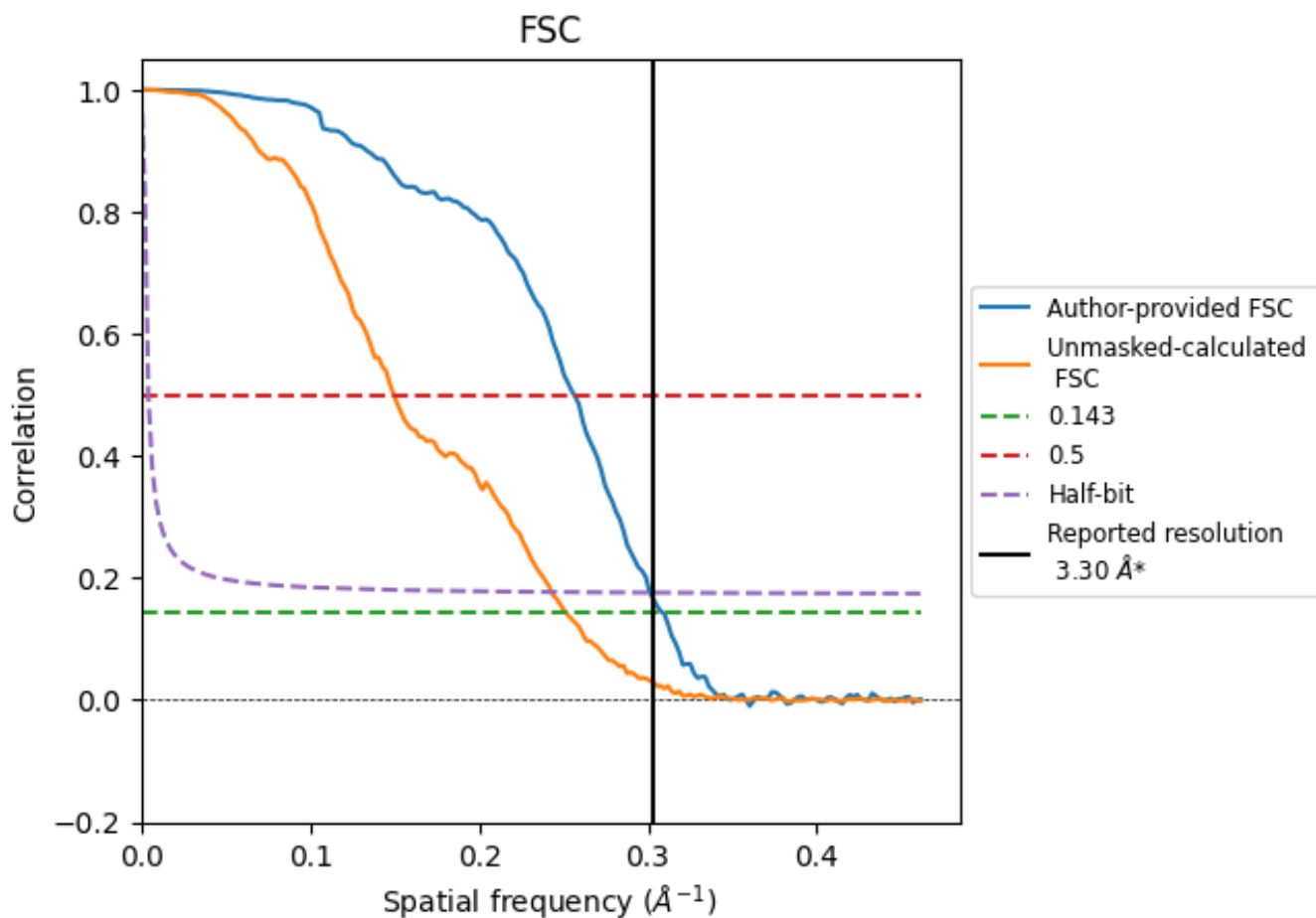


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

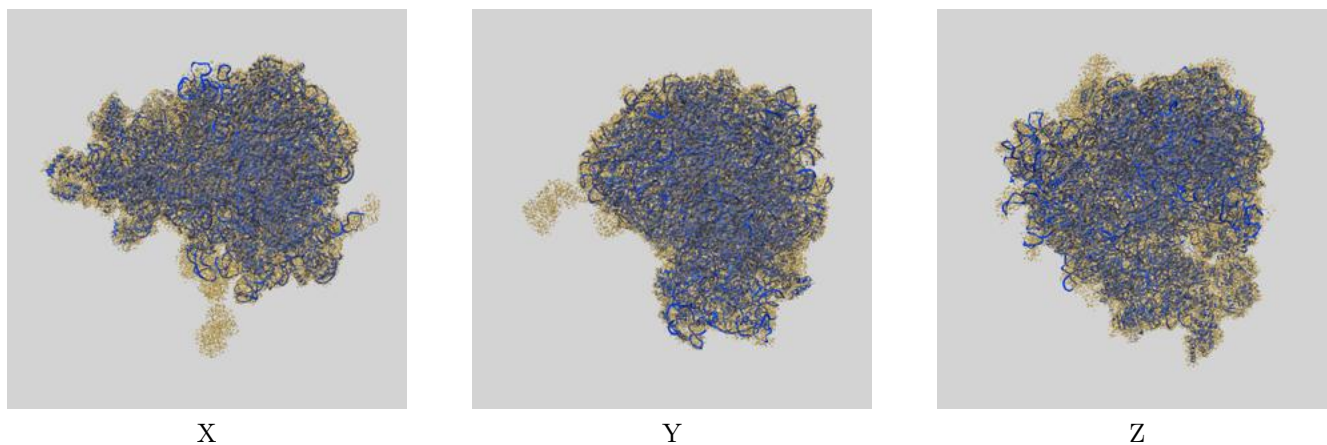
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.24	3.90	3.32
Unmasked-calculated*	3.98	6.68	4.12

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.3 by more than 10 %

## 9 Map-model fit [i](#)

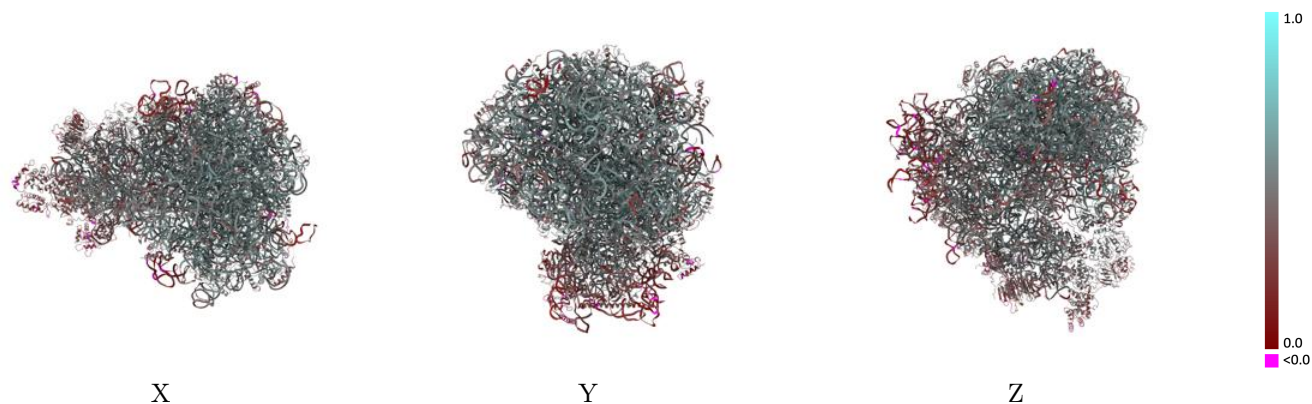
This section contains information regarding the fit between EMDB map EMD-12081 and PDB model 7B7D. Per-residue inclusion information can be found in section 3 on page 20.

### 9.1 Map-model overlay [i](#)



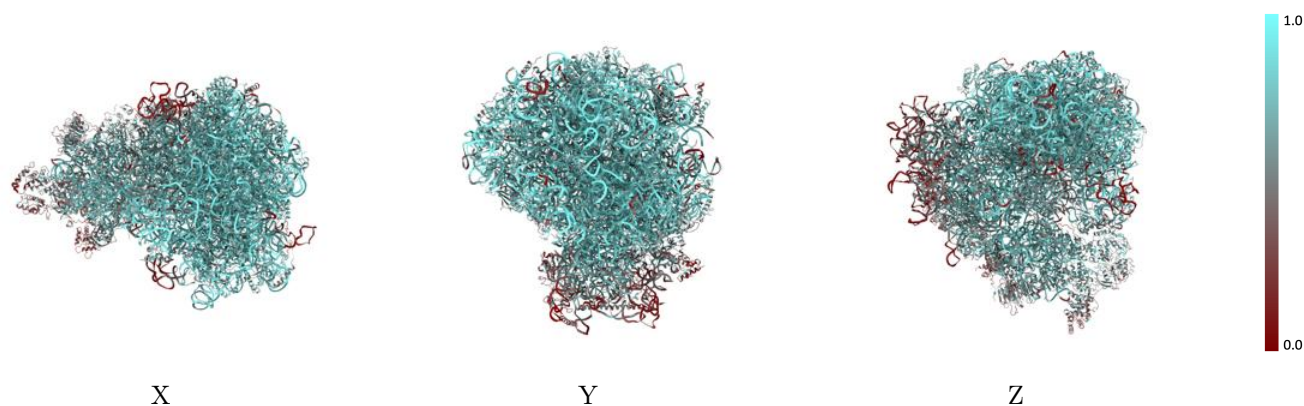
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



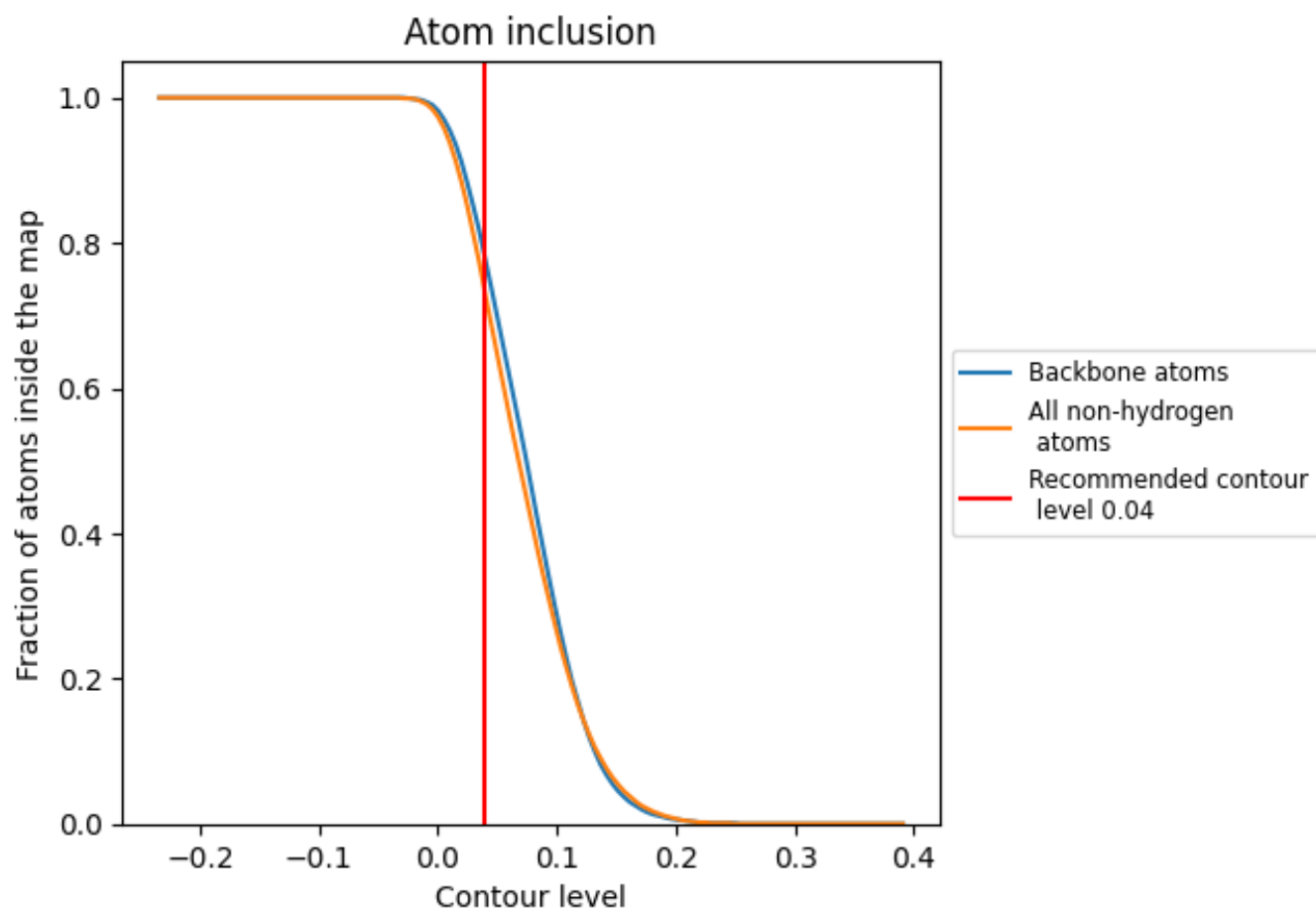
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 73% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7290	 0.4640
1	 0.7920	 0.5060
2	 0.7210	 0.4320
A	 0.5500	 0.3880
B	 0.6250	 0.4200
C	 0.5240	 0.3600
D	 0.1780	 0.1740
E	 0.5960	 0.3720
EF	 0.5300	 0.3800
F	 0.6830	 0.4600
G	 0.5620	 0.3970
H	 0.6630	 0.4310
I	 0.6900	 0.4610
J	 0.5550	 0.3880
K	 0.5510	 0.3510
L	 0.5730	 0.3960
LA	 0.8460	 0.5110
LB	 0.9010	 0.5280
LC	 0.8830	 0.5340
LD	 0.8060	 0.5400
LE	 0.7770	 0.5110
LF	 0.7670	 0.5080
LG	 0.7200	 0.4630
LH	 0.6570	 0.4420
LI	 0.7670	 0.5060
LJ	 0.6720	 0.4510
LK	 0.7140	 0.4790
LL	 0.6820	 0.4670
LM	 0.7090	 0.4590
LN	 0.7380	 0.5010
LO	 0.7240	 0.4810
LP	 0.8140	 0.5480
LQ	 0.7650	 0.5150
LR	 0.7690	 0.5070
LS	 0.5130	 0.3850















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Chain	Atom inclusion	Q-score
LT	 0.7530	 0.5070
LU	 0.7470	 0.5030
LV	 0.7140	 0.4740
LW	 0.7950	 0.5280
LX	 0.7210	 0.4960
LY	 0.6730	 0.4670
LZ	 0.7210	 0.4880
La	 0.7690	 0.5240
Lb	 0.7980	 0.5420
Lc	 0.7230	 0.5140
Ld	 0.7210	 0.4930
Le	 0.6820	 0.4630
Lf	 0.8400	 0.5520
Lg	 0.6330	 0.4260
Lh	 0.7660	 0.5160
Li	 0.7200	 0.4920
Lj	 0.6680	 0.4970
Lk	 0.7580	 0.5130
Ll	 0.7400	 0.5190
Lm	 0.7630	 0.5190
Ln	 0.7010	 0.4730
Lo	 0.7500	 0.5100
Lp	 0.7480	 0.5080
Lq	 0.6610	 0.4310
Lr	 0.7100	 0.4990
M	 0.7560	 0.4810
N	 0.2840	 0.2210
O	 0.4890	 0.3320
P	 0.6060	 0.4190
Q	 0.5690	 0.4120
R	 0.6370	 0.4490
S	 0.4670	 0.3650
Sm	 0.3710	 0.3140
Sn	 0.5750	 0.3680
T	 0.3780	 0.2810
U	 0.4310	 0.3330
V	 0.6210	 0.4270
W	 0.4410	 0.3450
X	 0.5830	 0.4370
Y	 0.6330	 0.4370
Z	 0.6660	 0.4590
a	 0.6100	 0.4220

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Chain	Atom inclusion	Q-score
b	 0.6780	 0.4810
c	 0.5630	 0.4070
d	 0.4090	 0.3280
e	 0.7120	 0.4760
f	 0.5490	 0.3830
g	 0.4100	 0.2890