



wwPDB EM Validation Summary Report ⓘ

Aug 26, 2026 – 07:54 pm BST

PDB ID : 9T7T / pdb_00009t7t
EMDB ID : EMD-55657
Title : CryoEM structure of Candida auris 80S ribosome in complex with Blasticidin S
Authors : Atamas, A.; Stetsenko, A.; Incarnato, D.; Macia Valero, A.; Rogachev, A.; Billerbeck, S.; Guskov, A.
Deposited on : 2025-11-11
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

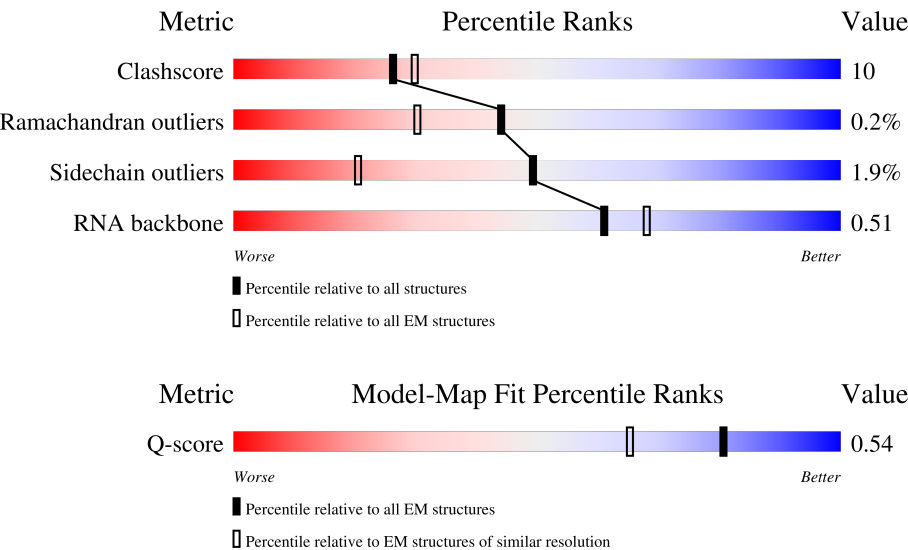
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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.



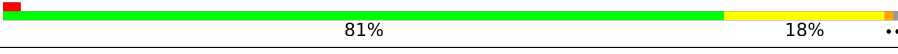
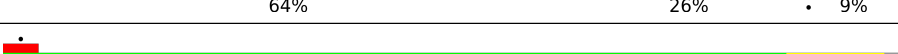
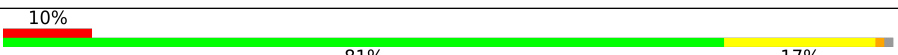
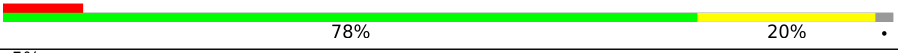
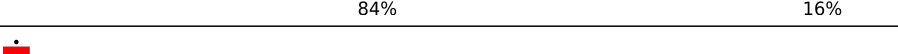
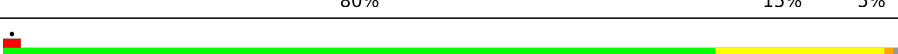
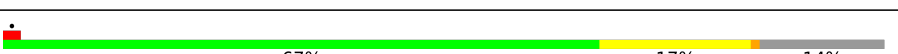
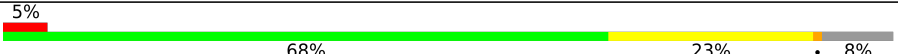
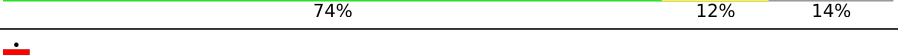
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	A	3283	
2	B	122	
3	C	158	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	254	
5	E	389	
6	F	363	
7	G	298	
8	H	165	
9	I	241	
10	J	263	
11	K	191	
12	L	220	
13	M	172	
14	N	198	
15	O	131	
16	P	204	
17	Q	200	
18	R	185	
19	S	186	
20	T	208	
21	U	186	
22	V	160	
23	W	119	
24	X	137	
25	Y	156	
26	Z	140	
27	CA	1775	
28	ZA	204	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	ZB	189	
30	a	127	
31	b	136	
32	c	149	
33	d	76	
34	e	105	
35	f	113	
36	g	149	
37	h	107	
38	i	115	
39	j	120	
40	k	99	
41	l	85	
42	m	78	
43	n	51	
44	o	52	
45	q	106	
46	r	99	
47	1	76	
48	2	7	
49	3	17	
50	ZC	123	
51	ZD	155	
52	ZE	151	
53	ZF	132	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	ZG	141	
55	ZH	142	
56	ZI	137	
57	ZJ	145	
58	ZK	145	
59	ZL	118	
60	ZM	87	
61	ZO	130	
62	ZP	145	
63	ZQ	135	
64	ZR	130	
65	ZS	182	
66	ZT	82	
67	ZU	67	
68	ZV	56	
69	ZW	63	
70	ZY	315	
71	p	25	
72	s	264	
73	t	256	
74	u	249	
75	v	250	
76	w	264	
77	x	223	
78	y	236	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	z	188	18% 62% 32%

2 Entry composition

There are 83 unique types of molecules in this entry. The entry contains 193216 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3030	Total	C	N	O	P	0	0
			64825	28944	11716	21135	3030		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	122	Total	C	N	O	P	0	0
			2609	1164	470	853	122		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	154	Total	C	N	O	P	0	0
			3274	1464	577	1079	154		

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	247	Total	C	N	O	S	0	0
			1873	1170	377	324	2		

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	387	Total	C	N	O	S	0	0
			3087	1957	579	544	7		

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	361	Total	C	N	O	S	0	0
			2786	1751	534	498	3		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	291	Total	C	N	O	S	0	0
			2370	1506	411	449	4		

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	150	Total	C	N	O	S	0	0
			1183	761	214	208			

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	237	Total	C	N	O	S	0	0
			1913	1230	345	336	2		

- Molecule 10 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	233	Total	C	N	O	S	0	0
			1847	1182	339	322	4		

- Molecule 11 is a protein called 60S ribosomal protein L9-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	190	Total	C	N	O	S	0	0
			1519	965	272	278	4		

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	211	Total	C	N	O	S	0	0
			1720	1087	327	298	8		

- Molecule 13 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	170	Total	C	N	O	S	0	0
			1364	854	261	244	5		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	194	Total	C	N	O	S	0	0
			1538	962	306	269	1		

- Molecule 15 is a protein called Large ribosomal subunit protein eL14 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	129	Total	C	N	O	S	0	0
			1030	657	194	178	1		

- Molecule 16 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	203	Total	C	N	O	S	0	0
			1703	1066	356	279	2		

- Molecule 17 is a protein called 60S ribosomal protein L16-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1587	1020	299	266	2		

- Molecule 18 is a protein called 60S ribosomal protein L17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	176	Total	C	N	O		0	0
			1418	882	286	250			

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	185	Total	C	N	O		0	0
			1456	919	293	244			

- Molecule 20 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	178	Total	C	N	O	S	0	0
			1435	888	307	236	4		

- Molecule 21 is a protein called 60S ribosomal protein eL20 (formerly L20).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	172	Total	C	N	O	S	0	0
			1448	941	261	242	4		

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	159	Total	C	N	O	S	0	0
			1282	816	242	221	3		

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	107	Total	C	N	O		0	0
			871	566	148	157			

- Molecule 24 is a protein called 60S ribosomal protein L23-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	137	Total	C	N	O	S	0	0
			1013	636	189	179	9		

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	62	Total	C	N	O	S	0	0
			517	330	103	83	1		

- Molecule 26 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	120	Total	C	N	O		0	0
			955	607	175	173			

- Molecule 27 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CA	1636	Total	C	N	O	P	0	0
			34938	15612	6249	11441	1636		

- Molecule 28 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	ZA	194	Total	C	N	O	S	0	0
			1545	958	309	276	2		

- Molecule 29 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	ZB	178	Total	C	N	O	S	0	0
			1459	921	287	249	2		

- Molecule 30 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	126	Total	C	N	O	S	0	0
			994	624	188	181	1		

- Molecule 31 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	135	Total	C	N	O	S	0	0
			1081	691	207	182	1		

- Molecule 32 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	148	Total	C	N	O	S	0	0
			1174	742	234	196	2		

- Molecule 33 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	d	60	Total	C	N	O	0	0
			498	302	114	82		

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	99	Total	C	N	O	S	0	0
			744	476	125	139	4		

- Molecule 35 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	109	Total	C	N	O	S	0	0
			895	563	173	156	3		

- Molecule 36 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	123	Total	C	N	O	S	0	0
			1002	629	201	170	2		

- Molecule 37 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	106	Total	C	N	O	S	0	0
			859	544	168	146	1		

- Molecule 38 is a protein called 60S ribosomal protein L34-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	113	Total	C	N	O	S	0	0
			897	558	179	156	4		

- Molecule 39 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	j	118	Total	C	N	O	0	0
			956	603	191	162		

- Molecule 40 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	98	Total	C	N	O	S	0	0
			774	479	163	131	1		

- Molecule 41 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	83	Total	C	N	O	S	0	0
			654	396	142	109	7		

- Molecule 42 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	m	77	Total	C	N	O	0	0
			617	396	112	109		

- Molecule 43 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	n	50	Total	C	N	O	0	0
			442	277	98	67		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	50	ASN	GLY	conflict	UNP A0A1D8PDT4

- Molecule 44 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	52	Total	C	N	O	S	0	0
			419	260	86	67	6		

- Molecule 45 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	103	Total	C	N	O	S	0	0
			822	517	164	136	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	90	Total	C	N	O	S	0	0
			691	425	141	121	4		

- Molecule 47 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1	35	Total	C	N	O	P	0	0
			750	335	138	242	35		

- Molecule 48 is a RNA chain called RNA (5'-R(P*CP*GP*AP*UP*UP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
48	2	7	Total	C	N	O	P	0	0
			147	66	25	49	7		

- Molecule 49 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3	17	Total	C	N	O	P	0	0
			365	163	68	117	17		

- Molecule 50 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	ZC	91	Total	C	N	O		0	0
			770	502	126	142			

- Molecule 51 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	ZD	142	Total	C	N	O	S	0	0
			1145	732	218	192	3		

- Molecule 52 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	ZE	149	Total	C	N	O	S	0	0
			1184	755	220	208	1		

- Molecule 53 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	ZF	127	Total	C	N	O	S	0	0
			945	578	188	176	3		

- Molecule 54 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	ZG	116	Total	C	N	O	S	0	0
			904	582	161	156	5		

- Molecule 55 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	ZH	140	Total	C	N	O	S	0	0
			1091	700	200	190	1		

- Molecule 56 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	ZI	126	Total	C	N	O	S	0	0
			1012	636	185	190	1		

- Molecule 57 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	ZJ	142	Total	C	N	O	S	0	0
			1170	733	229	204	4		

- Molecule 58 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	ZK	141	Total	C	N	O		0	0
			1101	691	208	202			

- Molecule 59 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	ZL	100	Total	C	N	O	S	0	0
			782	496	142	142	2		

- Molecule 60 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	ZM	87	Total	C	N	O	S	0	0
			678	415	127	134	2		

- Molecule 61 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	ZO	129	Total	C	N	O	S	0	0
			1032	656	190	183	3		

- Molecule 62 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	ZP	143	Total	C	N	O	S	0	0
			1109	698	219	190	2		

- Molecule 63 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	ZQ	132	Total	C	N	O	S	0	0
			1073	677	207	189			

- Molecule 64 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	ZR	71	Total	C	N	O	S	0	0
			564	360	104	99	1		

- Molecule 65 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	ZS	98	Total	C	N	O	S	0	0
			785	484	166	129	6		

- Molecule 66 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	ZT	81	Total	C	N	O	S	0	0
			617	383	112	115	7		

- Molecule 67 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	ZU	61	Total	C	N	O	S	0	0
			477	293	94	88	2		

- Molecule 68 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	ZV	54	Total	C	N	O	S	0	0
			449	278	93	74	4		

- Molecule 69 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	ZW	54	Total	C	N	O	S	0	0
			432	270	87	73	2		

- Molecule 70 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	ZY	308	Total	C	N	O	S	0	0
			2383	1510	405	464	4		

- Molecule 71 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	p	8	Total	C	N	O	S	0	0
			79	50	18	10	1		

- Molecule 72 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	s	217	Total	C	N	O	S	0	0
			1705	1087	297	318	3		

- Molecule 73 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	t	212	Total	C	N	O	S	0	0
			1703	1082	312	305	4		

- Molecule 74 is a protein called Rps21 ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	u	216	Total	C	N	O	S	0	0
			1636	1048	287	296	5		

- Molecule 75 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	v	224	Total	C	N	O	S	0	0
			1737	1109	314	309	5		

- Molecule 76 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	w	260	Total	C	N	O	S	0	0
			2056	1303	386	361	6		

- Molecule 77 is a protein called 40S ribosomal protein uS7 (formerly S5).

Mol	Chain	Residues	Atoms					AltConf	Trace
77	x	206	Total	C	N	O	S	0	0
			1610	1008	300	298	4		

- Molecule 78 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	y	226	Total	C	N	O	S	0	0
			1819	1128	355	331	5		

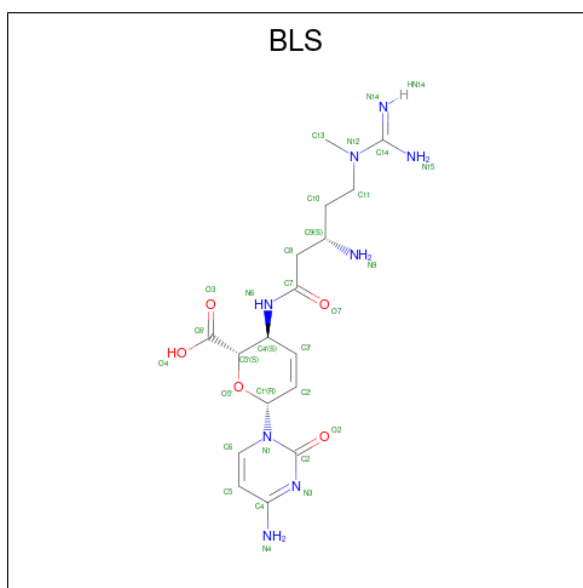
- Molecule 79 is a protein called 40S ribosomal protein eS7 (formerly S7).

Mol	Chain	Residues	Atoms				AltConf	Trace
79	z	183	Total	C	N	O	0	0
			1471	942	265	264		

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	A	152	Total	Mg	0
			152	152	
80	B	3	Total	Mg	0
			3	3	
80	C	1	Total	Mg	0
			1	1	
80	D	1	Total	Mg	0
			1	1	
80	L	2	Total	Mg	0
			2	2	
80	X	1	Total	Mg	0
			1	1	
80	CA	58	Total	Mg	0
			58	58	
80	h	1	Total	Mg	0
			1	1	
80	n	1	Total	Mg	0
			1	1	

- Molecule 81 is BLASTICIDIN S (CCD ID: BLS) (formula: $C_{17}H_{26}N_8O_5$).



Mol	Chain	Residues	Atoms				AltConf
81	A	1	Total	C	N	O	0
			30	17	8	5	

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	i	1	Total	Zn	0
			1	1	
82	l	1	Total	Zn	0
			1	1	
82	o	1	Total	Zn	0
			1	1	
82	q	1	Total	Zn	0
			1	1	
82	r	1	Total	Zn	0
			1	1	
82	ZS	1	Total	Zn	0
			1	1	
82	ZV	1	Total	Zn	0
			1	1	

- Molecule 83 is water.

Mol	Chain	Residues	Atoms		AltConf
83	A	83	Total	O	0
			83	83	

Continued on next page...

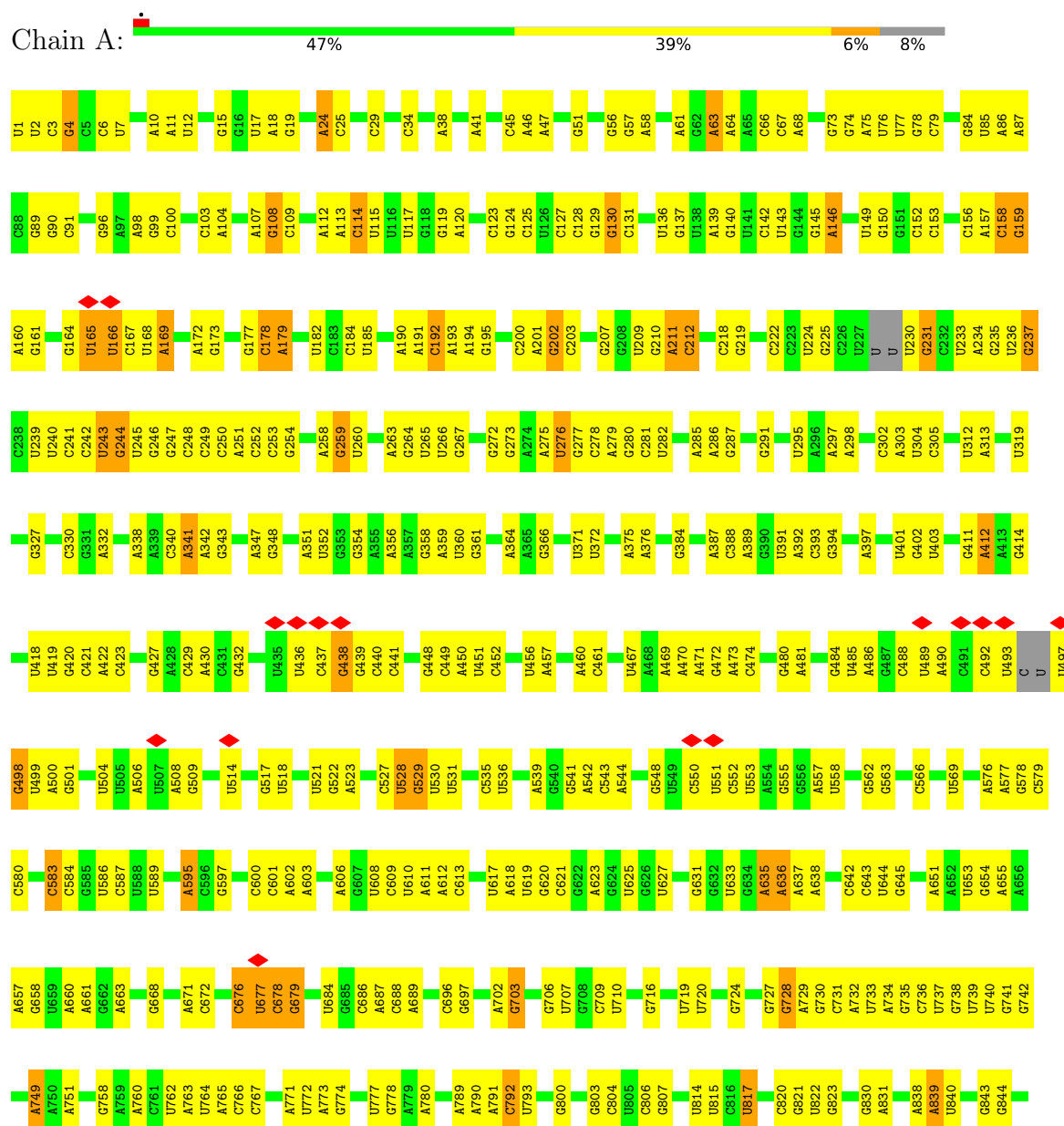
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
83	B	2	Total 2	O 2	0
83	C	3	Total 3	O 3	0
83	E	1	Total 1	O 1	0
83	P	2	Total 2	O 2	0
83	d	1	Total 1	O 1	0
83	i	1	Total 1	O 1	0
83	q	1	Total 1	O 1	0

3 Residue-property plots

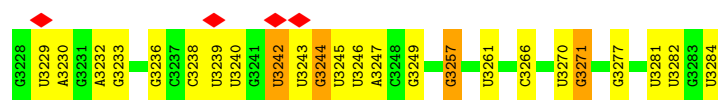
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 25S rRNA

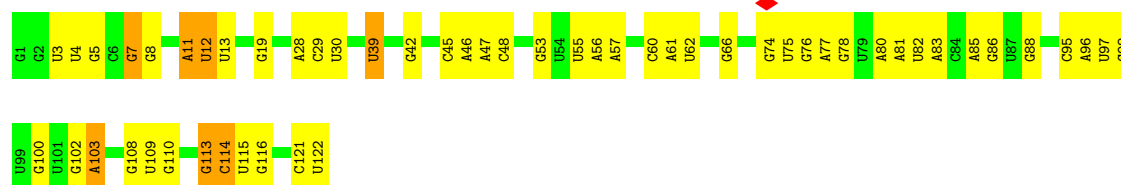


U	A1826	G1729	U1537	C1451	A1350	G1253	A	U115	A1012	A936	G850
C	C1827	A1730	C1538	A1452	C1353	G1254	U	A1116	G1019	U937	G851
G	A1828	U1738	U1539	A1453	U1358	A1255	G	C1122	U1029	C854	C854
C	A1829	G1739	G1540	U1454	C1359	U1256	A	C1123	G1030	A857	A857
C	U1830	A1740	A1544	U1455	G1360	G1257	C	G1124	A1031	A858	A858
A	A1835	A1741	A1547	A1458	A1361	G1260	U	A1127	A1032	A860	A860
A	U1836	A1742	A1547	A1458	A1362	A1265	C	U1128	U1035	A864	A864
A	U1837	U1744	C1551	G1466	C1363	G1266	C	G1129	G1036	G867	G867
C	A1838	C1745	A1552	A1467	G1364	C1267	G	U1130	U1041	C871	C871
U	G1839	C1746	A1552	A1468	G1365	G1267	G	C1131	A1042	A872	A872
U	G1840	G1747	U1557	G1471	G1368	U1272	A	U1132	G1043	U873	U873
G	G1841	C1748	U1558	G1477	U1368	A1273	U	C1133	A1044	G880	G880
G	A	A1749	G1559	A1478	G1377	A1276	C	G1134	A1045	C881	C881
A	G	G1750	G1560	C1479	U1378	U1276	C	U1135	A1050	C887	C887
G	C	A1751	A1561	C1479	U1379	A1277	C	G1136	U1051	C888	C888
C	C	A1752	U1562	C1480	C1380	U1278	G	U1137	U1052	U889	U889
C	A	A1753	G1563	C1481	U1389	A1279	U	U1138	G1053	G890	G890
C	A	A1754	C1564	U1486	A1402	C1280	A	U1139	C1054	C891	C891
C	A	G1755	G1565	U1487	A1403	A1290	A	A1140	U1055	C887	C887
C	A	G1756	G1566	U1487	A1404	G1291	G	A1141	U1056	C888	C888
C	A	A1756	G1567	C1491	A1406	U1296	G	A1142	U1057	U897	U897
C	A	A1757	A1568	C1492	G1407	U1297	U	C1143	U1058	U898	U898
C	A	U1758	U1570	G1495	A1410	U1298	U	U1148	G1064	U899	U899
C	A	U1759	C1571	A1496	U1413	U1299	U	A1149	C1065	A895	A895
C	A	U1760	U1571	A1497	U1414	C1300	U	A1150	C1066	G896	G896
C	A	U1761	G1575	A1498	U1415	G1301	U	A1151	U1067	U897	U897
C	A	U1762	A1578	A1499	U1420	G1302	U	U1155	U1068	C902	C902
C	A	U1763	C1579	G1502	A1421	U1305	U	U1156	G1074	G806	G806
C	A	U1764	A1582	U1503	U1422	G1306	U	U1157	U1075	U909	U909
C	A	U1765	C1584	C1504	A1424	C1307	U	U1167	A1077	A910	A910
C	A	U1766	U1585	G1505	A1425	G1317	U	C1166	G1078	G911	G911
C	A	U1767	G1586	U1506	G1429	U1320	U	U1167	U1081	C912	C912
C	A	U1768	G1587	U1507	U1430	G1321	U	U1168	C1084	U919	U919
C	A	U1769	U1591	C	G1431	U1322	U	U1169	C1088	C920	C920
C	A	U1770	G1592	U1508	U1432	G1323	U	U1170	U1089	G921	G921
C	A	U1771	A1596	U1508	U1433	G1327	U	U1171	A1090	U922	U922
C	A	U1772	C1597	U1508	U1434	U1328	U	U1172	U1091	U923	U923
C	A	U1773	U1598	U1508	U1435	G1329	U	U1173	U1099	A924	A924
C	A	U1774	G1598	U1508	U1436	G1332	U	U1175	A1100	C925	C925
C	A	U1775	C1599	U1508	U1437	G1333	U	U1176	A1101	A926	A926
C	A	U1776	U1600	U1508	U1438	C1334	U	U1177	U1103	A927	A927
C	A	U1777	G1601	U1508	U1439	U1335	U	U1178	G1104	A928	A928
C	A	U1778	G1602	U1508	U1440	G1336	U	U1179	A1105	C929	C929
C	A	U1779	G1603	U1508	U1441	U1337	U	U1180	A1106	A930	A930
C	A	U1780	G1604	U1508	U1442	U1338	U	U1181	A1107	G931	G931
C	A	U1781	U1605	U1508	U1443	U1339	U	U1182	A1108	U932	U932
C	A	U1782	G1606	U1508	U1444	U1340	U	U1183	A1109	U933	U933
C	A	U1783	G1607	U1508	U1445	U1341	U	U1184	A1110	U934	U934
C	A	U1784	G1608	U1508	U1446	U1342	U	U1185	A1111	U935	U935
C	A	U1785	U1609	U1508	U1447	U1343	U	U1186	A1112		
C	A	U1786	G1610	U1508	U1448	U1344	U	U1187			
C	A	U1787	G1611	U1508	U1449	U1345	U	U1188			
C	A	U1788	U1612	U1508	U1450	U1346	U	U1189			
C	A	U1789	G1613	U1508	U1451	U1347	U	U1190			
C	A	U1790	U1614	U1508	U1452	U1348	U	U1191			
C	A	U1791	G1615	U1508	U1453	U1349	U	U1192			
C	A	U1792	U1616	U1508	U1454	U1350	U	U1193			
C	A	U1793	G1617	U1508	U1455	U1351	U	U1194			
C	A	U1794	U1618	U1508	U1456	U1352	U	U1195			
C	A	U1795	G1619	U1508	U1457	U1353	U	U1196			
C	A	U1796	U1620	U1508	U1458	U1354	U	U1197			
C	A	U1797	G1621	U1508	U1459	U1355	U	U1198			
C	A	U1798	U1622	U1508	U1460	U1356	U	U1199			
C	A	U1799	G1623	U1508	U1461	U1357	U	U1200			
C	A	U1800	U1624	U1508	U1462	U1358	U	U1201			
C	A	U1801	G1625	U1508	U1463	U1359	U	U1202			
C	A	U1802	U1626	U1508	U1464	U1360	U	U1203			
C	A	U1803	G1627	U1508	U1465	U1361	U	U1204			
C	A	U1804	U1628	U1508	U1466	U1362	U	U1205			
C	A	U1805	G1629	U1508	U1467	U1363	U	U1206			
C	A	U1806	U1629	U1508	U1468	U1364	U	U1207			
C	A	U1807	G1630	U1508	U1469	U1365	U	U1208			
C	A	U1808	U1631	U1508	U1470	U1366	U	U1209			
C	A	U1809	G1632	U1508	U1471	U1367	U	U1210			
C	A	U1810	U1633	U1508	U1472	U1368	U	U1211			
C	A	U1811	G1634	U1508	U1473	U1369	U	U1212			
C	A	U1812	U1635	U1508	U1474	U1370	U	U1213			
C	A	U1813	G1636	U1508	U1475	U1371	U	U1214			
C	A	U1814	U1637	U1508	U1476	U1372	U	U1215			
C	A	U1815	G1638	U1508	U1477	U1373	U	U1216			
C	A	U1816	U1639	U1508	U1478	U1374	U	U1217			
C	A	U1817	G1640	U1508	U1479	U1375	U	U1218			
C	A	U1818	U1641	U1508	U1480	U1376	U	U1219			
C	A	U1819	G1642	U1508	U1481	U1377	U	U1220			
C	A	U1820	U1643	U1508	U1482	U1378	U	U1221			
C	A	U1821	G1644	U1508	U1483	U1379	U	U1222			
C	A	U1822	U1645	U1508	U1484	U1380	U	U1223			
C	A	U1823	G1646	U1508	U1485	U1381	U	U1224			
C	A	U1824	U1647	U1508	U1486	U1382	U	U1225			
C	A	U1825	G1648	U1508	U1487	U1383	U	U1226			
C	A	U1826	U1649	U1508	U1488	U1384	U	U1227			
C	A	U1827	G1650	U1508	U1489	U1385	U	U1228			
C	A	U1828	U1651	U1508	U1490	U1386	U	U1229			
C	A	U1829	G1652	U1508	U1491	U1387	U	U1230			
C	A	U1830	U1653	U1508	U1492	U1388	U	U1231			
C	A	U1831	G1654	U1508	U1493	U1389	U	U1232			
C	A	U1832	U1655	U1508	U1494	U1390	U	U1233			
C	A	U1833	G1656	U1508	U1495	U1391	U	U1234			
C	A	U1834	U1657	U1508	U1496	U1392	U	U1235			
C	A	U1835	G1658	U1508	U1497	U1393	U	U1236			
C	A	U1836	U1659	U1508	U1498	U1394	U	U1237			
C	A	U1837	G1660	U1508	U1499	U1395	U	U1238			
C	A	U1838	U1661	U1508	U1500	U1396	U	U1239			
C	A	U1839	G1662	U1508	U1501	U1397	U	U1240			
C	A	U1840	U1663	U1508	U1502	U1398	U	U1241			
C	A	U1841	G1664	U1508	U1503	U1399	U	U1242			
C	A	U1842	U1665	U1508	U1504	U1400	U	U1243			
C	A	U1843	G1666	U1508	U1505	U1401	U	U1244			
C	A	U1844	U1667	U1508	U1506	U1402	U	U1245			
C	A	U1845	G1668	U1508	U1507	U1403	U	U1246			
C	A	U1846	U1669	U1508	U1508	U1404	U	U1247			
C	A	U1847	G1670	U1508	U1509	U1405	U	U1248			
C	A	U1848	U1671	U1508	U1510	U1406	U	U1249			
C	A	U1849	G1672	U1508	U1511	U1407	U	U1250			
C	A	U1850	U1673	U1508	U1512	U1408	U	U1251			
C	A	U1851	G1674	U1508	U1513	U1409	U	U1252			
C	A	U1852	U1675	U1508	U1514	U1410	U	U1253			
C	A	U1853	G1676	U1508	U1515	U1411	U	U1254			
C	A	U1854	U1677	U1508	U1516	U1412	U	U1255			
C	A	U1855	G1678	U1508	U1517	U1413	U	U1256			
C	A	U1856	U1679	U1508	U1518	U1414	U	U1257			
C	A	U1857	G1680	U1508	U1519	U1415	U	U1258			
C	A	U1858	U1681	U1508	U1520	U1416	U	U1259			
C	A	U1859	G1682	U1508	U1521	U1417	U	U1260			
C	A	U1860	U1683	U1508	U1522	U1418	U	U1261			
C	A	U1861	G1684	U1508	U1523	U1419	U	U1262			
C	A	U1862	U1685	U1508	U1524	U1420	U	U1263			
C	A	U1863	G1686	U15							

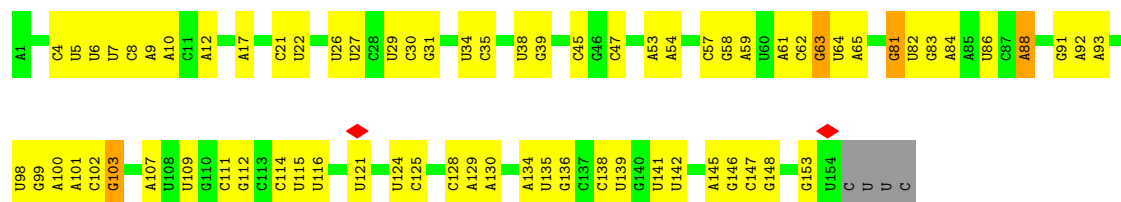




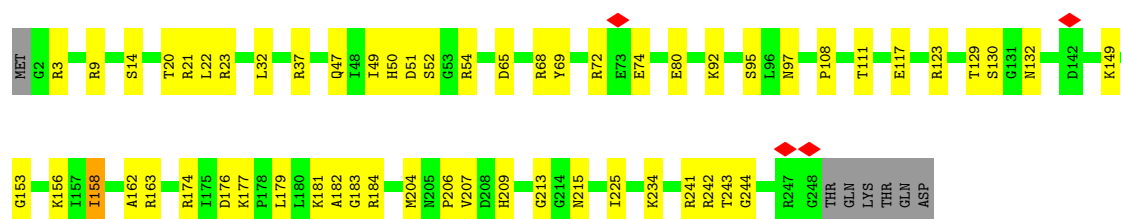
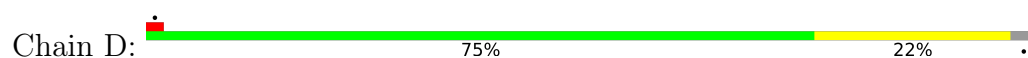
• Molecule 2: 5S rRNA



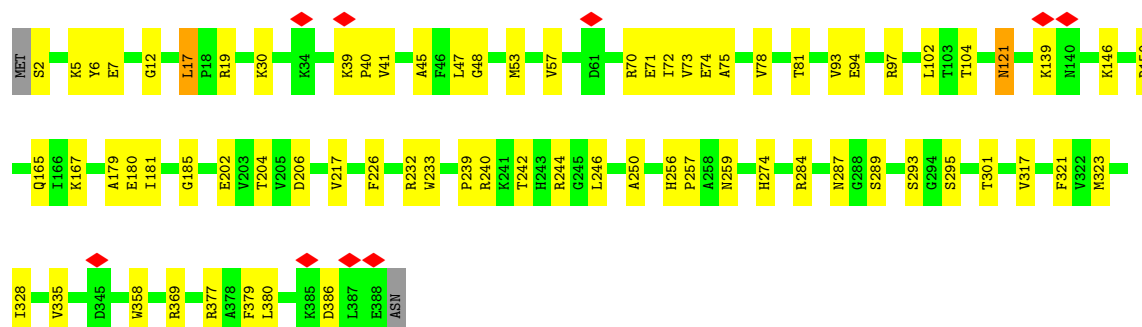
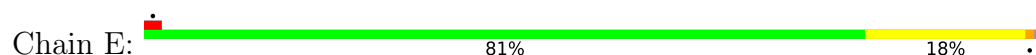
• Molecule 3: 5.8S rRNA



• Molecule 4: 60S ribosomal protein L2-A

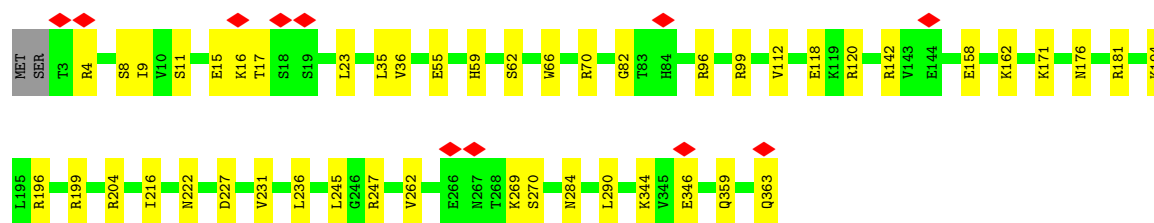


• Molecule 5: Large ribosomal subunit protein uL3



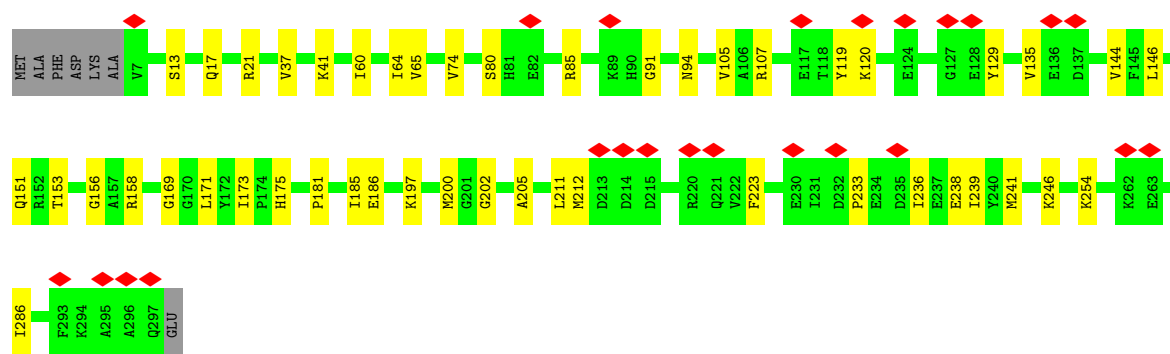
- Molecule 6: 60S ribosomal protein L4-A

Chain F:  87% 13% .



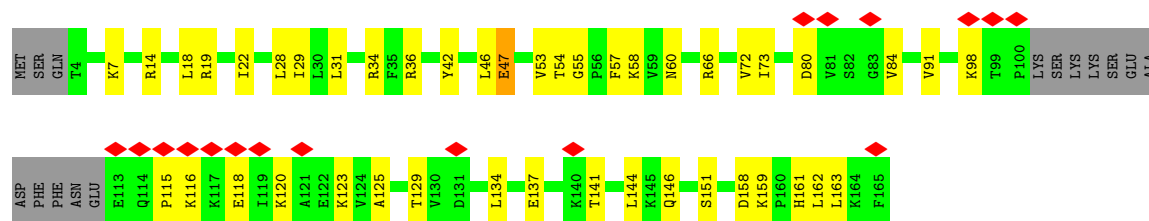
- Molecule 7: 60S ribosomal protein L5

Chain G:  8% 82% 16% .



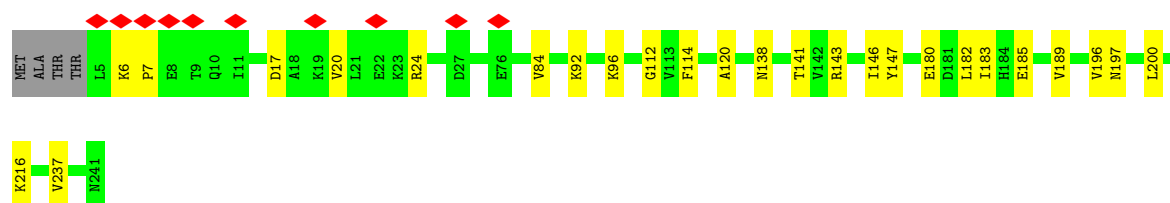
- Molecule 8: 60S ribosomal protein L6

Chain H:  10% 64% 26% 9% .

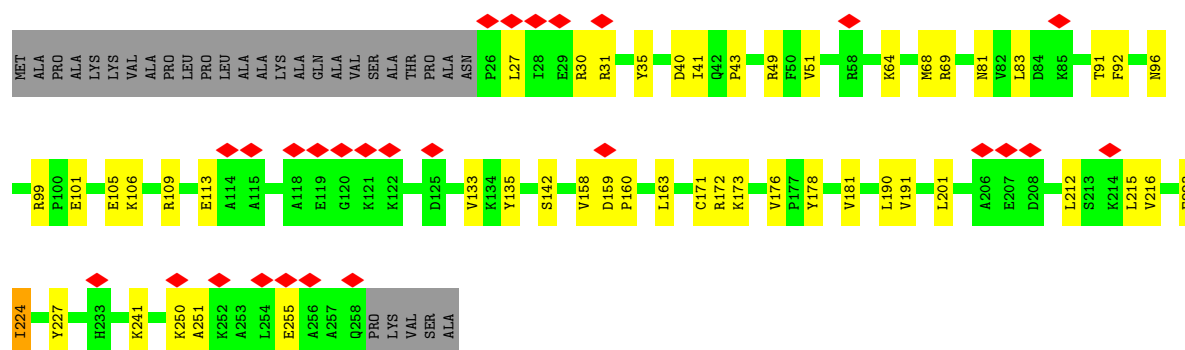


- Molecule 9: 60S ribosomal protein L7

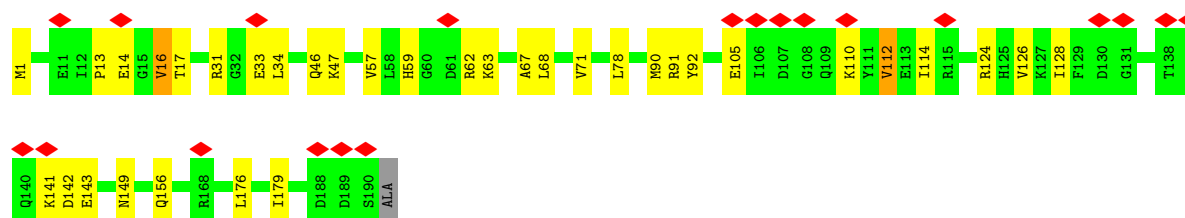
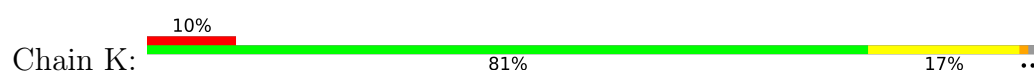
Chain I:  88% 11% .



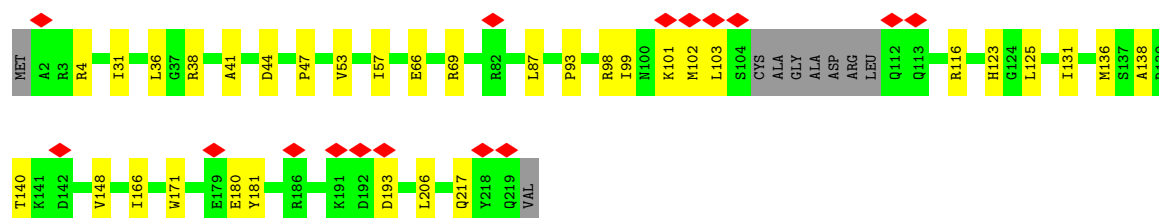
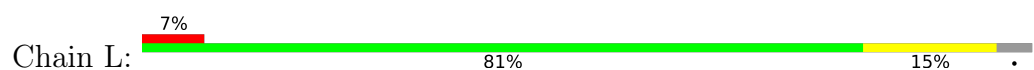
- Molecule 10: 60S ribosomal protein L8



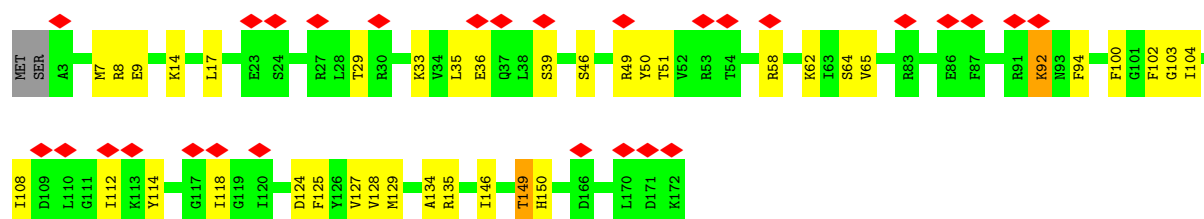
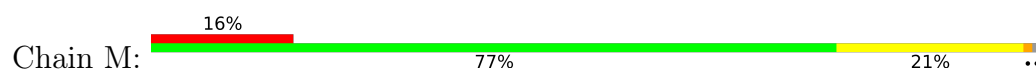
- Molecule 11: 60S ribosomal protein L9-B



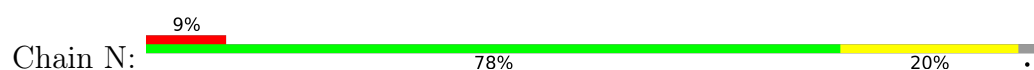
- Molecule 12: 60S ribosomal protein L10

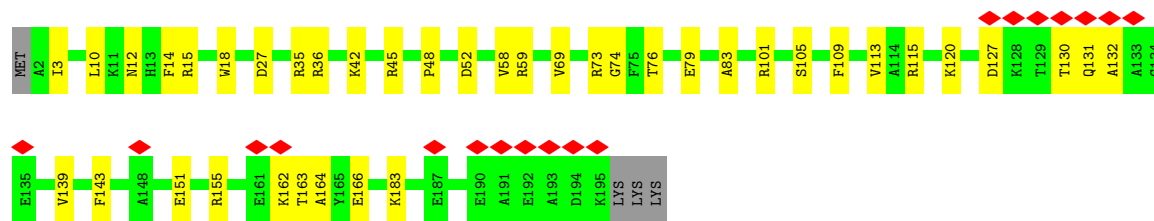


- Molecule 13: 60S ribosomal protein L11-A

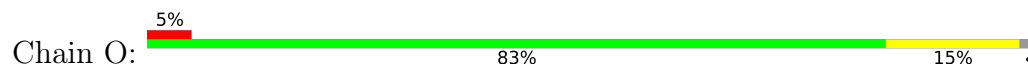


- Molecule 14: 60S ribosomal protein L13

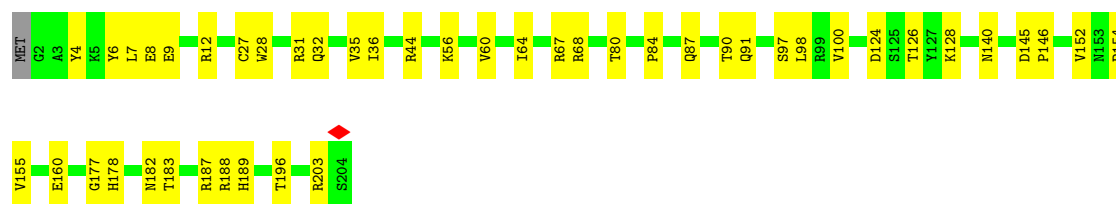
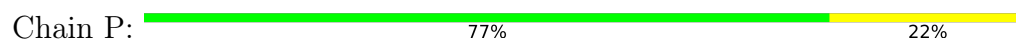




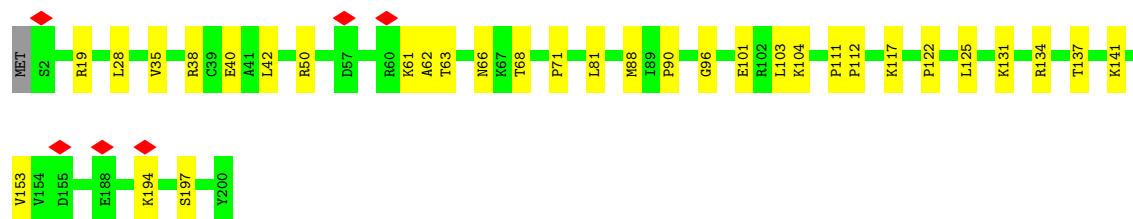
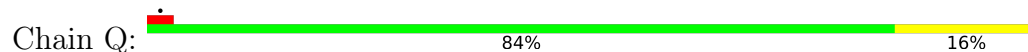
- Molecule 15: Large ribosomal subunit protein eL14 domain-containing protein



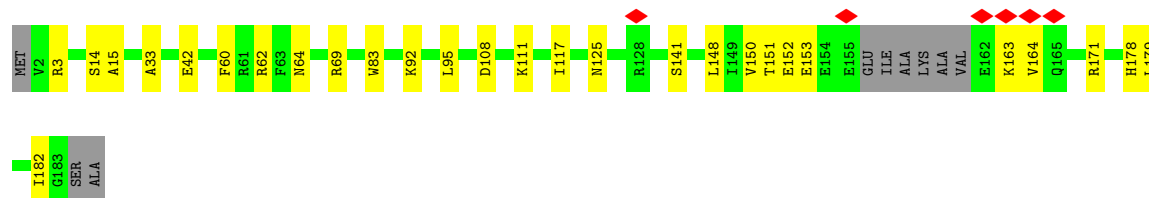
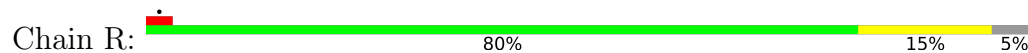
- Molecule 16: Ribosomal protein L15



- Molecule 17: 60S ribosomal protein L16-B

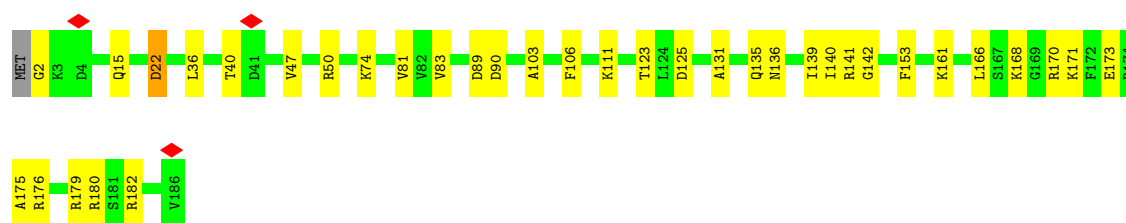


- Molecule 18: 60S ribosomal protein L17-B



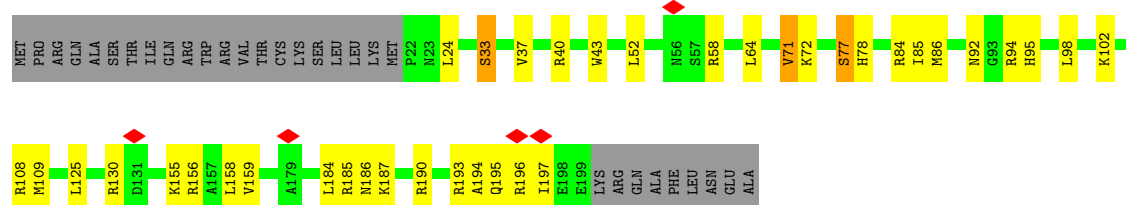
- Molecule 19: 60S ribosomal protein L18-A

Chain S:  80% 19% ..



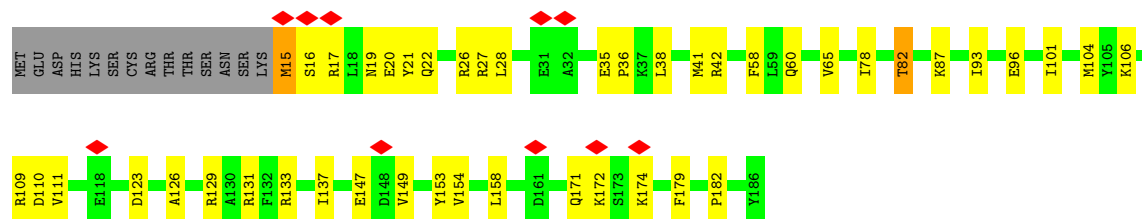
- Molecule 20: Ribosomal protein L19

Chain T:  67% 17% 14%



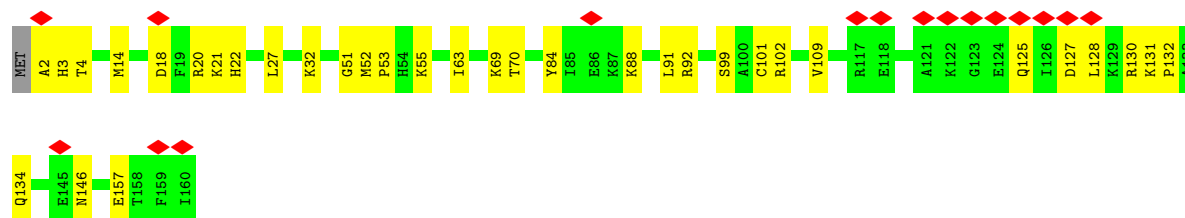
- Molecule 21: 60S ribosomal protein eL20 (formerly L20)

Chain U:  5% 68% 23% 8%



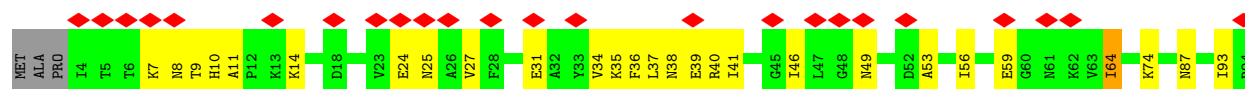
- Molecule 22: 60S ribosomal protein L21-A

Chain V:  10% 78% 21%

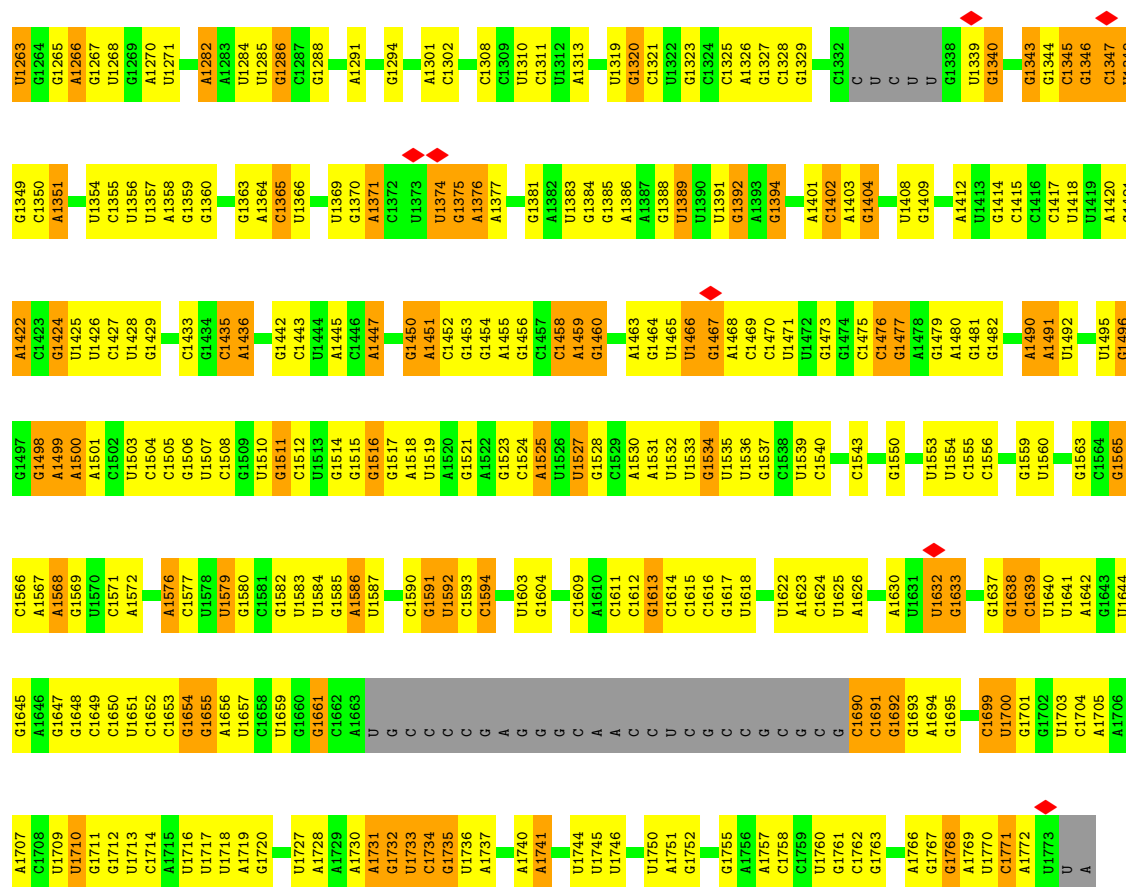


- Molecule 23: 60S ribosomal protein L22

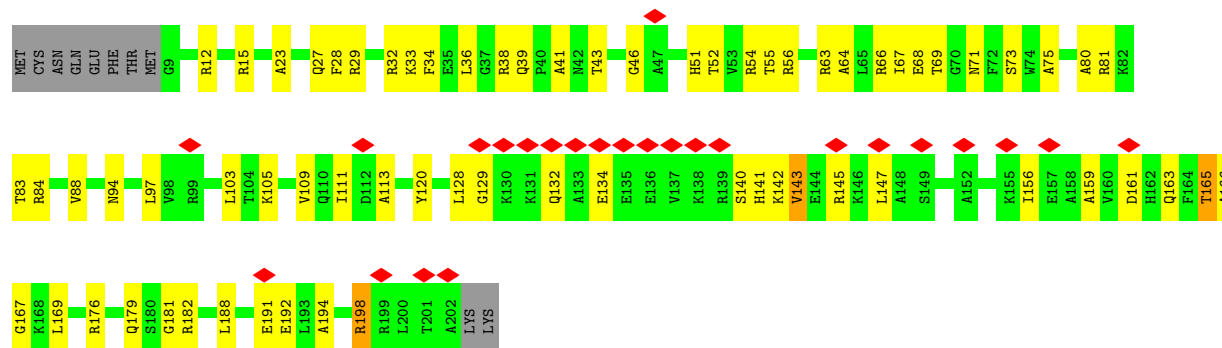
Chain W:  23% 66% 24% 10%



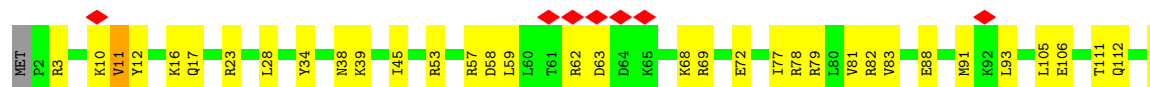


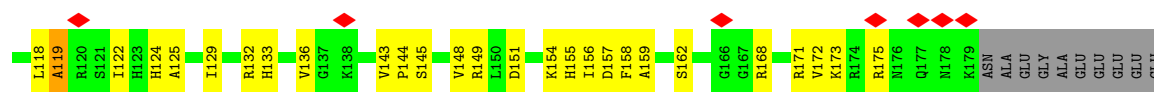


• Molecule 28: 40S ribosomal protein S8

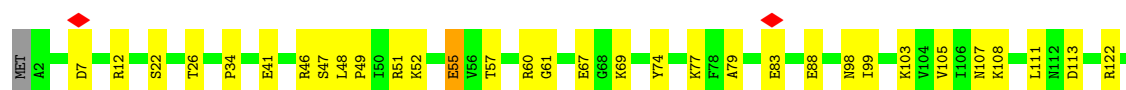


• Molecule 29: 40S ribosomal protein S9-A

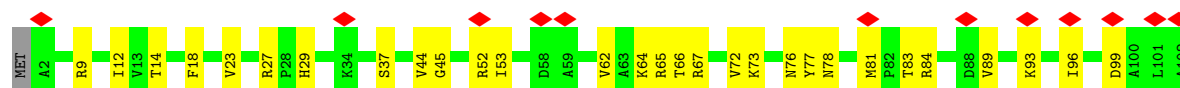
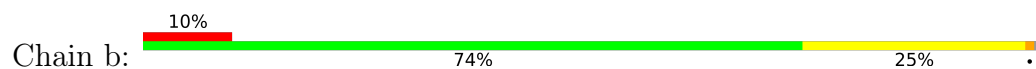




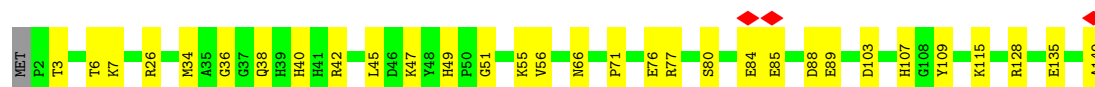
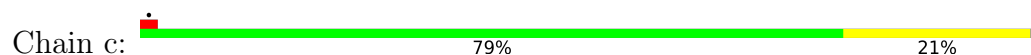
• Molecule 30: Ribosomal protein L24



• Molecule 31: 60S ribosomal protein L27



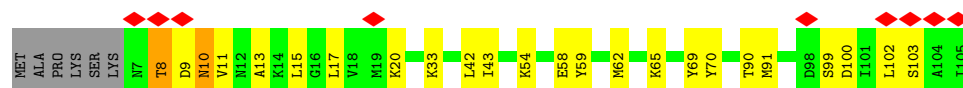
• Molecule 32: 60S ribosomal protein L28



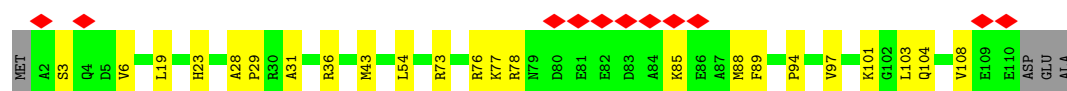
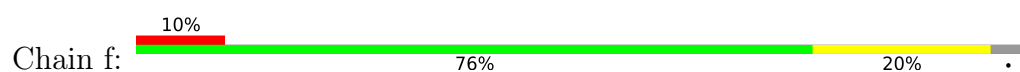
• Molecule 33: 60S ribosomal protein L29



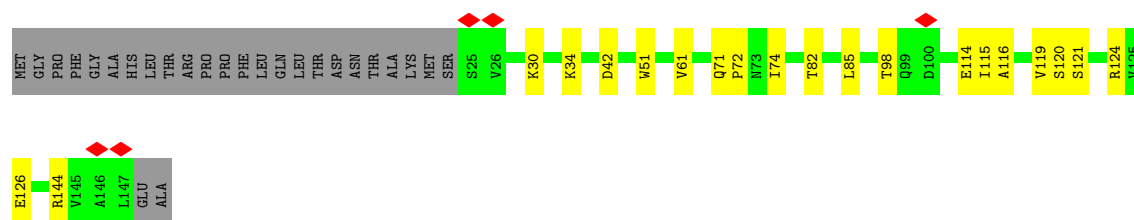
• Molecule 34: 60S ribosomal protein L30



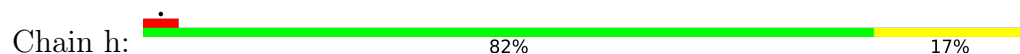
• Molecule 35: 60S ribosomal protein L31-A



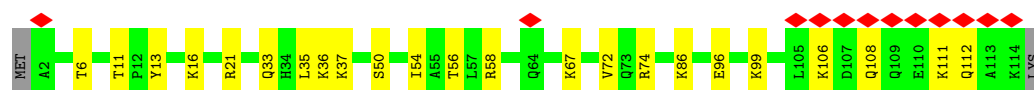
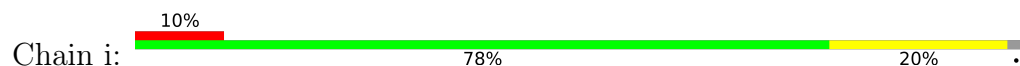
- Molecule 36: 60S ribosomal protein L32



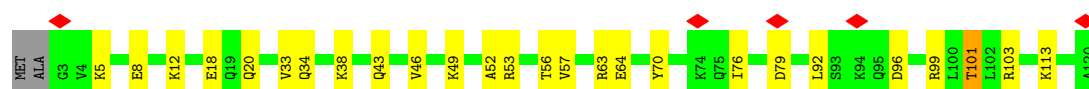
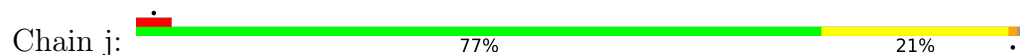
- Molecule 37: 60S ribosomal protein L33-A



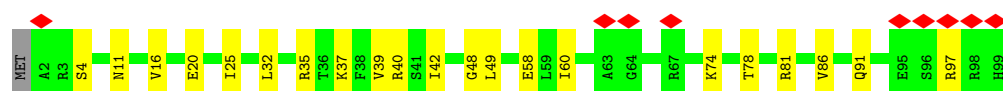
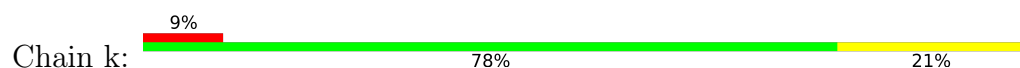
- Molecule 38: 60S ribosomal protein L34-B



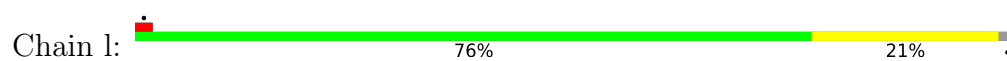
- Molecule 39: 60S ribosomal protein L35



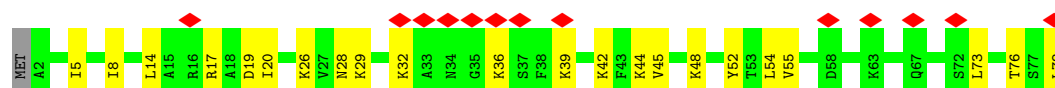
- Molecule 40: 60S ribosomal protein L36



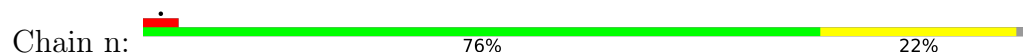
- Molecule 41: Ribosomal protein L37



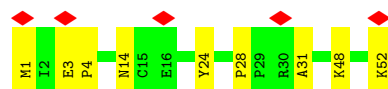
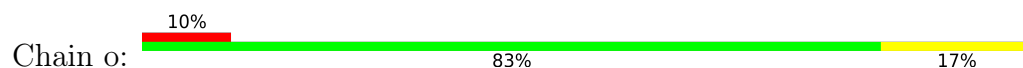
- Molecule 42: Large ribosomal subunit protein eL38



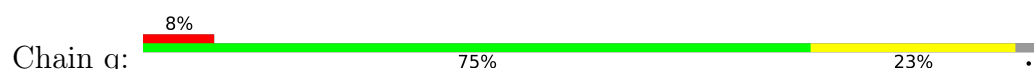
- Molecule 43: Large ribosomal subunit protein eL39



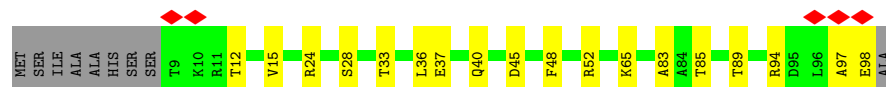
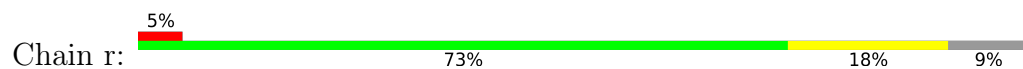
- Molecule 44: Large ribosomal subunit protein eL40



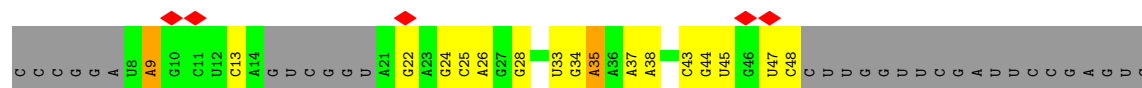
- Molecule 45: 60S ribosomal protein L44



- Molecule 46: 60S ribosomal protein L43



- Molecule 47: P-site tRNA



C
G
G
G
G
C
C
C
A
A

- Molecule 48: RNA (5'-R(P*CP*GP*AP*UP*UP*CP*A)-3')

Chain 2:

C1
G2
A3
U4
A7

- Molecule 49: A-site tRNA

Chain 3:

G28
G29
G30
A31
U32
U33
G34
A35
A36
A37
A38
U39
C40
C41
C42
C43
G44

- Molecule 50: 40S ribosomal protein S10-A

Chain ZC:

MET
LEU
I3
P4
K5
D6
R7
R8
K9
K10
I11
F16
G19
V20
V21
P30
K31
H32
E33
E34
I35
D36
T37
K38
N39
L40
Y41
K44
A45
L46
L49
V61
Q62
Y66
T67
L68
T69
D70
E71
E74
R77
N78
E79
L80
N81
I82
P83
E84
G85
I86
L87

P88
L89
T90
R91
L92
K93
GLY
ALA
PRO
ALA
ALA
GLN
ARG
PRO
ARG
PRO
ALA
ILE
ILE
GLY
GLY
PRO
PRO
ARG
ARG
PHE
GLY
ASP
SER
TYR
ARG
ARG
ALA
ALA
ASP

- Molecule 51: 40S ribosomal protein S11-A

Chain ZD:

MET
ALA
THR
GLU
L5
E10
K15
Q16
P17
T21
N28
K29
K30
K32
K33
W34
E37
L40
E50
Y53
I56
K69
I70
L71
T72
G73
T74
S77
T78
K79
M80
H81
R82
T83
I84
Y90
K96
E101
K105
P113
R116
V117

Q118
E119
G120
D121
P130
L140
K146
ALA
LYS
SER
LYS
GLN
PHE
THR
LYS
PHE

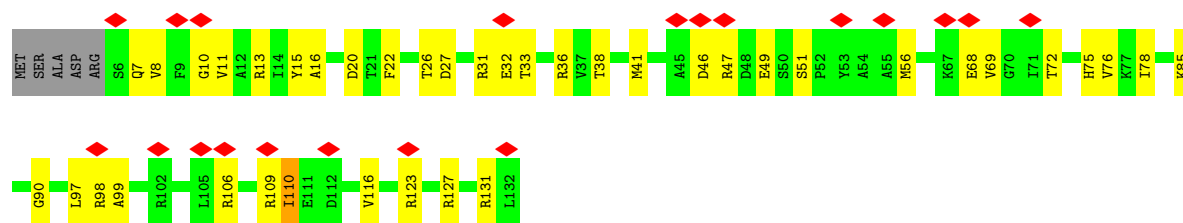
- Molecule 52: 40S ribosomal protein S13

Chain ZE:

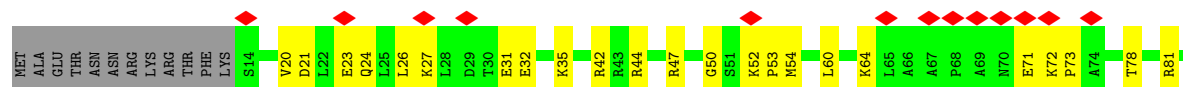
MET
G2
R3
M4
H5
S6
S7
S13
S14
A15
K27
L28
E32
E35
Q36
K43
T46
P47
I53
L54
R55
D56
V60
S61
Q62
E66
D67
L68
E103
R106
E119
I122
H123
R124
V132
A133
V134
L135
P136
V139
K140
Y141
V150
ASN

- Molecule 53: Small ribosomal subunit protein uS11

Chain ZF:



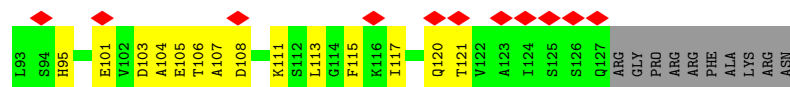
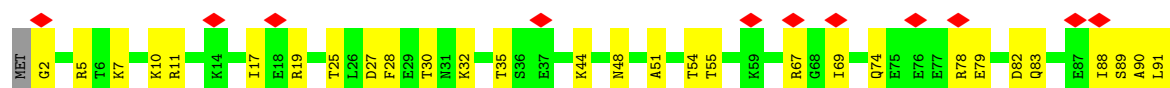
• Molecule 54: 40S ribosomal protein S15



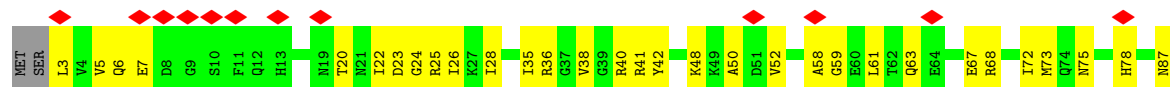
• Molecule 55: Small ribosomal subunit protein uS9



• Molecule 56: 40S ribosomal protein S17-B

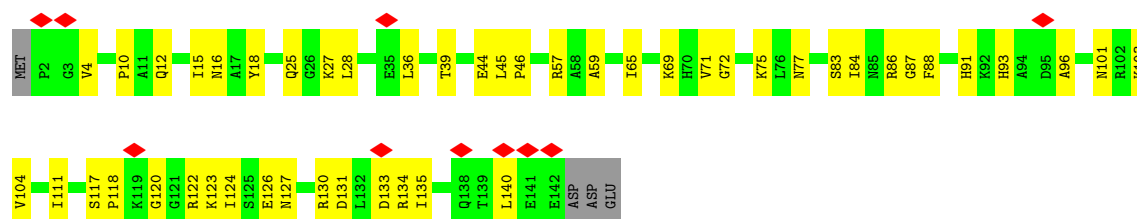


• Molecule 57: 40S ribosomal protein S18

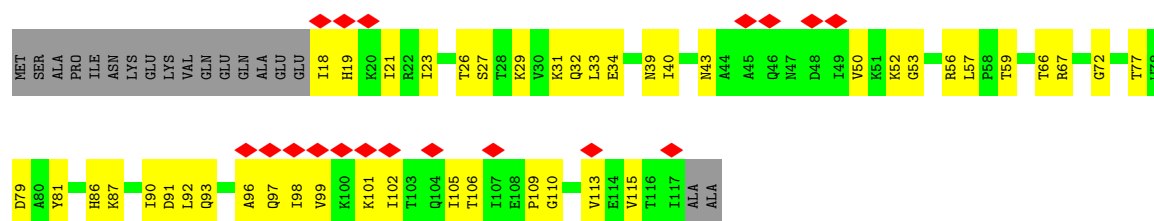




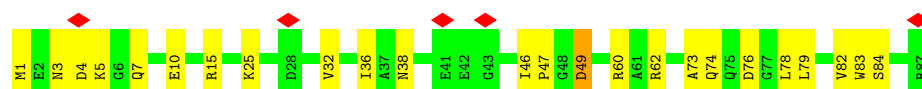
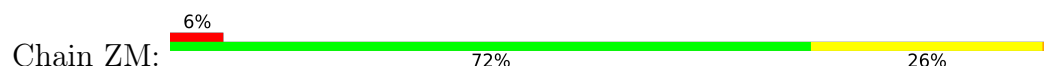
- Molecule 58: 40S ribosomal protein S19-A



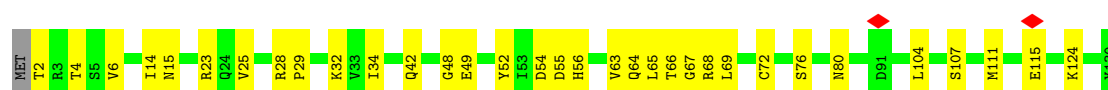
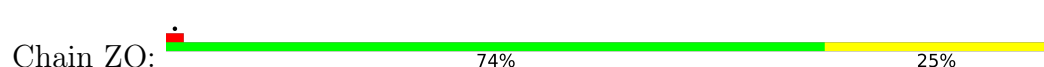
- Molecule 59: Small ribosomal subunit protein uS10



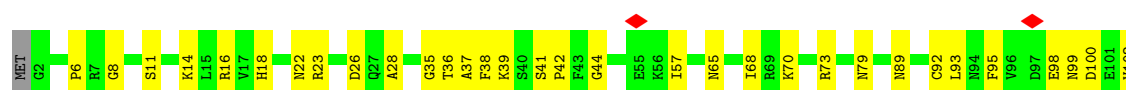
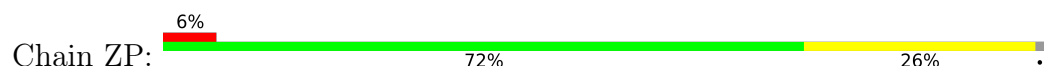
- Molecule 60: 40S ribosomal protein S21

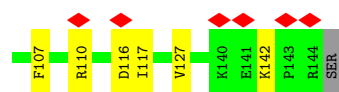


- Molecule 61: 40S ribosomal protein S22



- Molecule 62: 40S ribosomal protein S23

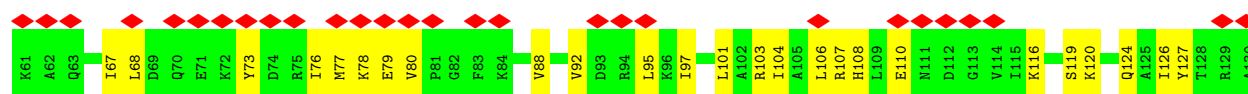
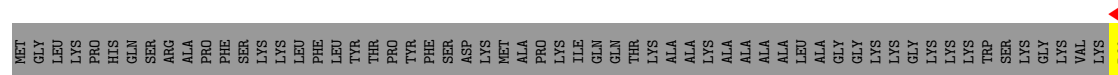
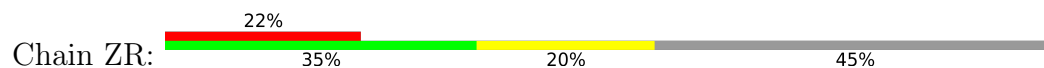




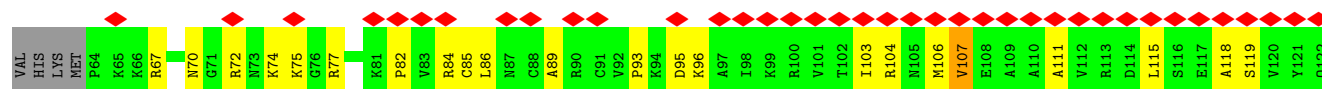
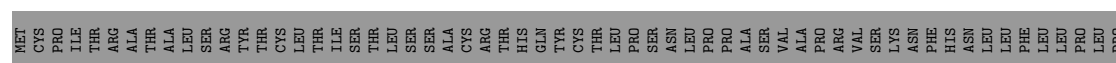
- Molecule 63: 40S ribosomal protein S24



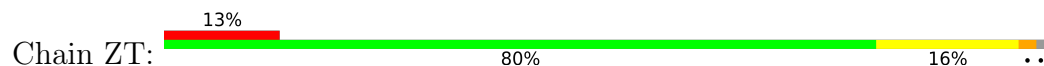
- Molecule 64: 40S ribosomal protein S25



- Molecule 65: 40S ribosomal protein S26

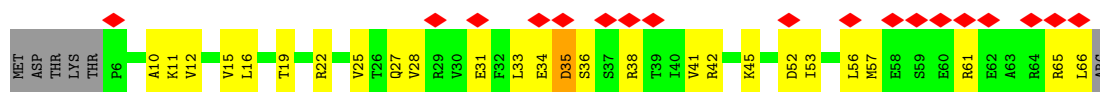


- Molecule 66: 40S ribosomal protein S27



- Molecule 67: 40S ribosomal protein S28-A





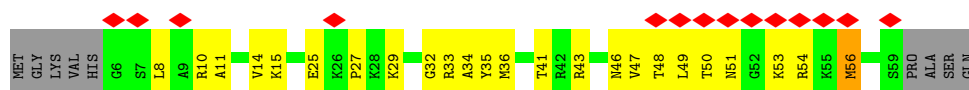
- Molecule 68: Small ribosomal subunit protein uS14

Chain ZV: 70% 23%



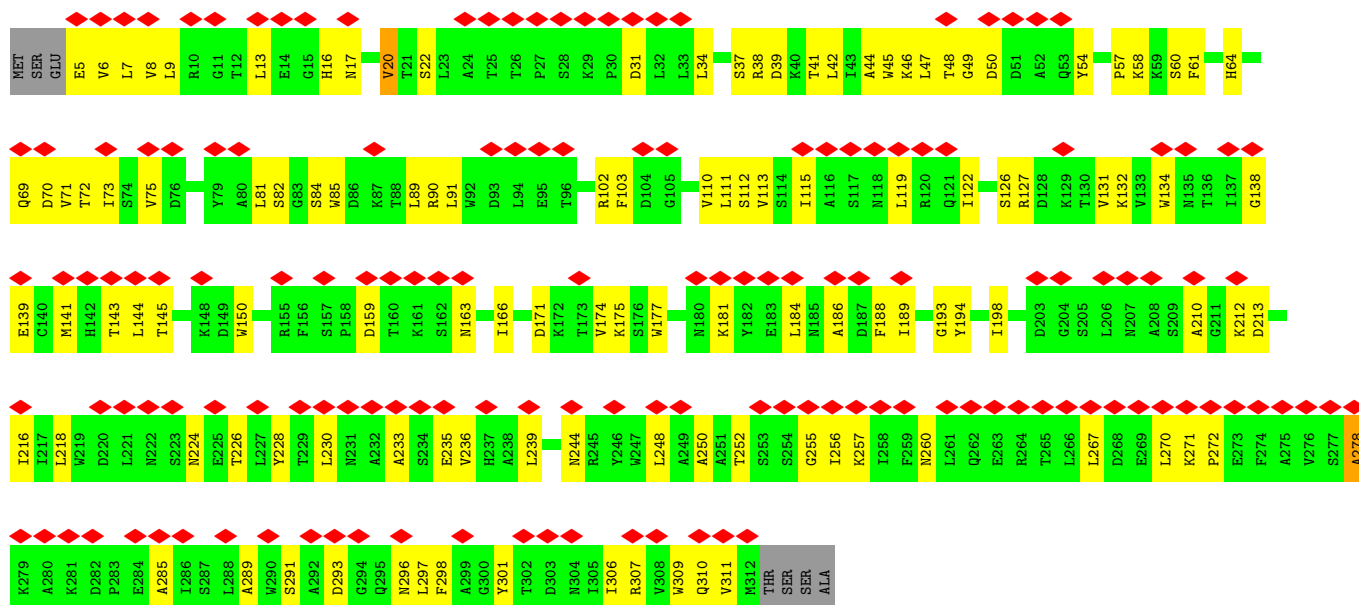
- Molecule 69: Small ribosomal subunit protein eS30

Chain ZW: 22% 48% 37% 14%



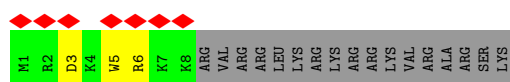
- Molecule 70: Small ribosomal subunit protein RACK1

Chain ZY: 47% 60% 37%

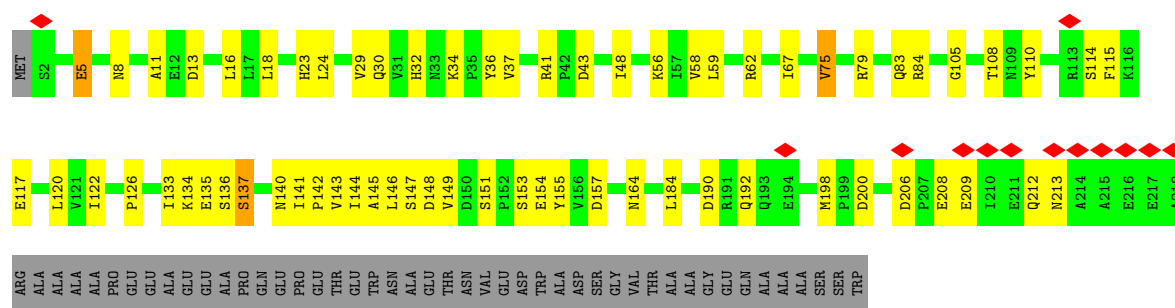


- Molecule 71: Small ribosomal subunit protein eS32

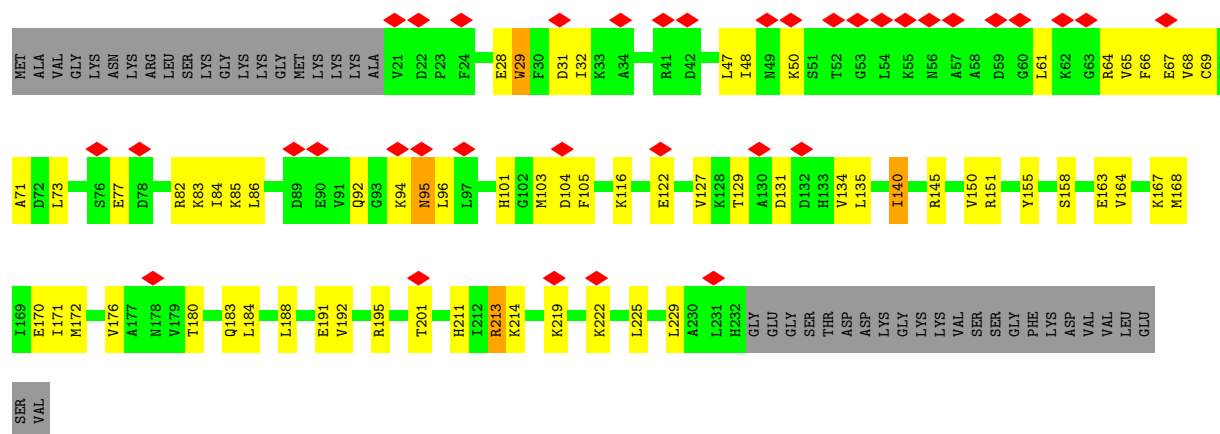
Chain p: 28% 20% 12% 68%



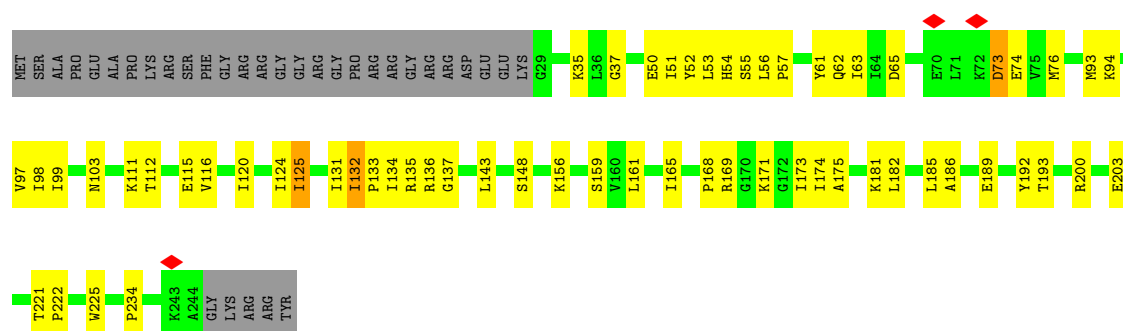
- Molecule 72: Small ribosomal subunit protein uS2



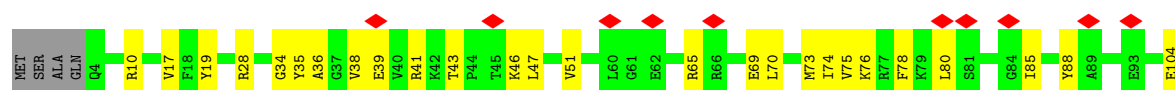
• Molecule 73: Small ribosomal subunit protein eS1

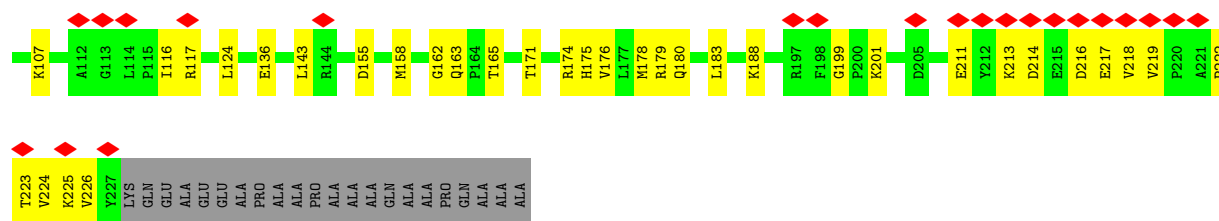


• Molecule 74: Rps21 ribosomal protein

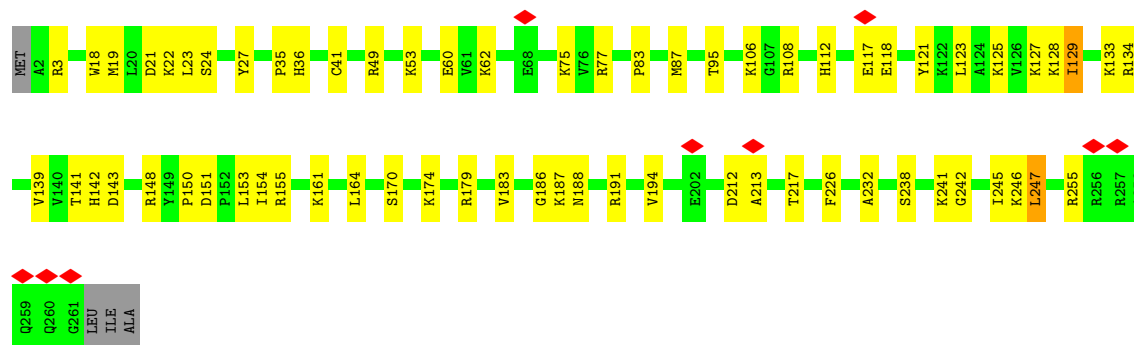
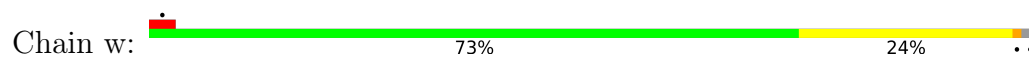


• Molecule 75: Small ribosomal subunit protein uS3

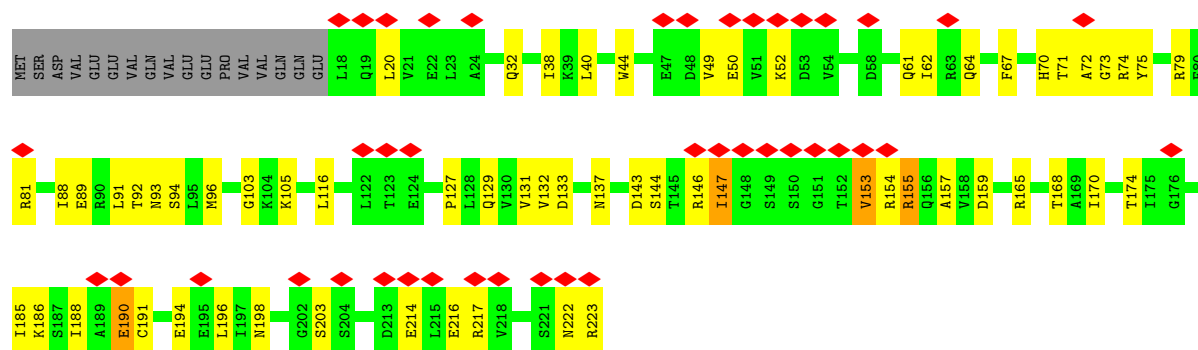




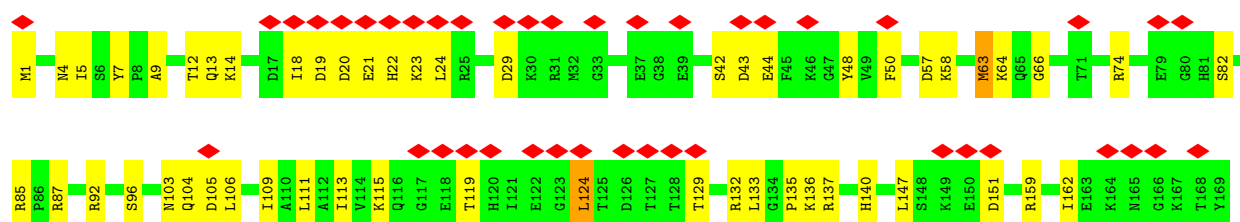
• Molecule 76: 40S ribosomal protein S4

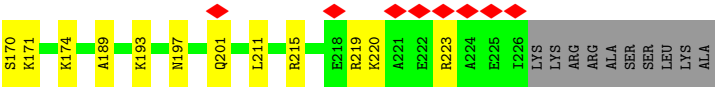


• Molecule 77: 40S ribosomal protein uS7 (formerly S5)

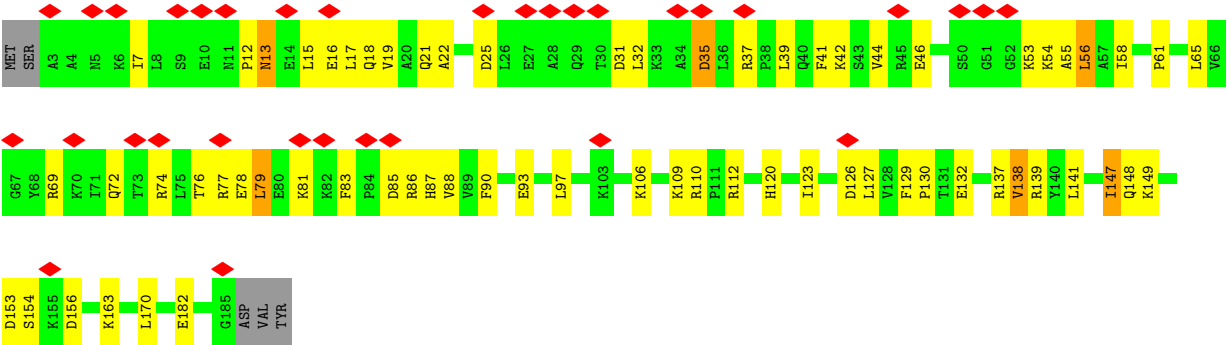


• Molecule 78: 40S ribosomal protein S6





• Molecule 79: 40S ribosomal protein eS7 (formerly S7)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37410	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.385	Depositor
Minimum map value	-0.465	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	401.28, 401.28, 401.28	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.836, 0.836, 0.836	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BLS, MG, ZN, B8N

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/72547	0.26	0/113096
2	B	0.14	0/2918	0.23	0/4548
3	C	0.15	0/3659	0.23	0/5698
4	D	0.18	0/1907	0.33	0/2560
5	E	0.14	0/3155	0.29	0/4246
6	F	0.13	0/2835	0.26	0/3823
7	G	0.12	0/2419	0.28	0/3253
8	H	0.16	0/1203	0.36	0/1621
9	I	0.13	0/1950	0.27	0/2621
10	J	0.13	0/1879	0.29	0/2525
11	K	0.14	0/1539	0.29	0/2068
12	L	0.14	0/1756	0.30	0/2355
13	M	0.13	0/1385	0.40	1/1854 (0.1%)
14	N	0.15	0/1564	0.31	0/2104
15	O	0.12	0/1044	0.31	0/1410
16	P	0.14	0/1743	0.26	0/2340
17	Q	0.15	0/1618	0.30	0/2169
18	R	0.15	0/1444	0.32	0/1943
19	S	0.15	0/1479	0.34	0/1985
20	T	0.14	0/1454	0.30	0/1937
21	U	0.15	0/1483	0.30	0/1996
22	V	0.14	0/1308	0.31	0/1758
23	W	0.13	0/887	0.35	0/1194
24	X	0.17	0/1030	0.34	0/1387
25	Y	0.14	0/530	0.26	0/704
26	Z	0.14	0/970	0.31	0/1311
27	CA	0.17	0/39053	0.29	0/60853
28	ZA	0.15	0/1571	0.36	0/2103
29	ZB	0.16	0/1485	0.35	0/1991
30	a	0.14	0/1005	0.33	0/1339
31	b	0.14	0/1104	0.32	0/1480
32	c	0.17	0/1203	0.38	0/1611

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.12	0/506	0.28	0/670
34	e	0.20	0/752	0.45	0/1011
35	f	0.15	0/911	0.30	0/1223
36	g	0.13	0/1019	0.26	0/1362
37	h	0.16	0/877	0.34	0/1180
38	i	0.16	0/906	0.36	0/1209
39	j	0.14	0/963	0.32	0/1284
40	k	0.12	0/780	0.31	0/1034
41	l	0.14	0/666	0.27	0/883
42	m	0.12	0/623	0.31	0/828
43	n	0.17	0/451	0.34	0/600
44	o	0.19	0/425	0.31	0/563
45	q	0.14	0/834	0.30	0/1103
46	r	0.16	0/699	0.30	0/933
47	1	0.12	0/838	0.23	0/1302
48	2	0.16	0/163	0.40	0/251
49	3	0.11	0/408	0.28	0/634
50	ZC	0.17	0/789	0.49	0/1067
51	ZD	0.16	0/1169	0.32	0/1571
52	ZE	0.17	0/1207	0.28	0/1626
53	ZF	0.20	0/956	0.42	0/1284
54	ZG	0.18	0/922	0.39	0/1239
55	ZH	0.18	0/1110	0.46	1/1488 (0.1%)
56	ZI	0.14	0/1024	0.38	0/1373
57	ZJ	0.15	0/1188	0.37	0/1591
58	ZK	0.13	0/1122	0.31	0/1510
59	ZL	0.21	0/791	0.47	0/1069
60	ZM	0.16	0/686	0.31	0/924
61	ZO	0.20	0/1049	0.37	0/1410
62	ZP	0.17	0/1127	0.38	0/1505
63	ZQ	0.13	0/1090	0.26	0/1457
64	ZR	0.19	0/572	0.38	0/767
65	ZS	0.14	0/797	0.43	0/1068
66	ZT	0.17	0/627	0.39	0/847
67	ZU	0.17	0/479	0.45	0/641
68	ZV	0.19	0/461	0.44	0/613
69	ZW	0.23	0/438	0.72	1/582 (0.2%)
70	ZY	0.13	0/2437	0.36	0/3320
71	p	0.13	0/80	0.46	0/102
72	s	0.16	0/1744	0.33	0/2379
73	t	0.14	0/1728	0.35	0/2322
74	u	0.17	0/1664	0.37	0/2253
75	v	0.19	0/1763	0.44	0/2368

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	w	0.14	0/2094	0.36	0/2816
77	x	0.15	0/1628	0.42	0/2195
78	y	0.14	0/1845	0.36	0/2467
79	z	0.16	0/1495	0.38	0/2011
All	All	0.16	0/207030	0.30	3/303818 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	ZH	77	VAL	N-CA-C	-7.84	106.26	113.71
69	ZW	15	LYS	N-CA-C	-7.21	105.66	114.75
13	M	118	ILE	N-CA-C	-5.33	107.18	113.42

There are no chirality outliers.

There are no planarity outliers.

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	A	64825	0	32616	1068	0
2	B	2609	0	1315	39	0
3	C	3274	0	1654	48	0
4	D	1873	0	1943	41	0
5	E	3087	0	3173	55	0
6	F	2786	0	2912	32	0
7	G	2370	0	2360	29	0
8	H	1183	0	1276	30	0
9	I	1913	0	1998	16	0
10	J	1847	0	1970	33	0
11	K	1519	0	1588	23	0
12	L	1720	0	1760	26	0
13	M	1364	0	1396	26	0
14	N	1538	0	1614	30	0
15	O	1030	0	1113	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	1703	0	1748	37	0
17	Q	1587	0	1695	23	0
18	R	1418	0	1446	22	0
19	S	1456	0	1570	27	0
20	T	1435	0	1540	30	0
21	U	1448	0	1511	35	0
22	V	1282	0	1341	24	0
23	W	871	0	903	16	0
24	X	1013	0	1057	31	0
25	Y	517	0	535	15	0
26	Z	955	0	1012	11	0
27	CA	34938	0	17569	717	0
28	ZA	1545	0	1580	56	0
29	ZB	1459	0	1531	49	0
30	a	994	0	1075	25	0
31	b	1081	0	1134	24	0
32	c	1174	0	1204	24	0
33	d	498	0	517	6	0
34	e	744	0	784	14	0
35	f	895	0	927	16	0
36	g	1002	0	1062	13	0
37	h	859	0	889	13	0
38	i	897	0	970	19	0
39	j	956	0	1067	22	0
40	k	774	0	848	15	0
41	l	654	0	668	14	0
42	m	617	0	685	13	0
43	n	442	0	478	11	0
44	o	419	0	460	7	0
45	q	822	0	886	15	0
46	r	691	0	723	15	0
47	1	750	0	380	13	0
48	2	147	0	76	8	0
49	3	365	0	185	8	0
50	ZC	770	0	774	31	0
51	ZD	1145	0	1213	19	0
52	ZE	1184	0	1246	22	0
53	ZF	945	0	979	33	0
54	ZG	904	0	944	31	0
55	ZH	1091	0	1147	35	0
56	ZI	1012	0	1064	35	0
57	ZJ	1170	0	1213	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	ZK	1101	0	1113	33	0
59	ZL	782	0	854	30	0
60	ZM	678	0	671	22	0
61	ZO	1032	0	1072	26	0
62	ZP	1109	0	1173	26	0
63	ZQ	1073	0	1126	31	0
64	ZR	564	0	598	19	0
65	ZS	785	0	835	29	0
66	ZT	617	0	631	12	0
67	ZU	477	0	510	23	0
68	ZV	449	0	425	12	0
69	ZW	432	0	471	14	0
70	ZY	2383	0	2344	99	0
71	p	79	0	90	2	0
72	s	1705	0	1711	47	0
73	t	1703	0	1796	50	0
74	u	1636	0	1743	50	0
75	v	1737	0	1835	52	0
76	w	2056	0	2145	49	0
77	x	1610	0	1687	49	0
78	y	1819	0	1882	46	0
79	z	1471	0	1559	52	0
80	A	152	0	0	0	0
80	B	3	0	0	0	0
80	C	1	0	0	0	0
80	CA	58	0	0	0	0
80	D	1	0	0	0	0
80	L	2	0	0	0	0
80	X	1	0	0	0	0
80	h	1	0	0	0	0
80	n	1	0	0	0	0
81	A	30	0	24	2	0
82	ZS	1	0	0	0	0
82	ZV	1	0	0	0	0
82	i	1	0	0	0	0
82	l	1	0	0	0	0
82	o	1	0	0	0	0
82	q	1	0	0	0	0
82	r	1	0	0	0	0
83	A	83	0	0	7	0
83	B	2	0	0	0	0
83	C	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	E	1	0	0	1	0
83	P	2	0	0	0	0
83	d	1	0	0	0	0
83	i	1	0	0	0	0
83	q	1	0	0	0	0
All	All	193216	0	143619	3322	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 10.

The worst 5 of 3322 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)
1:A:961:U:H3	1:A:983:G:H1	1.14	0.96
1:A:3126:G:H1	1:A:3145:U:H3	0.96	0.94
27:CA:1563:G:H1	27:CA:1583:U:H3	1.15	0.93
53:ZF:47:ARG:HG2	53:ZF:51:SER:HB3	1.55	0.88
1:A:161:G:H1	1:A:239:U:H3	1.23	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	245/254 (96%)	234 (96%)	11 (4%)	0	100	100
5	E	385/389 (99%)	374 (97%)	11 (3%)	0	100	100
6	F	359/363 (99%)	352 (98%)	7 (2%)	0	100	100
7	G	289/298 (97%)	278 (96%)	11 (4%)	0	100	100
8	H	146/165 (88%)	136 (93%)	9 (6%)	1 (1%)	18	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	235/241 (98%)	227 (97%)	7 (3%)	1 (0%)	30	60
10	J	231/263 (88%)	228 (99%)	3 (1%)	0	100	100
11	K	188/191 (98%)	181 (96%)	7 (4%)	0	100	100
12	L	207/220 (94%)	200 (97%)	7 (3%)	0	100	100
13	M	168/172 (98%)	161 (96%)	7 (4%)	0	100	100
14	N	192/198 (97%)	185 (96%)	7 (4%)	0	100	100
15	O	127/131 (97%)	123 (97%)	4 (3%)	0	100	100
16	P	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
17	Q	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
18	R	172/185 (93%)	170 (99%)	2 (1%)	0	100	100
19	S	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
20	T	176/208 (85%)	171 (97%)	4 (2%)	1 (1%)	21	51
21	U	170/186 (91%)	165 (97%)	5 (3%)	0	100	100
22	V	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
23	W	105/119 (88%)	98 (93%)	7 (7%)	0	100	100
24	X	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
25	Y	60/156 (38%)	60 (100%)	0	0	100	100
26	Z	118/140 (84%)	115 (98%)	3 (2%)	0	100	100
28	ZA	192/204 (94%)	180 (94%)	11 (6%)	1 (0%)	24	55
29	ZB	176/189 (93%)	165 (94%)	9 (5%)	2 (1%)	11	36
30	a	124/127 (98%)	124 (100%)	0	0	100	100
31	b	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
32	c	146/149 (98%)	138 (94%)	8 (6%)	0	100	100
33	d	58/76 (76%)	54 (93%)	4 (7%)	0	100	100
34	e	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	12	38
35	f	107/113 (95%)	107 (100%)	0	0	100	100
36	g	121/149 (81%)	120 (99%)	1 (1%)	0	100	100
37	h	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
38	i	111/115 (96%)	108 (97%)	3 (3%)	0	100	100
39	j	116/120 (97%)	113 (97%)	3 (3%)	0	100	100
40	k	96/99 (97%)	93 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	l	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
42	m	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
43	n	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
44	o	50/52 (96%)	50 (100%)	0	0	100	100
45	q	101/106 (95%)	97 (96%)	4 (4%)	0	100	100
46	r	88/99 (89%)	86 (98%)	2 (2%)	0	100	100
50	ZC	89/123 (72%)	78 (88%)	9 (10%)	2 (2%)	5	19
51	ZD	140/155 (90%)	135 (96%)	5 (4%)	0	100	100
52	ZE	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
53	ZF	125/132 (95%)	114 (91%)	11 (9%)	0	100	100
54	ZG	114/141 (81%)	111 (97%)	3 (3%)	0	100	100
55	ZH	138/142 (97%)	121 (88%)	17 (12%)	0	100	100
56	ZI	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
57	ZJ	140/145 (97%)	132 (94%)	8 (6%)	0	100	100
58	ZK	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
59	ZL	98/118 (83%)	93 (95%)	5 (5%)	0	100	100
60	ZM	85/87 (98%)	85 (100%)	0	0	100	100
61	ZO	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
62	ZP	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
63	ZQ	130/135 (96%)	128 (98%)	2 (2%)	0	100	100
64	ZR	69/130 (53%)	66 (96%)	3 (4%)	0	100	100
65	ZS	96/182 (53%)	89 (93%)	7 (7%)	0	100	100
66	ZT	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
67	ZU	59/67 (88%)	53 (90%)	5 (8%)	1 (2%)	7	25
68	ZV	52/56 (93%)	41 (79%)	10 (19%)	1 (2%)	6	22
69	ZW	52/63 (82%)	36 (69%)	14 (27%)	2 (4%)	2	9
70	ZY	306/315 (97%)	279 (91%)	26 (8%)	1 (0%)	36	66
71	p	6/25 (24%)	4 (67%)	2 (33%)	0	100	100
72	s	215/264 (81%)	211 (98%)	4 (2%)	0	100	100
73	t	210/256 (82%)	192 (91%)	18 (9%)	0	100	100
74	u	214/249 (86%)	207 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	v	222/250 (89%)	195 (88%)	24 (11%)	3 (1%)	9	30
76	w	258/264 (98%)	247 (96%)	11 (4%)	0	100	100
77	x	204/223 (92%)	187 (92%)	14 (7%)	3 (2%)	8	28
78	y	224/236 (95%)	206 (92%)	17 (8%)	1 (0%)	30	60
79	z	181/188 (96%)	166 (92%)	15 (8%)	0	100	100
All	All	10654/11662 (91%)	10165 (95%)	468 (4%)	21 (0%)	44	72

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	115	PRO
20	T	77	SER
34	e	8	THR
75	v	43	THR
77	x	153	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	186/193 (96%)	183 (98%)	3 (2%)	55	83
5	E	328/330 (99%)	325 (99%)	3 (1%)	70	89
6	F	298/300 (99%)	295 (99%)	3 (1%)	68	88
7	G	247/252 (98%)	244 (99%)	3 (1%)	63	87
8	H	131/145 (90%)	127 (97%)	4 (3%)	35	70
9	I	199/202 (98%)	199 (100%)	0	100	100
10	J	196/216 (91%)	194 (99%)	2 (1%)	68	88
11	K	168/168 (100%)	164 (98%)	4 (2%)	43	77
12	L	183/189 (97%)	181 (99%)	2 (1%)	65	87
13	M	143/145 (99%)	140 (98%)	3 (2%)	47	79
14	N	156/160 (98%)	155 (99%)	1 (1%)	78	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	110/111 (99%)	109 (99%)	1 (1%)	70	89
16	P	175/176 (99%)	172 (98%)	3 (2%)	53	83
17	Q	166/167 (99%)	164 (99%)	2 (1%)	63	87
18	R	146/152 (96%)	146 (100%)	0	100	100
19	S	153/154 (99%)	152 (99%)	1 (1%)	76	91
20	T	143/170 (84%)	140 (98%)	3 (2%)	47	79
21	U	154/168 (92%)	152 (99%)	2 (1%)	61	86
22	V	138/139 (99%)	134 (97%)	4 (3%)	37	73
23	W	96/106 (91%)	92 (96%)	4 (4%)	26	61
24	X	105/105 (100%)	101 (96%)	4 (4%)	29	64
25	Y	55/131 (42%)	54 (98%)	1 (2%)	51	82
26	Z	105/118 (89%)	103 (98%)	2 (2%)	50	81
28	ZA	157/167 (94%)	154 (98%)	3 (2%)	50	81
29	ZB	155/163 (95%)	153 (99%)	2 (1%)	61	86
30	a	111/112 (99%)	108 (97%)	3 (3%)	39	74
31	b	113/114 (99%)	110 (97%)	3 (3%)	39	74
32	c	119/120 (99%)	119 (100%)	0	100	100
33	d	50/66 (76%)	49 (98%)	1 (2%)	48	80
34	e	79/84 (94%)	74 (94%)	5 (6%)	16	45
35	f	97/100 (97%)	97 (100%)	0	100	100
36	g	109/130 (84%)	108 (99%)	1 (1%)	70	89
37	h	92/93 (99%)	91 (99%)	1 (1%)	65	87
38	i	97/99 (98%)	96 (99%)	1 (1%)	68	88
39	j	101/102 (99%)	100 (99%)	1 (1%)	68	88
40	k	80/81 (99%)	79 (99%)	1 (1%)	61	86
41	l	69/70 (99%)	69 (100%)	0	100	100
42	m	69/70 (99%)	67 (97%)	2 (3%)	37	73
43	n	47/48 (98%)	46 (98%)	1 (2%)	47	79
44	o	47/47 (100%)	46 (98%)	1 (2%)	47	79
45	q	87/90 (97%)	85 (98%)	2 (2%)	44	78
46	r	70/76 (92%)	69 (99%)	1 (1%)	59	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	ZC	85/108 (79%)	82 (96%)	3 (4%)	32	67
51	ZD	127/138 (92%)	121 (95%)	6 (5%)	23	57
52	ZE	129/131 (98%)	126 (98%)	3 (2%)	44	78
53	ZF	98/102 (96%)	97 (99%)	1 (1%)	68	88
54	ZG	97/118 (82%)	94 (97%)	3 (3%)	35	70
55	ZH	112/116 (97%)	109 (97%)	3 (3%)	39	74
56	ZI	112/121 (93%)	110 (98%)	2 (2%)	51	82
57	ZJ	126/129 (98%)	122 (97%)	4 (3%)	34	70
58	ZK	114/118 (97%)	109 (96%)	5 (4%)	25	59
59	ZL	90/104 (86%)	85 (94%)	5 (6%)	19	50
60	ZM	72/72 (100%)	70 (97%)	2 (3%)	38	73
61	ZO	113/114 (99%)	111 (98%)	2 (2%)	51	82
62	ZP	117/119 (98%)	113 (97%)	4 (3%)	32	68
63	ZQ	115/118 (98%)	112 (97%)	3 (3%)	40	75
64	ZR	62/107 (58%)	61 (98%)	1 (2%)	55	83
65	ZS	85/158 (54%)	84 (99%)	1 (1%)	63	87
66	ZT	72/73 (99%)	69 (96%)	3 (4%)	26	61
67	ZU	54/60 (90%)	53 (98%)	1 (2%)	50	81
68	ZV	47/48 (98%)	44 (94%)	3 (6%)	16	44
69	ZW	47/54 (87%)	45 (96%)	2 (4%)	26	60
70	ZY	261/267 (98%)	260 (100%)	1 (0%)	84	94
71	p	8/24 (33%)	8 (100%)	0	100	100
72	s	186/218 (85%)	181 (97%)	5 (3%)	39	74
73	t	188/223 (84%)	181 (96%)	7 (4%)	30	65
74	u	178/203 (88%)	174 (98%)	4 (2%)	45	78
75	v	179/192 (93%)	176 (98%)	3 (2%)	53	83
76	w	219/222 (99%)	216 (99%)	3 (1%)	59	85
77	x	175/192 (91%)	172 (98%)	3 (2%)	53	83
78	y	194/202 (96%)	191 (98%)	3 (2%)	57	84
79	z	163/168 (97%)	157 (96%)	6 (4%)	30	65
All	All	9155/9848 (93%)	8979 (98%)	176 (2%)	49	81

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	ZL	19	HIS
72	s	29	VAL
60	ZM	49	ASP
64	ZR	80	VAL
73	t	101	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
72	s	8	ASN
72	s	33	ASN
77	x	102	ASN
22	V	146	ASN
21	U	152	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3018/3283 (91%)	464 (15%)	18 (0%)
2	B	121/122 (99%)	15 (12%)	1 (0%)
27	CA	1629/1775 (91%)	467 (28%)	26 (1%)
3	C	153/158 (96%)	22 (14%)	0
47	1	33/76 (43%)	8 (24%)	0
48	2	6/7 (85%)	1 (16%)	0
49	3	16/17 (94%)	4 (25%)	0
All	All	4976/5438 (91%)	981 (19%)	45 (0%)

5 of 981 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	G
1	A	12	U
1	A	15	G
1	A	24	A
1	A	38	A

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	CA	865	G
27	CA	1244	C
27	CA	881	U
27	CA	1166	A
27	CA	1346	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
27	B8N	CA	1161	27	24,29,30	3.11	6 (25%)	29,42,45	1.94	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	B8N	CA	1161	27	-	11/16/34/35	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	CA	1161	B8N	C6-N1	7.82	1.55	1.36
27	CA	1161	B8N	C4-N3	-7.44	1.26	1.40
27	CA	1161	B8N	C6-C5	6.53	1.44	1.34
27	CA	1161	B8N	C2-N1	6.51	1.58	1.39
27	CA	1161	B8N	O4-C4	-3.22	1.16	1.23

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	CA	1161	B8N	C5-C4-N3	5.52	126.40	116.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	CA	1161	B8N	C4-N3-C2	-4.74	119.46	125.46
27	CA	1161	B8N	C31-N3-C2	3.51	122.92	117.67
27	CA	1161	B8N	N3-C2-N1	2.91	120.87	116.76
27	CA	1161	B8N	O4-C4-N3	-2.90	115.06	119.98

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	CA	1161	B8N	C32-C31-N3-C4
27	CA	1161	B8N	N3-C31-C32-C33
27	CA	1161	B8N	C31-C32-C33-N34
27	CA	1161	B8N	N34-C33-C34-O36
27	CA	1161	B8N	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	CA	1161	B8N	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 228 ligands modelled in this entry, 227 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	BLS	A	3453	-	30,31,31	0.65	1 (3%)	33,43,43	1.04	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	BLS	A	3453	-	-	4/25/38/38	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A	3453	BLS	O4-C6'	-2.88	1.21	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	A	3453	BLS	O5'-C1'-C2'	-4.30	110.81	113.13
81	A	3453	BLS	N15-C14-N12	2.05	121.00	118.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	A	3453	BLS	O7-C7-C8-C9
81	A	3453	BLS	N6-C7-C8-C9
81	A	3453	BLS	C3'-C4'-N6-C7
81	A	3453	BLS	C5'-C4'-N6-C7

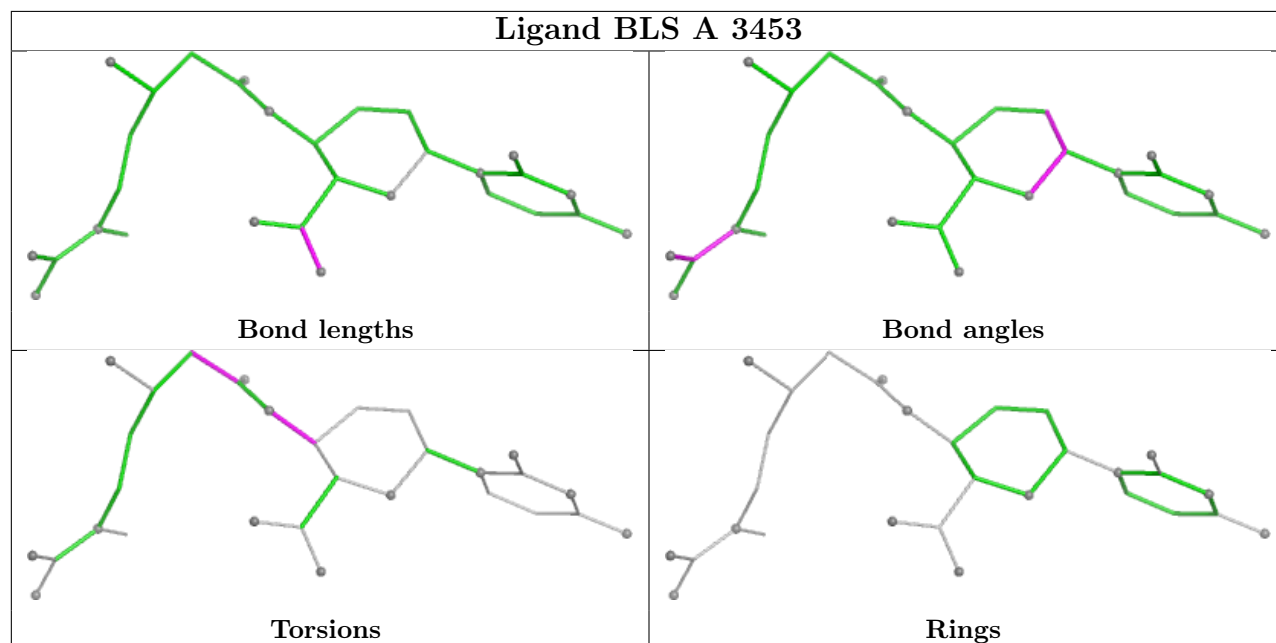
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	A	3453	BLS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

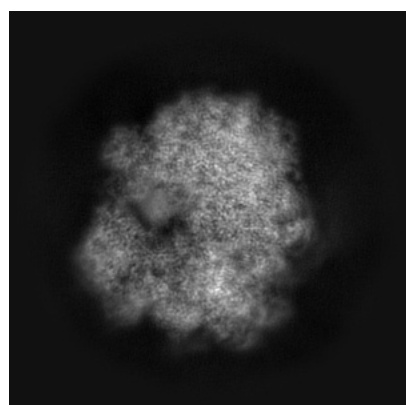
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55657. These allow visual inspection of the internal detail of the map and identification of artifacts.

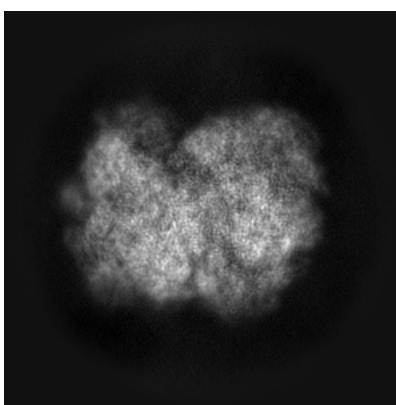
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

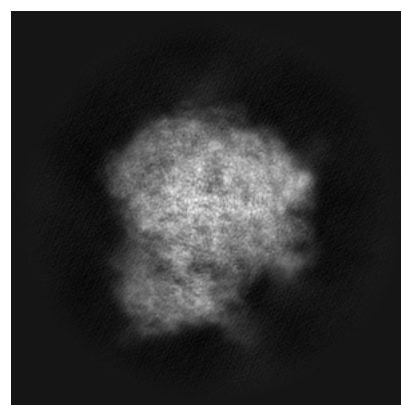
6.1.1 Primary map



X



Y

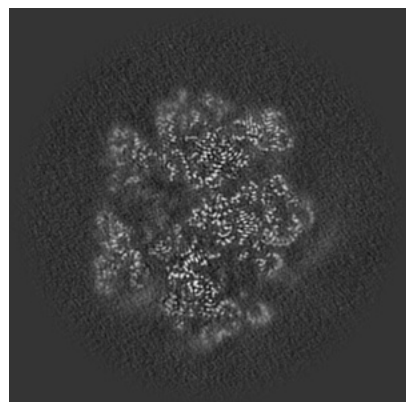


Z

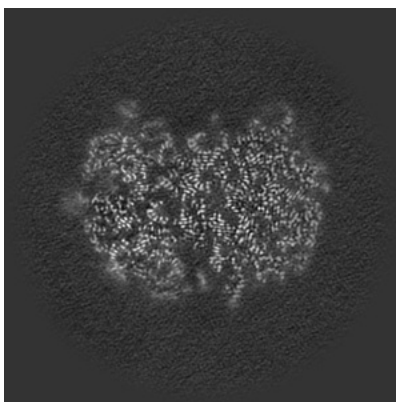
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

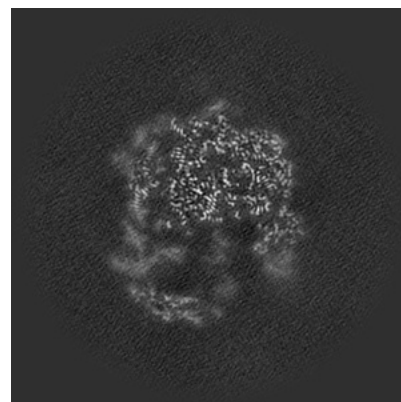
6.2.1 Primary map



X Index: 240



Y Index: 240

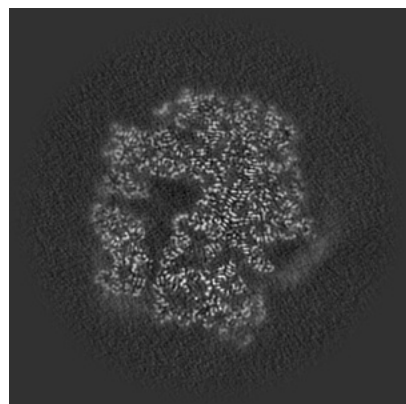


Z Index: 240

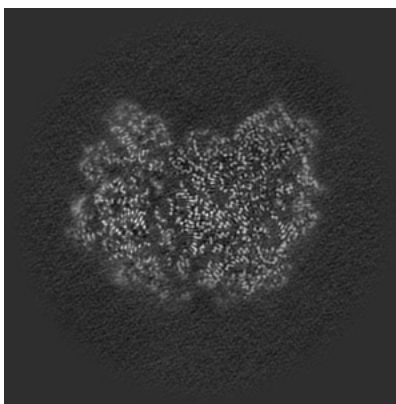
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

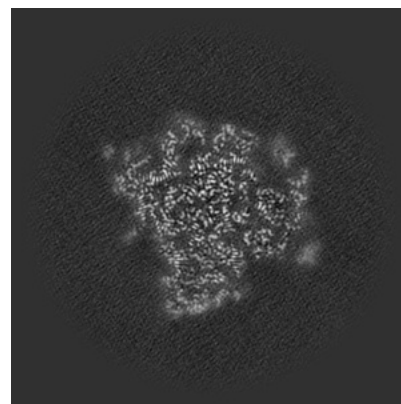
6.3.1 Primary map



X Index: 223



Y Index: 253

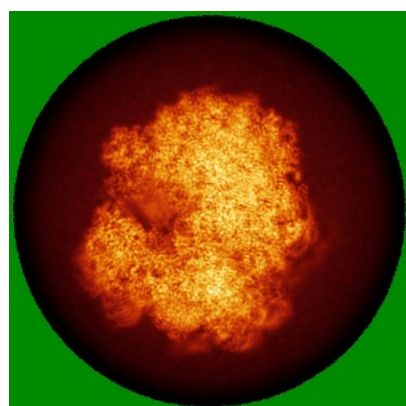


Z Index: 305

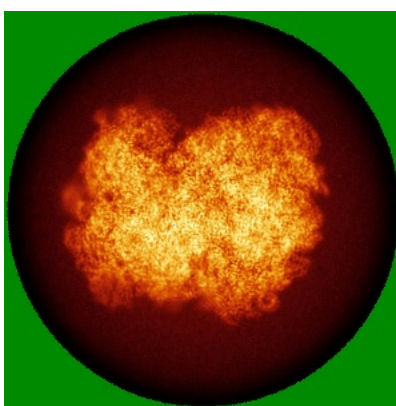
The images above show the largest variance slices of the map in three orthogonal directions.

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

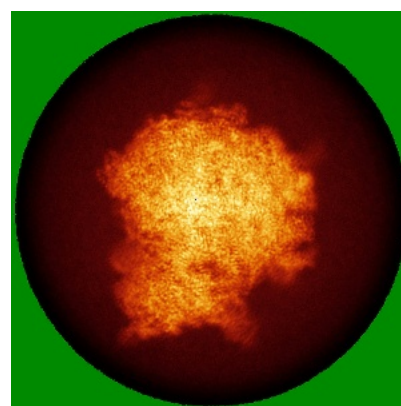
6.4.1 Primary map



X



Y

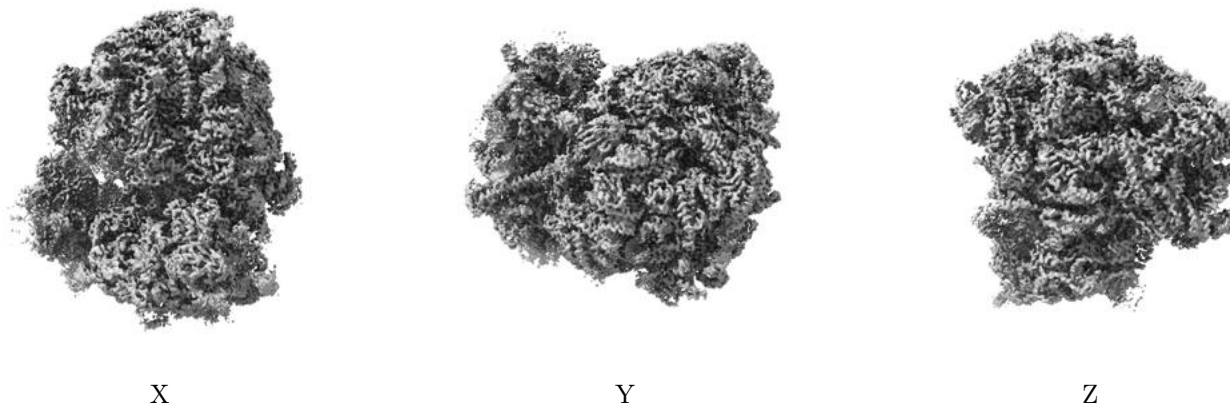


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

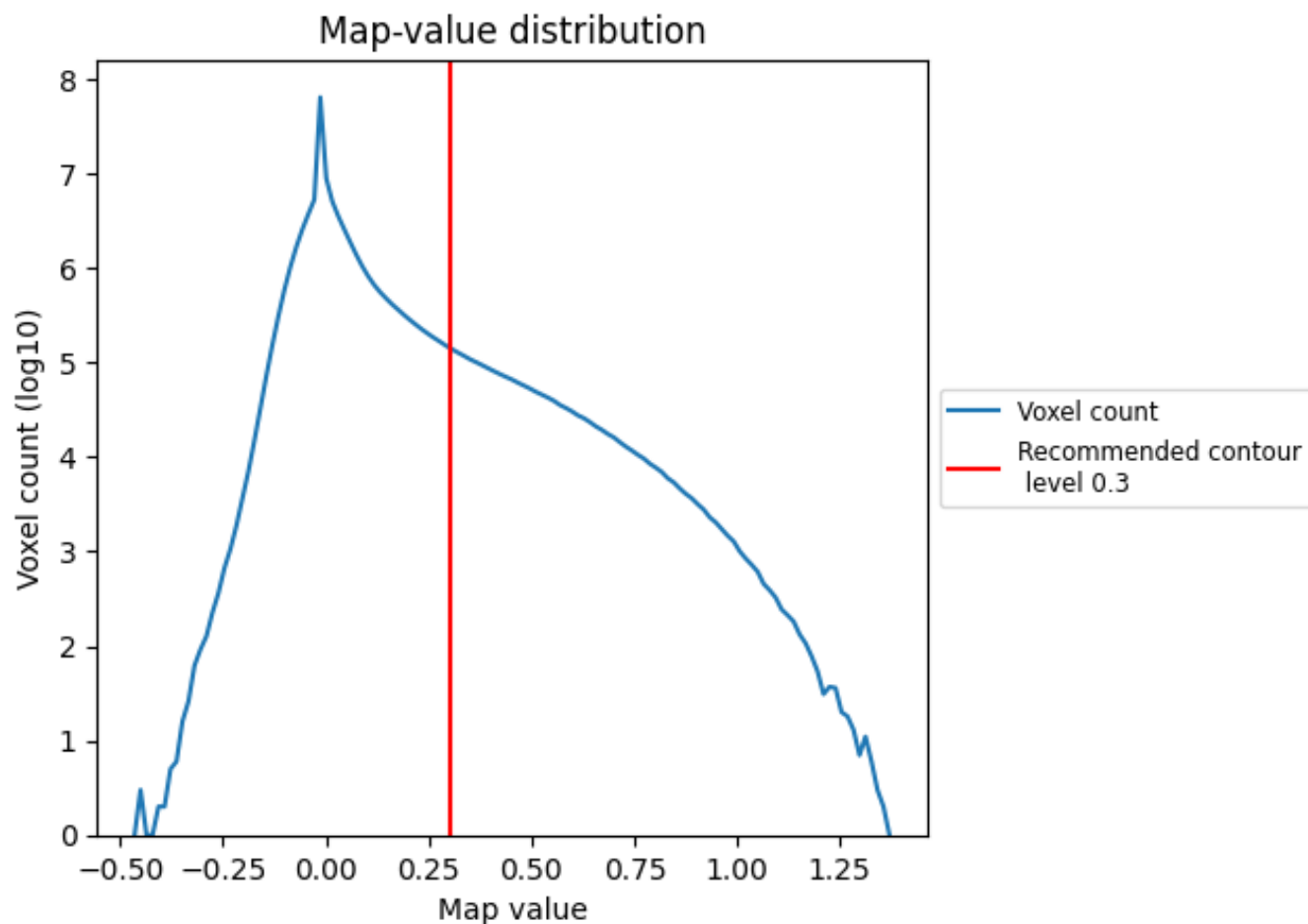
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

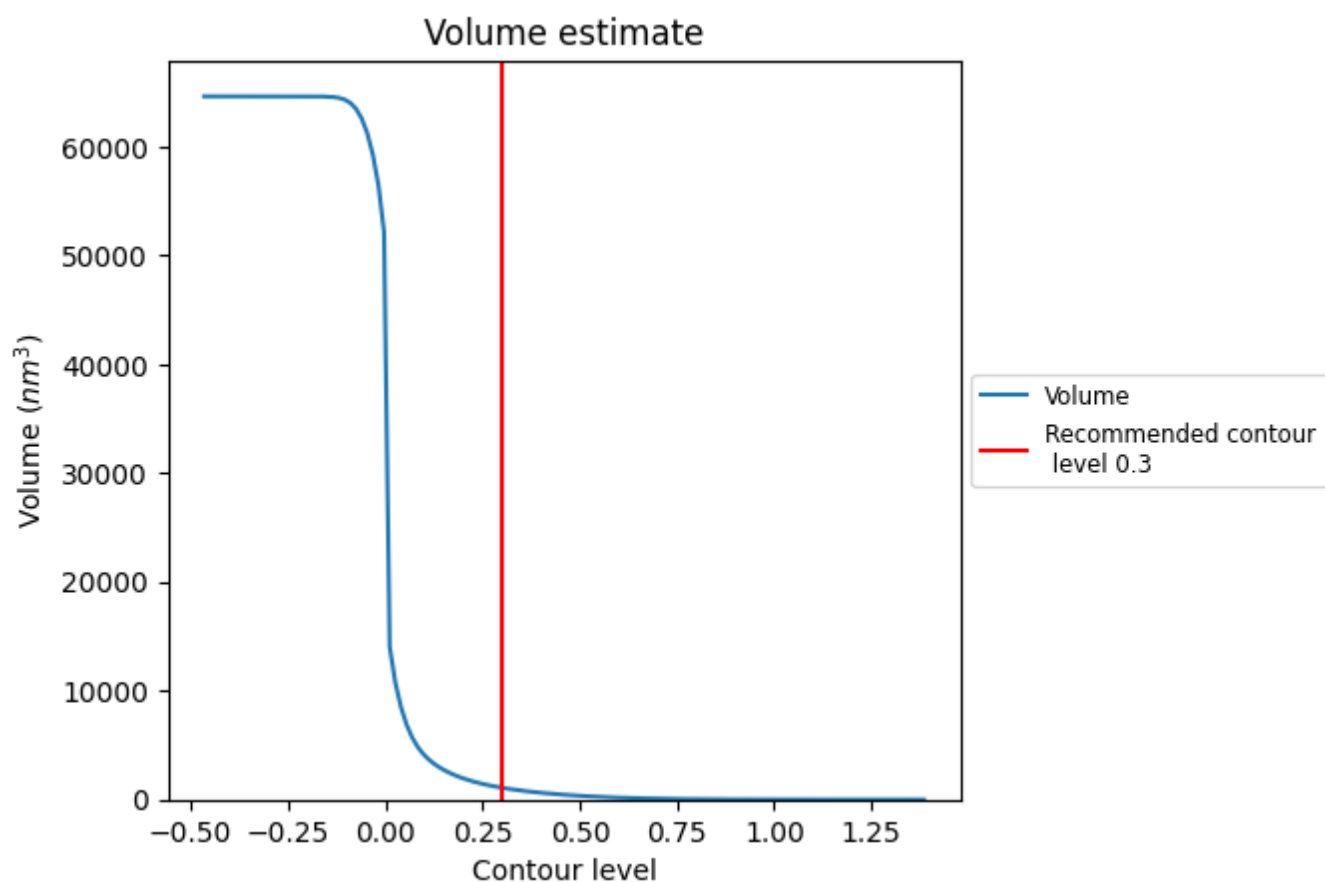
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

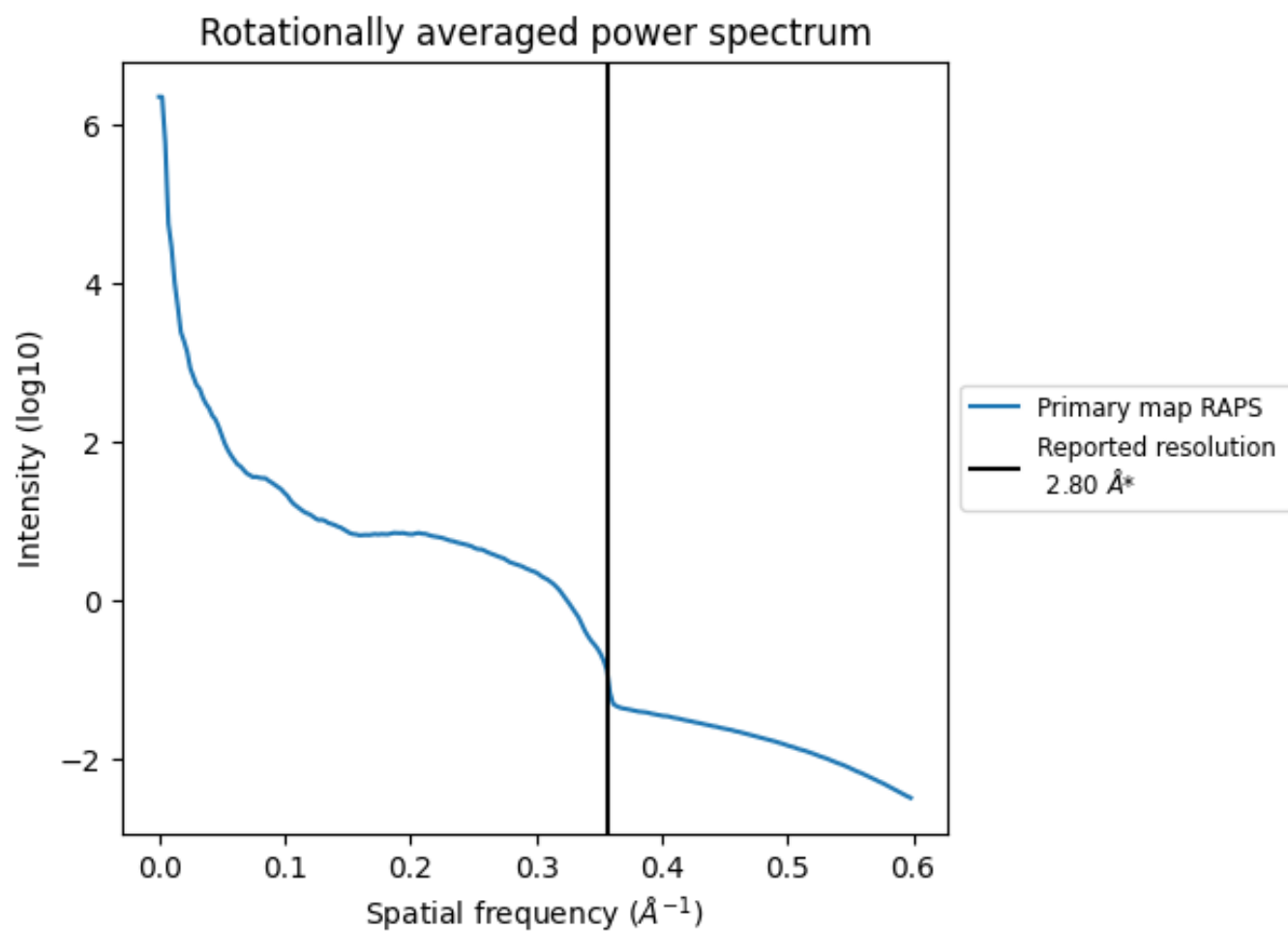
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1085 nm³; this corresponds to an approximate mass of 980 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

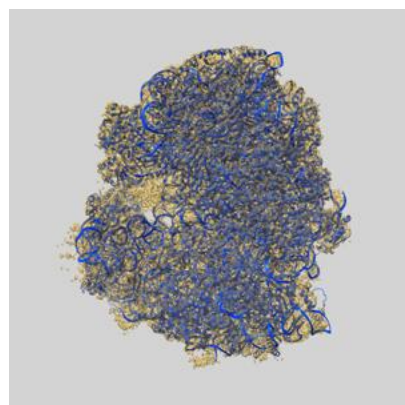
8 Fourier-Shell correlation ⓘ

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

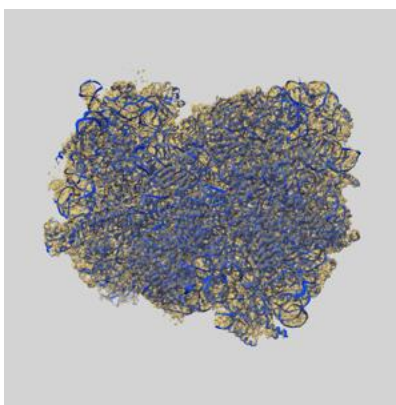
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55657 and PDB model 9T7T. Per-residue inclusion information can be found in section [3](#) on page [21](#).

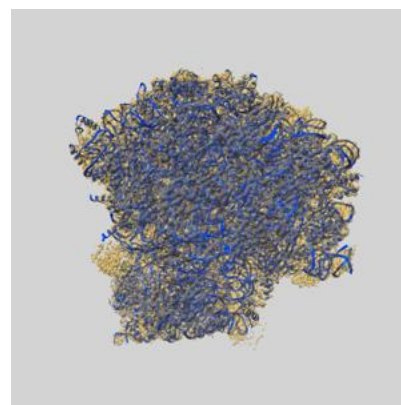
9.1 Map-model overlay [i](#)



X



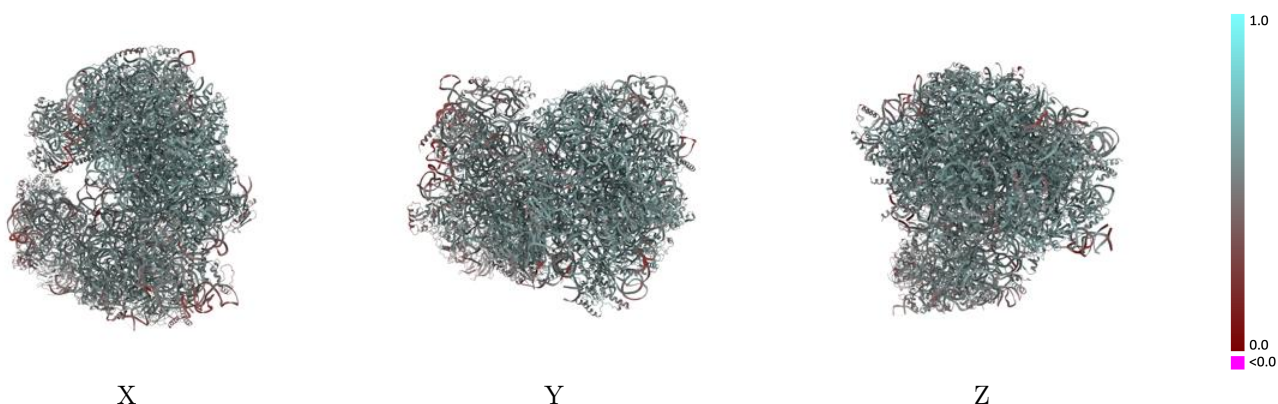
Y



Z

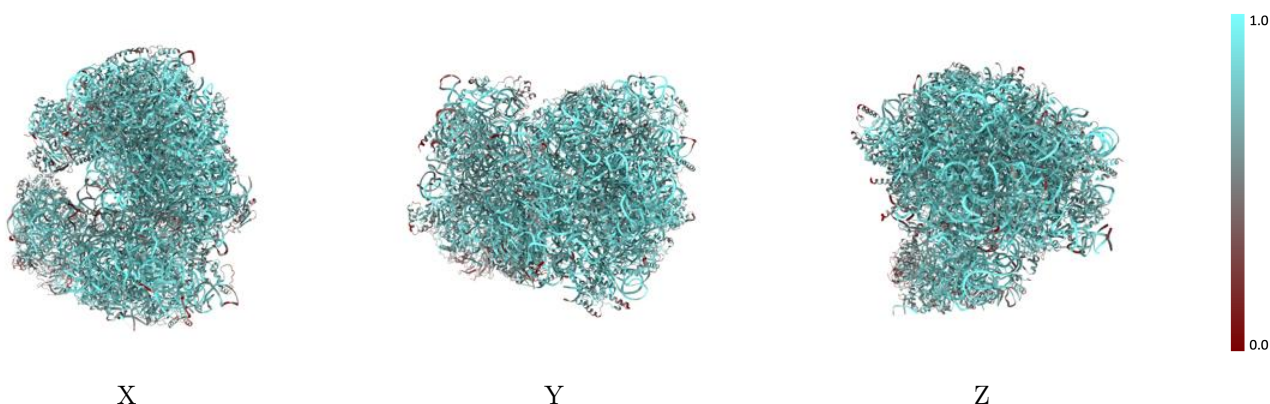
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



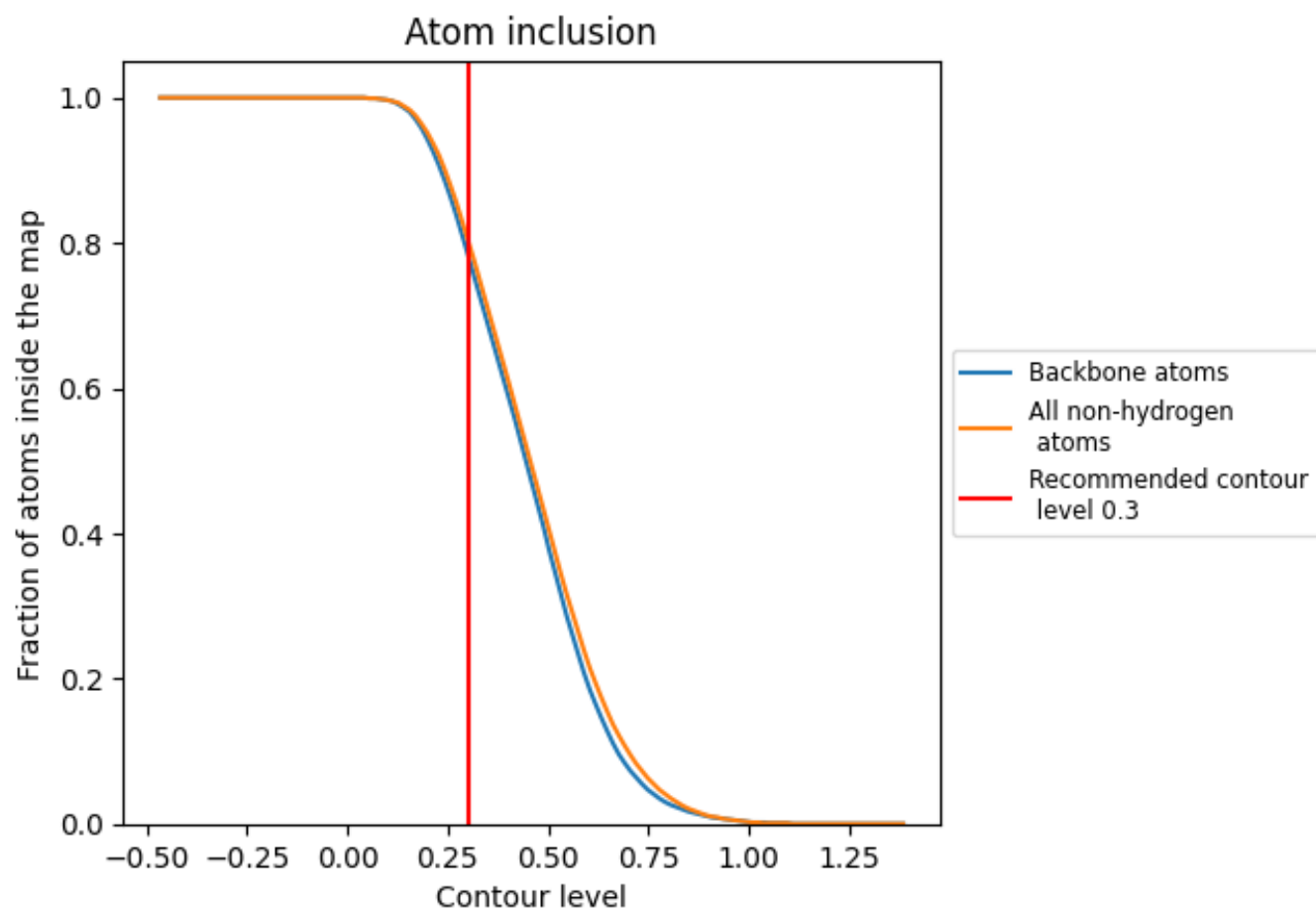
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8060	 0.5400
1	 0.6800	 0.4540
2	 0.7620	 0.5260
3	 0.3590	 0.4440
A	 0.9090	 0.5600
B	 0.9240	 0.5540
C	 0.9230	 0.5690
CA	 0.8700	 0.5110
D	 0.8100	 0.5950
E	 0.8030	 0.5870
F	 0.7870	 0.5740
G	 0.7020	 0.5150
H	 0.6860	 0.5240
I	 0.7580	 0.5660
J	 0.6750	 0.5320
K	 0.6630	 0.5610
L	 0.7090	 0.5700
M	 0.6140	 0.5030
N	 0.7700	 0.5640
O	 0.7250	 0.5580
P	 0.8330	 0.6030
Q	 0.7690	 0.5850
R	 0.8170	 0.5880
S	 0.8100	 0.5790
T	 0.7740	 0.5570
U	 0.7500	 0.5780
V	 0.7170	 0.5690
W	 0.5580	 0.4650
X	 0.7150	 0.5780
Y	 0.7770	 0.5840
Z	 0.7660	 0.5650
ZA	 0.6690	 0.5130
ZB	 0.7120	 0.5090
ZC	 0.6300	 0.4460
ZD	 0.7270	 0.5480



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
ZE	 0.7740	 0.5470
ZF	 0.6360	 0.4950
ZG	 0.6630	 0.4960
ZH	 0.6490	 0.4970
ZI	 0.6270	 0.4820
ZJ	 0.6890	 0.5010
ZK	 0.6910	 0.5020
ZL	 0.5960	 0.4820
ZM	 0.7600	 0.5440
ZO	 0.7960	 0.5690
ZP	 0.7080	 0.5640
ZQ	 0.6680	 0.4900
ZR	 0.4730	 0.4680
ZS	 0.2860	 0.4920
ZT	 0.7430	 0.5210
ZU	 0.5290	 0.4760
ZV	 0.8130	 0.5300
ZW	 0.5620	 0.4670
ZY	 0.4090	 0.4190
a	 0.7570	 0.5550
b	 0.7080	 0.5330
c	 0.8200	 0.5880
d	 0.7020	 0.5420
e	 0.7270	 0.5390
f	 0.7490	 0.5640
g	 0.7730	 0.5840
h	 0.7930	 0.5970
i	 0.7360	 0.5630
j	 0.7260	 0.5520
k	 0.6750	 0.5430
l	 0.8440	 0.6060
m	 0.6050	 0.5250
n	 0.7180	 0.5760
o	 0.7190	 0.5770
p	 0.1620	 0.3790
q	 0.7420	 0.5820
r	 0.7780	 0.5890
s	 0.7260	 0.5170
t	 0.6110	 0.4880
u	 0.7750	 0.5540
v	 0.6170	 0.4950
w	 0.7400	 0.5180

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
x	 0.5740	 0.4880
y	 0.5910	 0.4780
z	 0.6400	 0.4620