



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 03:11 AM UTC

PDB ID : 9NDP / pdb_00009ndp
EMDB ID : EMD-49275
Title : Structure of stalled ribosome and nascent chain in complex with NMT2 and NAC
Authors : Zdancewicz, S.; Jomaa, A.
Deposited on : 2025-02-18
Resolution : 2.82 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

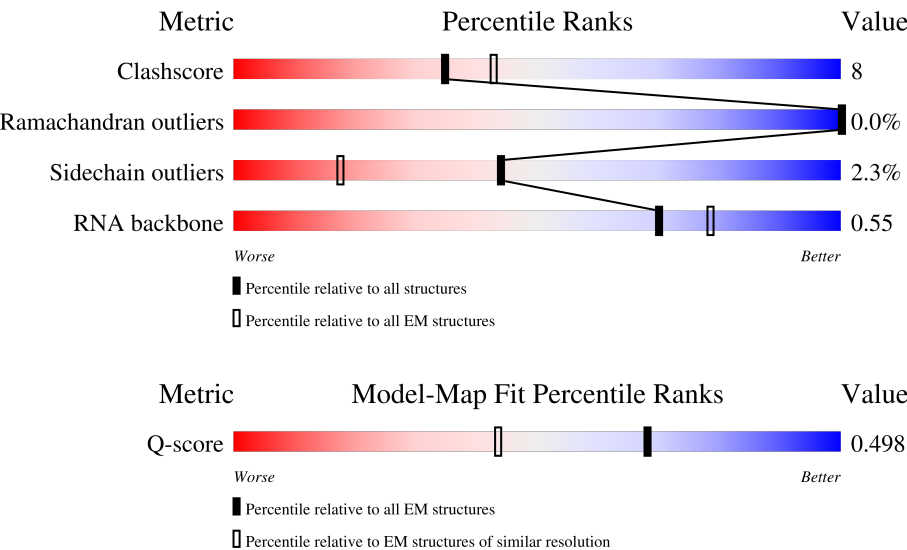
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.82 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.



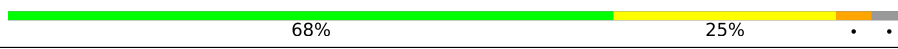
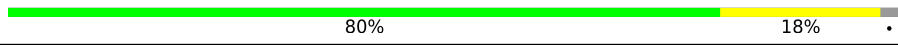
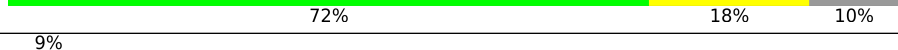
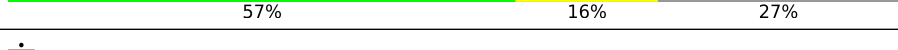
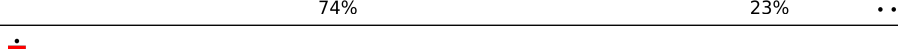
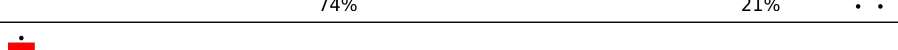
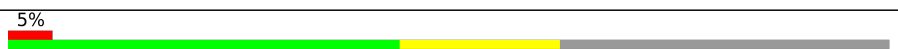
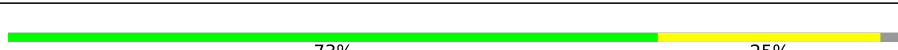
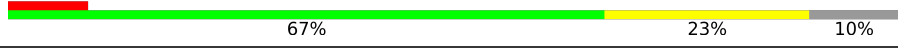
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11795 (2.32 - 3.32)

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	0	156	
2	4	6	
3	6	317	

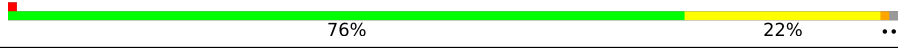
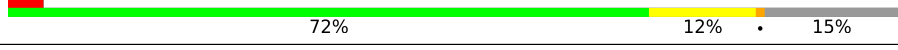
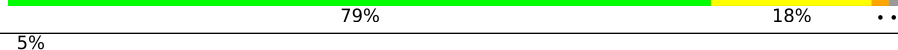
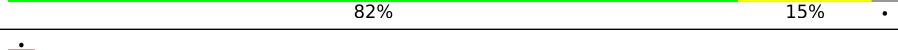
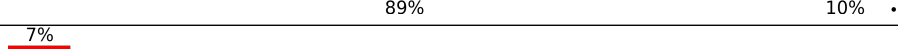
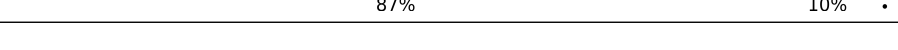
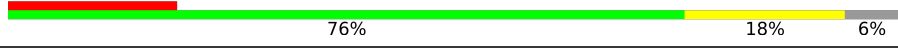
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Mol	Chain	Length	Quality of chain
4	7	120	
5	9	56	
6	A	257	
7	B	403	
8	C	413	
9	D	297	
10	F	249	
11	G	319	
12	H	192	
13	I	214	
14	J	178	
15	K	1698	
16	L	211	
17	M	218	
18	N	204	
19	O	203	
20	P	184	
21	Q	188	
22	R	181	
23	S	176	
24	T	160	
25	U	115	
26	V	140	
27	W	157	
28	X	156	

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Mol	Chain	Length	Quality of chain
29	Y	145	
30	Z	136	
31	a	148	
32	c	115	
33	d	125	
34	e	134	
35	f	110	
36	g	117	
37	h	123	
38	i	105	
39	j	97	
40	k	107	
41	l	51	
42	m	128	
43	n	25	
44	o	141	
45	p	92	
46	q	295	
47	r	137	
48	u	264	
49	v	255	
50	w	243	
51	x	263	
52	z	249	
53	s	318	

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Mol	Chain	Length	Quality of chain
54	t	165	
55	2	76	
56	5	3534	
57	8	151	
58	E	291	
59	b	245	
60	y	204	
61	BB	194	
62	CC	208	
63	DD	194	
64	SS	165	
65	EE	158	
66	RR	132	
67	QQ	151	
68	MM	151	
69	WW	145	
70	UU	146	
71	KK	135	
72	II	152	
73	PP	145	
74	GG	119	
75	HH	83	
76	TT	130	
77	VV	143	
78	NN	133	

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Mol	Chain	Length	Quality of chain
79	OO	124	
80	LL	117	
81	JJ	84	
82	FF	69	
83	AA	133	
84	EF	162	
85	EG	215	
86	NA	498	
87	NB	74	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 218587 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 protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	6	Total	C	N	O	P	0	0
			127	57	21	43	6		

- Molecule 3 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 5 is a protein called eS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	9	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 6 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 7 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 9 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

- Molecule 10 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

- Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 12 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 13 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 14 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 15 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	1698	Total	C	N	O	P	0	0
			36249	16180	6508	11864	1697		

- Molecule 16 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 18 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 19 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 20 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 21 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	187	Total	C	N	O	S	0	0
			1518	950	315	250	3		

- Molecule 22 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	180	Total	C	N	O	S	0	0
			1506	932	326	239	9		

- Molecule 23 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	176	Total	C	N	O	S	0	0
			1452	926	282	234	10		

- Molecule 24 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 25 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	104	Total	C	N	O	S	0	0
			846	541	147	156	2		

- Molecule 26 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 27 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 28 is a protein called eL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 29 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 31 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 32 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 33 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 34 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 35 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 36 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 37 is a protein called eL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 38 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 39 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 40 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 41 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 42 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 43 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 44 is a protein called Ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 45 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 46 is a protein called uS2 (SA).

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 47 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 48 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 49 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	221	Total	C	N	O	S	0	0
			1715	1111	295	300	9		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	57	ASN	ASP	conflict	UNP A0AAG1W6H3
v	97	PHE	CYS	conflict	UNP A0AAG1W6H3
v	141	VAL	LEU	conflict	UNP A0AAG1W6H3
v	181	PRO	LEU	conflict	UNP A0AAG1W6H3
v	191	VAL	-	insertion	UNP A0AAG1W6H3
v	215	MET	LEU	conflict	UNP A0AAG1W6H3
v	271	ASP	ASN	conflict	UNP A0AAG1W6H3
v	274	VAL	MET	conflict	UNP A0AAG1W6H3

- Molecule 50 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 51 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	262	Total	C	N	O	S	0	0
			2072	1323	384	357	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	25	GLY	SER	conflict	UNP G1TK17
x	156	VAL	MET	conflict	UNP G1TK17

- Molecule 52 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 53 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 54 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	t	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 55 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	2	76	Total	C	N	O	P	0	0
			1614	722	287	530	75		

- Molecule 56 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	5	3534	Total	C	N	O	P	0	0
			75786	33750	13880	24622	3534		

- Molecule 57 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 58 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 59 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	b	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 60 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	y	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 61 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BB	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 62 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	CC	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 63 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
63	DD	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 64 is a protein called S10_ plectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SS	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 65 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	EE	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 66 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	RR	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 67 is a protein called Ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	QQ	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 68 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	MM	135	Total	C	N	O	S	0	0
			1004	614	196	188	6		

- Molecule 69 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	WW	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 70 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	UU	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 71 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	KK	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 72 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	II	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 73 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	PP	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
PP	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 74 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	GG	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 75 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	HH	83	Total	C	N	O	S	0	0
			632	387	119	121	5		

- Molecule 76 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	TT	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 77 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	VV	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 78 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	NN	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 79 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	OO	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 80 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	LL	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 81 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	JJ	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 82 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	FF	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 83 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	AA	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 84 is a protein called Isoform 2 of Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	EF	110	Total	C	N	O	S	0	0
			854	534	158	158	4		

- Molecule 85 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	EG	67	Total	C	N	O	S	0	0
			531	335	97	98	1		

- Molecule 86 is a protein called Glycylpeptide N-tetradecanoyltransferase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	NA	361	Total	C	N	O	S	2	0
			2967	1920	503	530	14		

- Molecule 87 is a protein called Myristoylated alanine-rich C-kinase substrate,X-box-binding protein 1, luminal form.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	NB	37	Total	C	N	O	S	0	0
			288	187	50	48	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
NB	69	CYS	PRO	conflict	UNP P17861
NB	70	ALA	SER	conflict	UNP P17861

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	7	7	Total	Mg	0
			7	7	
88	A	1	Total	Mg	0
			1	1	
88	I	1	Total	Mg	0
			1	1	
88	K	77	Total	Mg	0
			77	77	
88	P	1	Total	Mg	0
			1	1	
88	V	1	Total	Mg	0
			1	1	
88	a	1	Total	Mg	0
			1	1	
88	e	1	Total	Mg	0
			1	1	
88	g	1	Total	Mg	0
			1	1	
88	5	198	Total	Mg	0
			198	198	
88	8	5	Total	Mg	0
			5	5	
88	y	1	Total	Mg	0
			1	1	

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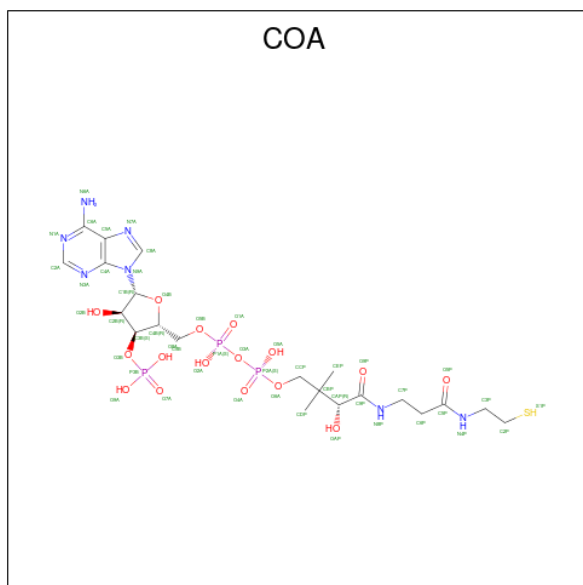
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
88	EE	1	Total	Mg	0
			1	1	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	g	1	Total	Zn	0
			1	1	
89	j	1	Total	Zn	0
			1	1	
89	m	1	Total	Zn	0
			1	1	
89	o	1	Total	Zn	0
			1	1	
89	p	1	Total	Zn	0
			1	1	
89	LL	1	Total	Zn	0
			1	1	

- Molecule 90 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).

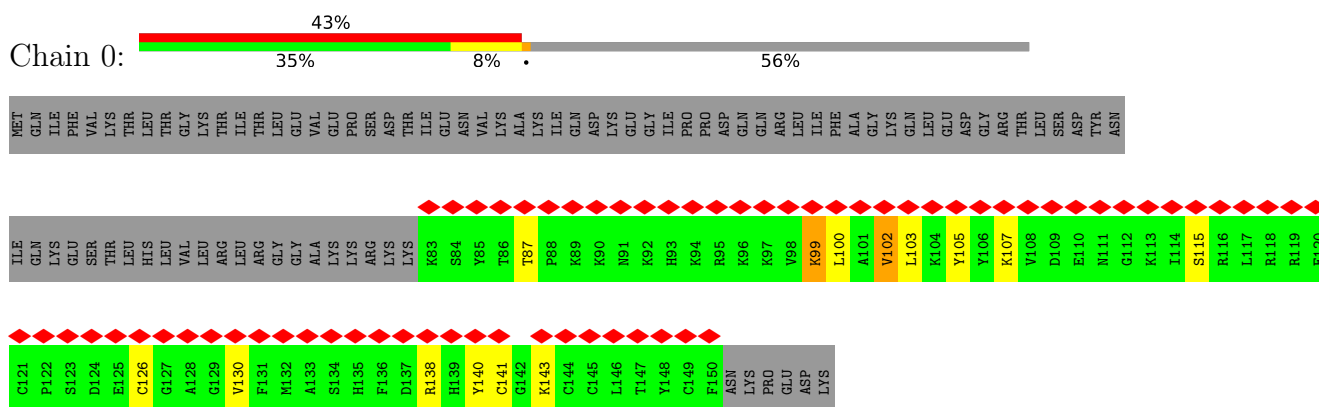


Mol	Chain	Residues	Atoms					AltConf	
90	NA	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	

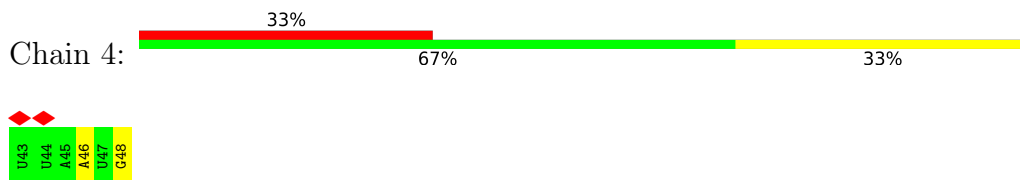
3 Residue-property plots [i](#)

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.

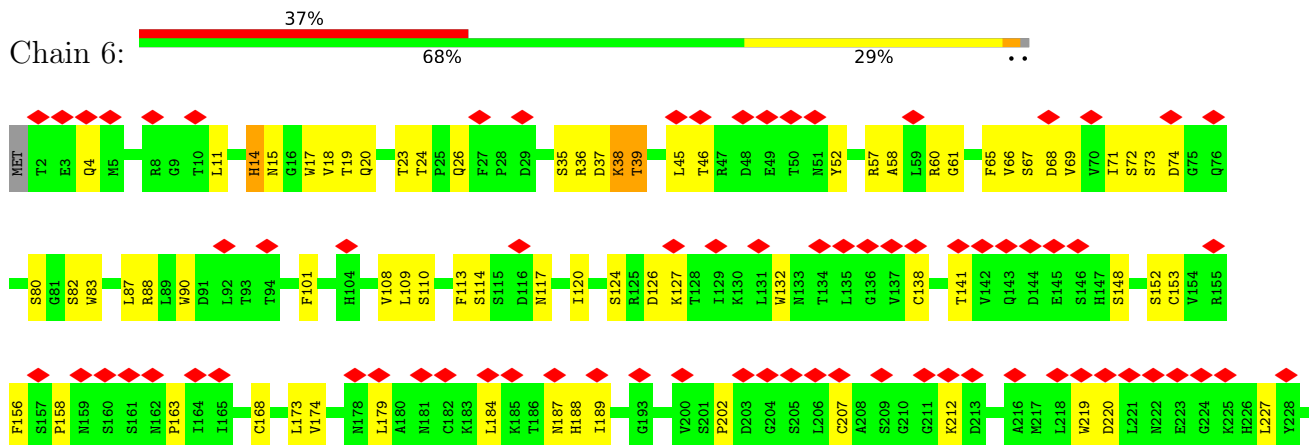
• Molecule 1: Ribosomal protein S27a

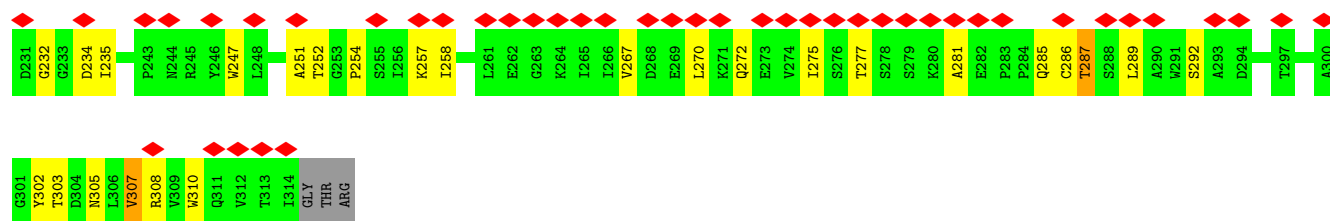


• Molecule 2: mRNA



• Molecule 3: RACK1

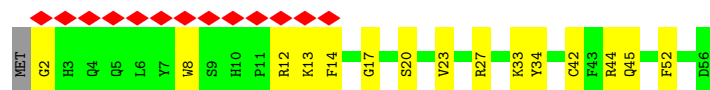




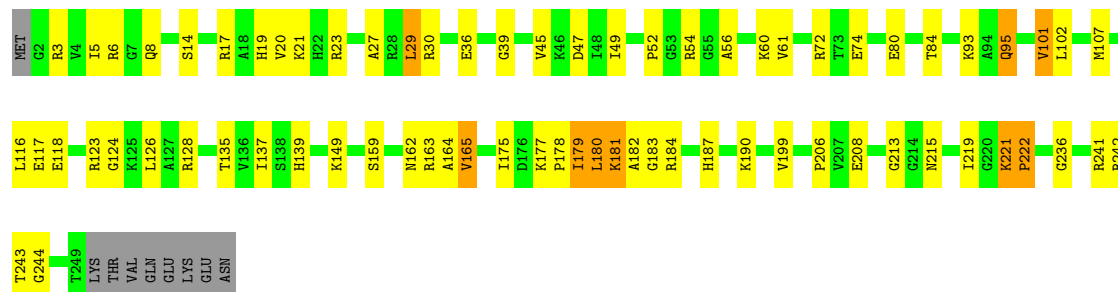
• Molecule 4: 5S rRNA



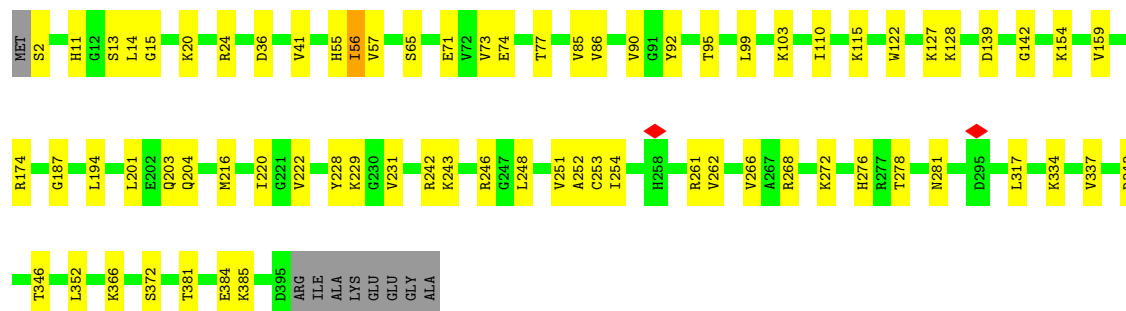
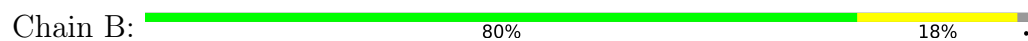
• Molecule 5: eS29



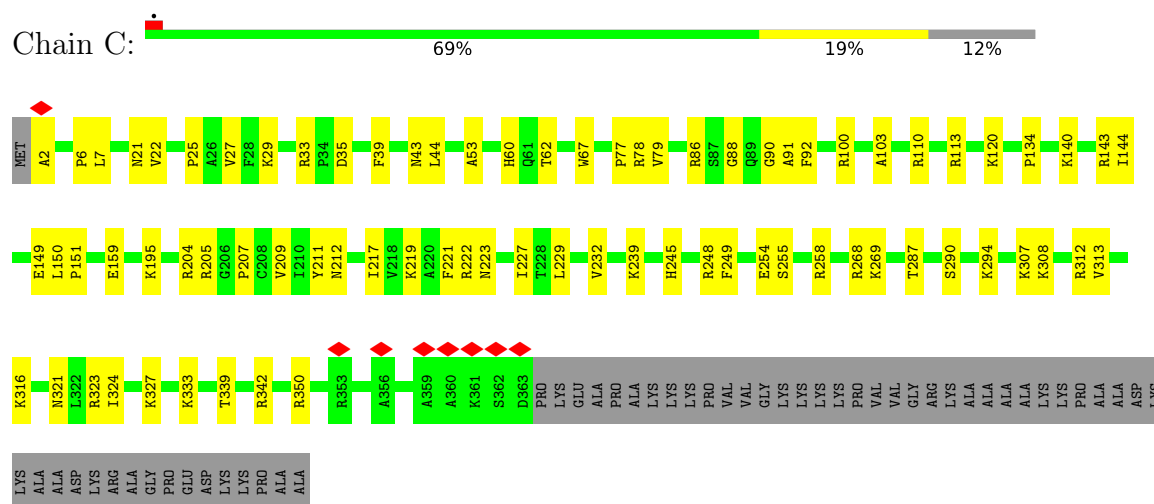
• Molecule 6: Ribosomal protein L8



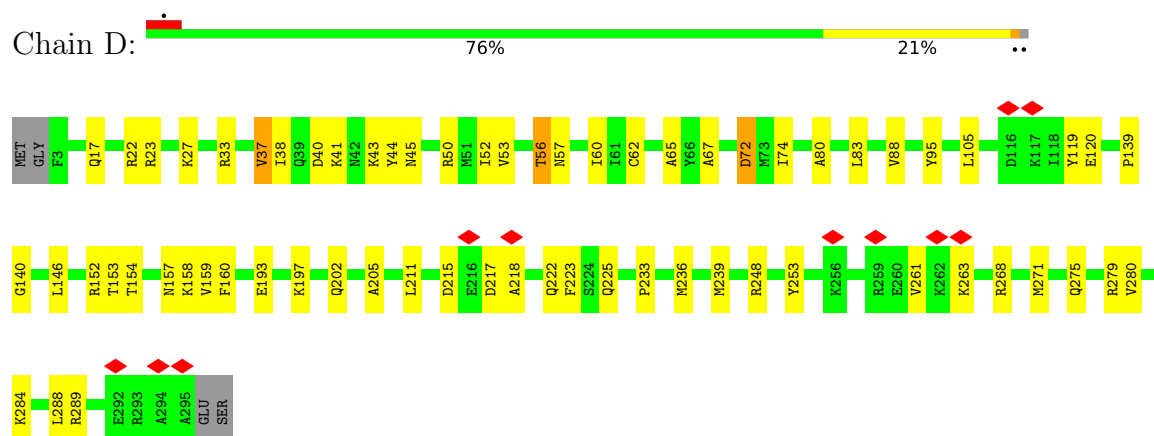
• Molecule 7: Ribosomal protein L3



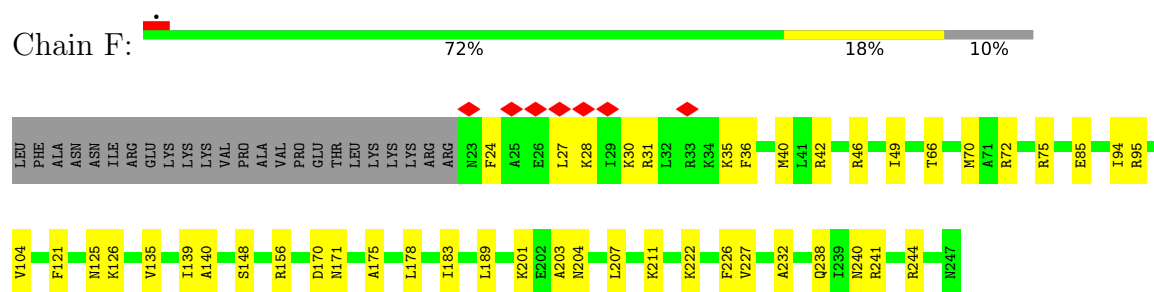
• Molecule 8: 60S ribosomal protein L4



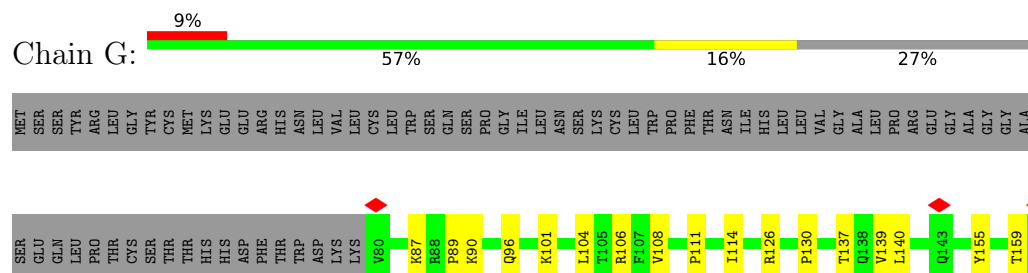
- Molecule 9: Large ribosomal subunit protein uL18

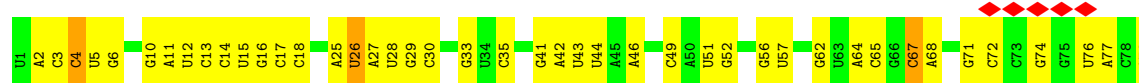


- Molecule 10: Large ribosomal subunit protein uL30

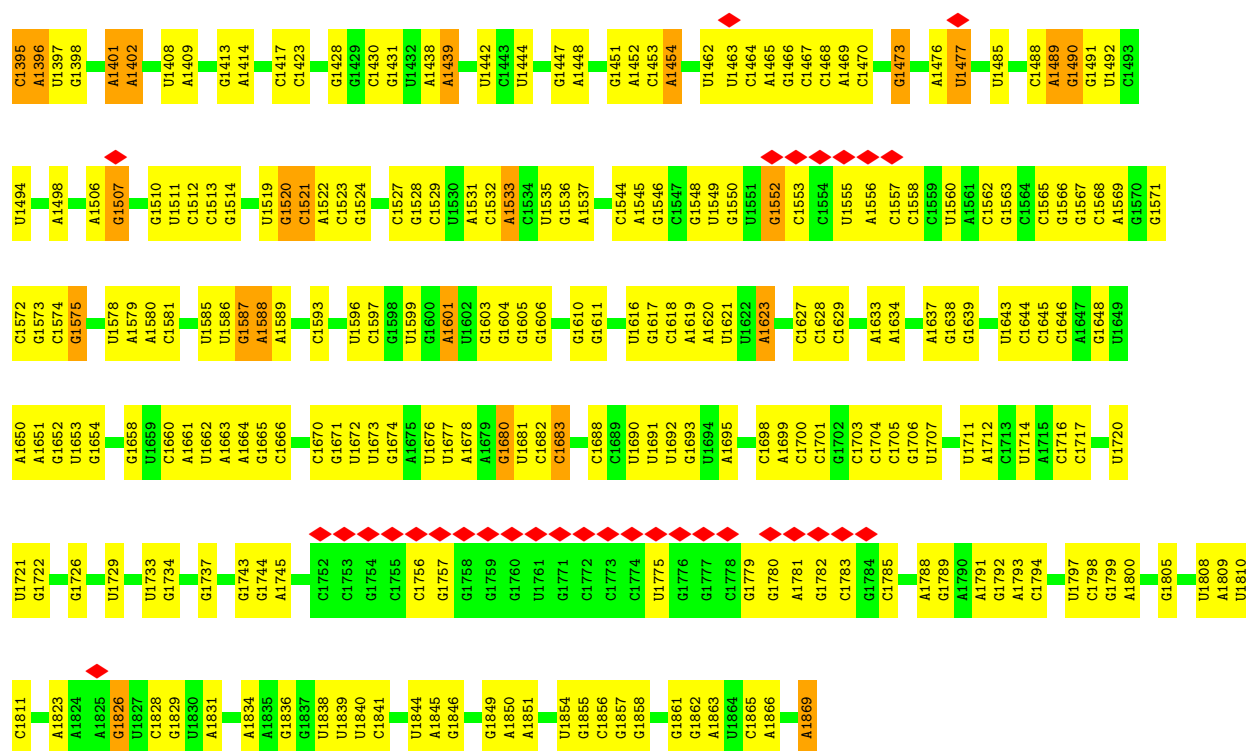


- Molecule 11: 60S ribosomal protein L7a

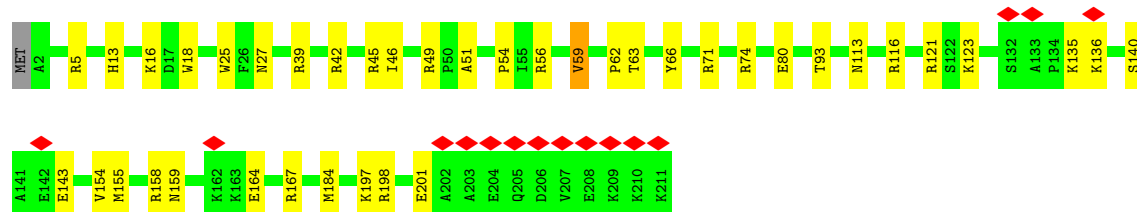
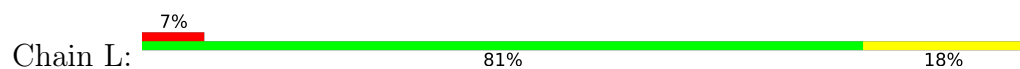




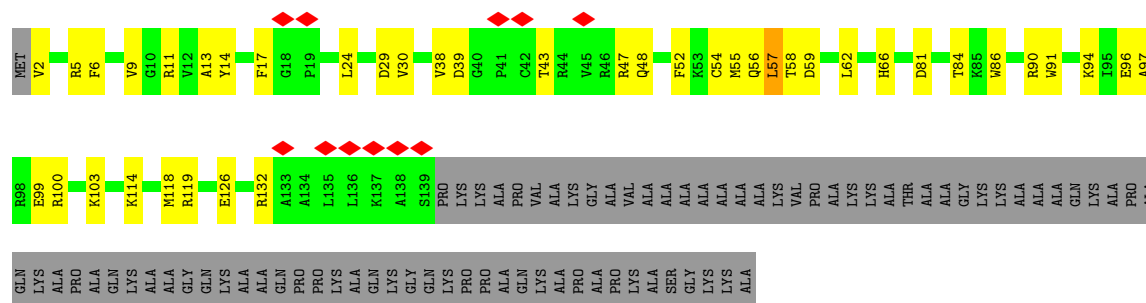
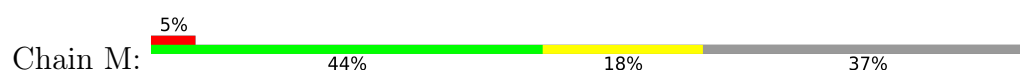




- Molecule 16: eL13

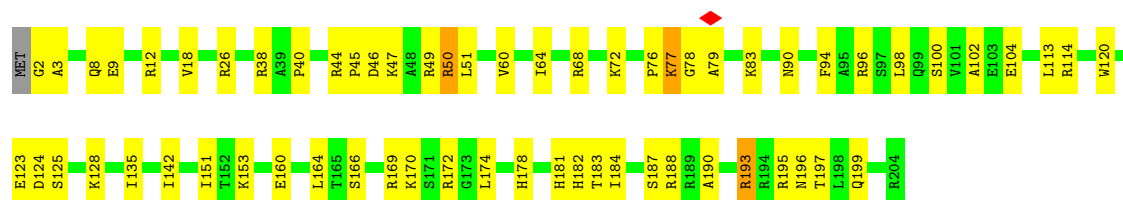


- Molecule 17: 60S ribosomal protein L14



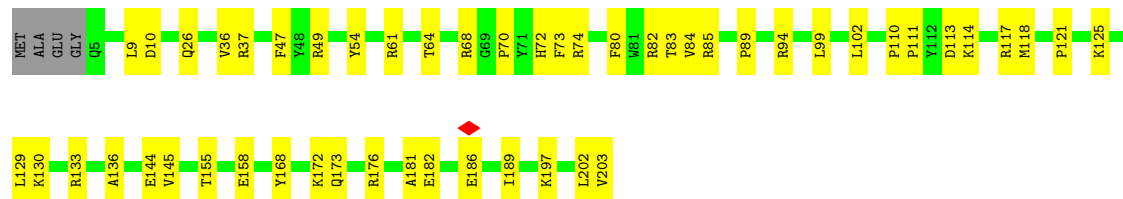
- Molecule 18: Ribosomal protein L15





• Molecule 19: Large ribosomal subunit protein uL13

Chain O: 73% 25%



• Molecule 20: Large ribosomal subunit protein uL22

Chain P: 71% 12% 17%



• Molecule 21: Ribosomal protein L18

Chain Q: 84% 15%



• Molecule 22: Ribosomal protein L19

Chain R: 7% 87% 12%



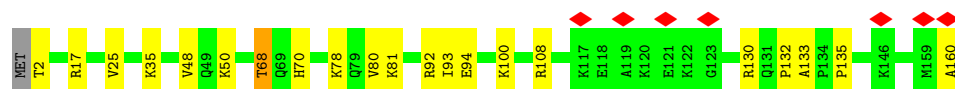
• Molecule 23: 60S ribosomal protein L18a

Chain S: 81% 18%



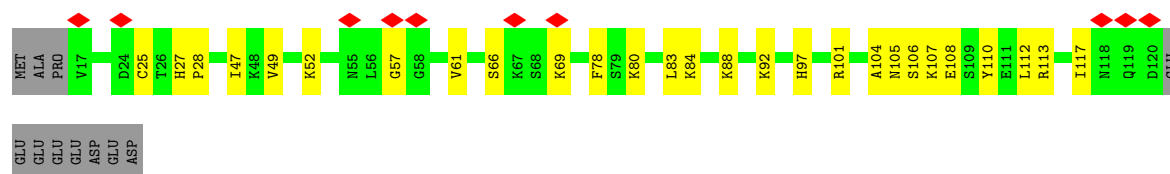
• Molecule 24: eL21

Chain T:  86% 12% ..



• Molecule 25: eL22

Chain U:  9% 67% 23% 10%



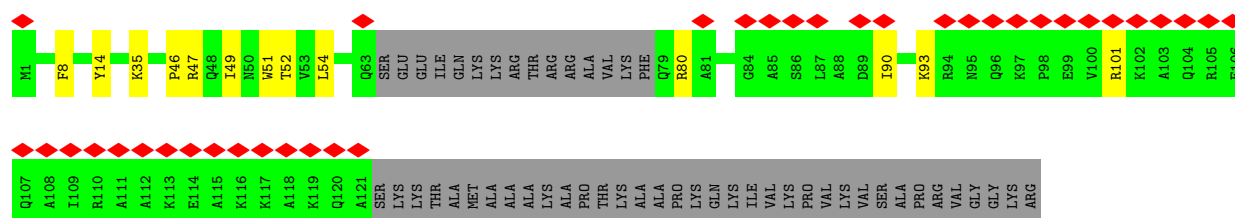
• Molecule 26: Ribosomal protein L23

Chain V:  78% 16% 6%



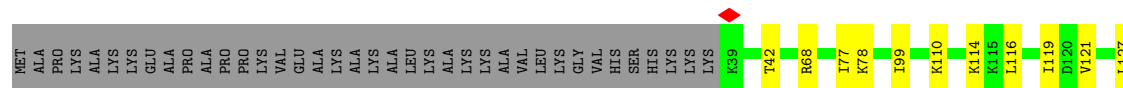
• Molecule 27: eL24

Chain W:  24% 59% 8% 32%



• Molecule 28: eL23

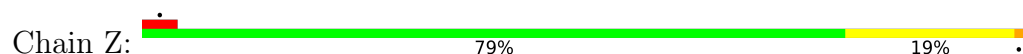
Chain X:  68% 8% 24%



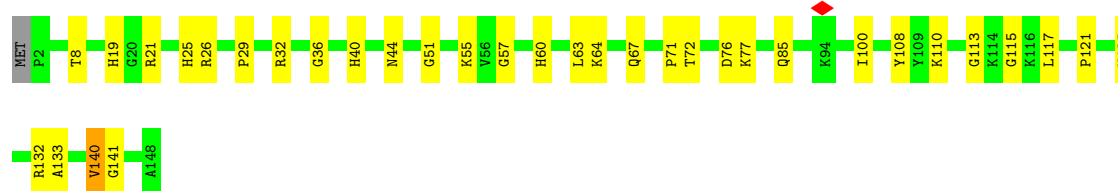
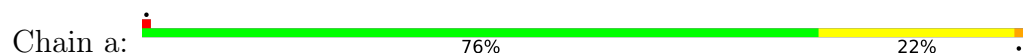
• Molecule 29: uL24

Chain Y:  74% 17% 8%

- Molecule 30: 60S ribosomal protein L27



- Molecule 31: 60S ribosomal protein L27a



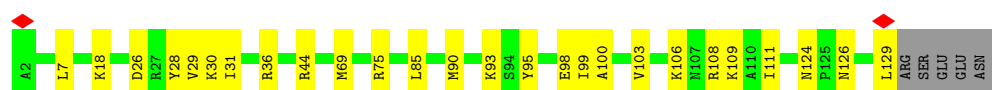
- Molecule 32: eL30



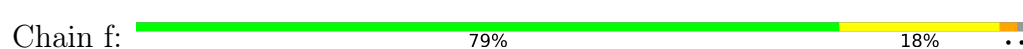
- Molecule 33: eL31

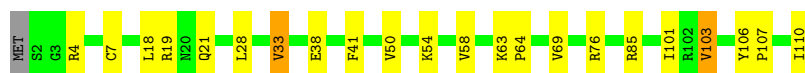


- Molecule 34: 60S ribosomal protein L32

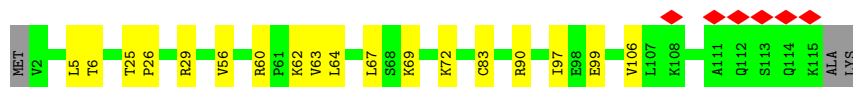
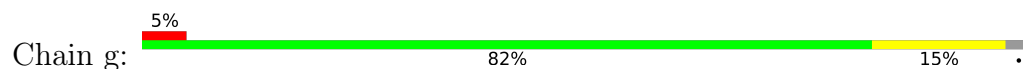


- Molecule 35: eL33

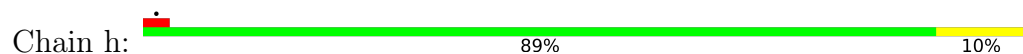




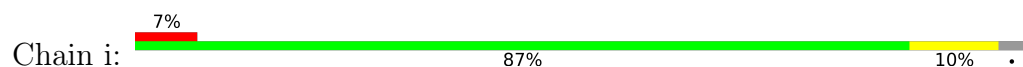
- Molecule 36: 60S ribosomal protein L34



- Molecule 37: eL35



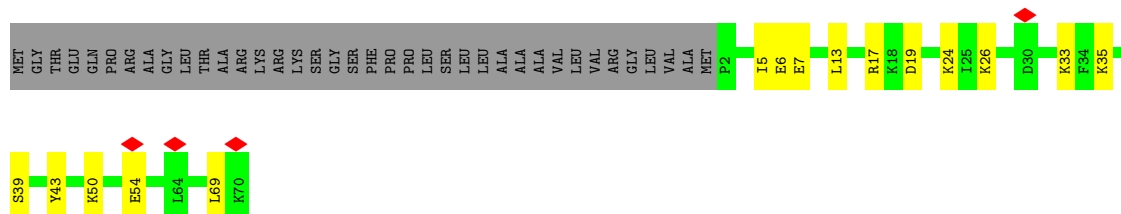
- Molecule 38: 60S ribosomal protein L36



- Molecule 39: Ribosomal protein L37



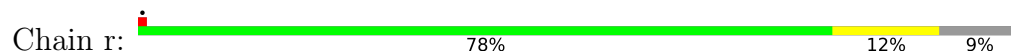
- Molecule 40: Large ribosomal subunit protein eL38



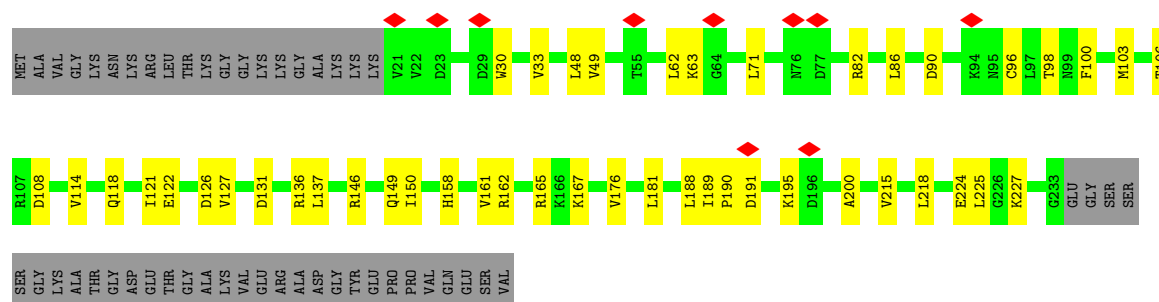
- Molecule 41: eL39



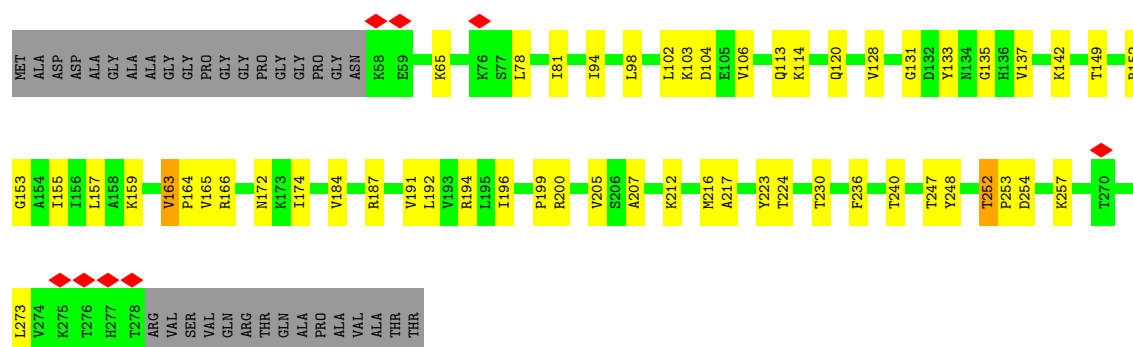
- Molecule 47: eL28



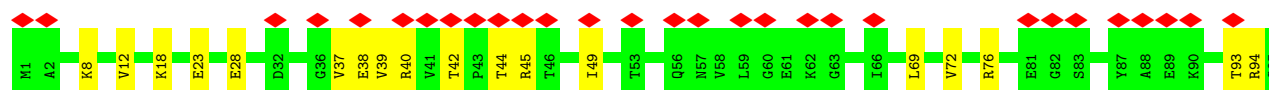
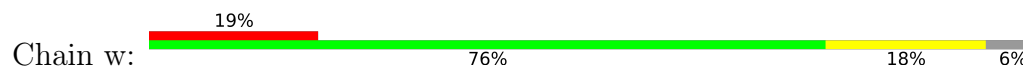
- Molecule 48: 40S ribosomal protein S3a

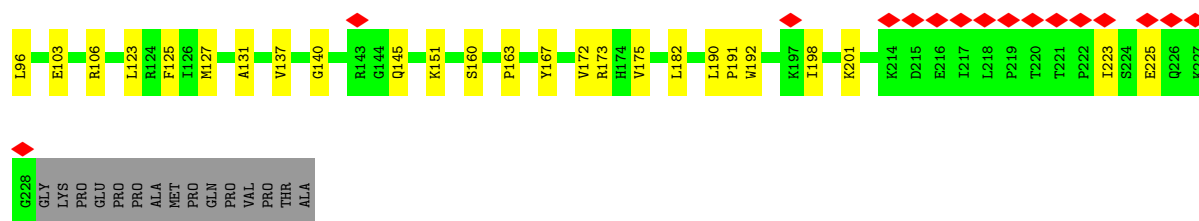


- Molecule 49: Small ribosomal subunit protein uS5

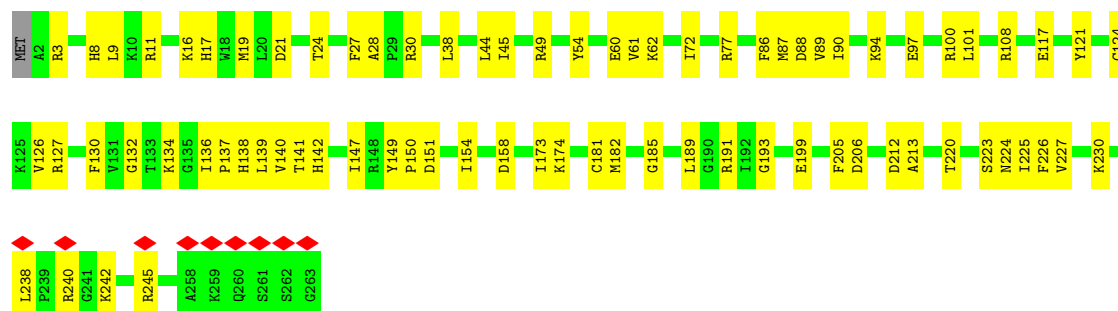


- Molecule 50: Ribosomal protein S3

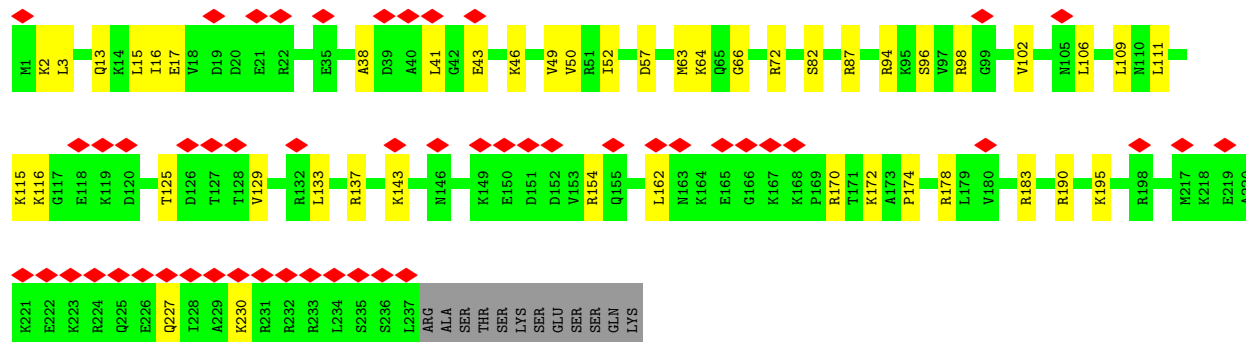
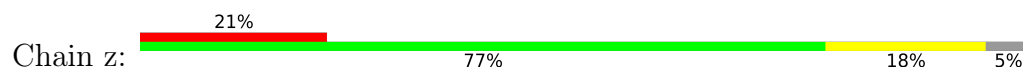




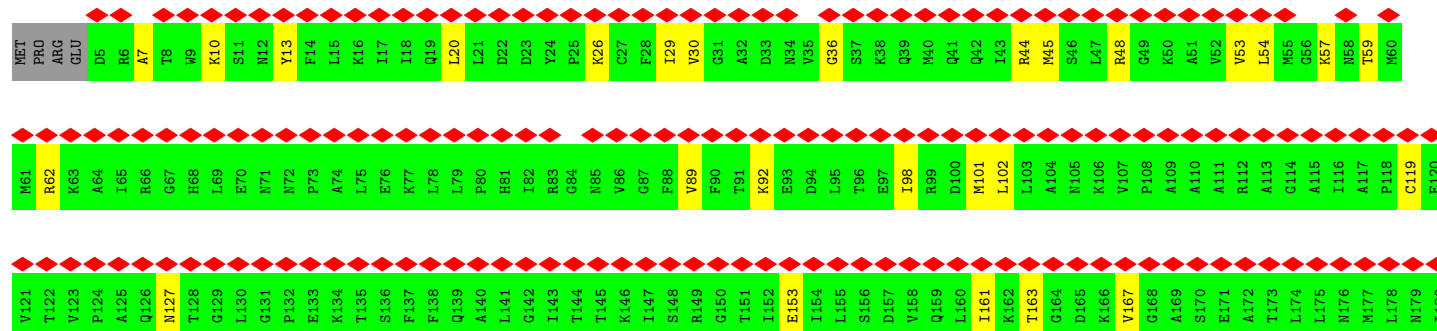
• Molecule 51: eS4

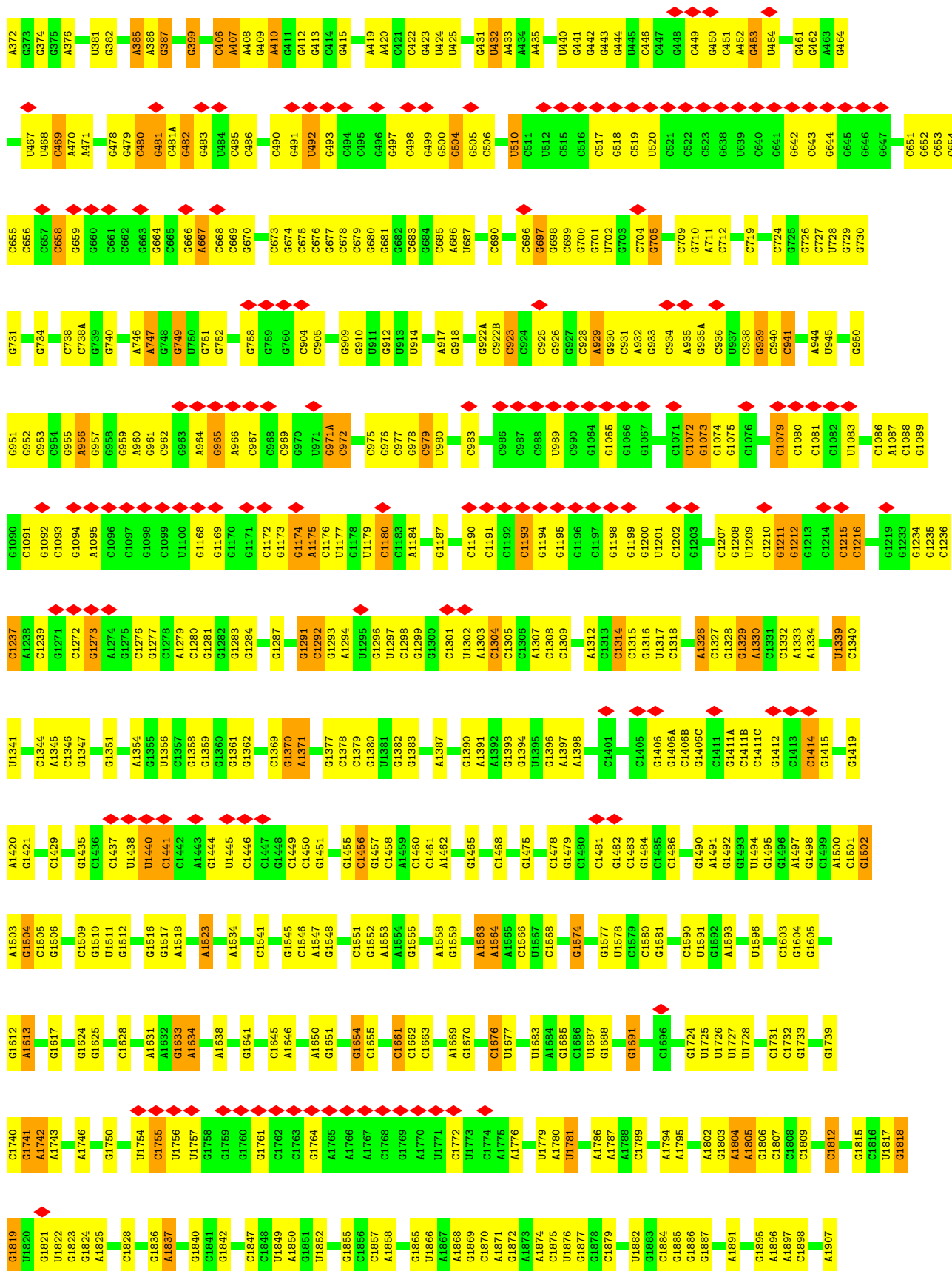


• Molecule 52: 40S ribosomal protein S6

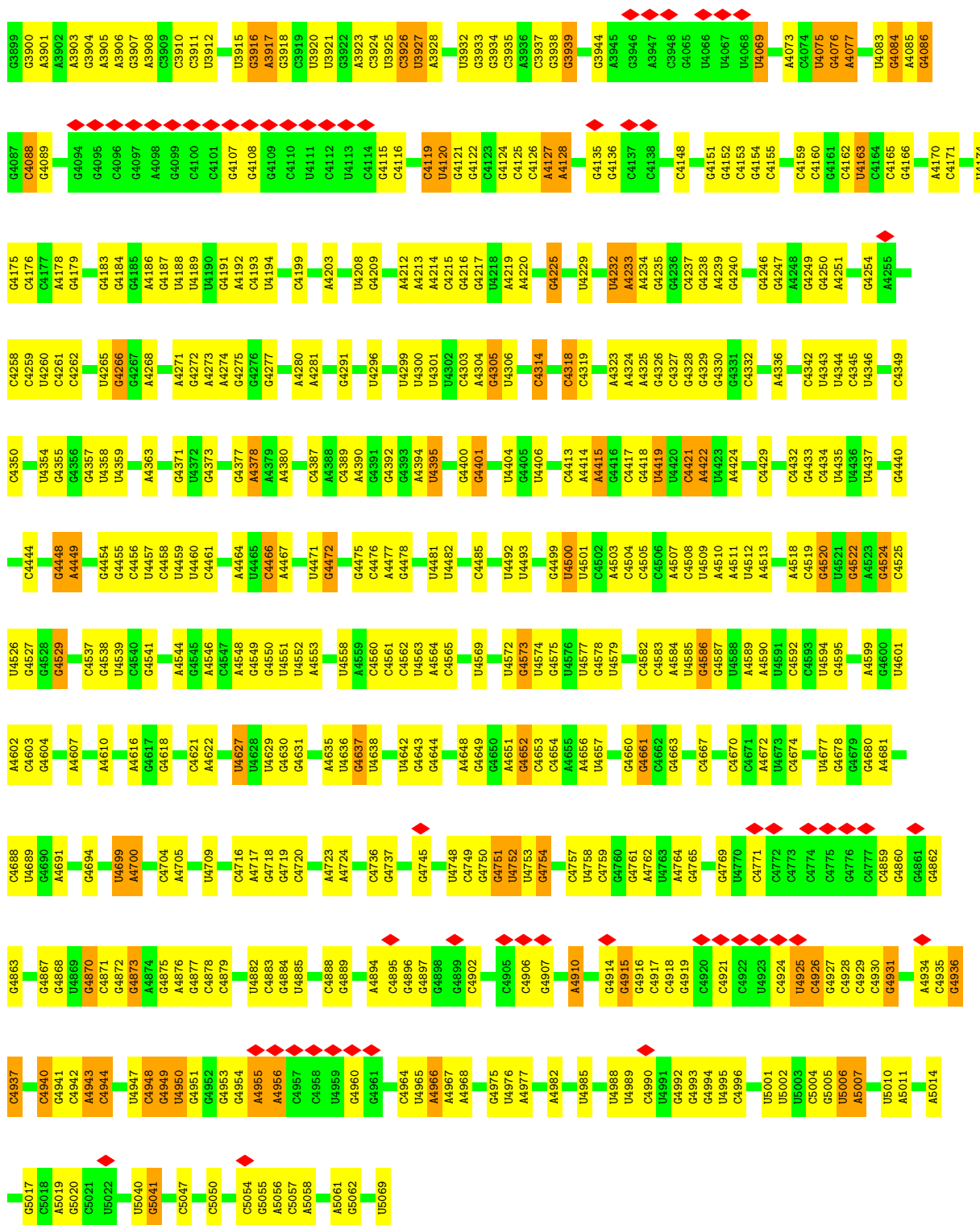


• Molecule 53: 60S acidic ribosomal protein P0



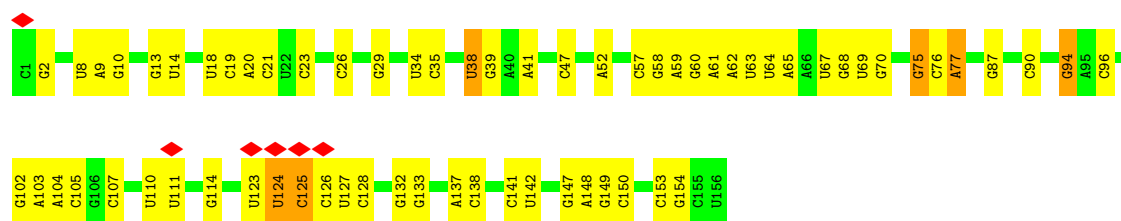


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A3723	A3724	G3725	A3726	A3727	A3728	C3731	A3732	A3733	C3739	G3740	A3746	A3747	A3748	C3753	G3754	A3759	A3760	G3765	C3771	U3772	U3773	A3774	A3775	G3776	G3777	C3782	A3783	A3784	A3785	U3786	G3787	C3788	C3789	U3790	U3796	U3805	G3806	C3807	G3809	C3810	C3811	C3812	A3813	A3814	C3815	A3816	C3817	U3818																																																																																																																																																																																																																																																																																																																																																																											
C3633	G3634	A3635	C3636	U3637	U3641	A3646	A3647	A3648	A3651	A3652	C3660	G3661	A3662	A3663	G3664	G3665	C3668	G3671	C3672	U3673	U3680	G3681	G3684	C3685	G3686	A3687	U3688	G3689	A3692	U3693	U3694	U3695	C3696	U3697	C3698	C3699	C3700	C3701	A3702	G3703	A3711	G3714	A3717	A3718	G3722																																																																																																																																																																																																																																																																																																																																																																														
A2832	A2833	C2834	A2835	A2836	U2837	U2838	U2839	G2842	U2843	A2844	A2845	G2848	G2855	C2856	A2857	U2858	G2859	G2863	U2869	C2875	G2876	G2877	G2878	G2879	U2880	A2881	G2898	C3598	A3599	G3600	G3603	A3604	C3605	U3606	U3607	C3609	A3610	A3611	G3615	C3619	G3620	A3621	C3622	C3623	A3624	A3717	A3718	G3722																																																																																																																																																																																																																																																																																																																																																																											
G2753	G2754	A2757	G2758	G2759	G2760	U2761	G2762	U2763	A2764	A2765	A2766	U2767	G2768	U2769	G2770	G2771	C2772	G2773	G2777	G2778	C2784	C2785	G2786	A2787	G2788	U2789	U2790	C2791	G2792	G2793	C2794	A2798	A2806	G2809	U2810	G2811	A2812	A2813	C2814	A2815	G2816	C2817	C2818	U2819	C2820	C2824	A2825	U2826	G2827	U2828																																																																																																																																																																																																																																																																																																																																																																									
C2668	C2669	A2674	G2675	A2676	G2682	C2683	G2686	U2687	G2688	C2689	C2690	U2691	G2692	G2693	C2694	A2695	A2697	C2704	G2705	G2706	U2707	U2708	C2709	C2710	G2711	G2712	C2713	G2714	C2719	A2725	G2726	U2730	C2731	U2734	G2735	C2736	C2737	C2738	C2739	U2740	U2741	G2742	A2743	A2744	A2745	A2746	U2747	C2748	G2750																																																																																																																																																																																																																																																																																																																																																																										
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G2481	C2482	G2483	A2484	U2485	G2486	G2487	C2488	C2489	U2490	U2491	C2492	G2493	U2494	U2495	G2496	C2497	C2498	A2502	G2503	C2504	G2506	A2513	A2517	U2519	C2520	G2521	G2522	C2526	A2527	G2528	A2529	U2530	A2537	U2538	C2539	C2540	G2541	G2542	A2543	U2544	U2545	G2546	G2547	A2553	G2557	C2558	G2559	C2560	C2561	G2562																																																																																																																																																																																																																																																																																																																																																																									
A2396	G2397	U2398	G2399	G2400	A2403	A2404	G2405	G2406	G2407	U2408	U2409	C2410	A2411	U2412	U2413	G2414	U2415	G2416	A2417	C2422	U2425	A2428	A2429	C2430	G2433	C2437	U2447	G2448	U2454	G2455	G2456	G2457	C2458	G2459	C2462	C2465	G2466	U2467	U2468	G2469	C2470	A2471	A2472	G2475	C2478	G2480																																																																																																																																																																																																																																																																																																																																																																													
A2268	C2269	C2274	G2275	G2283	C2289	A2300	G2301	C2306	G2309	A2313	G2316	C2317	G2318	G2321	C2322	C2323	C2324	C2325	G2331	A2332	C2333	C2334	C2335	G2336	G2345	G2348	C2351	A2360	G2361	U2362	A2363	G2378	A2381	U2386	G2387	A2388	A2389	G2394	A2395																																																																																																																																																																																																																																																																																																																																																																																				
U2048	G2049	G2052	G2055	G2056	G2060	U2061	G2062	G2063	G2064	A2069	G2076	G2077	C2078	G2079	U2080	G2081	G2082	U2084	G2085	G2089	U2090	C2091	G2092	G2093	C2094	A2095	G2096	A2097	G2098	G2099	G2100	A2101	G2102	A2103	A2104	A2105	G2106	A2107	G2108	A2109	G2110	U2111	G2112	G2113	C2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	G2193	G2194	G2195	G2196	G2197	G2198	G2199	G2200	G2201	G2202	G2203	G2204	G2205	G2206	G2207	G2208	G2209	G2210	G2211	G2212	G2213	G2214	G2215	G2216	G2217	G2218	G2219	G2220	G2221	G2222	G2223	G2224	G2225	G2226	G2227	G2228	G2229	G2230	G2231	G2232	G2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240	G2241	G2242	G2243	G2244	G2245	G2246	G2247	G2248	G2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	G2257	G2258	G2259	G2260	G2261	G2262	G2263	G2264	G2265	G2266	G2267	G2268	G2269	G2270	G2271	G2272	G2273	G2274	G2275	G2276	G2277	G2278	G2279	G2280	G2281	G2282	G2283	G2284	G2285	G2286	G2287	G2288	G2289	G2290	G2291	G2292	G2293	G2294	G2295	G2296	G2297	G2298	G2299	G2300	G2301	G2302	G2303	G2304	G2305	G2306	G2307	G2308	G2309	G2310	G2311	G2312	G2313	G2314	G2315	G2316	G2317	G2318	G2319	G2320	G2321	G2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2330	G2331	G2332	G2333	G2334	G2335	G2336	G2337	G2338	G2339	G2340	G2341	G2342	G2343	G2344	G2345	G2346	G2347	G2348	G2349	G2350	G2351	G2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2372	G2373	G2374	G2375	G2376	G2377	G2378	G2379	G2380	G2381	G2382	G2383	G2384	G2385	G2386	G2387	G2388	G2389	G2390	G2391	G2392	G2393	G2394	G2395	G2396	G2397	G2398	G2399	G2400	G2401	G2402	G2403	G2404	G2405	G2406	G2407	G2408	G2409	G2410	G2411	G2412	G2413	G2414	G2415	G2416	G2417	G2418	G2419	G2420	G2421	G2422	G2423	G2424	G2425	G2426	G2427	G2428	G2429	G2430	G2431	G2432	G2433	G2434	G2435	G2436	G2437	G2438	G2439	G2440	G2441	G2442	G2443	G2444	G2445	G2446	G2447	G2448	G2449	G2450	G2451	G2452	G2453	G2454	G2455	G2456	G2457	G2458	G2459	G2460	G2461	G2462	G2463	G2464	G2465	G2466	G2467	G2468	G2469	G2470	G2471	G2472	G2473	G2474	G2475	G2476	G2477	G2478	G2479	G2480
C1977	C1978	A1979	U1980	G1981	A1982	A1983	A1984	G1985	U1986	C1987	G1988	G1989	A1990	A1991	U1992	C1993	C1994	G1995	C1996	U1997	A1998	A1999	G2000	G2001	A2002	G2003	U2004	G2005	U2006	G2007	U2008	A2009	A2010	C2011	A2012	A2013	C2014	U2015	C2016	A2017	C2018	C2019	C2020	G2021	A2022	A2023	G2024	A2025	A2026	A2027	A2028	A2029	A2030	G2034	G2039	A2040	G2045	G2046	A2047																																																																																																																																																																																																																																																																																																																																																																
A1908	G1909	G1910	C1914	G1915	A1916	A1917	U1918	G1919	C1920	G1921	A1922	A1923	C1924	G1925	G1926	U1927	C1928	A1929	U1930	C1931	A1932	G1933	A1934	C1937	C1938	A1939	G1940	A1941	A1942	A1943	A1944	G1945	G1946	U1947	G1948	G1951	U1957	A1958	U1959	A1960	G1961	A1962	G1965	C1966	A1967	G1968	G1969	A1970	U1971	G1972	G1973	U1974	G1975	G1976																																																																																																																																																																																																																																																																																																																																																																					

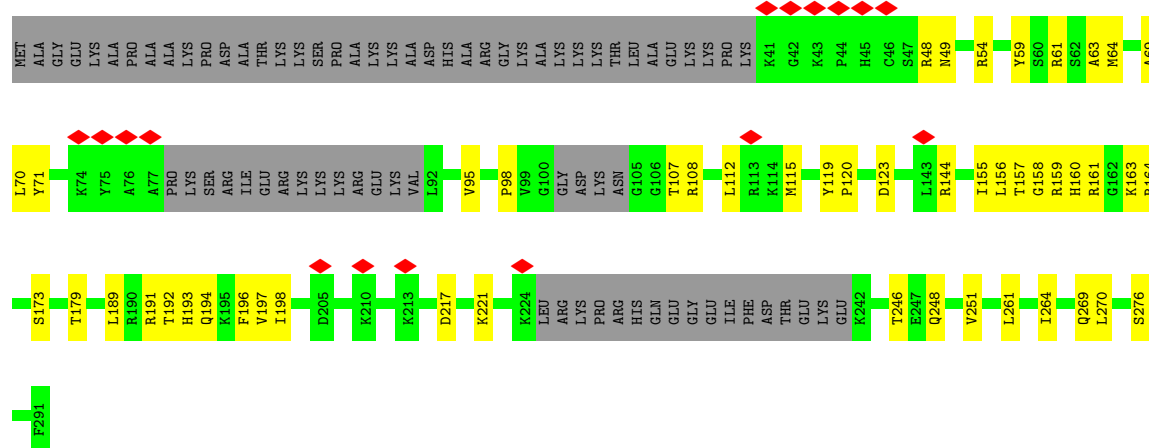


• Molecule 57: 5.8S rRNA

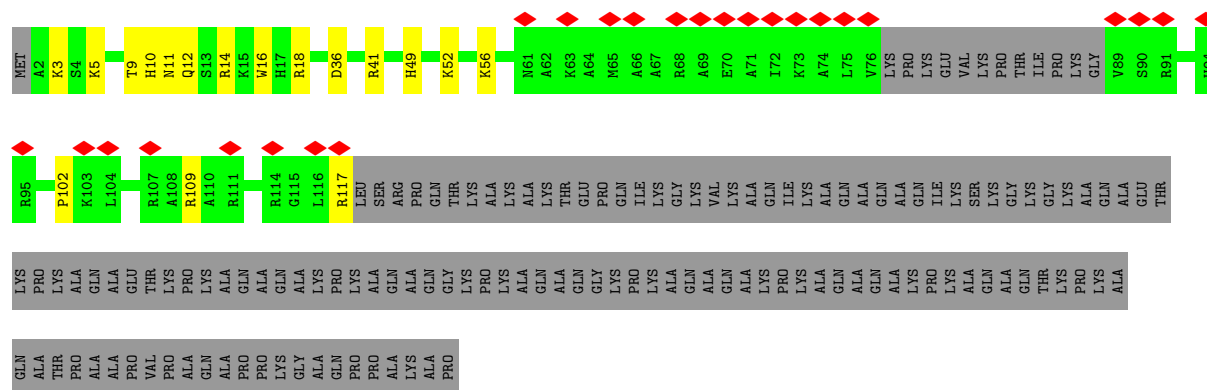
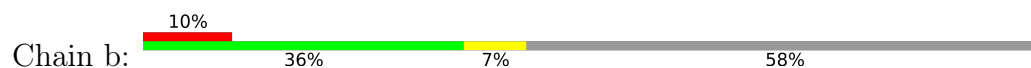
Chain 8: 56% 40%



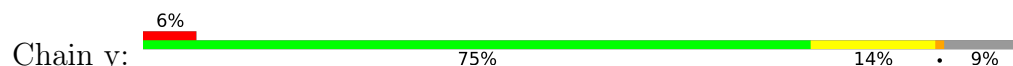
• Molecule 58: 60S ribosomal protein L6



• Molecule 59: Large ribosomal subunit protein eL29

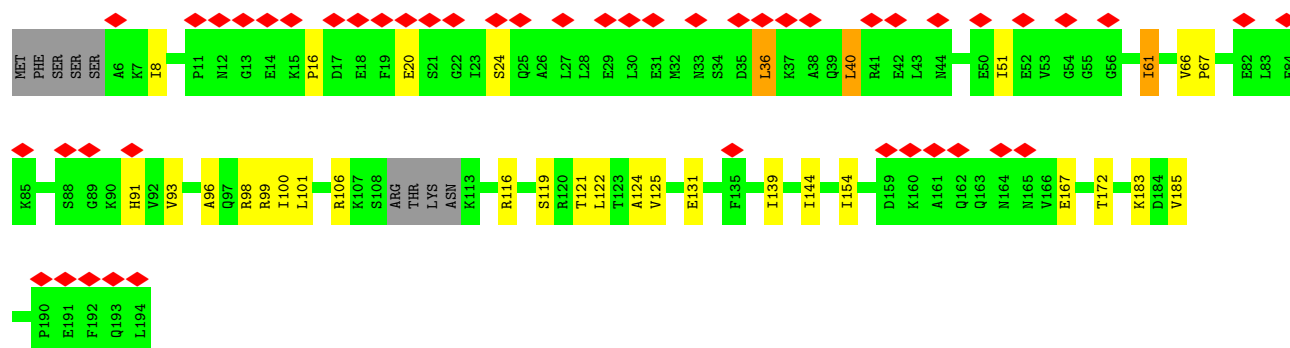
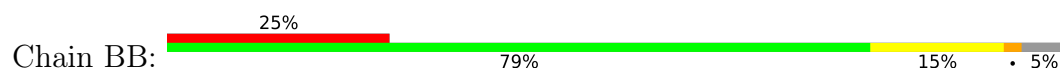


• Molecule 60: Ribosomal protein S5

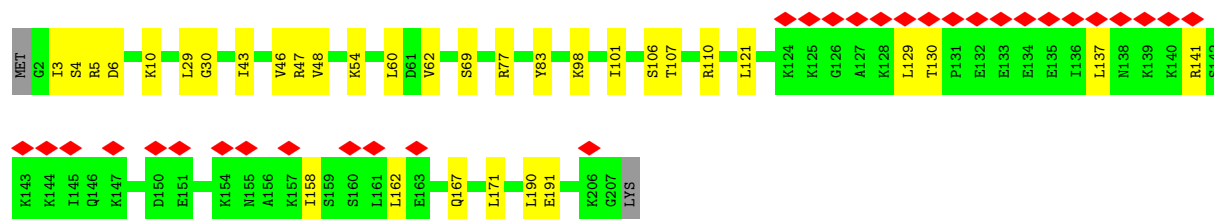
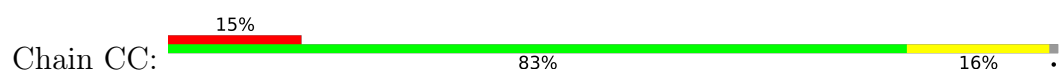




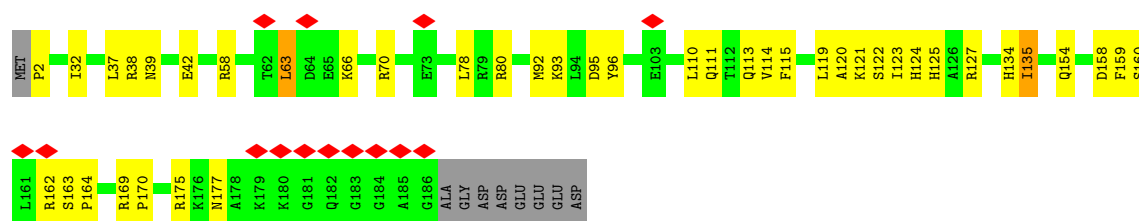
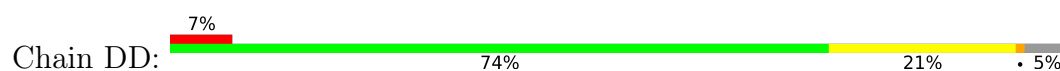
- Molecule 61: 40S ribosomal protein S7



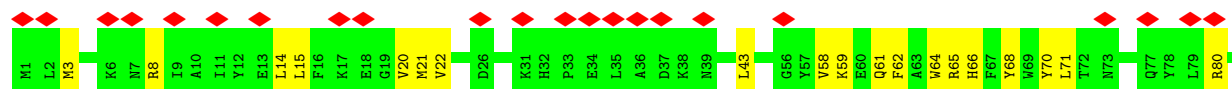
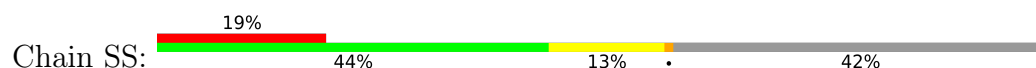
- Molecule 62: 40S ribosomal protein S8



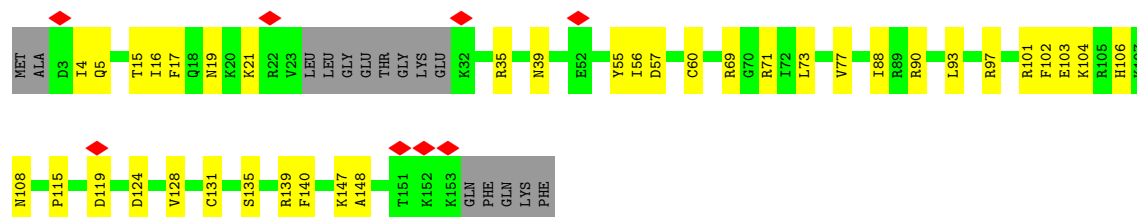
- Molecule 63: Ribosomal protein S9 (Predicted)



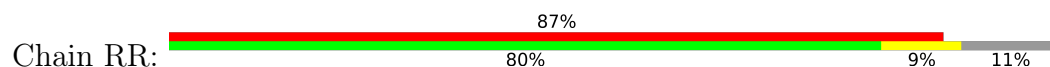
- Molecule 64: S10_ plectin domain-containing protein



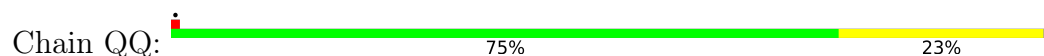
- Molecule 65: Ribosomal protein S11



- Molecule 66: 40S ribosomal protein S12

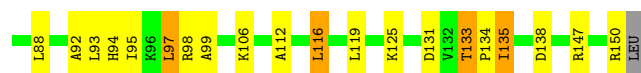


- Molecule 67: Ribosomal protein S13

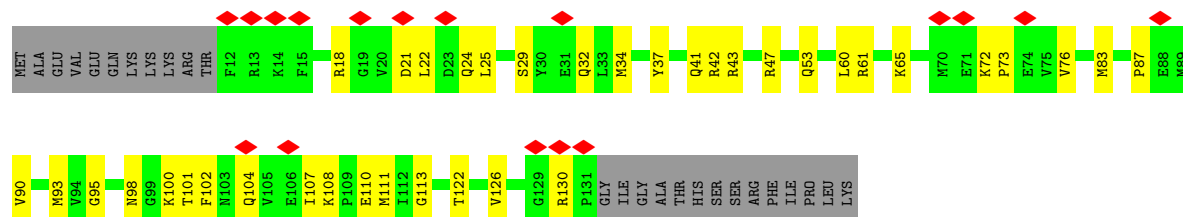


- Molecule 68: Small ribosomal subunit protein uS11

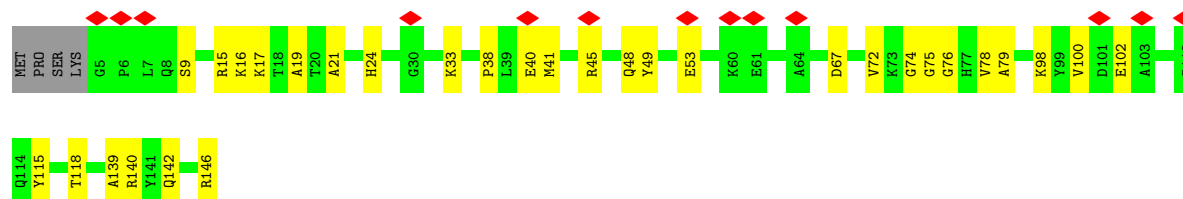
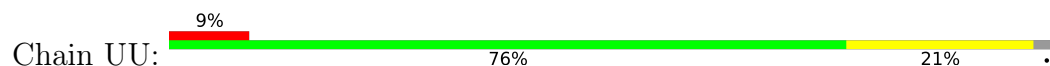




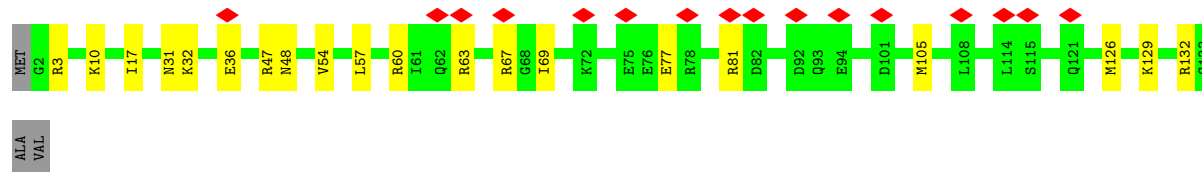
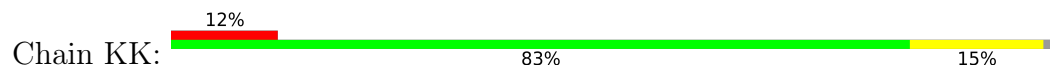
• Molecule 69: uS19



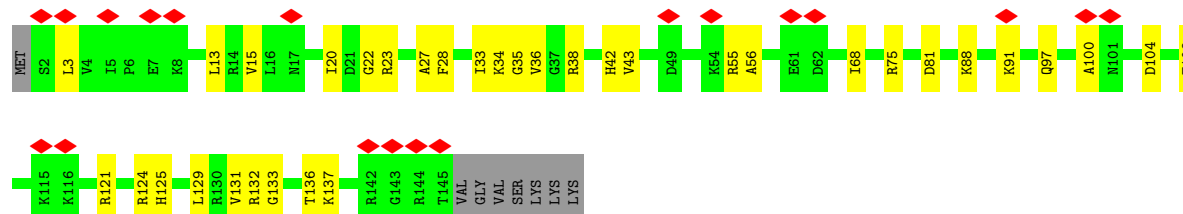
• Molecule 70: uS9



• Molecule 71: eS17

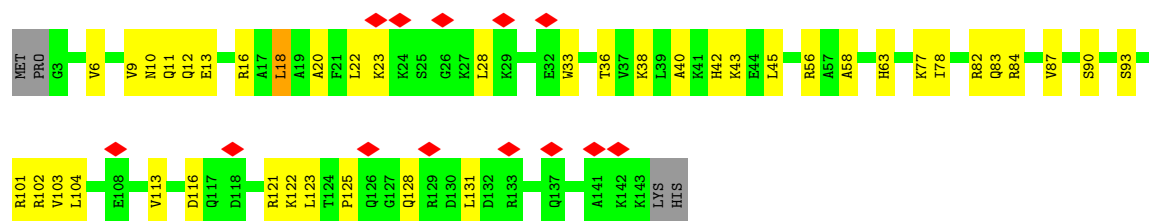


• Molecule 72: uS13

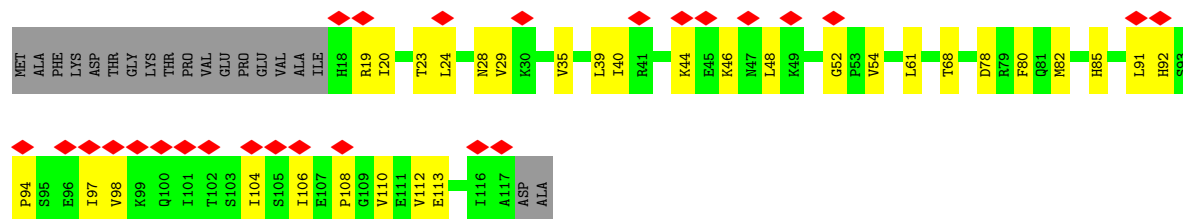


• Molecule 73: eS19

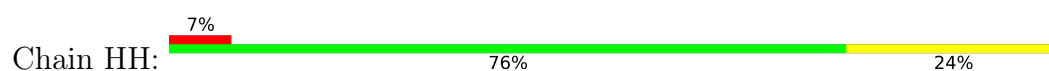




- Molecule 74: uS10



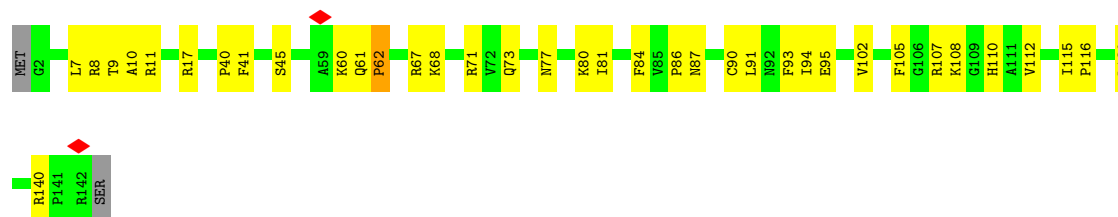
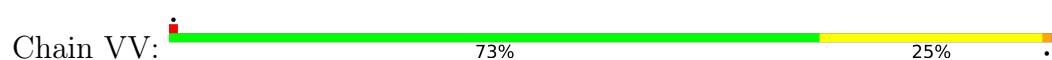
- Molecule 75: Small ribosomal subunit protein eS21



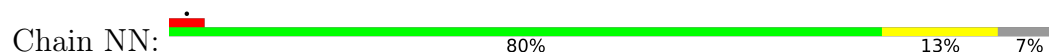
- Molecule 76: Ribosomal protein S15a

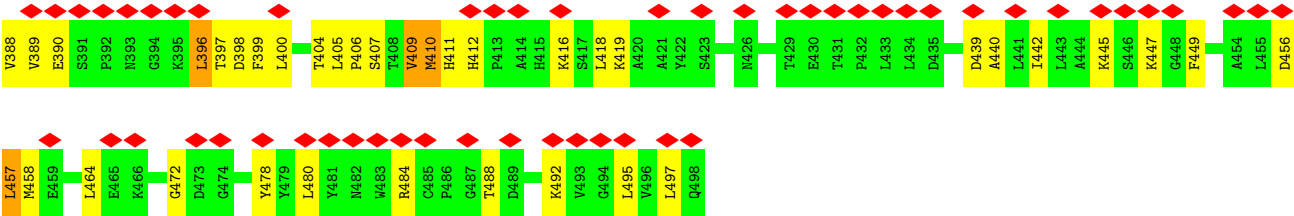


- Molecule 77: uS12

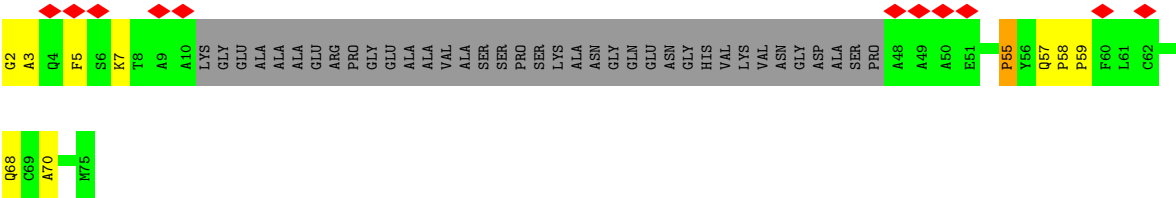
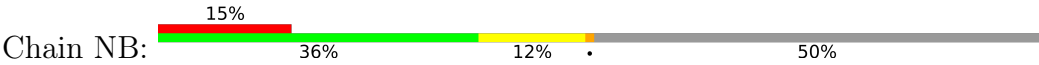


- Molecule 78: Small ribosomal subunit protein eS24





● Molecule 87: Myristoylated alanine-rich C-kinase substrate,X-box-binding protein 1, luminal form



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23479	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.610	Depositor
Minimum map value	-0.854	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.184	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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	0	0.13	0/567	0.29	0/753
2	4	0.09	0/141	0.26	0/217
3	6	0.13	0/2493	0.25	0/3394
4	7	0.08	0/2858	0.18	0/4455
5	9	0.07	0/470	0.20	0/623
6	A	0.20	0/1936	0.35	0/2596
7	B	0.08	0/3240	0.21	0/4339
8	C	0.08	0/2937	0.22	0/3946
9	D	0.07	0/2437	0.20	0/3264
10	F	0.08	0/1911	0.21	0/2549
11	G	0.08	0/1910	0.22	0/2569
12	H	0.07	0/1535	0.22	0/2063
13	I	0.13	0/1702	0.25	0/2272
14	J	0.08	0/1385	0.23	0/1852
15	K	0.11	0/40531	0.24	0/63162
16	L	0.08	0/1733	0.20	0/2316
17	M	0.08	0/1158	0.22	0/1547
18	N	0.08	0/1746	0.21	0/2338
19	O	0.09	0/1662	0.23	0/2222
20	P	0.08	0/1268	0.22	0/1700
21	Q	0.08	0/1543	0.22	0/2061
22	R	0.08	0/1522	0.19	0/2011
23	S	0.16	0/1492	0.33	0/2002
24	T	0.08	0/1326	0.22	0/1770
25	U	0.09	0/861	0.25	0/1157
26	V	0.07	0/993	0.20	0/1332
27	W	0.07	0/873	0.21	0/1158
28	X	0.07	0/984	0.20	0/1323
29	Y	0.20	0/1132	0.32	1/1504 (0.1%)
30	Z	0.07	0/1130	0.20	0/1507
31	a	0.07	0/1191	0.21	0/1590
32	c	0.06	0/771	0.17	0/1034

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.08	0/903	0.21	0/1216
34	e	0.07	0/1071	0.21	0/1429
35	f	0.08	0/895	0.23	0/1198
36	g	0.08	0/916	0.22	0/1220
37	h	0.07	0/1021	0.18	0/1348
38	i	0.08	0/841	0.20	0/1112
39	j	0.07	0/720	0.20	0/952
40	k	0.07	0/575	0.21	0/761
41	l	0.08	0/459	0.22	0/608
42	m	0.32	0/435	0.38	0/575
43	n	0.08	0/240	0.19	0/305
44	o	0.08	0/864	0.23	0/1140
45	p	0.07	0/718	0.19	0/953
46	q	0.07	0/1747	0.21	0/2374
47	r	0.08	0/1010	0.25	0/1354
48	u	0.08	0/1756	0.21	0/2350
49	v	0.08	0/1752	0.22	0/2368
50	w	0.08	0/1796	0.21	0/2417
51	x	0.07	0/2114	0.22	0/2843
52	z	0.07	0/1946	0.19	0/2590
53	s	0.08	0/1530	0.22	0/2064
54	t	0.08	0/1174	0.23	0/1582
55	2	0.08	0/1802	0.20	0/2804
56	5	0.11	0/84773	0.24	0/132212
57	8	0.08	0/3581	0.20	0/5577
58	E	0.07	0/1762	0.22	0/2362
59	b	0.19	0/861	0.28	0/1138
60	y	0.08	0/1492	0.22	0/2005
61	BB	0.07	0/1510	0.21	0/2022
62	CC	0.08	0/1715	0.23	0/2287
63	DD	0.07	0/1550	0.19	0/2069
64	SS	0.08	0/834	0.27	0/1125
65	EE	0.07	0/1195	0.21	0/1597
66	RR	0.08	0/918	0.24	0/1233
67	QQ	0.07	0/1226	0.19	0/1649
68	MM	0.07	0/1017	0.20	0/1365
69	WW	0.07	0/1017	0.21	0/1358
70	UU	0.20	0/1146	0.32	0/1534
71	KK	0.07	0/1082	0.19	0/1452
72	II	0.08	0/1208	0.23	0/1618
73	PP	0.07	0/1115	0.19	0/1493
74	GG	0.07	0/805	0.20	0/1081
75	HH	0.07	0/639	0.20	0/855

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	TT	0.09	0/1051	0.21	0/1406
77	VV	0.15	0/1116	0.38	0/1490
78	NN	0.06	0/1028	0.20	0/1366
79	OO	0.07	0/604	0.21	0/810
80	LL	0.07	0/828	0.21	0/1109
81	JJ	0.07	0/665	0.21	0/891
82	FF	0.05	0/490	0.18	0/656
83	AA	0.06	0/447	0.20	0/587
84	EF	0.09	0/862	0.30	0/1155
85	EG	0.07	0/536	0.24	0/715
86	NA	0.10	0/3048	0.29	0/4133
87	NB	0.08	0/299	0.30	0/407
All	All	0.10	0/234143	0.23	1/342946 (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
42	m	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y	9	SER	N-CA-C	-5.57	106.48	113.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	m	102	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	555	0	567	11	0
2	4	127	0	64	1	0
3	6	2436	0	2393	64	0
4	7	2558	0	1296	29	0
5	9	459	0	452	18	0
6	A	1898	0	1993	54	0
7	B	3172	0	3310	55	0
8	C	2883	0	3053	55	0
9	D	2391	0	2424	47	0
10	F	1875	0	1995	37	0
11	G	1879	0	2027	36	0
12	H	1516	0	1597	25	0
13	I	1664	0	1712	32	0
14	J	1362	0	1399	22	0
15	K	36249	0	18309	581	0
16	L	1702	0	1820	28	0
17	M	1137	0	1211	25	0
18	N	1701	0	1749	49	0
19	O	1630	0	1778	32	0
20	P	1242	0	1274	18	0
21	Q	1518	0	1640	21	0
22	R	1506	0	1659	17	0
23	S	1452	0	1496	24	0
24	T	1298	0	1366	18	0
25	U	846	0	861	20	0
26	V	979	0	1039	13	0
27	W	860	0	903	9	0
28	X	967	0	1040	10	0
29	Y	1115	0	1205	17	0
30	Z	1107	0	1182	16	0
31	a	1162	0	1209	27	0
32	c	761	0	794	9	0
33	d	888	0	930	9	0
34	e	1053	0	1147	21	0
35	f	876	0	912	18	0
36	g	906	0	998	10	0
37	h	1013	0	1147	11	0
38	i	830	0	916	6	0
39	j	705	0	737	15	0
40	k	569	0	637	8	0
41	l	447	0	480	11	0
42	m	429	0	465	6	0
43	n	239	0	289	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	o	851	0	920	23	0
45	p	708	0	757	13	0
46	q	1710	0	1708	35	0
47	r	994	0	1051	14	0
48	u	1729	0	1803	35	0
49	v	1715	0	1806	36	0
50	w	1768	0	1866	27	0
51	x	2072	0	2175	49	0
52	z	1923	0	2089	34	0
53	s	1507	0	1564	19	0
54	t	1160	0	1218	13	0
55	2	1614	0	822	16	0
56	5	75786	0	38289	1099	0
57	8	3208	0	1629	42	0
58	E	1729	0	1887	34	0
59	b	848	0	920	11	0
60	y	1471	0	1522	20	0
61	BB	1488	0	1582	21	0
62	CC	1686	0	1772	18	0
63	DD	1525	0	1640	29	0
64	SS	810	0	836	19	0
65	EE	1175	0	1249	27	0
66	RR	908	0	939	7	0
67	QQ	1202	0	1289	24	0
68	MM	1004	0	1023	25	0
69	WW	997	0	1045	25	0
70	UU	1128	0	1195	25	0
71	KK	1068	0	1121	16	0
72	II	1190	0	1249	24	0
73	PP	1097	0	1132	29	0
74	GG	795	0	862	17	0
75	HH	632	0	632	16	0
76	TT	1034	0	1080	25	0
77	VV	1098	0	1167	25	0
78	NN	1011	0	1083	14	0
79	OO	598	0	656	12	0
80	LL	814	0	863	9	0
81	JJ	651	0	672	13	0
82	FF	488	0	514	8	0
83	AA	443	0	492	8	0
84	EF	854	0	905	20	0
85	EG	531	0	573	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	NA	2967	0	2987	88	0
87	NB	288	0	271	8	0
88	5	198	0	0	0	0
88	7	7	0	0	0	0
88	8	5	0	0	0	0
88	A	1	0	0	0	0
88	EE	1	0	0	0	0
88	I	1	0	0	0	0
88	K	77	0	0	0	0
88	P	1	0	0	0	0
88	V	1	0	0	0	0
88	a	1	0	0	0	0
88	e	1	0	0	0	0
88	g	1	0	0	0	0
88	y	1	0	0	0	0
89	LL	1	0	0	0	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	NA	48	0	32	1	0
All	All	218587	0	164362	3005	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 8.

The worst 5 of 3005 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)
56:5:3692:A:N6	56:5:3823:G:H21	1.51	1.07
56:5:3692:A:H62	56:5:3823:G:N2	1.51	1.07
15:K:1452:A:H61	15:K:1473:G:H21	1.17	0.91
56:5:2639:U:HO2'	56:5:2694:G:H1	1.14	0.90
15:K:677:G:H21	15:K:1028:A:H62	1.17	0.90

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	
1	0	66/156 (42%)	64 (97%)	2 (3%)	0	100	100
3	6	311/317 (98%)	301 (97%)	10 (3%)	0	100	100
5	9	53/56 (95%)	53 (100%)	0	0	100	100
6	A	246/257 (96%)	232 (94%)	13 (5%)	1 (0%)	30	58
7	B	392/403 (97%)	385 (98%)	7 (2%)	0	100	100
8	C	360/413 (87%)	350 (97%)	10 (3%)	0	100	100
9	D	291/297 (98%)	283 (97%)	8 (3%)	0	100	100
10	F	223/249 (90%)	216 (97%)	7 (3%)	0	100	100
11	G	229/319 (72%)	223 (97%)	6 (3%)	0	100	100
12	H	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
13	I	201/214 (94%)	196 (98%)	5 (2%)	0	100	100
14	J	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
16	L	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
17	M	136/218 (62%)	132 (97%)	4 (3%)	0	100	100
18	N	201/204 (98%)	190 (94%)	11 (6%)	0	100	100
19	O	197/203 (97%)	194 (98%)	3 (2%)	0	100	100
20	P	151/184 (82%)	149 (99%)	2 (1%)	0	100	100
21	Q	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
22	R	178/181 (98%)	174 (98%)	4 (2%)	0	100	100
23	S	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
24	T	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
25	U	102/115 (89%)	96 (94%)	6 (6%)	0	100	100
26	V	129/140 (92%)	129 (100%)	0	0	100	100
27	W	102/157 (65%)	99 (97%)	3 (3%)	0	100	100
28	X	116/156 (74%)	114 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Y	132/145 (91%)	132 (100%)	0	0	100	100
30	Z	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
31	a	145/148 (98%)	141 (97%)	4 (3%)	0	100	100
32	c	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
33	d	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
34	e	126/134 (94%)	124 (98%)	2 (2%)	0	100	100
35	f	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
36	g	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
37	h	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
38	i	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
39	j	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
40	k	67/107 (63%)	66 (98%)	1 (2%)	0	100	100
41	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
42	m	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
43	n	23/25 (92%)	23 (100%)	0	0	100	100
44	o	102/141 (72%)	100 (98%)	2 (2%)	0	100	100
45	p	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
46	q	215/295 (73%)	212 (99%)	3 (1%)	0	100	100
47	r	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
48	u	211/264 (80%)	207 (98%)	4 (2%)	0	100	100
49	v	219/255 (86%)	217 (99%)	2 (1%)	0	100	100
50	w	226/243 (93%)	221 (98%)	5 (2%)	0	100	100
51	x	260/263 (99%)	254 (98%)	6 (2%)	0	100	100
52	z	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
53	s	194/318 (61%)	185 (95%)	9 (5%)	0	100	100
54	t	151/165 (92%)	141 (93%)	10 (7%)	0	100	100
58	E	208/291 (72%)	201 (97%)	7 (3%)	0	100	100
59	b	100/245 (41%)	99 (99%)	1 (1%)	0	100	100
60	y	181/204 (89%)	175 (97%)	6 (3%)	0	100	100
61	BB	181/194 (93%)	176 (97%)	5 (3%)	0	100	100
62	CC	204/208 (98%)	198 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	DD	183/194 (94%)	182 (100%)	1 (0%)	0	100	100
64	SS	94/165 (57%)	87 (93%)	7 (7%)	0	100	100
65	EE	139/158 (88%)	133 (96%)	6 (4%)	0	100	100
66	RR	115/132 (87%)	105 (91%)	10 (9%)	0	100	100
67	QQ	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
68	MM	133/151 (88%)	129 (97%)	4 (3%)	0	100	100
69	WW	118/145 (81%)	113 (96%)	5 (4%)	0	100	100
70	UU	140/146 (96%)	136 (97%)	4 (3%)	0	100	100
71	KK	130/135 (96%)	128 (98%)	2 (2%)	0	100	100
72	II	142/152 (93%)	139 (98%)	3 (2%)	0	100	100
73	PP	139/145 (96%)	133 (96%)	6 (4%)	0	100	100
74	GG	98/119 (82%)	95 (97%)	3 (3%)	0	100	100
75	HH	81/83 (98%)	81 (100%)	0	0	100	100
76	TT	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
77	VV	139/143 (97%)	132 (95%)	6 (4%)	1 (1%)	18	45
78	NN	122/133 (92%)	121 (99%)	1 (1%)	0	100	100
79	OO	73/124 (59%)	72 (99%)	1 (1%)	0	100	100
80	LL	99/117 (85%)	94 (95%)	5 (5%)	0	100	100
81	JJ	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
82	FF	60/69 (87%)	60 (100%)	0	0	100	100
83	AA	53/133 (40%)	53 (100%)	0	0	100	100
84	EF	108/162 (67%)	100 (93%)	7 (6%)	1 (1%)	14	38
85	EG	65/215 (30%)	60 (92%)	5 (8%)	0	100	100
86	NA	361/498 (72%)	321 (89%)	39 (11%)	1 (0%)	36	64
87	NB	33/74 (45%)	29 (88%)	3 (9%)	1 (3%)	3	11
All	All	12090/14332 (84%)	11737 (97%)	348 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
77	VV	62	PRO
84	EF	53	VAL
86	NA	222	LYS

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Mol	Chain	Res	Type
6	A	179	ILE
87	NB	55	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	61/140 (44%)	59 (97%)	2 (3%)	33	67
3	6	272/275 (99%)	262 (96%)	10 (4%)	30	63
5	9	48/49 (98%)	48 (100%)	0	100	100
6	A	190/199 (96%)	179 (94%)	11 (6%)	18	47
7	B	342/348 (98%)	338 (99%)	4 (1%)	63	86
8	C	302/337 (90%)	299 (99%)	3 (1%)	68	88
9	D	247/250 (99%)	243 (98%)	4 (2%)	55	82
10	F	196/218 (90%)	196 (100%)	0	100	100
11	G	200/272 (74%)	196 (98%)	4 (2%)	48	79
12	H	169/171 (99%)	161 (95%)	8 (5%)	23	55
13	I	175/181 (97%)	172 (98%)	3 (2%)	53	81
14	J	143/149 (96%)	133 (93%)	10 (7%)	14	39
16	L	175/176 (99%)	169 (97%)	6 (3%)	32	66
17	M	117/161 (73%)	111 (95%)	6 (5%)	21	52
18	N	171/172 (99%)	165 (96%)	6 (4%)	32	65
19	O	171/173 (99%)	166 (97%)	5 (3%)	37	71
20	P	134/163 (82%)	134 (100%)	0	100	100
21	Q	165/166 (99%)	159 (96%)	6 (4%)	31	64
22	R	159/160 (99%)	158 (99%)	1 (1%)	78	92
23	S	154/154 (100%)	148 (96%)	6 (4%)	28	62
24	T	139/140 (99%)	136 (98%)	3 (2%)	45	77
25	U	93/103 (90%)	92 (99%)	1 (1%)	65	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	V	101/107 (94%)	100 (99%)	1 (1%)	68	88
27	W	86/126 (68%)	86 (100%)	0	100	100
28	X	106/134 (79%)	106 (100%)	0	100	100
29	Y	124/135 (92%)	119 (96%)	5 (4%)	28	61
30	Z	117/118 (99%)	112 (96%)	5 (4%)	26	58
31	a	119/120 (99%)	118 (99%)	1 (1%)	73	90
32	c	84/98 (86%)	82 (98%)	2 (2%)	43	75
33	d	98/110 (89%)	94 (96%)	4 (4%)	27	60
34	e	114/120 (95%)	114 (100%)	0	100	100
35	f	88/89 (99%)	86 (98%)	2 (2%)	44	76
36	g	98/100 (98%)	94 (96%)	4 (4%)	27	60
37	h	109/110 (99%)	109 (100%)	0	100	100
38	i	86/89 (97%)	84 (98%)	2 (2%)	44	76
39	j	73/80 (91%)	72 (99%)	1 (1%)	59	84
40	k	64/92 (70%)	63 (98%)	1 (2%)	55	82
41	l	47/48 (98%)	46 (98%)	1 (2%)	47	78
42	m	48/116 (41%)	48 (100%)	0	100	100
43	n	24/24 (100%)	24 (100%)	0	100	100
44	o	92/121 (76%)	89 (97%)	3 (3%)	33	67
45	p	74/75 (99%)	73 (99%)	1 (1%)	59	84
46	q	180/245 (74%)	176 (98%)	4 (2%)	45	77
47	r	108/121 (89%)	107 (99%)	1 (1%)	70	89
48	u	194/231 (84%)	194 (100%)	0	100	100
49	v	186/205 (91%)	181 (97%)	5 (3%)	39	72
50	w	190/202 (94%)	187 (98%)	3 (2%)	55	82
51	x	223/224 (100%)	218 (98%)	5 (2%)	45	77
52	z	207/218 (95%)	207 (100%)	0	100	100
53	s	164/258 (64%)	164 (100%)	0	100	100
54	t	126/137 (92%)	126 (100%)	0	100	100
58	E	190/251 (76%)	188 (99%)	2 (1%)	65	86
59	b	84/184 (46%)	81 (96%)	3 (4%)	31	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	y	158/170 (93%)	155 (98%)	3 (2%)	50	79
61	BB	165/174 (95%)	161 (98%)	4 (2%)	43	75
62	CC	178/180 (99%)	172 (97%)	6 (3%)	32	66
63	DD	161/168 (96%)	157 (98%)	4 (2%)	42	74
64	SS	87/136 (64%)	84 (97%)	3 (3%)	32	66
65	EE	130/142 (92%)	129 (99%)	1 (1%)	73	90
66	RR	99/108 (92%)	97 (98%)	2 (2%)	48	79
67	QQ	130/131 (99%)	128 (98%)	2 (2%)	57	83
68	MM	104/119 (87%)	98 (94%)	6 (6%)	18	47
69	WW	109/130 (84%)	107 (98%)	2 (2%)	51	80
70	UU	117/121 (97%)	115 (98%)	2 (2%)	53	81
71	KK	119/121 (98%)	118 (99%)	1 (1%)	73	90
72	II	125/132 (95%)	124 (99%)	1 (1%)	73	90
73	PP	111/115 (96%)	108 (97%)	3 (3%)	39	72
74	GG	92/107 (86%)	89 (97%)	3 (3%)	33	67
75	HH	68/68 (100%)	67 (98%)	1 (2%)	57	83
76	TT	112/113 (99%)	111 (99%)	1 (1%)	70	89
77	VV	113/115 (98%)	108 (96%)	5 (4%)	25	58
78	NN	107/115 (93%)	107 (100%)	0	100	100
79	OO	66/102 (65%)	64 (97%)	2 (3%)	36	69
80	LL	88/99 (89%)	88 (100%)	0	100	100
81	JJ	75/76 (99%)	74 (99%)	1 (1%)	61	85
82	FF	55/62 (89%)	55 (100%)	0	100	100
83	AA	46/106 (43%)	46 (100%)	0	100	100
84	EF	94/136 (69%)	91 (97%)	3 (3%)	34	68
85	EG	60/183 (33%)	60 (100%)	0	100	100
86	NA	331/446 (74%)	303 (92%)	28 (8%)	10	30
87	NB	28/52 (54%)	27 (96%)	1 (4%)	31	64
All	All	10555/12172 (87%)	10315 (98%)	240 (2%)	44	76

5 of 240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	d	119	THR
86	NA	322	LEU
50	w	44	THR
86	NA	250	LEU
86	NA	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
46	q	193	HIS
82	FF	45	ASN
53	s	42	GLN
80	LL	19	GLN
86	NA	234	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	K	1687/1698 (99%)	298 (17%)	17 (1%)
2	4	5/6 (83%)	1 (20%)	0
4	7	119/120 (99%)	11 (9%)	0
55	2	74/76 (97%)	10 (13%)	0
56	5	3512/3534 (99%)	650 (18%)	52 (1%)
57	8	149/151 (98%)	26 (17%)	1 (0%)
All	All	5546/5585 (99%)	996 (17%)	70 (1%)

5 of 996 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	4	46	A
4	7	7	G
4	7	22	A
4	7	33	U
4	7	53	U

5 of 70 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
56	5	3888	G
56	5	4075	U
56	5	4884	G

Continued on next page...

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Mol	Chain	Res	Type
56	5	480	C
56	5	406	C

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](#)

Of 303 ligands modelled in this entry, 302 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	$\# Z > 2$
90	COA	NA	501	-	47,50,50	3.39	19 (40%)	69,75,75	1.59	9 (13%)

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
90	COA	NA	501	-	-	1/48/64/64	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	NA	501	COA	C2B-C3B	-12.52	1.25	1.53
90	NA	501	COA	P2A-O3A	7.79	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	NA	501	COA	P1A-O3A	6.75	1.66	1.59
90	NA	501	COA	C9P-N8P	5.94	1.47	1.33
90	NA	501	COA	O4B-C1B	-5.60	1.29	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	NA	501	COA	C5A-C4A-N3A	-5.33	119.38	126.72
90	NA	501	COA	N3A-C2A-N1A	-4.24	122.16	128.58
90	NA	501	COA	N3A-C4A-N9A	4.03	134.02	127.17
90	NA	501	COA	N9A-C8A-N7A	-3.60	108.83	113.94
90	NA	501	COA	C2A-N3A-C4A	3.53	120.46	111.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

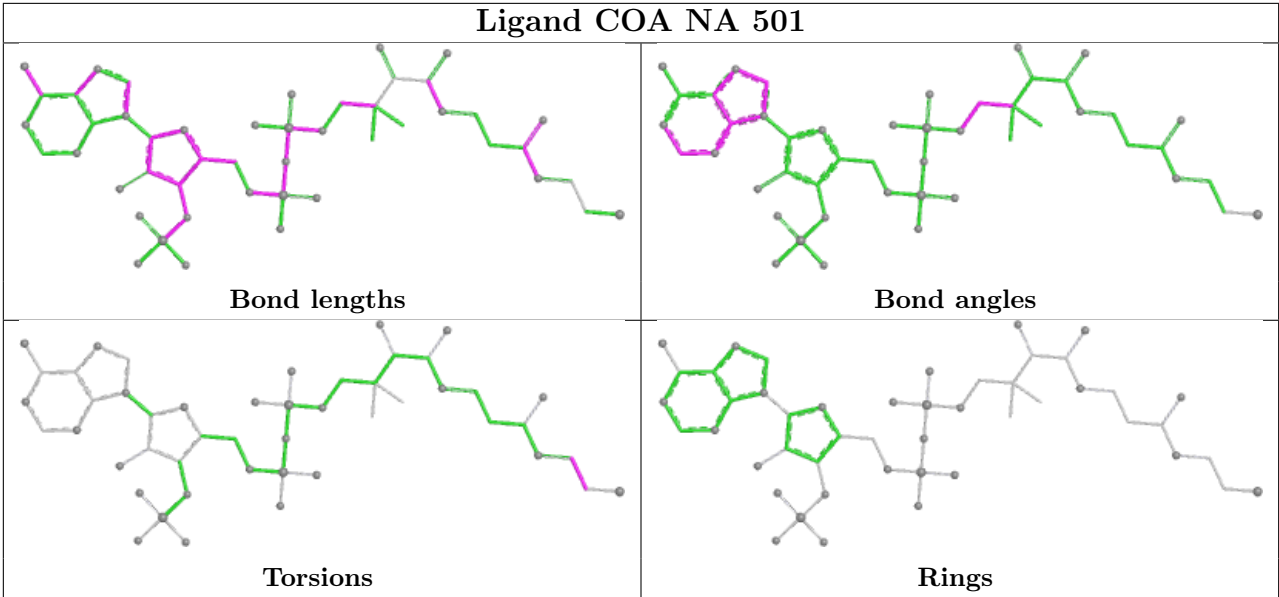
Mol	Chain	Res	Type	Atoms
90	NA	501	COA	S1P-C2P-C3P-N4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	NA	501	COA	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
56	5	24
15	K	11
57	8	1
55	2	1

The worst 5 of 37 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.50
1	5	1219:G	O3'	1233:G	P	22.32
1	5	1239:C	O3'	1271:G	P	19.49
1	5	3948:C	O3'	4065:G	P	19.05
1	K	697:G	O3'	729:C	P	18.82

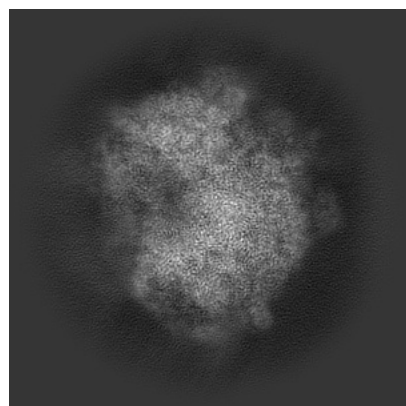
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49275. These allow visual inspection of the internal detail of the map and identification of artifacts.

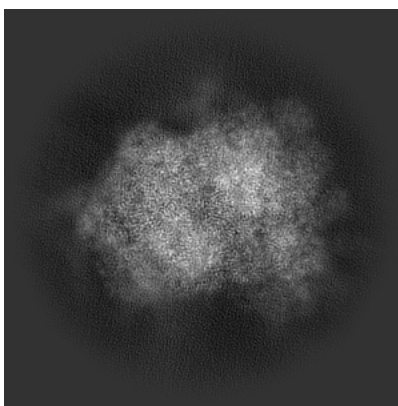
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

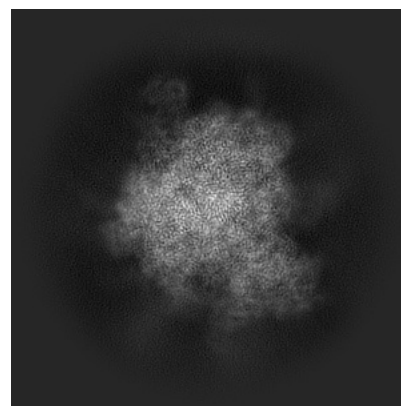
6.1.1 Primary map



X

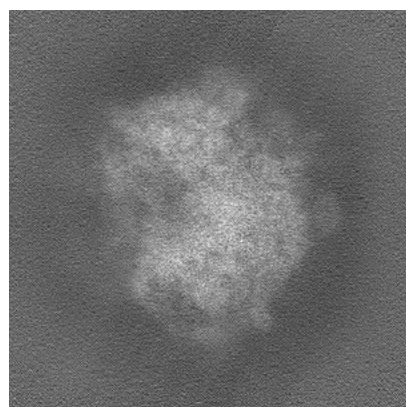


Y

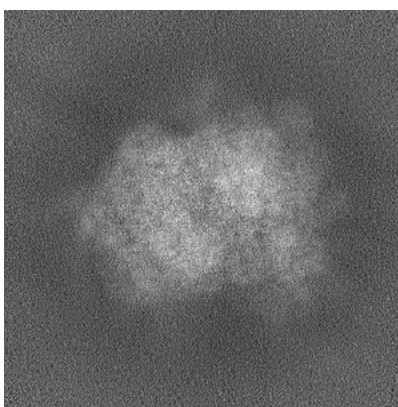


Z

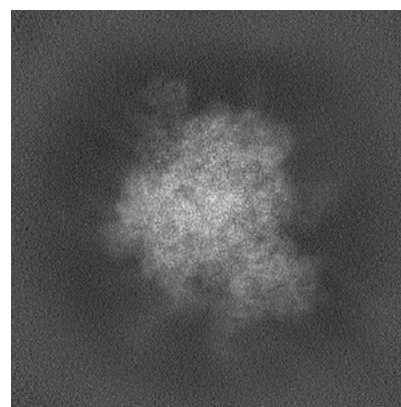
6.1.2 Raw map



X



Y

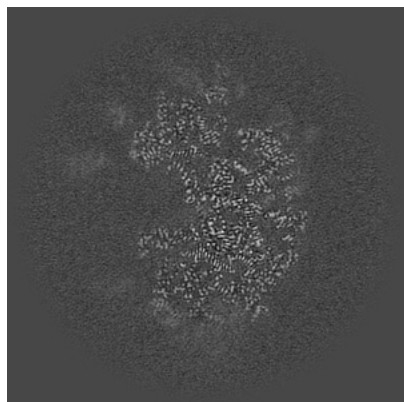


Z

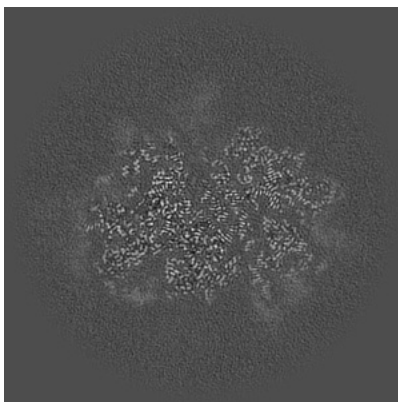
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

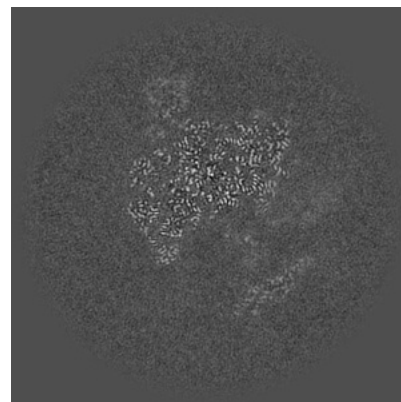
6.2.1 Primary map



X Index: 256

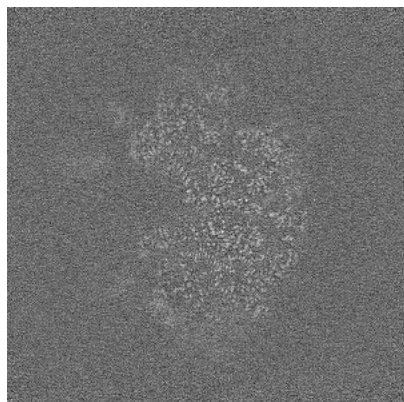


Y Index: 256

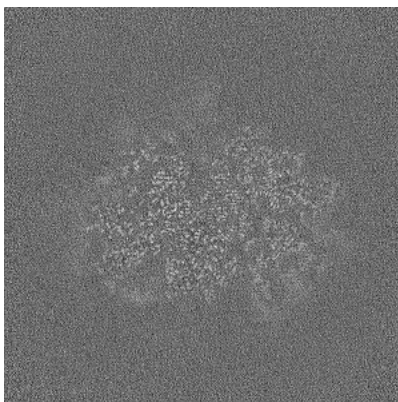


Z Index: 256

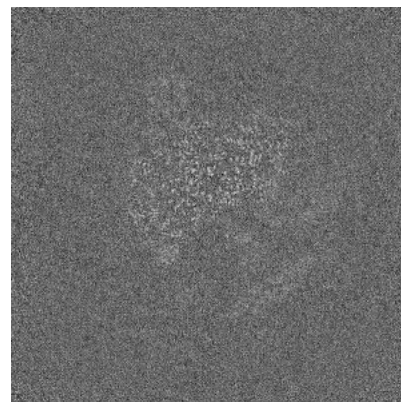
6.2.2 Raw map



X Index: 256



Y Index: 256

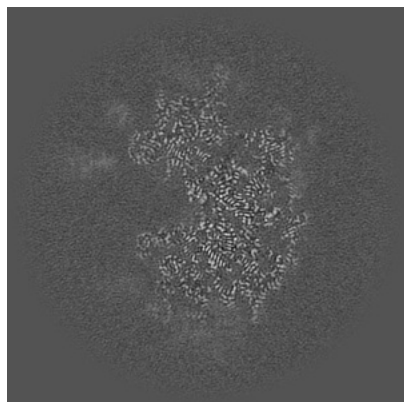


Z Index: 256

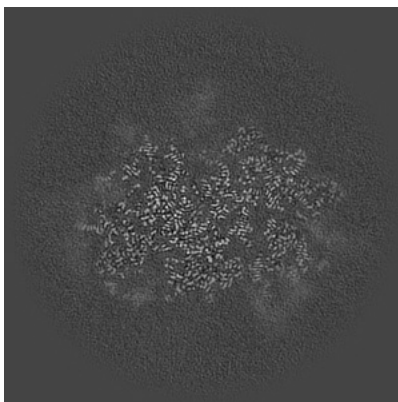
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

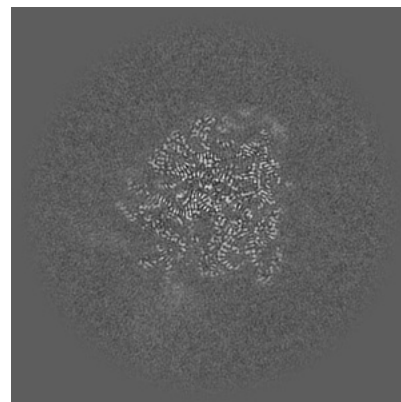
6.3.1 Primary map



X Index: 260

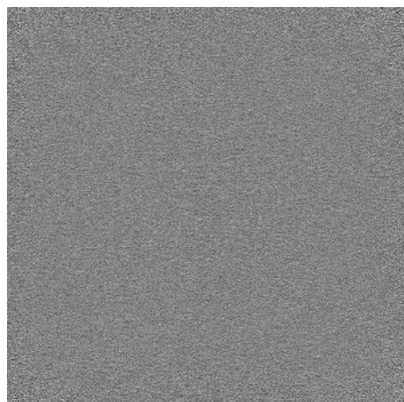


Y Index: 258

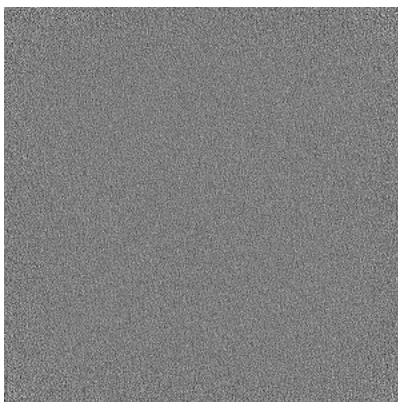


Z Index: 209

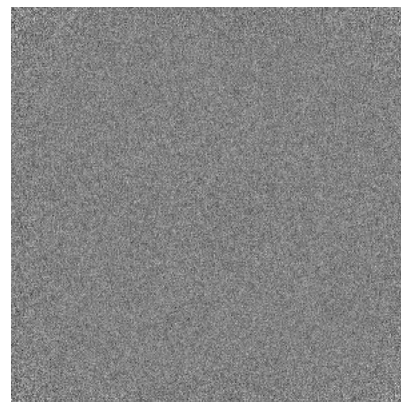
6.3.2 Raw map



X Index: 0



Y Index: 0

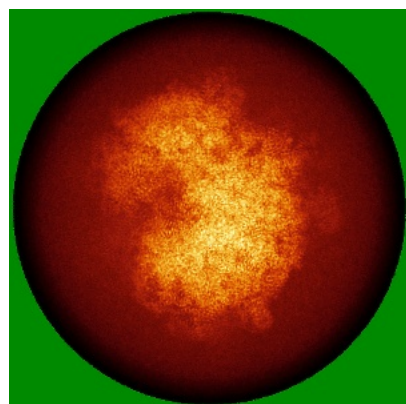


Z Index: 0

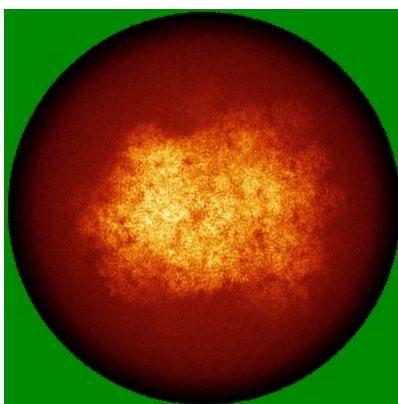
The images above show the largest variance slices of the map in three orthogonal directions.

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

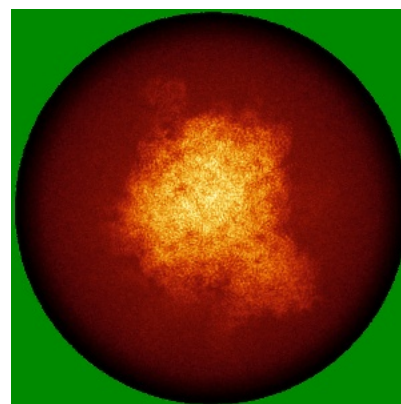
6.4.1 Primary map



X

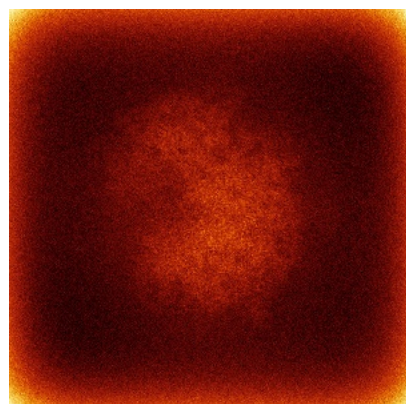


Y

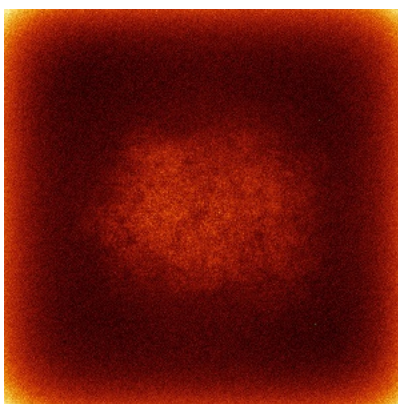


Z

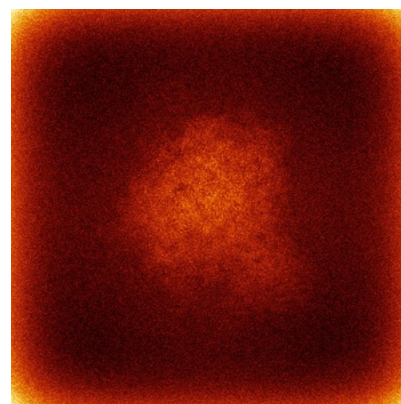
6.4.2 Raw map



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](#)

This section was not generated.

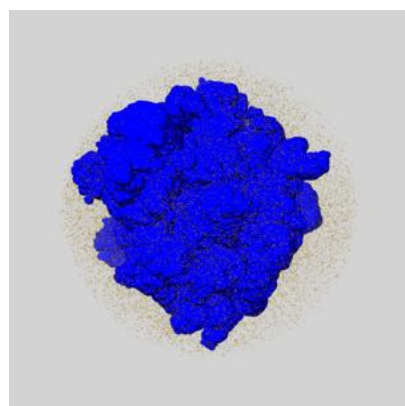
6.6 Mask visualisation [i](#)

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

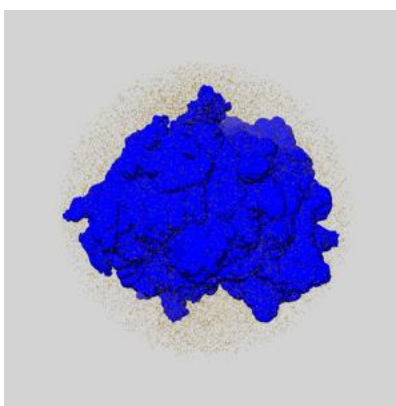
A mask typically either:

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

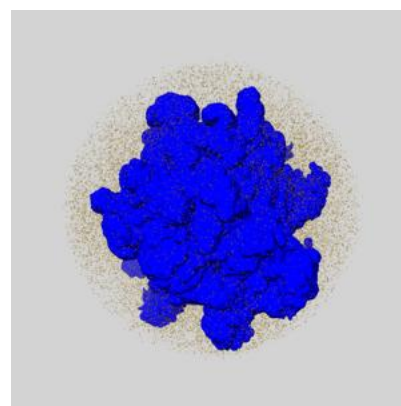
6.6.1 emd_49275_msk_1.map [i](#)



X



Y

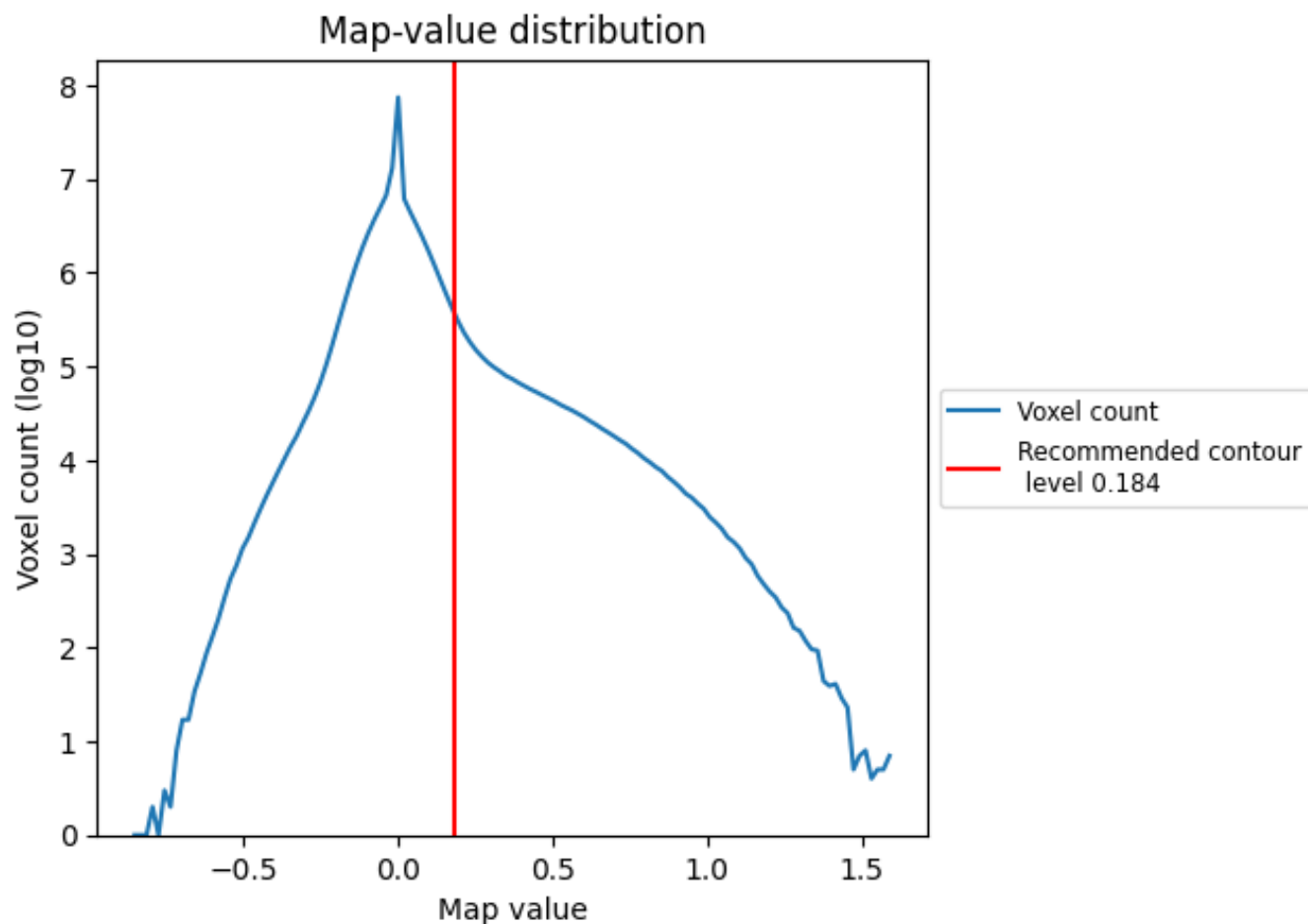


Z

7 Map analysis [i](#)

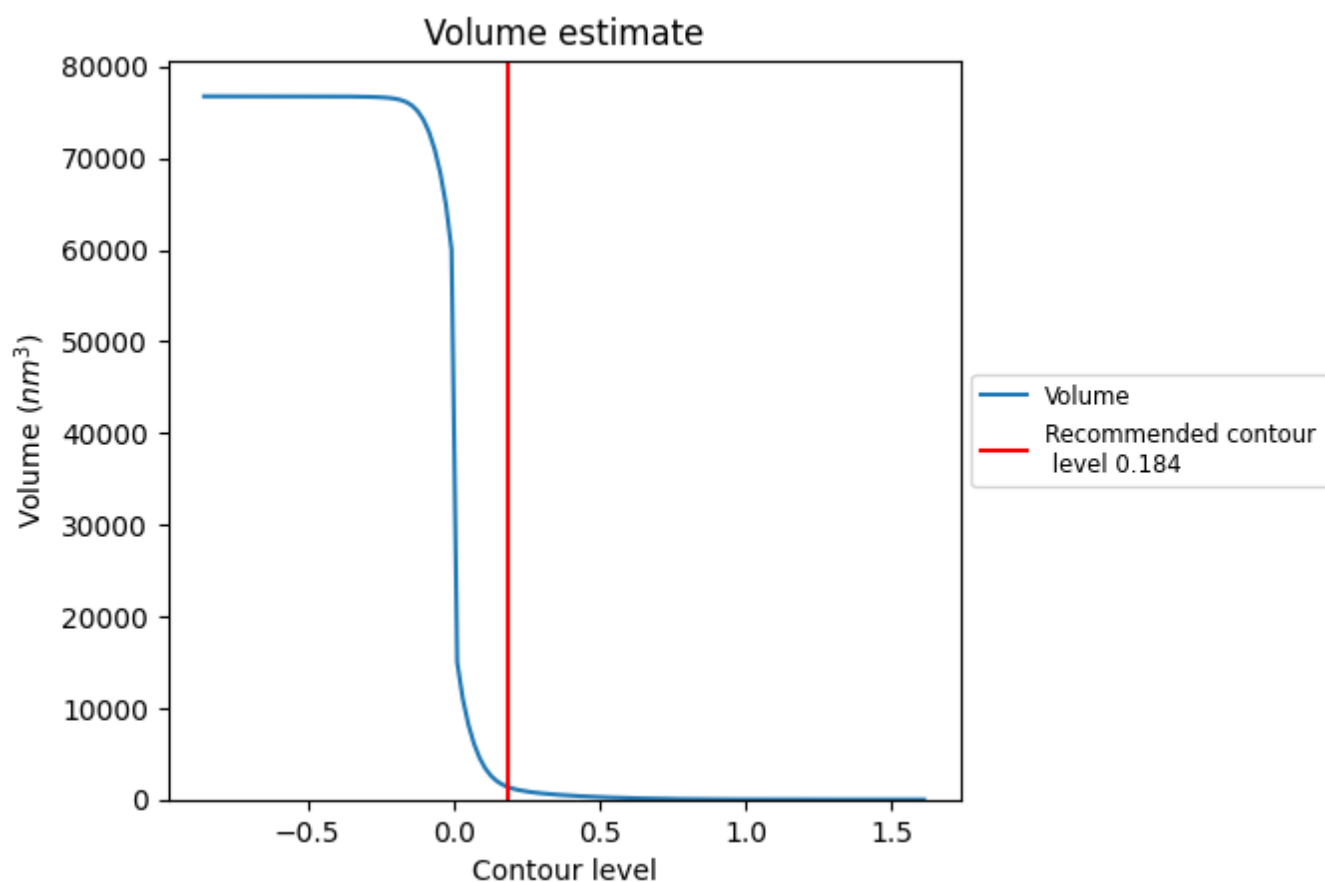
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

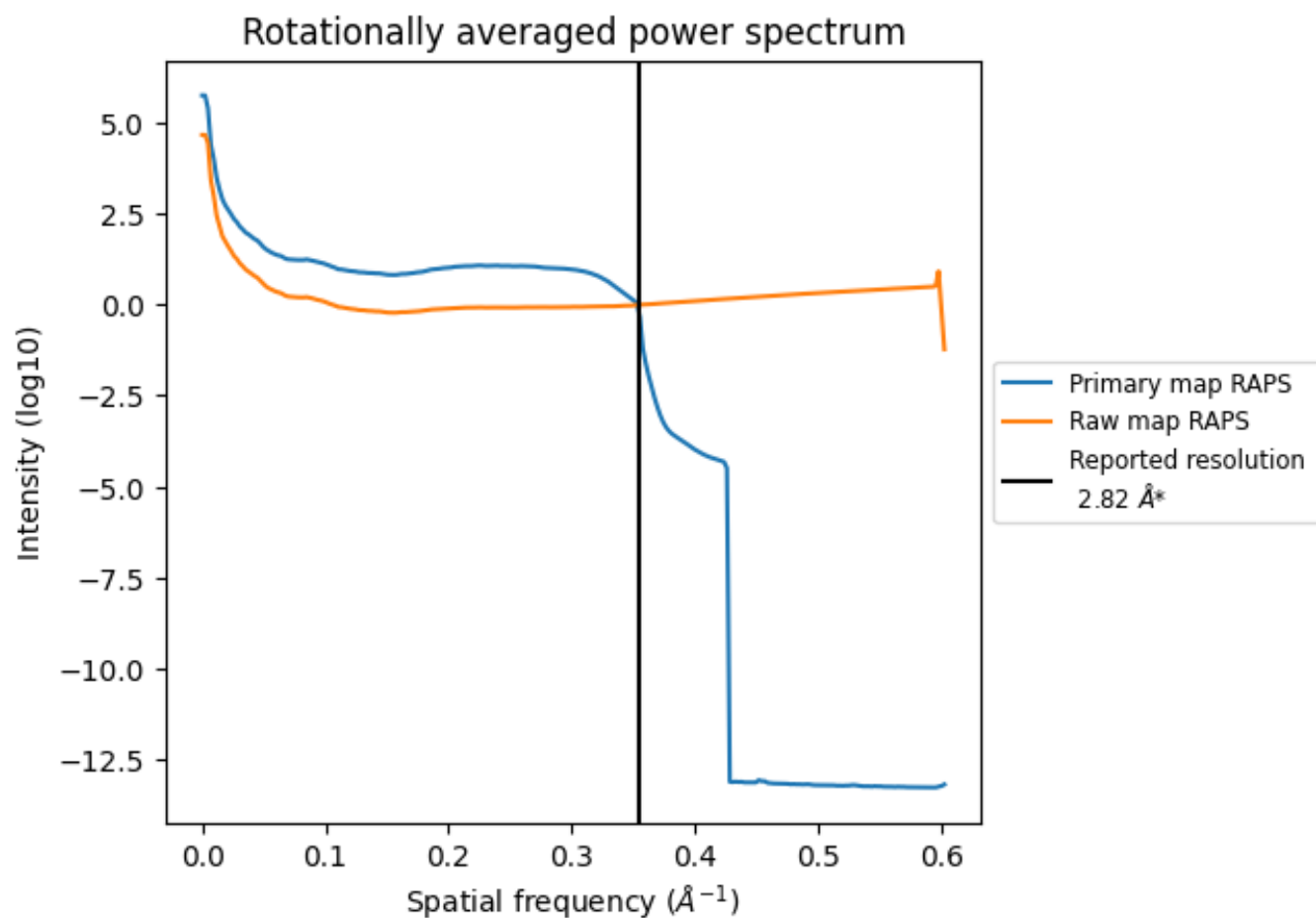
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1397 nm³; this corresponds to an approximate mass of 1262 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 ⓘ

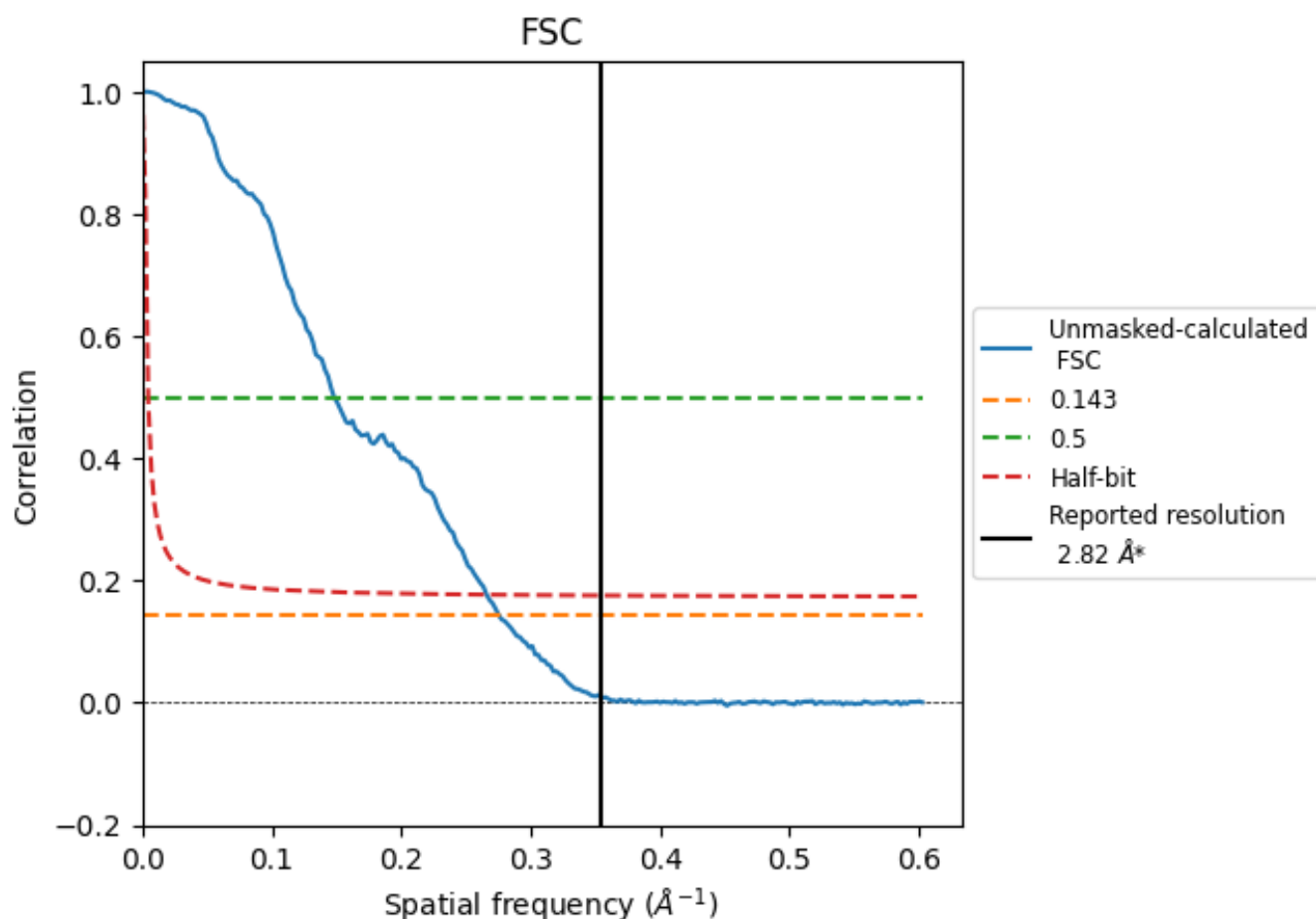


*Reported resolution corresponds to spatial frequency of $0.355 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.355 Å⁻¹

8.2 Resolution estimates [i](#)

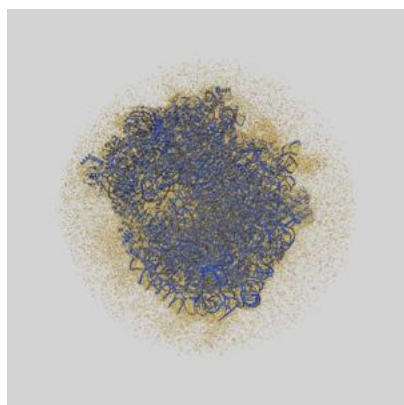
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.63	6.74	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.63 differs from the reported value 2.82 by more than 10 %

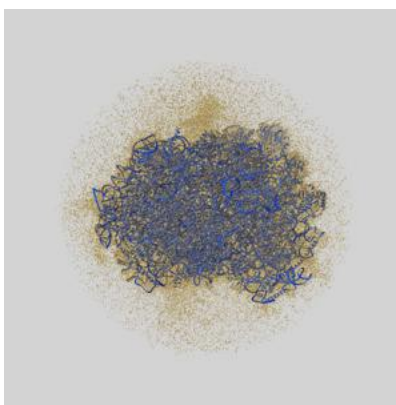
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49275 and PDB model 9NDP. Per-residue inclusion information can be found in section [3](#) on page [22](#).

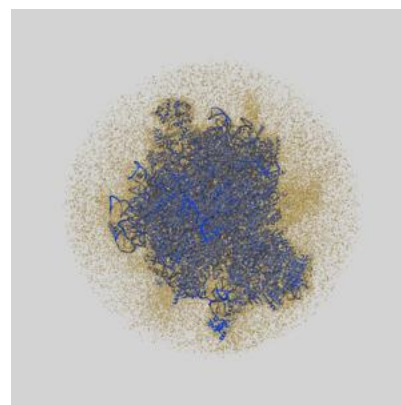
9.1 Map-model overlay [i](#)



X



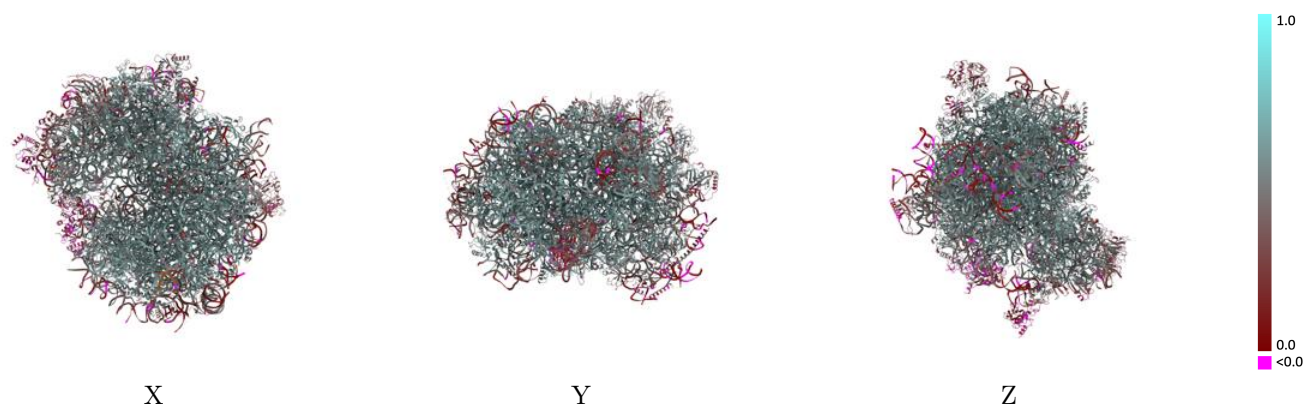
Y



Z

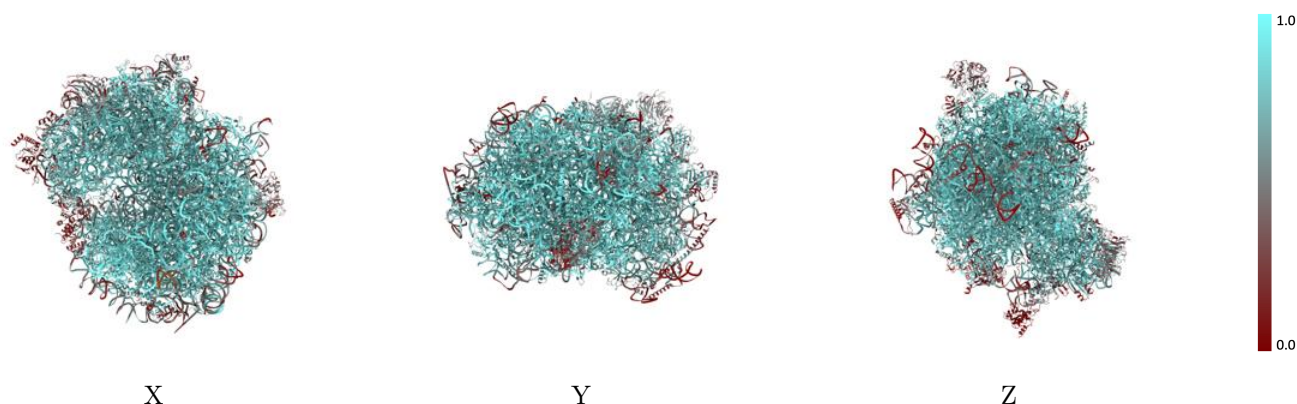
The images above show the 3D surface view of the map at the recommended contour level 0.184 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



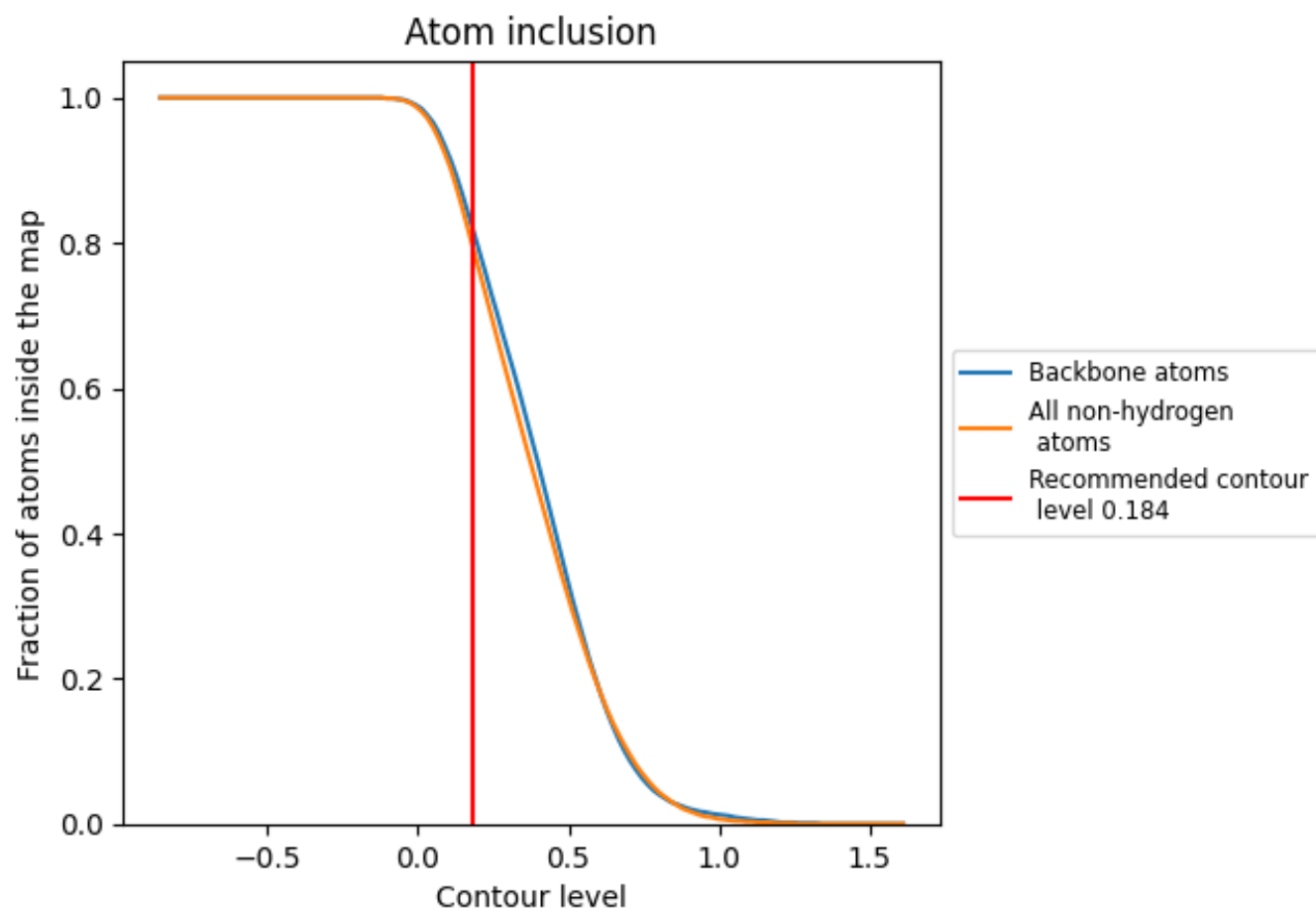
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.184).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.184) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7930	 0.4980
0	 0.0590	 0.0980
2	 0.7330	 0.4160
4	 0.5750	 0.4330
5	 0.8420	 0.5080
6	 0.4750	 0.3680
7	 0.9280	 0.5610
8	 0.8970	 0.5450
9	 0.6550	 0.4290
A	 0.9290	 0.6040
AA	 0.6240	 0.4380
B	 0.9000	 0.5860
BB	 0.6020	 0.4450
C	 0.8990	 0.5840
CC	 0.7460	 0.4920
D	 0.8410	 0.5490
DD	 0.7670	 0.5060
E	 0.7840	 0.5170
EE	 0.8340	 0.5410
EF	 0.4080	 0.3050
EG	 0.2410	 0.2000
F	 0.8850	 0.5810
FF	 0.6920	 0.4920
G	 0.7540	 0.5030
GG	 0.6020	 0.4070
H	 0.8360	 0.5520
HH	 0.7440	 0.5140
I	 0.8510	 0.5540
II	 0.6940	 0.4510
J	 0.7690	 0.5150
JJ	 0.6090	 0.4150
K	 0.8030	 0.4760
KK	 0.6860	 0.4700
L	 0.8360	 0.5430
LL	 0.8170	 0.5310



Continued on next page...

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Chain	Atom inclusion	Q-score
M	 0.8250	 0.5350
MM	 0.7960	 0.5270
N	 0.9330	 0.6040
NA	 0.3900	 0.2890
NB	 0.6610	 0.4150
NN	 0.7320	 0.4760
O	 0.9000	 0.5870
OO	 0.6380	 0.4330
P	 0.9020	 0.5960
PP	 0.7100	 0.4760
Q	 0.9110	 0.5960
QQ	 0.8420	 0.5640
R	 0.8260	 0.5470
RR	 0.0780	 0.1100
S	 0.9070	 0.5880
SS	 0.5350	 0.3290
T	 0.8480	 0.5600
TT	 0.8540	 0.5660
U	 0.7850	 0.5220
UU	 0.7360	 0.4970
V	 0.9050	 0.5930
VV	 0.8760	 0.5790
W	 0.6230	 0.4260
WW	 0.6190	 0.4170
X	 0.8570	 0.5710
Y	 0.8620	 0.5760
Z	 0.8370	 0.5480
a	 0.9140	 0.5940
b	 0.6960	 0.4640
c	 0.8560	 0.5680
d	 0.8440	 0.5630
e	 0.9160	 0.5960
f	 0.9390	 0.6050
g	 0.8620	 0.5630
h	 0.8470	 0.5640
i	 0.8050	 0.5380
j	 0.9330	 0.6030
k	 0.7560	 0.5340
l	 0.8710	 0.5780
m	 0.6420	 0.4820
n	 0.8850	 0.5760
o	 0.8460	 0.5530

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Chain	Atom inclusion	Q-score
p	 0.8900	 0.5900
q	 0.7940	 0.5240
r	 0.8800	 0.5820
s	 0.0900	 0.0550
t	 0.0480	 0.0630
u	 0.7870	 0.5330
v	 0.8180	 0.5410
w	 0.6170	 0.4450
x	 0.7890	 0.5190
y	 0.7430	 0.4930
z	 0.5910	 0.3830