



wwPDB EM Validation Summary Report ⓘ

Sep 17, 2026 – 02:24 pm BST

PDB ID : 9SMD / pdb_00009smd
EMDB ID : EMD-55029
Title : Ribosome-dome complex including the Sec-translocon (SecYEG-SecA-SecDF) from antibiotics treated Mycoplasma pneumoniae cells (Combined)
Authors : Xue, L.; Jensen, R.K.; Mahamid, J.
Deposited on : 2025-09-07
Resolution : 9.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

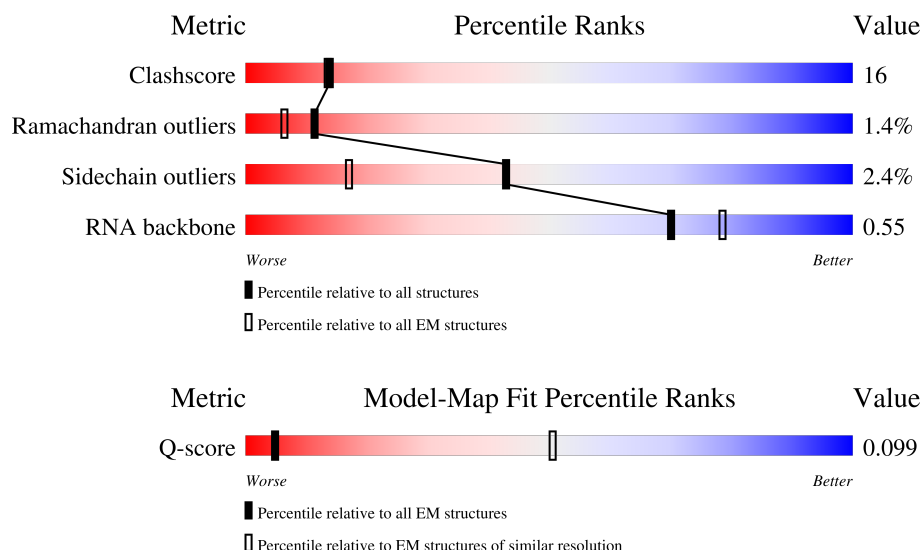
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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

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

The reported resolution of this entry is 9.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	224 (8.90 - 9.90)

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

Mol	Chain	Length	Quality of chain
1	0	48	
2	1	59	
3	10	477	

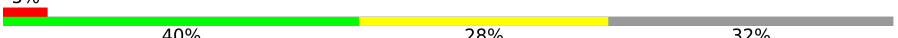
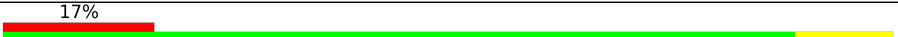
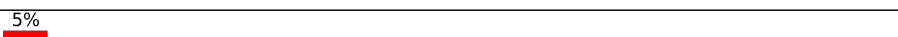
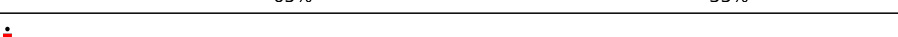
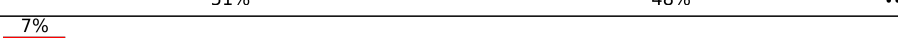
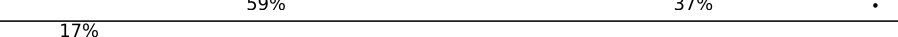
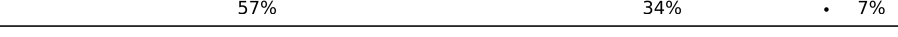
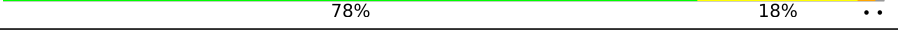
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Mol	Chain	Length	Quality of chain
4	11	76	
5	12	125	
6	17	971	
7	2	37	
8	3	2907	
9	4	108	
10	5	1523	
11	6	1523	
12	7	76	
13	8	76	
14	9	808	
15	A	294	
16	AA	219	
17	AB	21	
18	AC	97	
18	x	97	
19	C	205	
20	E	215	
21	F	155	
22	G	142	
23	H	132	
24	I	108	
25	J	121	
26	K	139	
27	L	124	

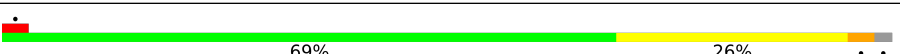
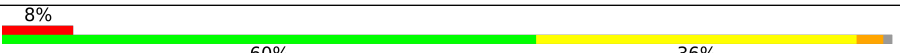
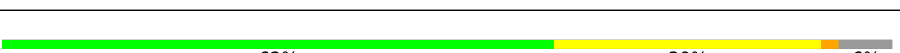
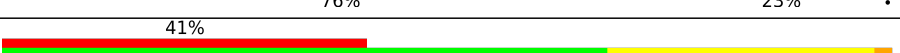
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Mol	Chain	Length	Quality of chain
28	M	61	
29	N	86	
30	O	94	
31	P	85	
32	Q	104	
33	R	87	
34	S	87	
35	T	60	
36	W	273	
37	Y	21	
38	Z	36	
39	a	287	
40	b	287	
41	c	212	
42	d	180	
43	e	184	
44	f	149	
45	g	161	
46	h	137	
47	i	146	
48	j	122	
49	k	151	
50	l	139	
51	m	124	
52	n	116	

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Mol	Chain	Length	Quality of chain
53	o	119	
54	p	127	
55	q	100	
56	r	159	
57	s	194	
58	t	111	
59	u	104	
60	v	65	
61	w	111	
62	y	57	
63	z	53	
64	13	1217	
65	14	1298	
66	15	1274	
67	16	276	
67	18	276	

2 Entry composition [i](#)

There are 72 unique types of molecules in this entry. The entry contains 202419 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 Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	47	Total	C	N	O	S	0	0
			380	236	81	61	2		

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			477	300	99	77	1		

- Molecule 3 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	10	454	Total	C	N	O	S	0	0
			3487	2284	568	628	7		

- Molecule 4 is a protein called Probable protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	11	76	Total	C	N	O	S	0	0
			585	391	93	96	5		

- Molecule 5 is a protein called SecE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	12	104	Total	C	N	O	S	0	0
			848	563	142	142	1		

- Molecule 6 is a protein called SecDF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	17	964	Total	C	N	O	S	0	0
			7613	4947	1255	1401	10		

- Molecule 7 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2	37	Total	C	N	O	S	0	0
			304	189	65	46	4		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3	2893	Total	C	N	O	P	0	0
			61992	27701	11293	20105	2893		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	4	108	Total	C	N	O	P	0	0
			2305	1030	415	752	108		

- Molecule 10 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	5	1507	Total	C	N	O	P	0	0
			32256	14418	5847	10484	1507		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	525	G7M	-	insertion	GB 26117688
5	1003	A	G	conflict	GB 26117688
5	1493	MA6	-	insertion	GB 26117688
5	1494	MA6	-	insertion	GB 26117688

- Molecule 11 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	6	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	574	7MG	-	insertion	GB 26117688
6	1053	A	G	conflict	GB 26117688
6	1543	MA6	-	insertion	GB 26117688

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Chain	Residue	Modelled	Actual	Comment	Reference
6	1544	MA6	-	insertion	GB 26117688

- Molecule 12 is a RNA chain called tRNA-Asp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
12	7	76	Total	C	N	O	P	S	0	0
			1638	734	291	535	76	2		

- Molecule 13 is a RNA chain called tRNA-Lys (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
13	8	76	Total	C	N	O	P	S	0	0
			1635	733	284	541	76	1		

- Molecule 14 is a protein called Protein translocase subunit SecA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	9	808	Total	C	N	O	S	0	0
			6467	4097	1141	1207	22		

- Molecule 15 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A	266	Total	C	N	O	S	0	0
			2138	1359	376	394	9		

- Molecule 16 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AA	155	Total	C	N	O	S	0	0
			1191	753	228	207	3		

- Molecule 17 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AB	21	Total	C	N	O	P	0	0
			440	198	75	146	21		

- Molecule 18 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AC	43	Total	C	N	O		0	0
			342	214	65	63			
18	x	46	Total	C	N	O	S	0	0
			366	235	59	68	4		

- Molecule 19 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	C	204	Total	C	N	O	S	0	0
			1669	1057	316	292	4		

- Molecule 20 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	184	Total	C	N	O	S	0	0
			1509	950	270	287	2		

- Molecule 21 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	F	155	Total	C	N	O	S	0	0
			1254	790	240	217	7		

- Molecule 22 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G	141	Total	C	N	O	S	0	0
			1110	723	193	192	2		

- Molecule 23 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	H	129	Total	C	N	O	S	0	0
			1041	661	196	183	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	27	HIS	LYS	conflict	UNP P75179

- Molecule 24 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	I	104	Total	C	N	O	S	0	0
			832	536	147	148	1		

- Molecule 25 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	J	114	Total	C	N	O	S	0	0
			829	514	153	156	6		

- Molecule 26 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	K	135	Total	C	N	O	S	0	0
			1071	677	212	180	2		

- Molecule 27 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	L	121	Total	C	N	O		0	0
			975	609	197	169			

- Molecule 28 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	M	60	Total	C	N	O	S	0	0
			474	302	96	72	4		

- Molecule 29 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	N	85	Total	C	N	O		0	0
			689	436	130	123			

- Molecule 30 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	O	87	Total	C	N	O	S	0	0
			705	453	130	118	4		

- Molecule 31 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	P	85	Total	C	N	O	S	0	0
			693	436	138	118	1		

- Molecule 32 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Q	71	Total	C	N	O	S	0	0
			590	378	115	93	4		

- Molecule 33 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	R	86	Total	C	N	O	S	0	0
			700	444	132	122	2		

- Molecule 34 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S	79	Total	C	N	O		0	0
			643	391	138	114			

- Molecule 35 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	T	59	Total	C	N	O	S	0	0
			519	326	111	80	2		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	W	224	Total	C	N	O	S	0	0
			1764	1116	326	317	5		

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Y	6	Total	C	N	O	P	0	0
			126	57	22	41	6		

- Molecule 38 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	Z	36	Total	C	N	O	0	0
			187	112	37	38		

- Molecule 39 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	a	285	Total	C	N	O	S	0	0
			2225	1385	437	397	6		

- Molecule 40 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	b	231	Total	C	N	O	S	0	0
			1778	1129	320	322	7		

- Molecule 41 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	c	211	Total	C	N	O	S	0	0
			1654	1053	299	299	3		

- Molecule 42 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	d	179	Total	C	N	O	S	0	0
			1416	910	251	251	4		

- Molecule 43 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	e	176	Total	C	N	O	0	0
			1396	899	247	250		

- Molecule 44 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	f	149	Total	C	N	O	S	0	0
			1208	779	212	214	3		

- Molecule 45 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	g	125	Total	C	N	O	S	0	0
			951	606	165	177	3		

- Molecule 46 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	h	128	Total	C	N	O	S	0	0
			959	616	160	177	6		

- Molecule 47 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	i	144	Total	C	N	O	S	0	0
			1164	737	213	209	5		

- Molecule 48 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	j	122	Total	C	N	O	S	0	0
			944	595	178	167	4		

- Molecule 49 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	k	150	Total	C	N	O	S	0	0
			1170	741	228	200	1		

- Molecule 50 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	l	136	Total	C	N	O	S	0	0
			1079	694	196	182	7		

- Molecule 51 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	m	119	Total	C	N	O	S	0	0
			958	609	175	171	3		

- Molecule 52 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	n	116	Total	C	N	O	S	0	0
			918	573	181	162	2		

- Molecule 53 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	o	118	Total	C	N	O	S	0	0
			966	609	186	170	1		

- Molecule 54 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	p	118	Total	C	N	O	S	0	0
			981	624	194	161	2		

- Molecule 55 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	q	99	Total	C	N	O	S	0	0
			811	525	148	134	4		

- Molecule 56 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	r	142	Total	C	N	O	S	0	0
			1091	677	212	195	7		

- Molecule 57 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	s	95	Total	C	N	O	S	0	0
			740	486	125	128	1		

- Molecule 58 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	t	111	Total	C	N	O	S	0	0
			871	550	166	152	3		

- Molecule 59 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	u	88	Total	C	N	O	S	0	0
			670	416	132	121	1		

- Molecule 60 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	v	64	Total	C	N	O	S	0	0
			520	320	109	90	1		

- Molecule 61 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	w	110	Total	C	N	O	S	0	0
			906	576	168	162			

- Molecule 62 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

- Molecule 63 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 64 is a protein called Uncharacterized lipoprotein MG307 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	13	1216	Total	C	N	O	S	0	0
			9604	6055	1627	1915	7		

- Molecule 65 is a protein called Uncharacterized lipoprotein MG309 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	14	1297	Total	C	N	O	S	0	0
			10101	6304	1723	2068	6		

- Molecule 66 is a protein called Uncharacterized lipoprotein MG338 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	15	1273	Total	C	N	O	S	0	0
			9894	6200	1706	1977	11		

- Molecule 67 is a protein called Uncharacterized lipoprotein MG348 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	18	275	Total	C	N	O	0	0
			2141	1329	379	433		
67	16	275	Total	C	N	O	0	0
			2141	1329	379	433		

- Molecule 68 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
68	2	1	Total	Zn	0
			1	1	
68	M	1	Total	Zn	0
			1	1	
68	Q	1	Total	Zn	0
			1	1	
68	x	2	Total	Zn	0
			2	2	
68	y	1	Total	Zn	0
			1	1	
68	z	1	Total	Zn	0
			1	1	

- Molecule 69 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

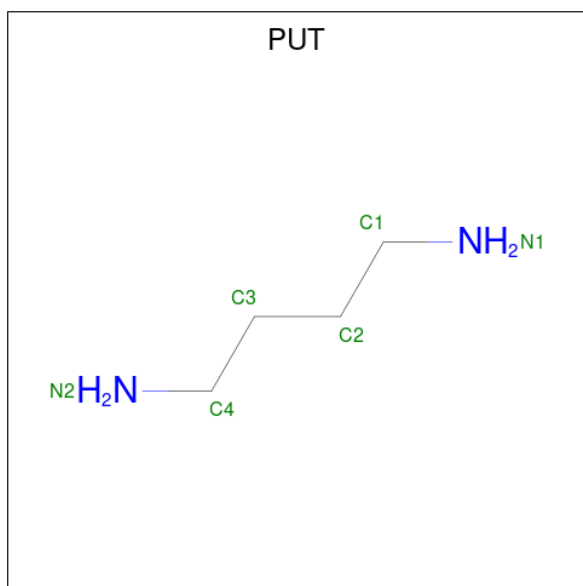
Mol	Chain	Residues	Atoms		AltConf
69	3	213	Total	Mg	0
			213	213	
69	4	1	Total	Mg	0
			1	1	
69	5	88	Total	Mg	0
			88	88	
69	6	1	Total	Mg	0
			1	1	
69	7	3	Total	Mg	0
			3	3	
69	8	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
69	AB	2	Total	Mg	0
			2	2	
69	K	1	Total	Mg	0
			1	1	
69	P	1	Total	Mg	0
			1	1	
69	Y	1	Total	Mg	0
			1	1	
69	b	2	Total	Mg	0
			2	2	
69	i	1	Total	Mg	0
			1	1	
69	y	2	Total	Mg	0
			2	2	

- Molecule 70 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
70	3	1	Total	C	N	0
			6	4	2	
70	3	1	Total	C	N	0
			6	4	2	
70	3	1	Total	C	N	0
			6	4	2	
70	3	1	Total	C	N	0
			6	4	2	

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Mol	Chain	Residues	Atoms			AltConf
70	3	1	Total	C	N	0
			6	4	2	
70	3	1	Total	C	N	0
			6	4	2	
70	5	1	Total	C	N	0
			6	4	2	
70	5	1	Total	C	N	0
			6	4	2	
70	5	1	Total	C	N	0
			6	4	2	
70	5	1	Total	C	N	0
			6	4	2	
70	b	1	Total	C	N	0
			6	4	2	

- Molecule 71 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
71	3	1	Total	K	0
			1	1	

- Molecule 72 is water.

Mol	Chain	Residues	Atoms		AltConf
72	3	16	Total	O	0
			16	16	
72	5	1	Total	O	0
			1	1	
72	A	1	Total	O	0
			1	1	
72	i	1	Total	O	0
			1	1	

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.

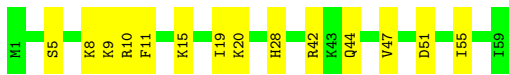
- Molecule 1: Large ribosomal subunit protein bL34

Chain 0: 



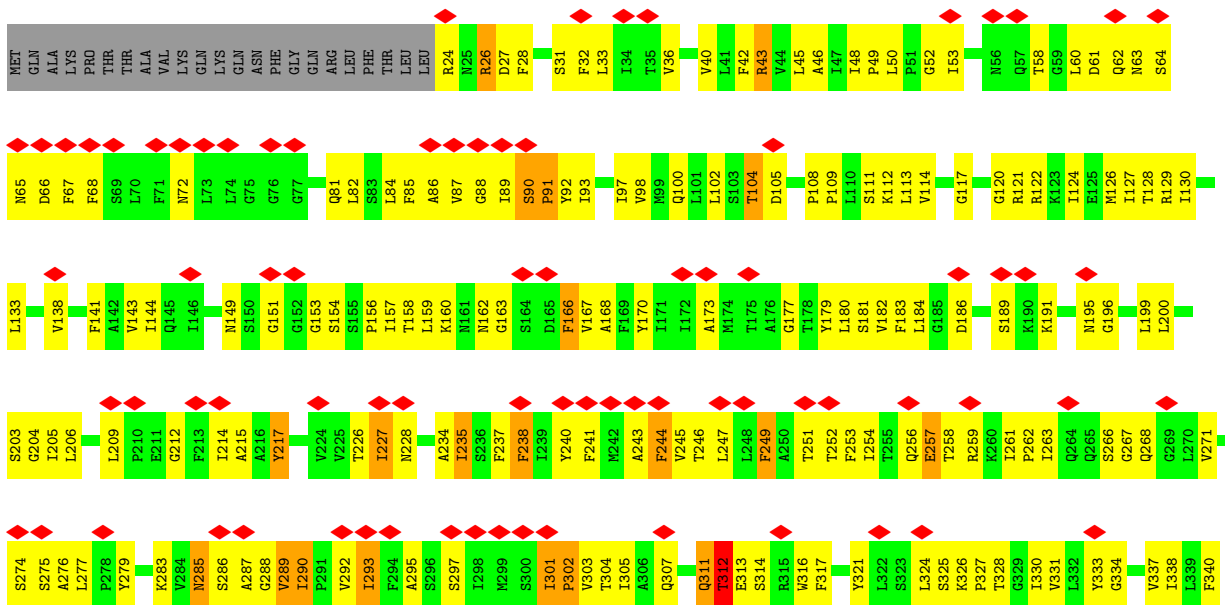
- Molecule 2: 50S ribosomal protein L35

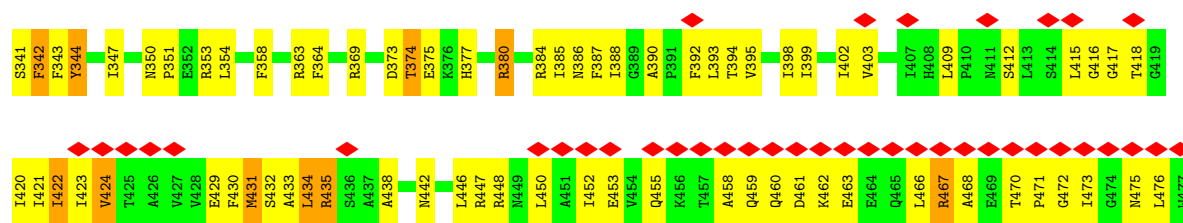
Chain 1: 



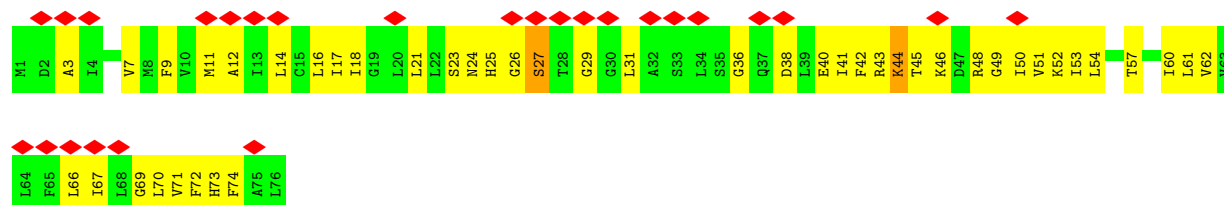
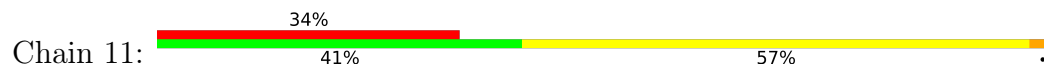
- Molecule 3: Protein translocase subunit SecY

Chain 10: 

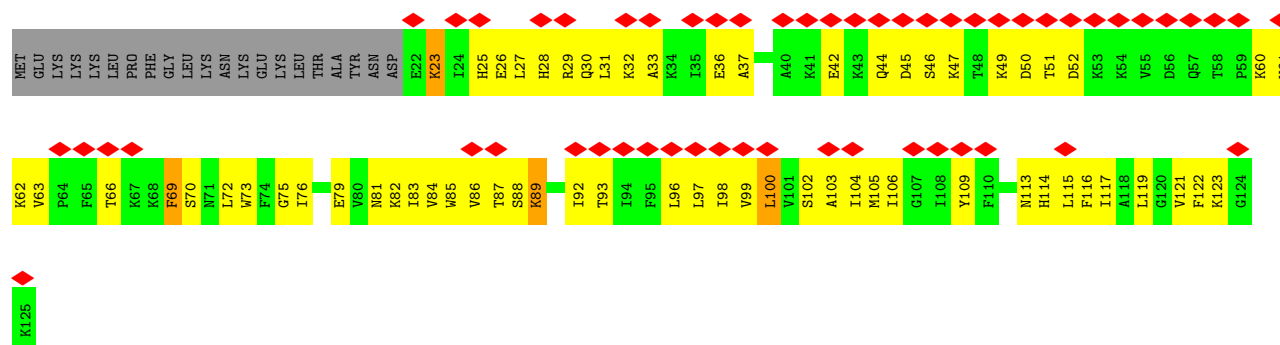




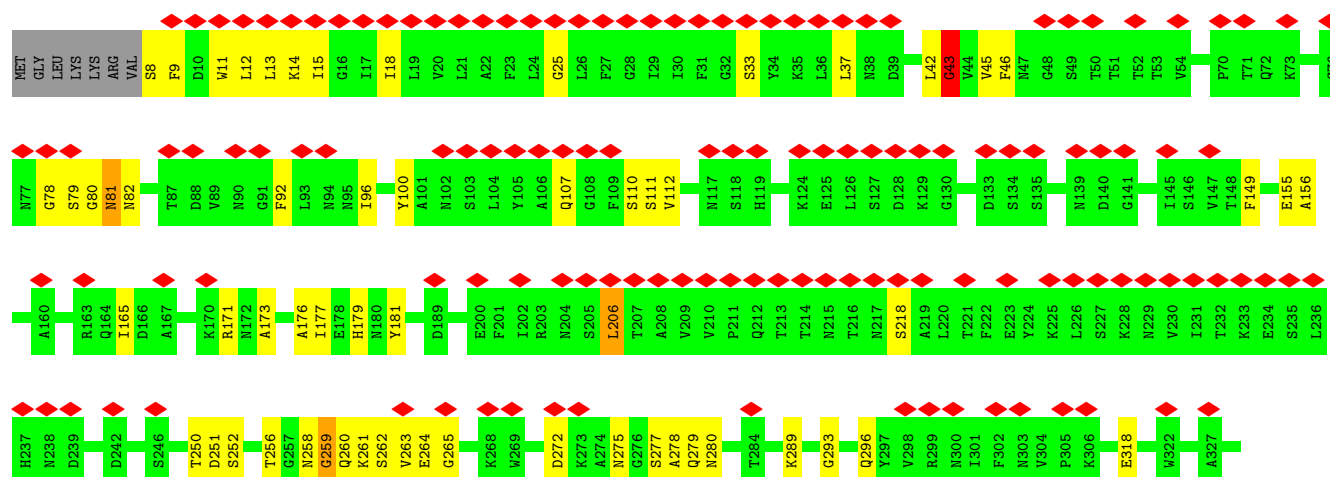
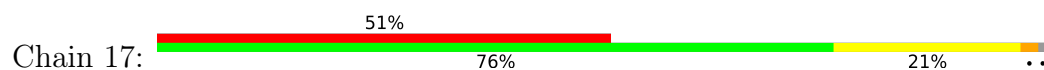
• Molecule 4: Probable protein-export membrane protein SecG

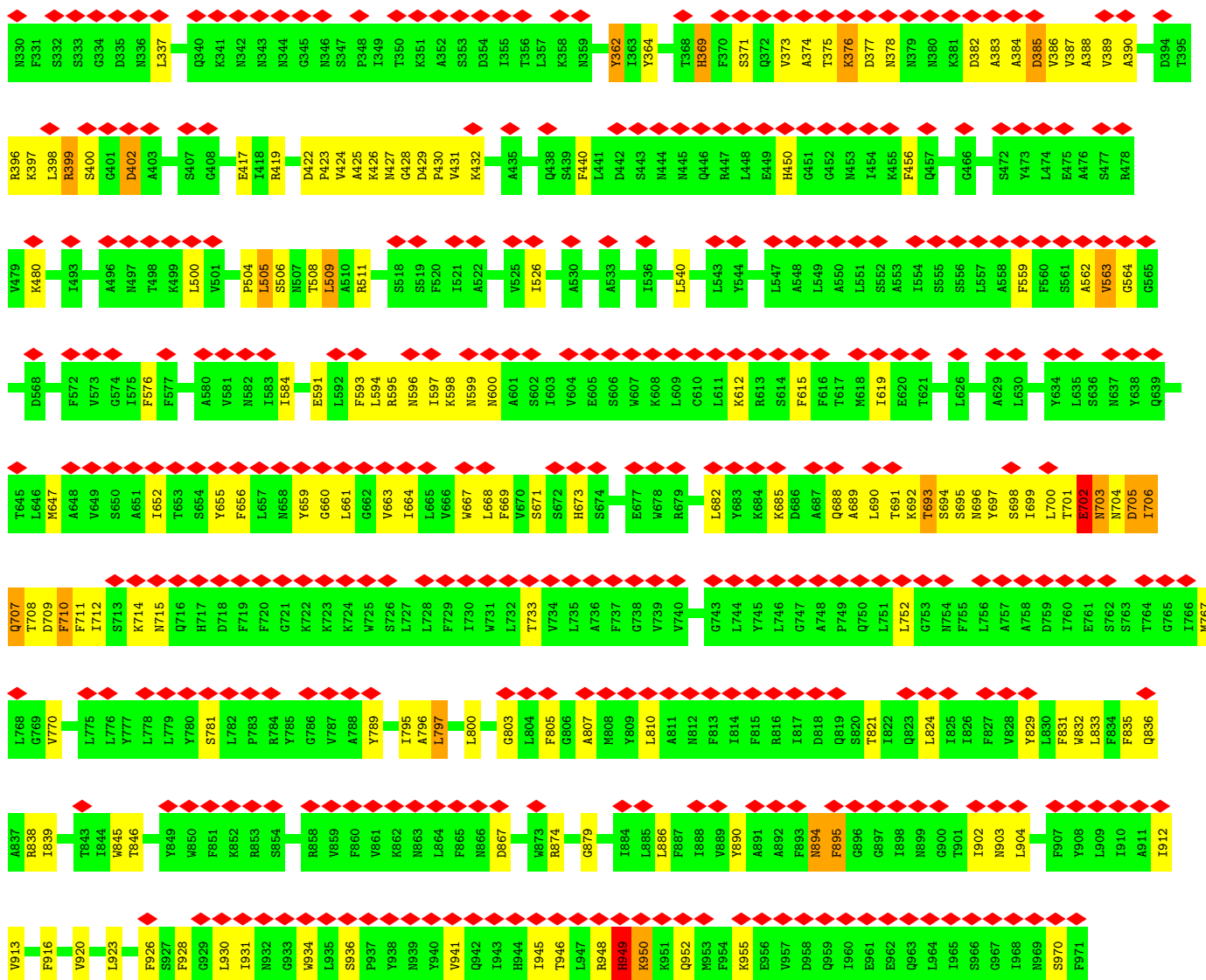


• Molecule 5: SecE



• Molecule 6: SecDF





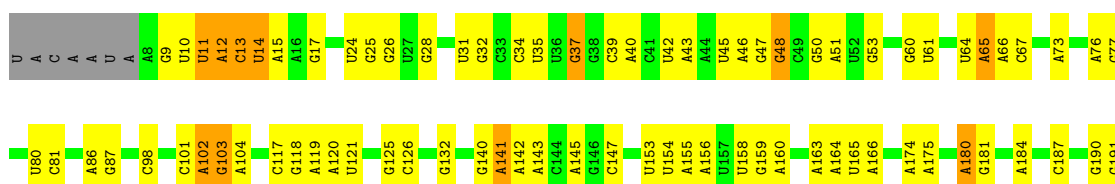
- Molecule 7: 50S ribosomal protein L36

Chain 2: 89% 11%



- Molecule 8: 23S ribosomal RNA

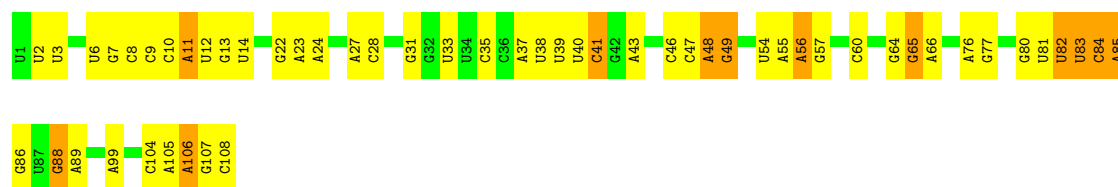
Chain 3: 55% 38% 7%



U1487	A1412	G1307	C1227	A1123	U1058	U963	C880	G788	U689	U607	G499	G300	U192
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A1493	A1414	G1309	G1229	U1125	G1060	A964	C882	U790	G691	A609	A502	U304	A194
U1494	A1415	U1310	U1229	A1062	A1061	U965	A883	G791	G695	G610	G512	A309	A195
A1496	A1420	G1313	G1231	G1128	A1063	U968	A887	U797	A698	C614	A515	U310	G196
A1497	U1422	U1318	U1232	U1129	A1064	A969	A888	G798	U699	G615	A516	G311	A200
A1502	A1423	C1317	A1233	A1131	U1068	U970	G889	U799	A700	G616	G517	U312	A201
A1503	U1424	U1318	U1235	C1132	G1069	A981	U890	C800	U701	A619	A518	G313	C202
G1504	A1431	C1321	G1236	G1134	G1071	A983	G891	G810	U702	G620	A519	A203	U204
G1508	C1432	A1322	U1239	C1135	A1072	C884	G892	G811	A703	U621	C520	A316	C207
U1509	U1433	A1323	U1240	U1136	A1073	A985	A893	G811	G704	U622	G524	U317	C207
A1510	A1436	C1325	U1241	C1137	A1074	G988	A897	A817	A705	A623	G527	U318	G219
A1512	U1437	U1329	G1245	C1139	U1076	U994	A898	U819	A712	A628	A527	A322	A220
A1513	A1438	U1330	U1246	U1141	C1078	A995	A899	U820	G714	U629	G529	A323	A223
U1514	U1439	U1334	C1247	G1142	U1079	A996	C901	A824	G716	A631	G531	C324	A225
U1515	U1440	A1335	A1248	C1143	A1080	G997	U902	A828	A720	A632	A532	A333	A226
A1518	A1441	A1336	A1249	U1144	A1081	U998	A903	A829	G721	U636	U539	C336	G230
A1519	G1442	A1337	G1250	A1145	A1082	U999	C904	A830	C722	U637	A540	U337	A231
A1520	U1444	G1337	G1251	A1146	A1083	U1000	U905	U831	G722	A638	A549	U339	A232
U1521	C1445	U1341	G1252	U1147	C1084	A1002	G906	C832	A728	C440	C440	U340	U233
U1522	G1446	C1342	U1254	G1149	A1089	U1003	U909	G840	C733	A648	A549	G447	G234
C1523	A1447	C1343	G1255	G1155	G1090	U1004	G910	U844	G739	A649	C558	G341	U235
G1525	U1448	U1344	A1256	U1156	A1092	U1006	G917	U845	A740	A651	C562	A343	G236
U1529	G1450	G1351	U1264	U1157	U1093	C1007	C918	U846	A741	U652	A451	A344	A237
G1530	A1451	G1352	U1265	U1158	G1094	A1008	G918	U847	U749	G653	C565	A345	U238
A1534	U1452	C1355	G1266	A1158	U1095	G1009	C922	U848	U750	A656	G566	U345	U245
A1535	A1457	U1356	A1267	C1170	G1097	A1016	A923	U849	C752	G656	U567	G353	G246
A1536	U1458	U1357	U1268	U1176	G1098	U1019	C924	C850	A756	A657	G568	C354	G252
A1537	A1459	U1369	C1269	U1176	C1099	A1019	C925	U851	C755	U660	U569	A355	C253
U1541	G1460	C1378	A1271	A1177	U1101	A1026	U926	C852	A757	G663	C570	A356	G254
G1542	A1461	U1379	A1271	U1178	U1102	A1026	A927	A854	G761	A663	A573	G363	G258
U1543	U1462	U1380	U1279	A1183	G1103	A1029	G928	A855	U761	G664	G574	A364	A259
G1544	G1463	A1381	G1280	U1184	A1104	U1030	C929	U858	G764	G666	C575	U365	G270
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G1550	C1470	U1387	U1284	A1201	A1108	A1033	A933	U862	C767	U670	U583	U382	A276
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A1548	C1472	C1390	G1286	G1203	C1110	A1037	U935	U863	A769	G672	U585	U386	U279
A1549	U1473	U1391	A1292	A1204	A1112	G1038	G936	G866	C775	A673	G586	U387	A280
U1550	C1474	G1392	U1293	U1208	C1113	G1039	U944	C867	U776	G674	C597	U388	U284
G1551	A1479	U1393	G1294	U1209	C1114	A1045	A947	U869	C777	U675	U598	C389	U284
A1552	A1480	A1401	U1295	U1210	G1115	A1048	A948	A870	U781	U676	U599	A392	G287
G1553	U1481	U1404	G1296	U1211	U1116	U1049	C949	G871	U781	A681	U600	G397	U295
U1564	U1482	C1404	G1301	C1212	U1117	U1054	U950	U874	U782	A682	G603	C398	U296
G1565	G1483	U1405	U1304	G1215	U1118	U1054	U952	G875	G783	A683	A604	G401	G297
A1566	U1484	U1407	G1305	U1219	A1120	A1055	G953	U879	A784	A694	A605	U298	U298
U1567	U1486		G1306		G1122		G957				G606	A402	A299

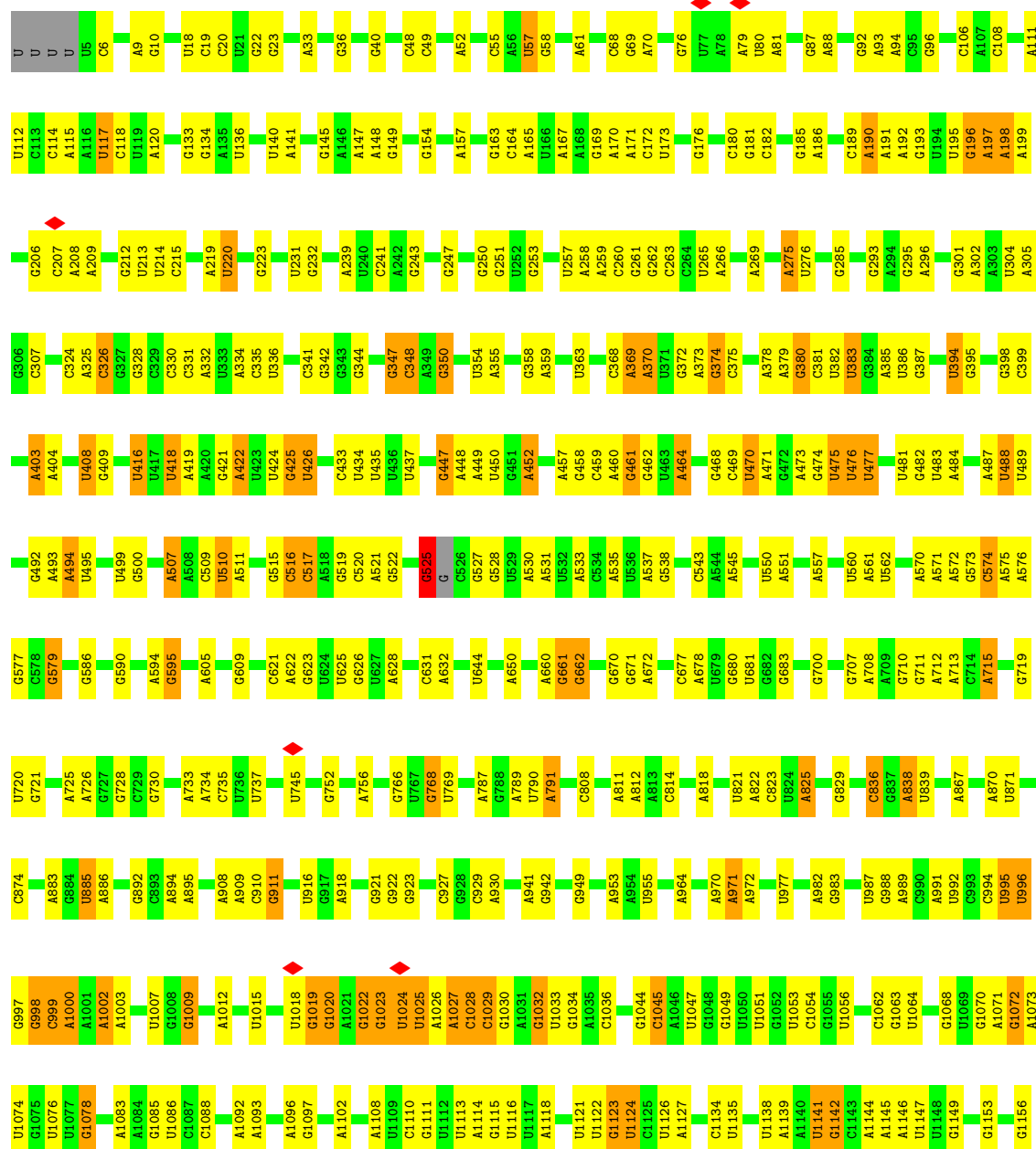
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A2854	A1573	A1652	C1789	U1894	G2017	A2096	A2181	A2276	U2356	G2452	G2558	U2655	C2763	U2655	A2854
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C2856	C1575	A1661	U1791	U1906	G2019	U2099	C2186	G2279	U2358	A2456	G2561	U2657	A2765	U2657	C2856
C2857	G1576	G1665	A1792	G1906	G2022	G2100	U2193	U2280	A2366	U2457	G2562	U2658	U2766	U2658	C2857
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U2862	U1581	U1670	A1798	G1910	C2024	A2107	G2195	U2282	G2373	U2459	C2564	U2660	U2771	C2564	U2862
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	A1641	U1764	U1764	A1966	A2071	A2160	U2246	U2325	U2418	G2521	U2623	U2709	U2825	U2709	
	A1643	U1764	U1764	A1967	A2072	U2160	U2247	U2326	U2419	G2522	U2624	U2710	G2829	U2710	
	A1644	U1767	U1767	A1968	A2073	U2161	U2248	U2327	U2420	G2523	U2625	U2711	U2830	U2711	
	C1645	U1768	U1768	A1969	A2074	U2162	U2249	U2328	U2421	G2524	U2626	U2712	U2831	U2712	
	A1647	U1769	U1769	A1970	A2075	U2163	U2250	U2329	U2422	G2525	U2627	U2713	U2832	U2713	
		A1770		A1971	A2076	U2164	U2251	U2330	U2423	G2526	U2628	U2714	U2833	U2714	
				A1972	A2077	U2165	U2252	U2331	U2424	G2527	U2629	U2715	U2834	U2715	
				A1973	A2078	U2166	U2253	U2332	U2425	G2528	U2630	U2716	U2835	U2716	
				A1974	A2079	U2167	U2254	U2333	U2426	G2529	U2631	U2717	U2836	U2717	
				A1975	A2080	U2168	U2255	U2334	U2427	G2530	U2632	U2718	U2837	U2718	
				A1976	A2081	U2169	U2256	U2335	U2428	G2531	U2633	U2719	U2838	U2719	
				A1977	A2082	U2170	U2257	U2336	U2429	G2532	U2634	U2720	U2839	U2720	
				A1978	A2083	U2171	U2258	U2337	U2430	G2533	U2635	U2721	U2840	U2721	
				A1979	A2084	U2172	U2259	U2338	U2431	G2534	U2636	U2722	U2841	U2722	
				A1980	A2085	U2173	U2260	U2339	U2432	G2535	U2637	U2723	U2842	U2723	
				A1981	A2086	U2174	U2261	U2340	U2433	G2536	U2638	U2724	U2843	U2724	
				A1982	A2087	U2175	U2262	U2341	U2434	G2537	U2639	U2725	U2844	U2725	
				A1983	A2088	U2176	U2263	U2342	U2435	G2538	U2640	U2726	U2845	U2726	
				A1984	A2089	U2177	U2264	U2343	U2436	G2539	U2641	U2727	U2846	U2727	
				A1985	A2090	U2178	U2265	U2344	U2437	G2540	U2642	U2728	U2847	U2728	
				A1986	A2091	U2179	U2266	U2345	U2438	G2541	U2643	U2729	U2848	U2729	
				A1987	A2092	U2180	U2267	U2346	U2439	G2542	U2644	U2730	U2849	U2730	
				A1988	A2093	U2181	U2268	U2347	U2440	G2543	U2645	U2731	U2850	U2731	
				A1989	A2094	U2182	U2269	U2348	U2441	G2544	U2646	U2732	U2851	U2732	
				A1990	A2095	U2183	U2270	U2349	U2442	G2545	U2647	U2733	U2852	U2733	
				A1991	A2096	U2184	U2271	U2350	U2443	G2546	U2648	U2734	U2853	U2734	
				A1992	A2097	U2185	U2272	U2351	U2444	G2547	U2649	U2735	U2854	U2735	
				A1993	A2098	U2186	U2273	U2352	U2445	G2548	U2650	U2736	U2855	U2736	
				A1994	A2099	U2187	U2274	U2353	U2446	G2549	U2651	U2737	U2856	U2737	
				A1995	A2100	U2188	U2275	U2354	U2447	G2550	U2652	U2738	U2857	U2738	
				A1996	A2101	U2189	U2276	U2355	U2448	G2551	U2653	U2739	U2858	U2739	
				A1997	A2102	U2190	U2277	U2356	U2449	G2552	U2654	U2740	U2859	U2740	
				A1998	A2103	U2191	U2278	U2357	U2450	G2553	U2655	U2741	U2860	U2741	
				A1999	A2104	U2192	U2279	U2358	U2451	G2554	U2656	U2742	U2861	U2742	
				A2000	A2105	U2193	U2280	U2359	U2452	G2555	U2657	U2743	U2862	U2743	
				A2001	A2106	U2194	U2281	U2360	U2453	G2556	U2658	U2744	U2863	U2744	
				A2002	A2107	U2195	U2282	U2361	U2454	G2557	U2659	U2745	U2864	U2745	
				A2003	A2108	U2196	U2283	U2362	U2455	G2558	U2660	U2746	U2865	U2746	
				A2004	A2109	U2197	U2284	U2363	U2456	G2559	U2661	U2747	U2866	U2747	
				A2005	A2110	U2198	U2285	U2364	U2457	G2560	U2662	U2748	U2867	U2748	
				A2006	A2111										

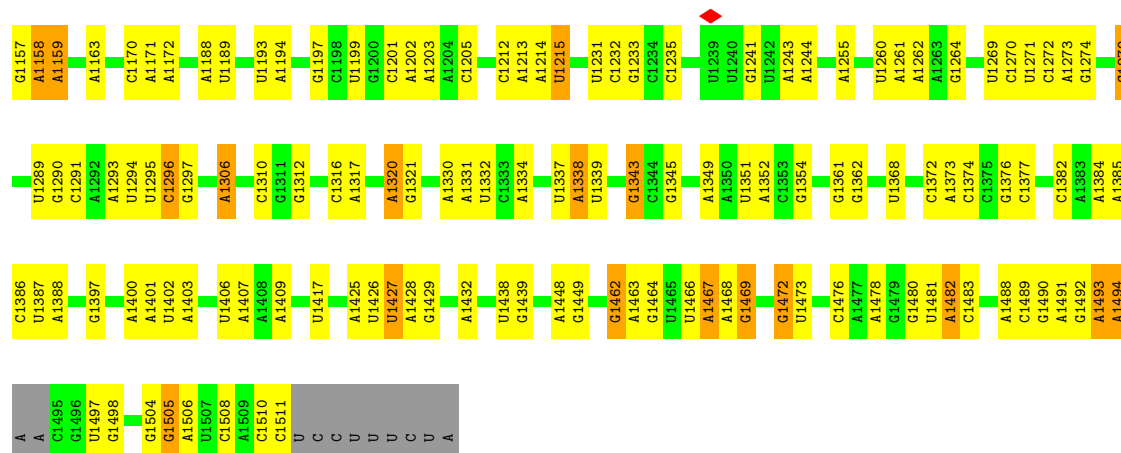
Chain 4:  50% 39% 11%



• Molecule 10: 16S ribosomal RNA

Chain 5:  62% 31% 6%

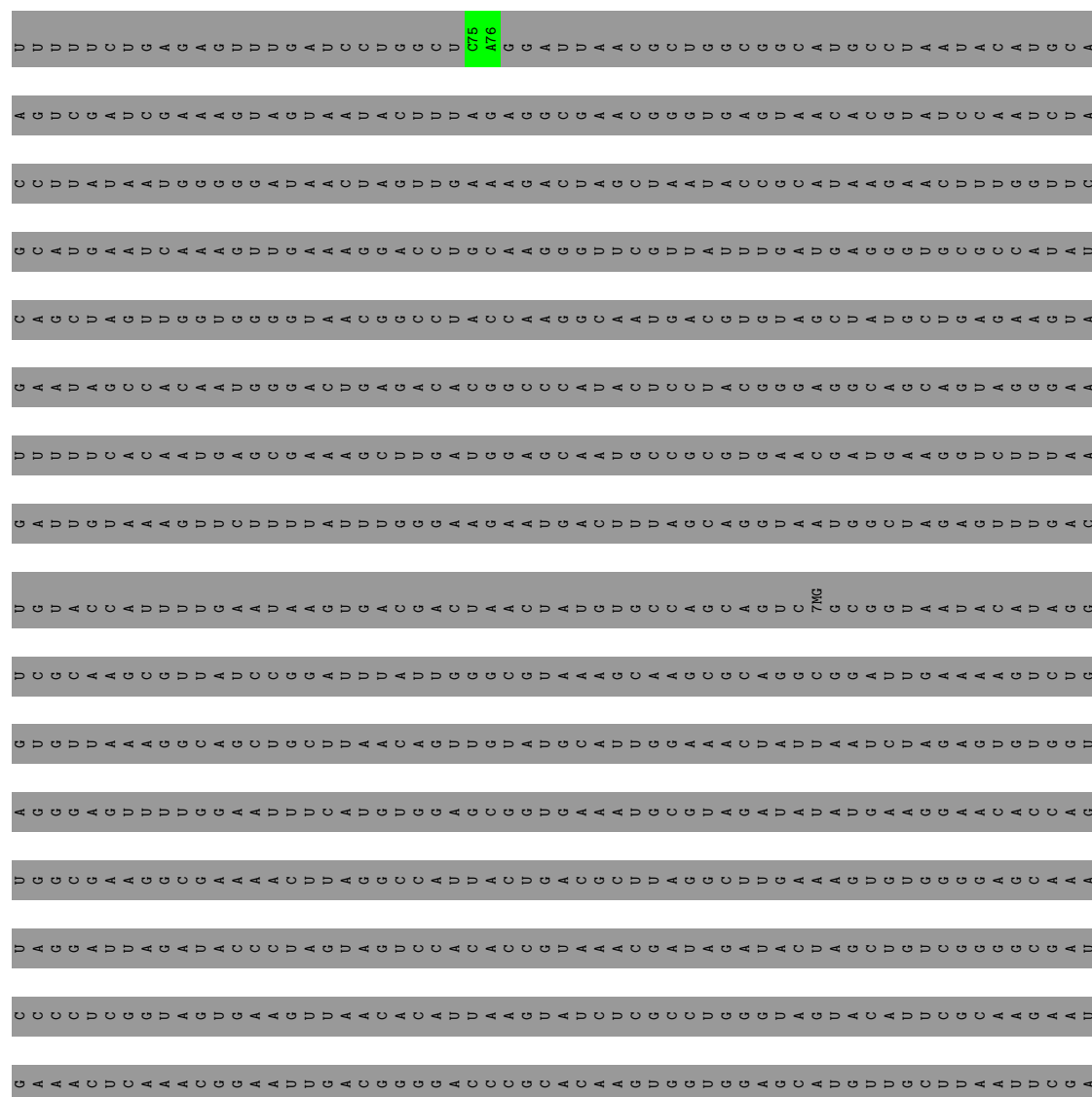


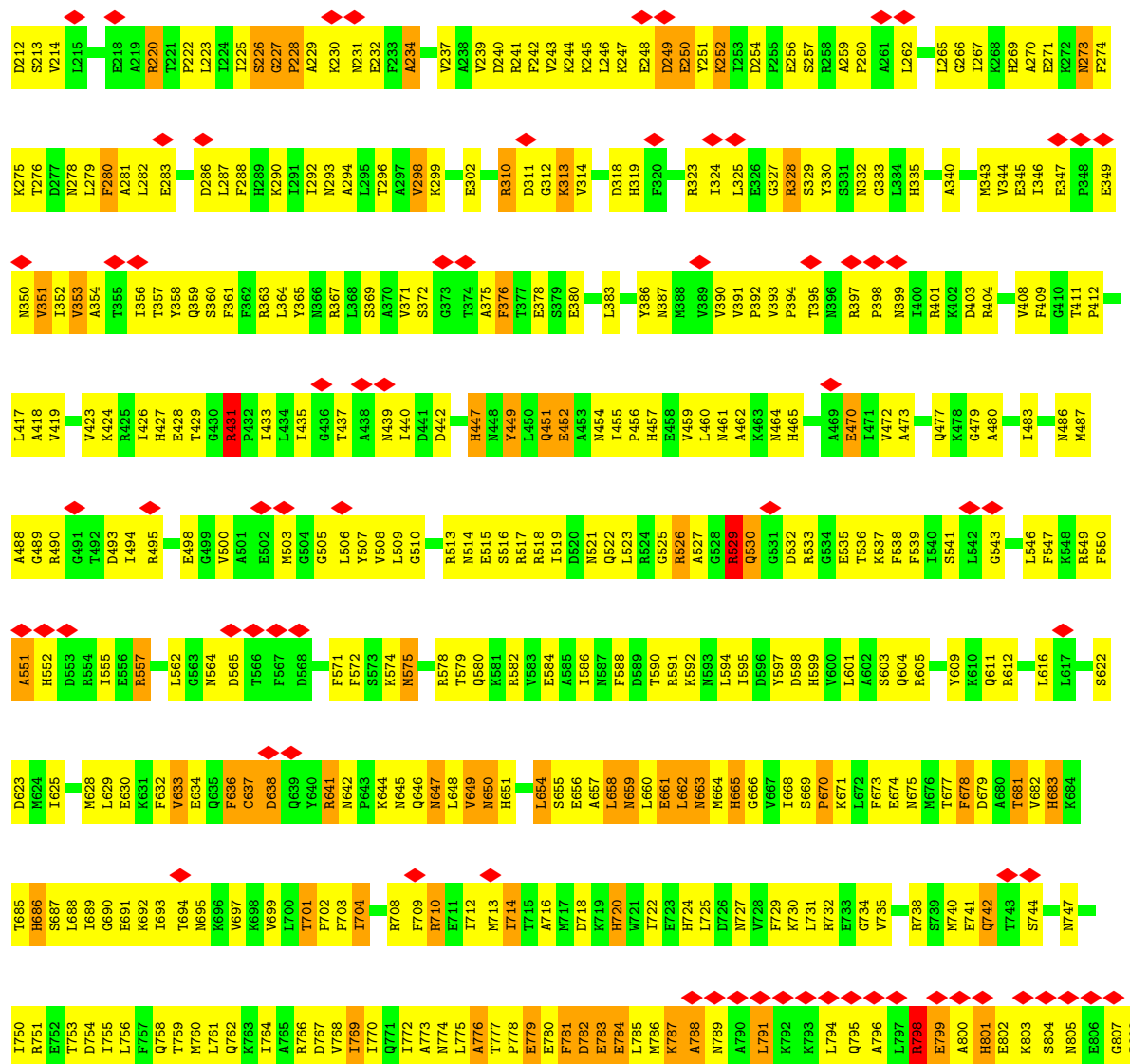


• Molecule 11: 16S ribosomal RNA

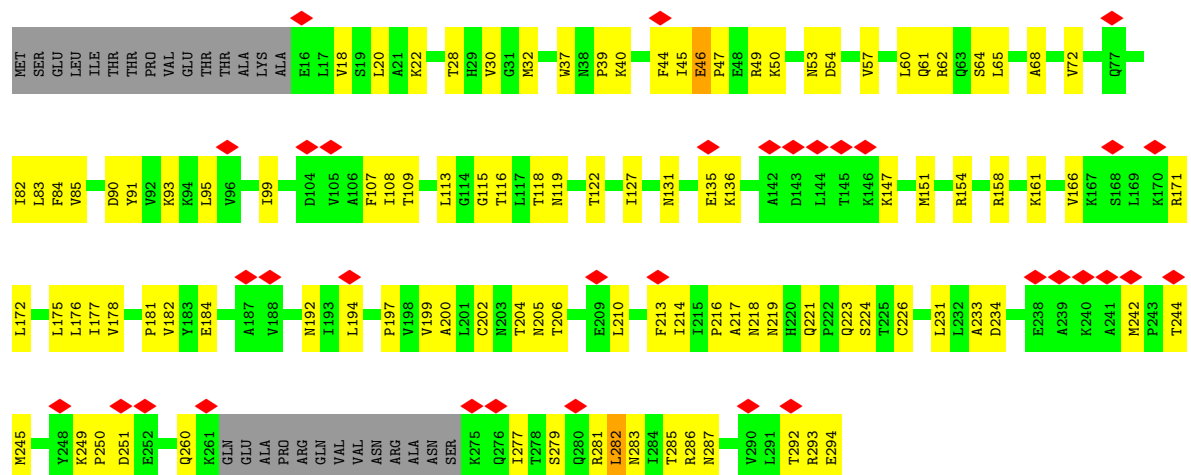
Chain 6:

100%

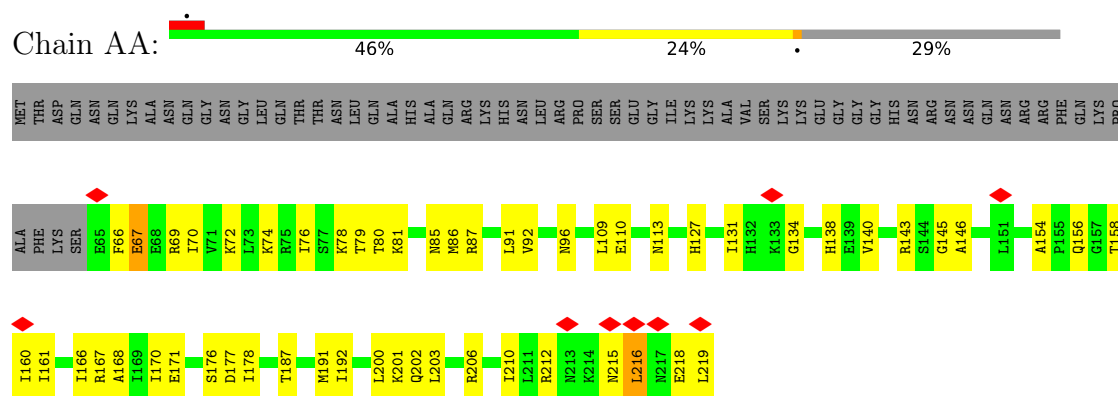




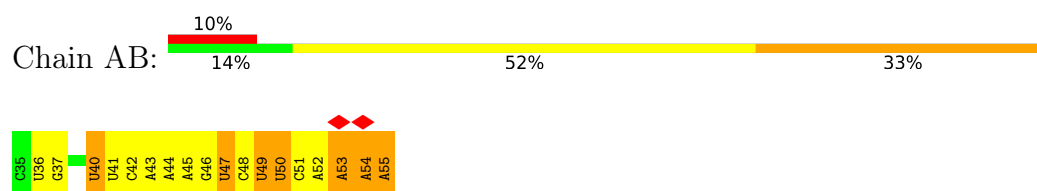
• Molecule 15: 30S ribosomal protein S2



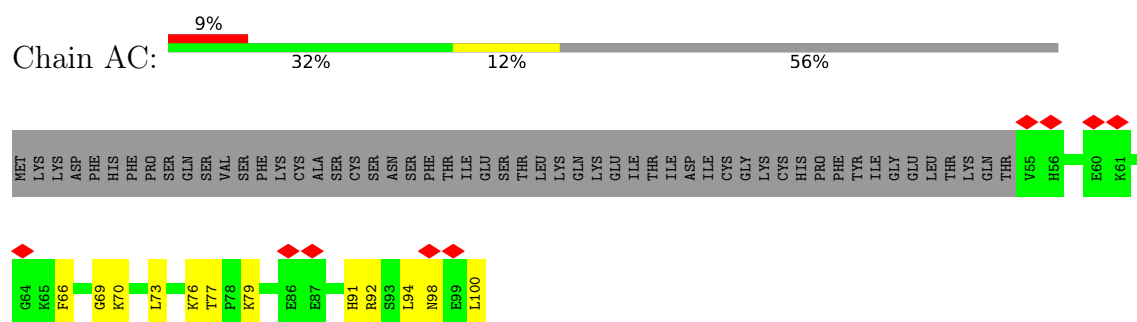
- Molecule 16: 30S ribosomal protein S5



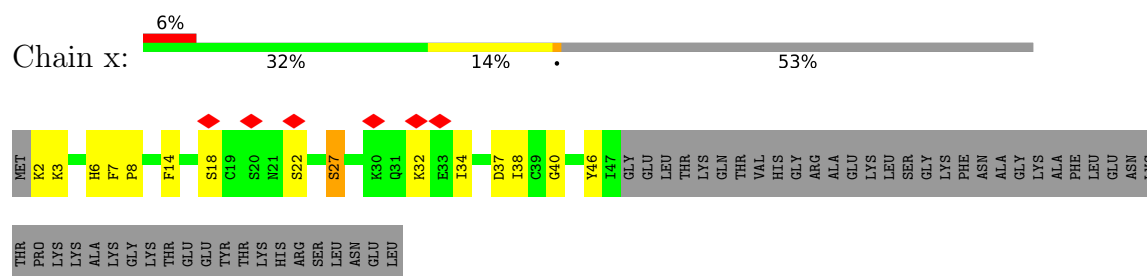
- Molecule 17: mRNA



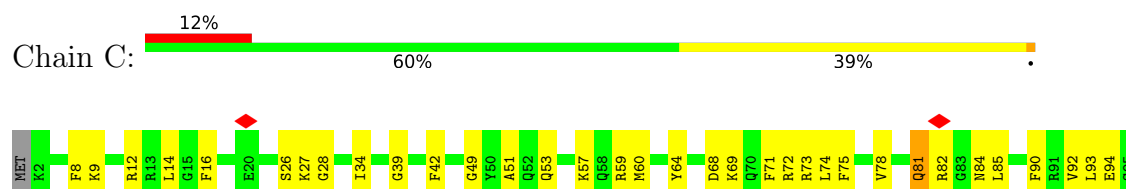
- Molecule 18: 50S ribosomal protein L31

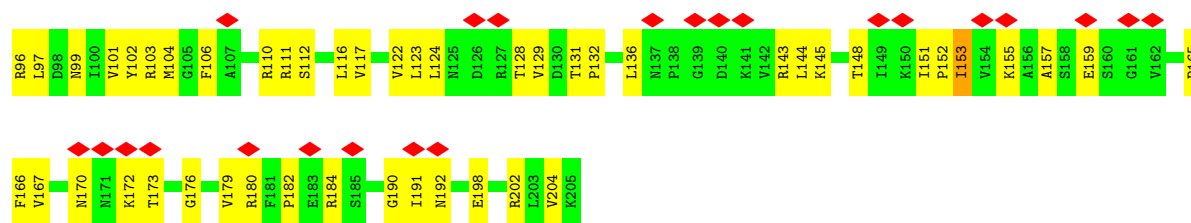


- Molecule 18: 50S ribosomal protein L31

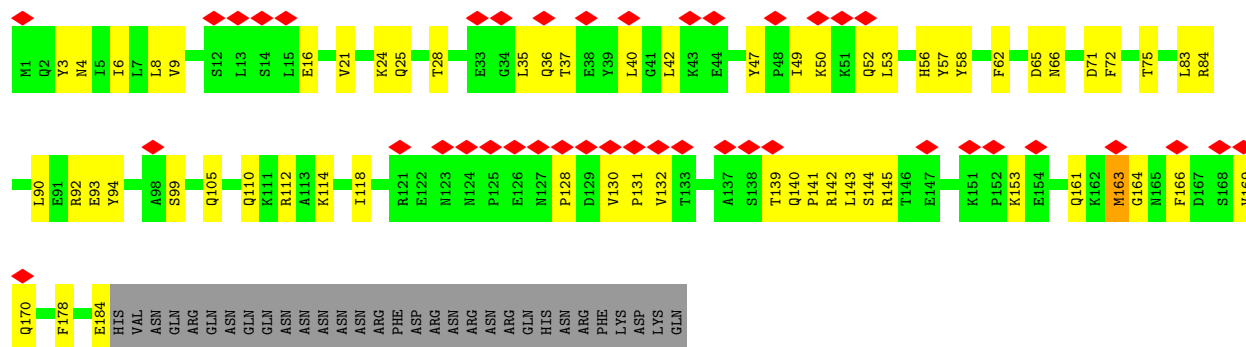


- Molecule 19: 30S ribosomal protein S4

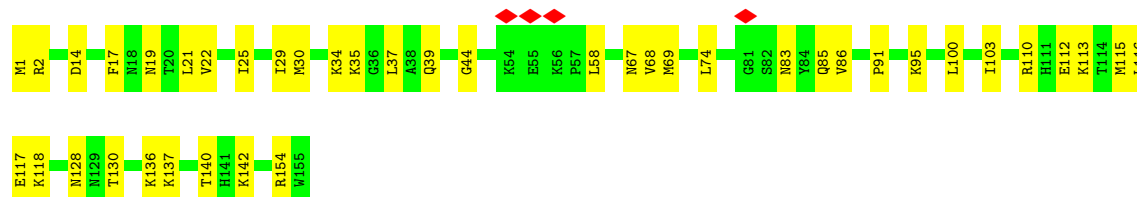
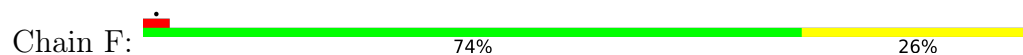




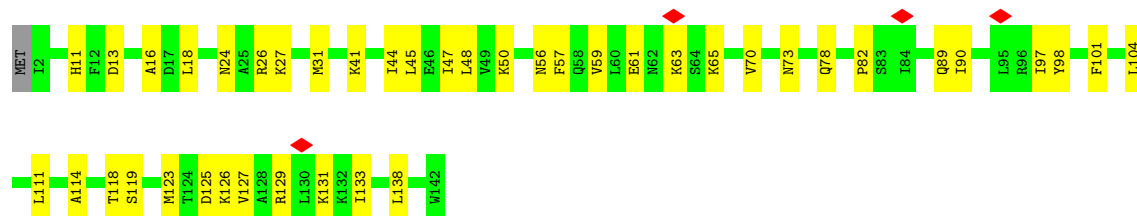
• Molecule 20: 30S ribosomal protein S6



• Molecule 21: 30S ribosomal protein S7

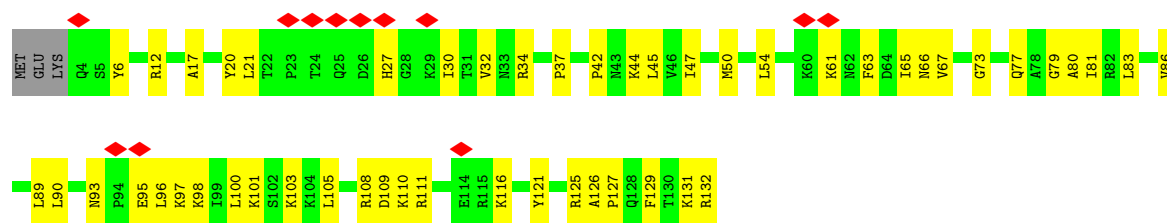


• Molecule 22: 30S ribosomal protein S8

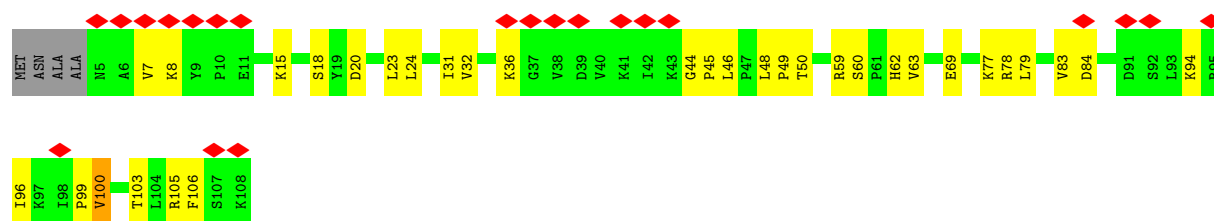


• Molecule 23: Small ribosomal subunit protein uS9

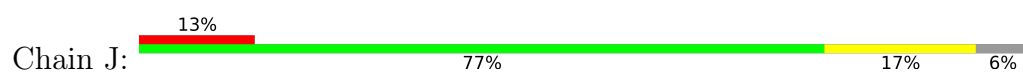




• Molecule 24: 30S ribosomal protein S10



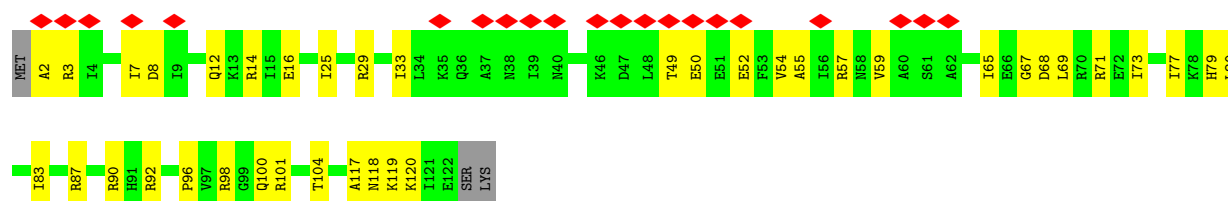
• Molecule 25: 30S ribosomal protein S11



• Molecule 26: 30S ribosomal protein S12



• Molecule 27: 30S ribosomal protein S13



• Molecule 28: 30S ribosomal protein S14 type Z

Chain M:  79% 20% .



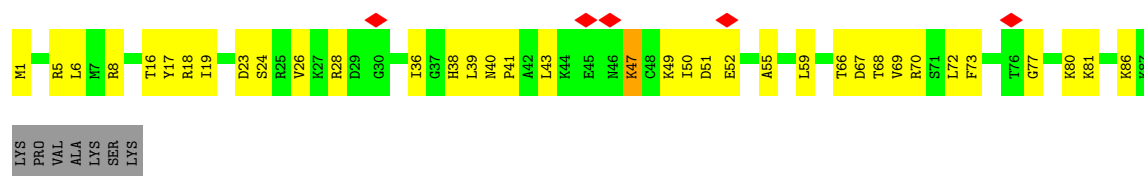
- Molecule 29: 30S ribosomal protein S15

Chain N:  81% 16% ..



- Molecule 30: 30S ribosomal protein S16

Chain O:  5% 54% 37% 7% .



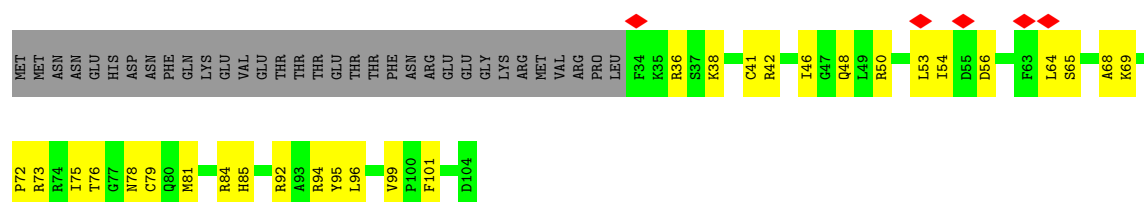
- Molecule 31: 30S ribosomal protein S17

Chain P:  18% 69% 31%



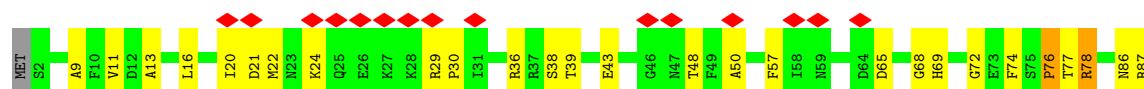
- Molecule 32: 30S ribosomal protein S18

Chain Q:  5% 40% 28% 32%

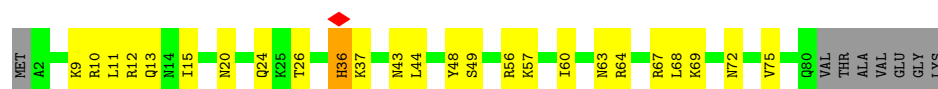


- Molecule 33: 30S ribosomal protein S19

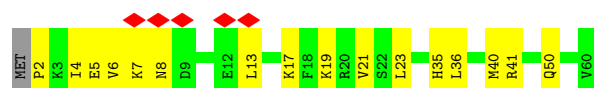
Chain R:  17% 68% 29% ..



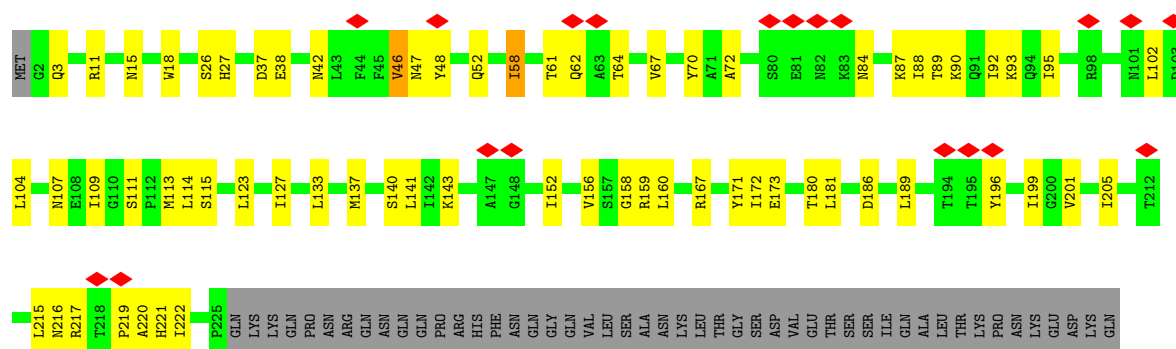
- Molecule 34: 30S ribosomal protein S20



- Molecule 35: 30S ribosomal protein S21



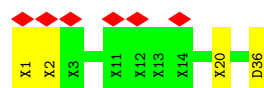
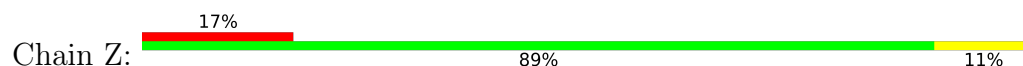
- Molecule 36: 30S ribosomal protein S3



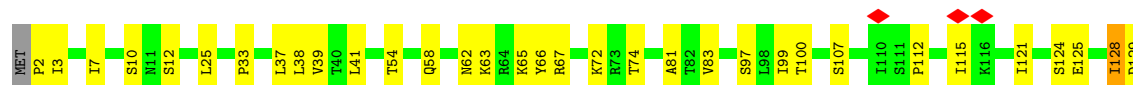
- Molecule 37: mRNA

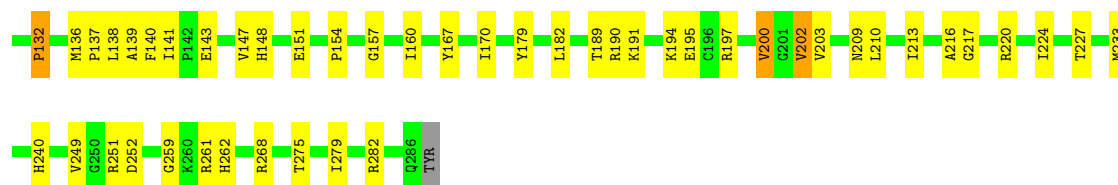


- Molecule 38: Nascent peptide

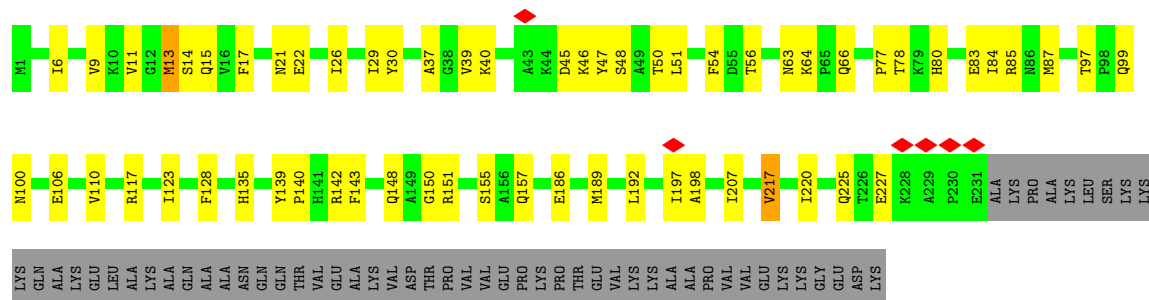


- Molecule 39: 50S ribosomal protein L2

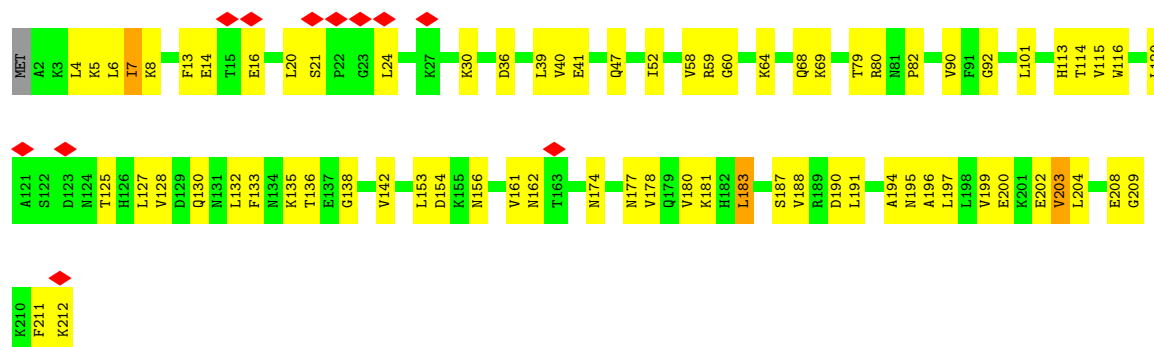




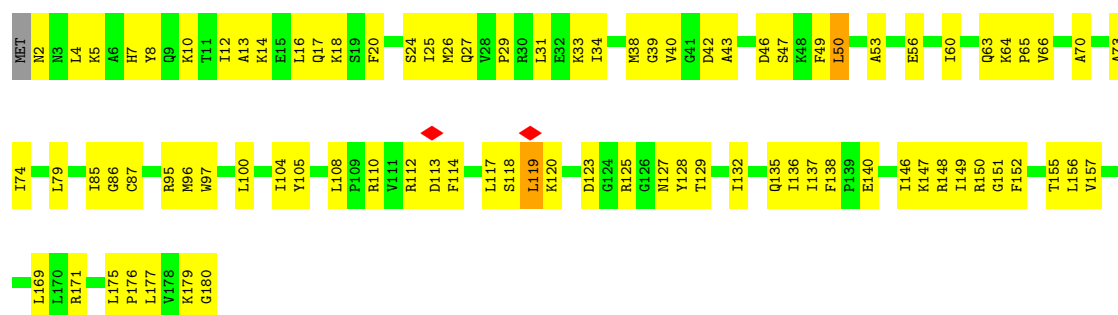
• Molecule 40: 50S ribosomal protein L3



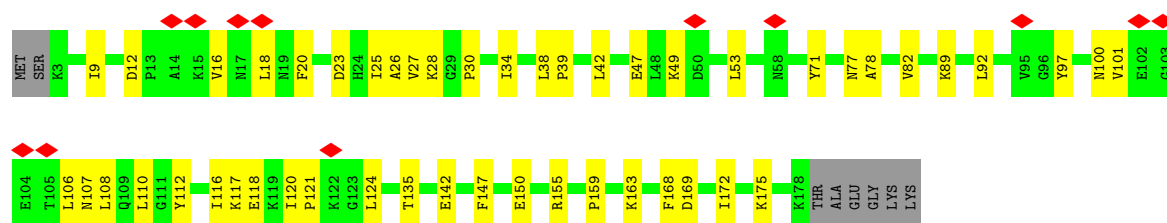
• Molecule 41: 50S ribosomal protein L4



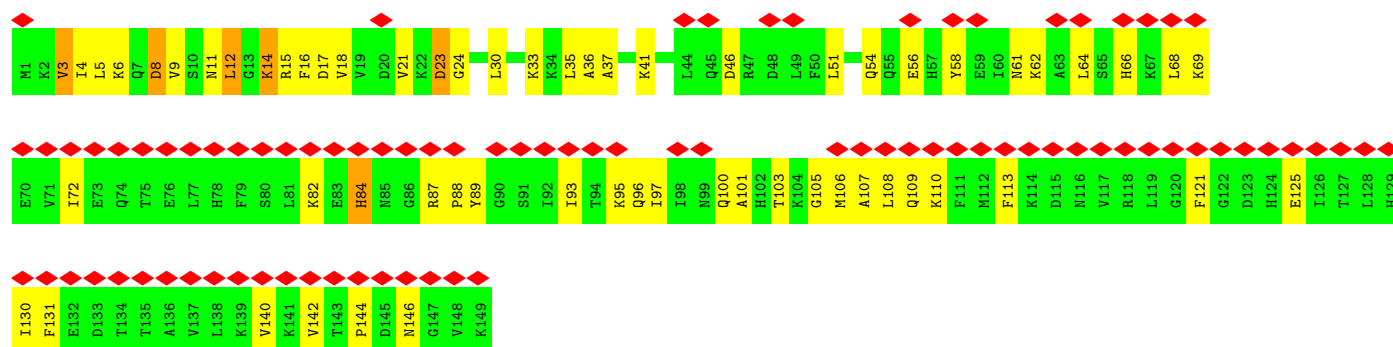
• Molecule 42: 50S ribosomal protein L5



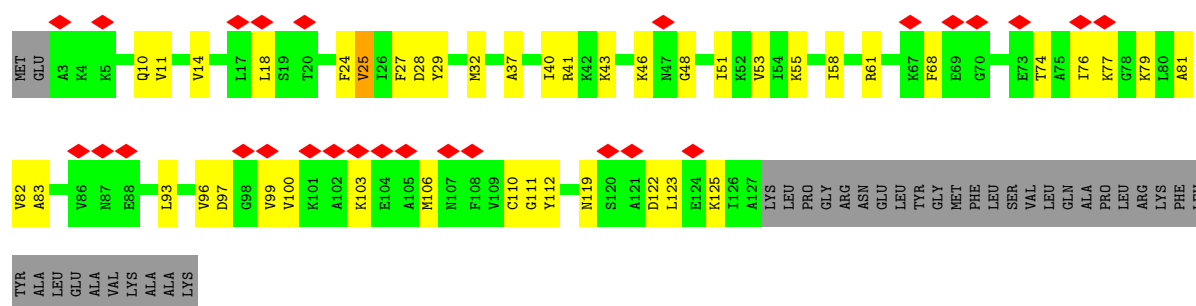
• Molecule 43: 50S ribosomal protein L6



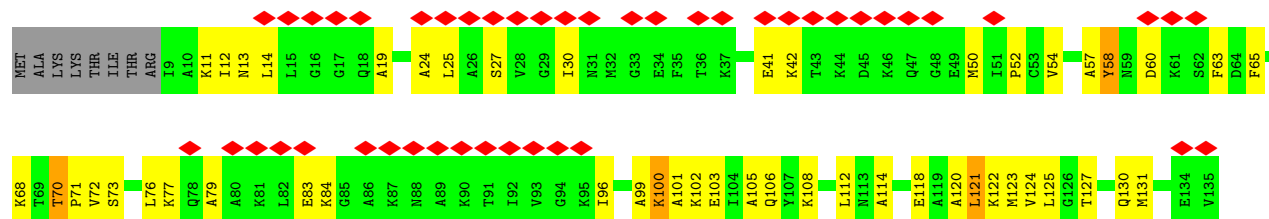
• Molecule 44: 50S ribosomal protein L9



• Molecule 45: 50S ribosomal protein L10



• Molecule 46: 50S ribosomal protein L11





- Molecule 47: 50S ribosomal protein L13

Chain i:  78% 18% ..



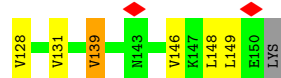
- Molecule 48: 50S ribosomal protein L14

Chain j:  70% 28% .



- Molecule 49: 50S ribosomal protein L15

Chain k:  71% 26% ..



- Molecule 50: 50S ribosomal protein L16

Chain l:  67% 30% ..



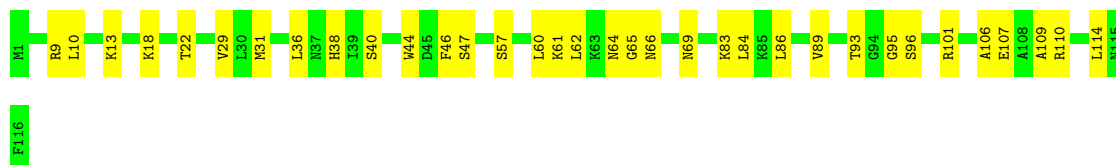
- Molecule 51: 50S ribosomal protein L17

Chain m:  73% 22% ..



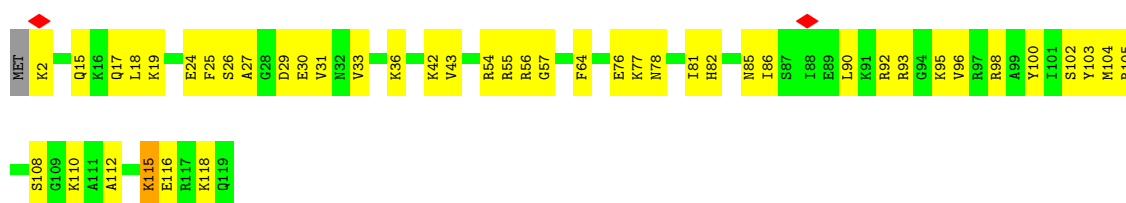
- Molecule 52: Large ribosomal subunit protein uL18

Chain n: 71% 29%



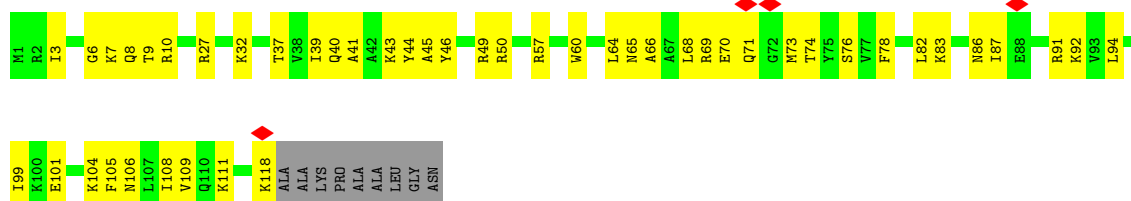
- Molecule 53: 50S ribosomal protein L19

Chain o: 61% 37% ..



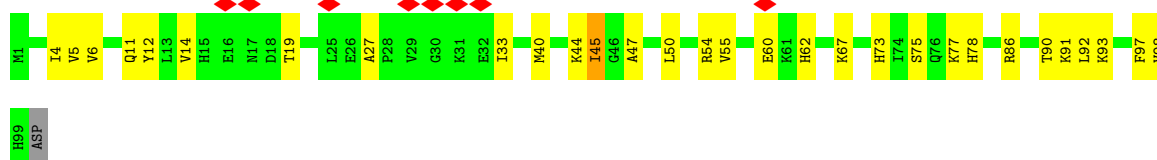
- Molecule 54: 50S ribosomal protein L20

Chain p: 56% 37% 7%



- Molecule 55: 50S ribosomal protein L21

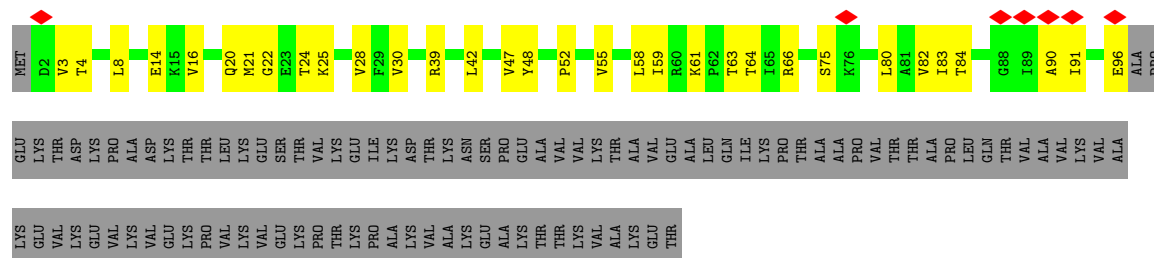
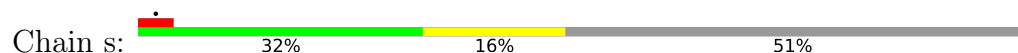
Chain q: 8% 69% 29% ..



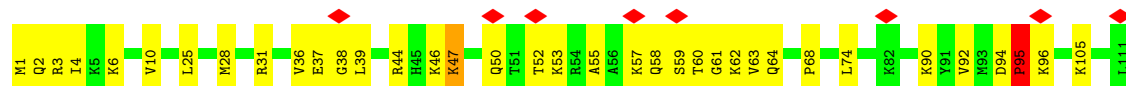
- Molecule 56: 50S ribosomal protein L22

Chain r: 68% 21% 11%

- Molecule 57: Large ribosomal subunit protein uL23



- Molecule 58: 50S ribosomal protein L24



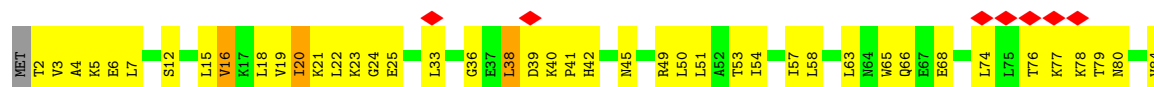
- Molecule 59: 50S ribosomal protein L27

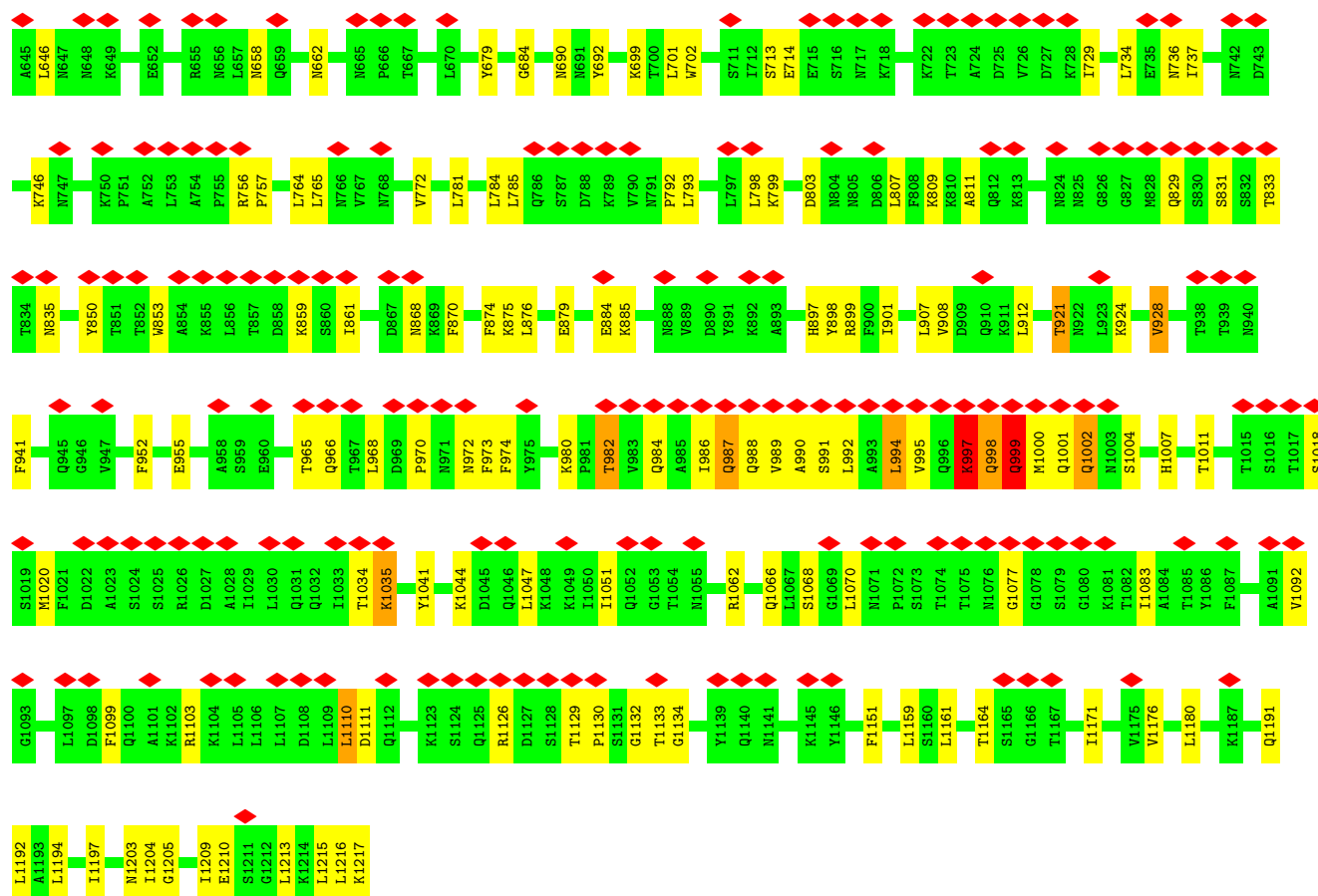


- Molecule 60: 50S ribosomal protein L28

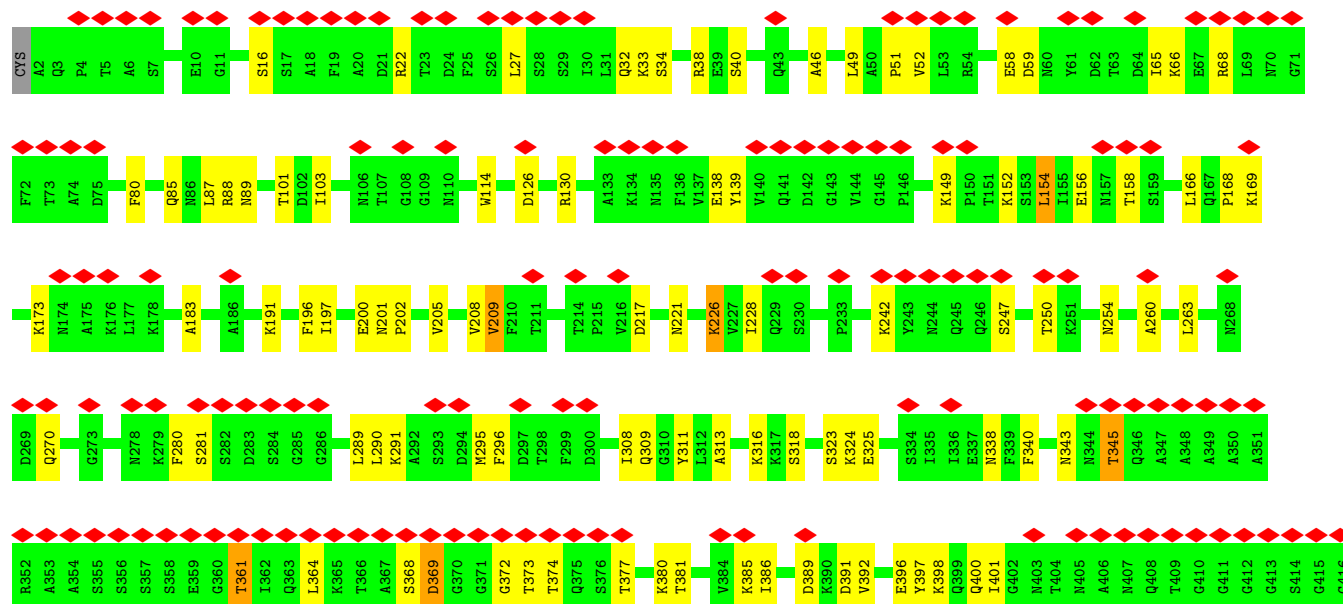
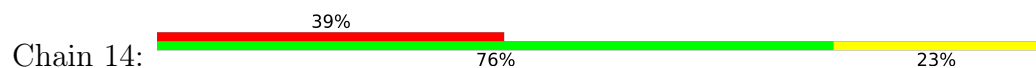


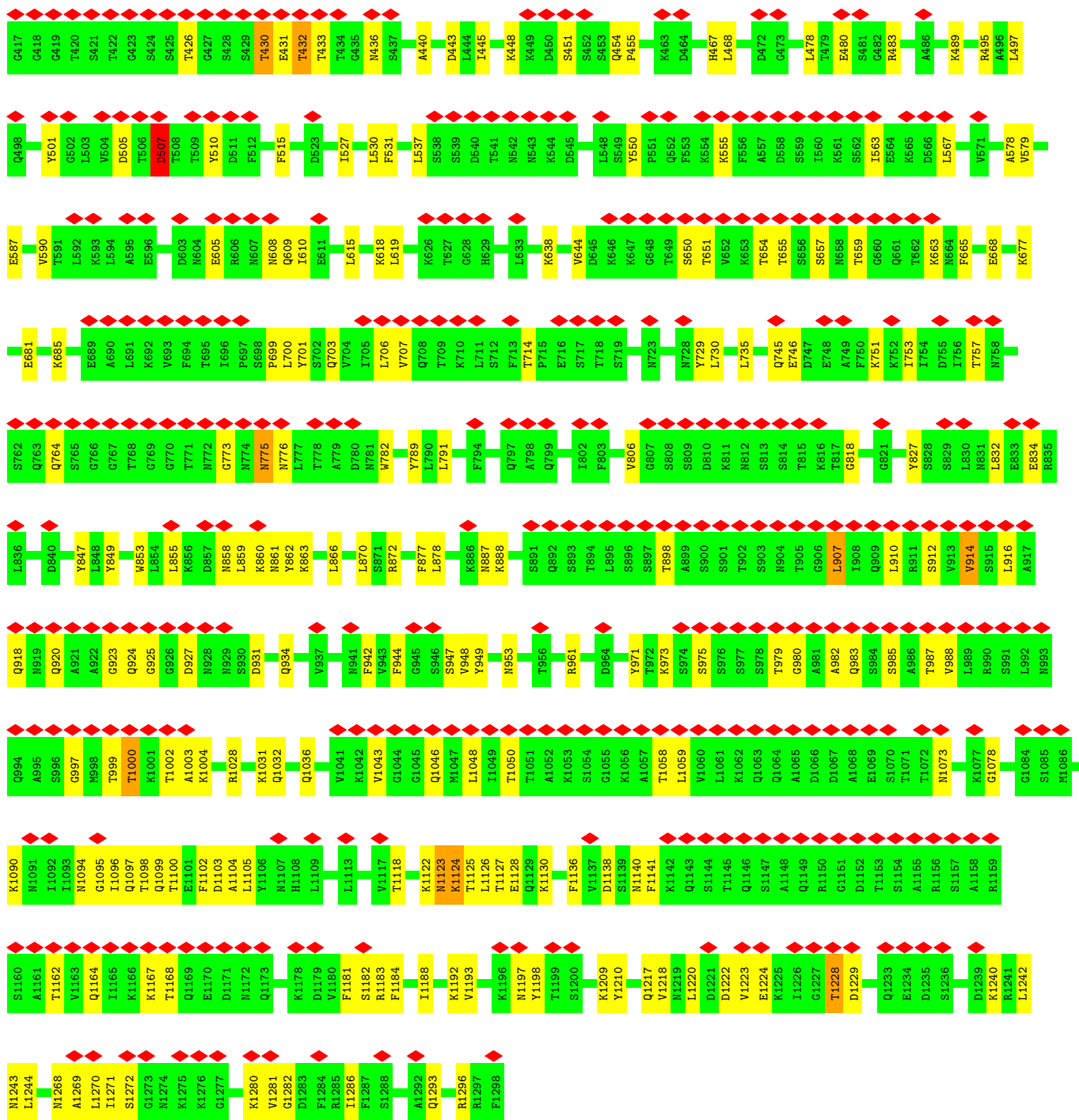
- Molecule 61: 50S ribosomal protein L29



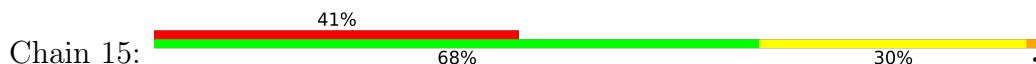


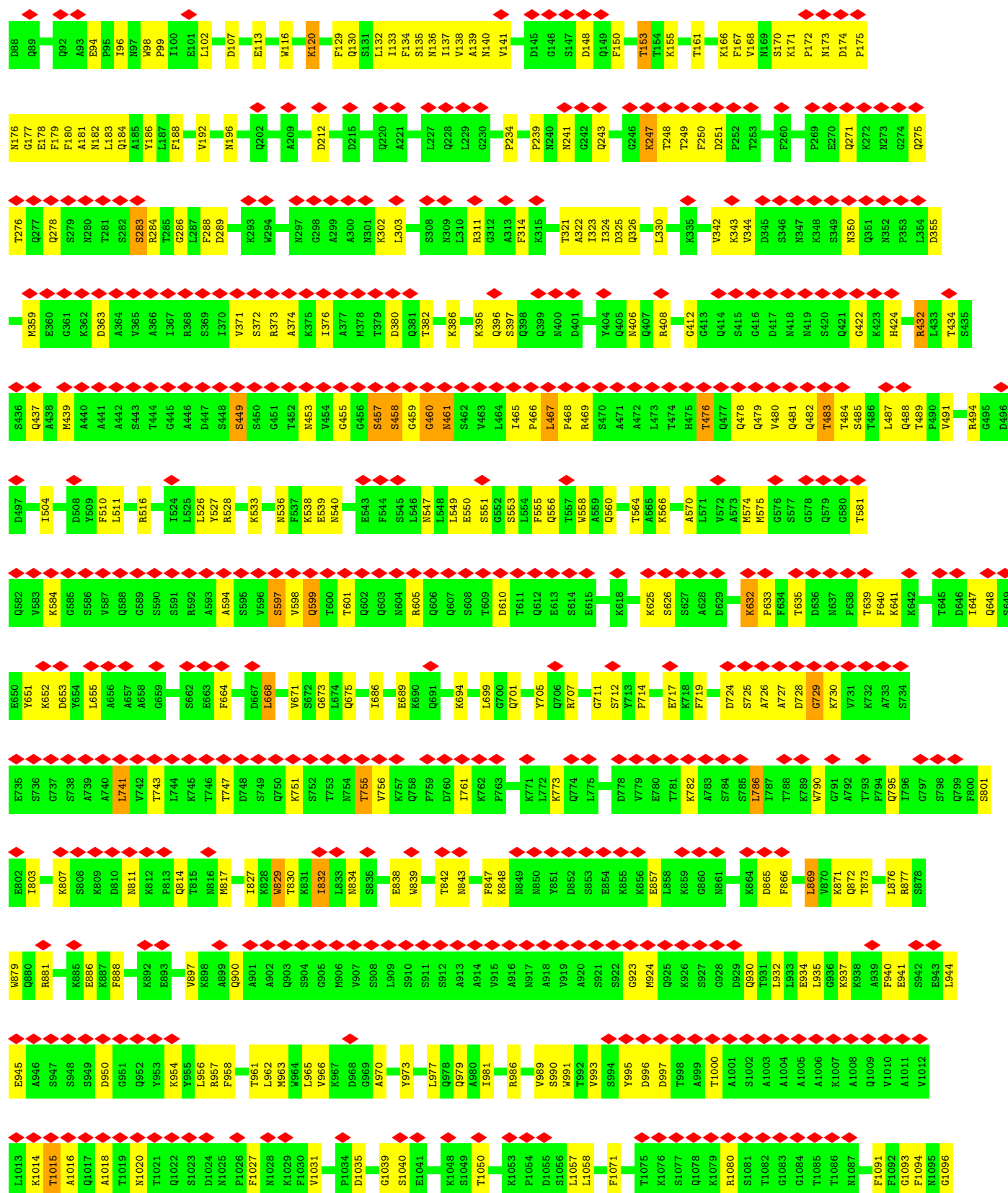
• Molecule 65: Uncharacterized lipoprotein MG309 homolog

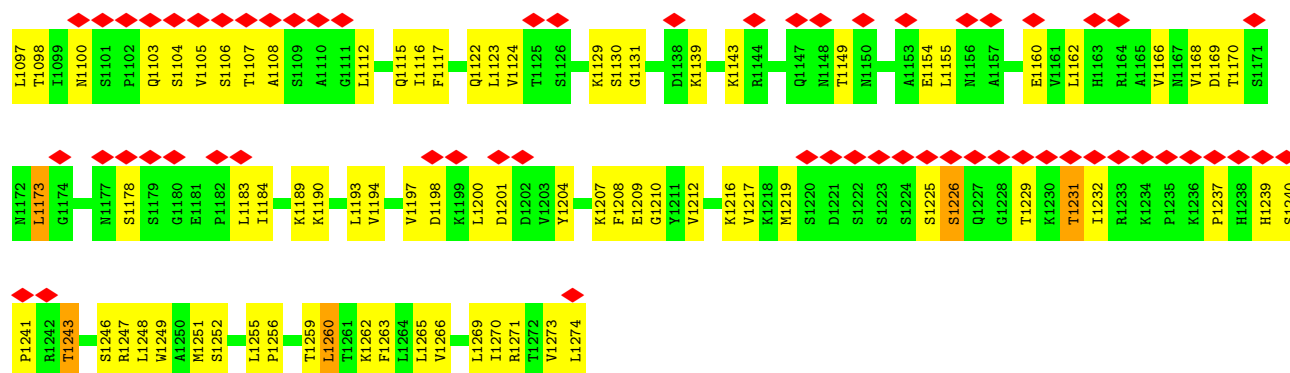




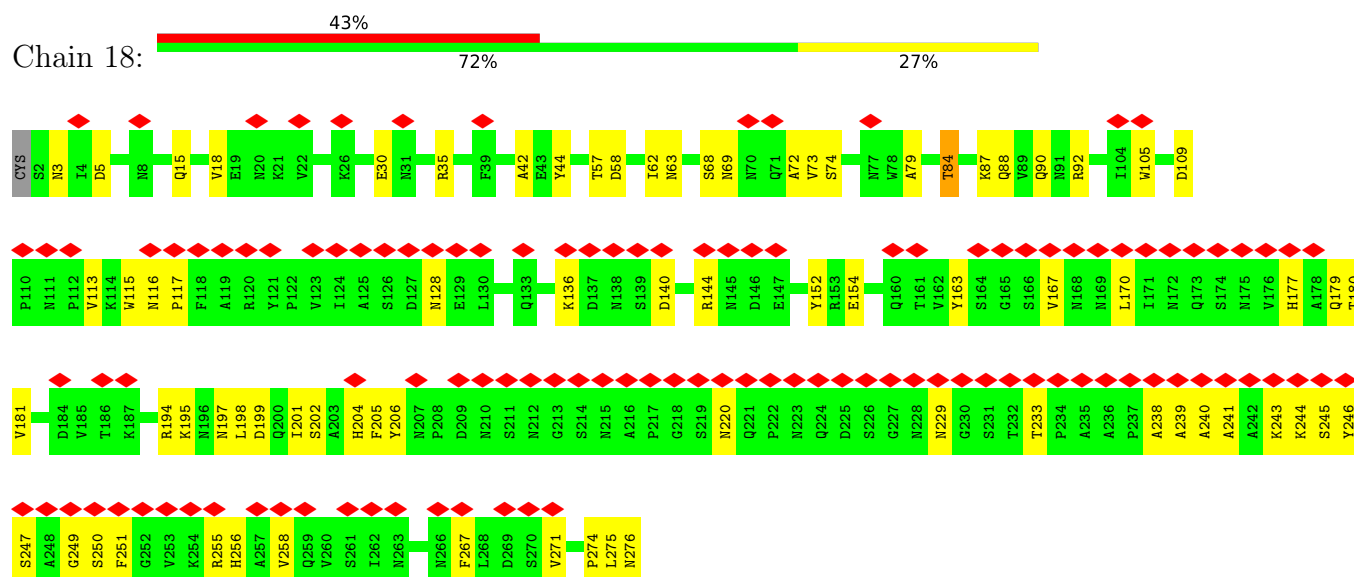
• Molecule 66: Uncharacterized lipoprotein MG338 homolog



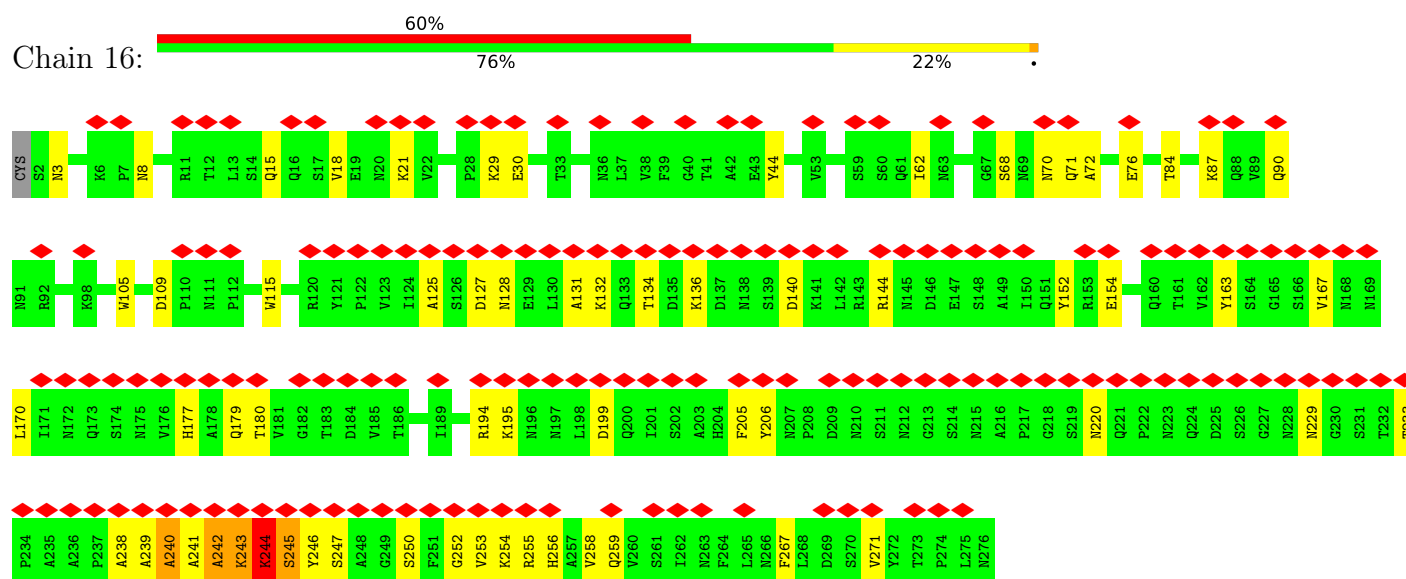




• Molecule 67: Uncharacterized lipoprotein MG348 homolog



• Molecule 67: Uncharacterized lipoprotein MG348 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	2304	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	130, 137	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.152	Depositor
Minimum map value	-1.126	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.137	Depositor
Recommended contour level	0.62	Depositor
Map size (Å)	742.4, 742.4, 742.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.9, 2.9, 2.9	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: T6A, K, PUT, PSU, 4SU, U8U, ZN, MA6, MIA, G7M, 3AU, MG, 5MU

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	0.12	0/383	0.25	0/504
2	1	0.12	0/484	0.31	0/637
3	10	2.25	120/3556 (3.4%)	2.54	249/4839 (5.1%)
4	11	2.30	24/592 (4.1%)	2.66	48/795 (6.0%)
5	12	2.17	24/864 (2.8%)	2.53	74/1154 (6.4%)
6	17	0.75	0/7779	1.29	16/10551 (0.2%)
7	2	0.13	0/306	0.36	0/401
8	3	0.12	0/69441	0.26	0/108286
9	4	0.15	0/2578	0.28	0/4016
10	5	0.10	0/36037	0.21	0/56183
11	6	0.07	0/46	0.14	0/69
12	7	0.19	0/1650	0.33	0/2565
13	8	0.58	9/1665 (0.5%)	0.33	0/2588
14	9	2.57	261/6575 (4.0%)	2.50	469/8870 (5.3%)
15	A	0.15	0/2172	0.42	0/2934
16	AA	0.13	0/1206	0.37	0/1616
17	AB	0.15	0/490	0.37	0/759
18	AC	0.14	0/347	0.54	0/457
18	x	0.15	0/375	0.38	0/502
19	C	0.15	0/1700	0.46	1/2278 (0.0%)
20	E	0.37	2/1536 (0.1%)	0.93	5/2072 (0.2%)
21	F	0.14	0/1274	0.40	0/1710
22	G	0.13	0/1126	0.37	0/1517
23	H	0.17	0/1058	0.49	0/1413
24	I	0.14	0/843	0.37	0/1132
25	J	0.13	0/844	0.36	0/1136
26	K	0.12	0/1089	0.40	0/1461
27	L	0.14	0/986	0.39	0/1321
28	M	0.11	0/483	0.29	0/643
29	N	0.14	0/695	0.41	0/926
30	O	0.22	0/718	0.62	1/962 (0.1%)
31	P	0.13	0/702	0.37	0/934

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Q	0.15	0/601	0.37	0/801
33	R	0.19	0/716	0.55	1/958 (0.1%)
34	S	0.14	0/645	0.38	0/857
35	T	0.14	0/524	0.37	0/685
36	W	0.16	0/1791	0.45	0/2421
37	Y	0.09	0/140	0.24	0/215
38	Z	0.09	0/26	0.33	0/33
39	a	0.54	1/2267 (0.0%)	0.48	2/3044 (0.1%)
40	b	0.29	1/1811 (0.1%)	0.40	0/2432
41	c	0.17	0/1681	0.42	0/2257
42	d	0.28	0/1437	0.56	0/1931
43	e	0.43	2/1420 (0.1%)	0.90	5/1912 (0.3%)
44	f	0.26	0/1231	0.55	0/1650
45	g	0.22	0/960	0.42	0/1284
46	h	0.30	0/968	0.51	0/1298
47	i	0.16	0/1186	0.36	0/1592
48	j	0.32	0/953	0.48	0/1275
49	k	0.16	0/1187	0.99	3/1581 (0.2%)
50	l	0.22	0/1104	0.45	0/1481
51	m	0.15	0/973	0.34	0/1309
52	n	0.15	0/927	0.38	0/1239
53	o	0.19	0/976	0.44	0/1296
54	p	0.20	0/996	0.42	0/1325
55	q	0.15	0/828	0.41	0/1111
56	r	0.15	0/1100	0.42	2/1471 (0.1%)
57	s	0.27	0/752	0.51	0/1015
58	t	0.53	2/878 (0.2%)	0.84	5/1165 (0.4%)
59	u	0.26	0/678	0.50	0/902
60	v	0.13	0/526	0.33	0/703
61	w	0.16	0/916	0.39	0/1222
62	y	0.13	0/457	0.37	0/601
63	z	0.13	0/412	0.36	0/547
64	13	0.85	4/9772 (0.0%)	1.05	3/13211 (0.0%)
65	14	0.88	9/10260 (0.1%)	1.06	4/13850 (0.0%)
66	15	0.91	9/10076 (0.1%)	1.10	9/13621 (0.1%)
67	16	0.90	3/2184 (0.1%)	1.08	1/2975 (0.0%)
67	18	0.78	0/2184	1.04	0/2975
All	All	0.70	471/215143 (0.2%)	0.79	898/313476 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	10	0	10
5	12	0	1
6	17	0	10
14	9	0	16
64	13	0	6
65	14	0	1
66	15	0	16
67	16	0	1
All	All	0	61

The worst 5 of 471 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	9	13	ARG	CZ-NH2	65.18	2.18	1.33
14	9	376	PHE	CG-CD2	31.25	2.04	1.38
14	9	376	PHE	CG-CD1	30.33	2.02	1.38
39	a	132	PRO	N-CD	24.41	1.81	1.47
14	9	376	PHE	CD2-CE2	23.05	2.07	1.38

The worst 5 of 898 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	k	37	LYS	N-CA-C	29.97	149.63	112.47
14	9	13	ARG	NE-CZ-NH1	-27.67	93.83	121.50
43	e	30	PRO	CB-CG-CD	23.05	179.86	106.10
20	E	128	PRO	CA-CB-CG	-20.56	65.43	104.50
20	E	128	PRO	N-CD-CG	-20.32	72.71	103.20

There are no chirality outliers.

5 of 61 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	10	129	ARG	Sidechain
3	10	166	PHE	Sidechain
3	10	217	TYR	Sidechain
3	10	26	ARG	Sidechain
3	10	43	ARG	Sidechain

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	0	380	0	429	7	0
2	1	477	0	530	11	0
3	10	3487	0	3650	95	0
4	11	585	0	646	0	0
5	12	848	0	924	113	0
6	17	7613	0	7589	1236	0
7	2	304	0	348	4	0
8	3	61992	0	31109	993	0
9	4	2305	0	1164	35	0
10	5	32256	0	16213	423	0
11	6	42	0	23	0	0
12	7	1638	0	841	57	0
13	8	1635	0	833	61	0
14	9	6467	0	6514	897	0
15	A	2138	0	2204	78	0
16	AA	1191	0	1284	37	0
17	AB	440	0	220	111	0
18	AC	342	0	354	12	0
18	x	366	0	356	18	0
19	C	1669	0	1729	65	0
20	E	1509	0	1520	52	0
21	F	1254	0	1320	32	0
22	G	1110	0	1226	32	0
23	H	1041	0	1101	48	0
24	I	832	0	918	29	0
25	J	829	0	855	18	0
26	K	1071	0	1165	53	0
27	L	975	0	1041	52	0
28	M	474	0	505	11	0
29	N	689	0	746	11	0
30	O	705	0	755	29	0
31	P	693	0	753	16	0
32	Q	590	0	625	30	0
33	R	700	0	708	23	0
34	S	643	0	694	18	0
35	T	519	0	578	13	0
36	W	1764	0	1833	55	0
37	Y	126	0	56	146	0
38	Z	187	0	65	14	0
39	a	2225	0	2301	58	0
40	b	1778	0	1821	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	c	1654	0	1744	55	0
42	d	1416	0	1500	92	0
43	e	1396	0	1481	38	0
44	f	1208	0	1254	56	0
45	g	951	0	1001	41	0
46	h	959	0	1039	56	0
47	i	1164	0	1192	29	0
48	j	944	0	1019	25	0
49	k	1170	0	1274	34	0
50	l	1079	0	1134	34	0
51	m	958	0	1011	20	0
52	n	918	0	979	28	0
53	o	966	0	1041	38	0
54	p	981	0	1062	47	0
55	q	811	0	858	19	0
56	r	1091	0	1178	27	0
57	s	740	0	819	41	0
58	t	871	0	964	103	0
59	u	670	0	704	15	0
60	v	520	0	565	16	0
61	w	906	0	976	164	0
62	y	452	0	467	27	0
63	z	408	0	436	12	0
64	13	9604	0	9522	377	0
65	14	10101	0	9885	511	0
66	15	9894	0	9743	814	0
67	16	2141	0	2059	113	0
67	18	2141	0	2060	182	0
68	2	1	0	0	0	0
68	M	1	0	0	0	0
68	Q	1	0	0	0	0
68	x	2	0	0	0	0
68	y	1	0	0	0	0
68	z	1	0	0	0	0
69	3	213	0	0	0	0
69	4	1	0	0	0	0
69	5	88	0	0	0	0
69	6	1	0	0	0	0
69	7	3	0	0	0	0
69	8	1	0	0	0	0
69	AB	2	0	0	0	0
69	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	P	1	0	0	0	0
69	Y	1	0	0	0	0
69	b	2	0	0	0	0
69	i	1	0	0	0	0
69	y	2	0	0	0	0
70	3	36	0	72	2	0
70	5	30	0	60	0	0
70	b	6	0	12	0	0
71	3	1	0	0	0	0
72	3	16	0	0	0	0
72	5	1	0	0	0	0
72	A	1	0	0	0	0
72	i	1	0	0	0	0
All	All	202419	0	154657	5578	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 16.

The worst 5 of 5578 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)
3:10:253:PHE:CE2	6:17:15:ILE:HD13	1.28	1.65
64:13:1192:LEU:CD2	67:18:88:GLN:HG2	1.19	1.63
14:9:795:GLN:CG	61:w:18:LEU:HD21	1.18	1.62
14:9:165:LEU:CD2	58:t:62:LYS:CE	1.75	1.62
14:9:165:LEU:HD23	58:t:62:LYS:CE	1.28	1.61

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	45/48 (94%)	45 (100%)	0	0	100	100
2	1	57/59 (97%)	57 (100%)	0	0	100	100
3	10	452/477 (95%)	444 (98%)	6 (1%)	2 (0%)	30	67
4	11	74/76 (97%)	70 (95%)	2 (3%)	2 (3%)	4	25
5	12	102/125 (82%)	98 (96%)	4 (4%)	0	100	100
6	17	962/971 (99%)	902 (94%)	44 (5%)	16 (2%)	7	36
7	2	35/37 (95%)	35 (100%)	0	0	100	100
14	9	806/808 (100%)	769 (95%)	32 (4%)	5 (1%)	21	59
15	A	262/294 (89%)	236 (90%)	24 (9%)	2 (1%)	16	54
16	AA	153/219 (70%)	145 (95%)	7 (5%)	1 (1%)	18	56
18	AC	41/97 (42%)	27 (66%)	14 (34%)	0	100	100
18	x	44/97 (45%)	36 (82%)	7 (16%)	1 (2%)	5	28
19	C	202/205 (98%)	169 (84%)	32 (16%)	1 (0%)	24	63
20	E	182/215 (85%)	157 (86%)	22 (12%)	3 (2%)	7	38
21	F	153/155 (99%)	140 (92%)	13 (8%)	0	100	100
22	G	139/142 (98%)	131 (94%)	8 (6%)	0	100	100
23	H	127/132 (96%)	114 (90%)	12 (9%)	1 (1%)	16	54
24	I	102/108 (94%)	88 (86%)	13 (13%)	1 (1%)	12	49
25	J	112/121 (93%)	105 (94%)	7 (6%)	0	100	100
26	K	133/139 (96%)	120 (90%)	12 (9%)	1 (1%)	16	54
27	L	119/124 (96%)	110 (92%)	8 (7%)	1 (1%)	16	54
28	M	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
29	N	83/86 (96%)	79 (95%)	4 (5%)	0	100	100
30	O	85/94 (90%)	78 (92%)	5 (6%)	2 (2%)	4	27
31	P	83/85 (98%)	71 (86%)	11 (13%)	1 (1%)	10	44
32	Q	69/104 (66%)	65 (94%)	4 (6%)	0	100	100
33	R	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
34	S	77/87 (88%)	74 (96%)	2 (3%)	1 (1%)	9	42
35	T	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
36	W	222/273 (81%)	197 (89%)	22 (10%)	3 (1%)	9	40
38	Z	3/36 (8%)	3 (100%)	0	0	100	100
39	a	283/287 (99%)	268 (95%)	14 (5%)	1 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	b	227/287 (79%)	219 (96%)	8 (4%)	0	100	100
41	c	209/212 (99%)	198 (95%)	11 (5%)	0	100	100
42	d	177/180 (98%)	169 (96%)	8 (4%)	0	100	100
43	e	174/184 (95%)	161 (92%)	13 (8%)	0	100	100
44	f	147/149 (99%)	131 (89%)	15 (10%)	1 (1%)	18	56
45	g	123/161 (76%)	115 (94%)	8 (6%)	0	100	100
46	h	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
47	i	142/146 (97%)	133 (94%)	9 (6%)	0	100	100
48	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
49	k	148/151 (98%)	138 (93%)	10 (7%)	0	100	100
50	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
51	m	117/124 (94%)	112 (96%)	5 (4%)	0	100	100
52	n	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
53	o	116/119 (98%)	107 (92%)	9 (8%)	0	100	100
54	p	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
55	q	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
56	r	140/159 (88%)	136 (97%)	4 (3%)	0	100	100
57	s	93/194 (48%)	89 (96%)	4 (4%)	0	100	100
58	t	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
59	u	86/104 (83%)	82 (95%)	4 (5%)	0	100	100
60	v	62/65 (95%)	62 (100%)	0	0	100	100
61	w	108/111 (97%)	102 (94%)	6 (6%)	0	100	100
62	y	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
63	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
64	13	1214/1217 (100%)	1119 (92%)	62 (5%)	33 (3%)	4	25
65	14	1295/1298 (100%)	1184 (91%)	75 (6%)	36 (3%)	4	24
66	15	1271/1274 (100%)	1147 (90%)	83 (6%)	41 (3%)	3	21
67	16	273/276 (99%)	241 (88%)	22 (8%)	10 (4%)	2	20
67	18	273/276 (99%)	243 (89%)	20 (7%)	10 (4%)	2	20
All	All	12719/13558 (94%)	11795 (93%)	748 (6%)	176 (1%)	11	40

5 of 176 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	17	398	LEU
6	17	715	ASN
6	17	950	LYS
14	9	742	GLN
16	AA	216	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	40/41 (98%)	40 (100%)	0	100	100
2	1	51/51 (100%)	51 (100%)	0	100	100
3	10	386/406 (95%)	375 (97%)	11 (3%)	38	60
4	11	65/65 (100%)	65 (100%)	0	100	100
5	12	94/113 (83%)	94 (100%)	0	100	100
6	17	828/834 (99%)	801 (97%)	27 (3%)	33	55
7	2	35/35 (100%)	35 (100%)	0	100	100
14	9	699/699 (100%)	678 (97%)	21 (3%)	36	57
15	A	238/262 (91%)	235 (99%)	3 (1%)	61	74
16	AA	125/178 (70%)	123 (98%)	2 (2%)	55	70
18	AC	35/86 (41%)	35 (100%)	0	100	100
18	x	44/86 (51%)	43 (98%)	1 (2%)	44	64
19	C	182/183 (100%)	180 (99%)	2 (1%)	65	76
20	E	165/196 (84%)	165 (100%)	0	100	100
21	F	132/132 (100%)	132 (100%)	0	100	100
22	G	123/124 (99%)	121 (98%)	2 (2%)	55	70
23	H	112/115 (97%)	112 (100%)	0	100	100
24	I	97/99 (98%)	97 (100%)	0	100	100
25	J	91/97 (94%)	91 (100%)	0	100	100
26	K	117/120 (98%)	113 (97%)	4 (3%)	32	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	L	102/105 (97%)	102 (100%)	0	100	100
28	M	47/48 (98%)	47 (100%)	0	100	100
29	N	77/78 (99%)	76 (99%)	1 (1%)	61	74
30	O	76/82 (93%)	76 (100%)	0	100	100
31	P	75/75 (100%)	75 (100%)	0	100	100
32	Q	62/94 (66%)	62 (100%)	0	100	100
33	R	76/77 (99%)	75 (99%)	1 (1%)	61	74
34	S	71/77 (92%)	69 (97%)	2 (3%)	38	60
35	T	55/56 (98%)	55 (100%)	0	100	100
36	W	187/232 (81%)	186 (100%)	1 (0%)	81	83
38	Z	2/2 (100%)	2 (100%)	0	100	100
39	a	241/243 (99%)	233 (97%)	8 (3%)	33	55
40	b	188/233 (81%)	183 (97%)	5 (3%)	39	61
41	c	183/184 (100%)	174 (95%)	9 (5%)	22	43
42	d	153/154 (99%)	148 (97%)	5 (3%)	33	55
43	e	153/159 (96%)	149 (97%)	4 (3%)	40	62
44	f	133/134 (99%)	127 (96%)	6 (4%)	24	46
45	g	100/129 (78%)	98 (98%)	2 (2%)	48	66
46	h	102/110 (93%)	97 (95%)	5 (5%)	22	43
47	i	126/128 (98%)	122 (97%)	4 (3%)	34	56
48	j	103/103 (100%)	100 (97%)	3 (3%)	37	58
49	k	125/126 (99%)	119 (95%)	6 (5%)	23	44
50	l	113/115 (98%)	111 (98%)	2 (2%)	51	68
51	m	105/109 (96%)	103 (98%)	2 (2%)	50	67
52	n	99/99 (100%)	95 (96%)	4 (4%)	28	49
53	o	104/105 (99%)	101 (97%)	3 (3%)	37	58
54	p	104/108 (96%)	102 (98%)	2 (2%)	50	67
55	q	90/91 (99%)	84 (93%)	6 (7%)	15	36
56	r	118/132 (89%)	116 (98%)	2 (2%)	53	69
57	s	84/169 (50%)	79 (94%)	5 (6%)	17	39
58	t	96/96 (100%)	92 (96%)	4 (4%)	26	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	u	70/85 (82%)	68 (97%)	2 (3%)	37	58
60	v	59/60 (98%)	56 (95%)	3 (5%)	21	42
61	w	97/98 (99%)	93 (96%)	4 (4%)	27	49
62	y	48/49 (98%)	47 (98%)	1 (2%)	47	65
63	z	47/50 (94%)	44 (94%)	3 (6%)	16	37
64	13	1068/1069 (100%)	1050 (98%)	18 (2%)	53	69
65	14	1128/1129 (100%)	1102 (98%)	26 (2%)	44	64
66	15	1085/1086 (100%)	1049 (97%)	36 (3%)	33	55
67	16	240/241 (100%)	236 (98%)	4 (2%)	53	69
67	18	240/241 (100%)	237 (99%)	3 (1%)	61	74
All	All	11091/11683 (95%)	10826 (98%)	265 (2%)	43	64

5 of 265 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
66	15	476	THR
66	15	639	THR
67	18	233	THR
41	c	183	LEU
41	c	79	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 181 such sidechains are listed below:

Mol	Chain	Res	Type
64	13	588	HIS
66	15	130	GLN
64	13	736	ASN
65	14	270	GLN
66	15	406	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	5	1506/1523 (98%)	255 (16%)	8 (0%)
11	6	1/1523 (0%)	0	0
12	7	75/76 (98%)	19 (25%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	8	75/76 (98%)	18 (24%)	1 (1%)
17	AB	20/21 (95%)	11 (55%)	3 (15%)
37	Y	5/21 (23%)	1 (20%)	0
8	3	2892/2907 (99%)	505 (17%)	13 (0%)
9	4	107/108 (99%)	29 (27%)	0
All	All	4681/6255 (74%)	838 (17%)	26 (0%)

5 of 838 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	3	11	U
8	3	12	A
8	3	13	C
8	3	14	U
8	3	28	G

5 of 26 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	5	571	A
10	5	1024	U
17	AB	51	C
10	5	995	U
10	5	1123	G

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

16 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	PSU	8	55	13	18,21,22	4.70	8 (44%)	22,30,33	1.80	5 (22%)
12	G7M	7	46	12	23,26,27	2.85	8 (34%)	35,39,42	1.93	8 (22%)
12	PSU	7	32	12	18,21,22	4.68	8 (44%)	22,30,33	1.80	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	3AU	8	47	13	24,28,29	2.88	8 (33%)	33,40,43	1.31	3 (9%)
12	3AU	7	47	12	24,28,29	2.86	7 (29%)	33,40,43	1.32	4 (12%)
13	PSU	8	39	13	18,21,22	4.70	8 (44%)	22,30,33	1.79	5 (22%)
12	PSU	7	55	12	18,21,22	4.68	8 (44%)	22,30,33	1.78	5 (22%)
13	5MU	8	54	13	19,22,23	1.46	6 (31%)	28,32,35	2.14	7 (25%)
12	MIA	7	37	12	28,31,32	2.42	5 (17%)	40,44,47	2.94	16 (40%)
10	MA6	5	1494	10	23,26,27	1.23	3 (13%)	34,38,41	2.89	14 (41%)
12	4SU	7	8	12	18,21,22	3.79	7 (38%)	26,30,33	2.23	5 (19%)
10	MA6	5	1493	10	23,26,27	1.25	4 (17%)	34,38,41	2.88	14 (41%)
12	PSU	7	39	12	18,21,22	4.67	8 (44%)	22,30,33	1.85	5 (22%)
13	U8U	8	34	37,13,17	19,24,25	3.27	7 (36%)	23,34,37	1.13	2 (8%)
10	G7M	5	525	10	23,26,27	3.63	12 (52%)	35,39,42	1.67	7 (20%)
13	T6A	8	37	13	31,34,35	2.00	7 (22%)	44,49,52	4.35	15 (34%)

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
13	PSU	8	55	13	-	0/7/25/26	0/2/2/2
12	G7M	7	46	12	-	4/7/25/26	0/3/3/3
12	PSU	7	32	12	-	0/7/25/26	0/2/2/2
13	3AU	8	47	13	-	2/16/34/35	0/2/2/2
12	3AU	7	47	12	-	4/16/34/35	0/2/2/2
13	PSU	8	39	13	-	0/7/25/26	0/2/2/2
12	PSU	7	55	12	-	0/7/25/26	0/2/2/2
13	5MU	8	54	13	-	2/7/25/26	0/2/2/2
12	MIA	7	37	12	-	4/15/33/34	0/3/3/3
10	MA6	5	1494	10	-	3/11/29/30	0/3/3/3
12	4SU	7	8	12	-	2/7/25/26	0/2/2/2
10	MA6	5	1493	10	-	0/11/29/30	0/3/3/3
12	PSU	7	39	12	-	0/7/25/26	0/2/2/2
13	U8U	8	34	37,13,17	-	1/9/28/29	0/2/2/2
10	G7M	5	525	10	-	2/7/25/26	0/3/3/3
13	T6A	8	37	13	-	4/23/41/42	0/3/3/3

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	8	55	PSU	C6-C5	12.38	1.49	1.35
13	8	39	PSU	C6-C5	12.28	1.49	1.35
12	7	32	PSU	C6-C5	12.24	1.49	1.35
12	7	55	PSU	C6-C5	12.23	1.49	1.35
12	7	39	PSU	C6-C5	12.17	1.49	1.35

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	8	37	T6A	C5-C6-N6	16.61	162.62	118.71
13	8	37	T6A	N6-C6-N1	-14.93	79.09	117.45
12	7	37	MIA	C11-S10-C2	11.16	110.60	102.27
13	8	37	T6A	N6-C10-N11	10.07	127.83	113.76
10	5	1493	MA6	N1-C6-N6	-8.83	107.43	117.08

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	5	525	G7M	O4'-C4'-C5'-O5'
10	5	525	G7M	C3'-C4'-C5'-O5'
10	5	1494	MA6	O4'-C4'-C5'-O5'
12	7	8	4SU	O4'-C4'-C5'-O5'
12	7	37	MIA	C5-C6-N6-C12

There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	8	55	PSU	2	0
13	8	47	3AU	1	0
13	8	54	5MU	2	0
12	7	37	MIA	6	0
12	7	8	4SU	1	0
10	5	1493	MA6	1	0
12	7	39	PSU	1	0
13	8	34	U8U	6	0
10	5	525	G7M	1	0
13	8	37	T6A	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 337 ligands modelled in this entry, 325 are monoatomic - leaving 12 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	$\# Z > 2$
70	PUT	3	3219	-	5,5,5	0.25	0	4,4,4	0.55	0
70	PUT	3	3180	-	5,5,5	0.25	0	4,4,4	0.55	0
70	PUT	3	3205	-	5,5,5	0.24	0	4,4,4	0.54	0
70	PUT	3	3210	-	5,5,5	0.24	0	4,4,4	0.53	0
70	PUT	5	1607	-	5,5,5	0.24	0	4,4,4	0.53	0
70	PUT	5	1631	-	5,5,5	0.25	0	4,4,4	0.54	0
70	PUT	3	3214	-	5,5,5	0.24	0	4,4,4	0.51	0
70	PUT	5	1602	-	5,5,5	0.25	0	4,4,4	0.52	0
70	PUT	3	3215	-	5,5,5	0.25	0	4,4,4	0.51	0
70	PUT	b	302	-	5,5,5	0.25	0	4,4,4	0.52	0
70	PUT	5	1605	-	5,5,5	0.25	0	4,4,4	0.54	0
70	PUT	5	1635	-	5,5,5	0.25	0	4,4,4	0.55	0

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
70	PUT	3	3219	-	-	0/3/3/3	-
70	PUT	3	3180	-	-	0/3/3/3	-
70	PUT	3	3205	-	-	0/3/3/3	-
70	PUT	3	3210	-	-	0/3/3/3	-
70	PUT	5	1607	-	-	0/3/3/3	-
70	PUT	5	1631	-	-	0/3/3/3	-
70	PUT	3	3214	-	-	0/3/3/3	-
70	PUT	5	1602	-	-	0/3/3/3	-

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Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PUT	3	3215	-	-	0/3/3/3	-
70	PUT	b	302	-	-	0/3/3/3	-
70	PUT	5	1605	-	-	0/3/3/3	-
70	PUT	5	1635	-	-	0/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	3	3214	PUT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	b	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	229:ALA	C	230:PRO	N	3.19

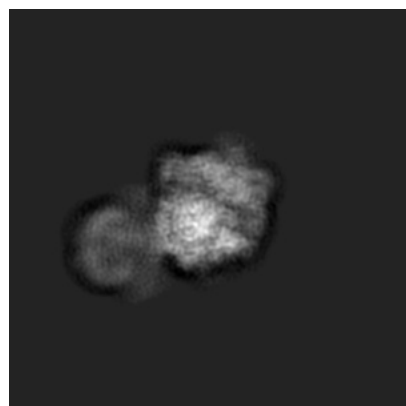
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55029. These allow visual inspection of the internal detail of the map and identification of artifacts.

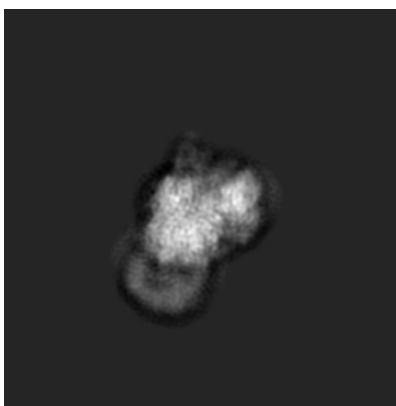
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

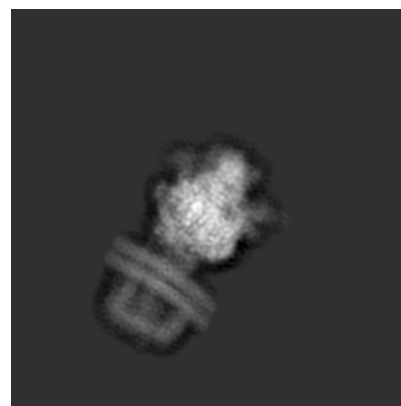
6.1.1 Primary map



X

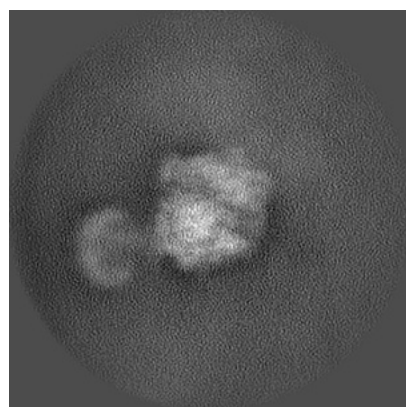


Y

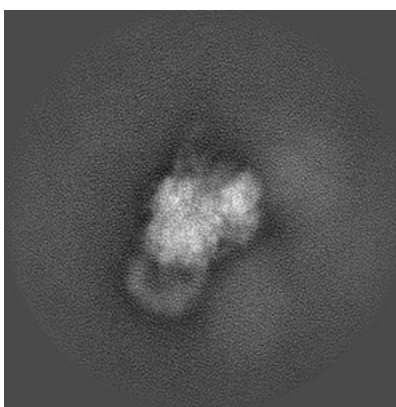


Z

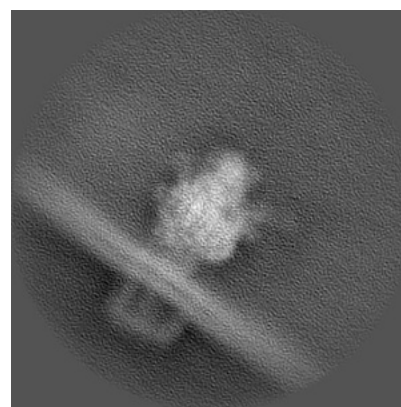
6.1.2 Raw map



X



Y

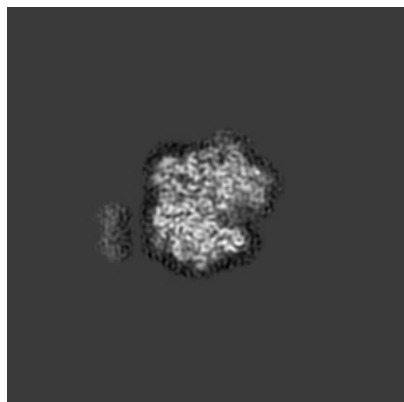


Z

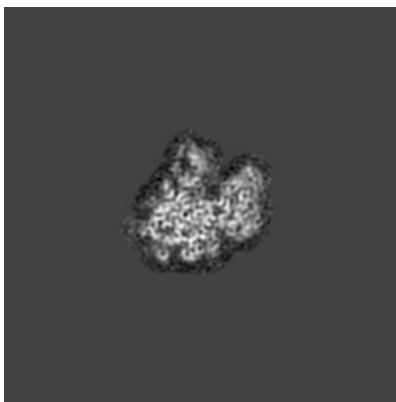
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

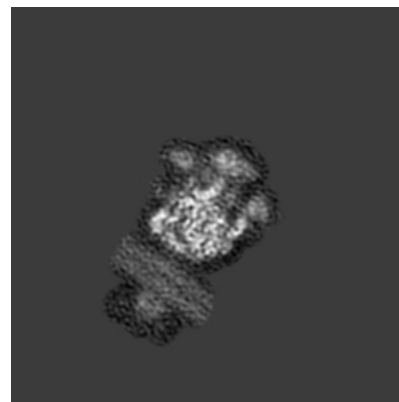
6.2.1 Primary map



X Index: 128

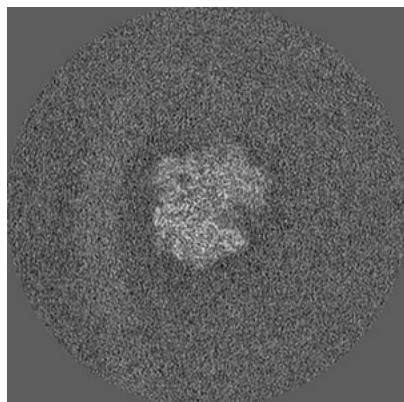


Y Index: 128

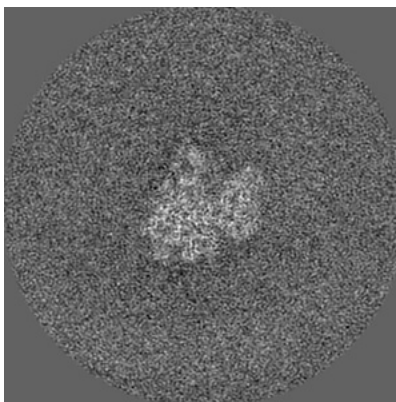


Z Index: 128

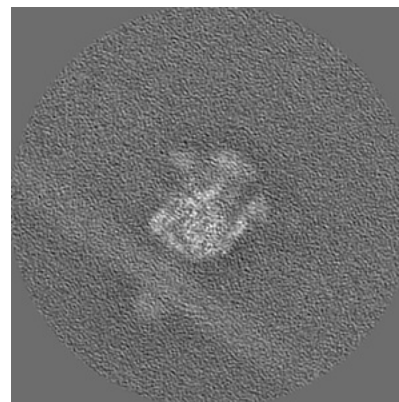
6.2.2 Raw map



X Index: 128



Y Index: 128

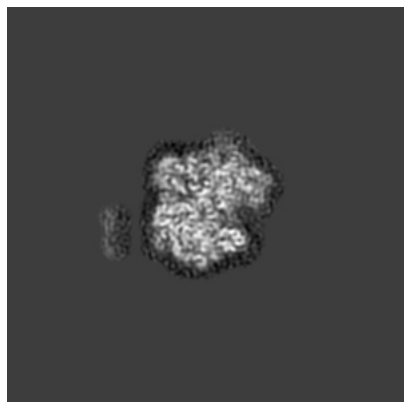


Z Index: 128

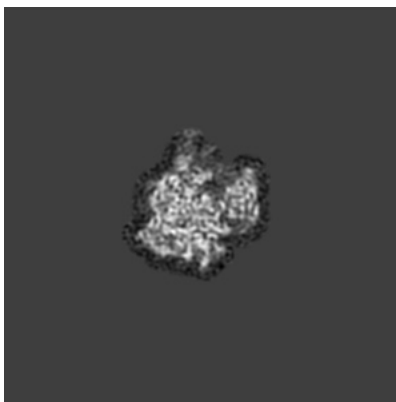
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

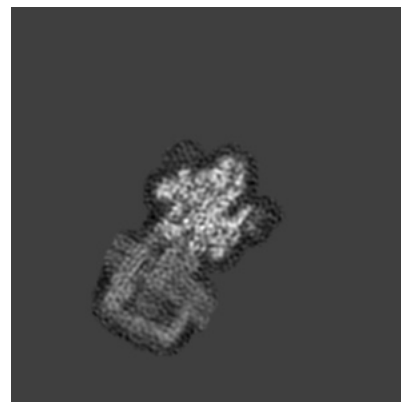
6.3.1 Primary map



X Index: 129

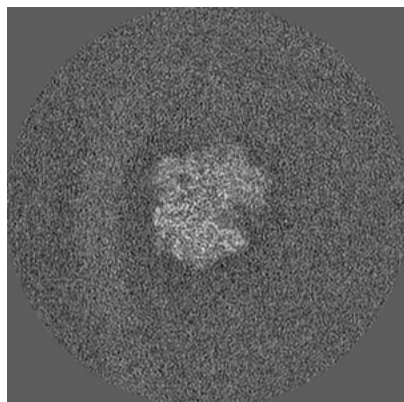


Y Index: 119

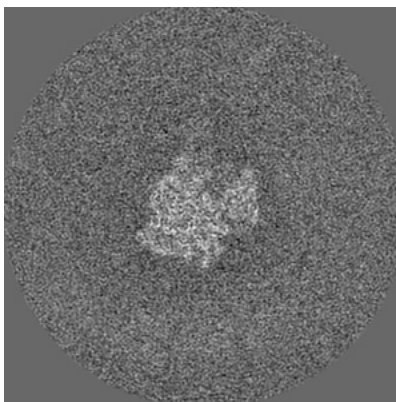


Z Index: 108

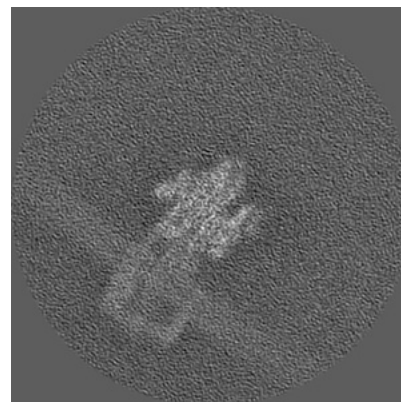
6.3.2 Raw map



X Index: 128



Y Index: 119

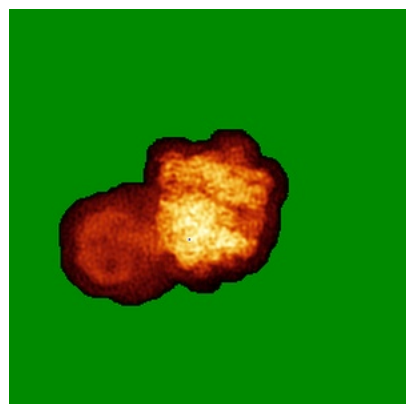


Z Index: 109

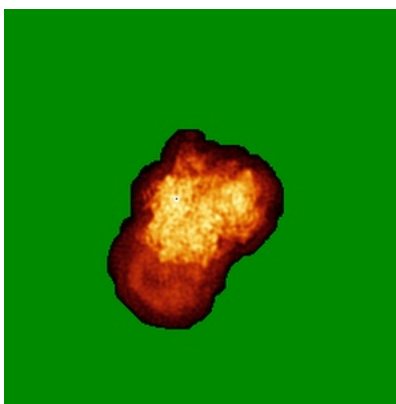
The images above show the largest variance slices of the map in three orthogonal directions.

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

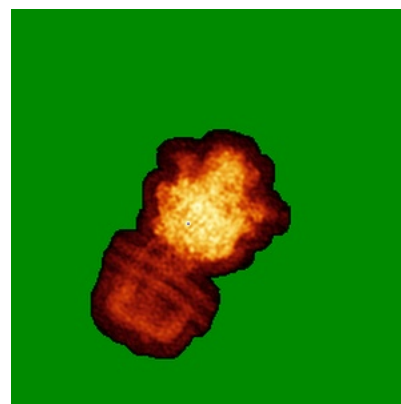
6.4.1 Primary map



X

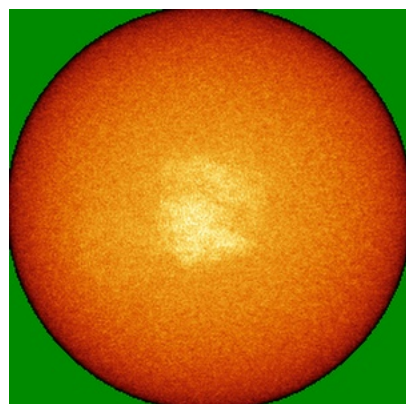


Y

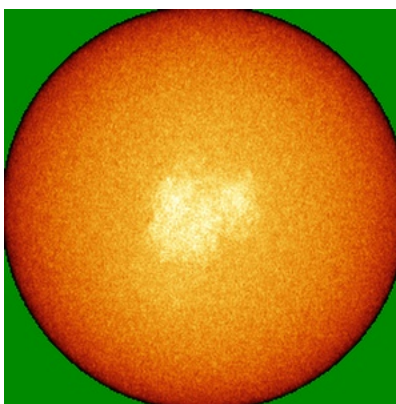


Z

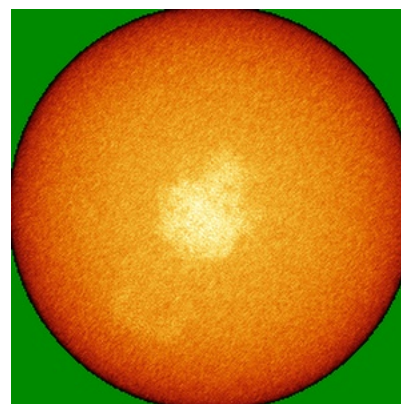
6.4.2 Raw map



X



Y

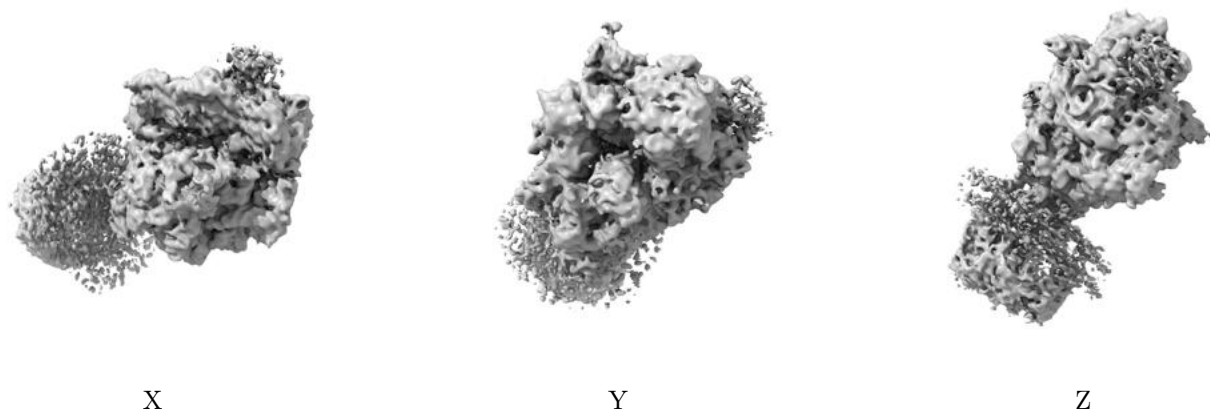


Z

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

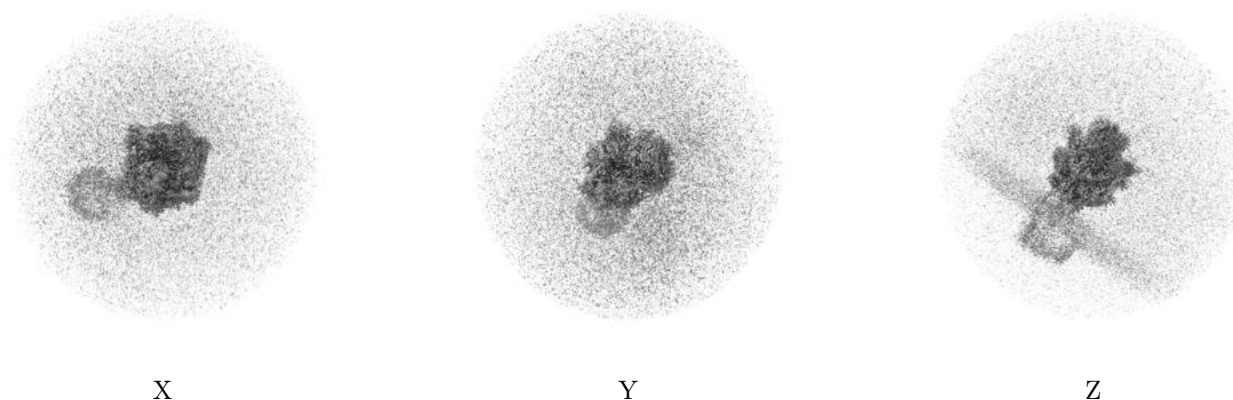
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.62. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

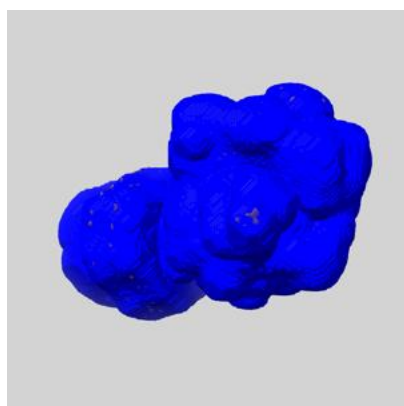
6.6 Mask visualisation [i](#)

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

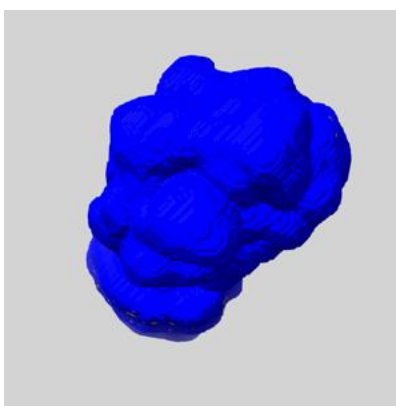
A mask typically either:

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

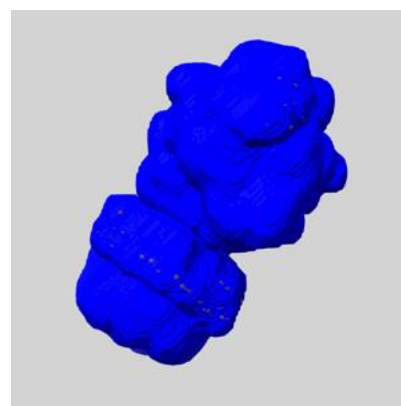
6.6.1 emd_55029_msk_1.map [i](#)



X



Y

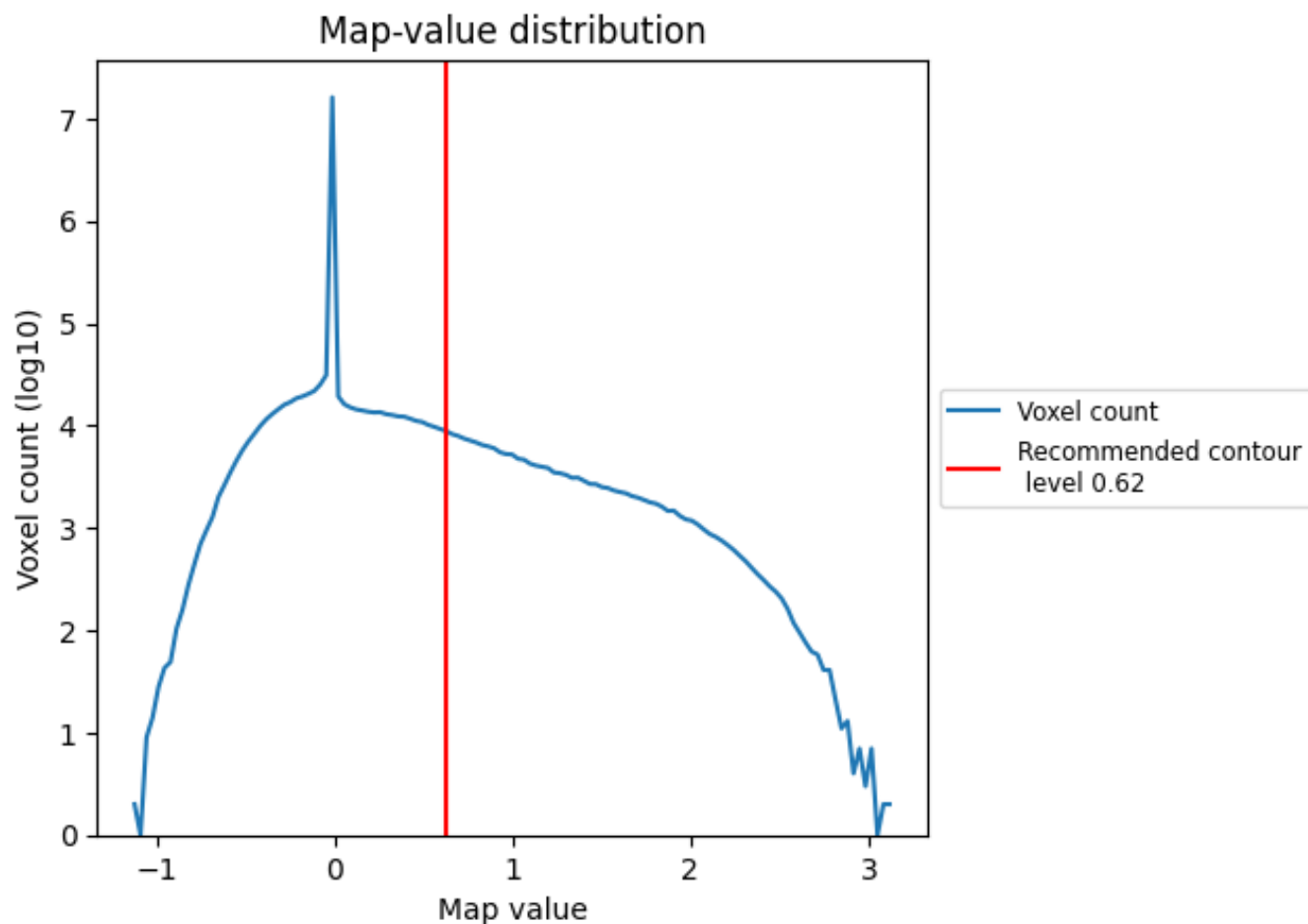


Z

7 Map analysis [i](#)

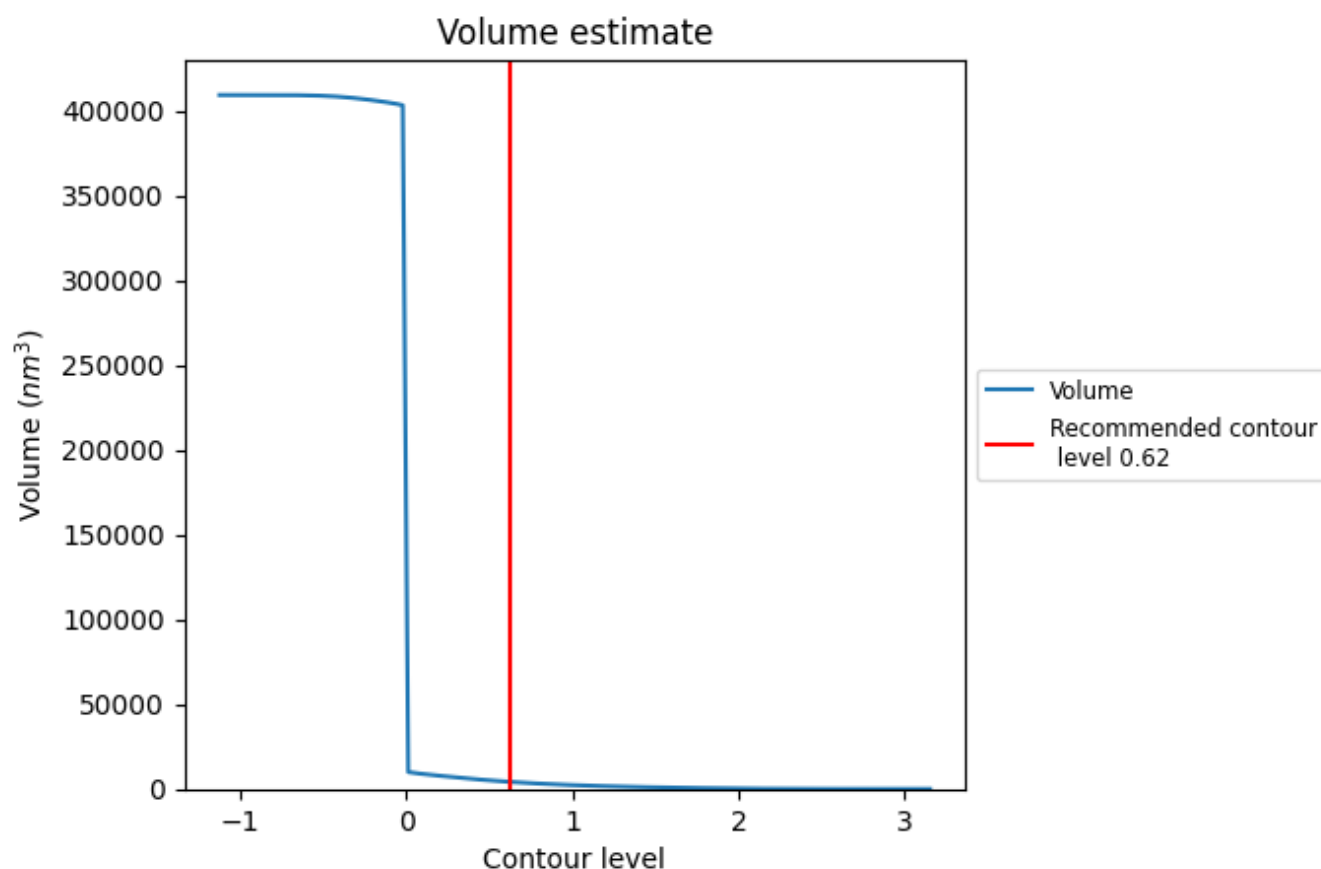
This section contains the results of statistical analysis of the map.

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.

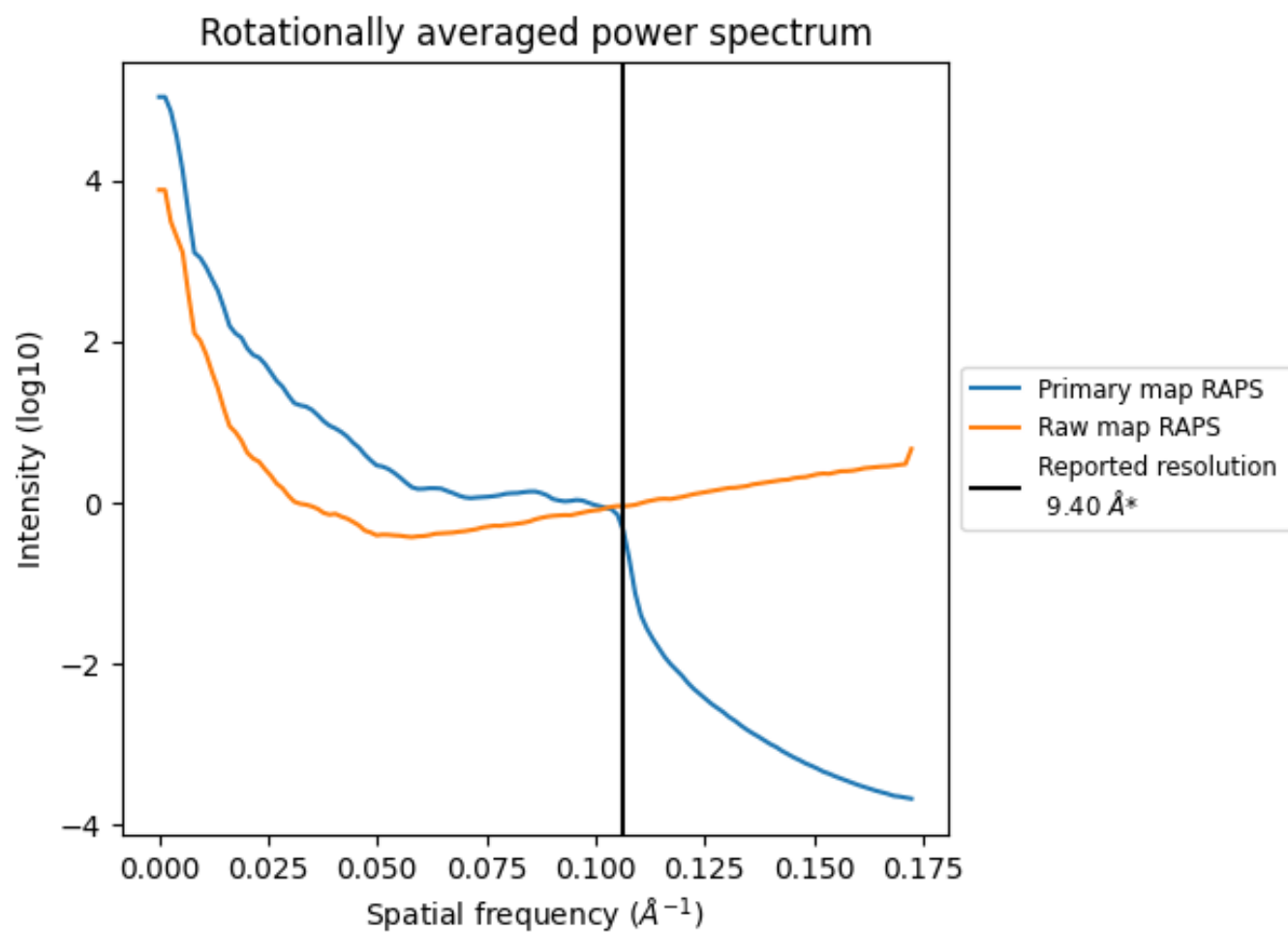
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4188 nm^3 ; this corresponds to an approximate mass of 3783 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 ⓘ

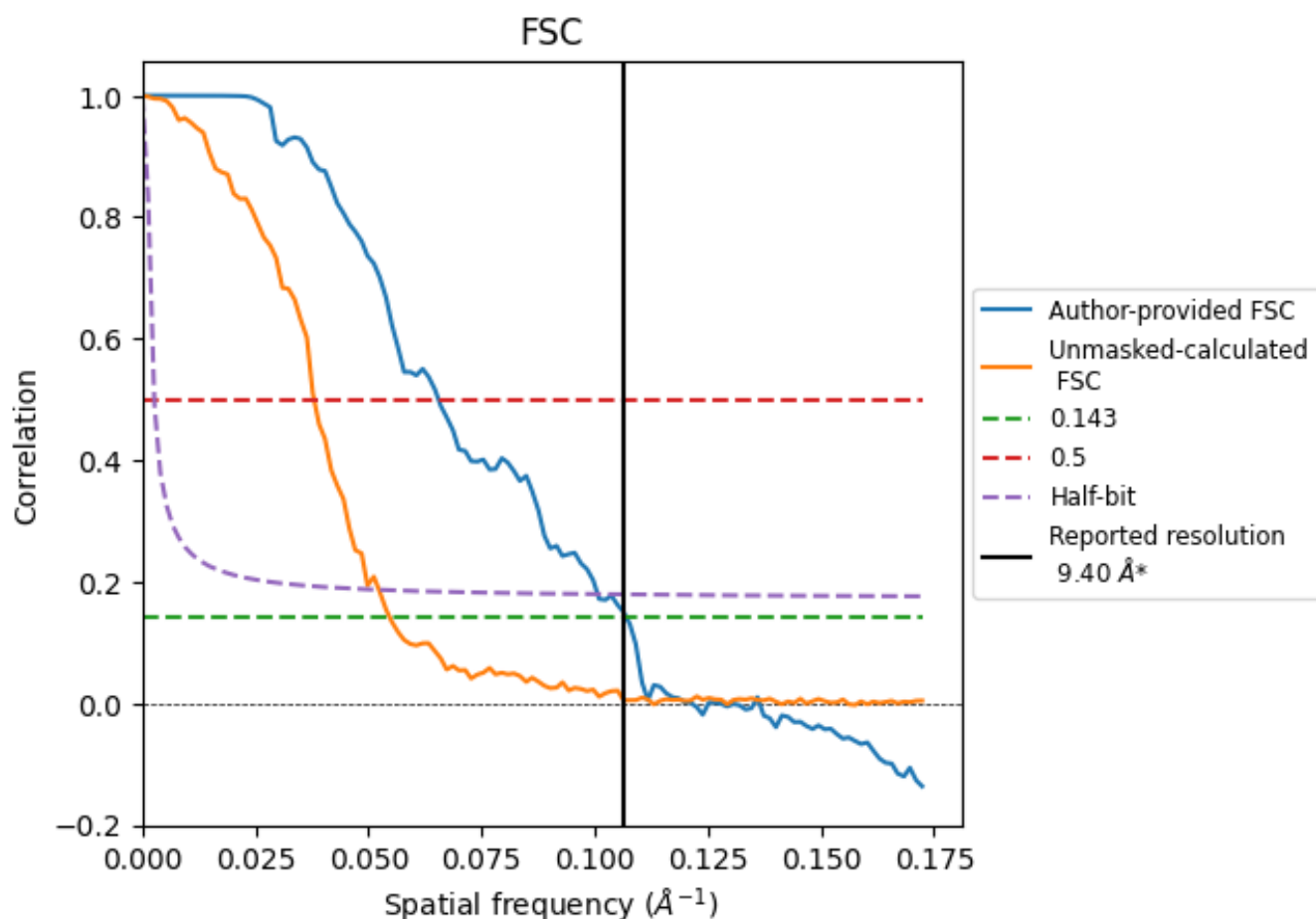


*Reported resolution corresponds to spatial frequency of 0.106 Å⁻¹

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 0.106 Å⁻¹

8.2 Resolution estimates [i](#)

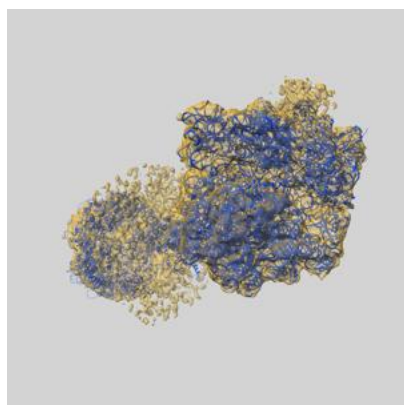
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.40	-	-
Author-provided FSC curve	9.35	15.27	9.93
Unmasked-calculated*	18.32	26.32	19.08

*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 18.32 differs from the reported value 9.4 by more than 10 %

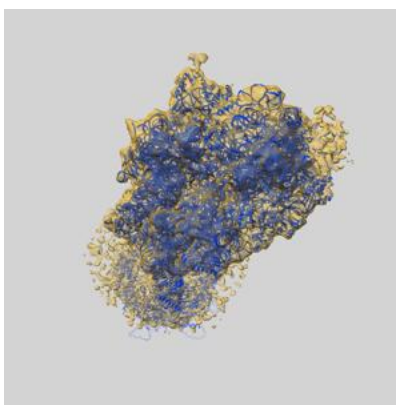
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55029 and PDB model 9SMD. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

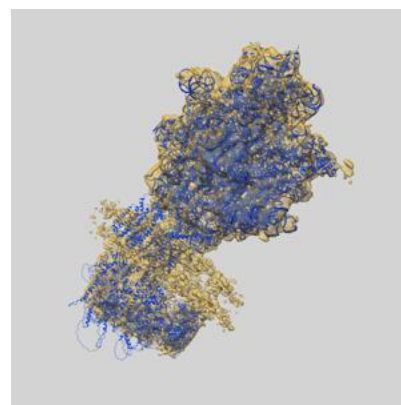
9.1 Map-model overlay [i](#)



X



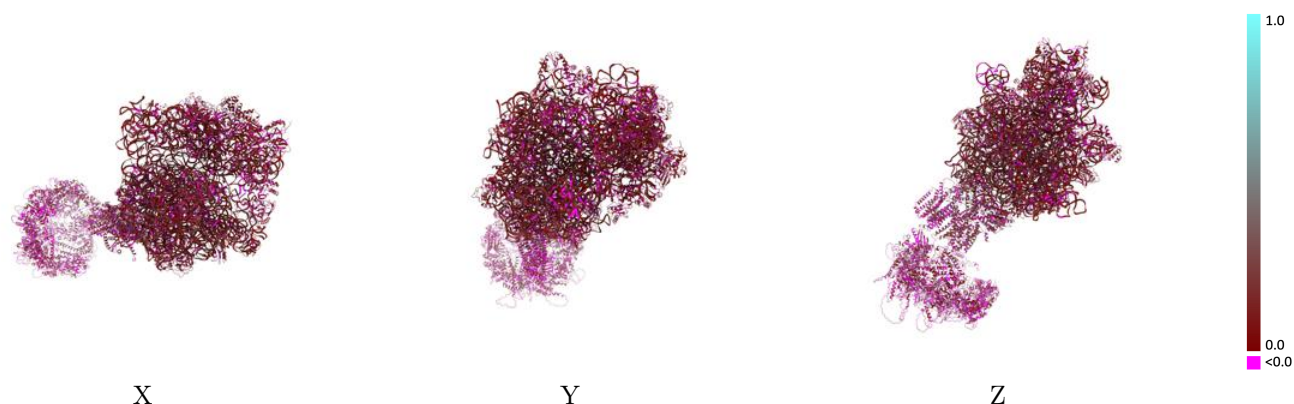
Y



Z

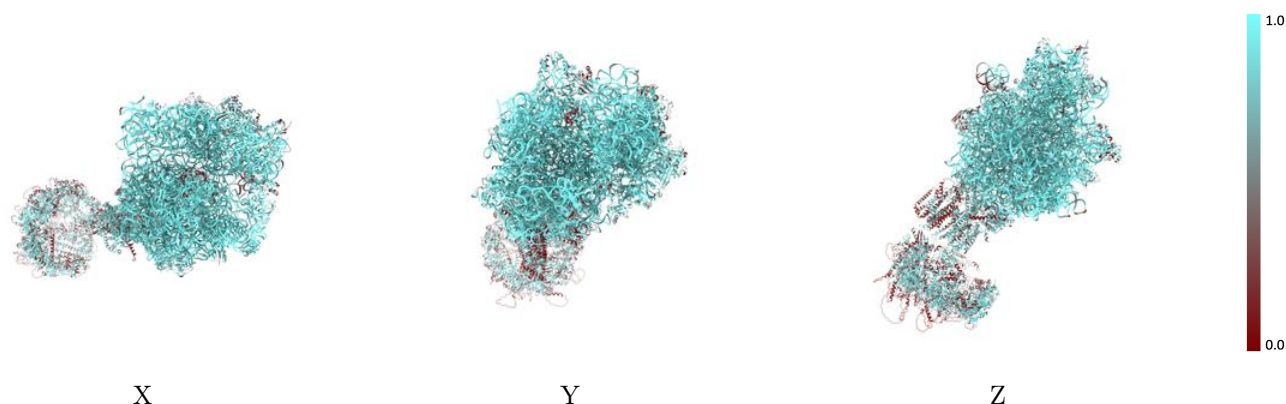
The images above show the 3D surface view of the map at the recommended contour level 0.62 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



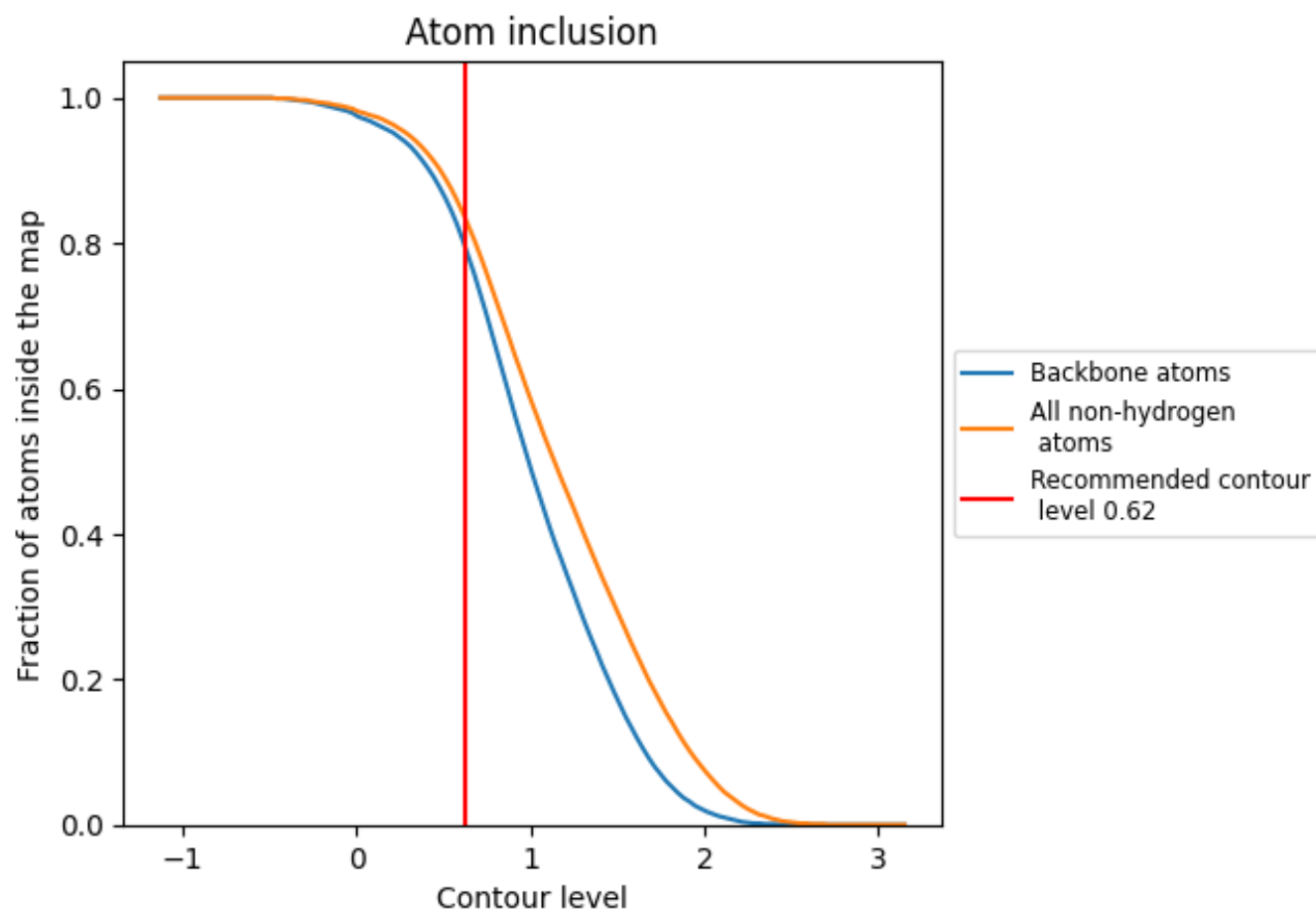
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.62).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 84% 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 (0.62) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.0990
0	 0.9640	 0.0770
1	 0.9510	 0.0760
10	 0.6260	 0.0850
11	 0.5660	 0.0800
12	 0.4200	 0.0840
13	 0.5870	 0.0280
14	 0.5730	 0.0480
15	 0.5590	 0.0390
16	 0.3780	 0.0120
17	 0.4410	 0.0140
18	 0.5300	 0.0090
2	 0.9560	 0.0490
3	 0.9820	 0.1380
4	 0.9940	 0.1530
5	 0.9750	 0.1220
6	 1.0000	 0.0500
7	 0.9720	 0.1250
8	 0.7490	 0.0980
9	 0.7650	 0.0930
A	 0.7710	 0.1100
AA	 0.8940	 0.0830
AB	 0.8850	 0.1010
AC	 0.6850	 0.1020
C	 0.8180	 0.0840
E	 0.6920	 0.1040
F	 0.9310	 0.0930
G	 0.8790	 0.1080
H	 0.8760	 0.0670
I	 0.7590	 0.0600
J	 0.7820	 0.0720
K	 0.9100	 0.0780
L	 0.7900	 0.0700
M	 0.9560	 0.0330
N	 0.8740	 0.0980



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Chain	Atom inclusion	Q-score
O	 0.8960	 0.0780
P	 0.7960	 0.0660
Q	 0.8560	 0.0870
R	 0.7540	 0.0410
S	 0.9330	 0.1120
T	 0.7920	 0.0980
W	 0.8410	 0.0800
Y	 1.0000	 0.1870
Z	 0.8340	 0.0360
a	 0.9440	 0.0720
b	 0.8980	 0.0790
c	 0.8780	 0.0950
d	 0.9260	 0.1110
e	 0.8190	 0.1150
f	 0.3830	 0.1020
g	 0.7490	 0.0950
h	 0.5990	 0.0740
i	 0.9080	 0.0910
j	 0.8710	 0.0820
k	 0.8880	 0.0820
l	 0.9350	 0.0920
m	 0.9290	 0.0940
n	 0.9180	 0.1000
o	 0.8950	 0.1030
p	 0.8960	 0.0920
q	 0.8220	 0.0990
r	 0.9340	 0.1100
s	 0.8530	 0.0880
t	 0.8380	 0.0820
u	 0.9170	 0.0540
v	 0.9140	 0.0930
w	 0.7930	 0.1300
x	 0.7850	 0.0980
y	 0.9410	 0.0650
z	 0.9500	 0.1040