



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 07:53 AM EST

PDB ID : 3J7Q
EMDB ID : EMD-2650
Title : Structure of the idle mammalian ribosome-Sec61 complex
Authors : Voorhees, R.M.; Fernandez, I.S.; Scheres, S.H.W.; Hegde, R.S.
Deposited on : 2014-08-01
Resolution : 3.50 Å(reported)
Based on initial models : 3J3B, 3J3F

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

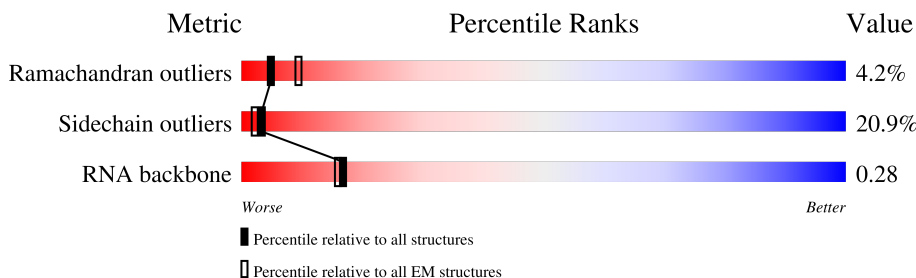
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.





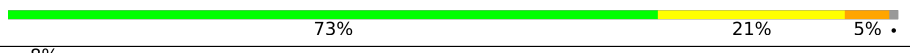
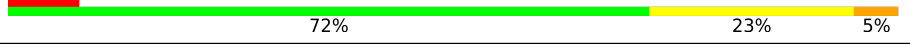



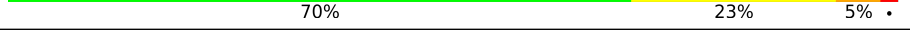
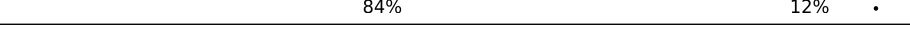
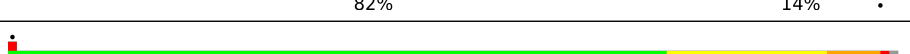
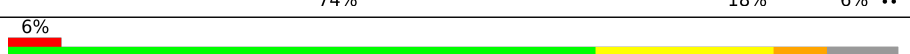

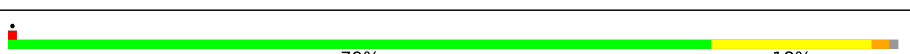
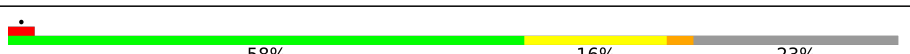
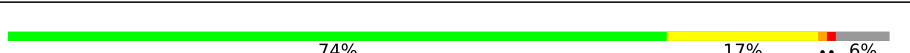




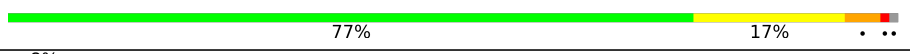





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	5	3722	
2	7	120	
3	8	156	
4	A	257	
5	B	394	
6	C	367	
7	D	297	
8	E	236	

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Mol	Chain	Length	Quality of chain
9	F	225	 72% 24%
10	G	266	 8% 69% 18% 9%
11	H	192	 73% 21% 5%
12	I	213	 8% 72% 23% 5%
13	J	178	 73% 20%
14	L	211	 7% 73% 19% 6%
15	M	213	 52% 11% 35%
16	N	204	 70% 23% 5%
17	O	201	 84% 12%
18	P	153	 82% 14%
19	Q	188	 74% 18% 6%
20	R	196	 6% 66% 20% 6% 8%
21	S	224	 57% 16% 5% 22%
22	T	160	 79% 18%
23	U	128	 58% 16% 23%
24	V	140	 74% 17% 6%
25	W	157	 31% 7% 60%
26	X	156	 62% 10% 24%
27	Y	145	 67% 19% 6% 8%
28	Z	136	 78% 18%
29	a	148	 77% 17%
30	b	160	 8% 33% 11% 53%
31	c	115	 63% 15% 18%
32	d	125	 5% 56% 22% 8% 14%
33	e	135	 68% 23% 5%

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Mol	Chain	Length	Quality of chain
34	f	110	 78% 15% 5% ..
35	g	117	 77% 19% . .
36	h	123	 80% 12% 6% ..
37	i	105	 76% 17% . .
38	j	86	 73% 21% 6%
39	k	70	 71% 27% .
40	l	51	 76% 20% ..
41	m	128	 31% 8% . 59%
42	n	25	 72% 20% 8%
43	o	106	 69% 23% 6% ..
44	p	91	 82% 15% .
45	r	125	 73% 23% ..
46	1	476	 65% 74% 8% 18%
47	2	68	 71% 82% 6% . 9%
48	3	36	 100% 100%

2 Entry composition i

There are 50 unique types of molecules in this entry. The entry contains 140540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	3662	78486	34947	14363	25515	3661	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	7	120	2558	1141	456	842	119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	8	156	3314	1480	585	1094	155	0	0

- Molecule 4 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	244	1868	1171	382	309	6	0	0

- Molecule 5 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	394	3147	2005	591	538	13	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ILE	VAL	conflict	UNP A0A480L253
B	86	VAL	ILE	conflict	UNP A0A480L253
B	140	ALA	GLU	conflict	UNP A0A480L253

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Chain	Residue	Modelled	Actual	Comment	Reference
B	141	ALA	ASP	conflict	UNP A0A480L253
B	143	ALA	LYS	conflict	UNP A0A480L253
B	144	ALA	LYS	conflict	UNP A0A480L253
B	145	ALA	GLN	conflict	UNP A0A480L253
B	147	ALA	GLU	conflict	UNP A0A480L253
B	148	ALA	ARG	conflict	UNP A0A480L253
B	155	ALA	LYS	conflict	UNP A0A480L253

- Molecule 6 is a protein called Ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	367	2919	1836	582	486	15	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	354	ALA	-	insertion	UNP A0A287AE76
C	355	ALA	-	insertion	UNP A0A287AE76
C	356	ALA	-	insertion	UNP A0A287AE76

- Molecule 7 is a protein called Ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	292	2380	1508	434	426	12	0	0

- Molecule 8 is a protein called Ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	236	1904	1219	364	316	5	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	62	MET	LYS	conflict	UNP Q2YGT9
E	64	MET	LEU	conflict	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	SER	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	VAL	deletion	UNP Q2YGT9
E	?	-	GLU	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	LYS	deletion	UNP Q2YGT9
E	?	-	VAL	deletion	UNP Q2YGT9
E	?	-	ARG	deletion	UNP Q2YGT9
E	176	VAL	SER	conflict	UNP Q2YGT9
E	206	LYS	GLU	conflict	UNP Q2YGT9

- Molecule 9 is a protein called Ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	225	1870	1202	358	301	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	31	LYS	ARG	conflict	UNP A0A480W0U3

- Molecule 10 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	241	1934	1232	372	326	4	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	53	ARG	CYS	conflict	UNP A0A4X1W808
G	172	ALA	SER	conflict	UNP A0A4X1W808
G	185	LYS	ASN	conflict	UNP A0A4X1W808
G	231	ASN	ASP	conflict	UNP A0A4X1W808

- Molecule 11 is a protein called Ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	H	190	1518	956	284	272	6	0	0

- Molecule 12 is a protein called Ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	213	1713	1083	331	284	15	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	49	GLY	CYS	conflict	UNP Q29195
I	82	ARG	LYS	conflict	UNP Q29195
I	87	MET	ILE	conflict	UNP Q29195
I	145	GLU	LYS	conflict	UNP Q29195
I	187	LYS	GLU	conflict	UNP Q29195
I	189	CYS	ARG	conflict	UNP Q29195
I	200	VAL	ILE	conflict	UNP Q29195
I	203	HIS	ARG	conflict	UNP Q29195
I	211	VAL	ALA	conflict	UNP Q29195

- Molecule 13 is a protein called Ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	170	1359	856	256	241	6	0	0

- Molecule 14 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	L	210	1703	1064	354	280	5	0	0

- Molecule 15 is a protein called Ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	M	138	1131	727	216	181	7	0	0

- Molecule 16 is a protein called Ribosomal protein eL15.

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

- Molecule 17 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	O	201	1651	1063	323	260	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	3	GLU	-	variant	UNP A0A481CAM4
O	4	GLY	-	variant	UNP A0A481CAM4

- Molecule 18 is a protein called Ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	P	153	1242	776	241	216	9	0	0

- Molecule 19 is a protein called Ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Q	187	1506	941	311	249	5	0	0

- Molecule 20 is a protein called Ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	R	180	1508	933	328	238	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	TYR	-	variant	UNP A0A480VXS3

- Molecule 21 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	S	175	1454	925	284	235	10	0	0

- Molecule 22 is a protein called Ribosomal protein eL21.

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

- Molecule 23 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	U	99	808	518	141	147	2	0	0

- Molecule 24 is a protein called Ribosomal protein uL14.

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

- Molecule 25 is a protein called Ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	W	63	528	337	103	85	3	0	0

- Molecule 26 is a protein called Ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	X	119	976	624	183	168	1	0	0

- Molecule 27 is a protein called Ribosomal protein uL24.

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

- Molecule 28 is a protein called Ribosomal protein eL27.

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

- Molecule 29 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	a	147	1163	735	239	185	4	0	0

- Molecule 30 is a protein called Ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	b	75	610	378	130	99	3	0	0

- Molecule 31 is a protein called Ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	c	94	732	465	130	131	6	0	0

- Molecule 32 is a protein called Ribosomal protein eL31.

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

- Molecule 33 is a protein called Ribosomal protein eL32.

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

- Molecule 34 is a protein called Ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	f	109	876	555	174	144	3	0	0

- Molecule 35 is a protein called Ribosomal protein eL34.

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

- Molecule 36 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	h	122	1015	642	205	167	1	0	0

- Molecule 37 is a protein called Ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	i	102	832	521	177	129	5	0	0

- Molecule 38 is a protein called Ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	j	86	706	436	155	110	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	82	ILE	THR	conflict	UNP A0A480UVT3

- Molecule 39 is a protein called Ribosomal protein eL38.

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

- Molecule 40 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	l	50	444	281	98	64	1	0	0

- Molecule 41 is a protein called Ribosomal protein eL40.

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

- Molecule 42 is a protein called Ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	23	Total	C	N	O	S	0	0
			222	134	61	25	2		

- Molecule 43 is a protein called Ribosomal protein eL42.

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

- Molecule 44 is a protein called Ribosomal protein eL43.

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

- Molecule 45 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	125	Total	C	N	O	S	0	0
			1001	622	206	168	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	64	ILE	MET	conflict	UNP A0A480YX24

- Molecule 46 is a protein called Sec61 alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1	392	Total	C	N	O	S	0	0
			3051	2007	493	532	19		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	343	HIS	TYR	conflict	UNP A0A480EHF8

- Molecule 47 is a protein called Sec61 gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	62	Total	C	N	O	S	0	0
			494	326	86	79	3		

- Molecule 48 is a protein called Sec61 beta subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	3	36	180	108	36	36	0	0

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	5	119	Total	Mg	0
			119	119	
49	7	5	Total	Mg	0
			5	5	
49	8	4	Total	Mg	0
			4	4	
49	P	1	Total	Mg	0
			1	1	
49	V	1	Total	Mg	0
			1	1	

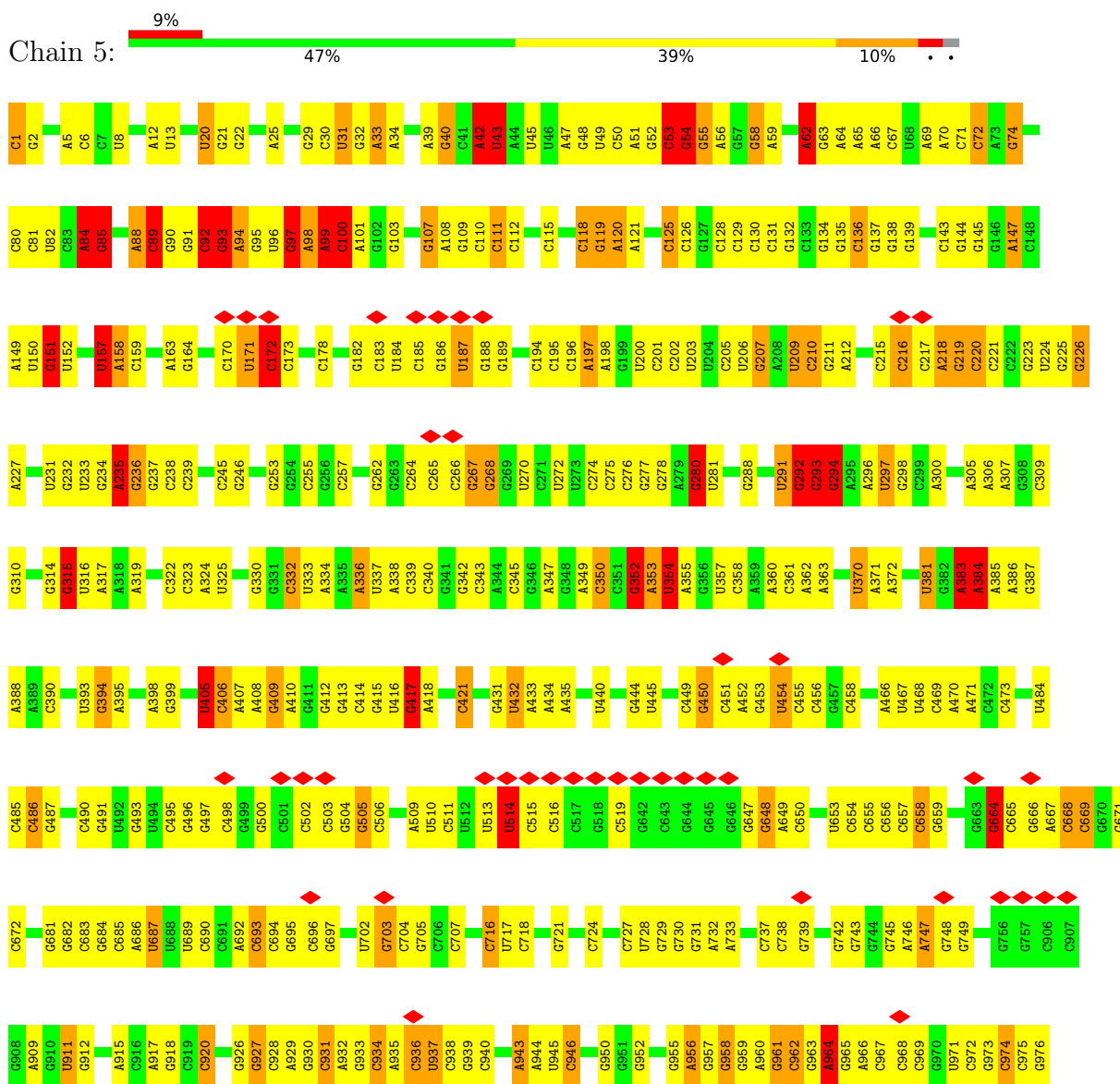
- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

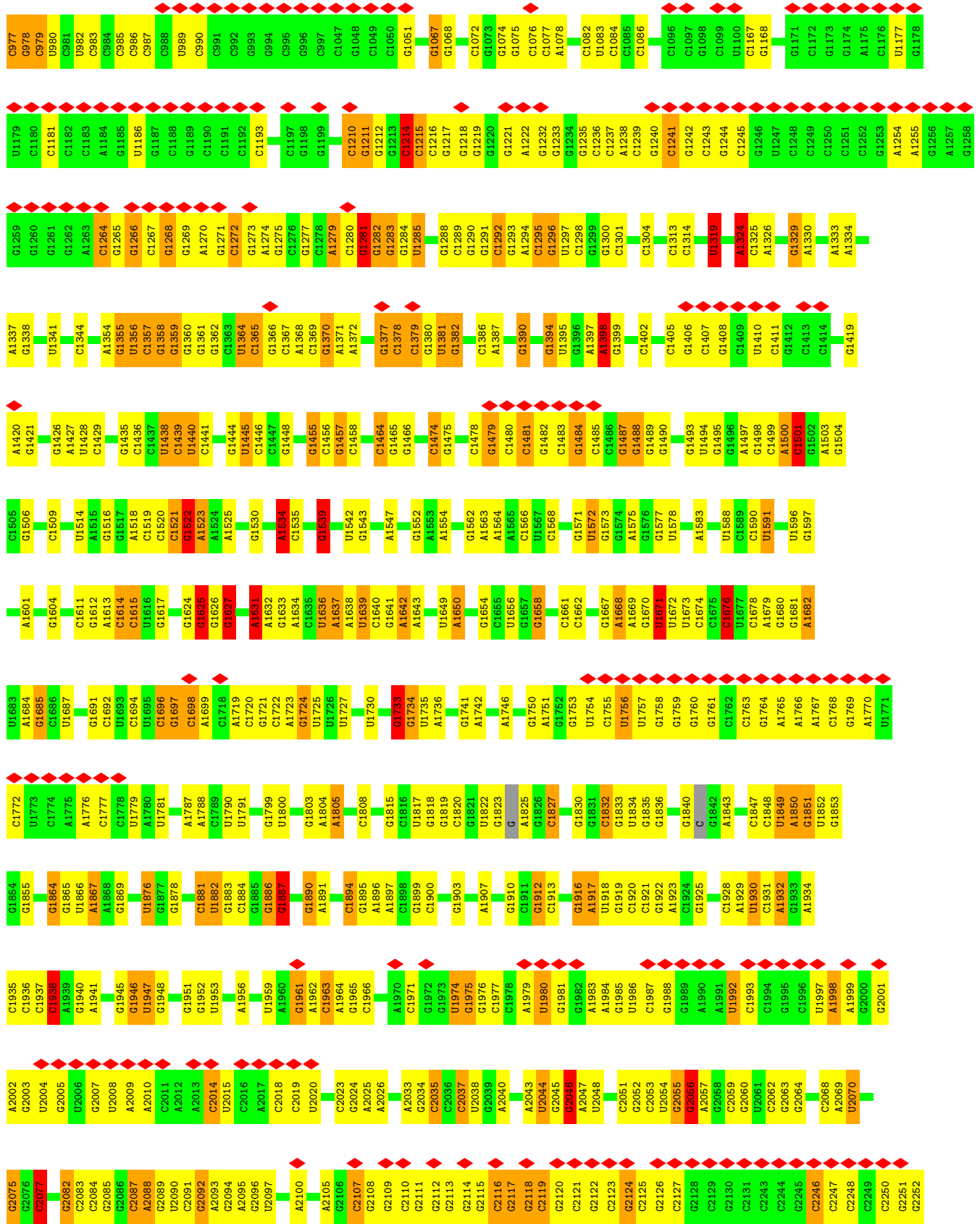
Mol	Chain	Residues	Atoms		AltConf
50	j	1	Total	Zn	0
			1	1	
50	m	1	Total	Zn	0
			1	1	
50	o	1	Total	Zn	0
			1	1	

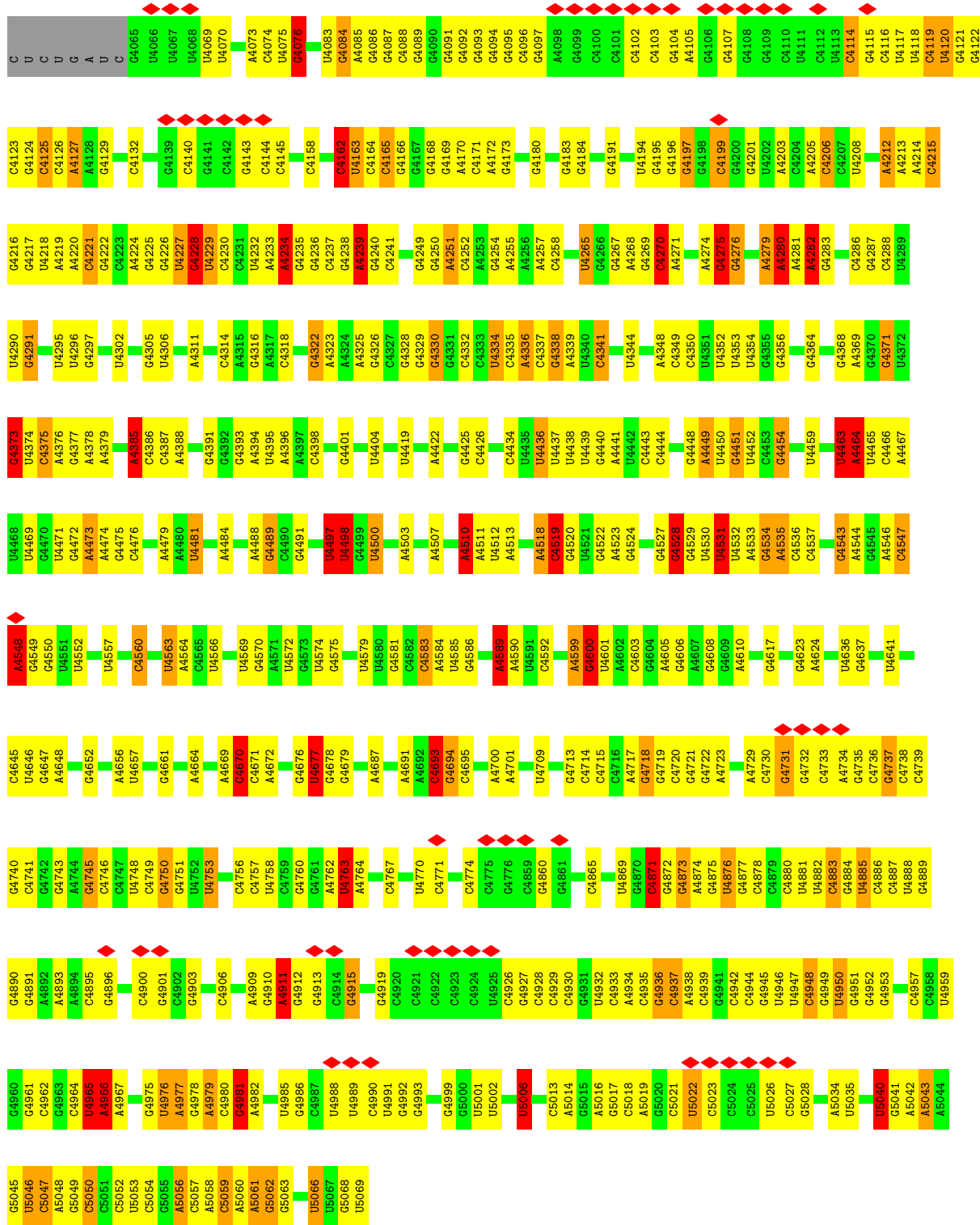
3 Residue-property plots [i](#)

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: 28S ribosomal RNA





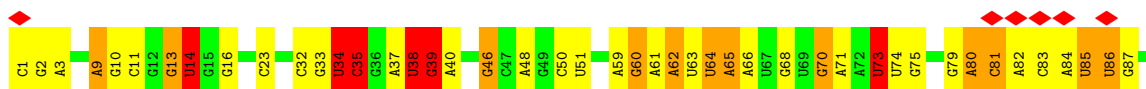


• Molecule 2: 5S ribosomal RNA

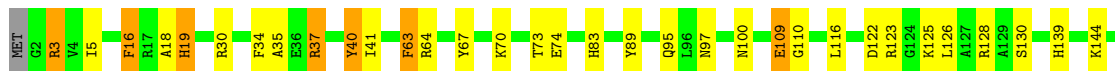




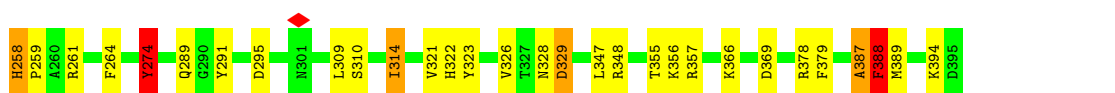
• Molecule 3: 5.8S ribosomal RNA



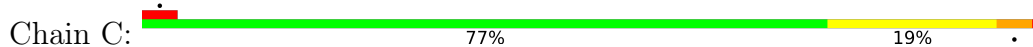
• Molecule 4: Ribosomal protein uL2



• Molecule 5: Ribosomal protein uL3

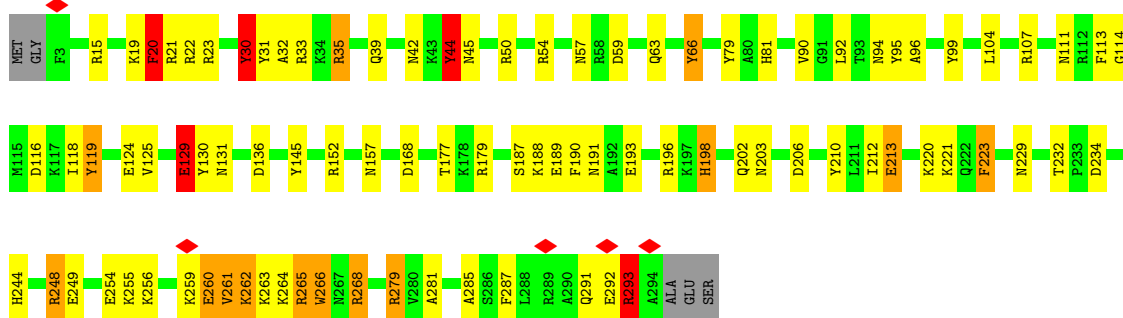


• Molecule 6: Ribosomal protein uL4

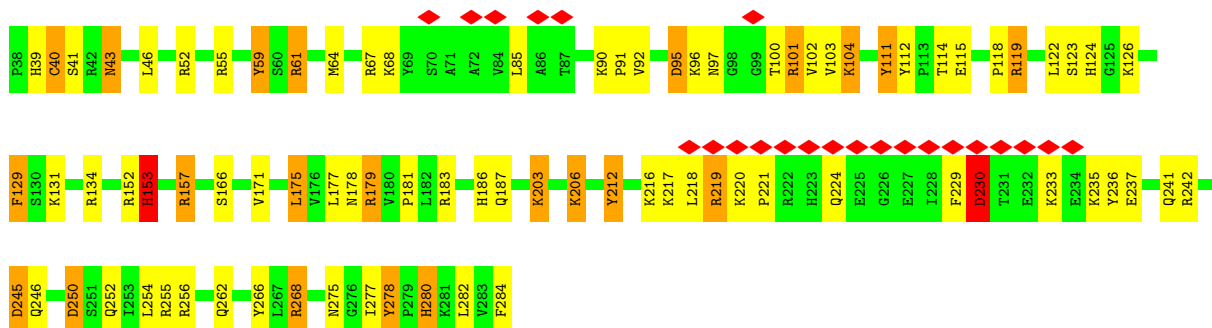




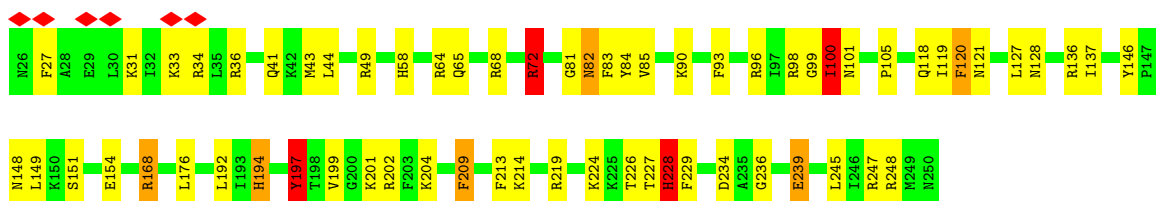
• Molecule 7: Ribosomal protein uL18



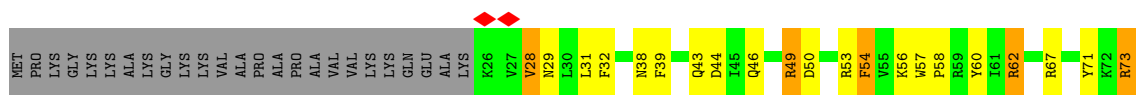
• Molecule 8: Ribosomal protein eL6

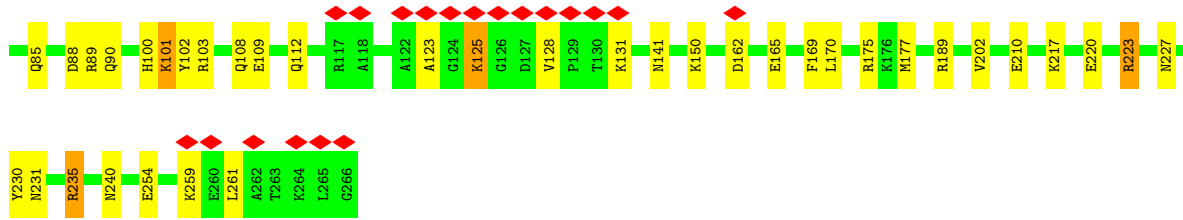


• Molecule 9: Ribosomal protein uL30

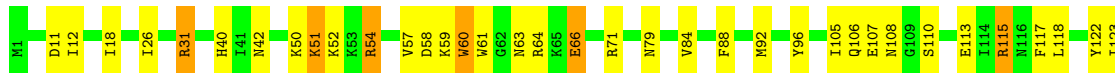


• Molecule 10: Ribosomal protein eL8





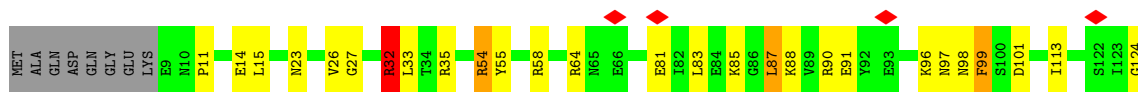
• Molecule 11: Ribosomal protein uL6



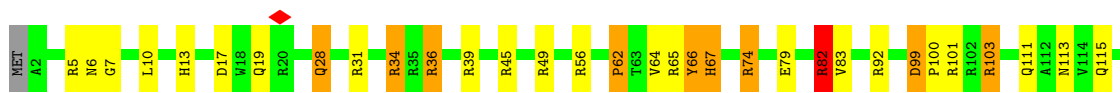
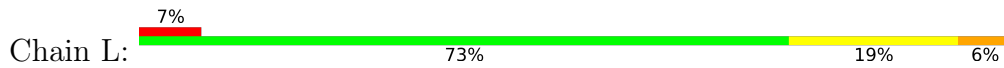
• Molecule 12: Ribosomal protein uL16



• Molecule 13: Ribosomal protein uL5

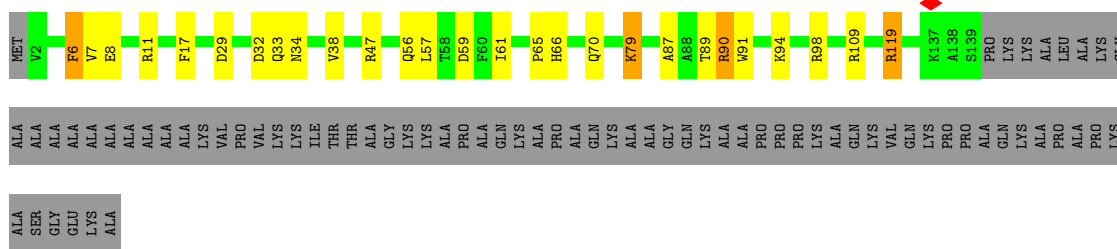


• Molecule 14: Ribosomal protein eL13



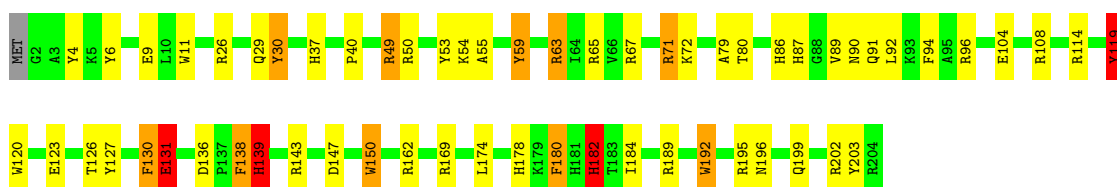
- Molecule 15: Ribosomal protein eL14

Chain M:  52% 11% 35%




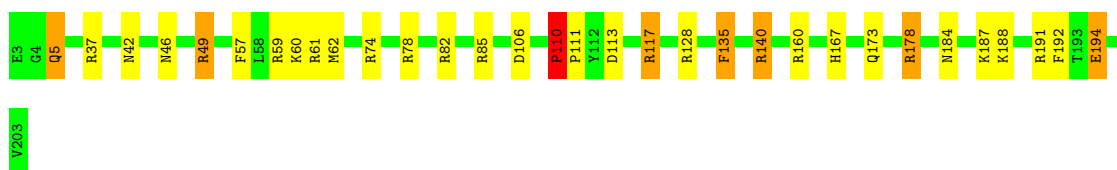
- Molecule 16: Ribosomal protein eL15

Chain N:  70% 23% 5%




- Molecule 17: Ribosomal protein uL13

Chain O:  84% 12%



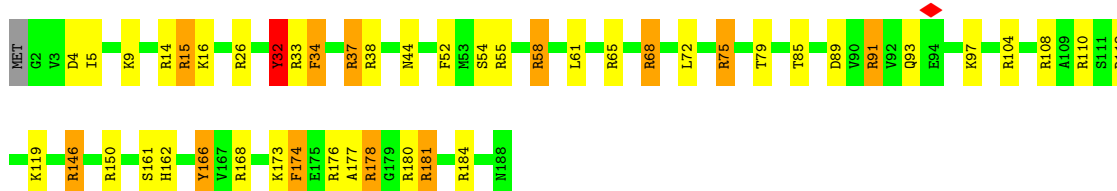
- Molecule 18: Ribosomal protein uL22

Chain P:  82% 14%

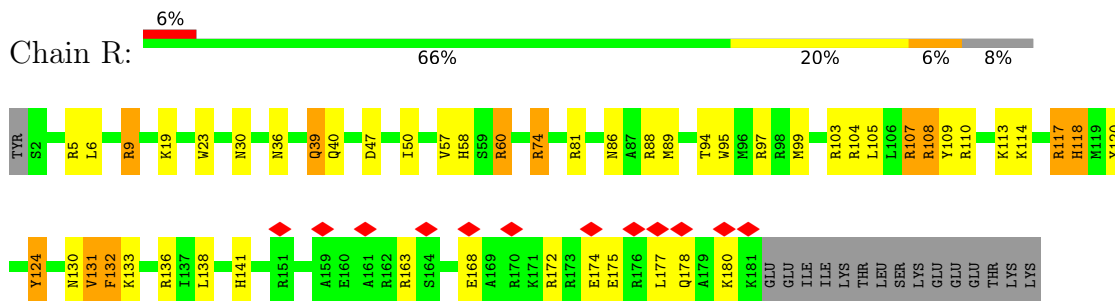


- Molecule 19: Ribosomal protein eL18

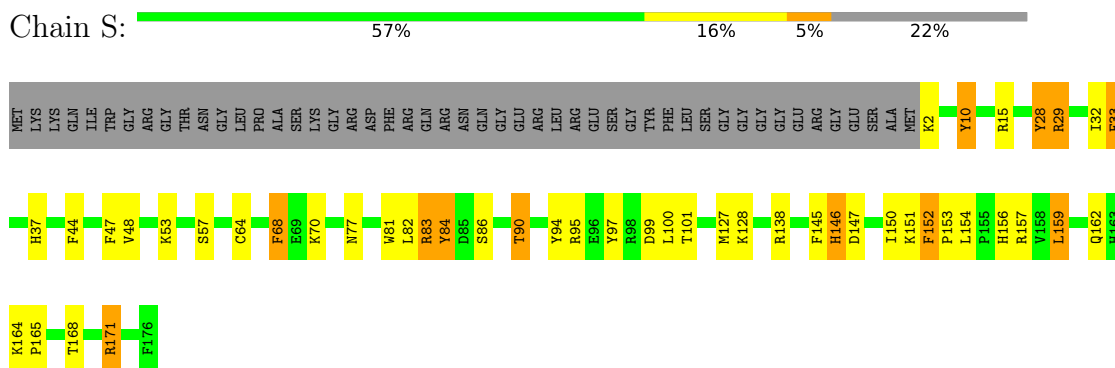
Chain Q:  74% 18% 6%



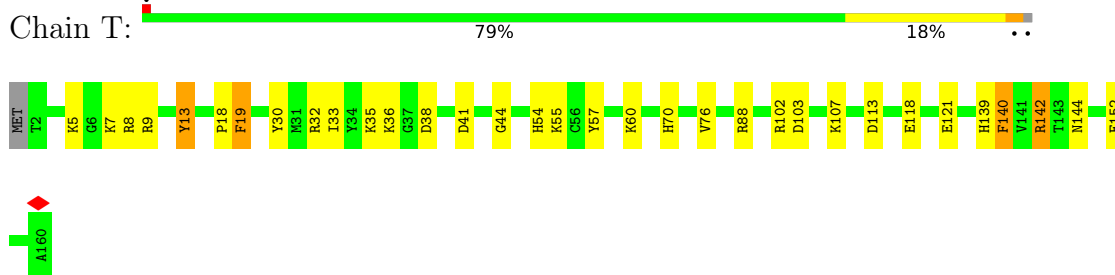
• Molecule 20: Ribosomal protein eL19



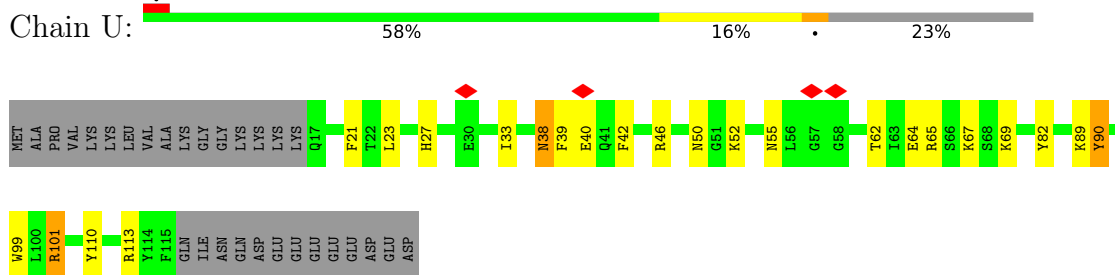
• Molecule 21: Ribosomal protein eL20



• Molecule 22: Ribosomal protein eL21

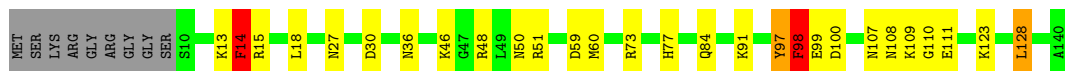


• Molecule 23: Ribosomal protein eL22

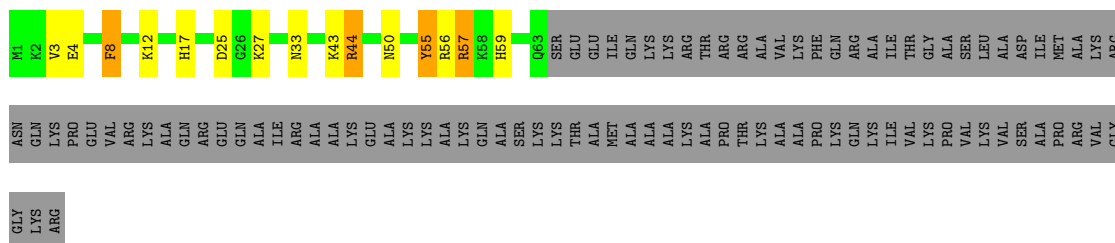


• Molecule 24: Ribosomal protein uL14

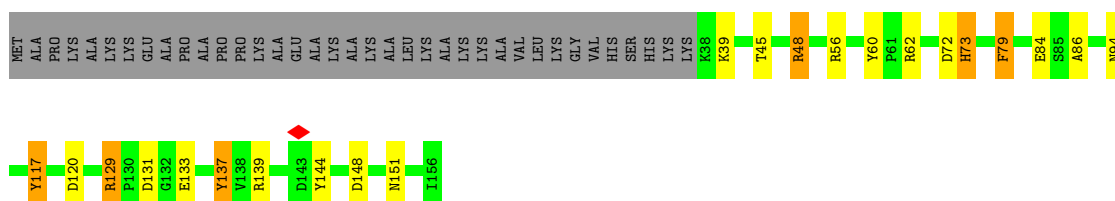




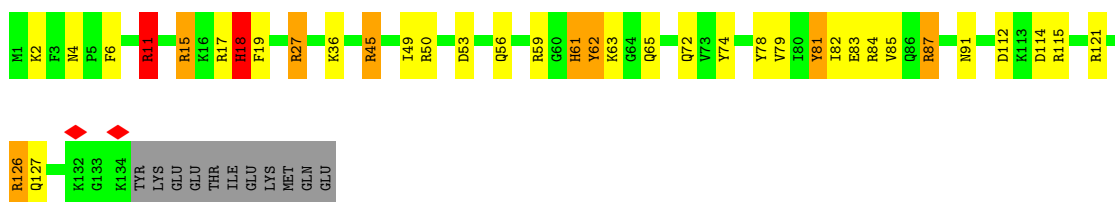
• Molecule 25: Ribosomal protein eL24



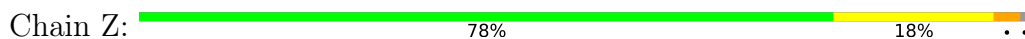
• Molecule 26: Ribosomal protein uL23



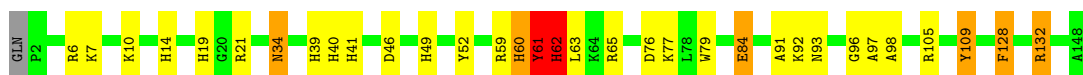
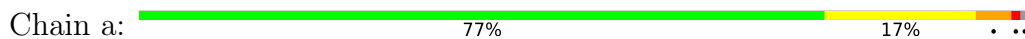
• Molecule 27: Ribosomal protein uL24



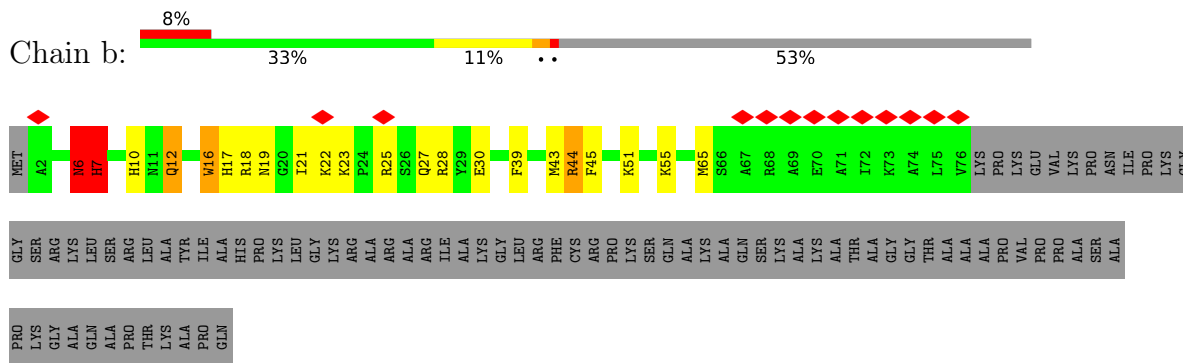
• Molecule 28: Ribosomal protein eL27



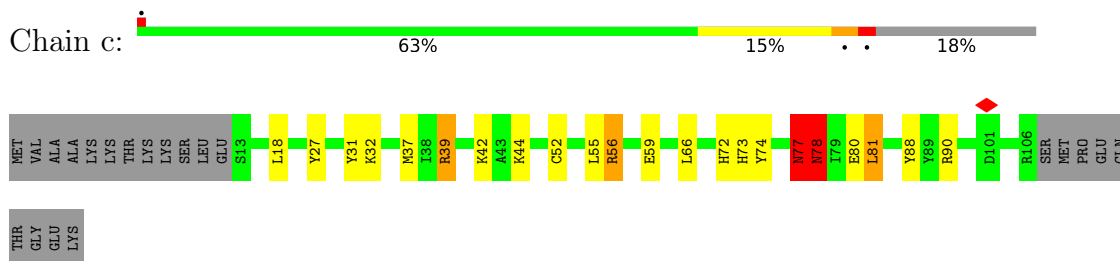
• Molecule 29: Ribosomal protein uL15



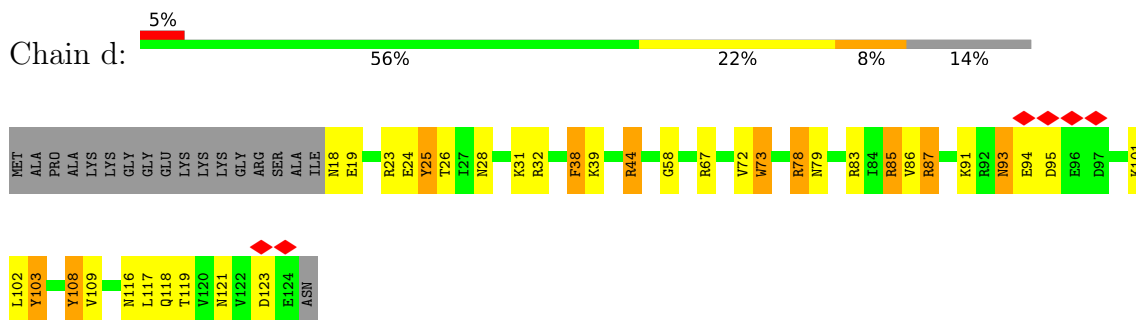
• Molecule 30: Ribosomal protein eL29



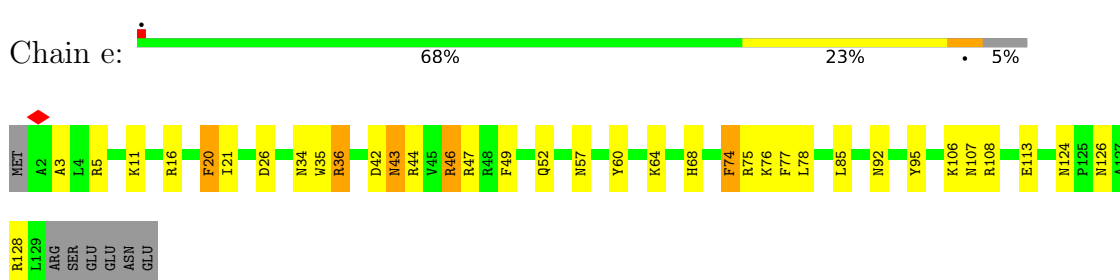
• Molecule 31: Ribosomal protein eL30



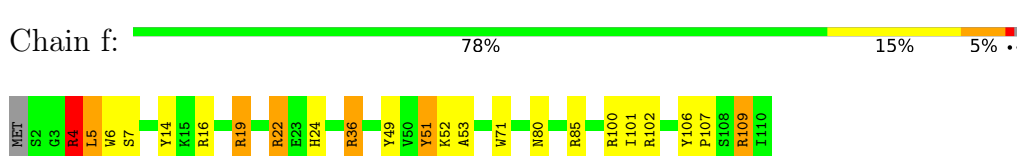
• Molecule 32: Ribosomal protein eL31



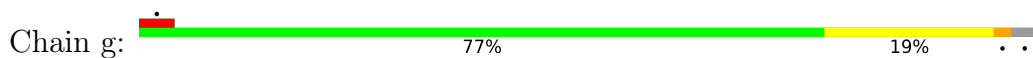
• Molecule 33: Ribosomal protein eL32



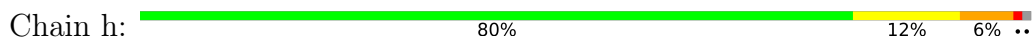
• Molecule 34: Ribosomal protein eL33



• Molecule 35: Ribosomal protein eL34



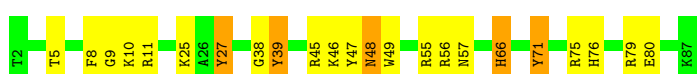
• Molecule 36: Ribosomal protein uL29



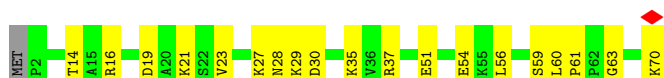
• Molecule 37: Ribosomal protein eL36



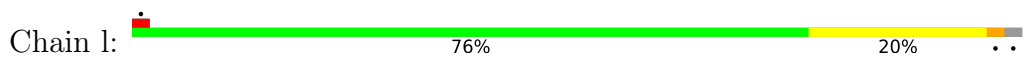
• Molecule 38: Ribosomal protein eL37



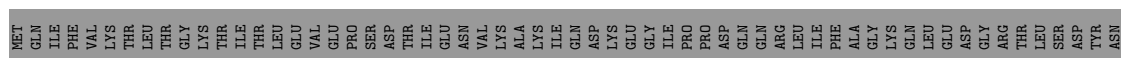
• Molecule 39: Ribosomal protein eL38



• Molecule 40: Ribosomal protein eL39

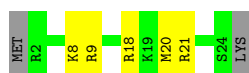


• Molecule 41: Ribosomal protein eL40

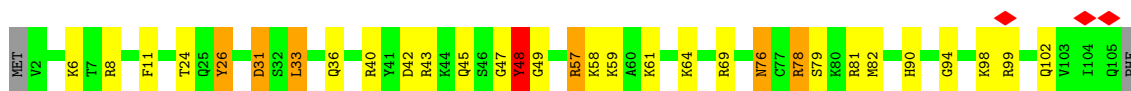




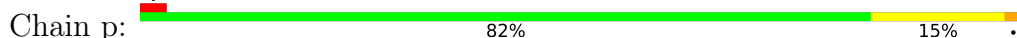
• Molecule 42: Ribosomal protein eL41



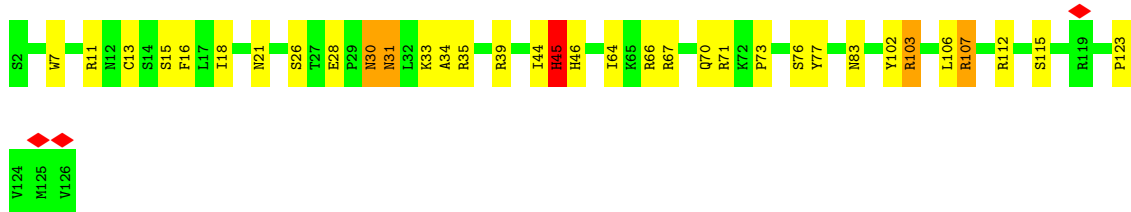
• Molecule 43: Ribosomal protein eL42



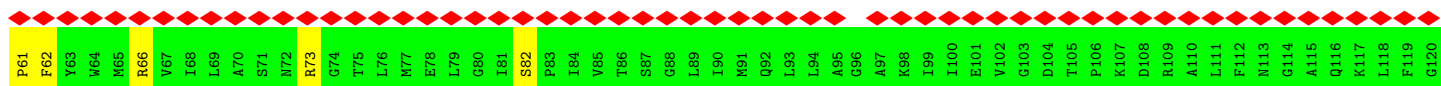
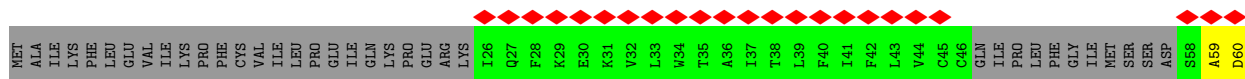
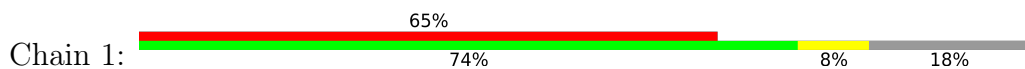
• Molecule 44: Ribosomal protein eL43

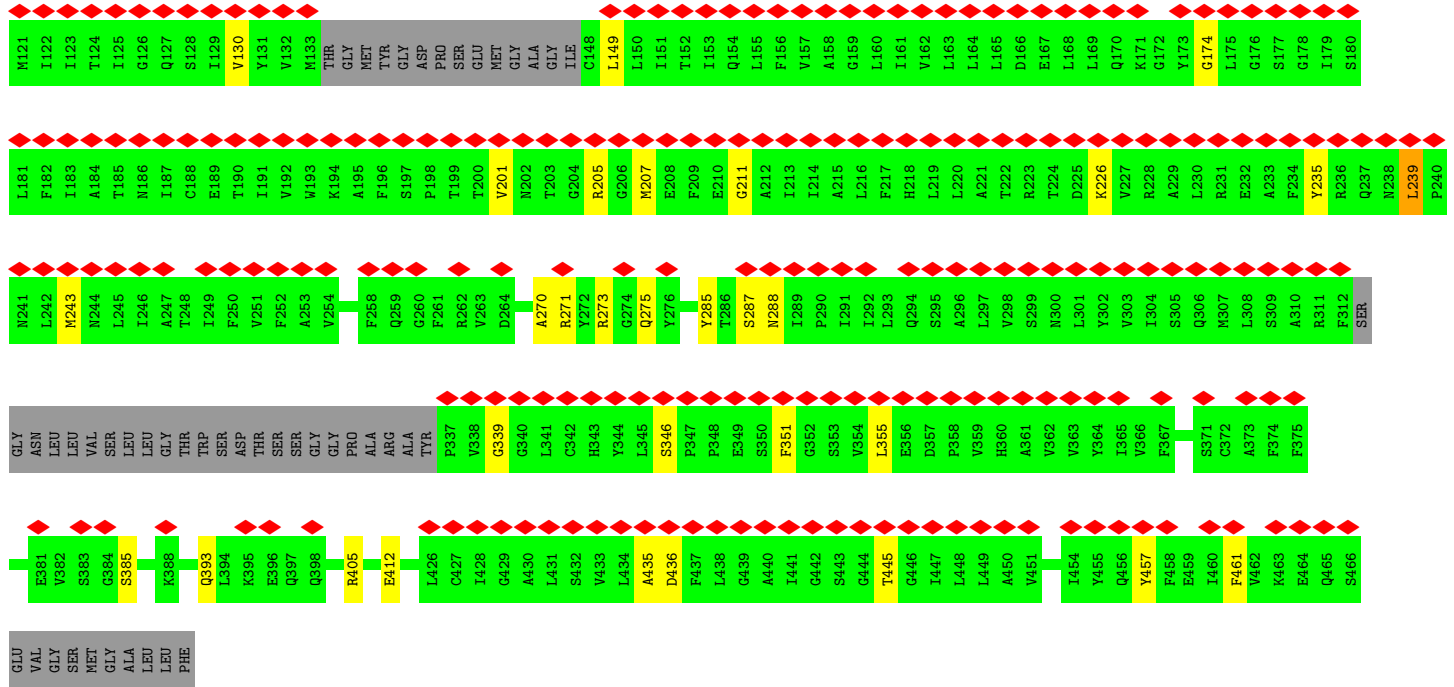


• Molecule 45: Ribosomal protein eL28

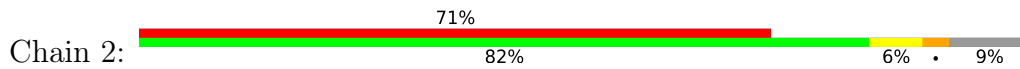


• Molecule 46: Sec61 alpha subunit

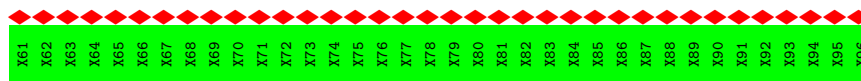




• Molecule 47: Sec61 gamma subunit



• Molecule 48: Sec61 beta subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80019	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.043	Depositor
Minimum map value	-0.599	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.09	Depositor
Map size (\AA)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3399999, 1.3399999, 1.3399999	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	5	0.64	80/87792 (0.1%)	1.13	742/136945 (0.5%)
2	7	0.54	1/2858 (0.0%)	0.96	9/4455 (0.2%)
3	8	0.68	3/3701 (0.1%)	1.20	42/5766 (0.7%)
4	A	0.80	3/1906 (0.2%)	1.26	21/2556 (0.8%)
5	B	0.81	8/3214 (0.2%)	1.16	26/4308 (0.6%)
6	C	0.73	4/2973 (0.1%)	1.12	18/3990 (0.5%)
7	D	0.73	2/2426 (0.1%)	1.23	27/3252 (0.8%)
8	E	0.73	5/1941 (0.3%)	1.21	20/2601 (0.8%)
9	F	0.80	2/1905 (0.1%)	1.27	26/2539 (1.0%)
10	G	0.76	4/1966 (0.2%)	1.09	14/2645 (0.5%)
11	H	0.77	3/1537 (0.2%)	1.17	10/2066 (0.5%)
12	I	0.66	1/1753 (0.1%)	1.11	12/2343 (0.5%)
13	J	0.63	1/1382 (0.1%)	1.04	11/1849 (0.6%)
14	L	0.71	2/1734 (0.1%)	1.12	15/2318 (0.6%)
15	M	0.76	2/1152 (0.2%)	1.11	5/1539 (0.3%)
16	N	0.84	4/1746 (0.2%)	1.33	23/2338 (1.0%)
17	O	0.72	3/1684 (0.2%)	1.11	12/2251 (0.5%)
18	P	0.74	2/1268 (0.2%)	1.10	9/1701 (0.5%)
19	Q	0.69	0/1530	1.35	31/2041 (1.5%)
20	R	0.79	3/1524 (0.2%)	1.27	21/2013 (1.0%)
21	S	0.95	8/1493 (0.5%)	1.30	19/2002 (0.9%)
22	T	0.67	1/1326 (0.1%)	1.04	7/1770 (0.4%)
23	U	0.63	1/822 (0.1%)	1.03	2/1103 (0.2%)
24	V	0.89	4/993 (0.4%)	1.11	7/1332 (0.5%)
25	W	0.71	0/541	1.23	5/720 (0.7%)
26	X	0.64	0/993	1.09	10/1334 (0.7%)
27	Y	0.72	0/1132	1.24	19/1504 (1.3%)
28	Z	0.63	0/1130	1.11	8/1507 (0.5%)
29	a	0.93	6/1192 (0.5%)	1.37	17/1591 (1.1%)
30	b	0.88	2/620 (0.3%)	1.17	5/819 (0.6%)
31	c	0.70	0/742	1.14	5/996 (0.5%)
32	d	0.84	3/903 (0.3%)	1.37	16/1216 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.90	3/1071 (0.3%)	1.23	15/1429 (1.0%)
34	f	1.02	2/895 (0.2%)	1.34	17/1198 (1.4%)
35	g	0.65	0/916	1.08	5/1220 (0.4%)
36	h	0.63	0/1023	1.21	13/1350 (1.0%)
37	i	0.63	0/843	1.19	8/1115 (0.7%)
38	j	0.97	1/721 (0.1%)	1.43	11/953 (1.2%)
39	k	0.59	0/575	0.97	1/761 (0.1%)
40	l	0.68	0/454	1.07	3/599 (0.5%)
41	m	0.57	0/435	1.02	3/575 (0.5%)
42	n	0.48	0/223	1.02	0/284
43	o	0.64	0/864	1.27	9/1140 (0.8%)
44	p	0.64	1/718 (0.1%)	1.00	3/953 (0.3%)
45	r	0.68	0/1017	1.12	8/1365 (0.6%)
46	1	0.45	0/3114	0.63	0/4218
47	2	0.47	0/504	0.71	1/673 (0.1%)
All	All	0.68	165/151252 (0.1%)	1.14	1311/223243 (0.6%)

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
1	5	1	158
2	7	0	2
3	8	0	11
4	A	0	6
5	B	0	13
6	C	0	5
7	D	0	8
8	E	0	12
9	F	0	5
10	G	0	3
11	H	0	3
12	I	0	5
13	J	0	2
14	L	0	5
15	M	0	4
16	N	0	11
17	O	0	3
18	P	0	1
19	Q	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	R	0	6
21	S	0	11
22	T	0	2
23	U	0	2
24	V	0	3
25	W	0	1
26	X	0	1
27	Y	0	4
29	a	0	9
30	b	0	1
31	c	0	2
32	d	0	4
33	e	0	4
34	f	0	2
35	g	0	1
36	h	0	3
37	i	0	3
38	j	0	4
39	k	0	1
43	o	0	6
44	p	0	1
45	r	0	5
46	1	0	1
47	2	0	1
All	All	1	340

The worst 5 of 165 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1823	G	O3'-P	41.48	2.10	1.61
10	G	109	GLU	CD-OE2	16.17	1.43	1.25
11	H	66	GLU	CD-OE1	15.86	1.43	1.25
34	f	6	TRP	CB-CG	-15.77	1.21	1.50
30	b	16	TRP	CB-CG	-13.52	1.25	1.50

The worst 5 of 1311 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	8	60	G	N9-C1'-C2'	16.16	135.01	114.00
38	j	11	ARG	NE-CZ-NH2	-13.83	113.38	120.30
19	Q	37	ARG	NE-CZ-NH2	12.90	126.75	120.30
1	5	92	C	N1-C1'-C2'	-12.62	97.59	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	139	ARG	CG-CD-NE	12.29	137.61	111.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	5	1992	U	C1'

5 of 340 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	5	22	G	Sidechain
1	5	31	U	Sidechain
1	5	42	A	Sidechain
1	5	43	U	Sidechain
1	5	53	C	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	242/257 (94%)	203 (84%)	30 (12%)	9 (4%)	3	26
5	B	392/394 (100%)	319 (81%)	40 (10%)	33 (8%)	1	9
6	C	365/367 (100%)	304 (83%)	46 (13%)	15 (4%)	3	23
7	D	290/297 (98%)	235 (81%)	33 (11%)	22 (8%)	1	10
8	E	232/236 (98%)	150 (65%)	51 (22%)	31 (13%)	0	4
9	F	223/225 (99%)	190 (85%)	23 (10%)	10 (4%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	G	239/266 (90%)	200 (84%)	32 (13%)	7 (3%)	4	31
11	H	188/192 (98%)	164 (87%)	20 (11%)	4 (2%)	7	38
12	I	211/213 (99%)	168 (80%)	30 (14%)	13 (6%)	1	15
13	J	168/178 (94%)	137 (82%)	23 (14%)	8 (5%)	2	20
14	L	208/211 (99%)	172 (83%)	25 (12%)	11 (5%)	2	17
15	M	136/213 (64%)	118 (87%)	16 (12%)	2 (2%)	10	45
16	N	201/204 (98%)	172 (86%)	23 (11%)	6 (3%)	4	30
17	O	199/201 (99%)	182 (92%)	14 (7%)	3 (2%)	10	45
18	P	151/153 (99%)	140 (93%)	9 (6%)	2 (1%)	12	48
19	Q	185/188 (98%)	160 (86%)	20 (11%)	5 (3%)	5	33
20	R	178/196 (91%)	153 (86%)	21 (12%)	4 (2%)	6	37
21	S	173/224 (77%)	146 (84%)	24 (14%)	3 (2%)	9	42
22	T	157/160 (98%)	128 (82%)	26 (17%)	3 (2%)	8	40
23	U	97/128 (76%)	74 (76%)	21 (22%)	2 (2%)	7	38
24	V	129/140 (92%)	112 (87%)	14 (11%)	3 (2%)	6	36
25	W	61/157 (39%)	57 (93%)	3 (5%)	1 (2%)	9	43
26	X	117/156 (75%)	108 (92%)	7 (6%)	2 (2%)	9	42
27	Y	132/145 (91%)	112 (85%)	14 (11%)	6 (4%)	2	21
28	Z	133/136 (98%)	113 (85%)	15 (11%)	5 (4%)	3	25
29	a	145/148 (98%)	111 (77%)	26 (18%)	8 (6%)	2	17
30	b	73/160 (46%)	58 (80%)	11 (15%)	4 (6%)	2	17
31	c	92/115 (80%)	78 (85%)	10 (11%)	4 (4%)	2	22
32	d	105/125 (84%)	85 (81%)	16 (15%)	4 (4%)	3	25
33	e	126/135 (93%)	110 (87%)	15 (12%)	1 (1%)	19	58
34	f	107/110 (97%)	95 (89%)	7 (6%)	5 (5%)	2	20
35	g	112/117 (96%)	103 (92%)	7 (6%)	2 (2%)	8	41
36	h	120/123 (98%)	103 (86%)	14 (12%)	3 (2%)	5	34
37	i	100/105 (95%)	91 (91%)	7 (7%)	2 (2%)	7	39
38	j	84/86 (98%)	67 (80%)	13 (16%)	4 (5%)	2	20
39	k	67/70 (96%)	55 (82%)	7 (10%)	5 (8%)	1	11
40	l	48/51 (94%)	42 (88%)	4 (8%)	2 (4%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	m	50/128 (39%)	44 (88%)	6 (12%)	0	100	100
42	n	21/25 (84%)	21 (100%)	0	0	100	100
43	o	102/106 (96%)	85 (83%)	11 (11%)	6 (6%)	1	15
44	p	89/91 (98%)	79 (89%)	9 (10%)	1 (1%)	14	52
45	r	123/125 (98%)	97 (79%)	20 (16%)	6 (5%)	2	19
46	1	384/476 (81%)	325 (85%)	42 (11%)	17 (4%)	2	21
47	2	60/68 (88%)	51 (85%)	6 (10%)	3 (5%)	2	19
All	All	6815/7601 (90%)	5717 (84%)	811 (12%)	287 (4%)	5	23

5 of 287 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	19	HIS
4	A	197	PRO
5	B	16	PHE
5	B	40	PRO
5	B	108	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	187/199 (94%)	139 (74%)	48 (26%)	0	3
5	B	335/335 (100%)	265 (79%)	70 (21%)	1	6
6	C	305/305 (100%)	239 (78%)	66 (22%)	1	5
7	D	246/250 (98%)	178 (72%)	68 (28%)	0	3
8	E	209/209 (100%)	157 (75%)	52 (25%)	0	4
9	F	194/194 (100%)	145 (75%)	49 (25%)	0	3
10	G	206/226 (91%)	158 (77%)	48 (23%)	1	4
11	H	169/171 (99%)	125 (74%)	44 (26%)	0	3
12	I	180/180 (100%)	136 (76%)	44 (24%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	J	143/149 (96%)	115 (80%)	28 (20%)	1	7
14	L	176/177 (99%)	135 (77%)	41 (23%)	1	4
15	M	116/160 (72%)	95 (82%)	21 (18%)	1	9
16	N	171/172 (99%)	129 (75%)	42 (25%)	0	4
17	O	172/172 (100%)	146 (85%)	26 (15%)	3	17
18	P	134/134 (100%)	112 (84%)	22 (16%)	2	13
19	Q	163/164 (99%)	132 (81%)	31 (19%)	1	8
20	R	159/175 (91%)	120 (76%)	39 (24%)	0	4
21	S	156/192 (81%)	121 (78%)	35 (22%)	1	4
22	T	139/140 (99%)	112 (81%)	27 (19%)	1	7
23	U	89/114 (78%)	67 (75%)	22 (25%)	0	4
24	V	101/107 (94%)	77 (76%)	24 (24%)	0	4
25	W	55/126 (44%)	42 (76%)	13 (24%)	1	4
26	X	107/133 (80%)	89 (83%)	18 (17%)	2	12
27	Y	124/135 (92%)	96 (77%)	28 (23%)	1	4
28	Z	117/118 (99%)	94 (80%)	23 (20%)	1	7
29	a	119/120 (99%)	102 (86%)	17 (14%)	3	19
30	b	63/123 (51%)	45 (71%)	18 (29%)	0	3
31	c	79/97 (81%)	60 (76%)	19 (24%)	0	4
32	d	98/110 (89%)	66 (67%)	32 (33%)	0	2
33	e	114/121 (94%)	89 (78%)	25 (22%)	1	5
34	f	88/89 (99%)	73 (83%)	15 (17%)	2	12
35	g	98/100 (98%)	79 (81%)	19 (19%)	1	7
36	h	109/110 (99%)	92 (84%)	17 (16%)	2	16
37	i	86/89 (97%)	71 (83%)	15 (17%)	2	11
38	j	73/73 (100%)	60 (82%)	13 (18%)	2	10
39	k	64/65 (98%)	52 (81%)	12 (19%)	1	8
40	l	47/48 (98%)	39 (83%)	8 (17%)	2	12
41	m	48/116 (41%)	36 (75%)	12 (25%)	0	4
42	n	22/24 (92%)	17 (77%)	5 (23%)	1	4
43	o	92/94 (98%)	70 (76%)	22 (24%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
44	p	74/74 (100%)	61 (82%)	13 (18%)	2 10
45	r	109/109 (100%)	85 (78%)	24 (22%)	1 5
46	1	330/398 (83%)	309 (94%)	21 (6%)	17 50
47	2	53/59 (90%)	50 (94%)	3 (6%)	20 53
All	All	5919/6456 (92%)	4680 (79%)	1239 (21%)	3 6

5 of 1239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	Z	121	ARG
41	m	104	HIS
30	b	23	LYS
28	Z	112	ARG
34	f	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 188 such sidechains are listed below:

Mol	Chain	Res	Type
22	T	58	HIS
31	c	73	HIS
24	V	36	ASN
28	Z	79	HIS
33	e	126	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3647/3722 (97%)	1611 (44%)	629 (17%)
2	7	119/120 (99%)	31 (26%)	9 (7%)
3	8	155/156 (99%)	61 (39%)	22 (14%)
All	All	3921/3998 (98%)	1703 (43%)	660 (16%)

5 of 1703 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	2	G
1	5	5	A
1	5	6	C

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Mol	Chain	Res	Type
1	5	8	U
1	5	12	A

5 of 660 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	3860	A
1	5	4645	C
1	5	4084	G
1	5	3856	A
1	5	4287	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 133 ligands modelled in this entry, 133 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	12
8	E	1

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	72:ALA	C	84:VAL	N	23.51
1	5	4776:G	O3'	4859:C	P	17.87
1	5	757:G	O3'	906:C	P	16.89
1	5	519:C	O3'	642:G	P	16.61
1	5	2910:G	O3'	3583:U	P	16.04

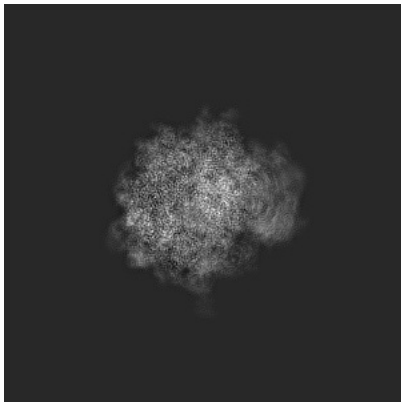
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2650. These allow visual inspection of the internal detail of the map and identification of artifacts.

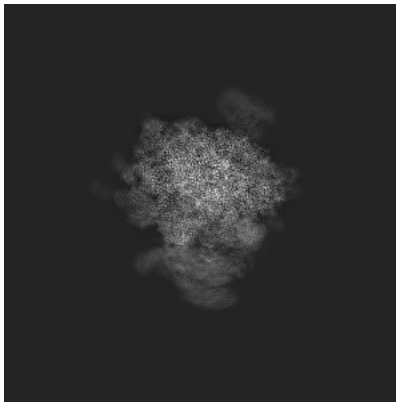
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

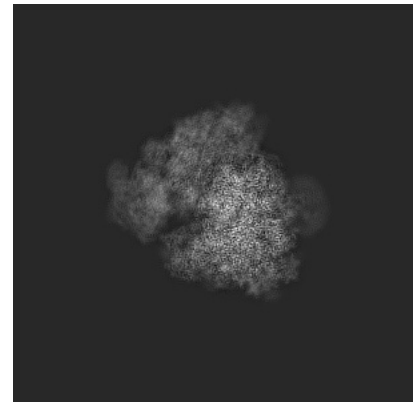
6.1.1 Primary map



X



Y

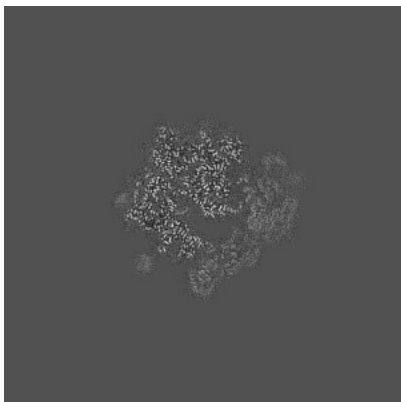


Z

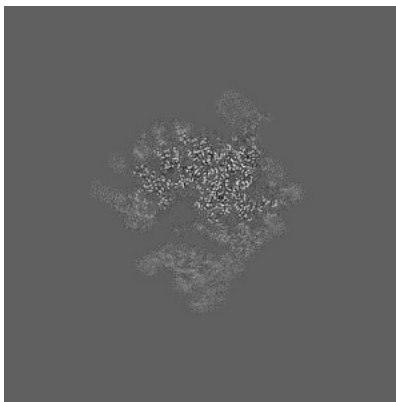
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

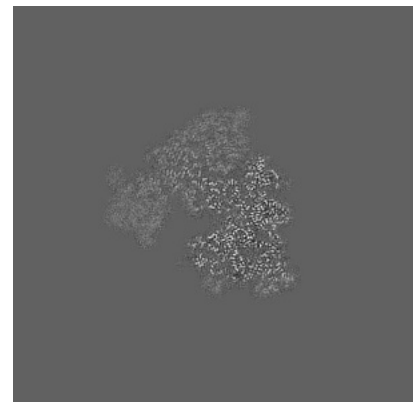
6.2.1 Primary map



X Index: 210



Y Index: 210

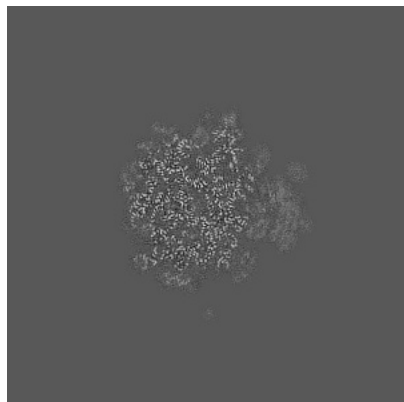


Z Index: 210

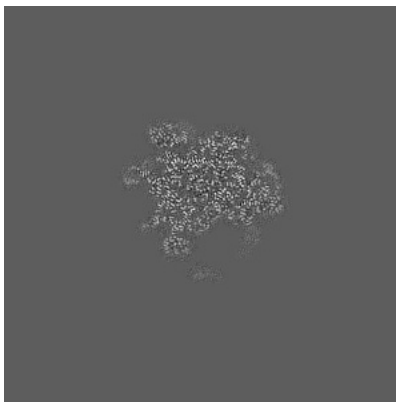
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

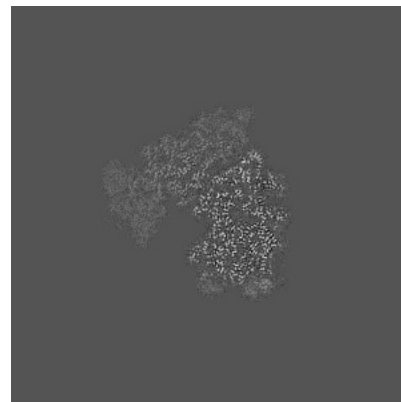
6.3.1 Primary map



X Index: 233



Y Index: 168



Z Index: 219

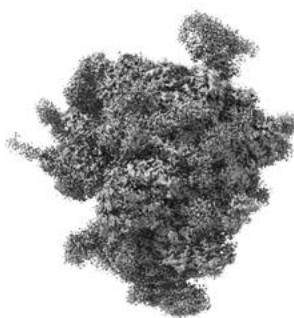
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

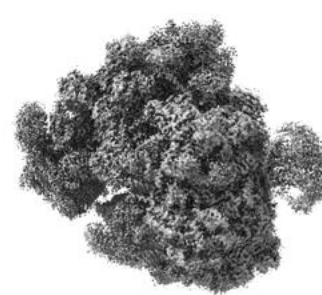
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

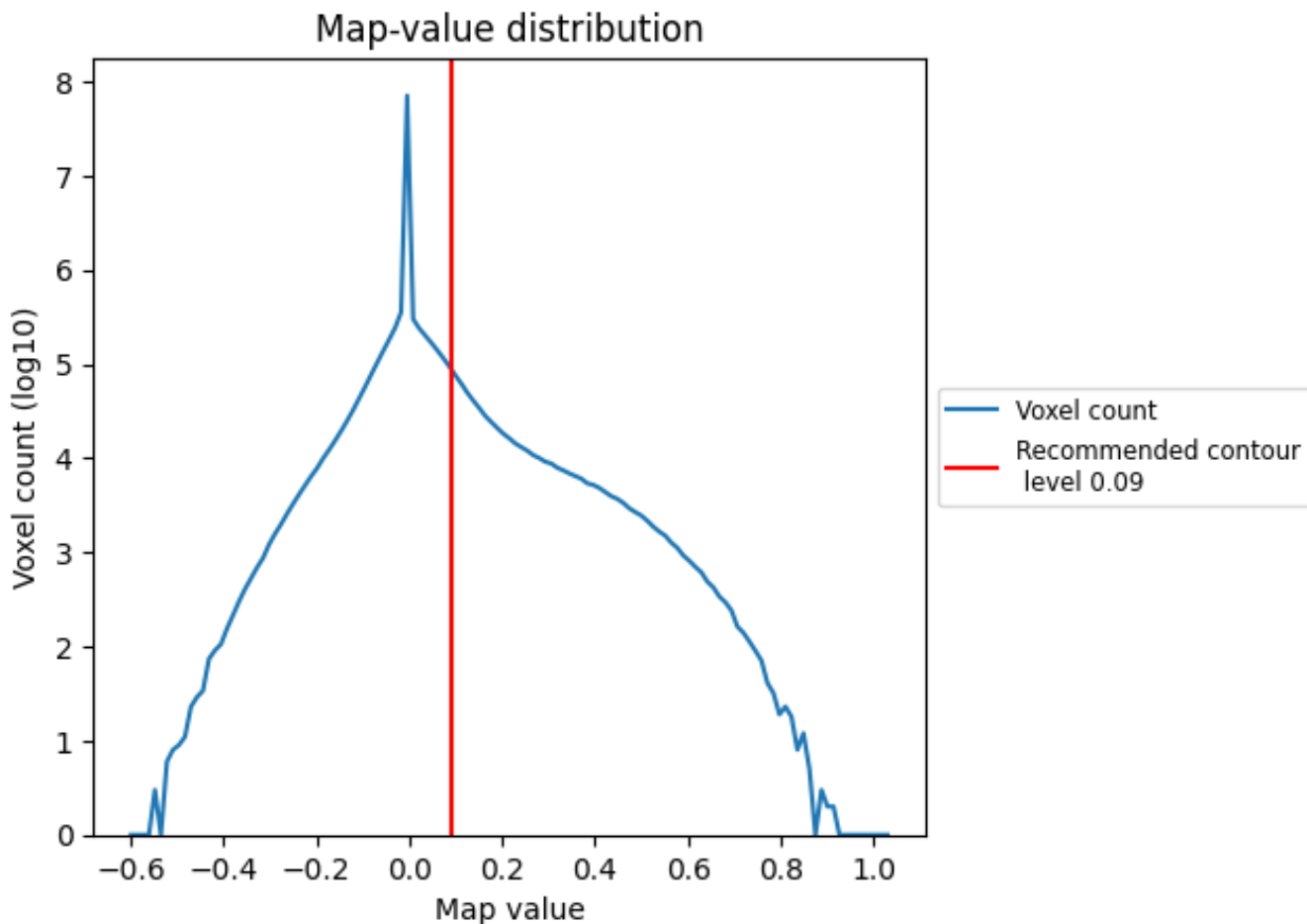
6.5 Mask visualisation

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

7 Map analysis [i](#)

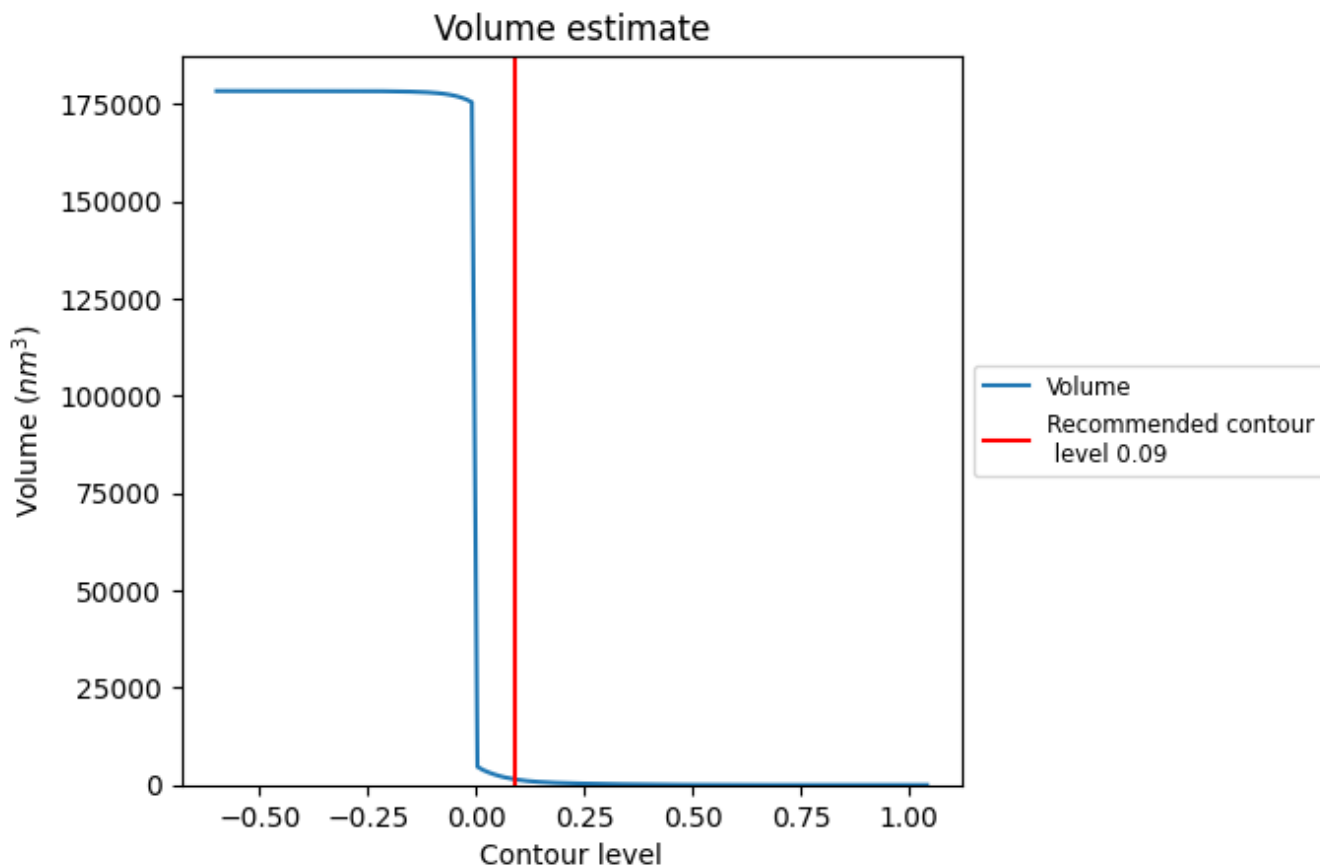
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

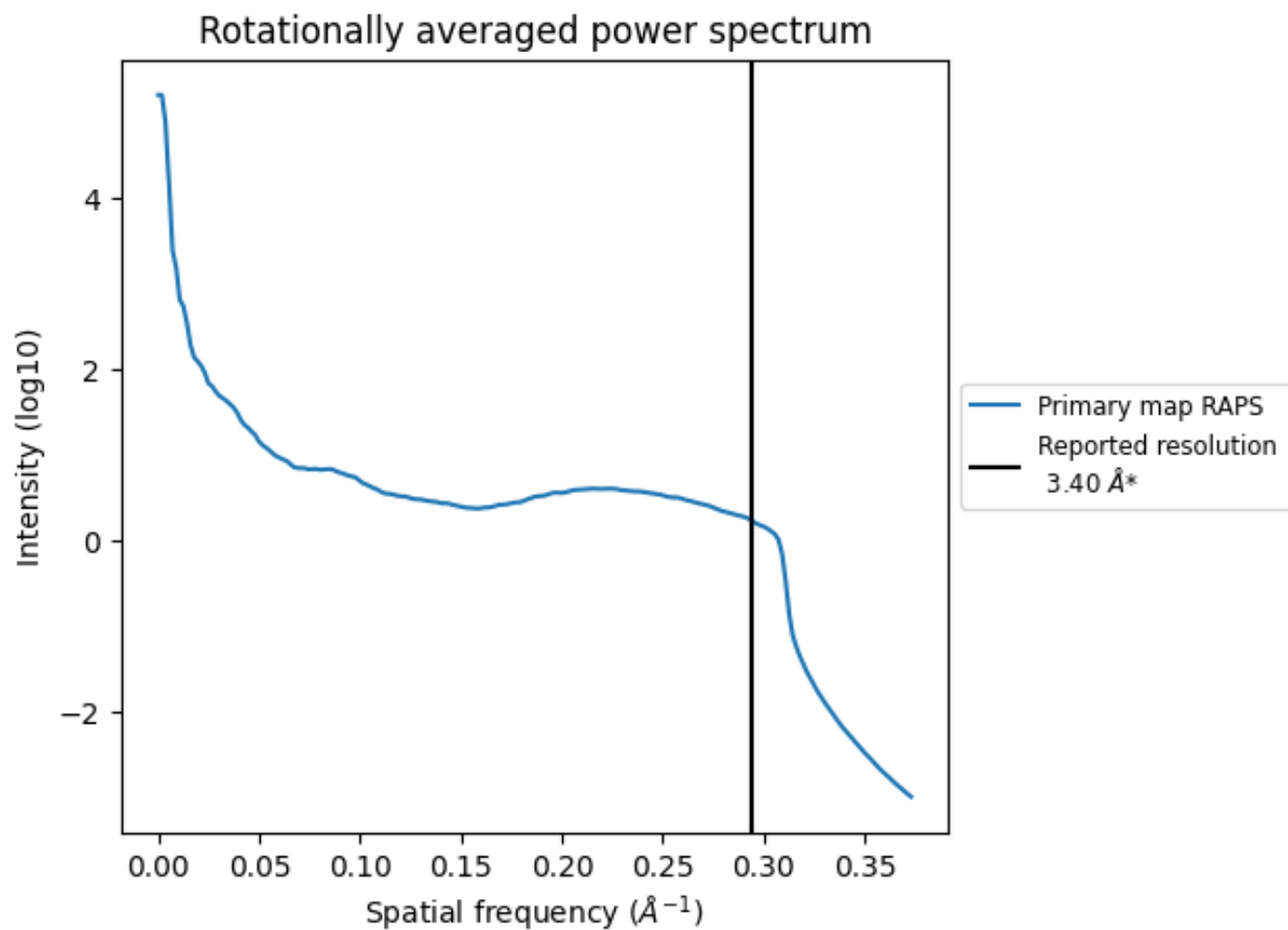
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1453 nm³; this corresponds to an approximate mass of 1312 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.294\AA^{-1}

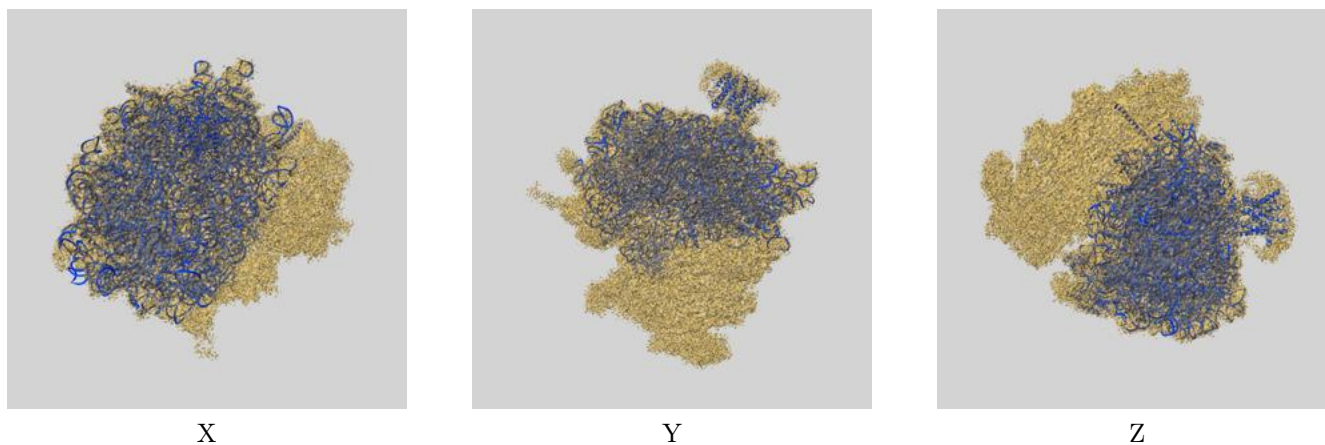
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

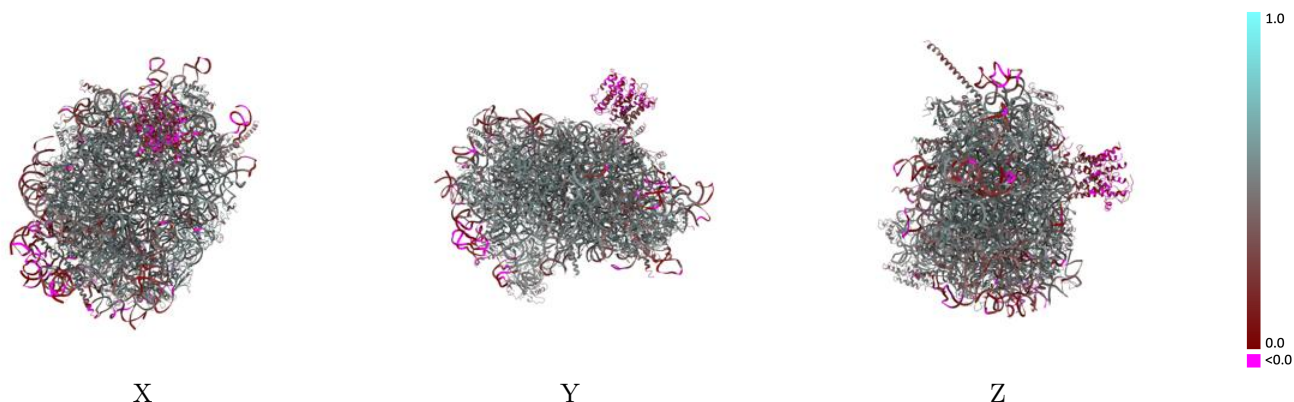
This section contains information regarding the fit between EMDB map EMD-2650 and PDB model 3J7Q. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



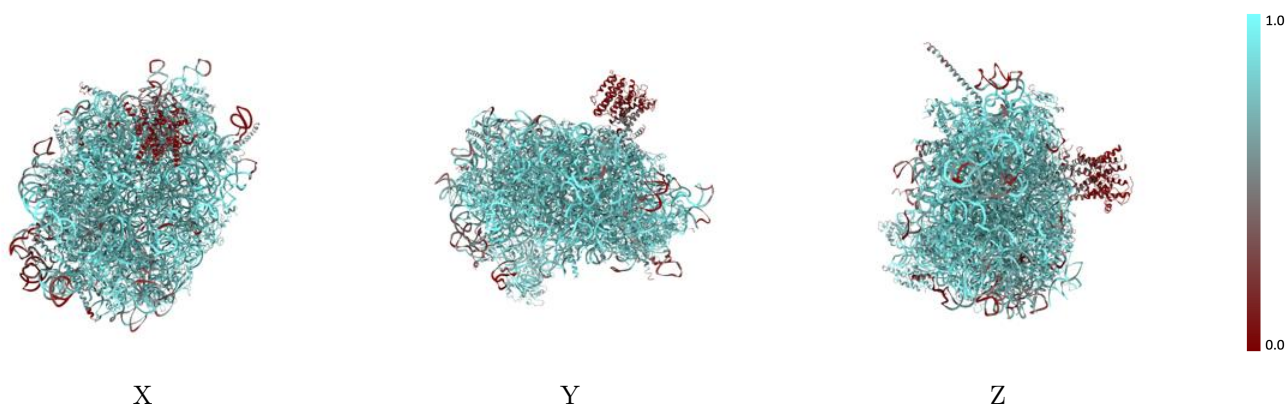
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



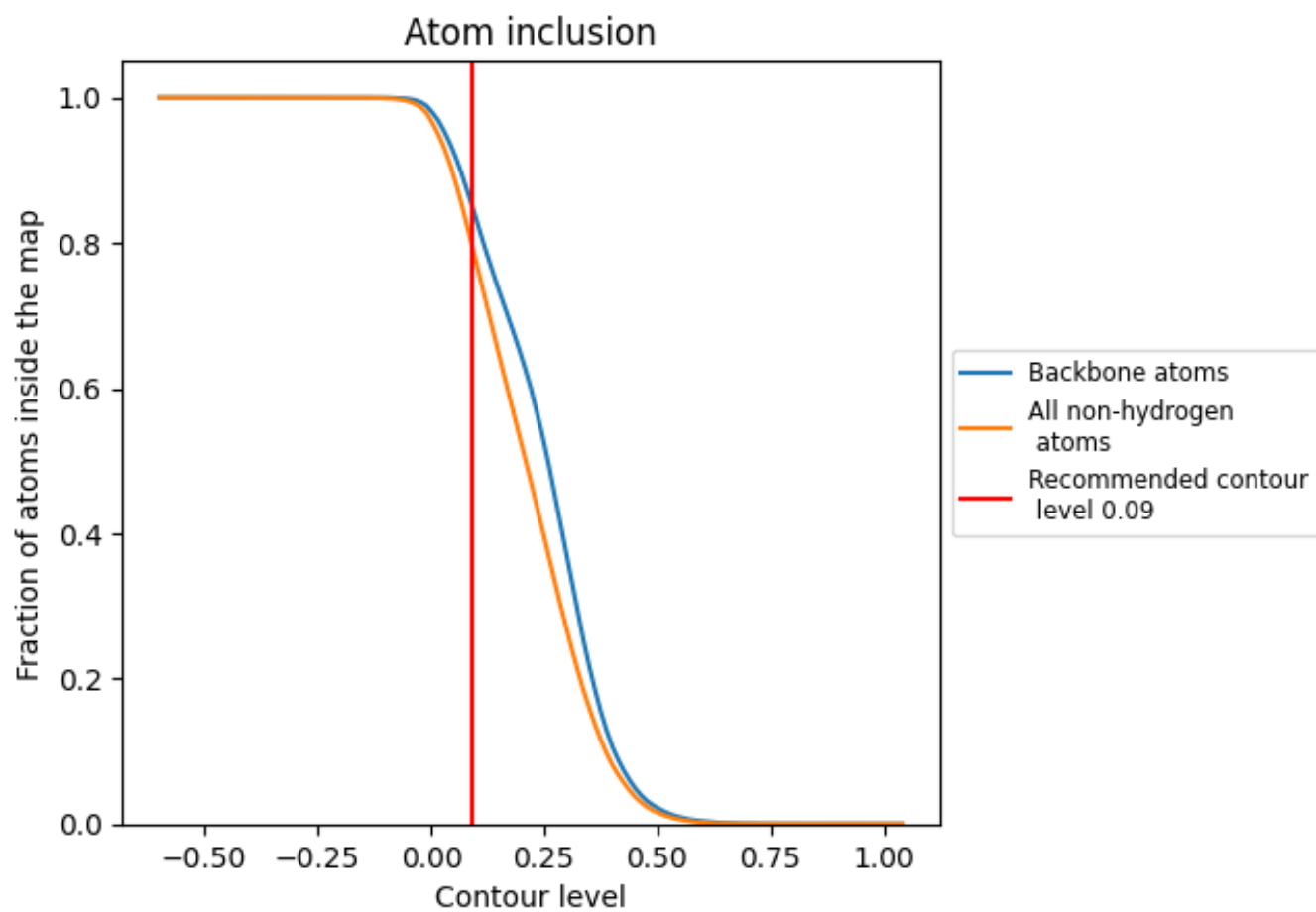
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8002	 0.4410
1	 0.2232	 0.1560
2	 0.2593	 0.1820
3	 0.0278	 0.0620
5	 0.8091	 0.4170
7	 0.9294	 0.4920
8	 0.8499	 0.4530
A	 0.8616	 0.5200
B	 0.8601	 0.5130
C	 0.8303	 0.5000
D	 0.8061	 0.4580
E	 0.7579	 0.4480
F	 0.8318	 0.5010
G	 0.7681	 0.4560
H	 0.8284	 0.5050
I	 0.8010	 0.4800
J	 0.7619	 0.4510
L	 0.7748	 0.4650
M	 0.8314	 0.5010
N	 0.8722	 0.5200
O	 0.8565	 0.5230
P	 0.8351	 0.5160
Q	 0.8614	 0.5230
R	 0.7786	 0.4670
S	 0.8614	 0.5190
T	 0.8250	 0.5020
U	 0.7203	 0.4230
V	 0.8434	 0.5190
W	 0.8212	 0.5040
X	 0.7871	 0.4910
Y	 0.8098	 0.4990
Z	 0.8313	 0.4950
a	 0.8627	 0.5160
b	 0.6785	 0.4120
c	 0.8084	 0.4850



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Chain	Atom inclusion	Q-score
d	 0.7993	 0.4790
e	 0.8466	 0.5210
f	 0.8777	 0.5260
g	 0.8147	 0.5080
h	 0.7892	 0.4880
i	 0.8045	 0.4890
j	 0.8472	 0.5010
k	 0.7540	 0.4600
l	 0.8345	 0.5180
m	 0.8486	 0.5220
n	 0.7711	 0.4760
o	 0.8015	 0.5020
p	 0.8198	 0.5160
r	 0.8392	 0.5060