



## wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 08:00 PM EST

PDB ID : 3JBV  
EMDB ID : EMD-6486  
Title : Mechanisms of Ribosome Stalling by SecM at Multiple Elongation Steps  
Authors : Zhang, J.; Pan, X.J.; Yan, K.G.; Sun, S.; Gao, N.; Sui, S.F.  
Deposited on : 2015-10-16  
Resolution : 3.32 Å(reported)  
Based on initial model : 4V7T

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
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) : 2.31.2

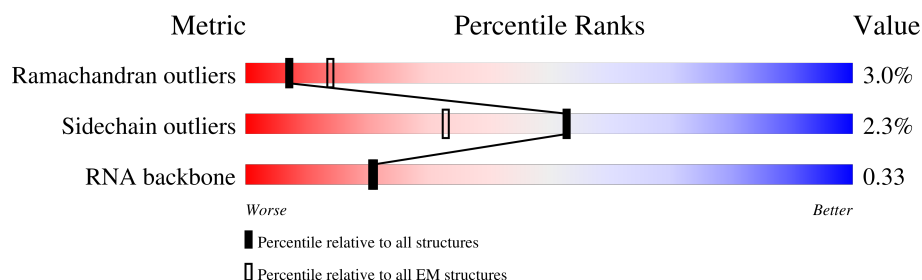
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.32 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1542	
2	B	241	
3	C	233	
4	D	206	
5	E	167	
6	F	131	
7	G	156	
8	H	130	

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Mol	Chain	Length	Quality of chain
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	V	76	
23	W	75	
24	X	11	
25	0	78	
26	1	63	
27	2	59	
28	3	57	
29	4	55	
30	6	46	
31	7	65	
32	8	38	
33	a	120	

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Mol	Chain	Length	Quality of chain
34	b	2904	
35	c	273	
36	i	142	
37	d	209	
38	e	201	
39	f	179	
40	g	177	
41	h	149	
42	j	142	
43	k	123	
44	l	144	
45	m	136	
46	n	127	
47	o	117	
48	p	115	
49	q	118	
50	r	103	
51	s	110	
52	t	100	
53	u	104	
54	w	94	
55	y	85	
56	z	27	

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145911 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 RNA (1530-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1530	Total	C	N	O	P	0	0
			32831	14642	6024	10635	1530		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	150	Total	C	N	O	S	0	0
			1174	730	226	214	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	113	Total	C	N	O	S	0	0
			876	541	177	155	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	79	ARG	GLN	conflict	UNP P0ADZ4

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a RNA chain called RNA (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	76	Total	C	N	O	P	0	0
			1620	723	290	532	75		

- Molecule 23 is a RNA chain called RNA (75-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total	C	N	O	P	0	0
			1599	713	287	525	74		

- Molecule 24 is a RNA chain called RNA (5'-R(P\*CP\*UP\*GP\*GP\*CP\*CP\*CP\*UP\*CP\*A P\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	11	Total	C	N	O	P	0	0
			231	103	39	78	11		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 27 is a protein called 50S ribosomal protein L30.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 33 is a RNA chain called RNA (118-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	117	Total	C	N	O	P	0	0
			2506	1116	459	814	117		

- Molecule 34 is a RNA chain called RNA (2903-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	2903	Total	C	N	O	P	0	0
			62321	27801	11467	20150	2903		

- Molecule 35 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 36 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	134	Total	C	N	O	S	0	0
			976	614	169	187	6		

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 38 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 39 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 42 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 43 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 44 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 45 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	135	Total	C	N	O	S	0	0
			1063	680	201	176	6		

- Molecule 46 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 47 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	o	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 48 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 49 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	117	Total	C	N	O		0	0
			947	604	192	151			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 51 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 52 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 53 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

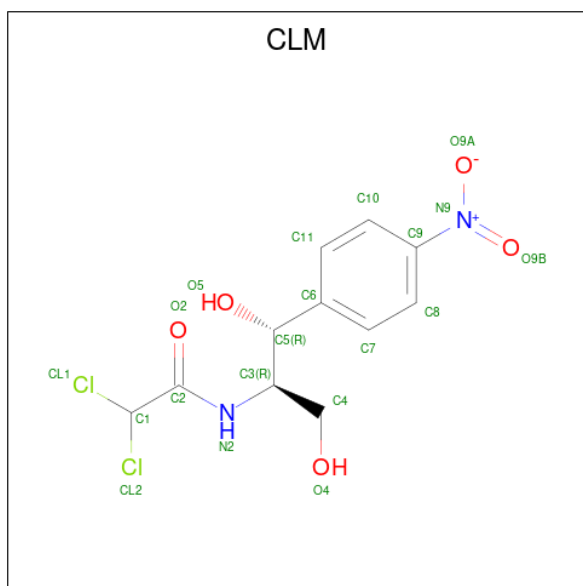
- Molecule 55 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 56 is a protein called Secretion monitor.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	z	27	Total	C	N	O	0	0
			211	134	35	42		

- Molecule 57 is CHLORAMPHENICOL (three-letter code: CLM) (formula:  $C_{11}H_{12}Cl_2N_2O_5$ ).

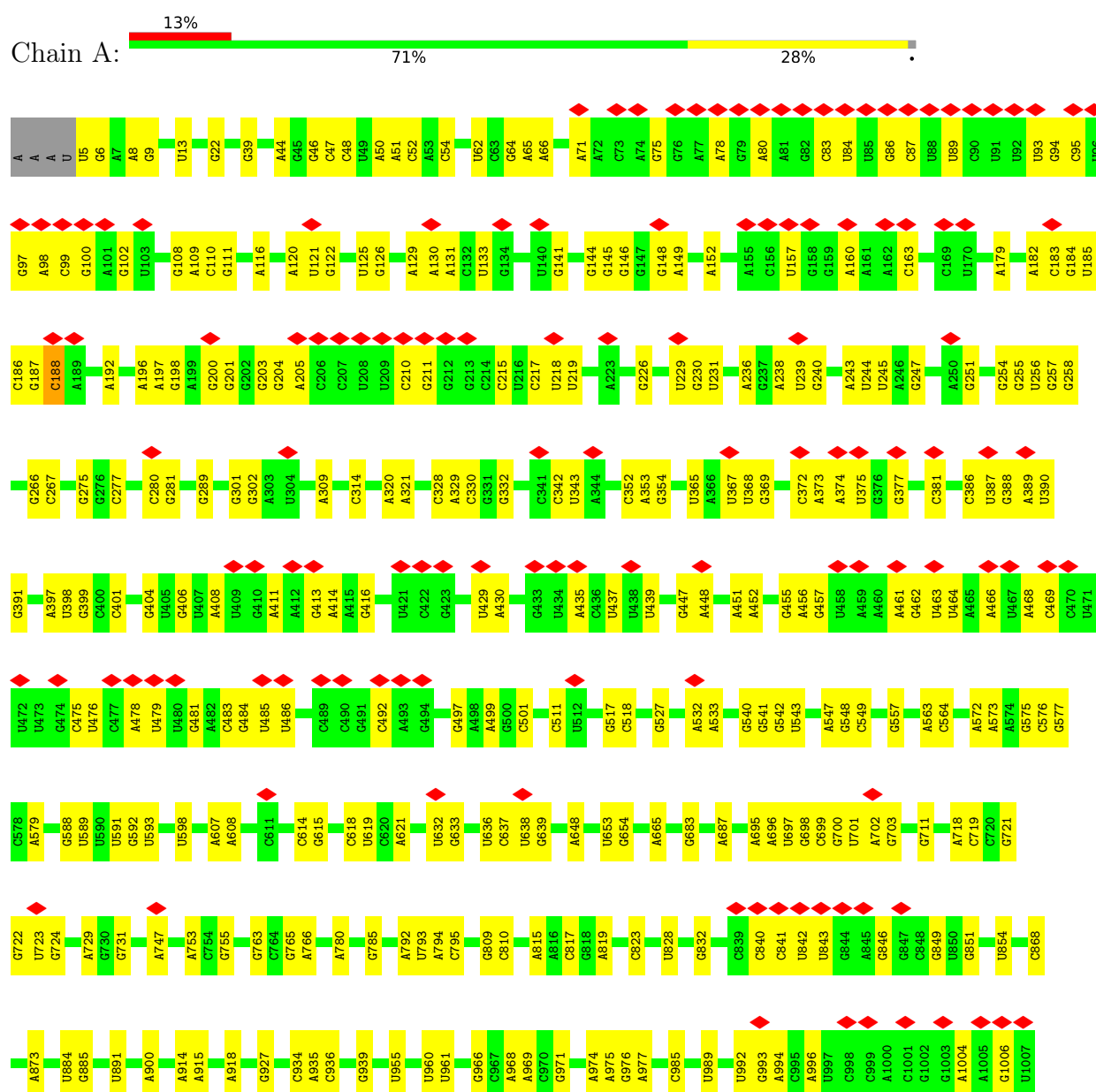


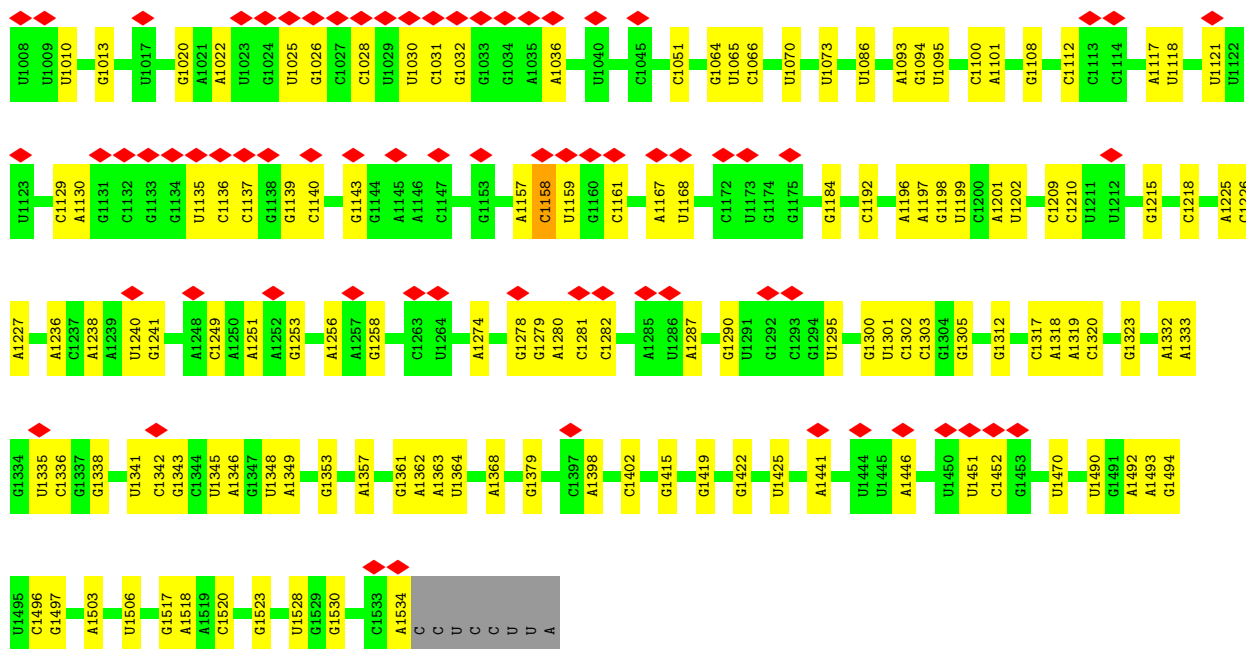
Mol	Chain	Residues	Atoms					AltConf
57	b	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

### 3 Residue-property plots

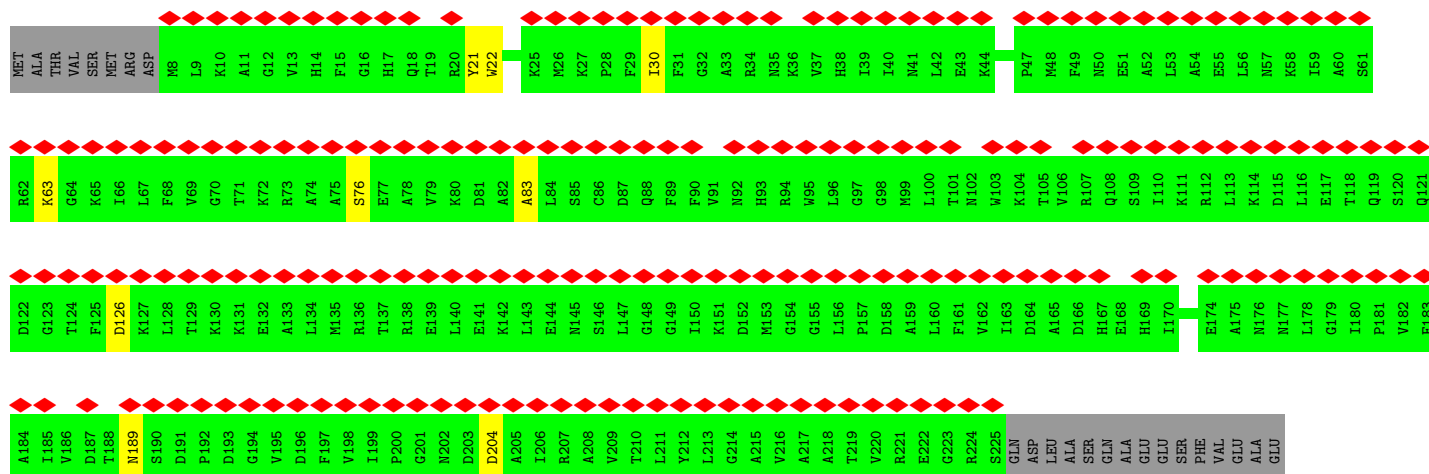
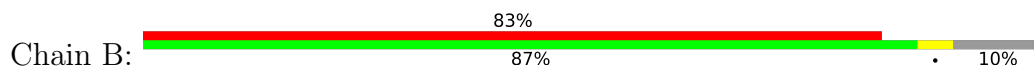
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RNA (1530-MER)

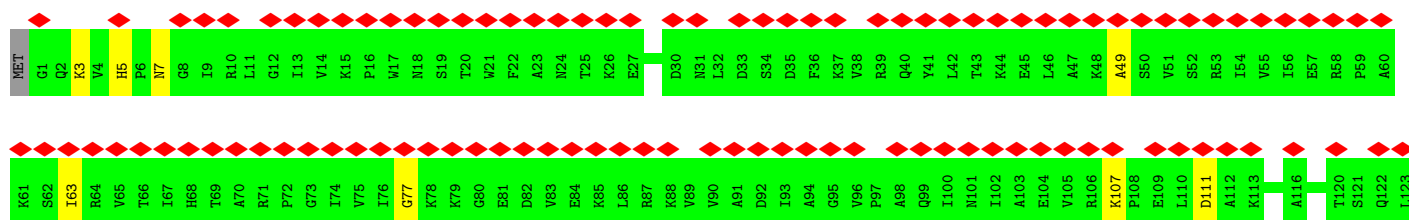
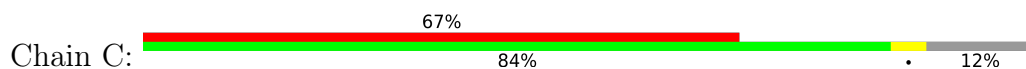


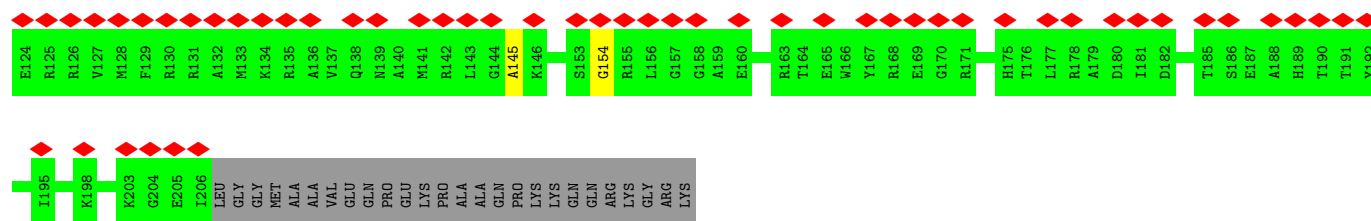


• Molecule 2: 30S ribosomal protein S2

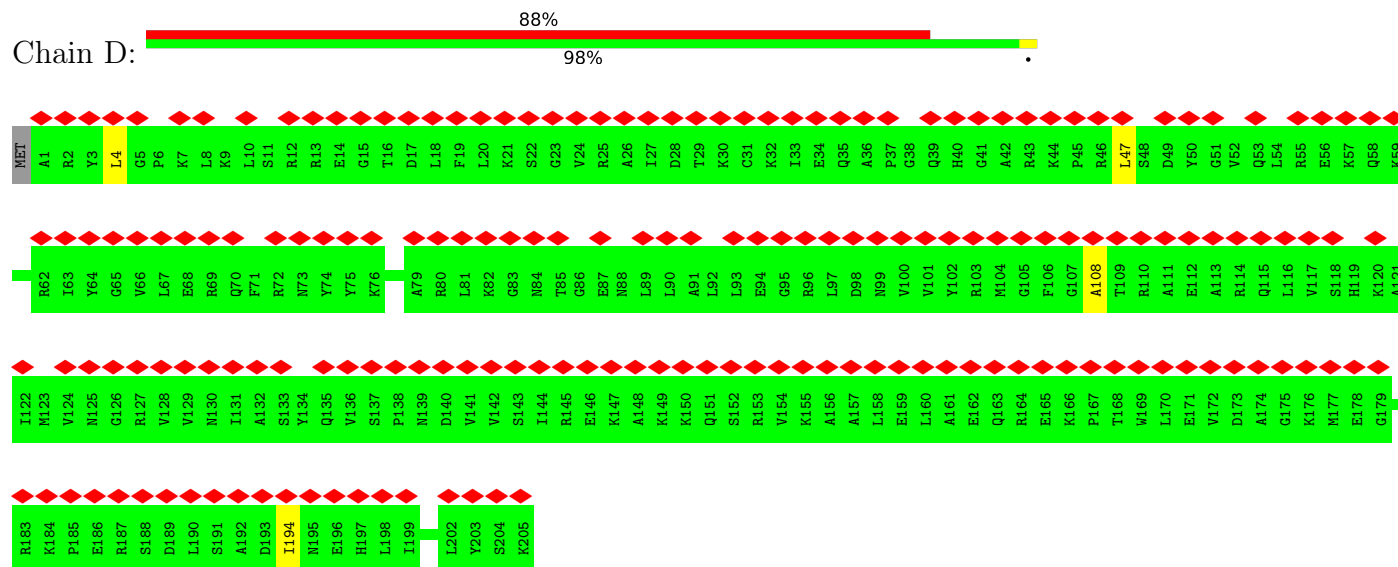


• Molecule 3: 30S ribosomal protein S3

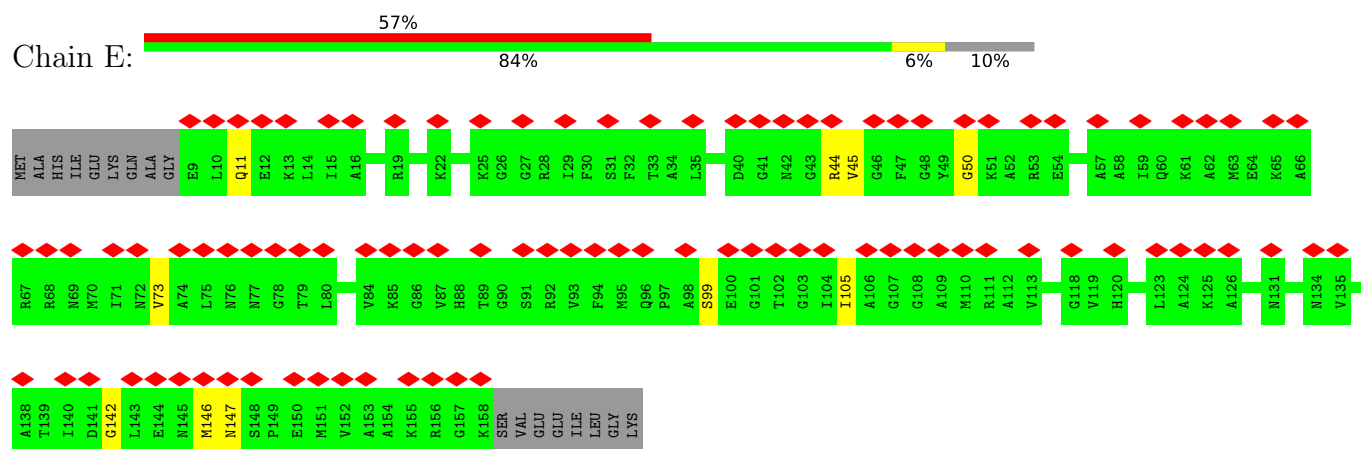




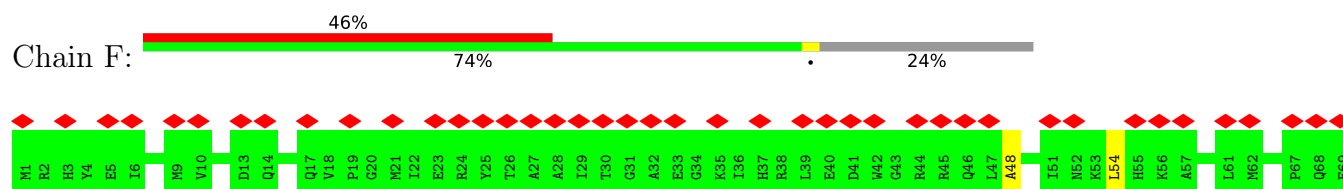
• Molecule 4: 30S ribosomal protein S4



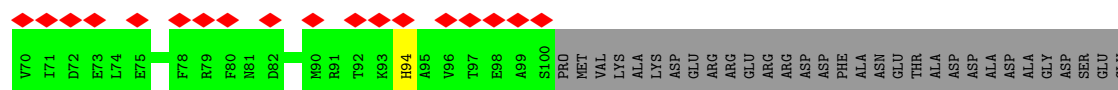
• Molecule 5: 30S ribosomal protein S5



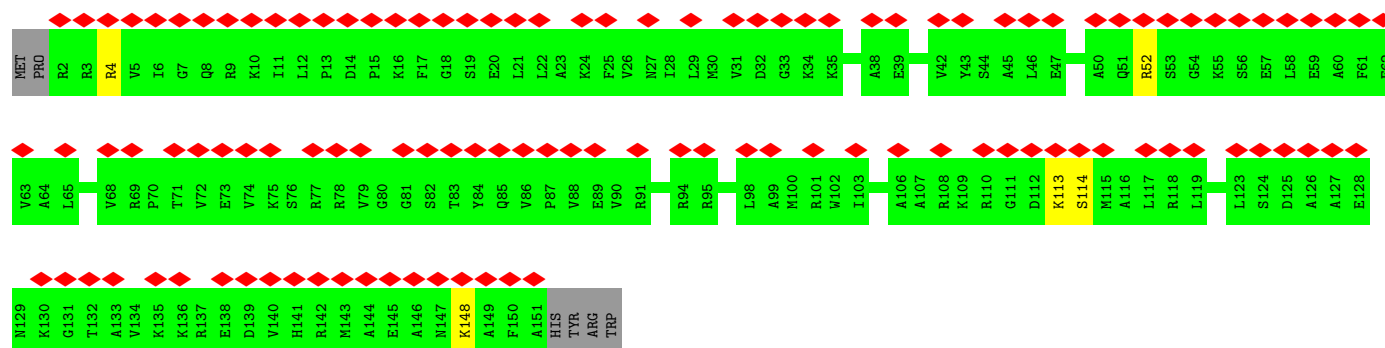
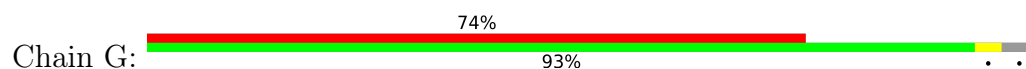
• Molecule 6: 30S ribosomal protein S6



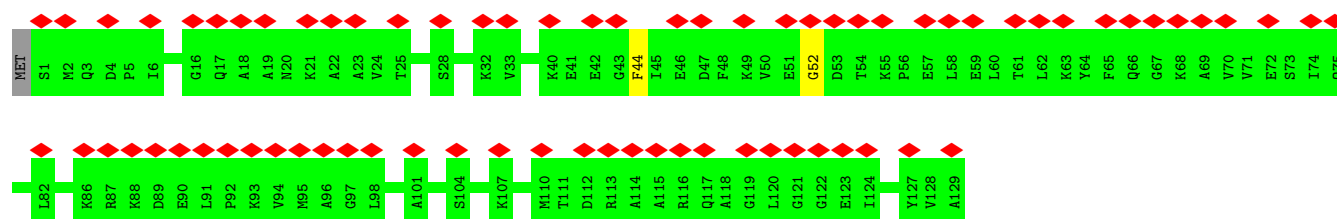


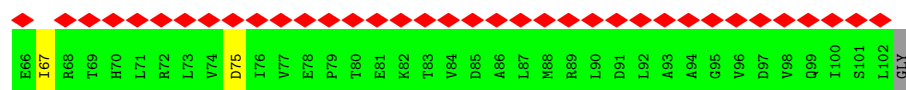


• Molecule 7: 30S ribosomal protein S7

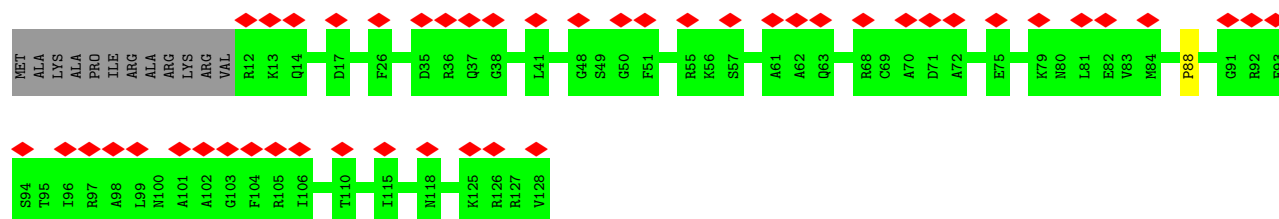
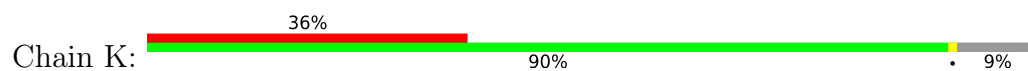


• Molecule 8: 30S ribosomal protein S8

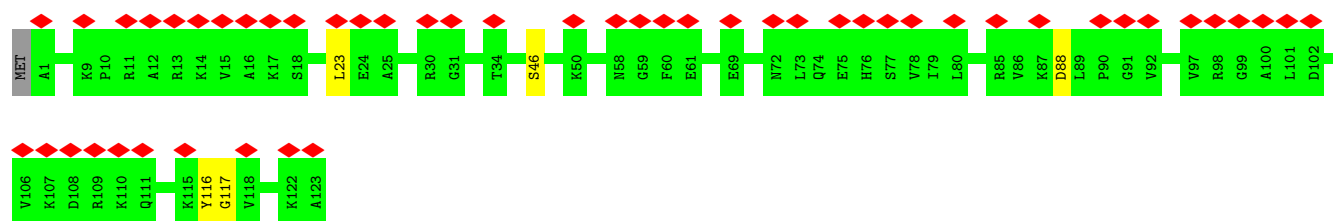




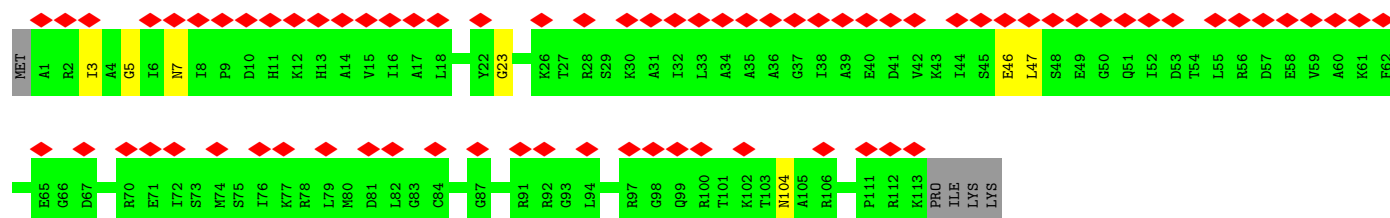
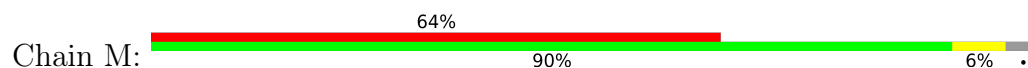
- Molecule 11: 30S ribosomal protein S11



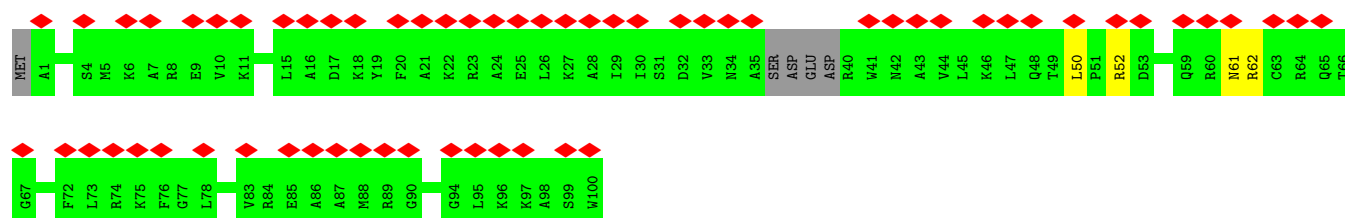
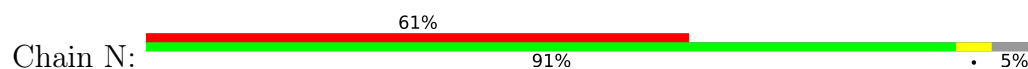
- Molecule 12: 30S ribosomal protein S12



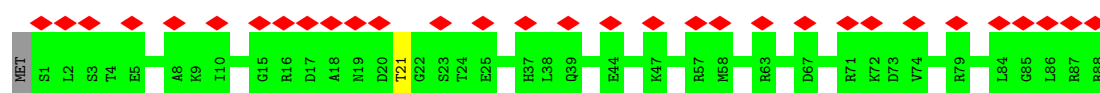
- Molecule 13: 30S ribosomal protein S13



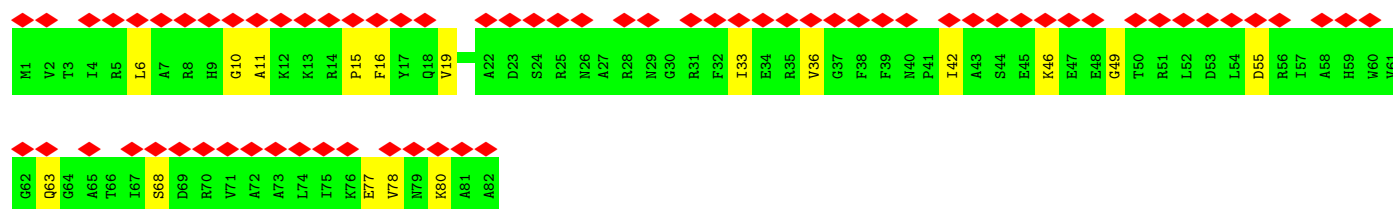
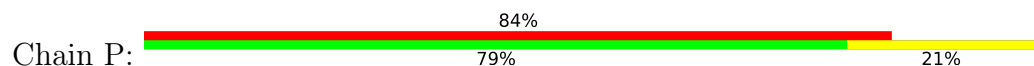
- Molecule 14: 30S ribosomal protein S14



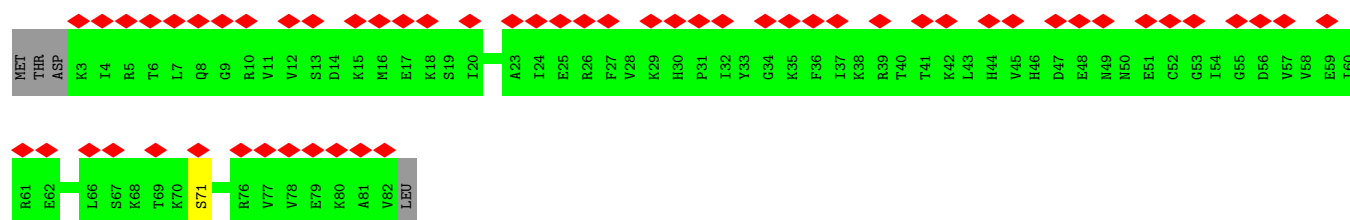
- Molecule 15: 30S ribosomal protein S15



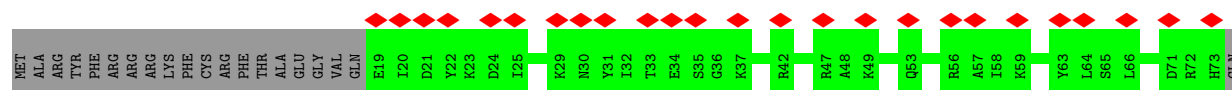
- Molecule 16: 30S ribosomal protein S16



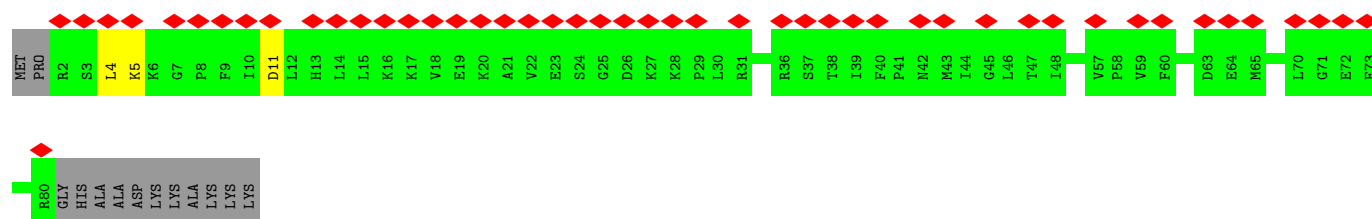
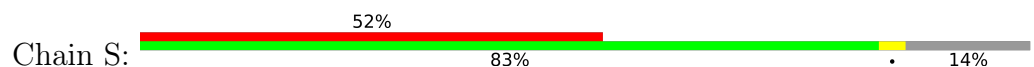
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

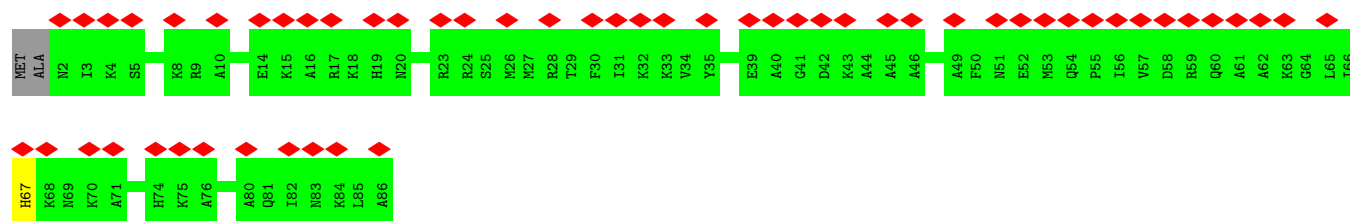


- Molecule 19: 30S ribosomal protein S19

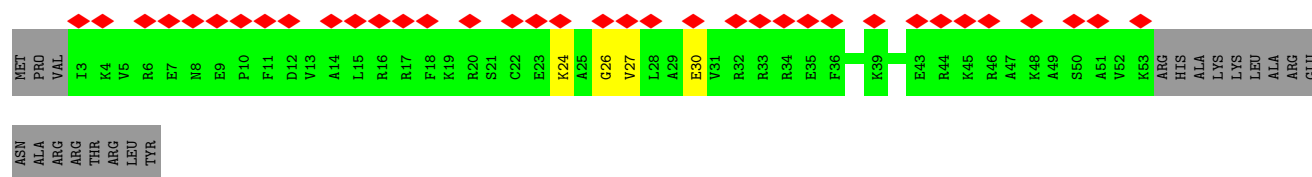


- Molecule 20: 30S ribosomal protein S20

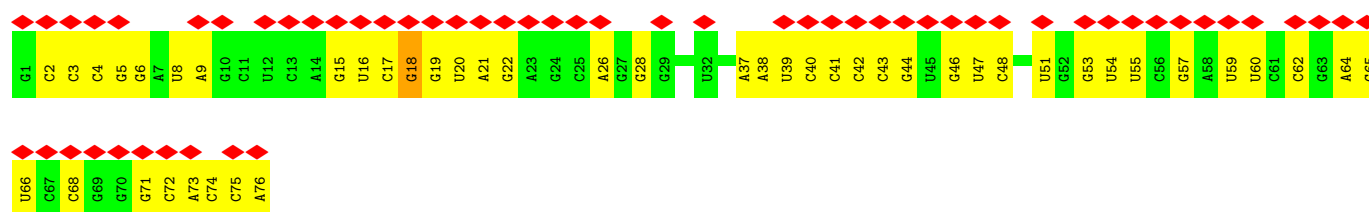
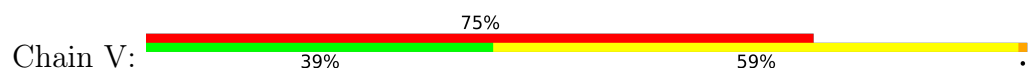




- Molecule 21: 30S ribosomal protein S21



- Molecule 22: RNA (76-MER)



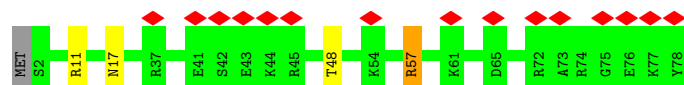
- Molecule 23: RNA (75-MER)



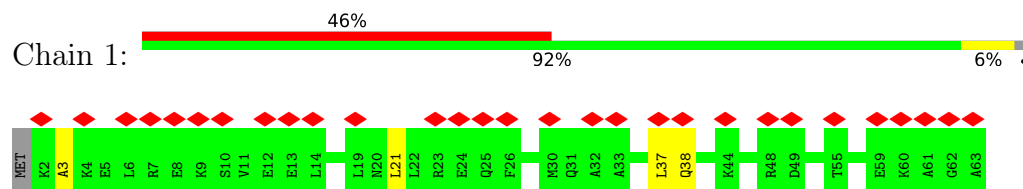
- Molecule 24: RNA (5'-R(P\*CP\*UP\*GP\*GP\*CP\*CP\*UP\*CP\*AP\*A)-3')



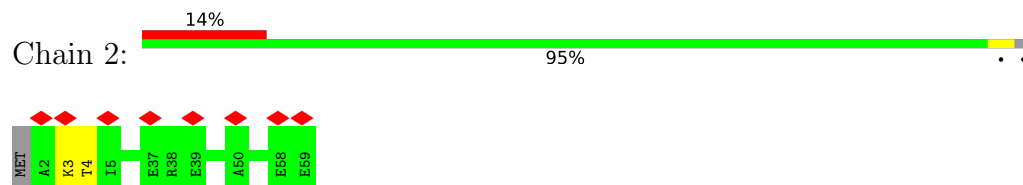
- Molecule 25: 50S ribosomal protein L28



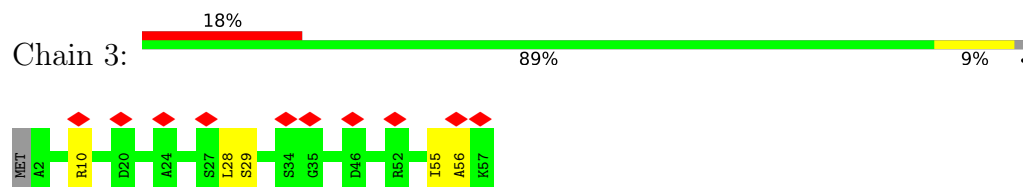
- Molecule 26: 50S ribosomal protein L29



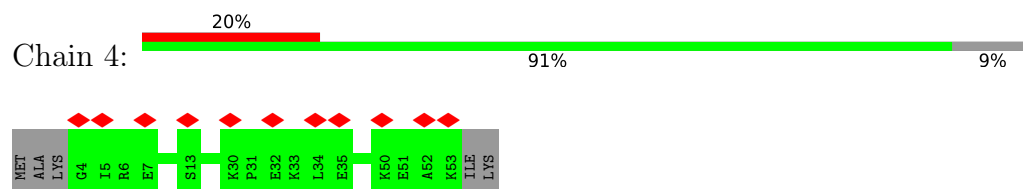
- Molecule 27: 50S ribosomal protein L30



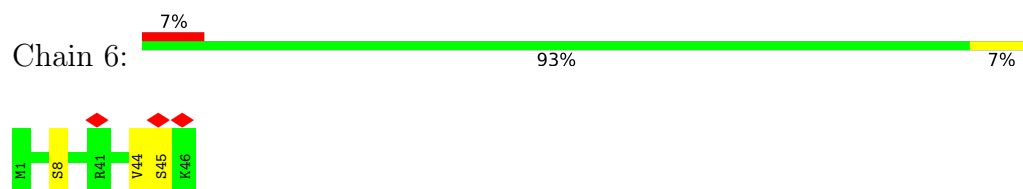
- Molecule 28: 50S ribosomal protein L32



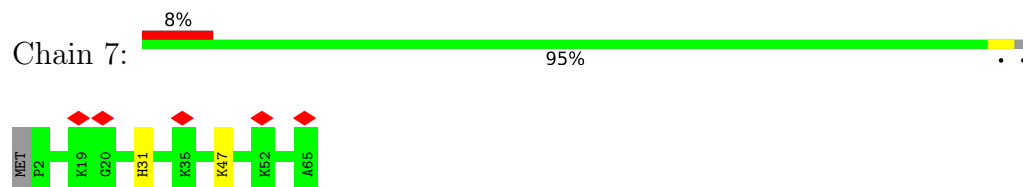
- Molecule 29: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L34

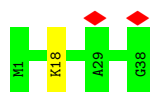


- Molecule 31: 50S ribosomal protein L35



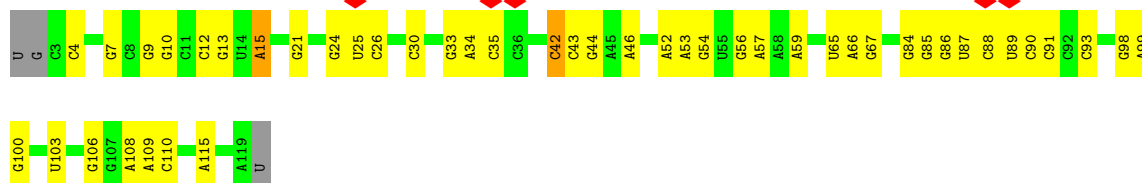
- Molecule 32: 50S ribosomal protein L36





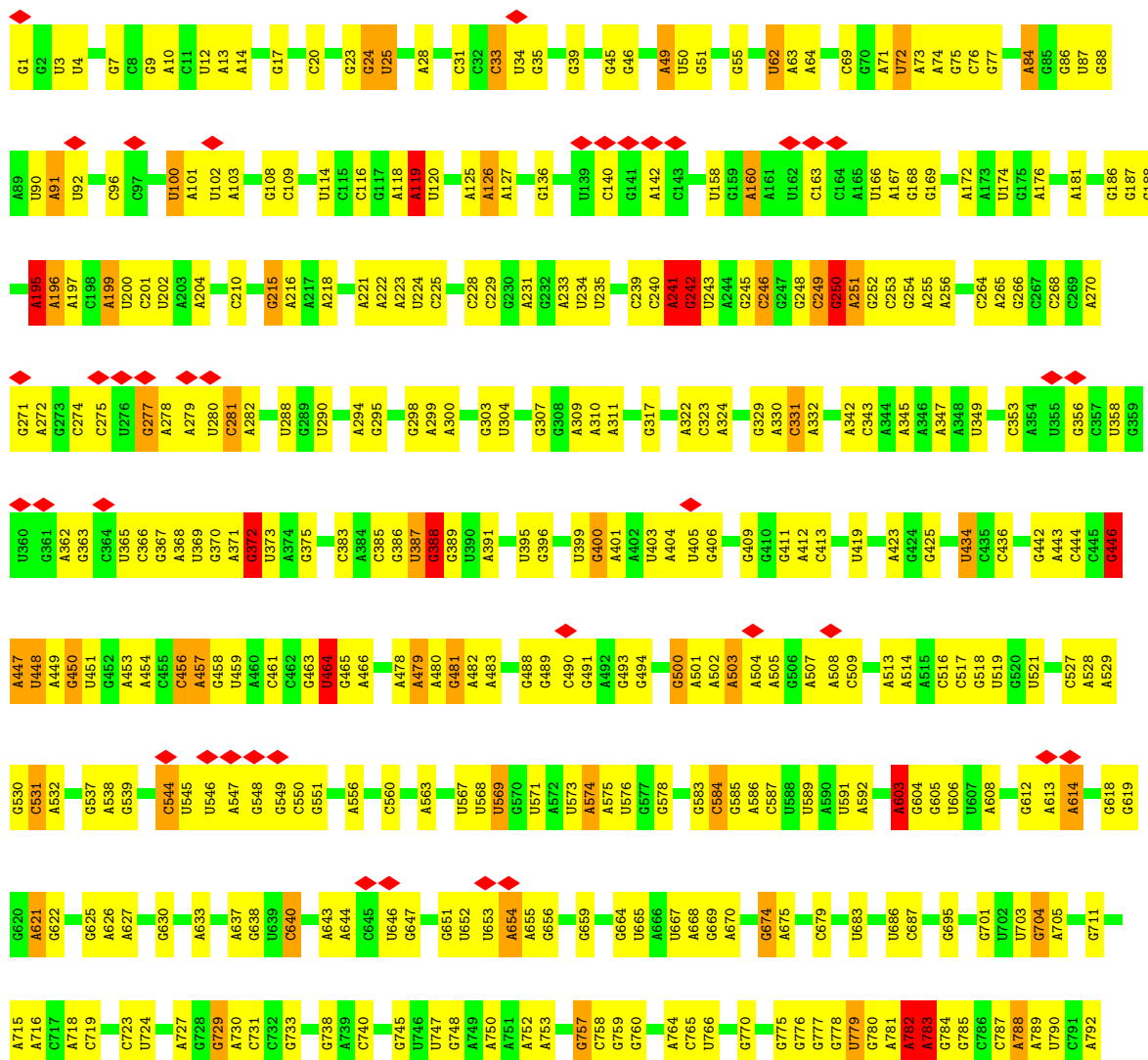
• Molecule 33: RNA (118-MER)

Chain a: 59% 37% ..

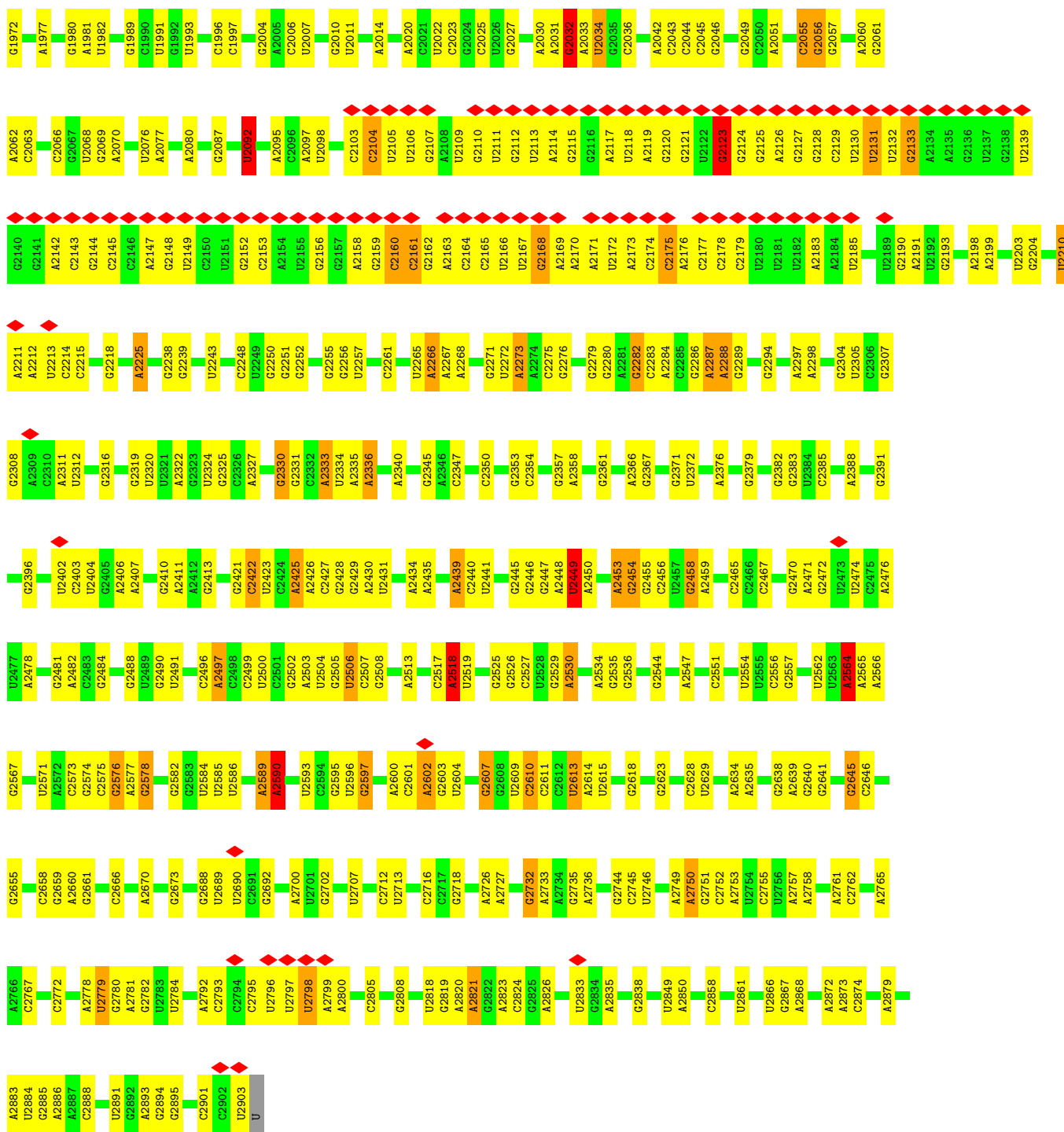


• Molecule 34: RNA (2903-MER)

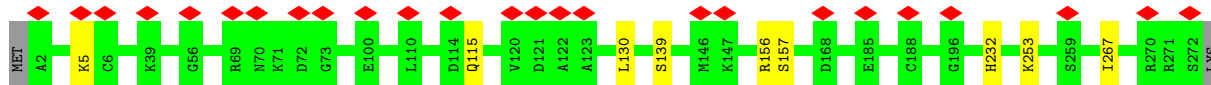
Chain b: 9% 55% 38% 5% .





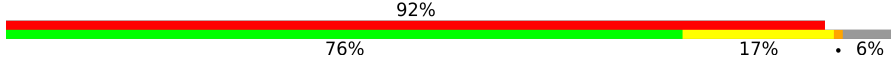


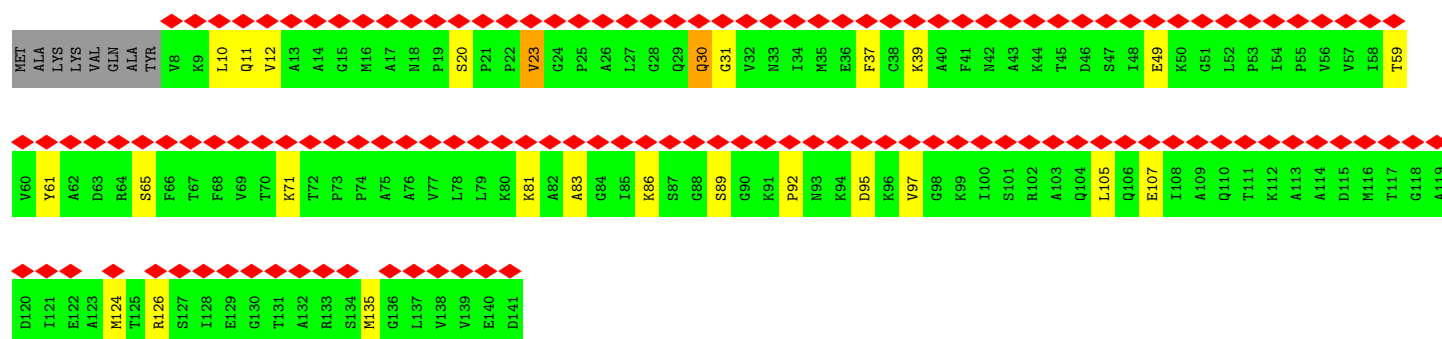
- Molecule 35: 50S ribosomal protein L2



- Molecule 36: 50S ribosomal protein L9

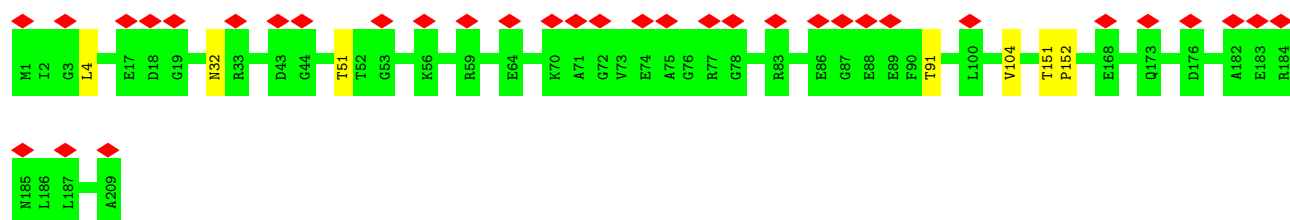


Chain i: 



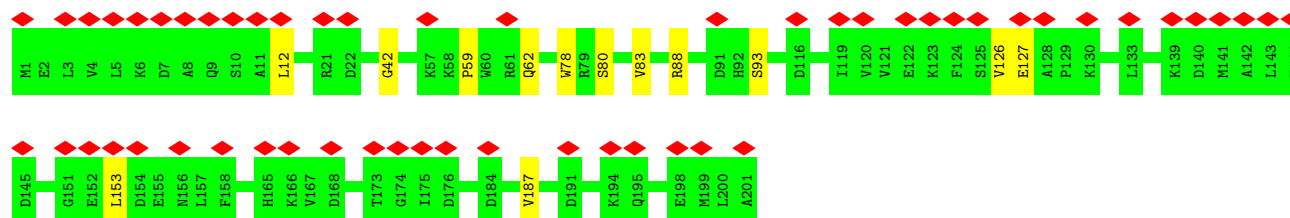
• Molecule 37: 50S ribosomal protein L11

Chain d: 

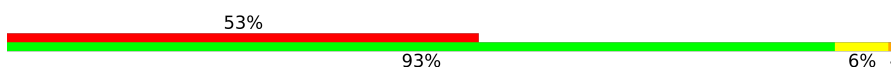


• Molecule 38: 50S ribosomal protein L3

Chain e: 

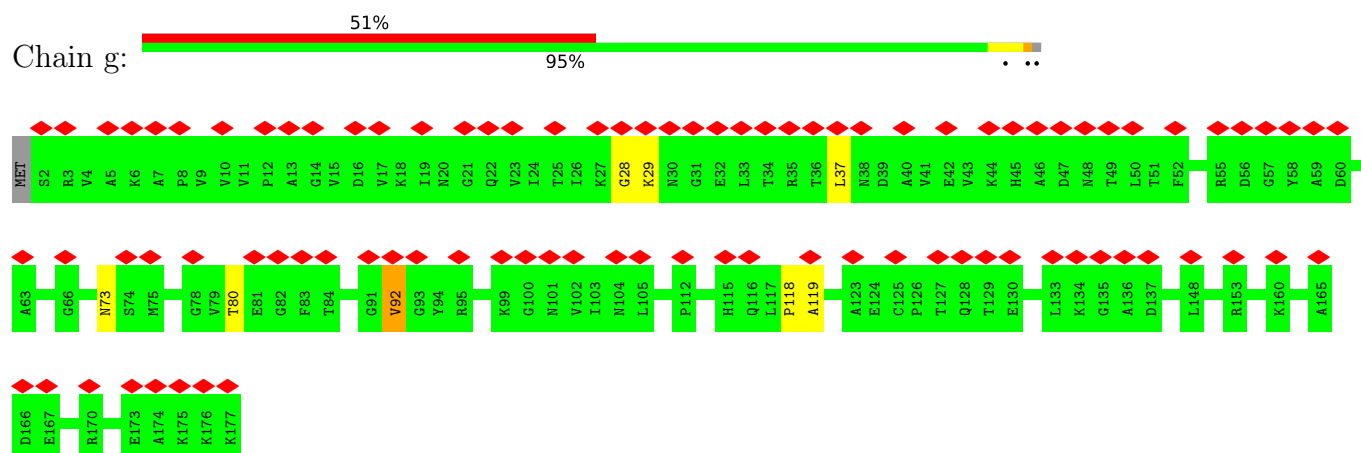


• Molecule 39: 50S ribosomal protein L4

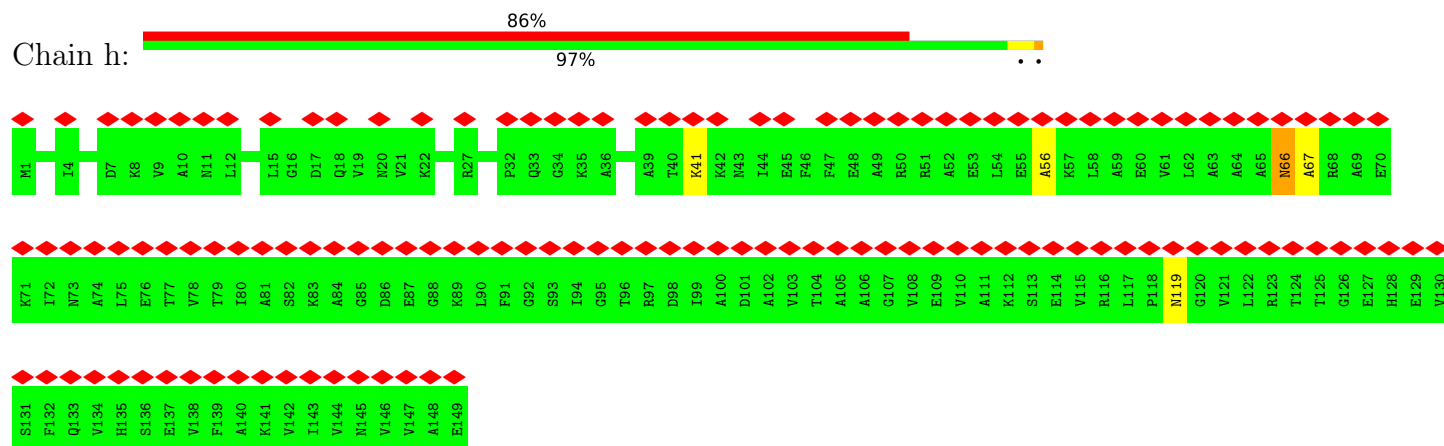
Chain f: 



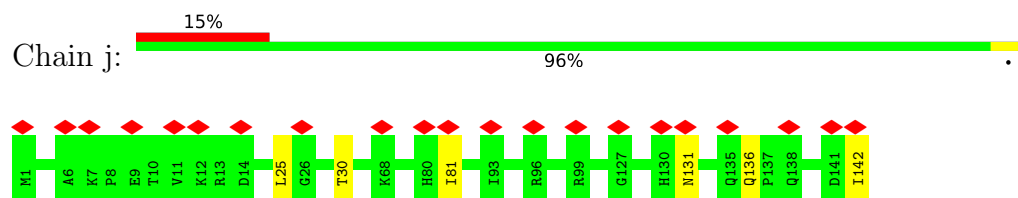
- Molecule 40: 50S ribosomal protein L5



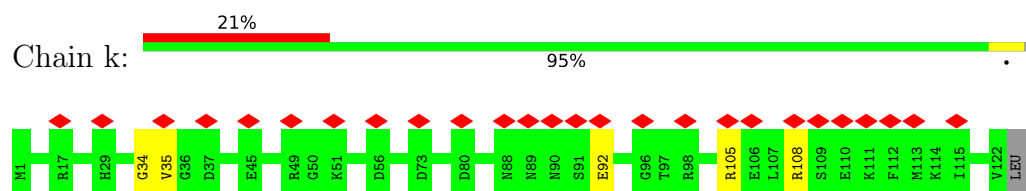
- Molecule 41: 50S ribosomal protein L6



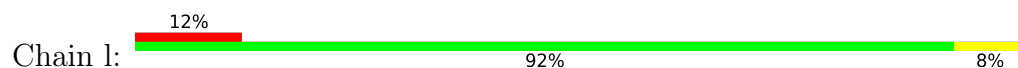
- Molecule 42: 50S ribosomal protein L13

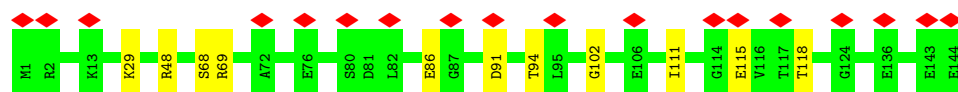


- Molecule 43: 50S ribosomal protein L14

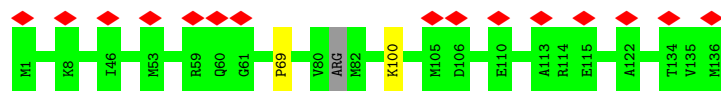


- Molecule 44: 50S ribosomal protein L15

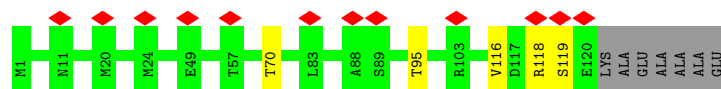
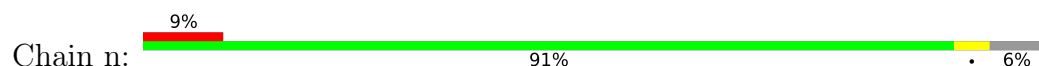




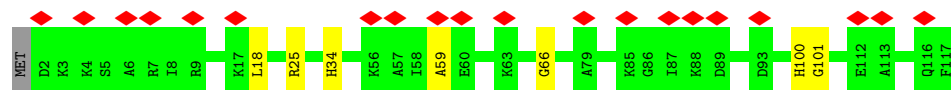
- Molecule 45: 50S ribosomal protein L16



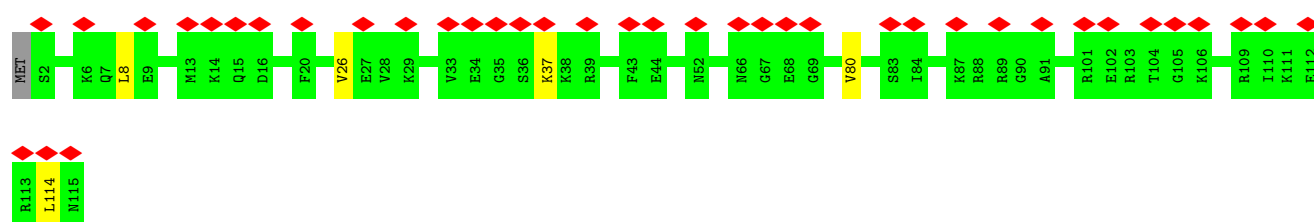
- Molecule 46: 50S ribosomal protein L17



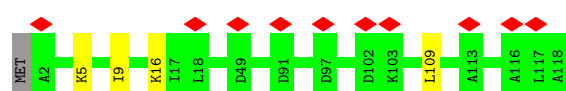
- Molecule 47: 50S ribosomal protein L18



- Molecule 48: 50S ribosomal protein L19

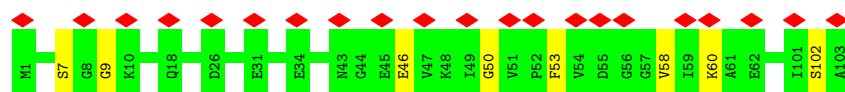


- Molecule 49: 50S ribosomal protein L20

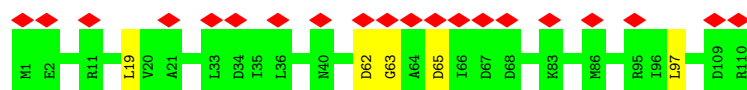


- Molecule 50: 50S ribosomal protein L21

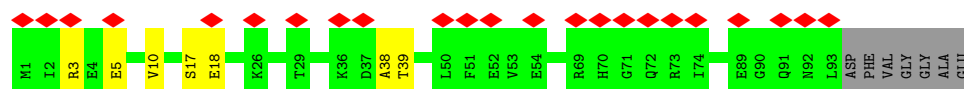
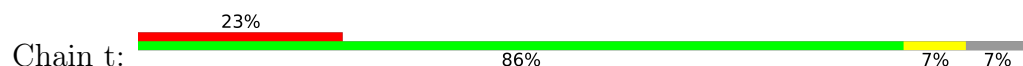




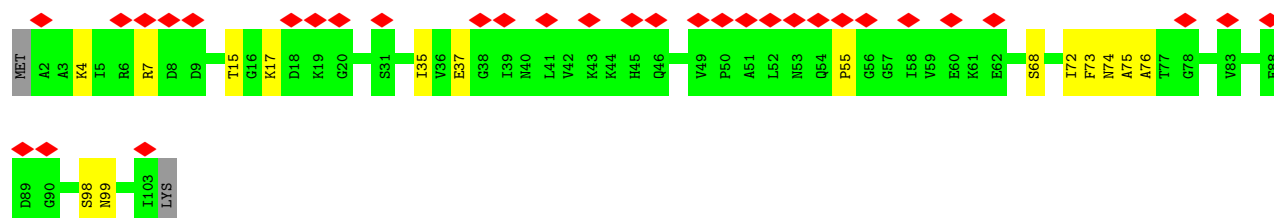
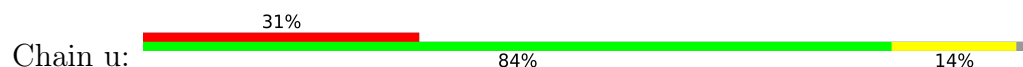
- Molecule 51: 50S ribosomal protein L22



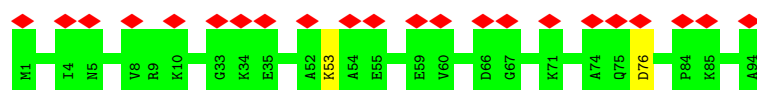
- Molecule 52: 50S ribosomal protein L23



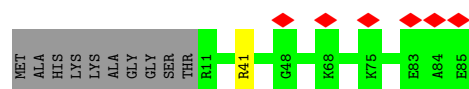
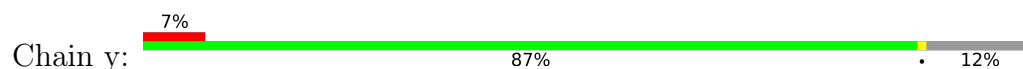
- Molecule 53: 50S ribosomal protein L24



- Molecule 54: 50S ribosomal protein L25



- Molecule 55: 50S ribosomal protein L27



- Molecule 56: Secretion monitor



E3	Q4	R5	L6	I7	S8	E9	E10	D11	L12	F13	S14	T15	P16	V17	W18	I19	S20	Q21	A22	Q23	G24	T25	R26	A27	G28	P29
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60354	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIND	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	16	Depositor
Minimum defocus (nm)	3500	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	37878	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.187	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size ( $\text{\AA}$ )	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.32, 1.32, 1.32	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.47	0/36762	0.79	8/57350 (0.0%)
2	B	0.28	0/1735	0.50	0/2338
3	C	0.32	0/1651	0.53	0/2225
4	D	0.31	0/1665	0.52	0/2227
5	E	0.34	0/1118	0.56	0/1504
6	F	0.28	0/835	0.53	0/1128
7	G	0.28	0/1187	0.51	0/1591
8	H	0.32	0/989	0.52	0/1326
9	I	0.31	0/1034	0.58	0/1375
10	J	0.29	0/796	0.56	0/1077
11	K	0.28	0/893	0.52	0/1205
12	L	0.32	0/969	0.56	0/1300
13	M	0.27	0/884	0.49	0/1181
14	N	0.30	0/785	0.50	0/1043
15	O	0.30	0/724	0.48	0/966
16	P	0.29	0/659	0.49	0/884
17	Q	0.31	0/657	0.49	0/881
18	R	0.29	0/462	0.50	0/621
19	S	0.30	0/652	0.51	0/877
20	T	0.31	0/671	0.49	0/888
21	U	0.29	0/430	0.60	0/570
22	V	0.33	0/1810	0.80	3/2821 (0.1%)
23	W	0.35	1/1786 (0.1%)	0.92	6/2784 (0.2%)
24	X	0.87	1/256 (0.4%)	0.81	0/394
25	0	0.41	0/635	0.76	1/848 (0.1%)
26	1	0.35	0/502	0.63	0/667
27	2	0.39	0/453	0.64	0/605
28	3	0.42	0/450	0.80	1/599 (0.2%)
29	4	0.38	0/416	0.61	0/554
30	6	0.48	0/380	0.86	0/498
31	7	0.40	0/513	0.65	0/676
32	8	0.40	0/303	0.77	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	a	0.45	1/2802 (0.0%)	0.89	4/4369 (0.1%)
34	b	0.59	84/69800 (0.1%)	1.02	432/108892 (0.4%)
35	c	0.42	0/2121	0.76	2/2852 (0.1%)
36	i	0.24	0/989	0.48	0/1334
37	d	0.39	0/1586	0.67	2/2134 (0.1%)
38	e	0.39	0/1571	0.64	1/2113 (0.0%)
39	f	0.39	0/1434	0.66	0/1926
40	g	0.36	0/1343	0.59	1/1816 (0.1%)
41	h	0.27	0/1122	0.60	1/1515 (0.1%)
42	j	0.39	0/1152	0.63	0/1551
43	k	0.41	0/947	0.71	0/1268
44	l	0.41	0/1062	0.71	0/1413
45	m	0.41	0/1081	0.67	0/1443
46	n	0.42	0/973	0.71	0/1301
47	o	0.38	0/902	0.73	2/1209 (0.2%)
48	p	0.38	0/929	0.67	0/1242
49	q	0.45	0/960	0.74	0/1278
50	r	0.43	0/829	0.65	0/1107
51	s	0.39	0/864	0.70	0/1156
52	t	0.41	0/744	0.67	1/994 (0.1%)
53	u	0.39	0/787	0.68	0/1051
54	w	0.36	0/766	0.59	0/1025
55	y	0.38	0/576	0.64	0/762
56	z	0.46	1/215 (0.5%)	0.91	1/291 (0.3%)
All	All	0.50	88/158617 (0.1%)	0.87	466/237442 (0.2%)

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
9	I	0	1
27	2	0	1
34	b	0	64
35	c	0	1
37	d	0	1
43	k	0	1
44	l	0	1
50	r	0	1
All	All	0	71

The worst 5 of 88 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	2610	C	O3'-P	18.27	1.83	1.61
34	b	2123	G	C6-N1	17.59	1.51	1.39
34	b	2504	U	O3'-P	16.95	1.81	1.61
34	b	2123	G	N3-C4	16.78	1.47	1.35
34	b	2123	G	N9-C8	14.57	1.48	1.37

The worst 5 of 466 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	36	C	O3'-P-O5'	22.33	146.43	104.00
34	b	2602	A	P-O3'-C3'	15.43	138.22	119.70
34	b	1275	A	N9-C1'-C2'	15.08	133.61	114.00
34	b	1096	A	N9-C1'-C2'	-14.60	95.02	114.00
34	b	400	G	N9-C1'-C2'	14.53	132.89	114.00

There are no chirality outliers.

5 of 71 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	2	3	LYS	Peptide
9	I	124	PRO	Peptide
34	b	119	A	Sidechain
34	b	195	A	Sidechain
34	b	25	U	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	
2	B	216/241 (90%)	188 (87%)	19 (9%)	9 (4%)	3	18
3	C	204/233 (88%)	171 (84%)	23 (11%)	10 (5%)	2	15
4	D	203/206 (98%)	190 (94%)	9 (4%)	4 (2%)	7	33
5	E	148/167 (89%)	131 (88%)	7 (5%)	10 (7%)	1	9
6	F	98/131 (75%)	81 (83%)	14 (14%)	3 (3%)	4	24
7	G	148/156 (95%)	135 (91%)	8 (5%)	5 (3%)	3	23
8	H	127/130 (98%)	110 (87%)	15 (12%)	2 (2%)	9	37
9	I	125/130 (96%)	106 (85%)	16 (13%)	3 (2%)	6	29
10	J	96/103 (93%)	84 (88%)	7 (7%)	5 (5%)	2	14
11	K	115/129 (89%)	104 (90%)	10 (9%)	1 (1%)	17	49
12	L	121/124 (98%)	94 (78%)	22 (18%)	5 (4%)	3	18
13	M	111/118 (94%)	99 (89%)	5 (4%)	7 (6%)	1	10
14	N	92/101 (91%)	80 (87%)	8 (9%)	4 (4%)	2	18
15	O	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	43
16	P	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	0	3
17	Q	78/84 (93%)	66 (85%)	11 (14%)	1 (1%)	12	40
18	R	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	S	77/92 (84%)	69 (90%)	5 (6%)	3 (4%)	3	20
20	T	83/87 (95%)	77 (93%)	5 (6%)	1 (1%)	13	43
21	U	49/71 (69%)	40 (82%)	5 (10%)	4 (8%)	1	6
25	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
26	1	60/63 (95%)	53 (88%)	5 (8%)	2 (3%)	4	23
27	2	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	8	35
28	3	54/57 (95%)	49 (91%)	3 (6%)	2 (4%)	3	21
29	4	48/55 (87%)	39 (81%)	9 (19%)	0	100	100
30	6	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	2	16
31	7	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
32	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
35	c	269/273 (98%)	251 (93%)	17 (6%)	1 (0%)	34	66
36	i	132/142 (93%)	83 (63%)	38 (29%)	11 (8%)	1	6
37	d	207/209 (99%)	194 (94%)	11 (5%)	2 (1%)	15	47
38	e	199/201 (99%)	186 (94%)	7 (4%)	6 (3%)	4	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	f	175/179 (98%)	157 (90%)	12 (7%)	6 (3%)	3	23
40	g	174/177 (98%)	139 (80%)	31 (18%)	4 (2%)	6	30
41	h	147/149 (99%)	122 (83%)	20 (14%)	5 (3%)	3	23
42	j	140/142 (99%)	128 (91%)	10 (7%)	2 (1%)	11	39
43	k	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	9	36
44	l	142/144 (99%)	126 (89%)	10 (7%)	6 (4%)	3	18
45	m	131/136 (96%)	123 (94%)	7 (5%)	1 (1%)	19	51
46	n	118/127 (93%)	111 (94%)	4 (3%)	3 (2%)	5	28
47	o	114/117 (97%)	104 (91%)	5 (4%)	5 (4%)	2	17
48	p	112/115 (97%)	106 (95%)	5 (4%)	1 (1%)	17	49
49	q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
50	r	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	4	25
51	s	108/110 (98%)	103 (95%)	2 (2%)	3 (3%)	5	26
52	t	91/100 (91%)	80 (88%)	8 (9%)	3 (3%)	4	23
53	u	100/104 (96%)	77 (77%)	12 (12%)	11 (11%)	0	3
54	w	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
55	y	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
56	z	25/27 (93%)	20 (80%)	5 (20%)	0	100	100
All	All	5630/5985 (94%)	5003 (89%)	458 (8%)	169 (3%)	7	25

5 of 169 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	7	ASN
5	E	99	SER
8	H	44	PHE
9	I	57	VAL
12	L	88	ASP

### 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	
2	B	180/199 (90%)	180 (100%)	0	100	100
3	C	170/190 (90%)	170 (100%)	0	100	100
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	113/126 (90%)	113 (100%)	0	100	100
6	F	87/112 (78%)	87 (100%)	0	100	100
7	G	123/129 (95%)	123 (100%)	0	100	100
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	90/99 (91%)	90 (100%)	0	100	100
12	L	103/104 (99%)	103 (100%)	0	100	100
13	M	91/96 (95%)	91 (100%)	0	100	100
14	N	79/84 (94%)	79 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	57 (88%)	8 (12%)	4	20
17	Q	74/78 (95%)	74 (100%)	0	100	100
18	R	48/65 (74%)	48 (100%)	0	100	100
19	S	70/79 (89%)	70 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	44/61 (72%)	44 (100%)	0	100	100
25	0	67/68 (98%)	63 (94%)	4 (6%)	19	50
26	1	54/55 (98%)	52 (96%)	2 (4%)	34	64
27	2	48/49 (98%)	48 (100%)	0	100	100
28	3	47/48 (98%)	45 (96%)	2 (4%)	29	61
29	4	45/49 (92%)	45 (100%)	0	100	100
30	6	38/38 (100%)	37 (97%)	1 (3%)	46	72
31	7	51/52 (98%)	49 (96%)	2 (4%)	32	63
32	8	34/34 (100%)	33 (97%)	1 (3%)	42	70
35	c	216/218 (99%)	210 (97%)	6 (3%)	43	71
36	i	104/110 (94%)	87 (84%)	17 (16%)	2	10
37	d	164/164 (100%)	161 (98%)	3 (2%)	59	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	e	165/165 (100%)	159 (96%)	6 (4%)	35	65
39	f	148/150 (99%)	142 (96%)	6 (4%)	30	62
40	g	137/138 (99%)	133 (97%)	4 (3%)	42	70
41	h	114/114 (100%)	114 (100%)	0	100	100
42	j	116/116 (100%)	112 (97%)	4 (3%)	37	66
43	k	103/104 (99%)	101 (98%)	2 (2%)	57	78
44	l	103/103 (100%)	99 (96%)	4 (4%)	32	63
45	m	108/109 (99%)	107 (99%)	1 (1%)	78	88
46	n	100/103 (97%)	98 (98%)	2 (2%)	55	77
47	o	86/87 (99%)	86 (100%)	0	100	100
48	p	99/100 (99%)	95 (96%)	4 (4%)	31	62
49	q	89/90 (99%)	85 (96%)	4 (4%)	27	60
50	r	84/84 (100%)	80 (95%)	4 (5%)	25	58
51	s	93/93 (100%)	91 (98%)	2 (2%)	52	76
52	t	80/84 (95%)	77 (96%)	3 (4%)	33	63
53	u	83/85 (98%)	79 (95%)	4 (5%)	25	58
54	w	78/78 (100%)	76 (97%)	2 (3%)	46	72
55	y	56/63 (89%)	55 (98%)	1 (2%)	59	79
56	z	23/23 (100%)	13 (56%)	10 (44%)	0	0
All	All	4678/4879 (96%)	4569 (98%)	109 (2%)	53	75

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	f	174	ASP
44	l	118	THR
56	z	4	GLN
40	g	73	ASN
42	j	142	ILE

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

Mol	Chain	Res	Type
41	h	28	ASN

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Mol	Chain	Res	Type
41	h	119	ASN
56	z	4	GLN
9	I	3	ASN
8	H	37	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1530/1542 (99%)	422 (27%)	30 (1%)
22	V	75/76 (98%)	45 (60%)	9 (12%)
23	W	75/75 (100%)	40 (53%)	10 (13%)
24	X	11/11 (100%)	8 (72%)	3 (27%)
33	a	116/120 (96%)	43 (37%)	0
34	b	2902/2904 (99%)	1204 (41%)	0
All	All	4709/4728 (99%)	1762 (37%)	52 (1%)

5 of 1762 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	22	G

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1348	U
22	V	40	C
24	X	12	C
1	A	1492	A
22	V	18	G

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

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	CLM	b	9000	-	19,20,20	0.88	1 (5%)	23,27,27	0.80	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
57	CLM	b	9000	-	-	10/20/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	b	9000	CLM	C9-N9	-2.07	1.40	1.45

There are no bond angle outliers.

There are no chirality outliers.

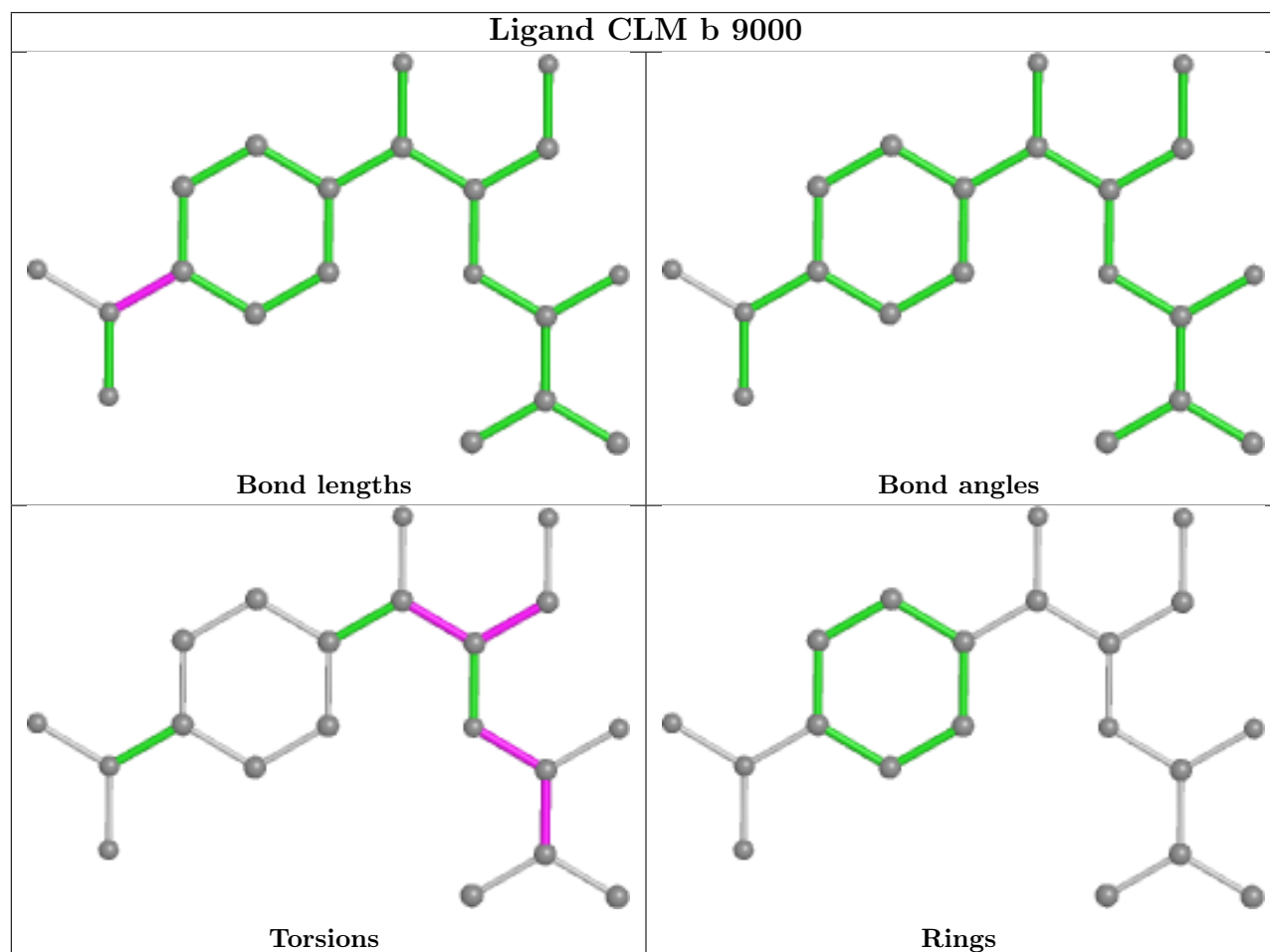
5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	b	9000	CLM	N2-C3-C5-O5
57	b	9000	CLM	N2-C3-C5-C6
57	b	9000	CLM	C4-C3-C5-O5
57	b	9000	CLM	O2-C2-N2-C3
57	b	9000	CLM	C1-C2-N2-C3

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	b	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	2610:C	O3'	2611:C	P	1.83
1	b	2504:U	O3'	2505:G	P	1.81
1	b	2248:C	O3'	2249:U	P	1.78
1	b	1323:C	O3'	1324:G	P	1.77

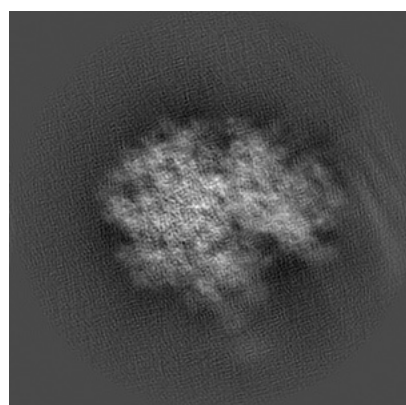
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6486. These allow visual inspection of the internal detail of the map and identification of artifacts.

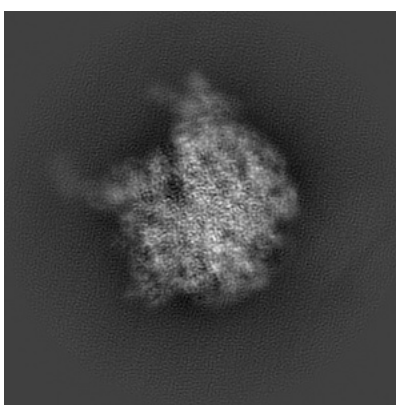
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

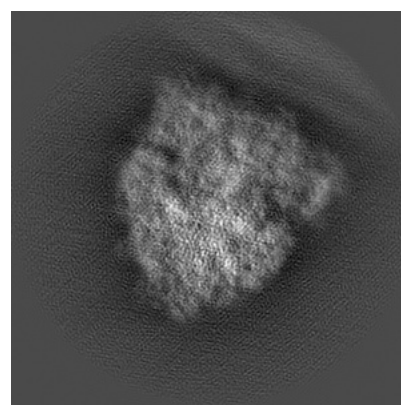
#### 6.1.1 Primary map



X



Y

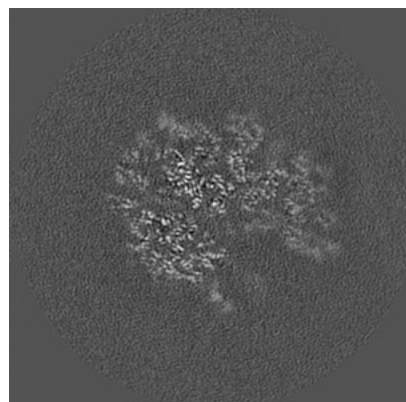


Z

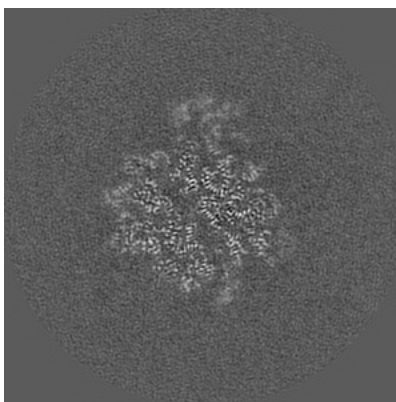
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

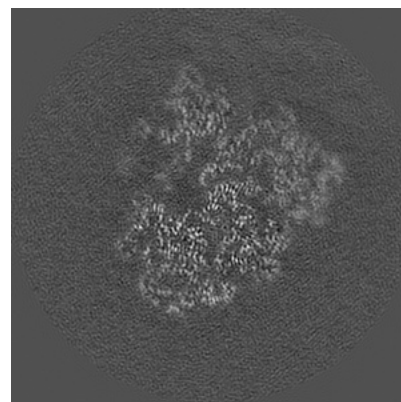
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

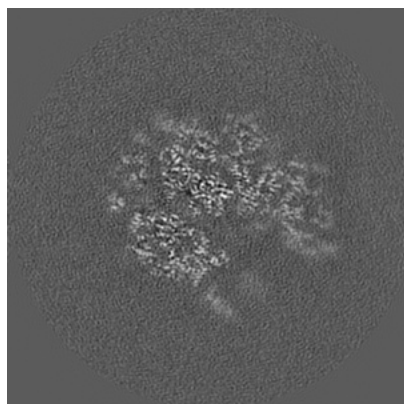


Z Index: 160

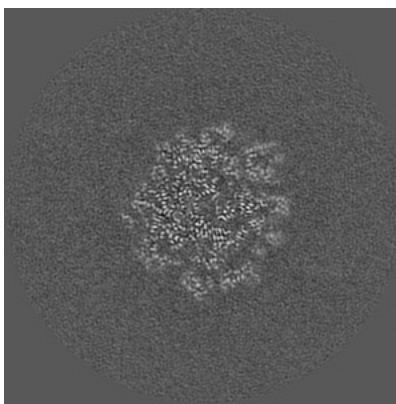
The images above show central slices of the map in three orthogonal directions.

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

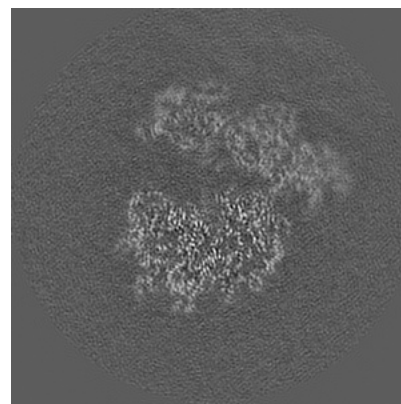
### 6.3.1 Primary map



X Index: 162



Y Index: 136



Z Index: 151

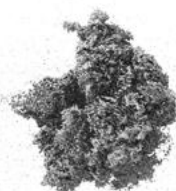
The images above show the largest variance slices of the map in three orthogonal directions.

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

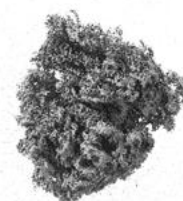
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

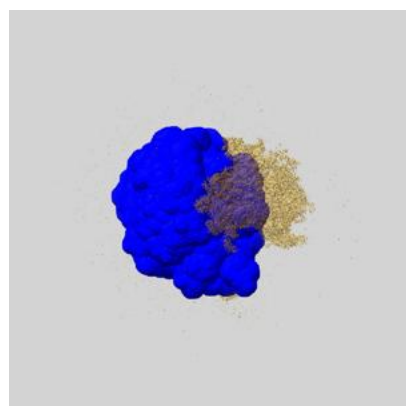
## 6.5 Mask visualisation [i](#)

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

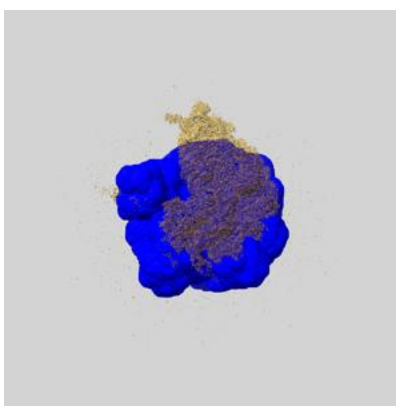
A mask typically either:

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

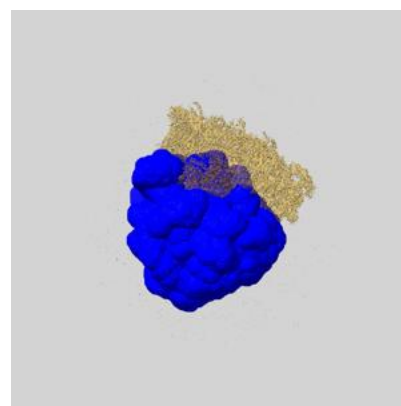
### 6.5.1 emd\_6486\_msk.map [i](#)



X



Y

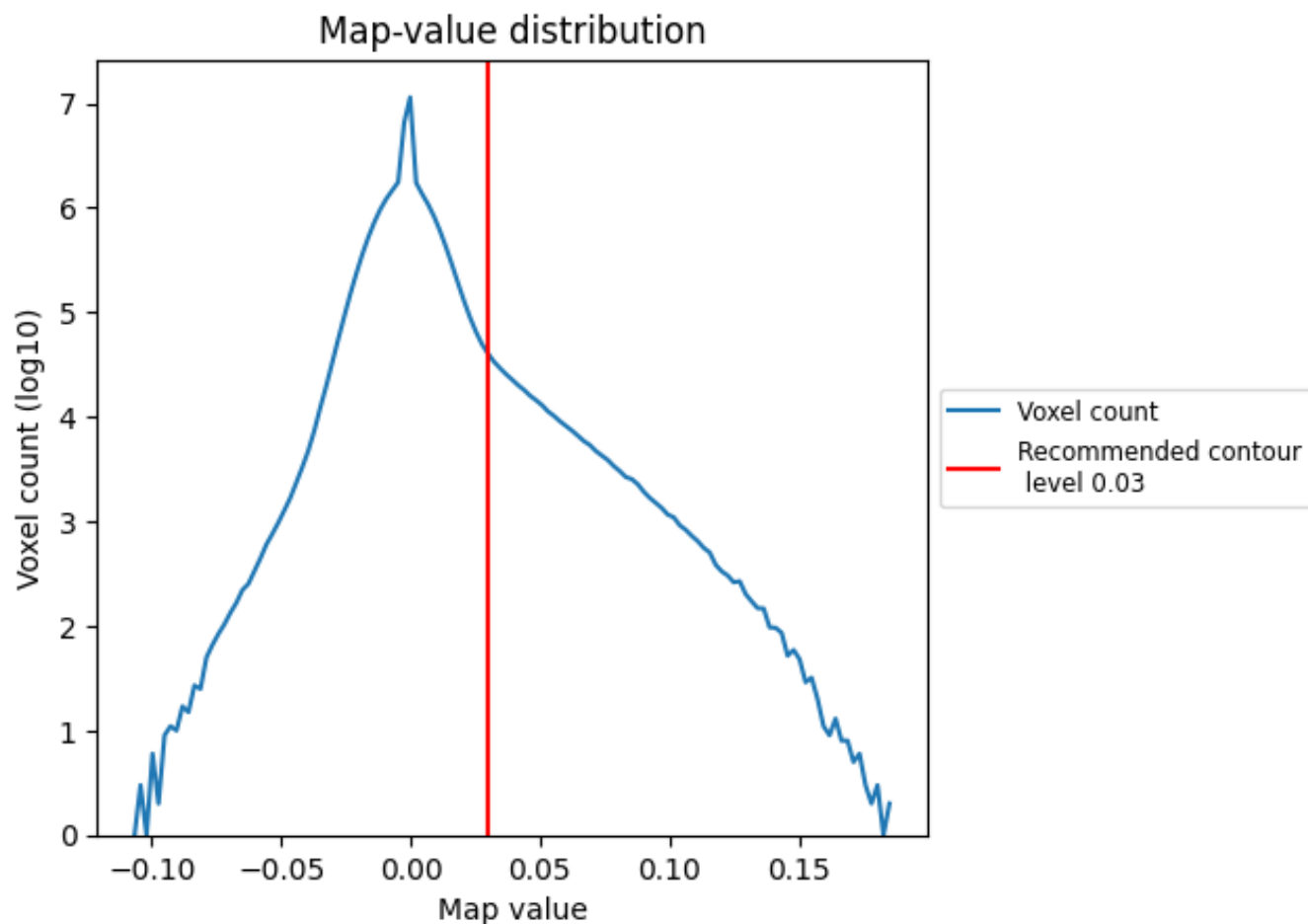


Z

## 7 Map analysis [i](#)

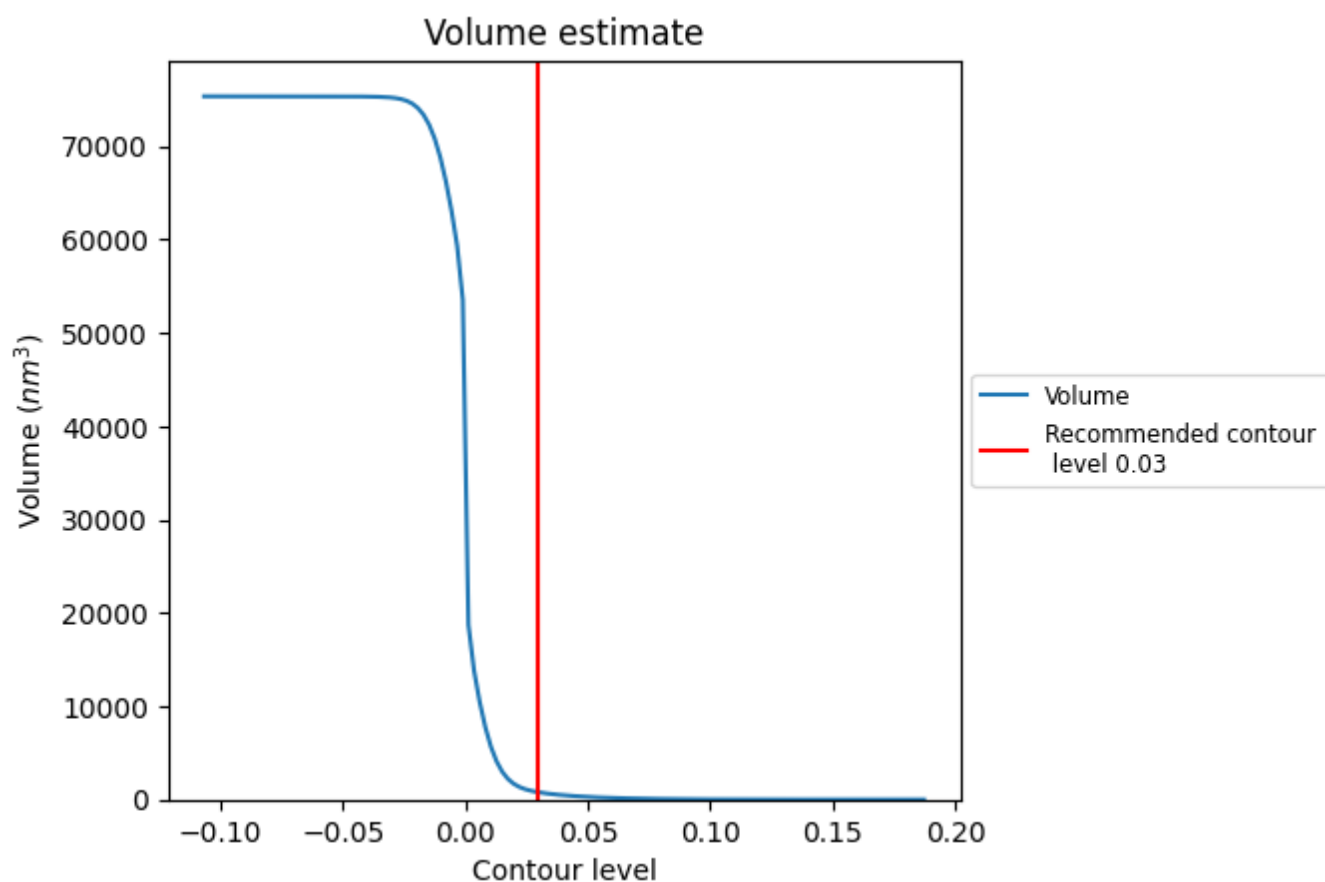
This section contains the results of statistical analysis of the map.

### 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.

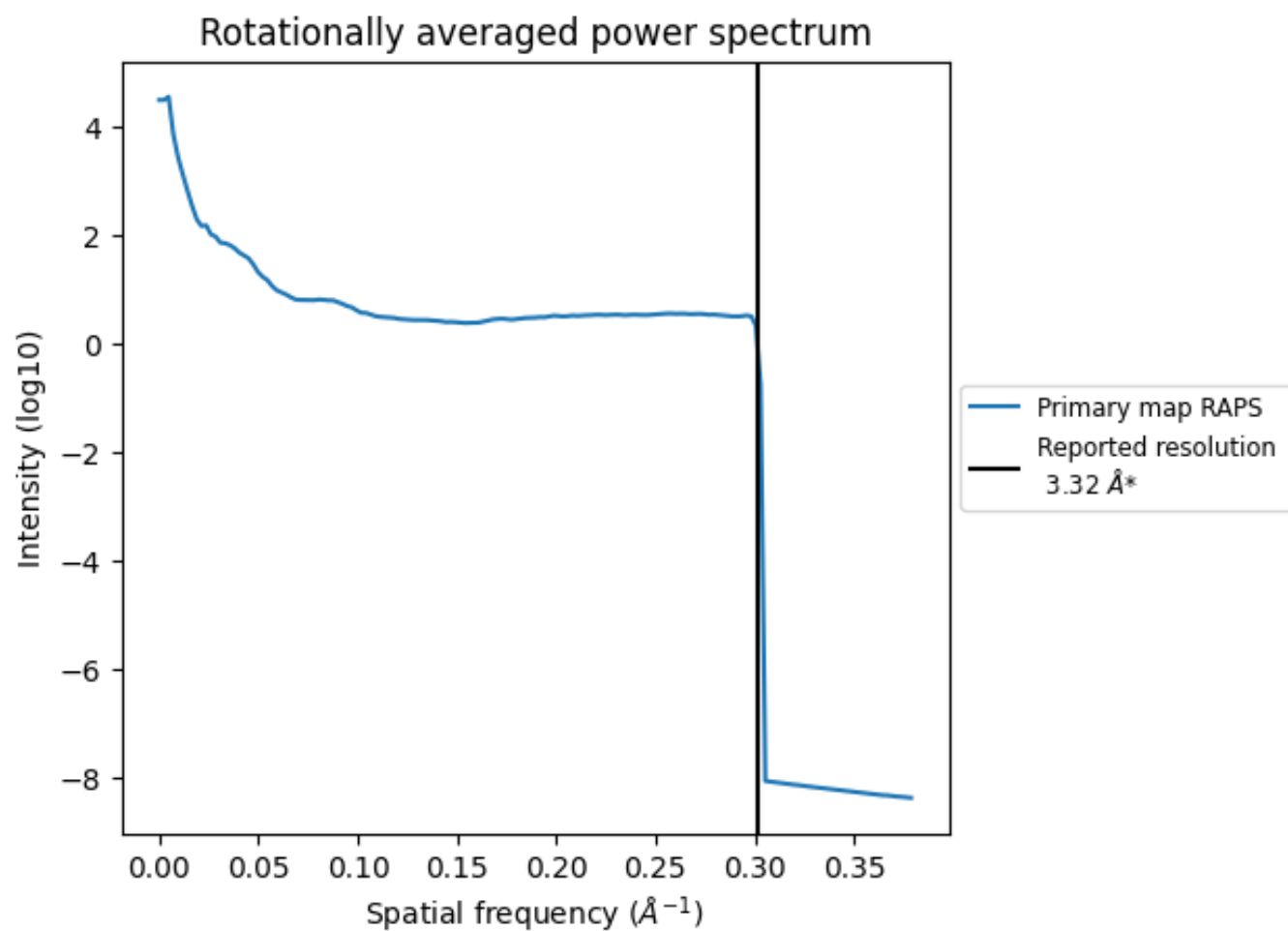
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 781 nm<sup>3</sup>; this corresponds to an approximate mass of 706 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 ⓘ

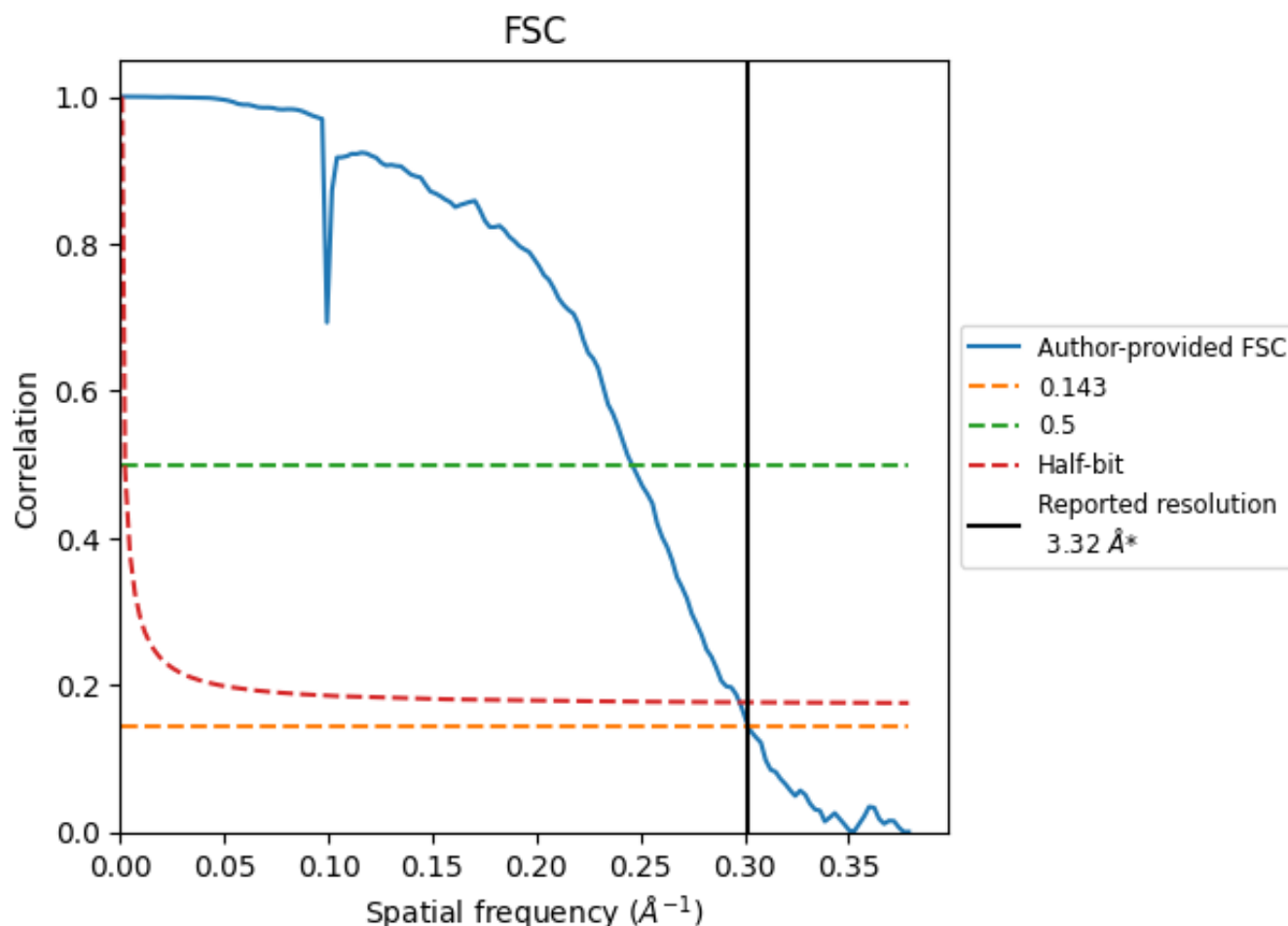


\*Reported resolution corresponds to spatial frequency of 0.301 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.301 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

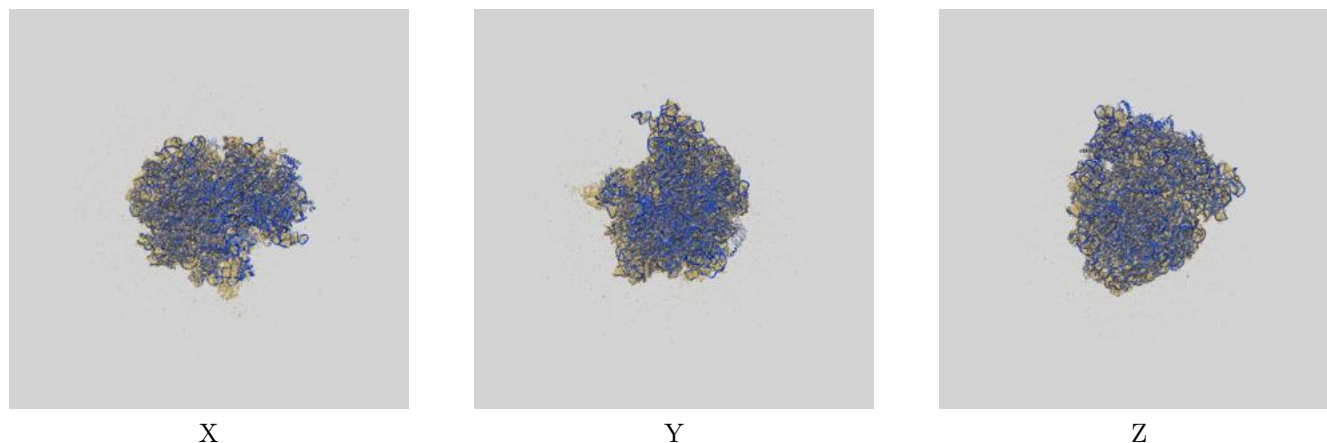
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.31	4.07	3.36
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

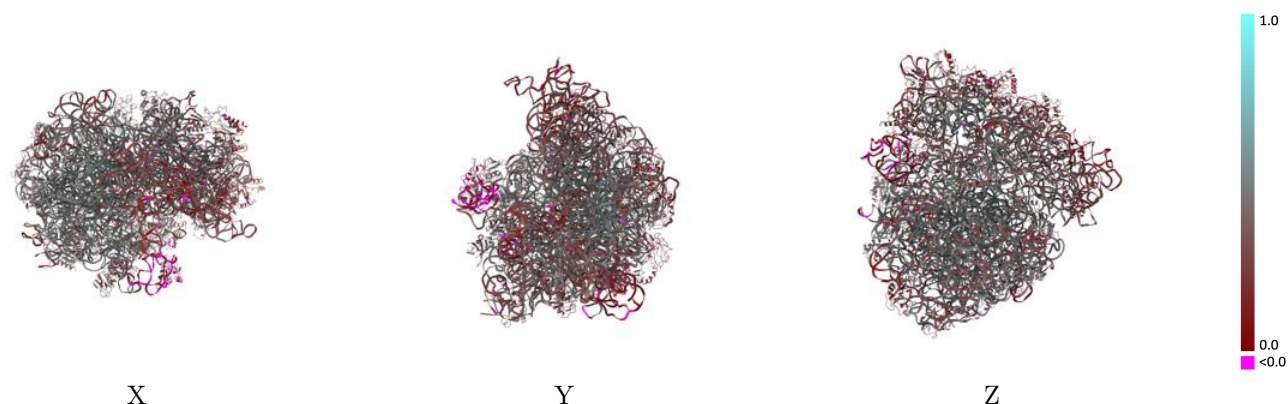
This section contains information regarding the fit between EMDB map EMD-6486 and PDB model 3JBV. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

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



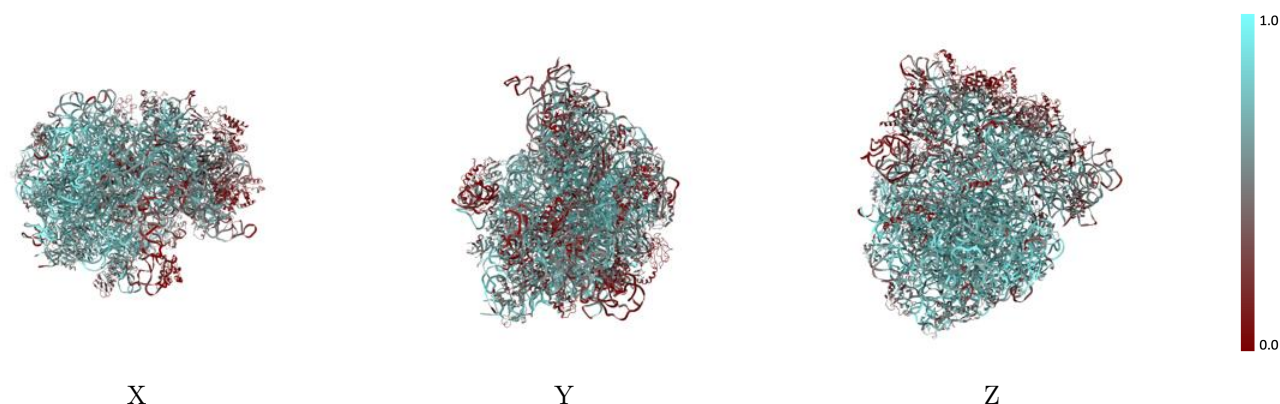
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



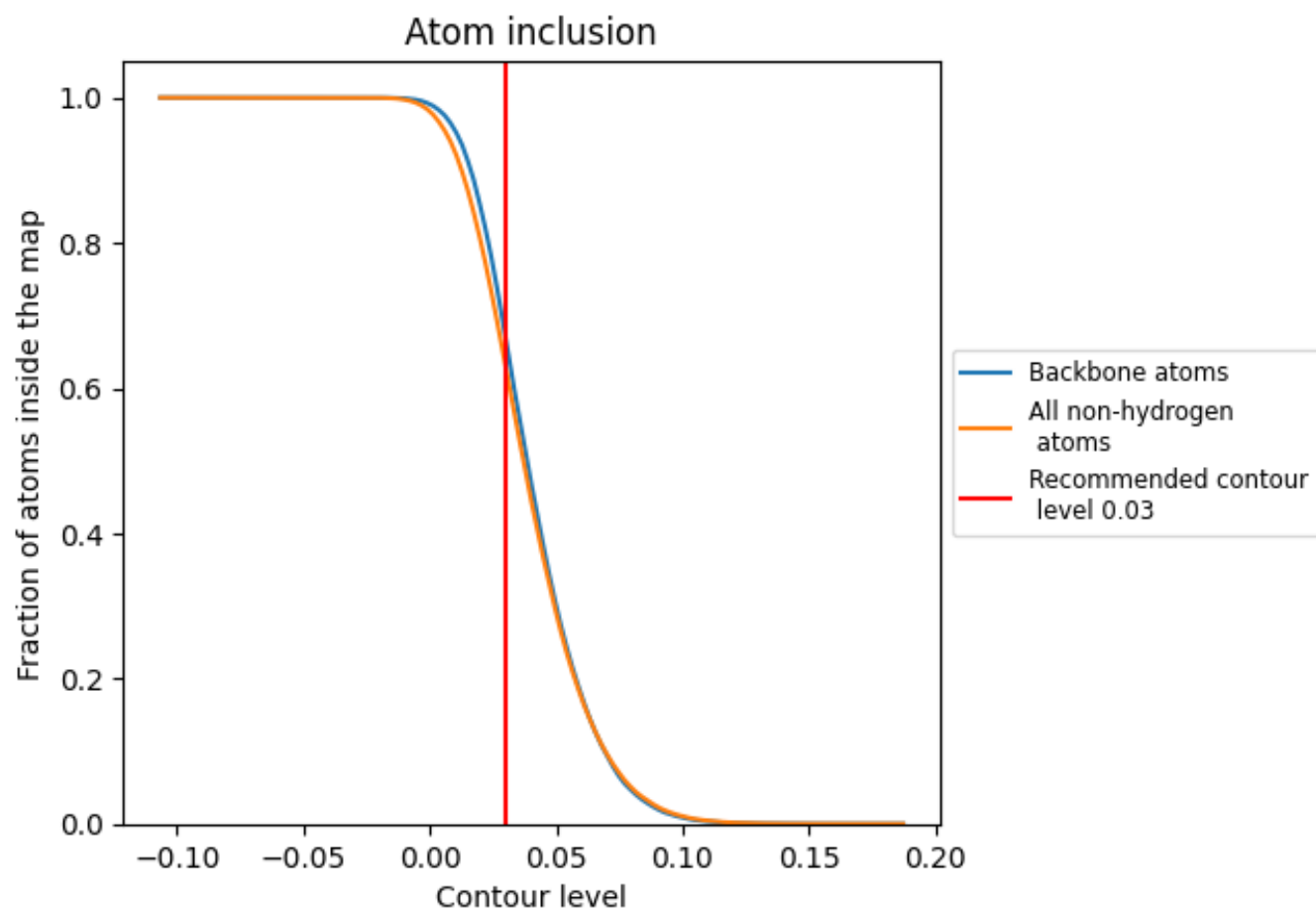
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 63% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6305	 0.3940
0	 0.5874	 0.4320
1	 0.4560	 0.3300
2	 0.6018	 0.4520
3	 0.6402	 0.4360
4	 0.5536	 0.3990
6	 0.7211	 0.4850
7	 0.6986	 0.5070
8	 0.6541	 0.4600
A	 0.6511	 0.3950
B	 0.1570	 0.2650
C	 0.2478	 0.3040
D	 0.1836	 0.2520
E	 0.3204	 0.3460
F	 0.3681	 0.3420
G	 0.2419	 0.2950
H	 0.3740	 0.3520
I	 0.2717	 0.2630
J	 0.2102	 0.2600
K	 0.4713	 0.3920
L	 0.4365	 0.3790
M	 0.3164	 0.3130
N	 0.3257	 0.3420
O	 0.5000	 0.3860
P	 0.2057	 0.1160
Q	 0.3418	 0.3360
R	 0.4450	 0.3770
S	 0.3688	 0.3650
T	 0.3354	 0.2890
U	 0.3153	 0.3170
V	 0.2704	 0.2560
W	 0.6123	 0.3470
X	 0.5368	 0.3990
a	 0.7502	 0.3890
b	 0.7591	 0.4220



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Chain	Atom inclusion	Q-score
c	 0.6771	 0.4680
d	 0.6027	 0.4520
e	 0.5474	 0.3900
f	 0.3860	 0.2860
g	 0.4133	 0.3360
h	 0.1496	 0.2440
i	 0.0620	 0.0360
j	 0.6227	 0.4430
k	 0.5608	 0.4450
l	 0.6279	 0.4350
m	 0.6137	 0.4560
n	 0.6432	 0.4500
o	 0.5701	 0.3650
p	 0.5169	 0.4020
q	 0.6729	 0.4670
r	 0.5822	 0.4160
s	 0.5909	 0.4500
t	 0.5277	 0.3770
u	 0.5059	 0.3570
w	 0.5528	 0.4050
y	 0.6685	 0.4770
z	 0.0625	 0.3120