



wwPDB EM Validation Summary Report ⓘ

Dec 7, 2022 – 09:44 AM JST

PDB ID : 5IMR
EMDB ID : EMD-6585
Title : Structure of ribosome bound to cofactor at 5.7 angstrom resolution
Authors : Kumar, V.; Ero, R.; Jian, G.K.; Ahmed, T.; Zhan, Y.; Bhushan, S.; Gao, Y.G.
Deposited on : 2016-03-06
Resolution : 5.70 Å(reported)
Based on initial models : 4W2E, 5AA0

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:

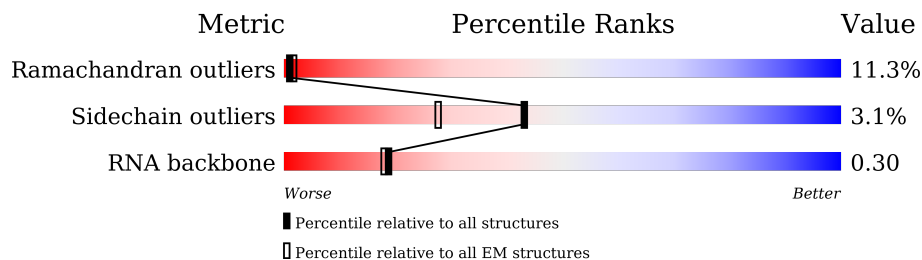
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 5.70 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	A	1522	
2	F	256	
3	G	239	
4	H	209	
5	I	162	
6	J	101	
7	K	156	
8	L	138	

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Mol	Chain	Length	Quality of chain
9	M	128	57% 88% 12%
10	N	105	58% 82% 11% 7%
11	O	129	33% 88% 5% 8%
12	P	132	35% 86% 8% 6%
13	Q	126	44% 78% 10% 10%
14	R	61	64% 89% 10%
15	S	89	43% 91% 8%
16	T	88	35% 88% 7% 6%
17	U	105	34% 92% 7%
18	V	88	41% 76% 7% 17%
19	W	93	41% 77% 6% 14%
20	X	106	49% 89% 5% 7%
21	Y	27	48% 78% 11% 11%
22	C	610	42% 55% 31% 7% 7%
23	D	2893	10% 45% 51%
24	E	123	20% 58% 42%
25	Z	229	85% 88% 10%
26	a	276	21% 84% 14%
27	b	206	45% 85% 15%
28	c	210	48% 90% 9%
29	d	182	54% 86% 13%
30	e	180	44% 82% 13%
31	f	140	52% 88% 11%
32	g	122	34% 89% 11%
33	h	150	43% 83% 14%

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Mol	Chain	Length	Quality of chain
34	i	141	40% 86% 10% . .
35	j	118	49% 92% 8% .
36	k	112	38% 89% 9% .
37	l	146	32% 70% 10% . 20%
38	m	118	52% 91% 8% .
39	n	101	53% 81% 18% .
40	o	113	50% 90% 6% . .
41	p	96	42% 91% 7% .
42	q	110	54% 78% 22%
43	r	206	58% 79% 8% 13%
44	s	85	47% 87% 6% 7%
45	t	67	49% 93% 7%
46	u	60	48% 92% 7% .
47	v	71	37% 76% 18% 6%
48	w	60	55% 82% 13% 5%
49	x	54	44% 69% 22% 9%
50	y	49	43% 86% 14%
51	z	65	54% 83% 14% . .
52	1	37	43% 95% 5%
53	2	173	73% 68% 7% 25%
54	3	147	50% 63% 24% 5% 9%
55	4	77	64% 61% 38% .
56	5	76	24% 49% 50% .

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 152879 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1515	32554	14490	6022	10527	1515	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	234	1900	1213	341	341	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	206	1612	1016	314	281	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	208	1703	1066	339	291	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	150	1146	724	217	201	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	101	843	531	155	154	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	K	155	1257	781	252	218	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	138	1116	705	215	193	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	M	127	1010	639	197	174	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	98	794	499	156	138	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	O	119	885	549	168	165	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	124	970	611	195	163	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Q	114	914	565	189	158	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	104	Total	C	N	O	S	0	0
			857	547	161	147	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	73	Total	C	N	O	0	0
			597	380	118	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	80	Total	C	N	O	S	0	0
			647	414	119	112	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a protein called Elongation factor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	C	570	Total	C	N	O	S	0	0
			4461	2858	768	826	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	2889	Total	C	N	O	P	0	0
			62218	27691	11629	20009	2889		

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	E	123	Total	C	N	O	P	0	0
			2641	1175	488	855	123		

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	228	Total	C	N	O	S	0	0
			1742	1102	318	319	3		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	272	Total	C	N	O	S	0	0
			2124	1339	424	358	3		

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	206	Total	C	N	O	S	0	0
			1578	997	302	273	6		

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	208	1625	1034	303	286	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	182	1482	947	269	261	5	0	0

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	174	1328	844	248	235	1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	139	1113	717	207	186	3	0	0

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	122	932	587	171	170	4	0	0

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	145	1106	688	226	190	2	0	0

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	136	1080	688	204	183	5	0	0

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	j	117	Total	C	N	O	0	0
			960	599	202	159		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	k	110	Total	C	N	O	0	0
			877	553	175	149		

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	117	Total	C	N	O	S	0	0
			976	614	197	164	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	117	Total	C	N	O	S	0	0
			964	610	202	151	1		

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	101	Total	C	N	O	S	0	0
			779	501	142	135	1		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	110	Total	C	N	O	S	0	0
			876	552	171	151	2		

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	p	94	Total	C	N	O	0	0
			742	483	133	126		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	110	Total	C	N	O	S	0	0
			844	539	158	141	6		

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	180	Total	C	N	O	S	0	0
			1435	916	256	260	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	79	Total	C	N	O	S	0	0
			625	387	131	106	1		

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	67	Total	C	N	O	S	0	0
			567	350	116	99	2		

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	u	59	Total	C	N	O	0	0
			469	298	90	81		

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	71	Total	C	N	O	S	0	0
			581	364	108	104	5		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	57	Total	C	N	O	S	0	0
			445	279	87	74	5		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	49	Total	C	N	O	S	0	0
			426	265	87	70	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	49	Total	C	N	O	S	0	0
			430	263	108	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	64	Total	C	N	O	S	0	0
			515	331	102	79	3		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	37	Total	C	N	O	S	0	0
			307	188	68	47	4		

- Molecule 53 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	2	130	Total	C	N	O	0	0
			641	381	130	130		

- Molecule 54 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	134	Total	C	N	O	S	0	0
			993	632	175	181	5		

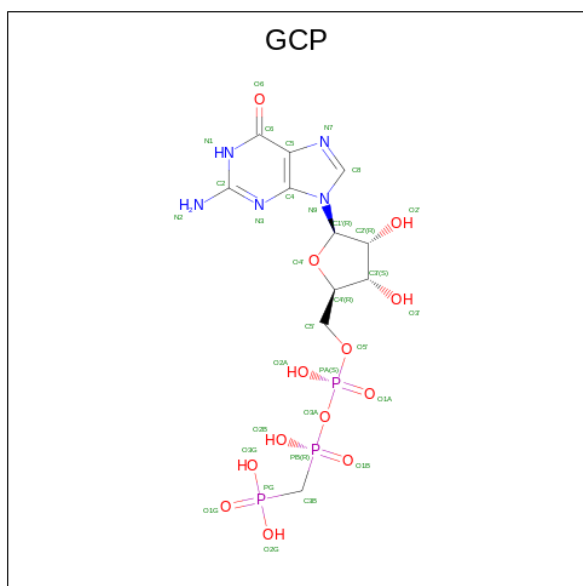
- Molecule 55 is a RNA chain called P site- tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 56 is a RNA chain called E site- tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	5	76	1623	723	290	534	76	0	0

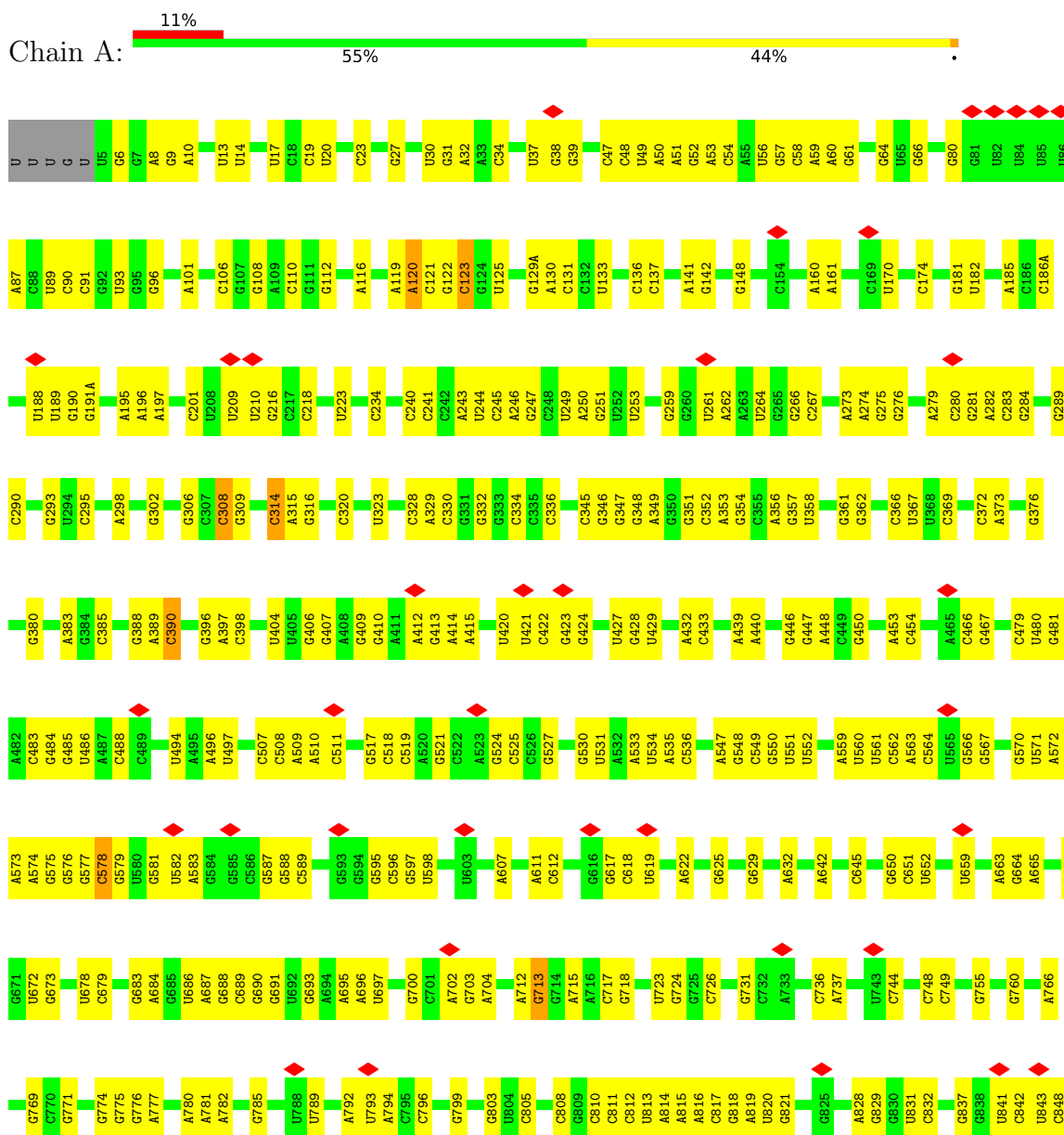
- Molecule 57 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

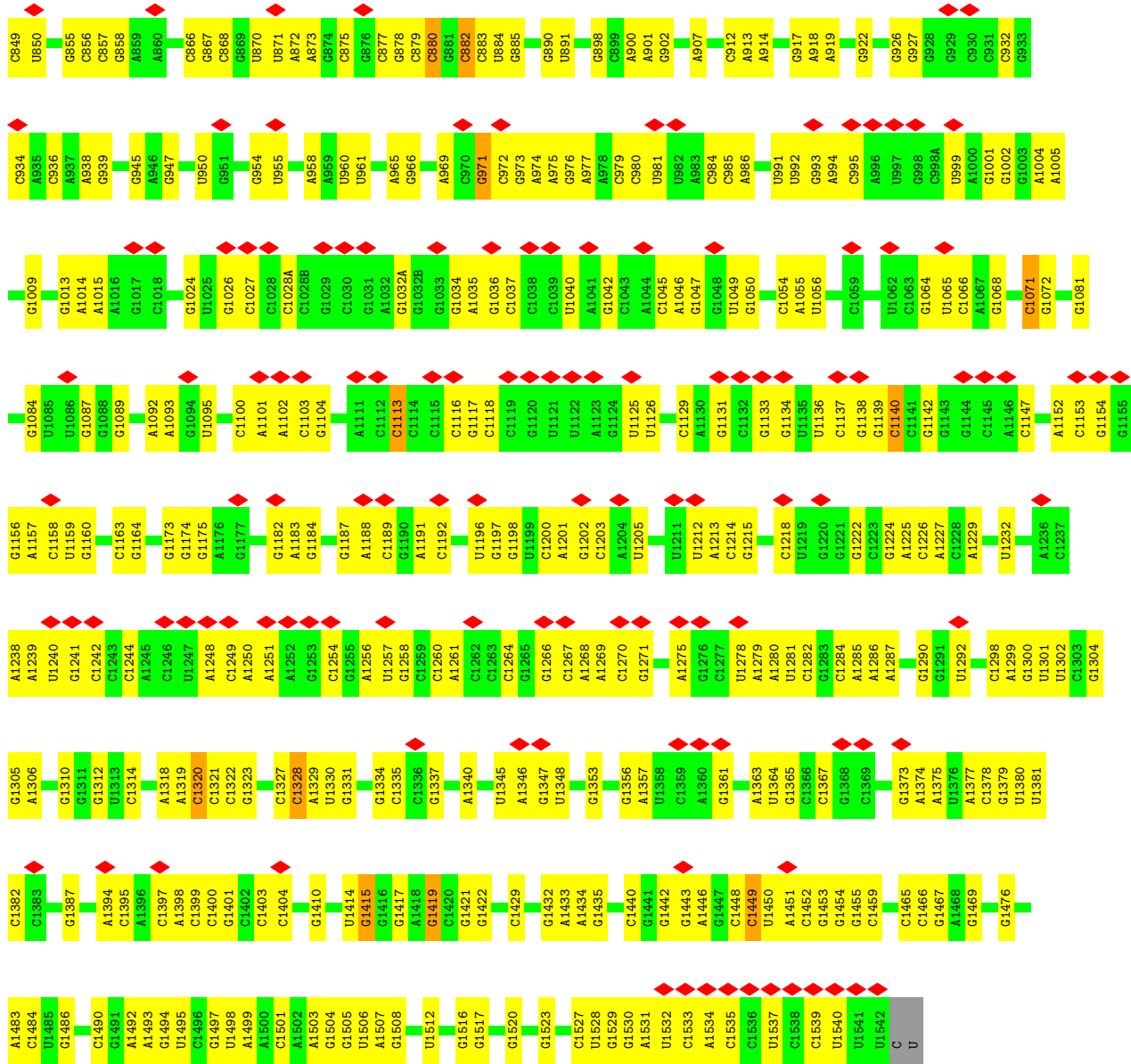


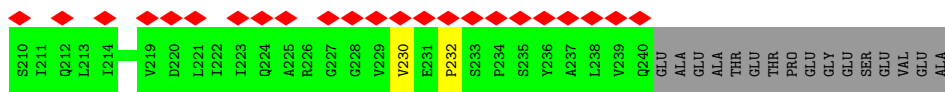
3 Residue-property plots

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.

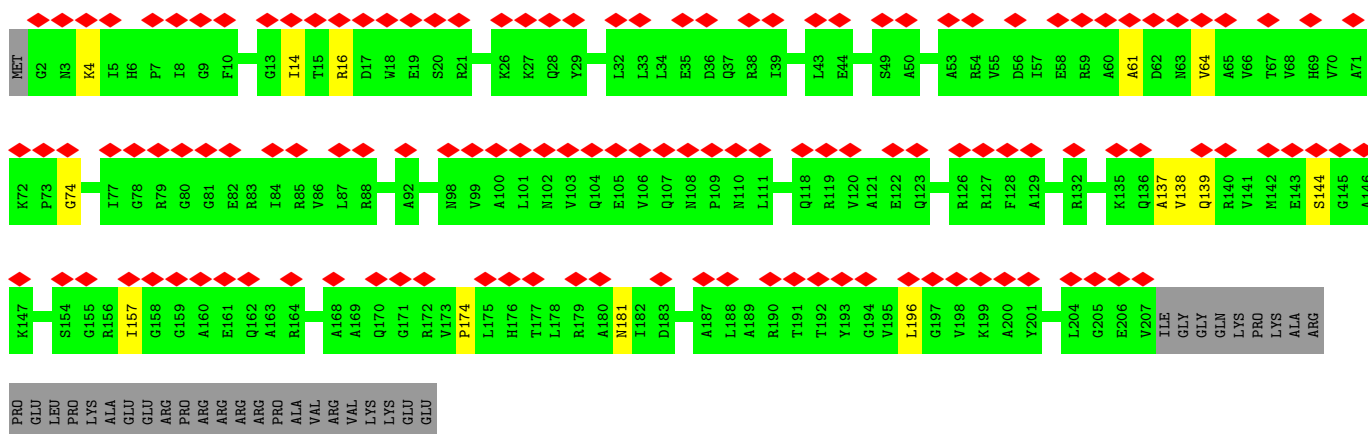
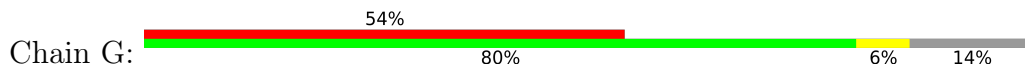
- Molecule 1: 16S ribosomal RNA



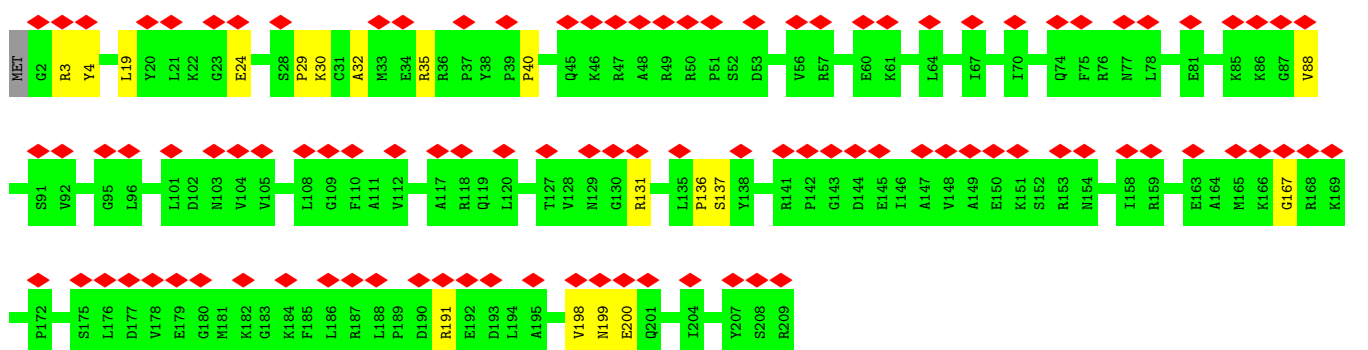
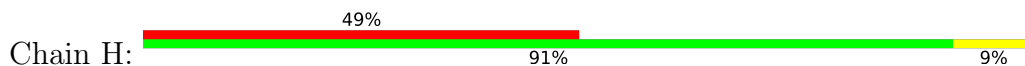




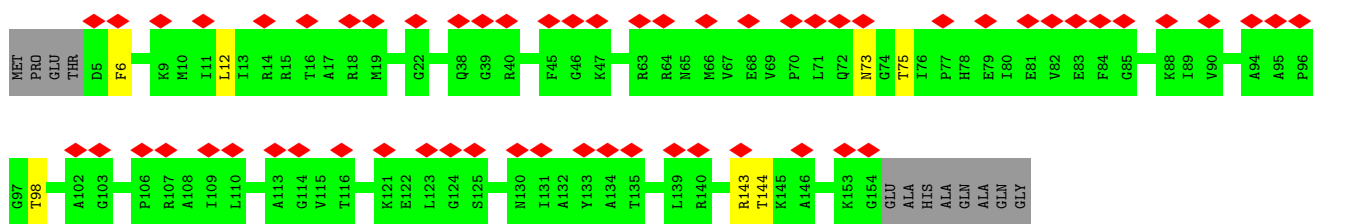
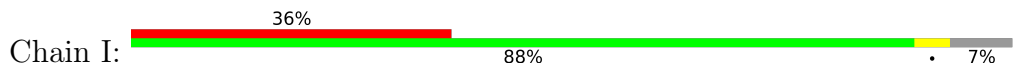
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

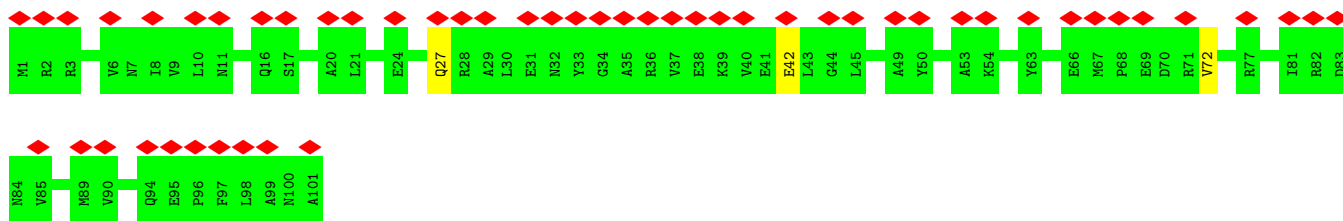


• Molecule 5: 30S ribosomal protein S5

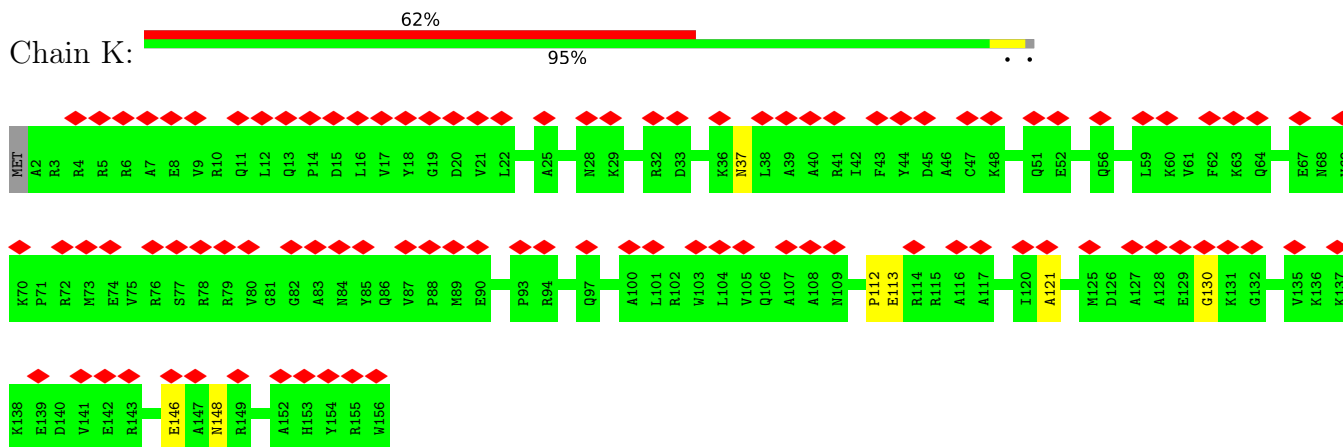


• Molecule 6: 30S ribosomal protein S6

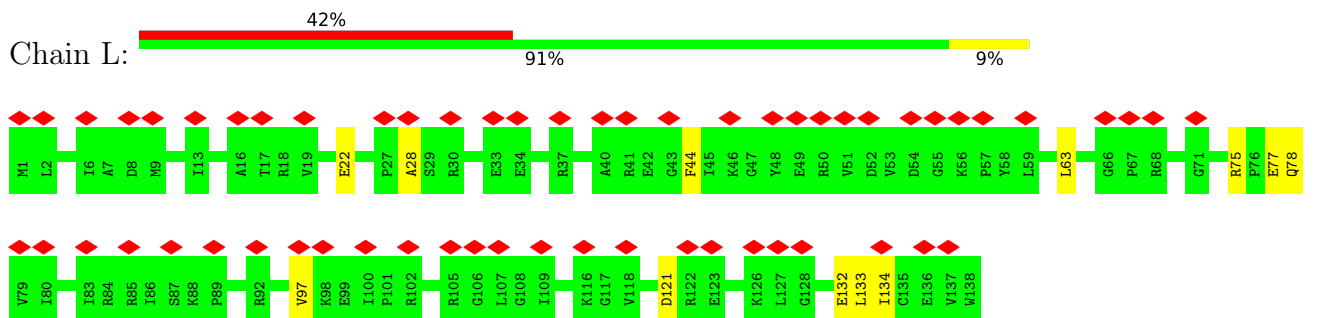




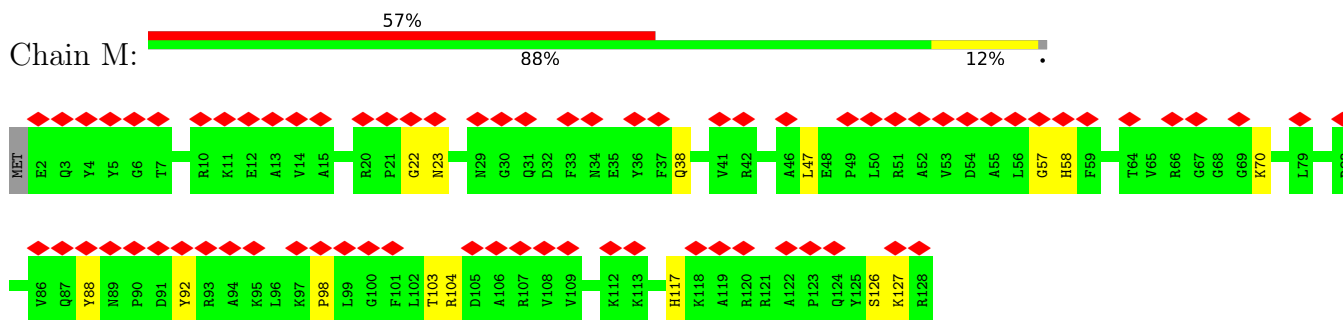
- Molecule 7: 30S ribosomal protein S7



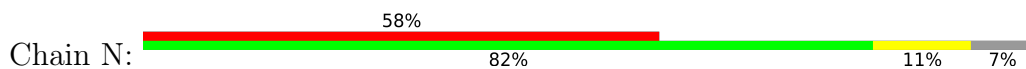
- Molecule 8: 30S ribosomal protein S8

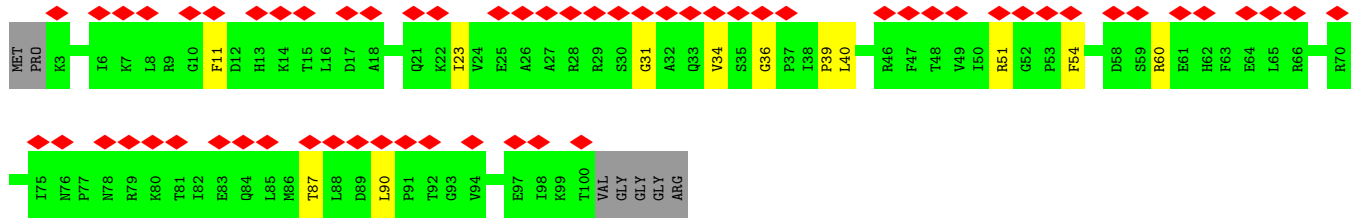


- Molecule 9: 30S ribosomal protein S9

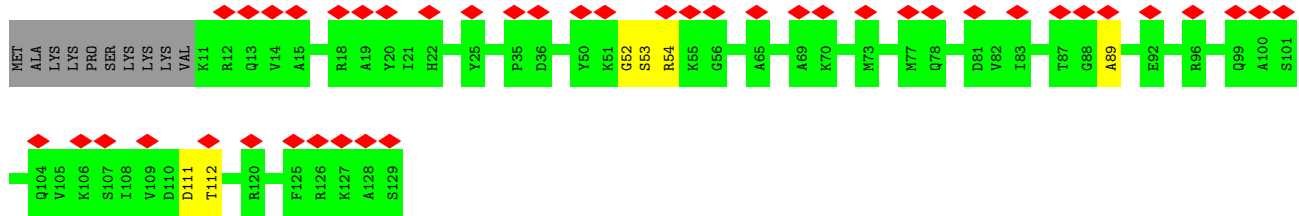
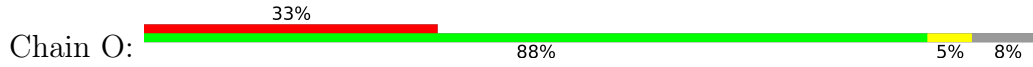


- Molecule 10: 30S ribosomal protein S10

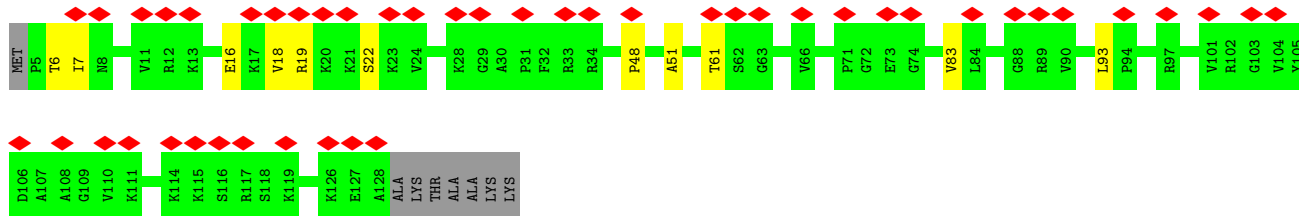
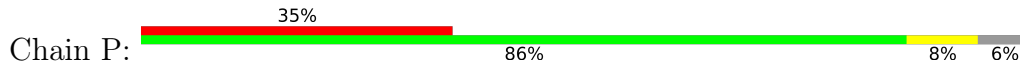




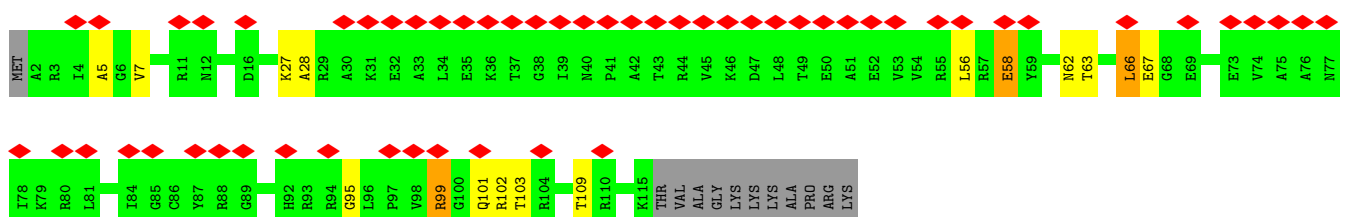
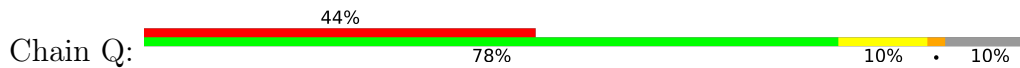
• Molecule 11: 30S ribosomal protein S11



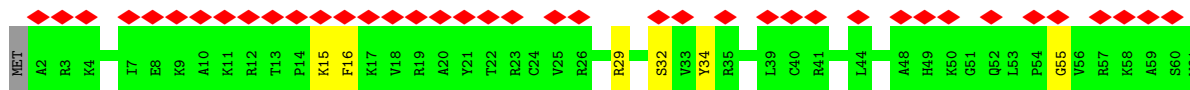
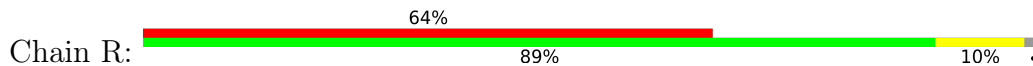
• Molecule 12: 30S ribosomal protein S12



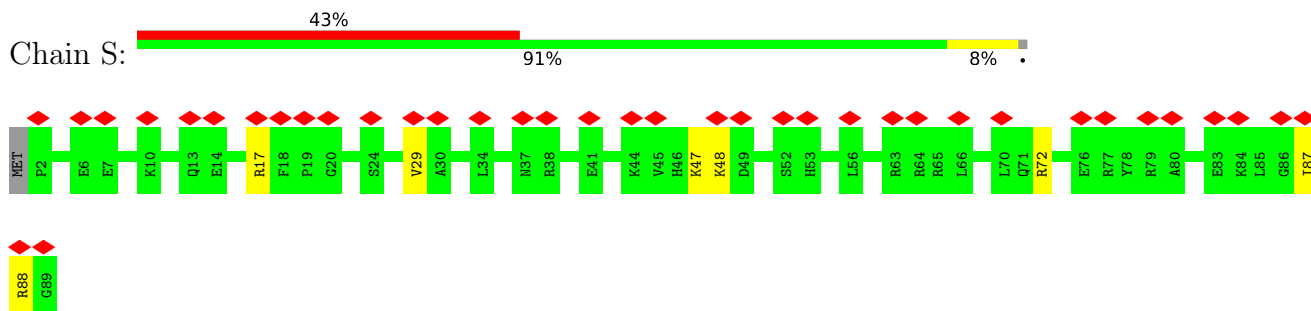
• Molecule 13: 30S ribosomal protein S13



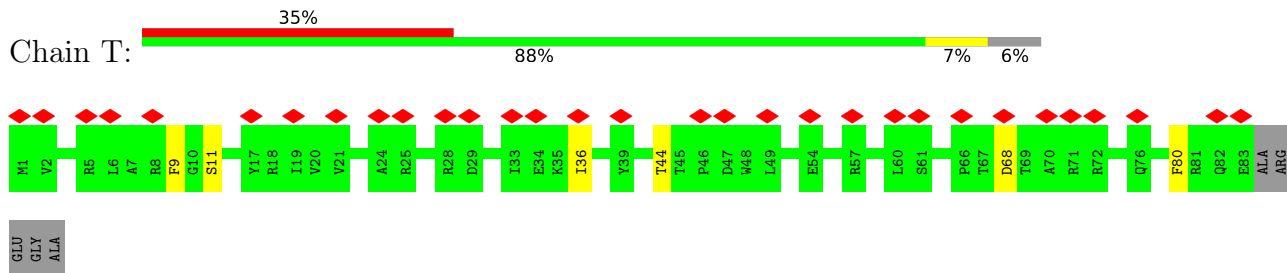
• Molecule 14: 30S ribosomal protein S14 type Z



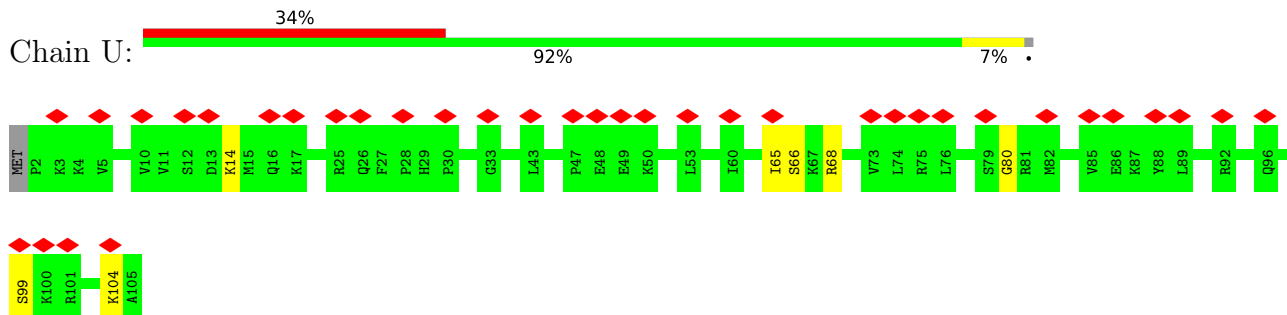
• Molecule 15: 30S ribosomal protein S15



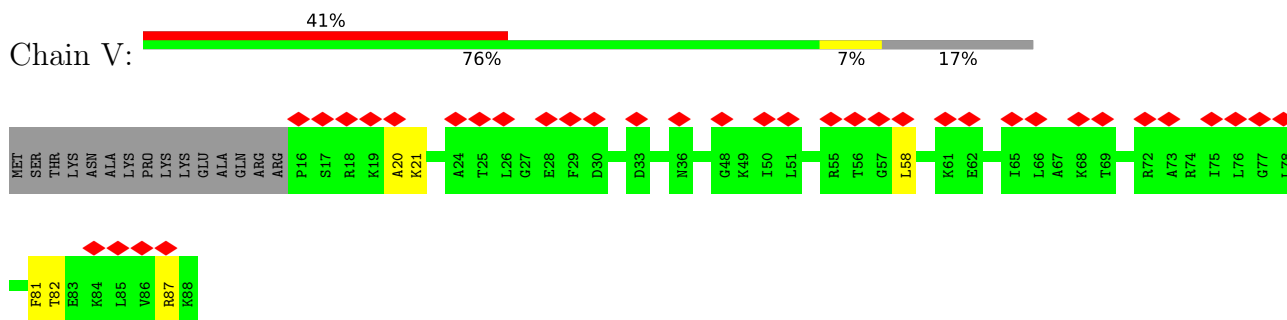
- Molecule 16: 30S ribosomal protein S16



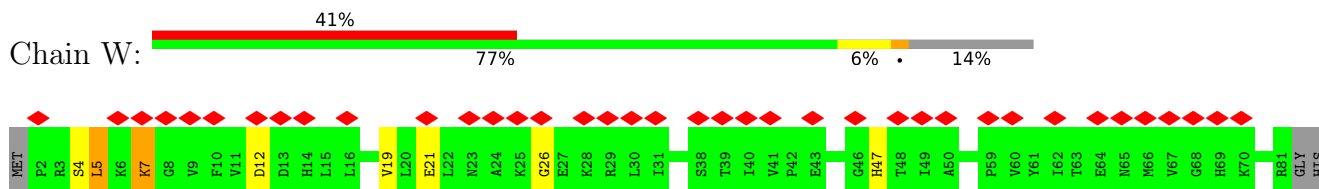
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

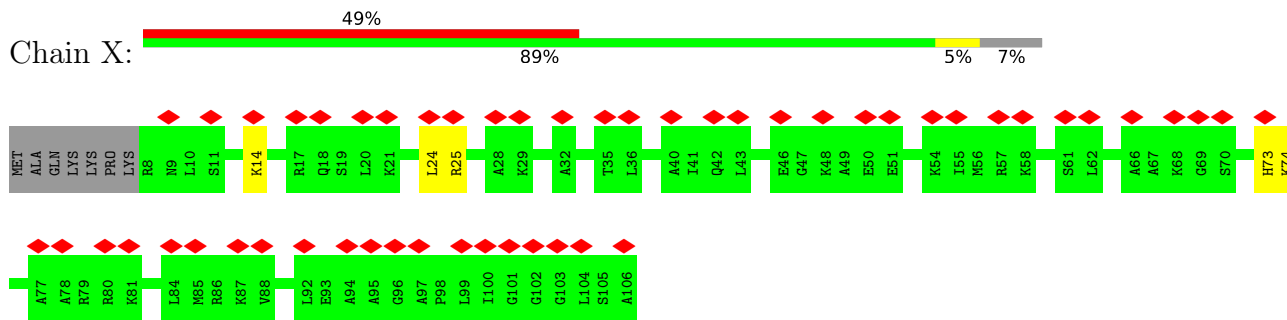


- Molecule 19: 30S ribosomal protein S19

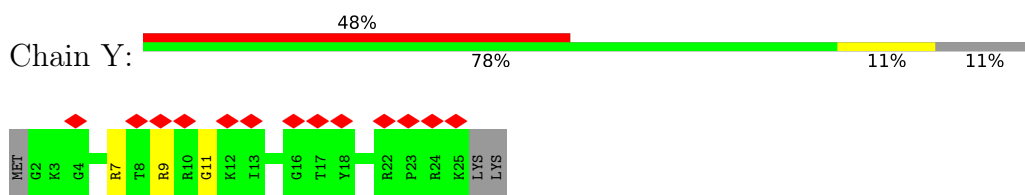


GLY
 LYS
 GLU
 ALA
 LYS
 LYS
 ALA
 THR
 LYS
 LYS

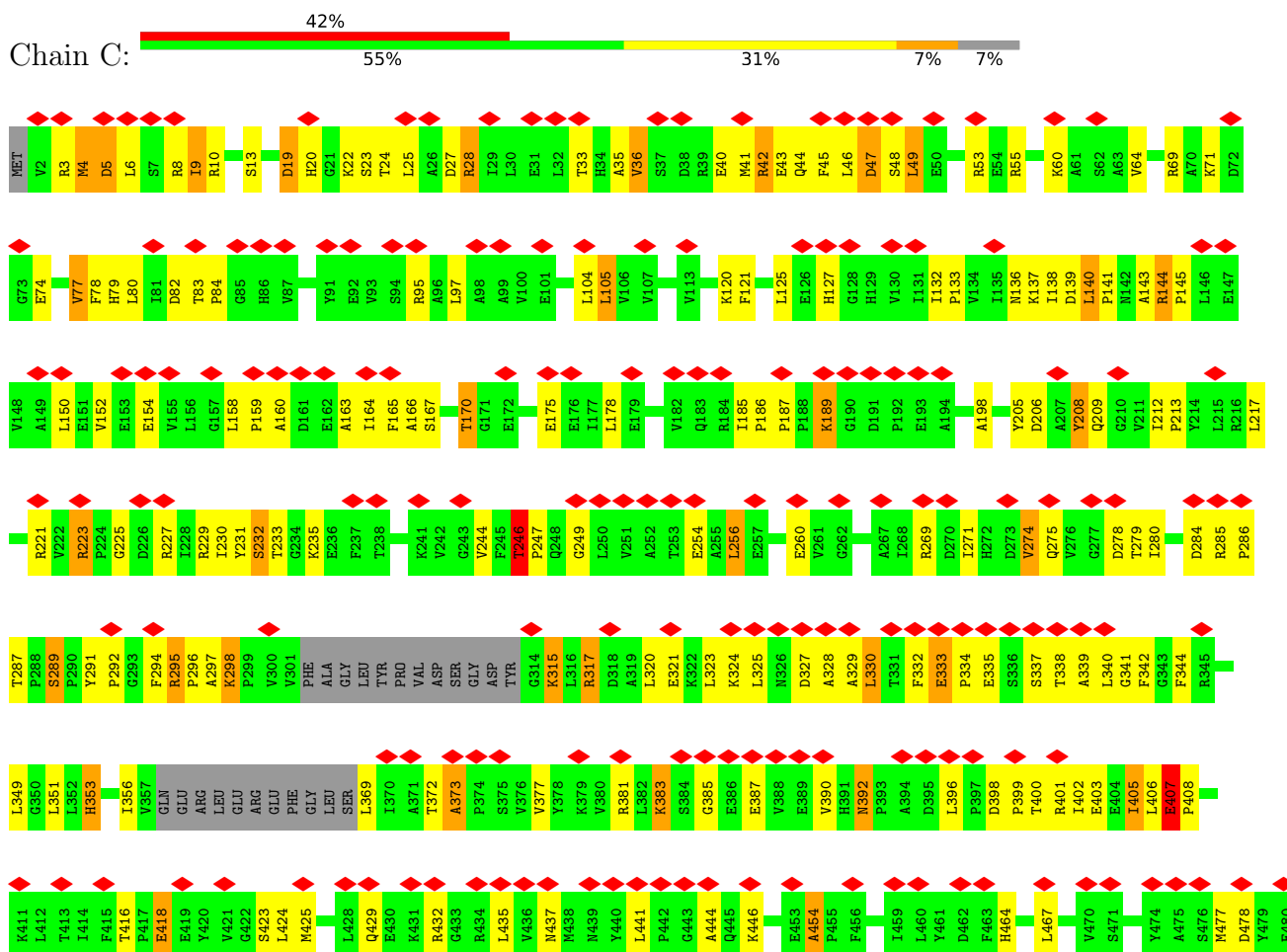
• Molecule 20: 30S ribosomal protein S20

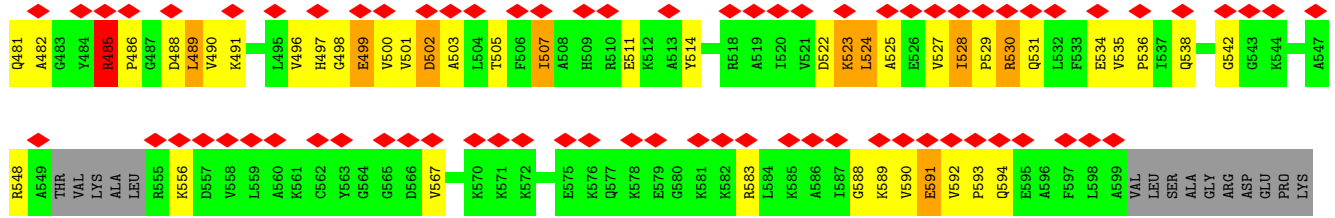


• Molecule 21: 30S ribosomal protein Thx



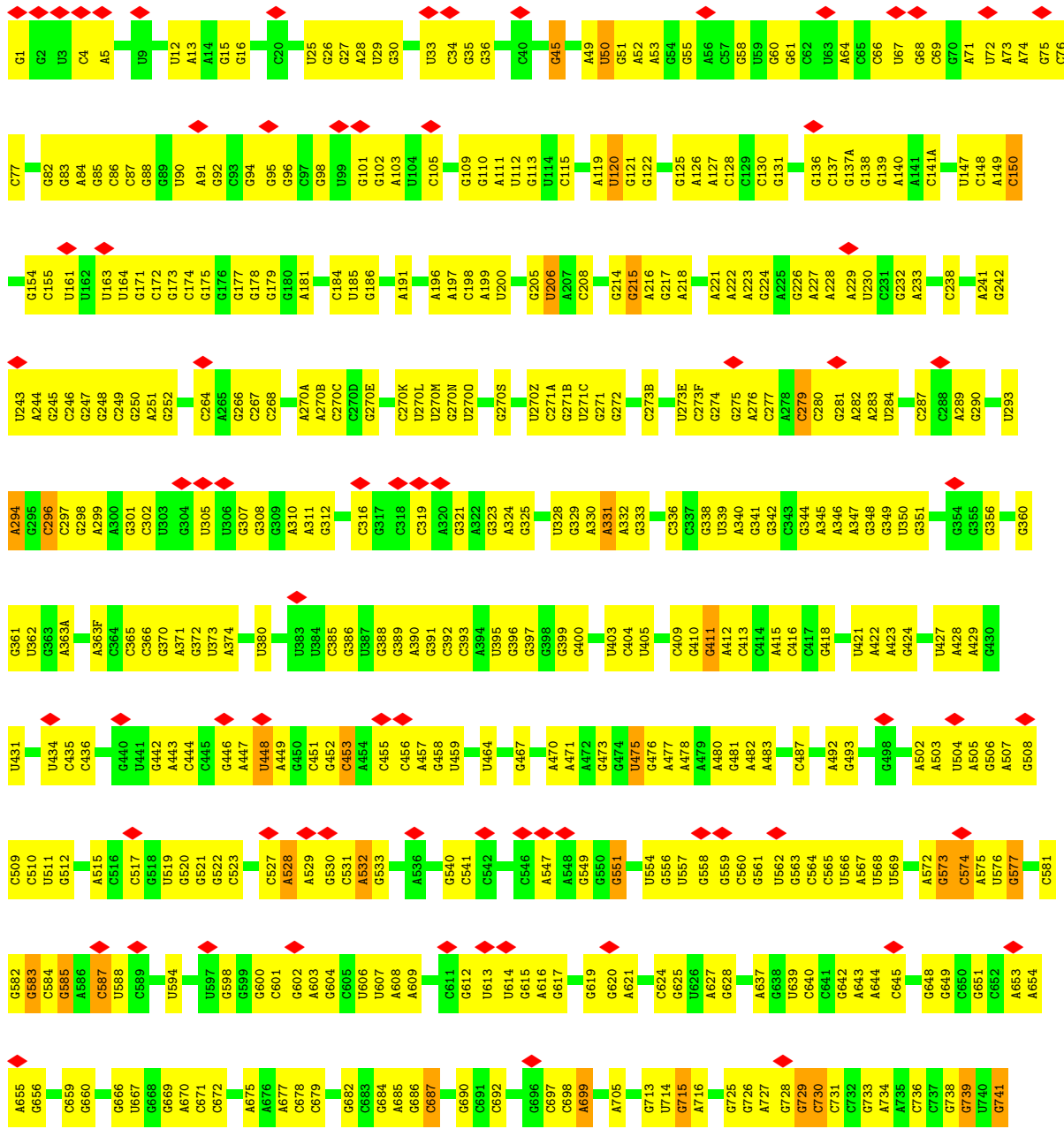
• Molecule 22: Elongation factor 4

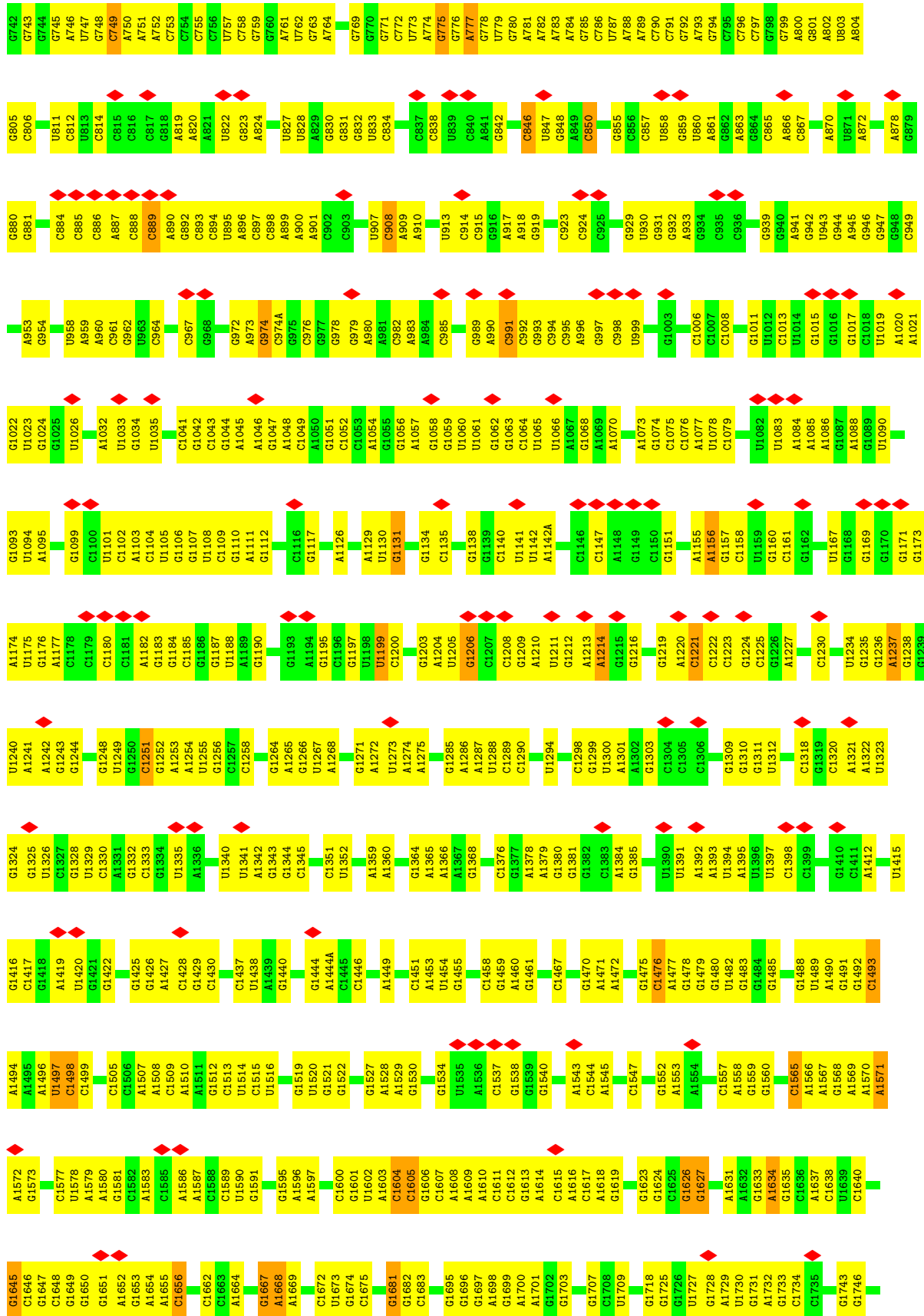


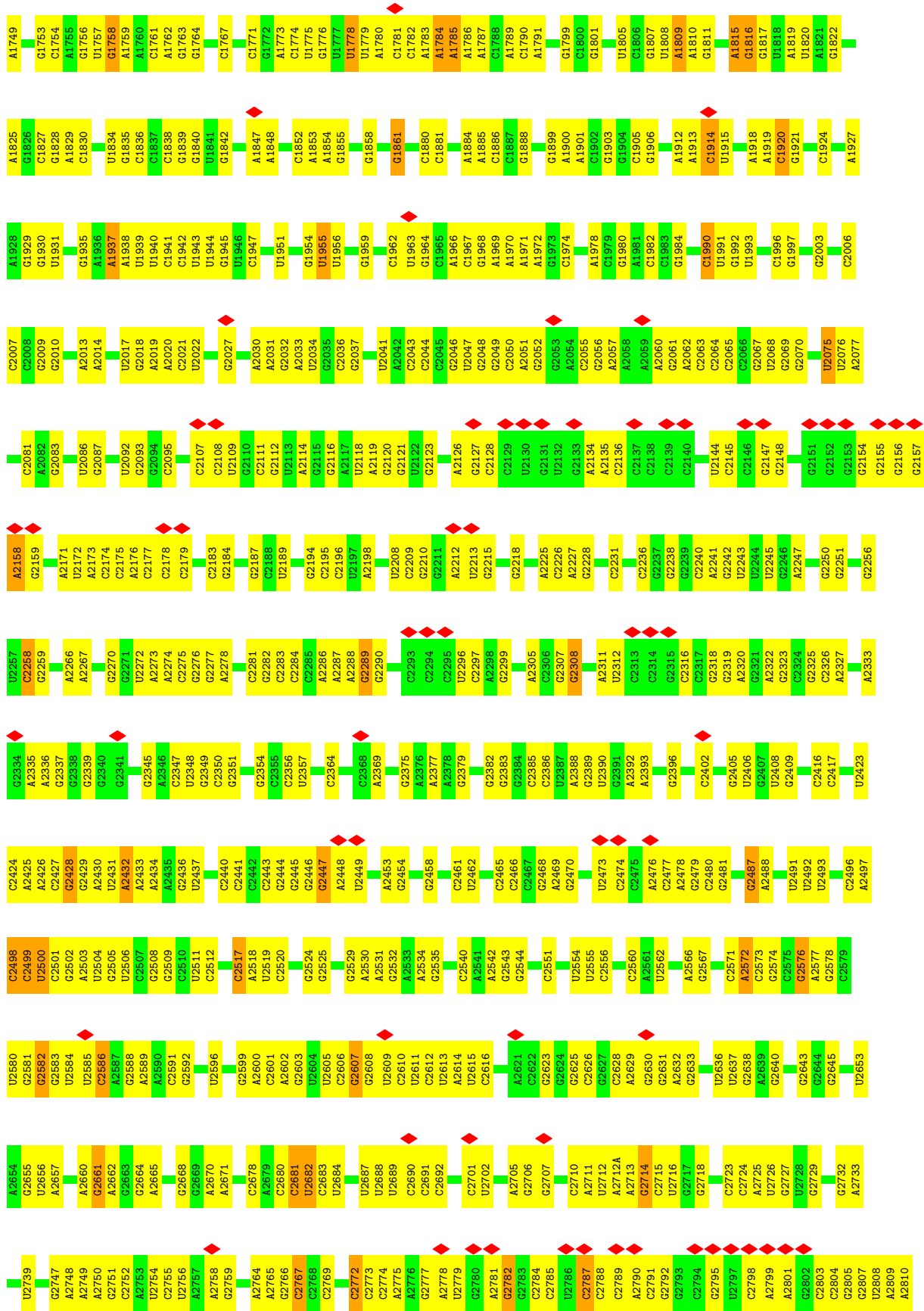


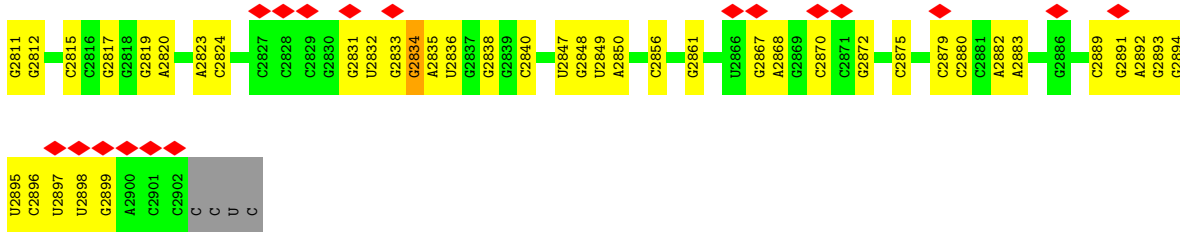
GLY

• Molecule 23: 23S ribosomal RNA

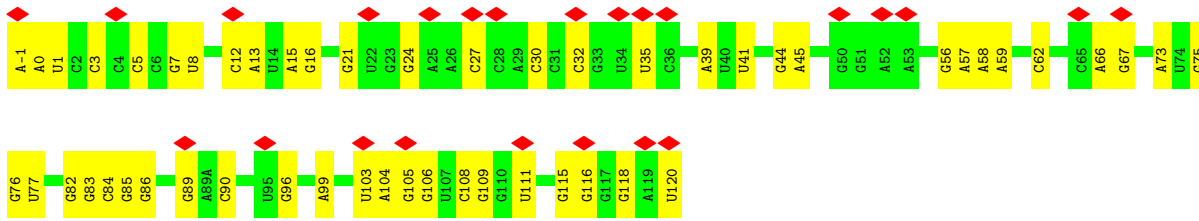




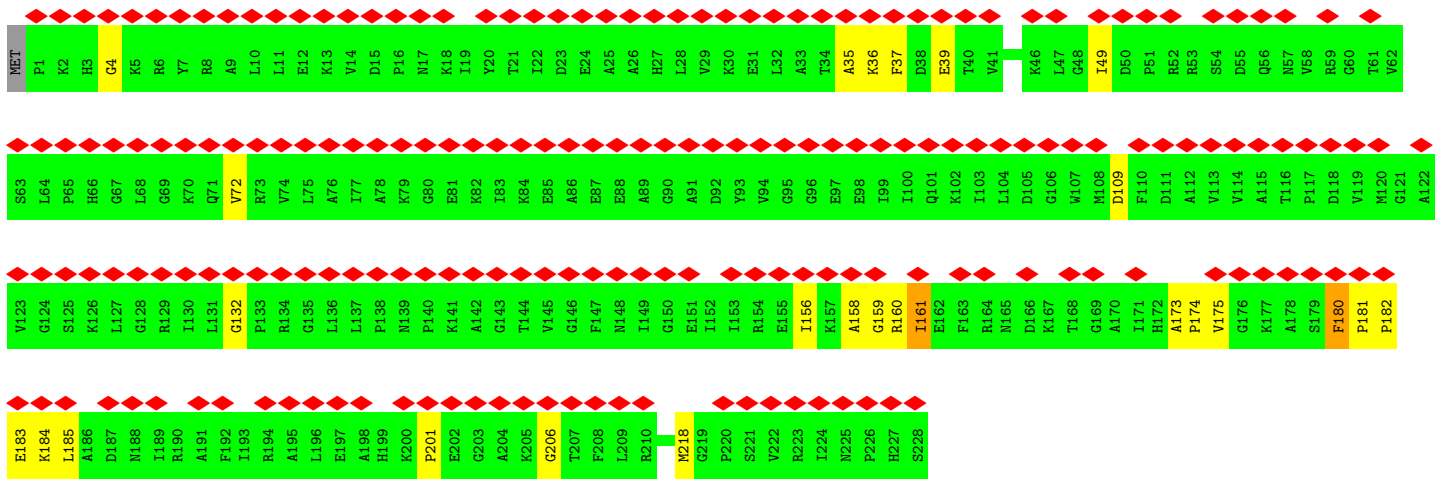
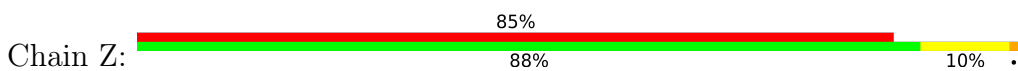




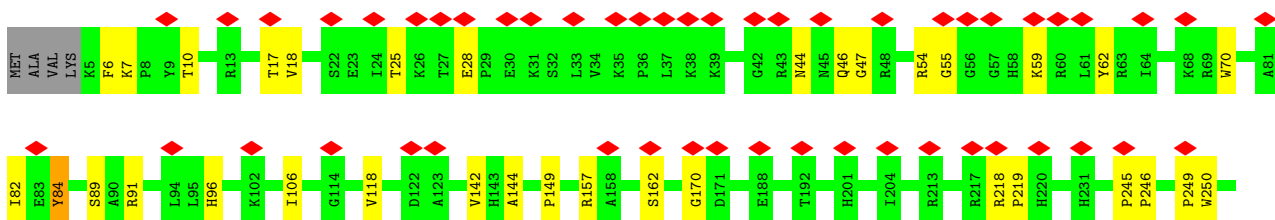
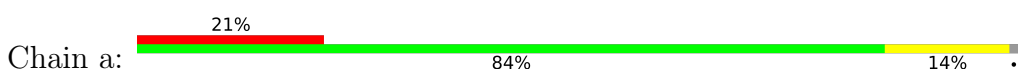
• Molecule 24: 5S ribosomal RNA

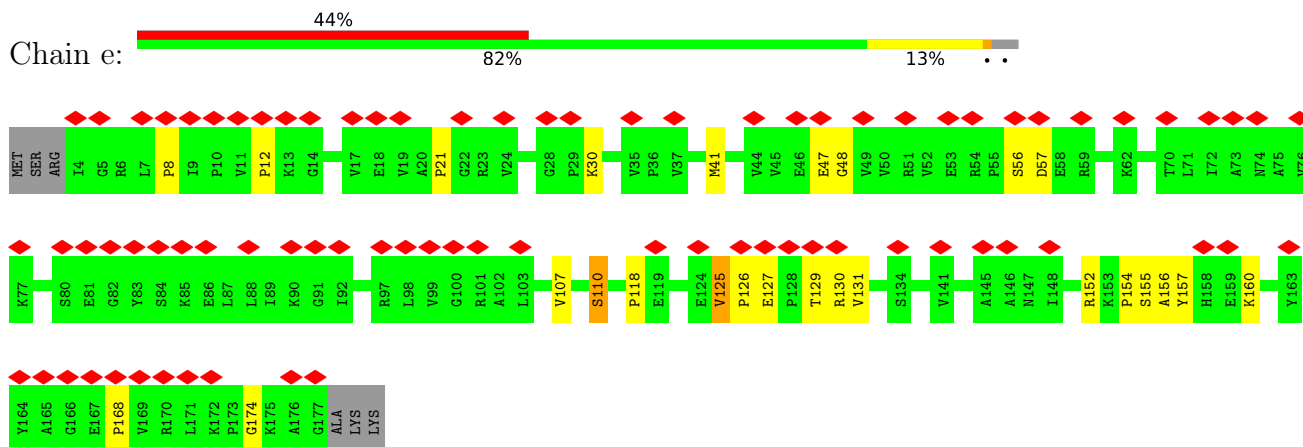


• Molecule 25: 50S ribosomal protein L1

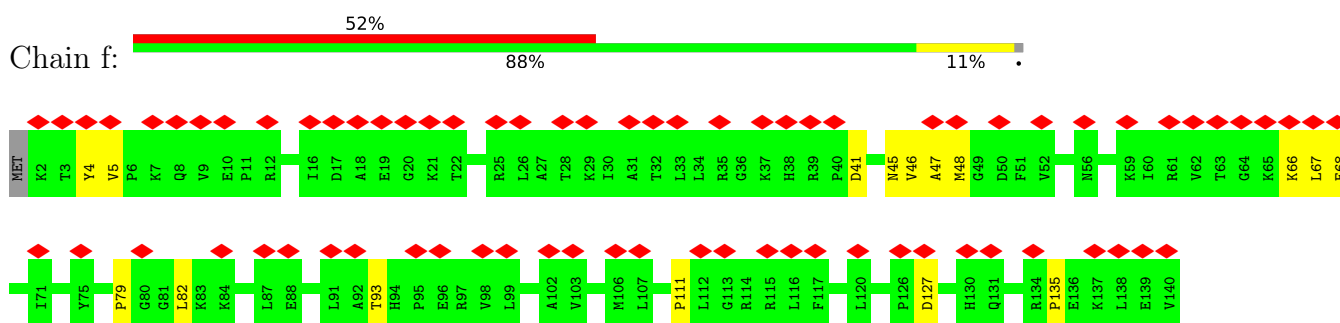


• Molecule 26: 50S ribosomal protein L2

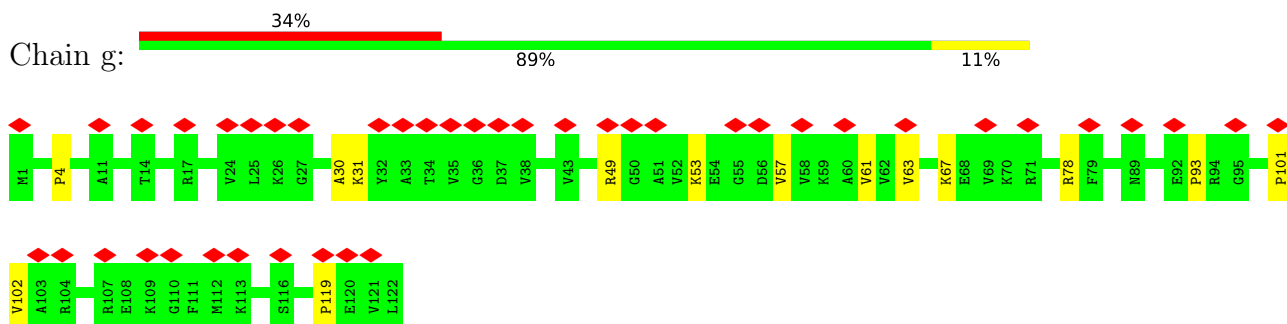




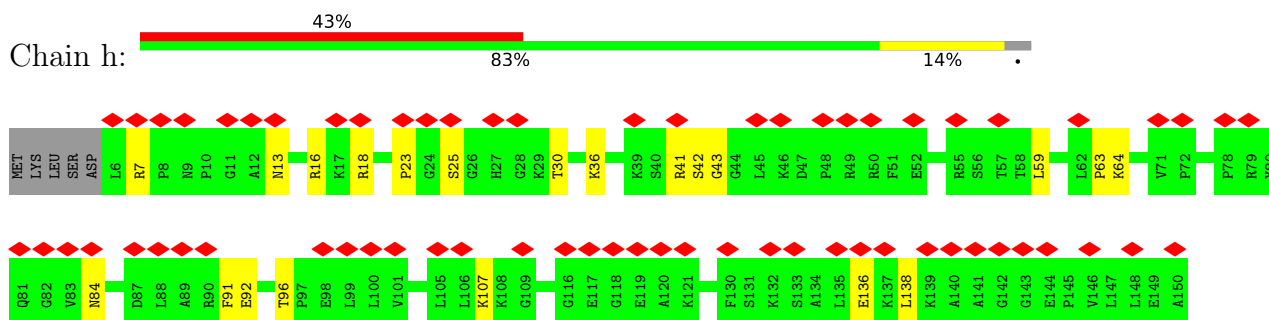
- Molecule 31: 50S ribosomal protein L13



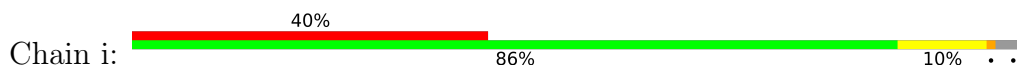
- Molecule 32: 50S ribosomal protein L14

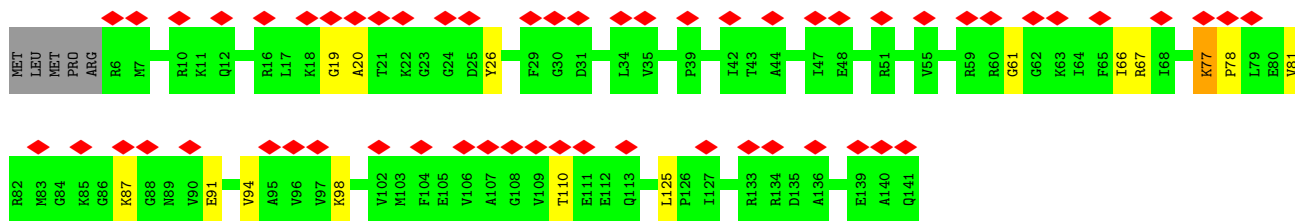


- Molecule 33: 50S ribosomal protein L15

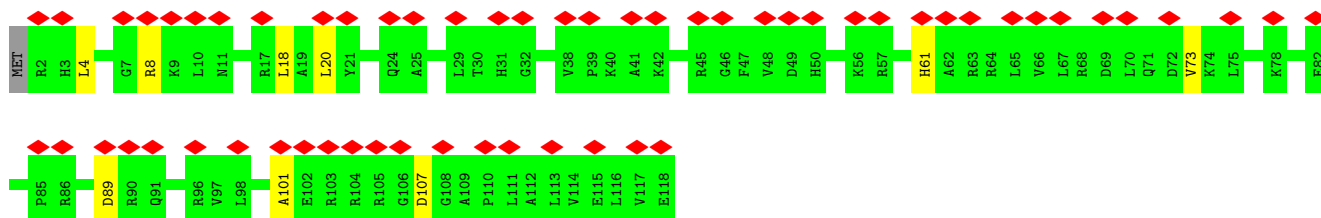
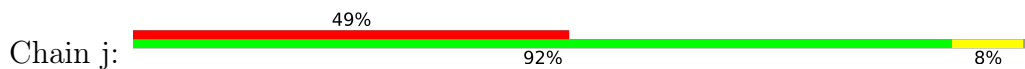


- Molecule 34: 50S ribosomal protein L16

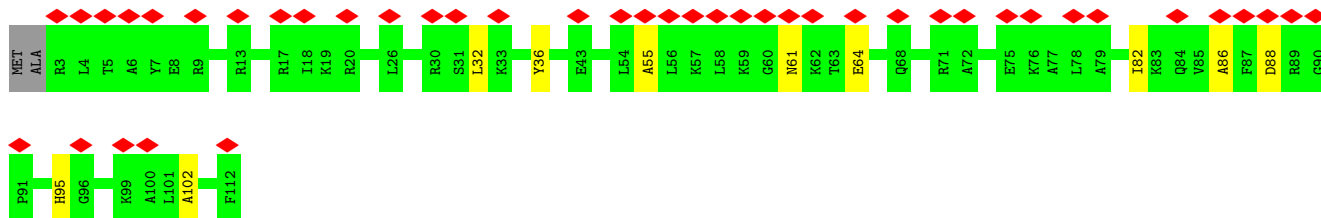
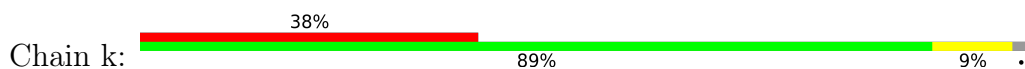




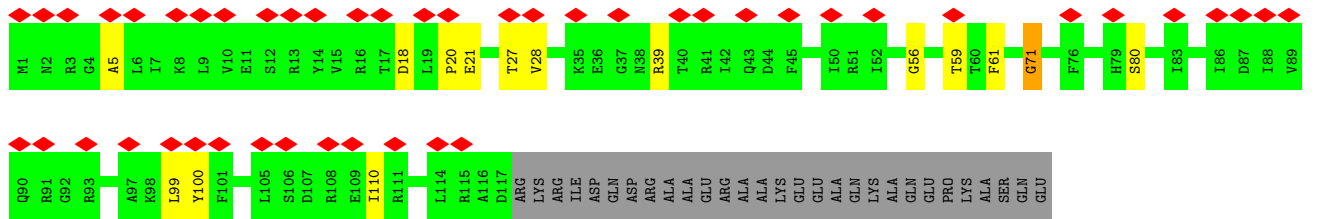
• Molecule 35: 50S ribosomal protein L17



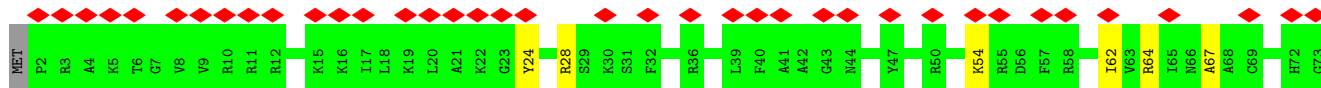
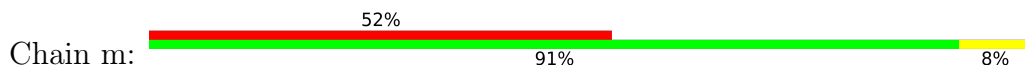
• Molecule 36: 50S ribosomal protein L18

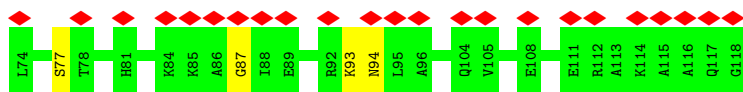


• Molecule 37: 50S ribosomal protein L19

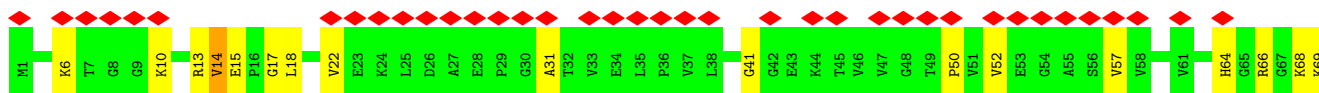
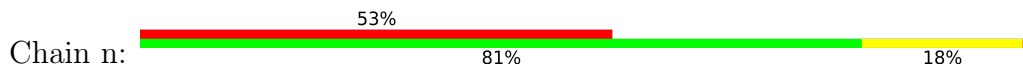


• Molecule 38: 50S ribosomal protein L20

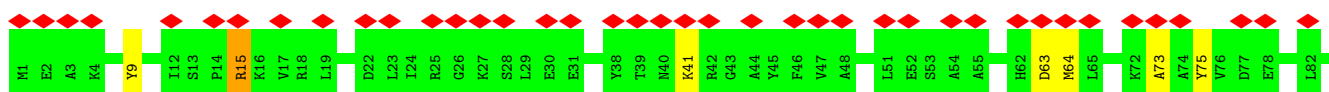
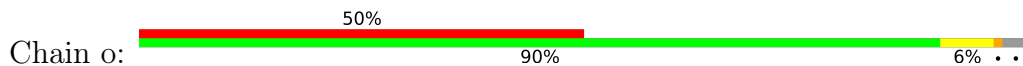




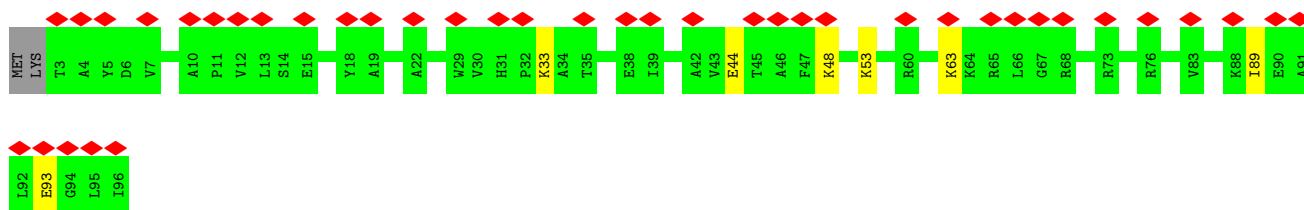
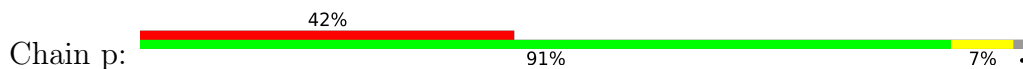
- Molecule 39: 50S ribosomal protein L21



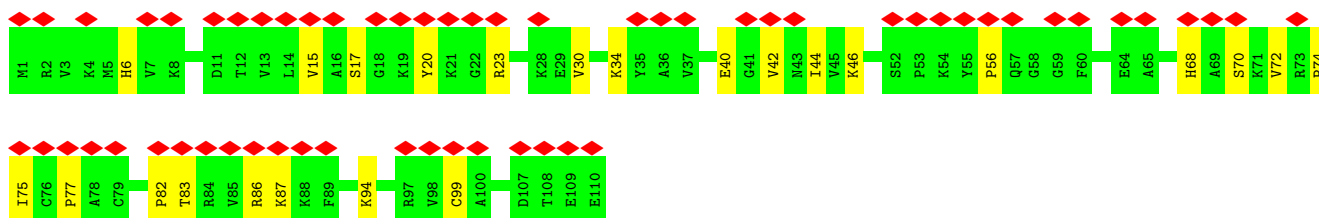
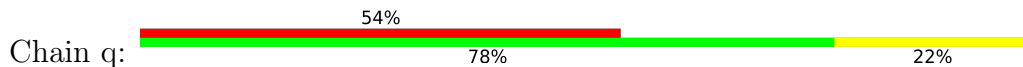
- Molecule 40: 50S ribosomal protein L22



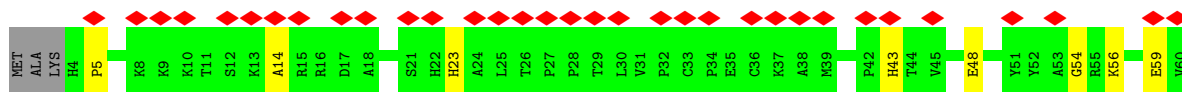
- Molecule 41: 50S ribosomal protein L23



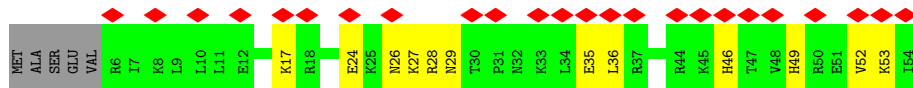
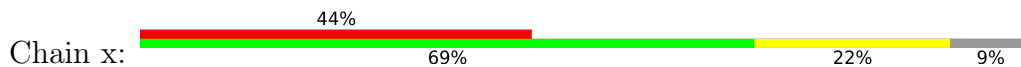
- Molecule 42: 50S ribosomal protein L24



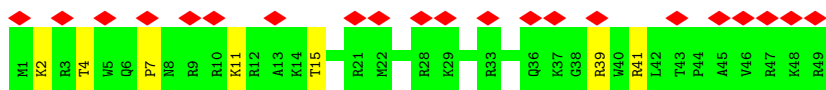
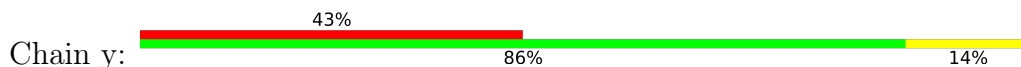
- Molecule 43: 50S ribosomal protein L25



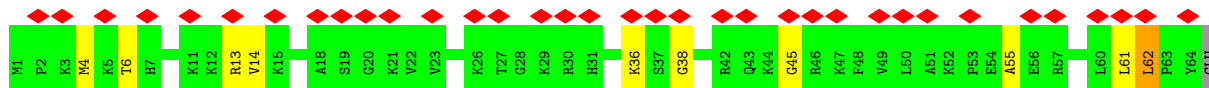
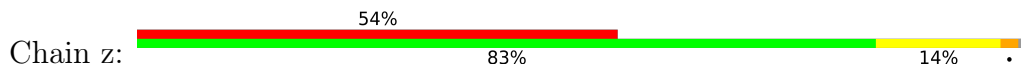
• Molecule 49: 50S ribosomal protein L33



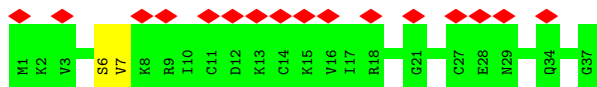
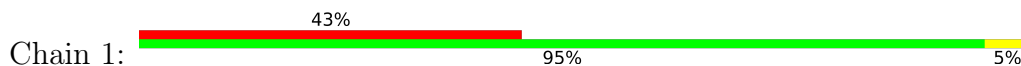
• Molecule 50: 50S ribosomal protein L34



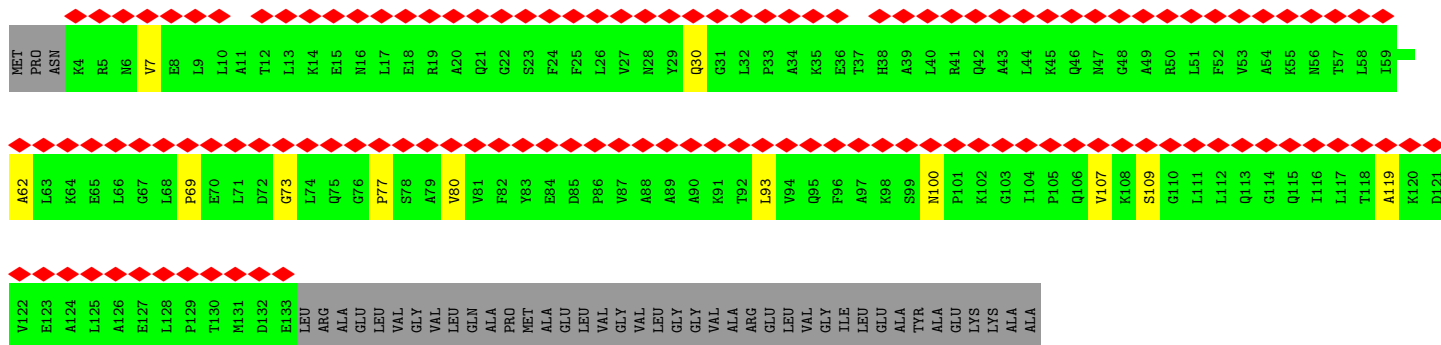
• Molecule 51: 50S ribosomal protein L35



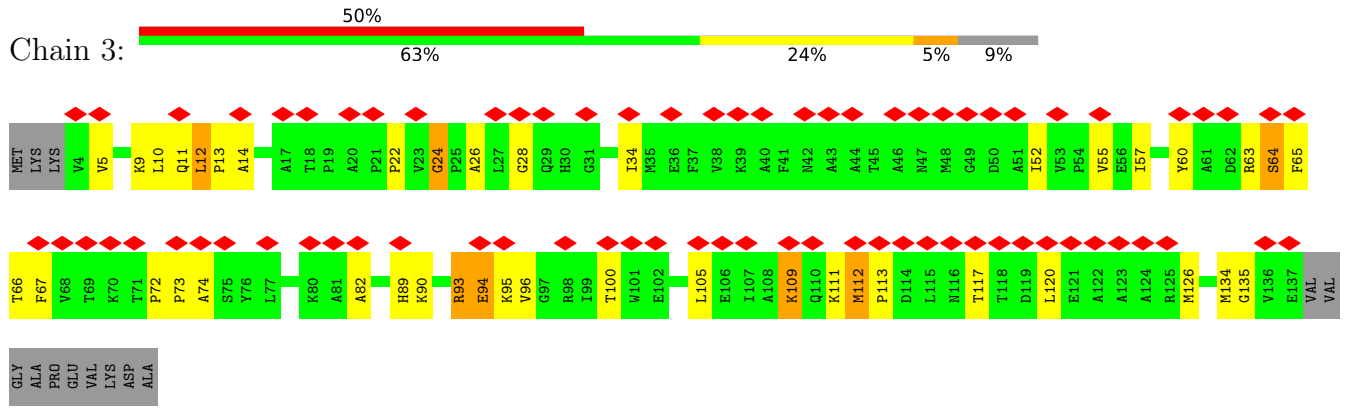
• Molecule 52: 50S ribosomal protein L36



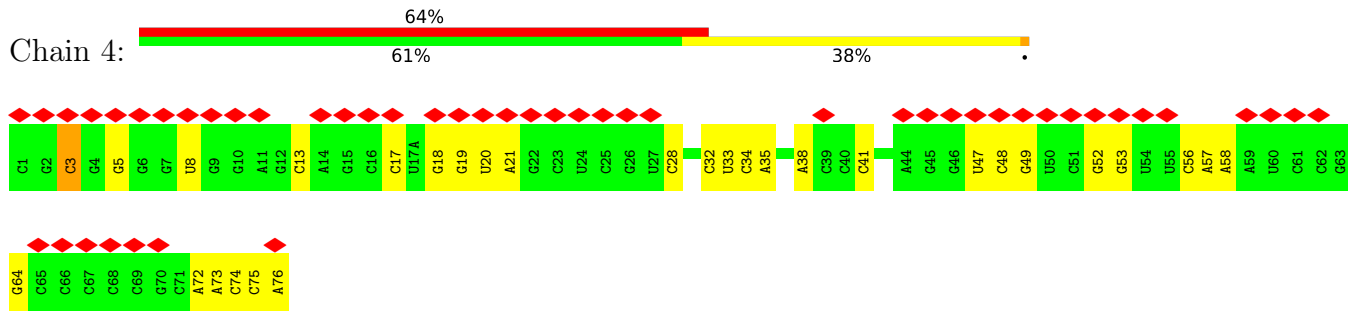
• Molecule 53: 50S ribosomal protein L10



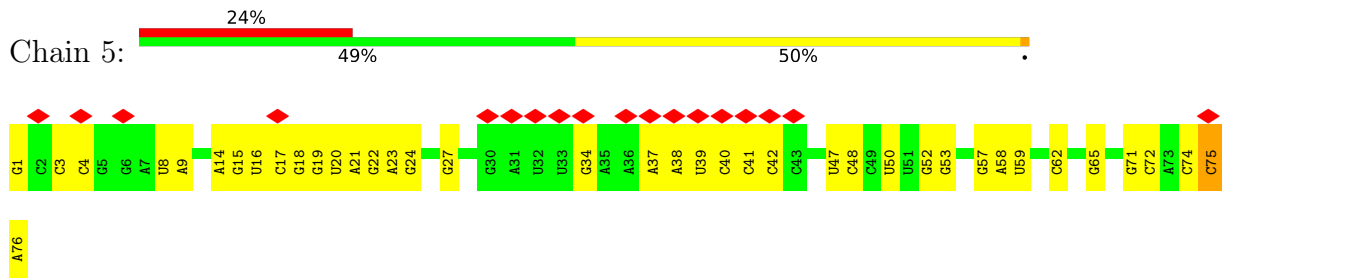
• Molecule 54: 50S ribosomal protein L11



• Molecule 55: P site- tRNA



• Molecule 56: E site- tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.959	Depositor
Minimum map value	-0.573	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.161	Depositor
Map size (\AA)	414.72, 414.72, 414.72	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.28, 1.28, 1.28	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: GCP

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	0.78	1/36438 (0.0%)	1.10	50/56869 (0.1%)
2	F	0.44	0/1935	0.72	1/2609 (0.0%)
3	G	0.42	0/1636	0.66	0/2205
4	H	0.49	0/1733	0.71	1/2318 (0.0%)
5	I	0.49	0/1162	0.76	0/1564
6	J	0.40	0/856	0.63	0/1154
7	K	0.38	0/1276	0.67	0/1709
8	L	0.48	0/1136	0.77	1/1527 (0.1%)
9	M	0.38	0/1029	0.65	0/1379
10	N	0.34	0/807	0.67	0/1085
11	O	0.39	0/900	0.63	0/1213
12	P	0.54	0/986	0.79	0/1320
13	Q	0.35	0/924	0.67	1/1238 (0.1%)
14	R	0.42	0/501	0.69	0/664
15	S	0.56	0/745	0.78	0/992
16	T	0.53	0/716	0.75	0/963
17	U	0.48	0/870	0.71	0/1159
18	V	0.41	0/603	0.72	1/799 (0.1%)
19	W	0.39	0/661	0.67	0/890
20	X	0.50	0/765	0.79	0/1007
21	Y	0.36	0/212	0.66	0/277
22	C	0.44	0/4545	0.57	25/6155 (0.4%)
23	D	0.97	10/69685 (0.0%)	1.24	293/108786 (0.3%)
24	E	0.82	1/2954 (0.0%)	1.09	2/4606 (0.0%)
25	Z	0.33	0/1775	0.58	2/2393 (0.1%)
26	a	0.57	1/2174 (0.0%)	0.80	1/2927 (0.0%)
27	b	0.54	0/1611	0.85	2/2171 (0.1%)
28	c	0.56	0/1660	0.78	0/2247
29	d	0.39	0/1507	0.73	2/2027 (0.1%)
30	e	0.47	0/1354	0.75	1/1831 (0.1%)
31	f	0.53	0/1140	0.79	2/1537 (0.1%)
32	g	0.52	0/942	0.80	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.48	0/1123	0.85	1/1493 (0.1%)
34	i	0.55	0/1100	0.81	1/1470 (0.1%)
35	j	0.52	0/974	0.73	0/1302
36	k	0.48	0/887	0.78	0/1180
37	l	0.52	0/990	0.81	1/1325 (0.1%)
38	m	0.60	0/982	0.79	0/1306
39	n	0.45	0/790	0.78	0/1057
40	o	0.52	0/886	0.71	0/1189
41	p	0.47	0/756	0.71	0/1015
42	q	0.43	0/857	0.78	0/1142
43	r	0.41	0/1467	0.70	0/1992
44	s	0.48	0/633	0.71	0/843
45	t	0.50	0/569	0.72	0/751
46	u	0.56	0/474	0.77	0/635
47	v	0.51	0/594	0.85	1/795 (0.1%)
48	w	0.56	0/459	0.76	0/621
49	x	0.49	0/433	0.87	0/576
50	y	0.58	0/438	0.78	0/575
51	z	0.57	0/523	0.83	0/690
52	1	0.46	0/310	0.72	0/407
53	2	0.23	0/640	0.45	0/889
54	3	0.43	0/1012	0.70	2/1373 (0.1%)
55	4	0.57	0/1832	0.96	1/2855 (0.0%)
56	5	1.93	7/1813 (0.4%)	1.02	3/2823 (0.1%)
All	All	0.81	20/165780 (0.0%)	1.07	395/247193 (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
2	F	0	1
8	L	0	1
26	a	0	5
28	c	0	3
30	e	0	1
31	f	0	1
32	g	0	1
37	l	0	2
38	m	0	1
39	n	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
40	o	0	1
41	p	0	1
42	q	0	1
46	u	0	1
47	v	0	1
49	x	0	1
51	z	0	1
54	3	0	2
All	All	0	26

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	5	75	C	N3-C4	39.72	1.61	1.33
56	5	75	C	N1-C6	36.95	1.59	1.37
56	5	75	C	C2-N3	36.64	1.65	1.35
56	5	75	C	C4-C5	26.84	1.64	1.43
56	5	75	C	N1-C2	25.86	1.66	1.40

The worst 5 of 395 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	2075	U	N1-C2-O2	10.51	130.16	122.80
23	D	1498	C	C2-N1-C1'	10.33	130.16	118.80
23	D	2498	C	N1-C2-O2	9.67	124.70	118.90
23	D	2498	C	N3-C2-O2	-9.54	115.22	121.90
23	D	1937	A	N1-C6-N6	-9.37	112.98	118.60

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	99	GLY	Peptide
8	L	28	ALA	Peptide
26	a	46	GLN	Peptide
26	a	82	ILE	Peptide
26	a	96	HIS	Peptide

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	F	232/256 (91%)	181 (78%)	33 (14%)	18 (8%)	1	12
3	G	204/239 (85%)	157 (77%)	33 (16%)	14 (7%)	1	14
4	H	206/209 (99%)	168 (82%)	21 (10%)	17 (8%)	1	12
5	I	148/162 (91%)	122 (82%)	19 (13%)	7 (5%)	2	21
6	J	99/101 (98%)	85 (86%)	11 (11%)	3 (3%)	4	28
7	K	153/156 (98%)	130 (85%)	16 (10%)	7 (5%)	2	21
8	L	136/138 (99%)	107 (79%)	19 (14%)	10 (7%)	1	13
9	M	125/128 (98%)	96 (77%)	14 (11%)	15 (12%)	0	5
10	N	96/105 (91%)	73 (76%)	11 (12%)	12 (12%)	0	5
11	O	117/129 (91%)	96 (82%)	15 (13%)	6 (5%)	2	19
12	P	122/132 (92%)	79 (65%)	33 (27%)	10 (8%)	1	12
13	Q	112/126 (89%)	80 (71%)	19 (17%)	13 (12%)	0	6
14	R	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	0	8
15	S	86/89 (97%)	70 (81%)	9 (10%)	7 (8%)	1	12
16	T	81/88 (92%)	65 (80%)	10 (12%)	6 (7%)	1	13
17	U	102/105 (97%)	82 (80%)	13 (13%)	7 (7%)	1	14
18	V	71/88 (81%)	57 (80%)	9 (13%)	5 (7%)	1	14
19	W	78/93 (84%)	53 (68%)	17 (22%)	8 (10%)	0	8
20	X	97/106 (92%)	85 (88%)	7 (7%)	5 (5%)	2	19
21	Y	22/27 (82%)	17 (77%)	2 (9%)	3 (14%)	0	4
22	C	562/610 (92%)	244 (43%)	187 (33%)	131 (23%)	0	1
25	Z	226/229 (99%)	180 (80%)	26 (12%)	20 (9%)	1	11
26	a	270/276 (98%)	188 (70%)	51 (19%)	31 (12%)	0	6
27	b	204/206 (99%)	147 (72%)	29 (14%)	28 (14%)	0	4
28	c	206/210 (98%)	160 (78%)	29 (14%)	17 (8%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	d	180/182 (99%)	119 (66%)	39 (22%)	22 (12%)	0	5
30	e	172/180 (96%)	121 (70%)	27 (16%)	24 (14%)	0	4
31	f	137/140 (98%)	106 (77%)	18 (13%)	13 (10%)	0	10
32	g	120/122 (98%)	86 (72%)	22 (18%)	12 (10%)	0	9
33	h	143/150 (95%)	98 (68%)	25 (18%)	20 (14%)	0	4
34	i	134/141 (95%)	89 (66%)	30 (22%)	15 (11%)	0	7
35	j	115/118 (98%)	93 (81%)	13 (11%)	9 (8%)	1	12
36	k	108/112 (96%)	78 (72%)	20 (18%)	10 (9%)	0	10
37	l	115/146 (79%)	70 (61%)	32 (28%)	13 (11%)	0	7
38	m	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	12
39	n	99/101 (98%)	59 (60%)	21 (21%)	19 (19%)	0	2
40	o	108/113 (96%)	82 (76%)	18 (17%)	8 (7%)	1	13
41	p	92/96 (96%)	74 (80%)	12 (13%)	6 (6%)	1	16
42	q	108/110 (98%)	61 (56%)	24 (22%)	23 (21%)	0	2
43	r	178/206 (86%)	128 (72%)	33 (18%)	17 (10%)	0	9
44	s	77/85 (91%)	60 (78%)	12 (16%)	5 (6%)	1	16
45	t	65/67 (97%)	58 (89%)	2 (3%)	5 (8%)	1	13
46	u	57/60 (95%)	43 (75%)	11 (19%)	3 (5%)	2	19
47	v	69/71 (97%)	39 (56%)	14 (20%)	16 (23%)	0	1
48	w	55/60 (92%)	35 (64%)	12 (22%)	8 (14%)	0	4
49	x	47/54 (87%)	21 (45%)	15 (32%)	11 (23%)	0	1
50	y	47/49 (96%)	30 (64%)	10 (21%)	7 (15%)	0	3
51	z	62/65 (95%)	38 (61%)	14 (23%)	10 (16%)	0	3
52	1	35/37 (95%)	25 (71%)	8 (23%)	2 (6%)	1	18
53	2	128/173 (74%)	95 (74%)	21 (16%)	12 (9%)	0	10
54	3	132/147 (90%)	82 (62%)	20 (15%)	30 (23%)	0	1
All	All	6511/6972 (93%)	4639 (71%)	1137 (18%)	735 (11%)	1	7

5 of 735 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	191	ASP
2	F	209	ARG

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Mol	Chain	Res	Type
3	G	64	VAL
4	H	30	LYS
4	H	191	ARG

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	
2	F	202/220 (92%)	202 (100%)	0	100	100
3	G	160/188 (85%)	160 (100%)	0	100	100
4	H	180/181 (99%)	180 (100%)	0	100	100
5	I	115/123 (94%)	115 (100%)	0	100	100
6	J	90/90 (100%)	90 (100%)	0	100	100
7	K	126/127 (99%)	126 (100%)	0	100	100
8	L	119/119 (100%)	119 (100%)	0	100	100
9	M	98/99 (99%)	98 (100%)	0	100	100
10	N	88/92 (96%)	88 (100%)	0	100	100
11	O	90/99 (91%)	90 (100%)	0	100	100
12	P	104/109 (95%)	103 (99%)	1 (1%)	76	86
13	Q	92/101 (91%)	87 (95%)	5 (5%)	22	47
14	R	49/50 (98%)	49 (100%)	0	100	100
15	S	79/80 (99%)	79 (100%)	0	100	100
16	T	72/74 (97%)	72 (100%)	0	100	100
17	U	96/97 (99%)	96 (100%)	0	100	100
18	V	64/77 (83%)	64 (100%)	0	100	100
19	W	71/80 (89%)	69 (97%)	2 (3%)	43	64
20	X	76/82 (93%)	76 (100%)	0	100	100
21	Y	19/22 (86%)	19 (100%)	0	100	100
22	C	473/505 (94%)	347 (73%)	126 (27%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	Z	180/181 (99%)	174 (97%)	6 (3%)	38	61
26	a	215/218 (99%)	213 (99%)	2 (1%)	78	87
27	b	166/166 (100%)	165 (99%)	1 (1%)	86	92
28	c	164/166 (99%)	164 (100%)	0	100	100
29	d	156/156 (100%)	153 (98%)	3 (2%)	57	75
30	e	143/148 (97%)	141 (99%)	2 (1%)	67	80
31	f	118/119 (99%)	118 (100%)	0	100	100
32	g	100/100 (100%)	99 (99%)	1 (1%)	76	86
33	h	111/116 (96%)	111 (100%)	0	100	100
34	i	106/111 (96%)	106 (100%)	0	100	100
35	j	100/101 (99%)	100 (100%)	0	100	100
36	k	87/88 (99%)	87 (100%)	0	100	100
37	l	105/127 (83%)	105 (100%)	0	100	100
38	m	93/94 (99%)	93 (100%)	0	100	100
39	n	82/82 (100%)	82 (100%)	0	100	100
40	o	90/92 (98%)	90 (100%)	0	100	100
41	p	76/78 (97%)	76 (100%)	0	100	100
42	q	91/91 (100%)	91 (100%)	0	100	100
43	r	159/179 (89%)	159 (100%)	0	100	100
44	s	63/67 (94%)	63 (100%)	0	100	100
45	t	62/62 (100%)	62 (100%)	0	100	100
46	u	51/52 (98%)	51 (100%)	0	100	100
47	v	63/63 (100%)	60 (95%)	3 (5%)	25	51
48	w	50/52 (96%)	50 (100%)	0	100	100
49	x	48/52 (92%)	48 (100%)	0	100	100
50	y	42/42 (100%)	42 (100%)	0	100	100
51	z	54/55 (98%)	54 (100%)	0	100	100
52	1	34/34 (100%)	34 (100%)	0	100	100
54	3	101/111 (91%)	86 (85%)	15 (15%)	3	15
All	All	5373/5618 (96%)	5206 (97%)	167 (3%)	43	62

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	C	489	LEU
29	d	25	TYR
22	C	507	ILE
22	C	583	ARG
47	v	31	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
26	a	44	ASN
54	3	116	ASN
31	f	94	HIS
54	3	42	ASN
47	v	47	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1514/1522 (99%)	640 (42%)	80 (5%)
23	D	2888/2893 (99%)	1464 (50%)	169 (5%)
24	E	122/123 (99%)	47 (38%)	4 (3%)
55	4	76/77 (98%)	30 (39%)	0
56	5	75/76 (98%)	36 (48%)	4 (5%)
All	All	4675/4691 (99%)	2217 (47%)	257 (5%)

5 of 2217 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	10	A
1	A	14	U

5 of 257 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	D	2576	G
23	D	2664	G
23	D	270(B)	A
23	D	227	A

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Mol	Chain	Res	Type
23	D	2725	A

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](#)

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	GCP	C	701	-	27,34,34	3.19	8 (29%)	34,54,54	2.76	9 (26%)

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	GCP	C	701	-	-	9/15/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	C	701	GCP	C3'-C4'	-9.42	1.28	1.53
57	C	701	GCP	O4'-C4'	7.70	1.62	1.45
57	C	701	GCP	O4'-C1'	-6.76	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	C	701	GCP	C2-N2	6.08	1.46	1.33
57	C	701	GCP	O2'-C2'	-3.10	1.35	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	C	701	GCP	N2-C2-N3	8.57	131.76	117.79
57	C	701	GCP	N2-C2-N1	-6.11	107.75	117.25
57	C	701	GCP	C1'-N9-C4	-6.03	116.05	126.64
57	C	701	GCP	N3-C2-N1	-5.05	120.48	127.22
57	C	701	GCP	PB-O3A-PA	-4.93	116.91	132.56

There are no chirality outliers.

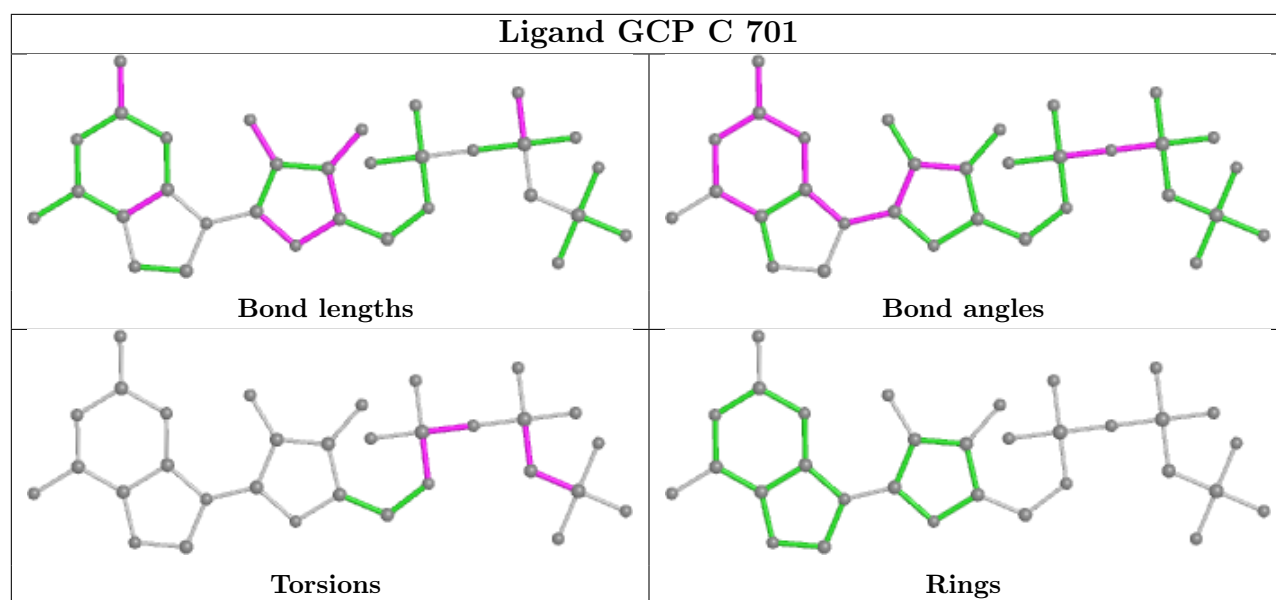
5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	C	701	GCP	PG-C3B-PB-O1B
57	C	701	GCP	PG-C3B-PB-O2B
57	C	701	GCP	PG-C3B-PB-O3A
57	C	701	GCP	C5'-O5'-PA-O3A
57	C	701	GCP	C5'-O5'-PA-O1A

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 [i](#)

There are no chain breaks in this entry.

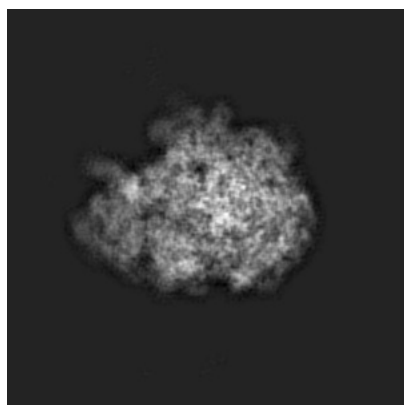
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6585. These allow visual inspection of the internal detail of the map and identification of artifacts.

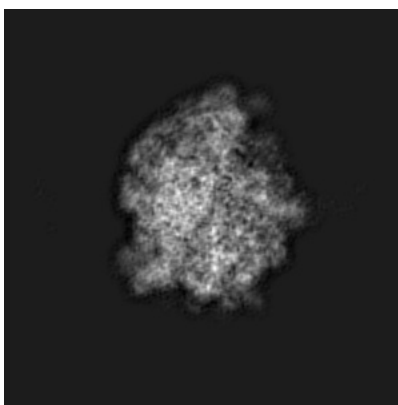
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

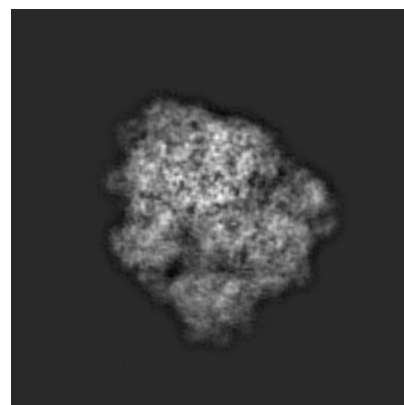
6.1.1 Primary map



X



Y

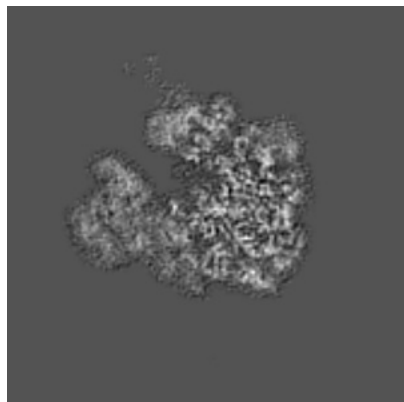


Z

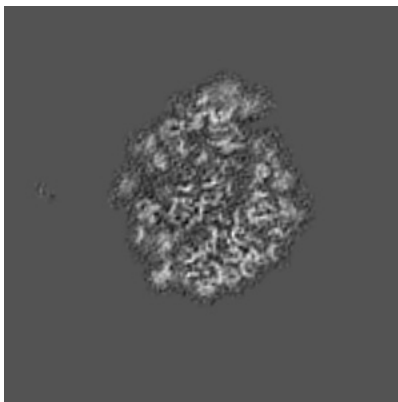
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

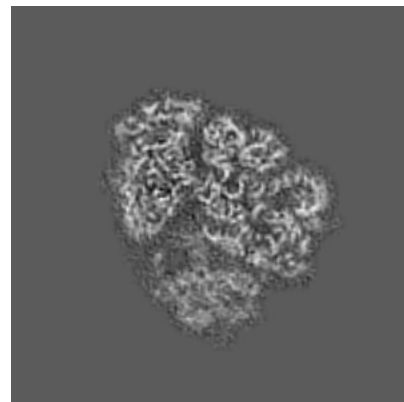
6.2.1 Primary map



X Index: 162



Y Index: 162

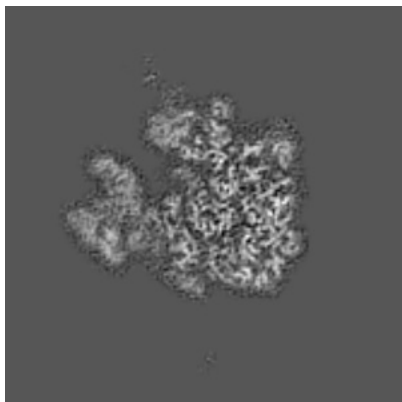


Z Index: 162

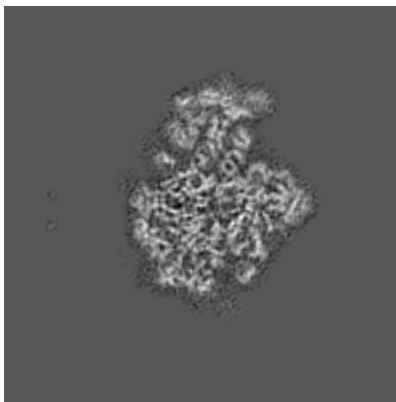
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

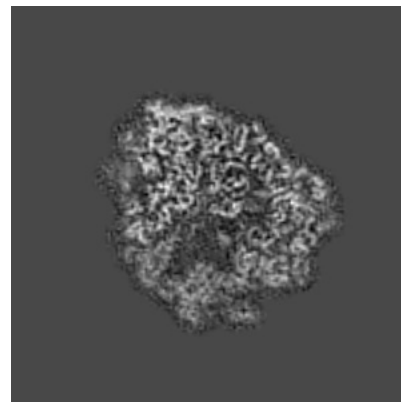
6.3.1 Primary map



X Index: 167



Y Index: 170



Z Index: 170

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

6.4 Orthogonal surface views [i](#)

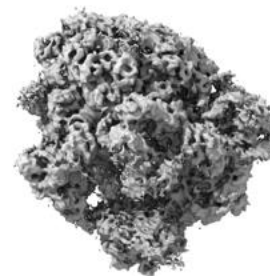
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.161. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

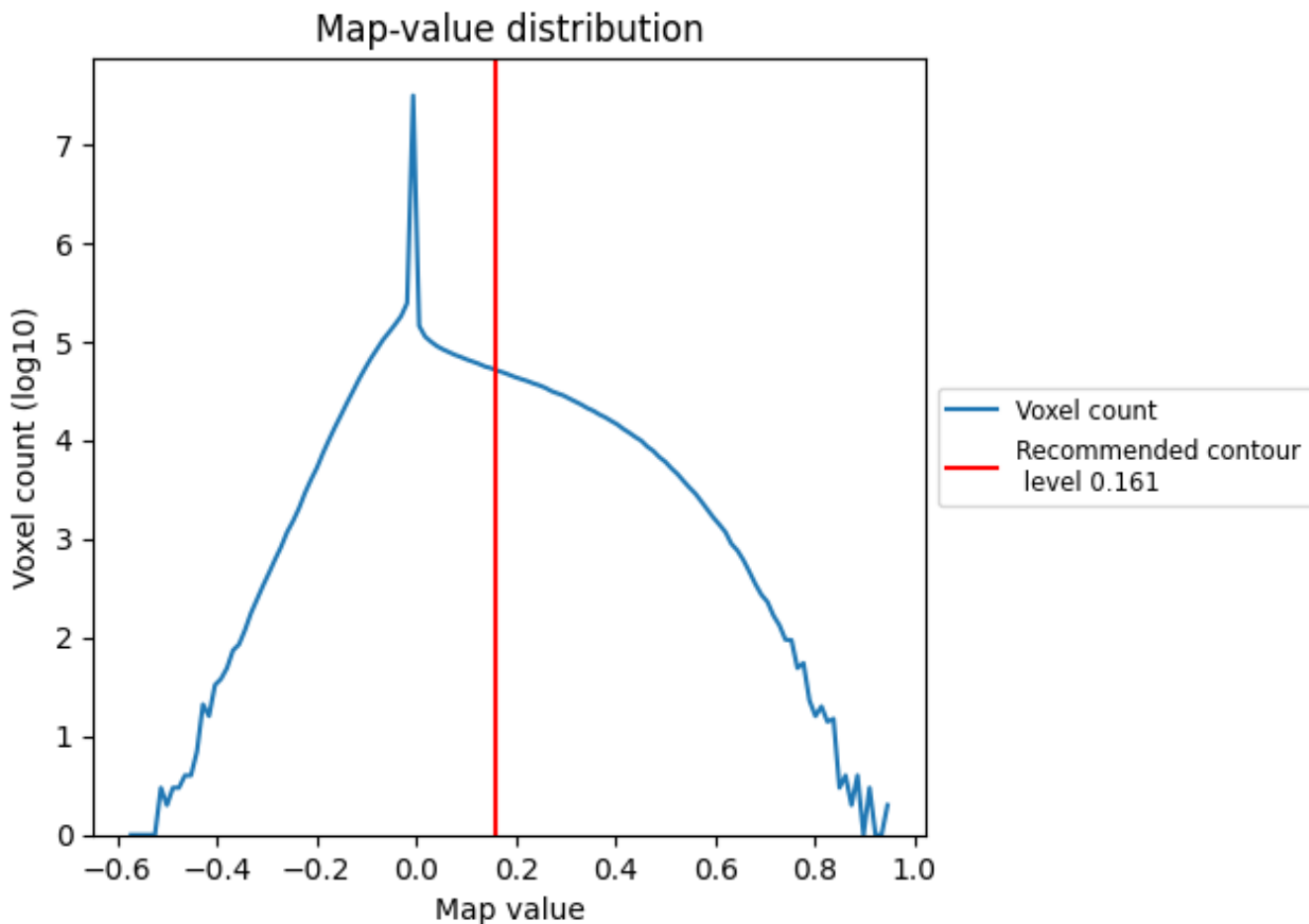
6.5 Mask visualisation

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

7 Map analysis [i](#)

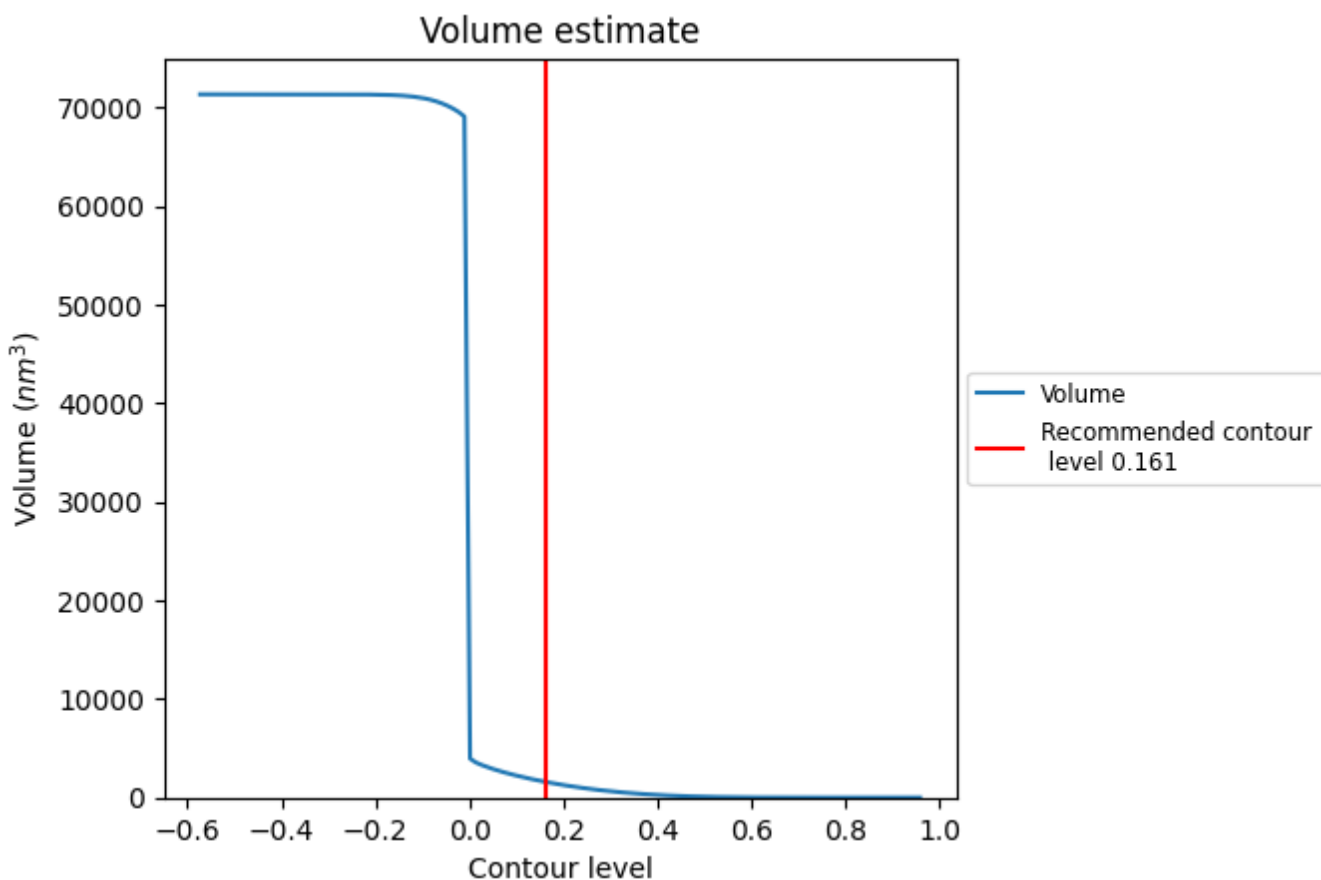
This section contains the results of statistical analysis of the map.

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.

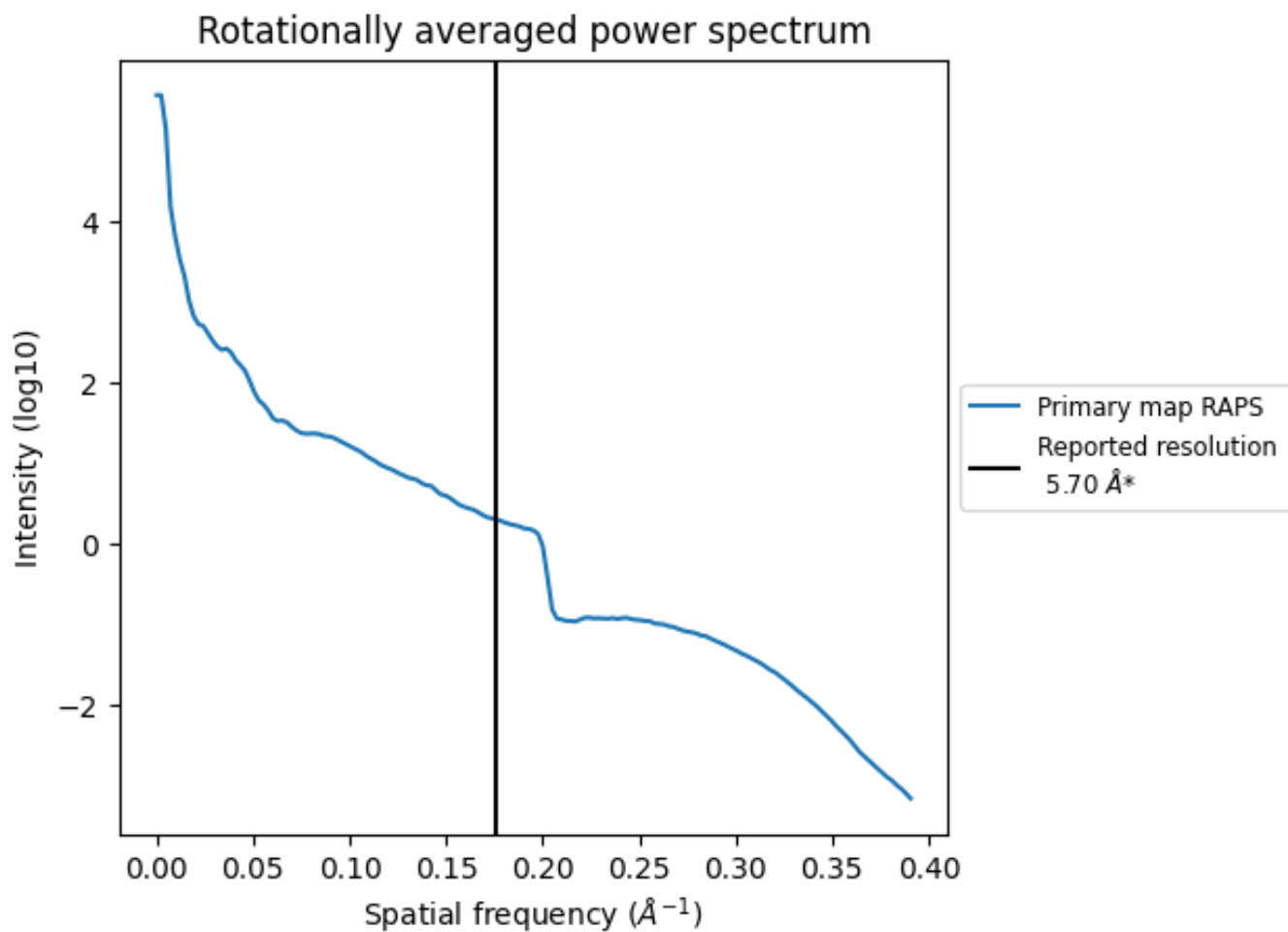
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1597 nm³; this corresponds to an approximate mass of 1443 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 0.175\AA^{-1}

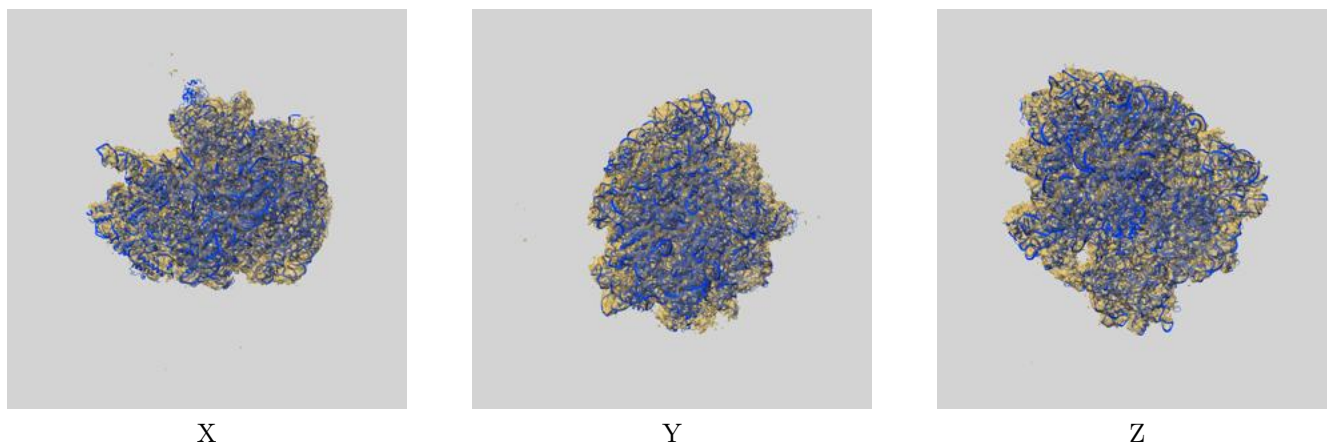
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

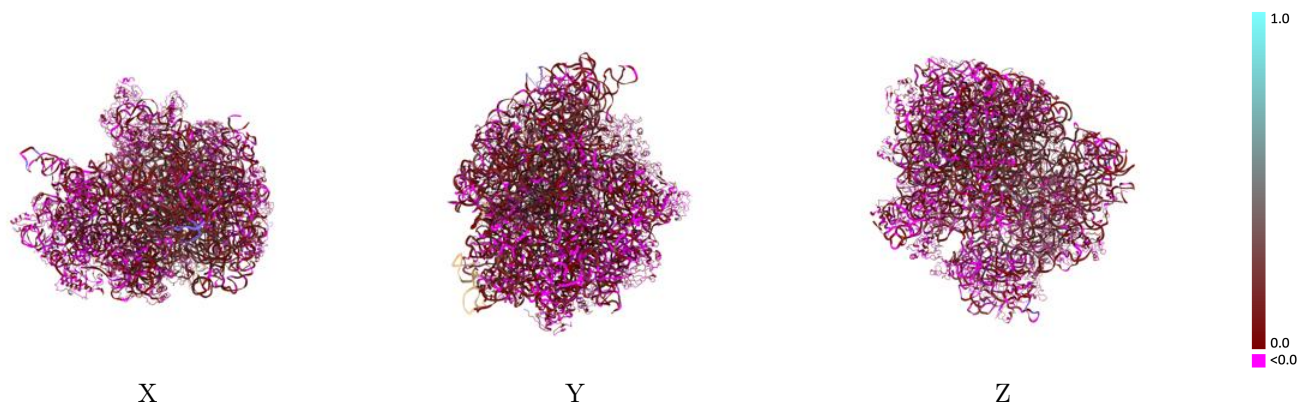
This section contains information regarding the fit between EMDB map EMD-6585 and PDB model 5IMR. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



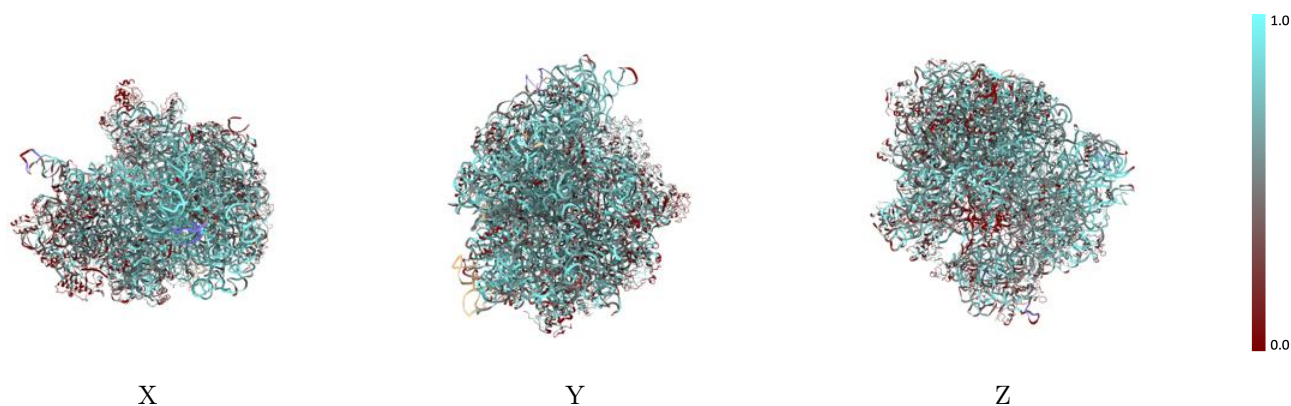
The images above show the 3D surface view of the map at the recommended contour level 0.161 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



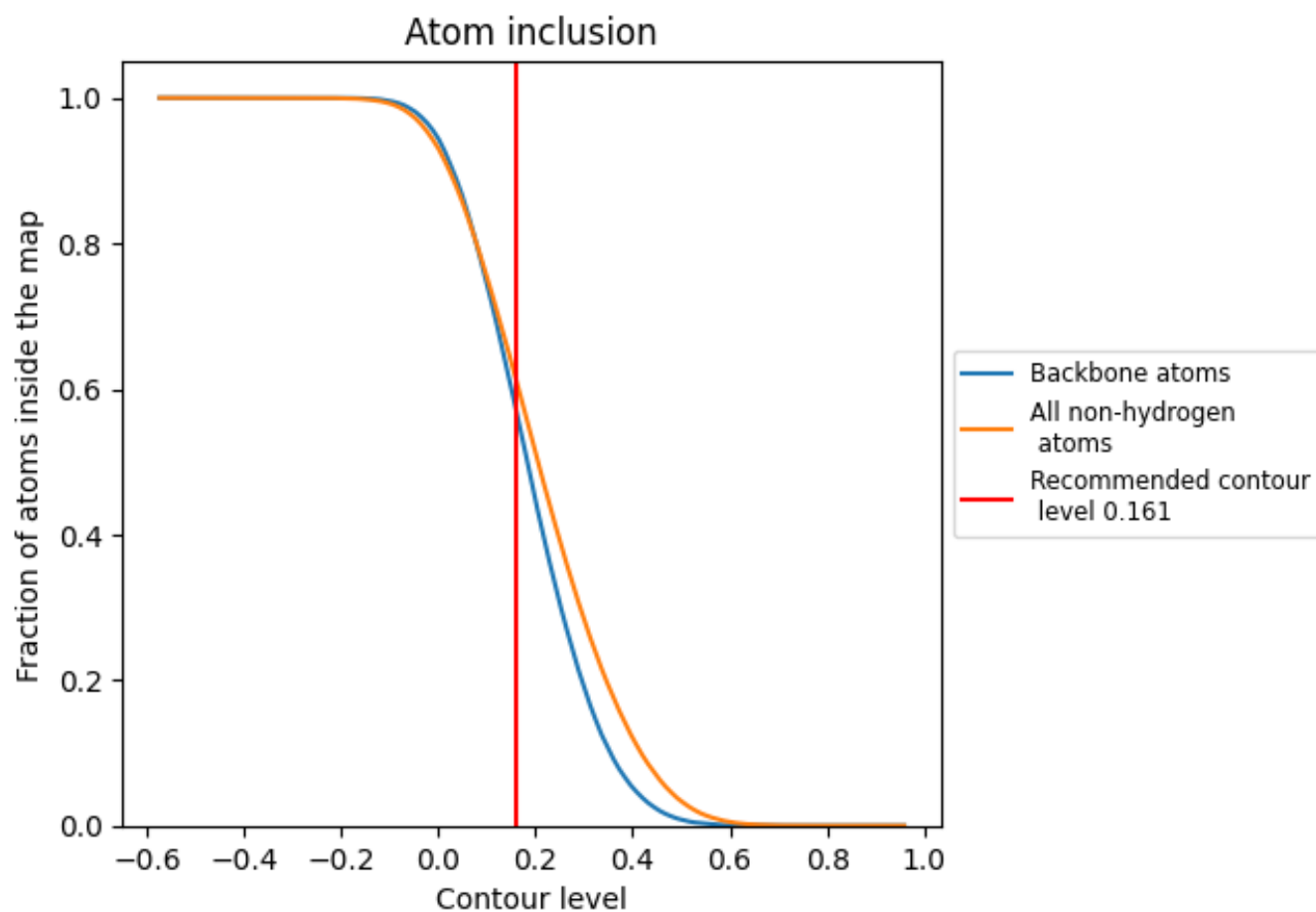
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.161).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 61% 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 (0.161) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6111	 0.1000
1	 0.5102	 0.0940
2	 0.0374	 0.0020
3	 0.3712	 0.0270
4	 0.3628	 0.1310
5	 0.5872	 0.1030
A	 0.7035	 0.1120
C	 0.4588	 0.0940
D	 0.7182	 0.1300
E	 0.6384	 0.0400
F	 0.3258	 0.0200
G	 0.3198	 0.0180
H	 0.4549	 0.0590
I	 0.4887	 0.0960
J	 0.4268	 0.0670
K	 0.3154	 0.0270
L	 0.4958	 0.0610
M	 0.3704	 0.0290
N	 0.3078	 0.0180
O	 0.5249	 0.1180
P	 0.5059	 0.1290
Q	 0.4455	 0.0260
R	 0.3233	 0.0250
S	 0.4633	 0.0880
T	 0.5337	 0.0280
U	 0.5289	 0.0990
V	 0.4286	 0.0820
W	 0.4517	 -0.0270
X	 0.4668	 0.0570
Y	 0.3508	 -0.0210
Z	 0.1617	 0.0120
a	 0.5875	 0.1510
b	 0.4922	 0.0860
c	 0.4517	 0.0640
d	 0.3993	 0.0230



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Chain	Atom inclusion	Q-score
e	 0.4795	 0.0370
f	 0.4253	 0.0370
g	 0.5088	 0.1400
h	 0.4841	 0.0750
i	 0.4459	 0.0850
j	 0.4483	 0.0250
k	 0.4958	 0.0120
l	 0.5075	 0.1240
m	 0.4165	 0.0340
n	 0.4081	 0.0160
o	 0.4270	 0.0540
p	 0.4677	 0.0670
q	 0.4281	 0.0270
r	 0.3178	 0.0200
s	 0.4338	 0.0550
t	 0.4461	 0.0290
u	 0.4254	 0.0400
v	 0.4857	 0.1120
w	 0.3880	 0.0100
x	 0.5159	 0.0970
y	 0.4648	 0.1110
z	 0.3738	 0.0400