



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 01:40 AM UTC

PDB ID : 3JCE / pdb_00003jce
EMDB ID : EMD-6550
Title : Structure of Escherichia coli EF4 in pretranslocational ribosomes (Pre EF4)
Authors : Zhang, D.; Yan, K.; Liu, G.; Song, G.; Luo, J.; Shi, Y.; Cheng, E.; Wu, S.;
Jiang, T.; Low, J.; Gao, N.; Qin, Y.
Deposited on : 2015-12-01
Resolution : 3.20 Å(reported)
Based on initial model : 4V9O

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

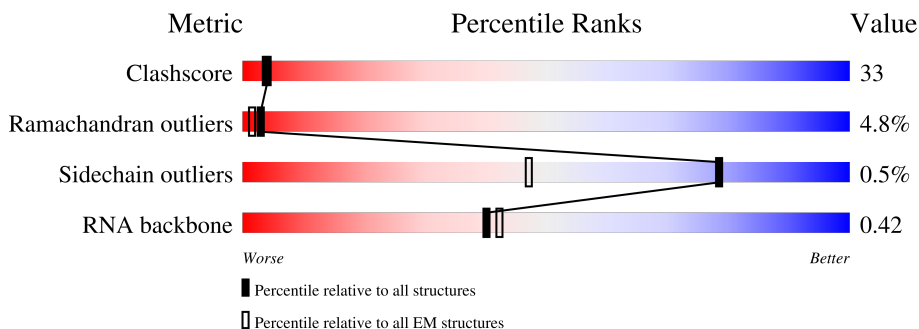
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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	1533	<div style="display: flex; justify-content: space-between;"> 62% 32% 55% 13% </div>
2	c	233	<div style="display: flex; justify-content: space-between;"> 73% 43% 43% 12% </div>
3	d	206	<div style="display: flex; justify-content: space-between;"> 82% 34% 63% </div>
4	e	167	<div style="display: flex; justify-content: space-between;"> 75% 35% 53% 10% </div>
5	f	135	<div style="display: flex; justify-content: space-between;"> 57% 30% 39% 7% 24% </div>
6	g	179	<div style="display: flex; justify-content: space-between;"> 70% 42% 40% 16% </div>
7	h	130	<div style="display: flex; justify-content: space-between;"> 71% 42% 55% </div>

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Mol	Chain	Length	Quality of chain
8	i	130	75% 28% 67% ..
9	j	103	71% 31% 57% 6% 5%
10	k	129	80% 42% 45% 9%
11	l	124	73% 44% 49% 6%
12	m	118	76% 33% 58% 6%
13	n	101	84% 31% 45% 20% ..
14	o	89	71% 47% 51% ..
15	p	82	74% 40% 55% 5%
16	q	84	67% 45% 50% 5%
17	r	75	60% 45% 25% 27%
18	s	92	63% 35% 48% 14%
19	t	87	75% 46% 49% ..
20	u	71	59% 30% 38% 28%
21	b	241	76% 30% 57% 10%
22	0	57	68% 51% 46% ..
23	1	55	73% 24% 58% 9% 9%
24	2	46	74% 67% 33%
25	3	65	77% 51% 45% ..
26	4	38	74% 37% 50% 13%
27	5	234	95% 18% 77% 5%
28	A	2904	62% 37% 50% 13%
29	B	120	57% 29% 57% 12%
30	C	273	78% 43% 52% ..
31	D	209	78% 45% 46% 8%
32	E	201	74% 42% 52% 5%


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Mol	Chain	Length	Quality of chain
33	F	179	82% 35% 59% 6%
34	G	177	77% 34% 61%
35	H	149	94% 23% 68% 9%
36	I	142	88% 31% 62% 6%
37	J	142	73% 44% 50% 6%
38	K	123	83% 45% 50%
39	L	144	65% 47% 46% 6%
40	M	136	82% 43% 52% 5%
41	N	127	68% 50% 43% 6%
42	O	117	56% 45% 54%
43	P	115	81% 49% 44% 6%
44	Q	118	70% 59% 39%
45	R	103	76% 45% 51%
46	S	110	75% 45% 53%
47	T	100	63% 27% 55% 9% 7%
48	U	104	65% 44% 49% 5%
49	V	94	70% 53% 44%
50	W	85	66% 19% 62% 12% 7%
51	X	78	68% 31% 62% 6%
52	Y	63	81% 32% 68%
53	Z	59	68% 51% 42% 5%
54	6	76	68% 34% 47% 17%
54	9	76	91% 5% 68% 26%
55	7	15	93% 53% 47%
56	8	77	60% 32% 43% 25%

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Mol	Chain	Length	Quality of chain
57	x	599	 <p>85% 33% 59% 6%</p>

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 154017 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	1533	32895	14671	6036	10655	1533	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3.

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

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

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

- Molecule 5 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	f	102	832	525	150	150	7	0	0

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	g	151	1181	735	227	215	4	0	0

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

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

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	m	114	883	546	178	156	3	0	0

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	n	100	805	499	164	139	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

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

- Molecule 21 is a protein called 30S ribosomal protein S2.

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

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 28 is a RNA chain called 23 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
28	A	2903	62320	27801	11467	20149	2903	0	0

- Molecule 29 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	B	118	2529	1126	464	821	118	0	0

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	C	270	2076	1285	422	362	7	0	0

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

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

- Molecule 35 is a protein called 50S ribosomal protein L9.

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

- Molecule 36 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

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

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 41 is a protein called 50S ribosomal protein L17.

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

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

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

- Molecule 48 is a protein called 50S ribosomal protein L24.

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

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 53 is a protein called 50S ribosomal protein L30.

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

- Molecule 54 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	6	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		
54	9	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	15	Total	C	N	O	P	0	0
			320	144	59	102	15		

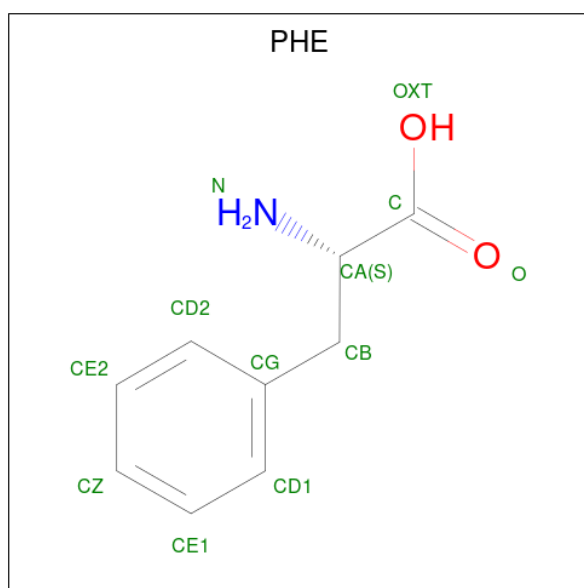
- Molecule 56 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	8	77	1640	732	297	535	76	0	0

- Molecule 57 is a protein called Elongation factor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	x	586	4573	2885	792	875	21	0	0

- Molecule 58 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



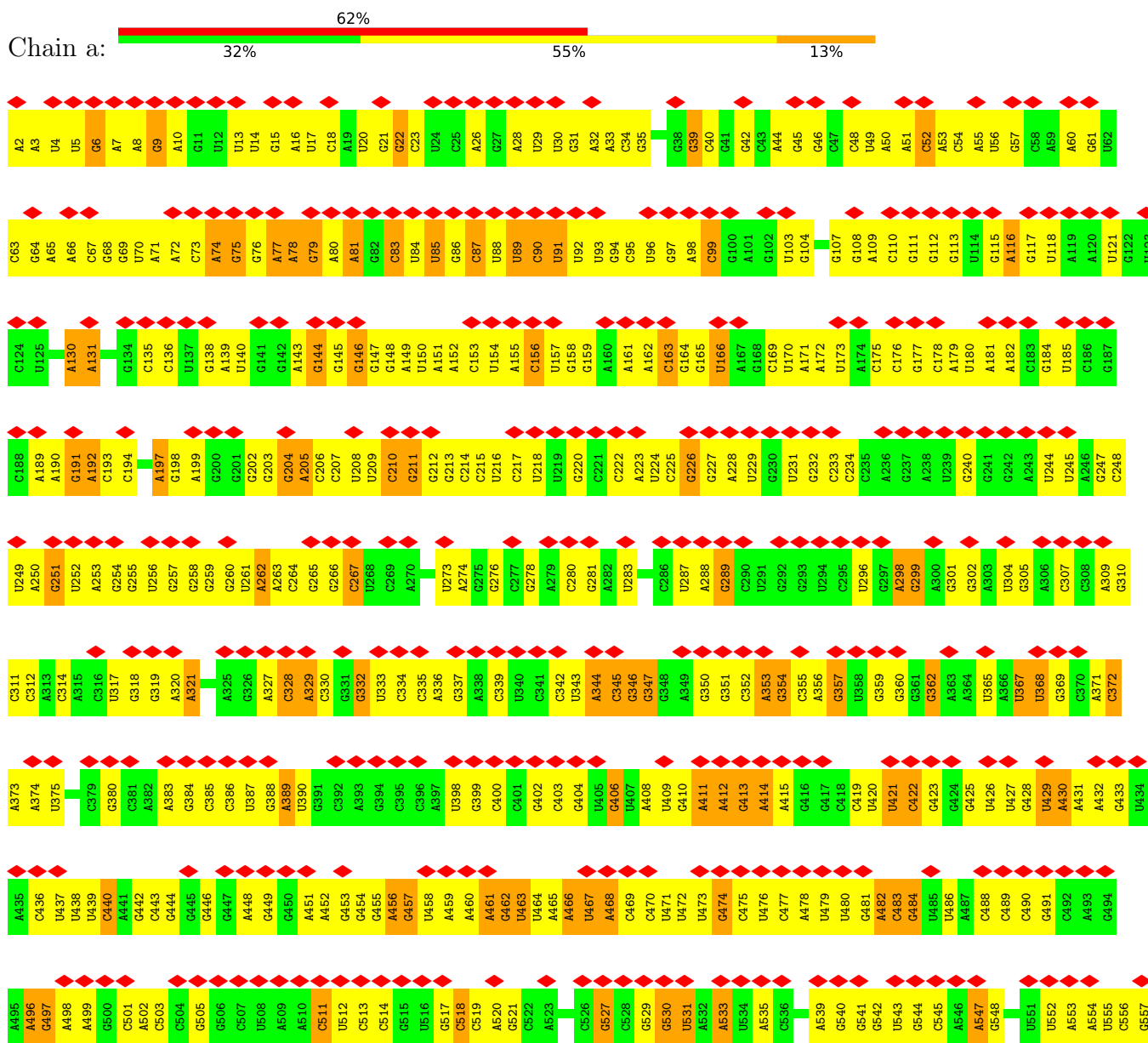
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
58	6	1	11	9	1	1	0

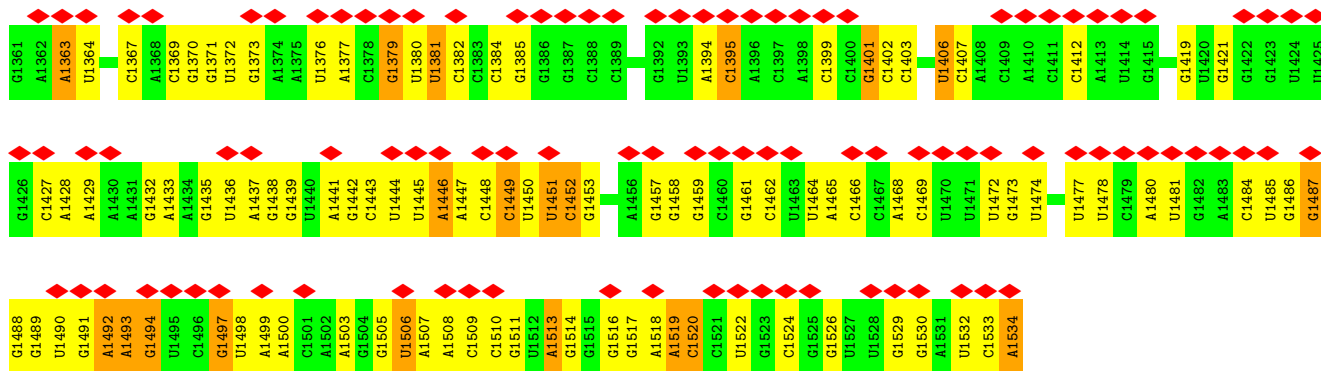
- Molecule 59 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

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





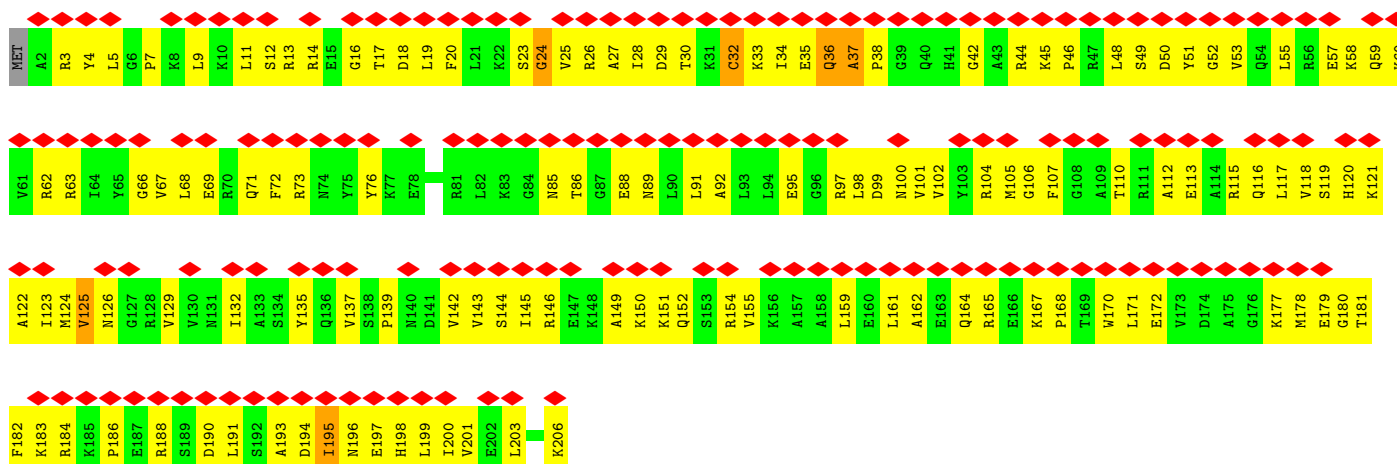
• Molecule 2: 30S ribosomal protein S3

Chain c: 43% 73% 43% 12%

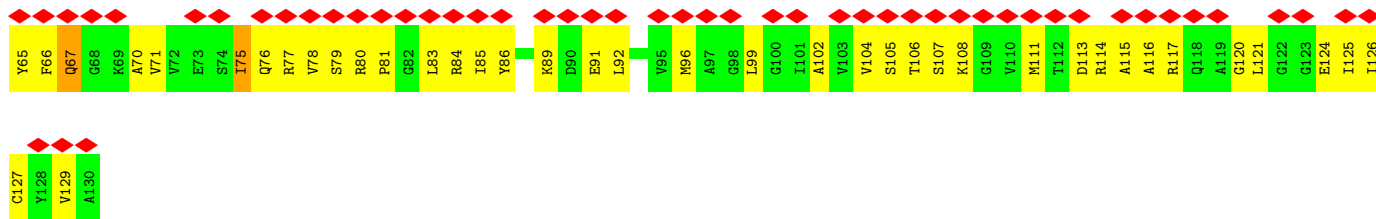


• Molecule 3: 30S ribosomal protein S4

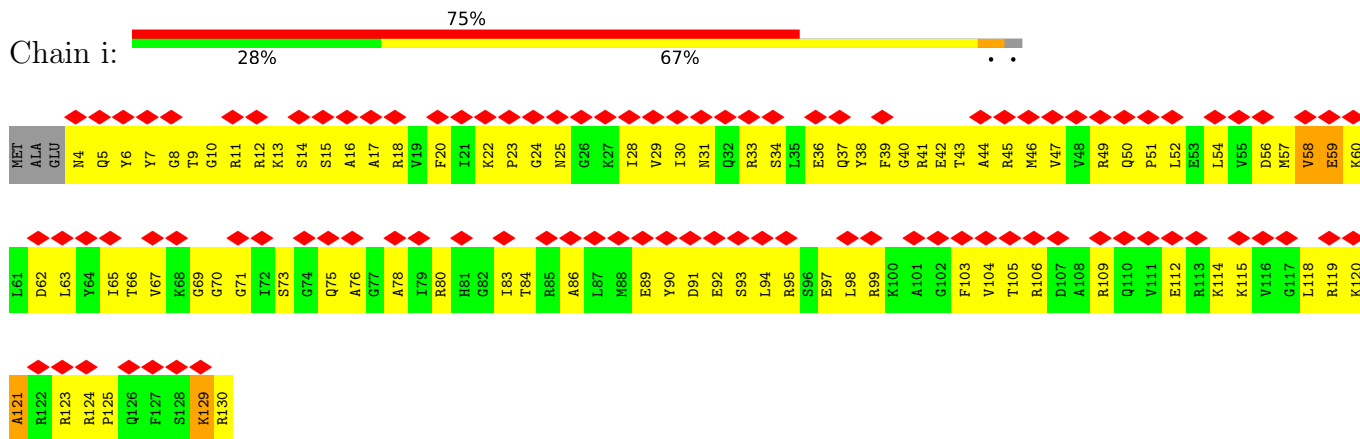
Chain d: 34% 82% 63%



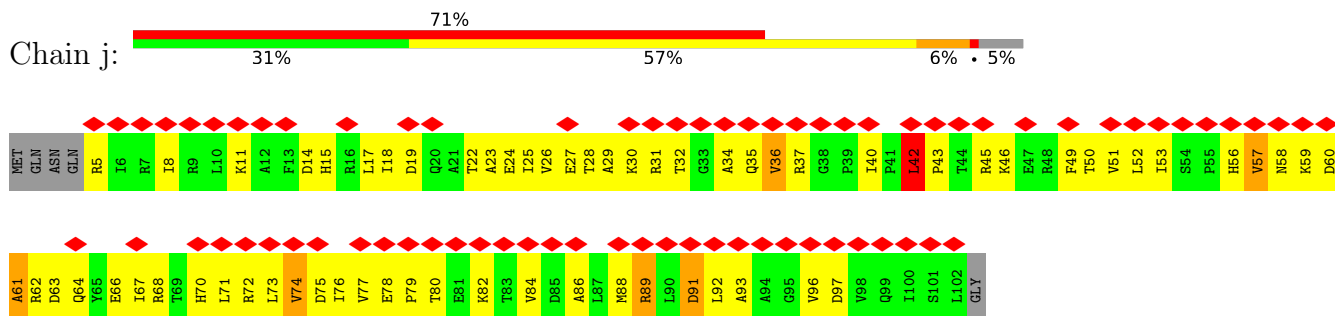
• Molecule 4: 30S ribosomal protein S5



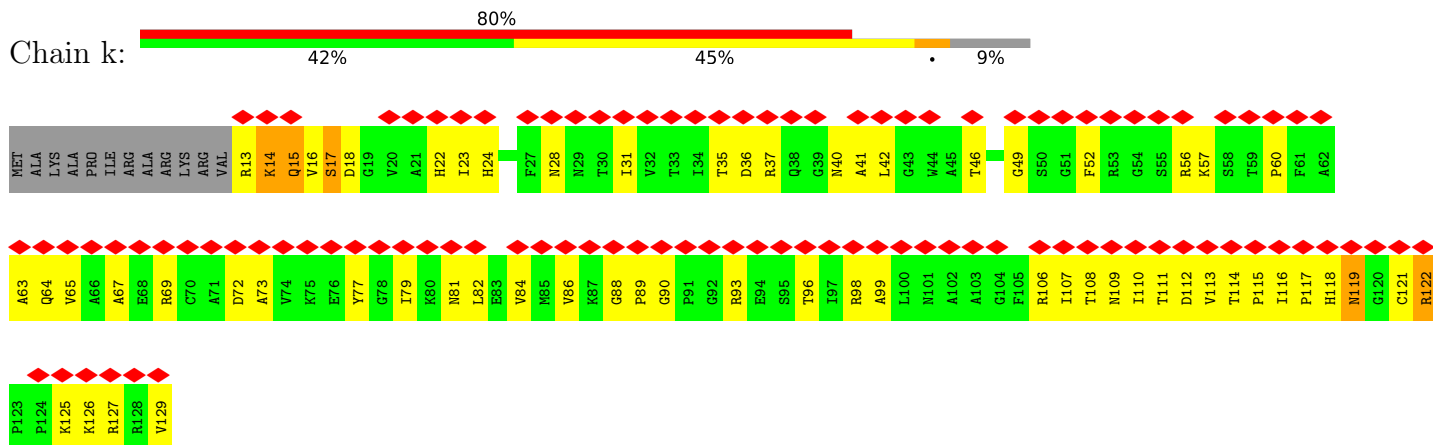
• Molecule 8: 30S ribosomal protein S9



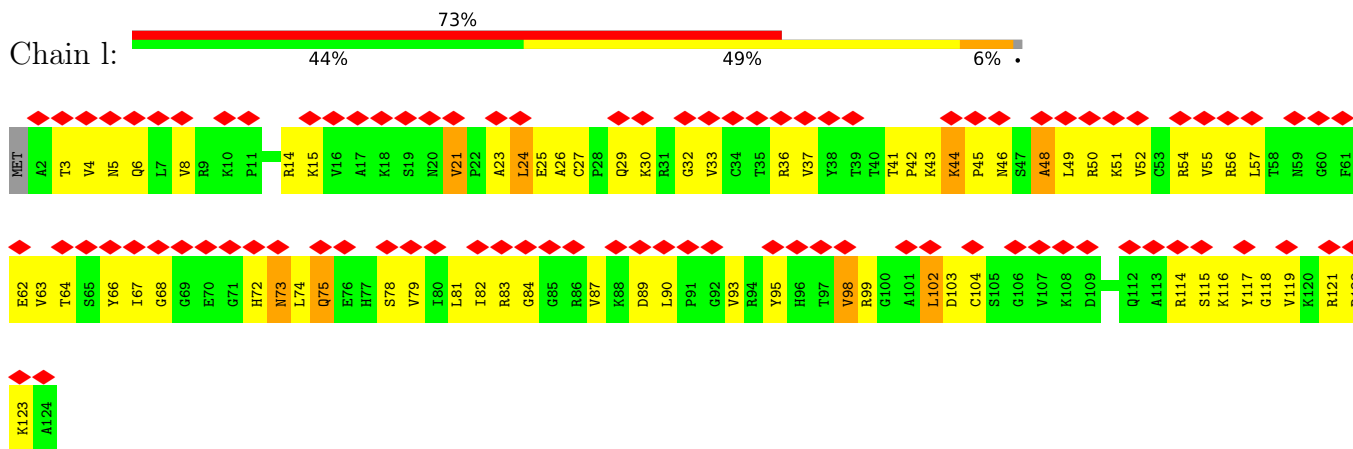
• Molecule 9: 30S ribosomal protein S10



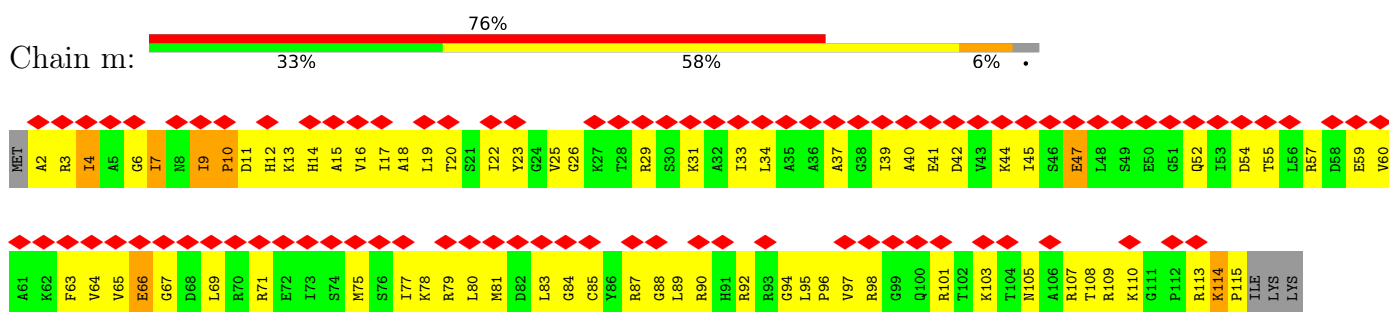
• Molecule 10: 30S ribosomal protein S11



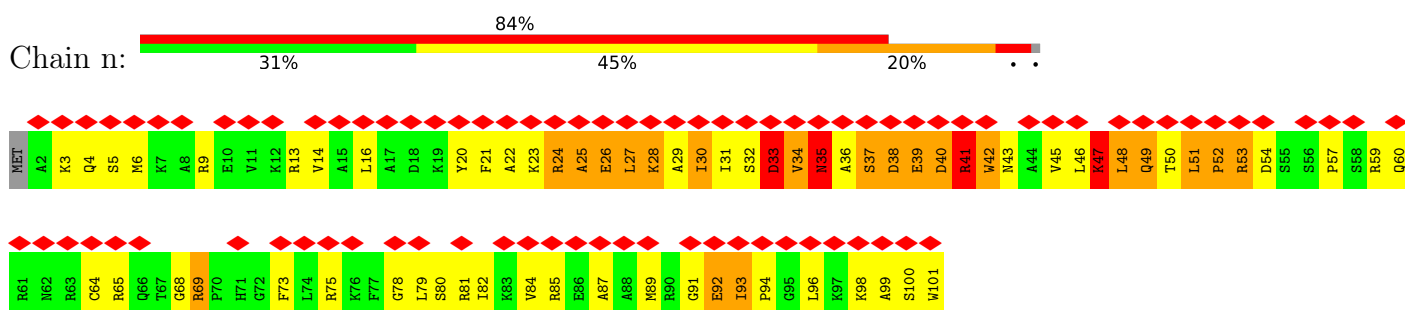
• Molecule 11: 30S ribosomal protein S12



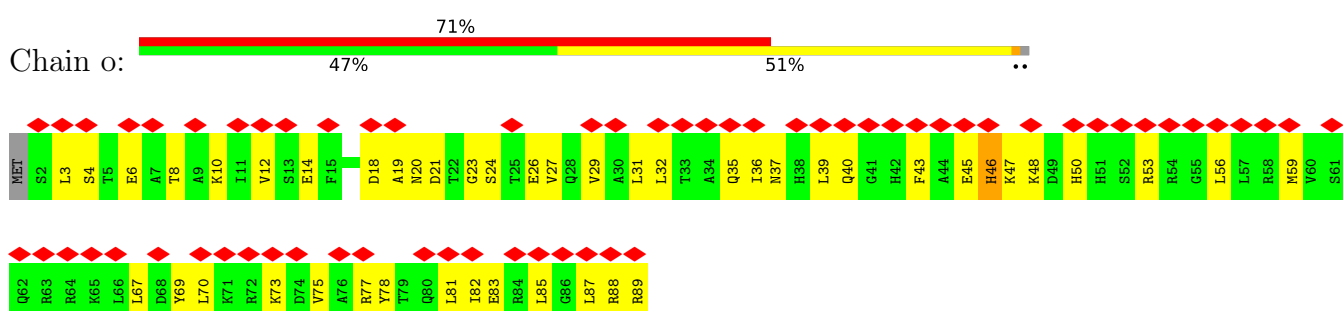
• Molecule 12: 30S ribosomal protein S13



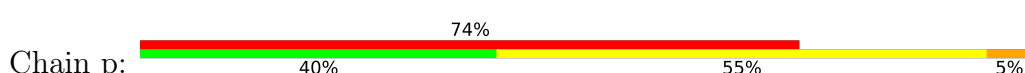
• Molecule 13: 30S ribosomal protein S14

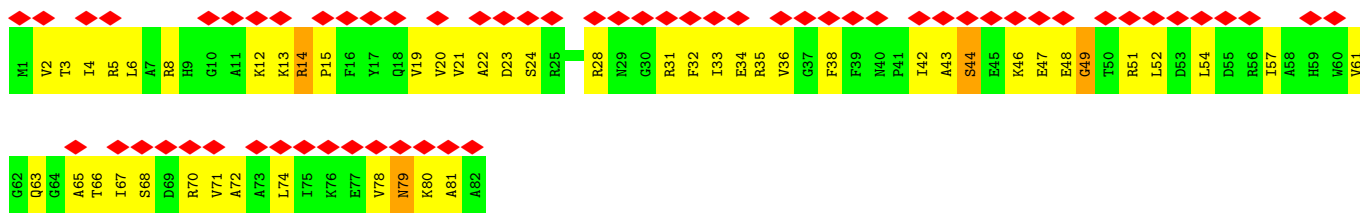


• Molecule 14: 30S ribosomal protein S15

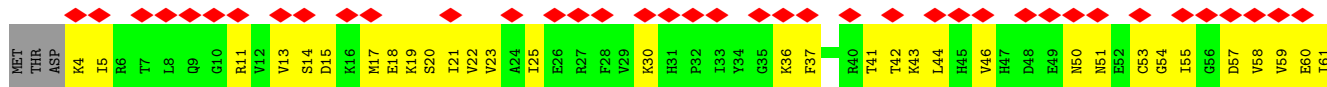
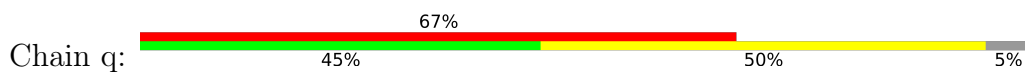


• Molecule 15: 30S ribosomal protein S16

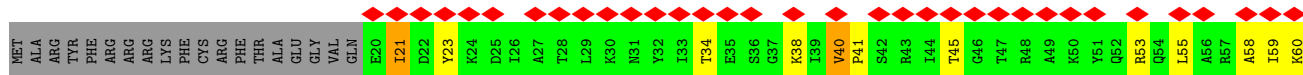
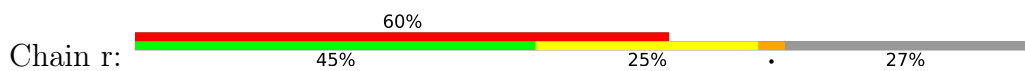




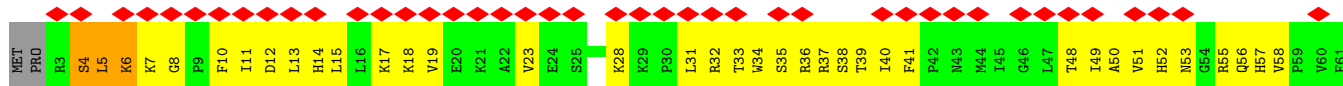
• Molecule 16: 30S ribosomal protein S17



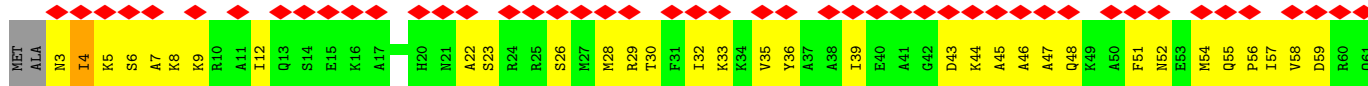
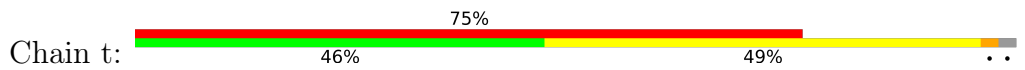
• Molecule 17: 30S ribosomal protein S18



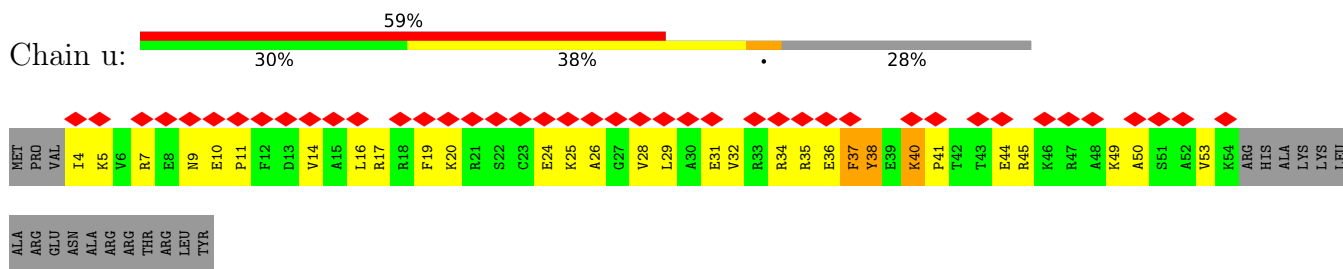
• Molecule 18: 30S ribosomal protein S19



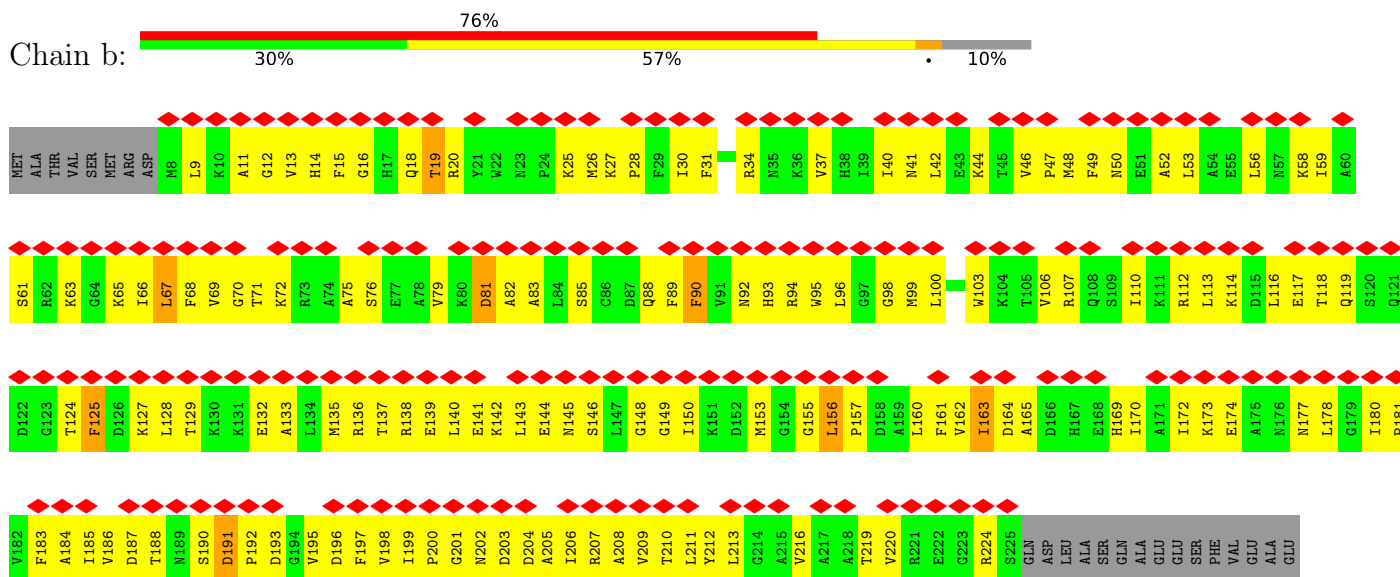
• Molecule 19: 30S ribosomal protein S20



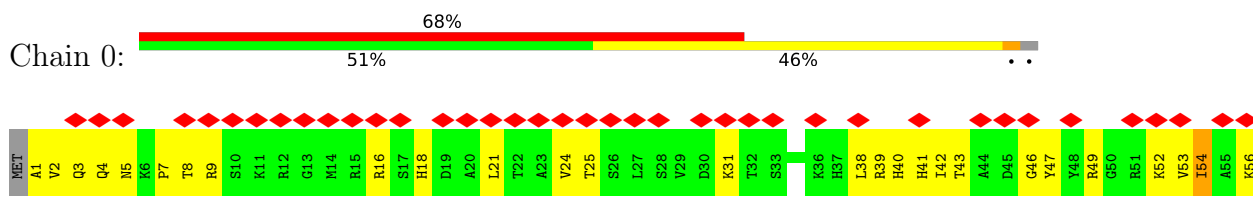
• Molecule 20: 30S ribosomal protein S21



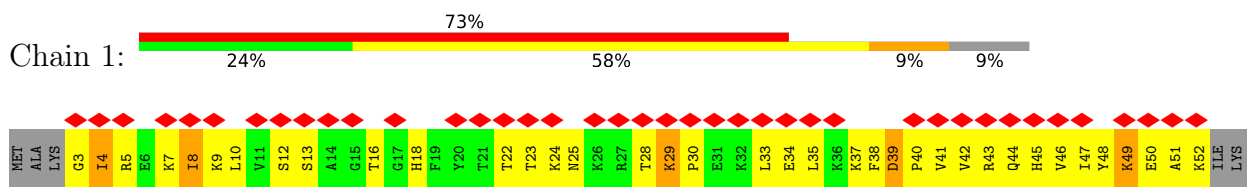
• Molecule 21: 30S ribosomal protein S2



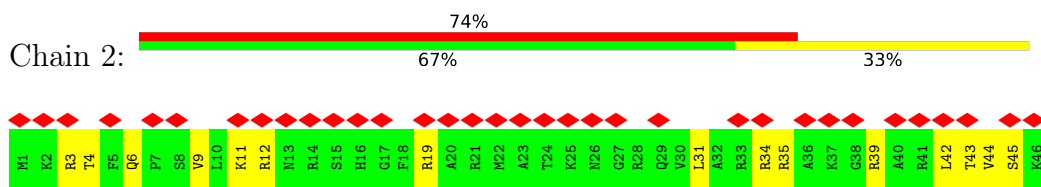
• Molecule 22: 50S ribosomal protein L32



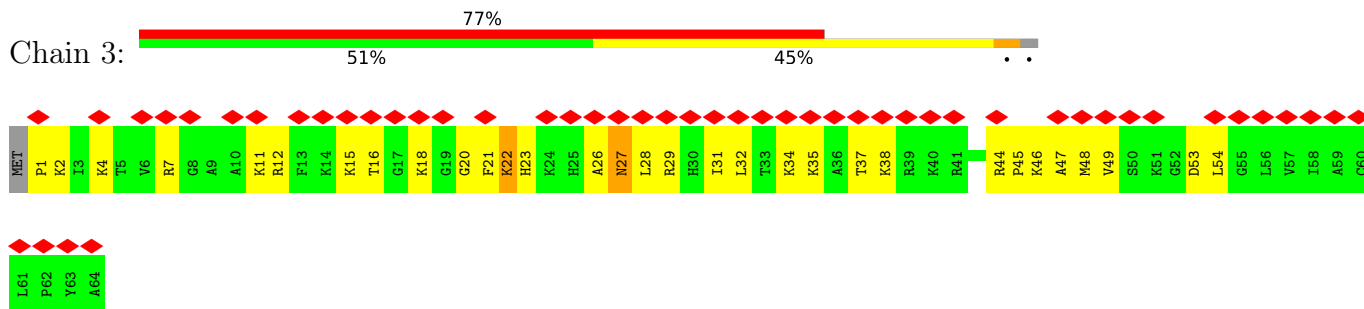
• Molecule 23: 50S ribosomal protein L33



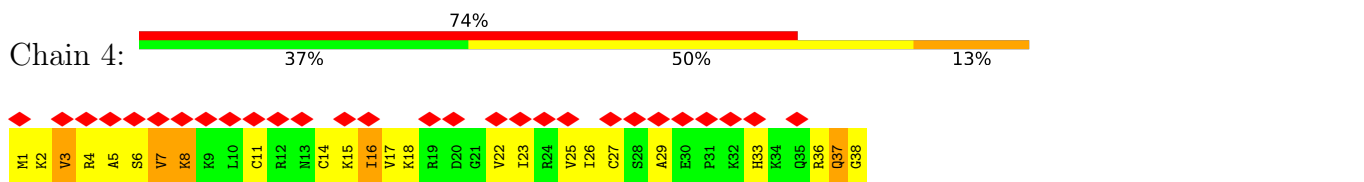
• Molecule 24: 50S ribosomal protein L34



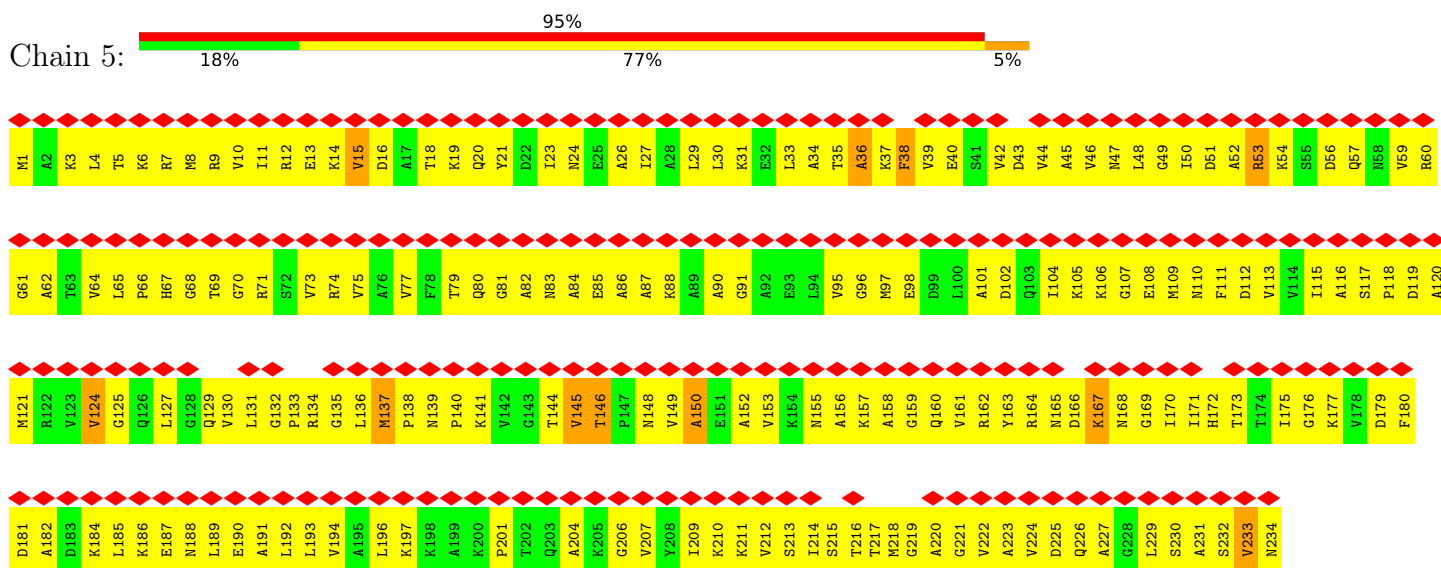
• Molecule 25: 50S ribosomal protein L35



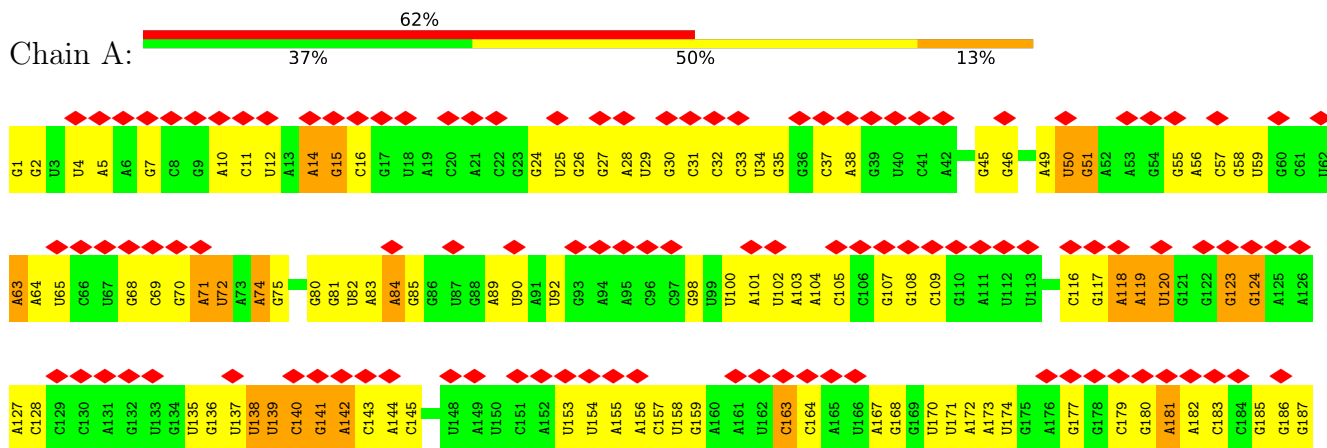
• Molecule 26: 50S ribosomal protein L36

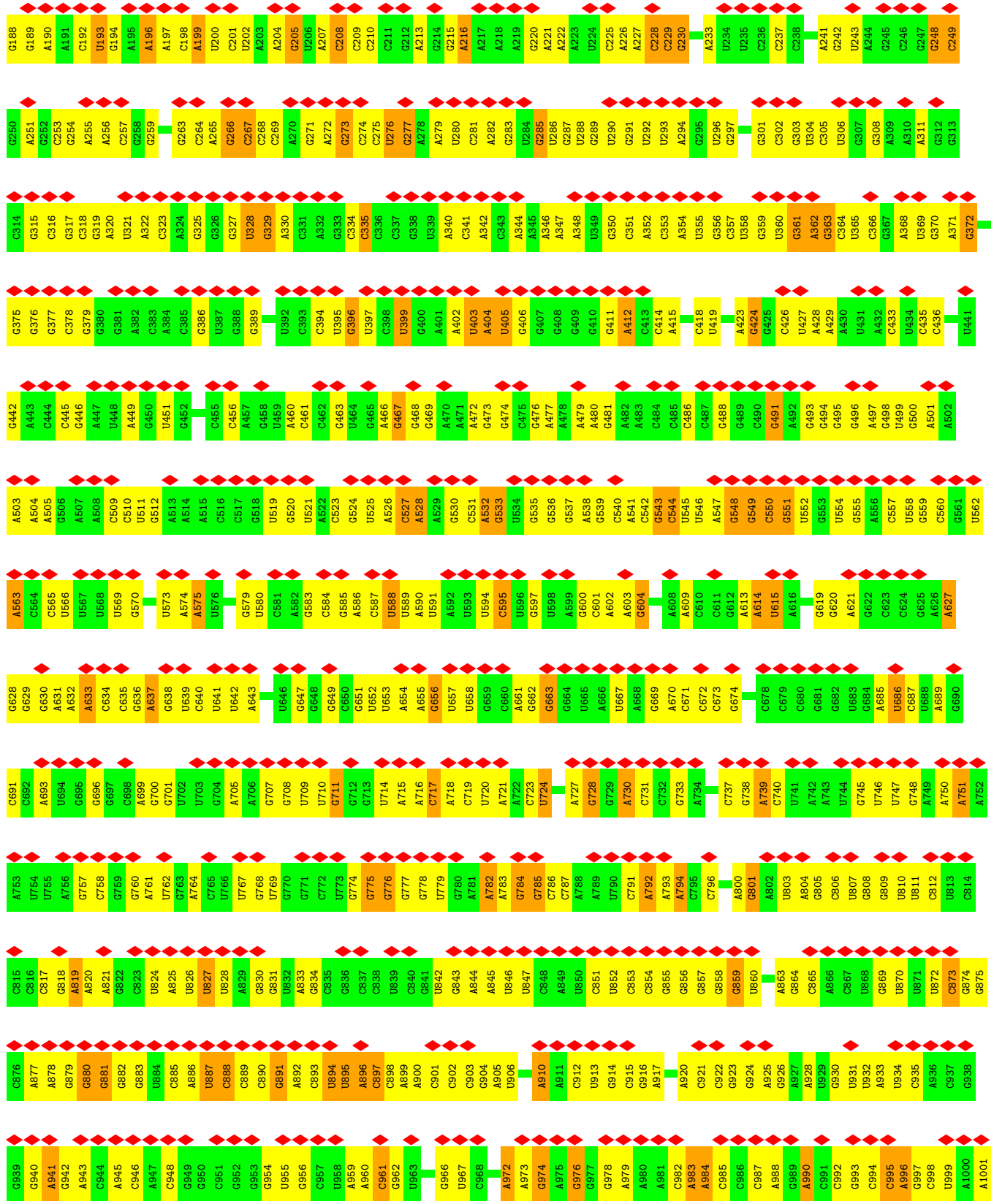


• Molecule 27: Large ribosomal subunit protein uL1



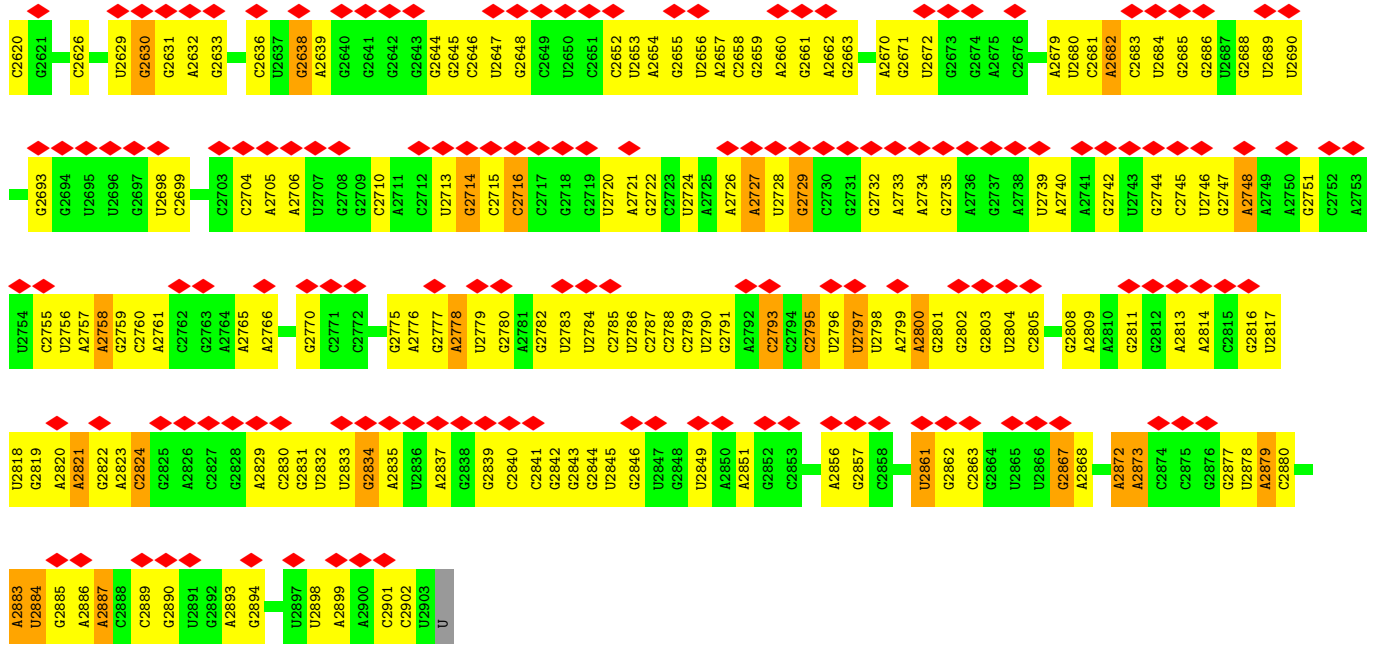
• Molecule 28: 23S ribosomal RNA



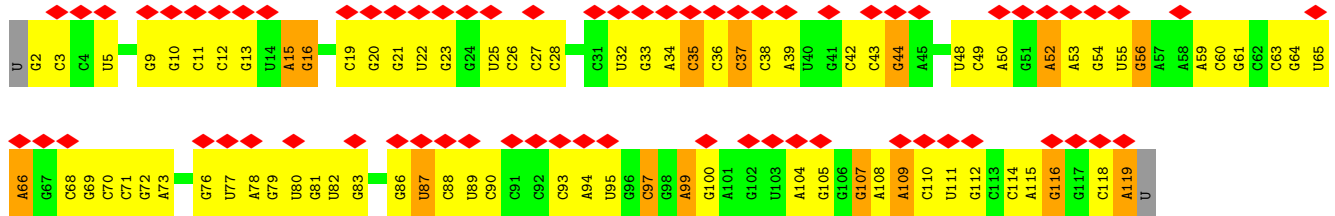


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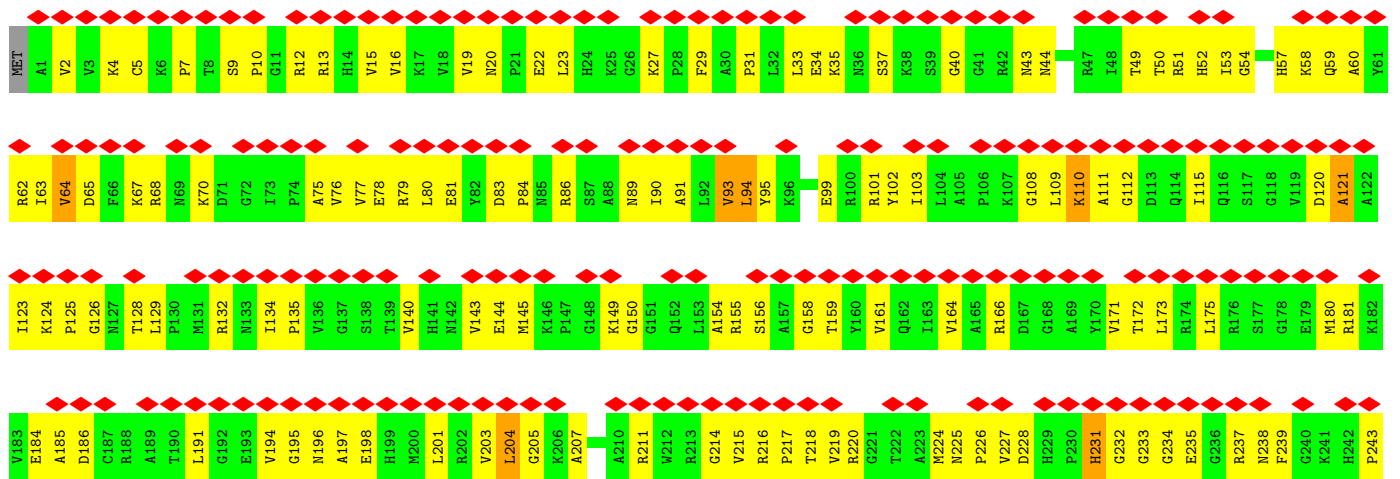
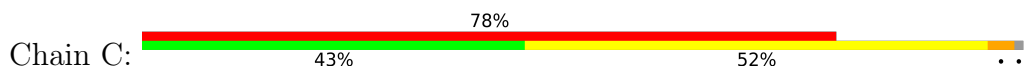
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• Molecule 29: 5S ribosomal RNA

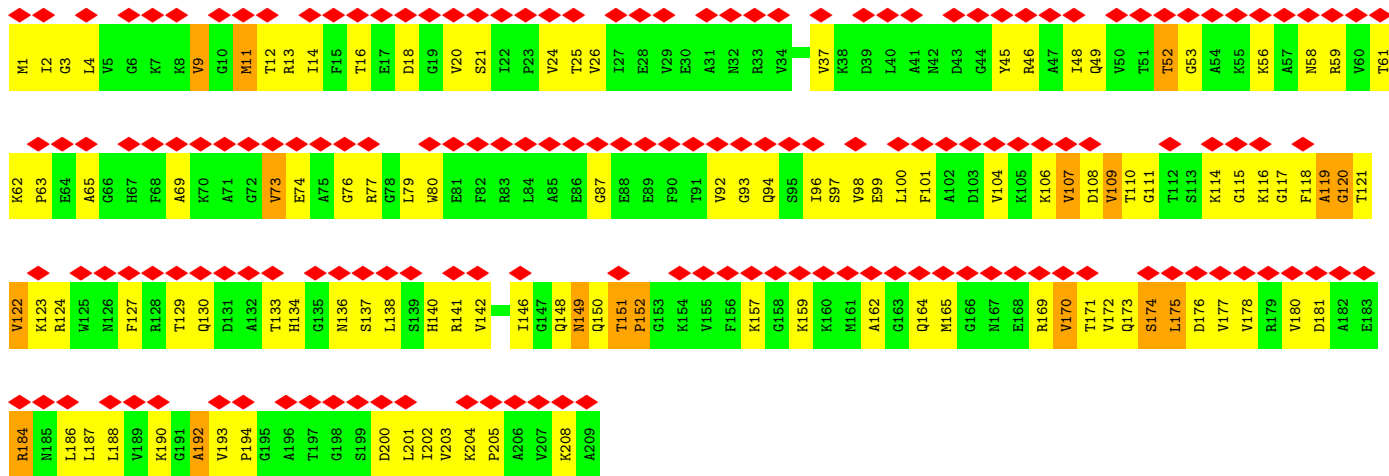
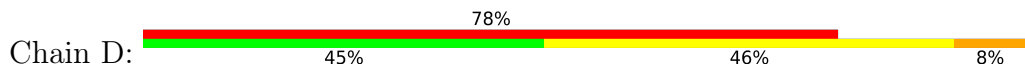


• Molecule 30: 50S ribosomal protein L2

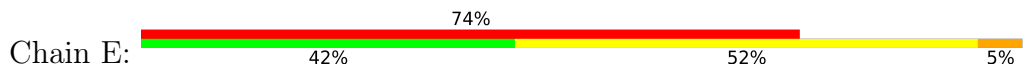




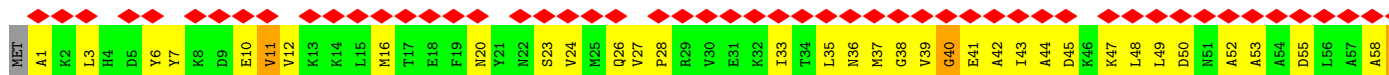
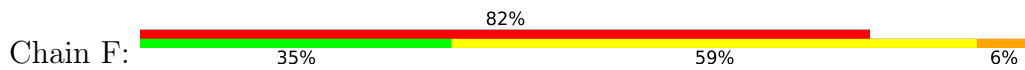
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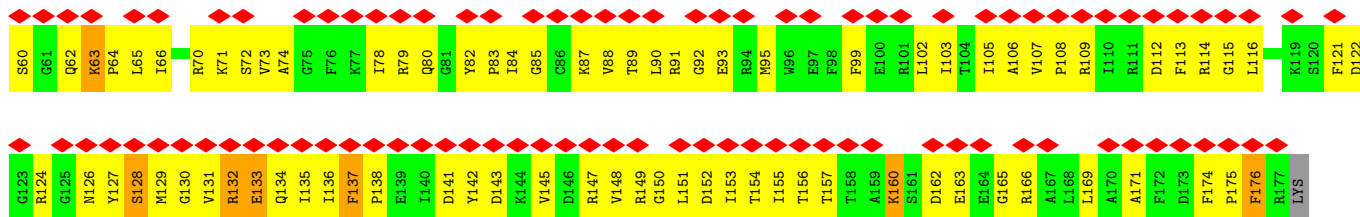


• Molecule 32: 50S ribosomal protein L4

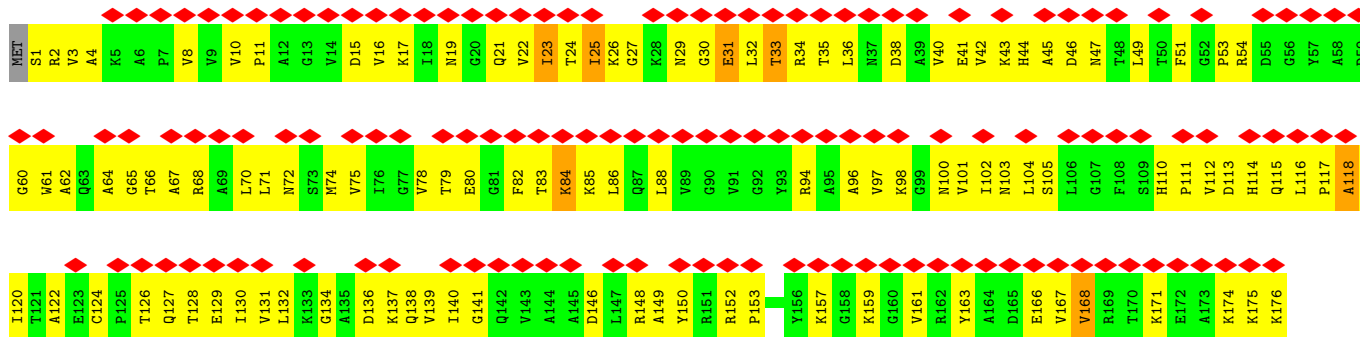
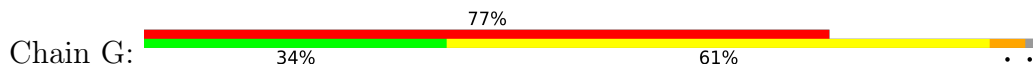


• Molecule 33: 50S ribosomal protein L5





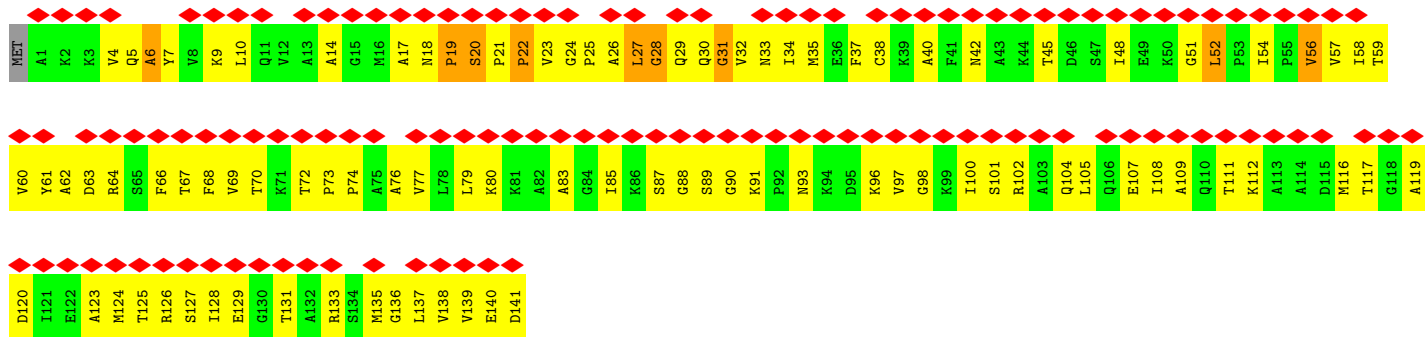
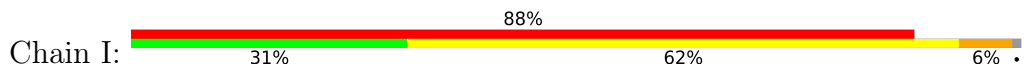
• Molecule 34: 50S ribosomal protein L6



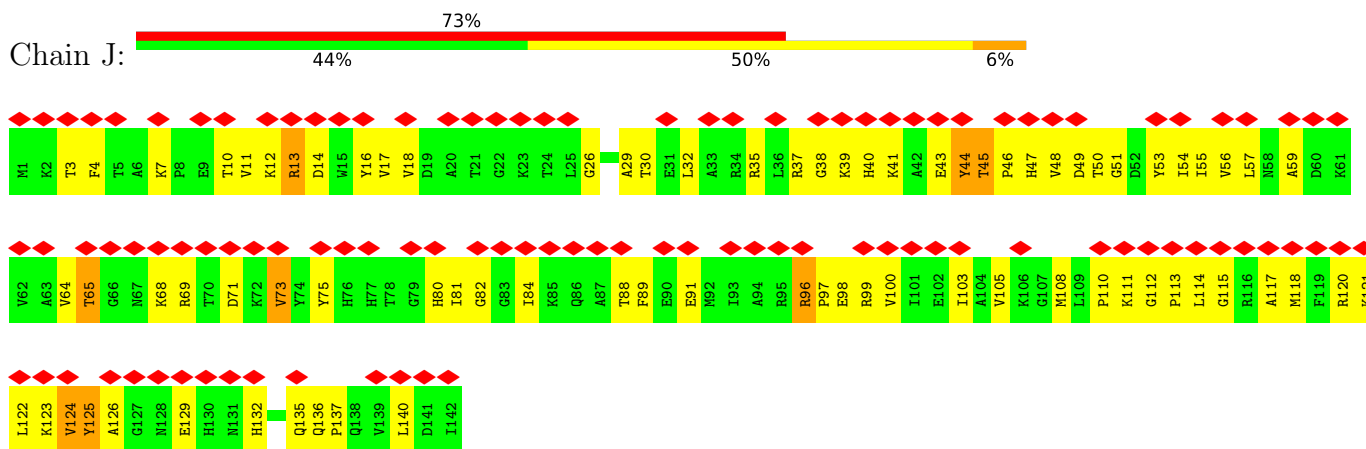
• Molecule 35: 50S ribosomal protein L9



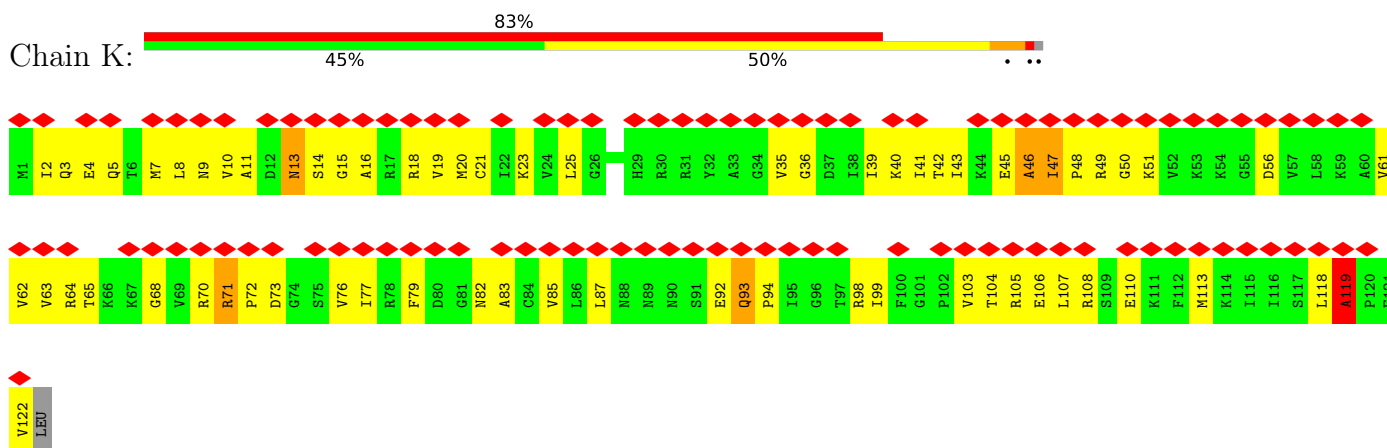
• Molecule 36: 50S ribosomal protein L11



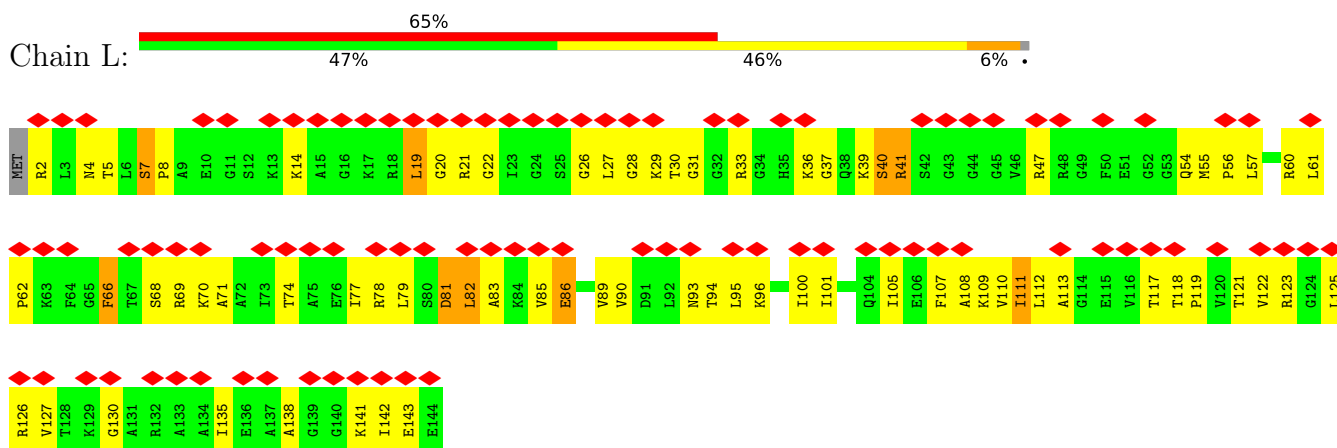
- Molecule 37: 50S ribosomal protein L13



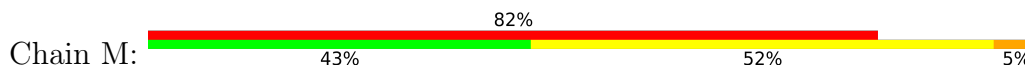
- Molecule 38: 50S ribosomal protein L14



- Molecule 39: 50S ribosomal protein L15

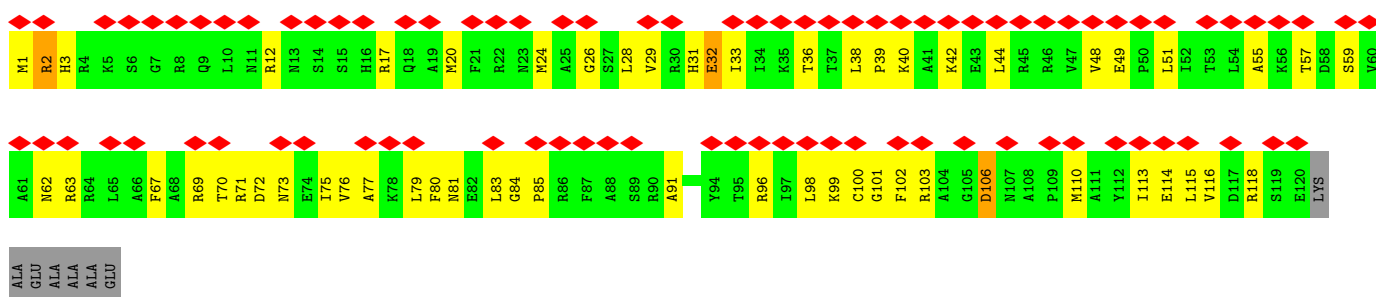


- Molecule 40: 50S ribosomal protein L16

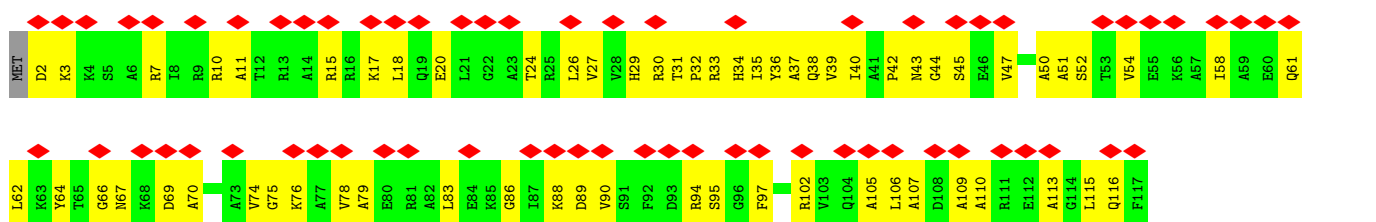




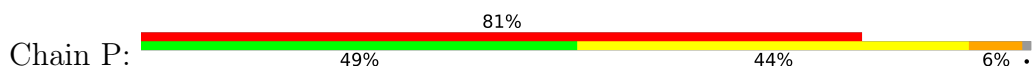
• Molecule 41: 50S ribosomal protein L17



• Molecule 42: 50S ribosomal protein L18

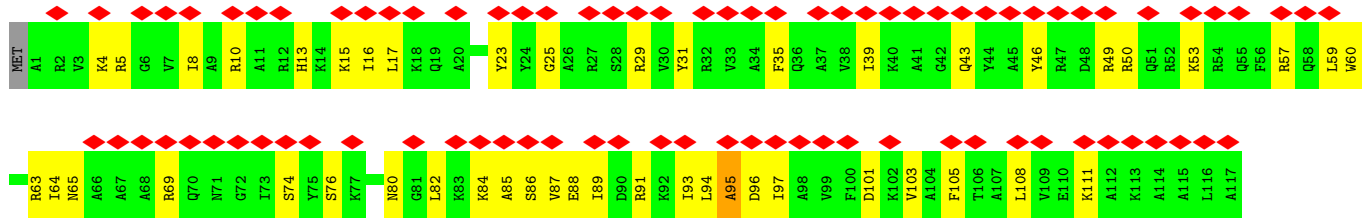


• Molecule 43: 50S ribosomal protein L19

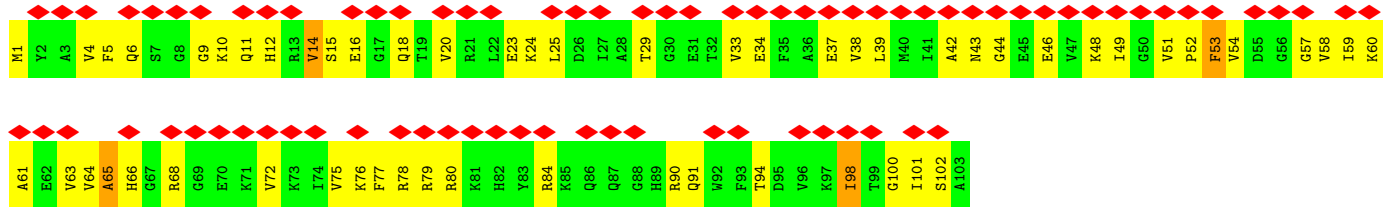
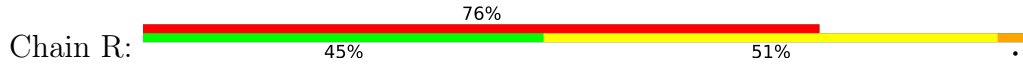


• Molecule 44: 50S ribosomal protein L20

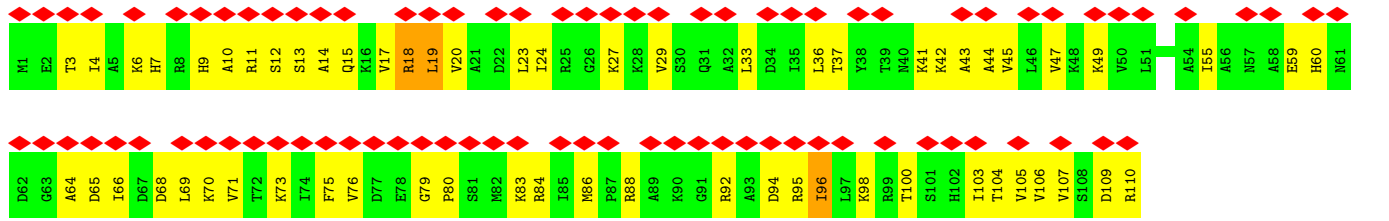
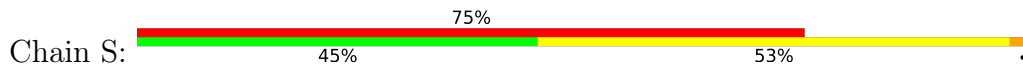




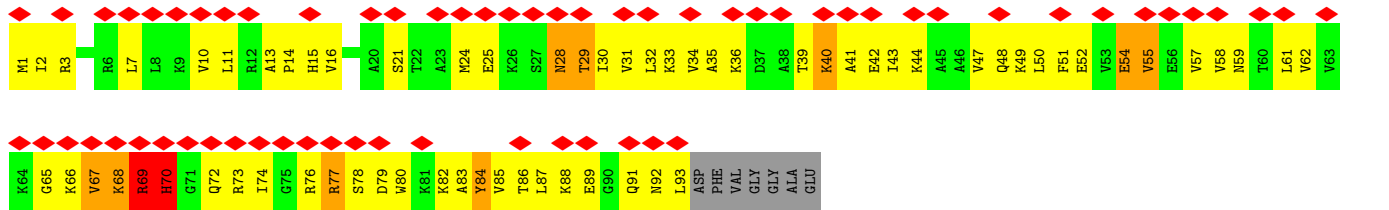
• Molecule 45: 50S ribosomal protein L21



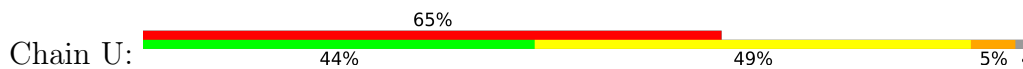
• Molecule 46: 50S ribosomal protein L22

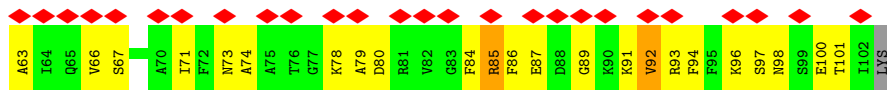


• Molecule 47: 50S ribosomal protein L23

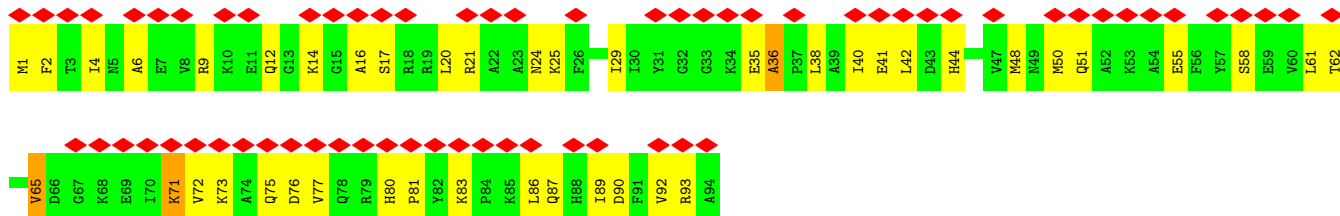


• Molecule 48: 50S ribosomal protein L24

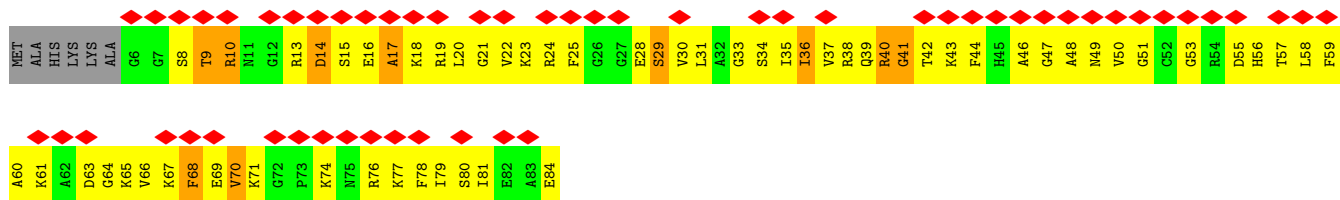




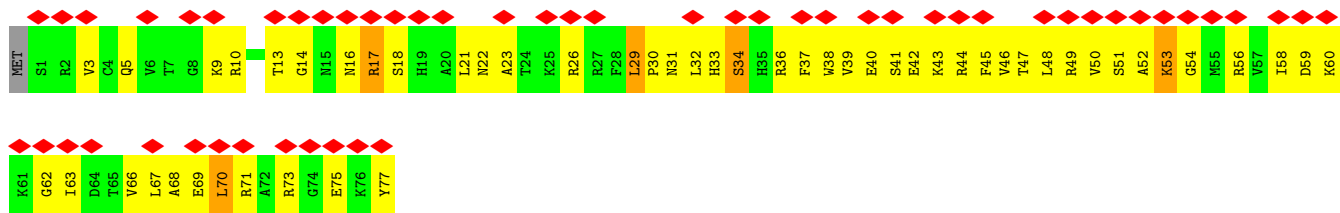
• Molecule 49: 50S ribosomal protein L25



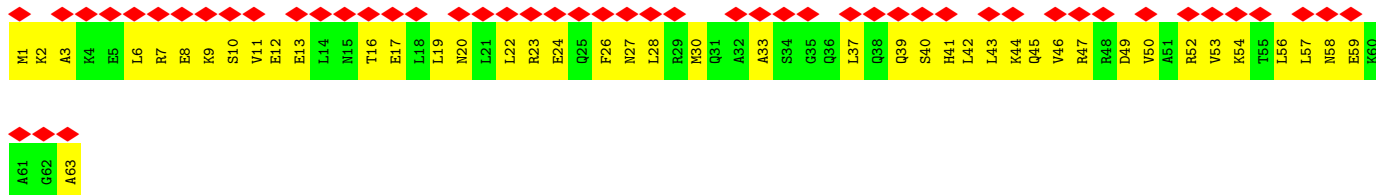
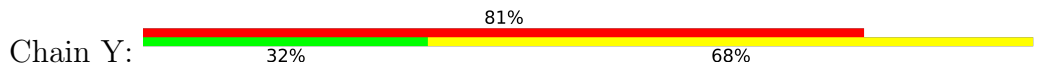
• Molecule 50: 50S ribosomal protein L27



• Molecule 51: 50S ribosomal protein L28



• Molecule 52: 50S ribosomal protein L29

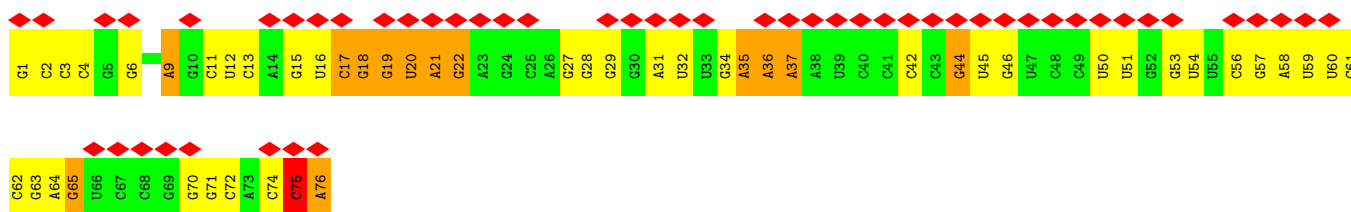


• Molecule 53: 50S ribosomal protein L30

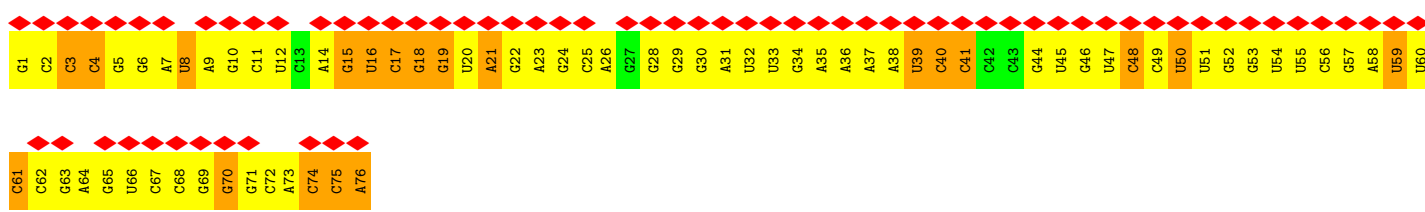
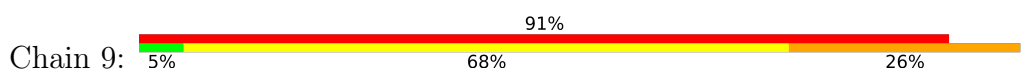




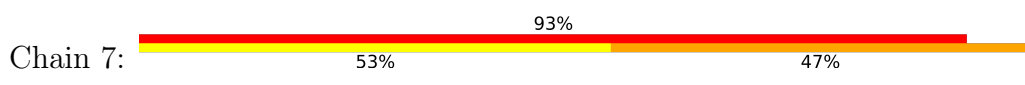
• Molecule 54: tRNA



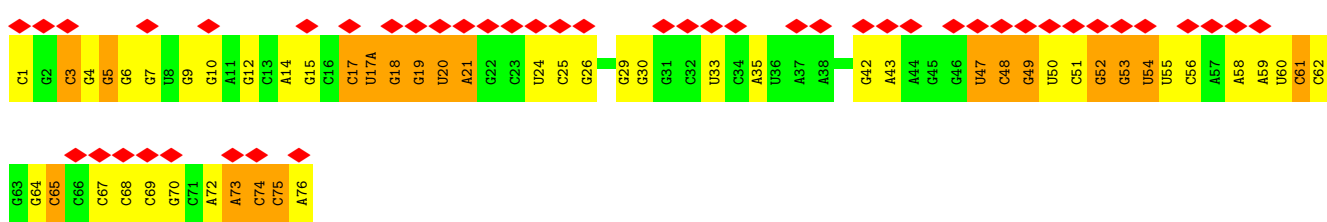
• Molecule 54: tRNA



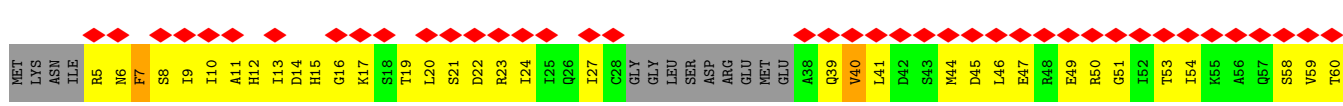
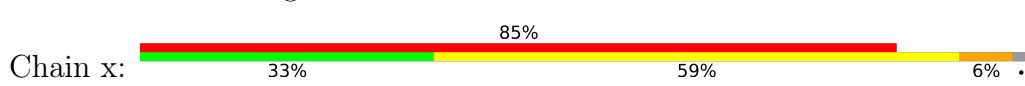
• Molecule 55: mRNA



• Molecule 56: tRNA



• Molecule 57: Elongation factor 4



V542	R482	C422	D362	V302	T241	P181	E121	L61
K543	V483	V423	L363	S303	P242	P182	E122	D62
Q544	D484	E424	L364	S304		P183	D123	Y63
L545	V485	K425	T365	D305	V245	E184	L124	K64
R546	L486	R426	T366	D306	D246	G185	E125	A65
K547	L487	C427	A367	D307	R247	R186	V126	S66
N548	M488	V428	P368	E308	T248	P187	P127	D67
V549	C489	Q429	T369	A309	E249	E188	P128	G68
L550	E490	T430	V370	F310	L250	G189	V129	E69
A551	R491	M431	V371	R311	K251	T70	L130	T70
K552	V492	M432	Y372	D312	C252	P190	M131	Y71
C553	D493	V433	E373	A313	G253	L191	K132	Q72
Y554	A494	Y434	V374	L314	E254	Q192	L133	L73
G555	L495	H435	E375	G315	V255	L194	D134	N74
D557	A496	C436	T376	K316	G256	I195	L135	F75
I558	L497	Q438	T377	L317	W257	I196	P136	I76
S559	T498	Q438	S378	S318	L258	D197	A137	D77
R560	T499	V439	R379	L319	C260	S198	A138	T78
R561	H500	A440	E380	N320	A261	W199	D139	P79
K561	R501	L441	V381	D321	I262	F200	P140	G80
K562	D502	T442	I382	A322	K263	D201	E141	H81
L564	N503	Y443	Y383	S323	D264	N202	R142	V82
L565	S504	E444	V384	L324	I265	Y203	A144	D83
Q566	O505	I445	D385	F325	H266	L204	E145	F84
K567	N506	P446	S386	Y326	G267	G205	E146	S85
Q568	R507	M447	E387	E327	A268	V206	I147	Y86
K569	G508	A448	S388	P328	P269	W207	E148	E87
E570	R509	E449	K389	E329	V270	S208	D149	V88
G571	E510	V450	L390	S330	G271	L209	I150	S89
K572	L511	V451	P391	S331	D272	I210	V151	R90
K573	V512	L452	A392	S332	T273	R211	G152	S91
R574	E513	D453	V393	S333	L274	I212	I153	L92
N575	K514	F454	N394	A333	T275	K213	D154	A93
K576	L515	F455	N395	L334	L276	N214	A155	A94
Q577	K516	D456	I396	G335	A277	G215	T156	C95
I578	D517	R457	T397	F336	R278	D157	D157	E96
G579	L518	L458	E398	G337	N279	L217	A158	G97
N580	V519	K459	L399	F338	P280	R218	A159	A98
V581	F620	S460	R400	R339	A281	K219	V159	L99
E582	R521	T461	E401	C340	E282	G220	R160	L100
L583	Q522	S462	P402	G341	K283	D221	C161	V101
F584	F524	R463	L403	F342	A284	K222	S162	V102
Q585	D525	Y465	A404	L343	L285	V223	A163	V103
E586	L526	A466	E405	G344	P286	K224	K164	D103
A587	A527	S467	C406	L345	G287	V225	L165	A104
F588	L528	L468	H407	L346	F288	M226	G166	G105
L589	Q529	D469	M408	H347	K289	S227	G168	G107
A590	A530	Y470	L409	M348	K290	V169	V169	V108
I591	A531	M471	L410	E349	V291	Q170	Q170	E109
L592	I532	F472	P411	I350	K292	D171	D171	A110
H593	S533	K473	Q412	I351	P293	Q230	V172	Q111
V594	G534	R474	A413	Q523	Q294	T231	L173	Q112
G595	H535	F475	Y414	R354	V295	Y232	E174	T112
K596	L536	Q476	L415	L355	A296	N233	R175	L113
D597	I537	A477	G416	G356	A297	A234	L114	A114
N598	V537	S478	M417	E356	A297	D235	V115	N115
K599	A538	S478	V418	R357	G298	R236	R178	C116
	R539	D479	T419	E358	L299	L237	D179	Y117
	S540	M480	T420	Y359	F300	G238	T118	T118
	T541	V481	L421	L361	P301	L239	L119	A119

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107706	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.036	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (\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 (\AA)	1.32, 1.32, 1.32	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: GNP, MG

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	0.34	0/36834	0.30	0/57462
2	c	0.57	0/1651	0.87	4/2225 (0.2%)
3	d	0.50	0/1665	0.82	2/2227 (0.1%)
4	e	0.64	0/1118	0.94	2/1504 (0.1%)
5	f	0.51	0/851	0.91	4/1150 (0.3%)
6	g	0.52	0/1195	0.86	3/1602 (0.2%)
7	h	0.59	0/989	0.88	2/1326 (0.2%)
8	i	0.50	0/1034	0.88	1/1375 (0.1%)
9	j	0.51	0/796	0.84	2/1077 (0.2%)
10	k	0.59	0/893	0.96	4/1205 (0.3%)
11	l	0.60	0/969	0.95	6/1300 (0.5%)
12	m	0.52	0/892	0.93	5/1193 (0.4%)
13	n	0.51	0/817	1.04	7/1088 (0.6%)
14	o	0.61	0/722	0.76	0/964
15	p	0.49	0/659	0.92	2/884 (0.2%)
16	q	0.53	0/657	0.84	0/881
17	r	0.55	0/462	0.92	4/621 (0.6%)
18	s	0.45	0/652	0.86	2/877 (0.2%)
19	t	0.55	0/671	0.77	0/888
20	u	0.51	0/430	0.84	0/570
21	b	0.49	0/1735	0.90	7/2338 (0.3%)
22	0	0.63	0/450	0.81	0/599
23	1	0.55	0/416	0.97	5/554 (0.9%)
24	2	0.71	0/380	0.90	2/498 (0.4%)
25	3	0.60	0/513	0.84	0/676
26	4	0.60	0/303	0.91	0/397
27	5	0.35	0/1748	0.94	6/2355 (0.3%)
28	A	0.39	0/69799	0.32	0/108892
29	B	0.29	0/2828	0.27	0/4410
30	C	0.68	0/2115	0.95	5/2844 (0.2%)
31	D	0.64	0/1586	0.98	9/2134 (0.4%)
32	E	0.58	0/1571	0.86	3/2113 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	F	0.46	0/1434	0.82	4/1926 (0.2%)
34	G	0.48	0/1343	0.82	1/1816 (0.1%)
35	H	0.42	0/1122	0.99	4/1515 (0.3%)
36	I	0.40	0/1046	0.89	3/1410 (0.2%)
37	J	0.63	0/1152	0.95	5/1551 (0.3%)
38	K	0.64	0/947	0.97	6/1268 (0.5%)
39	L	0.60	0/1054	0.94	2/1403 (0.1%)
40	M	0.65	0/1093	1.09	8/1460 (0.5%)
41	N	0.65	0/973	0.85	0/1301
42	O	0.53	0/902	0.81	0/1209
43	P	0.55	0/929	0.95	3/1242 (0.2%)
44	Q	0.75	0/960	0.84	1/1278 (0.1%)
45	R	0.59	0/829	0.84	3/1107 (0.3%)
46	S	0.68	0/864	0.96	5/1156 (0.4%)
47	T	0.56	0/744	0.90	2/994 (0.2%)
48	U	0.49	0/787	0.89	2/1051 (0.2%)
49	V	0.51	0/766	0.83	2/1025 (0.2%)
50	W	0.64	0/603	1.06	4/797 (0.5%)
51	X	0.61	0/635	0.93	3/848 (0.4%)
52	Y	0.57	0/510	0.80	0/677
53	Z	0.60	0/453	0.99	3/605 (0.5%)
54	6	0.37	1/1812 (0.1%)	0.40	2/2820 (0.1%)
54	9	0.15	0/1813	0.27	0/2823
55	7	0.32	0/358	0.39	0/555
56	8	0.30	0/1832	0.30	0/2855
57	x	0.49	0/4646	0.88	15/6285 (0.2%)
All	All	0.44	1/167008 (0.0%)	0.55	165/249206 (0.1%)

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
11	l	0	1
20	u	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	6	75	C	O3'-P	-9.67	1.46	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	M	71	LYS	CA-C-N	10.74	130.97	119.05
40	M	71	LYS	C-N-CA	10.74	130.97	119.05
15	p	14	ARG	CA-C-N	10.71	130.81	119.78
15	p	14	ARG	C-N-CA	10.71	130.81	119.78
39	L	7	SER	CA-C-N	10.41	130.50	119.78

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	l	23	ALA	Peptide
20	u	37	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32895	0	16553	1105	0
2	c	1624	0	1696	115	0
3	d	1643	0	1707	158	0
4	e	1105	0	1148	113	0
5	f	832	0	824	88	0
6	g	1181	0	1238	89	0
7	h	979	0	1031	108	0
8	i	1022	0	1070	129	0
9	j	786	0	828	93	0
10	k	877	0	887	83	0
11	l	955	0	1016	97	0
12	m	883	0	941	117	0
13	n	805	0	843	202	0
14	o	714	0	734	46	0
15	p	649	0	666	57	0
16	q	648	0	691	44	0
17	r	455	0	478	25	0
18	s	637	0	665	62	0
19	t	665	0	714	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	u	425	0	449	64	0
21	b	1704	0	1732	192	0
22	0	444	0	461	40	0
23	1	409	0	440	51	0
24	2	377	0	418	16	0
25	3	504	0	574	33	0
26	4	302	0	340	40	0
27	5	1733	0	1824	398	0
28	A	62320	0	31344	2050	0
29	B	2529	0	1281	96	0
30	C	2076	0	2152	170	0
31	D	1565	0	1616	141	0
32	E	1552	0	1619	139	0
33	F	1410	0	1447	130	0
34	G	1323	0	1374	156	0
35	H	1111	0	1148	237	0
36	I	1032	0	1088	166	0
37	J	1129	0	1162	119	0
38	K	938	0	1012	77	0
39	L	1045	0	1117	100	0
40	M	1074	0	1157	86	0
41	N	960	0	1000	58	0
42	O	892	0	923	84	0
43	P	917	0	965	90	0
44	Q	947	0	1022	101	0
45	R	816	0	839	96	0
46	S	857	0	922	60	0
47	T	738	0	807	99	0
48	U	779	0	834	53	0
49	V	753	0	780	48	0
50	W	596	0	610	120	0
51	X	625	0	655	64	0
52	Y	509	0	543	49	0
53	Z	449	0	491	34	0
54	6	1622	0	820	55	0
54	9	1623	0	821	163	0
55	7	320	0	162	22	0
56	8	1640	0	837	55	0
57	x	4573	0	4619	550	0
58	6	11	0	8	1	0
59	x	32	0	13	3	0
60	x	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	154017	0	105156	8213	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

The worst 5 of 8213 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:n:28:LYS:CE	13:n:48:LEU:HB3	1.52	1.39
13:n:32:SER:HB2	13:n:45:VAL:CG1	1.58	1.32
13:n:48:LEU:O	13:n:50:THR:N	1.61	1.29
13:n:35:ASN:OD1	13:n:42:TRP:CD1	1.89	1.25
57:x:12:HIS:CE1	57:x:109:GLU:OE2	1.85	1.25

There are no symmetry-related clashes.

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	c	204/233 (88%)	182 (89%)	16 (8%)	6 (3%)	3	24
3	d	203/206 (98%)	180 (89%)	16 (8%)	7 (3%)	3	20
4	e	148/167 (89%)	125 (84%)	19 (13%)	4 (3%)	4	25
5	f	100/135 (74%)	84 (84%)	9 (9%)	7 (7%)	1	6
6	g	149/179 (83%)	134 (90%)	11 (7%)	4 (3%)	4	25
7	h	127/130 (98%)	114 (90%)	11 (9%)	2 (2%)	7	36
8	i	125/130 (96%)	107 (86%)	14 (11%)	4 (3%)	3	21
9	j	96/103 (93%)	76 (79%)	11 (12%)	9 (9%)	0	3
10	k	115/129 (89%)	102 (89%)	9 (8%)	4 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	121/124 (98%)	104 (86%)	12 (10%)	5 (4%)	2	17
12	m	112/118 (95%)	101 (90%)	6 (5%)	5 (4%)	2	15
13	n	98/101 (97%)	70 (71%)	15 (15%)	13 (13%)	0	1
14	o	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	10	42
15	p	80/82 (98%)	66 (82%)	8 (10%)	6 (8%)	1	5
16	q	78/84 (93%)	62 (80%)	14 (18%)	2 (3%)	4	26
17	r	53/75 (71%)	50 (94%)	2 (4%)	1 (2%)	6	33
18	s	77/92 (84%)	68 (88%)	5 (6%)	4 (5%)	1	12
19	t	83/87 (95%)	78 (94%)	3 (4%)	2 (2%)	4	28
20	u	49/71 (69%)	39 (80%)	7 (14%)	3 (6%)	1	9
21	b	216/241 (90%)	189 (88%)	20 (9%)	7 (3%)	3	21
22	0	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	6	33
23	1	48/55 (87%)	41 (85%)	6 (12%)	1 (2%)	5	31
24	2	44/46 (96%)	43 (98%)	0	1 (2%)	5	29
25	3	62/65 (95%)	55 (89%)	5 (8%)	2 (3%)	3	21
26	4	36/38 (95%)	25 (69%)	5 (14%)	6 (17%)	0	0
27	5	232/234 (99%)	190 (82%)	34 (15%)	8 (3%)	3	20
30	C	268/273 (98%)	228 (85%)	28 (10%)	12 (4%)	2	15
31	D	207/209 (99%)	169 (82%)	23 (11%)	15 (7%)	1	6
32	E	199/201 (99%)	171 (86%)	14 (7%)	14 (7%)	1	6
33	F	175/179 (98%)	146 (83%)	21 (12%)	8 (5%)	2	15
34	G	174/177 (98%)	140 (80%)	21 (12%)	13 (8%)	1	5
35	H	147/149 (99%)	114 (78%)	22 (15%)	11 (8%)	1	5
36	I	139/142 (98%)	119 (86%)	11 (8%)	9 (6%)	1	8
37	J	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	2	16
38	K	120/123 (98%)	100 (83%)	14 (12%)	6 (5%)	1	13
39	L	141/144 (98%)	115 (82%)	17 (12%)	9 (6%)	1	8
40	M	134/136 (98%)	112 (84%)	15 (11%)	7 (5%)	1	12
41	N	118/127 (93%)	104 (88%)	10 (8%)	4 (3%)	3	20
42	O	114/117 (97%)	104 (91%)	10 (9%)	0	100	100
43	P	112/115 (97%)	93 (83%)	13 (12%)	6 (5%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	Q	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
45	R	101/103 (98%)	81 (80%)	15 (15%)	5 (5%)	1	13
46	S	108/110 (98%)	94 (87%)	11 (10%)	3 (3%)	4	25
47	T	91/100 (91%)	61 (67%)	18 (20%)	12 (13%)	0	1
48	U	100/104 (96%)	81 (81%)	11 (11%)	8 (8%)	1	4
49	V	92/94 (98%)	81 (88%)	9 (10%)	2 (2%)	5	29
50	W	77/85 (91%)	49 (64%)	17 (22%)	11 (14%)	0	1
51	X	75/78 (96%)	64 (85%)	7 (9%)	4 (5%)	1	12
52	Y	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
53	Z	56/59 (95%)	51 (91%)	3 (5%)	2 (4%)	2	19
57	x	582/599 (97%)	496 (85%)	58 (10%)	28 (5%)	2	14
All	All	6442/6818 (94%)	5465 (85%)	667 (10%)	310 (5%)	3	14

5 of 310 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	125	VAL
5	f	98	GLU
5	f	101	PRO
9	j	57	VAL
9	j	61	ALA

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	c	170/190 (90%)	170 (100%)	0	100	100
3	d	172/173 (99%)	172 (100%)	0	100	100
4	e	113/126 (90%)	113 (100%)	0	100	100
5	f	89/116 (77%)	89 (100%)	0	100	100
6	g	124/147 (84%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	104/105 (99%)	104 (100%)	0	100	100
8	i	105/107 (98%)	105 (100%)	0	100	100
9	j	86/90 (96%)	86 (100%)	0	100	100
10	k	90/99 (91%)	90 (100%)	0	100	100
11	l	103/104 (99%)	103 (100%)	0	100	100
12	m	92/96 (96%)	92 (100%)	0	100	100
13	n	83/84 (99%)	70 (84%)	13 (16%)	2	13
14	o	76/77 (99%)	76 (100%)	0	100	100
15	p	65/65 (100%)	65 (100%)	0	100	100
16	q	74/78 (95%)	74 (100%)	0	100	100
17	r	48/65 (74%)	48 (100%)	0	100	100
18	s	70/79 (89%)	70 (100%)	0	100	100
19	t	65/66 (98%)	65 (100%)	0	100	100
20	u	44/61 (72%)	44 (100%)	0	100	100
21	b	180/199 (90%)	180 (100%)	0	100	100
22	0	47/48 (98%)	47 (100%)	0	100	100
23	1	45/49 (92%)	44 (98%)	1 (2%)	45	71
24	2	38/38 (100%)	38 (100%)	0	100	100
25	3	51/52 (98%)	51 (100%)	0	100	100
26	4	34/34 (100%)	34 (100%)	0	100	100
27	5	181/181 (100%)	181 (100%)	0	100	100
30	C	215/218 (99%)	215 (100%)	0	100	100
31	D	164/164 (100%)	164 (100%)	0	100	100
32	E	165/165 (100%)	165 (100%)	0	100	100
33	F	148/150 (99%)	148 (100%)	0	100	100
34	G	137/138 (99%)	137 (100%)	0	100	100
35	H	114/114 (100%)	114 (100%)	0	100	100
36	I	109/110 (99%)	109 (100%)	0	100	100
37	J	116/116 (100%)	116 (100%)	0	100	100
38	K	103/104 (99%)	103 (100%)	0	100	100
39	L	102/103 (99%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	M	109/109 (100%)	109 (100%)	0	100	100
41	N	100/103 (97%)	100 (100%)	0	100	100
42	O	86/87 (99%)	86 (100%)	0	100	100
43	P	99/100 (99%)	99 (100%)	0	100	100
44	Q	89/90 (99%)	89 (100%)	0	100	100
45	R	84/84 (100%)	84 (100%)	0	100	100
46	S	93/93 (100%)	93 (100%)	0	100	100
47	T	80/84 (95%)	74 (92%)	6 (8%)	12	42
48	U	83/85 (98%)	83 (100%)	0	100	100
49	V	78/78 (100%)	78 (100%)	0	100	100
50	W	59/63 (94%)	59 (100%)	0	100	100
51	X	67/68 (98%)	67 (100%)	0	100	100
52	Y	55/55 (100%)	55 (100%)	0	100	100
53	Z	48/49 (98%)	48 (100%)	0	100	100
57	x	500/511 (98%)	495 (99%)	5 (1%)	68	80
All	All	5352/5570 (96%)	5327 (100%)	25 (0%)	78	85

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	T	66	LYS
47	T	70	HIS
57	x	589	LEU
47	T	69	ARG
47	T	73	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
37	J	135	GLN
46	S	60	HIS
57	x	548	ASN
39	L	54	GLN
43	P	9	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1532/1533 (99%)	302 (19%)	0
28	A	2902/2904 (99%)	566 (19%)	24 (0%)
29	B	117/120 (97%)	18 (15%)	0
54	6	75/76 (98%)	16 (21%)	3 (4%)
54	9	75/76 (98%)	24 (32%)	2 (2%)
55	7	14/15 (93%)	7 (50%)	1 (7%)
56	8	76/77 (98%)	20 (26%)	0
All	All	4791/4801 (99%)	953 (19%)	30 (0%)

5 of 953 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	9	G
1	a	13	U

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	A	1331	G
55	7	20	U
28	A	1905	C
54	9	74	C
54	6	17	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PHE	6	101	54	10,11,12	0.48	0	8,13,15	0.51	0
59	GNP	x	701	60	34,34,34	2.02	7 (20%)	47,54,54	1.22	5 (10%)

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
58	PHE	6	101	54	-	4/5/6/8	0/1/1/1
59	GNP	x	701	60	-	6/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	x	701	GNP	PA-O3A	-7.50	1.51	1.59
59	x	701	GNP	PB-O3A	-5.83	1.51	1.59
59	x	701	GNP	PB-O2B	-3.28	1.48	1.56
59	x	701	GNP	PG-O1G	3.28	1.51	1.46
59	x	701	GNP	PG-O2G	-2.30	1.50	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	x	701	GNP	O2B-PB-O1B	4.13	118.72	109.87
59	x	701	GNP	O1B-PB-N3B	-4.02	105.85	111.77
59	x	701	GNP	O1G-PG-N3B	-3.55	106.54	111.77
59	x	701	GNP	O3G-PG-O1G	-3.09	105.70	113.45
59	x	701	GNP	O2G-PG-O3G	2.62	114.62	107.59

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

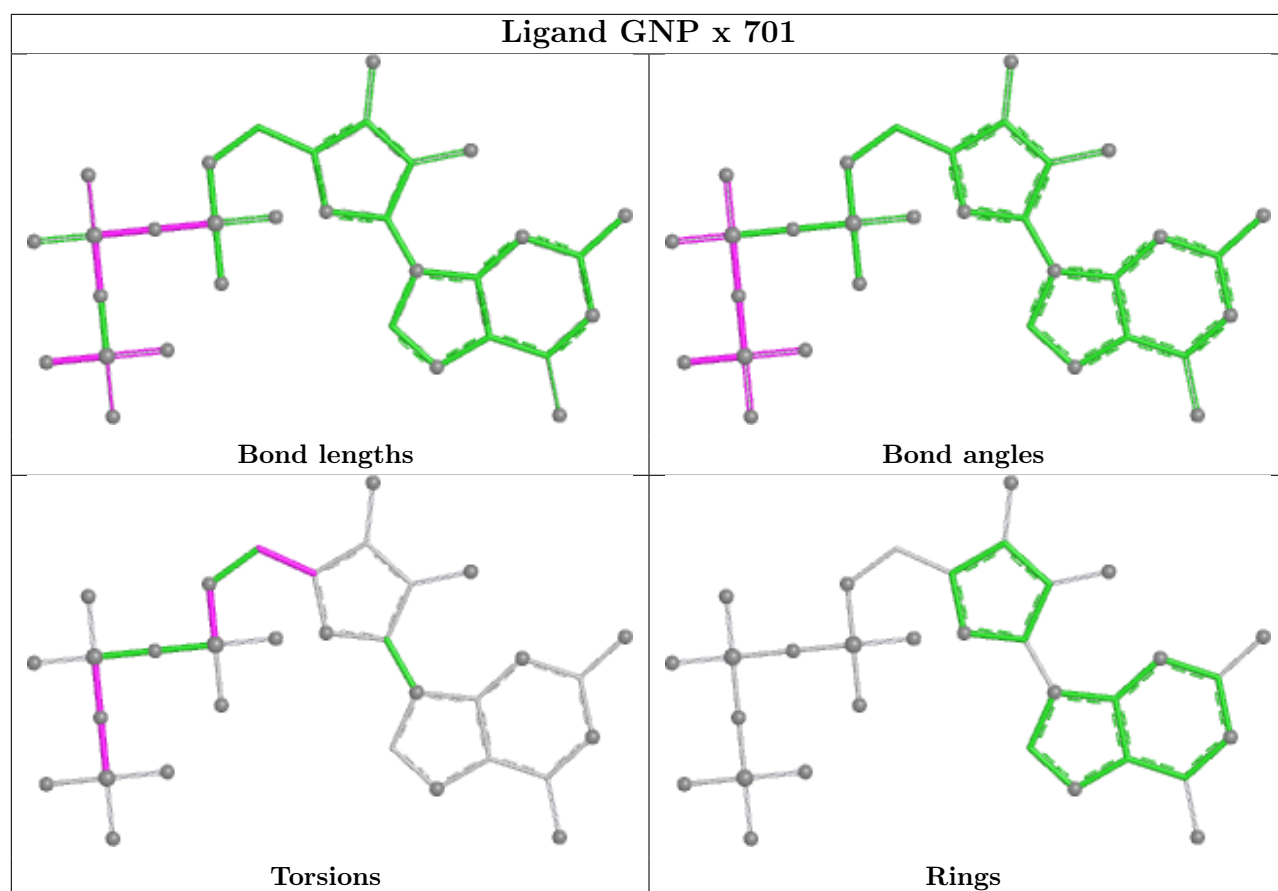
Mol	Chain	Res	Type	Atoms
58	6	101	PHE	C-CA-CB-CG
59	x	701	GNP	PB-N3B-PG-O1G
59	x	701	GNP	PG-N3B-PB-O1B
59	x	701	GNP	PG-N3B-PB-O3A
59	x	701	GNP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	6	101	PHE	1	0
59	x	701	GNP	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

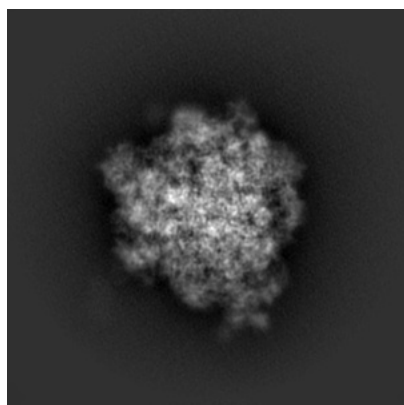
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6550. These allow visual inspection of the internal detail of the map and identification of artifacts.

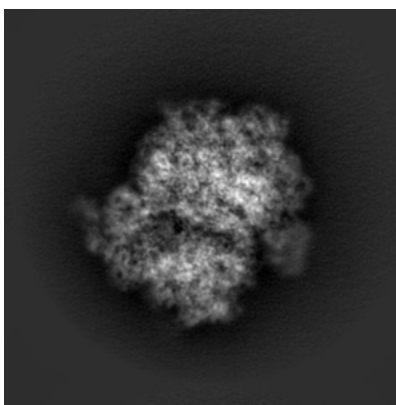
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

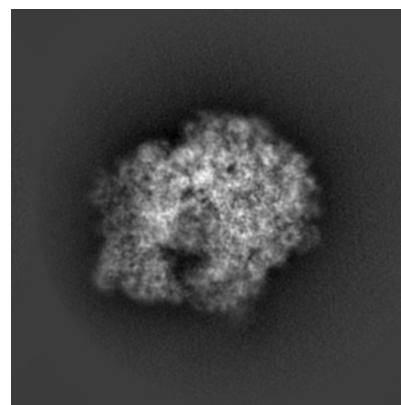
6.1.1 Primary map



X



Y

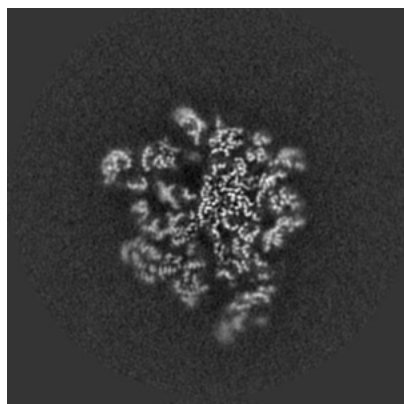


Z

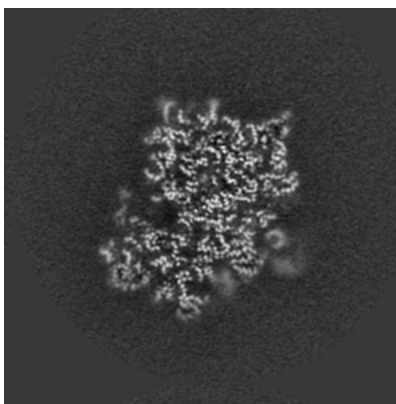
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

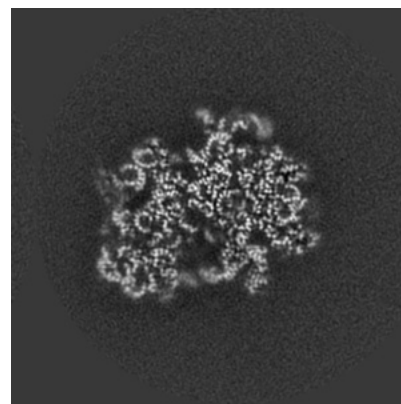
6.2.1 Primary map



X Index: 160



Y Index: 160

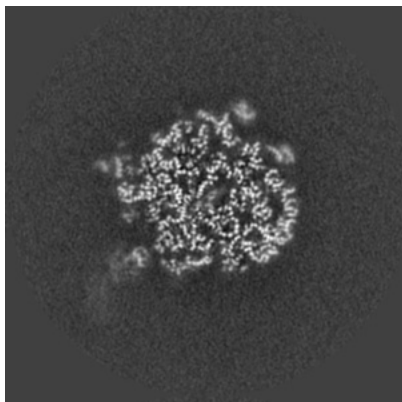


Z Index: 160

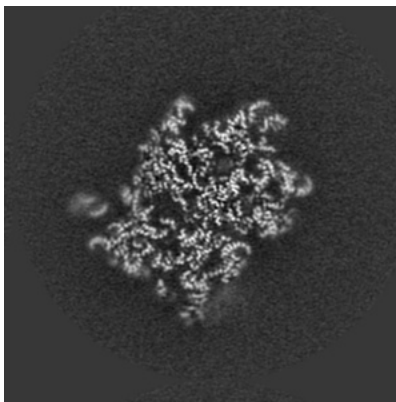
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

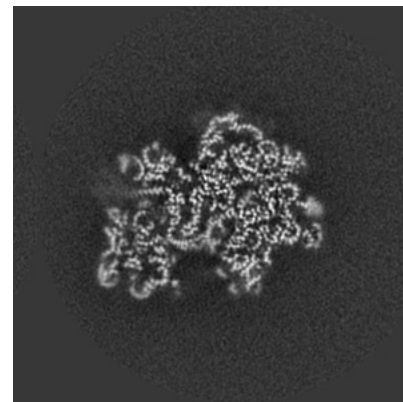
6.3.1 Primary map



X Index: 186



Y Index: 178

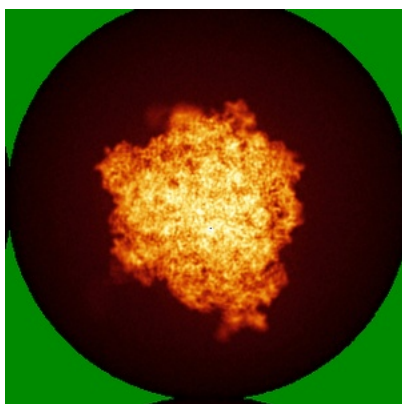


Z Index: 167

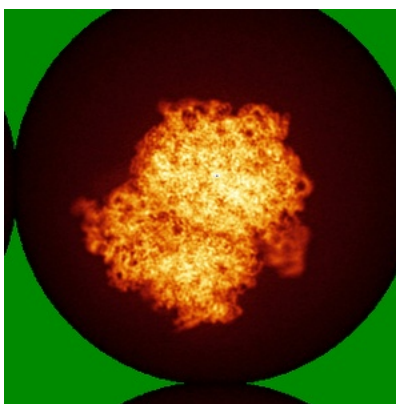
The images above show the largest variance slices of the map in three orthogonal directions.

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

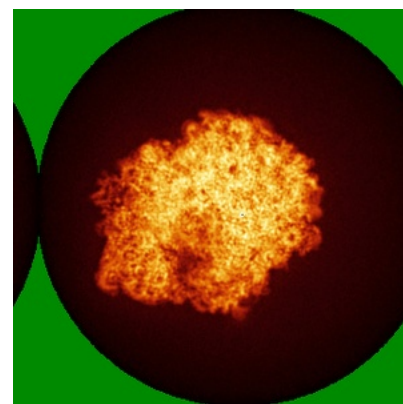
6.4.1 Primary map



X



Y

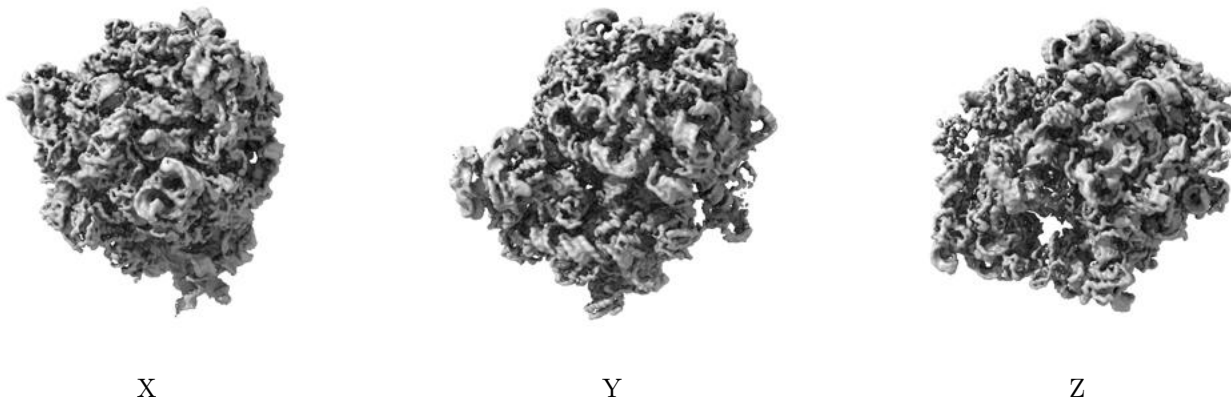


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

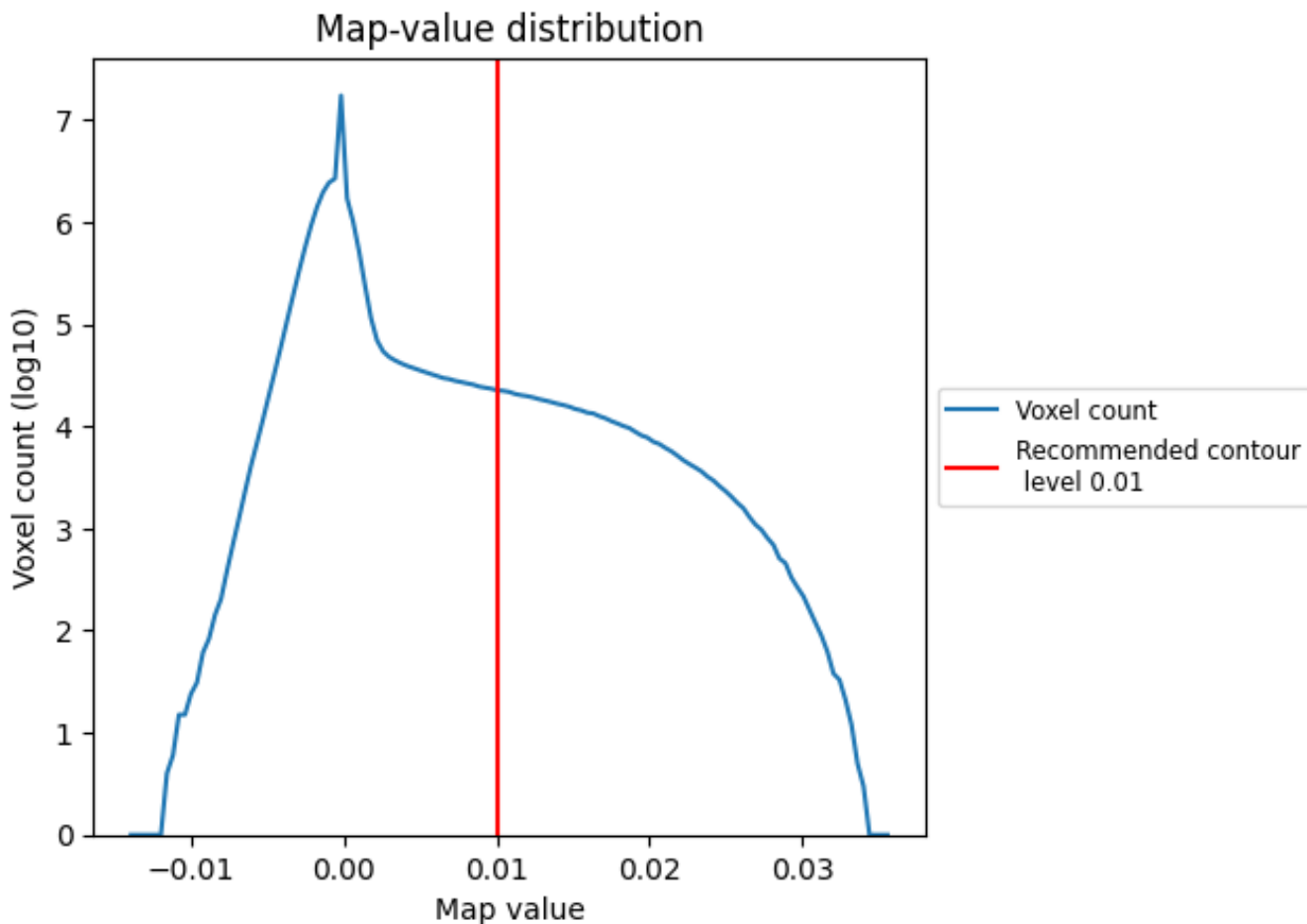
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

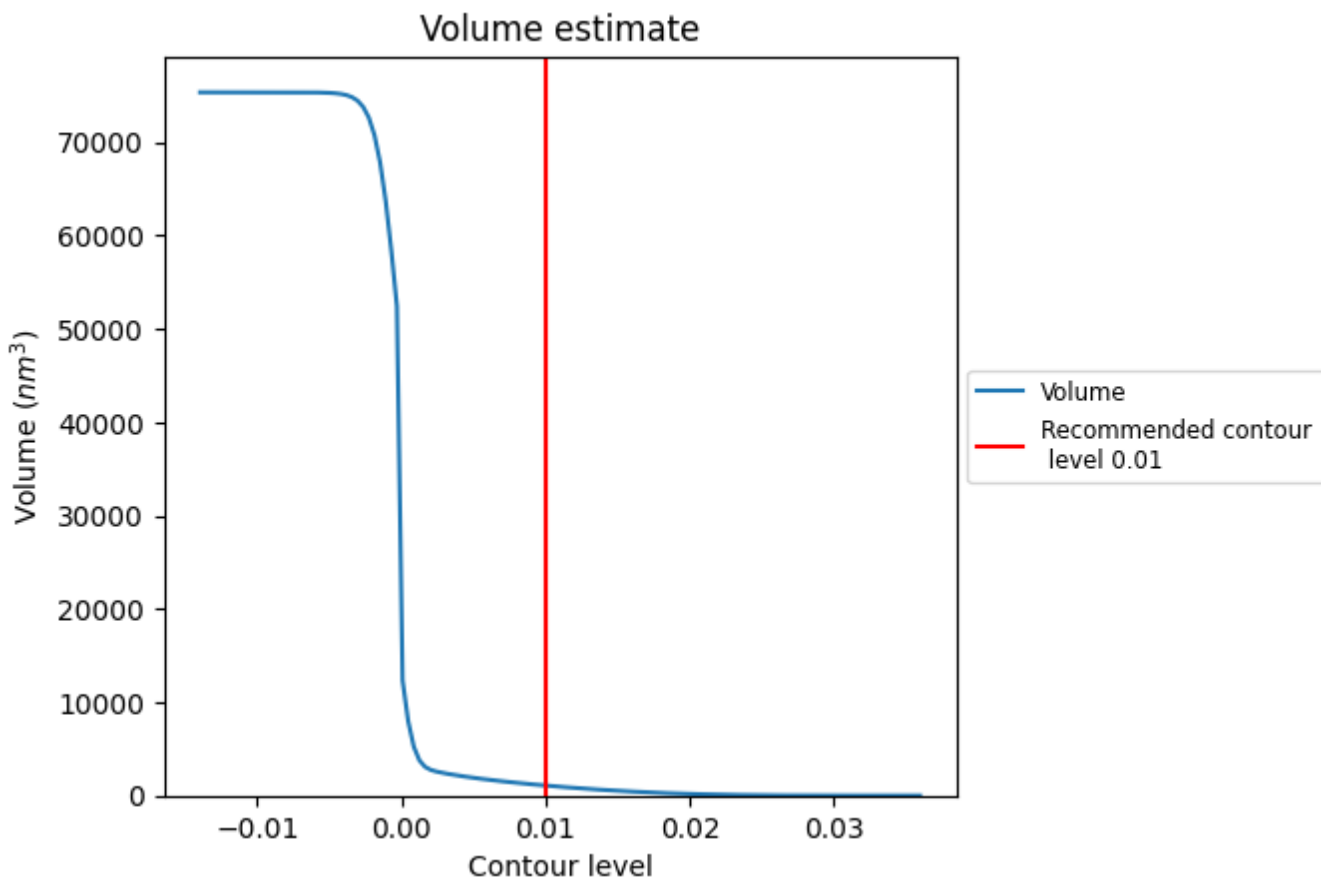
This section contains the results of statistical analysis of the map.

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.

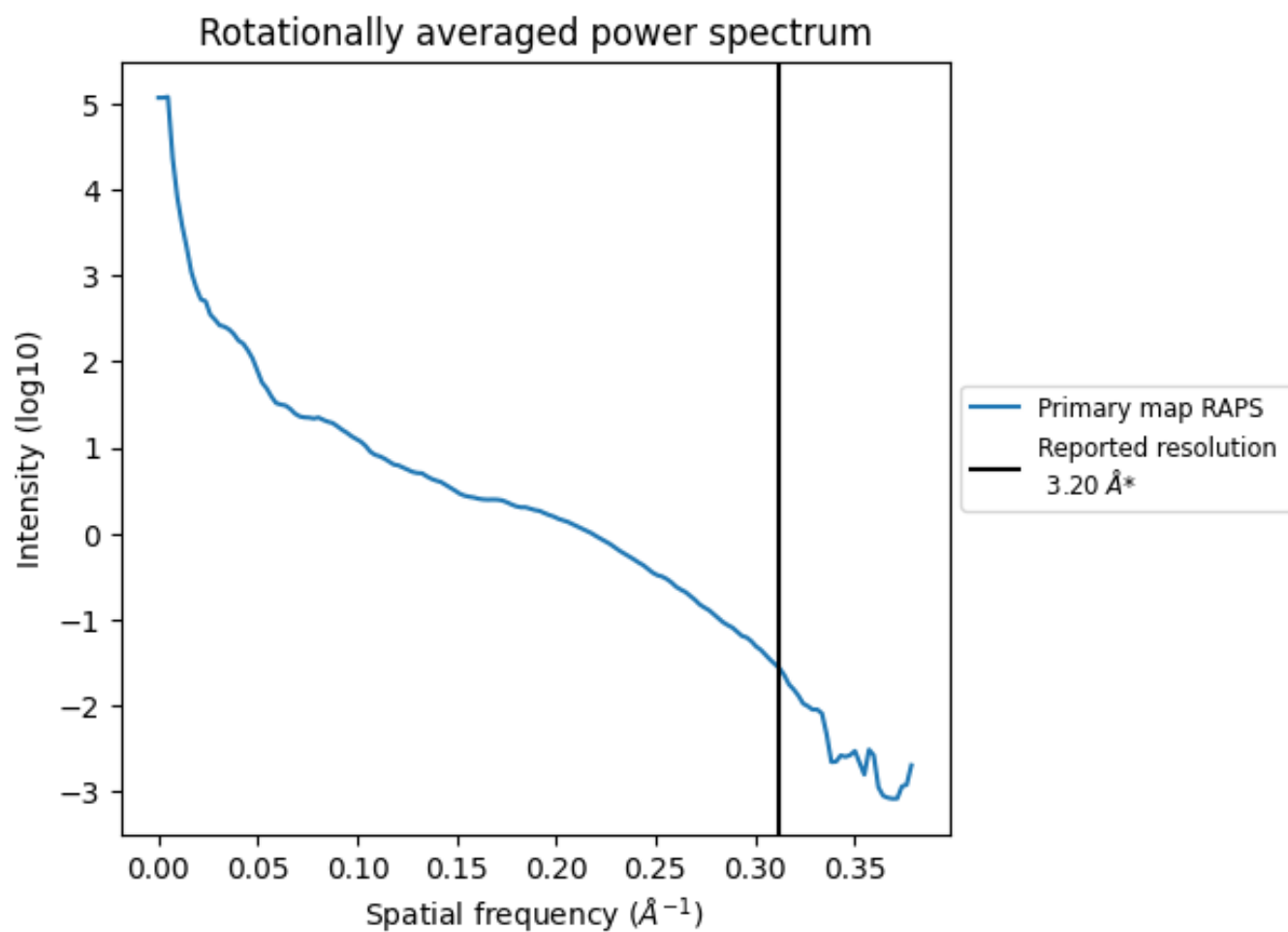
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1075 nm³; this corresponds to an approximate mass of 971 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 [\(i\)](#)

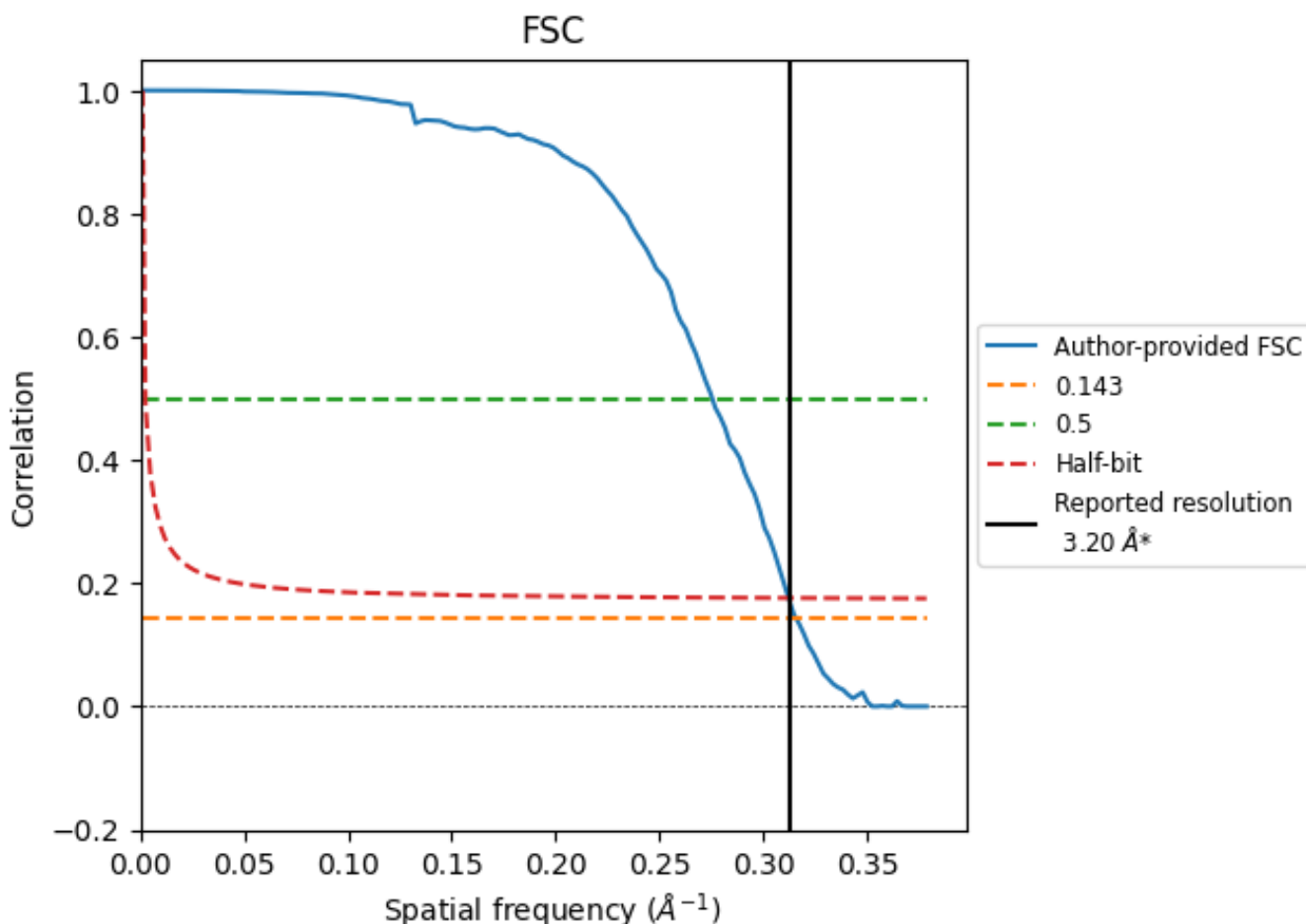


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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

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

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

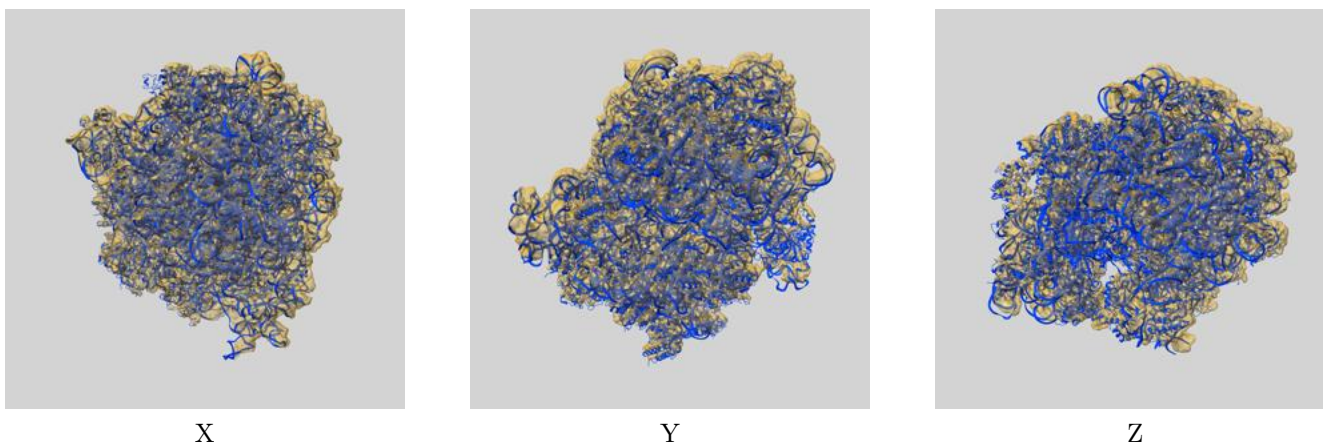
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.17	3.63	3.20
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

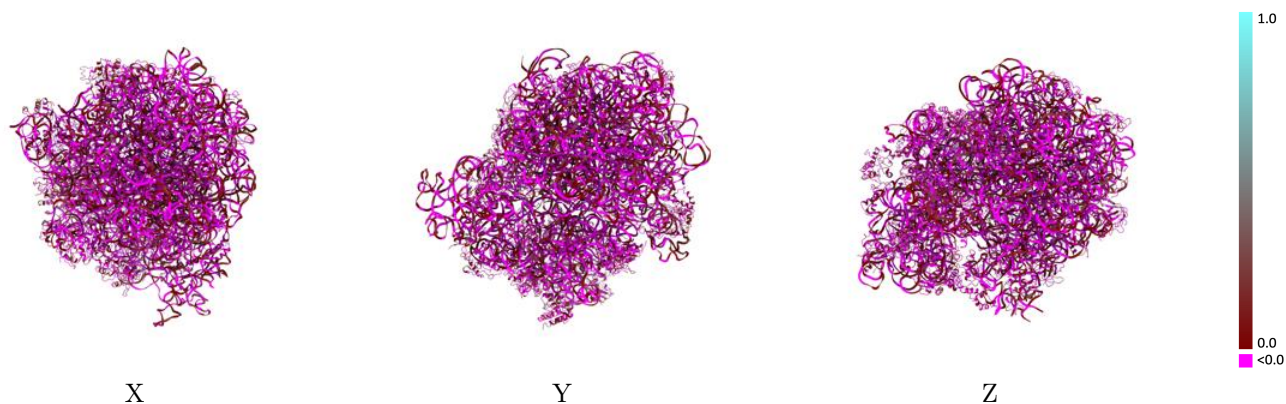
This section contains information regarding the fit between EMDB map EMD-6550 and PDB model 3JCE. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



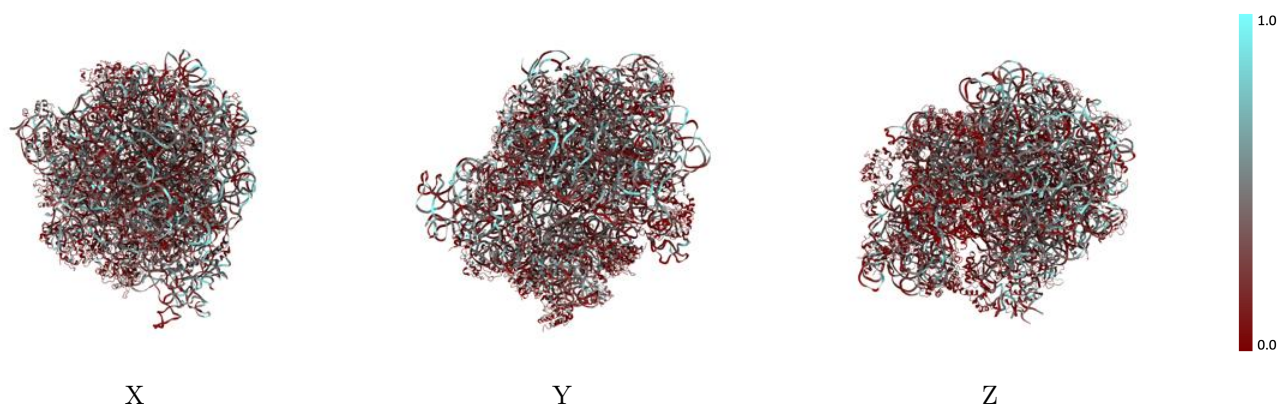
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



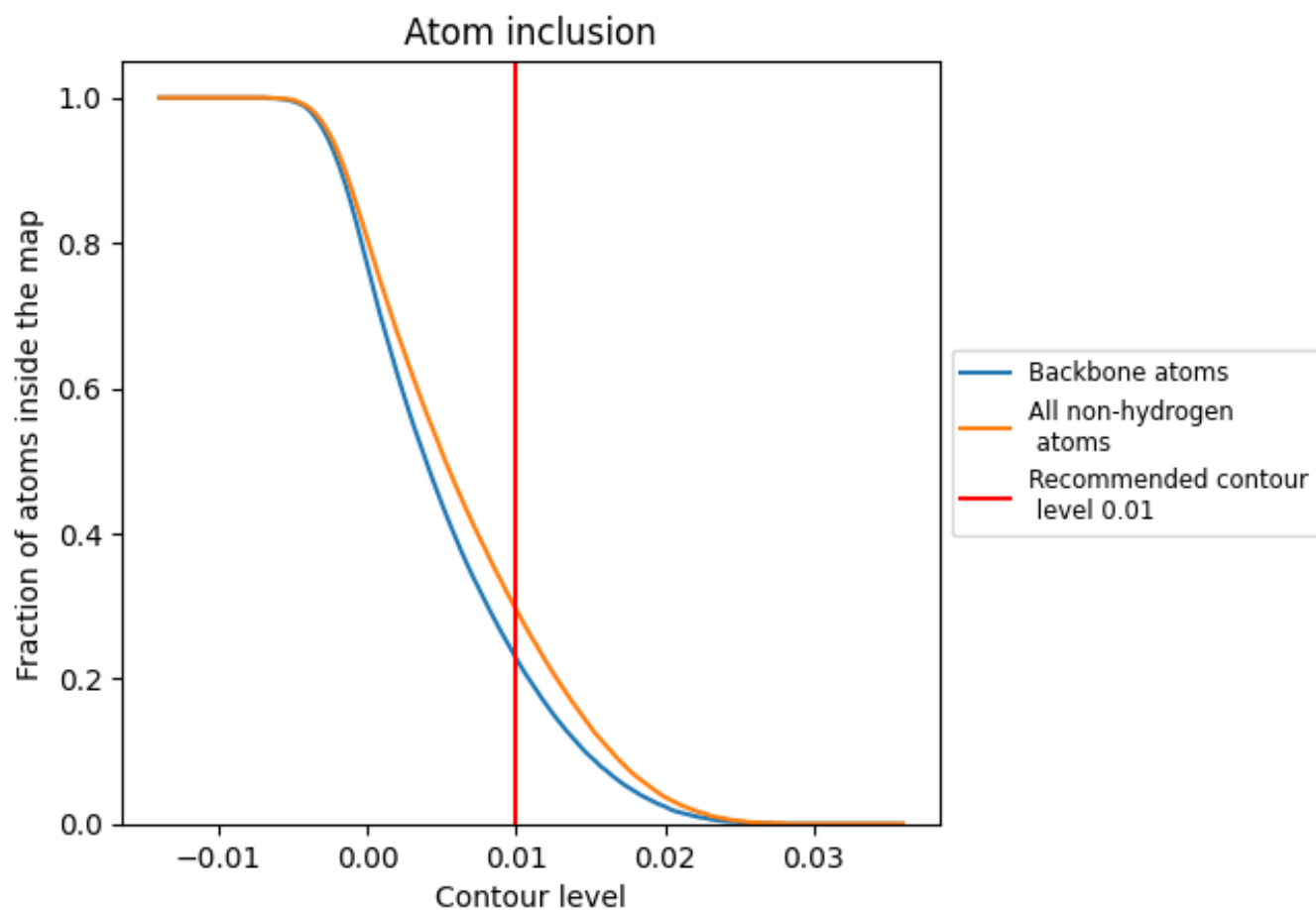
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 23% of all backbone atoms, 30% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2950	 -0.0160
0	 0.2500	 -0.0710
1	 0.1840	 -0.0080
2	 0.2200	 -0.0580
3	 0.2380	 -0.0330
4	 0.2330	 -0.0340
5	 0.0470	 0.0240
6	 0.2770	 0.0080
7	 0.1380	 -0.0660
8	 0.3170	 0.0250
9	 0.1150	 0.0280
A	 0.3460	 -0.0170
B	 0.3770	 -0.0130
C	 0.1920	 -0.0390
D	 0.2220	 -0.0230
E	 0.2340	 -0.0220
F	 0.1530	 -0.0490
G	 0.1980	 -0.0270
H	 0.0580	 0.0200
I	 0.1050	 -0.0080
J	 0.2370	 -0.0310
K	 0.1990	 -0.0050
L	 0.2880	 -0.0050
M	 0.1760	 -0.0140
N	 0.2550	 -0.0380
O	 0.3460	 0.0420
P	 0.1970	 -0.0010
Q	 0.2670	 -0.0250
R	 0.2520	 -0.0370
S	 0.2430	 -0.0400
T	 0.2780	 -0.0040
U	 0.2880	 -0.0080
V	 0.2760	 0.0170
W	 0.2790	 -0.0120
X	 0.2560	 -0.0360



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Chain	Atom inclusion	Q-score
Y	 0.2030	 -0.0360
Z	 0.2650	 -0.0170
a	 0.3490	 -0.0200
b	 0.1430	 -0.0020
c	 0.1860	 -0.0380
d	 0.1760	 -0.0060
e	 0.1590	 -0.0490
f	 0.2160	 -0.0120
g	 0.1840	 -0.0270
h	 0.2330	 0.0260
i	 0.1990	 -0.0310
j	 0.2310	 0.0510
k	 0.1550	 -0.0580
l	 0.2430	 -0.0190
m	 0.1970	 -0.0140
n	 0.1770	 -0.0250
o	 0.2590	 -0.0290
p	 0.2300	 0.0270
q	 0.2480	 -0.0090
r	 0.1880	 -0.0310
s	 0.2160	 -0.0360
t	 0.2340	 -0.0390
u	 0.1550	 0.0270
x	 0.1390	 -0.0120