



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 11:16 am BST

PDB ID : 6YAM
EMDB ID : EMD-10761
Title : Mammalian 48S late-stage translation initiation complex (LS48S+eIF3 IC)
with beta-globin mRNA
Authors : Bochler, A.; Simonetti, A.; Guca, E.; Hashem, Y.
Deposited on : 2020-03-12
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

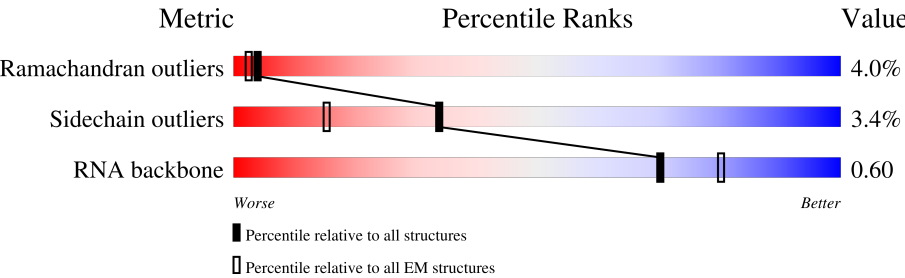
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.60 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	75	<div> <div>69%</div> <div> <div>77%</div> <div>16%</div> </div> </div>
2	l	25	<div> <div>28%</div> <div>96%</div> </div>
3	C	208	<div> <div>14%</div> <div>95%</div> <div>5%</div> </div>
4	D	264	<div> <div>22%</div> <div>77%</div> <div>5%</div> <div>19%</div> </div>
5	E	226	<div> <div>14%</div> <div>97%</div> </div>
6	F	227	<div> <div>32%</div> <div>95%</div> <div>5%</div> </div>
7	G	263	<div> <div>17%</div> <div>98%</div> </div>
8	H	191	<div> <div>21%</div> <div>97%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	237	<div>46%</div> <div>96%</div> <div>.</div>
10	J	190	<div>56%</div> <div>94%</div> <div>6%</div>
11	K	206	<div>29%</div> <div>95%</div> <div>.</div>
12	L	182	<div>18%</div> <div>97%</div> <div>..</div>
13	M	98	<div>29%</div> <div>89%</div> <div>9%</div> <div>.</div>
14	N	158	<div>26%</div> <div>94%</div> <div>5%</div> <div>.</div>
15	O	132	<div>85%</div> <div>88%</div> <div>6%</div> <div>6%</div>
16	P	150	<div>21%</div> <div>93%</div> <div>6%</div> <div>.</div>
17	Q	151	<div>18%</div> <div>86%</div> <div>.</div> <div>10%</div>
18	S	141	<div>18%</div> <div>96%</div> <div>.</div>
19	T	135	<div>36%</div> <div>90%</div> <div>.</div> <div>7%</div>
20	V	145	<div>17%</div> <div>95%</div> <div>..</div>
21	W	119	<div>29%</div> <div>87%</div> <div>.</div> <div>13%</div>
22	X	82	<div>17%</div> <div>95%</div> <div>..</div>
23	Y	130	<div>.</div> <div>96%</div> <div>..</div>
24	Z	142	<div>10%</div> <div>96%</div> <div>.</div>
25	a	133	<div>26%</div> <div>83%</div> <div>8%</div> <div>5%</div> <div>5%</div>
26	b	115	<div>7%</div> <div>83%</div> <div>.</div> <div>14%</div>
27	c	84	<div>39%</div> <div>83%</div> <div>14%</div> <div>.</div>
28	d	69	<div>26%</div> <div>91%</div> <div>.</div> <div>7%</div>
29	e	53	<div>36%</div> <div>81%</div> <div>19%</div>
30	f	71	<div>87%</div> <div>86%</div> <div>14%</div>
31	g	313	<div>47%</div> <div>98%</div> <div>.</div>
32	n	75	<div>41%</div> <div>96%</div> <div>.</div>
33	i	59	<div>49%</div> <div>92%</div> <div>7%</div> <div>.</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	2	1863	
35	A	266	
36	B	422	
37	j	144	
38	k	595	
39	U	152	
40	R	145	
41	3	45	
42	m	548	
43	y	1350	
44	v	913	
45	w	445	
46	q	272	
47	r	352	
48	s	218	
49	t	564	
50	u	374	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	C4J	2	1244	X	-	-	-

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 118536 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 initiator methionylated tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1614	722	299	519	74		

- Molecule 2 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 3 is a protein called 40S ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	208	Total	C	N	O	S	0	0
			1643	1045	289	301	8		

- Molecule 4 is a protein called 40S ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1741	1107	309	310	15		

- Molecule 5 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	226	Total	C	N	O	S	0	0
			1743	1127	300	307	9		

- Molecule 6 is a protein called 40S ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	227	Total	C	N	O	S	0	0
			1765	1124	317	316	8		

- Molecule 7 is a protein called 40S ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

- Molecule 8 is a protein called 40S ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 9 is a protein called 40S ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	237	Total	C	N	O	S	0	0
			1924	1200	387	330	7		

- Molecule 10 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	190	Total	C	N	O	S	0	0
			1530	975	281	273	1		

- Molecule 11 is a protein called 40S ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1680	1054	329	292	5		

- Molecule 12 is a protein called 40S ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	182	Total	C	N	O	S	0	0
			1499	952	300	245	2		

- Molecule 13 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	98	Total	C	N	O	S	0	0
			828	539	148	135	6		

- Molecule 14 is a protein called 40S ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 15 is a protein called 40S ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 16 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 17 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 18 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 19 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	126	Total	C	N	O	S	0	0
			1019	639	188	187	5		

- Molecule 20 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	141	Total	C	N	O	S	0	0
			1112	701	213	195	3		

- Molecule 21 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 22 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	82	Total	C	N	O	S	0	0
			620	378	117	120	5		

- Molecule 23 is a protein called 40S ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 24 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	142	Total	C	N	O	S	0	0
			1107	698	220	185	4		

- Molecule 25 is a protein called 40S ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	126	Total	C	N	O	S	0	0
			1021	645	198	173	5		

- Molecule 26 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	99	Total	C	N	O	S	0	0
			789	491	162	130	6		

- Molecule 27 is a protein called 40S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

- Molecule 28 is a protein called 40S ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 29 is a protein called ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 30 is a protein called ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	71	Total	C	N	O	S	0	0
			582	367	109	99	7		

- Molecule 31 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	313	Total	C	N	O	S	0	0
			2437	1535	424	466	12		

- Molecule 32 is a protein called ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	75	Total	C	N	O	S	0	0
			599	382	111	105	1		

- Molecule 33 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	59	Total	C	N	O	S	0	0
			473	293	104	75	1		

- Molecule 34 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	2	1743	Total	C	N	O	P	0	0
			37187	16605	6660	12182	1740		

- Molecule 35 is a protein called eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A	266	Total	C	N	O	S	0	0
			2147	1354	376	406	11		

- Molecule 36 is a protein called eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B	422	Total	C	N	O	S	0	0
			3214	2044	561	592	17		

- Molecule 37 is a protein called eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	109	Total	C	N	O	S	0	0
			882	549	168	161	4		

- Molecule 38 is a protein called ATP-binding cassette sub-family E member 1 (ABCE1).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	595	Total	C	N	O	S	0	0
			4693	2995	802	865	31		

- Molecule 39 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	U	145	Total	C	N	O	S	0	0
			1194	747	243	203	1		

- Molecule 40 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	R	140	Total	C	N	O	S	0	0
			1154	733	219	195	7		

- Molecule 41 is a RNA chain called beta-globin mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3	45	Total	C	N	O	P	0	0
			960	430	179	306	45		

- Molecule 42 is a protein called eukaryotic translation initiation factor 3 subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	365	Total	C	N	O	S	0	0
			2955	1856	517	564	18		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	y	603	Total	C	N	O	S	0	0
			4971	3133	897	920	21		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	554	Total	C	N	O	S	0	0
			4508	2830	800	845	33		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	w	419	Total	C	N	O	S	0	0
			3465	2220	586	639	20		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	272	Total	C	N	O	S	0	0
			2111	1330	359	410	12		

- Molecule 47 is a protein called eukaryotic translation initiation factor 3 subunit h.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	324	Total	C	N	O	S	0	0
			2624	1654	452	503	15		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	215	Total	C	N	O	S	0	0
			1737	1109	285	330	13		

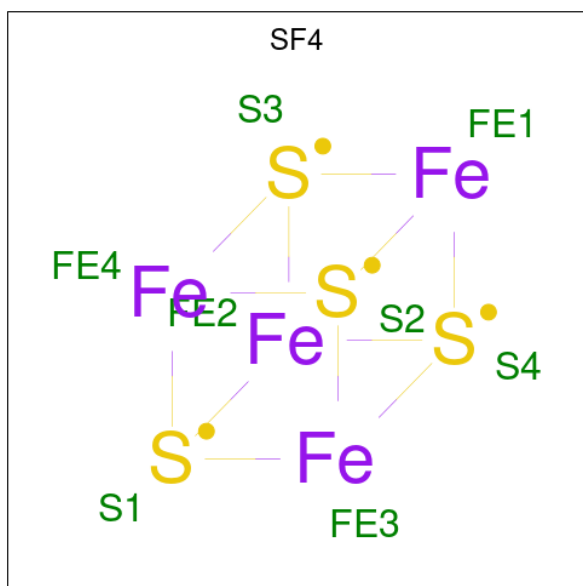
- Molecule 49 is a protein called eukaryotic translation initiation factor 3 subunit l.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	372	Total	C	N	O	S	0	0
			3109	2010	519	563	17		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	365	Total	C	N	O	S	0	0
			2918	1850	493	558	17		

- Molecule 51 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

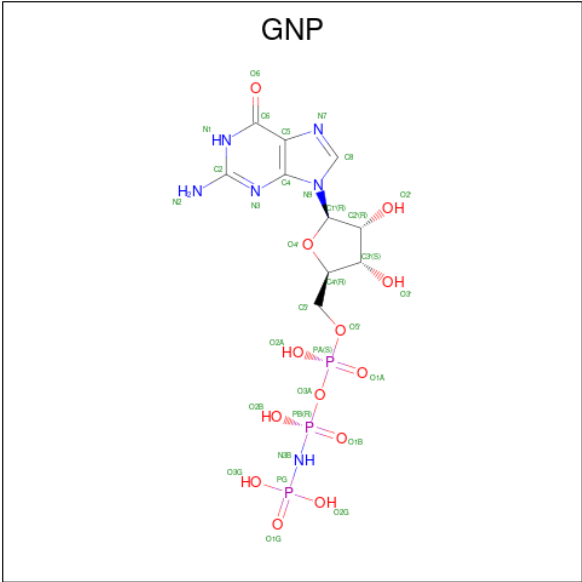


Mol	Chain	Residues	Atoms			AltConf
51	k	1	Total	Fe	S	0
			8	4	4	
51	k	1	Total	Fe	S	0
			8	4	4	

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	k	1	Total	Mg	0
			1	1	

- Molecule 53 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

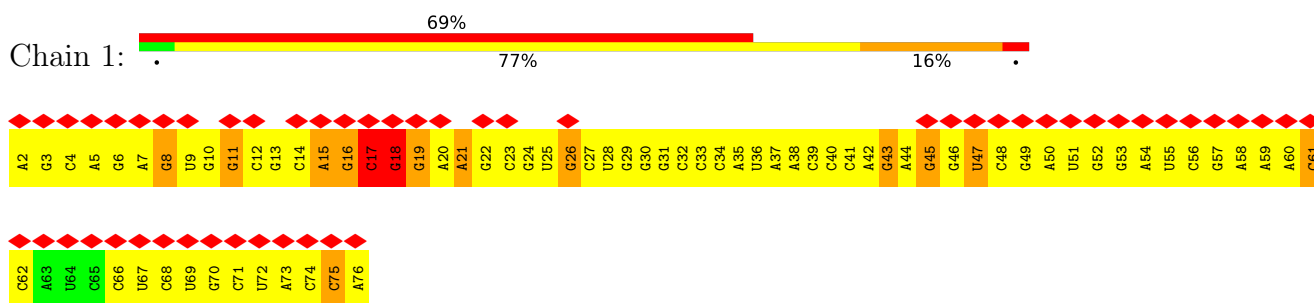


Mol	Chain	Residues	Atoms					AltConf
53	k	1	Total	C	N	O	P	0
			32	10	6	13	3	
53	k	1	Total	C	N	O	P	0
			32	10	6	13	3	

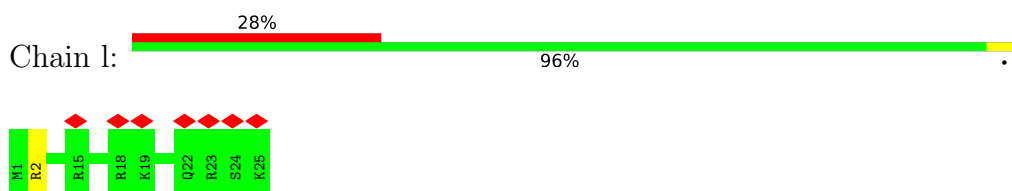
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

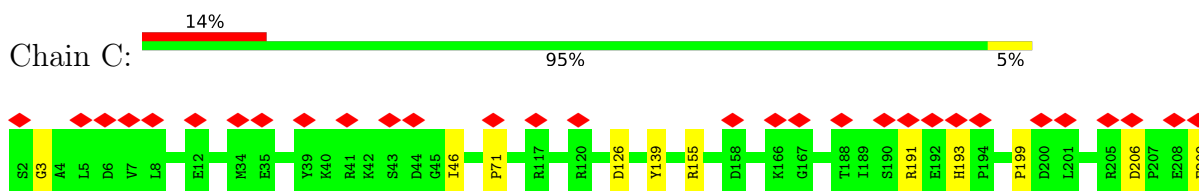
- Molecule 1: initiator methionylated tRNA



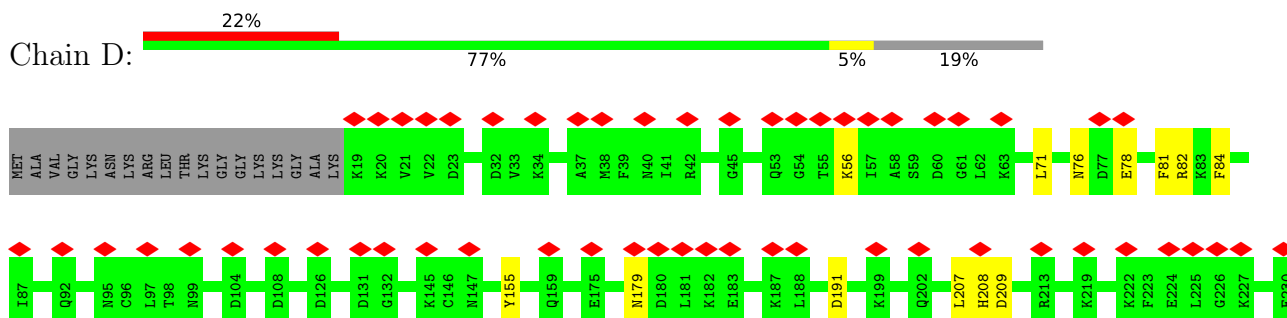
- Molecule 2: 60s ribosomal protein l41

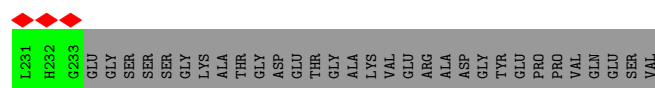


- Molecule 3: 40S ribosomal protein uS2

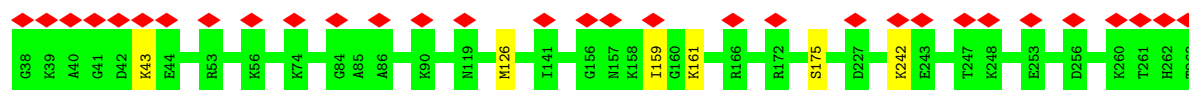


- Molecule 4: 40S ribosomal protein eS1

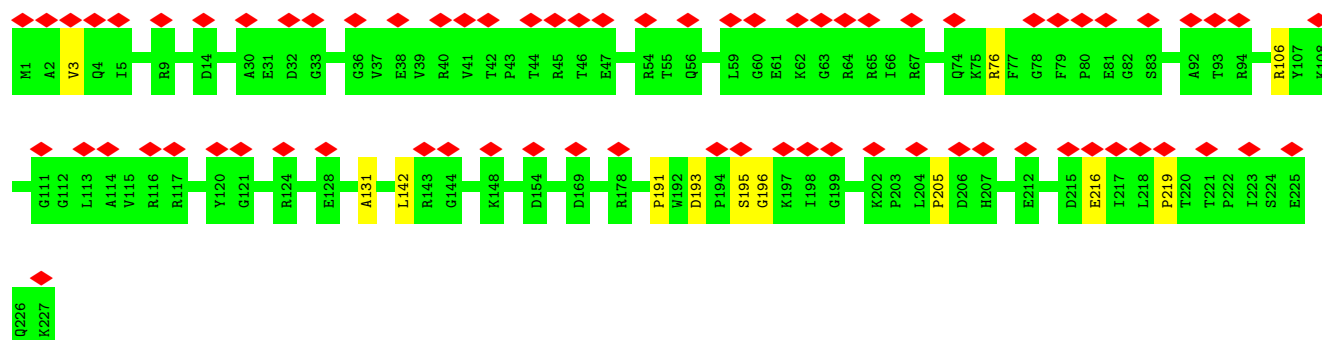




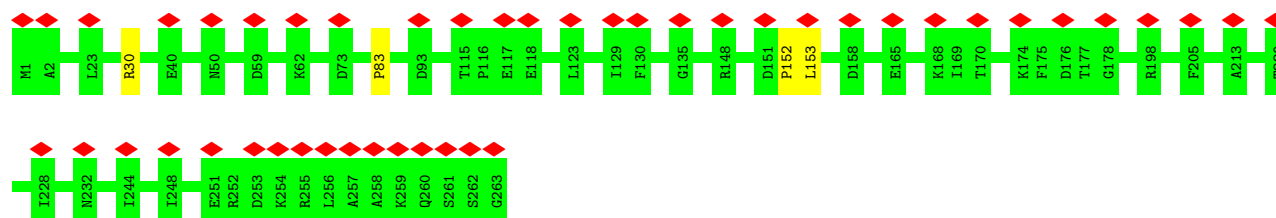
- Molecule 5: 40S ribosomal protein uS5



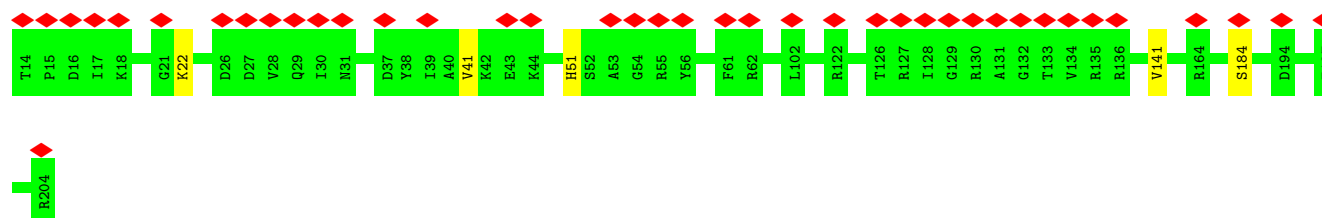
- Molecule 6: 40S ribosomal protein uS3



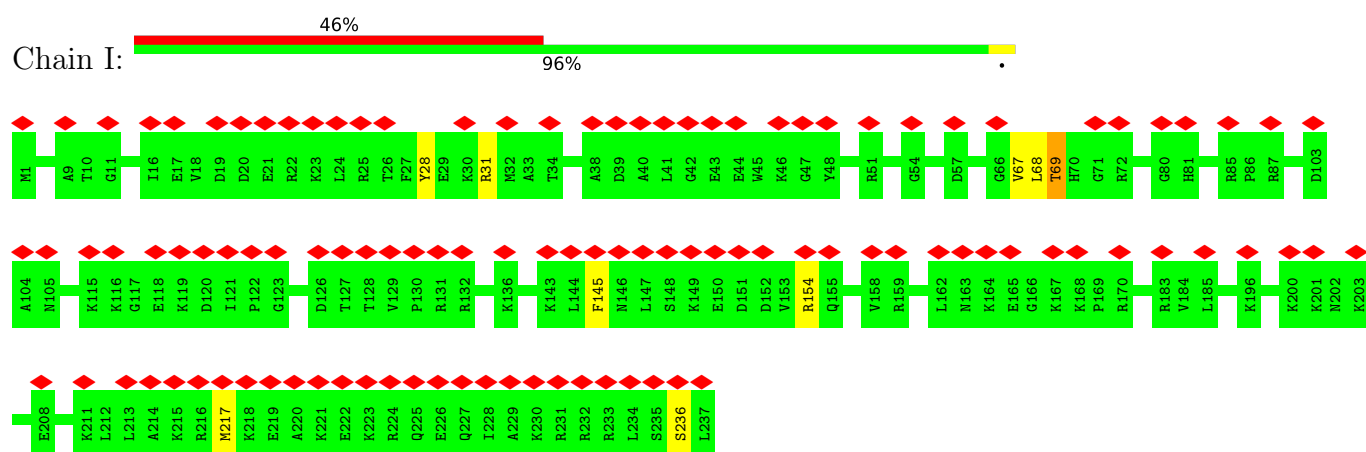
- Molecule 7: 40S ribosomal protein eS4



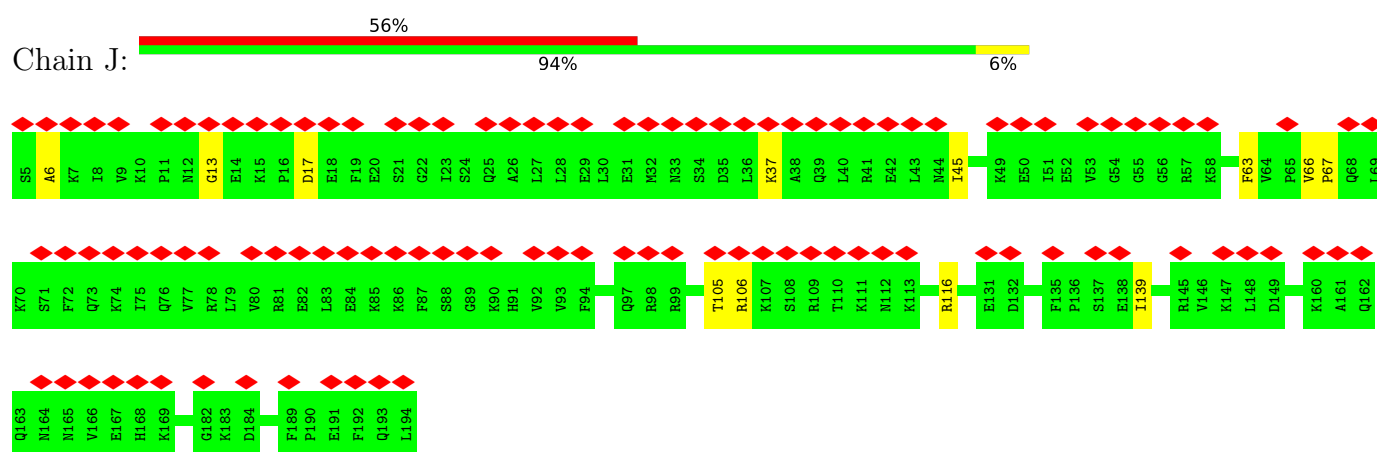
- Molecule 8: 40S ribosomal protein uS7



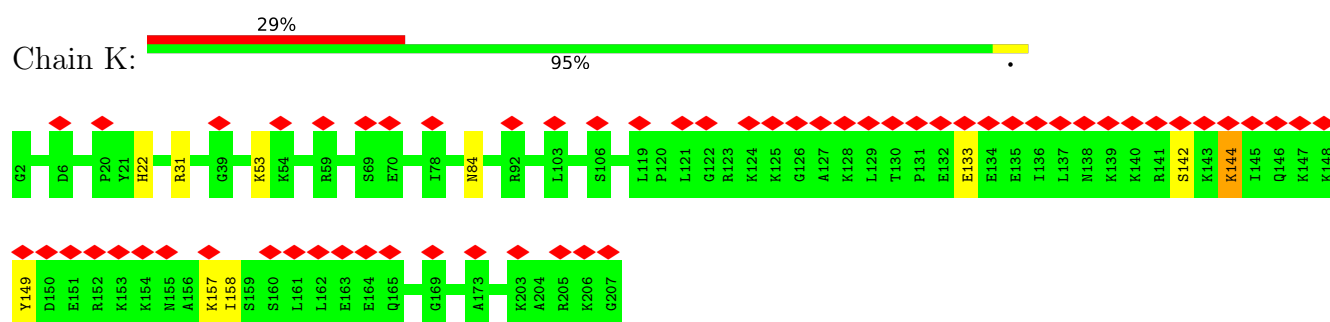
- Molecule 9: 40S ribosomal protein eS6



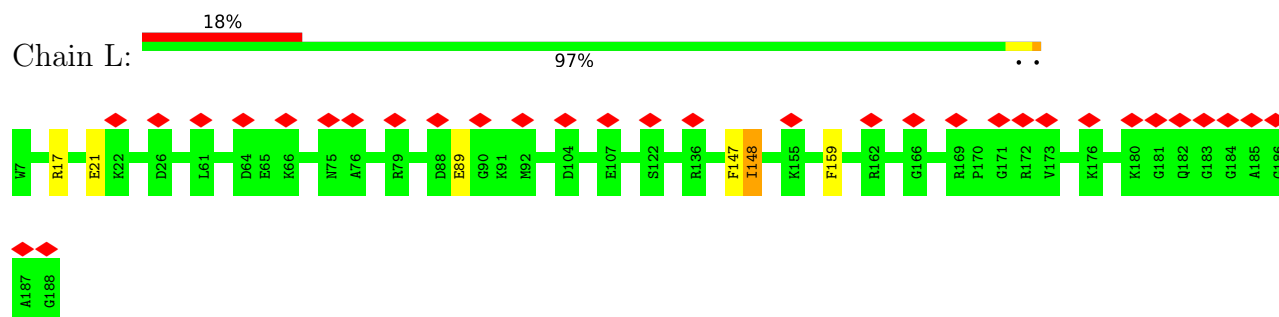
• Molecule 10: ribosomal protein eS7



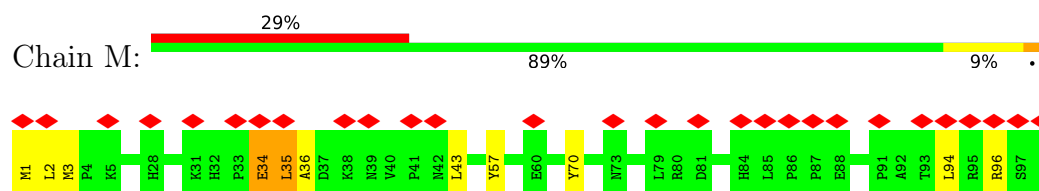
• Molecule 11: 40S ribosomal protein eS8



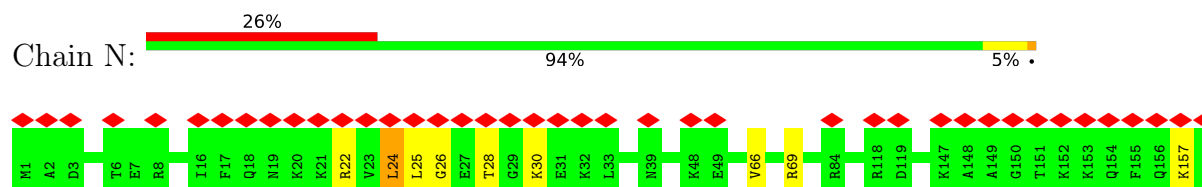
• Molecule 12: 40S ribosomal protein uS4



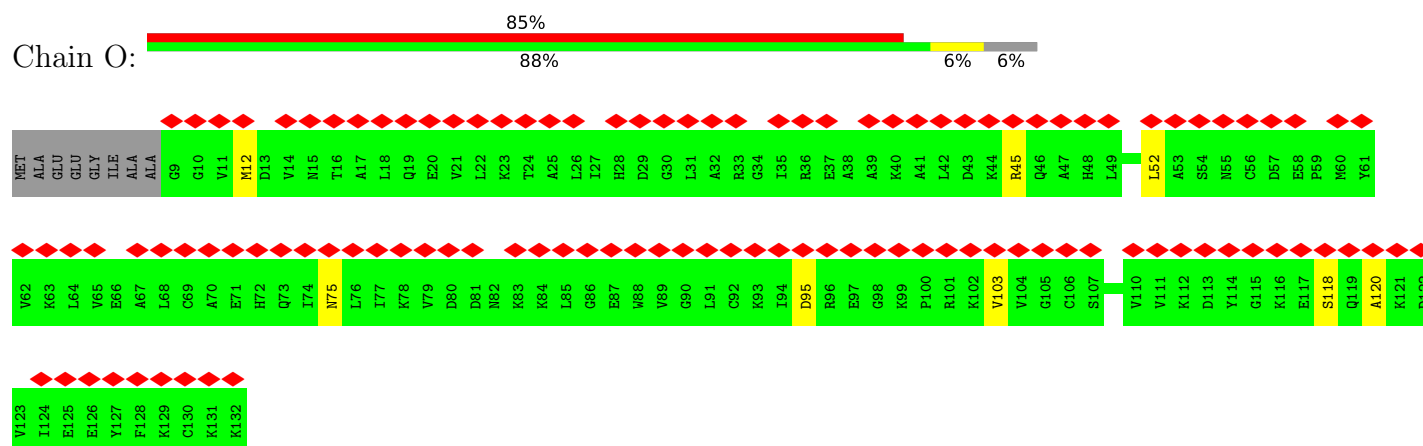
- Molecule 13: 40S ribosomal protein eS10



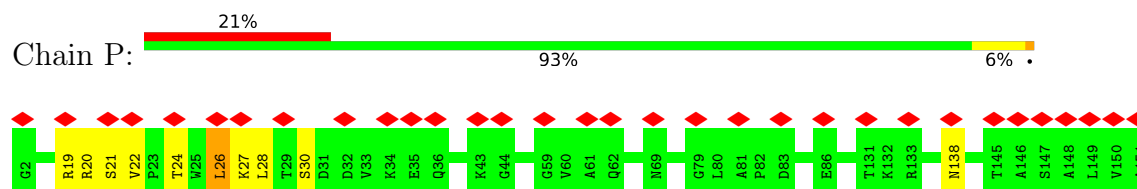
- Molecule 14: 40S ribosomal protein uS17



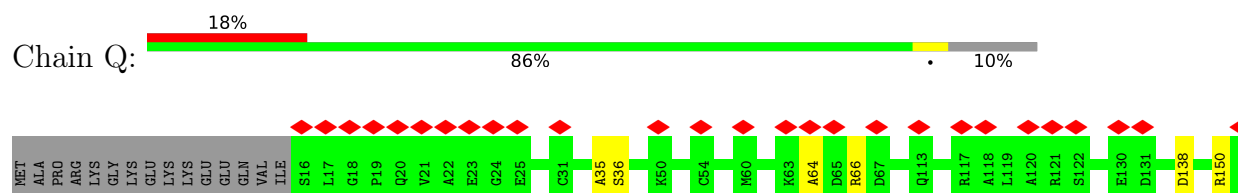
- Molecule 15: 40S ribosomal protein eS12



- Molecule 16: ribosomal protein uS15

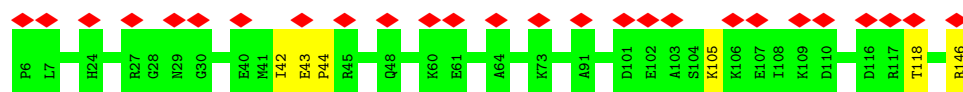


- Molecule 17: 40S ribosomal protein uS11

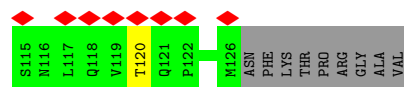
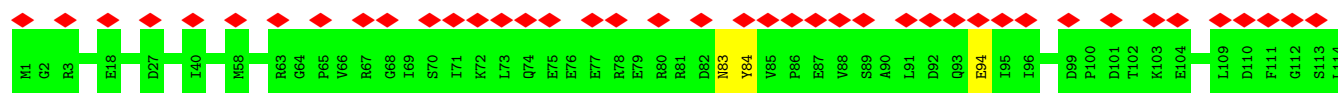
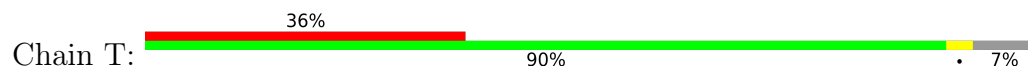


- Molecule 18: 40S ribosomal protein uS9

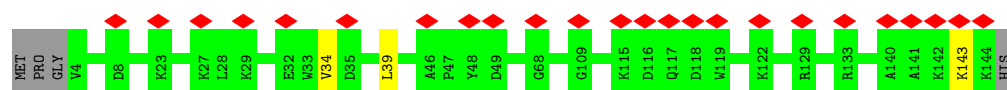




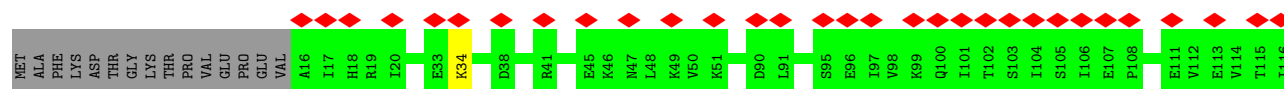
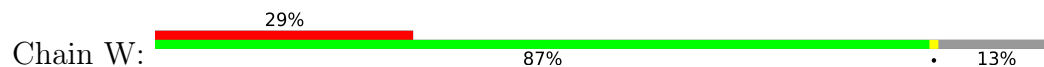
- Molecule 19: 40S ribosomal protein eS17



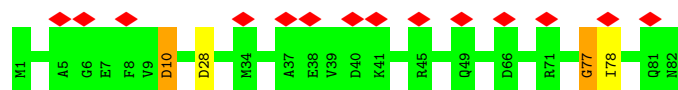
- Molecule 20: 40S ribosomal protein eS19



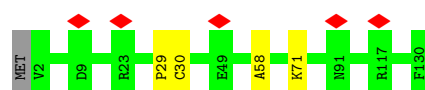
- Molecule 21: 40S ribosomal protein uS10



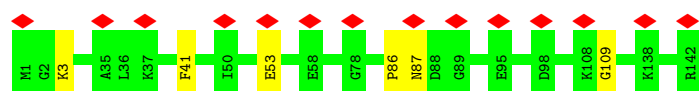
- Molecule 22: 40S ribosomal protein eS21



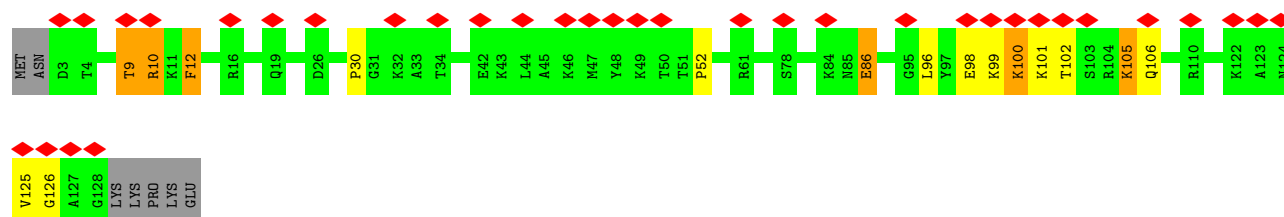
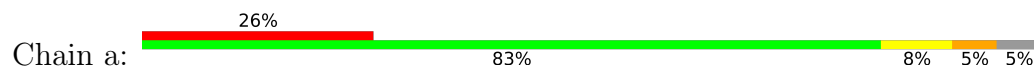
- Molecule 23: 40S ribosomal protein uS8



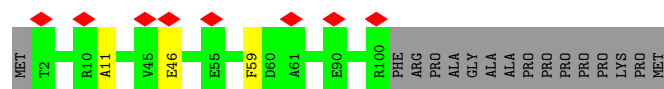
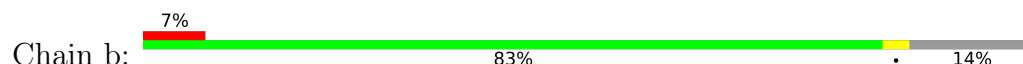
- Molecule 24: 40S ribosomal protein uS12



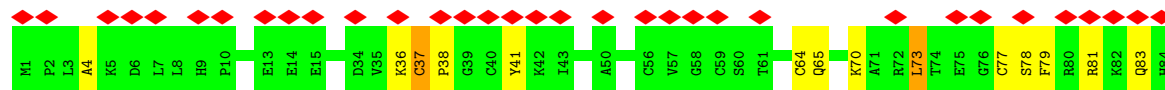
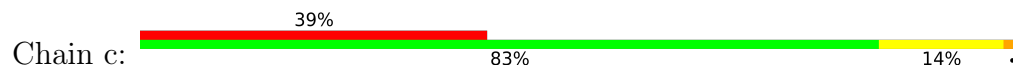
- Molecule 25: 40S ribosomal protein eS24



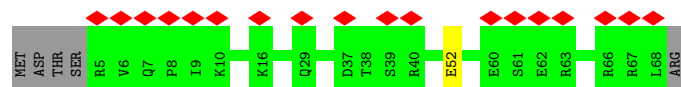
- Molecule 26: 40S ribosomal protein eS26



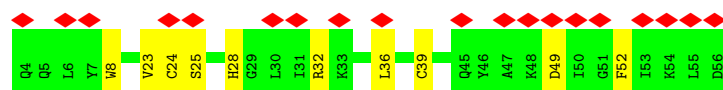
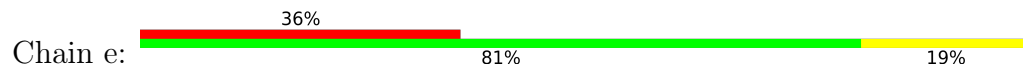
- Molecule 27: 40S ribosomal protein eS27



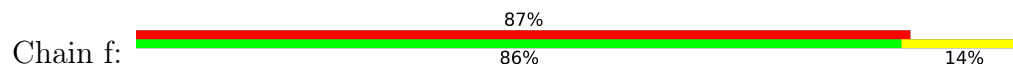
- Molecule 28: 40S ribosomal protein eS28

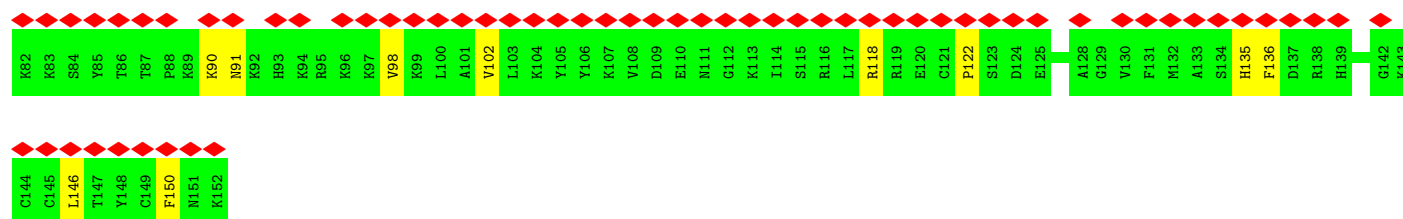


- Molecule 29: ribosomal protein uS14

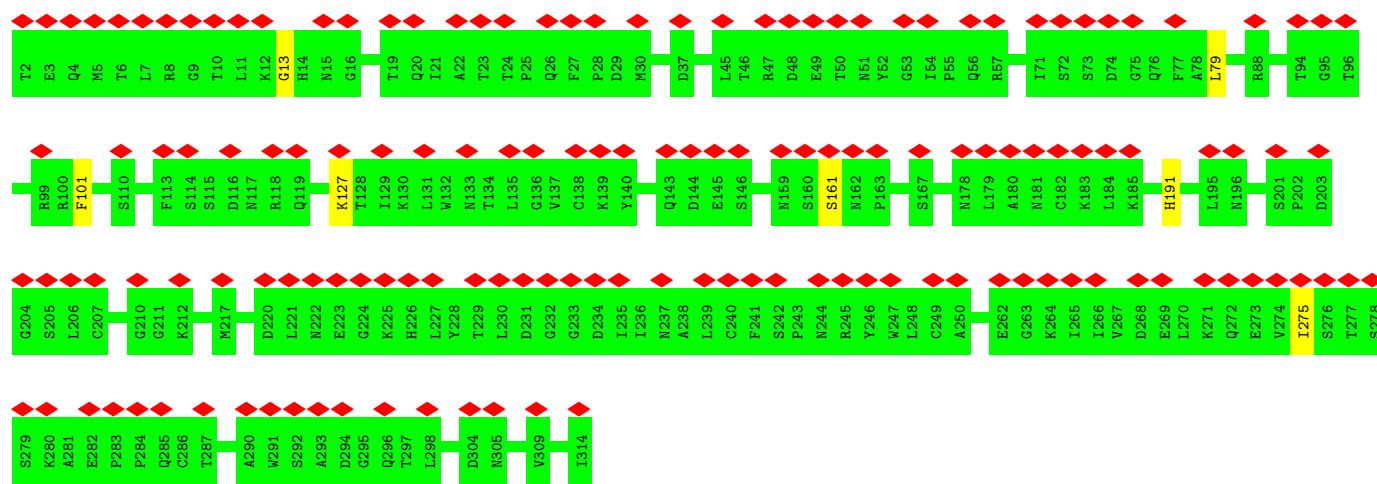


- Molecule 30: ribosomal protein eS31

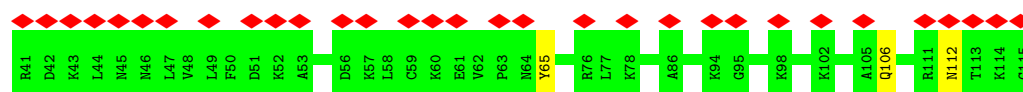
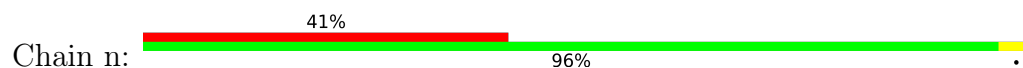




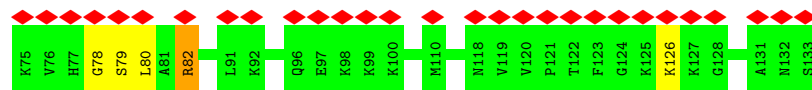
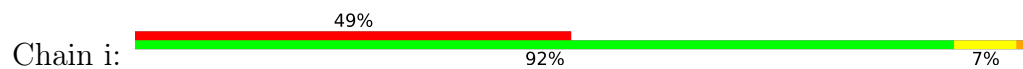
• Molecule 31: ribosomal protein RACK1



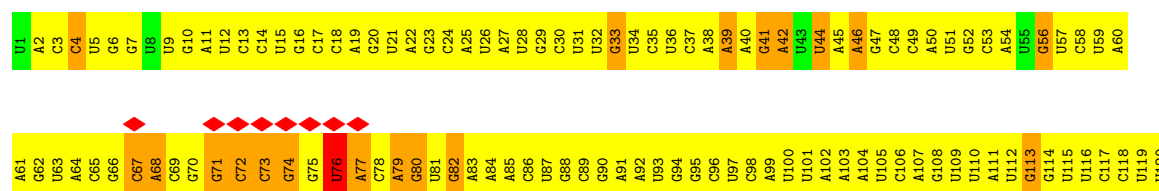
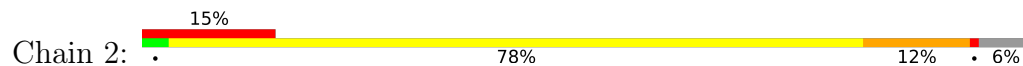
• Molecule 32: ribosomal protein eS25



• Molecule 33: 40S ribosomal protein eS30

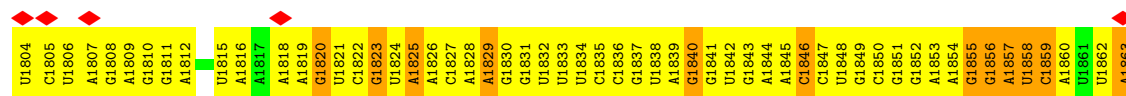


• Molecule 34: 18S ribosomal RNA

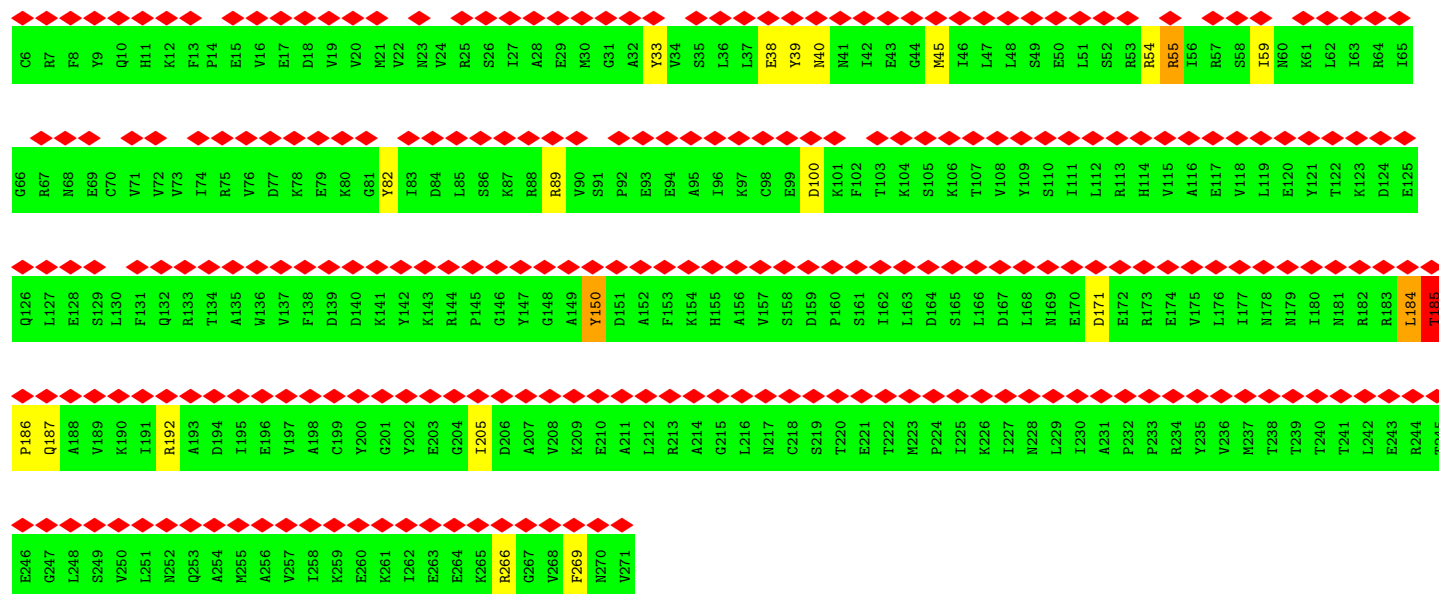
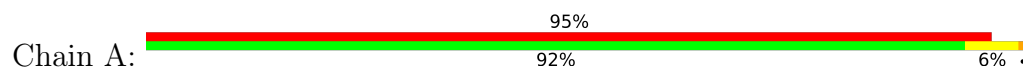




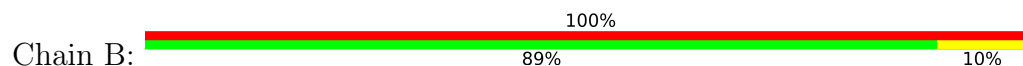
WORLDWIDE
PDB
PROTEIN DATA BANK

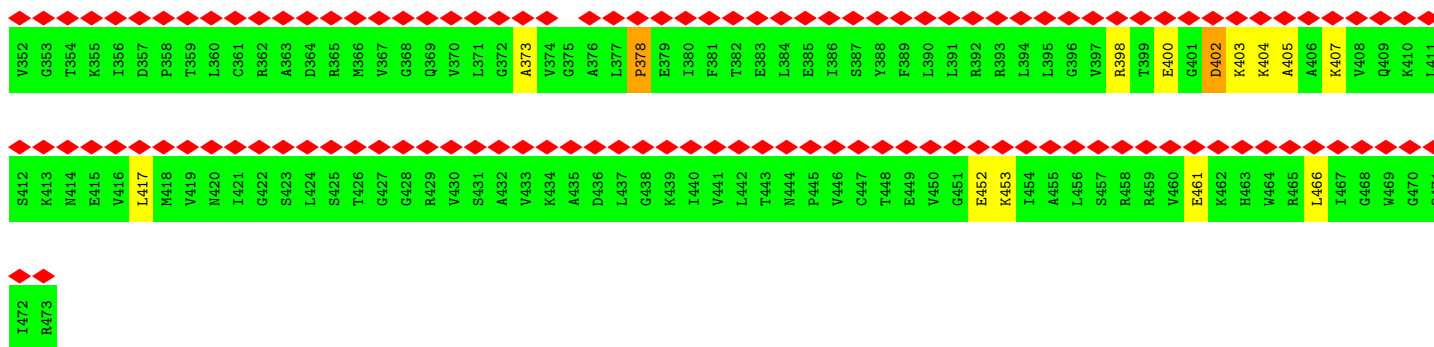


• Molecule 35: eukaryotic translation initiation factor 2 subunit alpha

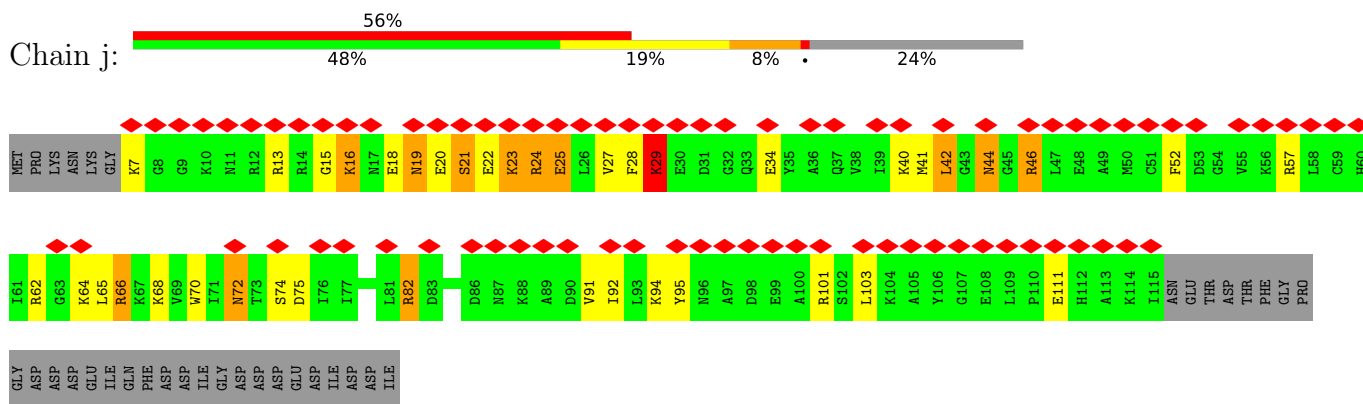


• Molecule 36: eukaryotic translation initiation factor 2 subunit gamma

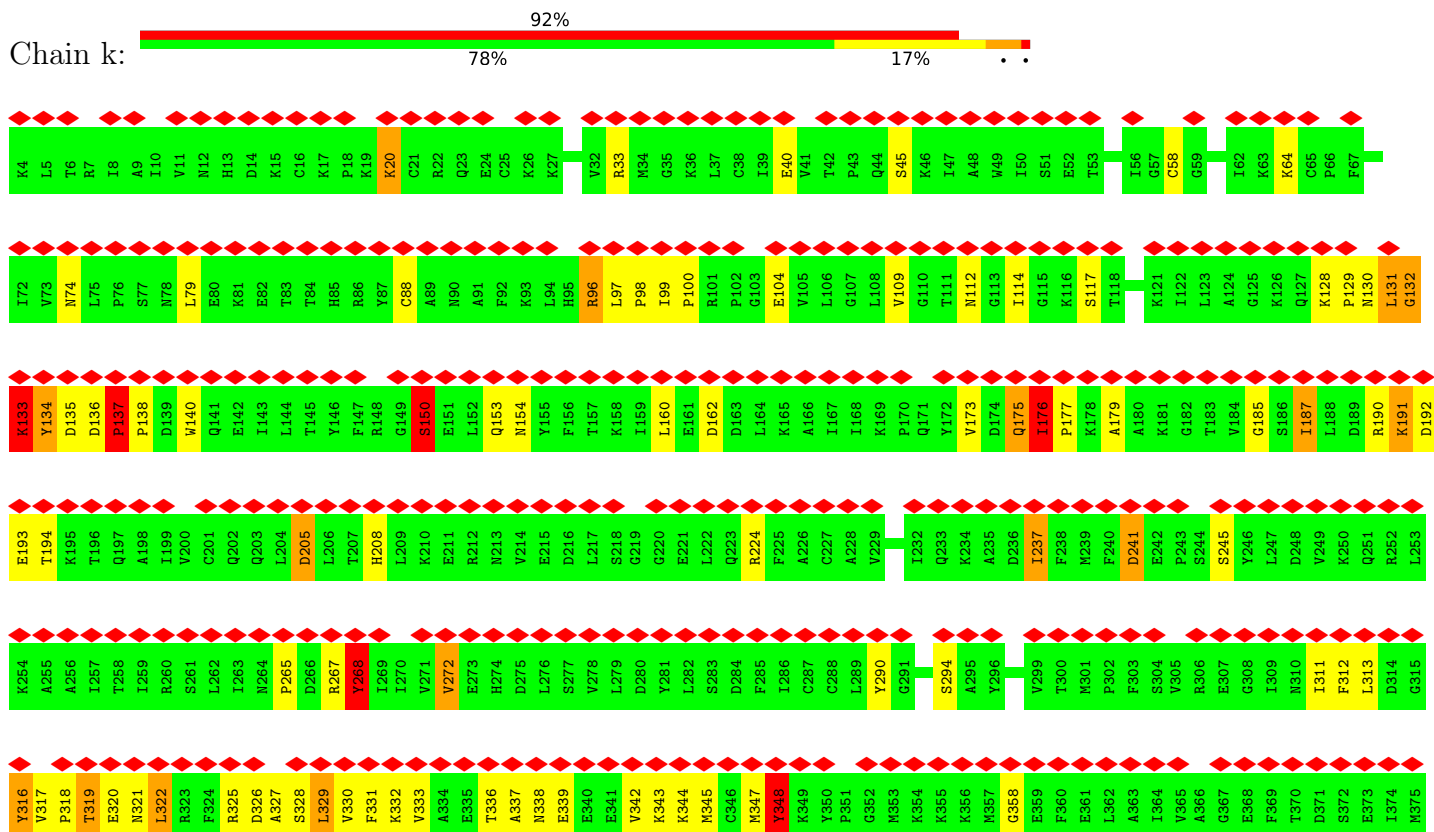


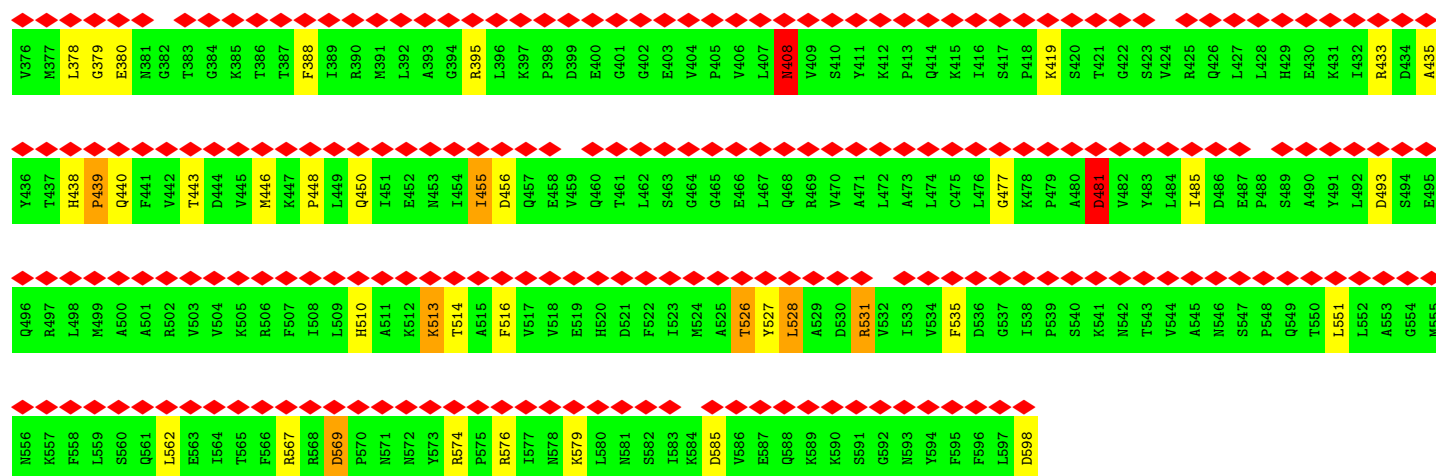


- Molecule 37: eukaryotic translation initiation factor 1A

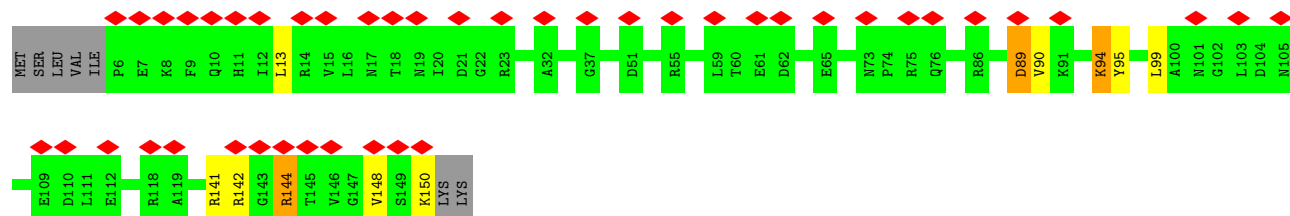
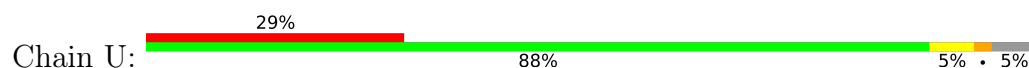


- Molecule 38: ATP-binding cassette sub-family E member 1 (ABCE1)

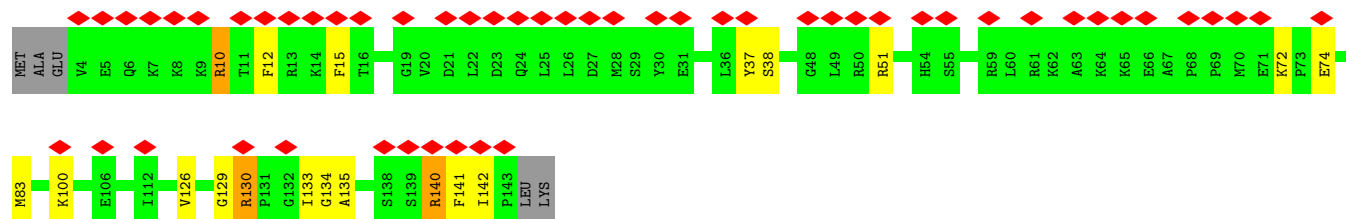
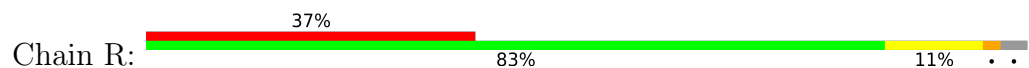




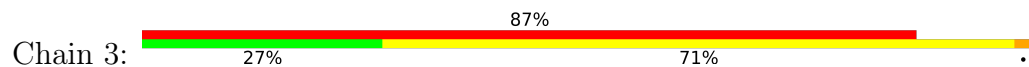
• Molecule 39: 40S ribosomal protein uS13



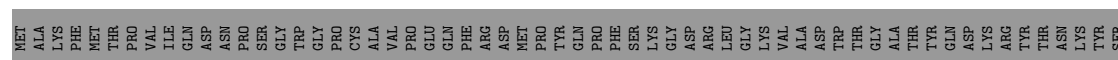
• Molecule 40: 40S ribosomal protein uS19



• Molecule 41: beta-globin mRNA



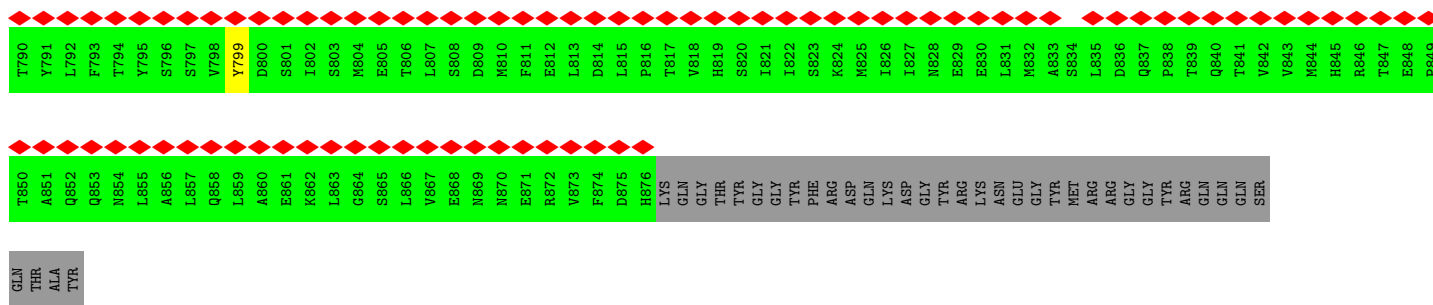
• Molecule 42: eukaryotic translation initiation factor 3 subunit d



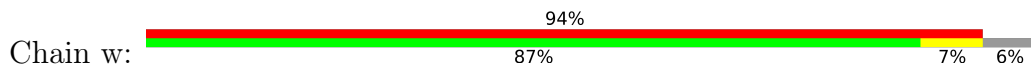


Chain v:



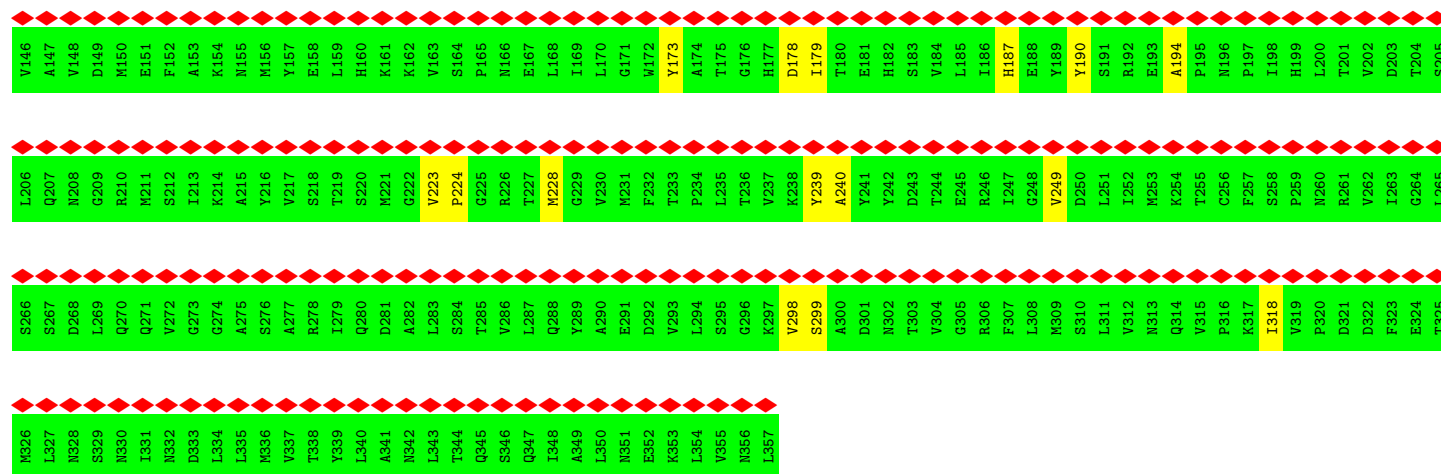


• Molecule 45: Eukaryotic translation initiation factor 3 subunit E

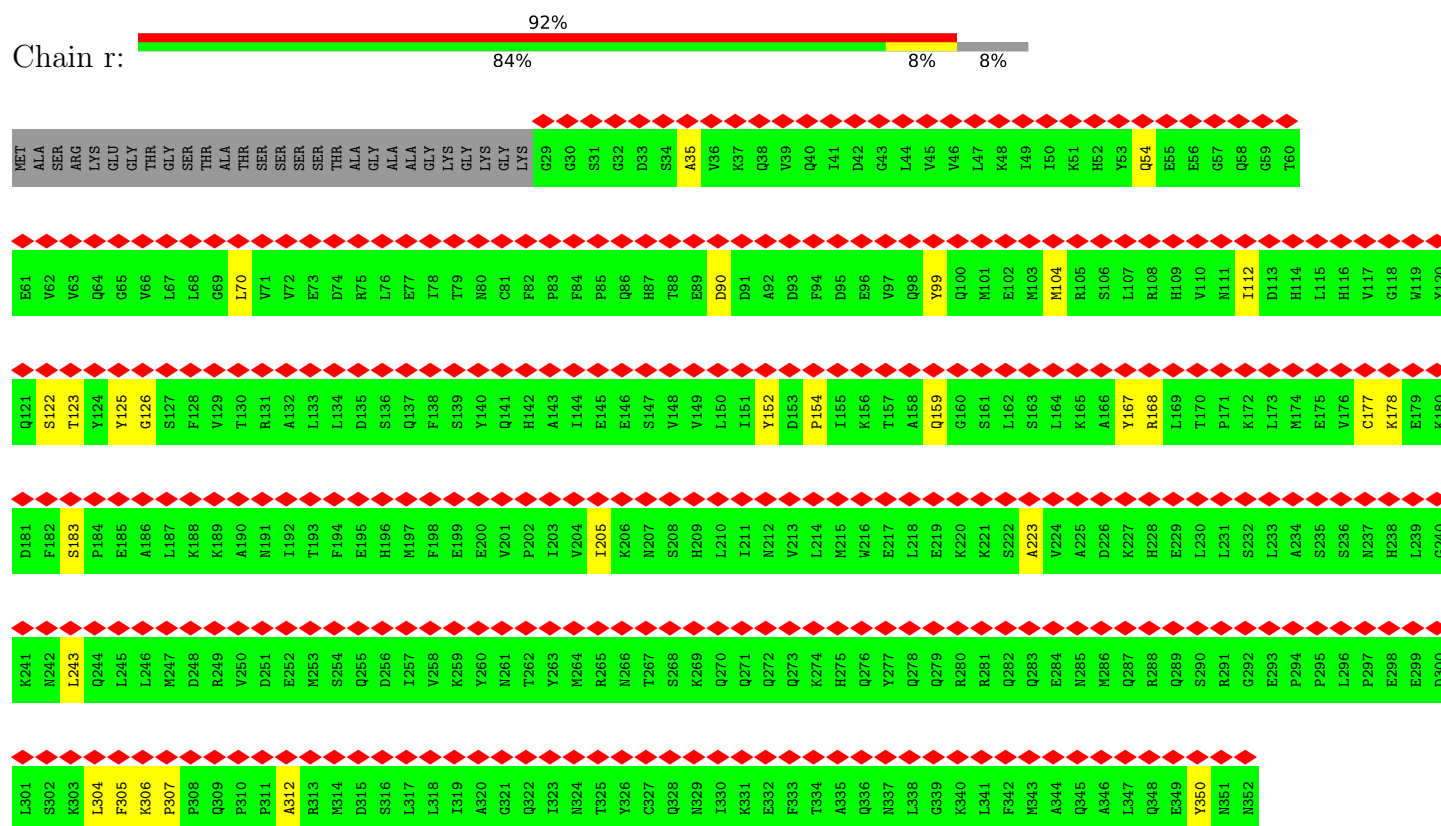


• Molecule 46: Eukaryotic translation initiation factor 3 subunit F

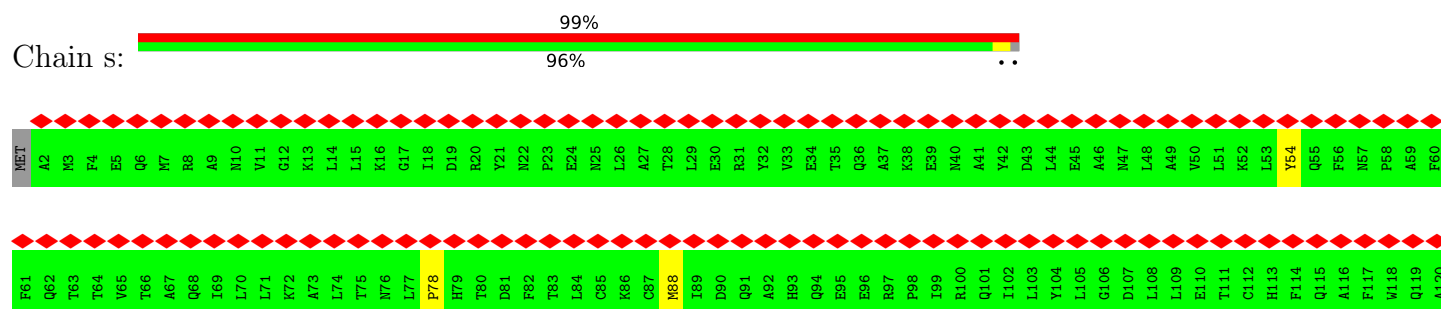


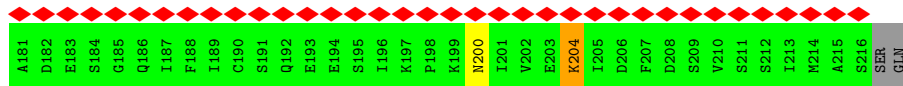


- Molecule 47: eukaryotic translation initiation factor 3 subunit h

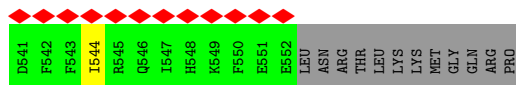
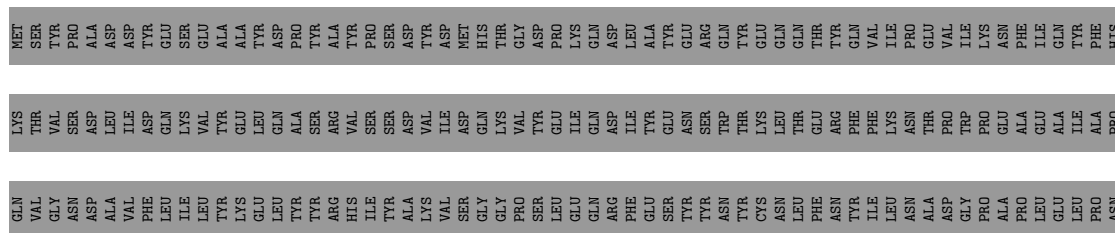


- Molecule 48: Eukaryotic translation initiation factor 3 subunit K

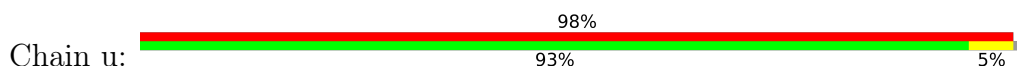




- Molecule 49: eukaryotic translation initiation factor 3 subunit 1



- Molecule 50: Eukaryotic translation initiation factor 3 subunit M





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26	Depositor
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	0.119	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, T6A, SF4, C4J, 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	1	1.99	11/1770 (0.6%)	2.43	176/2759 (6.4%)
2	l	1.36	0/241	0.93	0/305
3	C	0.97	0/1680	0.97	1/2283 (0.0%)
4	D	0.86	0/1769	0.96	2/2367 (0.1%)
5	E	0.91	0/1779	0.94	1/2399 (0.0%)
6	F	0.97	0/1793	0.98	0/2412
7	G	0.97	0/2125	0.97	0/2856
8	H	0.99	0/1531	0.93	0/2059
9	I	1.01	0/1947	0.98	4/2590 (0.2%)
10	J	0.96	0/1553	1.00	2/2079 (0.1%)
11	K	1.03	0/1709	1.00	3/2278 (0.1%)
12	L	1.07	0/1523	0.91	2/2031 (0.1%)
13	M	0.96	0/852	1.03	4/1147 (0.3%)
14	N	0.97	0/1319	0.95	0/1761
15	O	0.90	0/968	0.95	0/1296
16	P	0.94	0/1232	0.84	0/1656
17	Q	1.03	0/1029	0.98	0/1380
18	S	1.03	0/1142	0.98	0/1528
19	T	0.99	0/1031	0.93	0/1383
20	V	0.99	0/1132	0.91	0/1517
21	W	0.97	0/832	1.00	0/1117
22	X	1.05	1/627 (0.2%)	1.02	3/839 (0.4%)
23	Y	1.00	0/1051	0.96	0/1406
24	Z	0.99	0/1125	0.95	2/1500 (0.1%)
25	a	1.04	1/1038 (0.1%)	1.06	3/1380 (0.2%)
26	b	1.03	0/802	0.94	0/1076
27	c	0.85	0/673	0.89	2/902 (0.2%)
28	d	1.12	0/508	0.95	0/680
29	e	1.11	0/455	1.08	0/603
30	f	0.98	0/594	1.06	2/786 (0.3%)
31	g	0.91	0/2494	1.04	2/3394 (0.1%)
32	n	0.98	0/605	1.01	2/810 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	1.09	0/478	0.98	0/628
34	2	1.58	72/41548 (0.2%)	2.39	4296/64753 (6.6%)
35	A	0.79	1/2178 (0.0%)	1.15	11/2935 (0.4%)
36	B	0.91	2/3267 (0.1%)	1.00	4/4415 (0.1%)
37	j	0.72	1/892 (0.1%)	1.16	7/1186 (0.6%)
38	k	1.53	16/4772 (0.3%)	1.71	58/6428 (0.9%)
39	U	1.04	0/1211	0.95	0/1618
40	R	0.99	0/1177	1.00	3/1571 (0.2%)
41	3	0.54	0/1074	1.03	17/1671 (1.0%)
42	m	0.97	0/3015	0.96	4/4078 (0.1%)
43	y	0.70	1/5059 (0.0%)	0.79	13/6832 (0.2%)
44	v	0.86	2/4585 (0.0%)	1.01	12/6185 (0.2%)
45	w	0.95	0/3538	1.01	15/4786 (0.3%)
46	q	0.91	0/2149	0.97	1/2920 (0.0%)
47	r	0.91	0/2675	0.96	3/3609 (0.1%)
48	s	0.88	0/1772	0.88	4/2396 (0.2%)
49	t	0.95	0/3185	0.95	7/4296 (0.2%)
50	u	0.88	0/2963	0.97	3/3998 (0.1%)
All	All	1.23	108/124467 (0.1%)	1.68	4669/176884 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	3	2
3	C	0	1
4	D	0	1
9	I	0	3
10	J	0	2
11	K	0	2
12	L	0	2
13	M	0	5
17	Q	0	2
18	S	0	2
22	X	0	1
25	a	0	1
26	b	0	1
27	c	0	1
29	e	0	4
30	f	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
33	i	0	3
34	2	1	46
35	A	0	7
36	B	0	8
37	j	0	12
38	k	0	33
39	U	0	3
43	y	0	8
44	v	0	53
45	w	0	10
46	q	0	6
47	r	0	10
48	s	0	1
49	t	0	5
50	u	0	9
All	All	4	245

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	k	455	ILE	C-N	-38.75	0.45	1.34
38	k	562	LEU	C-N	-35.45	0.52	1.34
38	k	378	LEU	C-N	34.34	1.94	1.33
1	1	17	C	O3'-P	32.10	1.99	1.61
38	k	408	ASN	C-N	-28.67	0.68	1.34

The worst 5 of 4669 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	k	160	LEU	O-C-N	35.04	178.76	122.70
38	k	531	ARG	C-N-CA	-34.40	35.70	121.70
38	k	531	ARG	CA-C-N	-33.55	43.38	117.20
44	v	762	ASN	C-N-CA	-29.30	60.77	122.30
38	k	378	LEU	CA-C-N	-27.37	61.45	116.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	17	C	C3',C2'
1	1	18	G	C3'
34	2	1244	C4J	C4'

5 of 245 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	18	G	Sidechain
1	1	26	G	Sidechain
3	C	193	HIS	Peptide
4	D	208	HIS	Peptide
9	I	68	LEU	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	1	23/25 (92%)	23 (100%)	0	0	100	100
3	C	206/208 (99%)	177 (86%)	21 (10%)	8 (4%)	2	21
4	D	213/264 (81%)	186 (87%)	21 (10%)	6 (3%)	4	27
5	E	224/226 (99%)	208 (93%)	14 (6%)	2 (1%)	14	48
6	F	225/227 (99%)	202 (90%)	14 (6%)	9 (4%)	2	21
7	G	261/263 (99%)	233 (89%)	24 (9%)	4 (2%)	8	39
8	H	189/191 (99%)	169 (89%)	17 (9%)	3 (2%)	8	38
9	I	235/237 (99%)	209 (89%)	22 (9%)	4 (2%)	7	37
10	J	188/190 (99%)	161 (86%)	18 (10%)	9 (5%)	2	17
11	K	204/206 (99%)	178 (87%)	20 (10%)	6 (3%)	3	27
12	L	180/182 (99%)	167 (93%)	11 (6%)	2 (1%)	12	45
13	M	96/98 (98%)	74 (77%)	16 (17%)	6 (6%)	1	13
14	N	156/158 (99%)	130 (83%)	22 (14%)	4 (3%)	4	28
15	O	122/132 (92%)	105 (86%)	13 (11%)	4 (3%)	3	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	148/150 (99%)	130 (88%)	11 (7%)	7 (5%)	2	18
17	Q	134/151 (89%)	119 (89%)	12 (9%)	3 (2%)	5	32
18	S	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9	40
19	T	124/135 (92%)	112 (90%)	8 (6%)	4 (3%)	3	25
20	V	139/145 (96%)	128 (92%)	8 (6%)	3 (2%)	5	32
21	W	102/119 (86%)	93 (91%)	9 (9%)	0	100	100
22	X	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	4	29
23	Y	127/130 (98%)	117 (92%)	6 (5%)	4 (3%)	3	26
24	Z	140/142 (99%)	129 (92%)	7 (5%)	4 (3%)	3	27
25	a	124/133 (93%)	104 (84%)	10 (8%)	10 (8%)	1	8
26	b	97/115 (84%)	86 (89%)	10 (10%)	1 (1%)	13	46
27	c	82/84 (98%)	56 (68%)	16 (20%)	10 (12%)	0	4
28	d	62/69 (90%)	57 (92%)	4 (6%)	1 (2%)	8	38
29	e	51/53 (96%)	40 (78%)	7 (14%)	4 (8%)	1	9
30	f	69/71 (97%)	51 (74%)	12 (17%)	6 (9%)	0	7
31	g	311/313 (99%)	273 (88%)	33 (11%)	5 (2%)	8	38
32	n	73/75 (97%)	69 (94%)	3 (4%)	1 (1%)	9	40
33	i	57/59 (97%)	49 (86%)	7 (12%)	1 (2%)	7	35
35	A	264/266 (99%)	233 (88%)	25 (10%)	6 (2%)	5	31
36	B	420/422 (100%)	352 (84%)	48 (11%)	20 (5%)	2	17
37	j	107/144 (74%)	64 (60%)	27 (25%)	16 (15%)	0	2
38	k	577/595 (97%)	431 (75%)	95 (16%)	51 (9%)	0	7
39	U	141/152 (93%)	123 (87%)	12 (8%)	6 (4%)	2	19
40	R	138/145 (95%)	107 (78%)	18 (13%)	13 (9%)	0	6
42	m	363/548 (66%)	336 (93%)	25 (7%)	2 (1%)	22	55
43	y	601/1350 (44%)	457 (76%)	85 (14%)	59 (10%)	0	6
44	v	548/913 (60%)	446 (81%)	72 (13%)	30 (6%)	1	15
45	w	417/445 (94%)	349 (84%)	57 (14%)	11 (3%)	4	28
46	q	270/272 (99%)	226 (84%)	32 (12%)	12 (4%)	2	19
47	r	322/352 (92%)	267 (83%)	42 (13%)	13 (4%)	2	21
48	s	213/218 (98%)	201 (94%)	10 (5%)	2 (1%)	14	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	t	370/564 (66%)	328 (89%)	38 (10%)	4 (1%)	12	45
50	u	363/374 (97%)	308 (85%)	47 (13%)	8 (2%)	5	32
All	All	9695/11534 (84%)	8260 (85%)	1047 (11%)	388 (4%)	4	21

5 of 388 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	191	ARG
4	D	78	GLU
4	D	209	ASP
6	F	3	VAL
6	F	193	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	24/24 (100%)	23 (96%)	1 (4%)	25	54
3	C	174/174 (100%)	173 (99%)	1 (1%)	84	92
4	D	196/231 (85%)	192 (98%)	4 (2%)	50	72
5	E	187/187 (100%)	184 (98%)	3 (2%)	58	76
6	F	190/190 (100%)	187 (98%)	3 (2%)	58	76
7	G	225/225 (100%)	225 (100%)	0	100	100
8	H	161/161 (100%)	159 (99%)	2 (1%)	67	82
9	I	207/207 (100%)	206 (100%)	1 (0%)	86	93
10	J	170/170 (100%)	170 (100%)	0	100	100
11	K	177/177 (100%)	176 (99%)	1 (1%)	84	92
12	L	157/157 (100%)	155 (99%)	2 (1%)	65	81
13	M	89/89 (100%)	89 (100%)	0	100	100
14	N	142/142 (100%)	136 (96%)	6 (4%)	25	54
15	O	104/108 (96%)	100 (96%)	4 (4%)	28	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	130/130 (100%)	126 (97%)	4 (3%)	35	62
17	Q	106/119 (89%)	105 (99%)	1 (1%)	75	87
18	S	117/117 (100%)	115 (98%)	2 (2%)	56	75
19	T	114/121 (94%)	114 (100%)	0	100	100
20	V	113/116 (97%)	113 (100%)	0	100	100
21	W	94/107 (88%)	93 (99%)	1 (1%)	70	83
22	X	67/67 (100%)	67 (100%)	0	100	100
23	Y	112/113 (99%)	112 (100%)	0	100	100
24	Z	114/114 (100%)	113 (99%)	1 (1%)	75	87
25	a	108/115 (94%)	101 (94%)	7 (6%)	14	42
26	b	87/99 (88%)	86 (99%)	1 (1%)	70	83
27	c	76/76 (100%)	73 (96%)	3 (4%)	27	57
28	d	57/62 (92%)	57 (100%)	0	100	100
29	e	47/47 (100%)	45 (96%)	2 (4%)	25	54
30	f	64/64 (100%)	63 (98%)	1 (2%)	58	76
31	g	272/272 (100%)	271 (100%)	1 (0%)	89	95
32	n	66/66 (100%)	65 (98%)	1 (2%)	60	78
33	i	49/49 (100%)	47 (96%)	2 (4%)	26	55
35	A	238/238 (100%)	231 (97%)	7 (3%)	37	63
36	B	354/354 (100%)	328 (93%)	26 (7%)	11	38
37	j	92/123 (75%)	69 (75%)	23 (25%)	0	3
38	k	523/523 (100%)	466 (89%)	57 (11%)	5	25
39	U	125/132 (95%)	120 (96%)	5 (4%)	27	56
40	R	126/130 (97%)	119 (94%)	7 (6%)	17	47
42	m	329/494 (67%)	327 (99%)	2 (1%)	84	92
43	y	554/1233 (45%)	467 (84%)	87 (16%)	2	14
44	v	501/812 (62%)	489 (98%)	12 (2%)	44	67
45	w	384/406 (95%)	380 (99%)	4 (1%)	73	85
46	q	239/239 (100%)	237 (99%)	2 (1%)	79	88
47	r	293/310 (94%)	290 (99%)	3 (1%)	73	85
48	s	190/193 (98%)	190 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	t	342/515 (66%)	341 (100%)	1 (0%)	91	96
50	u	327/335 (98%)	327 (100%)	0	100	100
All	All	8613/10133 (85%)	8322 (97%)	291 (3%)	34	60

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	y	237	LEU
46	q	249	VAL
43	y	265	LYS
43	y	347	ILE
37	j	52	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
44	v	701	HIS
45	w	348	HIS
49	t	495	HIS
42	m	377	HIS
42	m	296	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	74/75 (98%)	13 (17%)	3 (4%)
34	2	1735/1863 (93%)	248 (14%)	8 (0%)
41	3	44/45 (97%)	29 (65%)	2 (4%)
All	All	1853/1983 (93%)	290 (15%)	13 (0%)

5 of 290 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	9	U
1	1	11	G
1	1	15	A
1	1	16	G
1	1	17	C

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	2	1112	C
34	2	1270	G
41	3	39	U
34	2	1857	A
41	3	36	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
34	C4J	2	1244	34	24,29,30	0.78	1 (4%)	29,42,45	1.03	1 (3%)
1	T6A	1	37	1	27,34,35	1.05	2 (7%)	29,49,52	2.65	9 (31%)

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
34	C4J	2	1244	34	1/1/7/7	9/16/34/35	0/2/2/2
1	T6A	1	37	1	-	6/19/41/42	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	37	T6A	C5-C4	2.54	1.47	1.40
1	1	37	T6A	O4'-C1'	2.20	1.44	1.41
34	2	1244	C4J	C1'-C5	-2.10	1.45	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	37	T6A	C12-N11-C10	8.53	136.15	121.94
1	1	37	T6A	C2-N1-C6	7.05	122.64	116.59
1	1	37	T6A	C14-C12-C13	3.72	116.53	110.19
1	1	37	T6A	N3-C2-N1	-3.61	123.04	128.68
34	2	1244	C4J	C4-N3-C2	-3.45	121.10	125.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	2	1244	C4J	C4'

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	37	T6A	C14-C12-N11-C10
34	2	1244	C4J	C31-C3-N3-C2
34	2	1244	C4J	C31-C3-N3-C4
34	2	1244	C4J	N3-C3-C31-C32
34	2	1244	C4J	C3-C31-C32-C34

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
53	GNP	k	705	-	29,34,34	1.77	6 (20%)	33,54,54	2.16	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	SF4	k	701	38	0,12,12	-	-	-		
53	GNP	k	704	52	29,34,34	1.76	6 (20%)	33,54,54	2.15	6 (18%)
51	SF4	k	702	38	0,12,12	-	-	-		

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
53	GNP	k	705	-	-	5/14/38/38	0/3/3/3
51	SF4	k	701	38	-	-	0/6/5/5
53	GNP	k	704	52	-	6/14/38/38	0/3/3/3
51	SF4	k	702	38	-	-	0/6/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	k	705	GNP	PG-O2G	-4.55	1.44	1.56
53	k	704	GNP	PG-O2G	-4.54	1.44	1.56
53	k	704	GNP	C6-N1	4.07	1.40	1.33
53	k	705	GNP	PB-O2B	-4.01	1.45	1.56
53	k	705	GNP	C6-N1	3.84	1.39	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	k	704	GNP	C5-C6-N1	-7.91	112.62	123.43
53	k	705	GNP	C5-C6-N1	-7.87	112.67	123.43
53	k	705	GNP	C2-N1-C6	6.08	125.59	115.93
53	k	704	GNP	C2-N1-C6	6.02	125.49	115.93
53	k	705	GNP	N3-C2-N1	-3.76	122.21	127.22

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	k	704	GNP	PG-N3B-PB-O1B
53	k	704	GNP	PG-N3B-PB-O3A
53	k	704	GNP	PA-O3A-PB-O1B
53	k	704	GNP	PA-O3A-PB-O2B

Continued on next page...

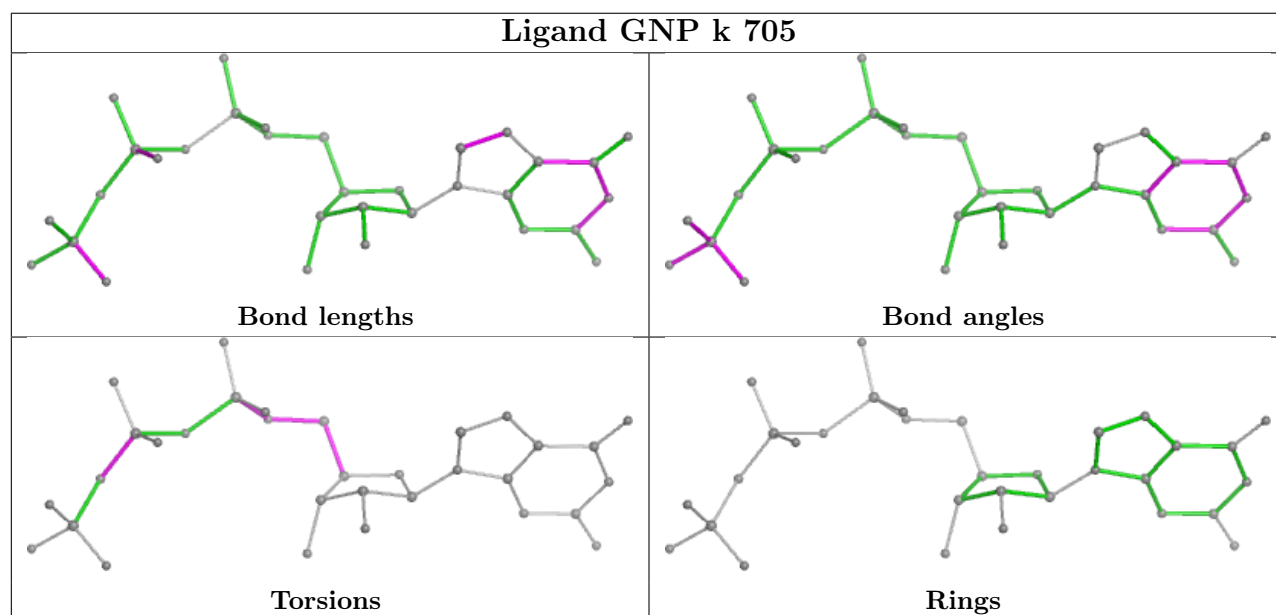
Continued from previous page...

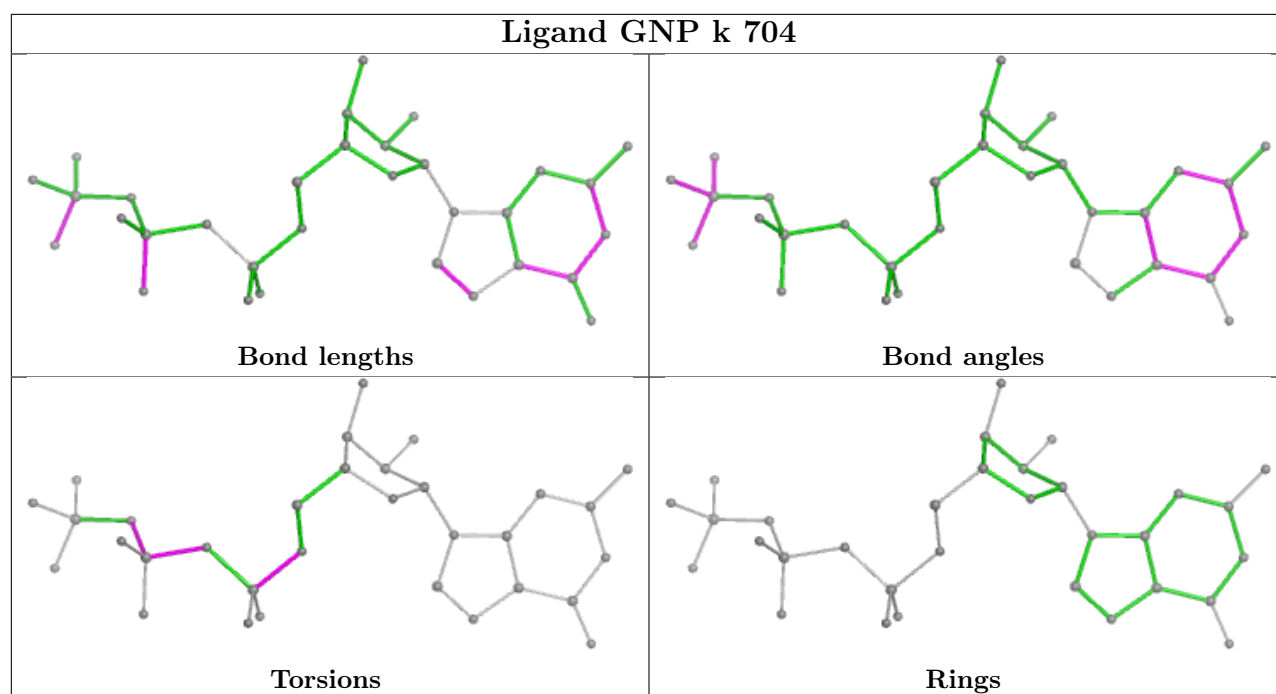
Mol	Chain	Res	Type	Atoms
53	k	705	GNP	PG-N3B-PB-O1B

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	k	23
34	2	4
44	v	4
1	1	2
39	U	1
25	a	1
37	j	1

The worst 5 of 36 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	730:C	O3'	731:C	P	8.58
1	k	521:ASP	C	522:PHE	N	2.98
1	U	142:ARG	C	143:GLY	N	2.92
1	k	451:ILE	C	452:GLU	N	2.79
1	k	373:GLU	C	374:ILE	N	2.70

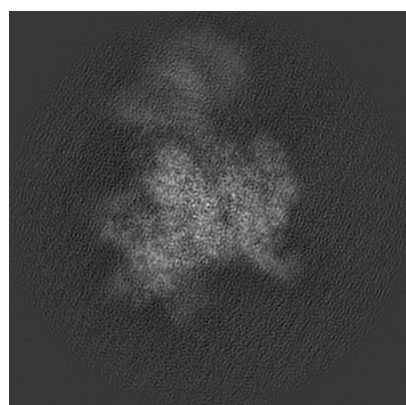
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10761. These allow visual inspection of the internal detail of the map and identification of artifacts.

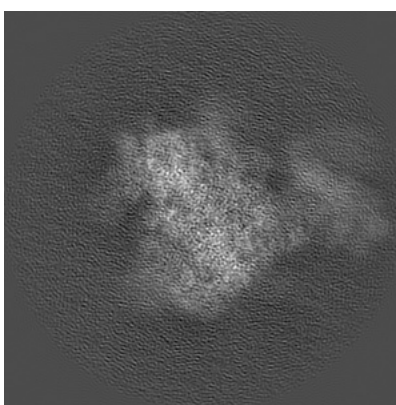
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

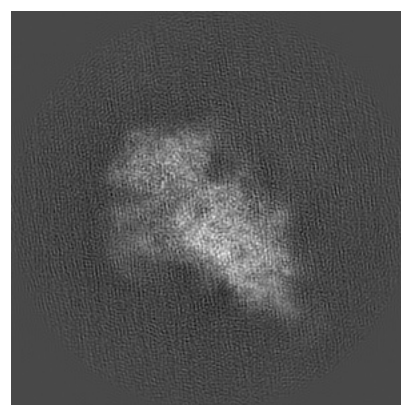
6.1.1 Primary map



X



Y

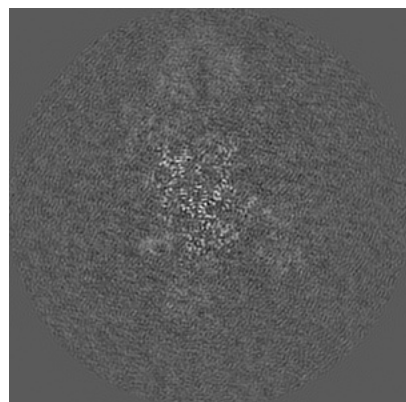


Z

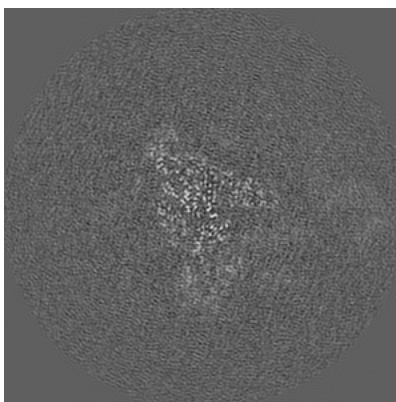
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

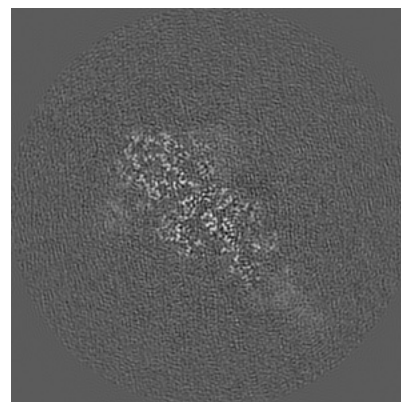
6.2.1 Primary map



X Index: 192



Y Index: 192

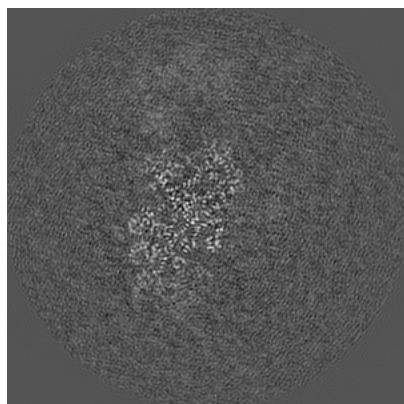


Z Index: 192

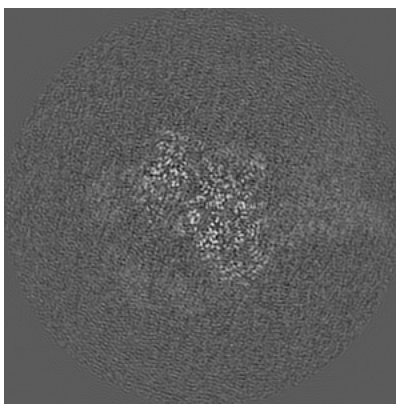
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

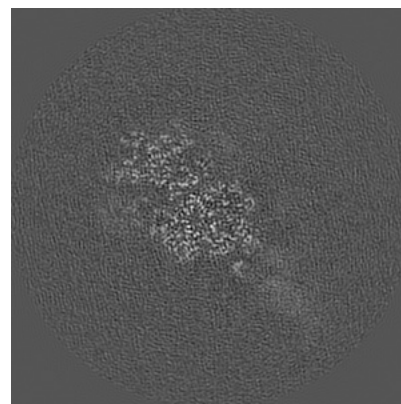
6.3.1 Primary map



X Index: 210



Y Index: 165

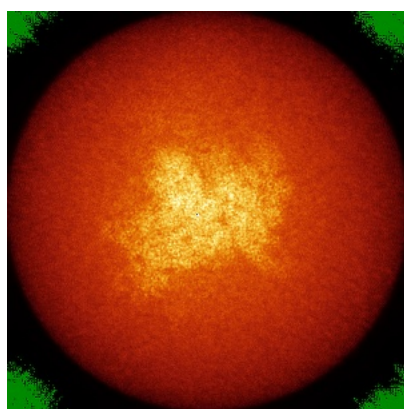


Z Index: 199

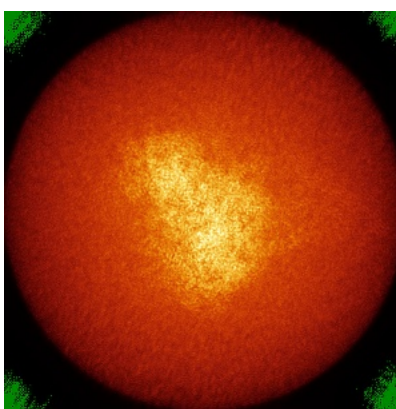
The images above show the largest variance slices of the map in three orthogonal directions.

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

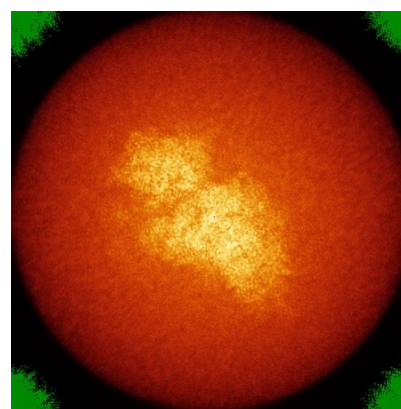
6.4.1 Primary map



X



Y

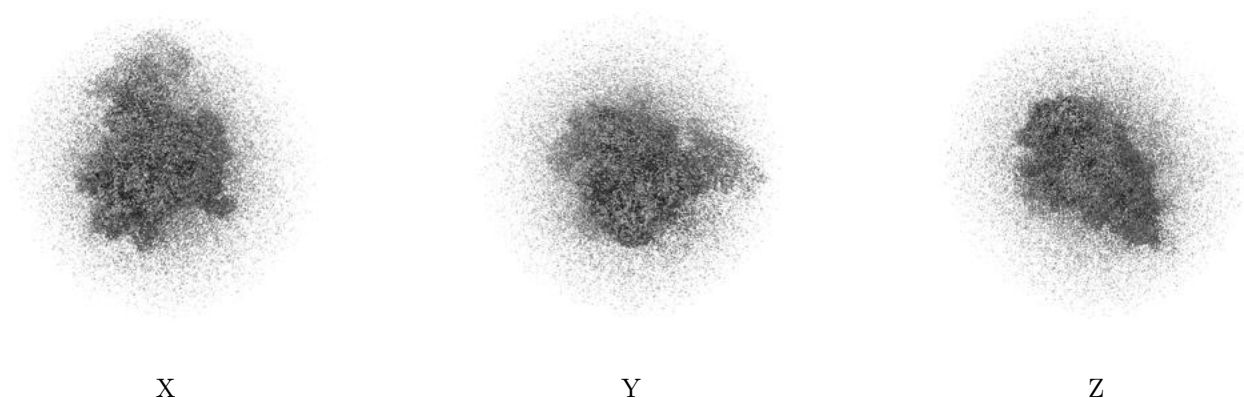


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

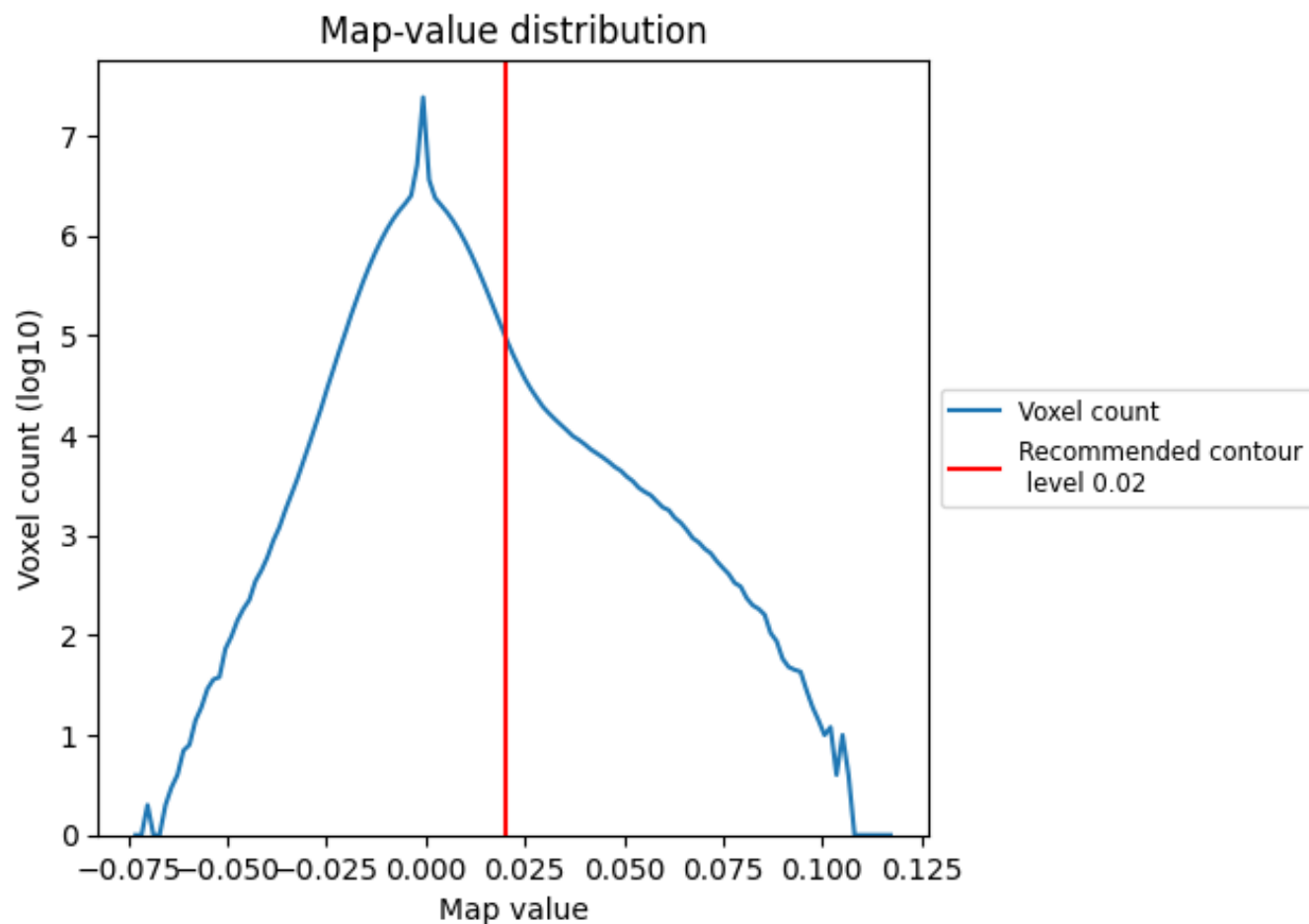
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

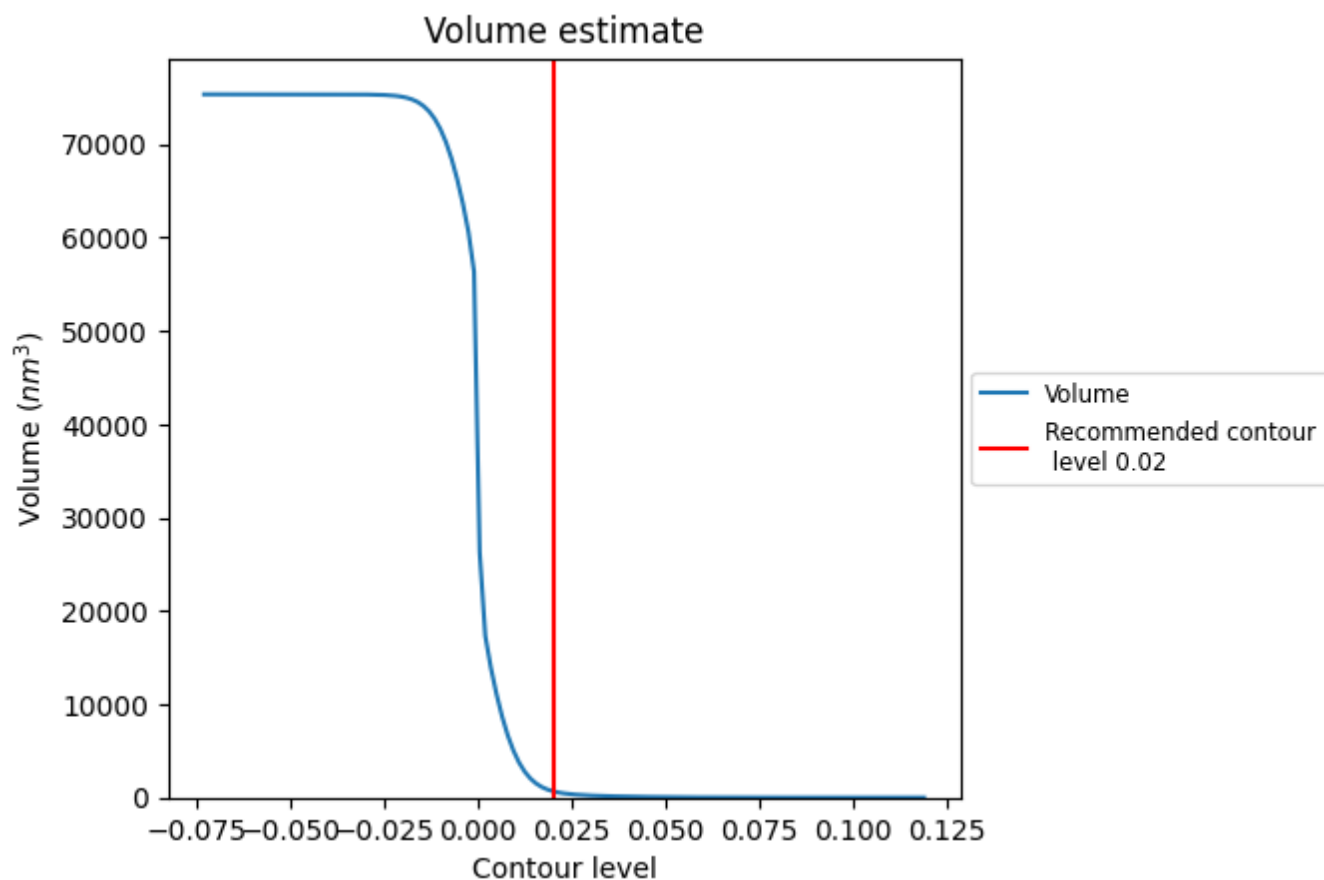
This section contains the results of statistical analysis of the map.

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.

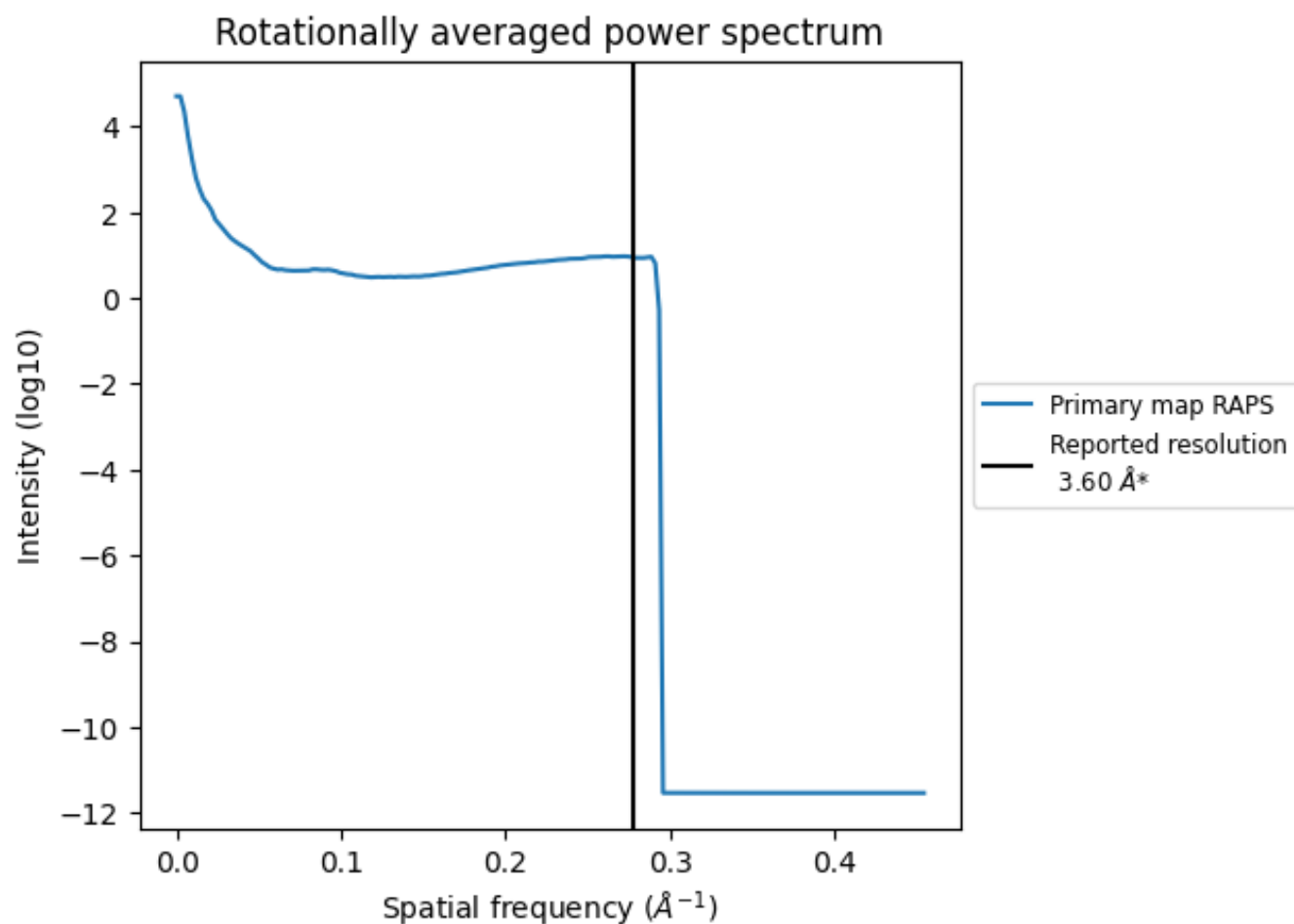
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 665 nm³; this corresponds to an approximate mass of 600 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

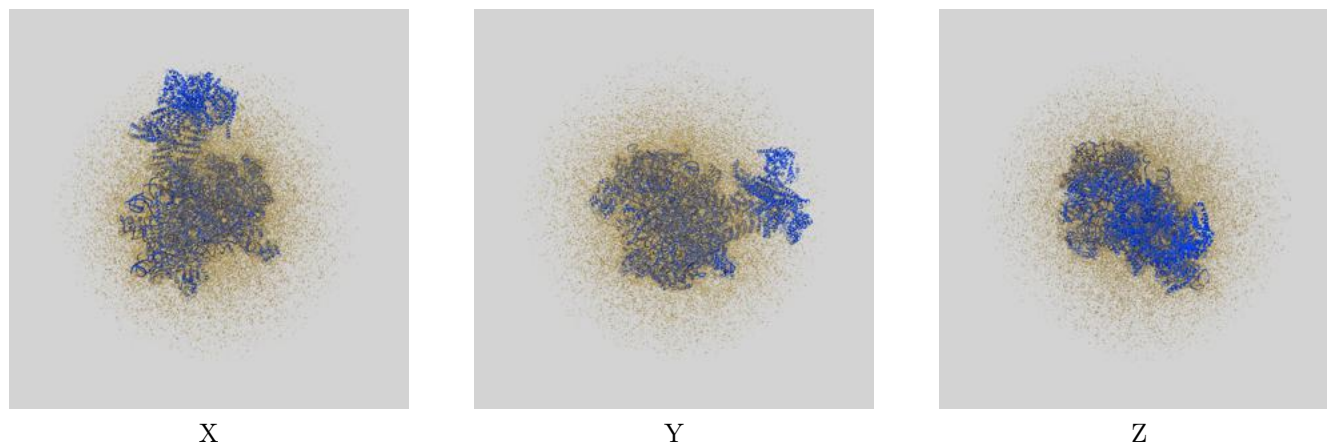
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

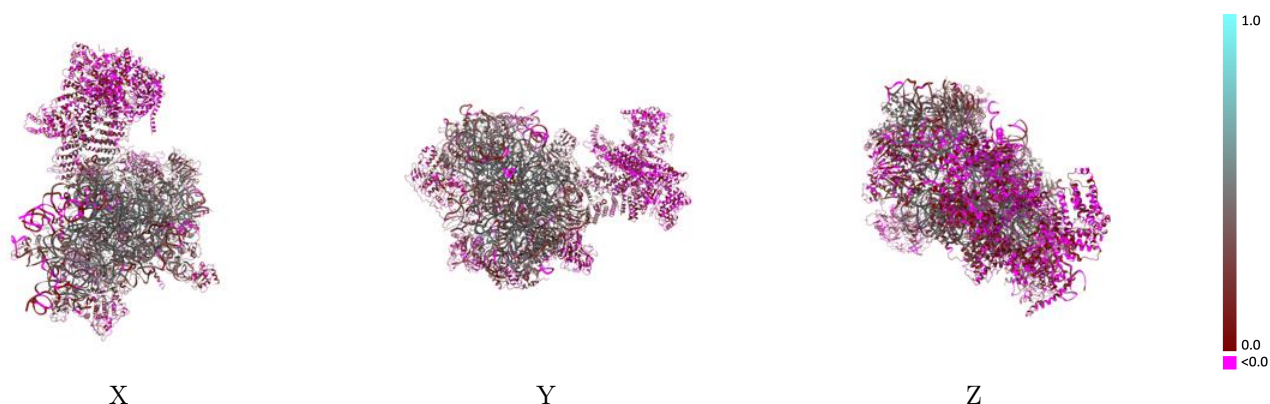
This section contains information regarding the fit between EMDB map EMD-10761 and PDB model 6YAM. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



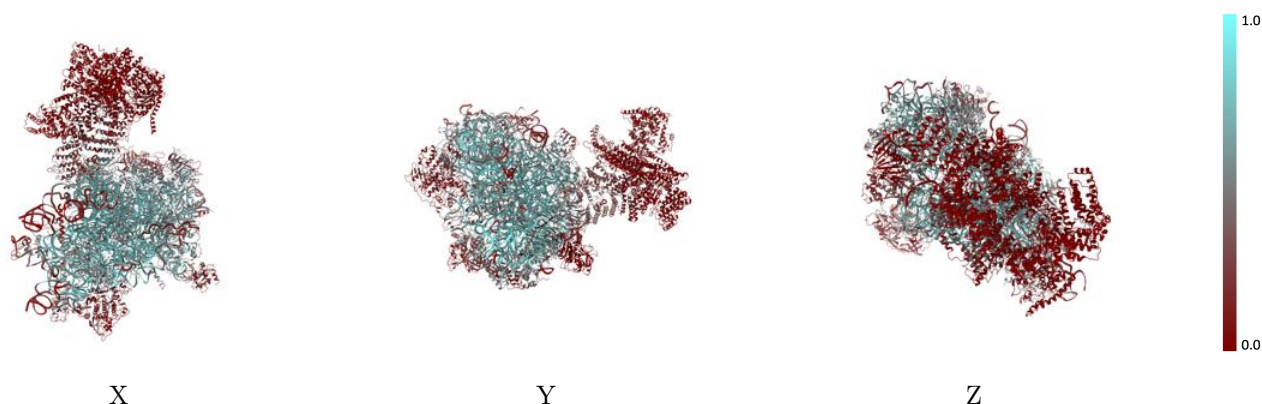
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



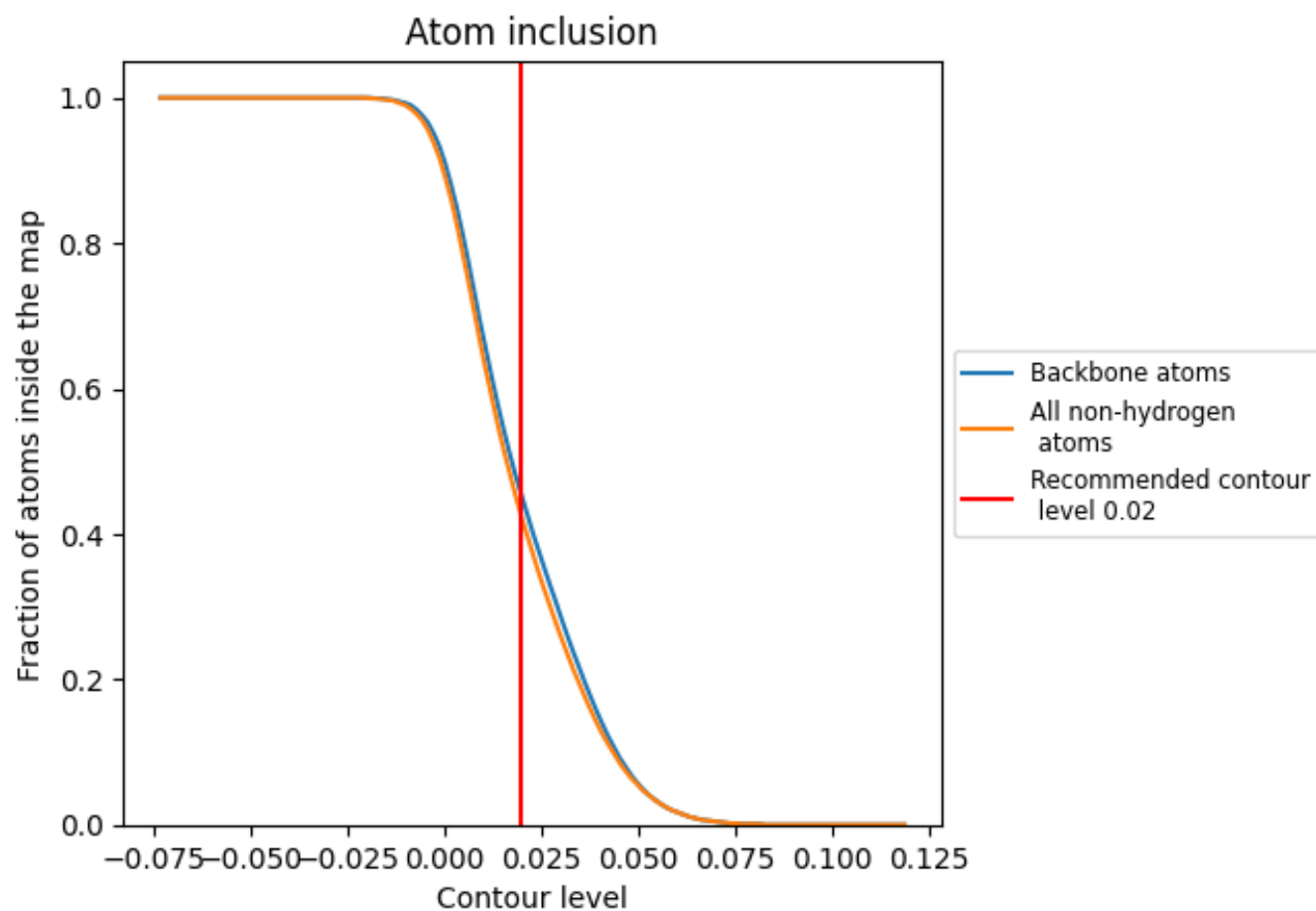
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 42% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4230	 0.2570
1	 0.3490	 0.1490
2	 0.6960	 0.3870
3	 0.1620	 0.0600
A	 0.1180	 0.1080
B	 0.0240	 0.0050
C	 0.6030	 0.3790
D	 0.5460	 0.3610
E	 0.6360	 0.4040
F	 0.5000	 0.3230
G	 0.6070	 0.3860
H	 0.5760	 0.3590
I	 0.4210	 0.2830
J	 0.3600	 0.2360
K	 0.5100	 0.3180
L	 0.6150	 0.3760
M	 0.4890	 0.2770
N	 0.5550	 0.3550
O	 0.1390	 0.0940
P	 0.5750	 0.3590
Q	 0.5710	 0.3550
R	 0.4470	 0.2960
S	 0.6060	 0.3790
T	 0.4870	 0.2970
U	 0.5170	 0.3340
V	 0.5880	 0.3760
W	 0.4870	 0.3130
X	 0.5810	 0.3810
Y	 0.6950	 0.4320
Z	 0.6580	 0.4060
a	 0.5160	 0.3190
b	 0.6540	 0.4120
c	 0.4990	 0.3270
d	 0.5230	 0.3360
e	 0.5150	 0.2410



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.1920	 0.1410
g	 0.4210	 0.2840
i	 0.4080	 0.2680
j	 0.2650	 0.2090
k	 0.1380	 0.1510
l	 0.5110	 0.3240
m	 0.0210	 0.0430
n	 0.4280	 0.2780
q	 0.0160	 0.0020
r	 0.0150	 -0.0050
s	 0.0010	 0.0140
t	 0.0030	 0.0140
u	 0.0090	 0.0180
v	 0.1510	 0.1240
w	 0.0330	 0.0340
y	 0.1500	 0.1290