



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 04:36 pm GMT

PDB ID : 6GSN
EMDB ID : EMD-0058
Title : Structure of a partial yeast 48S preinitiation complex in closed conformation
Authors : Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on : 2018-06-14
Resolution : 5.75 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

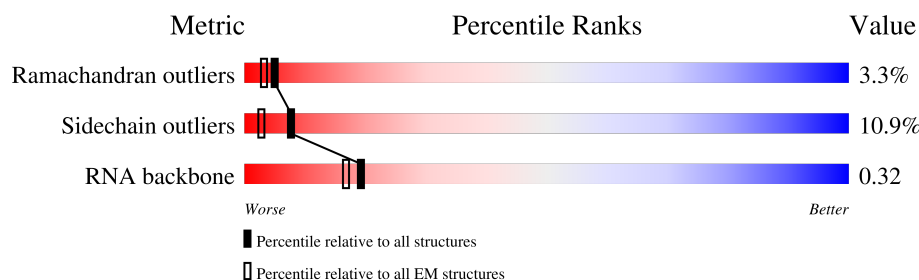
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.75 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.









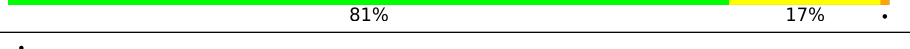
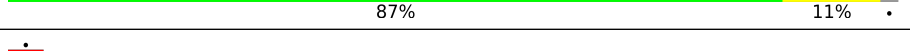
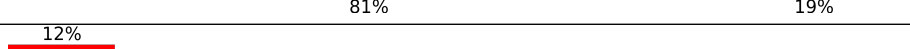
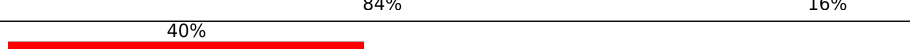
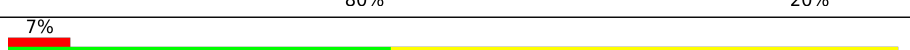

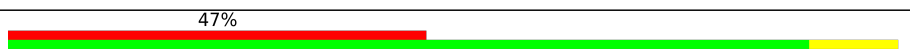







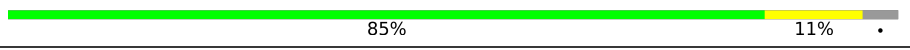
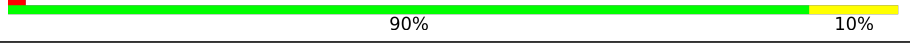
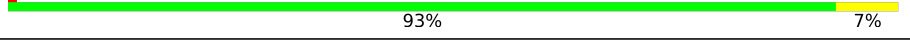


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	2	1798	
2	C	217	
3	D	223	
4	F	206	
5	K	96	
6	M	118	
7	P	117	
8	Q	141	

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Mol	Chain	Length	Quality of chain
9	R	130	
10	S	145	
11	T	143	
12	U	106	
13	Z	70	
14	c	62	
15	f	69	
16	g	324	
17	d	53	
18	e	58	
19	h	25	
20	3	14	
21	i	111	
22	m	90	
23	o	567	
24	q	699	
25	k	430	
26	l	144	
27	j	263	
28	1	75	
29	A	219	
30	B	231	
31	E	260	
32	G	226	
33	H	184	

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Mol	Chain	Length	Quality of chain
34	I	200	 82%10%6%
35	J	182	 82%18%
36	L	155	 8%81%18%
37	N	150	 87%12%
38	O	127	 86%13%
39	V	87	 89%8%
40	W	129	 90%9%
41	Y	134	 91%9%
42	X	144	 5%84%15%
43	a	98	 91%9%
44	b	81	 89%11%
45	p	666	 36%92%6%
46	s	342	 95%96%98%
47	r	49	 100%

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 103798 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 18S rRNA (1798-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1798	Total	C	N	O	P	0	0
			38175	17061	6721	12595	1798		

- Molecule 2 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 3 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 4 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 5 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 6 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	117	Total	C	N	O	0	0
			885	553	161	171		

- Molecule 7 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	117	Total	C	N	O	S	0	0
			927	595	166	161	5		

- Molecule 8 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	141	Total	C	N	O		0	0
			1105	709	204	192			

- Molecule 9 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	130	Total	C	N	O	S	0	0
			1027	640	191	193	3		

- Molecule 10 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 11 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	143	Total	C	N	O		0	0
			1110	693	210	207			

- Molecule 12 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 13 is a protein called KLLA0B06182p.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	70	Total	C	N	O	S	0	0
			558	355	104	98	1		

- Molecule 14 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	62	Total	C	N	O	S	0	0
			487	301	97	88	1		

- Molecule 15 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	69	Total	C	N	O	S	0	0
			546	351	101	90	4		

- Molecule 16 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 17 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 18 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	58	Total	C	N	O	S	0	0
			463	290	94	78	1		

- Molecule 19 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 20 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3	14	Total	C	N	O	P	0	0
			287	129	42	102	14		

- Molecule 21 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	i	111	Total	C	N	O	S	0	0
			884	542	170	167	5		

- Molecule 22 is a protein called Eukaryotic translation initiation factor eIF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	m	90	Total	C	N	O	S	0	0
			716	452	132	128	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	20	ALA	THR	conflict	UNP P32911
m	23	ALA	SER	conflict	UNP P32911

- Molecule 23 is a protein called Eukaryotic translation initiation factor 3 subunit A, eIF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	521	Total	C	N	O	S	0	0
			3996	2554	685	750	7		

- Molecule 24 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	q	675	Total	C	N	O	S	0	0
			5179	3309	874	984	12		

- Molecule 25 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	k	414	Total	C	N	O	S	0	0
			3123	1985	560	562	16		

- Molecule 26 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	l	126	Total	C	N	O	S	0	0
			1016	646	183	180	7		

- Molecule 27 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 28 is a RNA chain called tRNAi (75-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	75	Total	C	N	O	P	0	0
			1607	716	296	520	75		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	31	U	G	conflict	GB 176433
1	39	A	C	conflict	GB 176433

- Molecule 29 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A	219	Total	C	N	O	S	0	0
			1702	1085	299	316	2		

- Molecule 30 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B	222	Total	C	N	O	S	0	0
			1769	1117	324	325	3		

- Molecule 31 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 32 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 33 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	H	184	Total	C	N	O		
			1483	950	270	263	0	0

- Molecule 34 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	I	188	Total	C	N	O	S		
			1489	923	300	265	1	0	0

- Molecule 35 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	J	182	Total	C	N	O	S		
			1471	929	287	254	1	0	0

- Molecule 36 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L	155	Total	C	N	O	S		
			1248	798	237	210	3	0	0

- Molecule 37 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	150	Total	C	N	O	S		
			1187	756	223	206	2	0	0

- Molecule 38 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	127	Total	C	N	O	S		
			942	578	188	173	3	0	0

- Molecule 39 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	V	87	Total	C	N	O	S		
			687	424	126	135	2	0	0

- Molecule 40 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 41 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Y	134	Total	C	N	O	S	0	0
			1061	665	207	189			

- Molecule 42 is a protein called RPS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 43 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	a	98	Total	C	N	O	S	0	0
			779	480	165	129	5		

- Molecule 44 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	658	Total	C	N	O	S	0	0
			5147	3295	889	945	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	330	Total	C	N	O	S	0	0
			2606	1661	429	507	9		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	r	49	Total	C	N	O	0	0
			392	240	76	76		

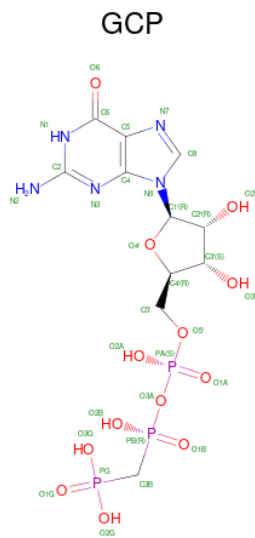
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	76	Total	Mg	0
			76	76	
48	C	1	Total	Mg	0
			1	1	
48	h	1	Total	Mg	0
			1	1	
48	k	1	Total	Mg	0
			1	1	
48	B	1	Total	Mg	0
			1	1	
48	a	1	Total	Mg	0
			1	1	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

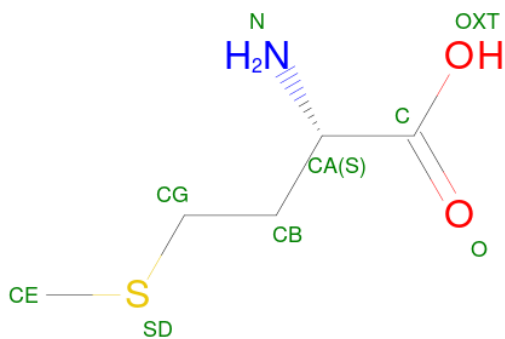
Mol	Chain	Residues	Atoms		AltConf
49	f	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	
49	a	1	Total	Zn	0
			1	1	
49	b	1	Total	Zn	0
			1	1	

- Molecule 50 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
50	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 51 is METHIONINE (three-letter code: MET) (formula: $\text{C}_5\text{H}_{11}\text{NO}_2\text{S}$).

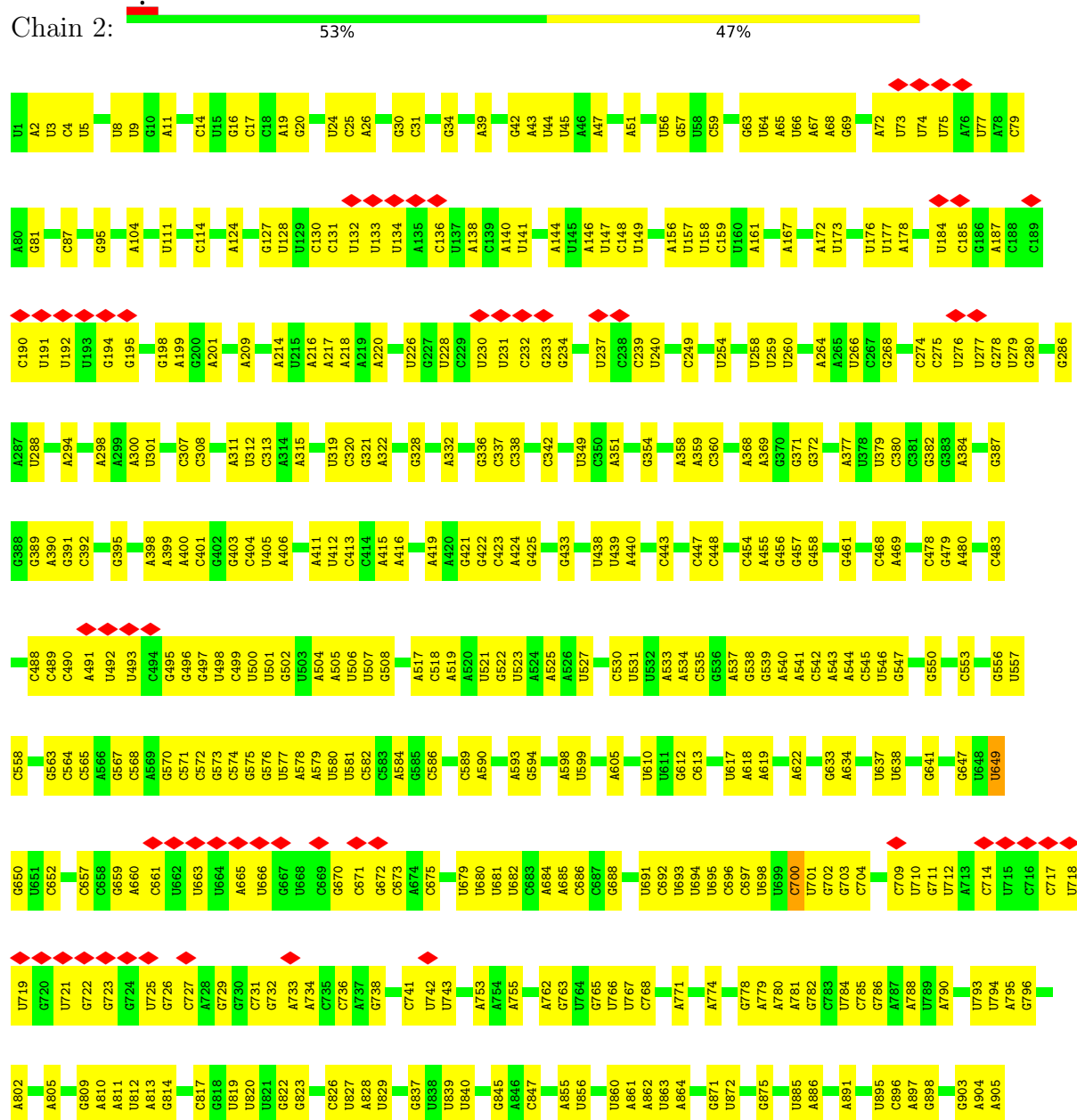


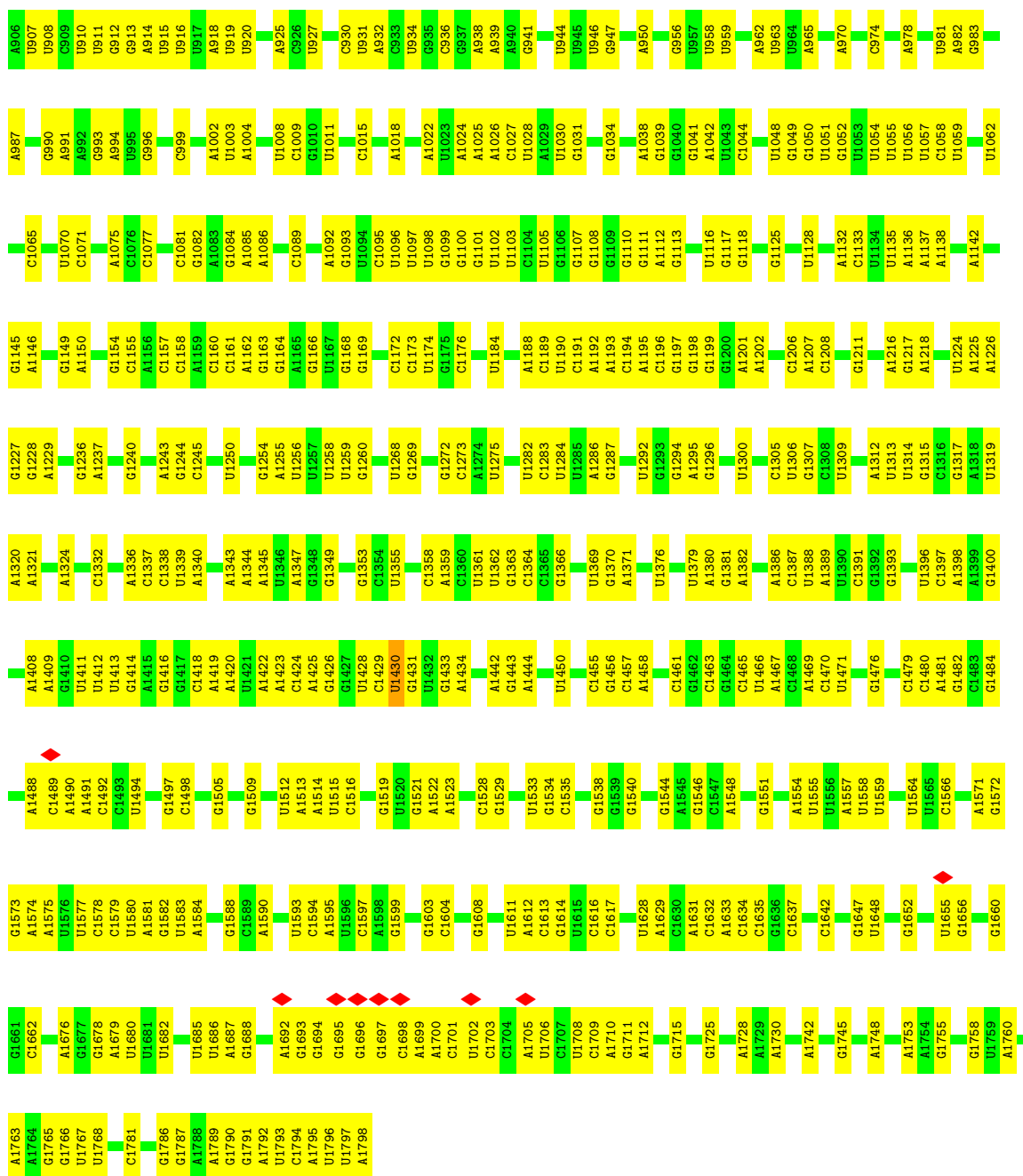
Mol	Chain	Residues	Atoms					AltConf
51	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

3 Residue-property plots

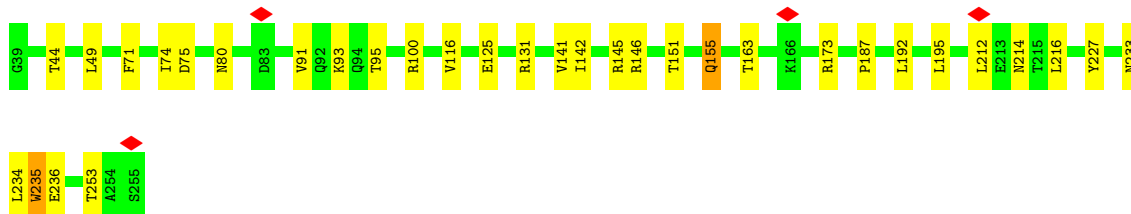
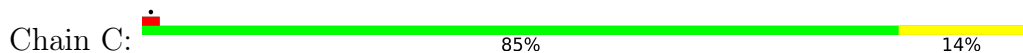
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 18S rRNA (1798-MER)




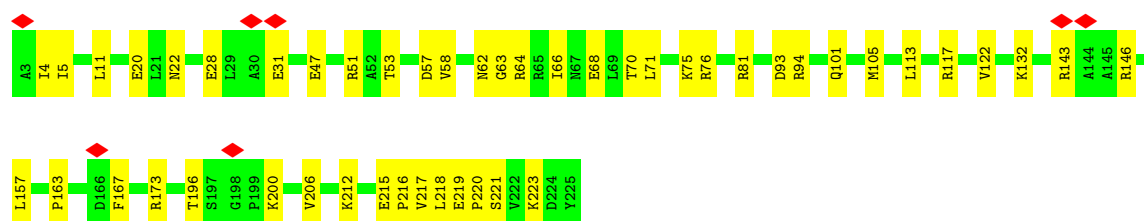


• Molecule 2: KLLA0F09812p

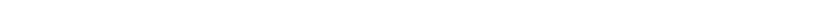


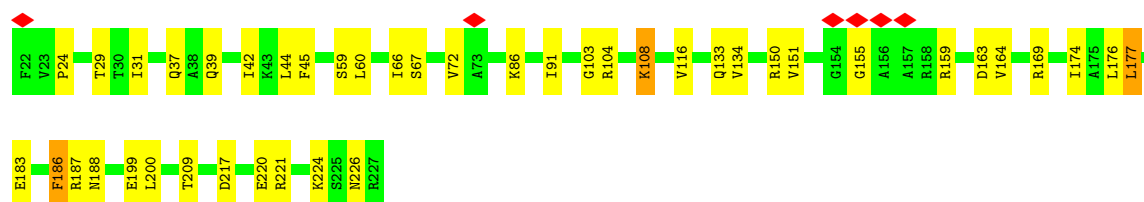
• Molecule 3: KLLA0D08305p

Chain D:  78% 22%

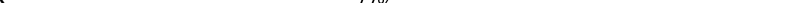


- Molecule 4: KLLA0D10659p

Chain F:  79% 19%




- Molecule 5: KLLA0B08173p

Chain K:  77% 23%




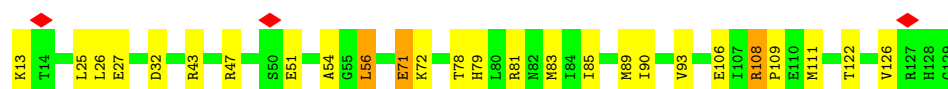
- Molecule 6: 40S ribosomal protein S12

Chain M:  12% 80% 19%

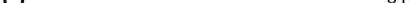


- Molecule 7: KLLA0F07843p

Chain P: 




- Molecule 8: 40S ribosomal protein S16

Chain Q:  81% 19%




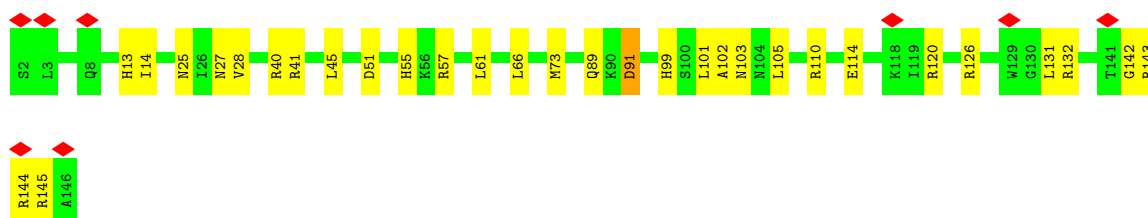
- Molecule 9: KLLA0B01474p

Chain R:  82% 17%




- Molecule 10: KLLA0B01562p

Chain S:  6% 79% 21%




- Molecule 11: KLLA0A07194p

Chain T:  82% 18%




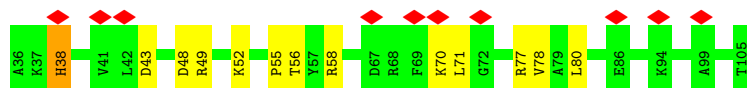
- Molecule 12: KLLA0F25542p

Chain U:  6% 85% 13%




- Molecule 13: KLLA0B06182p

Chain Z:  14% 81% 17%

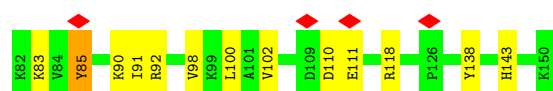
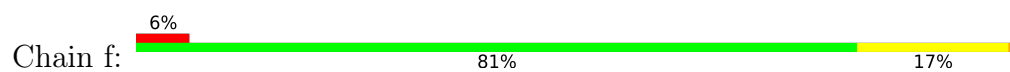


- Molecule 14: 40S ribosomal protein S28

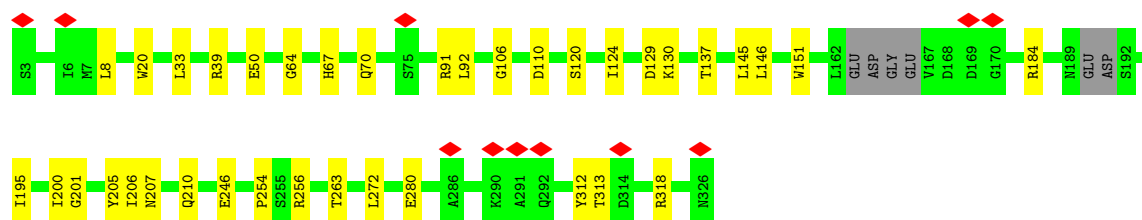
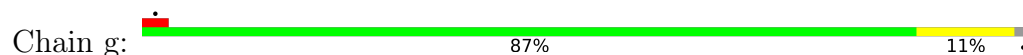
Chain c:  87% 13%



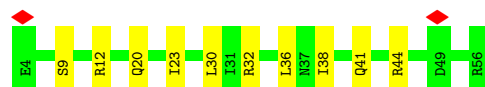
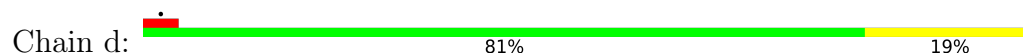
- Molecule 15: Ubiquitin-40S ribosomal protein S27a



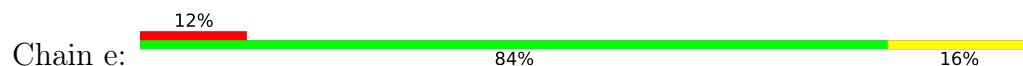
- Molecule 16: KLLA0E12277p



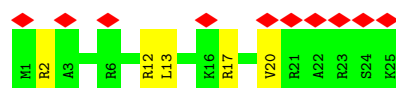
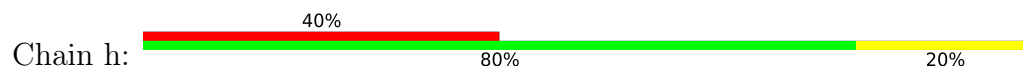
- Molecule 17: 40S ribosomal protein S29



- Molecule 18: 40S ribosomal protein S30



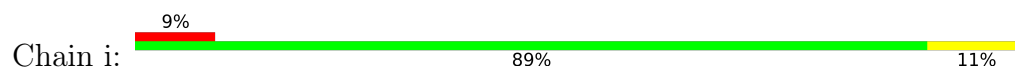
- Molecule 19: 60S ribosomal protein L41-A



- Molecule 20: mRNA

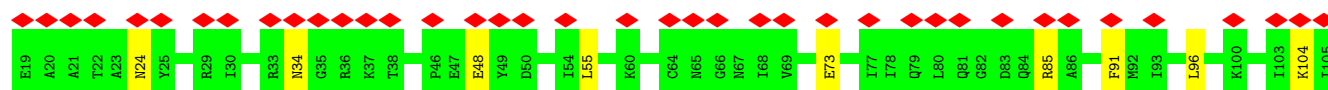
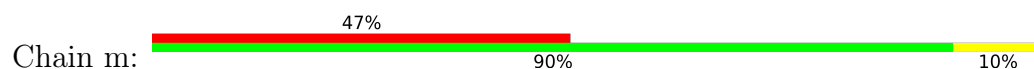


- Molecule 21: Eukaryotic translation initiation factor 1A

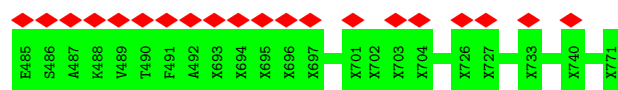
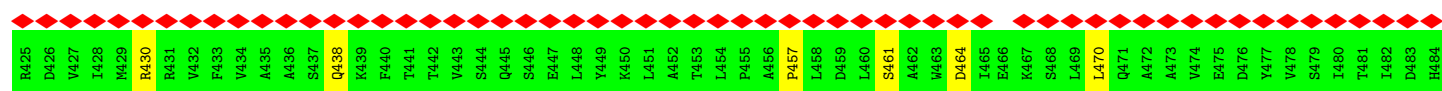
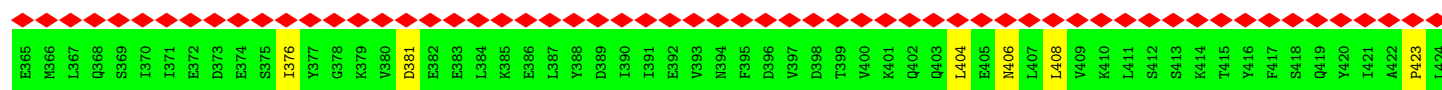
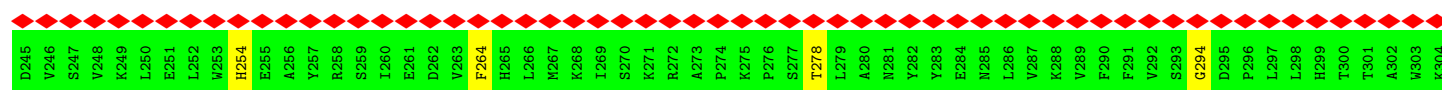
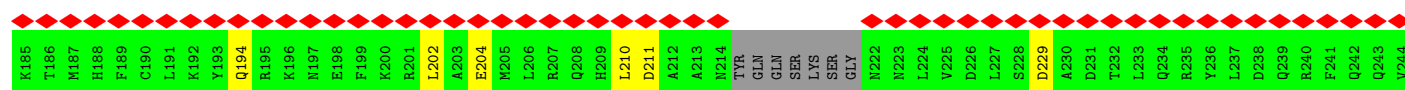
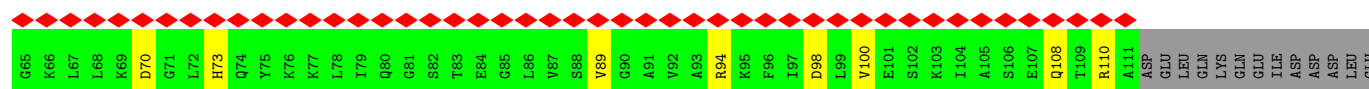
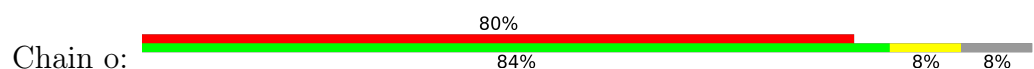




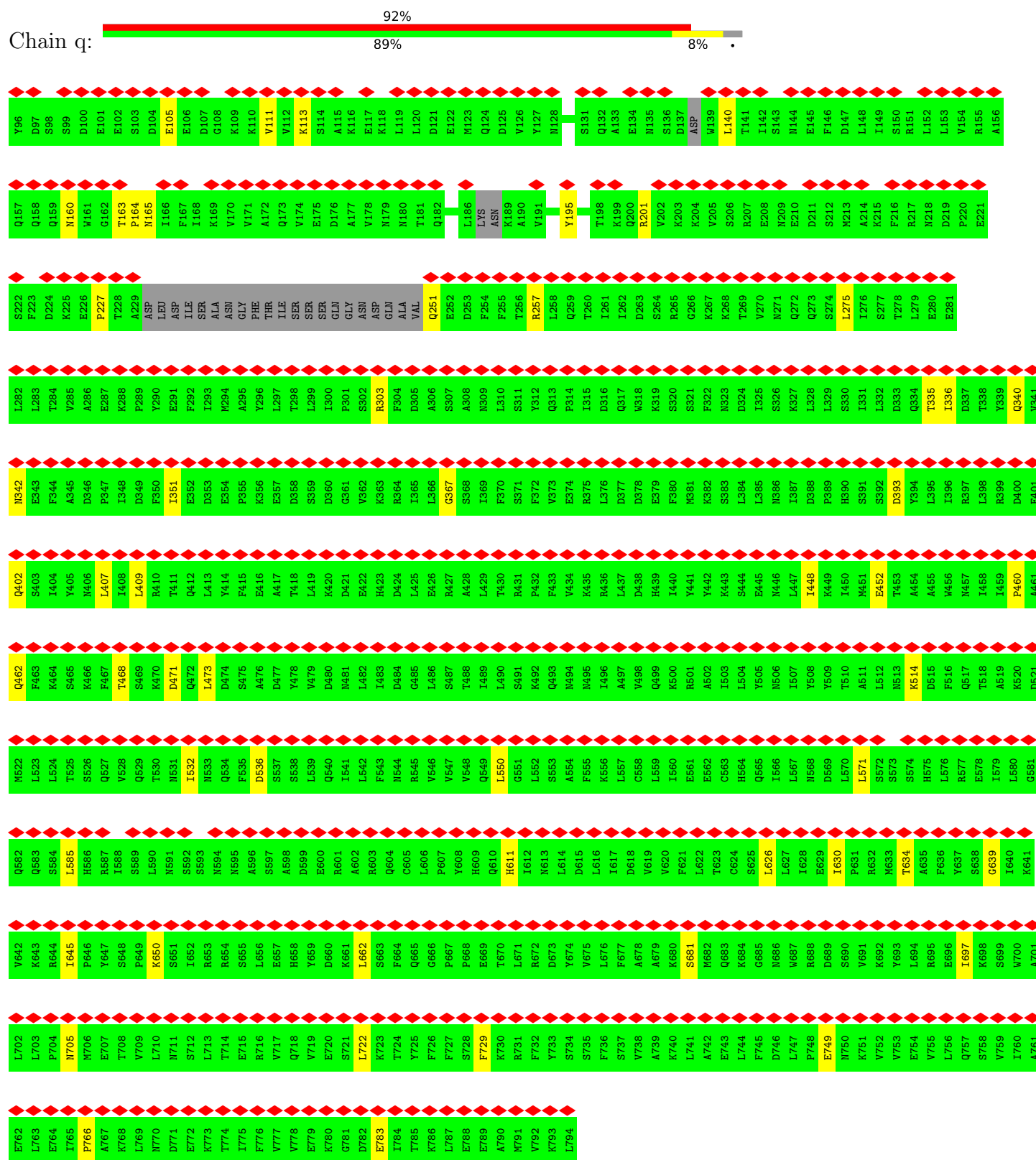
- Molecule 22: Eukaryotic translation initiation factor eIF-1



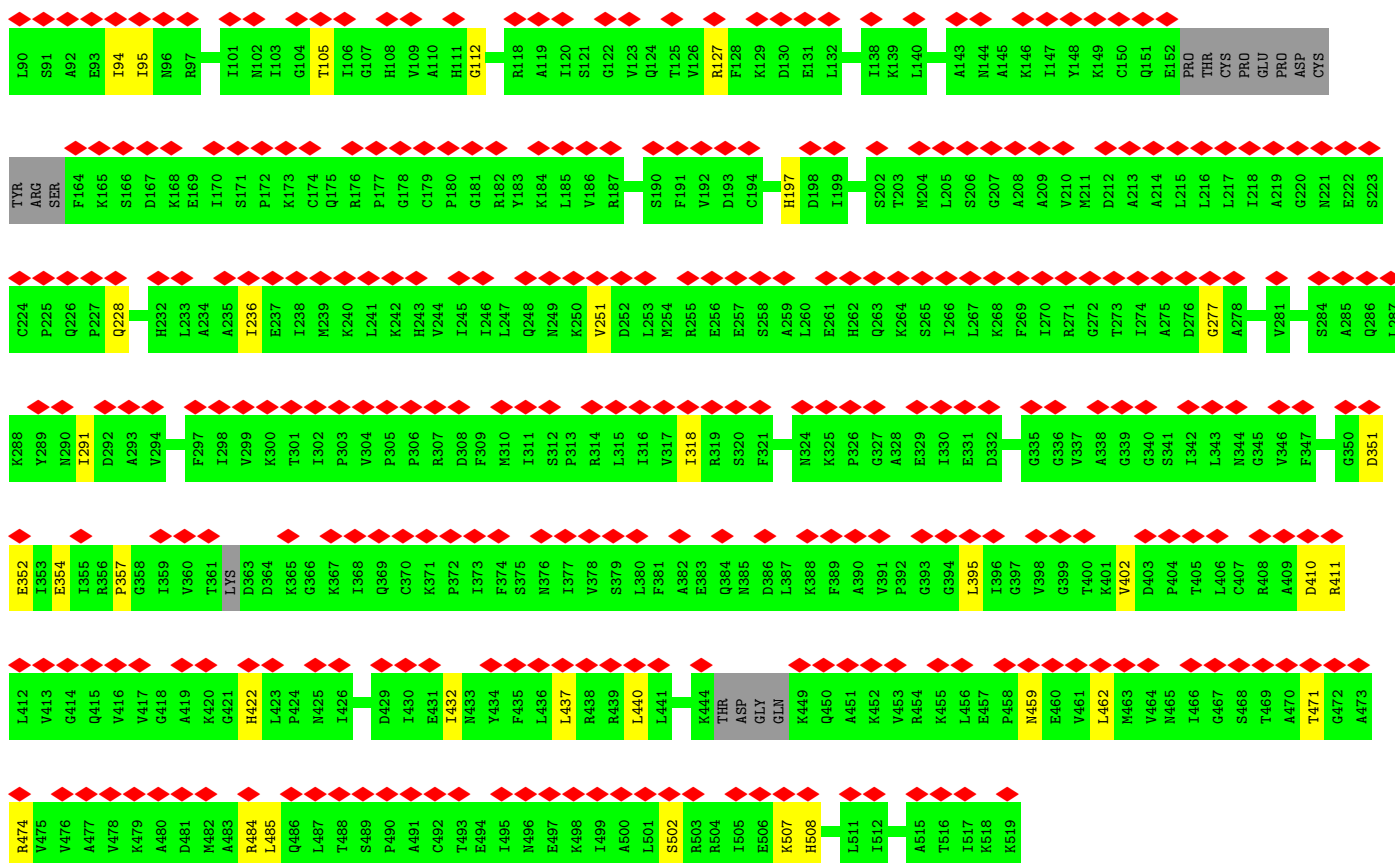
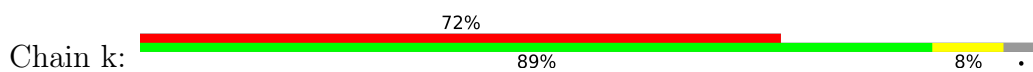
- Molecule 23: Eukaryotic translation initiation factor 3 subunit A, eIF3a



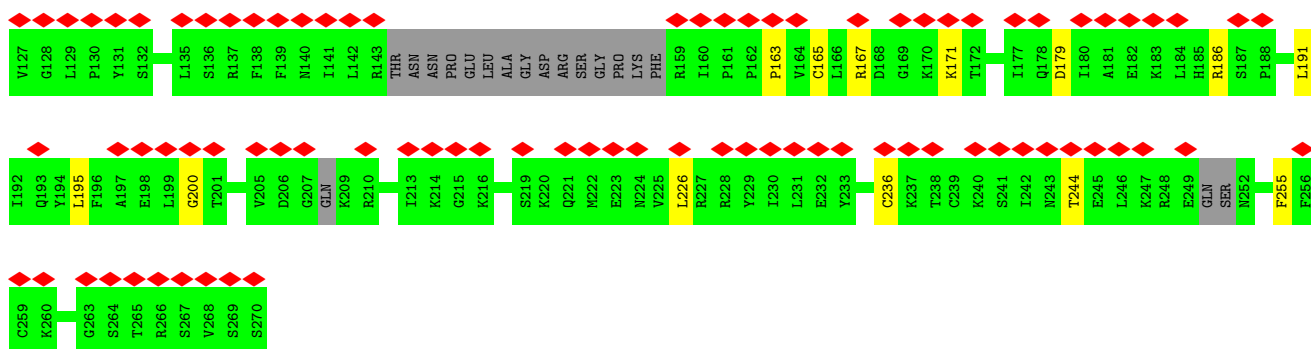
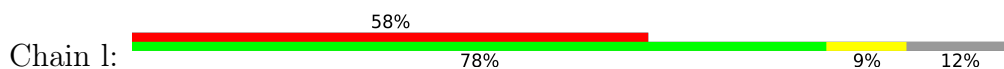
• Molecule 24: Eukaryotic translation initiation factor 3 subunit C



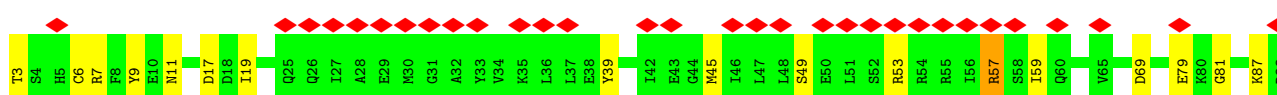
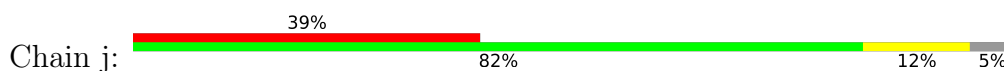
• Molecule 25: Eukaryotic translation initiation factor 2 subunit gamma

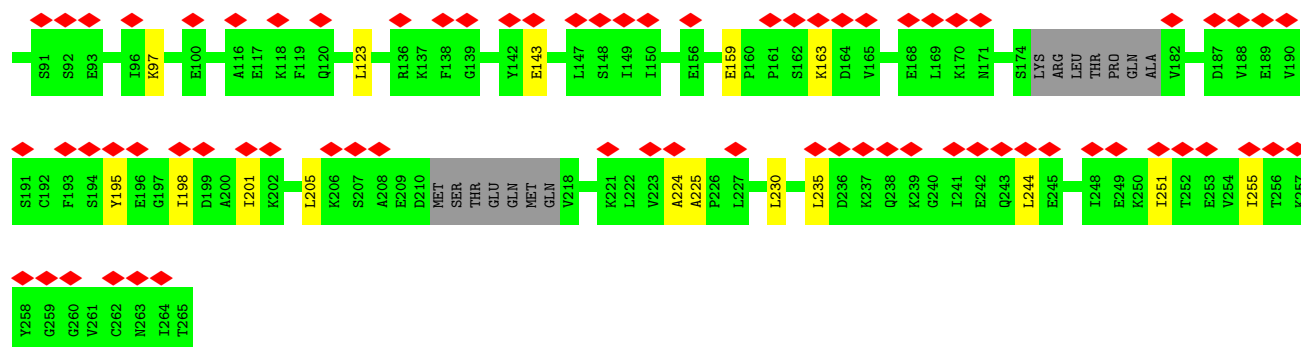


• Molecule 26: Eukaryotic translation initiation factor 2 subunit beta



• Molecule 27: Eukaryotic translation initiation factor 2 subunit alpha

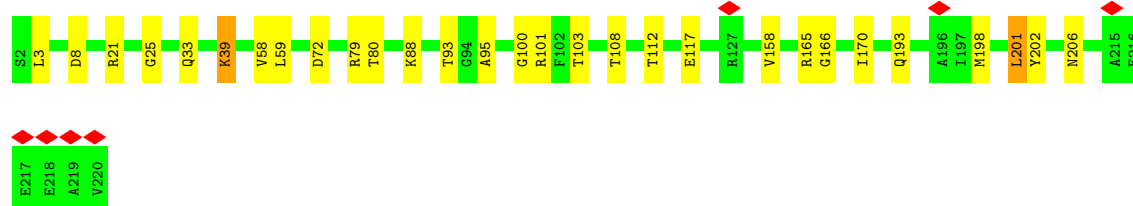




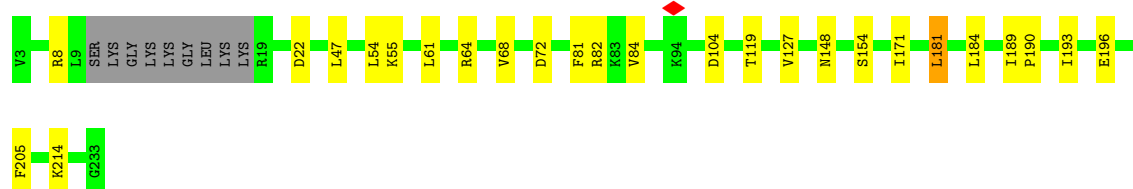
• Molecule 28: tRNAi (75-MER)



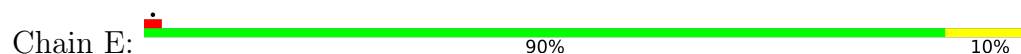
• Molecule 29: 40S ribosomal protein S0



• Molecule 30: 40S ribosomal protein S1

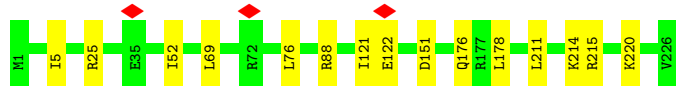


• Molecule 31: 40S ribosomal protein S4

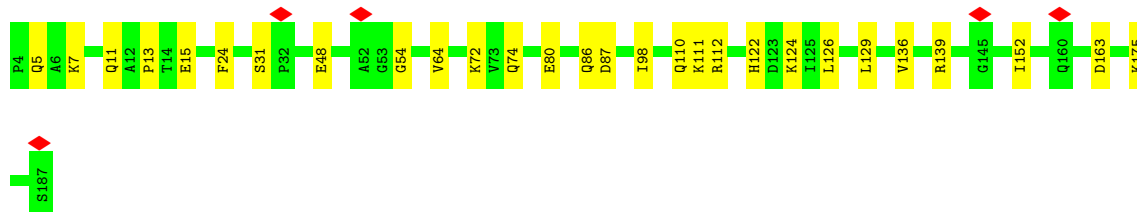
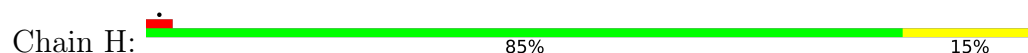




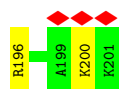
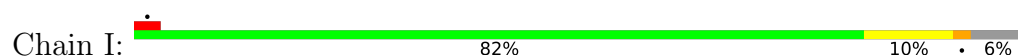
- Molecule 32: 40S ribosomal protein S6



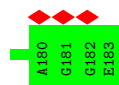
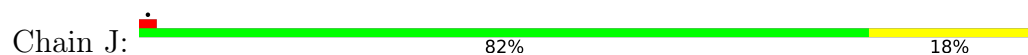
- Molecule 33: 40S ribosomal protein S7



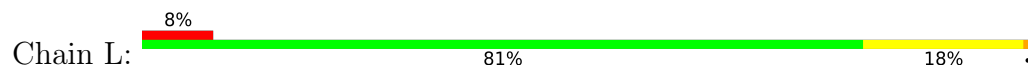
- Molecule 34: 40S ribosomal protein S8



- Molecule 35: KLLA0E23673p

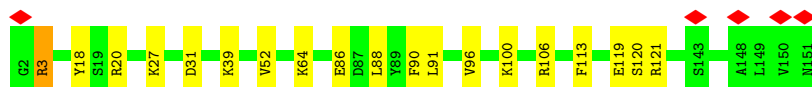
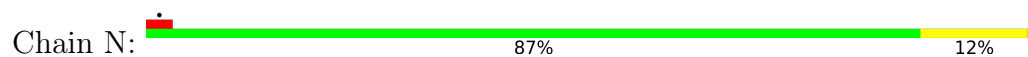


- Molecule 36: KLLA0A10483p

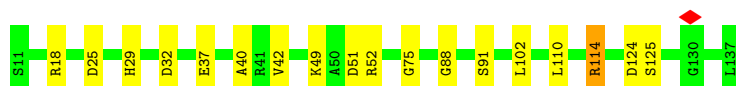
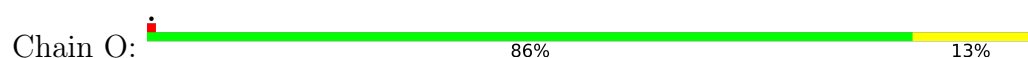




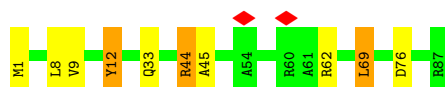
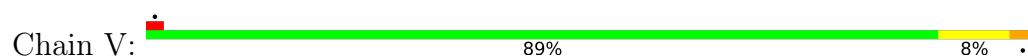
- Molecule 37: KLLA0F18040p



- Molecule 38: 40S ribosomal protein S14



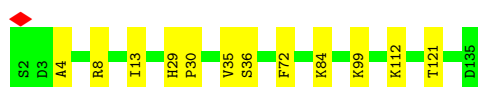
- Molecule 39: 40S ribosomal protein S21



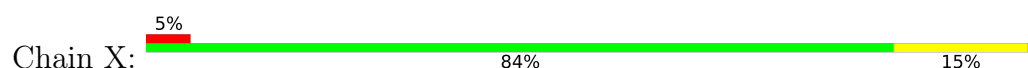
- Molecule 40: 40S ribosomal protein S22

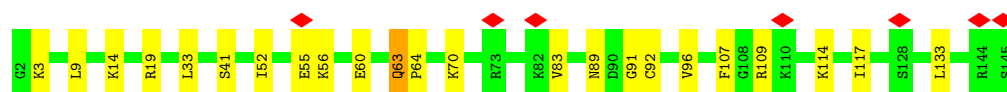


- Molecule 41: 40S ribosomal protein S24

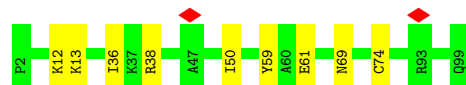
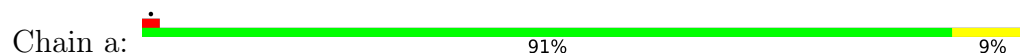


- Molecule 42: RPS23





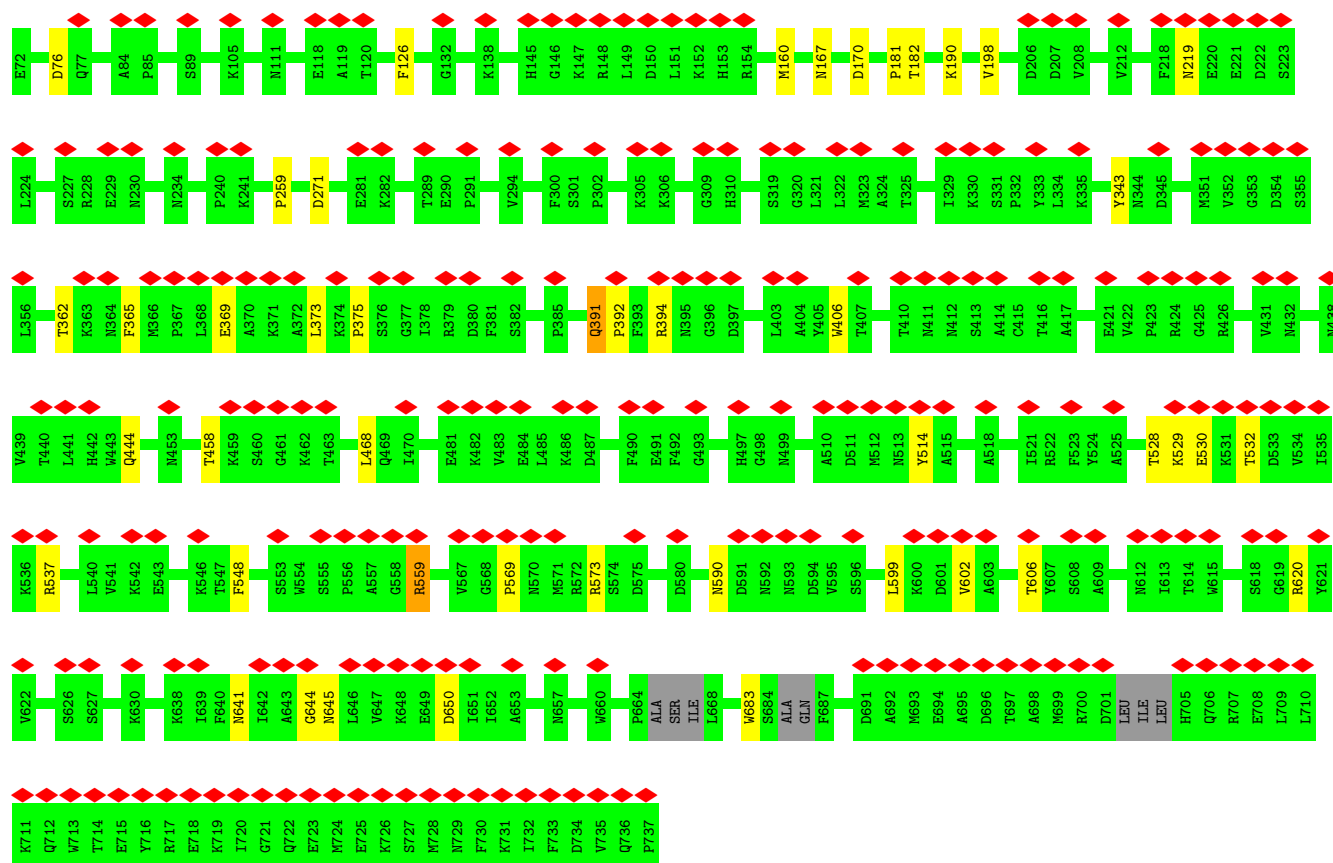
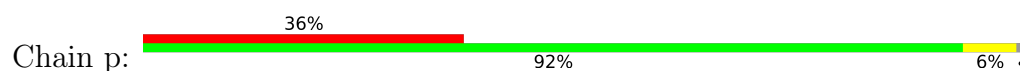
- Molecule 43: 40S ribosomal protein S26



- Molecule 44: 40S ribosomal protein S27

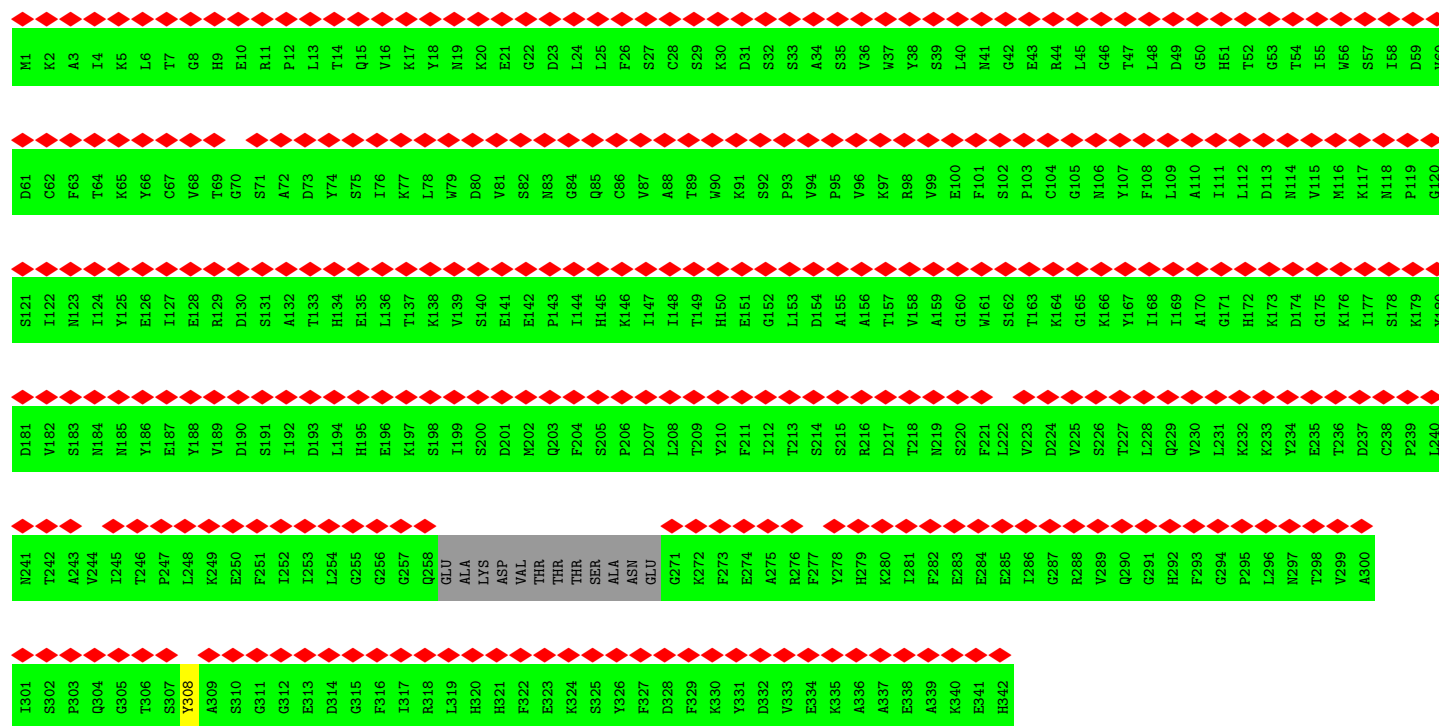


- Molecule 45: Eukaryotic translation initiation factor 3 subunit B



- Molecule 46: Eukaryotic translation initiation factor 3 subunit I

Chain s:  95% 96% .



- Molecule 47: Eukaryotic translation initiation factor 3 subunit G

Chain r: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12586	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.275	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, ZN, 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	2	0.23	0/42691	0.65	3/66521 (0.0%)
2	C	0.40	0/1659	0.68	0/2252
3	D	0.41	0/1769	0.71	0/2378
4	F	0.40	0/1628	0.74	1/2198 (0.0%)
5	K	0.45	0/831	0.70	0/1123
6	M	0.44	0/891	0.75	0/1201
7	P	0.43	0/946	0.72	1/1273 (0.1%)
8	Q	0.43	0/1125	0.72	0/1510
9	R	0.42	0/1038	0.80	1/1395 (0.1%)
10	S	0.41	0/1212	0.76	0/1629
11	T	0.39	0/1129	0.71	0/1520
12	U	0.39	0/857	0.68	0/1158
13	Z	0.41	0/567	0.67	0/762
14	c	0.39	0/489	0.71	0/655
15	f	0.48	0/559	0.69	0/747
16	g	0.41	0/2521	0.59	0/3431
17	d	0.42	0/457	0.62	0/607
18	e	0.40	0/471	0.65	0/628
19	h	0.36	0/234	0.64	0/300
20	3	0.26	0/317	0.68	0/489
21	i	0.36	0/894	0.61	0/1188
22	m	0.41	0/723	0.59	0/965
23	o	0.50	0/3671	0.61	0/4961
24	q	0.50	0/5270	0.62	0/7154
25	k	0.44	0/3167	0.63	1/4278 (0.0%)
26	l	0.47	0/1030	0.61	0/1375
27	j	0.44	0/2034	0.63	1/2737 (0.0%)
28	1	0.34	1/1796 (0.1%)	0.64	0/2795
29	A	0.41	0/1742	0.70	1/2383 (0.0%)
30	B	0.40	0/1793	0.69	2/2414 (0.1%)
31	E	0.39	0/2122	0.65	1/2861 (0.0%)
32	G	0.39	0/1835	0.69	1/2451 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	H	0.41	0/1507	0.69	0/2028
34	I	0.40	0/1515	0.70	2/2029 (0.1%)
35	J	0.40	0/1495	0.77	1/2001 (0.0%)
36	L	0.42	0/1276	0.65	0/1718
37	N	0.40	0/1210	0.74	0/1628
38	O	0.40	0/953	0.66	0/1279
39	V	0.37	0/696	0.66	1/938 (0.1%)
40	W	0.38	0/1039	0.70	2/1399 (0.1%)
41	Y	0.39	0/1075	0.67	0/1433
42	X	0.41	0/1137	0.70	1/1516 (0.1%)
43	a	0.37	0/791	0.65	0/1059
44	b	0.39	0/619	0.63	0/837
45	p	0.45	0/5282	0.57	0/7178
46	s	0.35	0/2669	0.53	0/3611
47	r	0.29	0/399	0.45	0/535
All	All	0.36	1/109131 (0.0%)	0.65	20/156528 (0.0%)

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
41	Y	0	1
42	X	0	1
45	p	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	1	A	OP3-P	-10.05	1.49	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	I	190	LEU	CA-CB-CG	7.41	132.35	115.30
7	P	56	LEU	CA-CB-CG	6.99	131.37	115.30
9	R	109	LEU	CA-CB-CG	6.17	129.50	115.30
40	W	26	LEU	CA-CB-CG	6.08	129.29	115.30
1	2	1430	U	C2'-C3'-O3'	6.07	123.41	113.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	X	63	GLN	Peptide
41	Y	29	HIS	Peptide
45	p	391	GLN	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	C	215/217 (99%)	194 (90%)	14 (6%)	7 (3%)	3	21
3	D	221/223 (99%)	196 (89%)	14 (6%)	11 (5%)	1	16
4	F	204/206 (99%)	171 (84%)	22 (11%)	11 (5%)	1	14
5	K	94/96 (98%)	84 (89%)	7 (7%)	3 (3%)	3	21
6	M	113/118 (96%)	86 (76%)	17 (15%)	10 (9%)	0	8
7	P	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	1	15
8	Q	139/141 (99%)	118 (85%)	11 (8%)	10 (7%)	1	10
9	R	128/130 (98%)	107 (84%)	15 (12%)	6 (5%)	2	16
10	S	143/145 (99%)	118 (82%)	17 (12%)	8 (6%)	1	14
11	T	141/143 (99%)	132 (94%)	7 (5%)	2 (1%)	9	40
12	U	104/106 (98%)	91 (88%)	8 (8%)	5 (5%)	2	16
13	Z	68/70 (97%)	56 (82%)	9 (13%)	3 (4%)	2	17
14	c	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	7	36
15	f	67/69 (97%)	51 (76%)	7 (10%)	9 (13%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	g	312/324 (96%)	271 (87%)	33 (11%)	8 (3%)	4	25
17	d	51/53 (96%)	39 (76%)	11 (22%)	1 (2%)	6	31
18	e	56/58 (97%)	45 (80%)	9 (16%)	2 (4%)	3	20
19	h	23/25 (92%)	23 (100%)	0	0	100	100
21	i	109/111 (98%)	90 (83%)	18 (16%)	1 (1%)	14	51
22	m	86/90 (96%)	76 (88%)	7 (8%)	3 (4%)	3	20
23	o	435/567 (77%)	366 (84%)	62 (14%)	7 (2%)	8	38
24	q	667/699 (95%)	577 (86%)	70 (10%)	20 (3%)	3	22
25	k	404/430 (94%)	337 (83%)	60 (15%)	7 (2%)	7	36
26	l	118/144 (82%)	97 (82%)	20 (17%)	1 (1%)	16	55
27	j	243/263 (92%)	210 (86%)	27 (11%)	6 (2%)	4	26
29	A	217/219 (99%)	183 (84%)	24 (11%)	10 (5%)	2	16
30	B	218/231 (94%)	187 (86%)	23 (11%)	8 (4%)	2	20
31	E	258/260 (99%)	240 (93%)	13 (5%)	5 (2%)	6	32
32	G	224/226 (99%)	205 (92%)	18 (8%)	1 (0%)	30	68
33	H	182/184 (99%)	157 (86%)	15 (8%)	10 (6%)	1	14
34	I	184/200 (92%)	166 (90%)	11 (6%)	7 (4%)	2	19
35	J	180/182 (99%)	150 (83%)	25 (14%)	5 (3%)	4	24
36	L	153/155 (99%)	132 (86%)	17 (11%)	4 (3%)	4	25
37	N	148/150 (99%)	135 (91%)	12 (8%)	1 (1%)	19	57
38	O	125/127 (98%)	102 (82%)	12 (10%)	11 (9%)	0	8
39	V	85/87 (98%)	75 (88%)	7 (8%)	3 (4%)	3	20
40	W	127/129 (98%)	113 (89%)	9 (7%)	5 (4%)	2	18
41	Y	132/134 (98%)	116 (88%)	13 (10%)	3 (2%)	5	28
42	X	142/144 (99%)	119 (84%)	14 (10%)	9 (6%)	1	12
43	a	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	2	17
44	b	79/81 (98%)	70 (89%)	3 (4%)	6 (8%)	1	10
45	p	650/666 (98%)	538 (83%)	93 (14%)	19 (3%)	3	23
46	s	326/342 (95%)	318 (98%)	8 (2%)	0	100	100
47	r	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
All	All	7889/8271 (95%)	6814 (86%)	816 (10%)	259 (3%)	5	21

5 of 259 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	141	VAL
2	C	187	PRO
3	D	220	PRO
4	F	67	SER
6	M	82	VAL

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	C	176/176 (100%)	148 (84%)	28 (16%)	2	10
3	D	185/185 (100%)	148 (80%)	37 (20%)	1	6
4	F	174/174 (100%)	140 (80%)	34 (20%)	1	7
5	K	88/88 (100%)	69 (78%)	19 (22%)	1	5
6	M	93/94 (99%)	79 (85%)	14 (15%)	2	11
7	P	100/100 (100%)	78 (78%)	22 (22%)	1	5
8	Q	117/117 (100%)	100 (86%)	17 (14%)	2	12
9	R	115/118 (98%)	96 (84%)	19 (16%)	2	9
10	S	128/128 (100%)	104 (81%)	24 (19%)	1	7
11	T	117/117 (100%)	93 (80%)	24 (20%)	1	6
12	U	96/96 (100%)	83 (86%)	13 (14%)	3	13
13	Z	60/60 (100%)	49 (82%)	11 (18%)	1	8
14	c	54/54 (100%)	47 (87%)	7 (13%)	3	14
15	f	57/60 (95%)	52 (91%)	5 (9%)	8	25
16	g	265/270 (98%)	236 (89%)	29 (11%)	5	18
17	d	46/46 (100%)	37 (80%)	9 (20%)	1	7
18	e	51/51 (100%)	44 (86%)	7 (14%)	3	13
19	h	23/23 (100%)	18 (78%)	5 (22%)	1	5
21	i	93/93 (100%)	82 (88%)	11 (12%)	4	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	m	77/78 (99%)	71 (92%)	6 (8%)	10	29
23	o	398/438 (91%)	360 (90%)	38 (10%)	7	22
24	q	527/644 (82%)	493 (94%)	34 (6%)	14	35
25	k	332/364 (91%)	307 (92%)	25 (8%)	11	31
26	l	117/132 (89%)	105 (90%)	12 (10%)	6	20
27	j	224/237 (94%)	197 (88%)	27 (12%)	4	15
29	A	180/185 (97%)	160 (89%)	20 (11%)	5	17
30	B	198/210 (94%)	181 (91%)	17 (9%)	8	26
31	E	223/223 (100%)	201 (90%)	22 (10%)	6	21
32	G	192/192 (100%)	179 (93%)	13 (7%)	13	34
33	H	164/164 (100%)	146 (89%)	18 (11%)	5	18
34	I	147/158 (93%)	130 (88%)	17 (12%)	4	16
35	J	153/153 (100%)	125 (82%)	28 (18%)	1	8
36	L	136/136 (100%)	110 (81%)	26 (19%)	1	7
37	N	127/127 (100%)	108 (85%)	19 (15%)	2	11
38	O	96/96 (100%)	88 (92%)	8 (8%)	9	27
39	V	73/73 (100%)	64 (88%)	9 (12%)	4	15
40	W	110/110 (100%)	103 (94%)	7 (6%)	14	35
41	Y	108/108 (100%)	100 (93%)	8 (7%)	11	31
42	X	119/119 (100%)	106 (89%)	13 (11%)	5	18
43	a	83/83 (100%)	78 (94%)	5 (6%)	16	37
44	b	71/71 (100%)	68 (96%)	3 (4%)	25	46
45	p	537/597 (90%)	510 (95%)	27 (5%)	20	41
46	s	287/297 (97%)	286 (100%)	1 (0%)	91	92
47	r	40/40 (100%)	40 (100%)	0	100	100
All	All	6757/7085 (95%)	6019 (89%)	738 (11%)	8	18

5 of 738 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	j	87	LYS
34	I	72	VAL
27	j	255	ILE

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Mol	Chain	Res	Type
27	j	79	GLU
31	E	69	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
32	G	185	GLN
39	V	3	ASN
34	I	84	HIS
37	N	49	GLN
42	X	22	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1797/1798 (99%)	828 (46%)	69 (3%)
20	3	13/14 (92%)	8 (61%)	2 (15%)
28	1	73/75 (97%)	32 (43%)	6 (8%)
All	All	1883/1887 (99%)	868 (46%)	77 (4%)

5 of 868 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	5	U
1	2	8	U

5 of 77 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1411	U
28	1	7	G
1	2	1455	C
1	2	1613	C
28	1	59	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 85 are 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	$\# Z > 2$
50	GCP	k	602	-	27,34,34	2.16	9 (33%)	34,54,54	1.95	8 (23%)
51	MET	k	603	-	6,7,8	0.46	0	2,7,9	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	GCP	k	602	-	-	3/15/38/38	0/3/3/3
51	MET	k	603	-	-	3/5/6/8	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	k	602	GCP	PG-O1G	5.41	1.61	1.50
50	k	602	GCP	C5-C6	4.77	1.49	1.41
50	k	602	GCP	PB-O1B	4.16	1.61	1.51
50	k	602	GCP	PB-O2B	-3.39	1.48	1.56
50	k	602	GCP	PB-O3A	3.36	1.62	1.58

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	k	602	GCP	C2-N3-C4	5.53	121.67	115.36
50	k	602	GCP	C2-N1-C6	3.97	122.24	115.93
50	k	602	GCP	C4-C5-C6	-3.90	117.07	120.80
50	k	602	GCP	C5-C6-N1	-3.64	118.46	123.43
50	k	602	GCP	N3-C2-N1	-3.58	122.45	127.22

There are no chirality outliers.

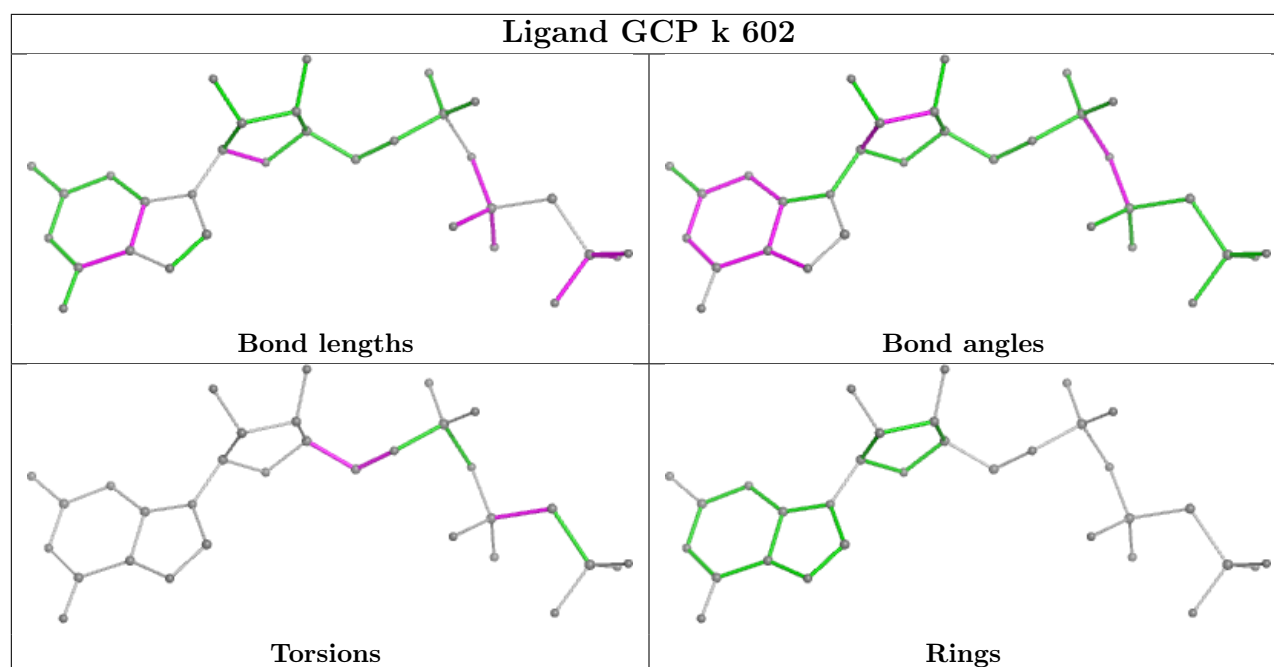
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	k	602	GCP	O4'-C4'-C5'-O5'
51	k	603	MET	O-C-CA-CB
51	k	603	MET	CA-CB-CG-SD
51	k	603	MET	N-CA-CB-CG
50	k	602	GCP	C4'-C5'-O5'-PA

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
23	o	2
28	1	1
22	m	1
25	k	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	492:ALA	C	693:UNK	N	230.47
1	1	16:U	O3'	18:G	P	5.21
1	m	75:GLY	C	76:GLU	N	4.38
1	k	372:PRO	C	373:ILE	N	3.76
1	o	5:PRO	C	6:PHE	N	3.57

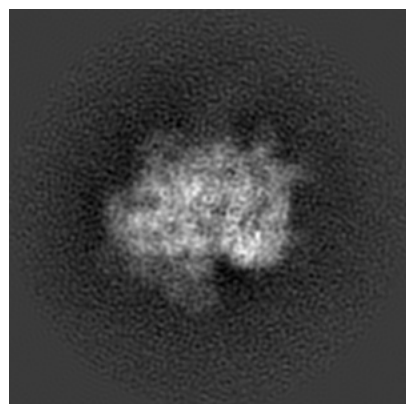
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0058. These allow visual inspection of the internal detail of the map and identification of artifacts.

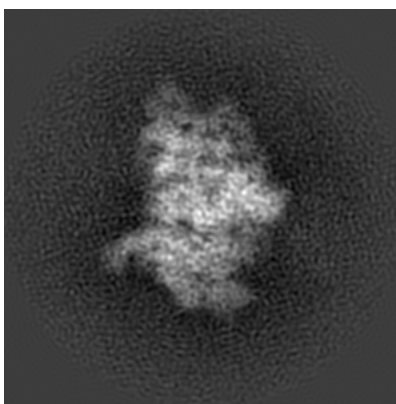
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

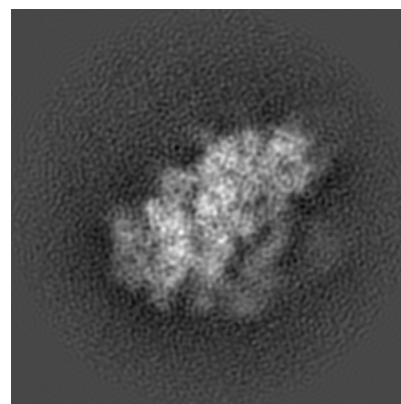
6.1.1 Primary map



X

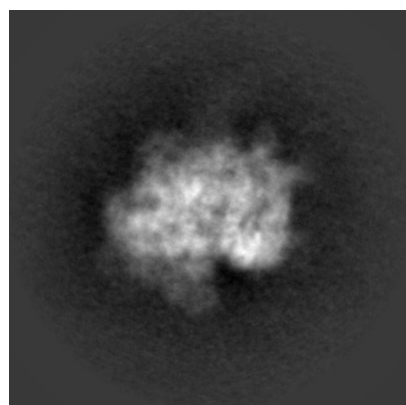


Y

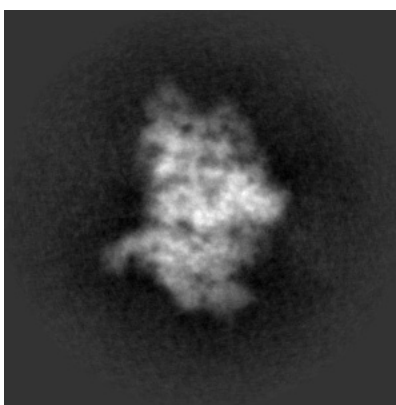


Z

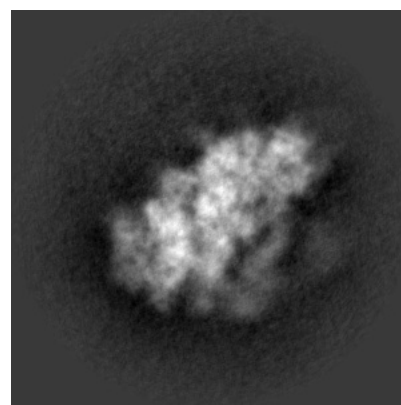
6.1.2 Raw map



X



Y

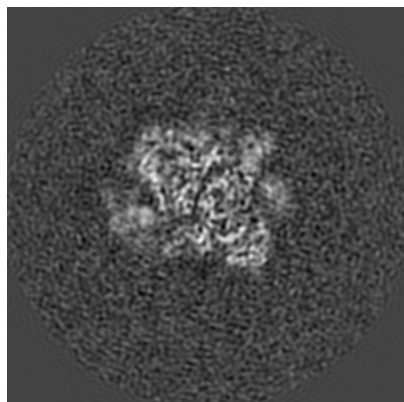


Z

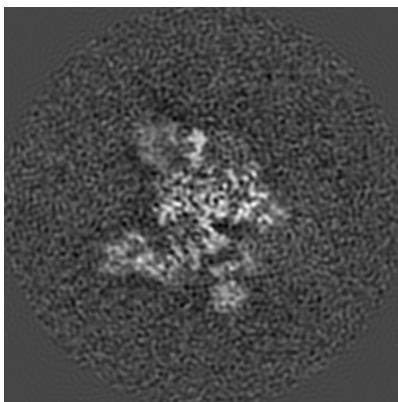
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

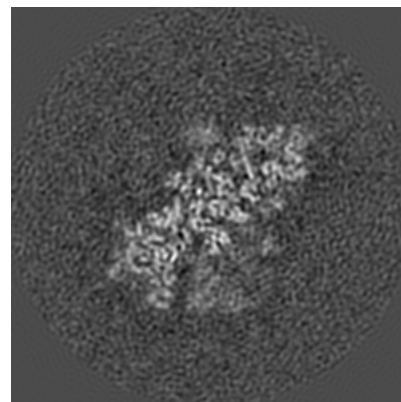
6.2.1 Primary map



X Index: 150

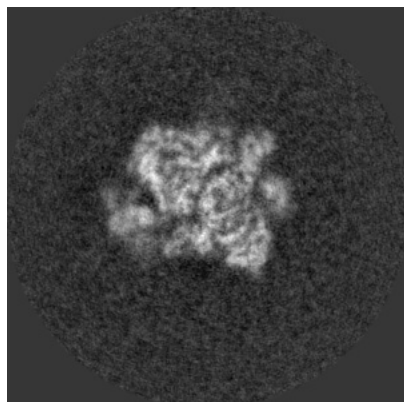


Y Index: 150

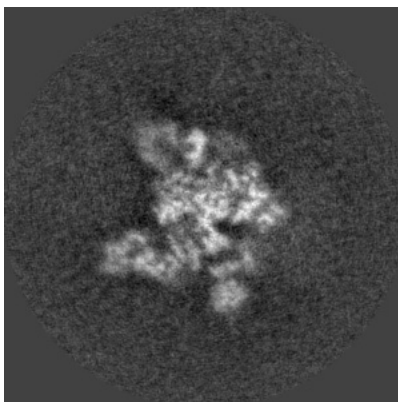


Z Index: 150

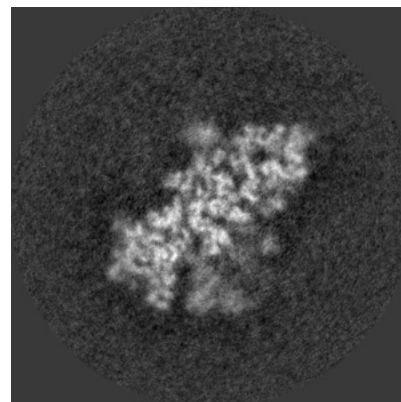
6.2.2 Raw map



X Index: 150



Y Index: 150

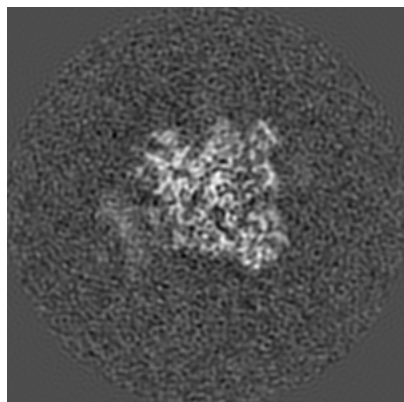


Z Index: 150

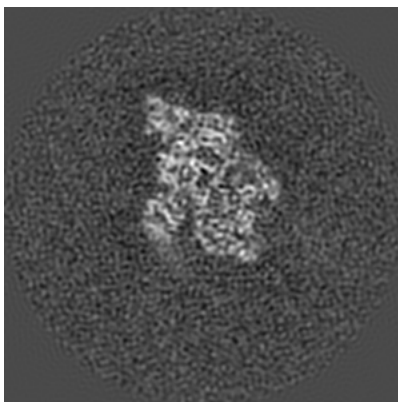
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

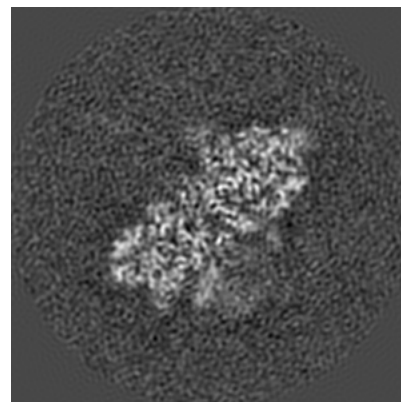
6.3.1 Primary map



X Index: 160

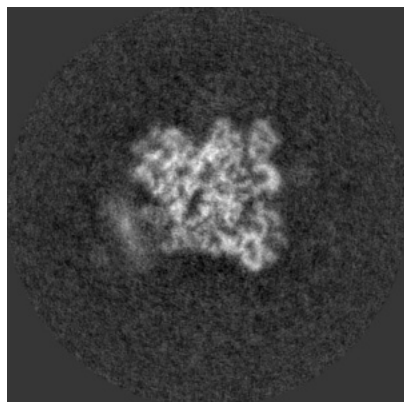


Y Index: 172

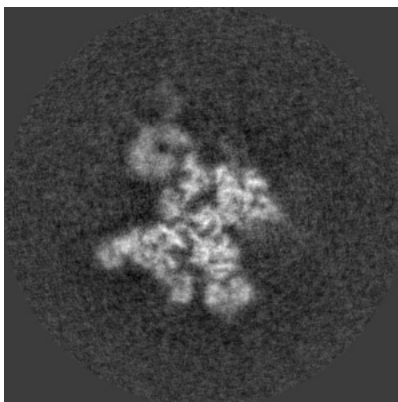


Z Index: 143

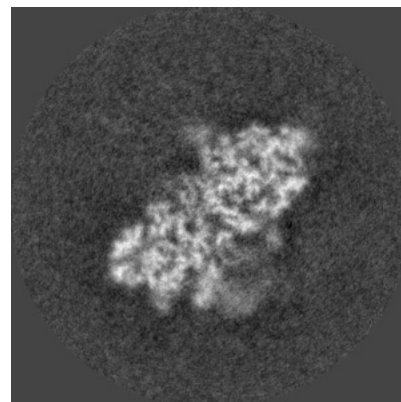
6.3.2 Raw map



X Index: 158



Y Index: 139

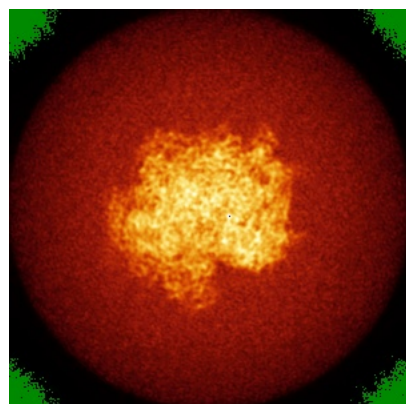


Z Index: 143

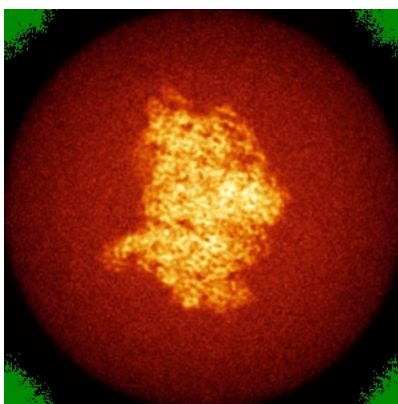
The images above show the largest variance slices of the map in three orthogonal directions.

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

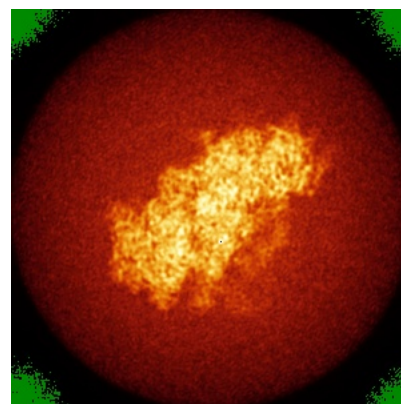
6.4.1 Primary map



X

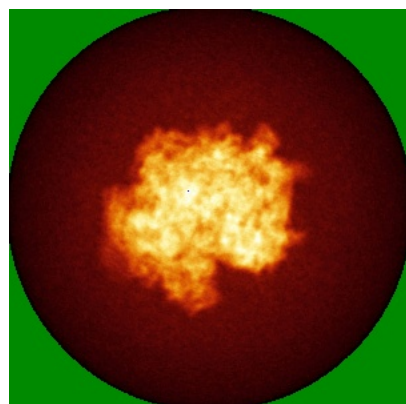


Y

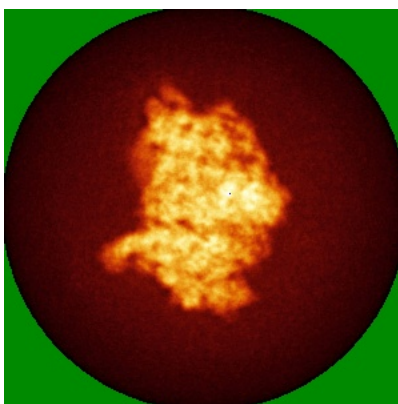


Z

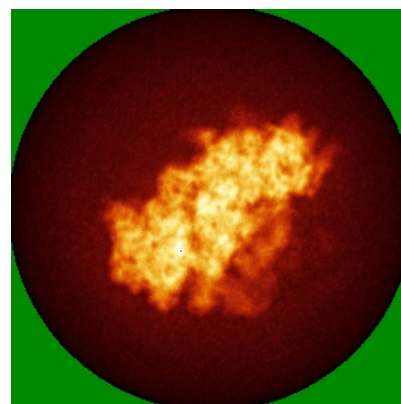
6.4.2 Raw map



X



Y

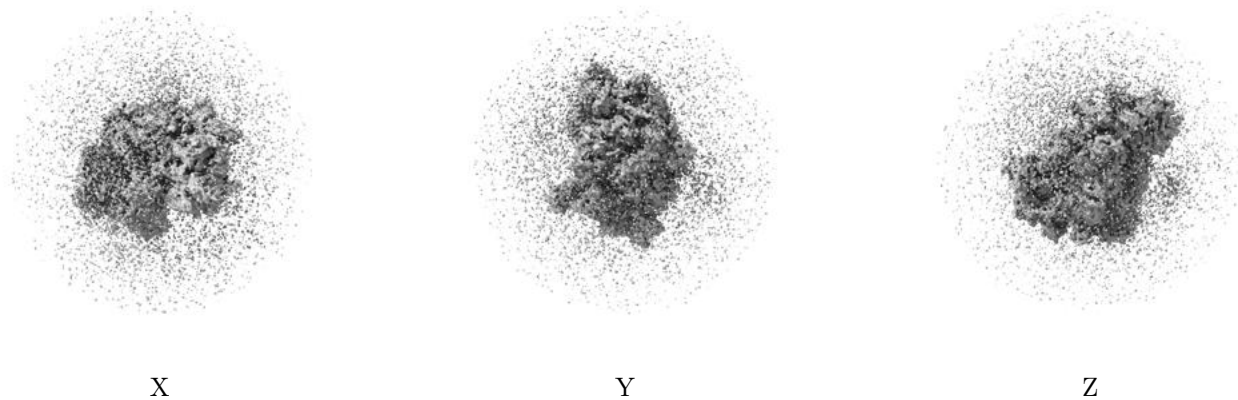


Z

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.

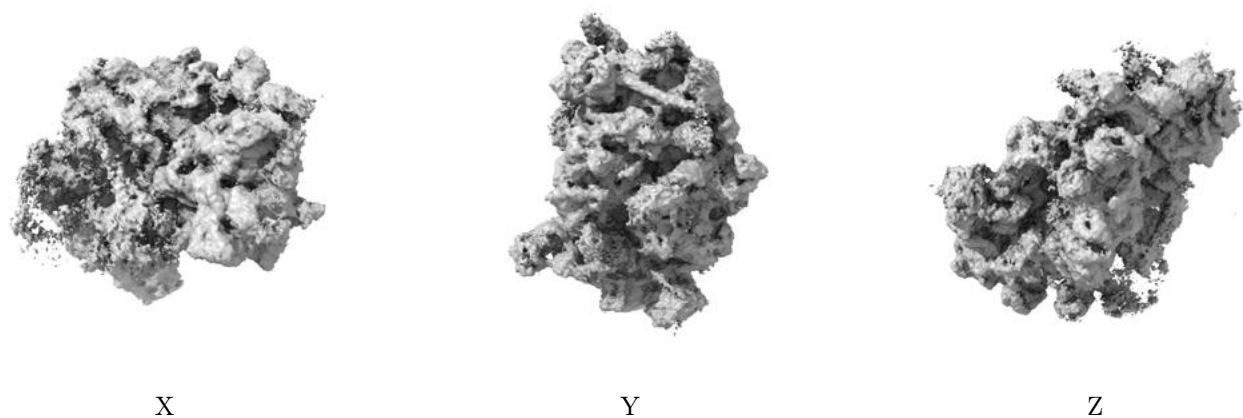
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

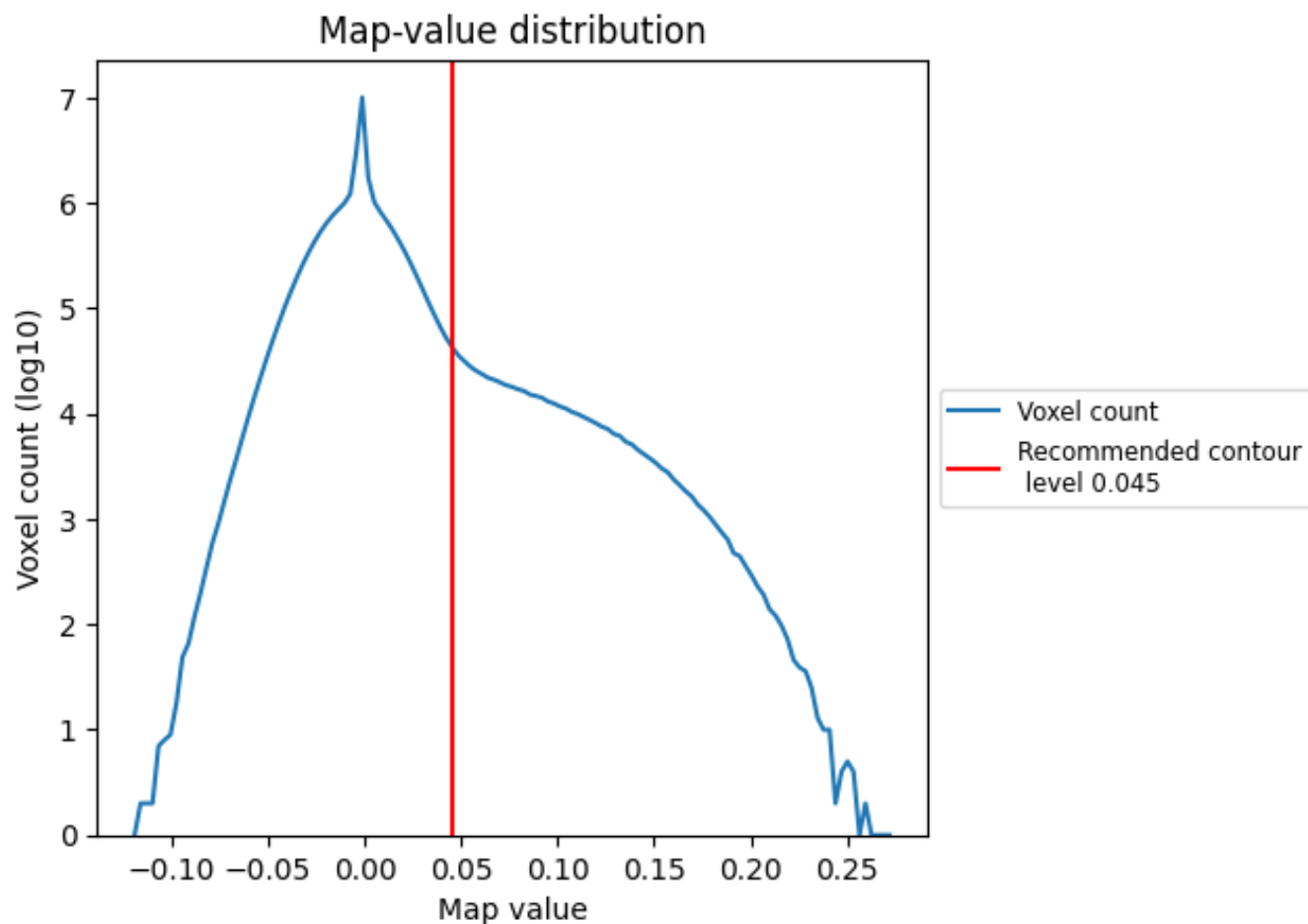
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

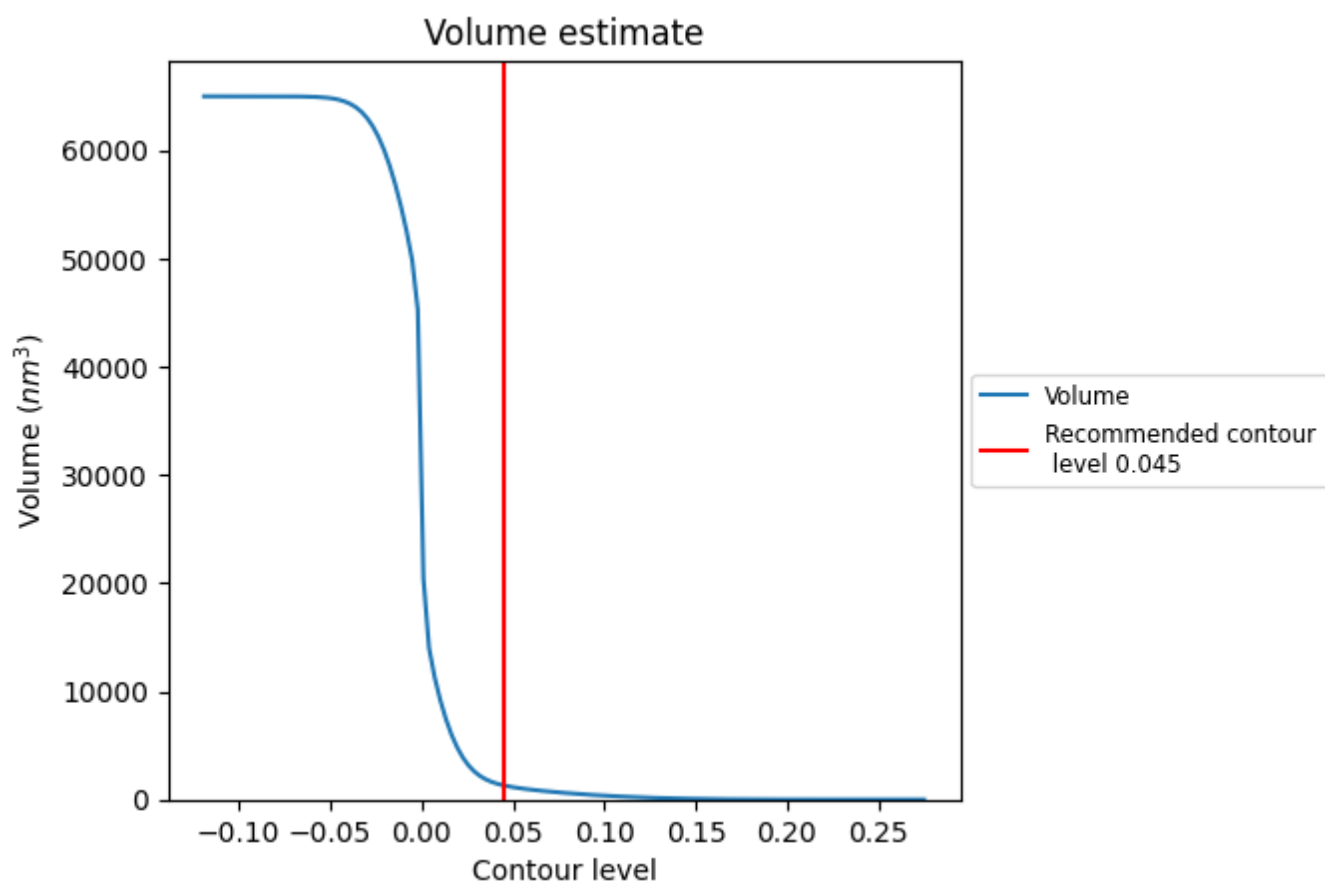
This section contains the results of statistical analysis of the map.

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.

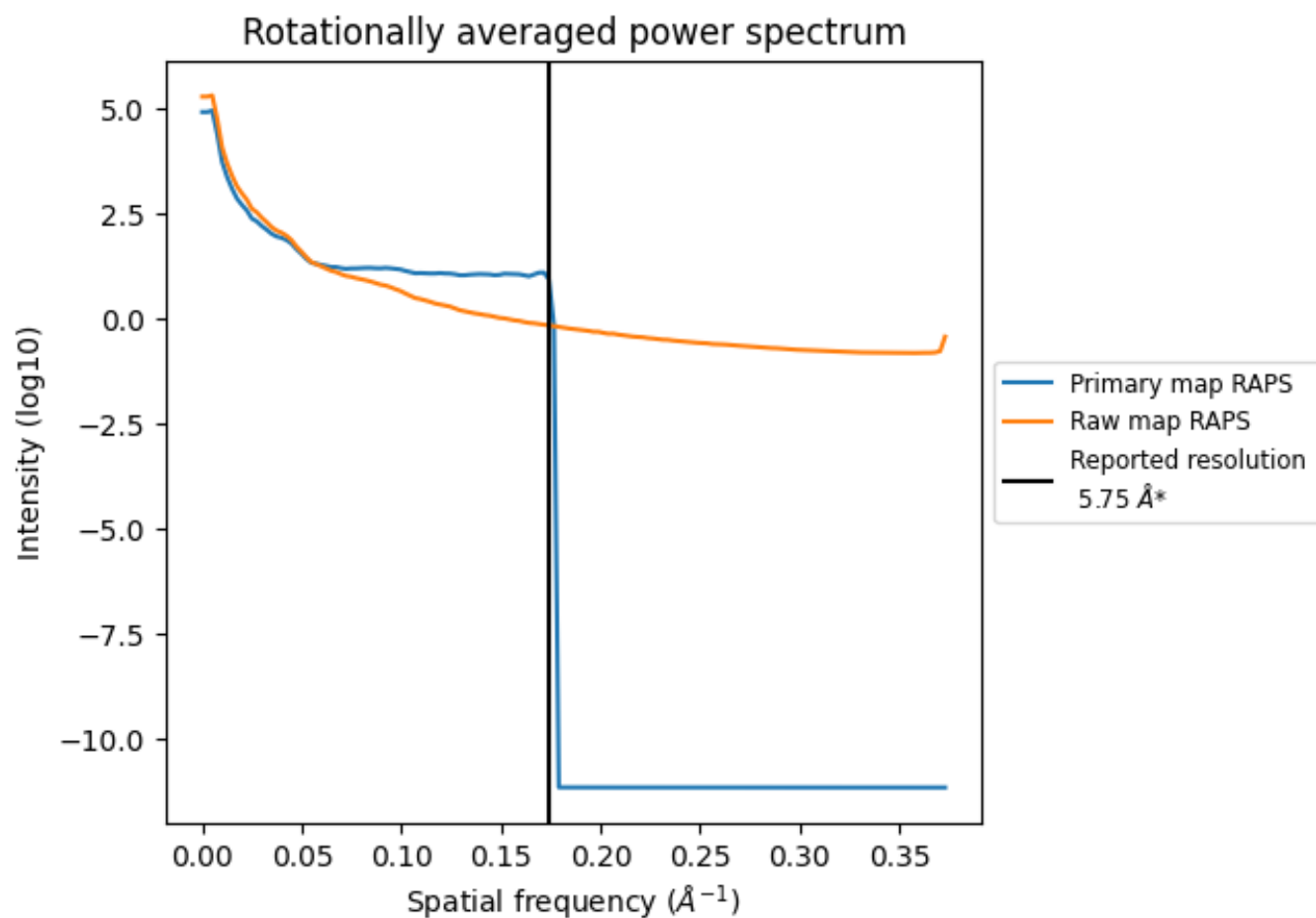
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1308 nm³; this corresponds to an approximate mass of 1181 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 ⓘ

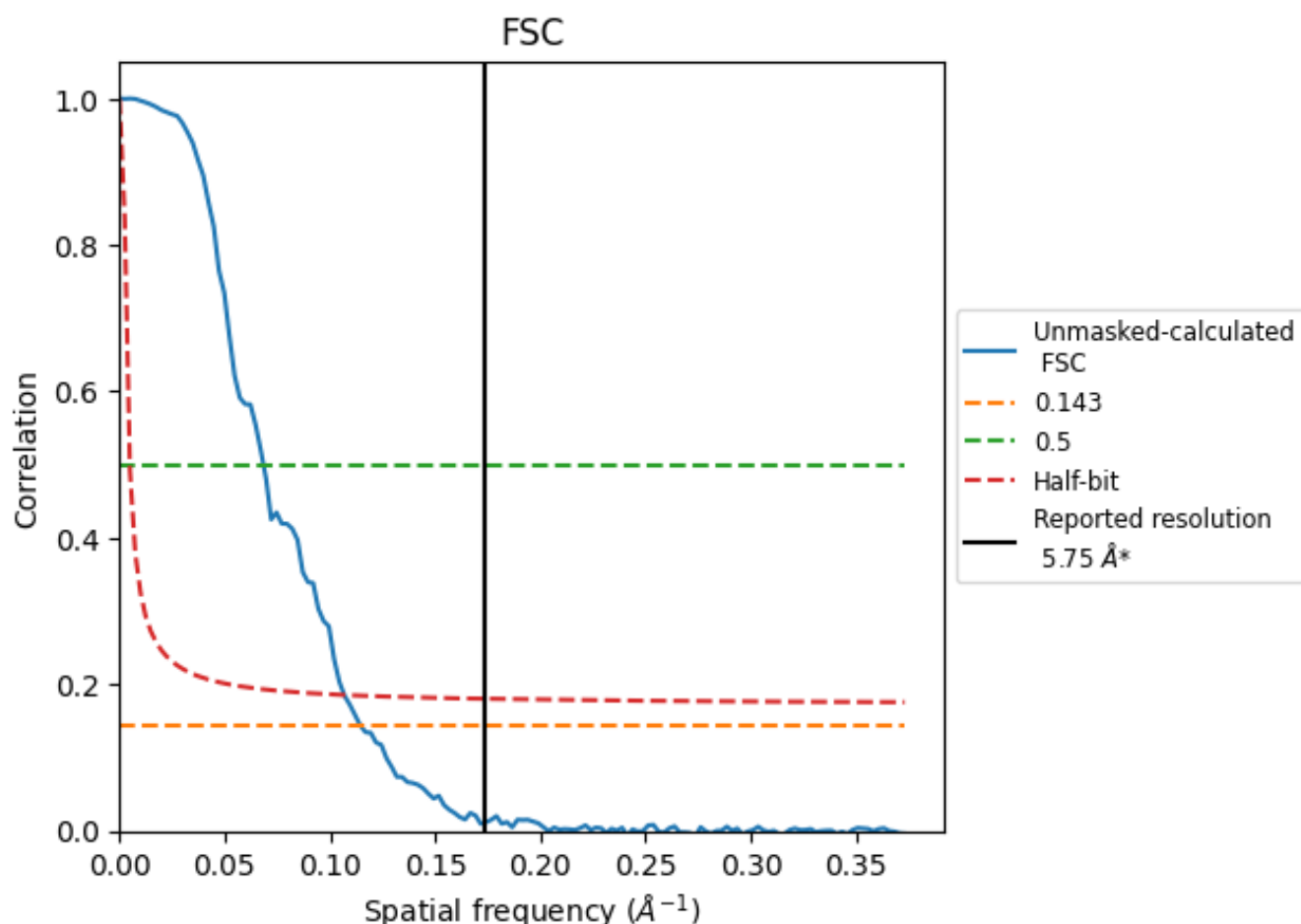


*Reported resolution corresponds to spatial frequency of 0.174 Å⁻¹

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 0.174 Å⁻¹

8.2 Resolution estimates [i](#)

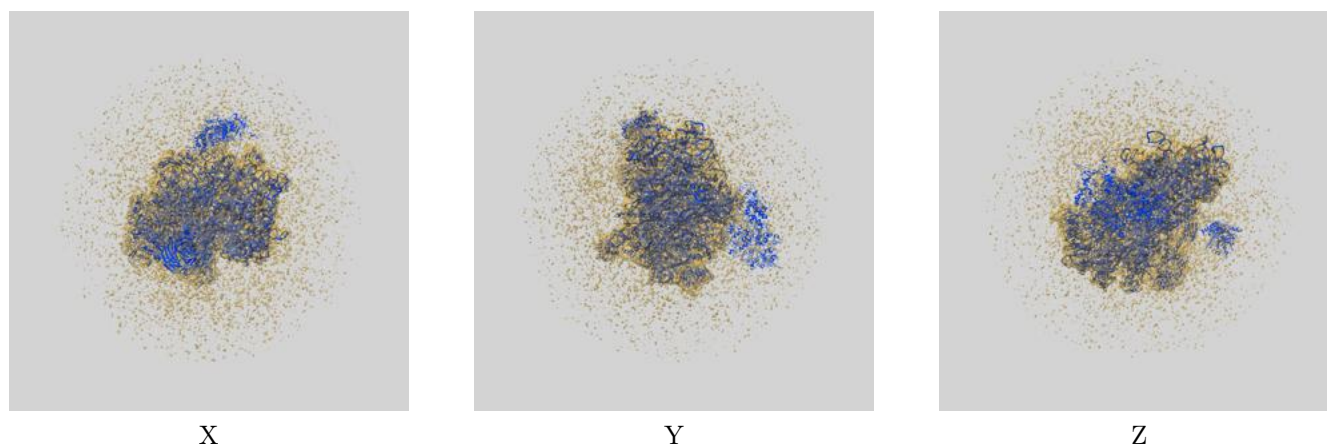
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.73	14.62	9.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.73 differs from the reported value 5.75 by more than 10 %

9 Map-model fit [i](#)

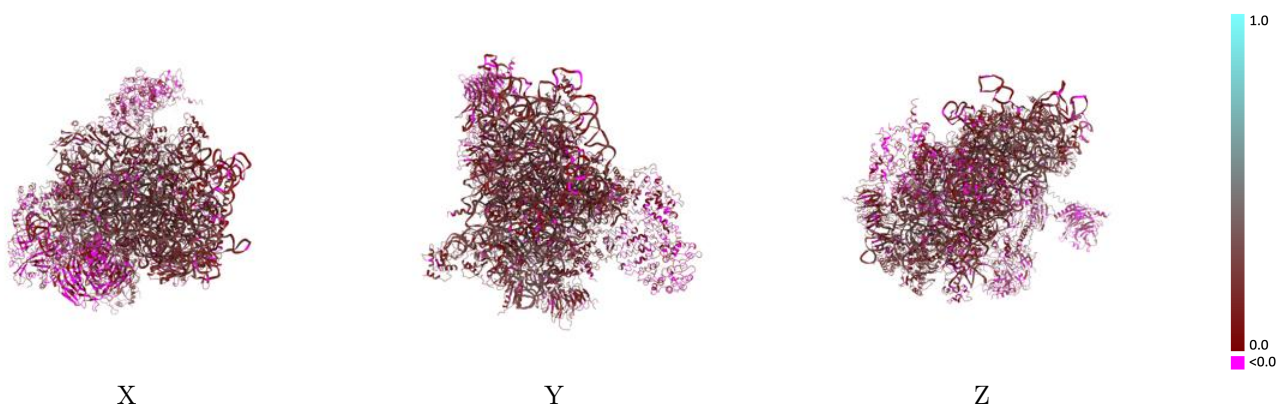
This section contains information regarding the fit between EMDB map EMD-0058 and PDB model 6GSN. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



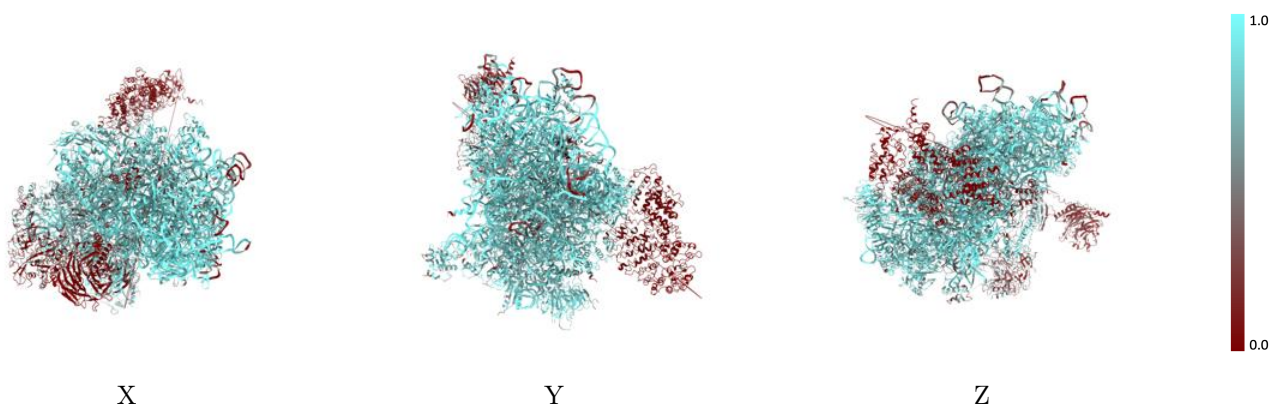
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



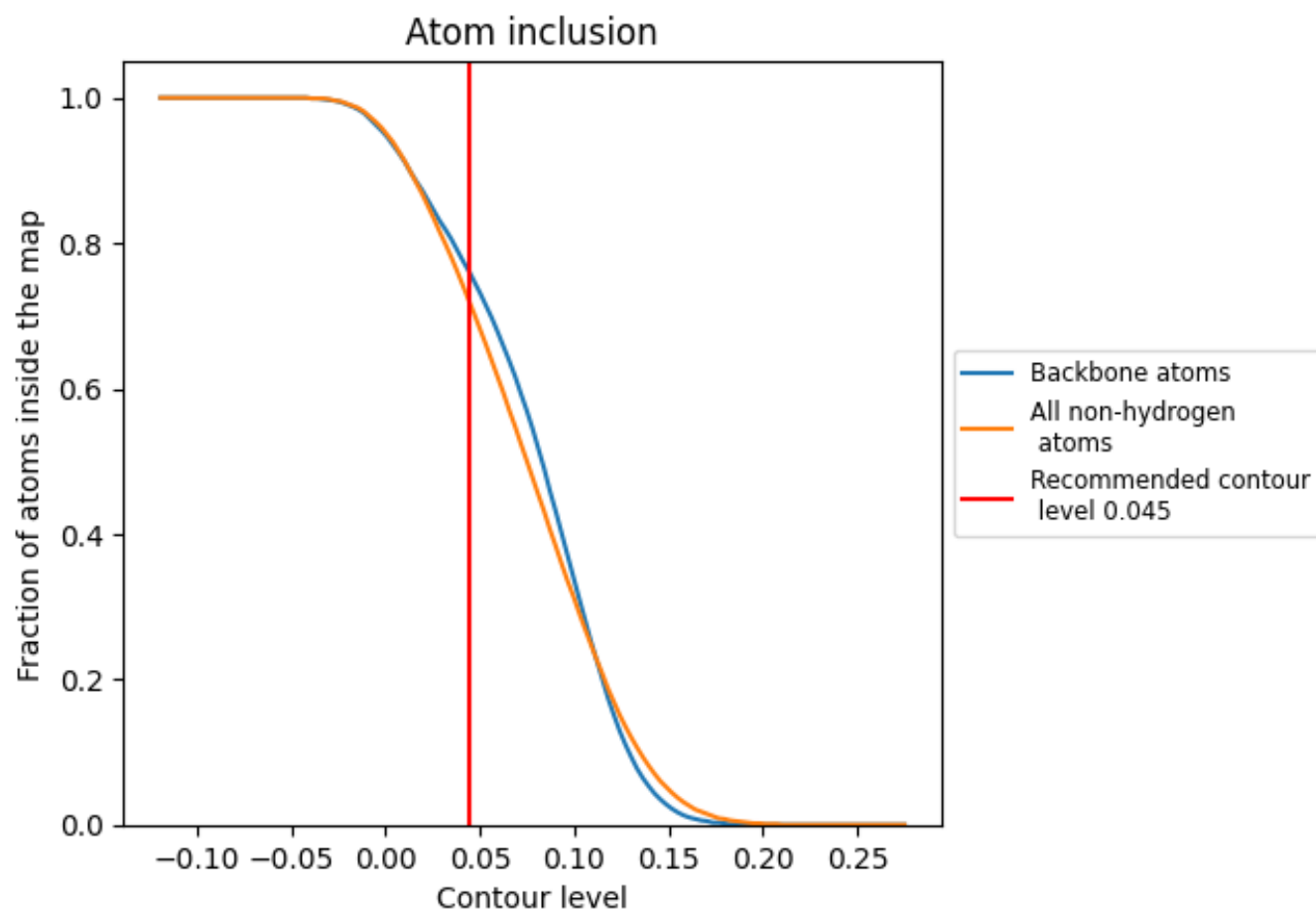
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7170	 0.1850
1	 0.8130	 0.1580
2	 0.9260	 0.2360
3	 0.7350	 0.1800
A	 0.8200	 0.2010
B	 0.8440	 0.1950
C	 0.7730	 0.2070
D	 0.7760	 0.2120
E	 0.7920	 0.1980
F	 0.7870	 0.1950
G	 0.8350	 0.1770
H	 0.8230	 0.1830
I	 0.8020	 0.1920
J	 0.7920	 0.2000
K	 0.8250	 0.1880
L	 0.7670	 0.2080
M	 0.6960	 0.1600
N	 0.8170	 0.1930
O	 0.8550	 0.2030
P	 0.8400	 0.1940
Q	 0.8150	 0.1760
R	 0.7820	 0.1940
S	 0.7940	 0.1800
T	 0.8270	 0.1810
U	 0.7510	 0.1810
V	 0.8430	 0.2120
W	 0.7920	 0.1980
X	 0.7260	 0.2060
Y	 0.8330	 0.2070
Z	 0.7350	 0.1580
a	 0.8330	 0.2220
b	 0.8410	 0.2140
c	 0.7940	 0.2100
d	 0.7840	 0.1930
e	 0.6930	 0.2070



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Chain	Atom inclusion	Q-score
f	 0.7900	 0.1870
g	 0.8280	 0.1720
h	 0.5400	 0.1350
i	 0.7160	 0.2200
j	 0.4780	 0.1290
k	 0.2490	 0.0930
l	 0.3020	 0.1060
m	 0.4460	 0.1650
o	 0.0950	 0.0710
p	 0.5480	 0.1290
q	 0.0460	 0.0870
r	 0.0210	 0.0550
s	 0.0230	 0.0020