



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 03:45 AM UTC

PDB ID : 6GSM / pdb_00006gsm
EMDB ID : EMD-0057
Title : Structure of a partial yeast 48S preinitiation complex in open conformation.
Authors : Llacer, J.L.; Hussain, T.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on : 2018-06-14
Resolution : 5.15 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:

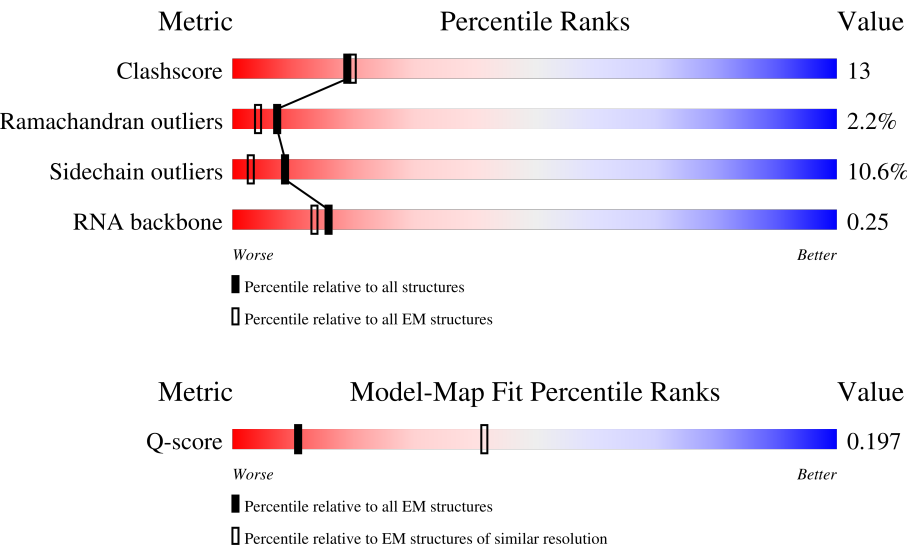
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 5.15 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	694 (4.65 - 5.65)

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	76	17% 45% 34% 14% . .
2	2	1798	11% 41% 50% 9%
3	A	208	35% 62% 33% 5%

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Mol	Chain	Length	Quality of chain
4	3	3	100% 100%
5	B	231	38% 66% 24% 6% .
6	C	217	37% 70% 24% 6%
7	D	223	49% 68% 27% 5%
8	E	260	28% 66% 32% .
9	F	206	47% 63% 33% 5%
10	G	226	38% 73% 23% .
11	H	184	43% 61% 28% 10% .
12	I	200	38% 68% 22% . 6%
13	J	182	27% 67% 27% 5%
14	K	96	58% 53% 40% 6% .
15	L	155	39% 79% 18% .
16	M	118	86% 68% 26% 5% .
17	N	150	25% 77% 22% .
18	O	127	28% 77% 20% ..
19	P	119	69% 74% 23% .
20	Q	141	38% 66% 30% .
21	R	125	46% 54% 24% 10% . 11%
22	S	145	51% 58% 37% 6%
23	T	143	36% 71% 27% .
24	U	106	64% 66% 30% .
25	V	87	38% 70% 26% ..
26	W	129	28% 74% 21% . .
27	X	144	41% 60% 32% 8%
28	Y	134	25% 62% 32% 6%

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Mol	Chain	Length	Quality of chain
29	Z	70	
30	a	98	
31	b	81	
32	c	62	
33	d	53	
34	e	58	
35	f	69	
36	g	324	
37	h	25	
38	i	95	
39	j	263	
40	k	430	
41	l	144	
42	m	96	
43	o	567	
44	p	651	
45	q	665	
46	s	342	
47	r	49	

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 103158 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 Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	74	Total	C	N	O	P	0	0
			1617	724	293	525	75		

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

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

- Molecule 3 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	208	Total	C	N	O	S	0	0
			1626	1040	286	298	2		

- Molecule 4 is a RNA chain called mRNA (5'-R(P*AP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	3	Total	C	N	O	P	0	0
			64	29	12	20	3		

- Molecule 5 is a protein called 40S ribosomal protein S1.

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

- Molecule 6 is a protein called KLLA0F09812p.

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

- Molecule 7 is a protein called KLLA0D08305p.

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

- Molecule 8 is a protein called 40S ribosomal protein S4.

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

- Molecule 9 is a protein called KLLA0D10659p.

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

- Molecule 10 is a protein called 40S ribosomal protein S6.

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

- Molecule 11 is a protein called 40S ribosomal protein S7.

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

- Molecule 12 is a protein called 40S ribosomal protein S8.

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

- Molecule 13 is a protein called KLLA0E23673p.

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

- Molecule 14 is a protein called KLLA0B08173p.

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

- Molecule 15 is a protein called KLLA0A10483p.

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

- Molecule 16 is a protein called 40S ribosomal protein S12.

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

- Molecule 17 is a protein called KLLA0F18040p.

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

- Molecule 18 is a protein called 40S ribosomal protein S14.

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

- Molecule 19 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	119	Total	C	N	O	S	0	0
			943	604	171	163	5		

- Molecule 20 is a protein called 40S ribosomal protein S16.

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

- Molecule 21 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	111	Total	C	N	O	S	0	0
			892	554	165	170	3		

- Molecule 22 is a protein called KLLA0B01562p.

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

- Molecule 23 is a protein called KLLA0A07194p.

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

- Molecule 24 is a protein called KLLA0F25542p.

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

- Molecule 25 is a protein called 40S ribosomal protein S21.

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

- Molecule 26 is a protein called 40S ribosomal protein S22.

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

- Molecule 27 is a protein called KLLA0B11231p.

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

- Molecule 28 is a protein called 40S ribosomal protein S24.

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

- Molecule 29 is a protein called KLLA0B06182p.

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

- Molecule 30 is a protein called 40S ribosomal protein S26.

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

- Molecule 31 is a protein called 40S ribosomal protein S27.

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

- Molecule 32 is a protein called 40S ribosomal protein S28.

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

- Molecule 33 is a protein called 40S ribosomal protein S29.

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

- Molecule 34 is a protein called 40S ribosomal protein S30.

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

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 36 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	309	Total	C	N	O	S	0	0
			2403	1526	419	453	5		

- Molecule 37 is a protein called 60S ribosomal protein L41-A.

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

- Molecule 38 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	95	Total	C	N	O	S	0	0
			765	475	142	143	5		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

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

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

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

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	130	Total	C	N	O	S	0	0
			1048	669	188	184	7		

- Molecule 42 is a protein called Eukaryotic translation initiation factor eIF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	96	Total	C	N	O	S	0	0
			736	464	134	134	4		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit A, Eukaryotic translation initiation factor 3 subunit A, eIF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	528	Total	C	N	O	S	0	0
			4051	2587	695	762	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	651	Total	C	N	O	S	0	0
			5092	3259	881	935	17		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	?	-	ALA	deletion	UNP P06103
p	?	-	SER	deletion	UNP P06103
p	?	-	ILE	deletion	UNP P06103
p	?	-	ALA	deletion	UNP P06103
p	?	-	GLN	deletion	UNP P06103
p	?	-	PHE	deletion	UNP P06103
p	?	-	ASP	deletion	UNP P06103
p	?	-	LEU	deletion	UNP P06103
p	?	-	ILE	deletion	UNP P06103
p	?	-	LEU	deletion	UNP P06103

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	665	Total	C	N	O	S	0	0
			5051	3212	857	970	12		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	?	-	ASP	deletion	UNP P32497
q	?	-	LYS	deletion	UNP P32497
q	?	-	ASN	deletion	UNP P32497

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Chain	Residue	Modelled	Actual	Comment	Reference
q	?	-	PRO	deletion	UNP P32497
q	?	-	GLU	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	PHE	deletion	UNP P32497
q	?	-	ASP	deletion	UNP P32497
q	?	-	LYS	deletion	UNP P32497
q	?	-	GLU	deletion	UNP P32497
q	?	-	PRO	deletion	UNP P32497
q	?	-	THR	deletion	UNP P32497
q	?	-	ALA	deletion	UNP P32497
q	?	-	ASP	deletion	UNP P32497
q	?	-	LEU	deletion	UNP P32497
q	?	-	ASP	deletion	UNP P32497
q	?	-	ILE	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	ALA	deletion	UNP P32497
q	?	-	ASN	deletion	UNP P32497
q	?	-	GLY	deletion	UNP P32497
q	?	-	PHE	deletion	UNP P32497
q	?	-	THR	deletion	UNP P32497
q	?	-	ILE	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	GLN	deletion	UNP P32497
q	?	-	GLY	deletion	UNP P32497
q	?	-	ASN	deletion	UNP P32497
q	?	-	ASP	deletion	UNP P32497
q	?	-	GLN	deletion	UNP P32497
q	?	-	ALA	deletion	UNP P32497
q	?	-	VAL	deletion	UNP P32497

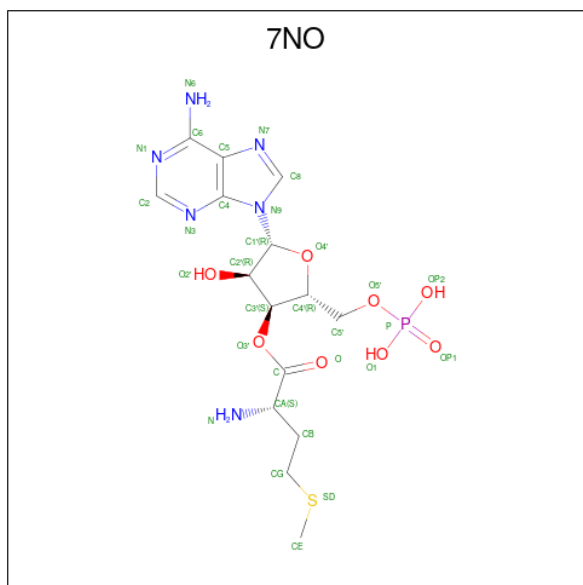
- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit I.

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 [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-4-oxidanyl-2-(phosphonoxy)methyl)oxolan-3-yl] (2 {S})-2-azanyl-4-methylsulfanyl-butanoate (CCD ID: 7NO) (formula: C₁₅H₂₃N₆O₈PS).



Mol	Chain	Residues	Atoms						AltConf
48	1	1	Total	C	N	O	P	S	0
			30	15	6	7	1	1	

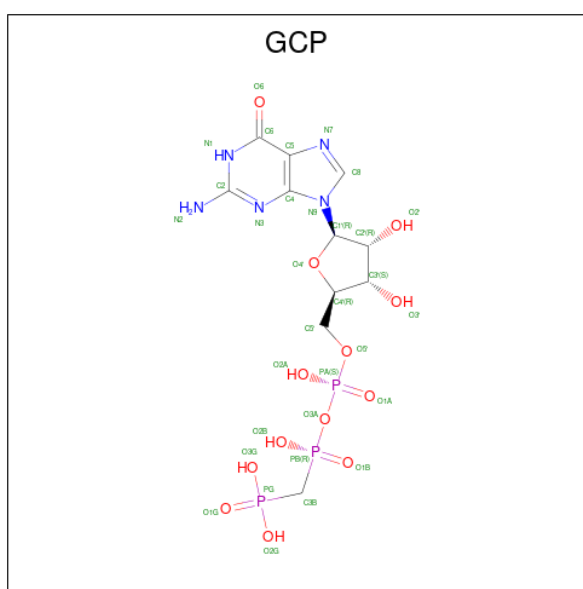
- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	2	76	Total	Mg	0
			76	76	
49	C	3	Total	Mg	0
			3	3	
49	O	1	Total	Mg	0
			1	1	
49	Q	1	Total	Mg	0
			1	1	
49	k	1	Total	Mg	0
			1	1	

- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
50	O	1	Total	Zn	0
			1	1	
50	b	1	Total	Zn	0
			1	1	
50	f	1	Total	Zn	0
			1	1	
50	l	1	Total	Zn	0
			1	1	

- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

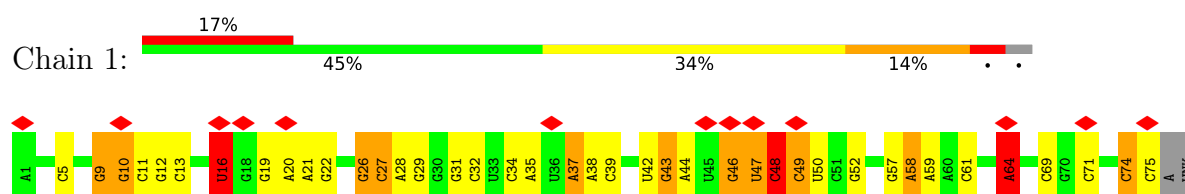


Mol	Chain	Residues	Atoms					AltConf
51	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

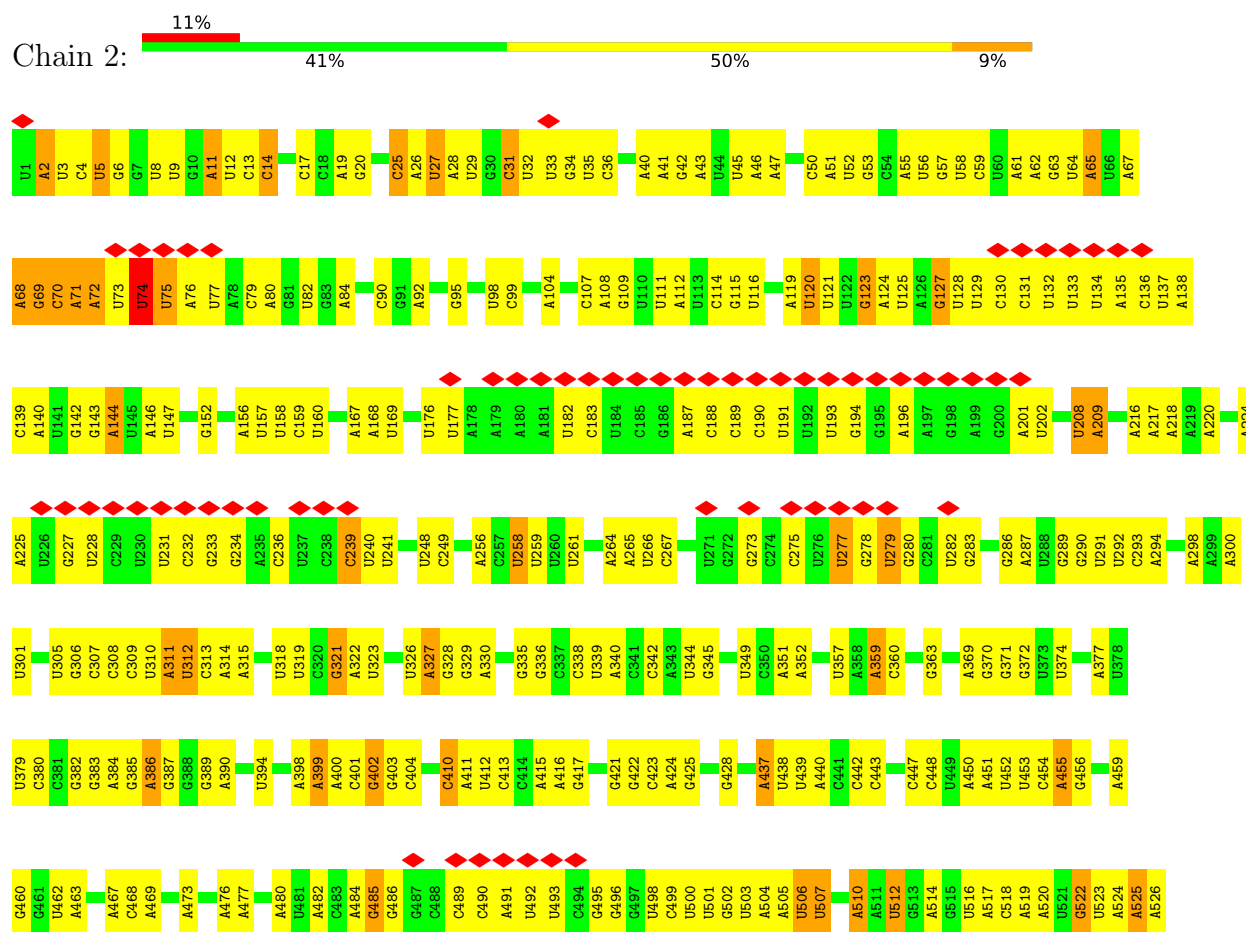
3 Residue-property plots [i](#)

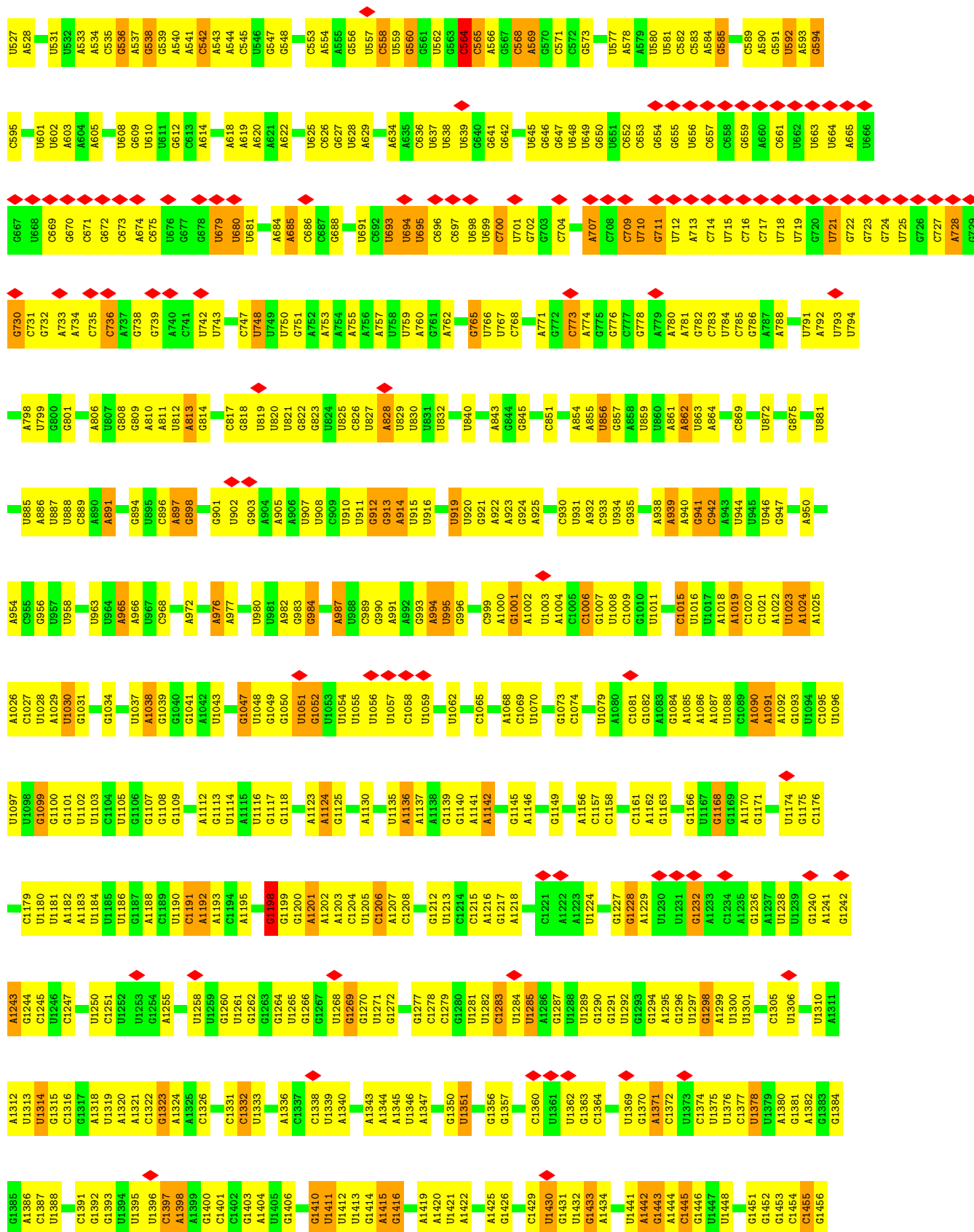
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

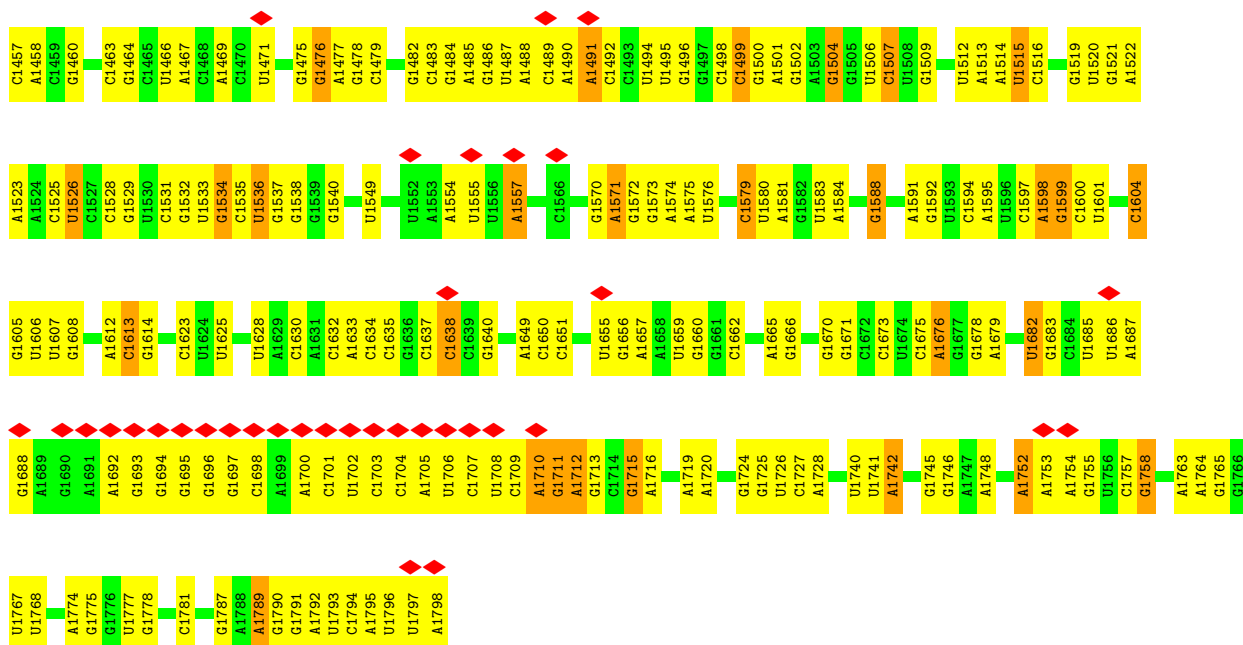
• Molecule 1: Met-tRNAi



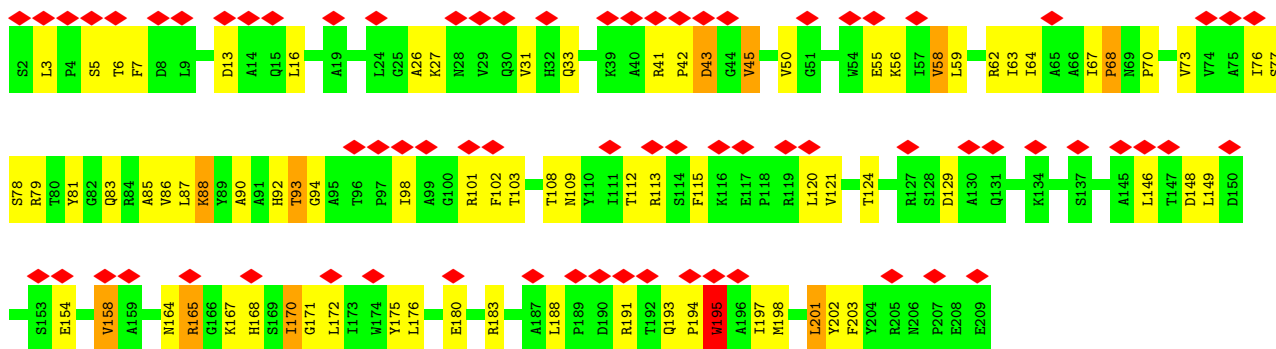
• Molecule 2: 18S ribosomal RNA







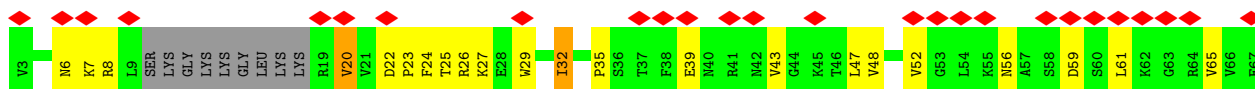
• Molecule 3: 40S ribosomal protein S0

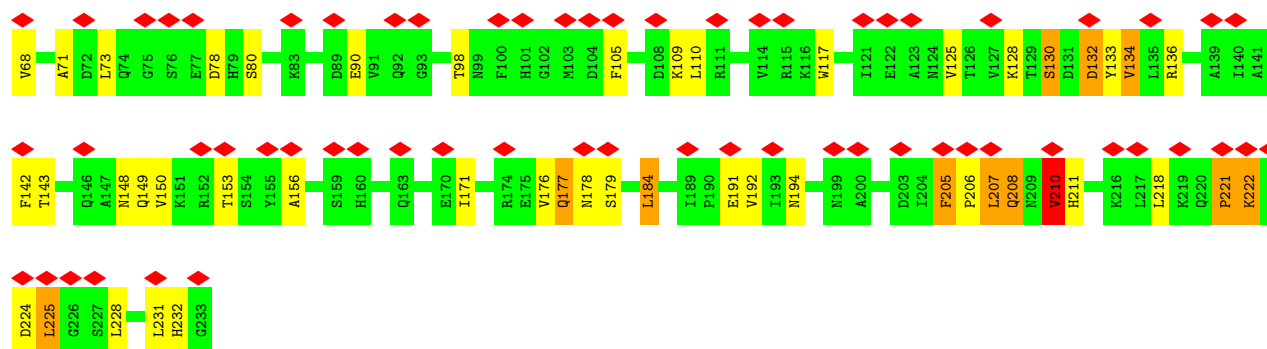


• Molecule 4: mRNA (5'-R(P*AP*AP*U)-3')

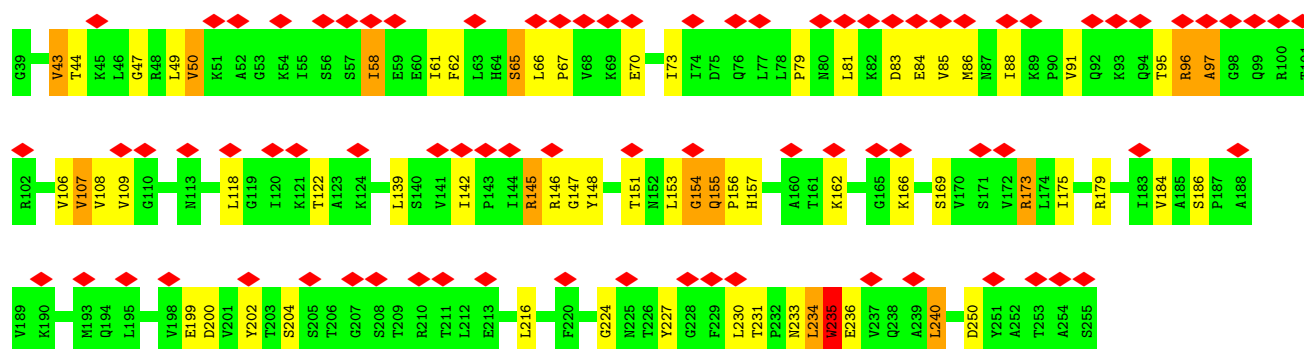


• Molecule 5: 40S ribosomal protein S1

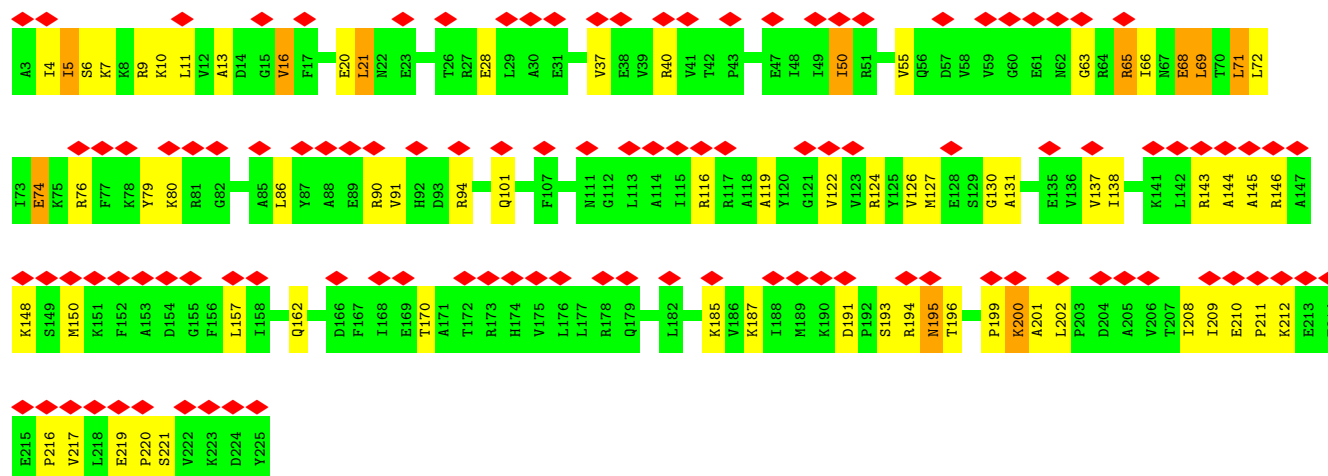




• Molecule 6: KLLA0F09812p

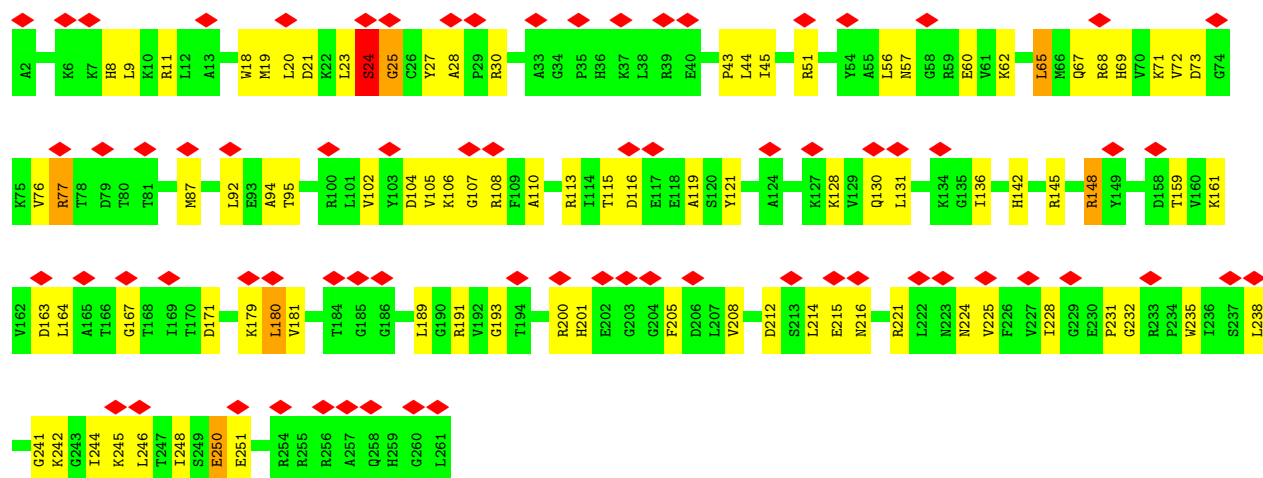


• Molecule 7: KLLA0D08305p

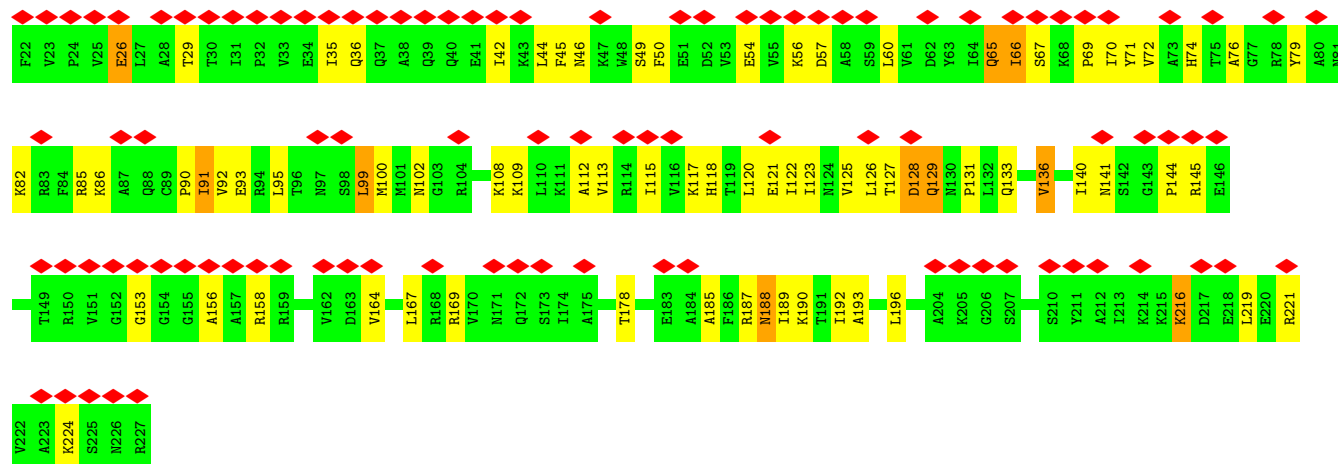


• Molecule 8: 40S ribosomal protein S4

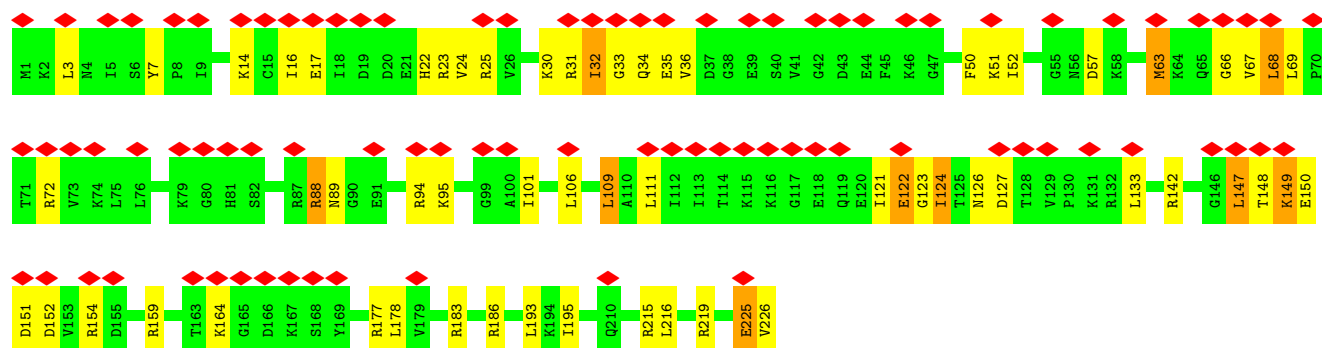
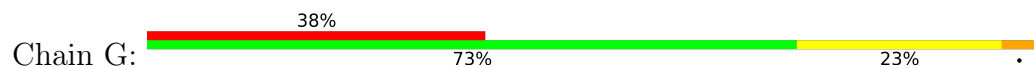




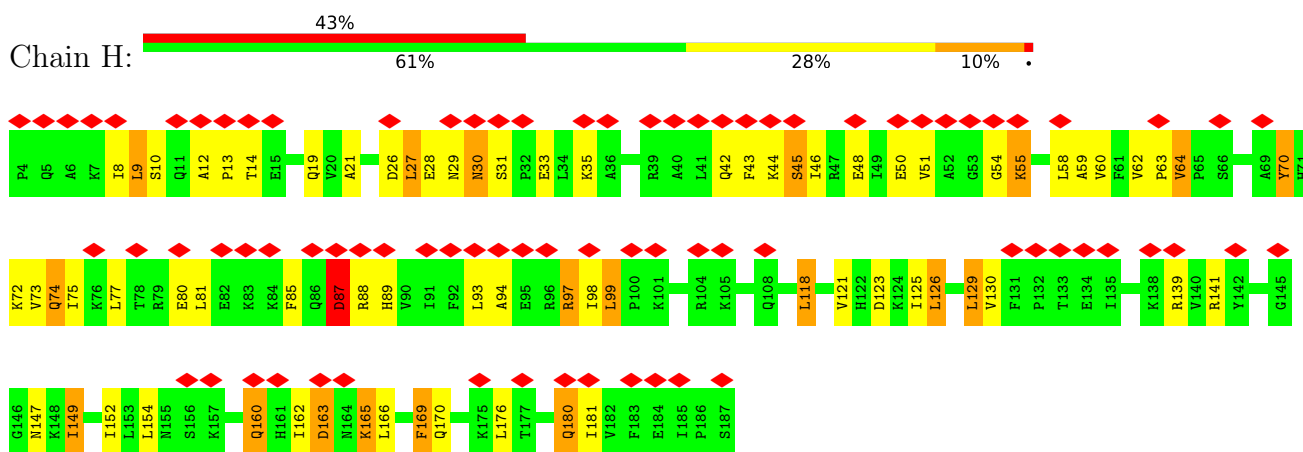
• Molecule 9: KLLA0D10659p



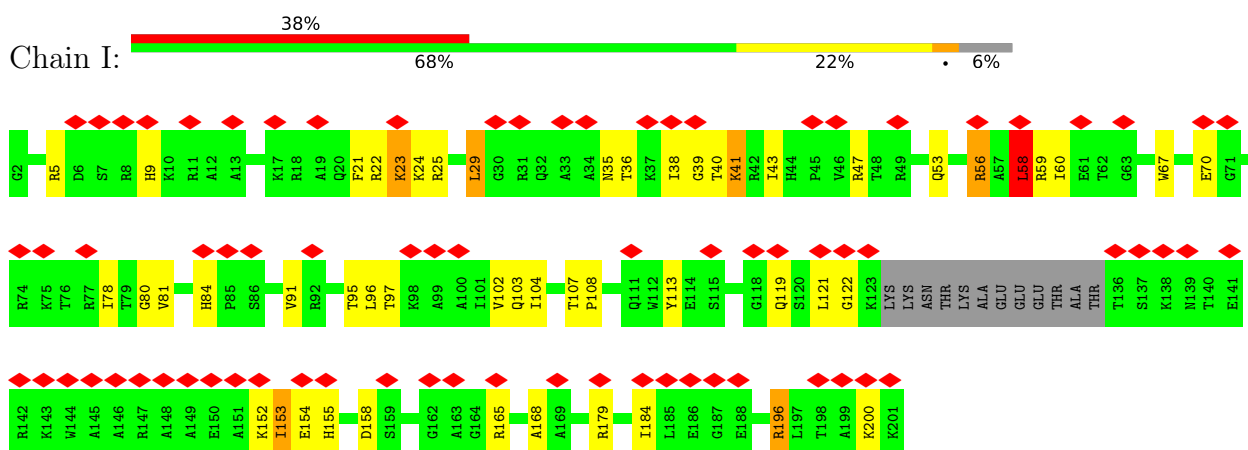
• Molecule 10: 40S ribosomal protein S6



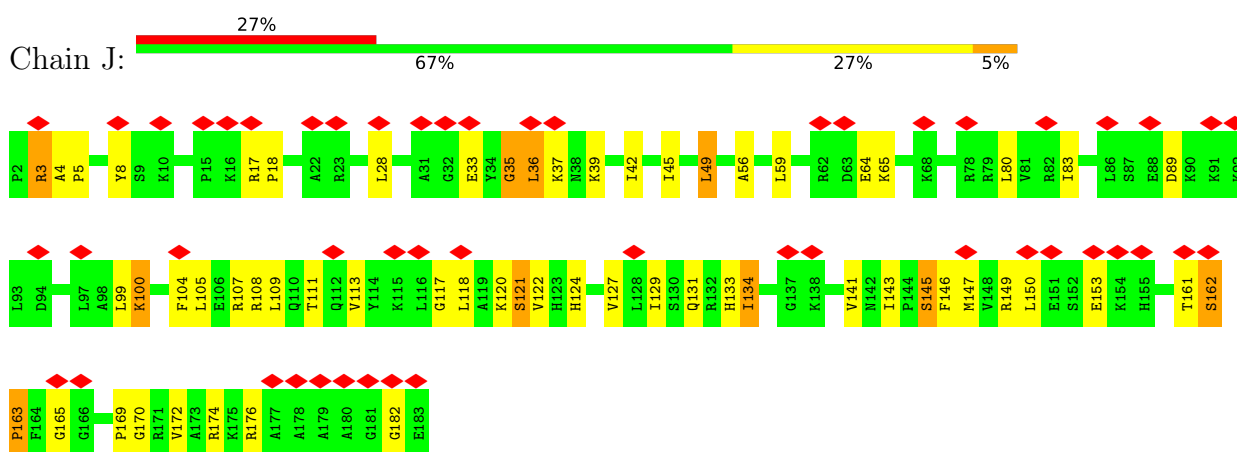
• Molecule 11: 40S ribosomal protein S7



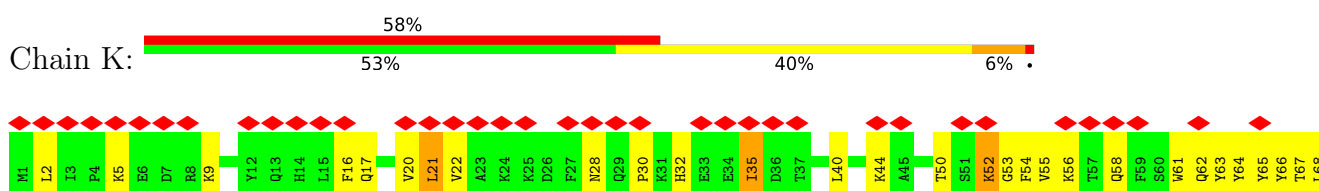
• Molecule 12: 40S ribosomal protein S8

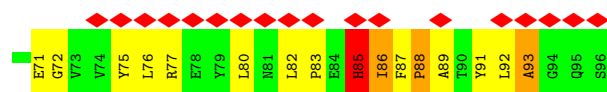


• Molecule 13: KLLA0E23673p

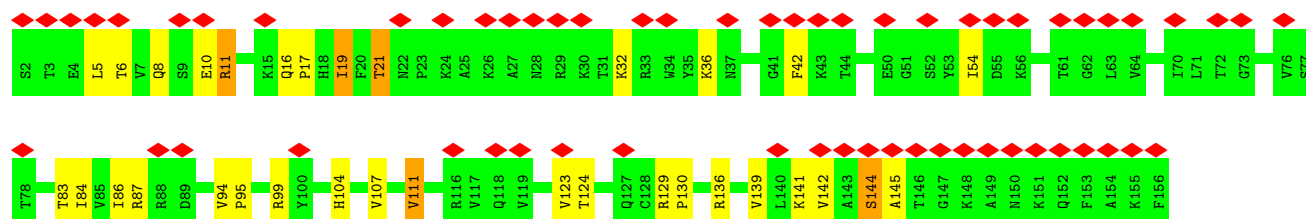
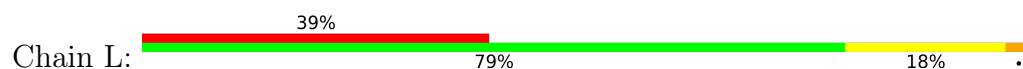


• Molecule 14: KLLA0B08173p

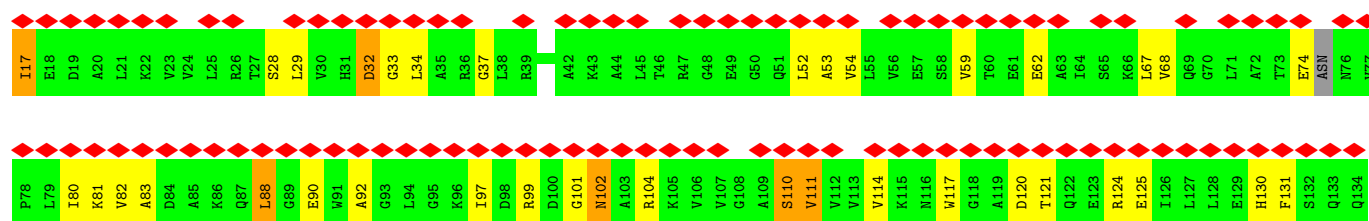
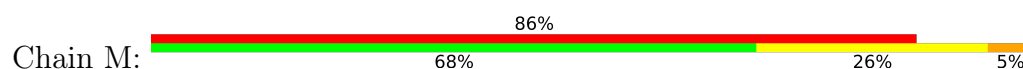




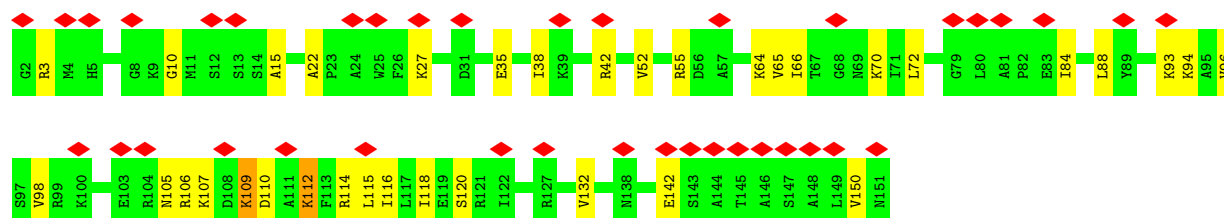
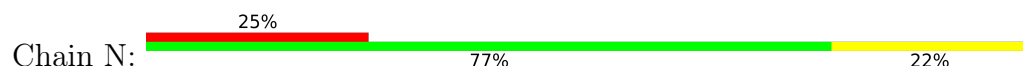
• Molecule 15: KLLA0A10483p



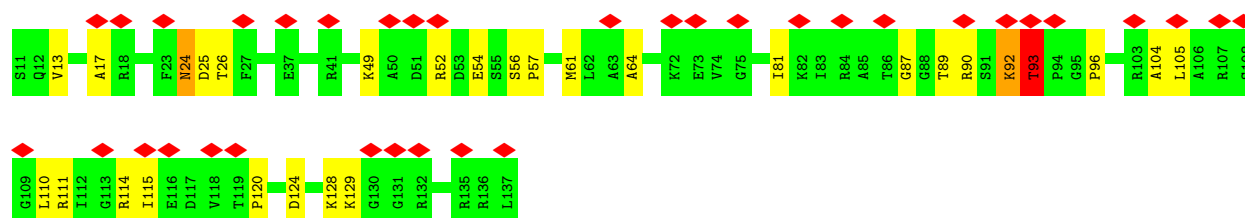
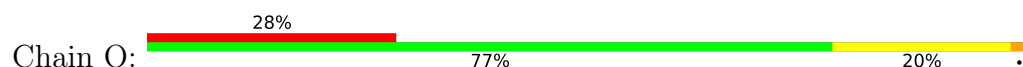
• Molecule 16: 40S ribosomal protein S12



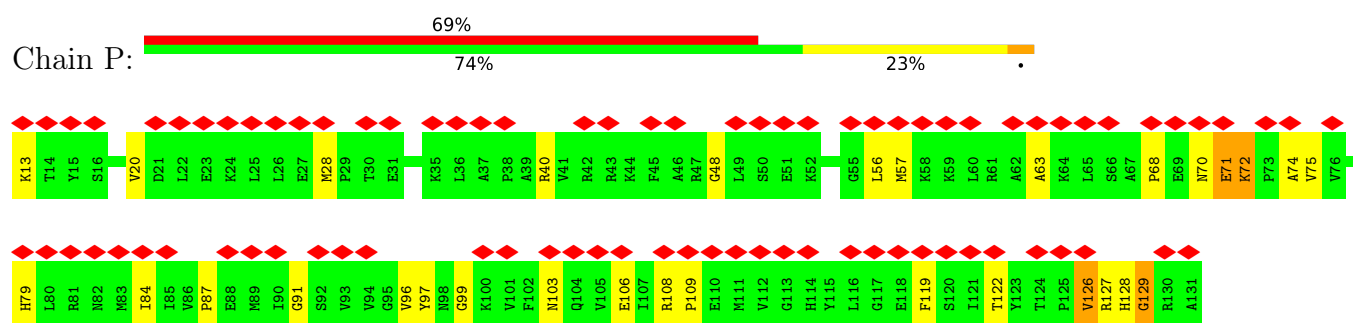
• Molecule 17: KLLA0F18040p



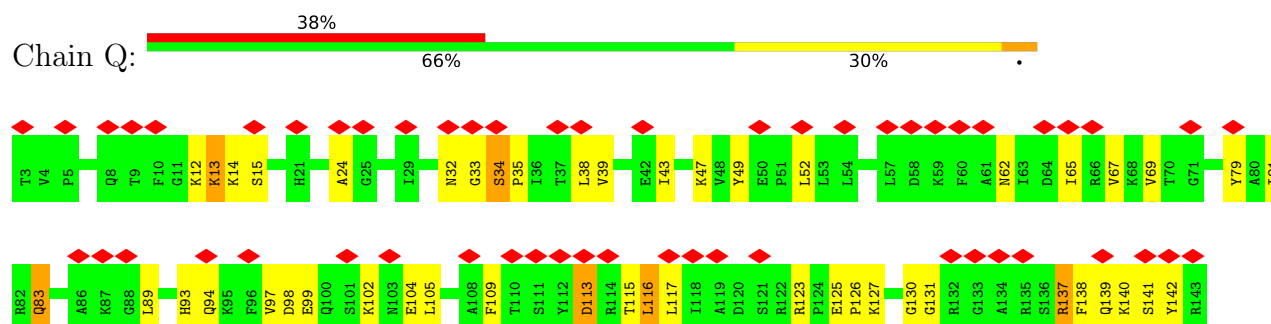
• Molecule 18: 40S ribosomal protein S14



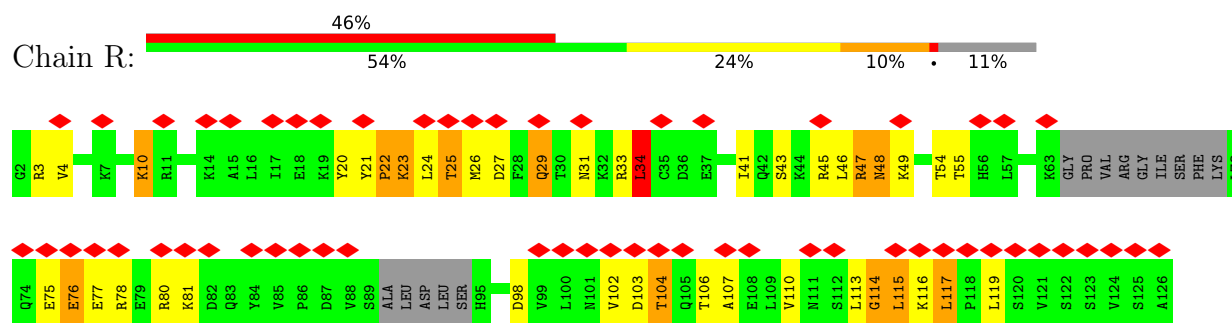
• Molecule 19: KLLA0F07843p



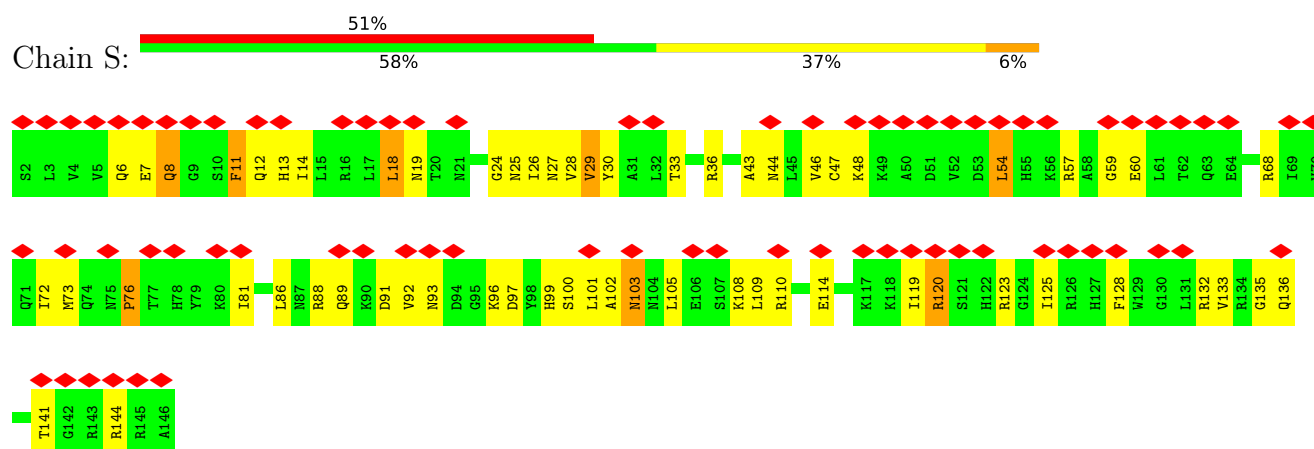
- Molecule 20: 40S ribosomal protein S16



- Molecule 21: KLLA0B01474p

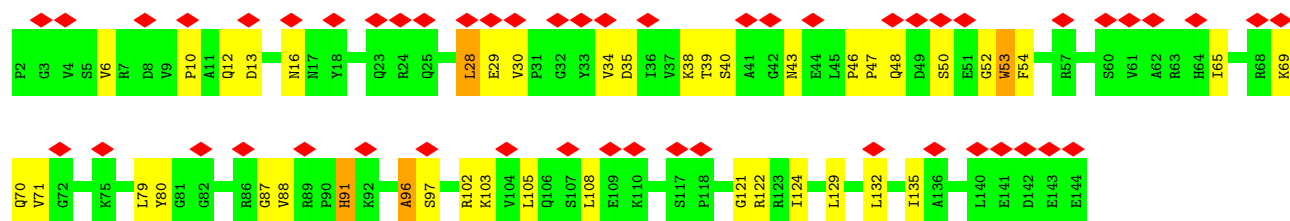


- Molecule 22: KLLA0B01562p

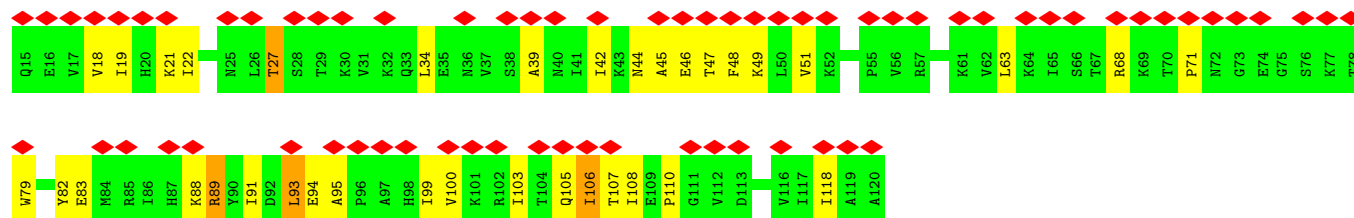


- Molecule 23: KLLA0A07194p

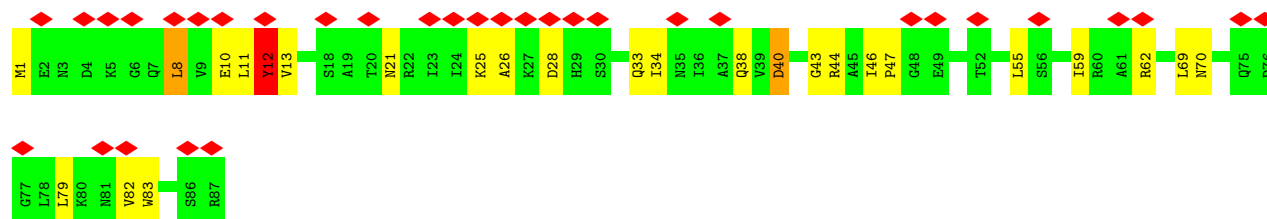
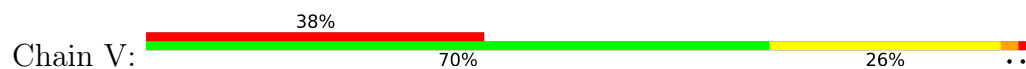




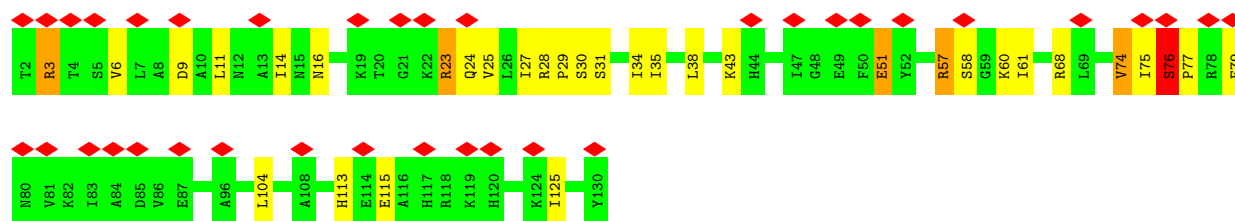
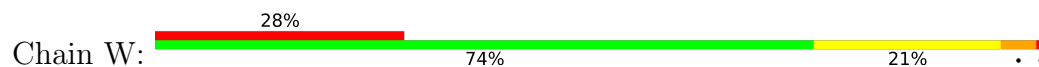
• Molecule 24: KLLA0F25542p



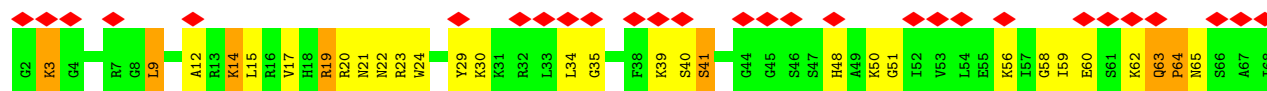
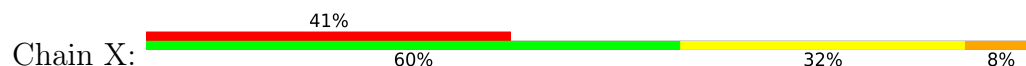
• Molecule 25: 40S ribosomal protein S21

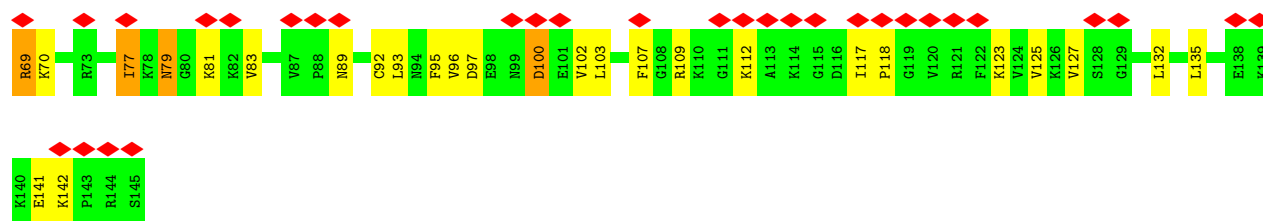


• Molecule 26: 40S ribosomal protein S22

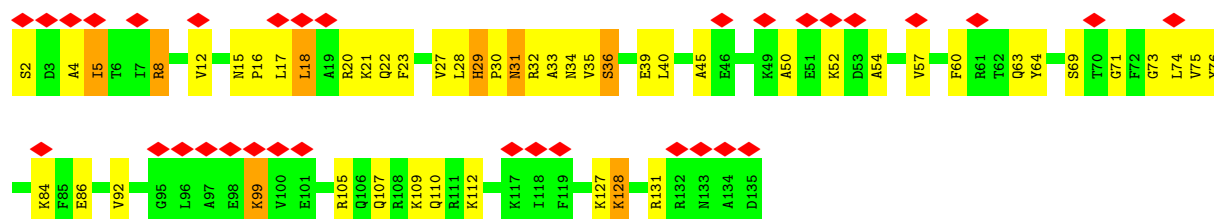


• Molecule 27: KLLA0B11231p

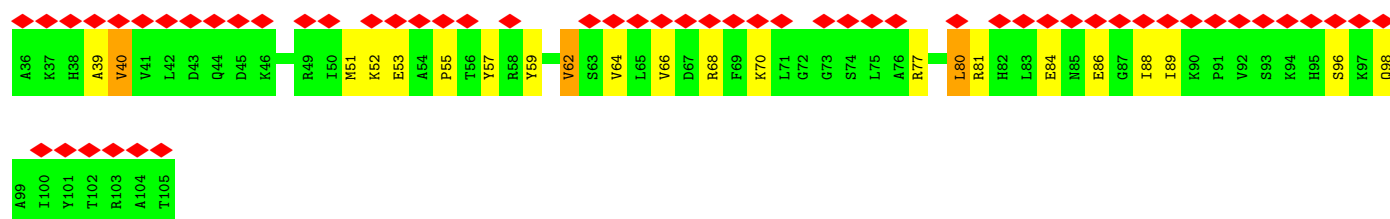
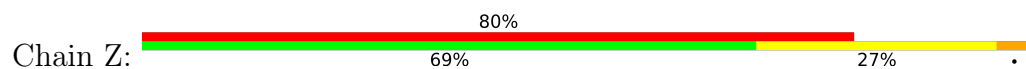




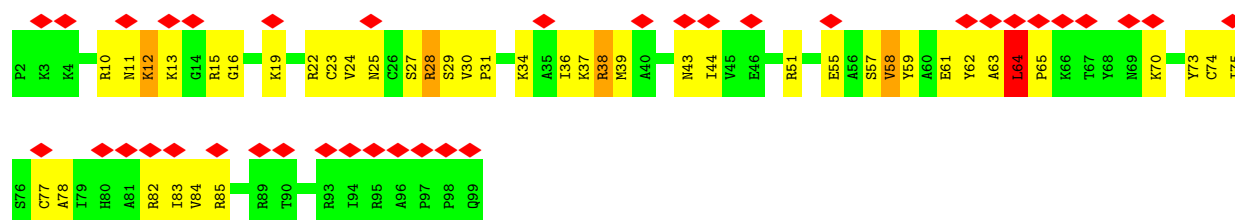
• Molecule 28: 40S ribosomal protein S24



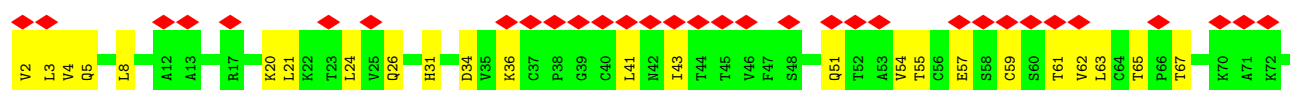
• Molecule 29: KLLA0B06182p

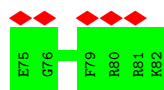


• Molecule 30: 40S ribosomal protein S26

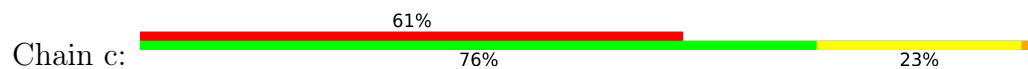


• Molecule 31: 40S ribosomal protein S27





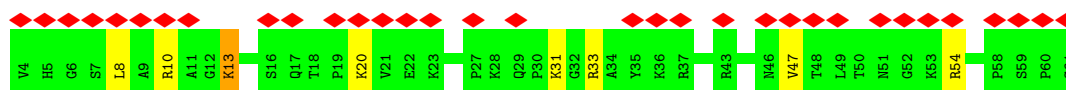
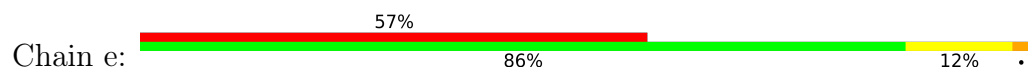
- Molecule 32: 40S ribosomal protein S28



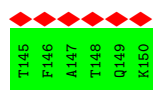
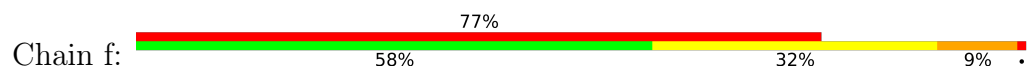
- Molecule 33: 40S ribosomal protein S29



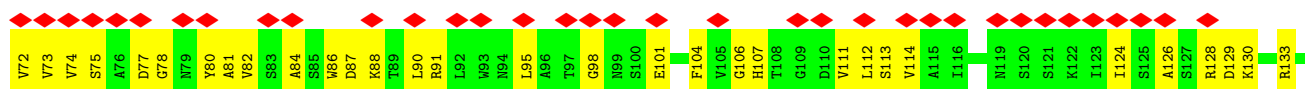
- Molecule 34: 40S ribosomal protein S30

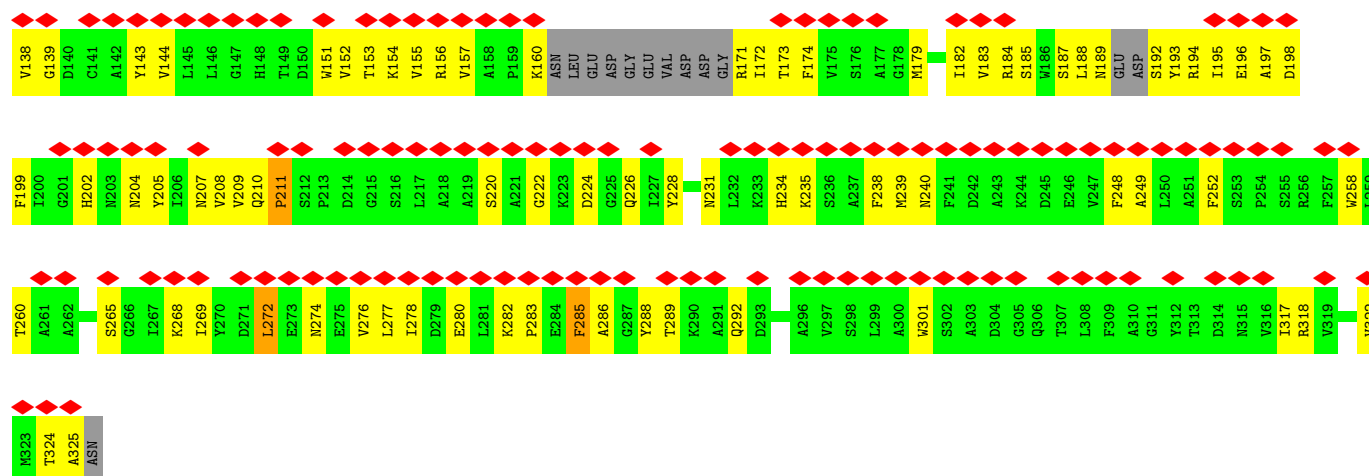


- Molecule 35: Ubiquitin-40S ribosomal protein S27a

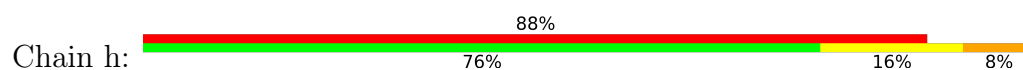


- Molecule 36: KLLA0E12277p

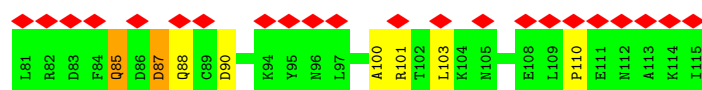
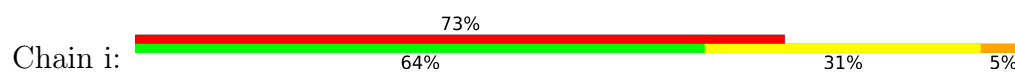




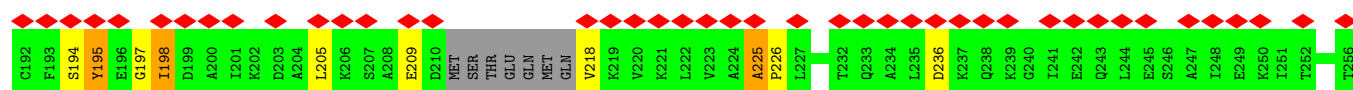
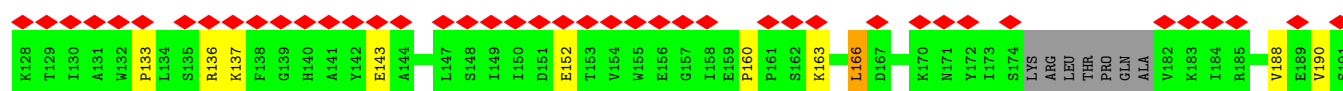
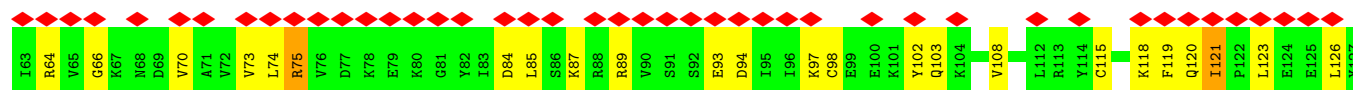
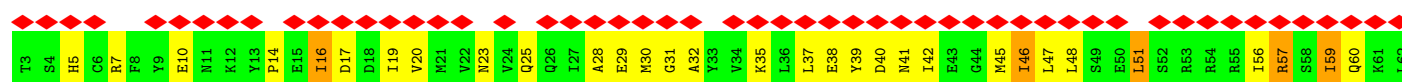
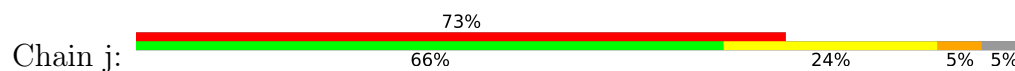
- Molecule 37: 60S ribosomal protein L41-A

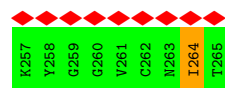


- Molecule 38: Eukaryotic translation initiation factor 1A

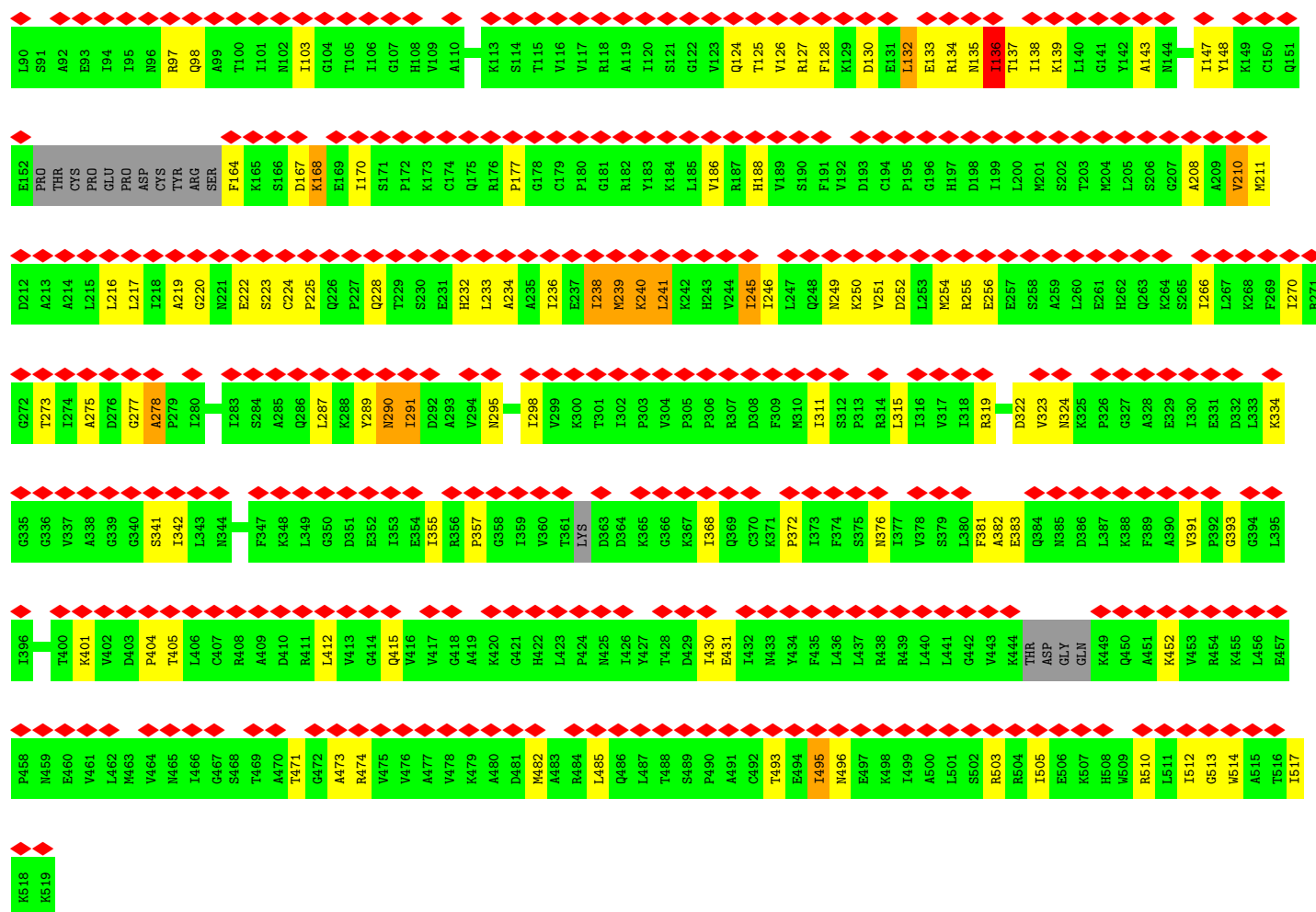
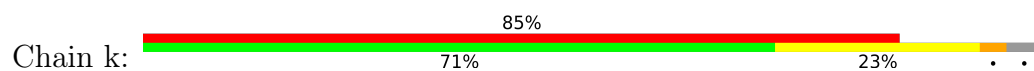


- Molecule 39: Eukaryotic translation initiation factor 2 subunit alpha

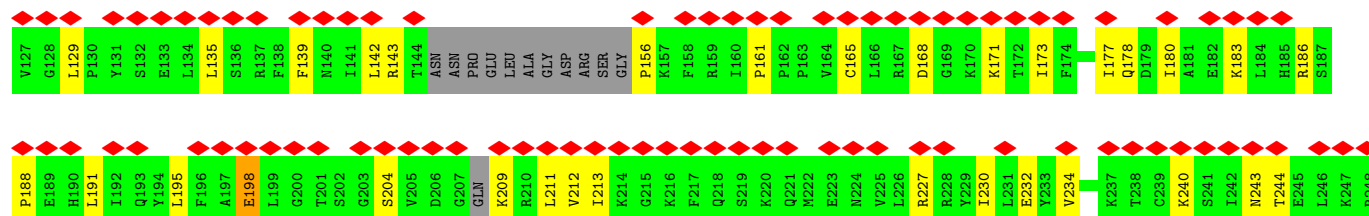


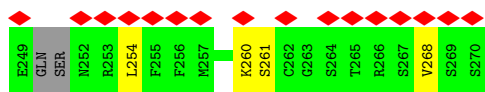


• Molecule 40: Eukaryotic translation initiation factor 2 subunit gamma

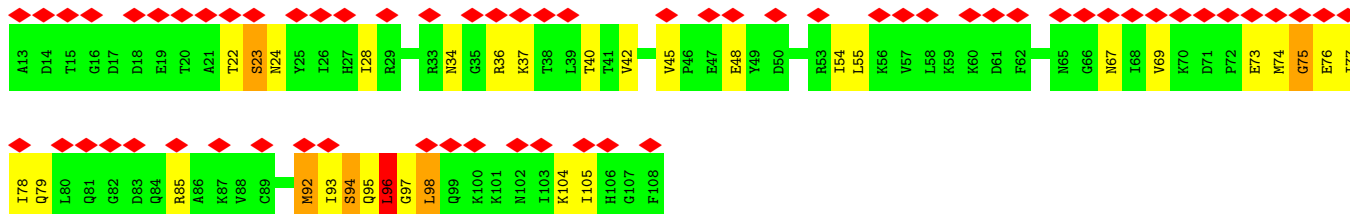


• Molecule 41: Eukaryotic translation initiation factor 2 subunit beta

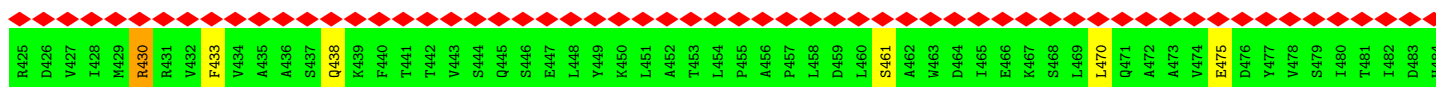
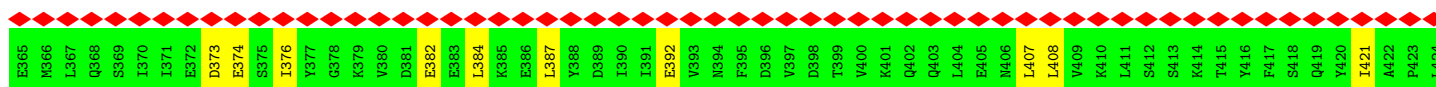
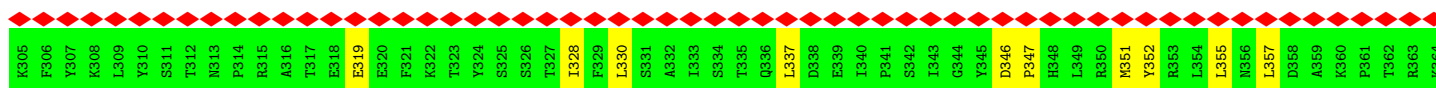
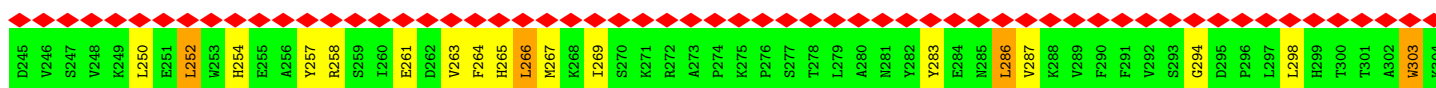
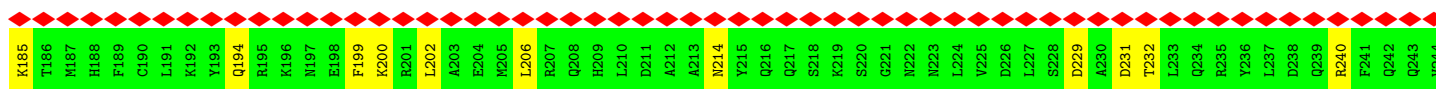
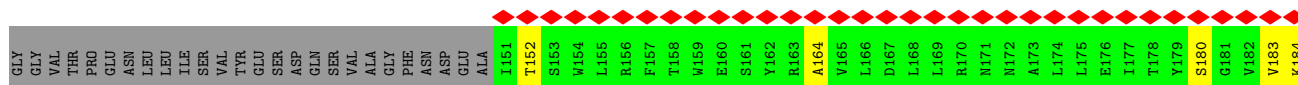
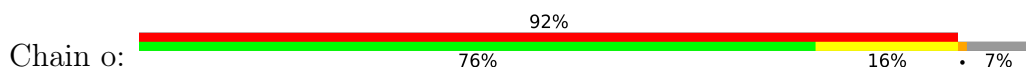


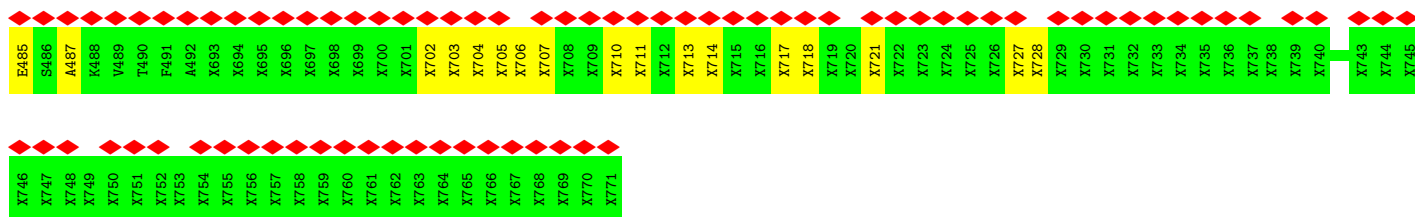


• Molecule 42: Eukaryotic translation initiation factor eIF-1

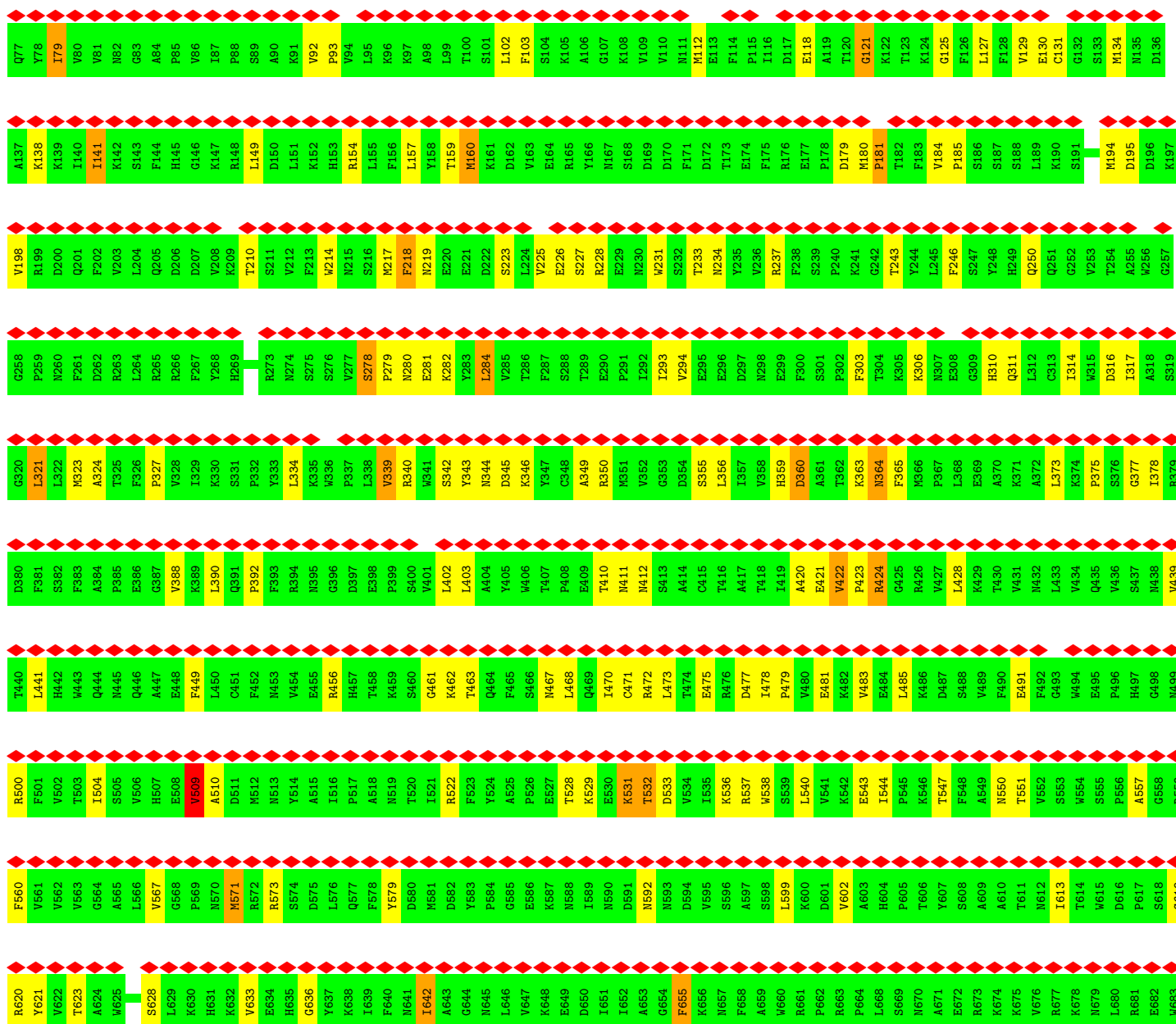
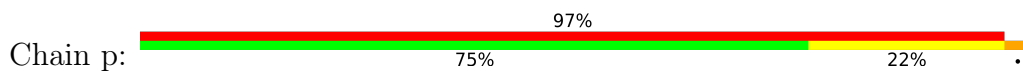


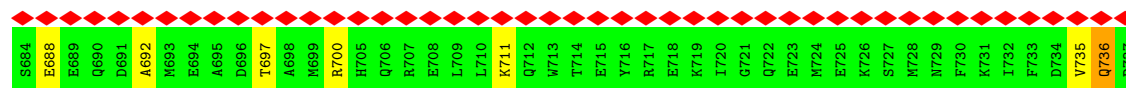
• Molecule 43: Eukaryotic translation initiation factor 3 subunit A, Eukaryotic translation initiation factor 3 subunit A, eIF3a



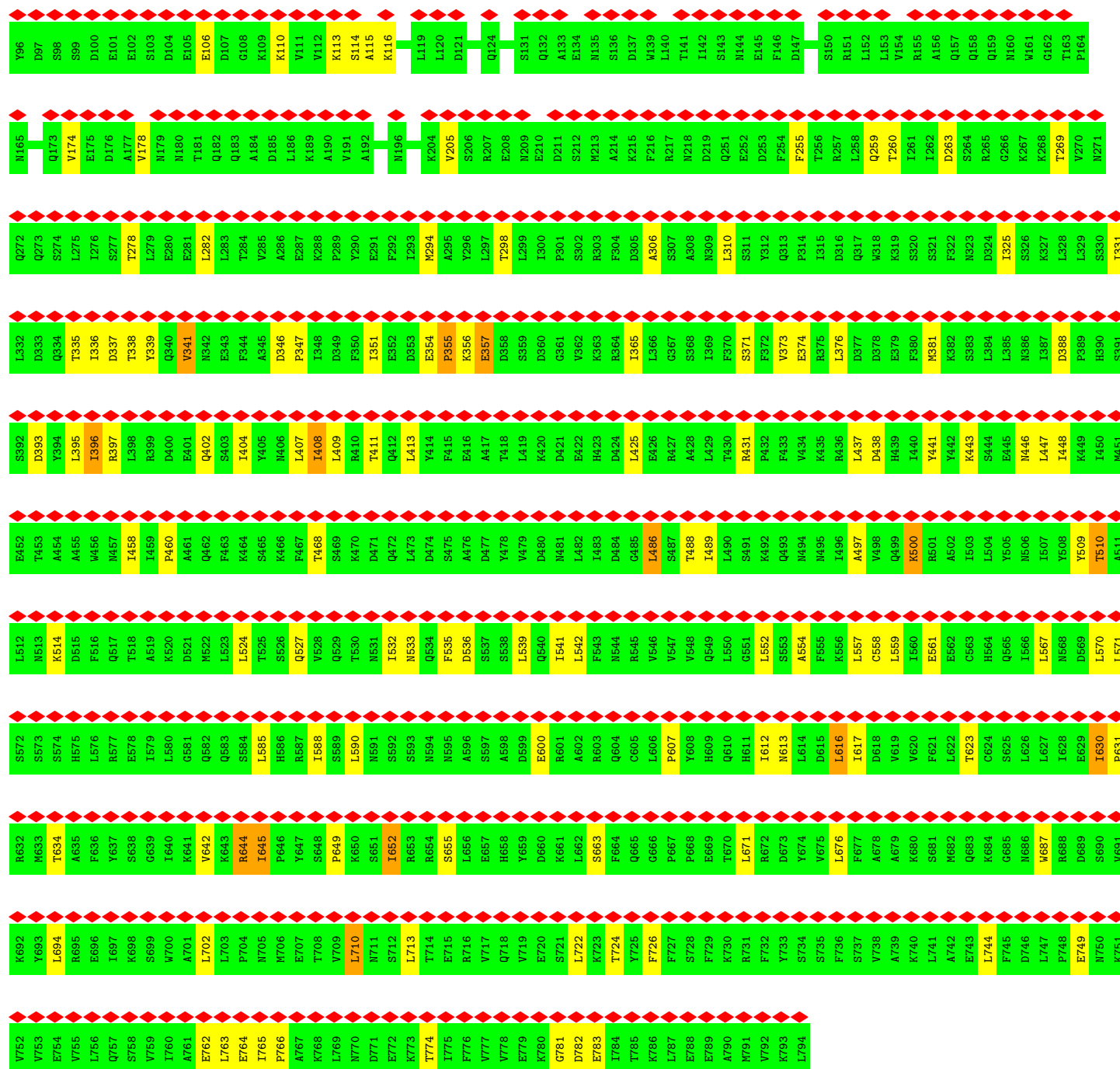
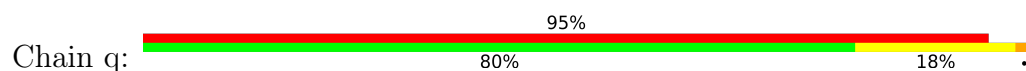


• Molecule 44: Eukaryotic translation initiation factor 3 subunit B





• Molecule 45: Eukaryotic translation initiation factor 3 subunit C



• Molecule 46: Eukaryotic translation initiation factor 3 subunit I

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5750	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.249	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.07	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: 1MA, M2G, RIA, 1MG, GCP, T6A, 7NO, 2MG, H2U, 5MC, 7MG, MG, ZN

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	0.46	1/1504 (0.1%)	0.78	2/2337 (0.1%)
2	2	0.39	0/42691	0.74	33/66521 (0.0%)
3	A	0.61	0/1666	0.99	0/2279
4	3	0.43	0/71	0.72	0/108
5	B	0.61	0/1793	0.97	1/2414 (0.0%)
6	C	0.59	0/1659	1.03	5/2252 (0.2%)
7	D	0.64	0/1769	0.98	0/2378
8	E	0.57	0/2122	0.94	4/2861 (0.1%)
9	F	0.62	0/1628	1.09	0/2198
10	G	0.56	0/1835	0.92	1/2451 (0.0%)
11	H	0.62	0/1507	1.02	4/2028 (0.2%)
12	I	0.58	0/1515	0.95	2/2029 (0.1%)
13	J	0.55	0/1495	1.08	3/2001 (0.1%)
14	K	0.65	0/831	1.03	2/1123 (0.2%)
15	L	0.61	0/1276	0.90	2/1718 (0.1%)
16	M	0.66	0/891	0.98	1/1201 (0.1%)
17	N	0.55	0/1210	1.07	2/1628 (0.1%)
18	O	0.61	0/953	1.00	1/1279 (0.1%)
19	P	0.70	0/962	0.99	1/1294 (0.1%)
20	Q	0.62	0/1125	1.04	2/1510 (0.1%)
21	R	0.65	0/899	1.06	3/1204 (0.2%)
22	S	0.65	0/1212	1.01	1/1629 (0.1%)
23	T	0.63	0/1129	1.10	2/1520 (0.1%)
24	U	0.63	0/857	1.01	2/1158 (0.2%)
25	V	0.52	0/696	0.93	0/938
26	W	0.55	0/1039	1.00	2/1399 (0.1%)
27	X	0.66	0/1137	1.03	2/1516 (0.1%)
28	Y	0.58	0/1075	1.00	3/1433 (0.2%)
29	Z	0.67	0/567	1.05	1/762 (0.1%)
30	a	0.69	0/791	1.11	6/1059 (0.6%)
31	b	0.60	0/619	0.89	0/837
32	c	0.68	0/489	0.88	0/655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.61	0/457	0.88	1/607 (0.2%)
34	e	0.64	0/471	0.95	0/628
35	f	0.81	0/562	1.20	7/751 (0.9%)
36	g	0.40	0/2459	0.74	4/3348 (0.1%)
37	h	0.58	0/234	0.95	0/300
38	i	0.66	0/775	1.02	5/1034 (0.5%)
39	j	0.71	0/2034	0.95	1/2737 (0.0%)
40	k	0.81	1/3168 (0.0%)	0.98	5/4281 (0.1%)
41	l	0.74	0/1064	0.87	0/1420
42	m	0.67	0/744	0.94	1/997 (0.1%)
43	o	0.82	0/3729	0.92	0/5041
44	p	0.78	1/5225 (0.0%)	0.94	4/7101 (0.1%)
45	q	0.82	0/5132	0.96	4/6965 (0.1%)
46	s	0.52	0/2669	0.71	0/3611
47	r	0.43	0/399	0.68	0/535
All	All	0.57	3/108135 (0.0%)	0.87	120/155076 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	k	254	MET	N-CA	5.15	1.52	1.46
1	1	37	T6A	O3'-P	5.12	1.61	1.56
44	p	532	THR	C-O	-5.03	1.17	1.24

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	k	238	ILE	N-CA-C	12.25	122.19	110.30
13	J	161	THR	N-CA-C	11.98	124.08	111.14
40	k	256	GLU	N-CA-C	11.04	123.06	111.14
23	T	53	TRP	N-CA-C	10.54	122.85	111.36
40	k	239	MET	N-CA-C	10.40	122.37	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1617	0	841	9	0
2	2	38175	0	19208	307	0
3	A	1626	0	1633	85	0
4	3	64	0	33	0	0
5	B	1769	0	1829	49	0
6	C	1629	0	1710	51	0
7	D	1744	0	1826	35	0
8	E	2078	0	2157	79	0
9	F	1609	0	1679	49	0
10	G	1812	0	1911	52	0
11	H	1483	0	1579	60	0
12	I	1489	0	1504	52	0
13	J	1471	0	1554	40	0
14	K	809	0	810	75	0
15	L	1248	0	1311	20	0
16	M	885	0	917	31	0
17	N	1187	0	1251	13	0
18	O	942	0	979	13	0
19	P	943	0	989	15	0
20	Q	1105	0	1170	32	0
21	R	892	0	932	50	0
22	S	1193	0	1217	76	0
23	T	1110	0	1124	41	0
24	U	845	0	913	36	0
25	V	687	0	682	34	0
26	W	1021	0	1056	38	0
27	X	1119	0	1198	66	0
28	Y	1061	0	1110	55	0
29	Z	558	0	585	42	0
30	a	779	0	830	72	0
31	b	609	0	631	13	0
32	c	487	0	528	16	0
33	d	446	0	436	35	0
34	e	463	0	503	7	0
35	f	549	0	563	62	0
36	g	2403	0	2352	259	0
37	h	233	0	284	4	0
38	i	765	0	769	40	0
39	j	2006	0	2066	86	0
40	k	3123	0	3235	136	0
41	l	1048	0	1090	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	m	736	0	744	20	0
43	o	4051	0	3794	30	0
44	p	5092	0	4865	111	0
45	q	5051	0	4764	48	0
46	s	2606	0	2528	0	0
47	r	392	0	382	0	0
48	1	30	0	0	3	0
49	2	76	0	0	0	0
49	C	3	0	0	0	0
49	O	1	0	0	0	0
49	Q	1	0	0	0	0
49	k	1	0	0	0	0
50	O	1	0	0	0	0
50	b	1	0	0	0	0
50	f	1	0	0	0	0
50	l	1	0	0	0	0
51	k	32	0	14	6	0
All	All	103158	0	84086	2312	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 2312 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:157:VAL:HG22	36:g:174:PHE:CE1	1.10	1.62
27:X:92:CYS:CA	27:X:95:PHE:CD1	1.86	1.56
40:k:128:PHE:CE1	40:k:132:LEU:HD11	1.37	1.55
28:Y:29:HIS:CD2	28:Y:34:ASN:O	1.64	1.50
36:g:154:LYS:NZ	36:g:208:VAL:HB	1.20	1.47

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	206/208 (99%)	185 (90%)	16 (8%)	5 (2%)	4	26
5	B	218/231 (94%)	190 (87%)	20 (9%)	8 (4%)	2	19
6	C	215/217 (99%)	196 (91%)	12 (6%)	7 (3%)	3	20
7	D	221/223 (99%)	193 (87%)	19 (9%)	9 (4%)	2	17
8	E	258/260 (99%)	231 (90%)	26 (10%)	1 (0%)	30	66
9	F	204/206 (99%)	182 (89%)	17 (8%)	5 (2%)	4	25
10	G	224/226 (99%)	204 (91%)	19 (8%)	1 (0%)	30	66
11	H	182/184 (99%)	158 (87%)	16 (9%)	8 (4%)	2	16
12	I	184/200 (92%)	165 (90%)	16 (9%)	3 (2%)	7	36
13	J	180/182 (99%)	161 (89%)	12 (7%)	7 (4%)	2	18
14	K	94/96 (98%)	82 (87%)	9 (10%)	3 (3%)	3	20
15	L	153/155 (99%)	140 (92%)	13 (8%)	0	100	100
16	M	113/118 (96%)	88 (78%)	22 (20%)	3 (3%)	4	24
17	N	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
18	O	125/127 (98%)	112 (90%)	11 (9%)	2 (2%)	7	36
19	P	117/119 (98%)	86 (74%)	24 (20%)	7 (6%)	1	12
20	Q	139/141 (99%)	120 (86%)	16 (12%)	3 (2%)	5	27
21	R	105/125 (84%)	87 (83%)	11 (10%)	7 (7%)	1	11
22	S	143/145 (99%)	125 (87%)	16 (11%)	2 (1%)	9	38
23	T	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	9	38
24	U	104/106 (98%)	94 (90%)	9 (9%)	1 (1%)	12	47
25	V	85/87 (98%)	76 (89%)	8 (9%)	1 (1%)	10	42
26	W	127/129 (98%)	115 (91%)	9 (7%)	3 (2%)	4	26
27	X	142/144 (99%)	124 (87%)	13 (9%)	5 (4%)	3	20
28	Y	132/134 (98%)	118 (89%)	11 (8%)	3 (2%)	5	27
29	Z	68/70 (97%)	62 (91%)	5 (7%)	1 (2%)	8	38
30	a	96/98 (98%)	82 (85%)	11 (12%)	3 (3%)	3	21
31	b	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
32	c	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
33	d	51/53 (96%)	41 (80%)	9 (18%)	1 (2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	e	56/58 (97%)	45 (80%)	10 (18%)	1 (2%)	6	32
35	f	67/69 (97%)	46 (69%)	17 (25%)	4 (6%)	1	12
36	g	305/324 (94%)	289 (95%)	16 (5%)	0	100	100
37	h	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
38	i	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	11	45
39	j	243/263 (92%)	207 (85%)	32 (13%)	4 (2%)	7	36
40	k	406/430 (94%)	345 (85%)	52 (13%)	9 (2%)	5	27
41	l	122/144 (85%)	100 (82%)	20 (16%)	2 (2%)	7	36
42	m	94/96 (98%)	74 (79%)	16 (17%)	4 (4%)	2	16
43	o	445/567 (78%)	371 (83%)	68 (15%)	6 (1%)	9	40
44	p	643/651 (99%)	537 (84%)	86 (13%)	20 (3%)	3	21
45	q	657/665 (99%)	537 (82%)	98 (15%)	22 (3%)	3	20
46	s	326/342 (95%)	318 (98%)	8 (2%)	0	100	100
47	r	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
All	All	7841/8198 (96%)	6836 (87%)	831 (11%)	174 (2%)	7	27

5 of 174 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	26	ARG
5	B	210	VAL
6	C	235	TRP
7	D	195	ASN
9	F	46	ASN

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	
3	A	174/176 (99%)	148 (85%)	26 (15%)	3	13
5	B	198/210 (94%)	170 (86%)	28 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	C	176/176 (100%)	151 (86%)	25 (14%)	3	14
7	D	185/185 (100%)	152 (82%)	33 (18%)	2	10
8	E	223/223 (100%)	187 (84%)	36 (16%)	2	12
9	F	174/174 (100%)	142 (82%)	32 (18%)	1	9
10	G	192/192 (100%)	165 (86%)	27 (14%)	3	14
11	H	164/164 (100%)	132 (80%)	32 (20%)	1	8
12	I	147/158 (93%)	134 (91%)	13 (9%)	9	29
13	J	153/153 (100%)	132 (86%)	21 (14%)	3	14
14	K	88/88 (100%)	76 (86%)	12 (14%)	3	15
15	L	136/136 (100%)	123 (90%)	13 (10%)	8	25
16	M	93/94 (99%)	85 (91%)	8 (9%)	10	29
17	N	127/127 (100%)	111 (87%)	16 (13%)	4	17
18	O	96/96 (100%)	86 (90%)	10 (10%)	7	22
19	P	101/101 (100%)	90 (89%)	11 (11%)	6	21
20	Q	117/117 (100%)	101 (86%)	16 (14%)	3	14
21	R	102/113 (90%)	91 (89%)	11 (11%)	6	21
22	S	128/128 (100%)	113 (88%)	15 (12%)	5	19
23	T	117/117 (100%)	106 (91%)	11 (9%)	8	26
24	U	96/96 (100%)	91 (95%)	5 (5%)	21	42
25	V	73/73 (100%)	64 (88%)	9 (12%)	4	17
26	W	110/110 (100%)	98 (89%)	12 (11%)	6	21
27	X	119/119 (100%)	105 (88%)	14 (12%)	5	18
28	Y	108/108 (100%)	94 (87%)	14 (13%)	4	16
29	Z	60/60 (100%)	58 (97%)	2 (3%)	33	55
30	a	83/83 (100%)	79 (95%)	4 (5%)	23	44
31	b	71/71 (100%)	63 (89%)	8 (11%)	5	20
32	c	54/54 (100%)	50 (93%)	4 (7%)	13	33
33	d	46/46 (100%)	46 (100%)	0	100	100
34	e	51/51 (100%)	46 (90%)	5 (10%)	7	24
35	f	58/60 (97%)	52 (90%)	6 (10%)	7	23
36	g	257/270 (95%)	255 (99%)	2 (1%)	73	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	h	23/23 (100%)	21 (91%)	2 (9%)	9	29
38	i	81/81 (100%)	71 (88%)	10 (12%)	4	17
39	j	224/237 (94%)	200 (89%)	24 (11%)	6	21
40	k	332/364 (91%)	311 (94%)	21 (6%)	16	37
41	l	120/132 (91%)	110 (92%)	10 (8%)	10	30
42	m	76/84 (90%)	68 (90%)	8 (10%)	6	22
43	o	404/438 (92%)	359 (89%)	45 (11%)	6	20
44	p	533/584 (91%)	486 (91%)	47 (9%)	9	29
45	q	509/615 (83%)	445 (87%)	64 (13%)	4	17
46	s	287/297 (97%)	286 (100%)	1 (0%)	86	84
47	r	40/40 (100%)	40 (100%)	0	100	100
All	All	6706/7024 (96%)	5993 (89%)	713 (11%)	9	22

5 of 713 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	b	67	THR
43	o	232	THR
35	f	108	VAL
31	b	65	THR
40	k	147	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
38	i	33	GLN
43	o	419	GLN
39	j	23	ASN
40	k	422	HIS
44	p	432	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	71/76 (93%)	33 (46%)	9 (12%)
2	2	1797/1798 (99%)	817 (45%)	70 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	3	2/3 (66%)	0	0
All	All	1870/1877 (99%)	850 (45%)	79 (4%)

5 of 850 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	5	C
1	1	9	1MG
1	1	10	2MG
1	1	11	C
1	1	12	G

5 of 79 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1123	A
2	2	1534	G
2	2	1198	G
2	2	1411	U
2	2	1678	G

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

11 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
1	H2U	1	47	1	18,21,22	0.73	0	19,30,33	1.36	2 (10%)
1	1MA	1	58	1	21,25,26	1.54	4 (19%)	30,37,40	1.87	5 (16%)
1	H2U	1	16	1	18,21,22	0.82	0	19,30,33	1.47	4 (21%)
1	1MG	1	9	1	23,26,27	1.45	3 (13%)	33,39,42	2.09	9 (27%)
1	T6A	1	37	1	31,34,35	1.54	4 (12%)	43,49,52	2.30	13 (30%)
1	RIA	1	64	1	35,38,39	1.34	4 (11%)	50,57,60	1.96	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	1	10	1	23,26,27	1.35	4 (17%)	33,38,41	2.31	7 (21%)
1	7MG	1	46	1	23,26,27	1.49	4 (17%)	27,39,42	2.66	7 (25%)
1	M2G	1	26	1	24,27,28	1.40	4 (16%)	33,40,43	2.03	7 (21%)
1	5MC	1	49	1	19,22,23	2.33	4 (21%)	26,32,35	1.53	2 (7%)
1	5MC	1	48	1	19,22,23	1.94	1 (5%)	26,32,35	1.54	6 (23%)

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
1	H2U	1	47	1	-	5/7/38/39	0/2/2/2
1	1MA	1	58	1	-	2/7/25/26	0/3/3/3
1	H2U	1	16	1	-	2/7/38/39	0/2/2/2
1	1MG	1	9	1	-	3/7/25/26	0/3/3/3
1	T6A	1	37	1	-	11/23/41/42	0/3/3/3
1	RIA	1	64	1	-	9/17/51/52	0/4/4/4
1	2MG	1	10	1	-	2/9/27/28	0/3/3/3
1	7MG	1	46	1	-	2/7/37/38	0/3/3/3
1	M2G	1	26	1	-	5/11/29/30	0/3/3/3
1	5MC	1	49	1	-	1/7/25/26	0/2/2/2
1	5MC	1	48	1	-	0/7/25/26	0/2/2/2

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	49	5MC	C5-C4	8.24	1.50	1.44
1	1	48	5MC	C5-C4	7.24	1.49	1.44
1	1	37	T6A	C5-C4	5.48	1.48	1.39
1	1	64	RIA	C5-C4	5.16	1.48	1.39
1	1	26	M2G	C2-N2	3.73	1.42	1.35

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	46	7MG	N9-C4-N3	8.78	138.32	125.46
1	1	10	2MG	C2-N3-C4	7.93	121.91	112.00
1	1	10	2MG	C5-C4-N3	-6.41	118.18	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	26	M2G	C5-C4-N3	-6.28	118.39	128.39
1	1	37	T6A	C5-C4-N3	-6.15	118.25	126.72

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	16	H2U	O4'-C4'-C5'-O5'
1	1	26	M2G	N1-C2-N2-CM1
1	1	26	M2G	N3-C2-N2-CM1
1	1	26	M2G	N3-C2-N2-CM2
1	1	37	T6A	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	16	H2U	1	0
1	1	64	RIA	2	0
1	1	48	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 86 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
51	GCP	k	602	49	32,34,34	1.56	7 (21%)	49,54,54	1.82	7 (14%)
48	7NO	1	101	1	29,32,33	1.42	1 (3%)	38,45,48	5.21	3 (7%)

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
51	GCP	k	602	49	-	7/19/38/38	0/3/3/3
48	7NO	1	101	1	-	6/19/37/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	1	101	7NO	O3'-C	7.35	1.51	1.34
51	k	602	GCP	C5-C4	3.46	1.48	1.38
51	k	602	GCP	PG-O2G	3.27	1.62	1.55
51	k	602	GCP	PA-O3A	3.18	1.62	1.59
51	k	602	GCP	PB-O3A	2.84	1.61	1.58

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	1	101	7NO	C3'-O3'-C	25.27	159.74	117.76
48	1	101	7NO	O3'-C-O	-16.42	94.30	123.95
48	1	101	7NO	O3'-C-CA	10.78	135.89	111.41
51	k	602	GCP	C5-C4-N3	-6.67	117.78	128.39
51	k	602	GCP	C2-N3-C4	5.48	121.74	112.30

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

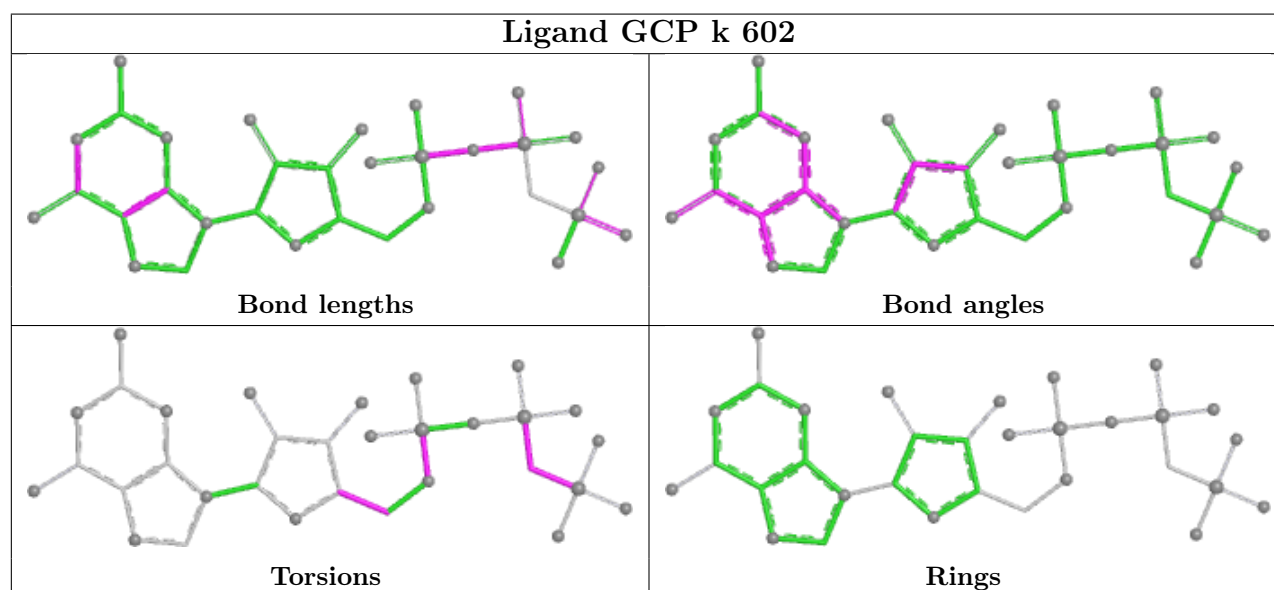
Mol	Chain	Res	Type	Atoms
48	1	101	7NO	C4'-C3'-O3'-C
48	1	101	7NO	CA-C-O3'-C3'
48	1	101	7NO	O-C-O3'-C3'
51	k	602	GCP	PG-C3B-PB-O2B
51	k	602	GCP	C5'-O5'-PA-O1A

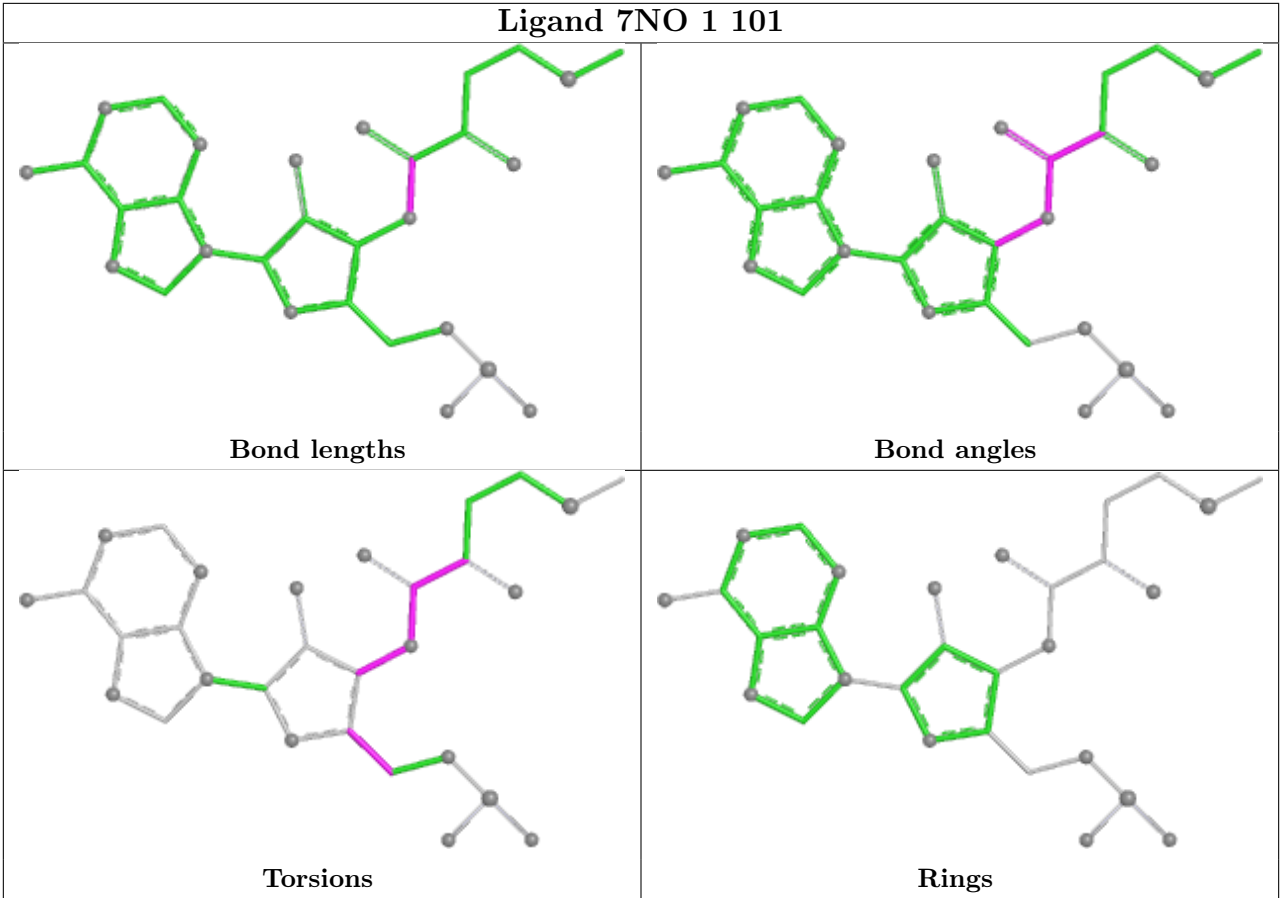
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	k	602	GCP	6	0
48	1	101	7NO	3	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
45	q	3
44	p	3
1	1	2
43	o	1

The worst 5 of 9 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	236.15
1	q	219:ASP	C	251:GLN	N	49.57
1	q	186:LEU	C	189:LYS	N	9.27

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	p	700:ARG	C	705:HIS	N	8.32
1	1	64:RIA	O3'	65:G	P	6.22

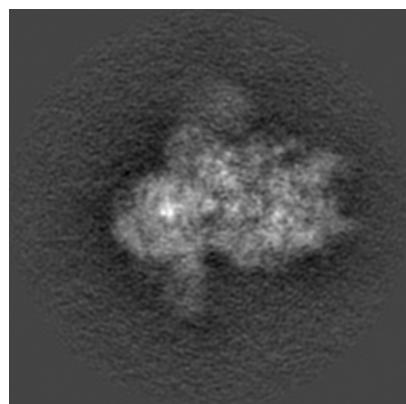
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0057. These allow visual inspection of the internal detail of the map and identification of artifacts.

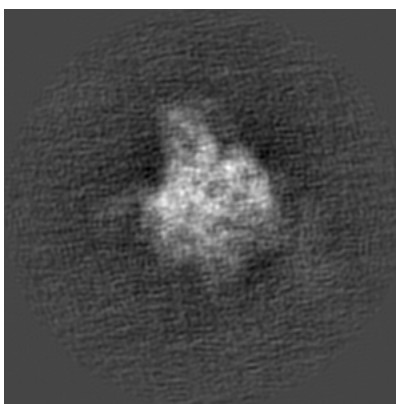
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

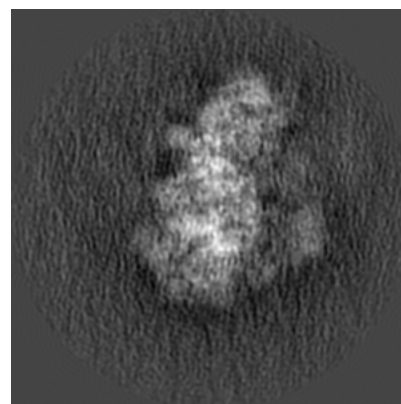
6.1.1 Primary map



X

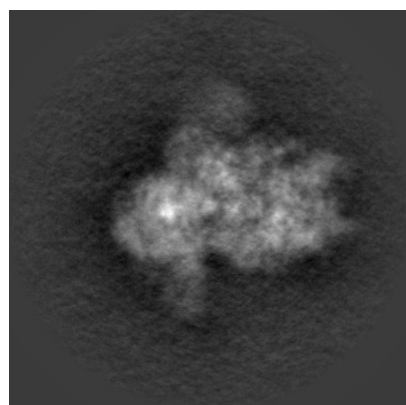


Y

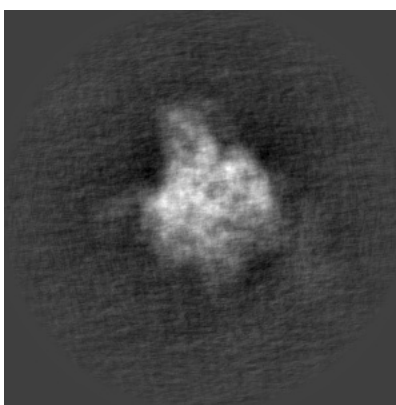


Z

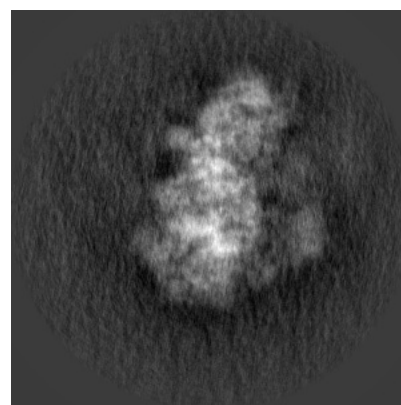
6.1.2 Raw map



X



Y

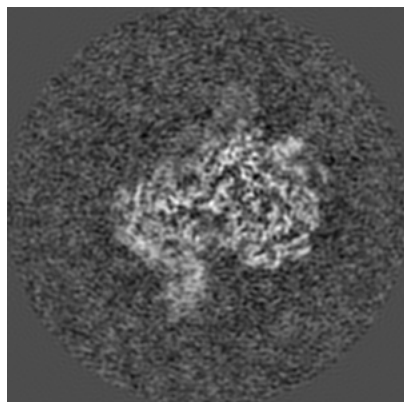


Z

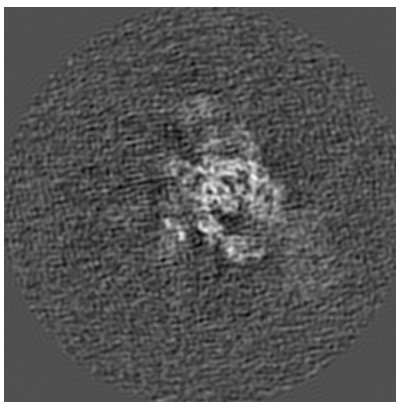
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

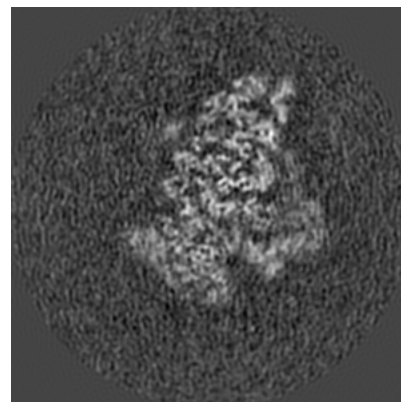
6.2.1 Primary map



X Index: 150

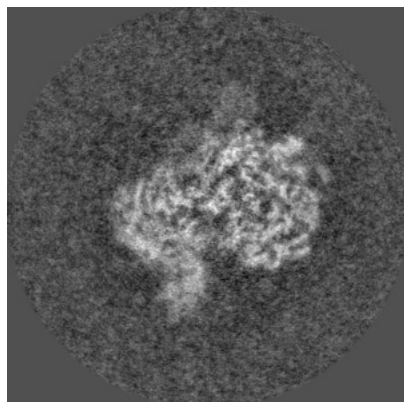


Y Index: 150

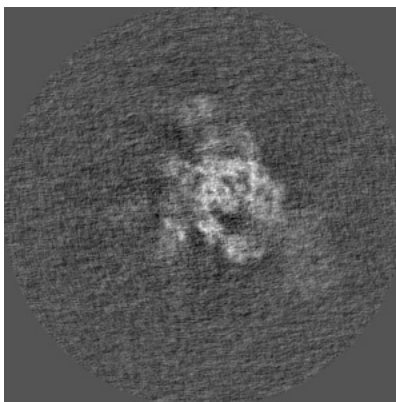


Z Index: 150

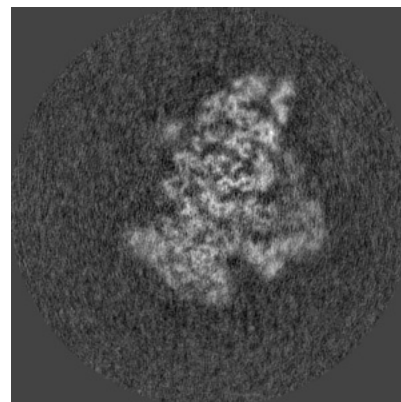
6.2.2 Raw map



X Index: 150



Y Index: 150

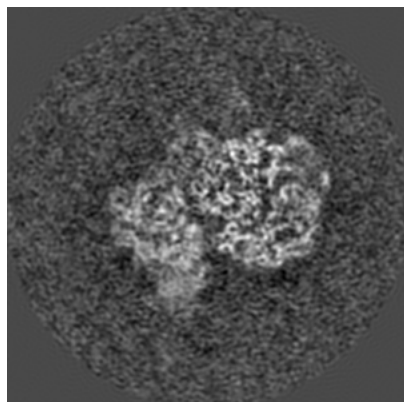


Z Index: 150

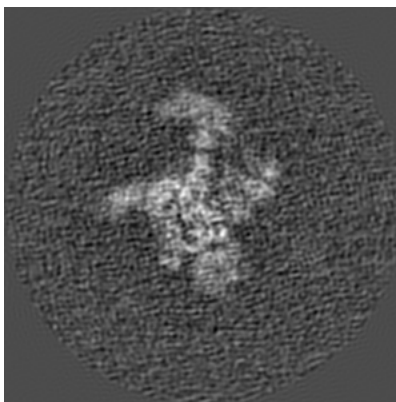
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

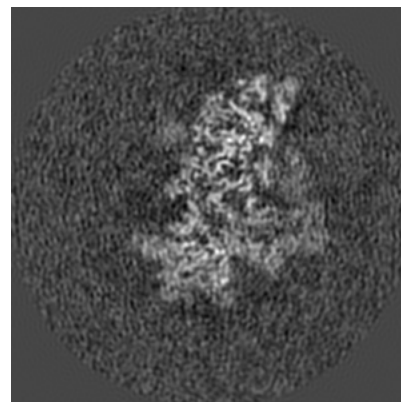
6.3.1 Primary map



X Index: 153

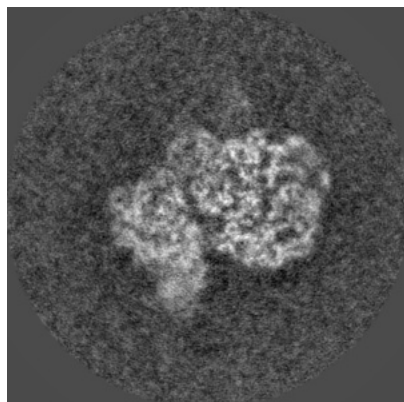


Y Index: 120

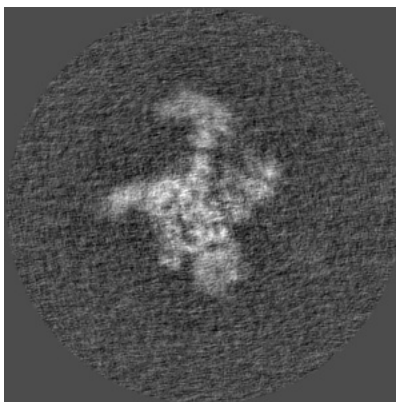


Z Index: 146

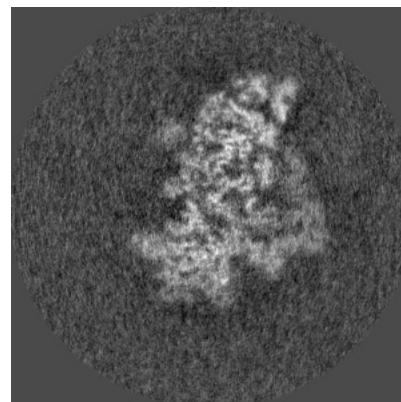
6.3.2 Raw map



X Index: 153



Y Index: 120

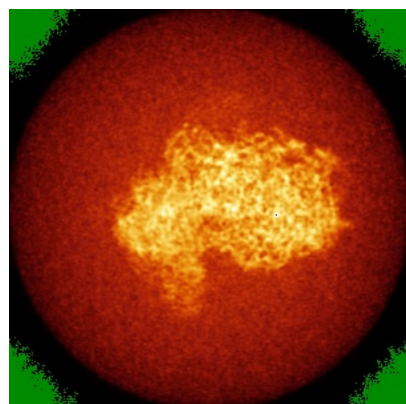


Z Index: 147

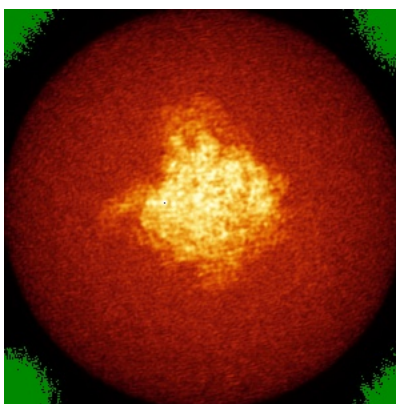
The images above show the largest variance slices of the map in three orthogonal directions.

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

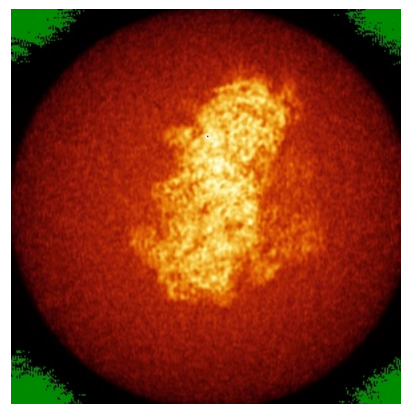
6.4.1 Primary map



X

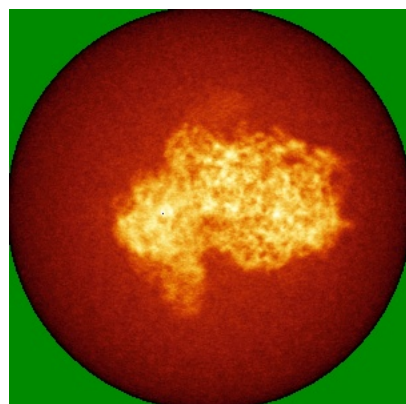


Y

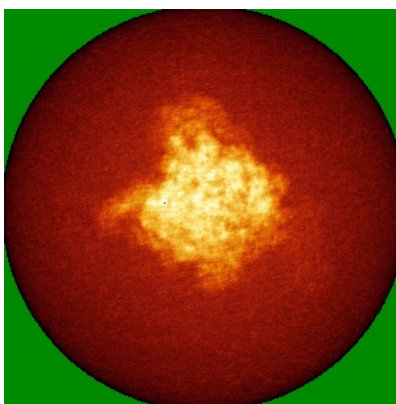


Z

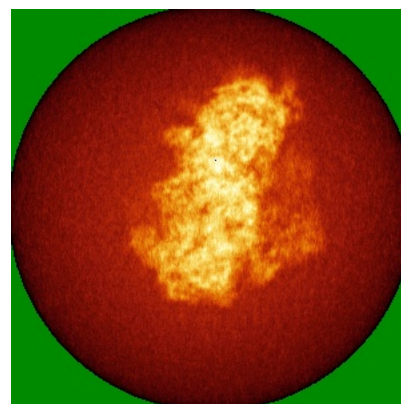
6.4.2 Raw map



X



Y

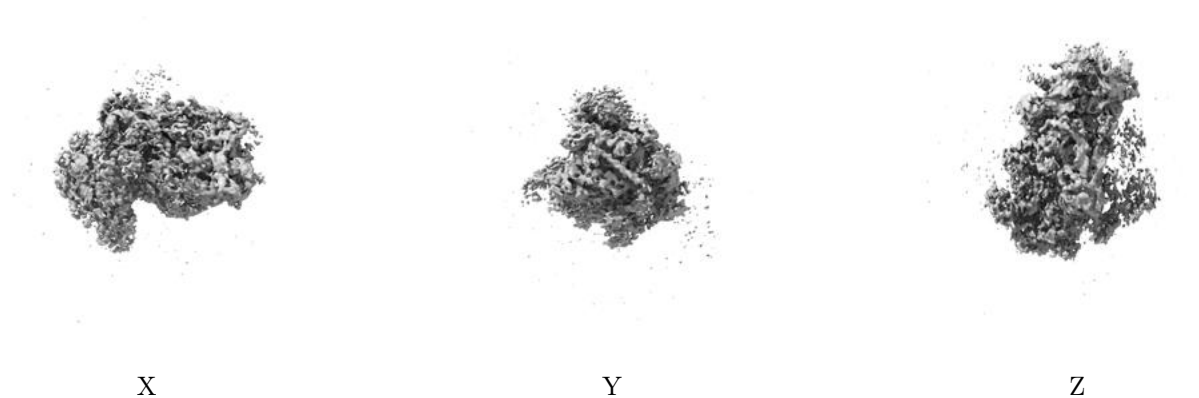


Z

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.

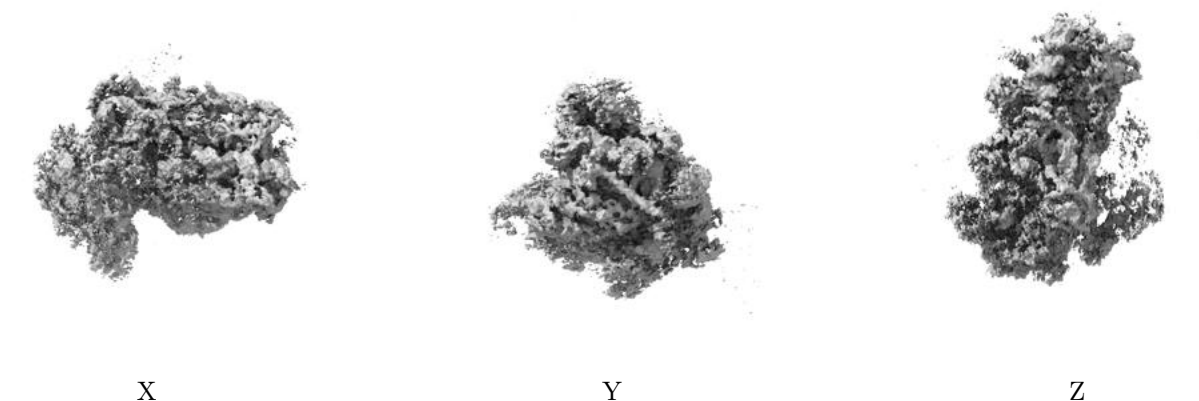
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

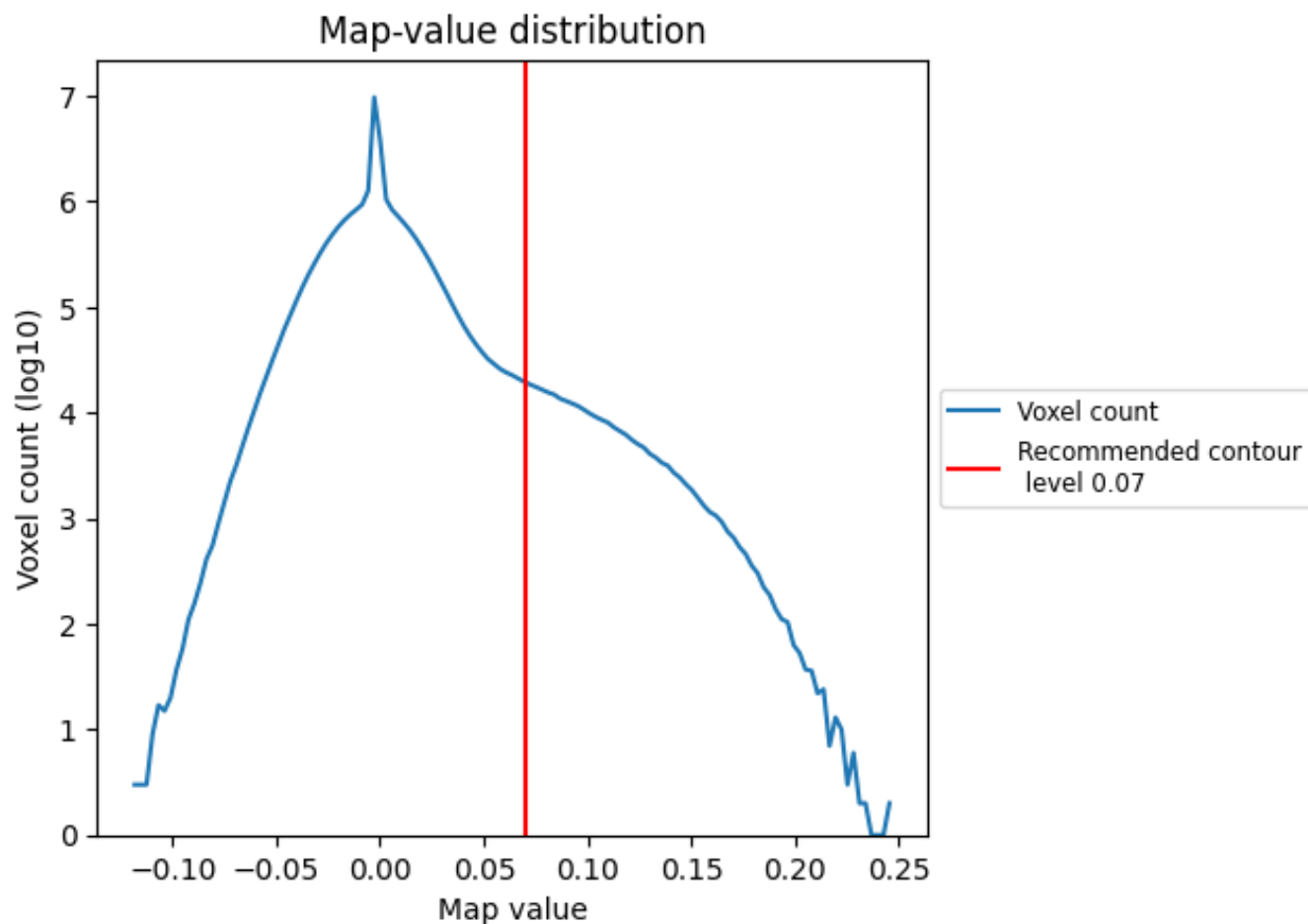
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

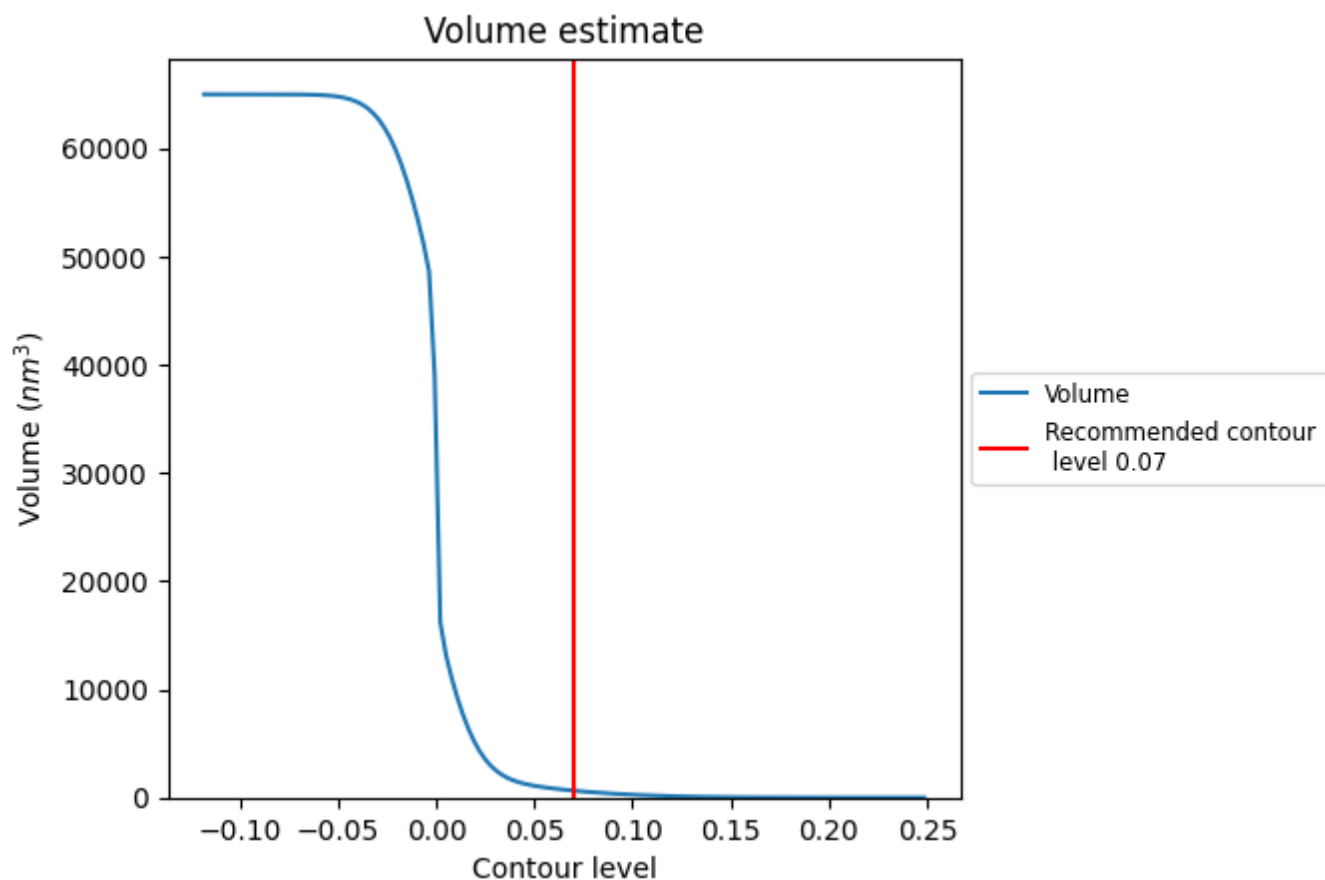
This section contains the results of statistical analysis of the map.

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.

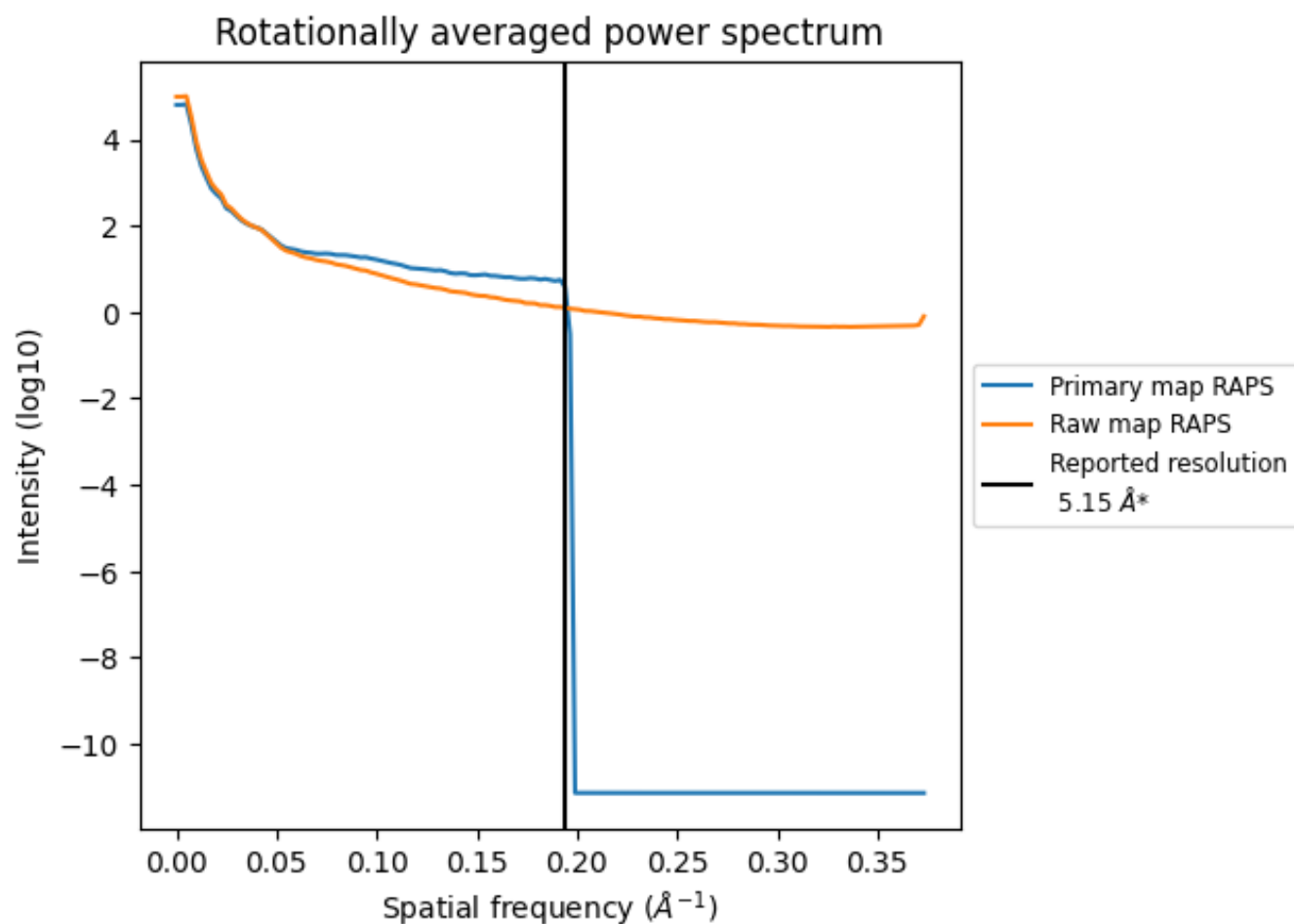
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638 nm³; this corresponds to an approximate mass of 576 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 ⓘ

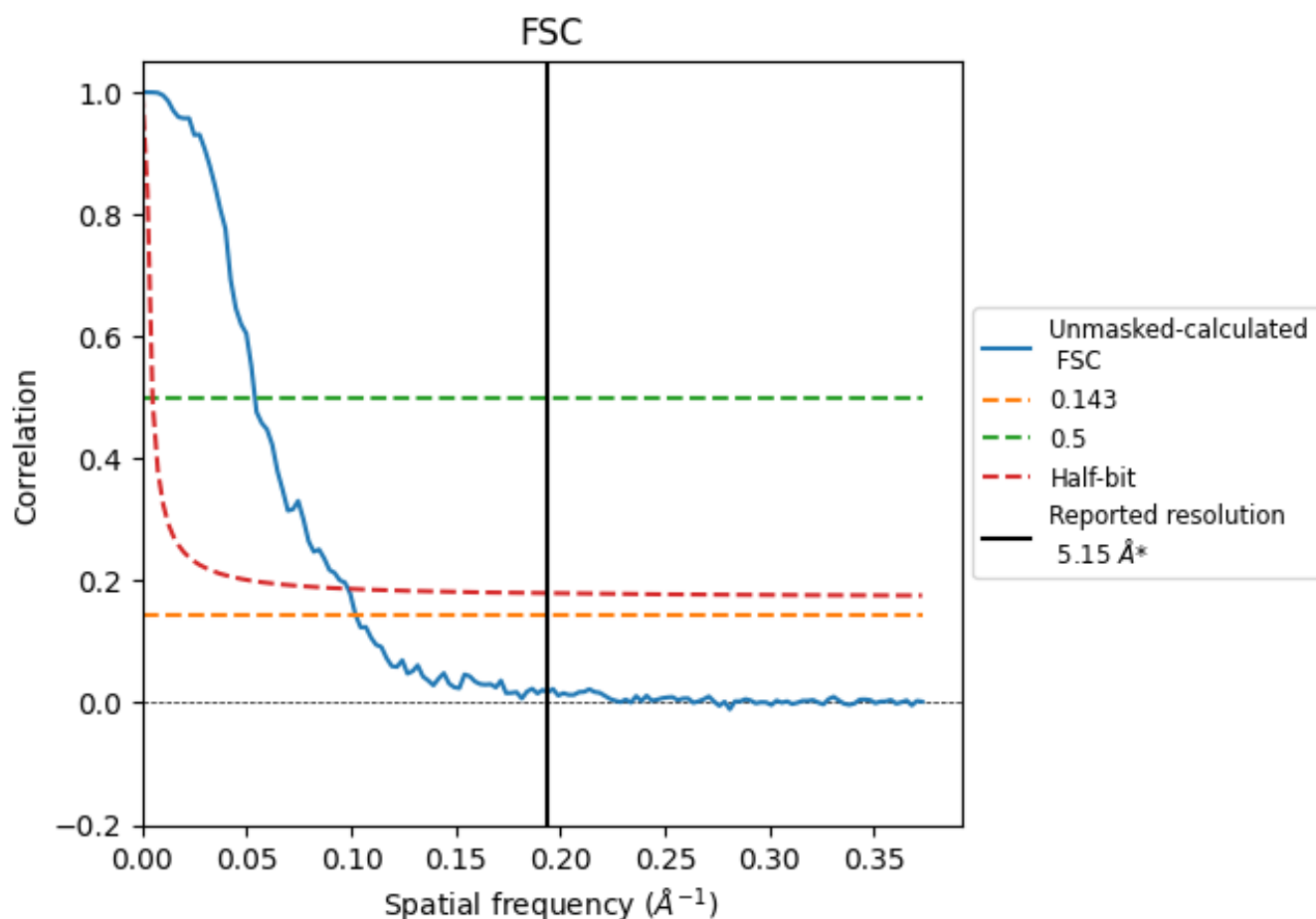


*Reported resolution corresponds to spatial frequency of 0.194 Å⁻¹

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 0.194 Å⁻¹

8.2 Resolution estimates [i](#)

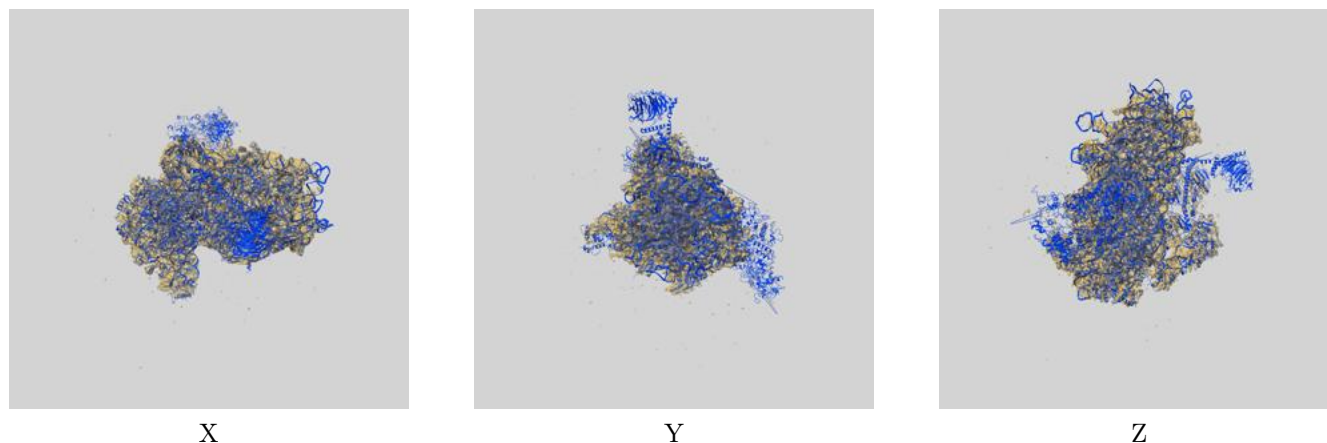
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.79	18.55	10.16

*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 9.79 differs from the reported value 5.15 by more than 10 %

9 Map-model fit [i](#)

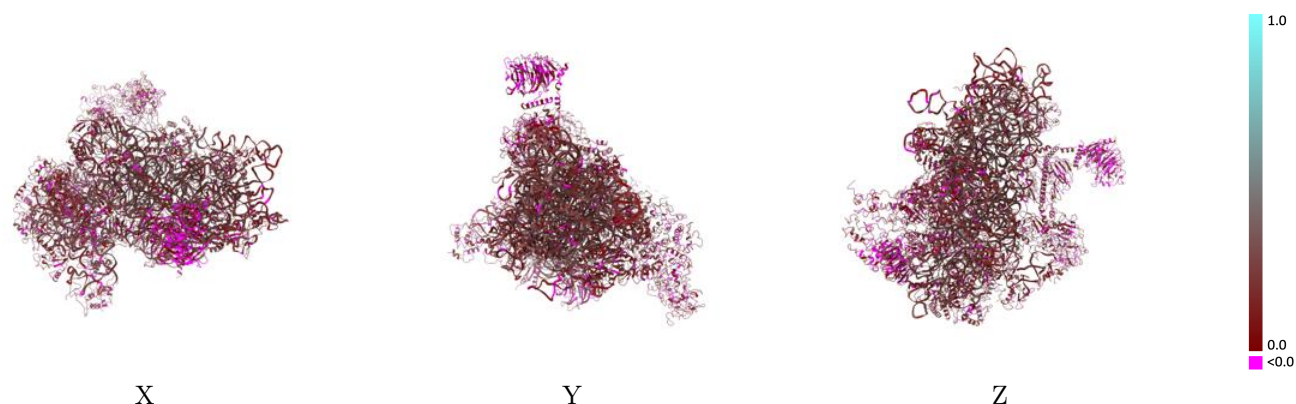
This section contains information regarding the fit between EMDB map EMD-0057 and PDB model 6GSM. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



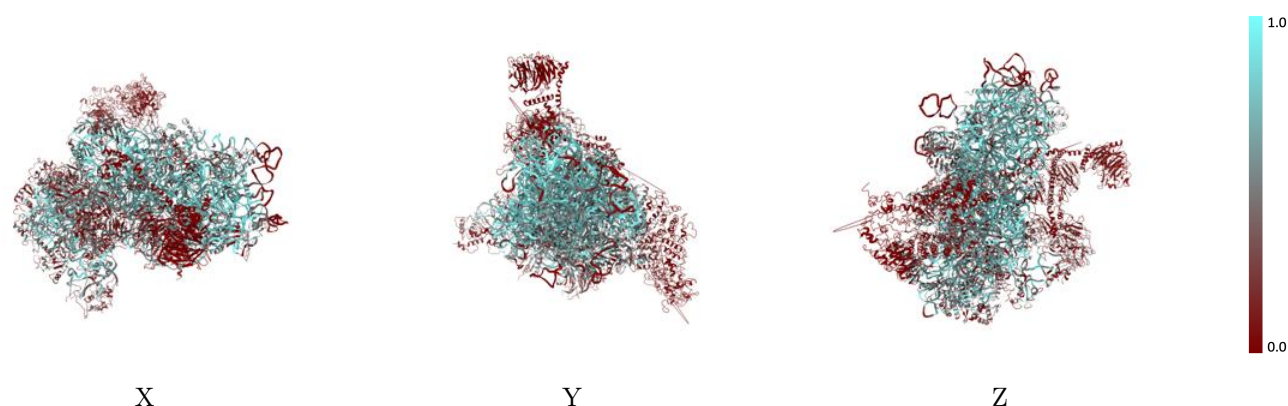
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



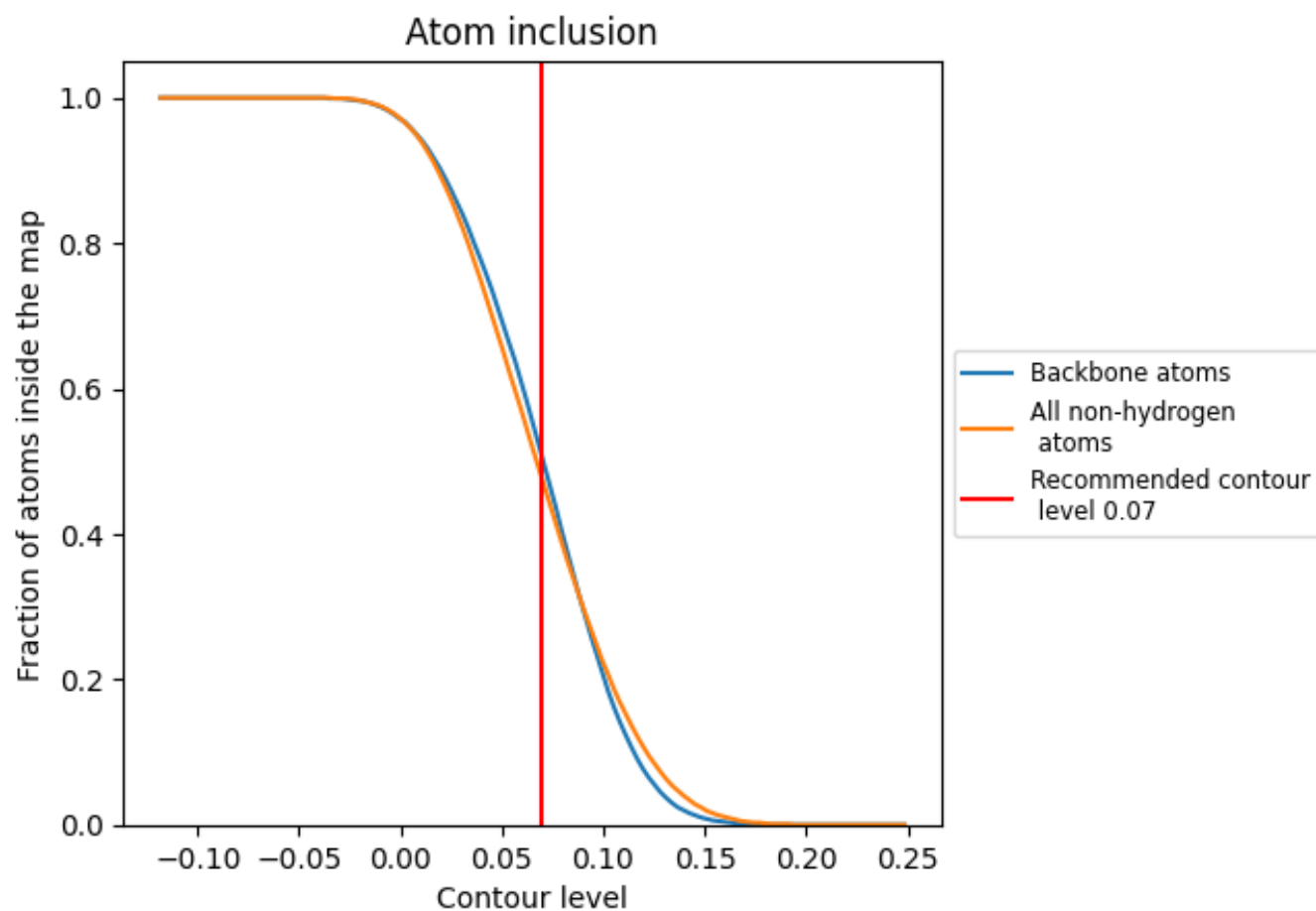
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 47% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4740	 0.1970
1	 0.6080	 0.1980
2	 0.7540	 0.2370
3	 0.2500	 0.1880
A	 0.4900	 0.2070
B	 0.4830	 0.2200
C	 0.4790	 0.2350
D	 0.3850	 0.2040
E	 0.5390	 0.2180
F	 0.4290	 0.1890
G	 0.4830	 0.1860
H	 0.4360	 0.1970
I	 0.4830	 0.2010
J	 0.5490	 0.2300
K	 0.3610	 0.1570
L	 0.4650	 0.2250
M	 0.1160	 0.1290
N	 0.5540	 0.2160
O	 0.5420	 0.1940
P	 0.3060	 0.1580
Q	 0.4640	 0.1840
R	 0.3890	 0.1990
S	 0.3990	 0.1750
T	 0.5270	 0.1740
U	 0.3340	 0.1690
V	 0.5130	 0.2130
W	 0.5260	 0.2270
X	 0.4330	 0.2240
Y	 0.5620	 0.2130
Z	 0.2250	 0.1680
a	 0.4890	 0.2410
b	 0.4440	 0.2110
c	 0.3300	 0.2070
d	 0.4500	 0.1660
e	 0.3590	 0.2060



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Chain	Atom inclusion	Q-score
f	 0.2300	 0.1300
g	 0.3120	 0.0840
h	 0.1890	 0.1960
i	 0.2450	 0.2080
j	 0.2220	 0.1810
k	 0.1410	 0.1520
l	 0.2150	 0.1960
m	 0.3210	 0.2410
o	 0.0190	 0.1410
p	 0.0490	 0.1440
q	 0.0430	 0.1570
r	 0.0000	 0.0030
s	 0.0000	 0.0140