



wwPDB EM Validation Summary Report ⓘ

Jun 21, 2026 – 12:10 pm BST

PDB ID : 8OZ0 / pdb_00008oz0
EMDB ID : EMD-17297
Title : Structure of a human 48S translation initiation complex with eIF4F and eIF4A
Authors : Brito Querido, J.; Sokabe, M.; Diaz-Lopez, I.; Gordiyenko, Y.; Fraser, C.S.;
Ramakrishnan, V.
Deposited on : 2023-05-06
Resolution : 3.50 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:

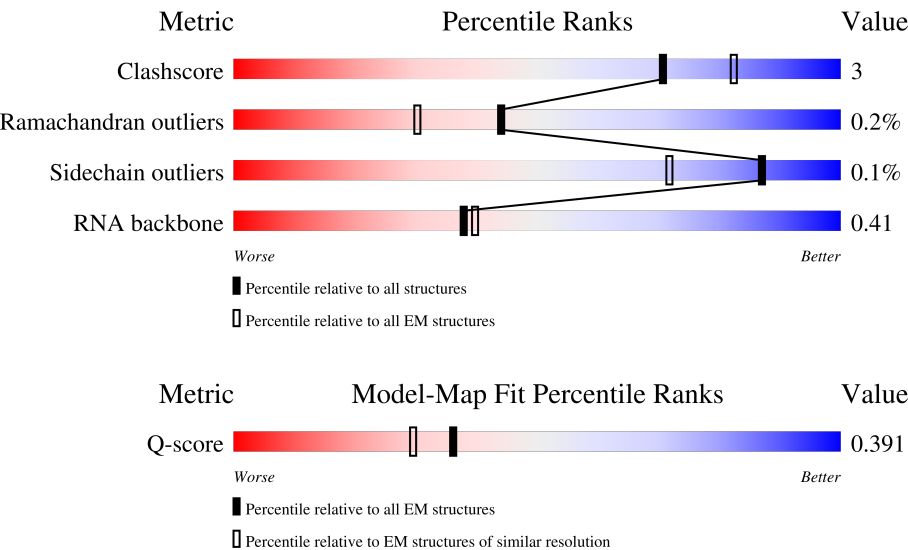
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 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.



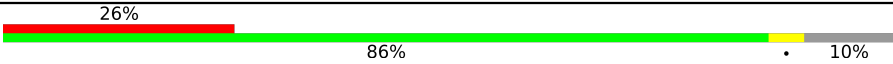
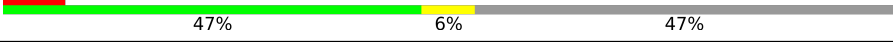
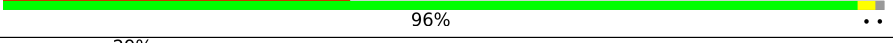
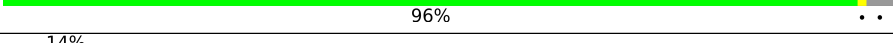
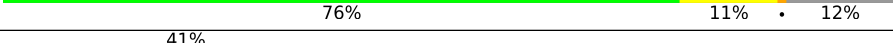
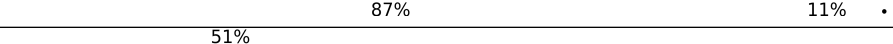
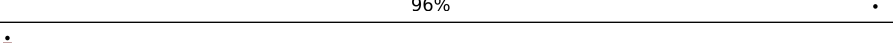
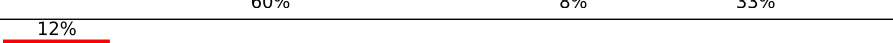
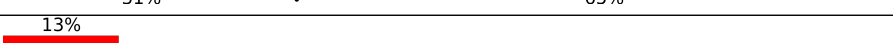
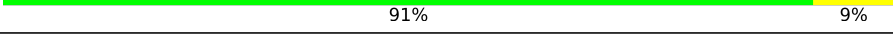
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	5	445	
2	6	357	
3	7	320	

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Mol	Chain	Length	Quality of chain
4	8	352	
5	9	25	
6	A	1382	
7	B	218	
8	C	374	
9	D	315	
10	E	472	
11	F	325	
12	G	144	
13	H	431	
14	I	814	
15	J	913	
16	K	564	
17	L	194	
18	M	84	
19	N	83	
20	O	293	
21	P	264	
22	Q	295	
23	R	115	
24	S	249	
25	T	151	
26	U	333	
27	V	151	
28	W	1719	

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Mol	Chain	Length	Quality of chain
29	X	158	
30	Y	263	
31	Z	194	
32	a	143	
33	b	59	
34	c	130	
35	d	208	
36	e	133	
37	f	204	
38	g	146	
39	h	243	
40	i	165	
41	j	145	
42	k	317	
43	l	145	
44	m	125	
45	n	151	
46	o	56	
47	p	156	
48	q	132	
49	s	69	
50	v	135	
51	w	119	
52	x	548	
53	y	75	

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Mol	Chain	Length	Quality of chain
54	z	207	
55	1	406	
55	3	406	
56	2	1404	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	JMH	W	1219	X	-	-	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 121610 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 protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	5	437	Total	C	N	O	0	0
			2175	1301	437	437		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	6	269	Total	C	N	O	0	0
			1330	791	269	270		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	7	77	Total	C	N	O	0	0
			616	389	111	116		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	8	316	Total	C	N	O	0	0
			1569	936	316	317		

- Molecule 5 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	733	Total	C	N	O	S	0	0
			5386	3376	979	1008	23		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	215	Total	C	N	O	0	0
			1066	636	215	215		

- Molecule 8 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	C	364	Total	C	N	O	0	0
			1809	1080	364	365		

- Molecule 9 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	278	Total	C	N	O	S	0	0
			2234	1410	390	421	13		

- Molecule 10 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	464	Total	C	N	O	S	0	0
			3540	2245	620	658	17		

- Molecule 11 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	F	325	Total	C	N	O	0	0
			1598	947	325	326		

- Molecule 12 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	97	Total	C	N	O	S	0	0
			789	492	147	146	4		

- Molecule 13 is a protein called Eukaryotic translation initiation factor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	149	Total	C	N	O	S	0	0
			1176	740	208	217	11		

- Molecule 14 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	575	Total	C	N	O	S	0	0
			4569	2935	788	828	18		

- Molecule 15 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	687	Total	C	N	O	S	0	0
			5207	3252	936	986	33		

- Molecule 16 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	531	Total	C	N	O	S	0	0
			2637	1574	531	532			

- Molecule 17 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	178	Total	C	N	O	S	0	0
			1439	923	262	253	1		

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 19 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 20 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 21 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	214	Total	C	N	O	S	0	0
			1695	1077	297	313	8		

- Molecule 23 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 24 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 25 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	133	Total	C	N	O	S	0	0
			997	610	196	185	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	139	Total	C	N	O	S	0	0
			689	411	139	139			

- Molecule 27 is a protein called 40S ribosomal protein S13.

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

- Molecule 28 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	1716	Total	C	N	O	P	0	0
			36639	16369	6570	11985	1715		

- Molecule 29 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	142	Total	C	N	O	S	0	0
			1166	743	218	199	6		

- Molecule 30 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

- Molecule 31 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

- Molecule 32 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 33 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	47	Total	C	N	O	S	0	0
			378	231	85	61	1		

- Molecule 34 is a protein called 40S ribosomal protein S15a.

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

- Molecule 35 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 36 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 37 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 38 is a protein called 40S ribosomal protein S16.

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

- Molecule 39 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 40 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 41 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	110	Total	C	N	O	S	0	0
			913	580	168	158	7		

- Molecule 42 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 43 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 44 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	66	Total	C	N	O	S	0	0
			523	338	93	91	1		

- Molecule 45 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	142	Total	C	N	O	S	0	0
			1176	737	239	199	1		

- Molecule 46 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	50	Total	C	N	O	S	0	0
			419	262	85	67	5		

- Molecule 47 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	53	Total	C	N	O	S	0	0
			435	276	82	70	7		

- Molecule 48 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 49 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	63	Total	C	N	O	S	0	0
			498	302	101	93	2		

- Molecule 50 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 51 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 52 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	440	Total	C	N	O	S	0	0
			2920	1798	539	574	9		

- Molecule 53 is a RNA chain called tRNAiMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	50	Total	C	N	O	P	0	0
			853	373	104	326	50		

- Molecule 55 is a protein called Eukaryotic initiation factor 4A-I.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	3	378	Total	C	N	O	0	0
			1869	1113	378	378		
55	1	371	Total	C	N	O	0	0
			1834	1092	371	371		

- Molecule 56 is a protein called Eukaryotic translation initiation factor 4 gamma 1.

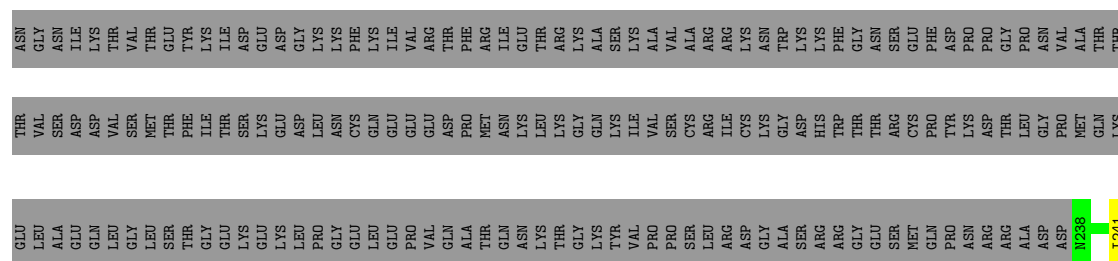
Mol	Chain	Residues	Atoms				AltConf	Trace
56	2	237	Total	C	N	O	0	0
			1178	704	237	237		

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

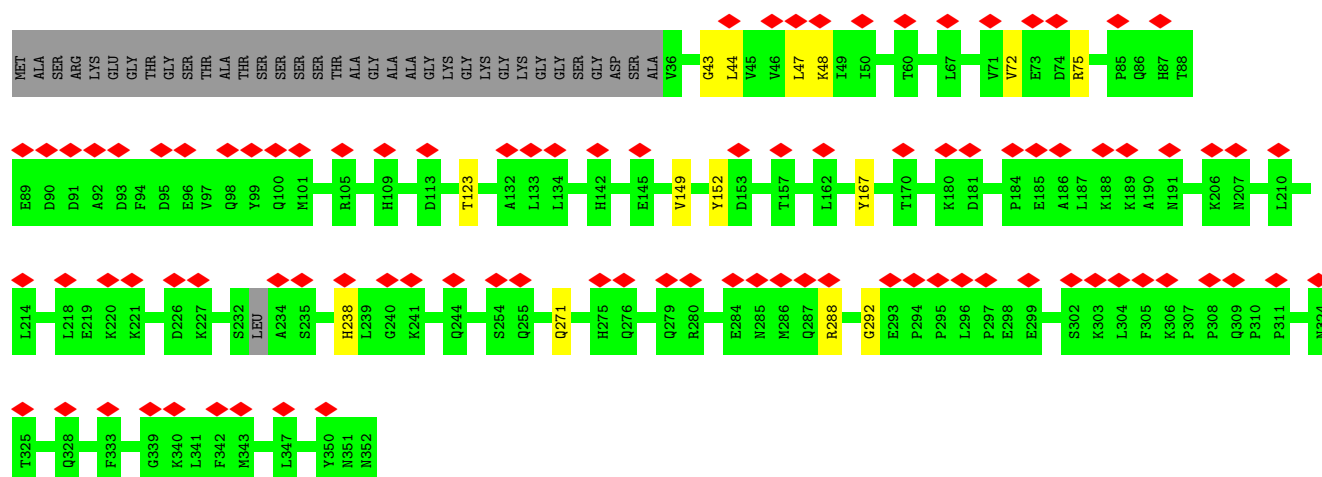
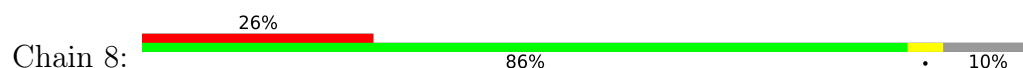
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	
57	p	1	Total	Zn	0
			1	1	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

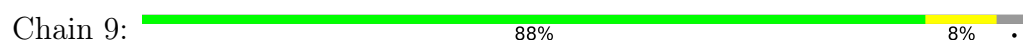
Mol	Chain	Residues	Atoms		AltConf
58	T	2	Total	Mg	0
			2	2	
58	W	86	Total	Mg	0
			86	86	
58	f	1	Total	Mg	0
			1	1	



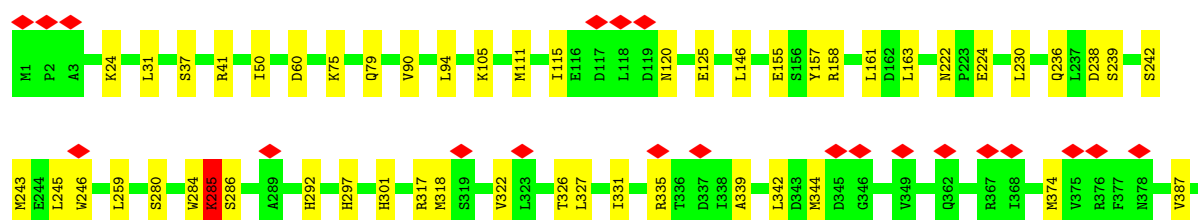
• Molecule 4: Eukaryotic translation initiation factor 3 subunit H

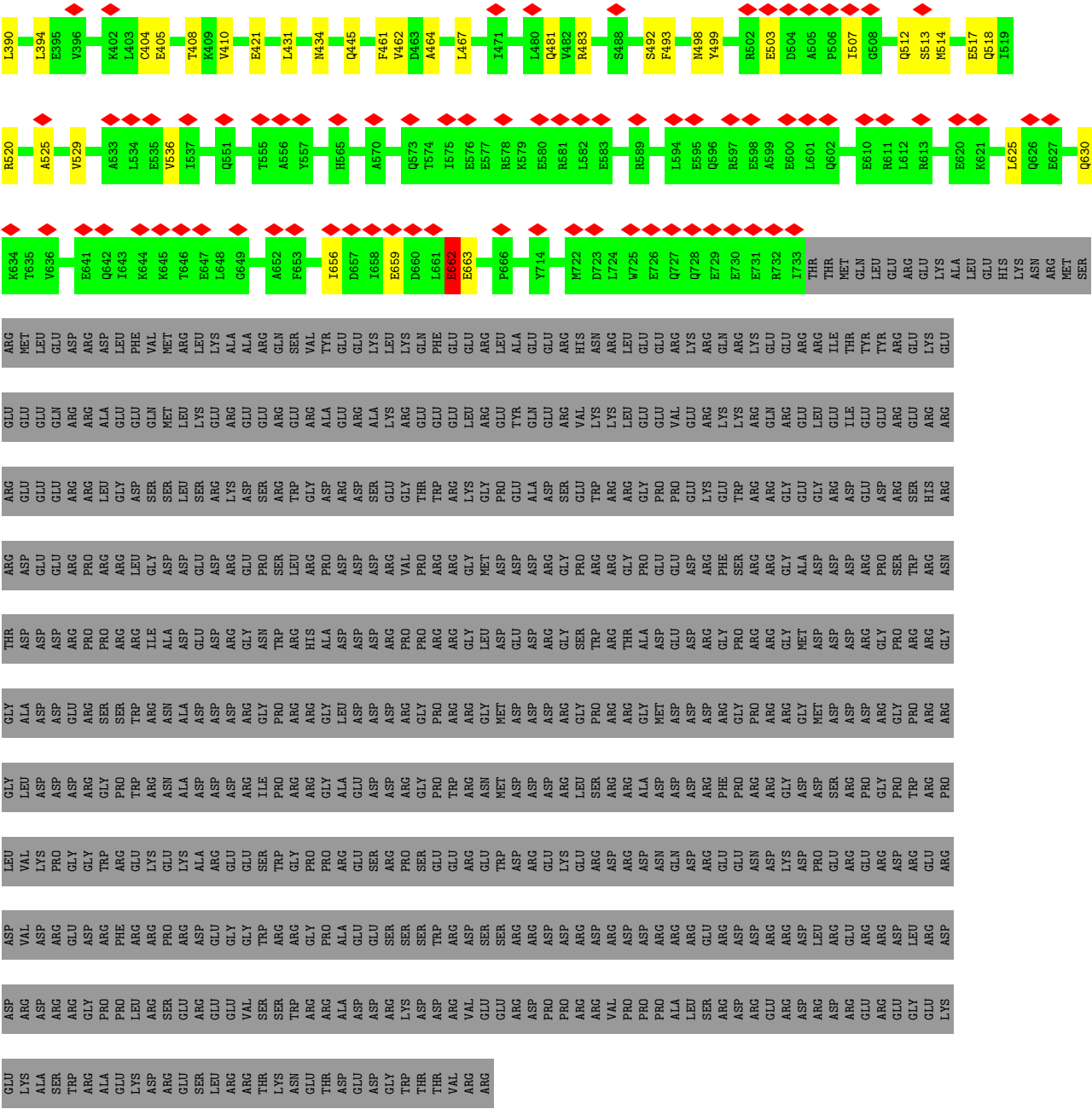


• Molecule 5: 60S ribosomal protein L41

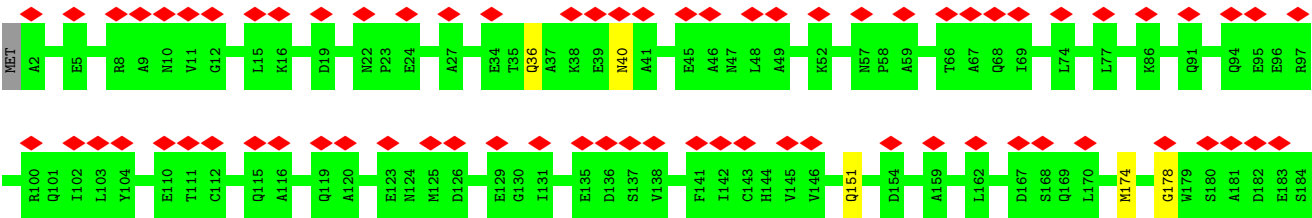


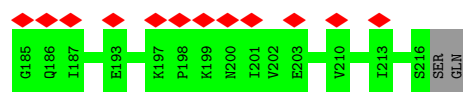
• Molecule 6: Eukaryotic translation initiation factor 3 subunit A



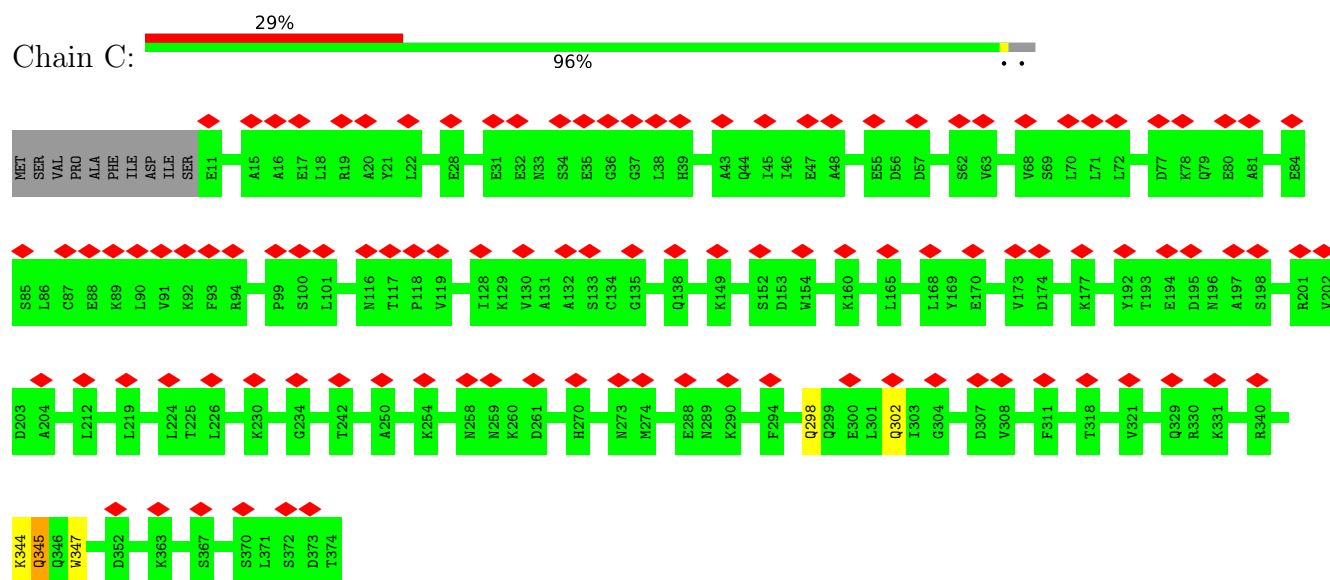


● Molecule 7: Eukaryotic translation initiation factor 3 subunit K

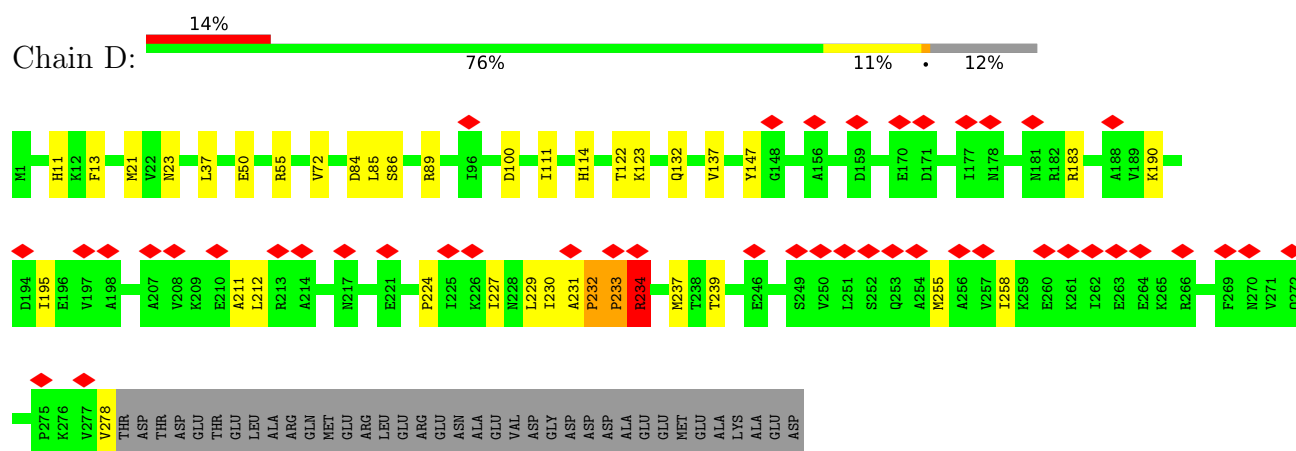




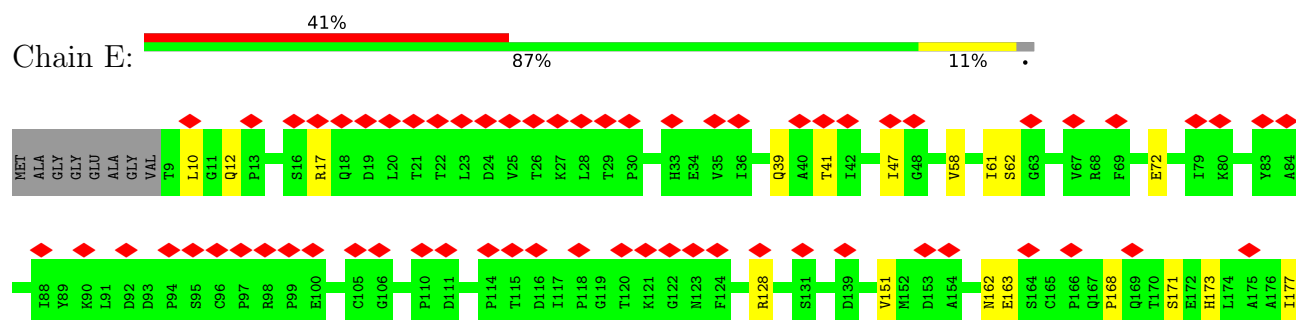
• Molecule 8: Eukaryotic translation initiation factor 3 subunit M

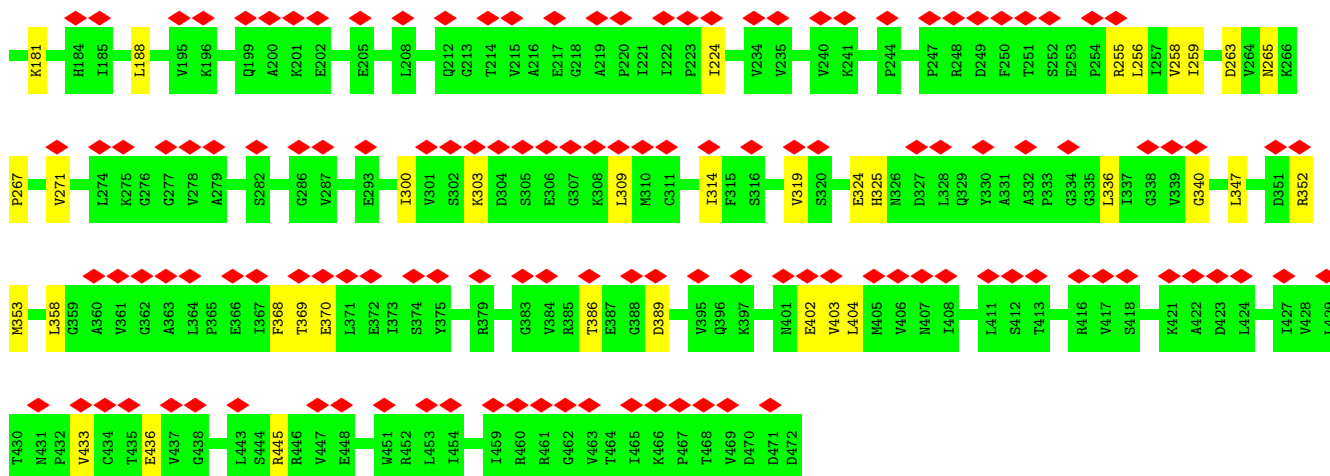


• Molecule 9: Eukaryotic translation initiation factor 2 subunit 1

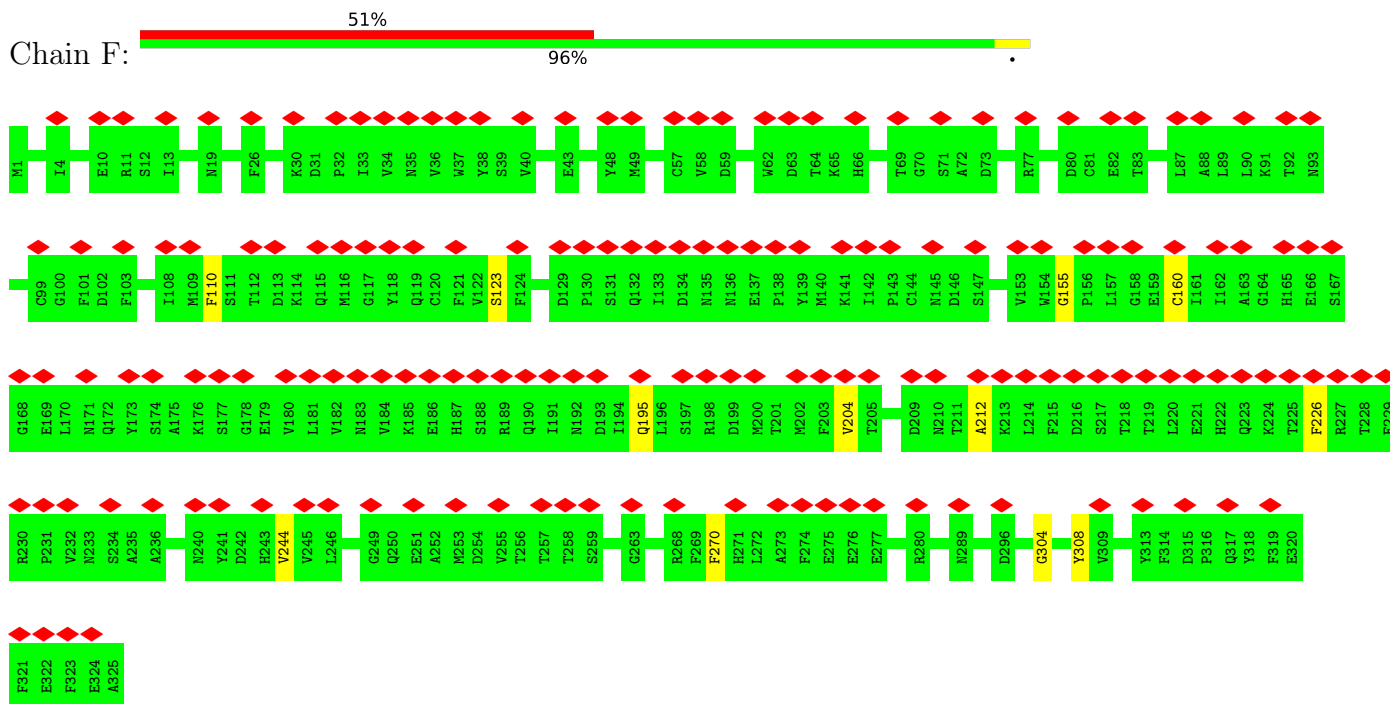


• Molecule 10: Eukaryotic translation initiation factor 2 subunit 3

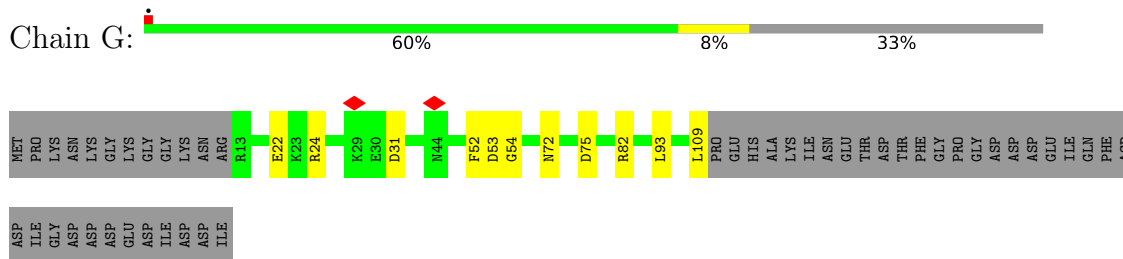




- Molecule 11: Eukaryotic translation initiation factor 3 subunit I

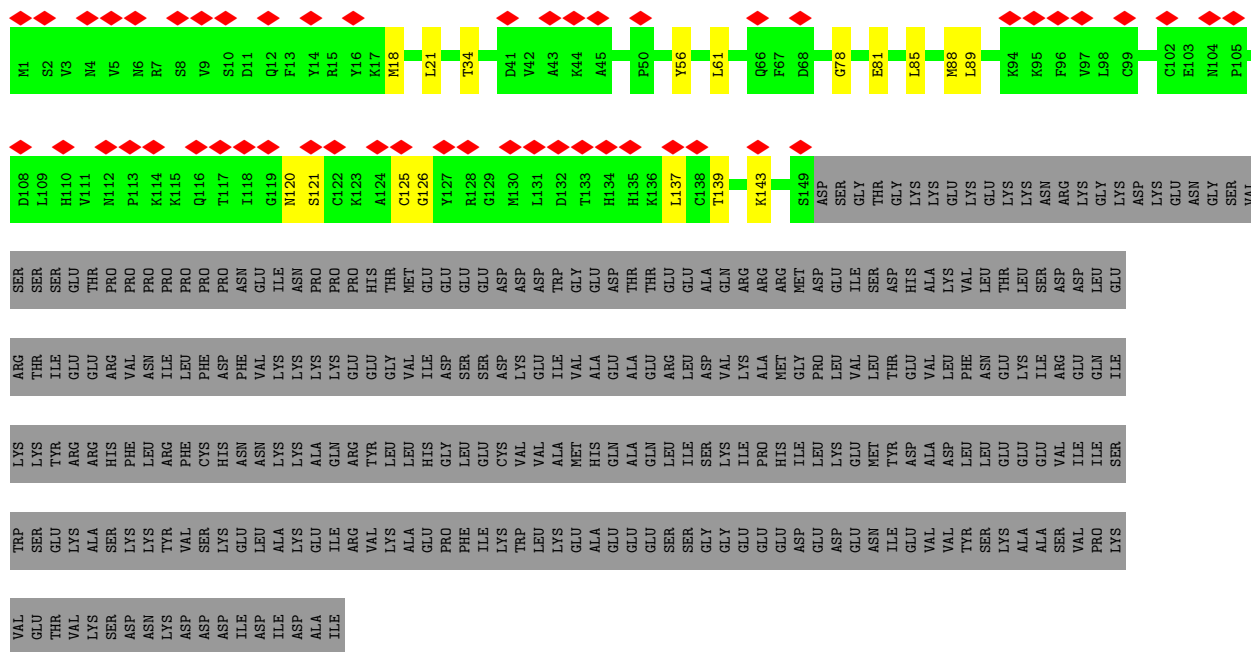


- Molecule 12: Eukaryotic translation initiation factor 1A, X-chromosomal

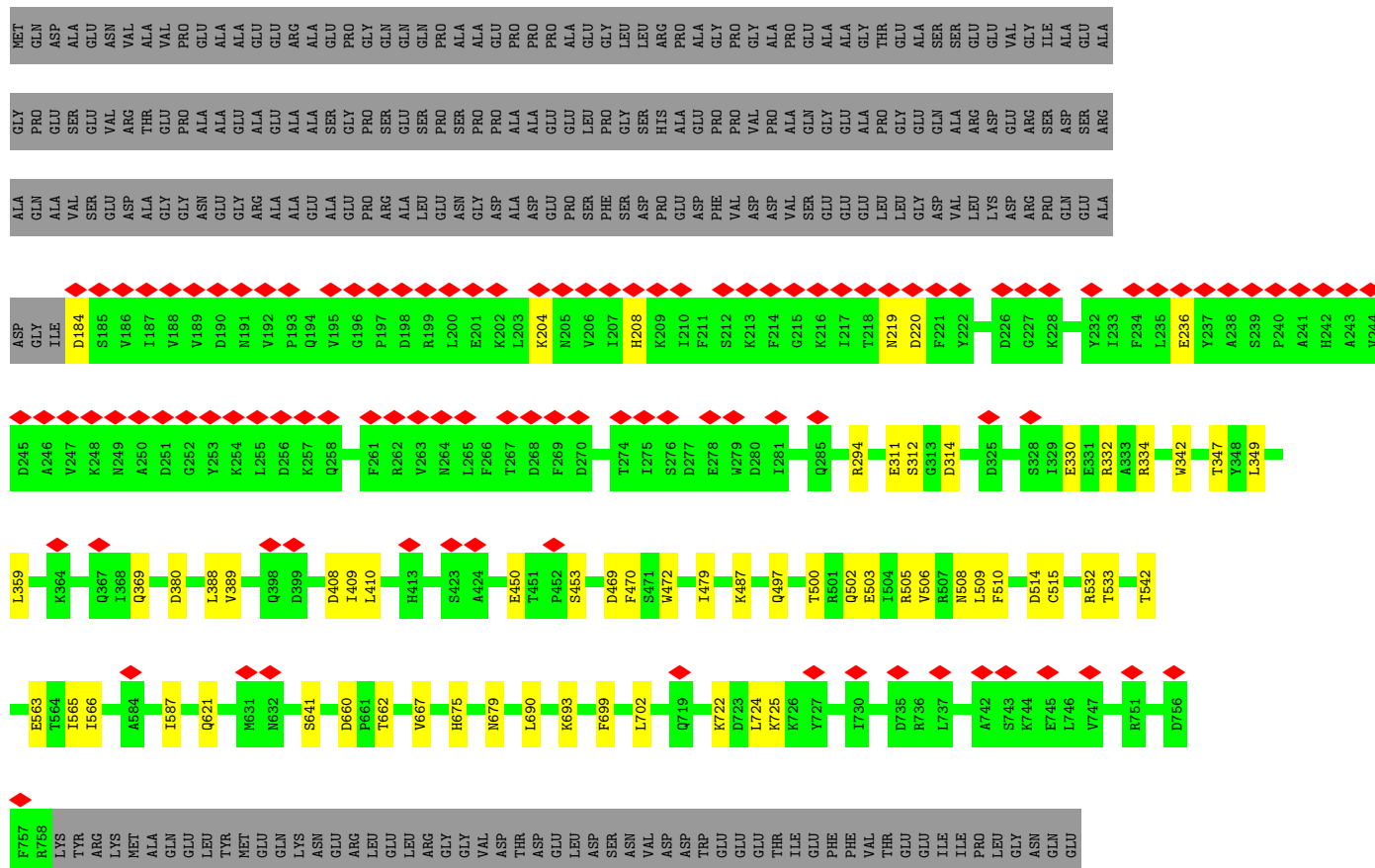


- Molecule 13: Eukaryotic translation initiation factor 5

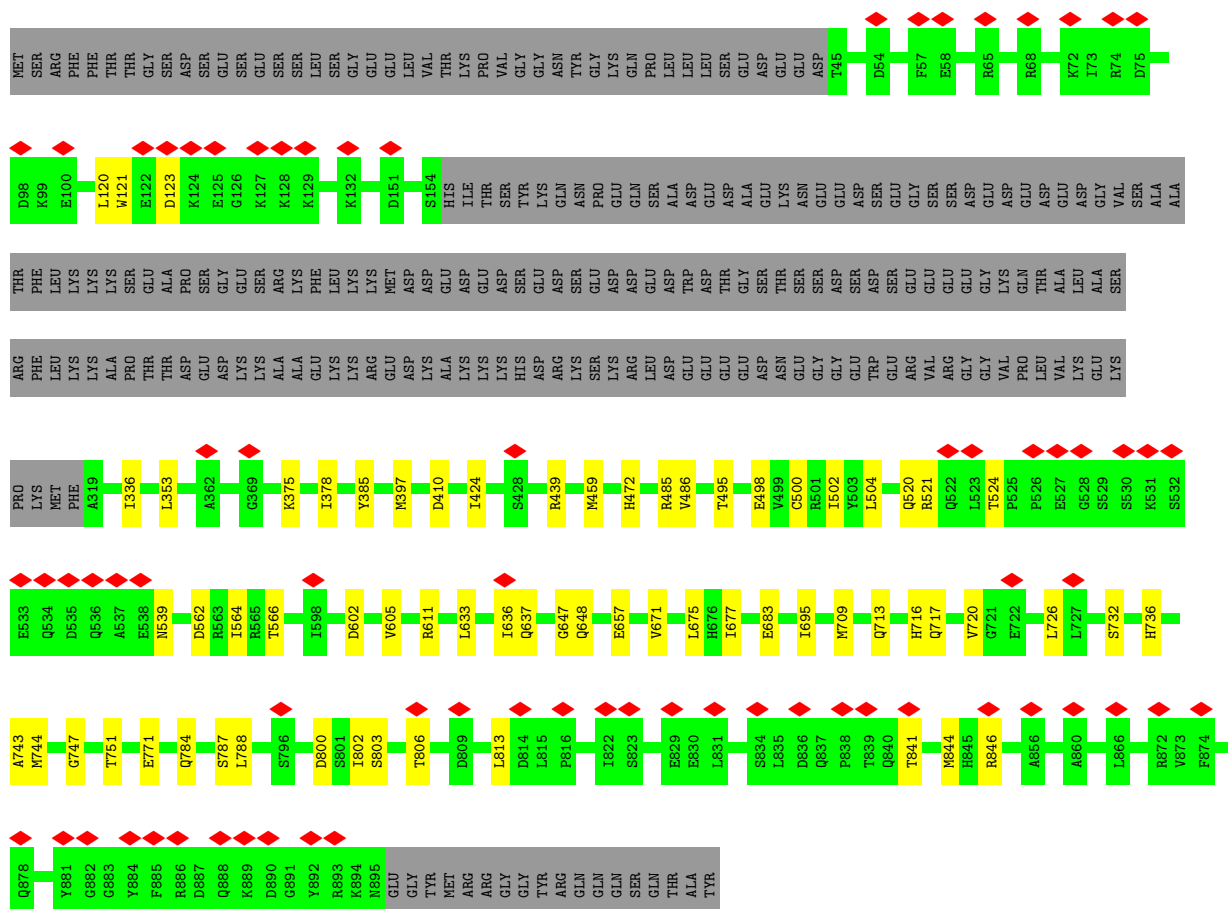




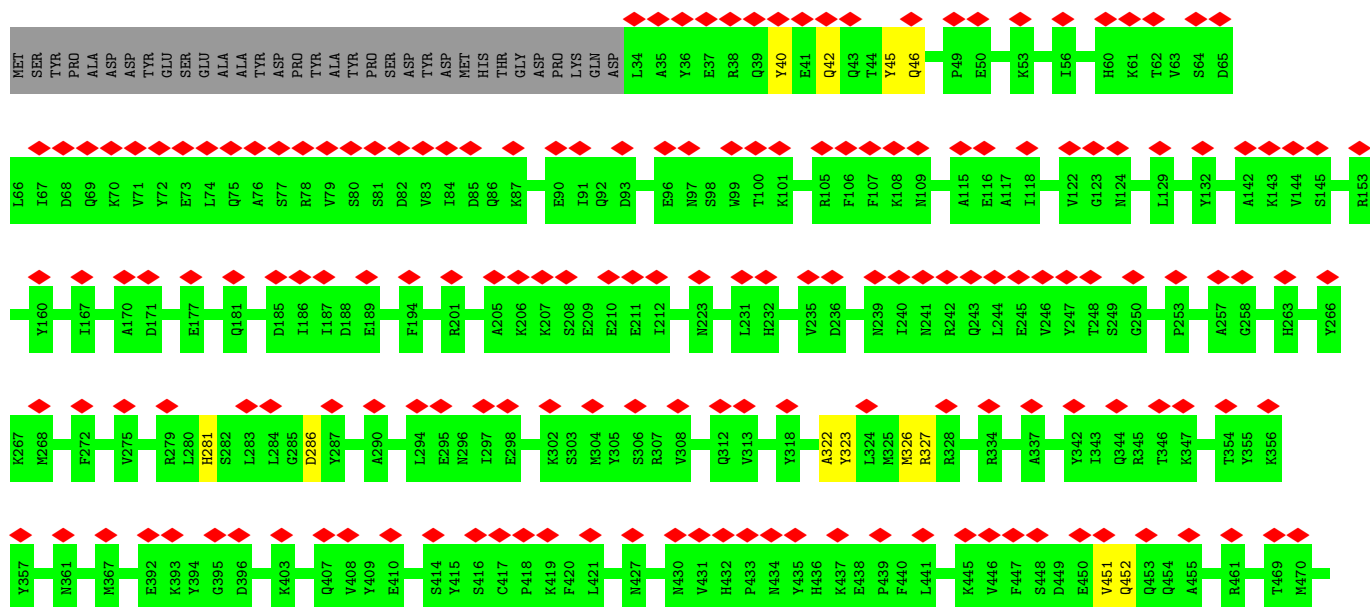
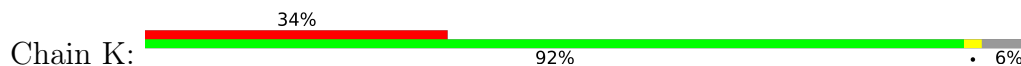
• Molecule 14: Eukaryotic translation initiation factor 3 subunit B

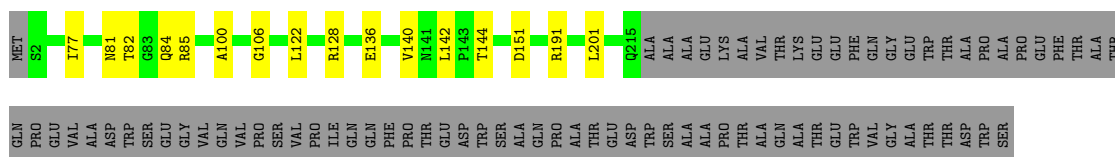


• Molecule 15: Eukaryotic translation initiation factor 3 subunit C

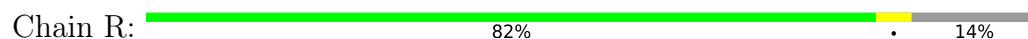


• Molecule 16: Eukaryotic translation initiation factor 3 subunit L

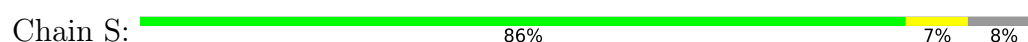




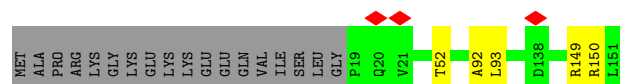
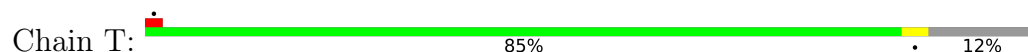
- Molecule 23: 40S ribosomal protein S26



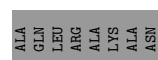
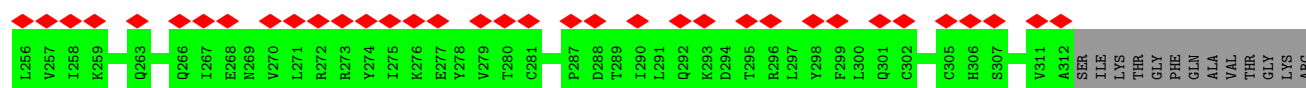
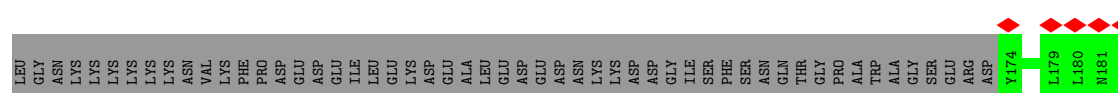
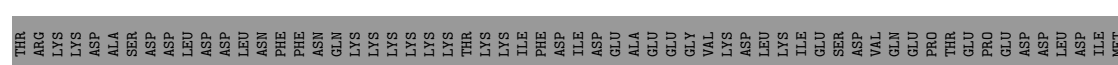
- Molecule 24: 40S ribosomal protein S6



- Molecule 25: 40S ribosomal protein S14

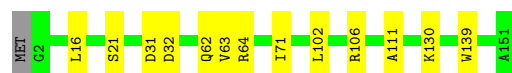


- Molecule 26: Eukaryotic translation initiation factor 2 subunit 2



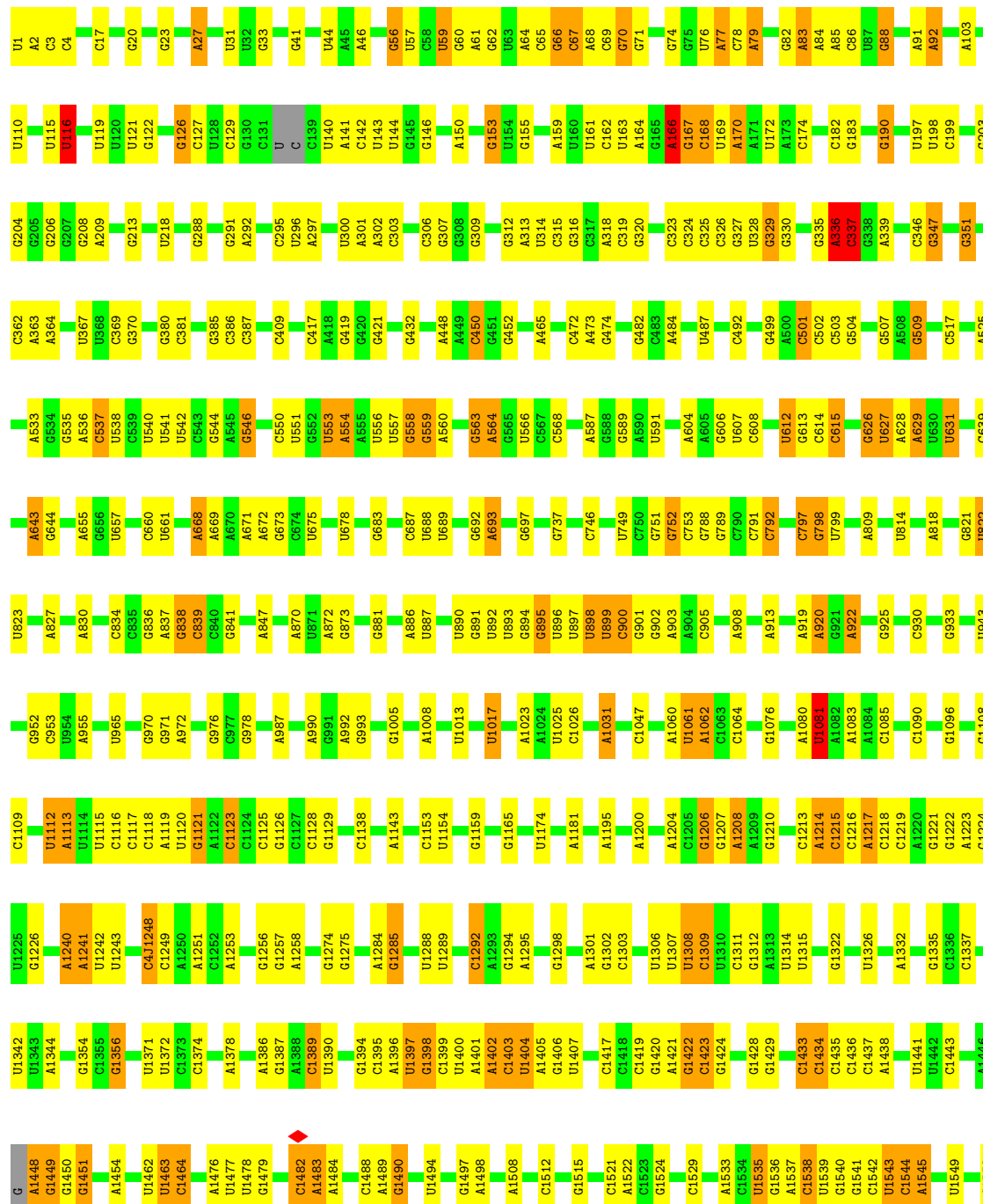
• Molecule 27: 40S ribosomal protein S13

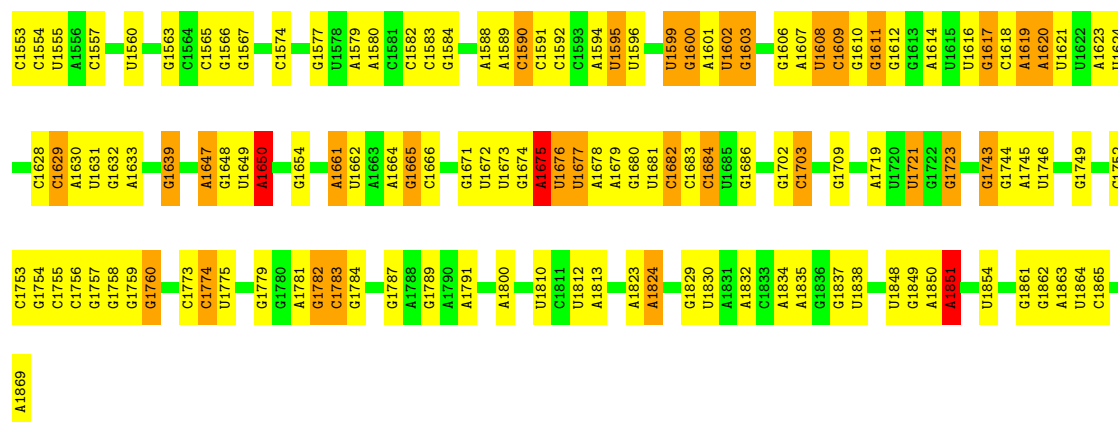
Chain V:  91% 9%



• Molecule 28: 18S rRNA

Chain W:  65% 27% 7%





- Molecule 29: 40S ribosomal protein S11

Chain X: 84% 6% 10%



- Molecule 30: 40S ribosomal protein S4, X isoform

Chain Y: 90% 8% 2%



- Molecule 31: 40S ribosomal protein S9

Chain Z: 88% 9% 3%



- Molecule 32: 40S ribosomal protein S23

Chain a: 91% 7% 2%



- Molecule 33: 40S ribosomal protein S30

Chain b: 78% 20% 2%



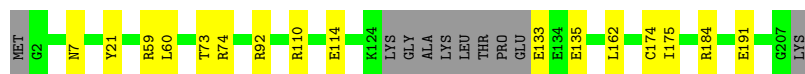
- Molecule 34: 40S ribosomal protein S15a

Chain c:  92% 7%



- Molecule 35: 40S ribosomal protein S8

Chain d:  88% 8% 5%



- Molecule 36: 40S ribosomal protein S24

Chain e:  86% 8% 6%



- Molecule 37: 40S ribosomal protein S5

Chain f:  83% 7% 10%



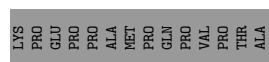
- Molecule 38: 40S ribosomal protein S16

Chain g:  84% 13%



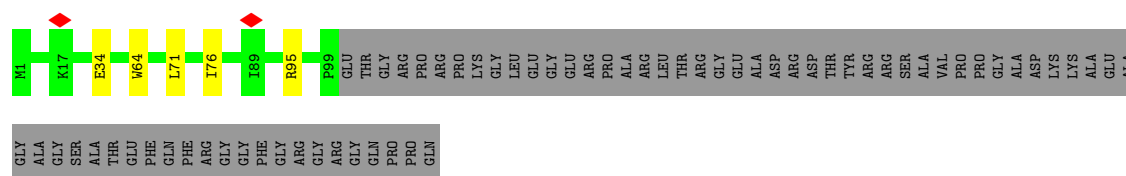
- Molecule 39: 40S ribosomal protein S3

Chain h:  81% 12% 7%



- Molecule 40: 40S ribosomal protein S10

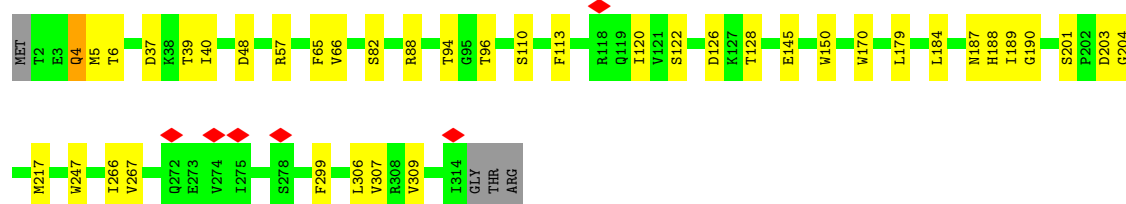
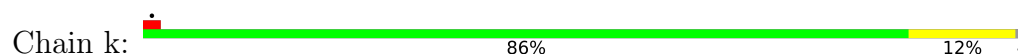
Chain i:  57% 40%



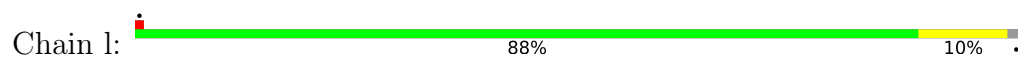
- Molecule 41: 40S ribosomal protein S15



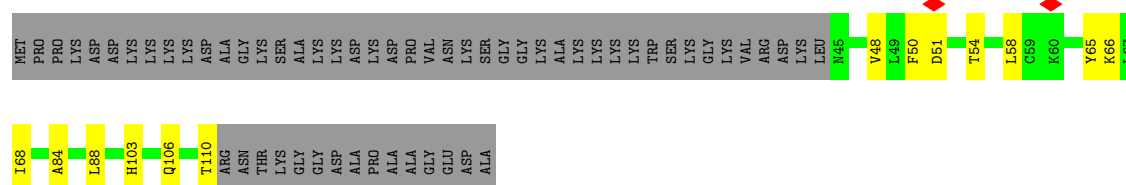
- Molecule 42: Receptor of activated protein C kinase 1



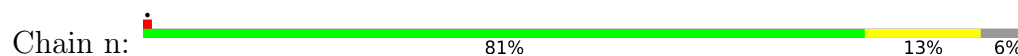
- Molecule 43: 40S ribosomal protein S19



- Molecule 44: 40S ribosomal protein S25

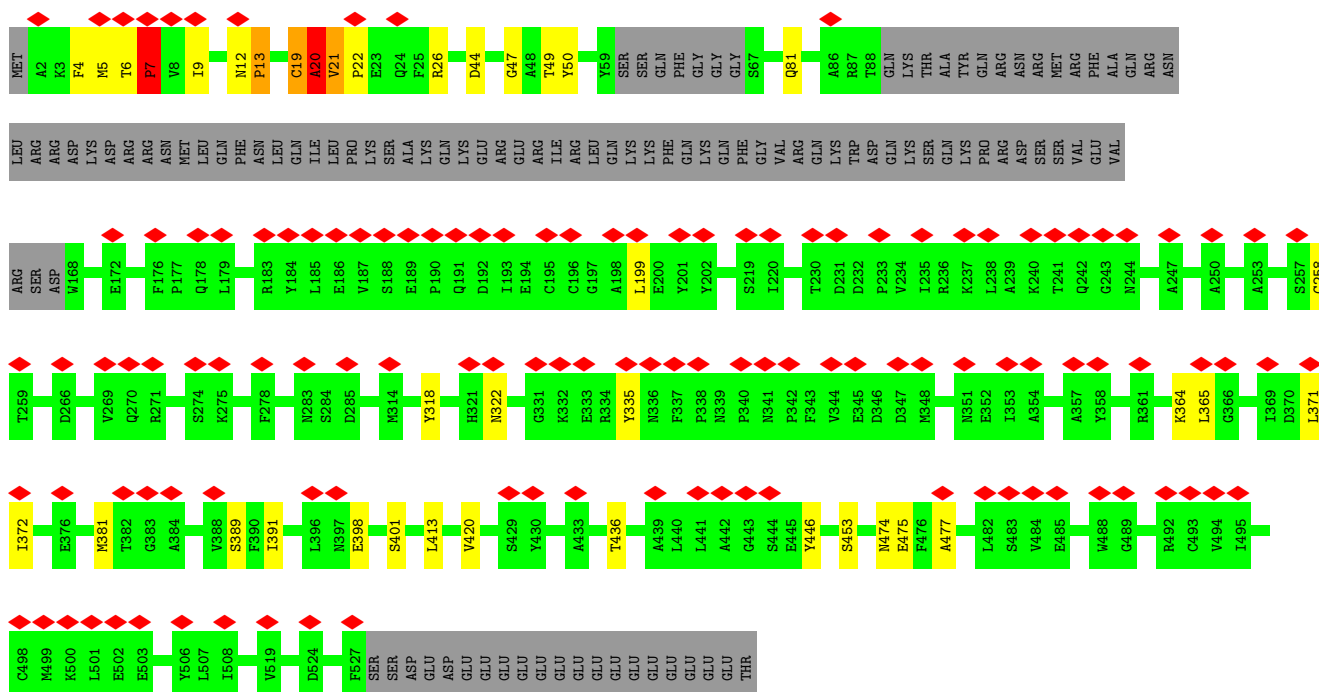


- Molecule 45: Small ribosomal subunit protein uS13



MET	ALA	PHE	LYS	ASP	THR	GLY	LYS	THR	PRO	VAL	GLU	PRO	GLU	VAL	ALA	I17	R21	N28	S31	K34	K46	P53	L88	I101	T102	S103	E107	A119
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------

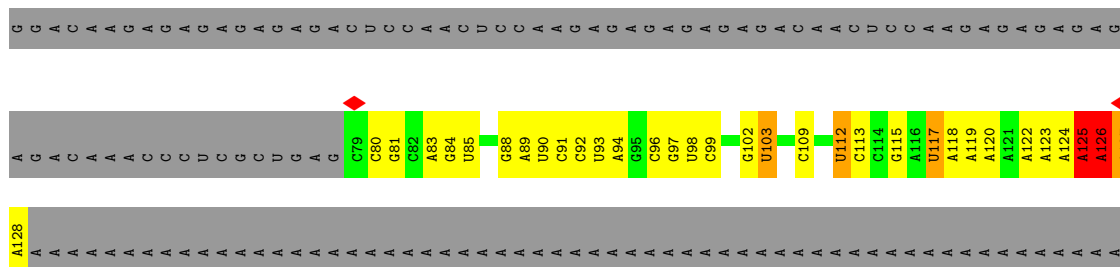
Chain x: 22% 73% 6% 20%



Chain y:

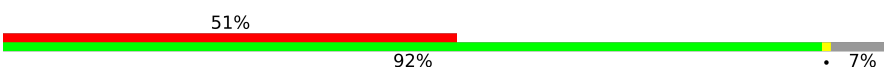


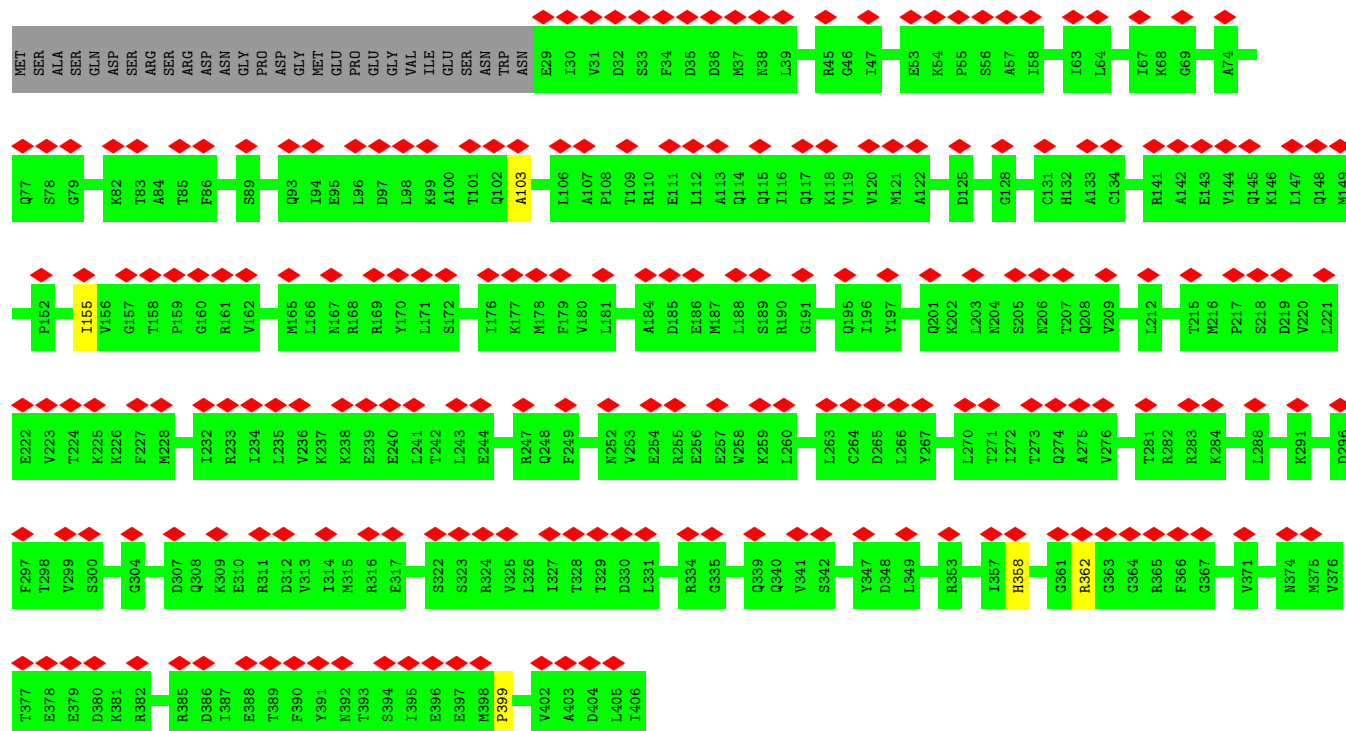
Chain z:



A A A A A A A A A A A A A A A A A

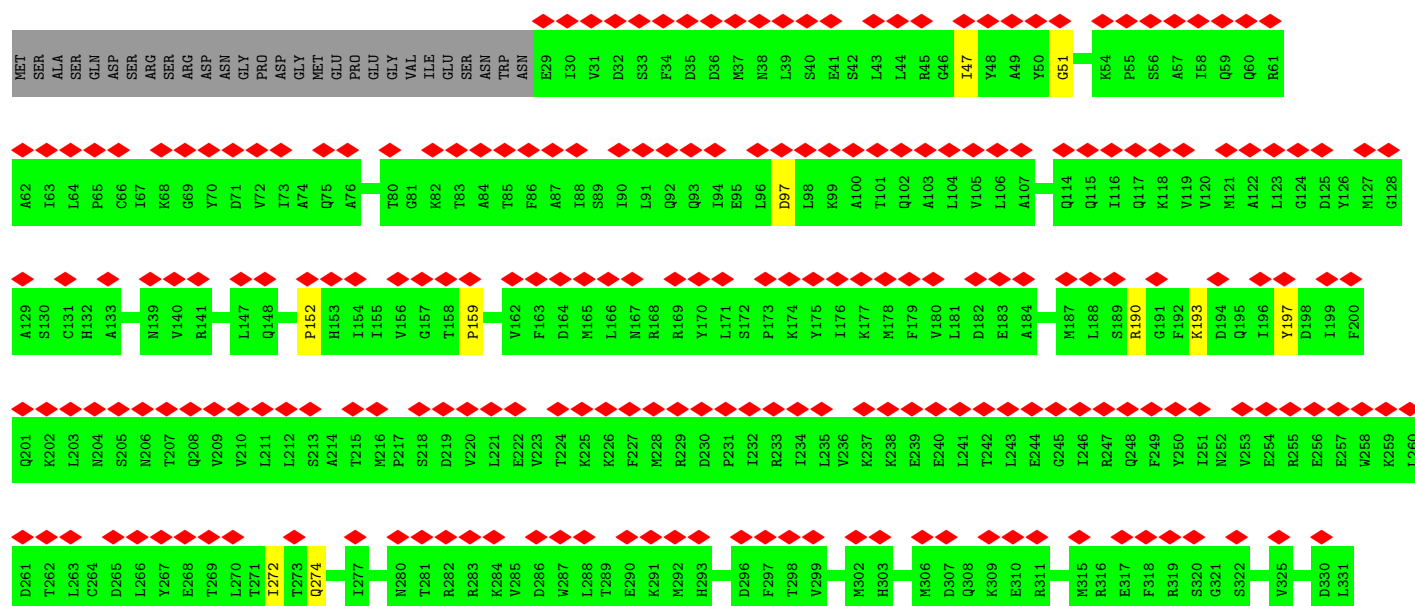
• Molecule 55: Eukaryotic initiation factor 4A-I

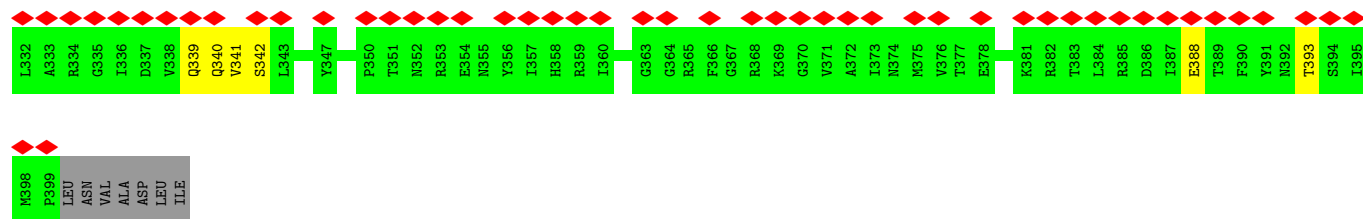
Chain 3: 



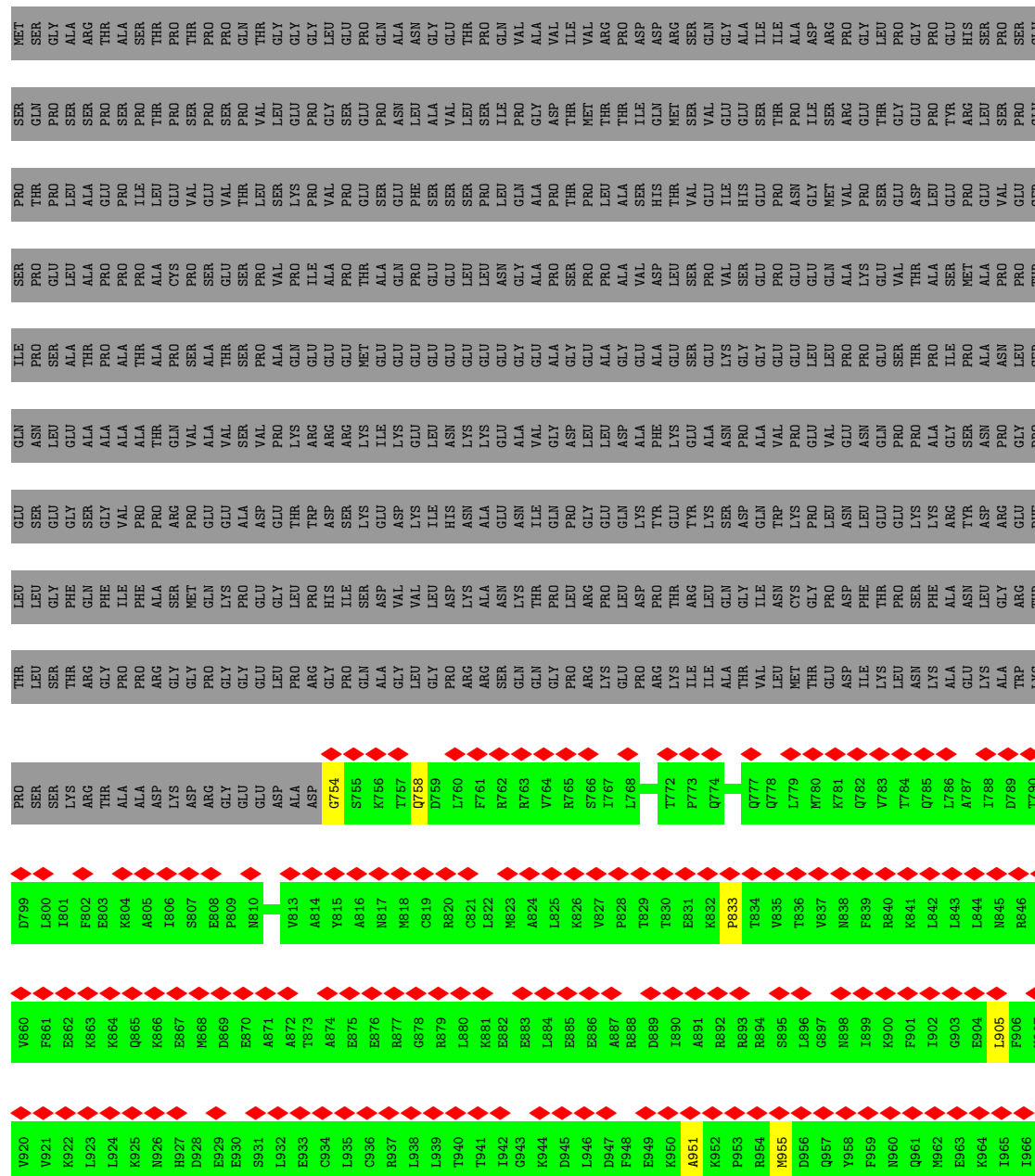
• Molecule 55: Eukaryotic initiation factor 4A-I

Chain 1: 





• Molecule 56: Eukaryotic translation initiation factor 4 gamma 1



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	241389	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 ($e^-/\text{\AA}^2$)	47.88	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, OMU, C4J, MA6, PSU, 5MU, 6MZ, JMH, A2M, 5MC, OMC, ZN, UR3

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	5	0.15	0/2174	0.40	0/3036
2	6	0.16	0/1329	0.33	0/1848
3	7	0.25	0/628	0.50	0/846
4	8	0.16	0/1567	0.35	0/2182
5	9	0.24	0/231	0.47	0/294
6	A	0.22	0/5470	0.47	3/7444 (0.0%)
7	B	0.15	0/1065	0.37	0/1484
8	C	0.22	0/1807	0.37	0/2518
9	D	0.28	0/2267	0.51	0/3056
10	E	0.20	0/3598	0.42	0/4868
11	F	0.15	0/1597	0.37	0/2216
12	G	0.24	0/797	0.52	0/1061
13	H	0.19	0/1200	0.41	0/1618
14	I	0.23	0/4695	0.44	0/6376
15	J	0.24	0/5288	0.49	0/7159
16	K	0.25	0/2636	0.39	0/3676
17	L	0.22	0/1460	0.46	0/1953
18	M	0.22	0/644	0.42	0/864
19	N	0.23	0/623	0.43	0/833
20	O	0.24	0/1743	0.44	0/2354
21	P	0.23	0/1742	0.44	0/2330
22	Q	0.23	0/1732	0.42	0/2353
23	R	0.24	0/805	0.44	0/1079
24	S	0.22	0/1885	0.47	0/2510
25	T	0.21	0/1010	0.45	0/1353
26	U	0.16	0/688	0.39	0/958
27	V	0.22	0/1232	0.41	0/1656
28	W	0.78	17/40246 (0.0%)	0.45	18/62715 (0.0%)
29	X	0.22	0/1186	0.40	0/1585
30	Y	0.22	0/2077	0.39	0/2796
31	Z	0.22	0/1502	0.42	0/2008
32	a	0.23	0/1105	0.39	0/1476

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.21	0/380	0.37	0/496
34	c	0.23	0/1051	0.40	0/1406
35	d	0.21	0/1654	0.41	0/2203
36	e	0.22	0/1032	0.42	0/1371
37	f	0.20	0/1481	0.46	0/1988
38	g	0.20	0/1142	0.45	0/1528
39	h	0.22	0/1793	0.45	0/2414
40	i	0.26	0/859	0.53	0/1159
41	j	0.21	0/929	0.44	0/1241
42	k	0.20	0/2493	0.44	0/3394
43	l	0.20	0/1123	0.44	0/1504
44	m	0.24	0/529	0.51	0/712
45	n	0.21	0/1194	0.49	0/1599
46	o	0.20	0/429	0.41	0/568
47	p	0.24	0/444	0.45	0/588
48	q	0.22	0/960	0.49	0/1286
49	s	0.21	0/500	0.47	0/669
50	v	0.23	0/1077	0.48	0/1444
51	w	0.19	0/827	0.46	0/1110
52	x	0.39	1/2963 (0.0%)	1.78	4/4050 (0.1%)
53	y	0.18	0/1795	0.39	0/2798
54	z	0.28	0/944	0.53	3/1463 (0.2%)
55	1	0.17	0/1833	0.39	0/2552
55	3	0.15	0/1868	0.37	0/2601
56	2	0.16	0/1177	0.32	0/1642
All	All	0.47	18/126506 (0.0%)	0.51	28/180291 (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
6	A	0	1
9	D	0	1
28	W	1	0
32	a	0	1
39	h	0	1
42	k	0	1
52	x	0	1
All	All	1	6

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	W	1675	A	C6-N1	56.51	2.48	1.35
28	W	1675	A	C2-N3	56.33	2.46	1.33
28	W	1675	A	N3-C4	54.78	2.44	1.34
28	W	1675	A	N1-C2	54.24	2.42	1.34
28	W	1675	A	C5-C6	49.15	2.39	1.41

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	x	20	ALA	O-C-N	-66.50	23.96	122.39
52	x	20	ALA	CA-C-N	-60.76	9.73	122.13
52	x	20	ALA	C-N-CA	-60.76	9.73	122.13
28	W	1650	A	N7-C8-N9	-25.84	36.27	113.80
28	W	1650	A	C4-C5-N7	-25.75	33.45	110.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	W	1219	JMH	C2'

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	662	GLU	Peptide
9	D	234	ARG	Sidechain
32	a	60	LYS	Peptide
39	h	161	GLY	Peptide
42	k	4	GLN	Peptide

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	5	2175	0	954	9	0
2	6	1330	0	591	2	0
3	7	616	0	600	5	0
4	8	1569	0	674	7	0
5	9	230	0	276	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	5386	0	4899	52	0
7	B	1066	0	481	3	0
8	C	1809	0	810	3	0
9	D	2234	0	2288	29	0
10	E	3540	0	3690	35	0
11	F	1598	0	723	6	0
12	G	789	0	806	8	0
13	H	1176	0	1182	10	0
14	I	4569	0	4316	35	0
15	J	5207	0	4893	39	0
16	K	2637	0	1135	7	0
17	L	1439	0	1533	5	0
18	M	631	0	657	5	0
19	N	617	0	622	7	0
20	O	1707	0	1794	13	0
21	P	1715	0	1785	17	0
22	Q	1695	0	1696	9	0
23	R	792	0	843	4	0
24	S	1862	0	2018	15	0
25	T	997	0	1021	4	0
26	U	689	0	290	0	0
27	V	1208	0	1294	9	0
28	W	36639	0	18516	237	0
29	X	1166	0	1233	5	0
30	Y	2035	0	2138	15	0
31	Z	1477	0	1589	5	0
32	a	1087	0	1154	7	0
33	b	378	0	417	1	0
34	c	1034	0	1080	6	0
35	d	1627	0	1706	15	0
36	e	1015	0	1086	6	0
37	f	1461	0	1511	10	0
38	g	1124	0	1193	13	0
39	h	1765	0	1865	20	0
40	i	834	0	861	4	0
41	j	913	0	952	9	0
42	k	2436	0	2393	27	0
43	l	1105	0	1138	9	0
44	m	523	0	573	7	0
45	n	1176	0	1233	15	0
46	o	419	0	415	6	0
47	p	435	0	434	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	q	950	0	987	7	0
49	s	498	0	525	3	0
50	v	1064	0	1117	8	0
51	w	817	0	882	6	0
52	x	2920	0	2231	30	0
53	y	1604	0	816	15	0
54	z	853	0	429	5	0
55	1	1834	0	821	5	0
55	3	1869	0	838	2	0
56	2	1178	0	511	3	0
57	R	1	0	0	0	0
57	p	1	0	0	0	0
58	T	2	0	0	0	0
58	W	86	0	0	0	0
58	f	1	0	0	0	0
All	All	121610	0	92515	727	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 3.

The worst 5 of 727 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)
28:W:1675:A:C5	28:W:1675:A:C4	2.27	1.22
1:5:12:HIS:HA	52:x:9:ILE:HA	1.16	1.11
28:W:1675:A:C5	28:W:1675:A:C6	2.39	1.10
9:D:231:ALA:HA	10:E:267:PRO:HB3	1.40	1.04
1:5:12:HIS:CA	52:x:9:ILE:HA	1.99	0.93

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	
1	5	435/445 (98%)	419 (96%)	16 (4%)	0	100	100
2	6	267/357 (75%)	252 (94%)	15 (6%)	0	100	100
3	7	75/320 (23%)	66 (88%)	9 (12%)	0	100	100
4	8	312/352 (89%)	294 (94%)	17 (5%)	1 (0%)	36	67
5	9	22/25 (88%)	22 (100%)	0	0	100	100
6	A	731/1382 (53%)	697 (95%)	32 (4%)	2 (0%)	36	67
7	B	213/218 (98%)	195 (92%)	18 (8%)	0	100	100
8	C	360/374 (96%)	340 (94%)	19 (5%)	1 (0%)	36	67
9	D	276/315 (88%)	257 (93%)	17 (6%)	2 (1%)	18	51
10	E	462/472 (98%)	442 (96%)	19 (4%)	1 (0%)	43	74
11	F	323/325 (99%)	290 (90%)	33 (10%)	0	100	100
12	G	95/144 (66%)	87 (92%)	8 (8%)	0	100	100
13	H	147/431 (34%)	139 (95%)	8 (5%)	0	100	100
14	I	571/814 (70%)	531 (93%)	38 (7%)	2 (0%)	30	62
15	J	683/913 (75%)	650 (95%)	32 (5%)	1 (0%)	48	79
16	K	529/564 (94%)	504 (95%)	24 (4%)	1 (0%)	43	74
17	L	172/194 (89%)	166 (96%)	6 (4%)	0	100	100
18	M	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
19	N	79/83 (95%)	73 (92%)	6 (8%)	0	100	100
20	O	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
21	P	209/264 (79%)	199 (95%)	10 (5%)	0	100	100
22	Q	212/295 (72%)	198 (93%)	14 (7%)	0	100	100
23	R	97/115 (84%)	94 (97%)	3 (3%)	0	100	100
24	S	228/249 (92%)	219 (96%)	9 (4%)	0	100	100
25	T	131/151 (87%)	123 (94%)	8 (6%)	0	100	100
26	U	137/333 (41%)	126 (92%)	11 (8%)	0	100	100
27	V	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
29	X	138/158 (87%)	135 (98%)	3 (2%)	0	100	100
30	Y	254/263 (97%)	245 (96%)	9 (4%)	0	100	100
31	Z	175/194 (90%)	173 (99%)	2 (1%)	0	100	100
32	a	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
33	b	43/59 (73%)	41 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	c	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
35	d	194/208 (93%)	190 (98%)	4 (2%)	0	100	100
36	e	123/133 (92%)	120 (98%)	3 (2%)	0	100	100
37	f	180/204 (88%)	167 (93%)	13 (7%)	0	100	100
38	g	139/146 (95%)	131 (94%)	8 (6%)	0	100	100
39	h	225/243 (93%)	220 (98%)	5 (2%)	0	100	100
40	i	97/165 (59%)	89 (92%)	8 (8%)	0	100	100
41	j	108/145 (74%)	103 (95%)	5 (5%)	0	100	100
42	k	311/317 (98%)	293 (94%)	18 (6%)	0	100	100
43	l	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
44	m	64/125 (51%)	62 (97%)	2 (3%)	0	100	100
45	n	140/151 (93%)	129 (92%)	11 (8%)	0	100	100
46	o	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
47	p	49/156 (31%)	45 (92%)	4 (8%)	0	100	100
48	q	120/132 (91%)	107 (89%)	13 (11%)	0	100	100
49	s	61/69 (88%)	52 (85%)	9 (15%)	0	100	100
50	v	127/135 (94%)	117 (92%)	9 (7%)	1 (1%)	16	49
51	w	101/119 (85%)	94 (93%)	7 (7%)	0	100	100
52	x	434/548 (79%)	361 (83%)	68 (16%)	5 (1%)	10	41
55	1	369/406 (91%)	304 (82%)	59 (16%)	6 (2%)	7	36
55	3	376/406 (93%)	353 (94%)	22 (6%)	1 (0%)	36	67
56	2	235/1404 (17%)	216 (92%)	18 (8%)	1 (0%)	30	62
All	All	11727/16023 (73%)	11003 (94%)	699 (6%)	25 (0%)	44	74

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	8	271	GLN
9	D	232	PRO
9	D	233	PRO
52	x	13	PRO
52	x	21	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	
3	7	64/277 (23%)	64 (100%)	0	100	100
5	9	23/24 (96%)	23 (100%)	0	100	100
6	A	495/1259 (39%)	493 (100%)	2 (0%)	84	81
9	D	249/280 (89%)	246 (99%)	3 (1%)	63	73
10	E	394/397 (99%)	394 (100%)	0	100	100
12	G	83/123 (68%)	83 (100%)	0	100	100
13	H	133/389 (34%)	133 (100%)	0	100	100
14	I	470/702 (67%)	470 (100%)	0	100	100
15	J	511/811 (63%)	509 (100%)	2 (0%)	84	81
17	L	160/174 (92%)	160 (100%)	0	100	100
18	M	73/76 (96%)	73 (100%)	0	100	100
19	N	65/67 (97%)	65 (100%)	0	100	100
20	O	186/225 (83%)	186 (100%)	0	100	100
21	P	192/231 (83%)	192 (100%)	0	100	100
22	Q	180/243 (74%)	180 (100%)	0	100	100
23	R	86/98 (88%)	86 (100%)	0	100	100
24	S	200/218 (92%)	200 (100%)	0	100	100
25	T	104/119 (87%)	104 (100%)	0	100	100
27	V	130/131 (99%)	130 (100%)	0	100	100
29	X	129/142 (91%)	129 (100%)	0	100	100
30	Y	220/225 (98%)	220 (100%)	0	100	100
31	Z	158/168 (94%)	158 (100%)	0	100	100
32	a	112/115 (97%)	112 (100%)	0	100	100
33	b	38/48 (79%)	38 (100%)	0	100	100
34	c	112/113 (99%)	112 (100%)	0	100	100
35	d	172/180 (96%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	e	107/115 (93%)	107 (100%)	0	100	100
37	f	156/170 (92%)	156 (100%)	0	100	100
38	g	117/121 (97%)	117 (100%)	0	100	100
39	h	190/202 (94%)	190 (100%)	0	100	100
40	i	90/136 (66%)	90 (100%)	0	100	100
41	j	100/130 (77%)	100 (100%)	0	100	100
42	k	272/275 (99%)	272 (100%)	0	100	100
43	l	112/115 (97%)	112 (100%)	0	100	100
44	m	58/103 (56%)	58 (100%)	0	100	100
45	n	123/131 (94%)	123 (100%)	0	100	100
46	o	44/49 (90%)	44 (100%)	0	100	100
47	p	47/140 (34%)	47 (100%)	0	100	100
48	q	104/108 (96%)	104 (100%)	0	100	100
49	s	56/62 (90%)	56 (100%)	0	100	100
50	v	119/122 (98%)	119 (100%)	0	100	100
51	w	94/107 (88%)	94 (100%)	0	100	100
52	x	205/494 (42%)	205 (100%)	0	100	100
All	All	6733/9415 (72%)	6726 (100%)	7 (0%)	87	87

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	D	123	LYS
9	D	234	ARG
15	J	123	ASP
15	J	120	LEU
9	D	122	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
42	k	104	HIS
52	x	326	GLN
44	m	106	GLN
45	n	135	HIS

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Mol	Chain	Res	Type
52	x	456	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	W	1706/1719 (99%)	467 (27%)	13 (0%)
53	y	74/75 (98%)	33 (44%)	0
54	z	49/207 (23%)	32 (65%)	0
All	All	1829/2001 (91%)	532 (29%)	13 (0%)

5 of 532 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	W	2	A
28	W	4	C
28	W	17	C
28	W	20	G
28	W	23	G

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	W	1463	U
28	W	1599	U
28	W	1782	G
28	W	1631	U
28	W	1675	A

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

29 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
28	OMC	W	517	28	19,22,23	2.54	3 (15%)	26,31,34	0.80	0
28	PSU	W	1243	28	18,21,22	3.82	5 (27%)	22,30,33	1.87	5 (22%)
28	A2M	W	166	28	22,25,26	2.93	8 (36%)	31,36,39	2.52	9 (29%)
28	PSU	W	1081	28	18,21,22	3.71	6 (33%)	22,30,33	1.77	4 (18%)
28	OMC	W	174	28	19,22,23	2.52	3 (15%)	26,31,34	0.77	0
28	A2M	W	27	28	22,25,26	2.94	9 (40%)	31,36,39	2.67	7 (22%)
28	C4J	W	1248	28	24,29,30	1.54	5 (20%)	29,42,45	1.50	4 (13%)
28	JMH	W	1219	58,28	18,22,23	2.89	6 (33%)	21,32,35	3.44	5 (23%)
28	OMU	W	116	28	19,22,23	2.78	5 (26%)	26,31,34	3.31	8 (30%)
28	MA6	W	1851	28	23,26,27	1.69	6 (26%)	34,38,41	2.69	10 (29%)
28	PSU	W	822	28	18,21,22	3.79	6 (33%)	22,30,33	1.80	4 (18%)
28	5MC	W	1374	28	18,22,23	2.73	4 (22%)	26,32,35	1.08	2 (7%)
28	A2M	W	484	28	22,25,26	2.80	8 (36%)	31,36,39	2.60	9 (29%)
28	OMG	W	509	58,28	23,26,27	2.45	6 (26%)	33,38,41	2.02	10 (30%)
28	A2M	W	668	58,28	22,25,26	2.86	7 (31%)	31,36,39	2.78	12 (38%)
28	PSU	W	612	28	18,21,22	3.72	6 (33%)	22,30,33	1.71	5 (22%)
28	PSU	W	823	28	18,21,22	3.72	5 (27%)	22,30,33	1.84	5 (22%)
28	A2M	W	159	28	22,25,26	2.94	8 (36%)	31,36,39	2.76	10 (32%)
28	5MU	W	814	28	19,22,23	2.92	6 (31%)	28,32,35	2.28	8 (28%)
28	OMC	W	1703	28	19,22,23	2.52	3 (15%)	26,31,34	0.78	1 (3%)
28	A2M	W	1678	28	22,25,26	2.79	5 (22%)	31,36,39	2.74	10 (32%)
28	6MZ	W	1832	58,28	22,25,26	2.56	6 (27%)	30,36,39	2.85	11 (36%)
28	A2M	W	1031	28	22,25,26	2.97	9 (40%)	31,36,39	2.74	10 (32%)
28	OMU	W	121	28	19,22,23	2.78	5 (26%)	26,31,34	3.36	8 (30%)
28	OMG	W	644	28	23,26,27	2.46	6 (26%)	33,38,41	2.04	10 (30%)
28	MA6	W	1850	28	23,26,27	1.64	6 (26%)	34,38,41	2.64	10 (29%)
28	PSU	W	119	28	18,21,22	3.79	5 (27%)	22,30,33	1.58	3 (13%)
28	UR3	W	1830	28	19,22,23	1.94	5 (26%)	26,32,35	1.59	4 (15%)
28	OMG	W	683	28	23,26,27	2.47	5 (21%)	33,38,41	2.01	9 (27%)

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
28	OMC	W	517	28	-	0/9/27/28	0/2/2/2
28	PSU	W	1243	28	-	1/7/25/26	0/2/2/2
28	A2M	W	166	28	-	7/9/27/28	0/3/3/3
28	PSU	W	1081	28	-	3/7/25/26	0/2/2/2
28	OMC	W	174	28	-	0/9/27/28	0/2/2/2
28	A2M	W	27	28	-	2/9/27/28	0/3/3/3
28	C4J	W	1248	28	-	2/16/34/35	0/2/2/2
28	JMH	W	1219	58,28	1/1/5/5	6/7/25/26	0/2/2/2
28	OMU	W	116	28	-	2/9/27/28	0/2/2/2
28	MA6	W	1851	28	-	3/11/29/30	0/3/3/3
28	PSU	W	822	28	-	1/7/25/26	0/2/2/2
28	5MC	W	1374	28	-	0/7/25/26	0/2/2/2
28	A2M	W	484	28	-	0/9/27/28	0/3/3/3
28	OMG	W	509	58,28	-	2/9/27/28	0/3/3/3
28	A2M	W	668	58,28	-	2/9/27/28	0/3/3/3
28	PSU	W	612	28	-	2/7/25/26	0/2/2/2
28	PSU	W	823	28	-	0/7/25/26	0/2/2/2
28	A2M	W	159	28	-	0/9/27/28	0/3/3/3
28	5MU	W	814	28	-	0/7/25/26	0/2/2/2
28	OMC	W	1703	28	-	2/9/27/28	0/2/2/2
28	A2M	W	1678	28	-	2/9/27/28	0/3/3/3
28	6MZ	W	1832	58,28	-	2/9/27/28	0/3/3/3
28	A2M	W	1031	28	-	2/9/27/28	0/3/3/3
28	OMU	W	121	28	-	0/9/27/28	0/2/2/2
28	OMG	W	644	28	-	1/9/27/28	0/3/3/3
28	MA6	W	1850	28	-	2/11/29/30	0/3/3/3
28	PSU	W	119	28	-	0/7/25/26	0/2/2/2
28	UR3	W	1830	28	-	2/7/25/26	0/2/2/2
28	OMG	W	683	28	-	0/9/27/28	0/3/3/3

The worst 5 of 167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	W	166	A2M	O3'-C3'	-10.28	1.18	1.43
28	W	1031	A2M	O3'-C3'	-10.20	1.19	1.43
28	W	159	A2M	O3'-C3'	-10.10	1.19	1.43
28	W	668	A2M	O3'-C3'	-10.02	1.19	1.43
28	W	27	A2M	O3'-C3'	-10.01	1.19	1.43

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	W	1219	JMH	C1'-N1-C2	11.47	136.35	116.99
28	W	121	OMU	N3-C2-N1	8.98	126.81	114.89
28	W	121	OMU	C4-N3-C2	-8.67	115.14	126.58
28	W	116	OMU	N3-C2-N1	8.61	126.32	114.89
28	W	159	A2M	C4-N9-C8	8.48	114.92	105.73

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	W	1219	JMH	C2'

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	W	166	A2M	C3'-C4'-C5'-O5'
28	W	509	OMG	O4'-C4'-C5'-O5'
28	W	509	OMG	C3'-C4'-C5'-O5'
28	W	668	A2M	O4'-C4'-C5'-O5'
28	W	668	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	W	166	A2M	2	0
28	W	1081	PSU	1	0
28	W	116	OMU	1	0
28	W	1851	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 91 ligands modelled in this entry, 91 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
28	W	7
8	C	1
14	I	1
50	v	1

The worst 5 of 10 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	753:C	O3'	788:G	P	16.10
1	W	1760:G	O3'	1771:G	P	15.61
1	W	697:G	O3'	733:C	P	15.25
1	W	225:G	O3'	287:U	P	11.87
1	W	740:C	O3'	746:C	P	6.05

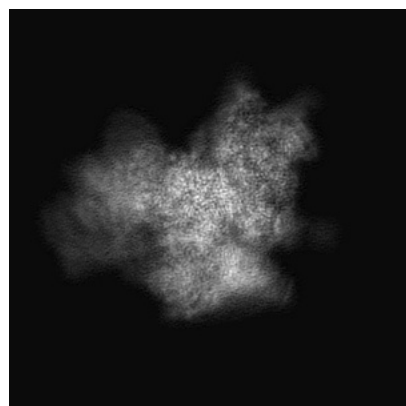
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17297. These allow visual inspection of the internal detail of the map and identification of artifacts.

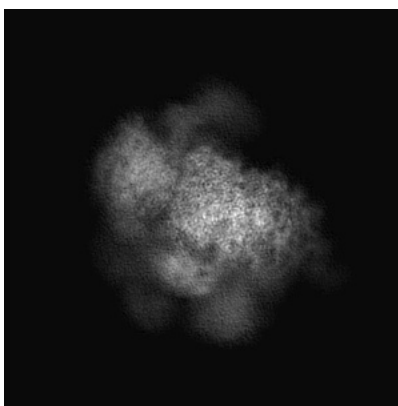
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

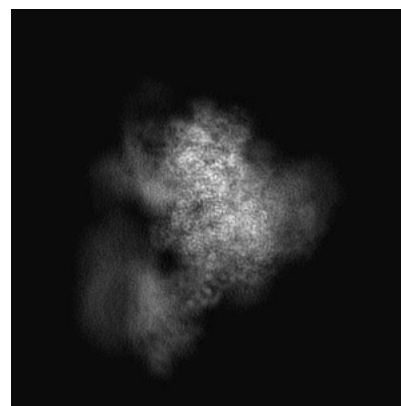
6.1.1 Primary map



X

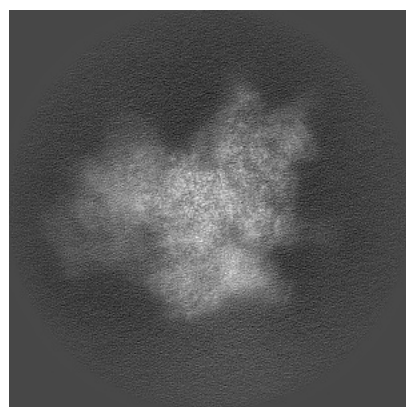


Y

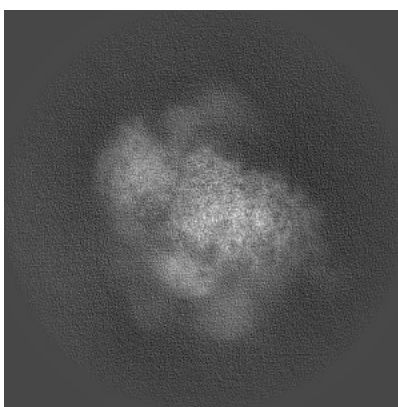


Z

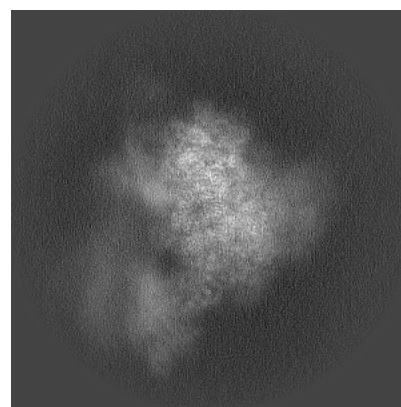
6.1.2 Raw map



X



Y

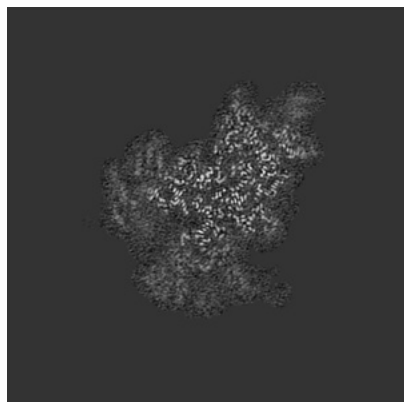


Z

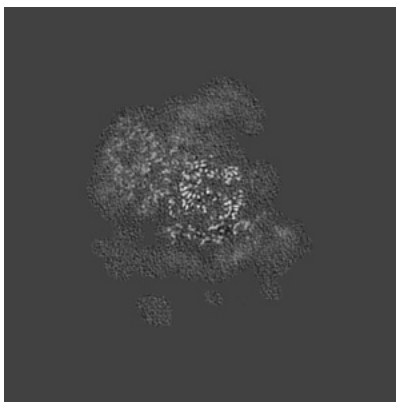
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

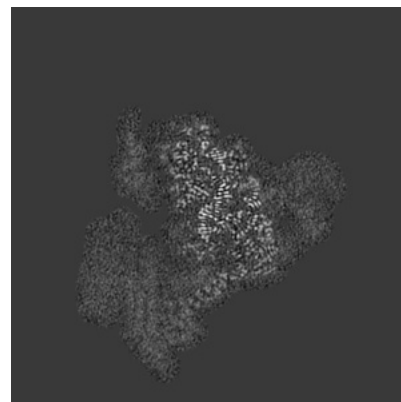
6.2.1 Primary map



X Index: 200

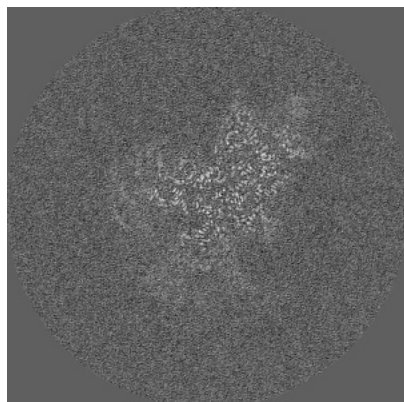


Y Index: 200

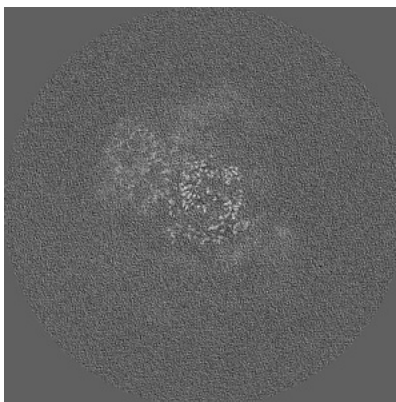


Z Index: 200

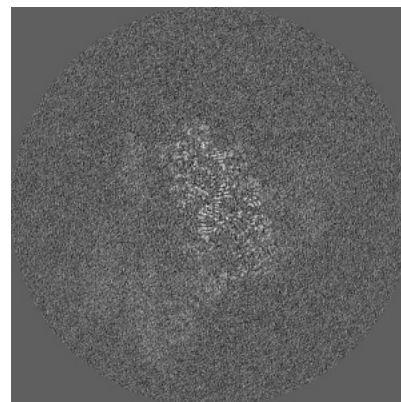
6.2.2 Raw map



X Index: 200



Y Index: 200

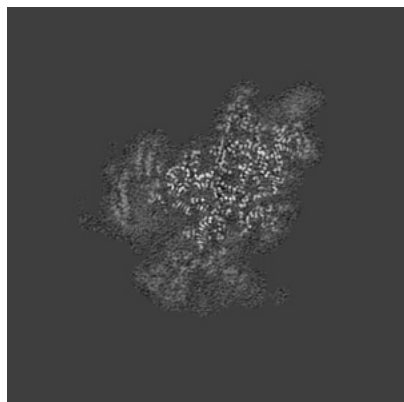


Z Index: 200

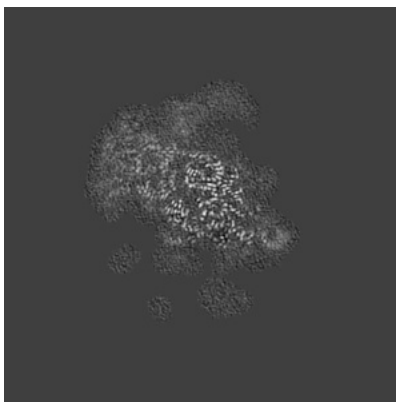
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

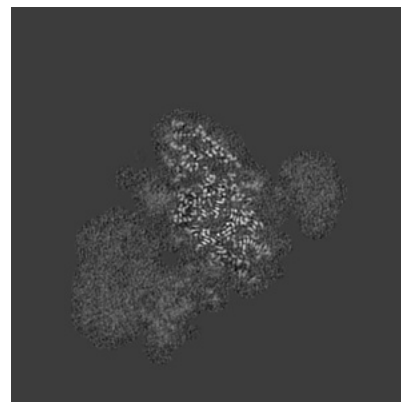
6.3.1 Primary map



X Index: 197

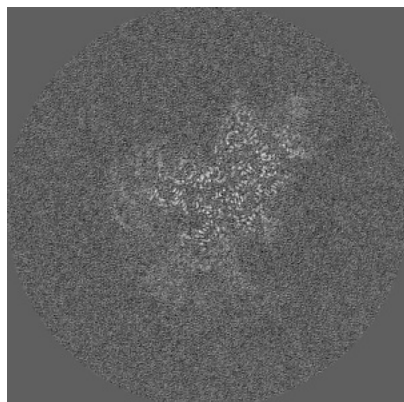


Y Index: 192

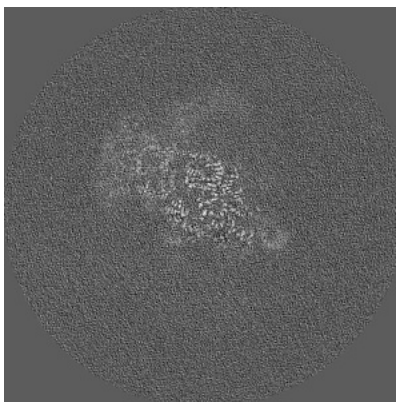


Z Index: 218

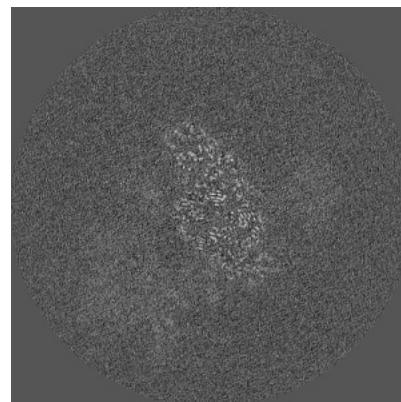
6.3.2 Raw map



X Index: 200



Y Index: 192

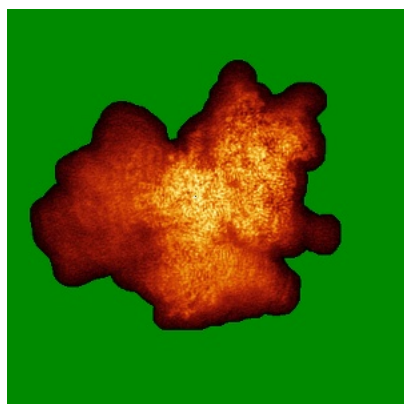


Z Index: 213

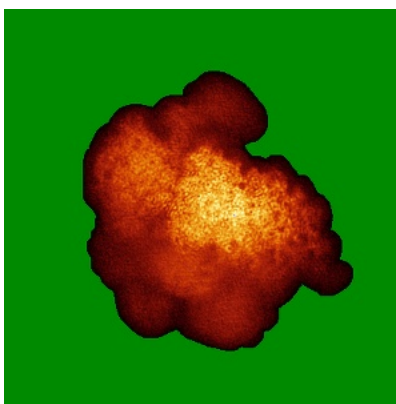
The images above show the largest variance slices of the map in three orthogonal directions.

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

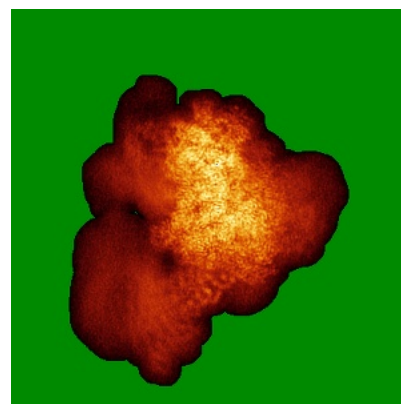
6.4.1 Primary map



X

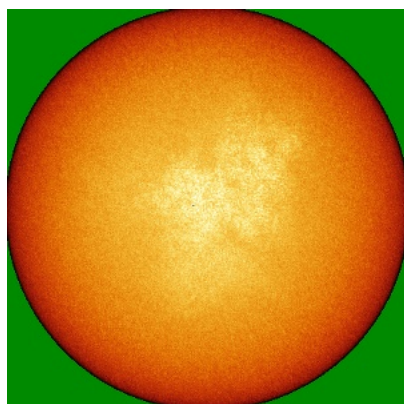


Y

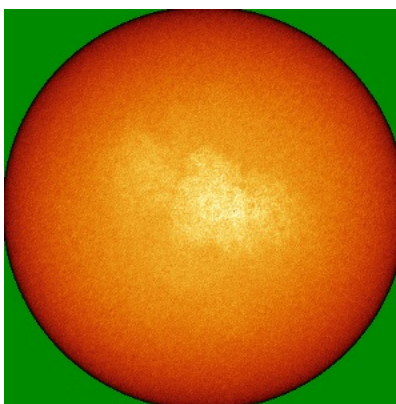


Z

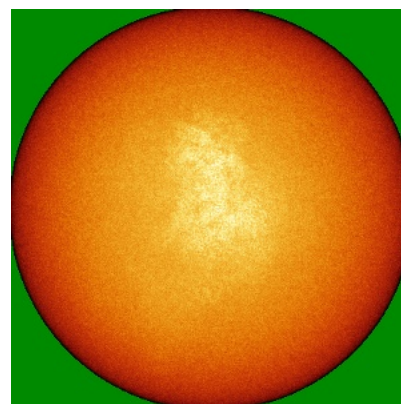
6.4.2 Raw map



X



Y

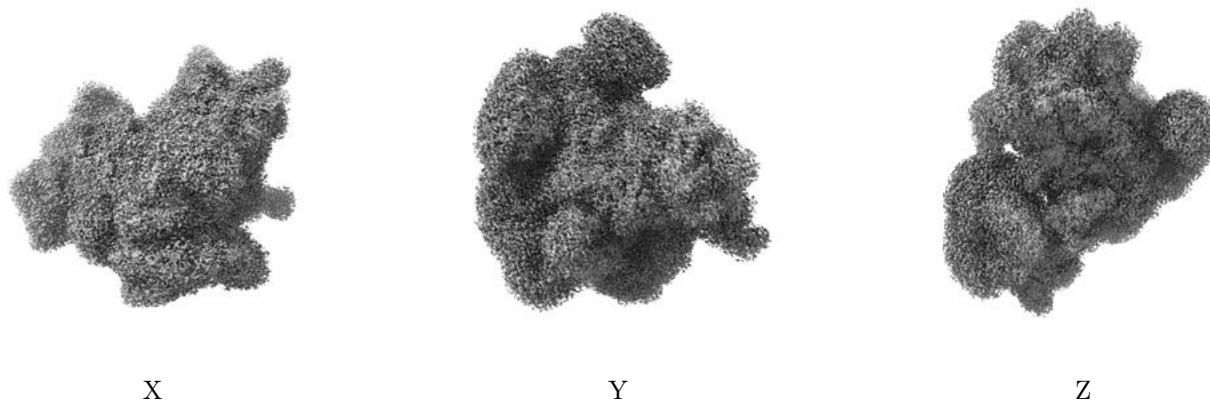


Z

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.

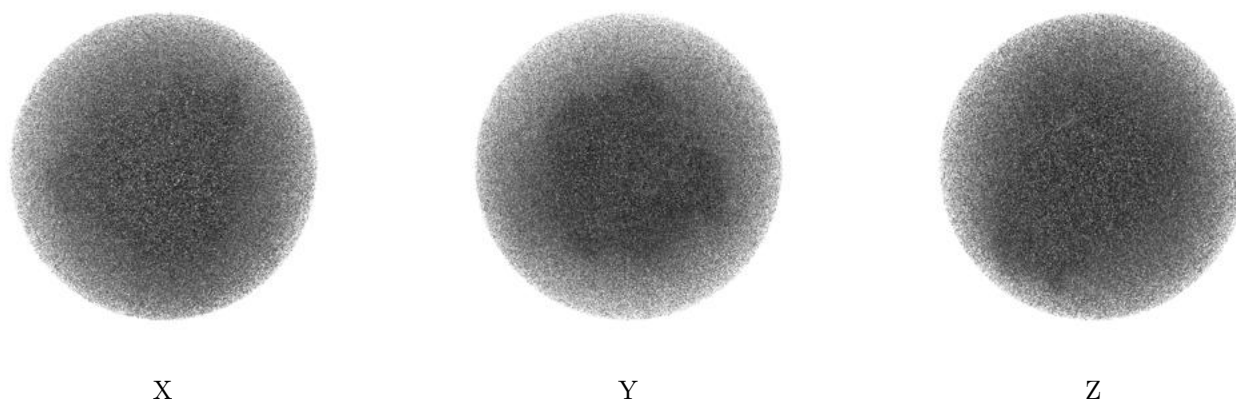
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

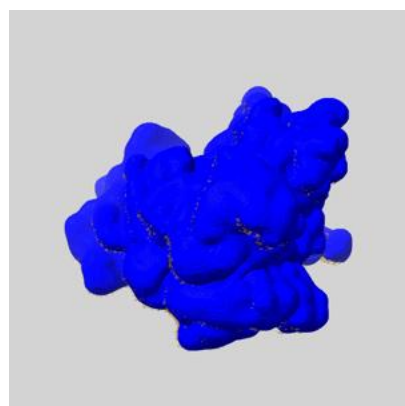
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

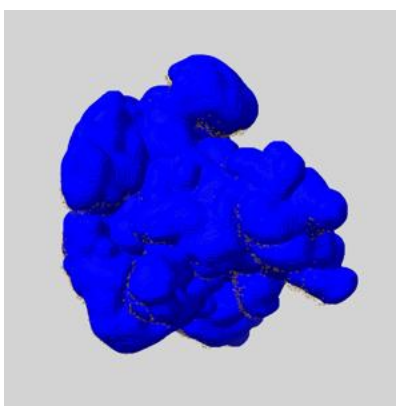
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

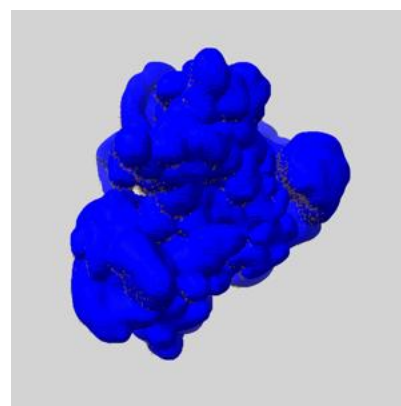
6.6.1 emd_17297_msk_1.map [i](#)



X



Y

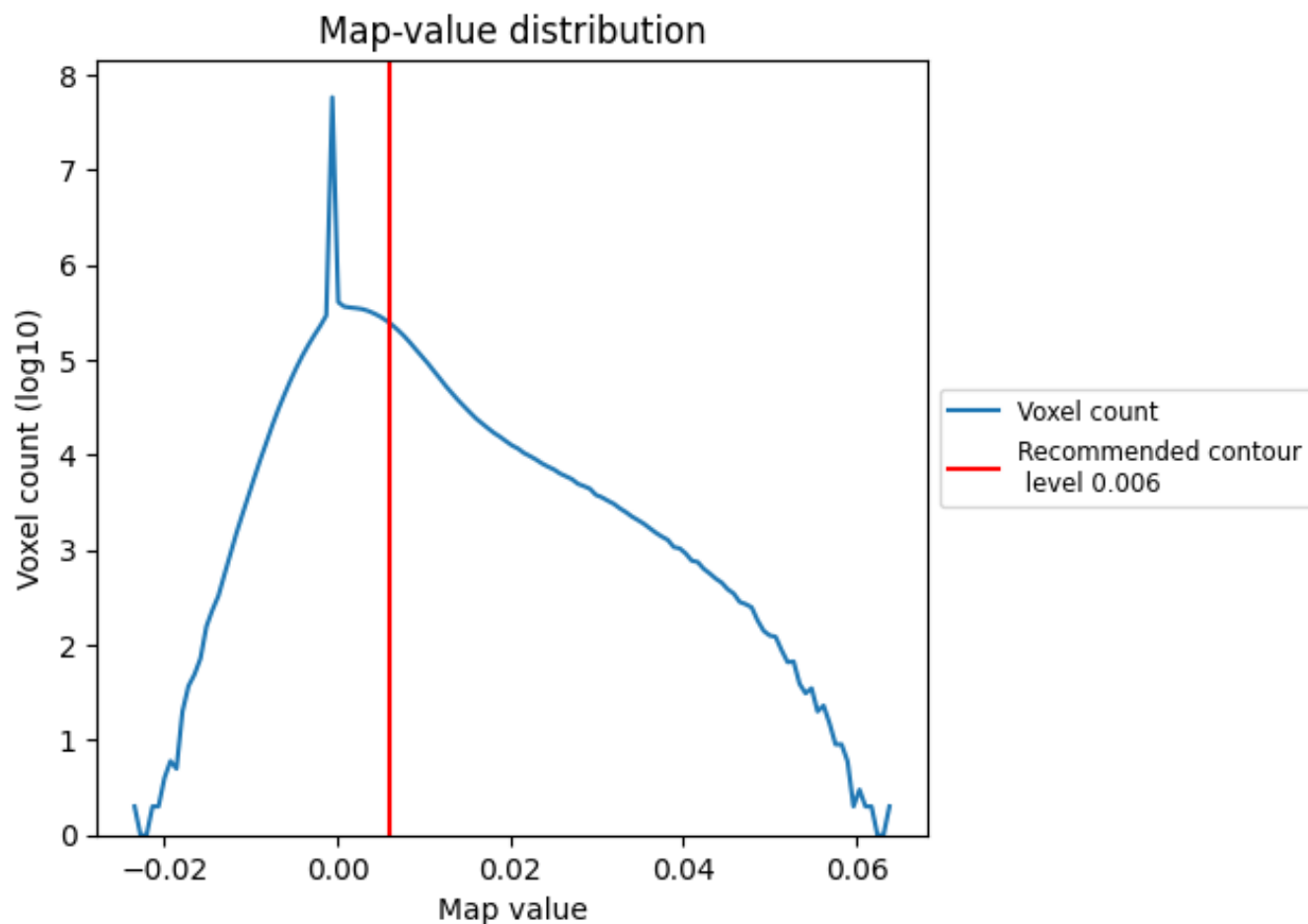


Z

7 Map analysis [i](#)

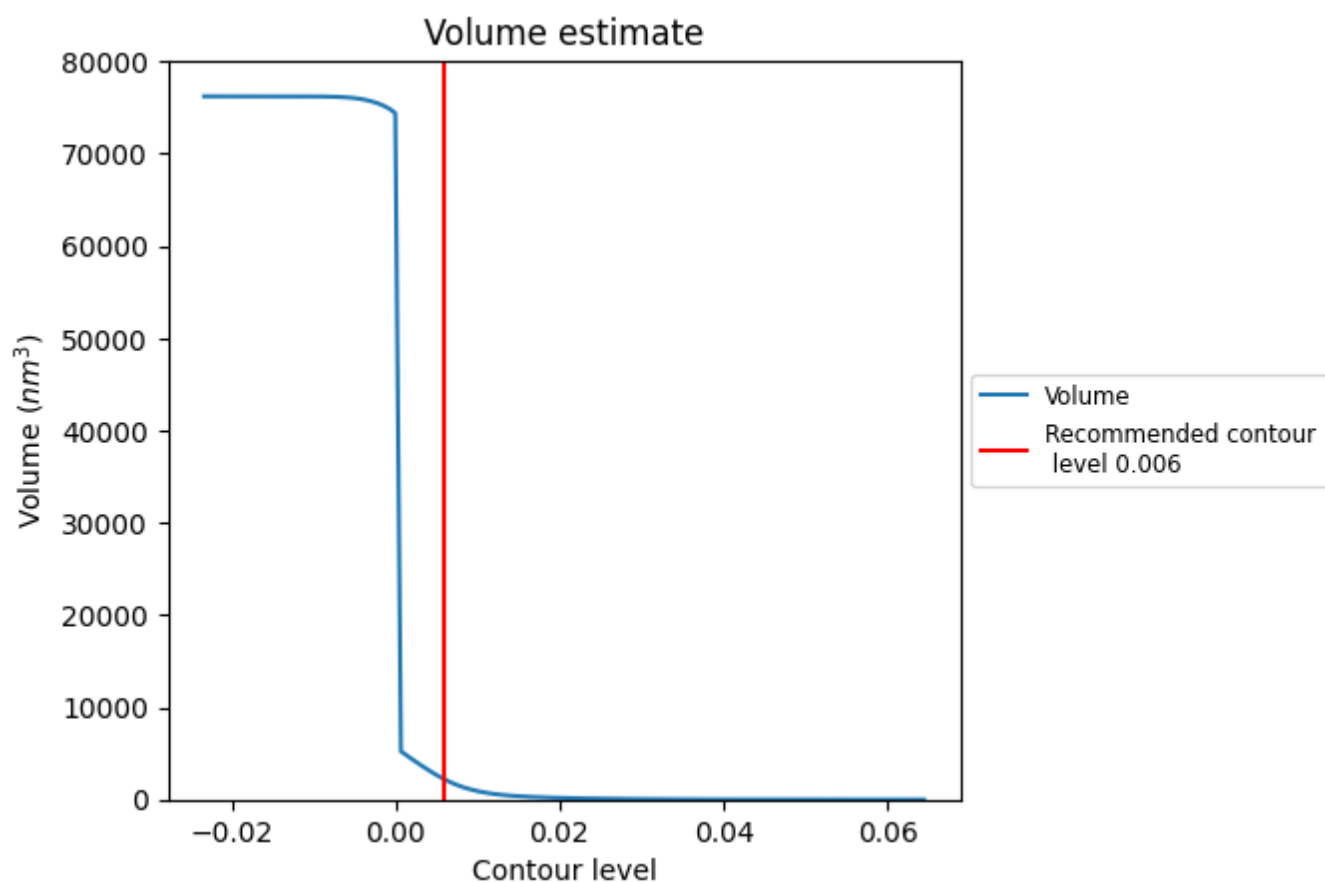
This section contains the results of statistical analysis of the map.

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.

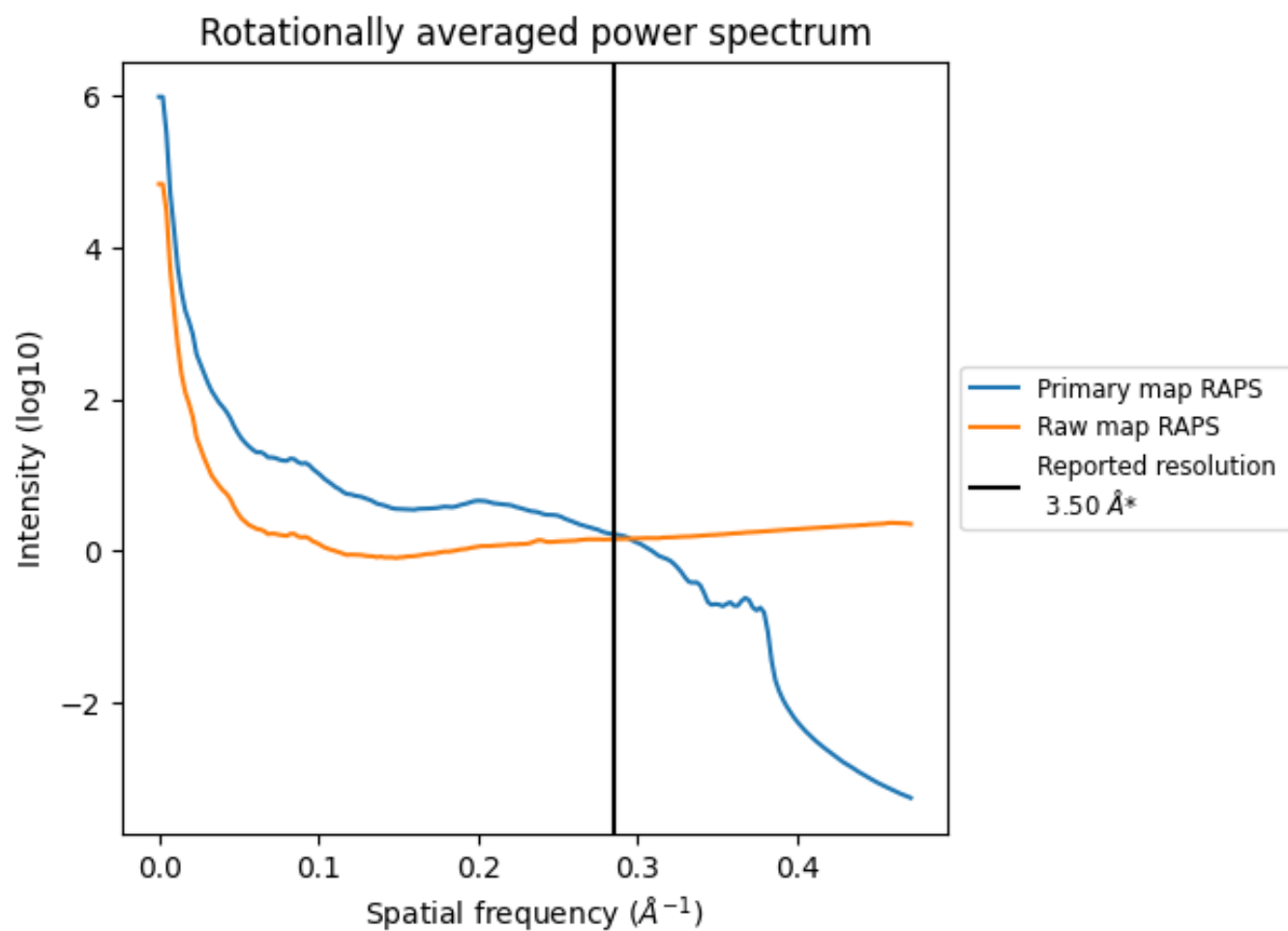
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2177 nm³; this corresponds to an approximate mass of 1966 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 ⓘ

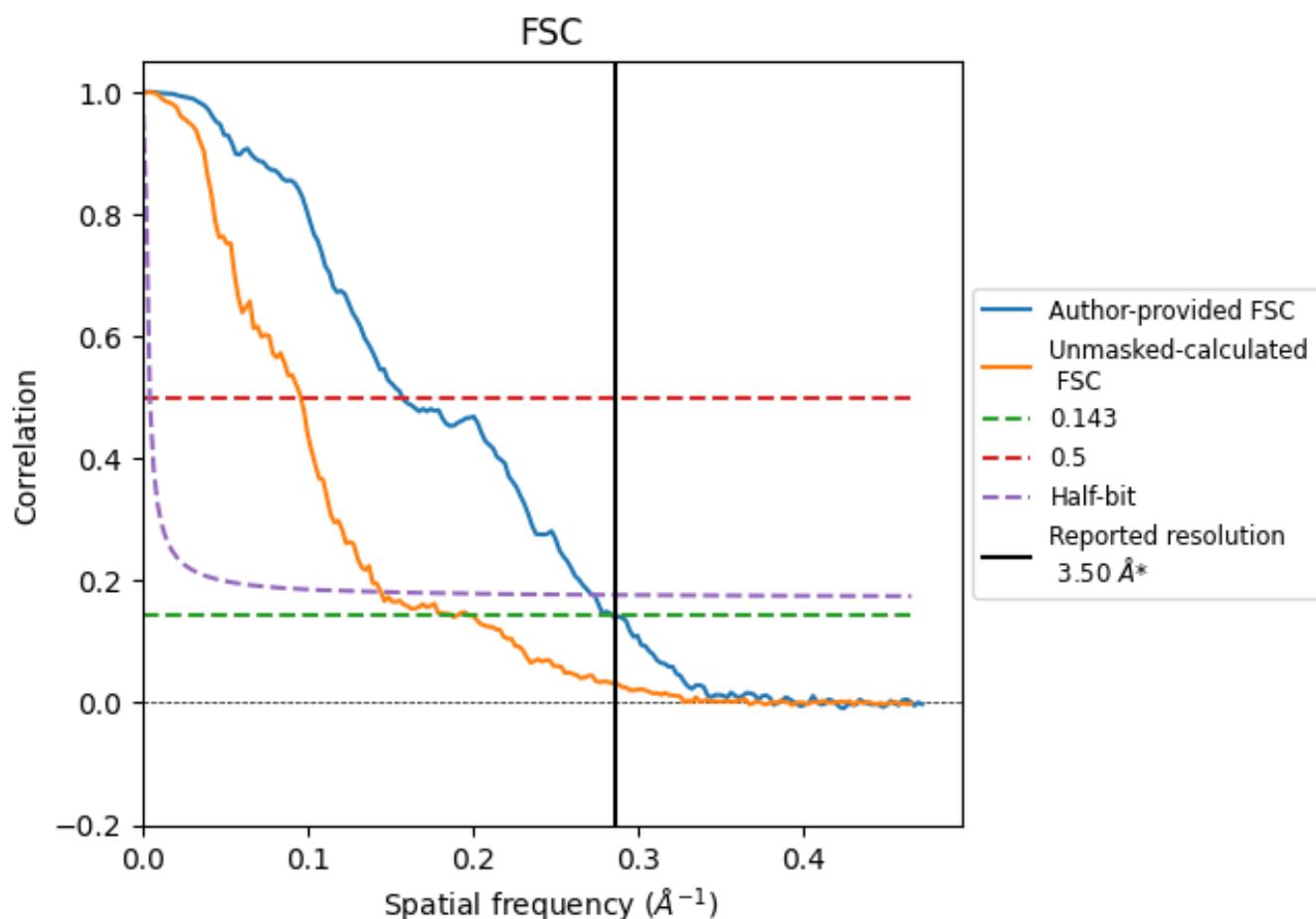


*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

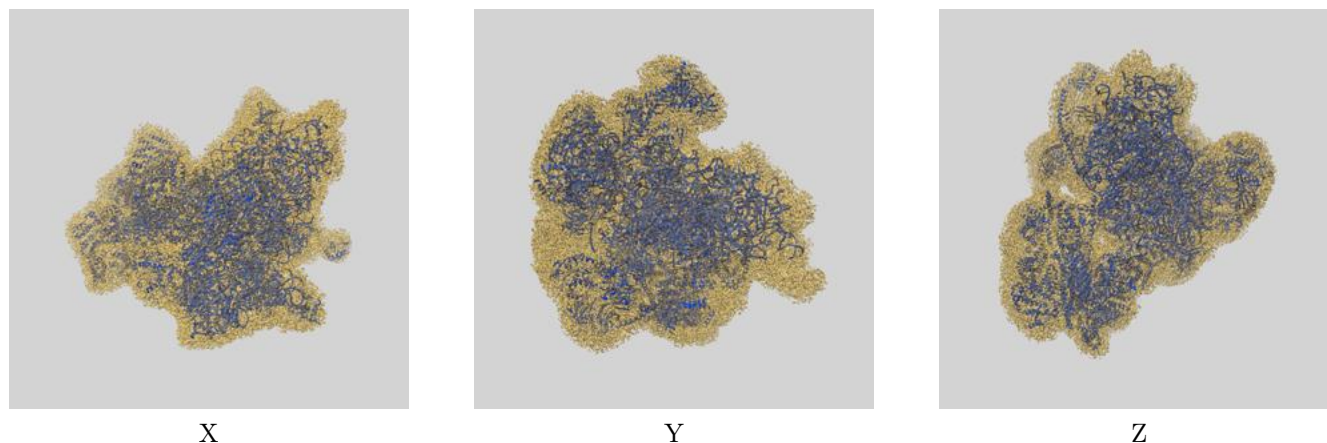
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.52	6.36	3.66
Unmasked-calculated*	5.35	10.43	6.93

*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 5.35 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

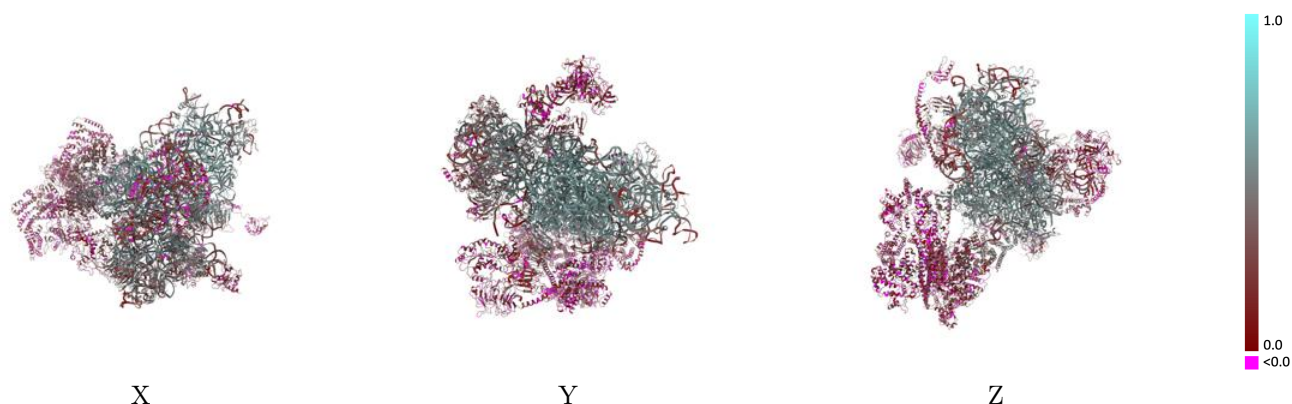
This section contains information regarding the fit between EMDB map EMD-17297 and PDB model 8OZ0. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



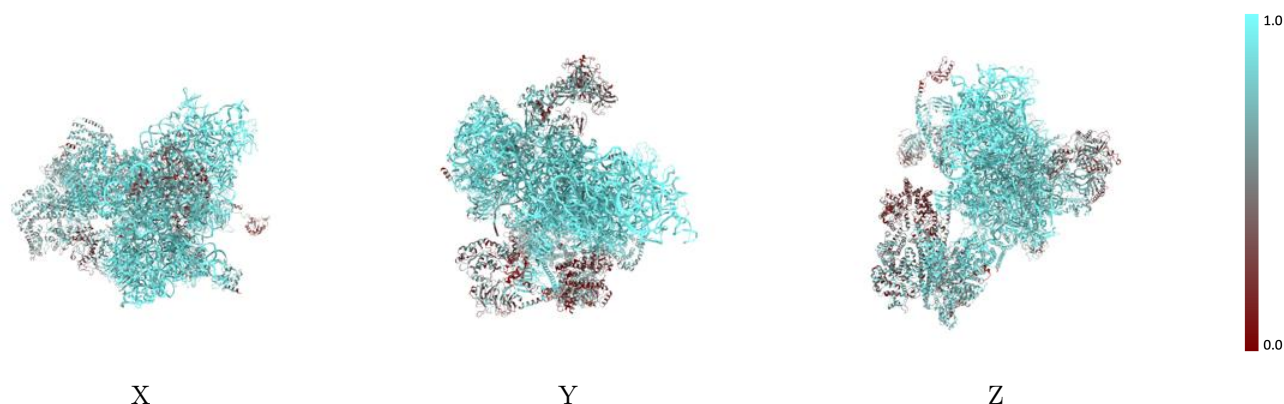
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



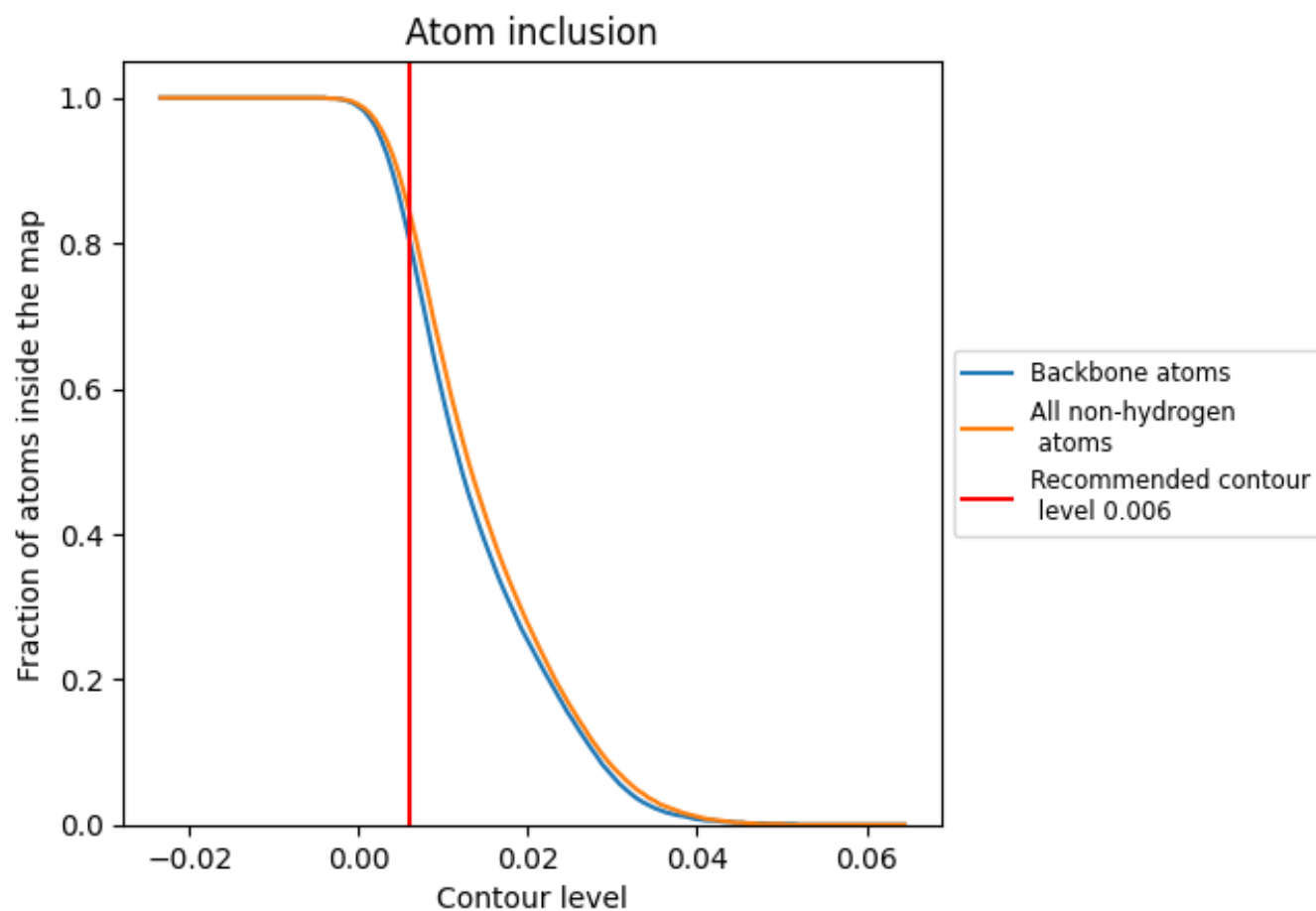
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 84% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8440	 0.3910
1	 0.3550	 0.1560
2	 0.2350	 0.1320
3	 0.4650	 0.1990
5	 0.7240	 0.1690
6	 0.6350	 0.1830
7	 0.7650	 0.2560
8	 0.6560	 0.1800
9	 0.9760	 0.5390
A	 0.7770	 0.2550
B	 0.5570	 0.1480
C	 0.6220	 0.1600
D	 0.7210	 0.2600
E	 0.4530	 0.1810
F	 0.4770	 0.1950
G	 0.8750	 0.3700
H	 0.5600	 0.2520
I	 0.7370	 0.2770
J	 0.8020	 0.2830
K	 0.5950	 0.1740
L	 0.9570	 0.4930
M	 0.9870	 0.5550
N	 0.9770	 0.5480
O	 0.9890	 0.5750
P	 0.9780	 0.5390
Q	 0.9840	 0.5580
R	 0.9910	 0.5650
S	 0.9490	 0.4490
T	 0.9620	 0.5230
U	 0.4310	 0.1720
V	 0.9860	 0.5450
W	 0.9780	 0.4960
X	 0.9850	 0.5730
Y	 0.9950	 0.5760
Z	 0.9890	 0.5690



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Chain	Atom inclusion	Q-score
a	 0.9940	 0.5880
b	 0.9950	 0.5600
c	 0.9890	 0.5880
d	 0.9840	 0.5310
e	 0.9840	 0.5450
f	 0.9670	 0.4750
g	 0.9590	 0.4650
h	 0.9580	 0.4450
i	 0.9290	 0.4260
j	 0.8950	 0.4160
k	 0.9030	 0.3770
l	 0.9530	 0.4250
m	 0.8930	 0.3980
n	 0.9040	 0.3970
o	 0.9900	 0.5110
p	 0.7610	 0.1950
q	 0.6560	 0.2460
s	 0.9310	 0.4720
v	 0.9640	 0.4920
w	 0.9440	 0.4450
x	 0.6540	 0.2610
y	 0.8600	 0.2650
z	 0.7990	 0.2440