wwPDB EM Validation Summary Report (i)

Apr 17, 2024 – 01:27 pm BST

PDB ID	:	7QP6
EMDB ID	:	EMD-14113
Title	:	Structure of the human 48S initiation complex in open state (h48S AUG open)
Authors	:	Yi, S.-H.; Petrychenko, V.; Schliep, J.E.; Goyal, A.; Linden, A.; Chari, A.; Urlaub, H.; Stark, H.; Rodnina, M.V.; Adio, S.; Fischer, N.
Deposited on	:	2022-01-03
Resolution	:	4.70 Å(reported)
Based on initial model	:	6ZMW

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 (i) 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 (i)) were used in the production of this report:

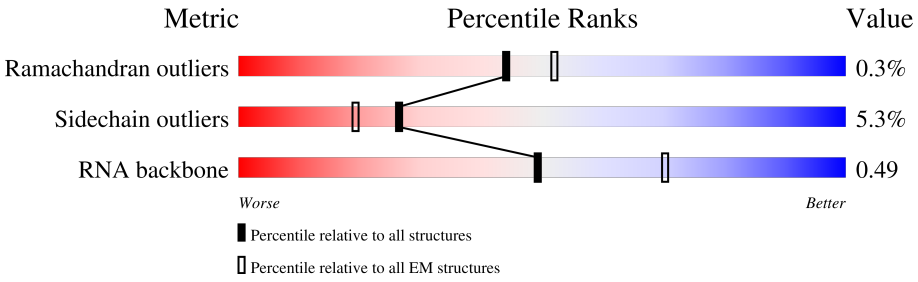
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	813	15% 51% · 48%
2	3	218	49% 98% ·
3	4	357	13% 71% · 28%
4	5	564	15% 57% 43%
5	6	374	26% 93% · 6%
6	7	20	5% 25% 75%
7	8	352	25% 90% 10%
8	9	25	92% · ·

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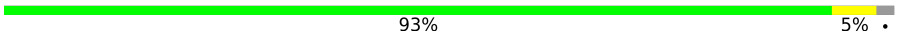
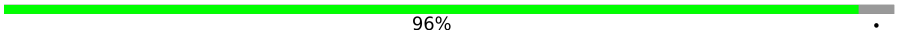
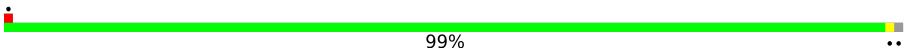
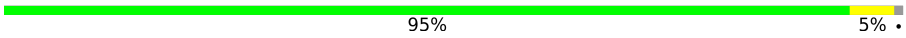
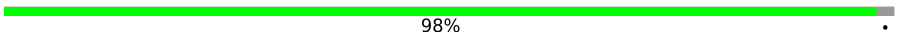
Mol	Chain	Length	Quality of chain
9	A	1869	
10	B	158	
11	C	263	
12	D	194	
13	E	143	
14	F	59	
15	G	194	
16	H	84	
17	I	151	
18	J	130	
19	K	83	
20	L	293	
21	M	135	
22	N	295	
23	O	264	
24	P	151	
25	Q	115	
26	R	208	
27	S	249	
28	T	133	
29	V	204	
30	Y	146	
31	Z	243	
32	a	165	
33	b	145	

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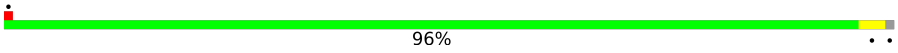
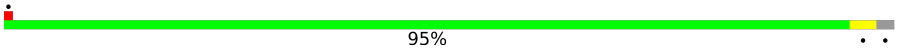
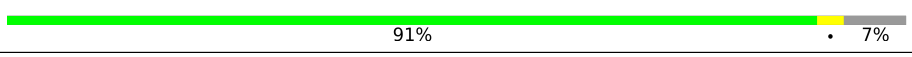
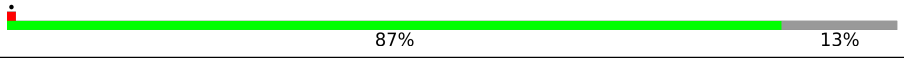
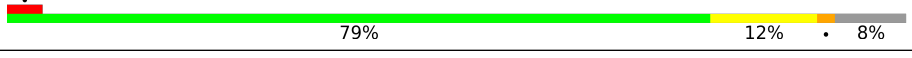
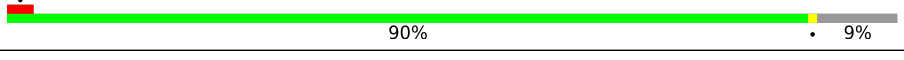
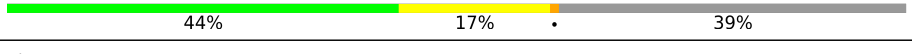
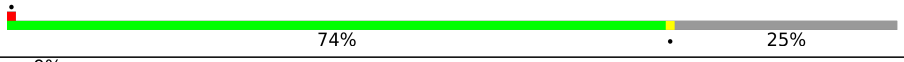
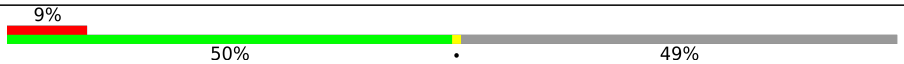
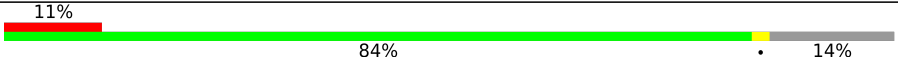
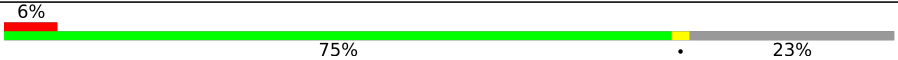
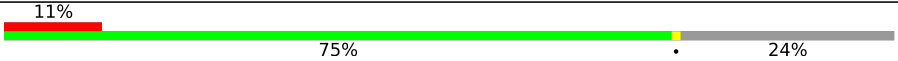
Mol	Chain	Length	Quality of chain
34	c	317	
35	d	145	
36	e	125	
37	f	152	
38	h	119	
39	i	56	
40	k	156	
41	m	132	
42	n	69	
43	o	320	
44	p	113	
45	q	144	
46	r	315	
47	s	333	
48	t	472	
49	u	1382	
50	v	445	
51	w	75	
52	x	548	
53	y	913	

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 109900 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 B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	424	2445	1501	469	470	5	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	3	213	1057	631	213	213	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	4	257	1272	757	257	258	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	5	319	1581	943	319	319	0	0

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	350	1917	1159	376	380	2	0	0

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	O	P		
6	7	20	240	100	120	20	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	8	317	Total	C	N	O	0	0
			1571	936	317	318		

- Molecule 8 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 9 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1719	Total	C	N	O	P	0	0
			36668	16378	6574	11998	1718		

- Molecule 10 is a protein called 40S ribosomal protein S11.

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

- Molecule 11 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 12 is a protein called 40S ribosomal protein S9.

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

- Molecule 13 is a protein called 40S ribosomal protein S23.

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

- Molecule 14 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	40	Total	C	N	O	S	0	0
			330	204	75	50	1		

- Molecule 15 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 16 is a protein called 40S ribosomal protein S27.

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

- Molecule 17 is a protein called 40S ribosomal protein S13.

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

- Molecule 18 is a protein called 40S ribosomal protein S15a.

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

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

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

- Molecule 21 is a protein called 40S ribosomal protein S17.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 23 is a protein called 40S ribosomal protein S3a.

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

- Molecule 24 is a protein called 40S ribosomal protein S14.

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

- Molecule 25 is a protein called 40S ribosomal protein S26.

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

- Molecule 26 is a protein called 40S ribosomal protein S8.

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

- Molecule 27 is a protein called 40S ribosomal protein S6.

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

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

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

- Molecule 29 is a protein called 40S ribosomal protein S5.

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

- Molecule 30 is a protein called 40S ribosomal protein S16.

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

- Molecule 31 is a protein called 40S ribosomal protein S3.

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

- Molecule 32 is a protein called 40S ribosomal protein S10.

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

- Molecule 33 is a protein called 40S ribosomal protein S15.

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

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 35 is a protein called 40S ribosomal protein S19.

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

- Molecule 36 is a protein called 40S ribosomal protein S25.

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

- Molecule 37 is a protein called 40S ribosomal protein S18.

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

- Molecule 38 is a protein called 40S ribosomal protein S20.

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

- Molecule 39 is a protein called 40S ribosomal protein S29.

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

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

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

- Molecule 41 is a protein called 40S ribosomal protein S12.

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

- Molecule 42 is a protein called 40S ribosomal protein S28.

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

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

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

- Molecule 44 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	85	Total	C	N	O	S	0	0
			691	438	125	126	2		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	88	Total	C	N	O	S	0	0
			714	451	129	130	4		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	275	Total	C	N	O	S	0	0
			2215	1398	387	418	12		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	138	Total	C	N	O	S	0	0
			1123	709	206	199	9		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	t	356	Total	C	N	O	0	0
			1750	1038	356	356		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	706	Total	C	N	O	S	1	0
			5383	3379	982	999	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	384	Total	C	N	O	S	0	0
			2635	1657	477	489	12		

- Molecule 51 is a RNA chain called Initiator Met-tRNA-i.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	421	Total	C	N	O	S	0	0
			2831	1746	521	555	9		

- Molecule 53 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	697	Total	C	N	O	S	0	0
			5470	3437	980	1018	35		

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	Q	1	Total	Zn	0
			1	1	
54	k	1	Total	Zn	0
			1	1	

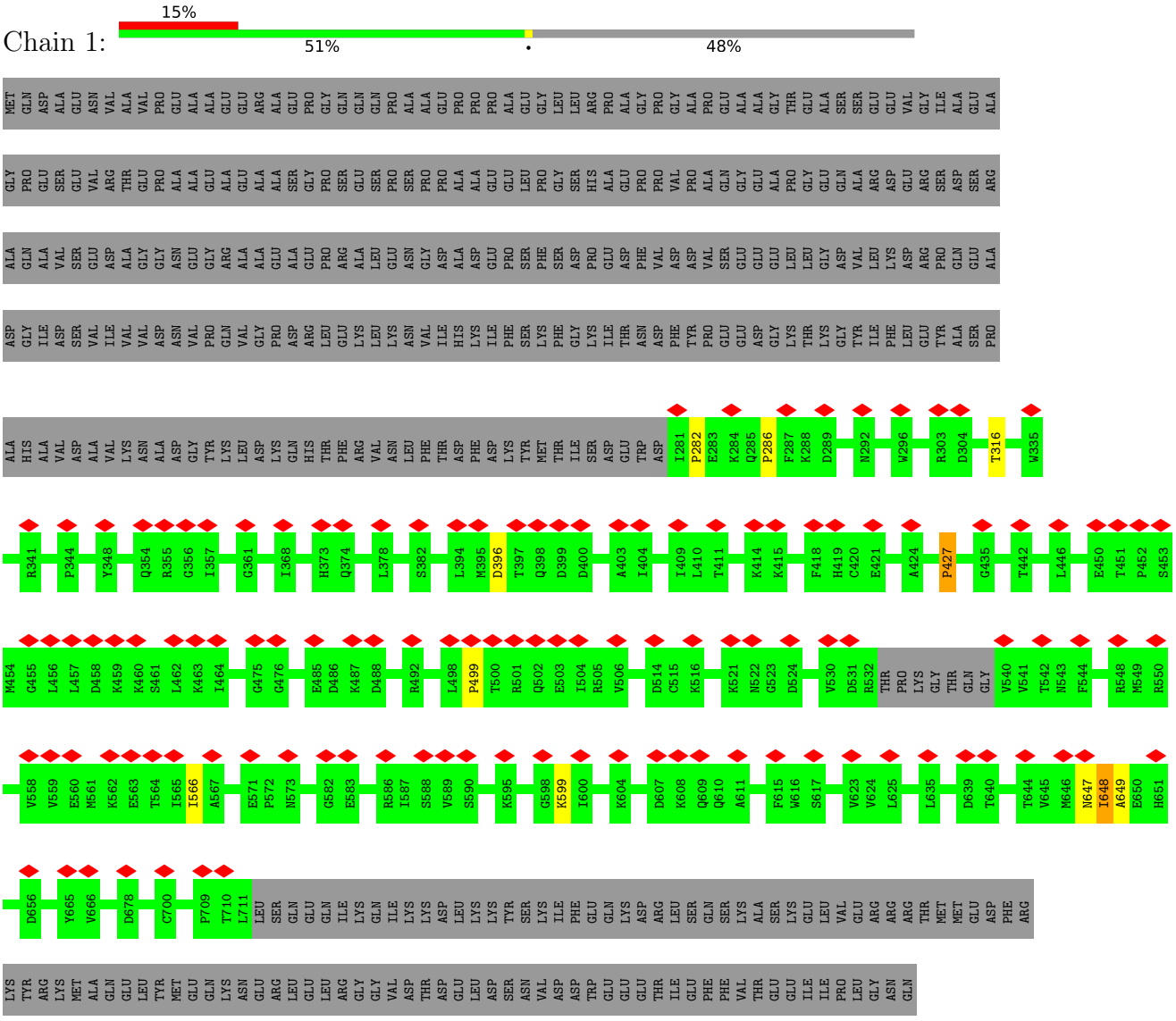
- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	d	1	Total	Mg	0
			1	1	
55	f	1	Total	Mg	0
			1	1	

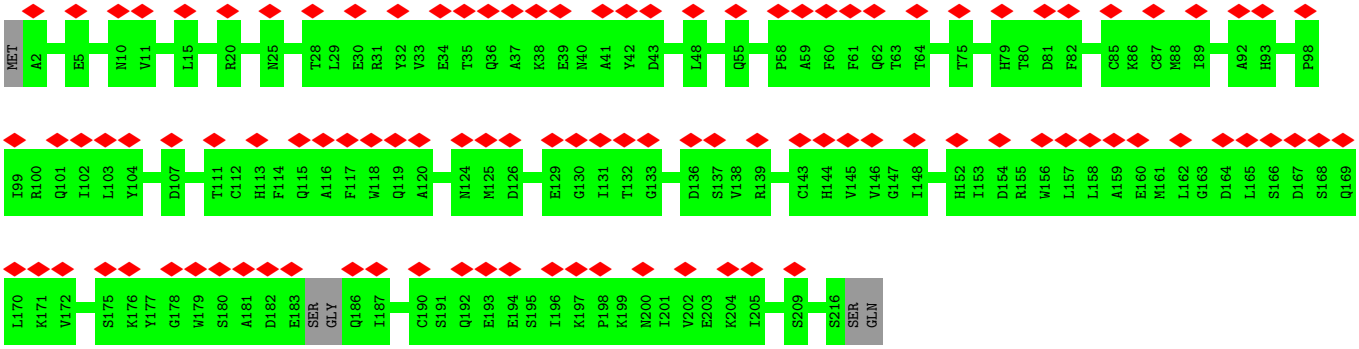
3 Residue-property plots (i)

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.

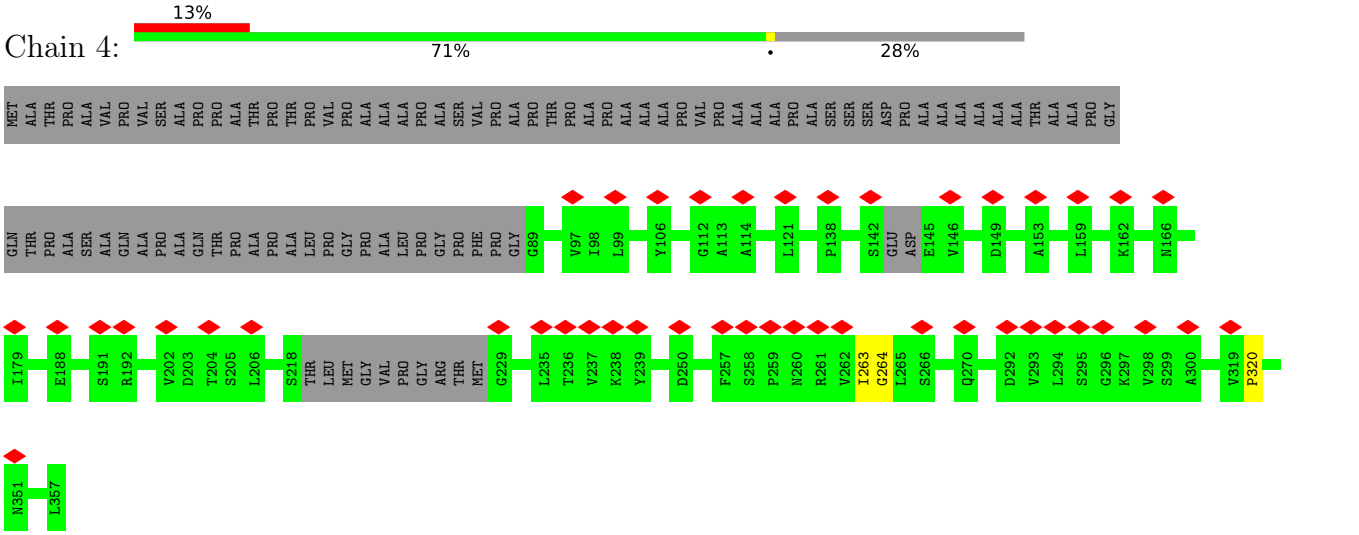
• Molecule 1: Eukaryotic translation initiation factor 3 subunit B



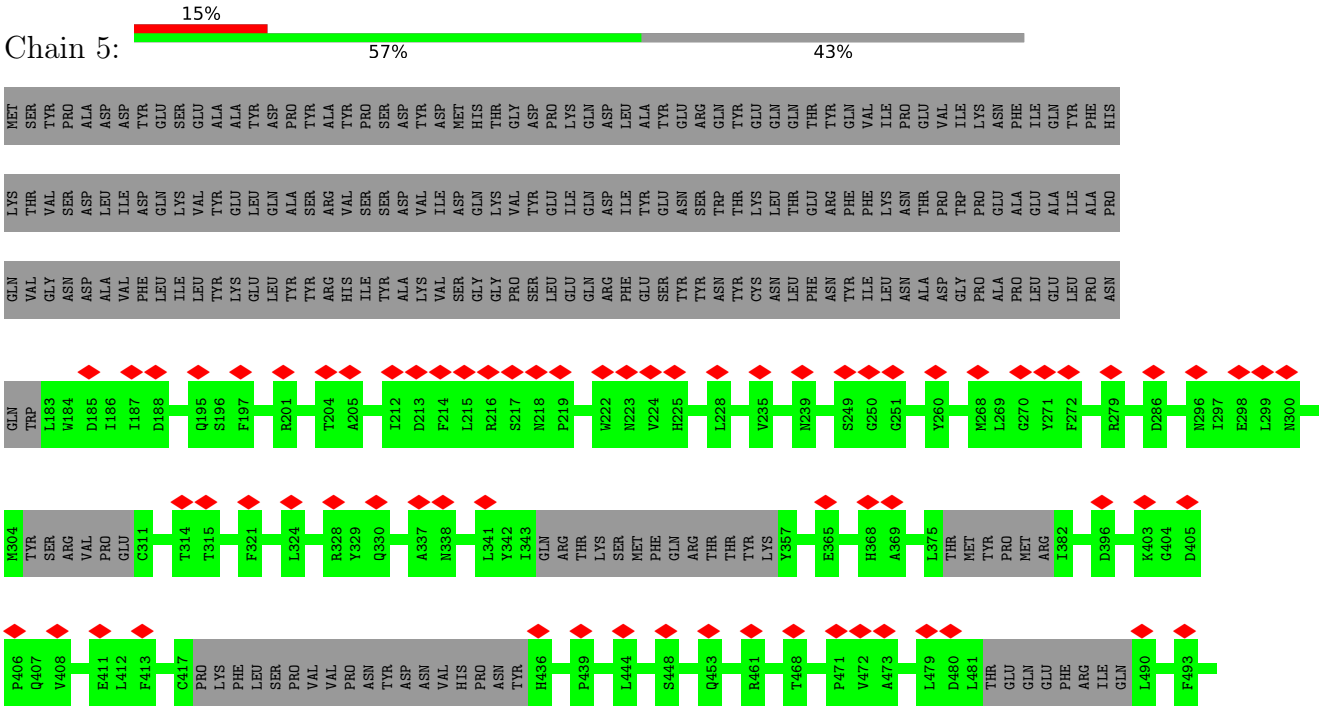
• Molecule 2: Eukaryotic translation initiation factor 3 subunit K

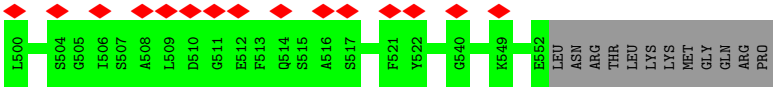


• Molecule 3: Eukaryotic translation initiation factor 3 subunit F

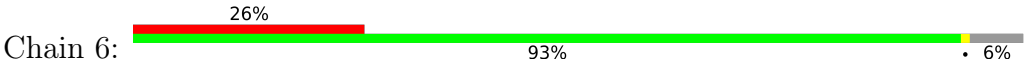


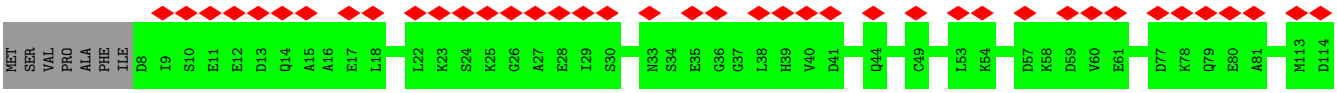
• Molecule 4: Eukaryotic translation initiation factor 3 subunit L

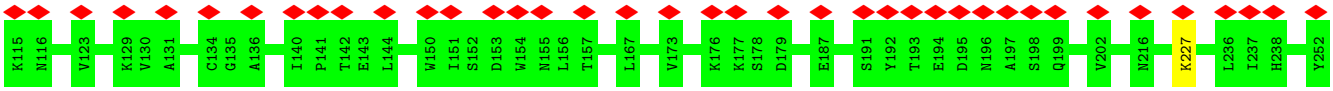


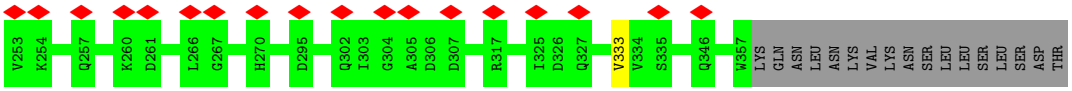


• Molecule 5: Eukaryotic translation initiation factor 3 subunit M



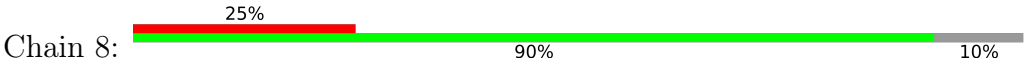


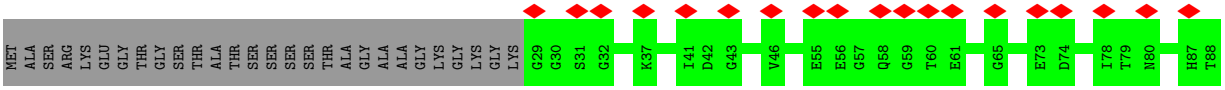


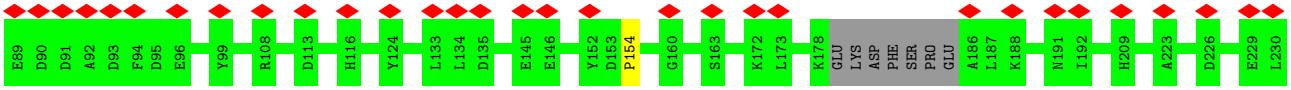


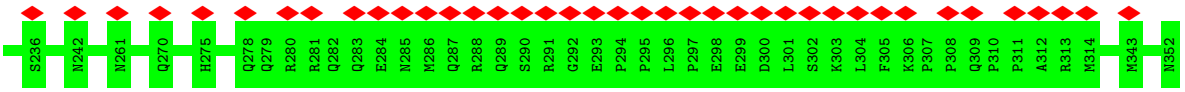
• Molecule 6: mRNA

• Molecule 7: Eukaryotic translation initiation factor 3 subunit H

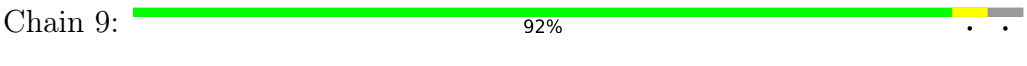


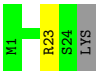




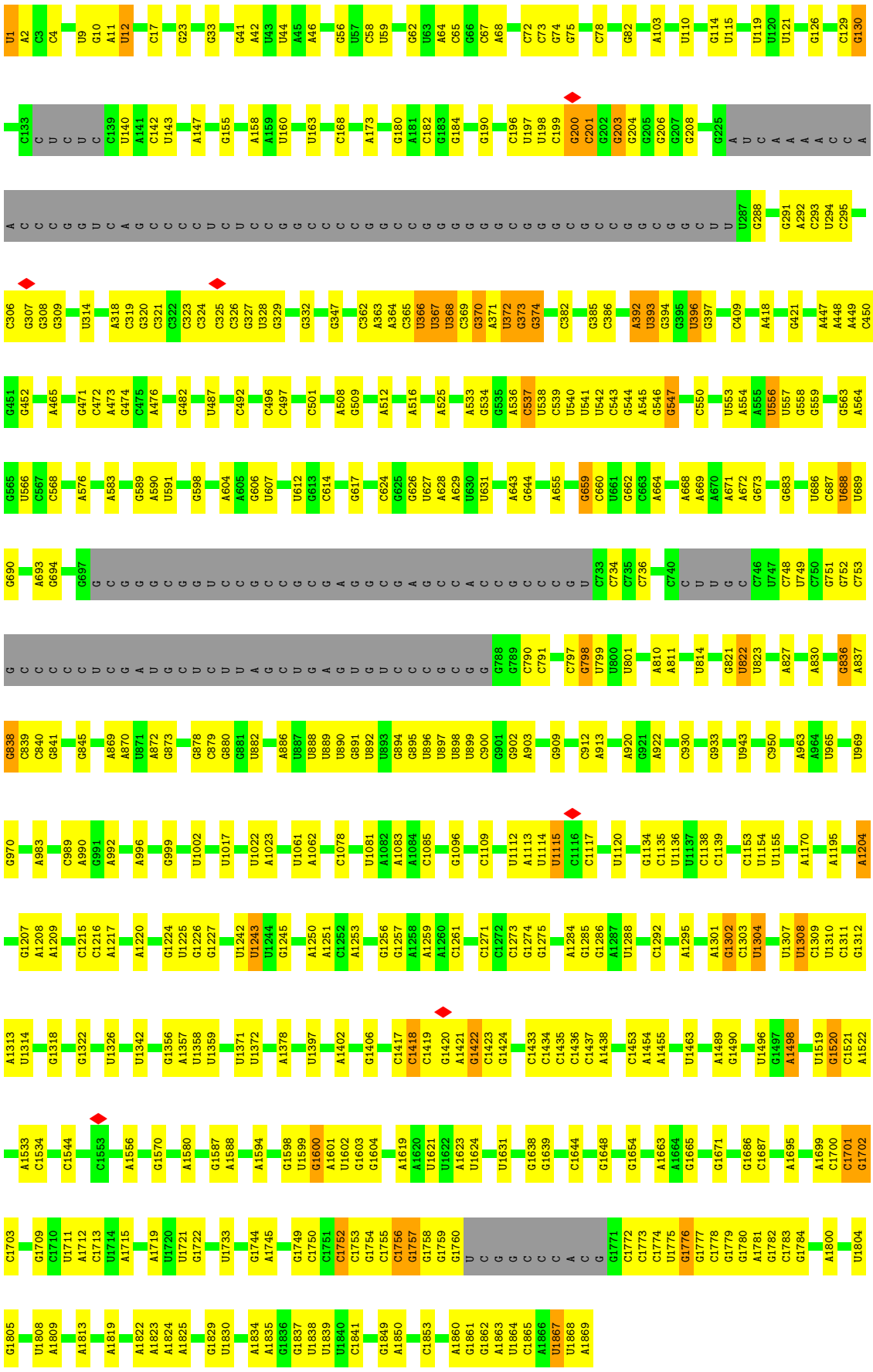


• Molecule 8: 60S ribosomal protein L41



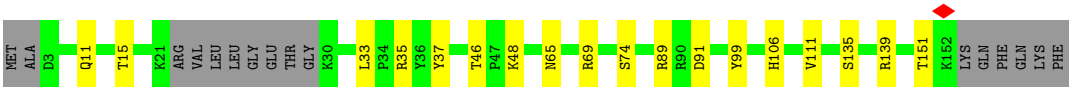


• Molecule 9: 18S rRNA



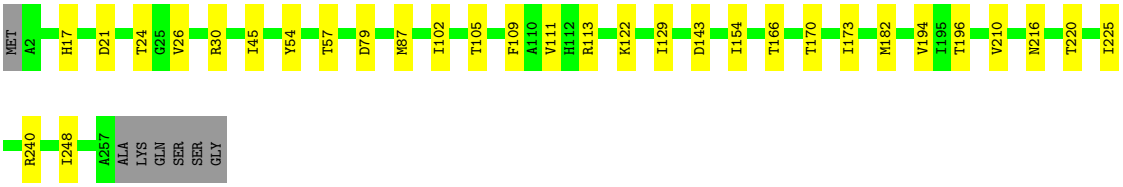
• Molecule 10: 40S ribosomal protein S11

Chain B:



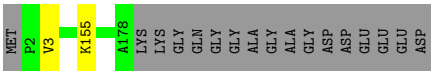
• Molecule 11: 40S ribosomal protein S4, X isoform

Chain C:



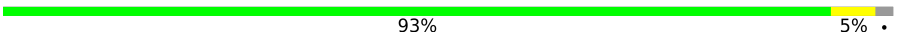
• Molecule 12: 40S ribosomal protein S9

Chain D:



• Molecule 13: 40S ribosomal protein S23

Chain E:

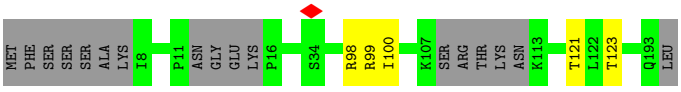


• Molecule 14: 40S ribosomal protein S30

Chain F:

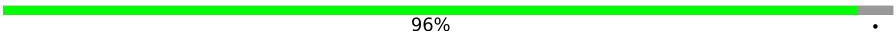
• Molecule 15: 40S ribosomal protein S7

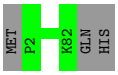
Chain G:



• Molecule 16: 40S ribosomal protein S27

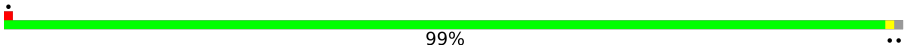
Chain H:

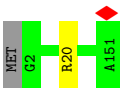




• Molecule 17: 40S ribosomal protein S13

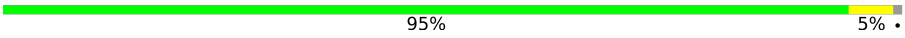
Chain I:

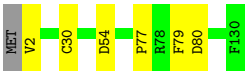




• Molecule 18: 40S ribosomal protein S15a

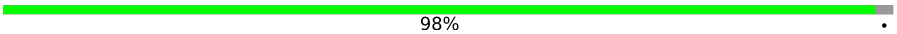
Chain J:





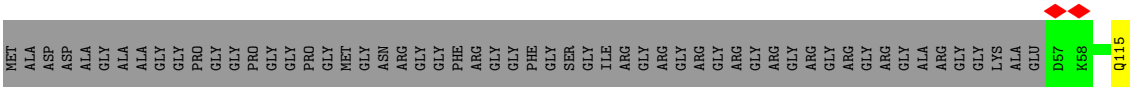
• Molecule 19: 40S ribosomal protein S21

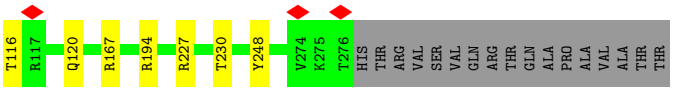
Chain K:



• Molecule 20: 40S ribosomal protein S2

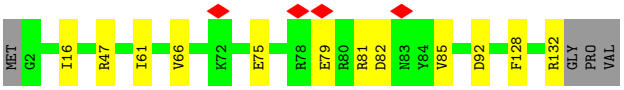
Chain L:





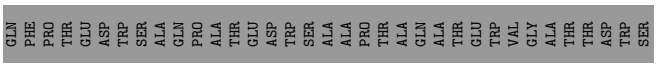
• Molecule 21: 40S ribosomal protein S17

Chain M:



• Molecule 22: 40S ribosomal protein SA

Chain N:



• Molecule 23: 40S ribosomal protein S3a

Chain O:

• Molecule 24: 40S ribosomal protein S14

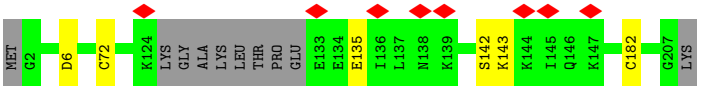
Chain P:

• Molecule 25: 40S ribosomal protein S26

Chain Q:

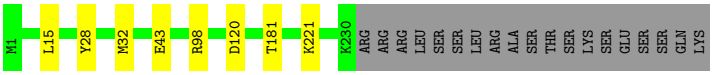
• Molecule 26: 40S ribosomal protein S8

Chain R:



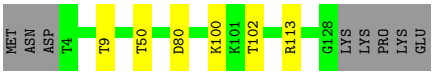
• Molecule 27: 40S ribosomal protein S6

Chain S:



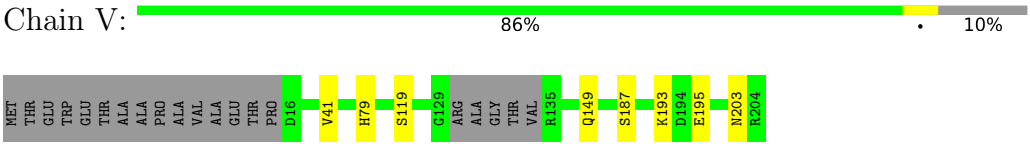
• Molecule 28: 40S ribosomal protein S24

Chain T:



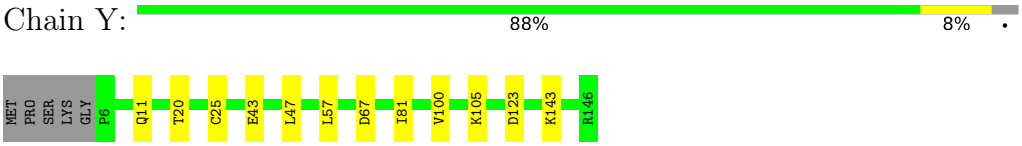
• Molecule 29: 40S ribosomal protein S5

Chain V:



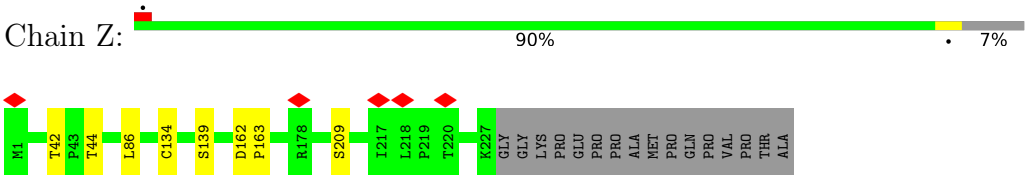
• Molecule 30: 40S ribosomal protein S16

Chain Y:



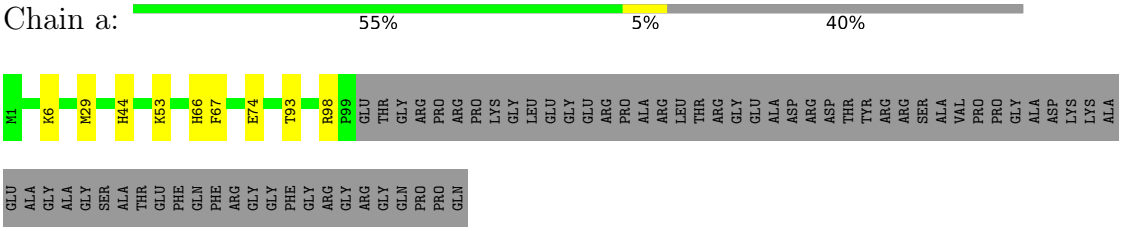
• Molecule 31: 40S ribosomal protein S3

Chain Z:



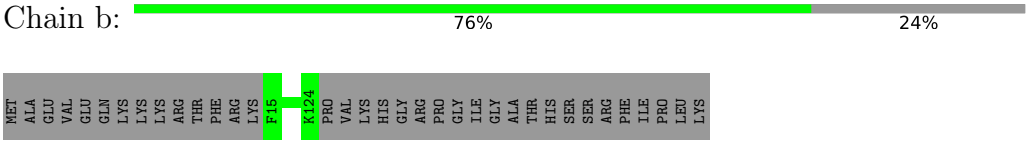
• Molecule 32: 40S ribosomal protein S10

Chain a:



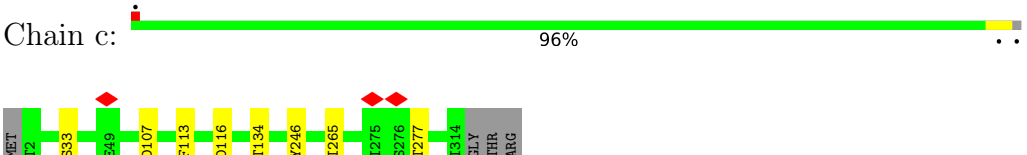
• Molecule 33: 40S ribosomal protein S15

Chain b:



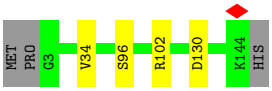
• Molecule 34: Receptor of activated protein C kinase 1

Chain c:



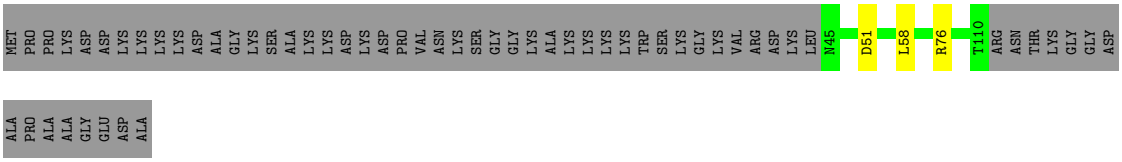
• Molecule 35: 40S ribosomal protein S19

Chain d:



• Molecule 36: 40S ribosomal protein S25

Chain e:

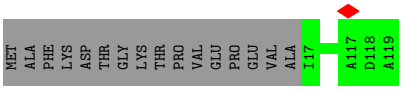


• Molecule 37: 40S ribosomal protein S18

Chain f:

• Molecule 38: 40S ribosomal protein S20

Chain h:

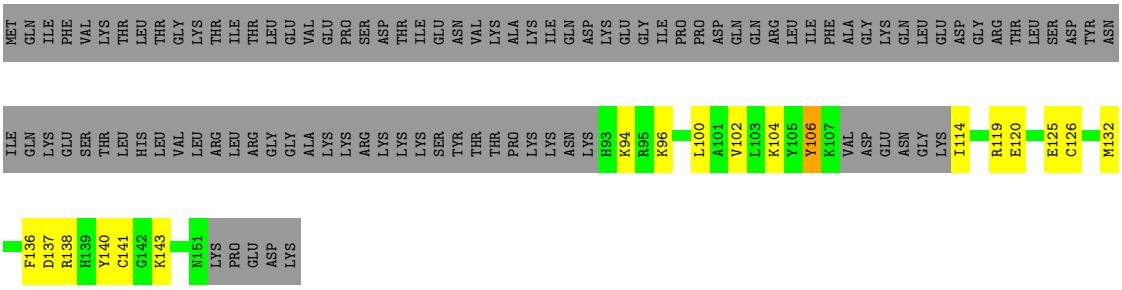


• Molecule 39: 40S ribosomal protein S29

Chain i:

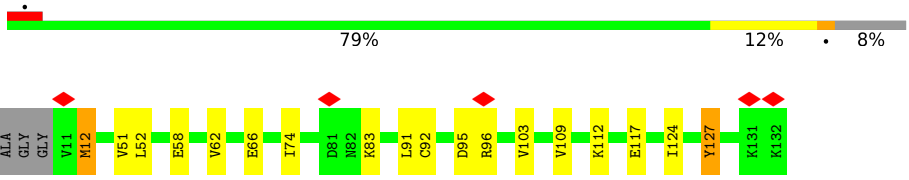
• Molecule 40: Ubiquitin-40S ribosomal protein S27a

Chain k:



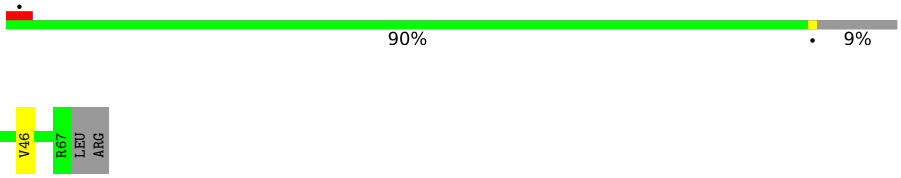
• Molecule 41: 40S ribosomal protein S12

Chain m:



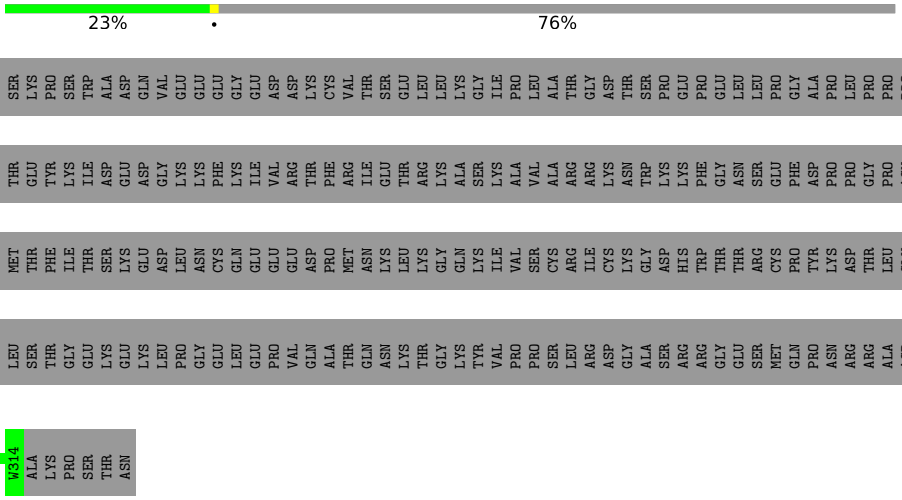
• Molecule 42: 40S ribosomal protein S28

Chain n:



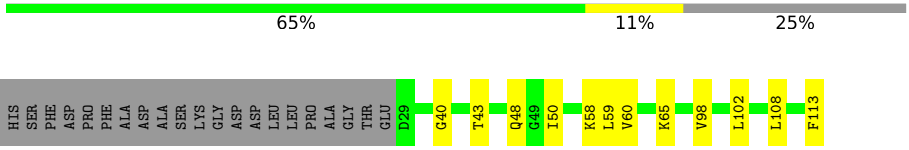
• Molecule 43: Eukaryotic translation initiation factor 3 subunit G

Chain o:



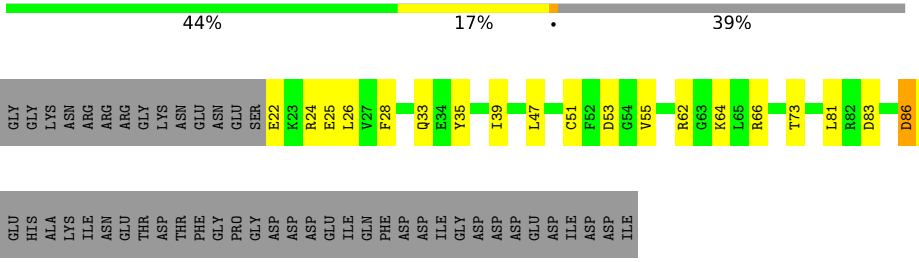
• Molecule 44: Eukaryotic translation initiation factor 1

Chain p:



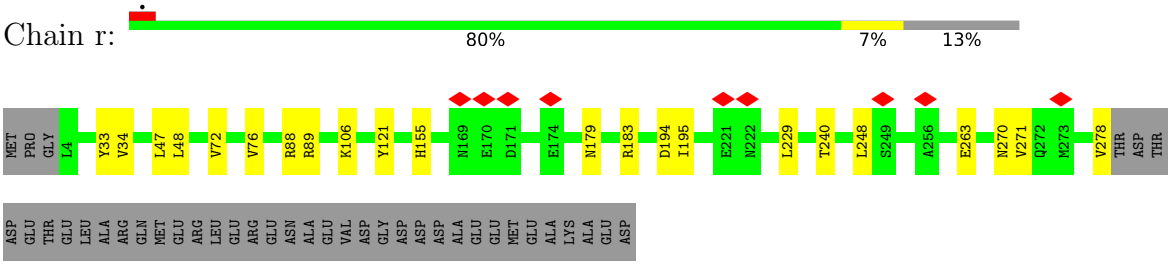
• Molecule 45: Eukaryotic translation initiation factor 1A, X-chromosomal

Chain q:



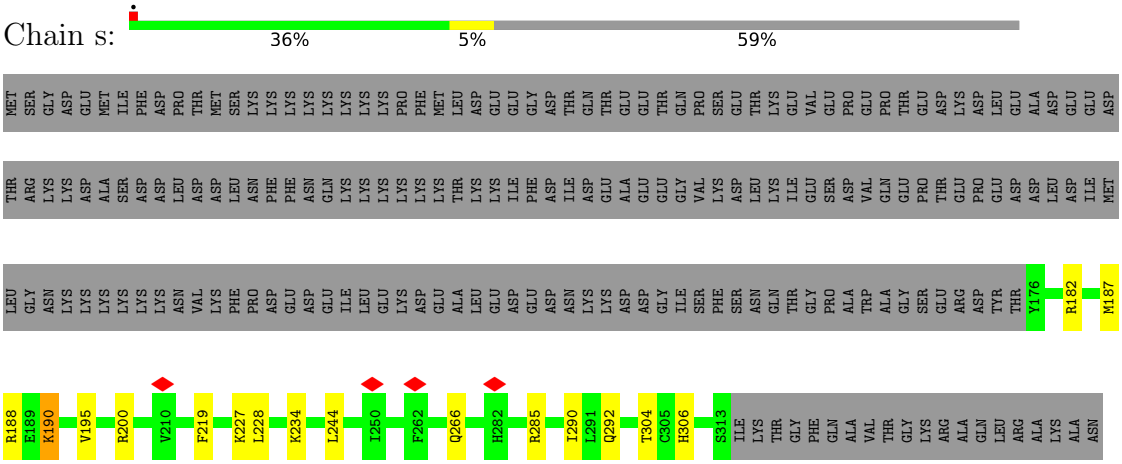
• Molecule 46: Eukaryotic translation initiation factor 2 subunit 1

Chain r:



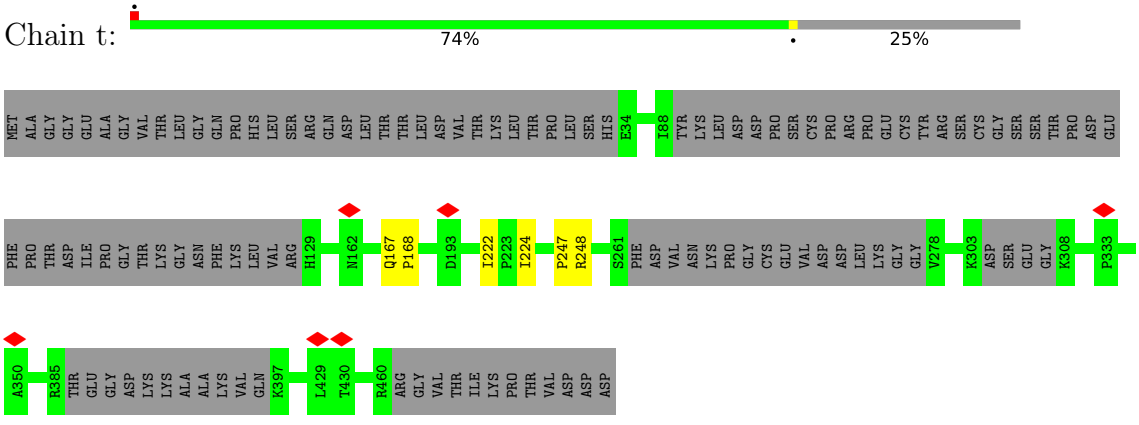
• Molecule 47: Eukaryotic translation initiation factor 2 subunit 2

Chain s:



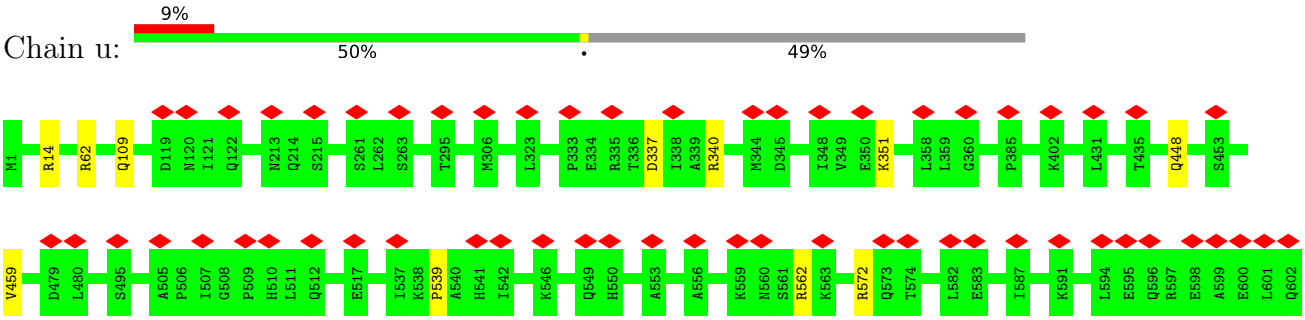
• Molecule 48: Eukaryotic translation initiation factor 2 subunit 3

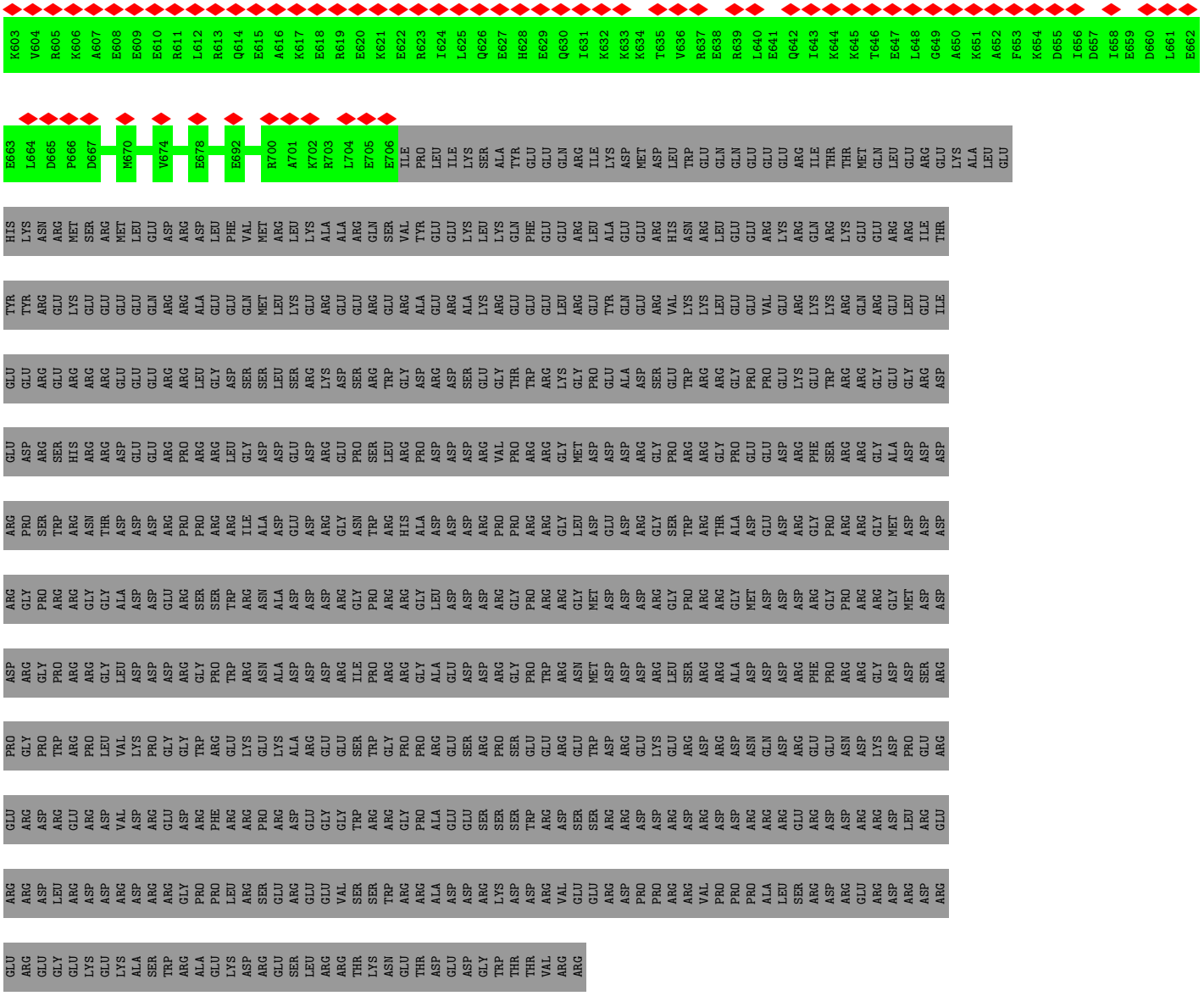
Chain t:



• Molecule 49: Eukaryotic translation initiation factor 3 subunit A

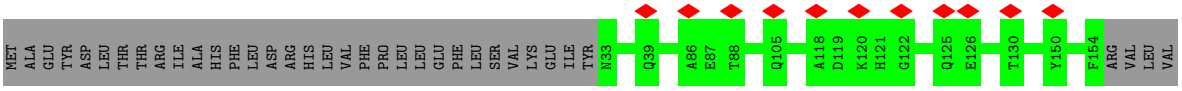
Chain u:

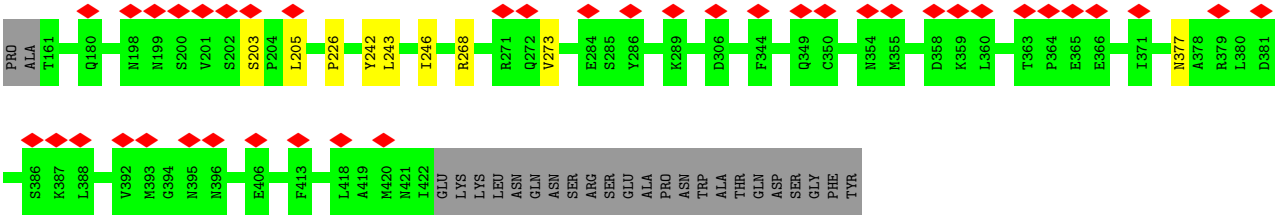




• Molecule 50: Eukaryotic translation initiation factor 3 subunit E

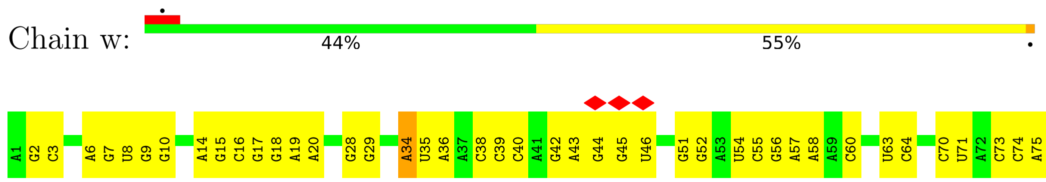
Chain v:





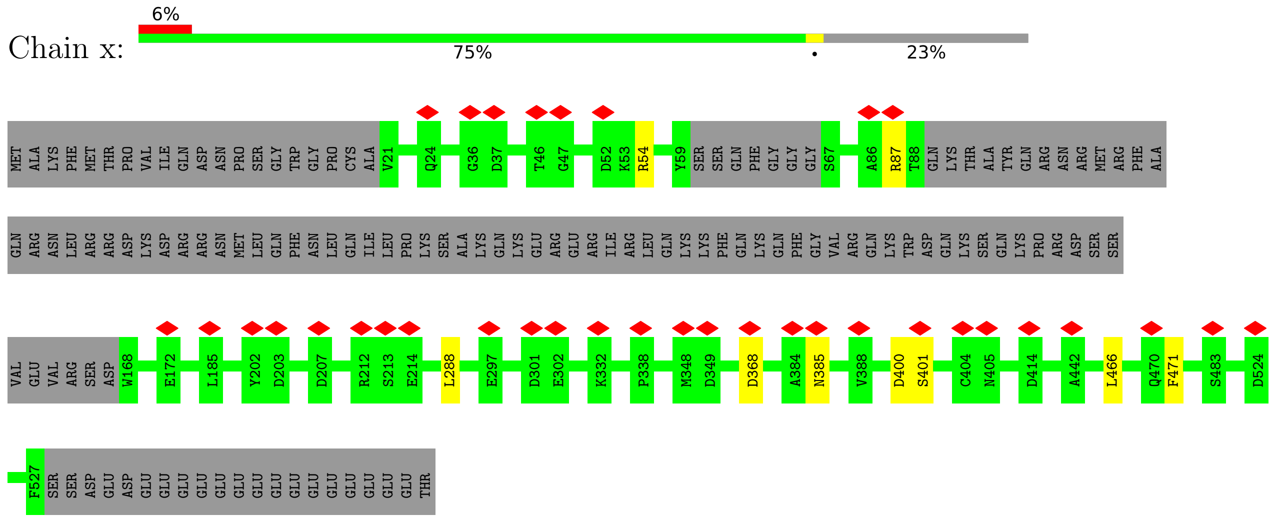
• Molecule 51: Initiator Met-tRNA-i

Chain w:



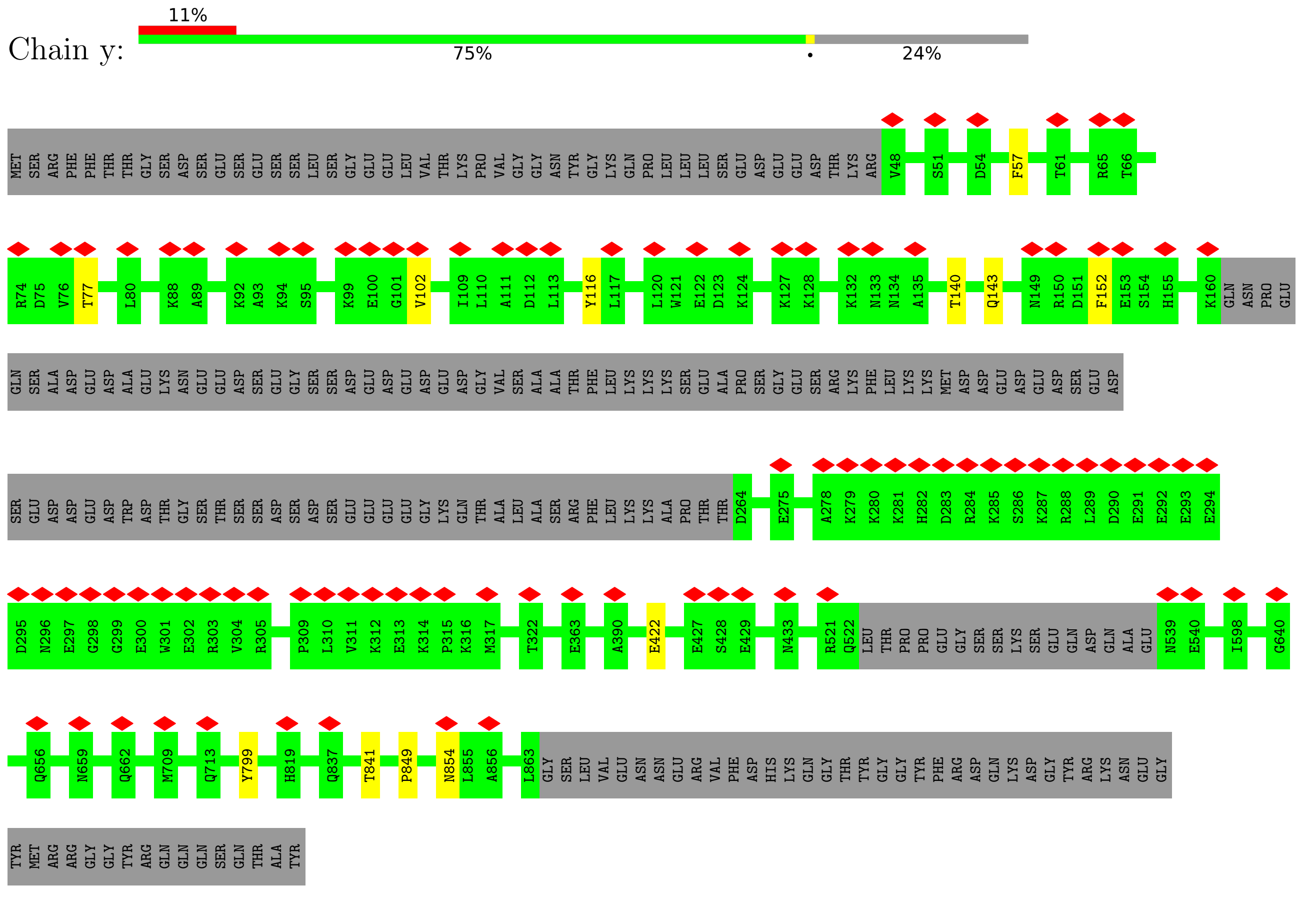
- Molecule 52: Eukaryotic translation initiation factor 3 subunit D

Chain x:



- Molecule 53: Eukaryotic translation initiation factor 3 subunit C

Chain y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57184	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	20.695	Depositor
Minimum map value	-7.349	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.3	Depositor
Map size (Å)	417.59998, 417.59998, 417.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.77	0/2466	1.15	9/3400 (0.3%)
2	3	0.68	0/1055	0.67	0/1469
3	4	0.73	0/1269	0.83	0/1762
4	5	0.72	0/1575	0.70	0/2187
5	6	0.68	0/1926	0.79	1/2669 (0.0%)
6	7	0.34	0/259	0.89	0/396
7	8	0.72	0/1569	0.81	0/2183
8	9	0.46	0/231	0.80	0/294
9	A	0.65	0/40362	0.90	90/62905 (0.1%)
10	B	0.56	0/1186	0.81	1/1585 (0.1%)
11	C	0.55	0/2077	0.79	0/2796
12	D	0.52	0/1502	0.67	0/2008
13	E	0.54	0/1105	0.80	1/1476 (0.1%)
14	F	0.53	0/332	0.76	0/434
15	G	0.54	0/1451	0.75	0/1942
16	H	0.56	0/644	0.76	0/864
17	I	0.57	0/1232	0.78	0/1656
18	J	0.55	0/1051	0.74	1/1406 (0.1%)
19	K	0.62	0/623	0.75	0/833
20	L	0.58	0/1743	0.82	1/2354 (0.0%)
21	M	0.59	0/1078	0.91	0/1447
22	N	0.57	1/1670 (0.1%)	0.74	0/2271
23	O	0.54	0/1742	0.74	0/2330
24	P	0.84	0/1010	1.24	3/1353 (0.2%)
25	Q	0.60	0/805	0.86	1/1079 (0.1%)
26	R	0.53	0/1654	0.71	0/2203
27	S	0.54	0/1885	0.72	0/2510
28	T	0.51	0/1032	0.68	0/1371
29	V	0.57	0/1481	0.78	0/1988
30	Y	0.56	0/1142	0.79	0/1528
31	Z	0.58	0/1793	0.80	0/2414
32	a	0.55	0/859	0.75	0/1159

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.53	0/929	0.71	0/1241
34	c	0.54	0/2493	0.76	0/3394
35	d	0.55	0/1123	0.74	1/1504 (0.1%)
36	e	0.55	0/529	0.73	0/712
37	f	0.52	0/1194	0.73	0/1599
38	h	0.56	0/827	0.76	0/1110
39	i	0.55	0/429	0.89	1/568 (0.2%)
40	k	0.58	0/444	1.08	1/588 (0.2%)
41	m	0.65	0/960	0.96	3/1286 (0.2%)
42	n	0.56	0/500	0.80	0/669
43	o	0.58	0/628	0.76	0/846
44	p	0.59	0/701	1.03	0/936
45	q	0.61	0/722	0.90	0/963
46	r	0.36	0/2247	0.67	0/3029
47	s	0.57	0/1142	0.79	0/1534
48	t	0.71	0/1745	0.75	0/2417
49	u	0.56	2/5475 (0.0%)	0.74	0/7432
50	v	0.59	0/2672	0.75	0/3647
51	w	0.39	0/1795	0.88	2/2798 (0.1%)
52	x	0.61	0/2874	0.77	0/3925
53	y	0.55	0/5557	0.70	1/7503 (0.0%)
All	All	0.61	3/114795 (0.0%)	0.84	117/163973 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	136	GLU	CD-OE2	-5.45	1.19	1.25
49	u	14[A]	ARG	C-O	5.12	1.33	1.23
49	u	14[B]	ARG	C-O	5.12	1.33	1.23

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1304	U	C2'-C3'-O3'	11.53	134.87	109.50
9	A	1155	U	O5'-P-OP1	-11.51	95.34	105.70
9	A	1273	C	O5'-P-OP2	-9.28	97.34	105.70
9	A	392	A	C2'-C3'-O3'	8.64	128.51	109.50
9	A	367	U	C2'-C3'-O3'	8.50	128.21	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	1	420/813 (52%)	394 (94%)	20 (5%)	6 (1%)	11 47
2	3	209/218 (96%)	205 (98%)	4 (2%)	0	100 100
3	4	251/357 (70%)	230 (92%)	18 (7%)	3 (1%)	13 50
4	5	307/564 (54%)	299 (97%)	8 (3%)	0	100 100
5	6	348/374 (93%)	320 (92%)	28 (8%)	0	100 100
7	8	313/352 (89%)	276 (88%)	36 (12%)	1 (0%)	41 76
8	9	22/25 (88%)	22 (100%)	0	0	100 100
10	B	138/158 (87%)	132 (96%)	6 (4%)	0	100 100
11	C	254/263 (97%)	246 (97%)	7 (3%)	1 (0%)	34 72
12	D	175/194 (90%)	175 (100%)	0	0	100 100
13	E	138/143 (96%)	136 (99%)	1 (1%)	1 (1%)	22 62
14	F	38/59 (64%)	37 (97%)	1 (3%)	0	100 100
15	G	171/194 (88%)	163 (95%)	8 (5%)	0	100 100
16	H	79/84 (94%)	77 (98%)	2 (2%)	0	100 100
17	I	148/151 (98%)	144 (97%)	4 (3%)	0	100 100
18	J	127/130 (98%)	123 (97%)	4 (3%)	0	100 100
19	K	79/83 (95%)	77 (98%)	2 (2%)	0	100 100
20	L	218/293 (74%)	210 (96%)	8 (4%)	0	100 100
21	M	129/135 (96%)	123 (95%)	5 (4%)	1 (1%)	19 60
22	N	205/295 (70%)	196 (96%)	9 (4%)	0	100 100
23	O	209/264 (79%)	198 (95%)	10 (5%)	1 (0%)	29 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	P	131/151 (87%)	120 (92%)	11 (8%)	0	100	100
25	Q	97/115 (84%)	94 (97%)	2 (2%)	1 (1%)	15	54
26	R	194/208 (93%)	192 (99%)	2 (1%)	0	100	100
27	S	228/249 (92%)	225 (99%)	3 (1%)	0	100	100
28	T	123/133 (92%)	123 (100%)	0	0	100	100
29	V	180/204 (88%)	173 (96%)	6 (3%)	1 (1%)	25	65
30	Y	139/146 (95%)	137 (99%)	2 (1%)	0	100	100
31	Z	225/243 (93%)	221 (98%)	4 (2%)	0	100	100
32	a	97/165 (59%)	94 (97%)	3 (3%)	0	100	100
33	b	108/145 (74%)	104 (96%)	4 (4%)	0	100	100
34	c	311/317 (98%)	304 (98%)	7 (2%)	0	100	100
35	d	140/145 (97%)	135 (96%)	5 (4%)	0	100	100
36	e	64/125 (51%)	62 (97%)	2 (3%)	0	100	100
37	f	140/152 (92%)	136 (97%)	4 (3%)	0	100	100
38	h	101/119 (85%)	98 (97%)	3 (3%)	0	100	100
39	i	48/56 (86%)	45 (94%)	2 (4%)	1 (2%)	7	38
40	k	49/156 (31%)	46 (94%)	2 (4%)	1 (2%)	7	40
41	m	120/132 (91%)	114 (95%)	5 (4%)	1 (1%)	19	60
42	n	61/69 (88%)	59 (97%)	2 (3%)	0	100	100
43	o	75/320 (23%)	74 (99%)	1 (1%)	0	100	100
44	p	83/113 (74%)	81 (98%)	1 (1%)	1 (1%)	13	50
45	q	86/144 (60%)	75 (87%)	9 (10%)	2 (2%)	6	36
46	r	273/315 (87%)	249 (91%)	23 (8%)	1 (0%)	34	72
47	s	136/333 (41%)	120 (88%)	15 (11%)	1 (1%)	22	62
48	t	346/472 (73%)	329 (95%)	11 (3%)	6 (2%)	9	43
49	u	705/1382 (51%)	676 (96%)	28 (4%)	1 (0%)	51	85
50	v	380/445 (85%)	349 (92%)	31 (8%)	0	100	100
52	x	415/548 (76%)	385 (93%)	30 (7%)	0	100	100
53	y	691/913 (76%)	661 (96%)	29 (4%)	1 (0%)	51	85
All	All	9724/13164 (74%)	9264 (95%)	428 (4%)	32 (0%)	44	76

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	282	PRO
1	1	427	PRO
1	1	648	ILE
3	4	264	GLY
23	O	117	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	97/701 (14%)	96 (99%)	1 (1%)	76 86
5	6	49/335 (15%)	48 (98%)	1 (2%)	55 73
8	9	23/24 (96%)	22 (96%)	1 (4%)	29 54
10	B	129/142 (91%)	112 (87%)	17 (13%)	4 20
11	C	220/225 (98%)	190 (86%)	30 (14%)	3 19
12	D	158/168 (94%)	156 (99%)	2 (1%)	69 82
13	E	112/115 (97%)	107 (96%)	5 (4%)	27 53
14	F	33/48 (69%)	26 (79%)	7 (21%)	1 7
15	G	159/174 (91%)	154 (97%)	5 (3%)	40 62
16	H	73/76 (96%)	73 (100%)	0	100 100
17	I	130/131 (99%)	129 (99%)	1 (1%)	81 89
18	J	112/113 (99%)	107 (96%)	5 (4%)	27 53
19	K	65/67 (97%)	65 (100%)	0	100 100
20	L	186/225 (83%)	179 (96%)	7 (4%)	33 58
21	M	119/122 (98%)	108 (91%)	11 (9%)	9 31
22	N	173/243 (71%)	172 (99%)	1 (1%)	86 92
23	O	192/231 (83%)	189 (98%)	3 (2%)	62 79
24	P	104/119 (87%)	98 (94%)	6 (6%)	20 47
25	Q	86/98 (88%)	83 (96%)	3 (4%)	36 60
26	R	172/180 (96%)	166 (96%)	6 (4%)	36 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	S	200/218 (92%)	192 (96%)	8 (4%)	31 56
28	T	107/115 (93%)	101 (94%)	6 (6%)	21 48
29	V	156/170 (92%)	149 (96%)	7 (4%)	27 53
30	Y	117/121 (97%)	105 (90%)	12 (10%)	7 27
31	Z	190/202 (94%)	182 (96%)	8 (4%)	30 55
32	a	90/136 (66%)	81 (90%)	9 (10%)	7 28
33	b	100/130 (77%)	100 (100%)	0	100 100
34	c	272/275 (99%)	264 (97%)	8 (3%)	42 64
35	d	112/115 (97%)	109 (97%)	3 (3%)	44 66
36	e	58/103 (56%)	55 (95%)	3 (5%)	23 50
37	f	123/132 (93%)	119 (97%)	4 (3%)	38 61
38	h	94/107 (88%)	94 (100%)	0	100 100
39	i	44/49 (90%)	34 (77%)	10 (23%)	1 6
40	k	47/140 (34%)	30 (64%)	17 (36%)	0 1
41	m	104/108 (96%)	87 (84%)	17 (16%)	2 14
42	n	56/62 (90%)	55 (98%)	1 (2%)	59 77
43	o	64/277 (23%)	60 (94%)	4 (6%)	18 44
44	p	74/96 (77%)	63 (85%)	11 (15%)	3 16
45	q	75/123 (61%)	51 (68%)	24 (32%)	0 2
46	r	247/280 (88%)	226 (92%)	21 (8%)	10 36
47	s	128/304 (42%)	111 (87%)	17 (13%)	4 20
49	u	528/1259 (42%)	519 (98%)	9 (2%)	60 78
50	v	206/406 (51%)	197 (96%)	9 (4%)	28 54
52	x	206/494 (42%)	197 (96%)	9 (4%)	28 54
53	y	564/811 (70%)	554 (98%)	10 (2%)	59 77
All	All	6354/9770 (65%)	6015 (95%)	339 (5%)	26 49

5 of 339 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	p	50	ILE
47	s	187	MET
44	p	108	LEU

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Mol	Chain	Res	Type
45	q	101	ARG
47	s	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
10	B	65	ASN
25	Q	86	ASN
31	Z	56	GLN
40	k	139	HIS
41	m	46	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	w	74/75 (98%)	41 (55%)	0
6	7	19/20 (95%)	15 (78%)	0
9	A	1708/1869 (91%)	442 (25%)	52 (3%)
All	All	1801/1964 (91%)	498 (27%)	52 (2%)

5 of 498 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	7	10	A
6	7	11	A
6	7	12	A
6	7	13	A
6	7	14	A

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	1313	A
9	A	1600	G
9	A	1863	A
9	A	1434	C
9	A	1521	C

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

26 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	$\#\|Z\| > 2$
9	PSU	A	1081	9	18,21,22	1.12	1 (5%)	22,30,33	1.19	2 (9%)
9	OMG	A	683	9	18,26,27	0.94	1 (5%)	19,38,41	0.81	0
9	PSU	A	822	9	18,21,22	1.13	1 (5%)	22,30,33	1.14	2 (9%)
9	OMC	A	174	9	19,22,23	0.61	0	26,31,34	0.44	0
9	OMG	A	509	9	18,26,27	1.10	1 (5%)	19,38,41	1.17	1 (5%)
9	A2M	A	668	9	18,25,26	0.67	0	18,36,39	0.77	0
9	OMC	A	1703	9	19,22,23	0.72	1 (5%)	26,31,34	0.50	0
9	OMC	A	517	9	19,22,23	0.63	0	26,31,34	0.45	0
9	MA6	A	1850	9	18,26,27	0.81	0	19,38,41	1.15	1 (5%)
9	5MU	A	814	9	19,22,23	0.94	1 (5%)	28,32,35	0.92	1 (3%)
9	OMG	A	644	9	18,26,27	0.90	1 (5%)	19,38,41	0.49	0
9	A2M	A	1678	9	18,25,26	0.63	0	18,36,39	0.64	0
9	5MC	A	1374	9	18,22,23	0.68	0	26,32,35	0.62	0
9	PSU	A	1243	9	18,21,22	1.28	2 (11%)	22,30,33	1.06	2 (9%)
9	OMU	A	121	9	19,22,23	0.89	0	26,31,34	0.84	1 (3%)
9	A2M	A	484	9	18,25,26	0.70	0	18,36,39	0.56	0
9	A2M	A	166	9	18,25,26	0.68	0	18,36,39	0.86	0
9	MA6	A	1851	9	18,26,27	0.63	0	19,38,41	0.69	0
9	PSU	A	612	9	18,21,22	1.07	1 (5%)	22,30,33	0.95	1 (4%)
9	PSU	A	119	9	18,21,22	1.11	2 (11%)	22,30,33	1.15	2 (9%)
9	A2M	A	159	9	18,25,26	0.79	0	18,36,39	0.60	0
9	A2M	A	27	9	18,25,26	0.72	0	18,36,39	0.69	0
9	PSU	A	823	9	18,21,22	1.15	2 (11%)	22,30,33	1.14	2 (9%)
9	OMU	A	116	9	19,22,23	0.72	0	26,31,34	0.77	0
9	UR3	A	1830	9	19,22,23	0.98	1 (5%)	26,32,35	1.84	5 (19%)
9	A2M	A	1031	9	18,25,26	0.74	0	18,36,39	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PSU	A	1081	9	-	1/7/25/26	0/2/2/2
9	OMG	A	683	9	-	0/5/27/28	0/3/3/3
9	PSU	A	822	9	-	0/7/25/26	0/2/2/2
9	OMC	A	174	9	-	0/9/27/28	0/2/2/2
9	OMG	A	509	9	-	1/5/27/28	0/3/3/3
9	A2M	A	668	9	-	2/5/27/28	0/3/3/3
9	OMC	A	1703	9	-	0/9/27/28	0/2/2/2
9	OMC	A	517	9	-	1/9/27/28	0/2/2/2
9	MA6	A	1850	9	-	3/7/29/30	0/3/3/3
9	5MU	A	814	9	-	0/7/25/26	0/2/2/2
9	OMG	A	644	9	-	1/5/27/28	0/3/3/3
9	A2M	A	1678	9	-	0/5/27/28	0/3/3/3
9	5MC	A	1374	9	-	0/7/25/26	0/2/2/2
9	PSU	A	1243	9	-	0/7/25/26	0/2/2/2
9	OMU	A	121	9	-	0/9/27/28	0/2/2/2
9	A2M	A	484	9	-	0/5/27/28	0/3/3/3
9	A2M	A	166	9	-	0/5/27/28	0/3/3/3
9	MA6	A	1851	9	-	5/7/29/30	0/3/3/3
9	PSU	A	612	9	-	0/7/25/26	0/2/2/2
9	PSU	A	119	9	-	0/7/25/26	0/2/2/2
9	A2M	A	159	9	-	2/5/27/28	0/3/3/3
9	A2M	A	27	9	-	0/5/27/28	0/3/3/3
9	PSU	A	823	9	-	0/7/25/26	0/2/2/2
9	OMU	A	116	9	-	1/9/27/28	0/2/2/2
9	UR3	A	1830	9	-	2/7/25/26	0/2/2/2
9	A2M	A	1031	9	-	0/5/27/28	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1243	PSU	C6-C5	3.36	1.39	1.35
9	A	822	PSU	C6-C5	3.32	1.39	1.35
9	A	119	PSU	C6-C5	3.25	1.39	1.35
9	A	509	OMG	C6-N1	-3.06	1.33	1.37
9	A	823	PSU	C6-C5	2.86	1.38	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1830	UR3	C4-N3-C2	-5.57	119.32	124.56
9	A	1850	MA6	N1-C6-N6	4.21	121.49	117.06
9	A	1830	UR3	C1'-N1-C2	3.51	122.91	116.99
9	A	1830	UR3	O4'-C1'-N1	3.17	115.60	108.36
9	A	1081	PSU	C6-C5-C4	-3.06	116.06	118.20

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	509	OMG	C1'-C2'-O2'-CM2
9	A	1830	UR3	O4'-C1'-N1-C6
9	A	1830	UR3	O4'-C1'-N1-C2
9	A	1850	MA6	C5-C6-N6-C10
9	A	1851	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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)

There are no chain breaks in this entry.

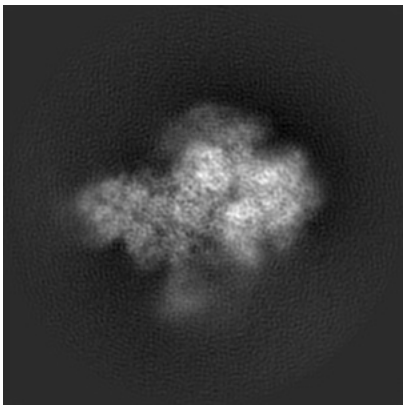
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14113. These allow visual inspection of the internal detail of the map and identification of artifacts.

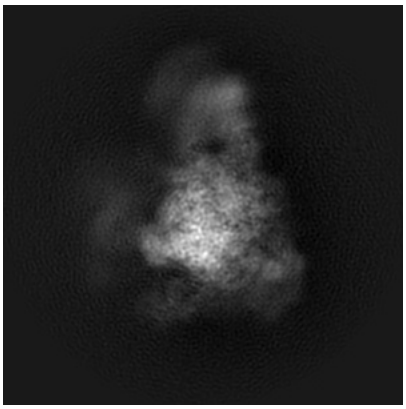
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

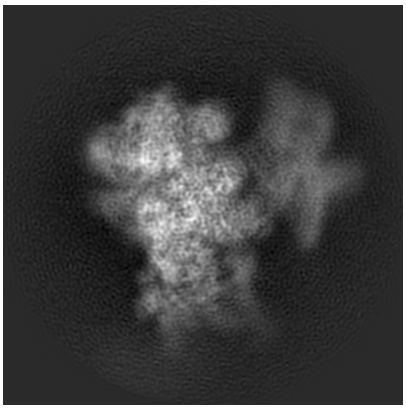
6.1.1 Primary map



X

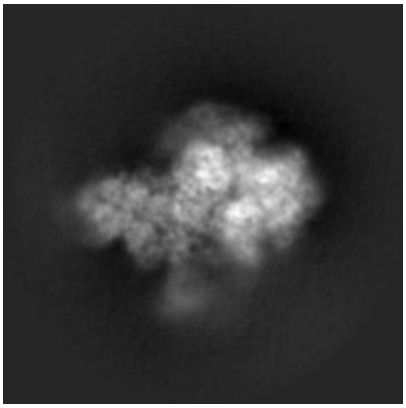


Y

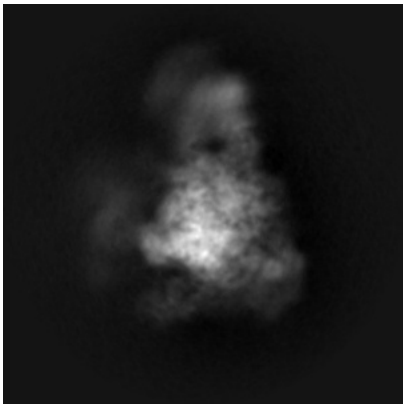


Z

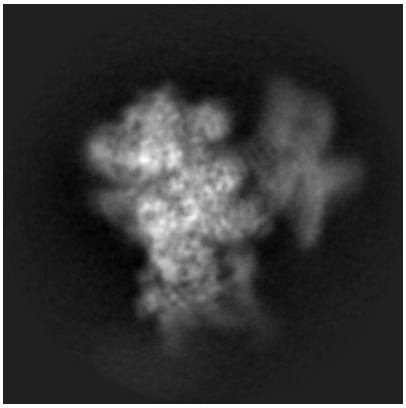
6.1.2 Raw map



X



Y

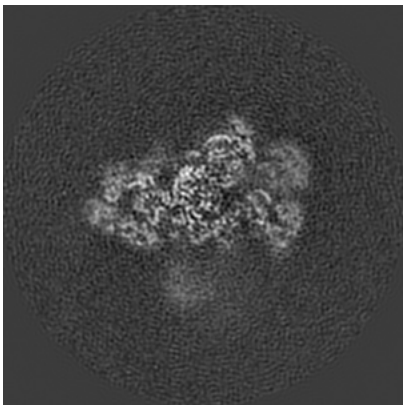


Z

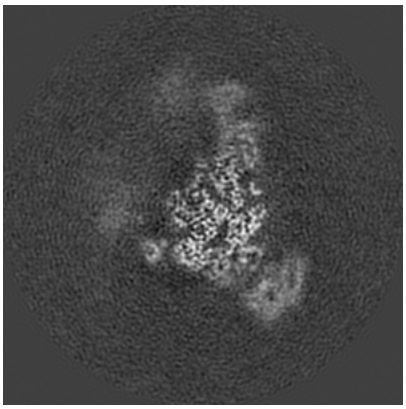
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

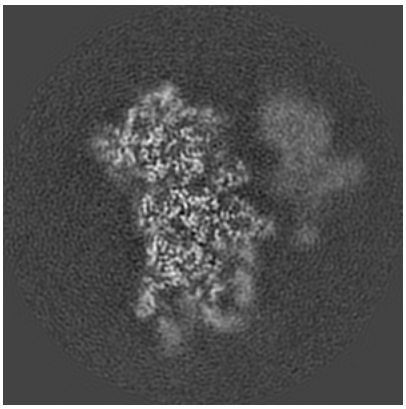
6.2.1 Primary map



X Index: 180

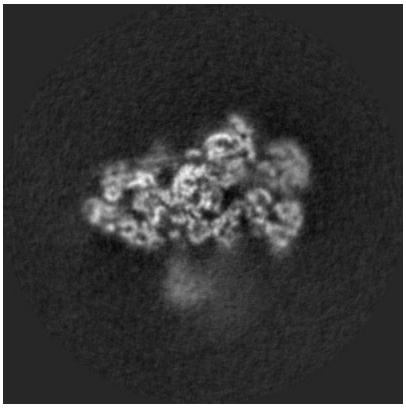


Y Index: 180

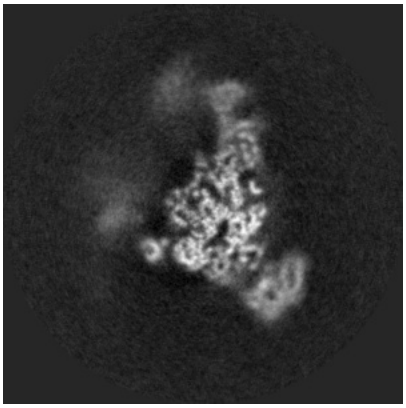


Z Index: 180

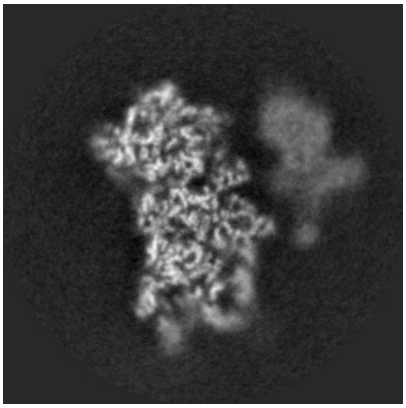
6.2.2 Raw map



X Index: 180



Y Index: 180

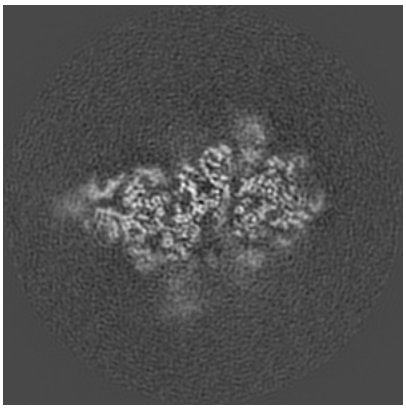


Z Index: 180

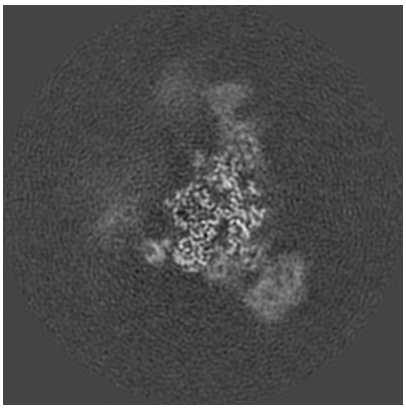
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

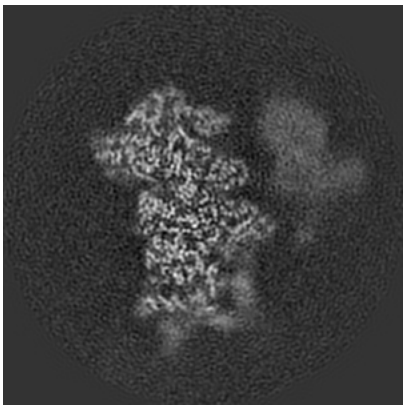
6.3.1 Primary map



X Index: 152

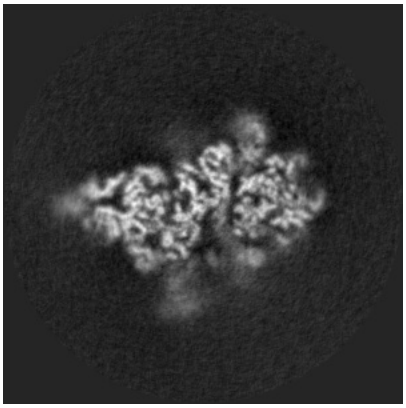


Y Index: 178

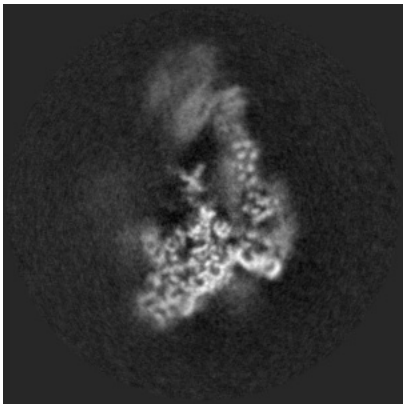


Z Index: 176

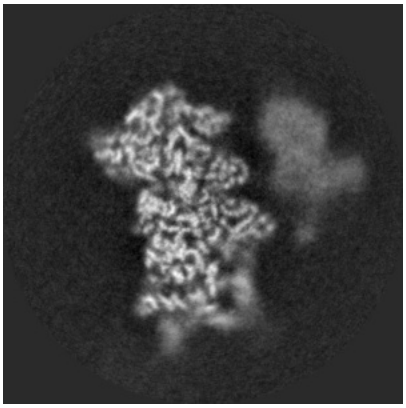
6.3.2 Raw map



X Index: 152



Y Index: 219

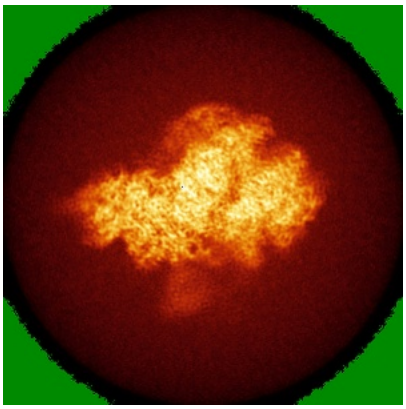


Z Index: 176

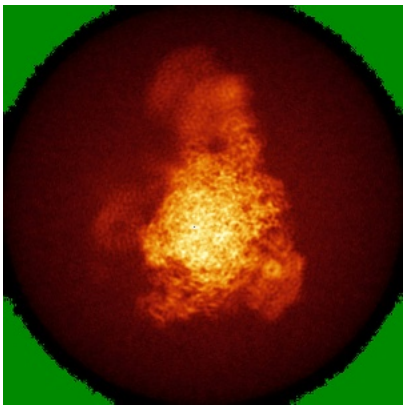
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

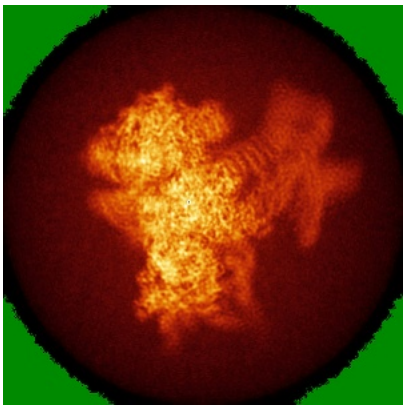
6.4.1 Primary map



X

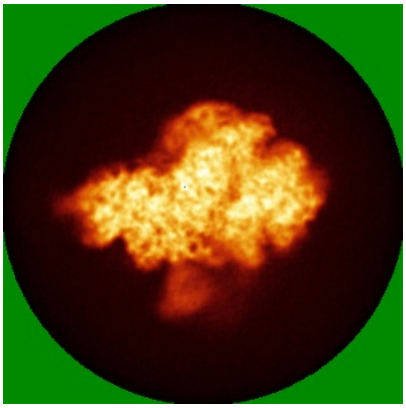


Y

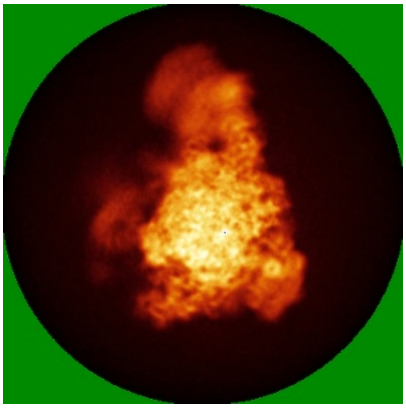


Z

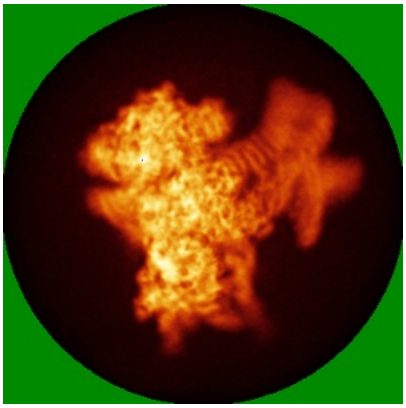
6.4.2 Raw map



X



Y

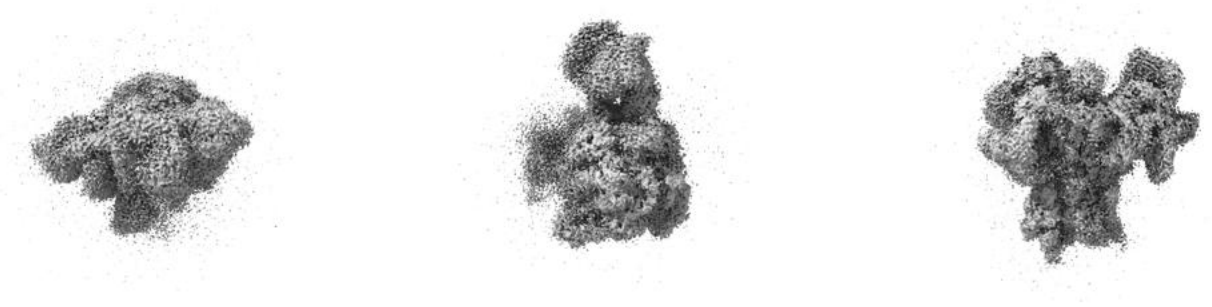


Z

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)

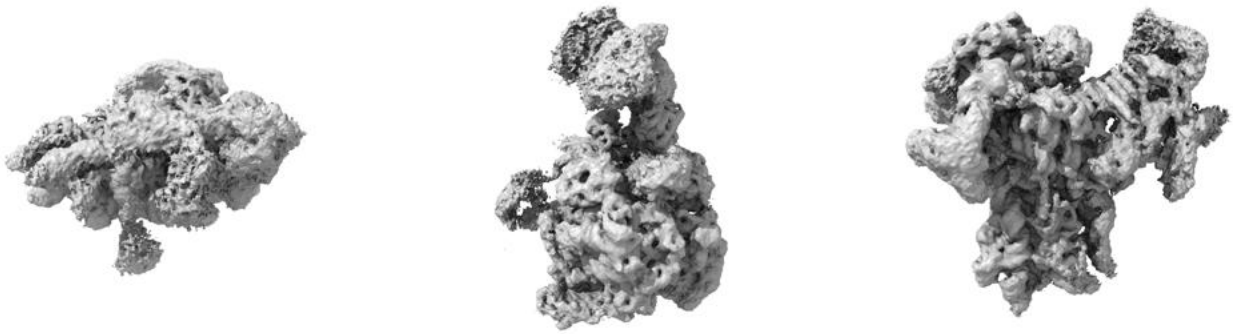
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.3. 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



X Y Z

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)

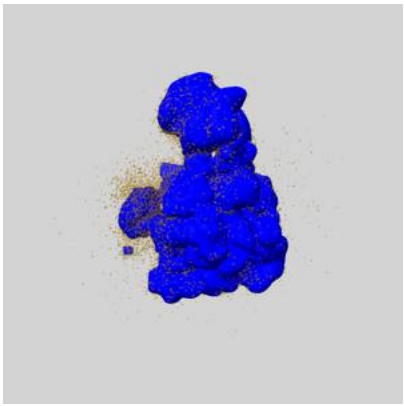
This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

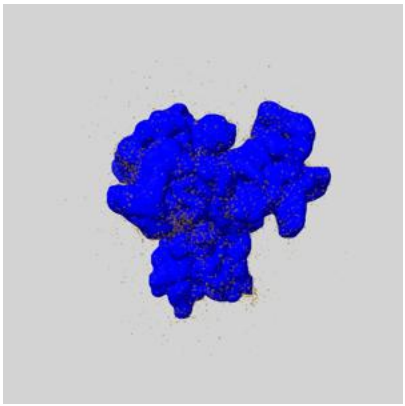
- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_14113_msk_1.map (i)

X



Y

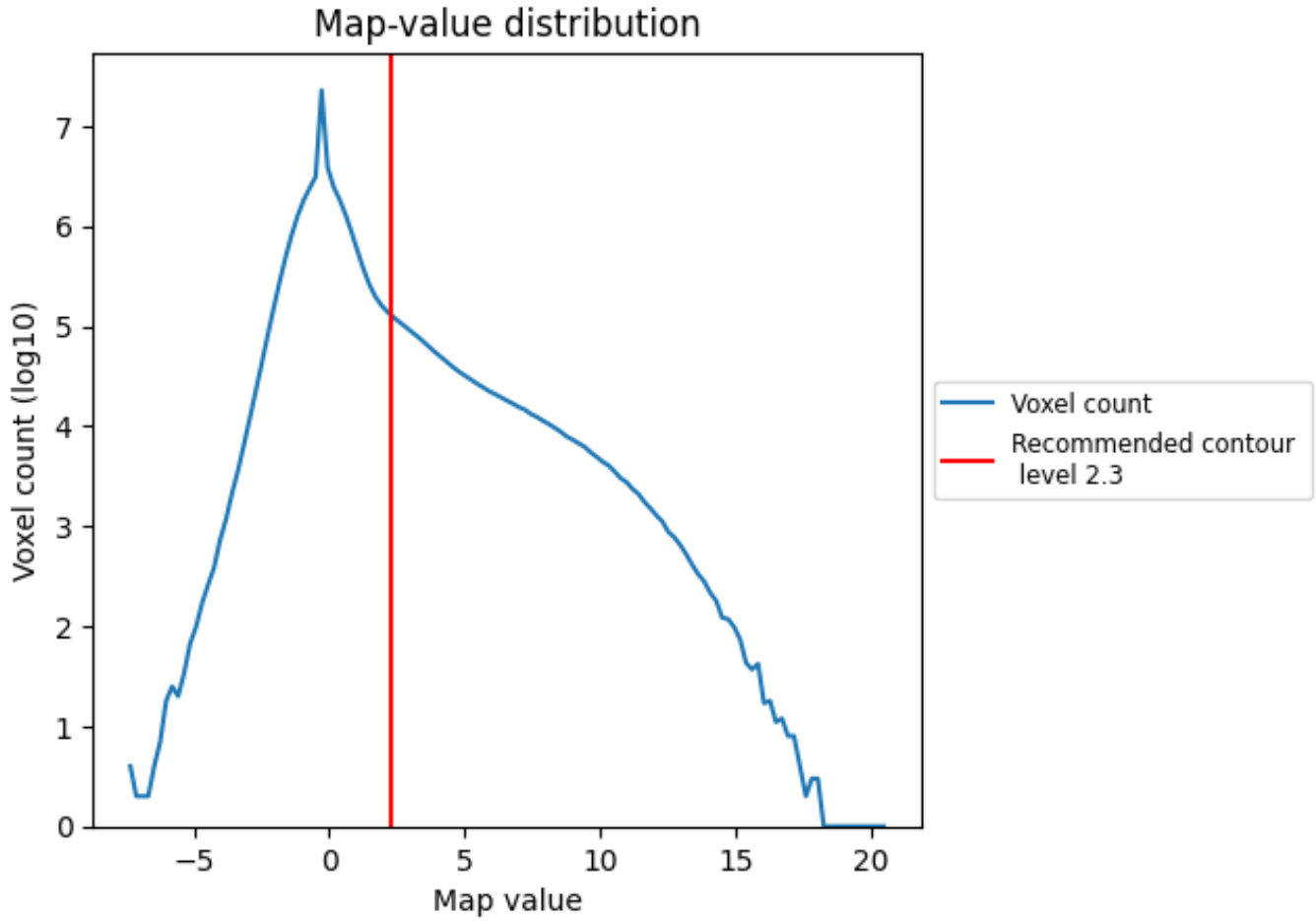


Z

7 Map analysis

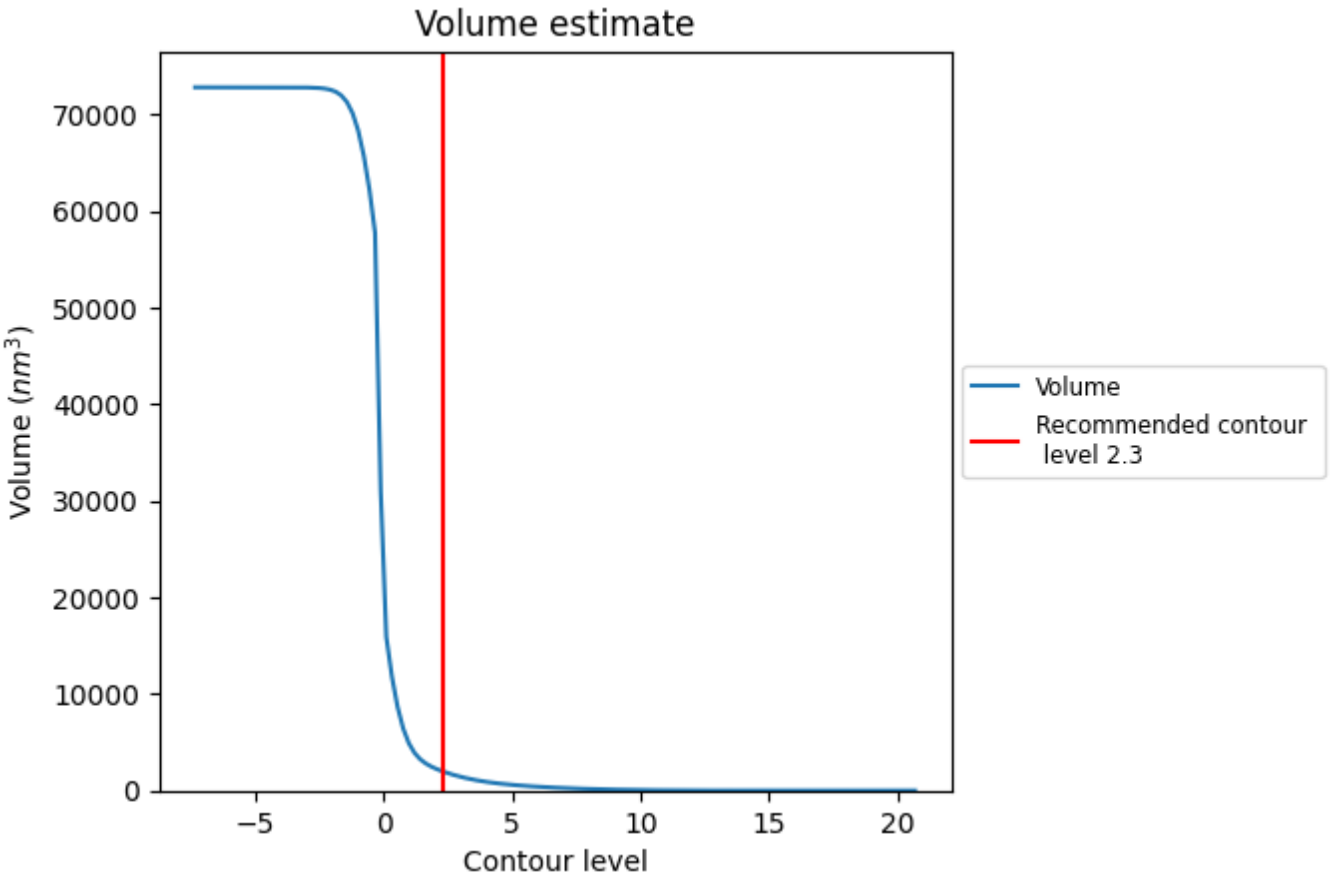
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

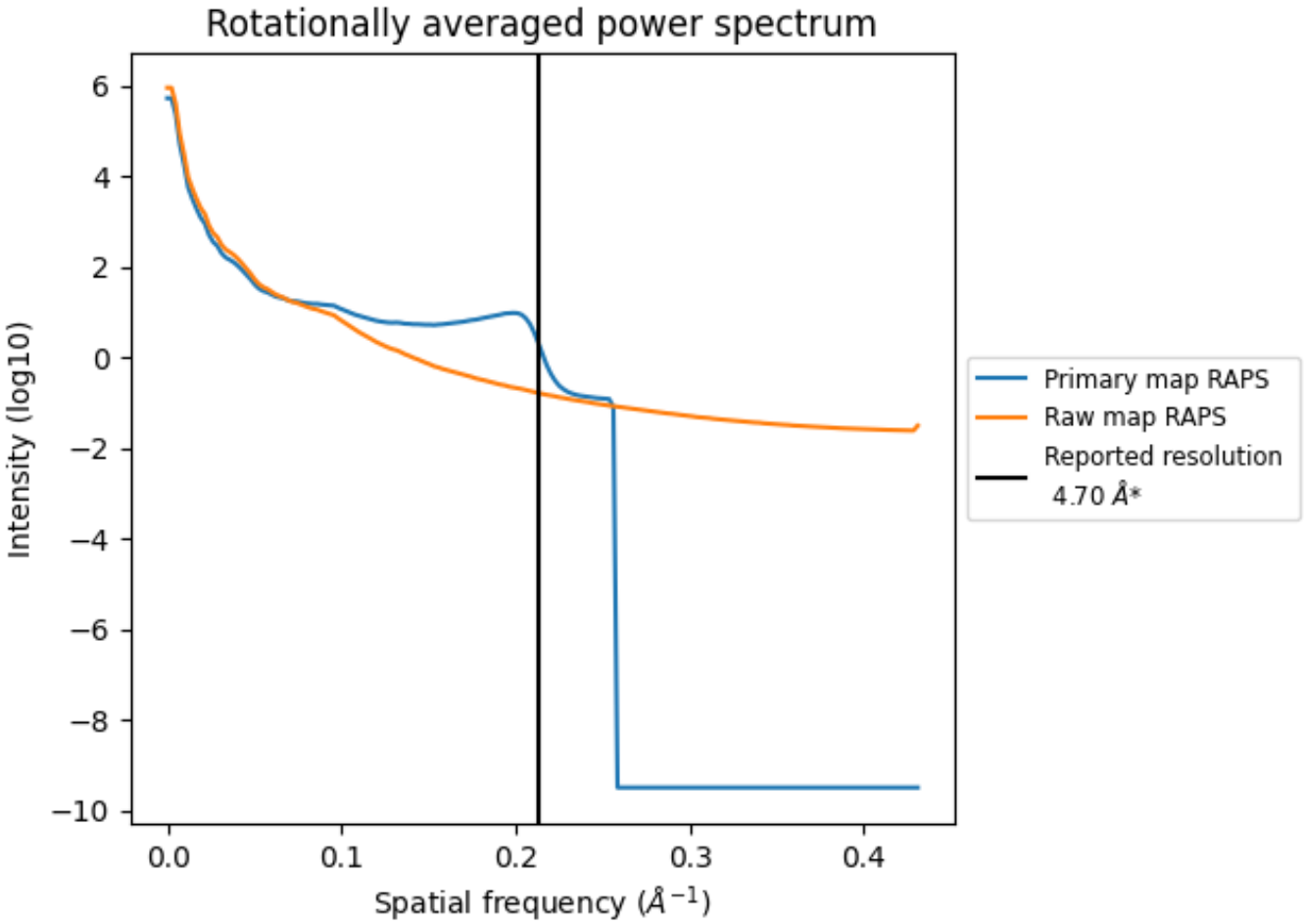
7.2 Volume estimate (i)



The volume at the recommended contour level is 1983 nm^3; this corresponds to an approximate mass of 1791 kDa.

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

7.3 Rotationally averaged power spectrum (i)

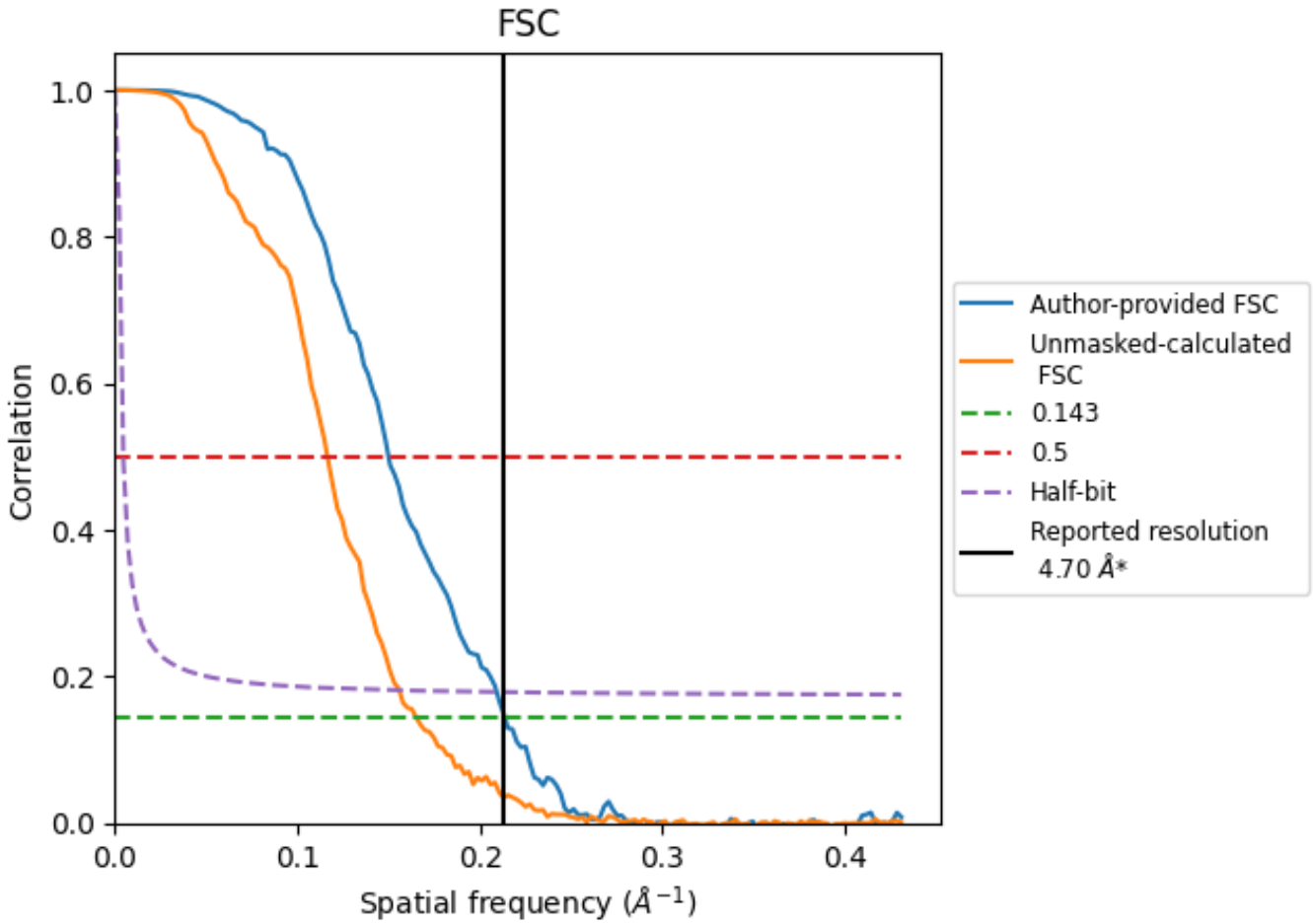


*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8.2 Resolution estimates (i)

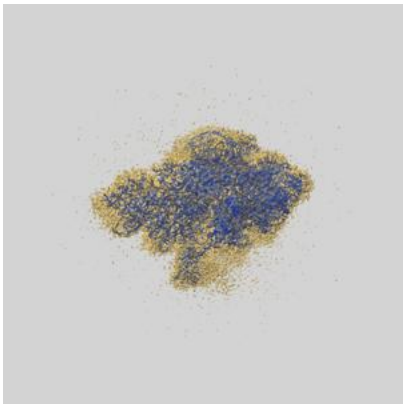
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.68	6.67	4.78
Unmasked-calculated*	6.05	8.58	6.41

*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 6.05 differs from the reported value 4.7 by more than 10 %

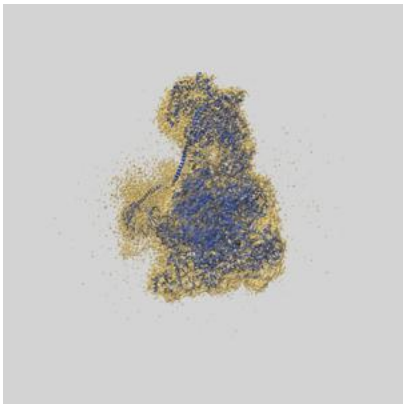
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14113 and PDB model 7QP6. Per-residue inclusion information can be found in section 3 on page 13.

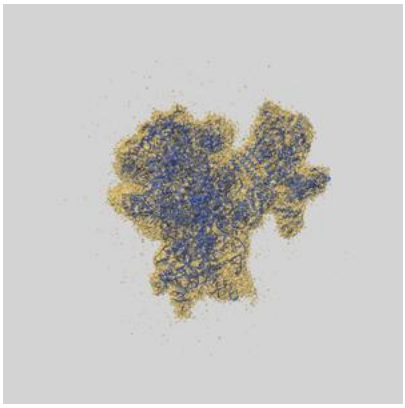
9.1 Map-model overlay



X



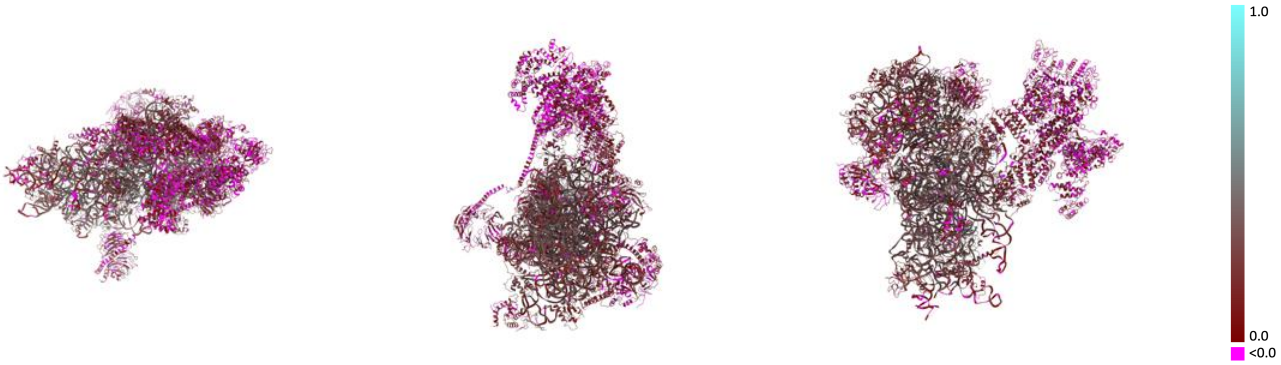
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.3 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.

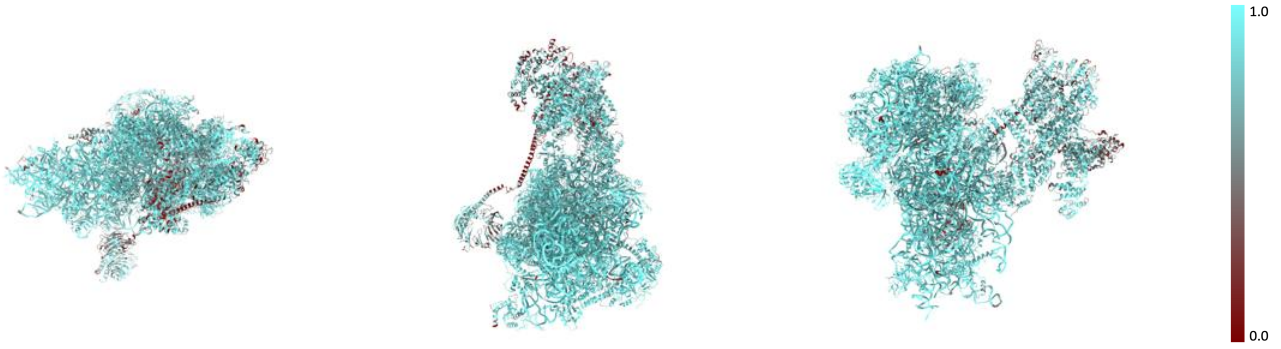
9.2 Q-score mapped to coordinate model



X Y Z

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.

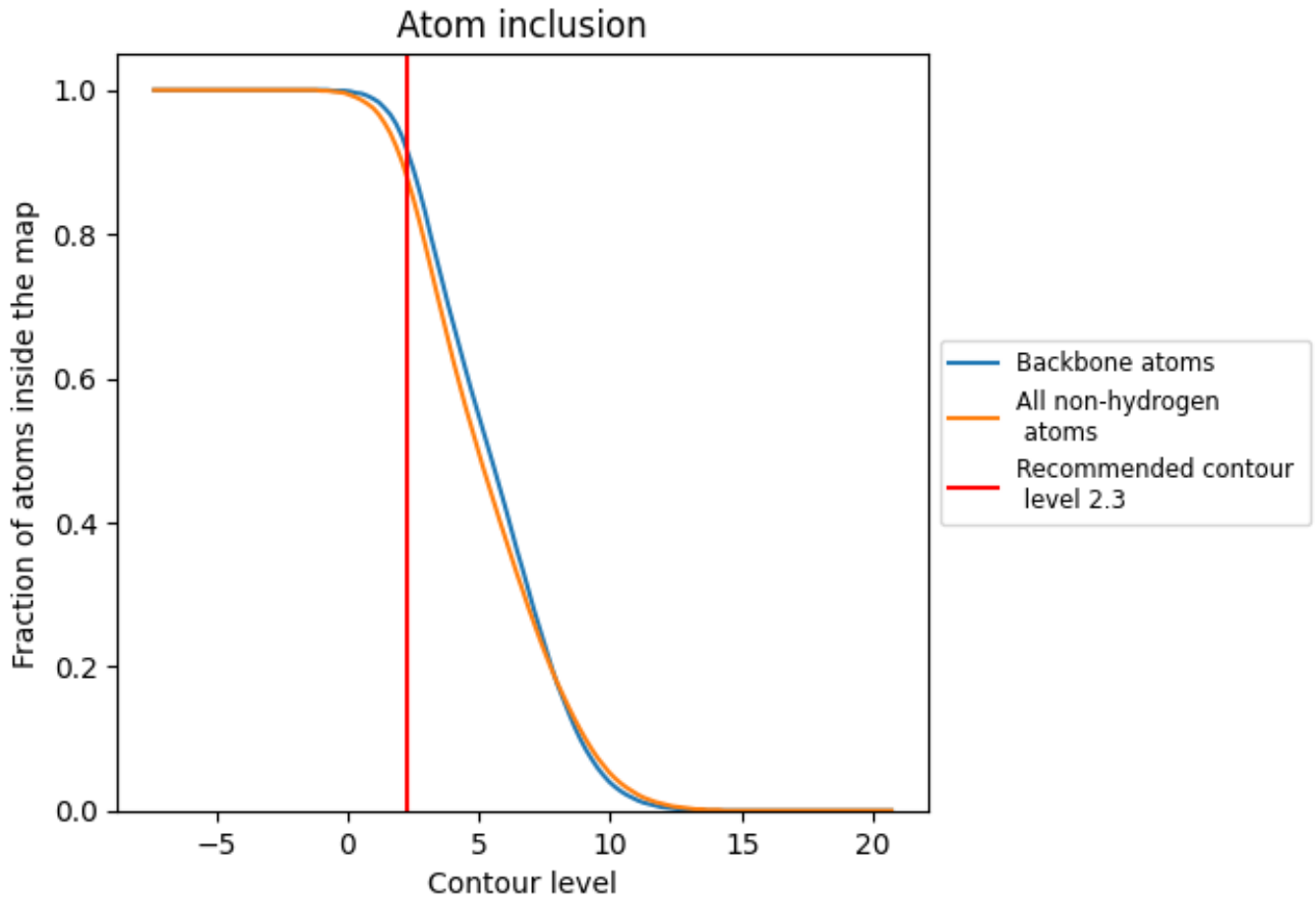
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (2.3).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 88% 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 (2.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8750	0.2330
1	0.6150	0.1310
3	0.5170	0.0340
4	0.7820	0.0690
5	0.6800	0.0350
6	0.6940	0.0470
7	0.7750	0.0750
8	0.6890	0.0500
9	0.9520	0.3600
A	0.9790	0.3000
B	0.9270	0.3770
C	0.9190	0.3440
D	0.8790	0.2860
E	0.9050	0.3440
F	0.9430	0.3260
G	0.8620	0.2610
H	0.8560	0.2960
I	0.8970	0.3010
J	0.8570	0.3270
K	0.8760	0.3220
L	0.8410	0.3060
M	0.8050	0.2890
N	0.8520	0.3010
O	0.8790	0.2790
P	0.9210	0.3330
Q	0.9110	0.3460
R	0.8730	0.2320
S	0.9110	0.2370
T	0.9310	0.2600
V	0.8600	0.2450
Y	0.9330	0.3310
Z	0.8200	0.2690
a	0.9170	0.3070
b	0.8880	0.2390
c	0.8820	0.2080

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.9120	0.2490
e	0.9020	0.2170
f	0.9040	0.2210
h	0.8870	0.2810
i	0.8850	0.3160
k	0.9600	0.2020
m	0.8250	0.1530
n	0.8240	0.2720
o	0.8700	0.1880
p	0.9040	0.3000
q	0.8660	0.2420
r	0.8270	0.1290
s	0.8410	0.1650
t	0.9630	0.1080
u	0.7060	0.1010
v	0.7540	0.0650
w	0.9330	0.1920
x	0.7950	0.1230
y	0.7390	0.1240