wwPDB EM Validation Summary Report (i)

Apr 20, 2024 – 07:12 pm BST

PDB ID	:	7QP7
EMDB ID	:	EMD-14114
Title	:	Structure of the human 48S initiation complex in closed state (h48S AUG closed)
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	:	3.70 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:

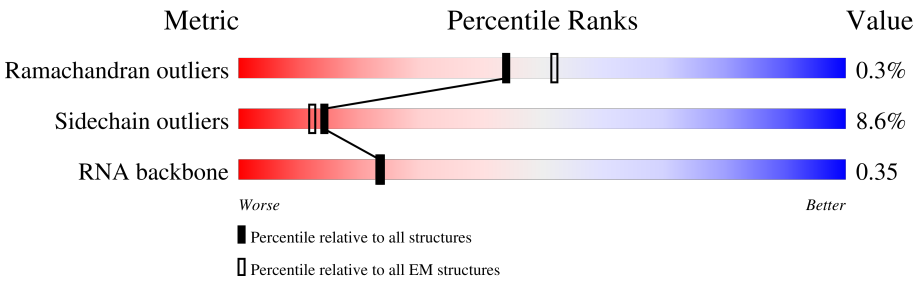
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.70 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	19% 55% 45%
2	3	218	64% 97%
3	4	357	15% 71% 28%
4	5	564	17% 57% 43%
5	6	374	32% 93% 6%
6	7	255	92%
7	8	352	21% 89% 10%
8	9	25	92%

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Mol	Chain	Length	Quality of chain
9	A	1869	63% 28% 8%
10	B	158	81% 9% 10%
11	C	263	90% 8%
12	D	194	87% 9%
13	E	143	88% 10%
14	F	59	75% 5% 20%
15	G	194	81% 10% 9%
16	H	84	83% 13%
17	I	151	97%
18	J	130	93% 5%
19	K	83	87% 11%
20	L	293	64% 11% 25%
21	M	135	82% 10% 7%
22	N	295	64% 5% 30%
23	O	264	80% 20%
24	P	151	74% 14% 12%
25	Q	115	76% 10% 14%
26	R	208	88% 8% 5%
27	S	249	81% 12% 8%
28	T	133	85% 9% 6%
29	V	204	83% 7% 10%
30	Y	146	90% 6%
31	Z	243	79% 14% 7%
32	a	165	56% 40%
33	b	145	67% 9% 24%

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Mol	Chain	Length	Quality of chain
34	c	317	85% 13%
35	d	145	90% 8%
36	e	125	46% 6% 47%
37	f	152	85% 9% 7%
38	h	119	75% 12% 13%
39	i	56	79% 11% 11%
40	k	156	26% 8% 66%
41	m	132	5% 85% 8% 8%
42	n	69	78% 12% 9%
43	o	320	23% 76%
44	q	144	53% 17% 30%
45	r	315	73% 14% 13%
46	t	472	75% 25%
47	u	1382	10% 50% 49%
48	v	445	10% 84% 14%
49	w	75	44% 56%
50	x	548	13% 74% 23%
51	y	913	69% 30%

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 108194 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	447	2560	1570	492	493	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	N	O	P		
6	7	21	441	199	78	144	20	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	M	125	1015	639	185	187	4	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 44 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	q	101	782	494	141	143	4	0	0

- Molecule 45 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

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

- Molecule 46 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

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

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

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

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

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

- Molecule 49 is a RNA chain called Initiator Met-tRNA-i.

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

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

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

- Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	y	642	5197	3274	925	963	35	0	0

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

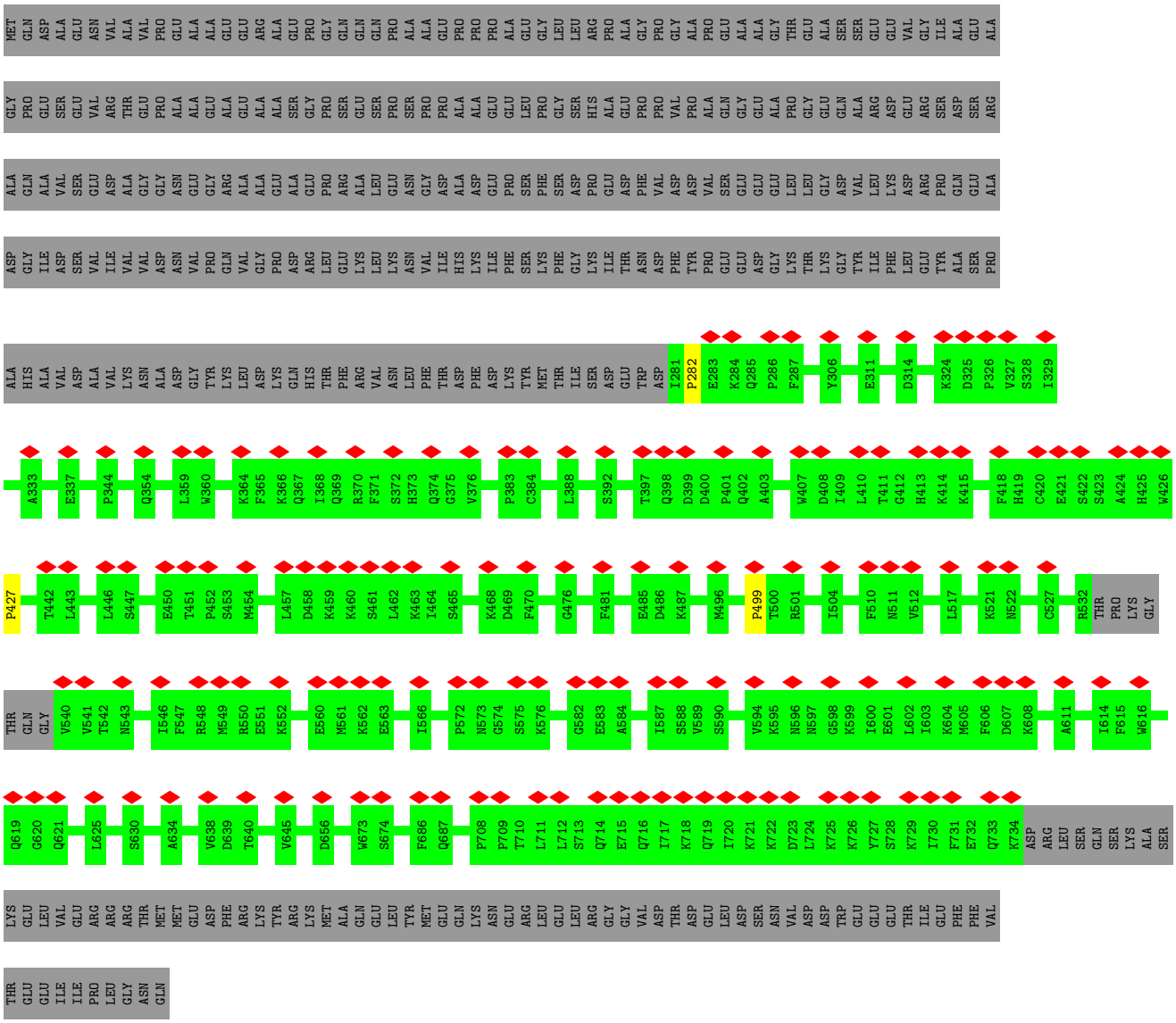
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
52	Q	1	1	1	0
52	k	1	1	1	0

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

Chain 1:



• Molecule 2: Eukaryotic translation initiation factor 3 subunit K

Chain 3: 64% 97%

MET A2 M3 F4 E5 Q6 M7 R8 A9 N10 L15 K16 P23 E24 N25 L26 A27 T28 Y32 V33 E34 T35 Q36 A37 K38 E39 N40 A41 Y42 D43 L44 L51 N57 P58 A59 F60 F61 Q62 T63 T64 V65 T66 K72 A73 L74 T75 N76 L77 P78 H79 T80 D81 D90

Q91 Q94 E95 E96 R97 P98 I99 R100 Q101 I102 L103 Y104 L108 L109 C112 H113 F114 Q115 A116 F117 W118 Q119 A120 L121 D122 E123 N124 M125 D126 E129 G130 I131 T132 G133 F134 E135 D136 S137 V138 R139 K140 F141 I142 C143 H144 V145 V146 T149 Y150 Q151 H152 I153 D154 R155 W156

L157 L158 A159 E160 M161 D164 L165 S166 D167 S168 Q169 L170 K171 V172 W173 M174 S175 K176 Y177 G178 W179 S180 A181 D182 E183 SER GLY Q186 I187 F188 I189 C190 S191 Q192 E193 E194 S195 I196 K197 P198 K199 N200 I201 V202 E203 K204 I205 D206 V210 S211 M214 A215 S216 SER GLN

- Molecule 3: Eukaryotic translation initiation factor 3 subunit F

Chain 4: 15% 71% 28%

MET ALA THR PRO ALA VAL PRO VAL SER ALA PRO PRO ALA THR PRO THR PRO VAL PRO ALA ALA ALA PRO ALA SER VAL PRO ALA PRO THR PRO ALA PRO ALA ALA ALA PRO VAL PRO ALA ALA ALA PRO ALA SER SER SER ASP PRO ALA ALA ALA ALA ALA ALA THR ALA ALA PRO GLY

GLN THR PRO ALA SER ALA GLN ALA PRO ALA GLN THR PRO ALA PRO ALA LEU PRO GLY PRO ALA LEU PRO GLY PRO PHE PRO GLY G89 R90 V91 A114 T132 N133 S142 GLU ASP E145 V146 A147 V148 D149 M150 E151 K154 N155 K161 S164 H182 S183 V184 S191

R192 E193 A194 P195 S205 L206 G209 R210 M211 S218 THR LEU MET GLY VAL PRO GLY ARG THR MET G229 P234 L235 T236 V237 K238 Y239 Y242 D243 T244 R261 V262 I263 G264 G273 V286 A290 E291 D292 V293 L294 S295 G296 K297 V298 S299 V304 K317 I318

V319 P320 D321 D322 N342 L357

- Molecule 4: Eukaryotic translation initiation factor 3 subunit L

Chain 5: 17% 57% 43%

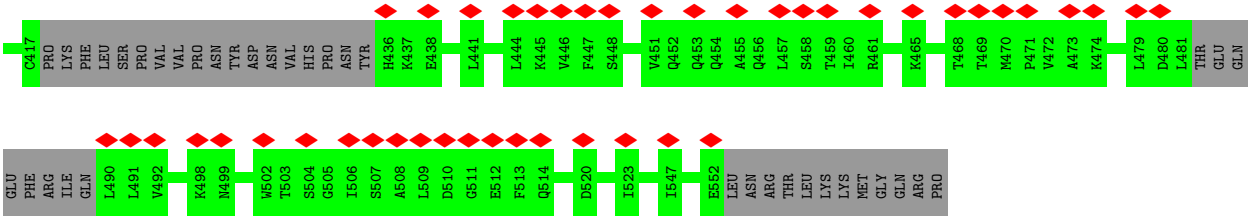
MET SER TYR PRO ALA ASP ASP TYR GLU SER GLU ALA ALA TYR ASP PRO TYR ALA TYR PRO SER ASP TYR ASP MET HIS THR GLY ASP PRO LYS GLN ASP LEU ALA TYR GLU ARG GLN TYR GLU GLN GLN THR TYR GLN VAL ILE PRO GLU VAL ILE LYS ASN PHE ILE GLN TYR PHE HIS

LYS THR VAL SER ASP LEU ILE ASP GLN LYS VAL TYR GLU LEU GLN ALA SER ARG VAL SER SER ASP VAL ILE ASP GLN LYS VAL TYR GLU ILE GLN ASP ILE TYR GLU ASN SER TRP THR LYS LEU THR GLU ARG PHE PHE LYS ASN THR PRO TRP PRO GLU ALA GLU ALA ILE ALA PRO

GLN VAL GLY ASN ASP ALA VAL PHE LEU ILE LEU TYR LYS GLU LEU TYR TYR ARG HIS ILE TYR ALA LYS VAL SER GLY GLY PRO SER LEU GLU GLN ARG PHE GLU SER TYR TYR ASN TYR CYS ASN LEU PHE ASN TYR ILE LEU ASN ALA ASP GLY PRO ALA PRO LEU GLU LEU PRO ASN

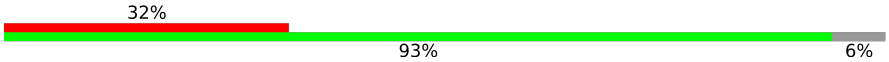
GLN TRP L183 D188 I191 K203 K207 S208 E209 E210 E211 F214 S217 N218 I221 L244 Y247 G250 P253 E254 S255 V256 L265 G270 Y271 F272 K292 V293 L294 I297 E298 K301 M304 TYR SER ARG VAL PRO GLU C311 Q312 V313

L324 M325 M326 R327 R328 N338 I339 L340 L341 Y342 I343 GLN ARG THR LYS SER MET PHE GLN ARG THR THR TYR LYS Y357 E358 N364 A372 I373 A374 L375 THR MET TYR PRO MET ARG I382 S385 I386 H387 L388 Q389 E392 D396 K397 R400 K403 Q407 F413



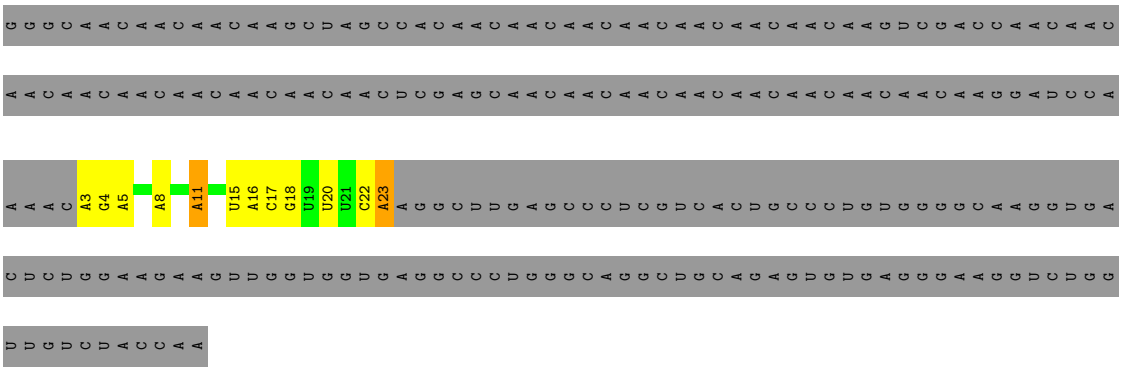
• Molecule 5: Eukaryotic translation initiation factor 3 subunit M

Chain 6:



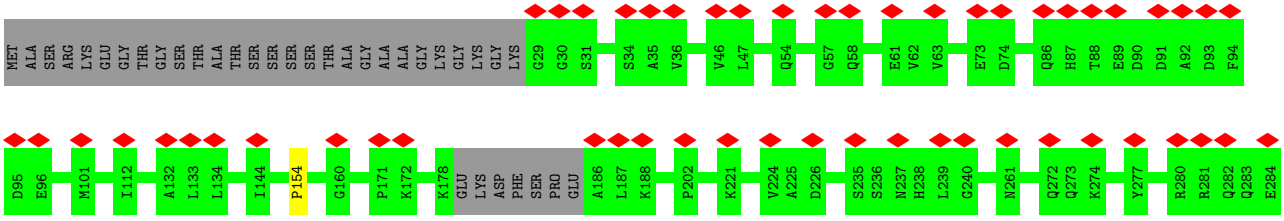
• Molecule 6: mRNA

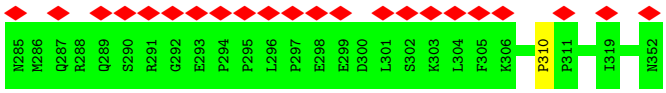
Chain 7:



• Molecule 7: Eukaryotic translation initiation factor 3 subunit H

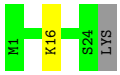
Chain 8:





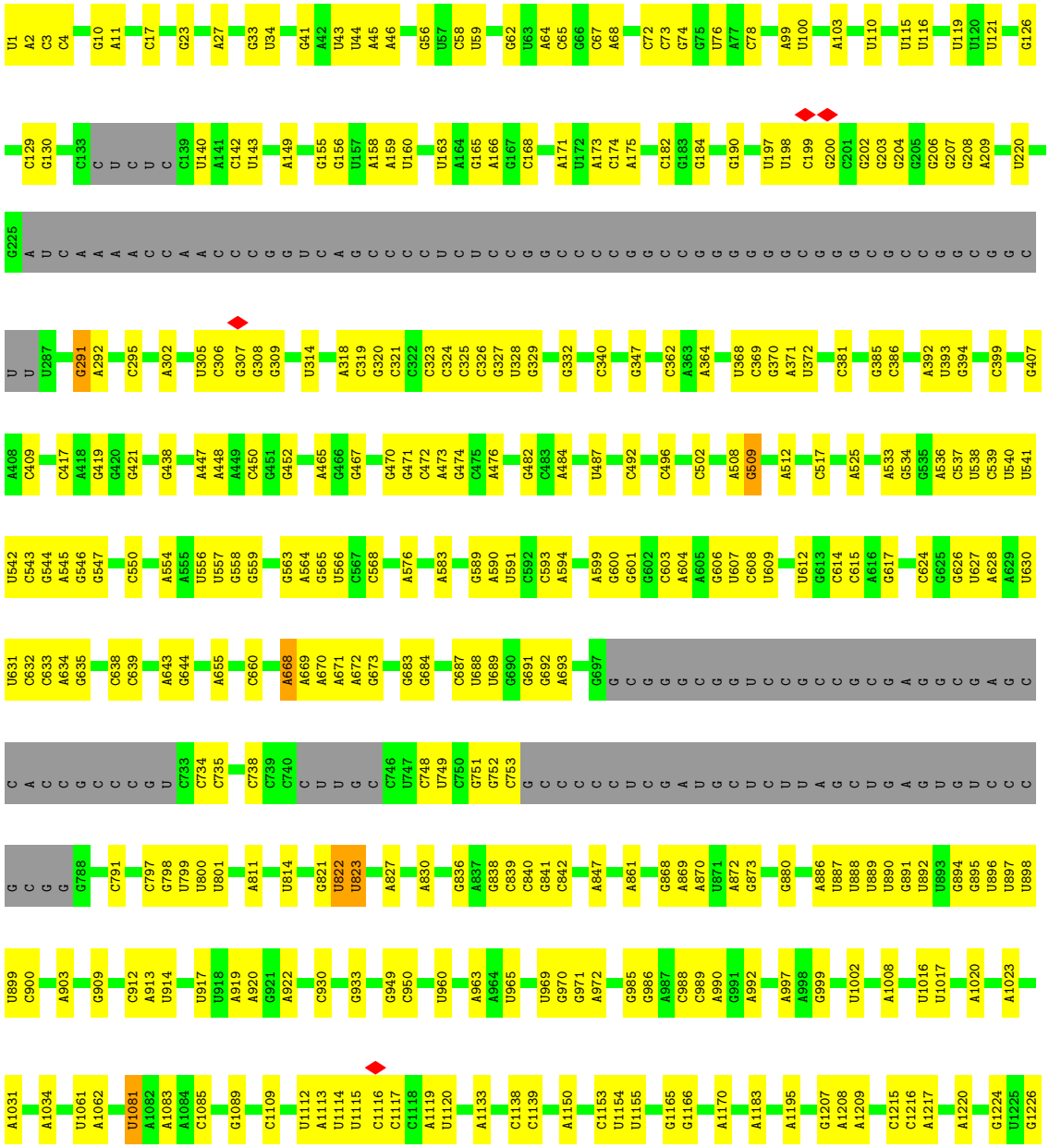
• Molecule 8: 60S ribosomal protein L41

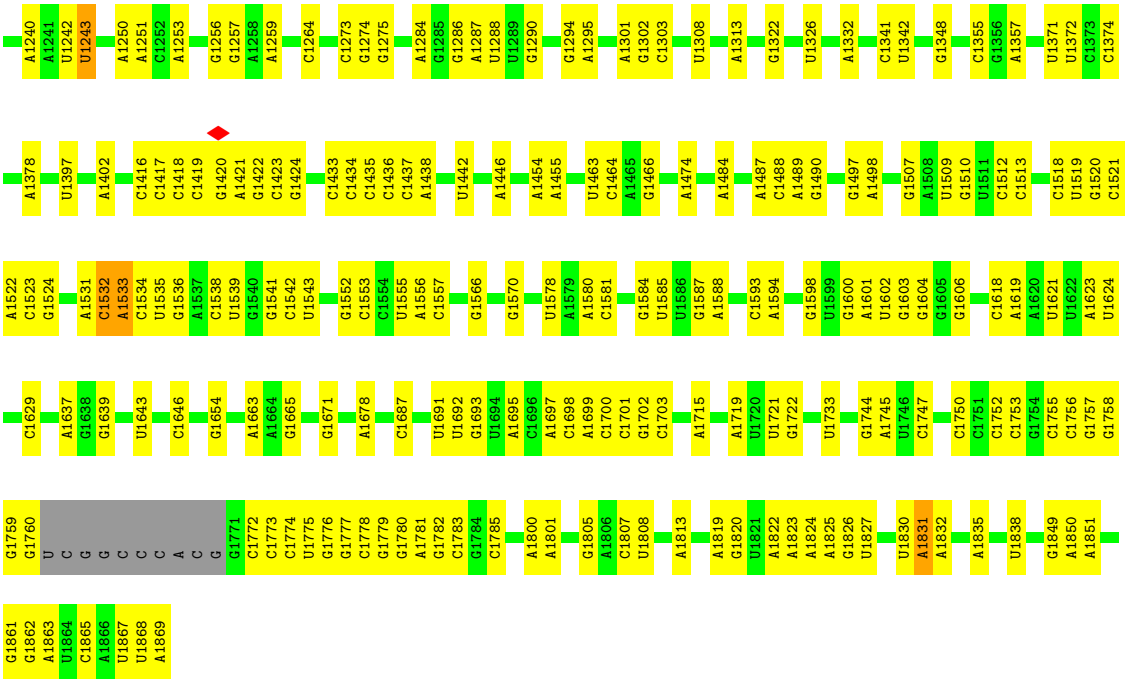
Chain 9:



• Molecule 9: 18S rRNA

Chain A:





- Molecule 10: 40S ribosomal protein S11

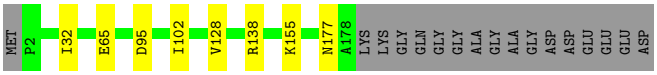
Chain B:

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

Chain C:

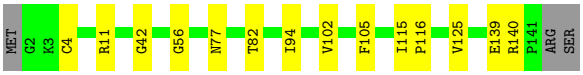
- Molecule 12: 40S ribosomal protein S9

Chain D:



- Molecule 13: 40S ribosomal protein S23

Chain E:



- Molecule 14: 40S ribosomal protein S30

Chain F: 75% 5% 20%

LYS VAL HIS GLY SER L80 A81 R82 V93 T103 V119 VAL PRO THR PHE GLY LYS LYS K127 S133

- Molecule 15: 40S ribosomal protein S7

Chain G: 81% 10% 9%

MET PHE SER SER SER ALA LYS I8 P11 ASN GLY GLU LYS P16 F19 Q25 E29 L30 N33 T46 I51 E52 V53 F72 V92 R98 K107 SER ARG THR LYS ASN K113 T121 V166 E171 L180 K183 D184 V185 P190 Q193

LEU

- Molecule 16: 40S ribosomal protein S27

Chain H: 83% 13%

MET P2 L8 E13 R23 Q26 D34 V35 C40 V53 C56 C59 S60 T61 K82 GLN HIS

- Molecule 17: 40S ribosomal protein S13

Chain I: 97%

MET G2 E35 D87 R106 K140 A151

- Molecule 18: 40S ribosomal protein S15a

Chain J: 93% 5%

MET V2 P29 D55 N64 C72 G73 V74 I75 S76 P77 F130

- Molecule 19: 40S ribosomal protein S21

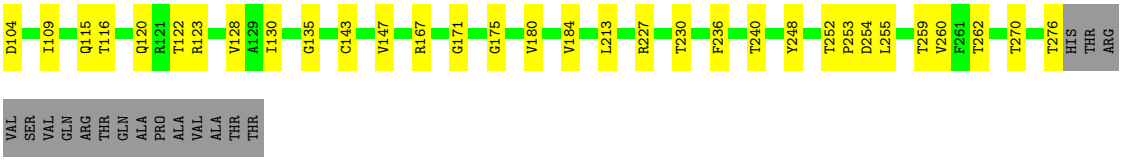
Chain K: 87% 11%

M1 D28 E38 V39 F50 K51 T52 E64 V79 S80 K81 ASN PHE

- Molecule 20: 40S ribosomal protein S2

Chain L: 64% 11% 25%

MET ALA ASP ASP ALA GLY ALA ALA GLY GLY PRO GLY GLY PRO GLY GLY PRO GLY MET GLY ASN ARG GLY GLY PHE ARG GLY GLY PHE GLY SER GLY ILE ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ALA ARG GLY GLY LYS ALA GLU D57 L83

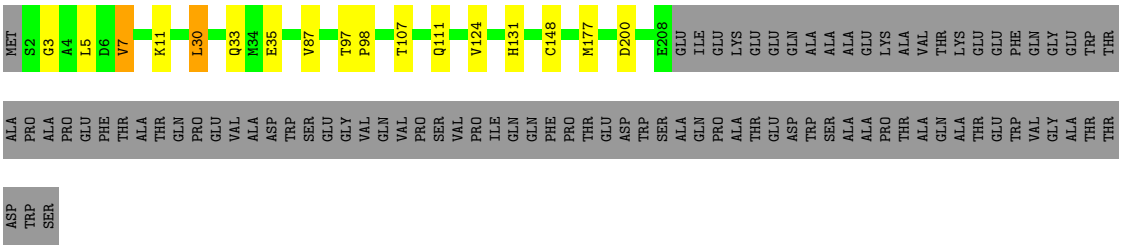


• Molecule 21: 40S ribosomal protein S17

Chain M:

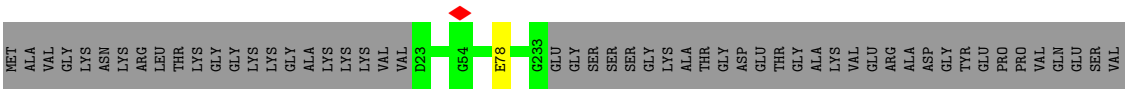
• Molecule 22: 40S ribosomal protein SA

Chain N:



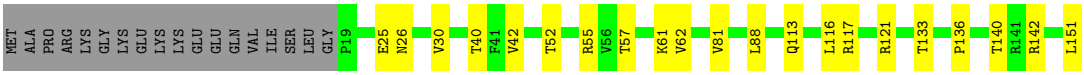
• Molecule 23: 40S ribosomal protein S3a

Chain O:



• Molecule 24: 40S ribosomal protein S14

Chain P:

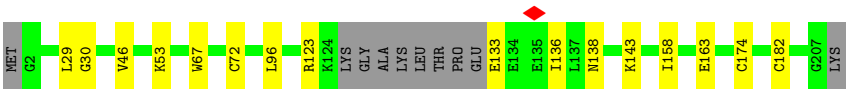


• Molecule 25: 40S ribosomal protein S26

Chain Q:

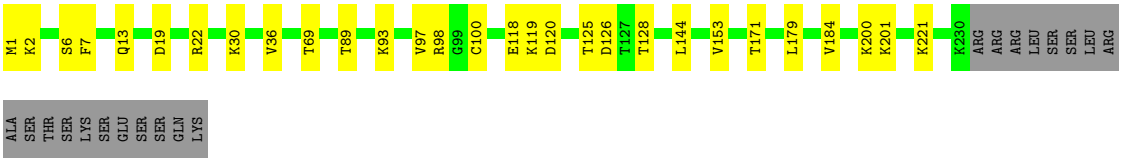
• Molecule 26: 40S ribosomal protein S8

Chain R:



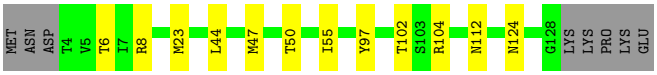
• Molecule 27: 40S ribosomal protein S6

Chain S:



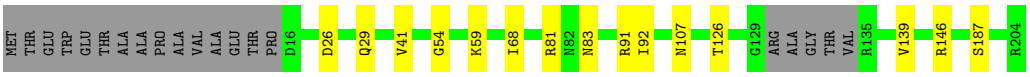
• Molecule 28: 40S ribosomal protein S24

Chain T:



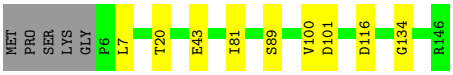
• Molecule 29: 40S ribosomal protein S5

Chain V:



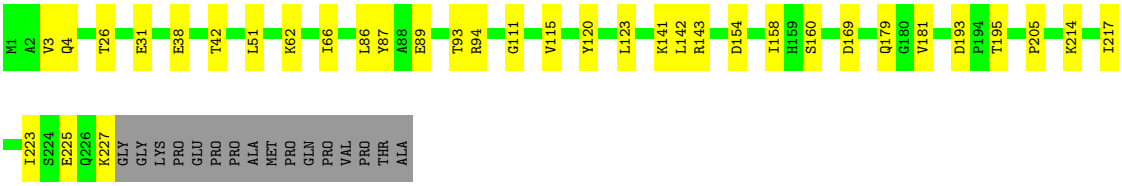
• Molecule 30: 40S ribosomal protein S16

Chain Y:



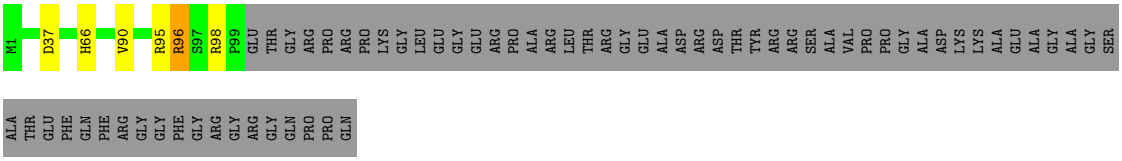
• Molecule 31: 40S ribosomal protein S3

Chain Z:



• Molecule 32: 40S ribosomal protein S10

Chain a:

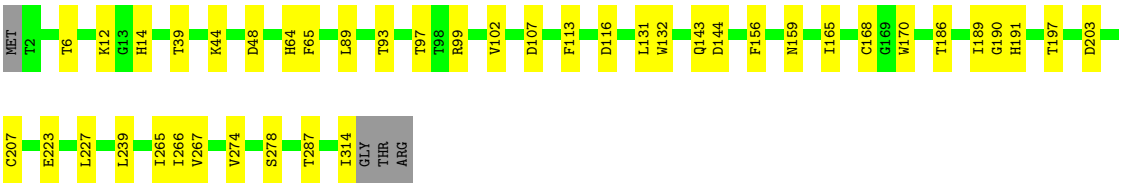


• Molecule 33: 40S ribosomal protein S15

Chain b:

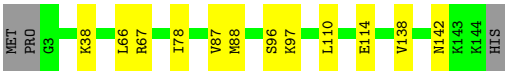
• Molecule 34: Receptor of activated protein C kinase 1

Chain c:



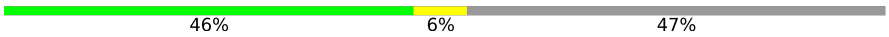
• Molecule 35: 40S ribosomal protein S19

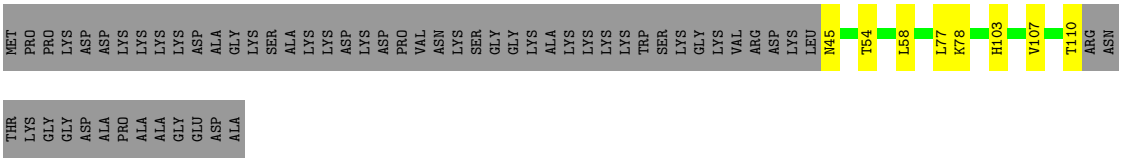
Chain d:



• Molecule 36: 40S ribosomal protein S25

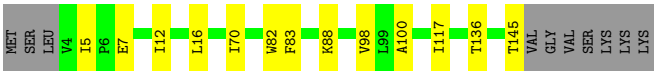
Chain e:





• Molecule 37: 40S ribosomal protein S18

Chain f:



• Molecule 38: 40S ribosomal protein S20

Chain h: 75% 12% 13%

MET ALA PHE LYS ASP THR GLY LYS THR PRO VAL GLU PRO GLU VAL ALA I17 H18 L39 V50 T58 T68 P69 C70 D78 L91 I101 I104 V112 E113 I116 A117 D118 A119

- Molecule 39: 40S ribosomal protein S29

Chain i: 79% 11% 11%

MET GLY HIS GLN GLN LEU Y7 H10 P11 R12 K13 R22 I53 D56

- Molecule 40: Ubiquitin-40S ribosomal protein S27a

Chain k: 26% 8% • 66%

MET GLN ILE PHE VAL LYS THR LEU THR GLY LYS THR ILE THR LEU GLU VAL GLU PRO SER ASP THR ILE GLU ASN VAL LYS ALA LYS ILE GLN ASP LYS GLU GLY ILE PRO PRO ASP GLN GLN ARG LEU ILE PHE ALA GLY LYS GLN LEU GLU ASP GLY ARG THR LEU SER ASP TYR ASN

ILE GLN LYS GLU SER THR LEU HIS LEU VAL LEU ARG LEU ARG GLY GLY ALA LYS LYS ARG LYS LYS LYS SER TYR THR THR PRO LYS LYS ASN LYS H93 K99 L100 A101 V102 Y106 K107 VAL ASP GLU ASN GLY LYS I114 S115 R116 L117 V130 F131 M132 H135 F136 D137 R138

N151 LYS PRO GLU ASP LYS

- Molecule 41: 40S ribosomal protein S12

Chain m: 5% 85% 8% 8%

MET ALA GLU GLU GLY ILE ALA ALA GLY GLY V11 M12 C50 V62 E66 I74 D80 L91 C92 K93 R96 K99 E117 V123 I124 Y127 C130 K131 K132

- Molecule 42: 40S ribosomal protein S28

Chain n: 78% 12% • 9%

MET ASP THR SER R5 V6 I9 V17 T28 V32 S39 V46 L58 E62 R67 LEU ARG

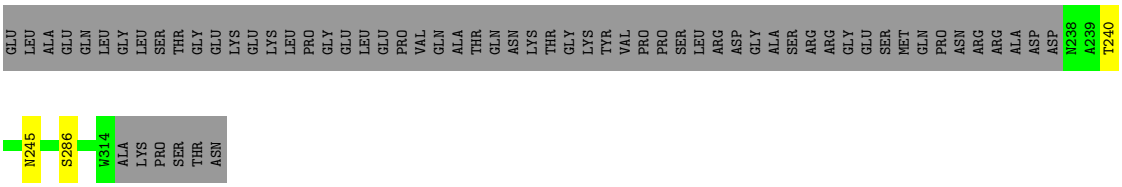
- Molecule 43: Eukaryotic translation initiation factor 3 subunit G

Chain o: 23% • 76%

MET PRO THR GLY ASP PHE ASP SER LYS PRO SER TRP ALA ASP GLN VAL GLU GLU GLU GLU GLY GLU ASP ASP LYS CYS VAL THR SER GLU LEU LEU LYS GLY ILE PRO LEU ALA THR GLY ASP THR SER PRO GLU PRO GLU LEU LEU PRO GLY ALA PRO LEU PRO PRO PRO LYS GLU VAL ILE

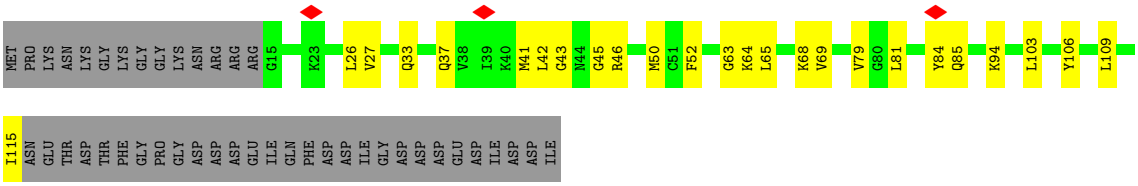
ASN GLY ASN ILE LYS THR VAL THR GLU TYR LYS ILE ASP GLU ASP GLY LYS LYS PHE LYS ILE VAL ARG ASP THR PHE ARG ILE GLU THR ARG LYS ALA SER LYS ALA VAL ALA ARG ARG LYS ASN TRP LYS LYS PHE GLY ASN SER GLU PHE ASP PRO PRO GLY PRO ASN VAL ALA THR THR

THR VAL SER ASP ASP VAL SER MET THR PHE ILE THR SER LYS GLU ASP LEU ASN CYS GLN GLU GLU GLU ASP PRO MET ASN LYS LEU LYS GLY GLN LYS ILE VAL SER CYS ARG ILE CYS LYS GLY ASP HIS TRP THR THR ARG CYS PRO TYR LYS ASP THR LEU GLY PRO MET GLN LYS



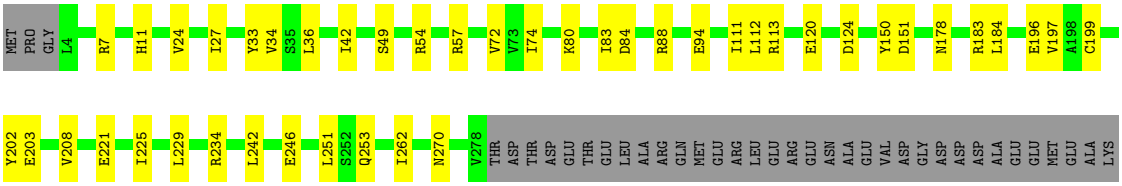
• Molecule 44: Eukaryotic translation initiation factor 1A, X-chromosomal

Chain q:



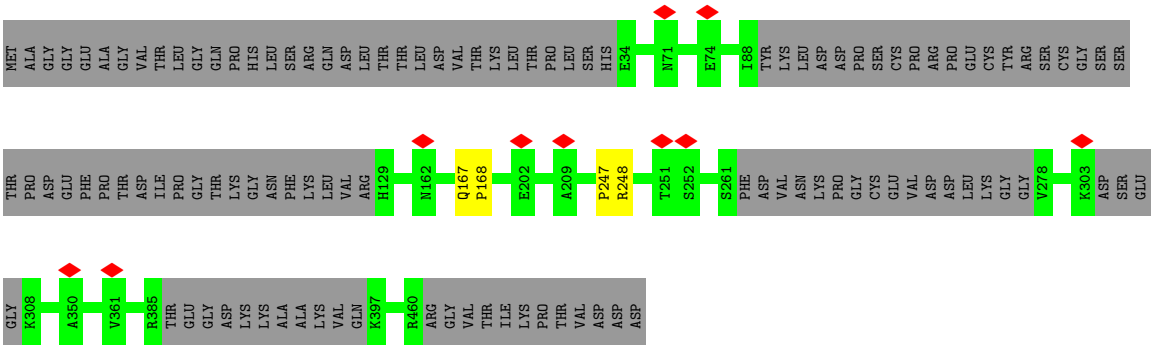
• Molecule 45: Eukaryotic translation initiation factor 2 subunit 1

Chain r:



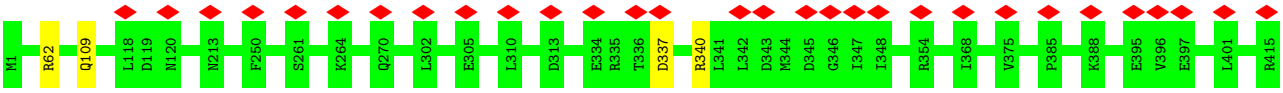
• Molecule 46: Eukaryotic translation initiation factor 2 subunit 3

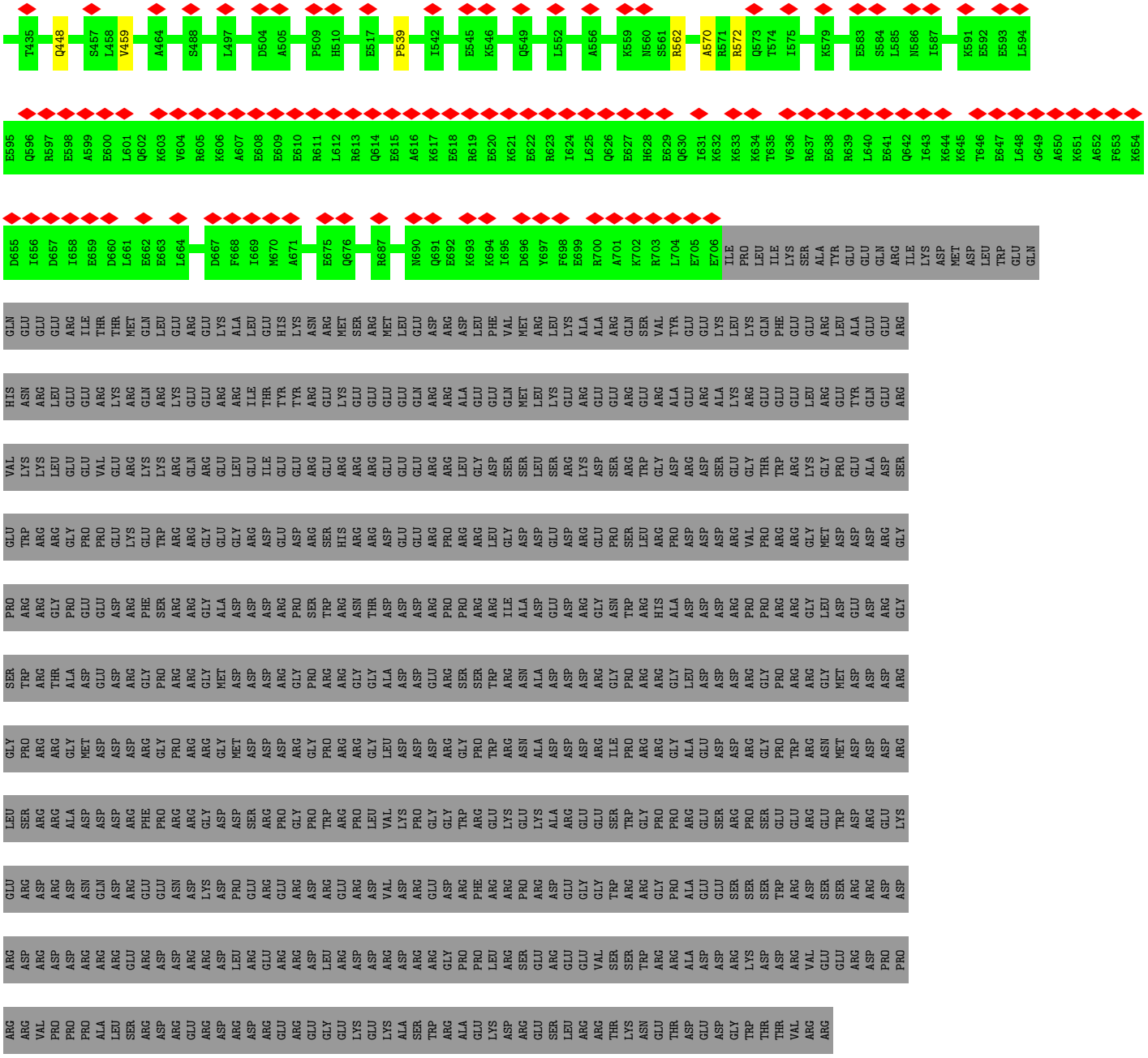
Chain t:



• Molecule 47: Eukaryotic translation initiation factor 3 subunit A

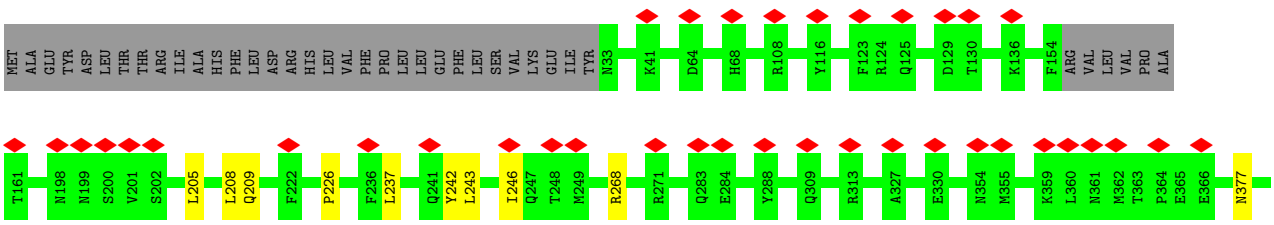
Chain u:

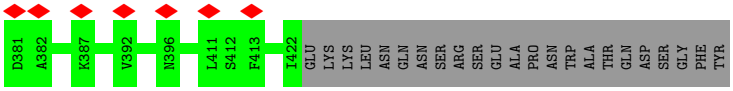




- Molecule 48: Eukaryotic translation initiation factor 3 subunit E

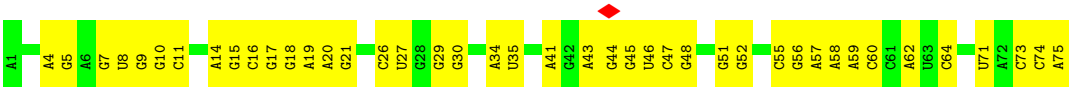
Chain v:





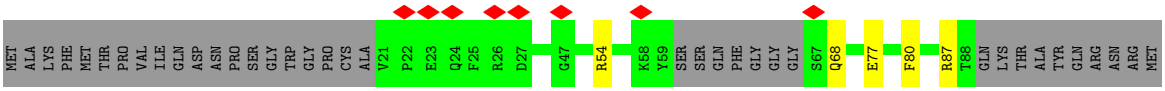
• Molecule 49: Initiator Met-tRNA-i

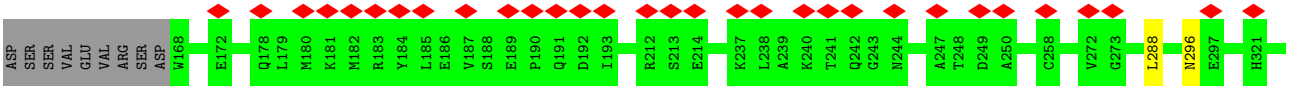
Chain w:

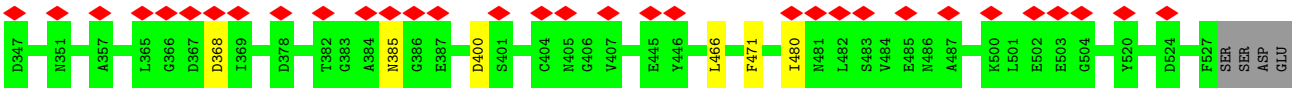


• Molecule 50: Eukaryotic translation initiation factor 3 subunit D

Chain x:

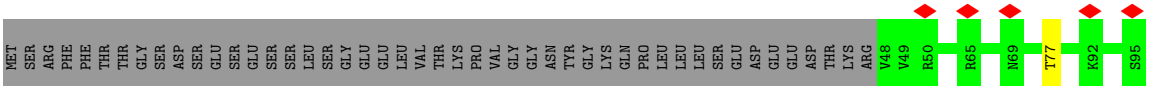


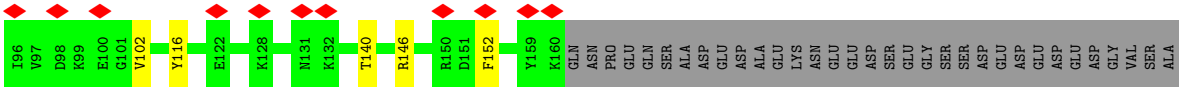


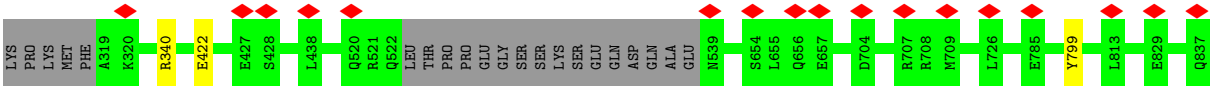


• Molecule 51: Eukaryotic translation initiation factor 3 subunit C

Chain y:







T841
P849
L863
GLY
SER
LEU
VAL
GLU
ASN
ASN
GLU
ARG
VAL
PHE
ASP
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ARG
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MET
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TYR
ARG
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GLN
GLN
SER
GLN
THR
ALA
TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	364950	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	24.271	Depositor
Minimum map value	-11.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.15	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: OMC, ZN, OMG, A2M, UR3, OMU, 5MU, MA6, PSU, 5MC

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	0.45	0/2581	0.71	0/3561
2	3	0.35	0/1055	0.54	0/1469
3	4	0.47	0/1269	0.68	0/1762
4	5	0.36	0/1575	0.52	0/2187
5	6	0.42	0/1926	0.64	1/2669 (0.0%)
6	7	0.87	2/492 (0.4%)	1.23	3/764 (0.4%)
7	8	0.44	0/1569	0.66	0/2183
8	9	0.96	0/231	0.74	0/294
9	A	0.41	0/40362	0.69	4/62905 (0.0%)
10	B	0.84	0/1186	0.86	2/1585 (0.1%)
11	C	0.83	0/2077	0.81	1/2796 (0.0%)
12	D	0.84	0/1502	0.79	0/2008
13	E	0.96	0/1105	0.95	2/1476 (0.1%)
14	F	0.83	0/380	0.88	0/496
15	G	0.74	0/1451	0.84	0/1942
16	H	0.82	0/644	0.82	0/864
17	I	0.84	0/1232	0.82	0/1656
18	J	1.03	0/1051	0.98	5/1406 (0.4%)
19	K	0.93	0/623	0.93	1/833 (0.1%)
20	L	1.01	0/1743	0.93	2/2354 (0.1%)
21	M	0.81	0/1029	0.85	0/1383
22	N	0.94	0/1670	0.94	3/2271 (0.1%)
23	O	0.40	0/1742	0.62	0/2330
24	P	0.98	0/1010	0.99	1/1353 (0.1%)
25	Q	0.87	0/805	0.91	1/1079 (0.1%)
26	R	0.70	0/1654	0.79	2/2203 (0.1%)
27	S	0.62	0/1885	0.77	0/2510
28	T	0.80	0/1032	0.75	0/1371
29	V	0.94	0/1481	0.86	2/1988 (0.1%)
30	Y	0.93	0/1142	0.89	2/1528 (0.1%)
31	Z	0.87	0/1793	0.92	3/2414 (0.1%)
32	a	0.82	0/859	0.79	1/1159 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.73	0/929	0.78	1/1241 (0.1%)
34	c	0.73	0/2493	0.85	3/3394 (0.1%)
35	d	0.87	0/1123	0.81	1/1504 (0.1%)
36	e	0.79	0/529	0.85	2/712 (0.3%)
37	f	0.79	0/1194	0.84	1/1599 (0.1%)
38	h	0.85	0/827	0.91	1/1110 (0.1%)
39	i	0.90	0/429	0.86	0/568
40	k	0.58	0/444	0.86	2/588 (0.3%)
41	m	0.42	0/960	0.67	0/1286
42	n	0.86	0/500	0.89	0/669
43	o	0.45	0/628	0.77	0/846
44	q	0.62	0/792	0.98	4/1062 (0.4%)
45	r	0.58	0/2247	0.81	2/3029 (0.1%)
46	t	0.39	0/1745	0.61	0/2417
47	u	0.42	0/5475	0.66	1/7432 (0.0%)
48	v	0.44	0/2672	0.70	2/3647 (0.1%)
49	w	0.33	0/1795	0.66	0/2798
50	x	0.42	0/2874	0.69	1/3925 (0.0%)
51	y	0.40	0/5284	0.67	3/7123 (0.0%)
All	All	0.59	2/113096 (0.0%)	0.75	60/161749 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	7	23	A	C1'-N9	-5.25	1.39	1.46
6	7	11	A	C5-C4	-5.14	1.35	1.38

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	y	146	ARG	NE-CZ-NH2	-13.68	113.46	120.30
22	N	7	VAL	N-CA-C	-12.54	77.15	111.00
51	y	146	ARG	NE-CZ-NH1	9.22	124.91	120.30
44	q	42	LEU	N-CA-C	-9.21	86.14	111.00
10	B	53	GLY	N-CA-C	9.19	136.07	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	443/813 (54%)	414 (94%)	26 (6%)	3 (1%)	22	59
2	3	209/218 (96%)	205 (98%)	3 (1%)	1 (0%)	29	66
3	4	251/357 (70%)	229 (91%)	19 (8%)	3 (1%)	13	48
4	5	307/564 (54%)	301 (98%)	6 (2%)	0	100	100
5	6	348/374 (93%)	318 (91%)	30 (9%)	0	100	100
7	8	313/352 (89%)	276 (88%)	35 (11%)	2 (1%)	25	62
8	9	22/25 (88%)	22 (100%)	0	0	100	100
10	B	138/158 (87%)	136 (99%)	2 (1%)	0	100	100
11	C	254/263 (97%)	249 (98%)	5 (2%)	0	100	100
12	D	175/194 (90%)	174 (99%)	1 (1%)	0	100	100
13	E	138/143 (96%)	134 (97%)	3 (2%)	1 (1%)	22	59
14	F	43/59 (73%)	43 (100%)	0	0	100	100
15	G	171/194 (88%)	163 (95%)	7 (4%)	1 (1%)	25	62
16	H	79/84 (94%)	76 (96%)	2 (2%)	1 (1%)	12	47
17	I	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
18	J	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	19	56
19	K	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
20	L	218/293 (74%)	215 (99%)	2 (1%)	1 (0%)	29	66
21	M	123/135 (91%)	121 (98%)	2 (2%)	0	100	100
22	N	205/295 (70%)	201 (98%)	3 (2%)	1 (0%)	29	66
23	O	209/264 (79%)	193 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	P	131/151 (87%)	123 (94%)	7 (5%)	1 (1%)	19	56
25	Q	97/115 (84%)	93 (96%)	4 (4%)	0	100	100
26	R	194/208 (93%)	194 (100%)	0	0	100	100
27	S	228/249 (92%)	223 (98%)	5 (2%)	0	100	100
28	T	123/133 (92%)	122 (99%)	1 (1%)	0	100	100
29	V	180/204 (88%)	175 (97%)	5 (3%)	0	100	100
30	Y	139/146 (95%)	136 (98%)	3 (2%)	0	100	100
31	Z	225/243 (93%)	223 (99%)	2 (1%)	0	100	100
32	a	97/165 (59%)	97 (100%)	0	0	100	100
33	b	108/145 (74%)	107 (99%)	1 (1%)	0	100	100
34	c	311/317 (98%)	301 (97%)	10 (3%)	0	100	100
35	d	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
36	e	64/125 (51%)	64 (100%)	0	0	100	100
37	f	140/152 (92%)	134 (96%)	6 (4%)	0	100	100
38	h	101/119 (85%)	97 (96%)	4 (4%)	0	100	100
39	i	48/56 (86%)	47 (98%)	0	1 (2%)	7	38
40	k	49/156 (31%)	44 (90%)	4 (8%)	1 (2%)	7	39
41	m	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
42	n	61/69 (88%)	59 (97%)	1 (2%)	1 (2%)	9	43
43	o	75/320 (23%)	73 (97%)	2 (3%)	0	100	100
44	q	99/144 (69%)	83 (84%)	12 (12%)	4 (4%)	3	26
45	r	273/315 (87%)	255 (93%)	17 (6%)	1 (0%)	34	69
46	t	346/472 (73%)	337 (97%)	5 (1%)	4 (1%)	13	48
47	u	705/1382 (51%)	672 (95%)	32 (4%)	1 (0%)	51	83
48	v	380/445 (85%)	350 (92%)	30 (8%)	0	100	100
50	x	415/548 (76%)	386 (93%)	29 (7%)	0	100	100
51	y	636/913 (70%)	610 (96%)	25 (4%)	1 (0%)	47	78
All	All	9485/12718 (75%)	9077 (96%)	378 (4%)	30 (0%)	44	74

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	282	PRO

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Mol	Chain	Res	Type
1	1	427	PRO
3	4	264	GLY
16	H	56	CYS
24	P	136	PRO

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%)	97 (100%)	0	100	100
5	6	49/335 (15%)	49 (100%)	0	100	100
8	9	23/24 (96%)	22 (96%)	1 (4%)	29	58
10	B	129/142 (91%)	117 (91%)	12 (9%)	9	35
11	C	220/225 (98%)	201 (91%)	19 (9%)	10	39
12	D	158/168 (94%)	150 (95%)	8 (5%)	24	55
13	E	112/115 (97%)	101 (90%)	11 (10%)	8	33
14	F	38/48 (79%)	35 (92%)	3 (8%)	12	42
15	G	159/174 (91%)	141 (89%)	18 (11%)	6	28
16	H	73/76 (96%)	63 (86%)	10 (14%)	3	21
17	I	130/131 (99%)	126 (97%)	4 (3%)	40	65
18	J	112/113 (99%)	108 (96%)	4 (4%)	35	63
19	K	65/67 (97%)	57 (88%)	8 (12%)	4	24
20	L	186/225 (83%)	156 (84%)	30 (16%)	2	15
21	M	114/122 (93%)	100 (88%)	14 (12%)	4	24
22	N	173/243 (71%)	158 (91%)	15 (9%)	10	38
23	O	192/231 (83%)	191 (100%)	1 (0%)	88	94
24	P	104/119 (87%)	85 (82%)	19 (18%)	1	10
25	Q	86/98 (88%)	75 (87%)	11 (13%)	4	23
26	R	172/180 (96%)	158 (92%)	14 (8%)	11	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	S	200/218 (92%)	171 (86%)	29 (14%)	3	18
28	T	107/115 (93%)	95 (89%)	12 (11%)	6	28
29	V	156/170 (92%)	143 (92%)	13 (8%)	11	40
30	Y	117/121 (97%)	110 (94%)	7 (6%)	19	50
31	Z	190/202 (94%)	158 (83%)	32 (17%)	2	14
32	a	90/136 (66%)	84 (93%)	6 (7%)	16	47
33	b	100/130 (77%)	88 (88%)	12 (12%)	5	25
34	c	272/275 (99%)	233 (86%)	39 (14%)	3	19
35	d	112/115 (97%)	101 (90%)	11 (10%)	8	33
36	e	58/103 (56%)	52 (90%)	6 (10%)	7	31
37	f	123/132 (93%)	111 (90%)	12 (10%)	8	33
38	h	94/107 (88%)	81 (86%)	13 (14%)	3	21
39	i	44/49 (90%)	39 (89%)	5 (11%)	5	27
40	k	47/140 (34%)	36 (77%)	11 (23%)	1	5
41	m	104/108 (96%)	94 (90%)	10 (10%)	8	34
42	n	56/62 (90%)	47 (84%)	9 (16%)	2	15
43	o	64/277 (23%)	61 (95%)	3 (5%)	26	56
44	q	77/123 (63%)	60 (78%)	17 (22%)	1	6
45	r	247/280 (88%)	206 (83%)	41 (17%)	2	14
47	u	528/1259 (42%)	520 (98%)	8 (2%)	65	81
48	v	206/406 (51%)	198 (96%)	8 (4%)	32	60
50	x	206/494 (42%)	194 (94%)	12 (6%)	20	52
51	y	563/811 (69%)	555 (99%)	8 (1%)	67	82
All	All	6153/9370 (66%)	5627 (92%)	526 (8%)	14	40

5 of 526 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	r	88	ARG
45	r	197	VAL
45	r	83	ILE
51	y	116	TYR
26	R	133	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
50	x	68	GLN
50	x	296	ASN
28	T	124	ASN
28	T	112	ASN
50	x	416	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	w	74/75 (98%)	42 (56%)	0
6	7	21/255 (8%)	11 (52%)	3 (14%)
9	A	1708/1869 (91%)	506 (29%)	69 (4%)
All	All	1803/2199 (81%)	559 (31%)	72 (3%)

5 of 559 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	7	4	G
6	7	5	A
6	7	8	A
6	7	11	A
6	7	15	U

5 of 72 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	1600	G
9	A	1831	A
9	A	1637	A
9	A	1757	G
9	A	839	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	612	9	18,21,22	1.50	5 (27%)	22,30,33	2.04	4 (18%)
9	PSU	A	119	9	18,21,22	1.46	4 (22%)	22,30,33	2.17	5 (22%)
9	A2M	A	668	9	18,25,26	0.98	0	18,36,39	1.54	2 (11%)
9	5MU	A	814	9	19,22,23	1.56	4 (21%)	28,32,35	2.34	9 (32%)
9	PSU	A	822	9	18,21,22	1.53	4 (22%)	22,30,33	2.22	5 (22%)
9	OMG	A	683	9	18,26,27	1.06	1 (5%)	19,38,41	1.24	2 (10%)
9	MA6	A	1851	9	18,26,27	1.23	2 (11%)	19,38,41	1.88	6 (31%)
9	OMC	A	174	9	19,22,23	0.93	0	26,31,34	1.12	2 (7%)
9	A2M	A	27	9	18,25,26	0.99	1 (5%)	18,36,39	1.30	2 (11%)
9	A2M	A	159	9	18,25,26	0.95	1 (5%)	18,36,39	1.23	2 (11%)
9	A2M	A	1031	9	18,25,26	0.98	1 (5%)	18,36,39	1.31	2 (11%)
9	PSU	A	823	9	18,21,22	1.59	5 (27%)	22,30,33	2.03	4 (18%)
9	OMU	A	116	9	19,22,23	1.33	3 (15%)	26,31,34	1.83	5 (19%)
9	OMG	A	644	9	18,26,27	1.10	1 (5%)	19,38,41	1.26	4 (21%)
9	5MC	A	1374	9	18,22,23	1.08	2 (11%)	26,32,35	1.51	5 (19%)
9	OMC	A	1703	9	19,22,23	1.05	1 (5%)	26,31,34	1.15	1 (3%)
9	A2M	A	166	9	18,25,26	1.05	1 (5%)	18,36,39	1.26	2 (11%)
9	PSU	A	1243	9	18,21,22	1.54	5 (27%)	22,30,33	2.05	4 (18%)
9	OMU	A	121	9	19,22,23	1.43	4 (21%)	26,31,34	1.85	6 (23%)
9	OMG	A	509	9	18,26,27	1.15	1 (5%)	19,38,41	1.19	2 (10%)
9	MA6	A	1850	9	18,26,27	1.26	1 (5%)	19,38,41	1.97	5 (26%)
9	A2M	A	1678	9	18,25,26	1.04	0	18,36,39	1.48	3 (16%)
9	UR3	A	1830	9	19,22,23	1.04	1 (5%)	26,32,35	2.02	7 (26%)
9	A2M	A	484	9	18,25,26	1.00	1 (5%)	18,36,39	1.20	2 (11%)
9	PSU	A	1081	9	18,21,22	1.72	5 (27%)	22,30,33	2.35	6 (27%)
9	OMC	A	517	9	19,22,23	0.98	1 (5%)	26,31,34	1.17	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PSU	A	612	9	-	1/7/25/26	0/2/2/2
9	PSU	A	119	9	-	1/7/25/26	0/2/2/2
9	A2M	A	668	9	-	2/5/27/28	0/3/3/3
9	5MU	A	814	9	-	0/7/25/26	0/2/2/2
9	PSU	A	822	9	-	0/7/25/26	0/2/2/2
9	OMG	A	683	9	-	1/5/27/28	0/3/3/3
9	MA6	A	1851	9	-	4/7/29/30	0/3/3/3
9	OMC	A	174	9	-	0/9/27/28	0/2/2/2
9	A2M	A	27	9	-	1/5/27/28	0/3/3/3
9	A2M	A	159	9	-	1/5/27/28	0/3/3/3
9	A2M	A	1031	9	-	1/5/27/28	0/3/3/3
9	PSU	A	823	9	-	1/7/25/26	0/2/2/2
9	OMU	A	116	9	-	1/9/27/28	0/2/2/2
9	OMG	A	644	9	-	2/5/27/28	0/3/3/3
9	5MC	A	1374	9	-	0/7/25/26	0/2/2/2
9	OMC	A	1703	9	-	2/9/27/28	0/2/2/2
9	A2M	A	166	9	-	0/5/27/28	0/3/3/3
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	OMG	A	509	9	-	2/5/27/28	0/3/3/3
9	MA6	A	1850	9	-	1/7/29/30	0/3/3/3
9	A2M	A	1678	9	-	0/5/27/28	0/3/3/3
9	UR3	A	1830	9	-	2/7/25/26	0/2/2/2
9	A2M	A	484	9	-	1/5/27/28	0/3/3/3
9	PSU	A	1081	9	-	2/7/25/26	0/2/2/2
9	OMC	A	517	9	-	1/9/27/28	0/2/2/2

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1081	PSU	C4-N3	-3.67	1.32	1.38
9	A	823	PSU	C4-N3	-3.44	1.32	1.38
9	A	814	5MU	C4-N3	-3.44	1.32	1.38
9	A	509	OMG	C6-N1	-3.35	1.32	1.37
9	A	121	OMU	C4-N3	-3.27	1.32	1.38

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	822	PSU	N1-C2-N3	6.57	122.58	115.13
9	A	1081	PSU	N1-C2-N3	6.48	122.47	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	119	PSU	N1-C2-N3	6.13	122.07	115.13
9	A	823	PSU	N1-C2-N3	6.09	122.03	115.13
9	A	1243	PSU	N1-C2-N3	6.03	121.96	115.13

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	27	A2M	C1'-C2'-O2'-CM'
9	A	116	OMU	C1'-C2'-O2'-CM2
9	A	159	A2M	C1'-C2'-O2'-CM'
9	A	484	A2M	C1'-C2'-O2'-CM'
9	A	517	OMC	C1'-C2'-O2'-CM2

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 2 ligands modelled in this entry, 2 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.

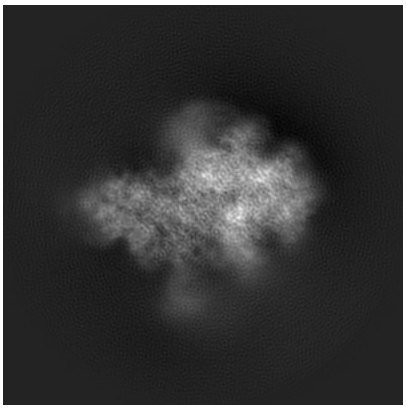
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14114. These allow visual inspection of the internal detail of the map and identification of artifacts.

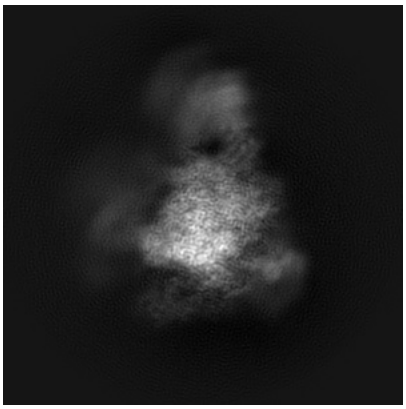
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

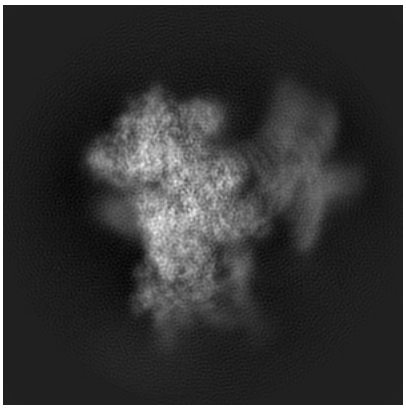
6.1.1 Primary map



X

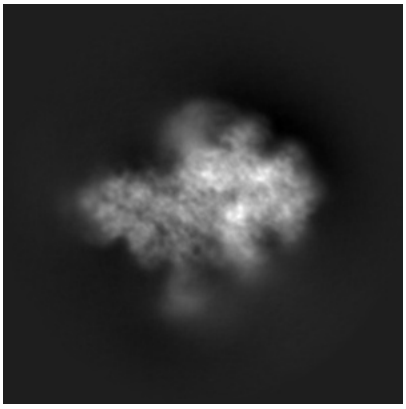


Y

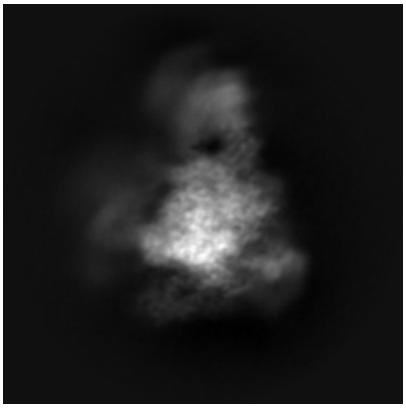


Z

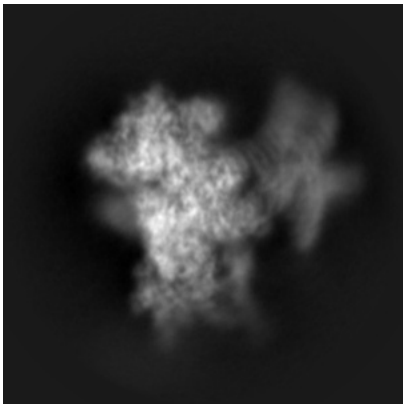
6.1.2 Raw map



X



Y

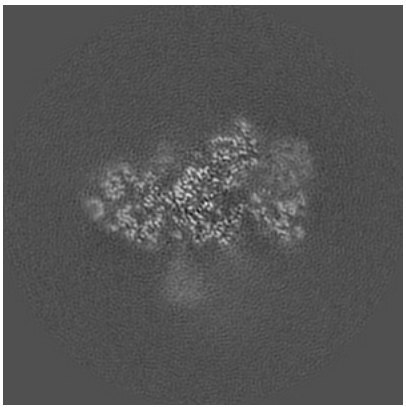


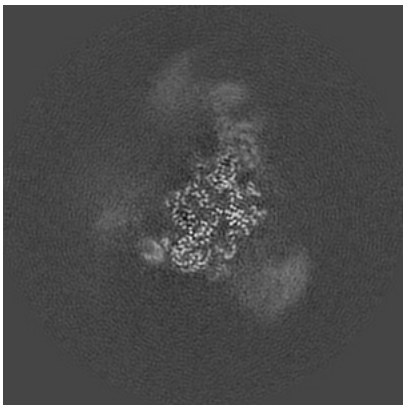
Z

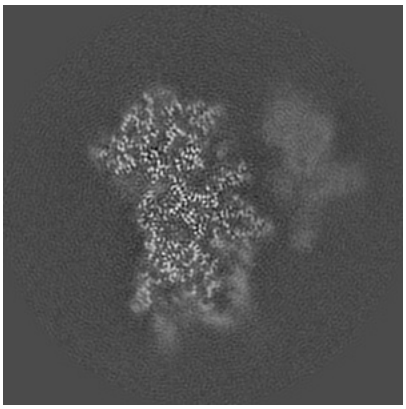
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

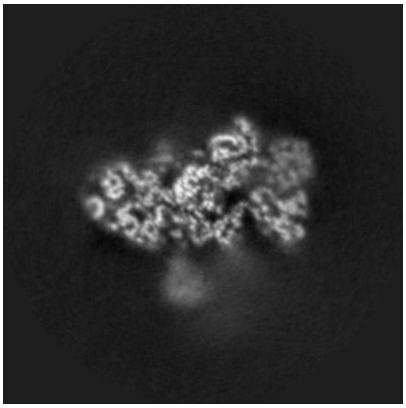
6.2.1 Primary map

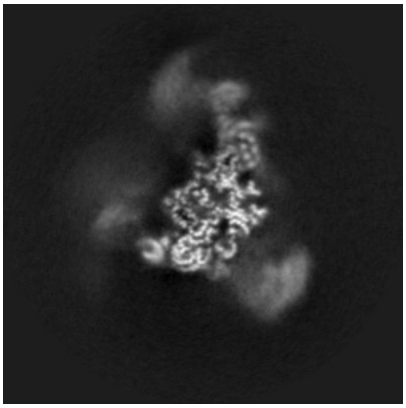

X Index: 180

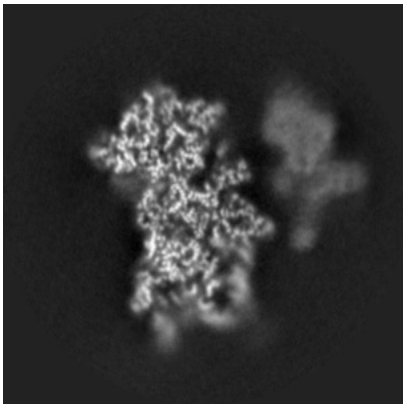

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

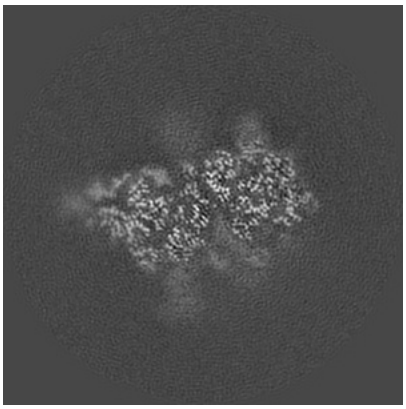

Y Index: 180


Z Index: 180

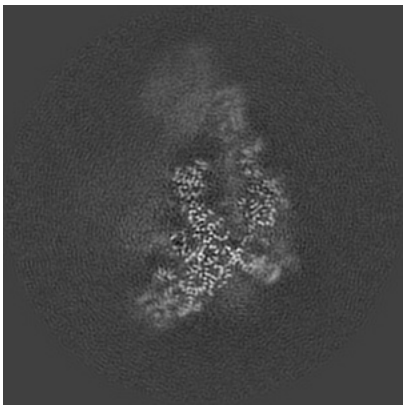
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

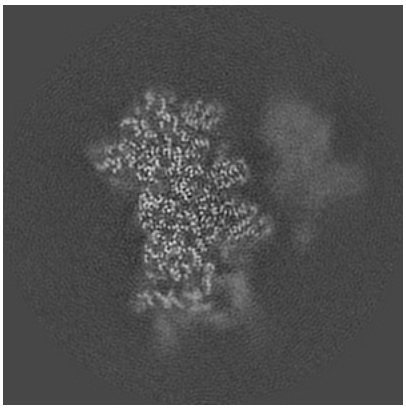
6.3.1 Primary map



X Index: 149

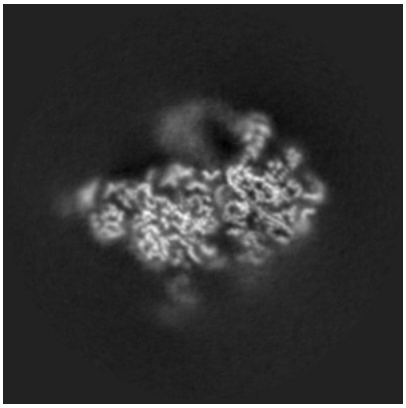


Y Index: 213

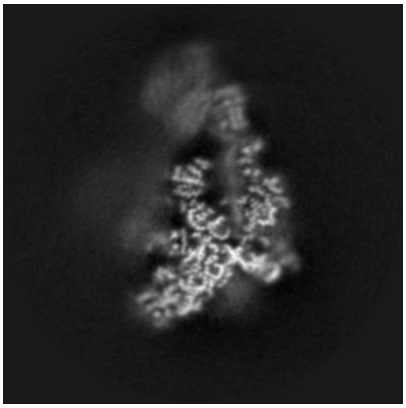


Z Index: 176

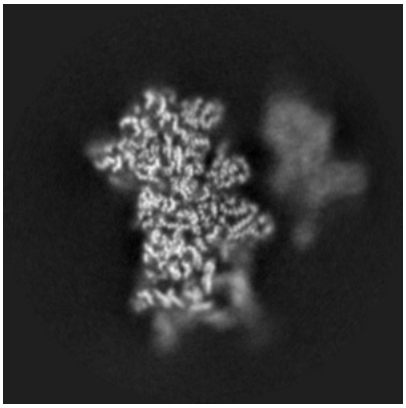
6.3.2 Raw map



X Index: 139



Y Index: 213

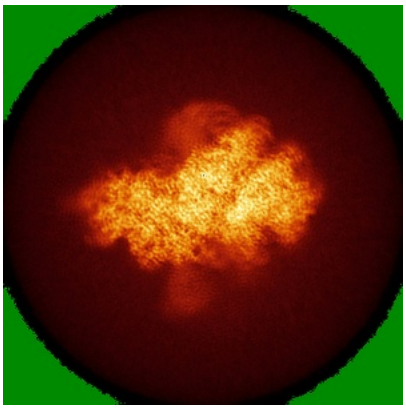


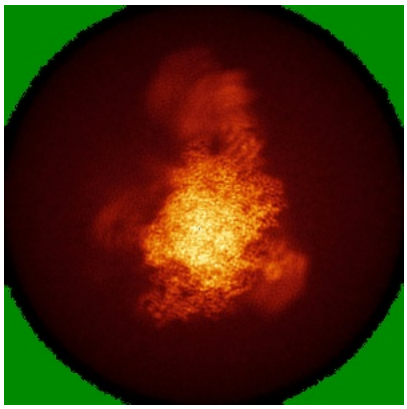
Z Index: 176

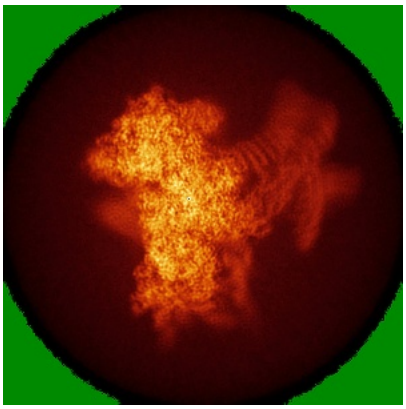
The images above show the largest variance slices of the map in three orthogonal directions.

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

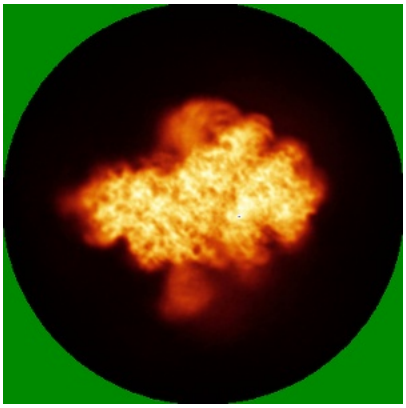
6.4.1 Primary map

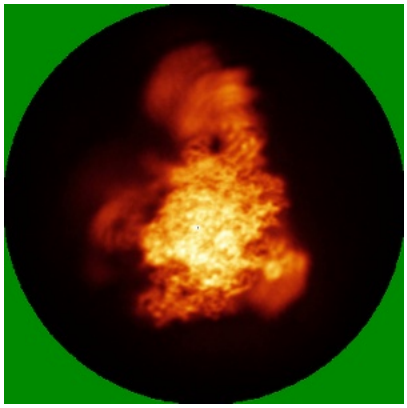

X


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 2.15. 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.

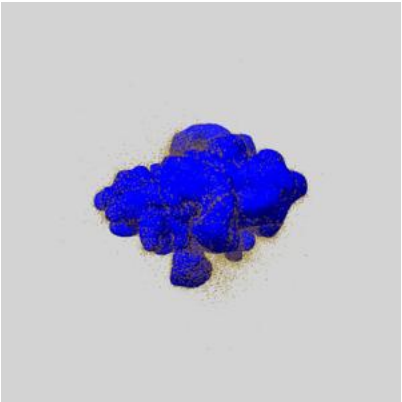
6.6 Mask visualisation (i)

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

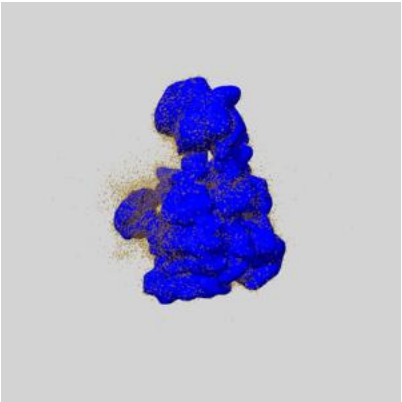
A mask typically either:

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

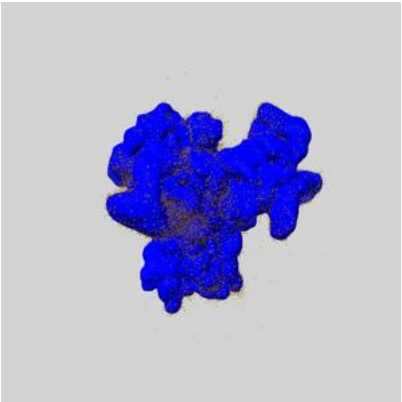
6.6.1 emd_14114_msk_1.map (i)



X



Y

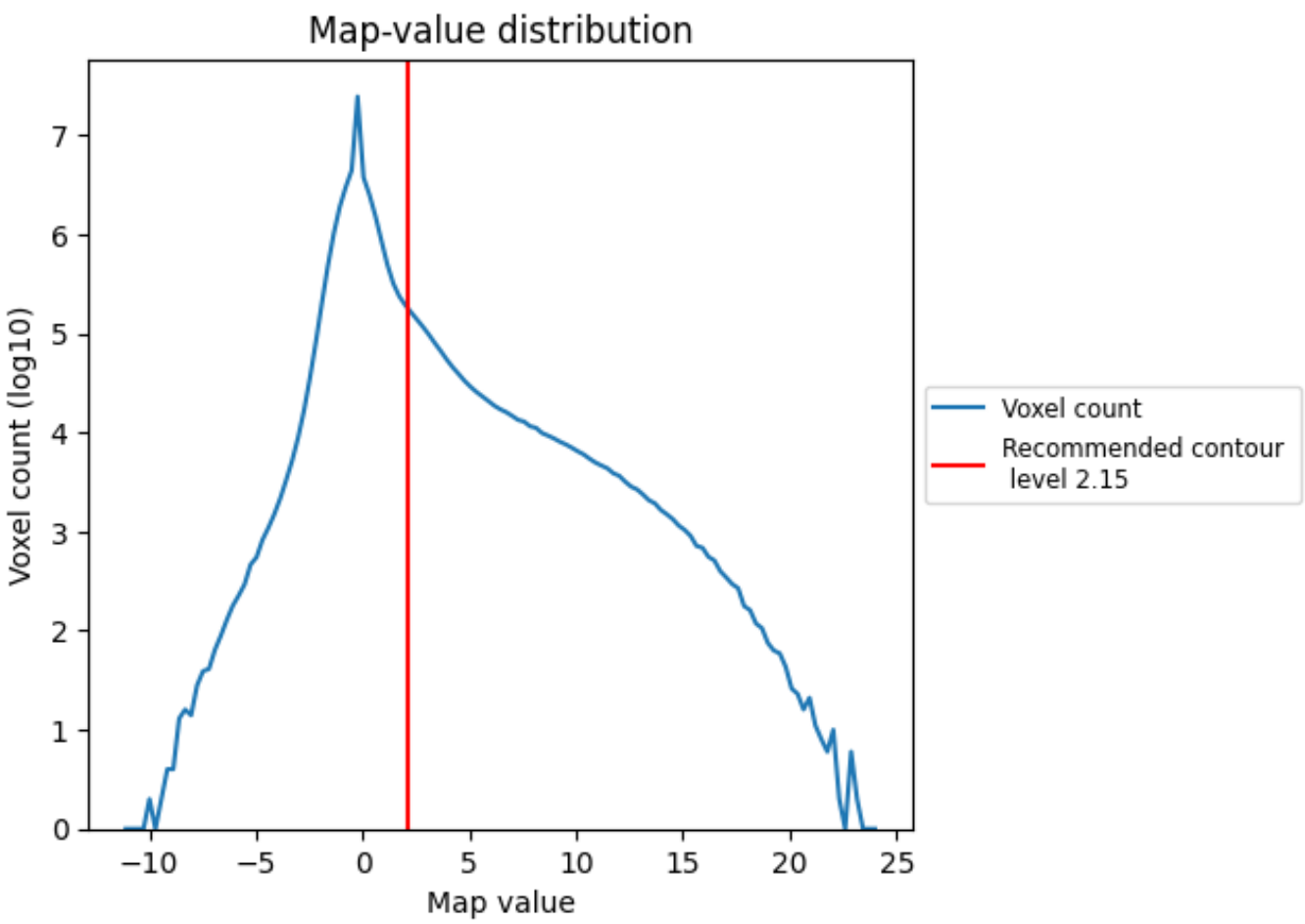


Z

7 Map analysis (i)

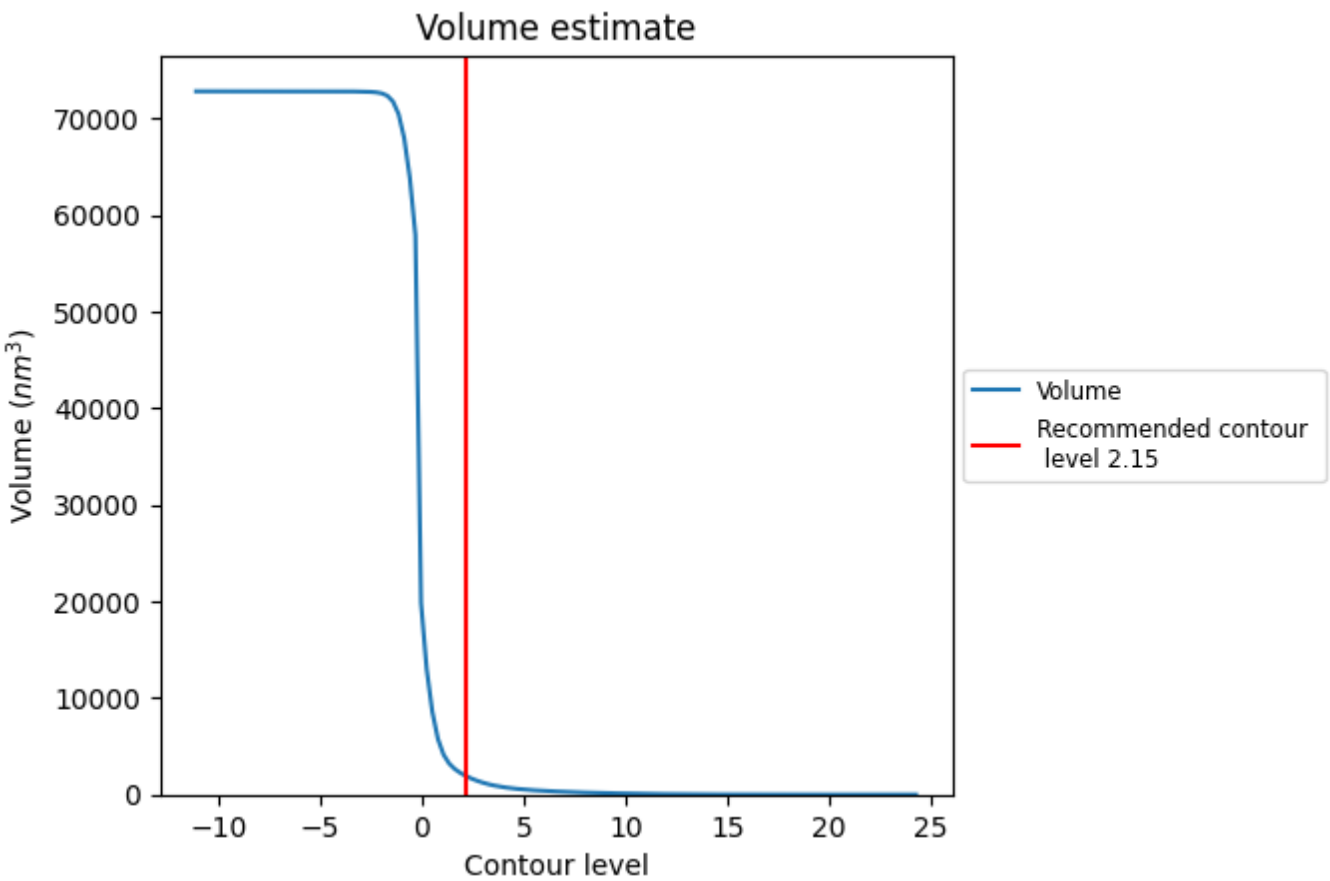
This section contains the results of statistical analysis of the map.

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.

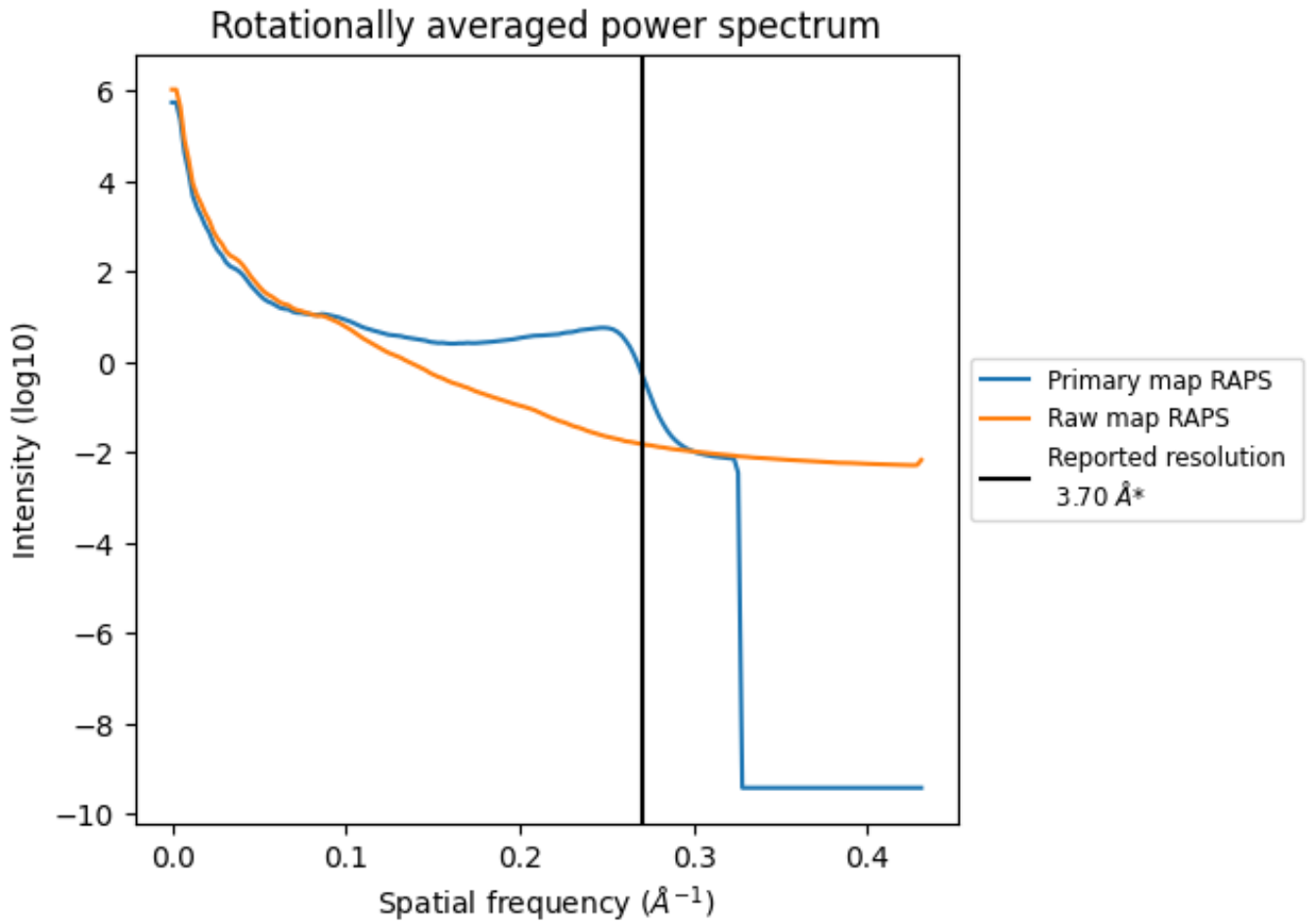
7.2 Volume estimate (i)



The volume at the recommended contour level is 1935 nm^3; this corresponds to an approximate mass of 1748 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)

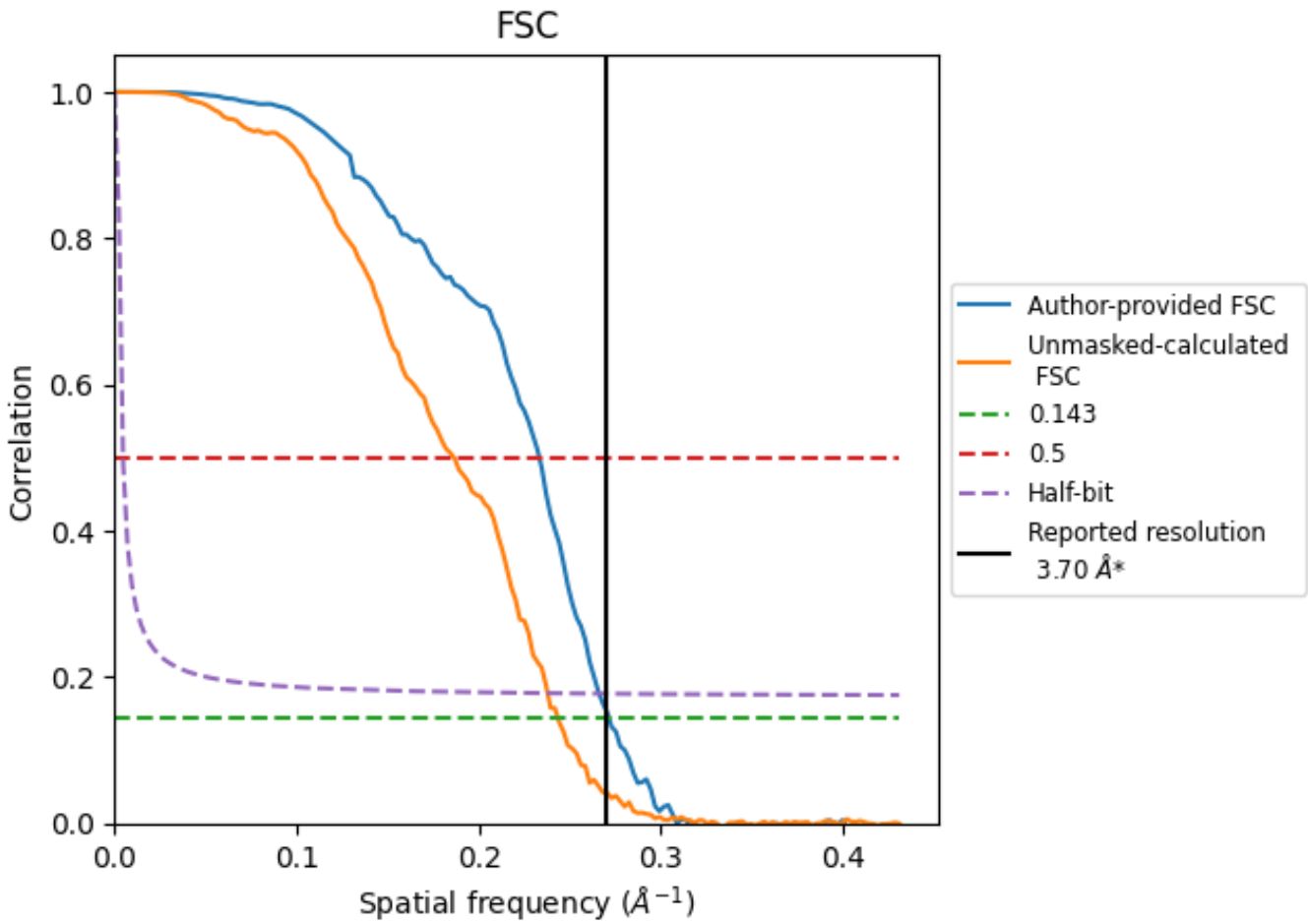


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

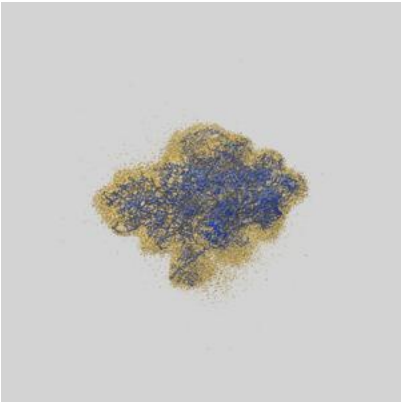
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.29	3.76
Unmasked-calculated*	4.11	5.36	4.20

*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 4.11 differs from the reported value 3.7 by more than 10 %

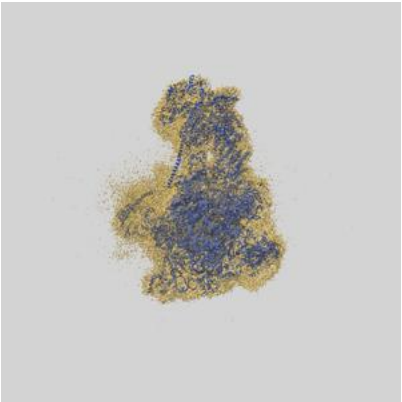
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14114 and PDB model 7QP7. Per-residue inclusion information can be found in section 3 on page 13.

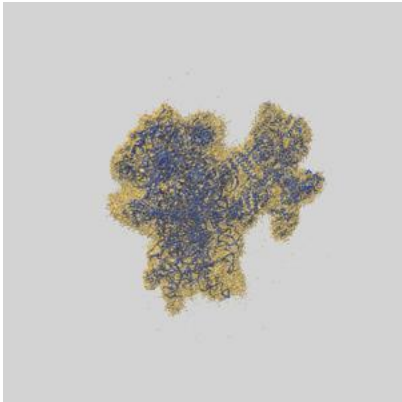
9.1 Map-model overlay (i)



X



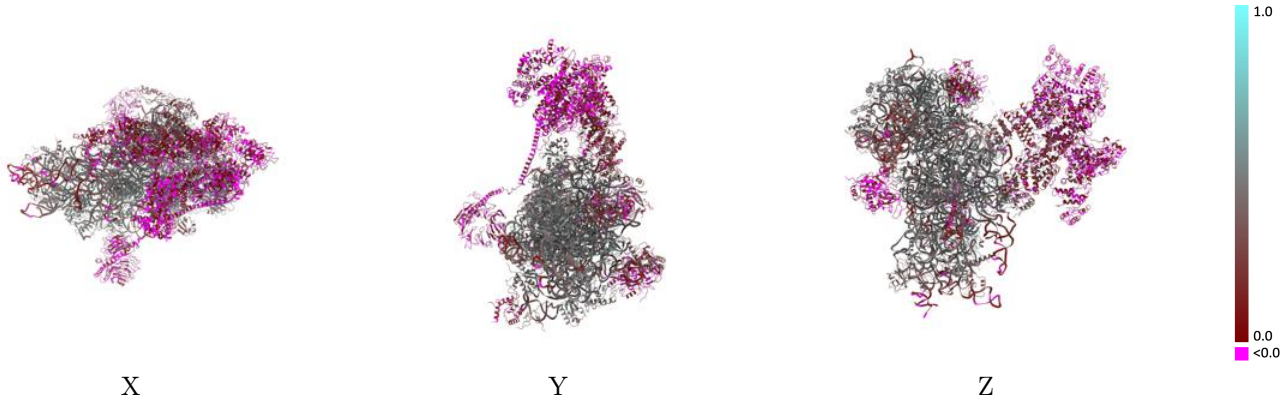
Y



Z

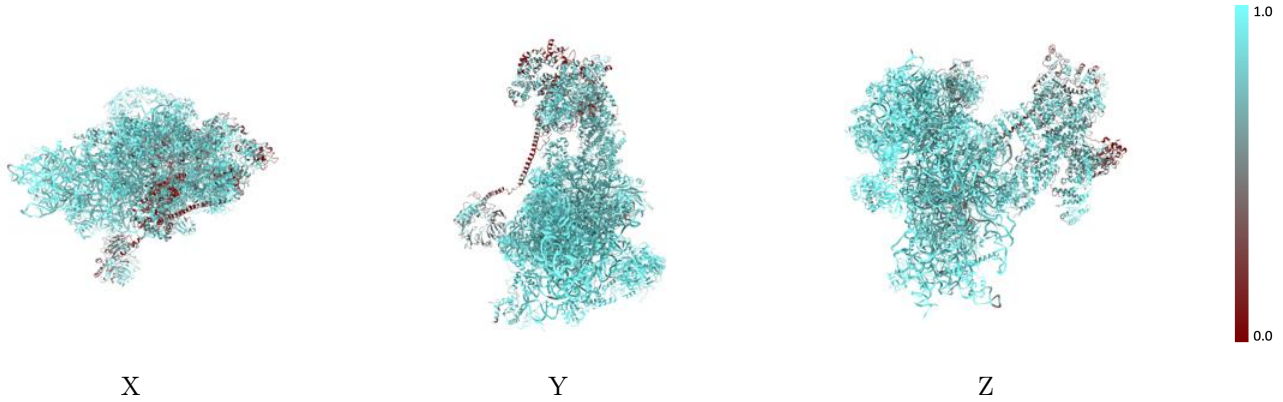
The images above show the 3D surface view of the map at the recommended contour level 2.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



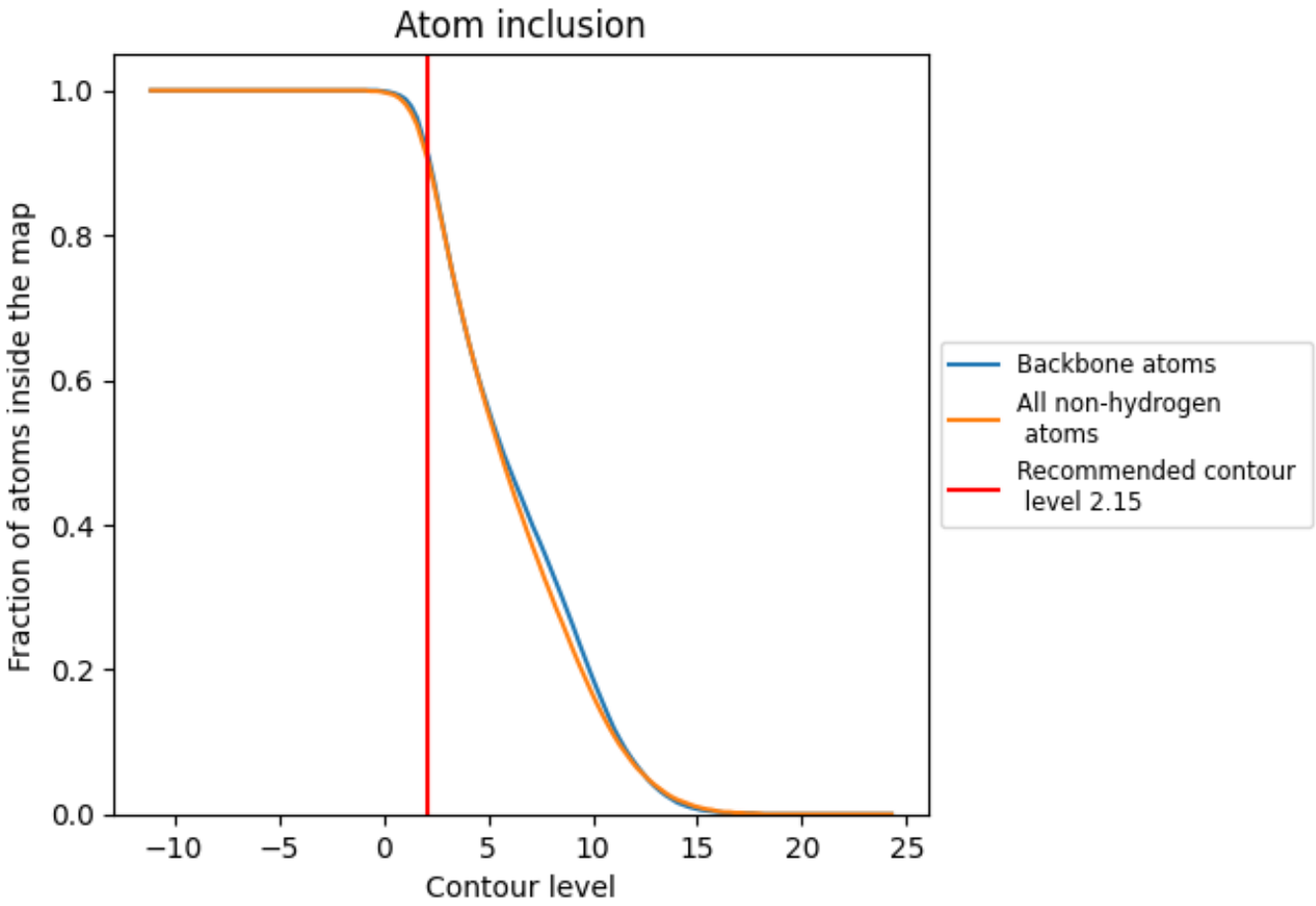
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.15).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9010	0.3370
1	0.5900	0.0480
3	0.4050	0.0230
4	0.7400	0.0390
5	0.6400	0.0290
6	0.6270	0.0200
7	0.8870	0.2360
8	0.6980	0.0350
9	0.9710	0.4920
A	0.9850	0.4050
B	0.9680	0.4940
C	0.9720	0.4950
D	0.9680	0.4890
E	0.9700	0.5100
F	0.9730	0.4820
G	0.9300	0.4390
H	0.9440	0.4800
I	0.9800	0.4910
J	0.9610	0.5170
K	0.9720	0.5040
L	0.9490	0.5010
M	0.9250	0.4600
N	0.9540	0.4940
O	0.9210	0.3930
P	0.9660	0.4860
Q	0.9590	0.5090
R	0.9640	0.4350
S	0.9660	0.4150
T	0.9850	0.4700
V	0.9650	0.4930
Y	0.9650	0.4950
Z	0.9400	0.4750
a	0.9580	0.4660
b	0.9610	0.4650
c	0.9590	0.4390

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Chain	Atom inclusion	Q-score
d	0.9780	0.4840
e	0.9590	0.4570
f	0.9580	0.4520
h	0.9670	0.4650
i	0.9530	0.4940
k	0.9430	0.3350
m	0.8100	0.1540
n	0.9370	0.4830
o	0.8600	0.2190
q	0.8380	0.3450
r	0.9560	0.3330
t	0.9320	0.0370
u	0.7040	0.1200
v	0.7640	0.0480
w	0.9740	0.2120
x	0.7010	0.1440
y	0.7970	0.1610