



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 11:39 AM UTC

PDB ID : 7QP6 / pdb_00007qp6
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

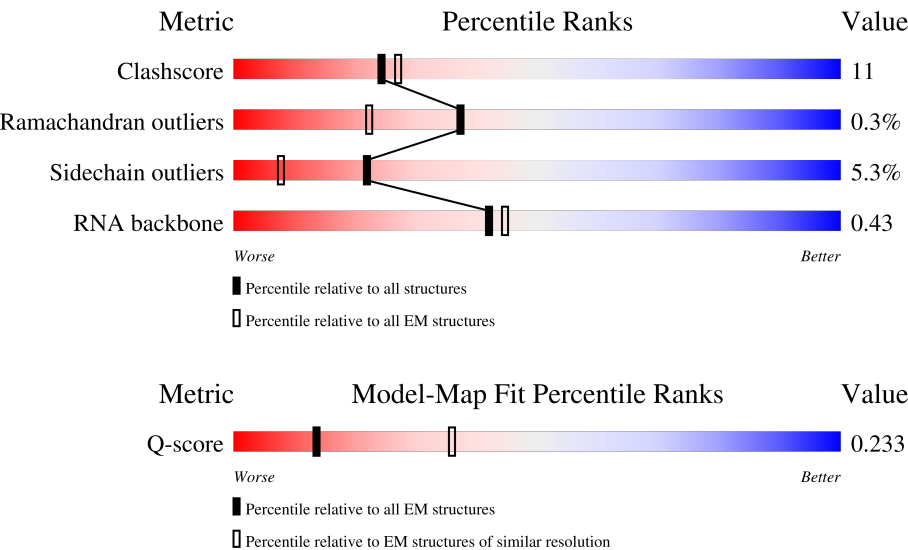
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1989 (4.20 - 5.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	813	
2	3	218	
3	4	357	

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Mol	Chain	Length	Quality of chain
4	5	564	
5	6	374	
6	7	20	
7	8	352	
8	9	25	
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	

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Mol	Chain	Length	Quality of chain
29	V	204	
30	Y	146	
31	Z	243	
32	a	165	
33	b	145	
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

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
1	1	424	Total	C	N	O	S	0	0
			2445	1501	469	470	5		

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

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

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

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

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

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

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

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

- Molecule 6 is a RNA chain called mRNA.

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

- 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 (CCD ID: ZN) (formula: Zn).

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

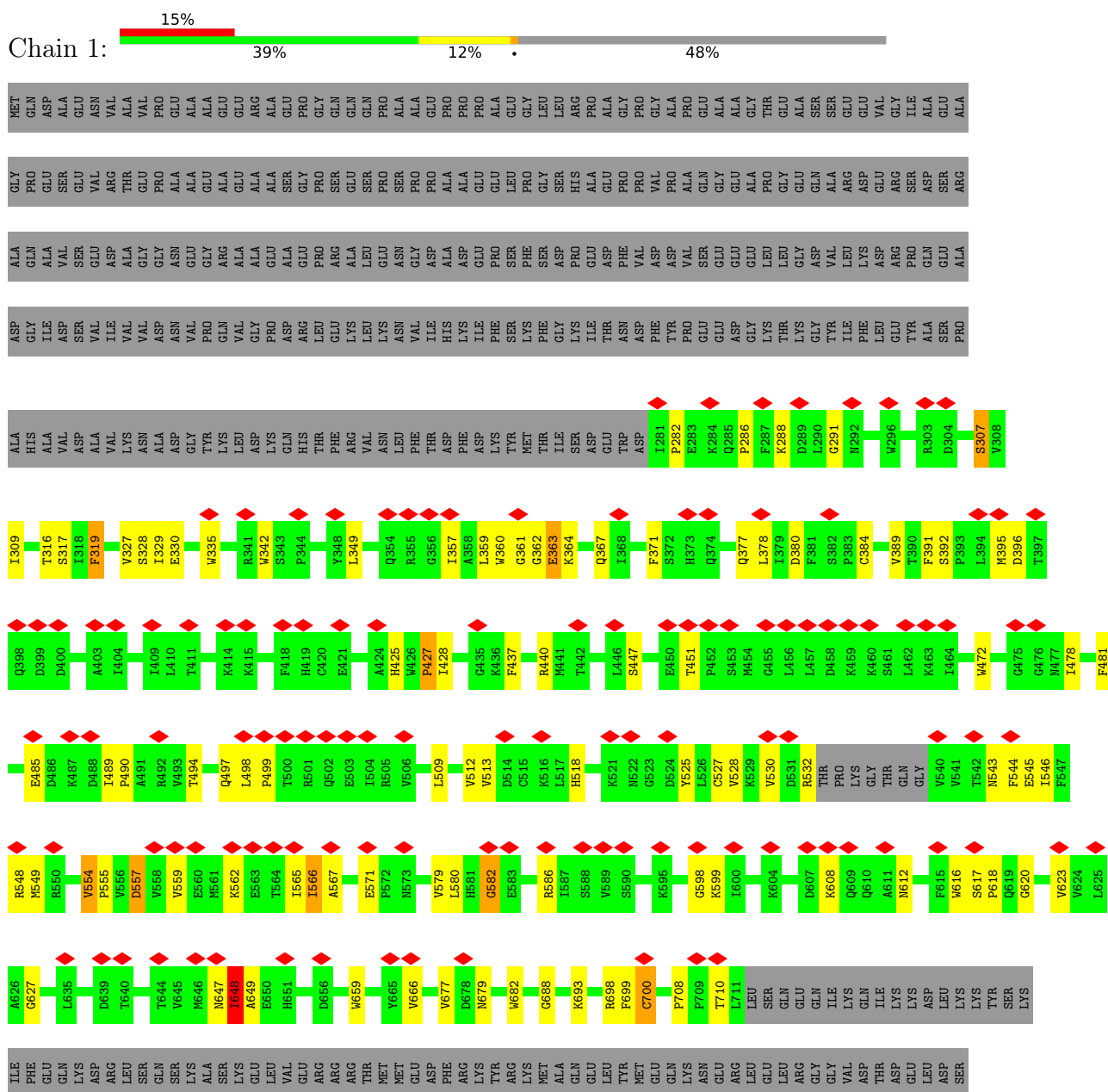
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

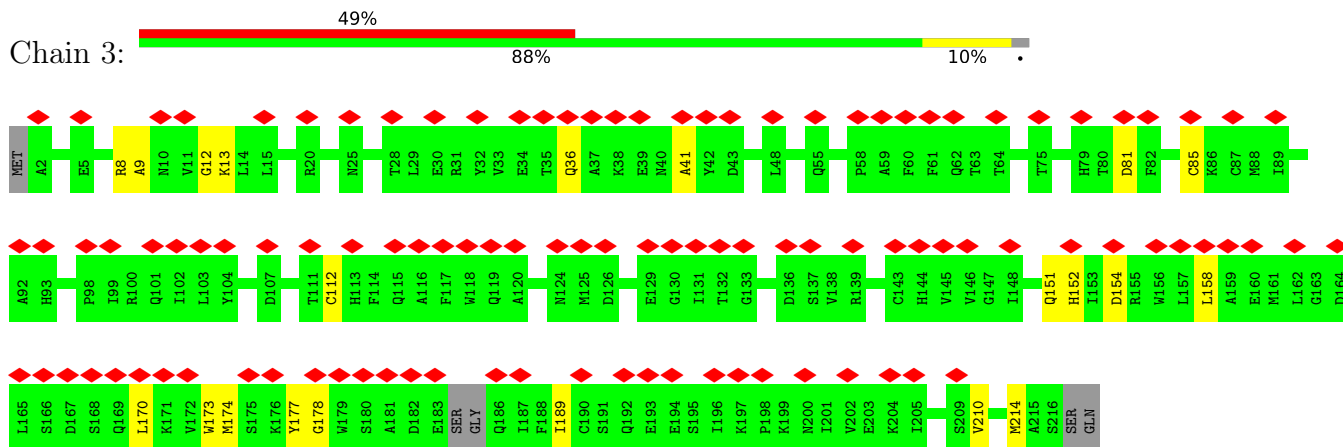
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

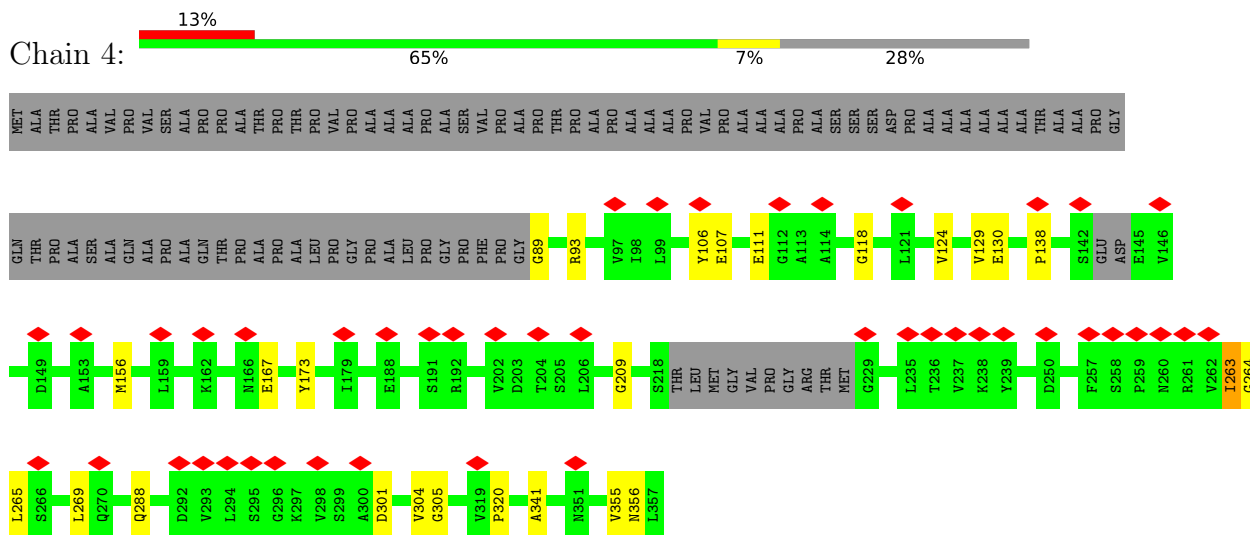


ASN VAL
VAL ASP
ASP TRP
TRP GLU
GLU GLU
GLU THR
THR ILE
ILE GLU
GLU PHE
PHE VAL
VAL THR
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GLU ILE
ILE PRO
PRO LEU
LEU GLY
GLY ASN
ASN GLN

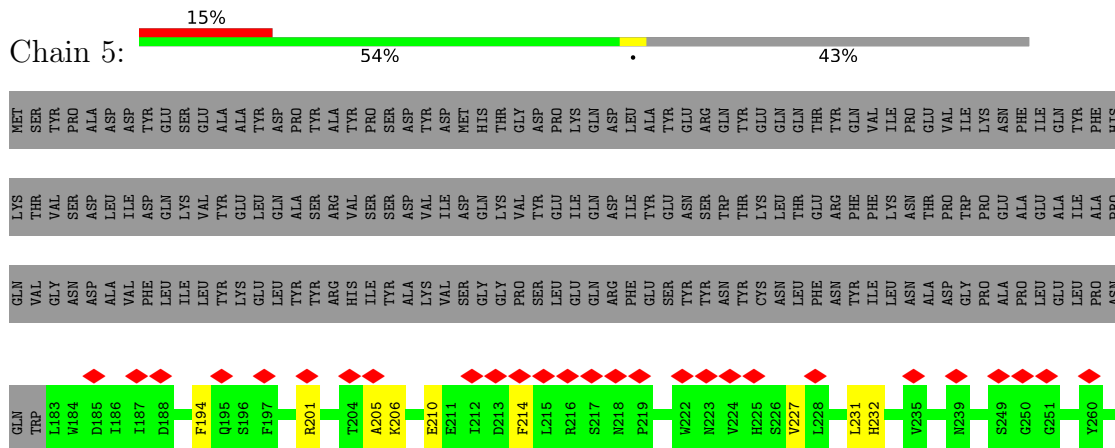
• Molecule 2: Eukaryotic translation initiation factor 3 subunit K

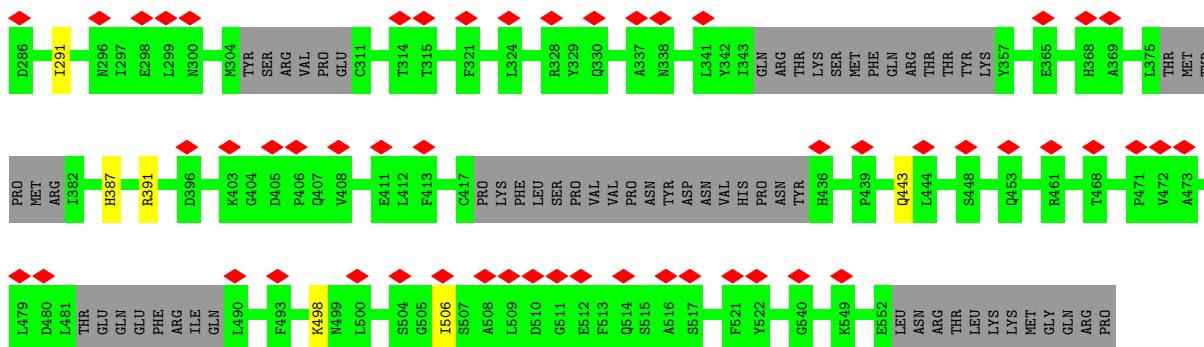


• Molecule 3: Eukaryotic translation initiation factor 3 subunit F

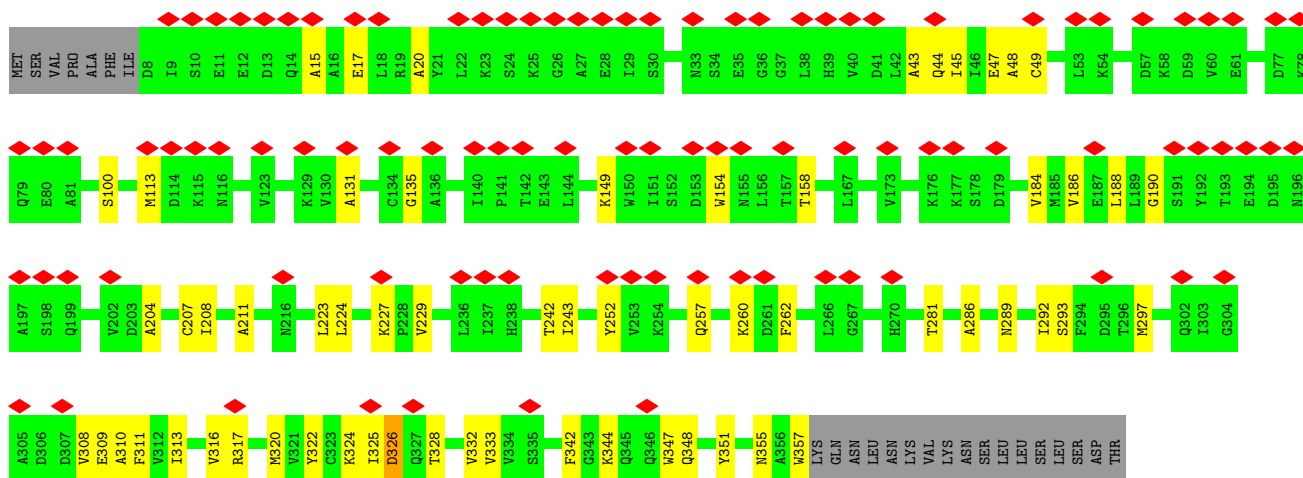
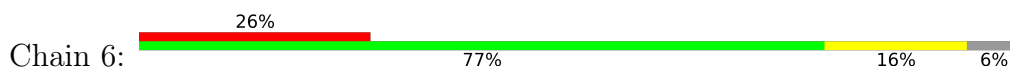


• Molecule 4: Eukaryotic translation initiation factor 3 subunit L





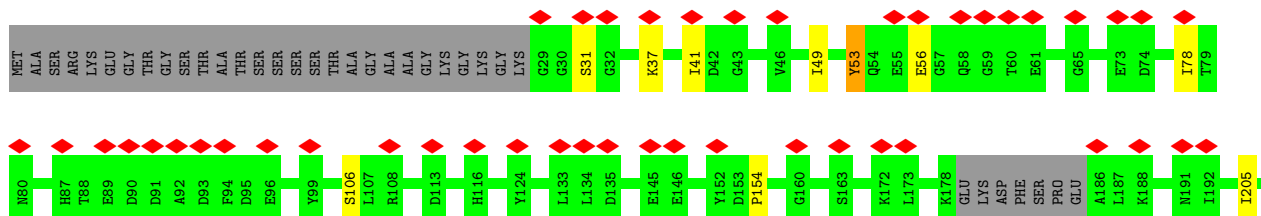
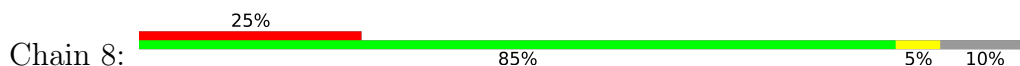
• Molecule 5: Eukaryotic translation initiation factor 3 subunit M

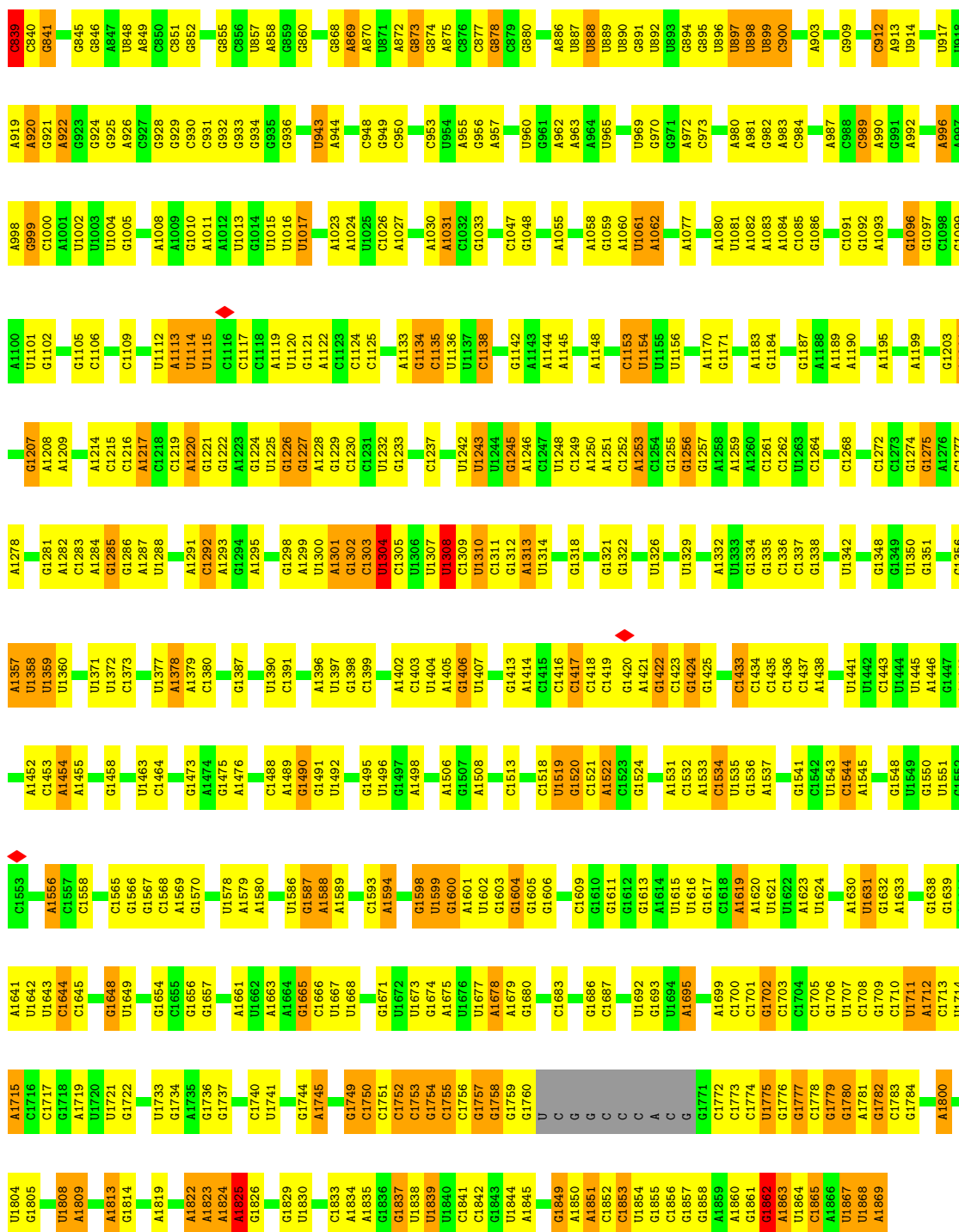


• Molecule 6: mRNA

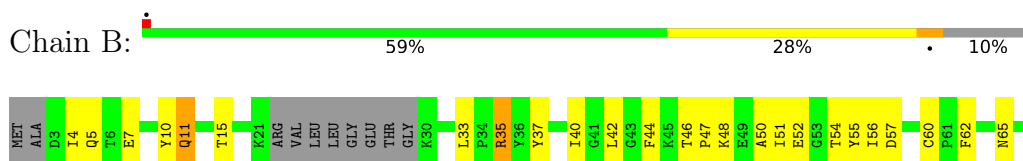


• Molecule 7: Eukaryotic translation initiation factor 3 subunit H





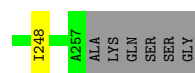
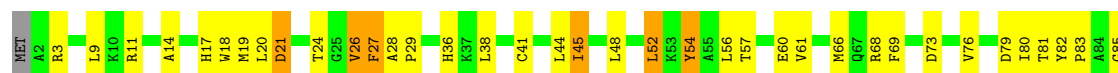
- Molecule 10: 40S ribosomal protein S11





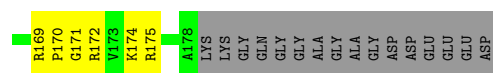
- Molecule 11: 40S ribosomal protein S4, X isoform

Chain C: 53% 39% 5%



- Molecule 12: 40S ribosomal protein S9

Chain D: 71% 20% 9%



- Molecule 13: 40S ribosomal protein S23

Chain E: 79% 19%



- Molecule 14: 40S ribosomal protein S30

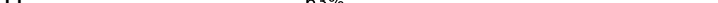
Chain F: 37% 29% 32%

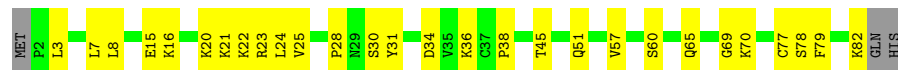


- Molecule 15: 40S ribosomal protein S7

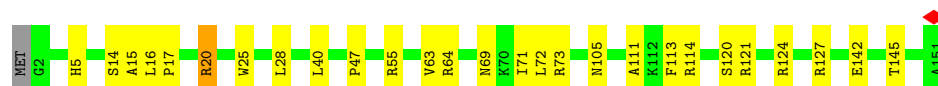
Chain G: 66% 24% 9%



- Chain H:  63% 33% .

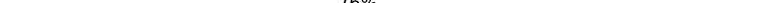


- Chain I: 81% 17% ..

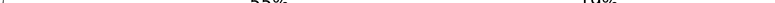


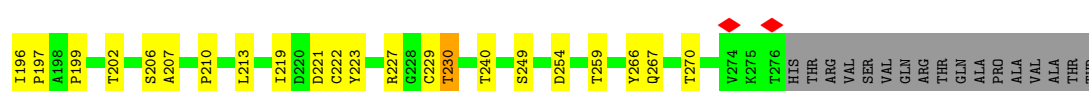
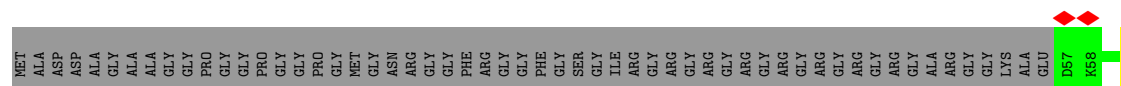
- Chain J: 81% 16% ..

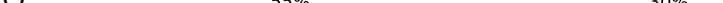


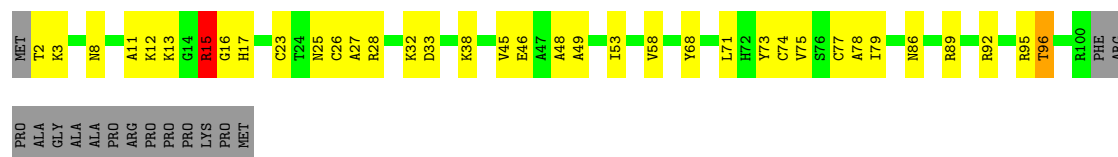
- Chain K:  76% 22%



- Chain L: 

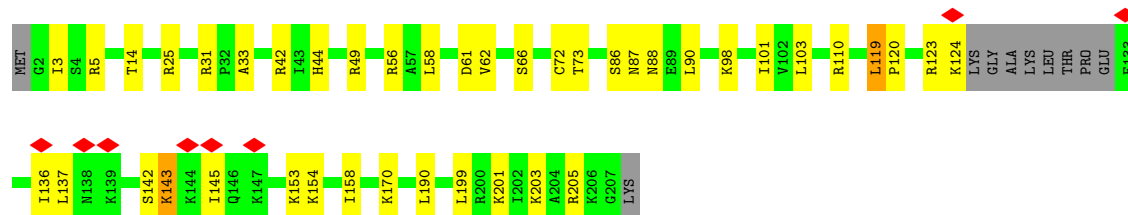


- Chain Q:  55% 30% 2% 14%



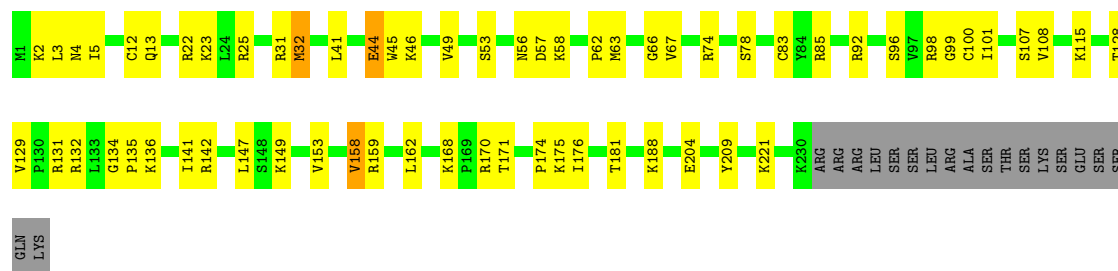
- Molecule 26: 40S ribosomal protein S8

Chain R: 75% 19% 5%



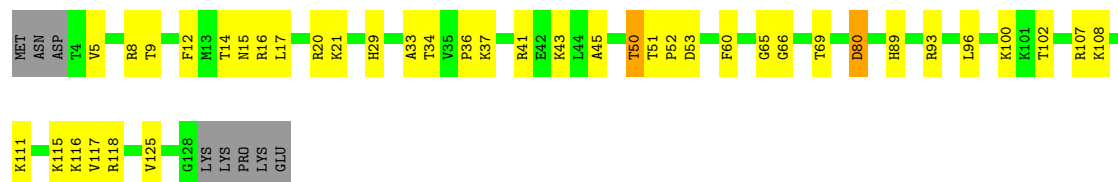
- Molecule 27: 40S ribosomal protein S6

Chain S: 67% 24% 8%



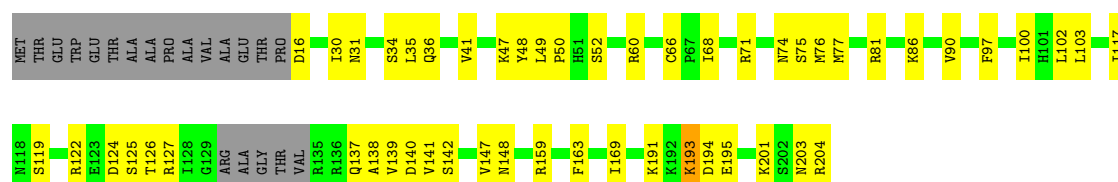
- Molecule 28: 40S ribosomal protein S24

Chain T: 64% 29% 6%



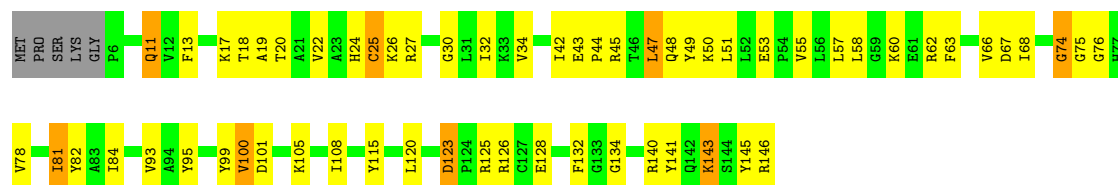
- Molecule 29: 40S ribosomal protein S5

Chain V: 65% 25% 10%



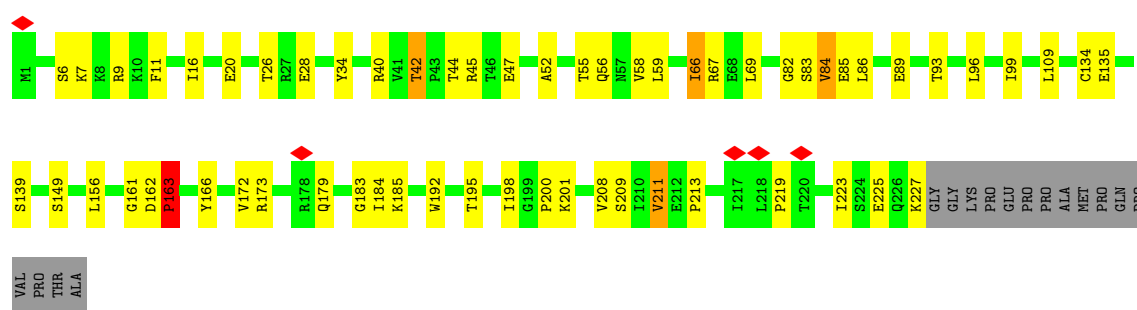
- Molecule 30: 40S ribosomal protein S16

Chain Y:  55% 36% 5% .

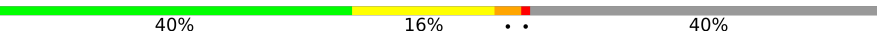


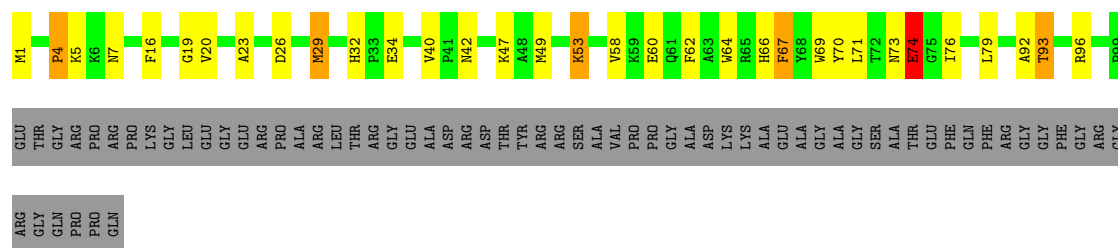
- Molecule 31: 40S ribosomal protein S3

Chain Z:  69% 23% 7% .



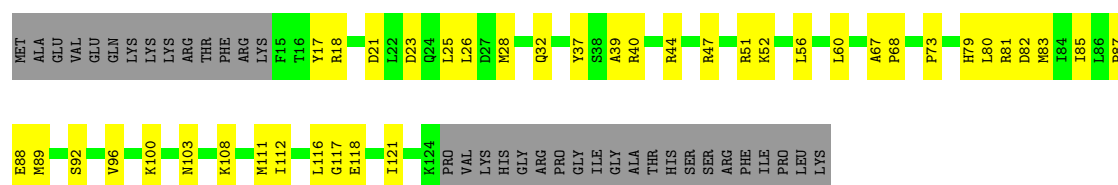
- Molecule 32: 40S ribosomal protein S10

Chain a:  40% 16% 40% . .



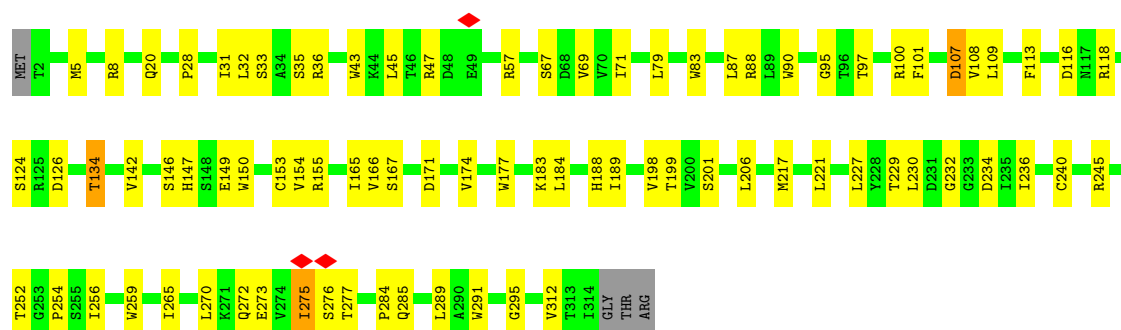
- Molecule 33: 40S ribosomal protein S15

Chain b:  48% 28% 24%

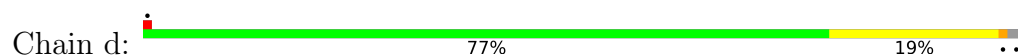


- Molecule 34: Receptor of activated protein C kinase 1

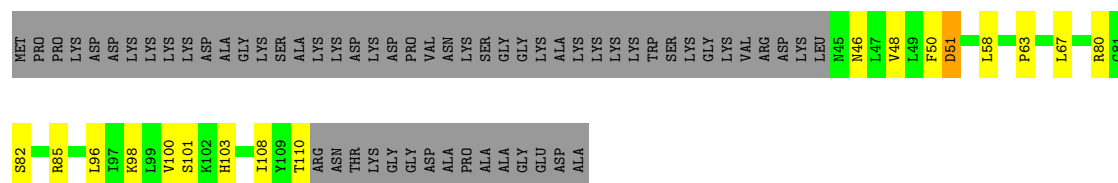
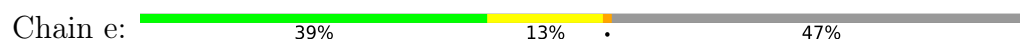
Chain c:  73% 25% . .



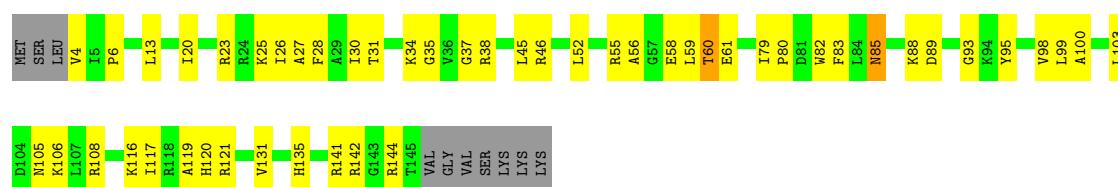
- Molecule 35: 40S ribosomal protein S19



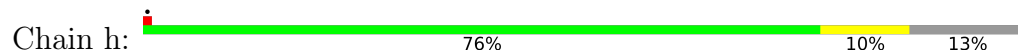
- Molecule 36: 40S ribosomal protein S25



- Molecule 37: 40S ribosomal protein S18



- Molecule 38: 40S ribosomal protein S20



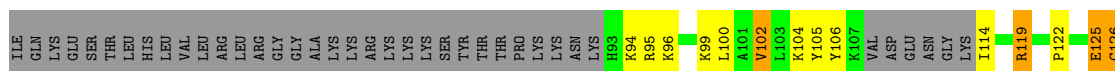
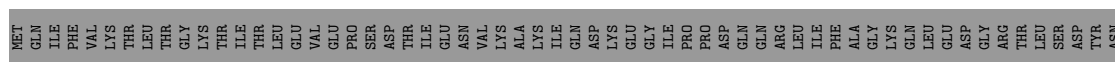
- Molecule 39: 40S ribosomal protein S29





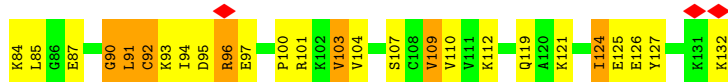
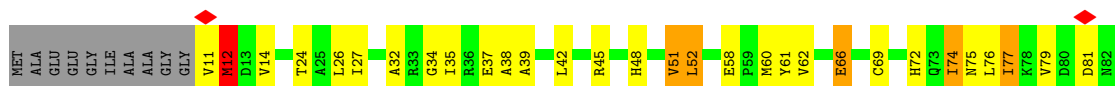
• Molecule 40: Ubiquitin-40S ribosomal protein S27a

Chain k: 14% 15% 5% 66%



• Molecule 41: 40S ribosomal protein S12

Chain m: 49% 33% 9% 8%



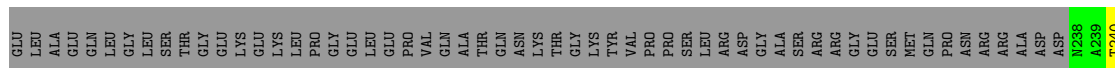
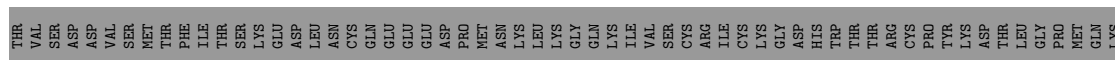
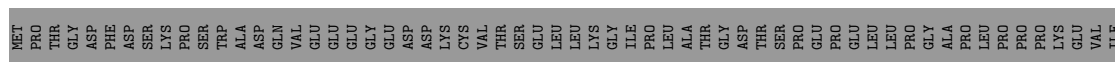
• Molecule 42: 40S ribosomal protein S28

Chain n: 55% 35% 9%

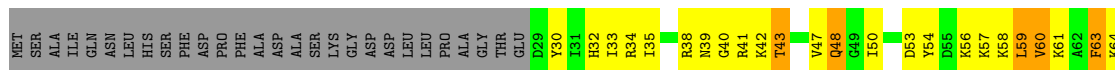


• Molecule 43: Eukaryotic translation initiation factor 3 subunit G

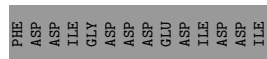
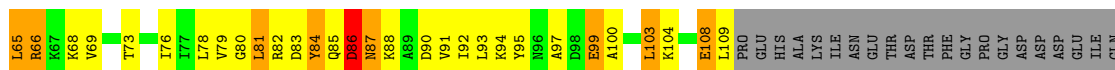
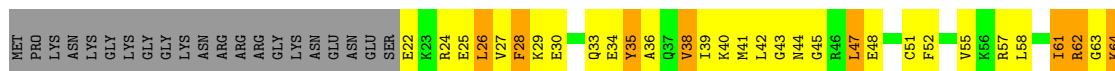
Chain o: 16% 8% 76%



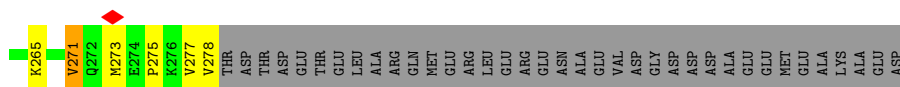
- Molecule 44: Eukaryotic translation initiation factor 1



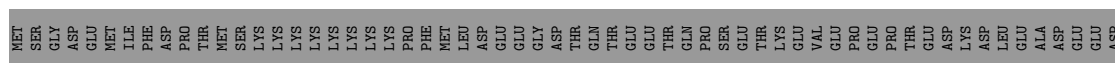
- Molecule 45: Eukaryotic translation initiation factor 1A, X-chromosomal



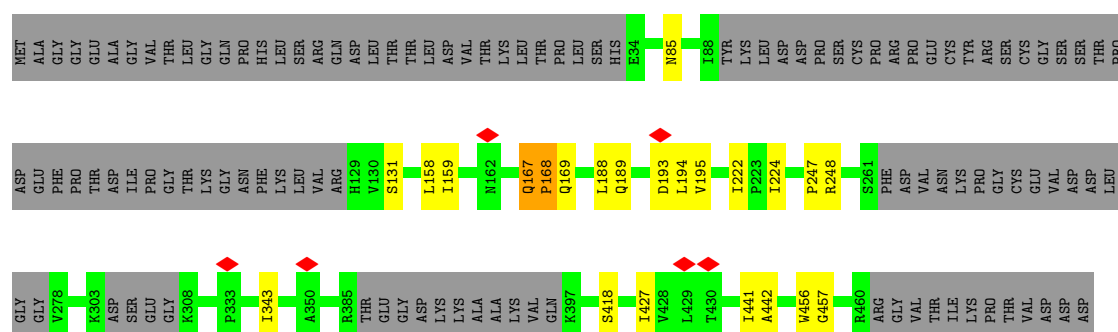
- Molecule 46: Eukaryotic translation initiation factor 2 subunit 1



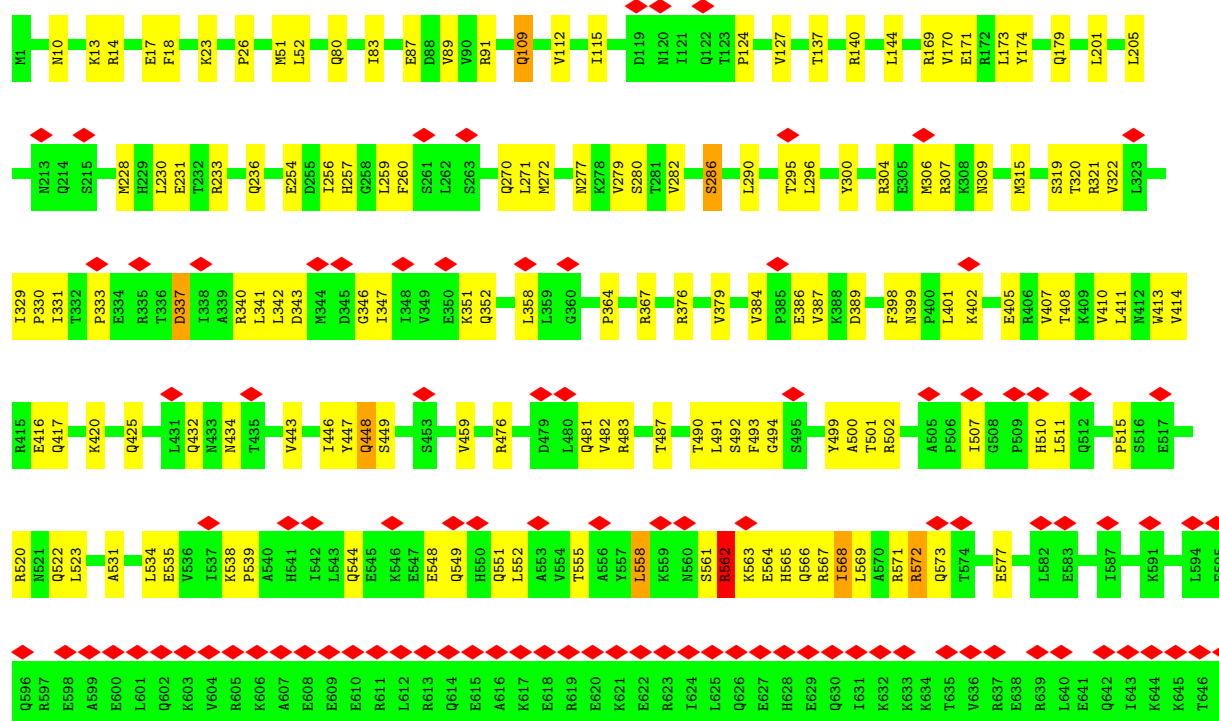
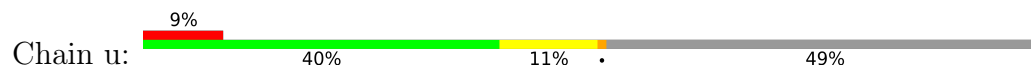
- Molecule 47: Eukaryotic translation initiation factor 2 subunit 2



- Molecule 48: Eukaryotic translation initiation factor 2 subunit 3



- Molecule 49: Eukaryotic translation initiation factor 3 subunit A





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.14	0/2466	1.82	53/3400 (1.6%)
2	3	1.02	0/1055	1.17	0/1469
3	4	1.08	0/1269	1.39	3/1762 (0.2%)
4	5	1.07	0/1575	1.24	0/2187
5	6	1.03	0/1926	1.39	13/2669 (0.5%)
6	7	0.53	0/259	1.14	2/396 (0.5%)
7	8	1.07	0/1569	1.37	4/2183 (0.2%)
8	9	0.64	0/231	1.51	1/294 (0.3%)
9	A	0.47	0/40362	0.68	50/62905 (0.1%)
10	B	0.85	0/1186	1.36	5/1585 (0.3%)
11	C	0.85	0/2077	1.38	3/2796 (0.1%)
12	D	0.72	0/1502	0.93	1/2008 (0.0%)
13	E	0.79	0/1105	1.16	1/1476 (0.1%)
14	F	0.78	0/332	1.34	1/434 (0.2%)
15	G	0.73	0/1451	1.13	1/1942 (0.1%)
16	H	0.77	0/644	1.11	1/864 (0.1%)
17	I	0.78	0/1232	1.13	0/1656
18	J	0.77	0/1051	1.06	1/1406 (0.1%)
19	K	0.82	0/623	1.09	0/833
20	L	0.78	0/1743	1.12	0/2354
21	M	0.85	0/1078	1.53	7/1447 (0.5%)
22	N	0.76	0/1670	1.04	2/2271 (0.1%)
23	O	0.74	0/1742	1.07	1/2330 (0.0%)
24	P	1.22	3/1010 (0.3%)	1.84	18/1353 (1.3%)
25	Q	0.84	0/805	1.24	1/1079 (0.1%)
26	R	0.72	0/1654	0.98	0/2203
27	S	0.75	0/1885	1.04	1/2510 (0.0%)
28	T	0.72	0/1032	1.00	0/1371
29	V	0.83	0/1481	1.15	6/1988 (0.3%)
30	Y	0.83	0/1142	1.38	2/1528 (0.1%)
31	Z	0.82	0/1793	1.17	6/2414 (0.2%)
32	a	0.83	0/859	1.34	3/1159 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.73	0/929	0.98	0/1241
34	c	0.76	0/2493	1.03	1/3394 (0.0%)
35	d	0.76	0/1123	1.03	0/1504
36	e	0.80	0/529	1.04	0/712
37	f	0.74	0/1194	1.05	1/1599 (0.1%)
38	h	0.78	0/827	1.07	0/1110
39	i	0.79	0/429	1.51	3/568 (0.5%)
40	k	0.87	0/444	1.52	3/588 (0.5%)
41	m	0.92	0/960	1.48	8/1286 (0.6%)
42	n	0.78	0/500	1.13	0/669
43	o	0.82	0/628	1.08	1/846 (0.1%)
44	p	0.85	0/701	1.70	7/936 (0.7%)
45	q	0.88	0/722	1.49	6/963 (0.6%)
46	r	0.44	1/2247 (0.0%)	0.86	1/3029 (0.0%)
47	s	0.85	0/1142	1.24	4/1534 (0.3%)
48	t	1.06	0/1745	1.24	1/2417 (0.0%)
49	u	0.81	2/5475 (0.0%)	1.14	10/7432 (0.1%)
50	v	0.86	0/2672	1.14	1/3647 (0.0%)
51	w	0.38	0/1795	0.76	5/2798 (0.2%)
52	x	0.88	0/2874	1.11	1/3925 (0.0%)
53	y	0.78	0/5557	1.04	5/7503 (0.1%)
All	All	0.73	6/114795 (0.0%)	1.03	245/163973 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	u	14[A]	ARG	C-O	7.72	1.33	1.24
49	u	14[B]	ARG	C-O	7.72	1.33	1.24
24	P	140	THR	CA-C	-5.49	1.45	1.52
24	P	48	SER	CA-CB	-5.12	1.45	1.53
46	r	231	ALA	N-CA	5.12	1.49	1.46

The worst 5 of 245 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1304	U	C2'-C3'-O3'	14.11	134.87	113.70
24	P	138	ASP	CA-CB-CG	14.02	126.62	112.60
24	P	103	ASN	N-CA-C	-12.11	98.51	113.28
47	s	202	PHE	N-CA-C	-12.06	98.09	112.92
9	A	368	U	C2'-C3'-O3'	11.08	126.12	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2445	0	1563	42	0
2	3	1057	0	475	12	0
3	4	1272	0	564	22	0
4	5	1581	0	689	9	0
5	6	1917	0	1096	36	0
6	7	240	0	121	0	0
7	8	1571	0	683	14	0
8	9	230	0	276	7	0
9	A	36668	0	18551	639	0
10	B	1166	0	1233	36	0
11	C	2035	0	2138	72	0
12	D	1477	0	1589	36	0
13	E	1087	0	1154	18	0
14	F	330	0	373	11	0
15	G	1430	0	1520	50	0
16	H	631	0	657	31	0
17	I	1208	0	1294	34	0
18	J	1034	0	1080	25	0
19	K	617	0	622	20	0
20	L	1707	0	1794	55	0
21	M	1064	0	1118	59	0
22	N	1633	0	1640	51	0
23	O	1715	0	1785	52	0
24	P	997	0	1021	62	0
25	Q	792	0	843	36	0
26	R	1627	0	1706	44	0
27	S	1862	0	2018	55	0
28	T	1015	0	1086	37	0
29	V	1461	0	1511	54	0
30	Y	1124	0	1193	53	0
31	Z	1765	0	1865	47	0
32	a	834	0	861	28	0
33	b	913	0	952	35	0
34	c	2436	0	2393	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	d	1105	0	1138	31	0
36	e	523	0	573	19	0
37	f	1176	0	1233	44	0
38	h	817	0	882	12	0
39	i	419	0	415	26	0
40	k	435	0	434	30	0
41	m	950	0	987	37	0
42	n	498	0	525	23	0
43	o	616	0	600	15	0
44	p	691	0	706	36	0
45	q	714	0	735	41	0
46	r	2215	0	2266	43	0
47	s	1123	0	1157	35	0
48	t	1750	0	806	14	0
49	u	5383	0	5085	112	0
50	v	2635	0	2207	54	0
51	w	1604	0	816	23	0
52	x	2831	0	2199	50	0
53	y	5470	0	5329	104	0
54	Q	1	0	0	0	0
54	k	1	0	0	0	0
55	d	1	0	0	0	0
55	f	1	0	0	0	0
All	All	109900	0	85557	1938	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1938 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:35:ARG:HH21	10:B:51:ILE:HA	1.09	1.16
41:m:100:PRO:HB2	41:m:103:VAL:HB	1.38	1.05
10:B:35:ARG:NH2	10:B:51:ILE:HG23	1.71	1.03
10:B:35:ARG:HH22	10:B:51:ILE:HG23	1.23	0.96
24:P:66:ARG:HH12	46:r:53:ARG:HB2	1.30	0.93

There are no symmetry-related clashes.

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%)	9	39
2	3	209/218 (96%)	205 (98%)	4 (2%)	0	100	100
3	4	251/357 (70%)	230 (92%)	18 (7%)	3 (1%)	10	43
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%)	36	72
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%)	30	67
12	D	175/194 (90%)	175 (100%)	0	0	100	100
13	E	138/143 (96%)	136 (99%)	1 (1%)	1 (1%)	18	55
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%)	16	53
22	N	205/295 (70%)	196 (96%)	9 (4%)	0	100	100
23	O	209/264 (79%)	198 (95%)	10 (5%)	1 (0%)	24	63
24	P	131/151 (87%)	120 (92%)	11 (8%)	0	100	100
25	Q	97/115 (84%)	94 (97%)	2 (2%)	1 (1%)	12	47
26	R	194/208 (93%)	192 (99%)	2 (1%)	0	100	100
27	S	228/249 (92%)	225 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	T	123/133 (92%)	123 (100%)	0	0	100	100
29	V	180/204 (88%)	173 (96%)	6 (3%)	1 (1%)	21	59
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%)	5	29
40	k	49/156 (31%)	46 (94%)	2 (4%)	1 (2%)	6	31
41	m	120/132 (91%)	114 (95%)	5 (4%)	1 (1%)	16	53
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%)	10	43
45	q	86/144 (60%)	75 (87%)	9 (10%)	2 (2%)	5	28
46	r	273/315 (87%)	249 (91%)	23 (8%)	1 (0%)	30	67
47	s	136/333 (41%)	120 (88%)	15 (11%)	1 (1%)	18	55
48	t	346/472 (73%)	329 (95%)	11 (3%)	6 (2%)	7	35
49	u	705/1382 (51%)	676 (96%)	28 (4%)	1 (0%)	48	83
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%)	48	83
All	All	9724/13164 (74%)	9264 (95%)	428 (4%)	32 (0%)	37	72

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	282	PRO
1	1	427	PRO
1	1	648	ILE

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Mol	Chain	Res	Type
3	4	264	GLY
23	O	117	TRP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	97/701 (14%)	95 (98%)	2 (2%)	47	65
5	6	49/335 (15%)	47 (96%)	2 (4%)	27	49
8	9	23/24 (96%)	22 (96%)	1 (4%)	26	48
10	B	129/142 (91%)	115 (89%)	14 (11%)	6	21
11	C	220/225 (98%)	188 (86%)	32 (14%)	3	14
12	D	158/168 (94%)	155 (98%)	3 (2%)	50	66
13	E	112/115 (97%)	109 (97%)	3 (3%)	39	60
14	F	33/48 (69%)	25 (76%)	8 (24%)	1	5
15	G	159/174 (91%)	155 (98%)	4 (2%)	42	62
16	H	73/76 (96%)	72 (99%)	1 (1%)	59	72
17	I	130/131 (99%)	129 (99%)	1 (1%)	73	78
18	J	112/113 (99%)	108 (96%)	4 (4%)	31	52
19	K	65/67 (97%)	65 (100%)	0	100	100
20	L	186/225 (83%)	181 (97%)	5 (3%)	39	60
21	M	119/122 (98%)	106 (89%)	13 (11%)	6	21
22	N	173/243 (71%)	172 (99%)	1 (1%)	78	81
23	O	192/231 (83%)	189 (98%)	3 (2%)	55	69
24	P	104/119 (87%)	98 (94%)	6 (6%)	18	40
25	Q	86/98 (88%)	83 (96%)	3 (4%)	32	54
26	R	172/180 (96%)	165 (96%)	7 (4%)	27	49
27	S	200/218 (92%)	194 (97%)	6 (3%)	36	57
28	T	107/115 (93%)	101 (94%)	6 (6%)	19	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	V	156/170 (92%)	152 (97%)	4 (3%)	40	61
30	Y	117/121 (97%)	106 (91%)	11 (9%)	8	26
31	Z	190/202 (94%)	178 (94%)	12 (6%)	16	38
32	a	90/136 (66%)	83 (92%)	7 (8%)	11	32
33	b	100/130 (77%)	98 (98%)	2 (2%)	48	66
34	c	272/275 (99%)	262 (96%)	10 (4%)	30	51
35	d	112/115 (97%)	106 (95%)	6 (5%)	20	42
36	e	58/103 (56%)	56 (97%)	2 (3%)	32	55
37	f	123/132 (93%)	119 (97%)	4 (3%)	33	55
38	h	94/107 (88%)	94 (100%)	0	100	100
39	i	44/49 (90%)	35 (80%)	9 (20%)	1	7
40	k	47/140 (34%)	31 (66%)	16 (34%)	0	2
41	m	104/108 (96%)	89 (86%)	15 (14%)	3	14
42	n	56/62 (90%)	55 (98%)	1 (2%)	51	67
43	o	64/277 (23%)	58 (91%)	6 (9%)	8	26
44	p	74/96 (77%)	59 (80%)	15 (20%)	1	8
45	q	75/123 (61%)	52 (69%)	23 (31%)	0	2
46	r	247/280 (88%)	225 (91%)	22 (9%)	9	28
47	s	128/304 (42%)	116 (91%)	12 (9%)	8	26
49	u	528/1259 (42%)	517 (98%)	11 (2%)	47	65
50	v	206/406 (51%)	197 (96%)	9 (4%)	25	47
52	x	206/494 (42%)	201 (98%)	5 (2%)	43	63
53	y	564/811 (70%)	555 (98%)	9 (2%)	55	69
All	All	6354/9770 (65%)	6018 (95%)	336 (5%)	22	42

5 of 336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	p	43	THR
46	r	248	LEU
44	p	85	LEU
45	q	73	THR
47	s	290	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
40	k	139	HIS
53	y	467	GLN
49	u	44	GLN
53	y	460	GLN
53	y	717	GLN

5.3.3 RNA ⓘ

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	1710/1869 (91%)	445 (26%)	52 (3%)
All	All	1803/1964 (91%)	501 (27%)	52 (2%)

5 of 501 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 ⓘ

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	A2M	A	159	9	22,25,26	0.98	2 (9%)	30,36,39	0.97	3 (10%)
9	PSU	A	1243	9	18,21,22	1.29	2 (11%)	21,30,33	1.11	2 (9%)
9	A2M	A	1678	9	22,25,26	0.77	0	30,36,39	0.98	2 (6%)
9	A2M	A	27	9	22,25,26	0.94	1 (4%)	30,36,39	0.90	1 (3%)
9	PSU	A	119	9	18,21,22	1.13	2 (11%)	21,30,33	1.22	3 (14%)
9	5MC	A	1374	9	19,22,23	0.68	0	26,32,35	0.62	0
9	OMC	A	174	9	19,22,23	0.59	0	25,31,34	0.45	0
9	A2M	A	668	9	22,25,26	1.02	2 (9%)	30,36,39	0.97	1 (3%)
9	OMC	A	1703	9	19,22,23	0.70	0	25,31,34	0.52	0
9	UR3	A	1830	9	19,22,23	0.98	1 (5%)	26,32,35	2.11	6 (23%)
9	MA6	A	1850	9	23,26,27	0.98	1 (4%)	33,38,41	1.41	3 (9%)
9	A2M	A	484	9	22,25,26	0.86	1 (4%)	30,36,39	0.96	2 (6%)
9	MA6	A	1851	9	23,26,27	0.92	2 (8%)	33,38,41	1.22	2 (6%)
9	OMU	A	116	9	19,22,23	0.73	0	25,31,34	0.82	0
9	OMC	A	517	9	19,22,23	0.59	0	25,31,34	0.46	0
9	A2M	A	1031	9	22,25,26	0.98	2 (9%)	30,36,39	0.89	1 (3%)
9	PSU	A	823	9	18,21,22	1.17	2 (11%)	21,30,33	1.21	2 (9%)
9	OMU	A	121	9	19,22,23	0.88	0	25,31,34	0.89	1 (4%)
9	A2M	A	166	9	22,25,26	0.83	1 (4%)	30,36,39	1.12	2 (6%)
9	OMG	A	644	9	23,26,27	0.82	0	32,38,41	0.73	0
9	PSU	A	612	9	18,21,22	1.08	1 (5%)	21,30,33	1.00	1 (4%)
9	PSU	A	1081	9	18,21,22	1.13	1 (5%)	21,30,33	1.20	2 (9%)
9	OMG	A	683	9	23,26,27	0.90	1 (4%)	32,38,41	0.89	1 (3%)
9	5MU	A	814	9	19,22,23	0.92	1 (5%)	27,32,35	0.94	1 (3%)
9	OMG	A	509	9	23,26,27	1.29	3 (13%)	32,38,41	2.15	7 (21%)
9	PSU	A	822	9	18,21,22	1.13	1 (5%)	21,30,33	1.18	2 (9%)

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	A2M	A	159	9	-	2/9/27/28	0/3/3/3
9	PSU	A	1243	9	-	0/7/25/26	0/2/2/2
9	A2M	A	1678	9	-	0/9/27/28	0/3/3/3
9	A2M	A	27	9	-	0/9/27/28	0/3/3/3
9	PSU	A	119	9	-	0/7/25/26	0/2/2/2
9	5MC	A	1374	9	-	0/7/25/26	0/2/2/2
9	OMC	A	174	9	-	0/9/27/28	0/2/2/2
9	A2M	A	668	9	-	2/9/27/28	0/3/3/3
9	OMC	A	1703	9	-	0/9/27/28	0/2/2/2
9	UR3	A	1830	9	-	2/7/25/26	0/2/2/2
9	MA6	A	1850	9	-	3/11/29/30	0/3/3/3
9	A2M	A	484	9	-	0/9/27/28	0/3/3/3
9	MA6	A	1851	9	-	5/11/29/30	0/3/3/3
9	OMU	A	116	9	-	1/9/27/28	0/2/2/2
9	OMC	A	517	9	-	1/9/27/28	0/2/2/2
9	A2M	A	1031	9	-	0/9/27/28	0/3/3/3
9	PSU	A	823	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	166	9	-	0/9/27/28	0/3/3/3
9	OMG	A	644	9	-	2/9/27/28	0/3/3/3
9	PSU	A	612	9	-	0/7/25/26	0/2/2/2
9	PSU	A	1081	9	-	1/7/25/26	0/2/2/2
9	OMG	A	683	9	-	0/9/27/28	0/3/3/3
9	5MU	A	814	9	-	0/7/25/26	0/2/2/2
9	OMG	A	509	9	-	1/9/27/28	0/3/3/3
9	PSU	A	822	9	-	0/7/25/26	0/2/2/2

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1243	PSU	C6-C5	3.56	1.39	1.35
9	A	822	PSU	C6-C5	3.52	1.39	1.35
9	A	119	PSU	C6-C5	3.45	1.39	1.35
9	A	823	PSU	C6-C5	3.04	1.38	1.35
9	A	509	OMG	C5-C4	2.98	1.46	1.38

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1830	UR3	C4-N3-C2	-6.53	119.32	124.58
9	A	509	OMG	C5-C4-N3	-6.32	118.33	128.39
9	A	509	OMG	C2'-C1'-N9	-4.95	104.84	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	509	OMG	C2-N3-C4	4.69	120.38	112.30
9	A	509	OMG	N9-C4-N3	4.64	135.24	125.95

There are no chirality outliers.

5 of 20 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.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	159	A2M	1	0
9	A	1678	A2M	2	0
9	A	174	OMC	1	0
9	A	1703	OMC	1	0
9	A	116	OMU	3	0
9	A	517	OMC	1	0
9	A	1031	A2M	3	0
9	A	121	OMU	1	0
9	A	683	OMG	1	0
9	A	509	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

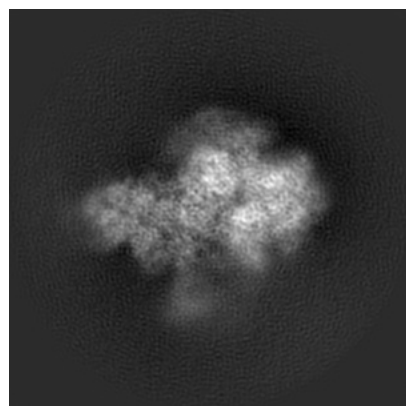
6 Map visualisation [i](#)

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.

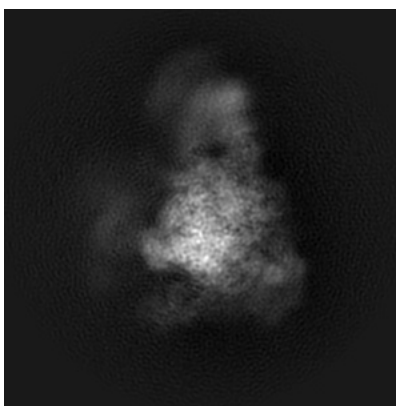
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

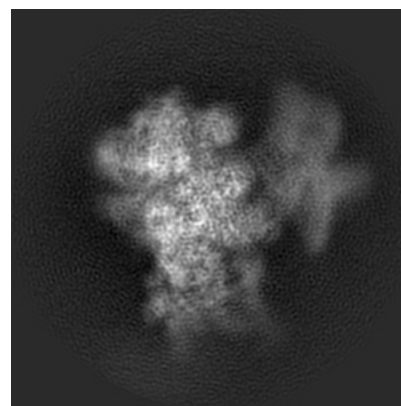
6.1.1 Primary map



X

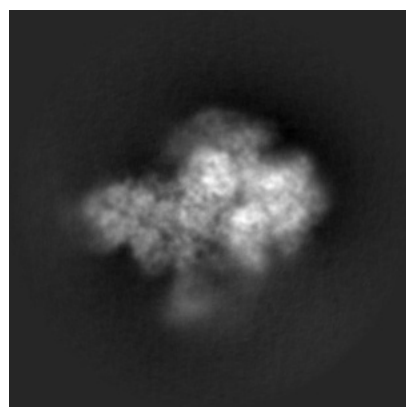


Y

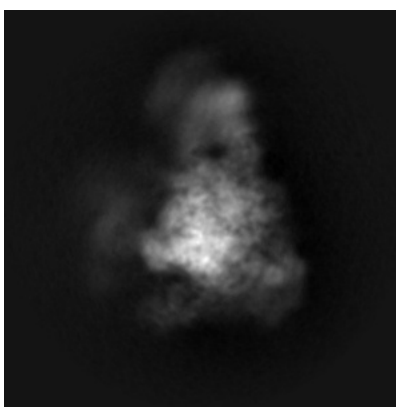


Z

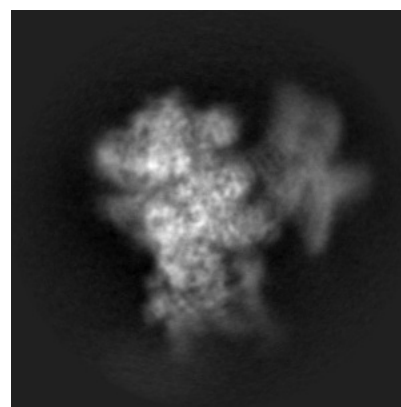
6.1.2 Raw map



X



Y

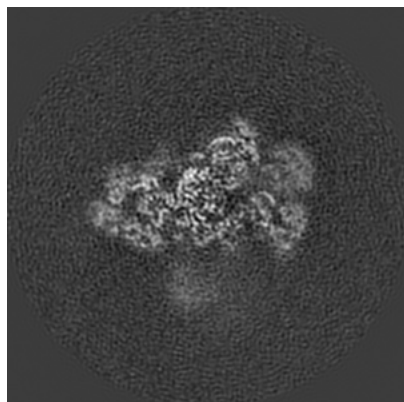


Z

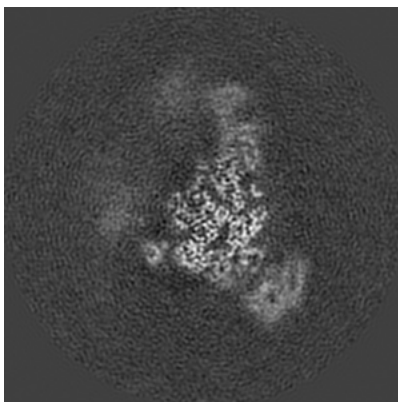
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

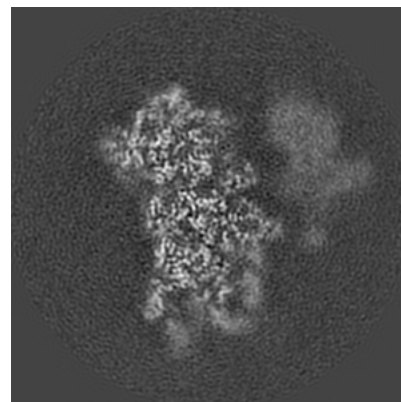
6.2.1 Primary map



X Index: 180

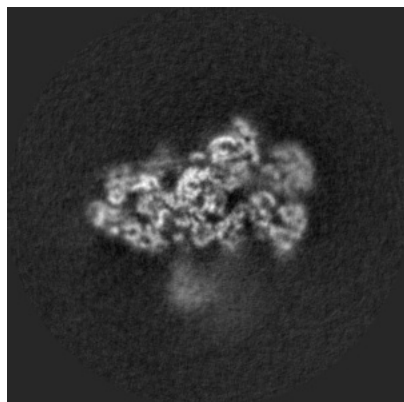


Y Index: 180

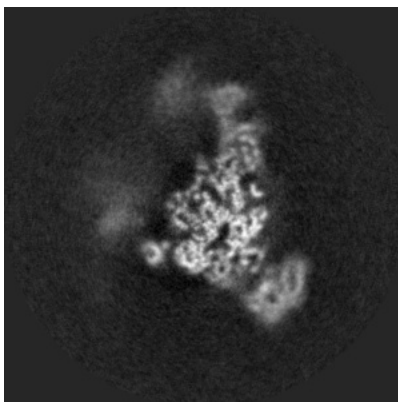


Z Index: 180

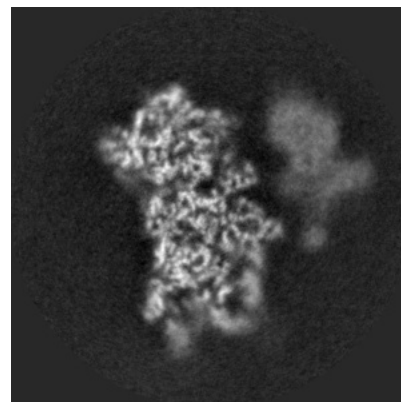
6.2.2 Raw map



X Index: 180



Y Index: 180

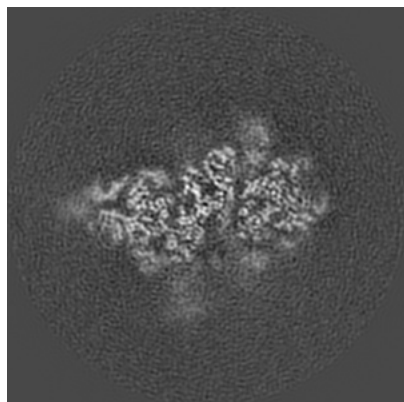


Z Index: 180

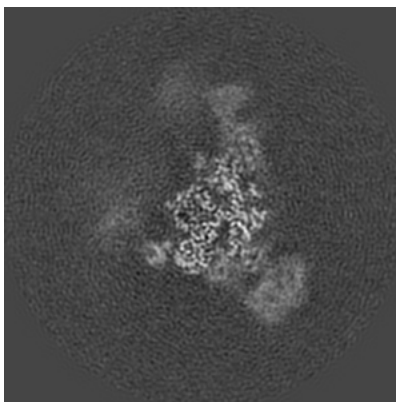
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

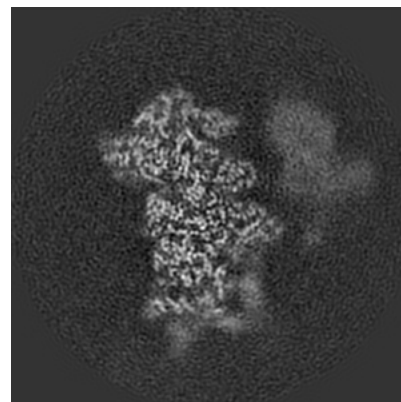
6.3.1 Primary map



X Index: 152

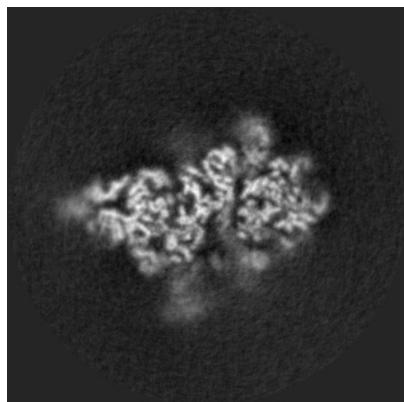


Y Index: 178

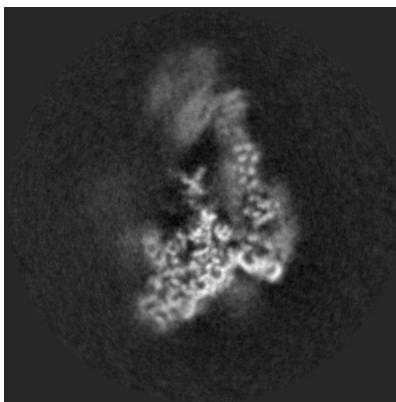


Z Index: 176

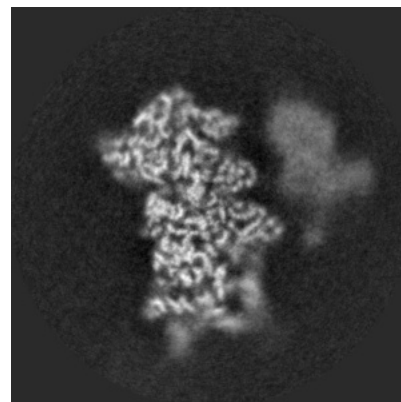
6.3.2 Raw map



X Index: 152



Y Index: 219

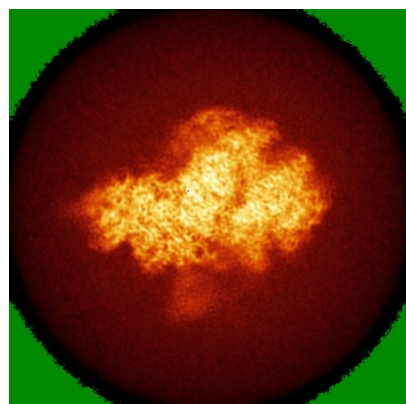


Z Index: 176

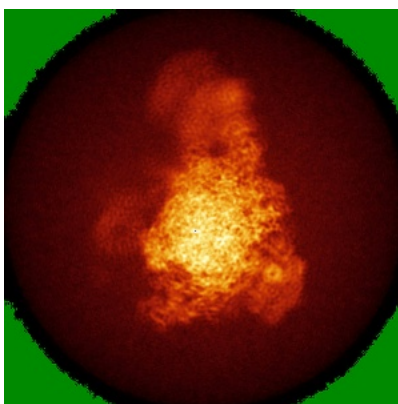
The images above show the largest variance slices of the map in three orthogonal directions.

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

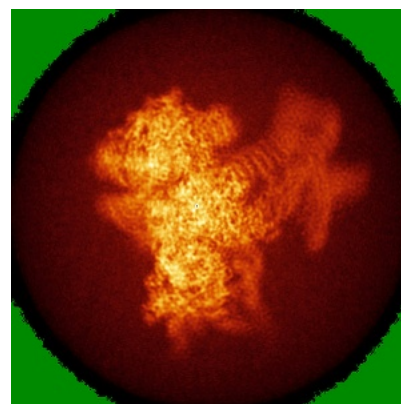
6.4.1 Primary map



X

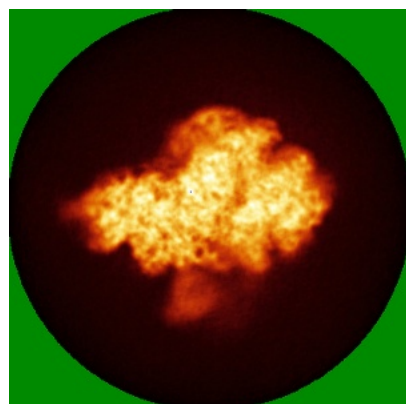


Y

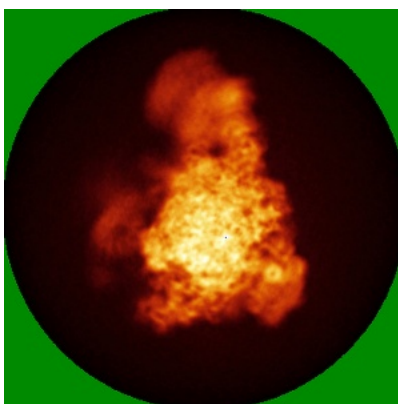


Z

6.4.2 Raw map



X



Y

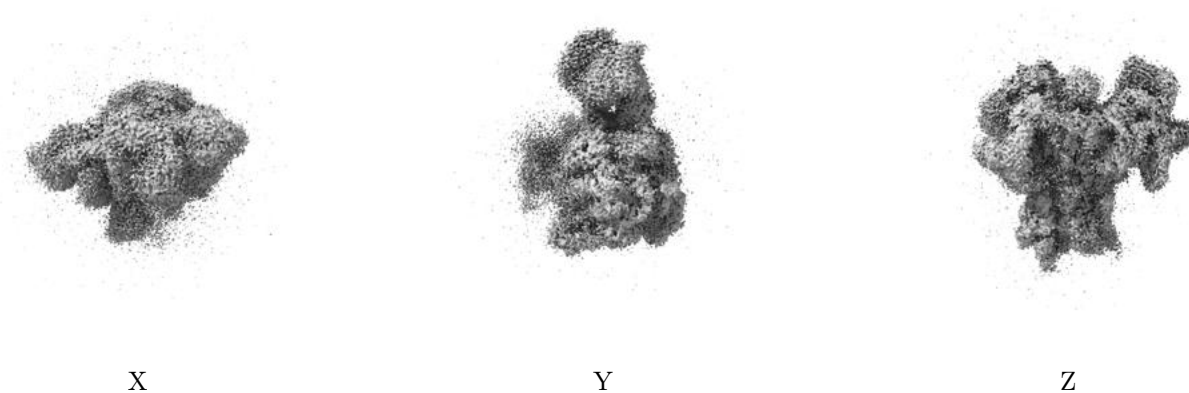


Z

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



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.

6.6 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

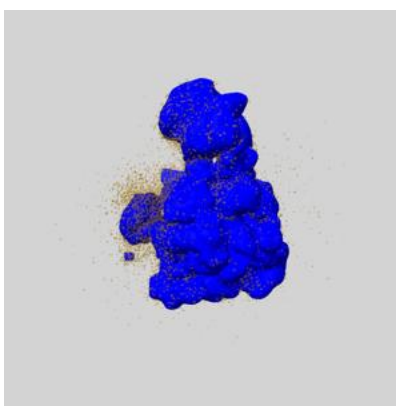
A mask typically either:

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

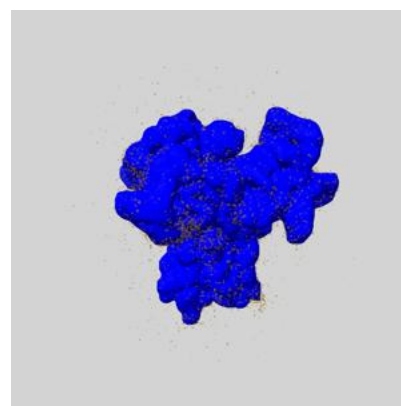
6.6.1 emd_14113_msk_1.map [i](#)



X



Y

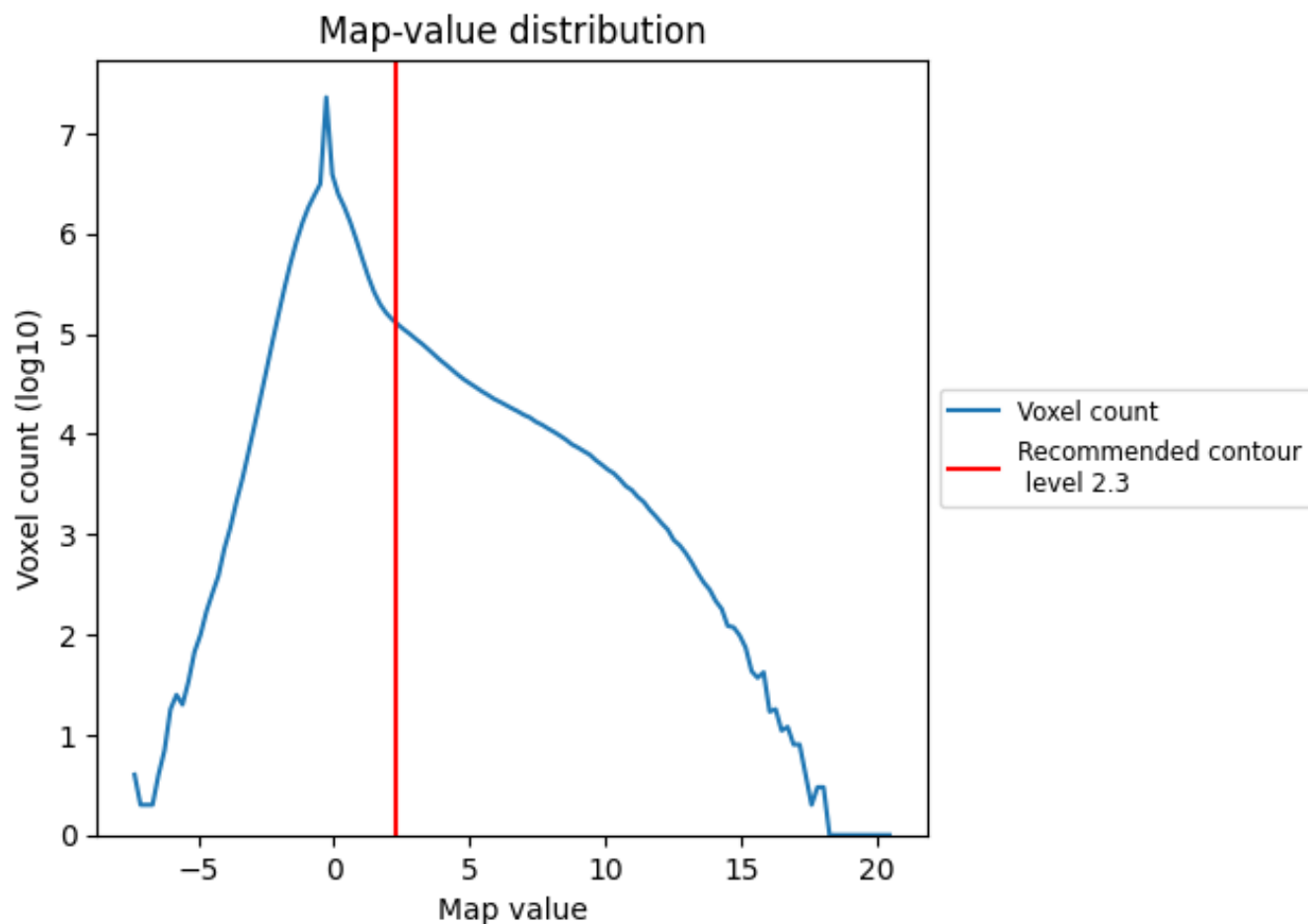


Z

7 Map analysis [i](#)

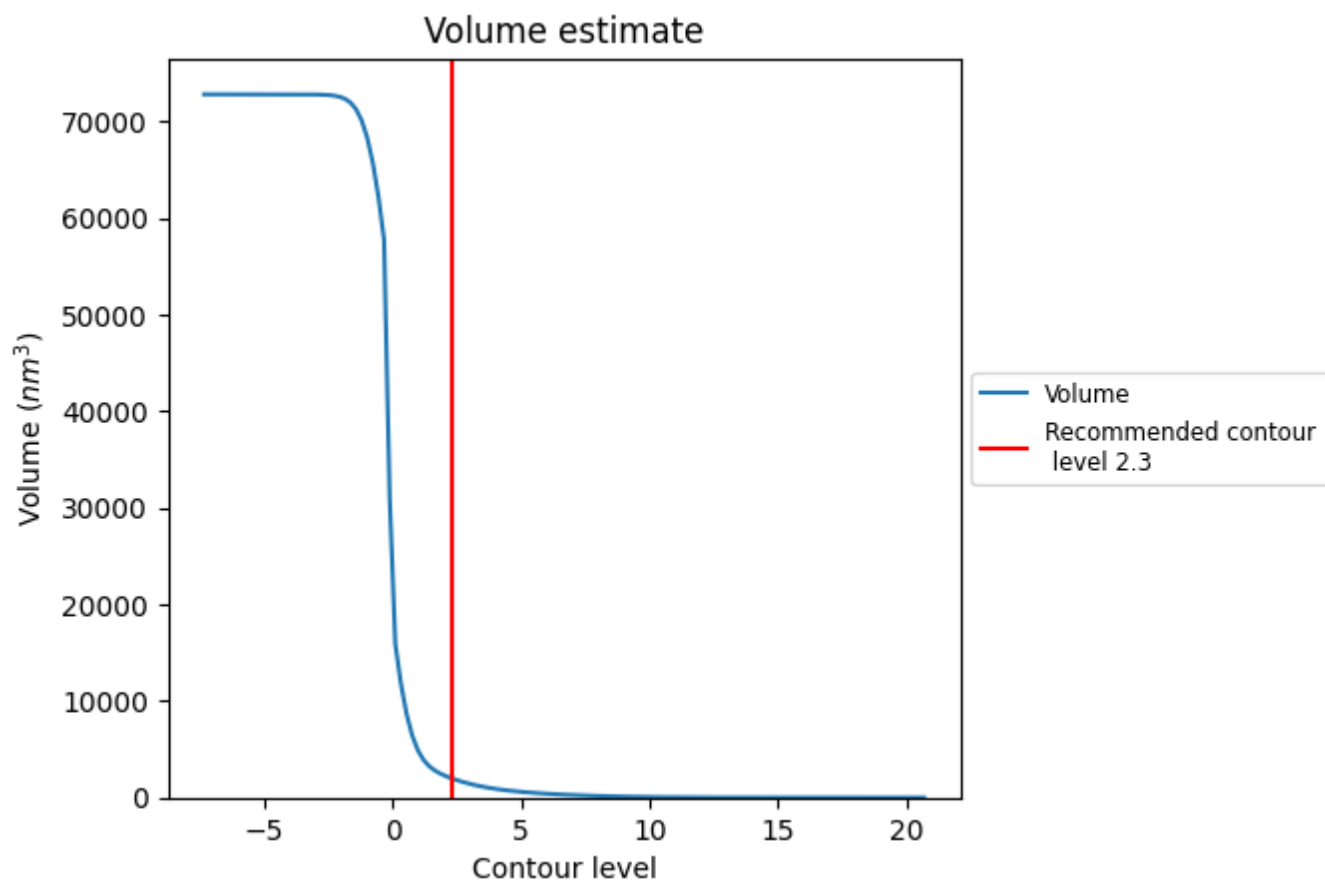
This section contains the results of statistical analysis of the map.

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.

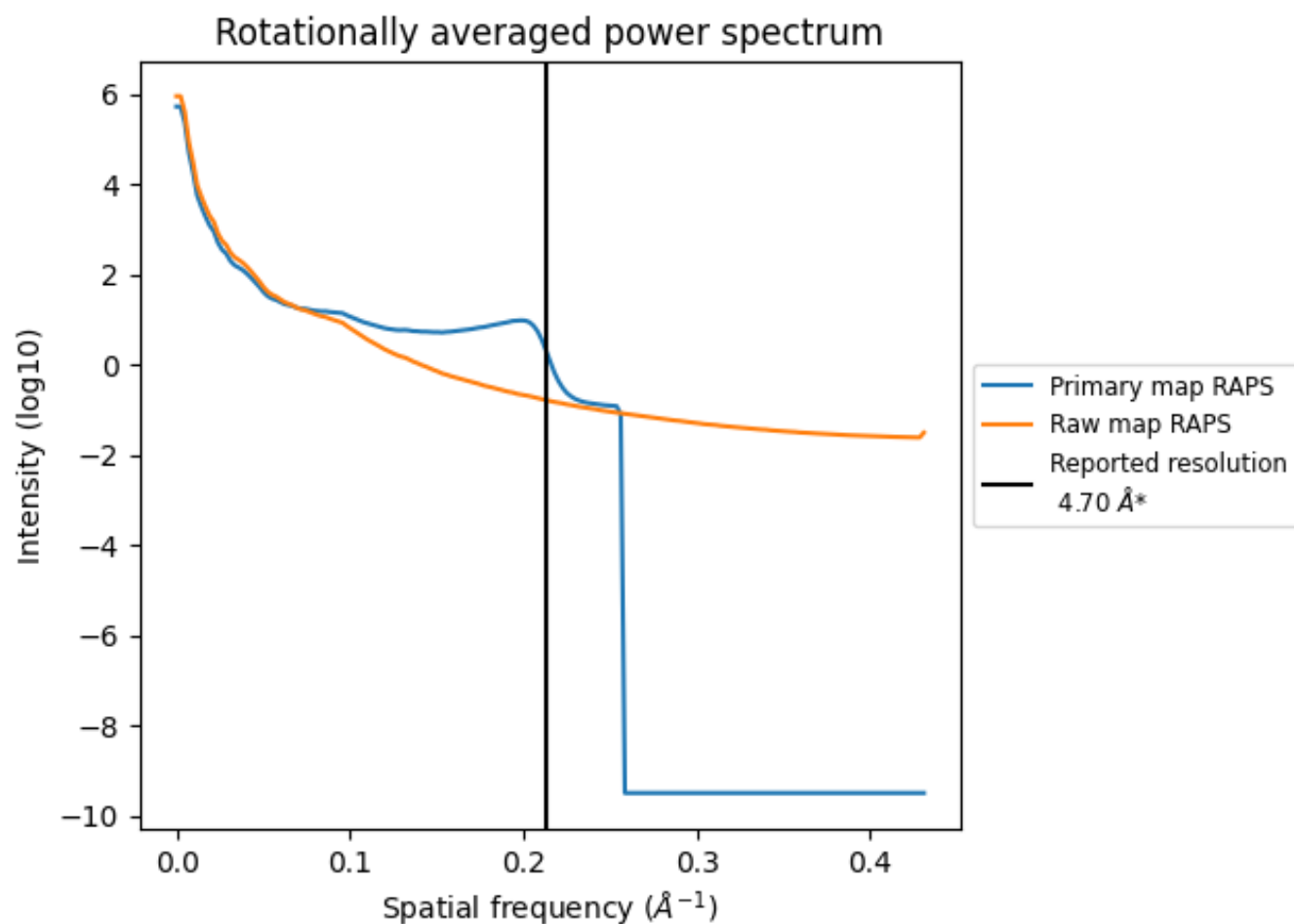
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1983 nm³; 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 ⓘ

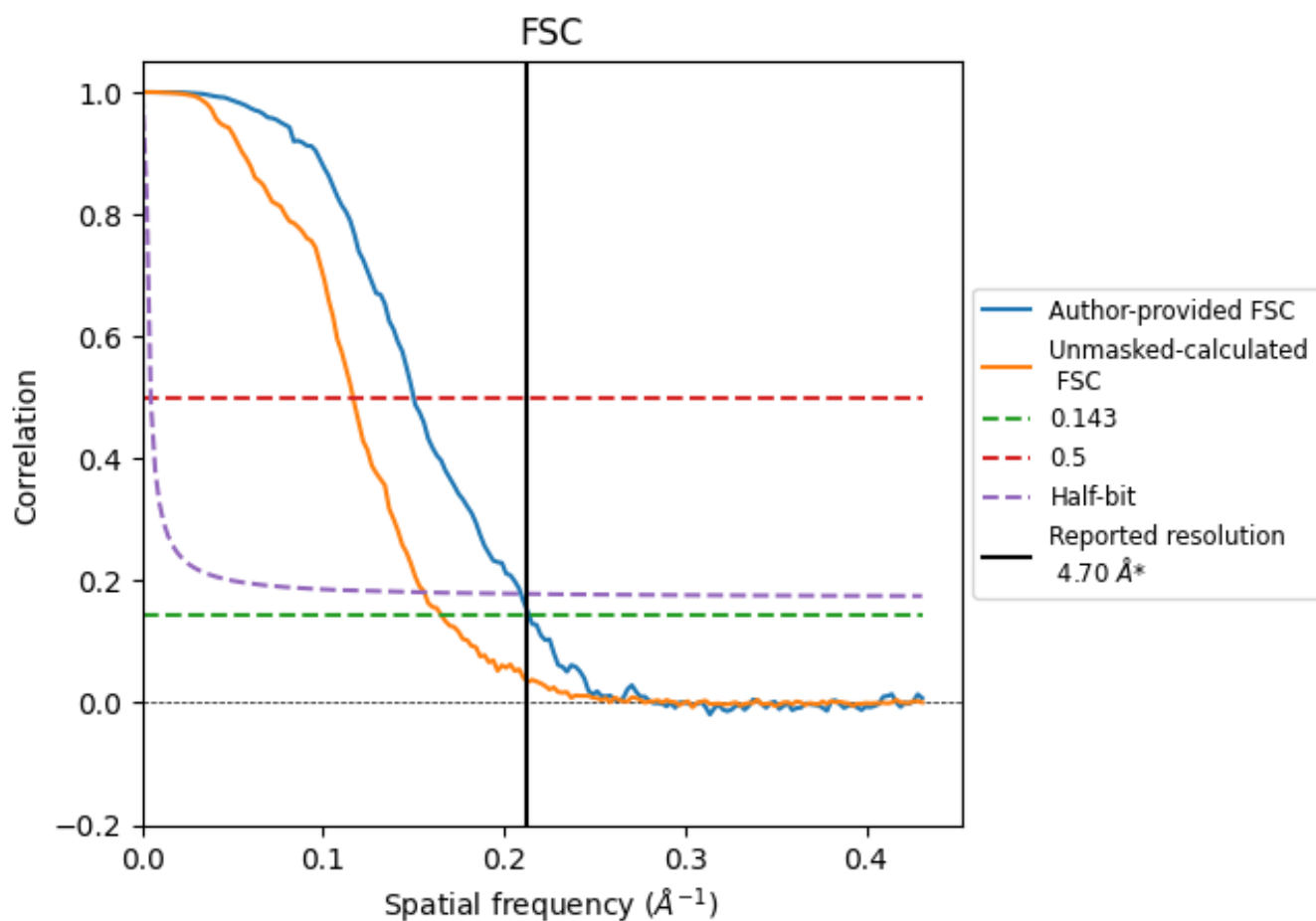


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 $0.213 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

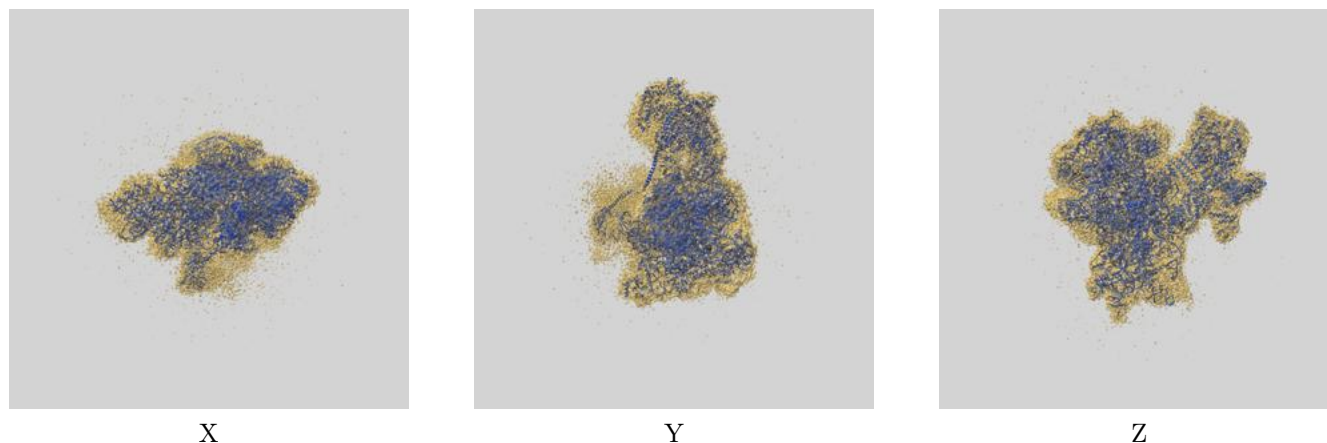
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.68	6.67	4.78
Unmasked-calculated*	6.05	8.58	6.41

*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 [i](#)

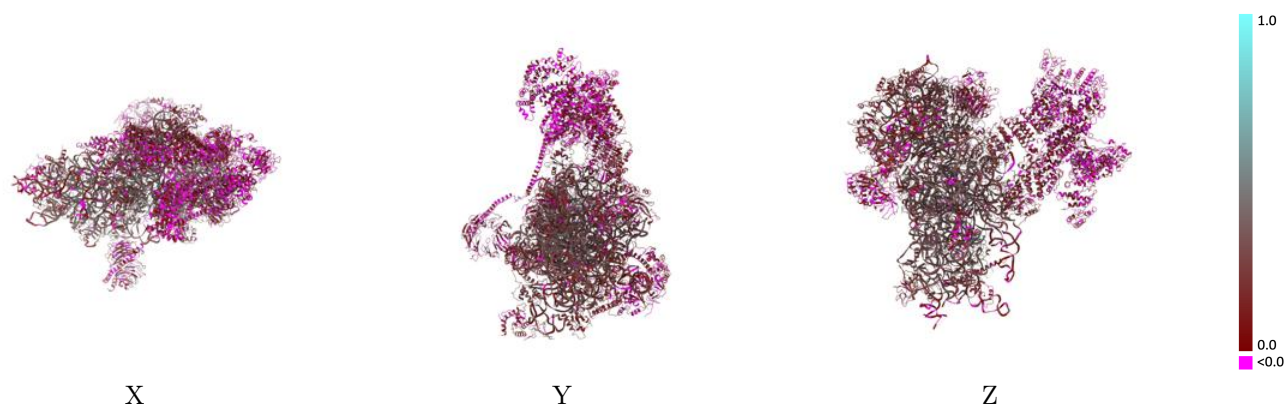
This section contains information regarding the fit between EMDB map EMD-14113 and PDB model 7QP6. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



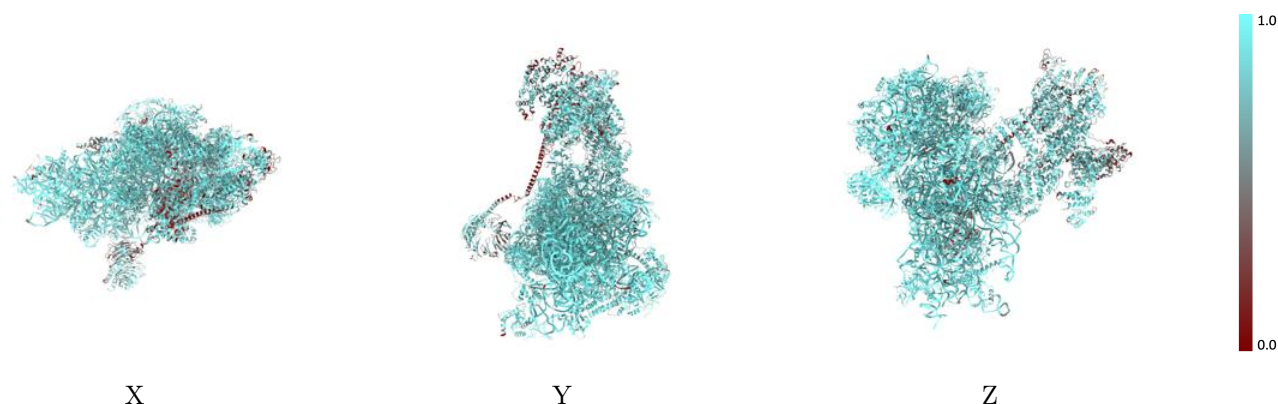
The images above show the 3D surface view of the map at the recommended contour level 2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



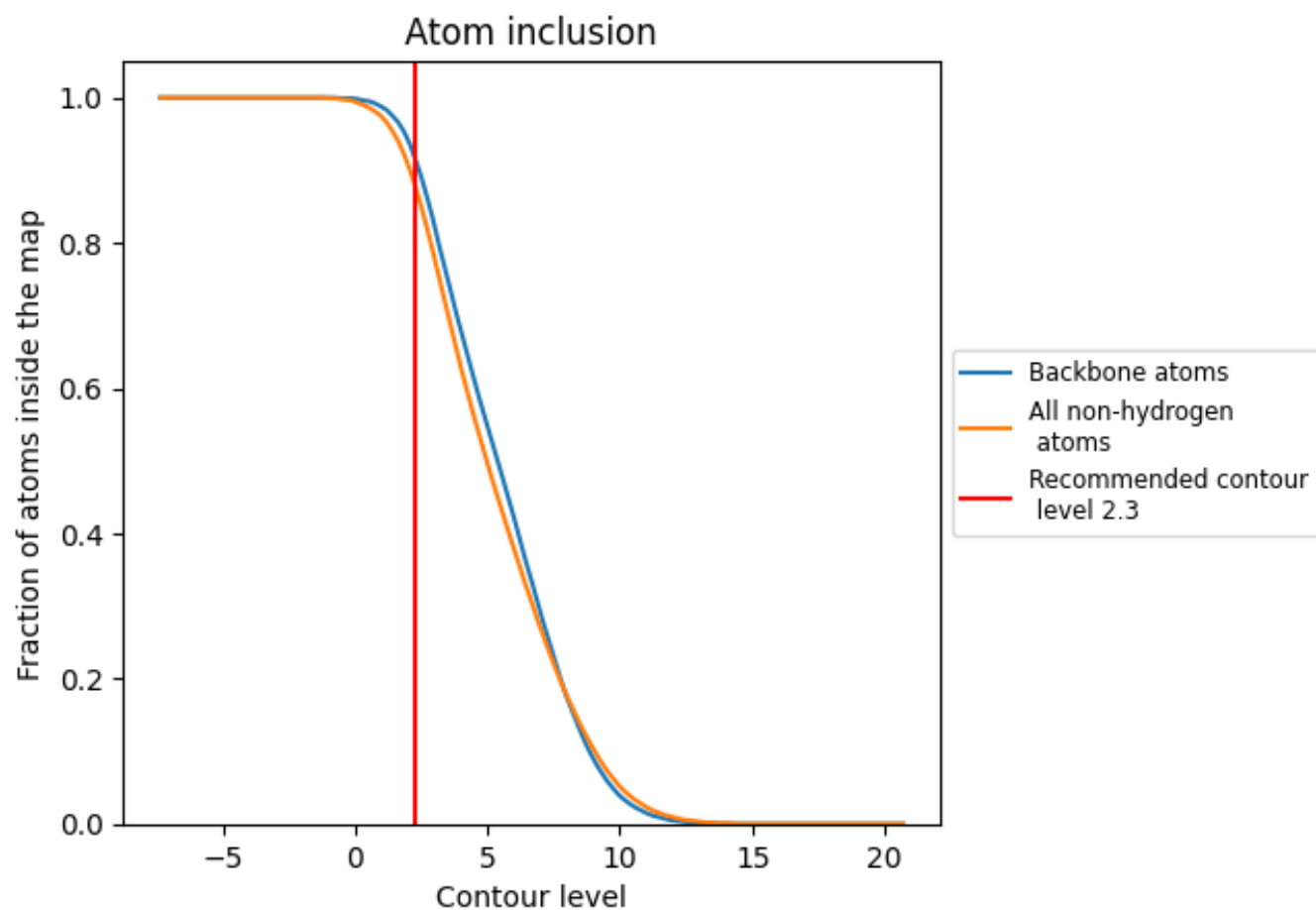
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.3).

9.4 Atom inclusion ⓘ



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



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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