



Full wwPDB EM Validation Report ⓘ

Apr 17, 2024 – 01:27 pm BST

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

This is a Full wwPDB EM Validation 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:

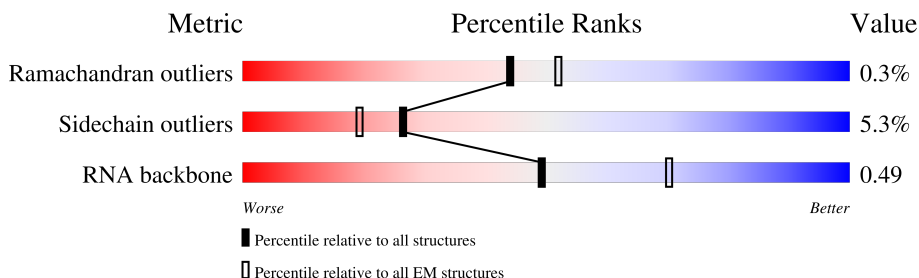
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 Å.

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







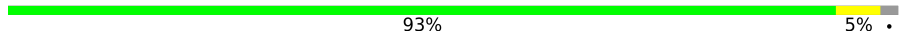


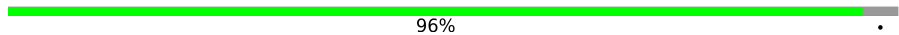
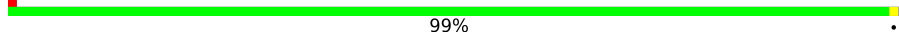
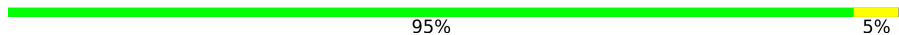
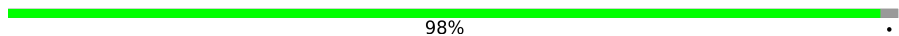






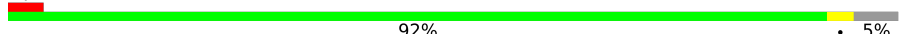







Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
4	5	564	
5	6	374	
6	7	20	
7	8	352	
8	9	25	

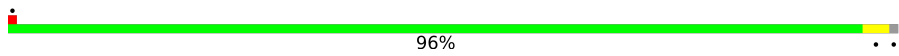
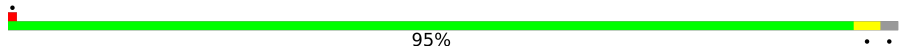
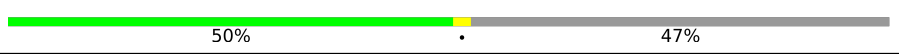
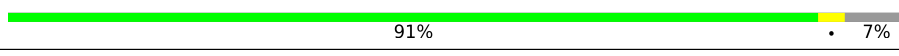




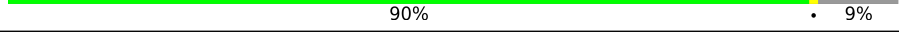
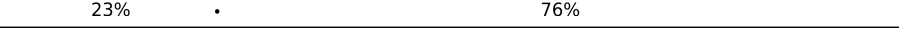
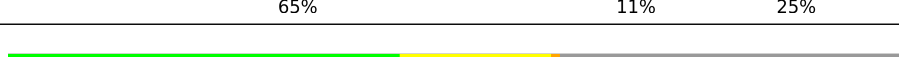
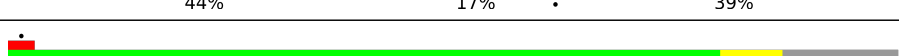

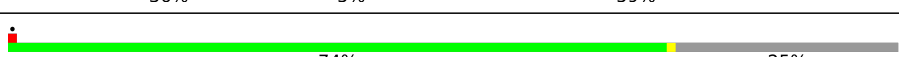
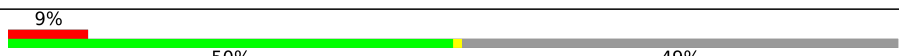
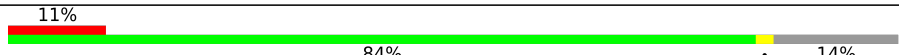
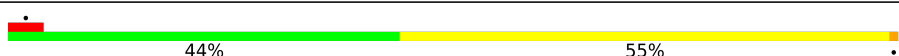



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	A	1869	 66% 23% 8%
10	B	158	 78% 11% 10%
11	C	263	 86% 12%
12	D	194	 90% 9%
13	E	143	 93% 5%
14	F	59	 56% 12% 32%
15	G	194	 89% 9%
16	H	84	 96%
17	I	151	 99%
18	J	130	 95% 5%
19	K	83	 98%
20	L	293	 72% 25%
21	M	135	 88% 9%
22	N	295	 69% 30%
23	O	264	 78% 20%
24	P	151	 83% 5% 12%
25	Q	115	 83% 14%
26	R	208	 92% 5%
27	S	249	 89% 8%
28	T	133	 89% 5% 6%
29	V	204	 86% 10%
30	Y	146	 88% 8%
31	Z	243	 90% 7%
32	a	165	 55% 5% 40%
33	b	145	 76% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	c	317	 96%
35	d	145	 95%
36	e	125	 50% 47%
37	f	152	 91% 7%
38	h	119	 87% 13%
39	i	56	 70% 18% 11%
40	k	156	 22% 11% 66%
41	m	132	 79% 12% 8%
42	n	69	 90% 9%
43	o	320	 23% 76%
44	p	113	 65% 11% 25%
45	q	144	 44% 17% 39%
46	r	315	 80% 7% 13%
47	s	333	 36% 5% 59%
48	t	472	 74% 25%
49	u	1382	 9% 50% 49%
50	v	445	 11% 84% 14%
51	w	75	 44% 55%
52	x	548	 6% 75% 23%
53	y	913	 11% 75% 24%

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 109900 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Eukaryotic translation initiation factor 3 subunit B.

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

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

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

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

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

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

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

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

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

- Molecule 6 is a RNA chain called mRNA.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			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
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
			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
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
			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 1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

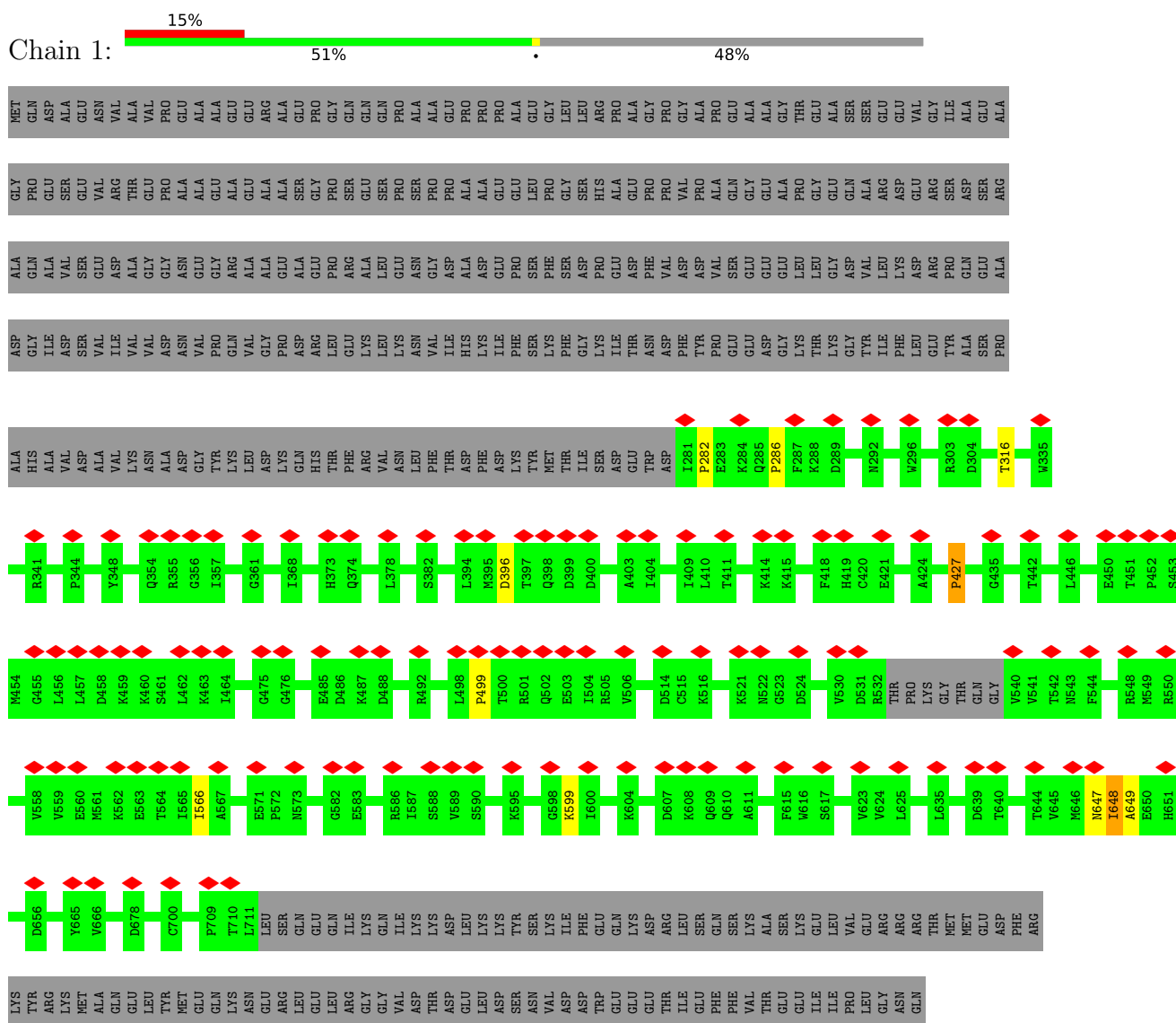
- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots [i](#)

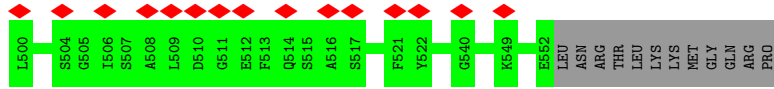
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Eukaryotic translation initiation factor 3 subunit B

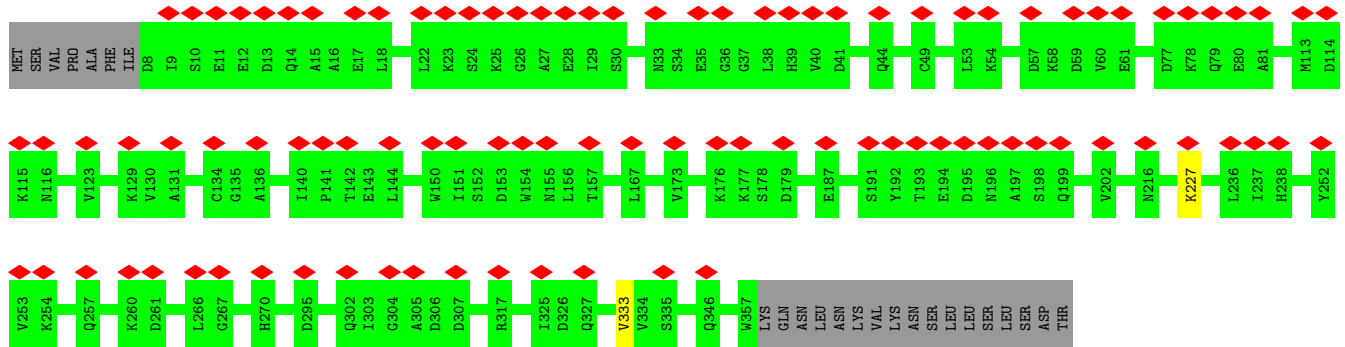
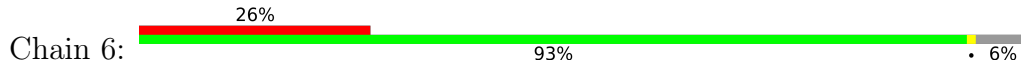


- Molecule 2: Eukaryotic translation initiation factor 3 subunit K





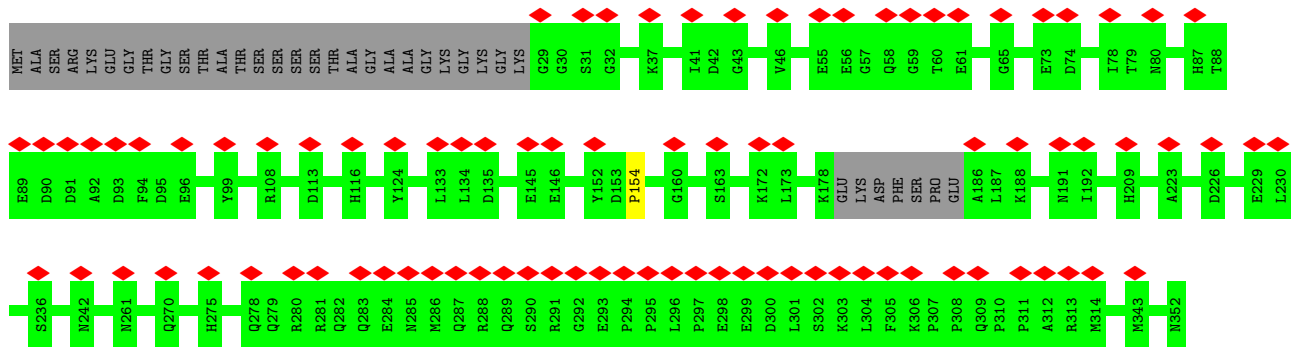
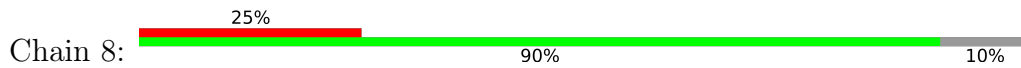
• Molecule 5: Eukaryotic translation initiation factor 3 subunit M



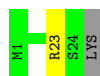
• Molecule 6: mRNA



• Molecule 7: Eukaryotic translation initiation factor 3 subunit H

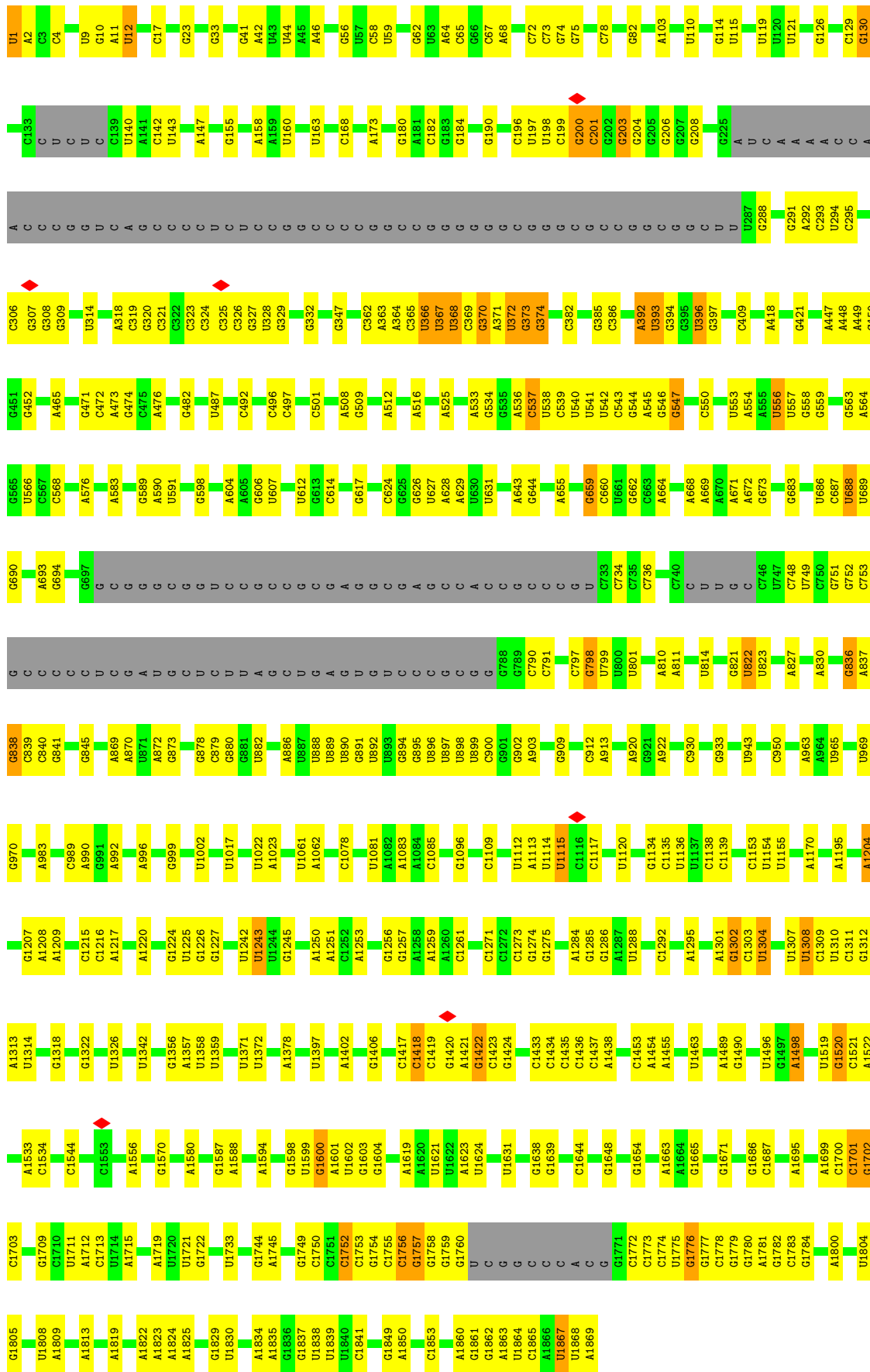


• Molecule 8: 60S ribosomal protein L41




• Molecule 9: 18S rRNA






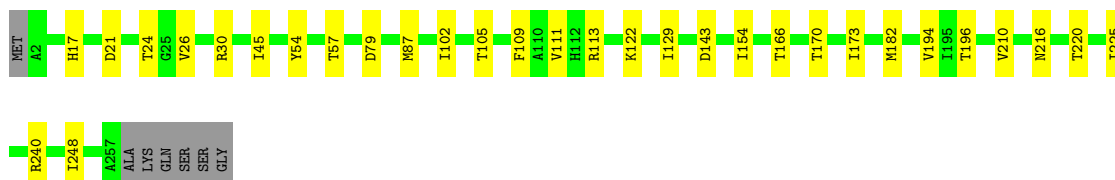
- Molecule 10: 40S ribosomal protein S11

Chain B:  78% 11% 10%




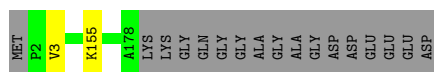
- Molecule 11: 40S ribosomal protein S4, X isoform

Chain C:  86% 12%



- Molecule 12: 40S ribosomal protein S9

Chain D:  90% 9%



- Molecule 13: 40S ribosomal protein S23

Chain E:  93% 5%




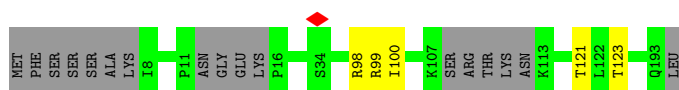
- Molecule 14: 40S ribosomal protein S30

Chain F:  56% 12% 32%



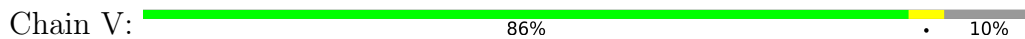
- Molecule 15: 40S ribosomal protein S7

Chain G:  89% 9%

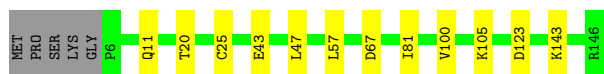
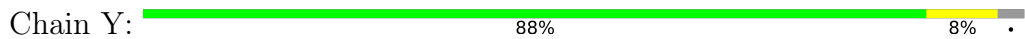


- Molecule 16: 40S ribosomal protein S27

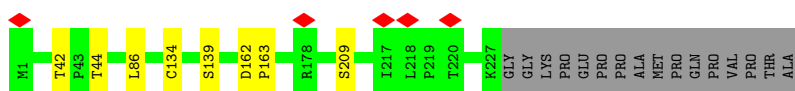
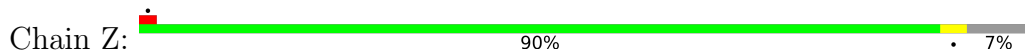
Chain H:  96%



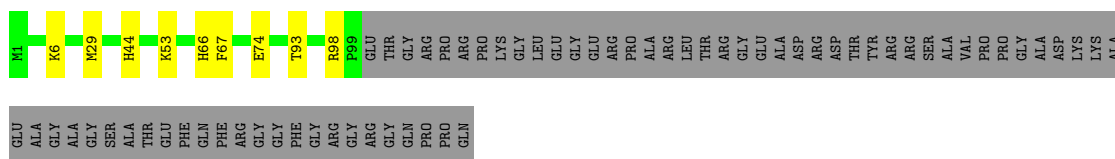
• Molecule 30: 40S ribosomal protein S16



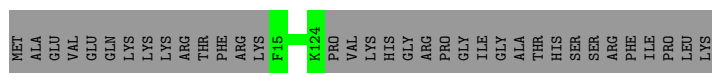
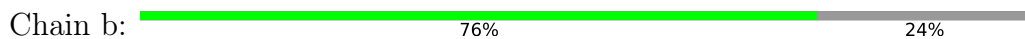
• Molecule 31: 40S ribosomal protein S3



• Molecule 32: 40S ribosomal protein S10



• Molecule 33: 40S ribosomal protein S15

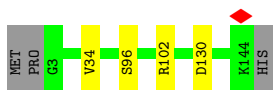


• Molecule 34: Receptor of activated protein C kinase 1

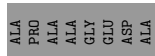
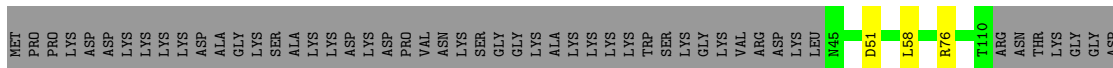


• Molecule 35: 40S ribosomal protein S19

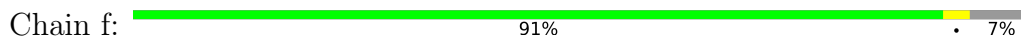




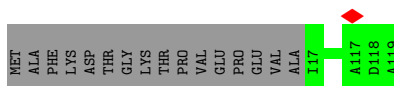
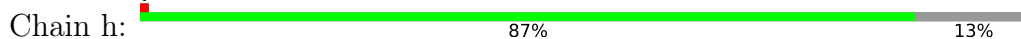
- Molecule 36: 40S ribosomal protein S25



- Molecule 37: 40S ribosomal protein S18



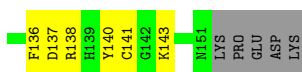
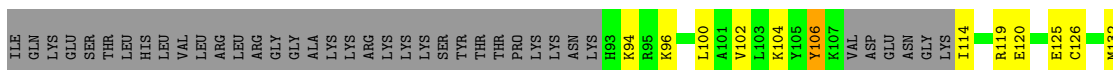
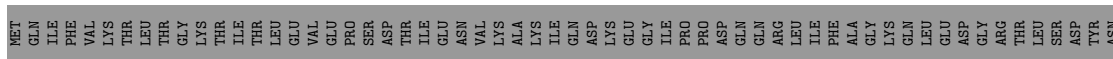
- Molecule 38: 40S ribosomal protein S20



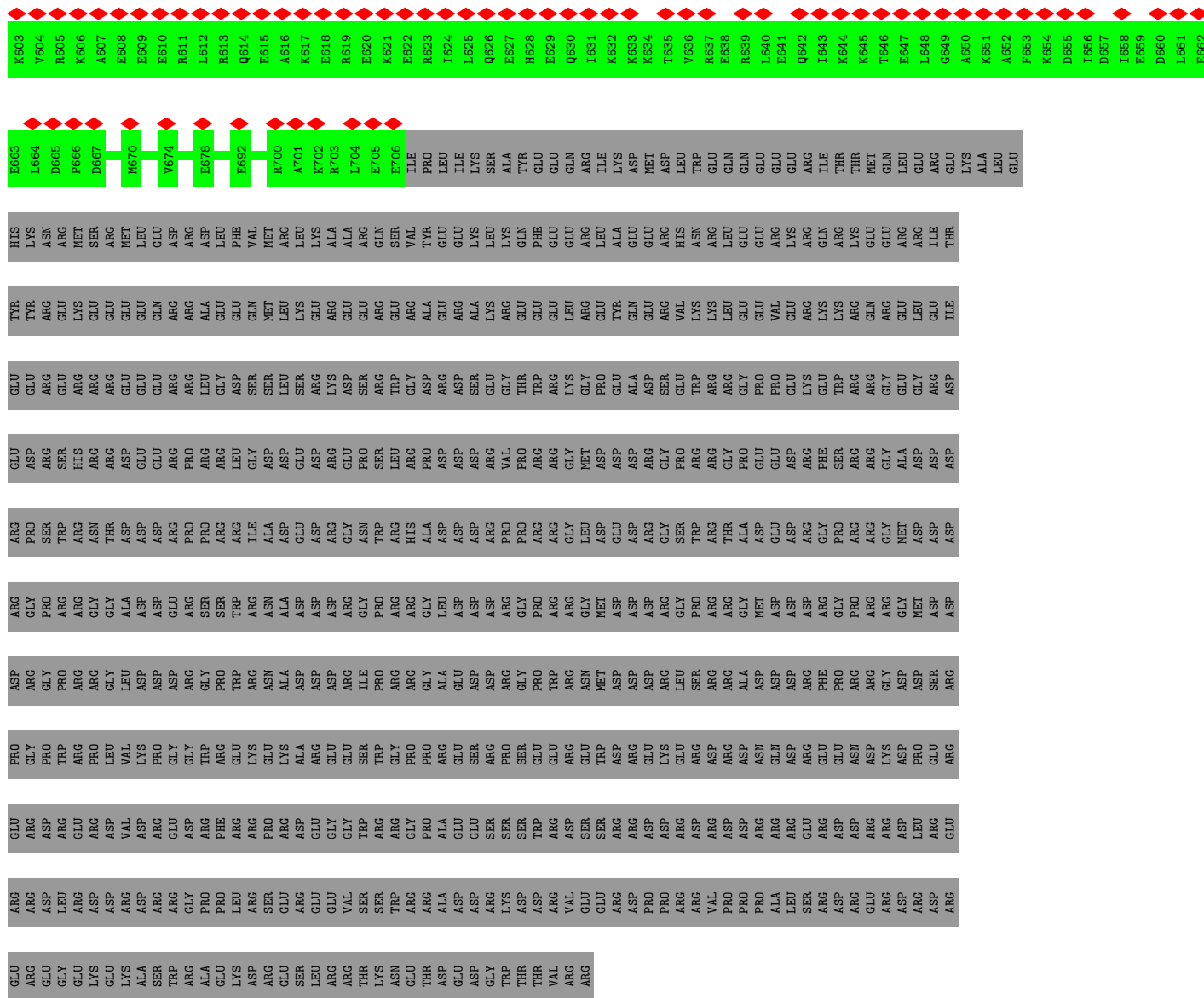
- Molecule 39: 40S ribosomal protein S29



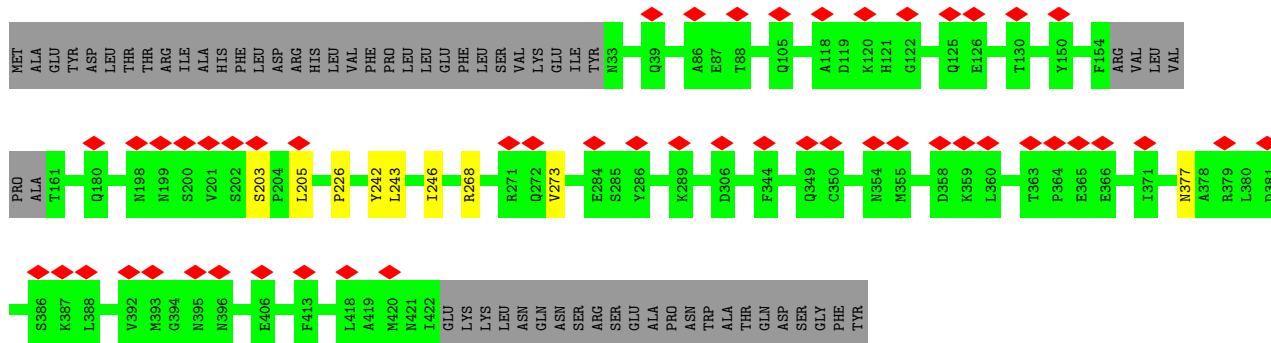
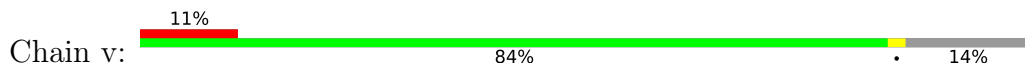
- Molecule 40: Ubiquitin-40S ribosomal protein S27a



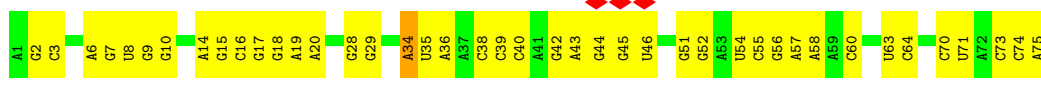
- Molecule 41: 40S ribosomal protein S12



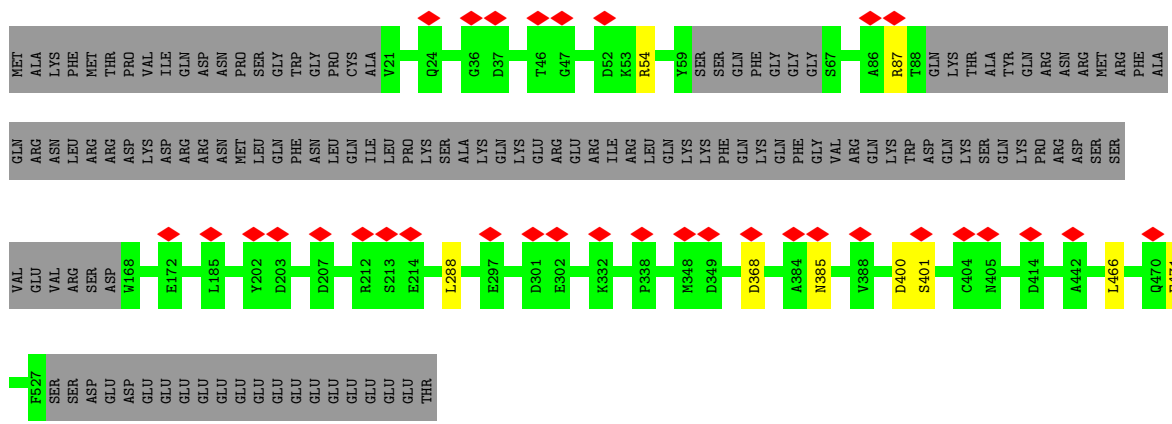
• Molecule 50: Eukaryotic translation initiation factor 3 subunit E



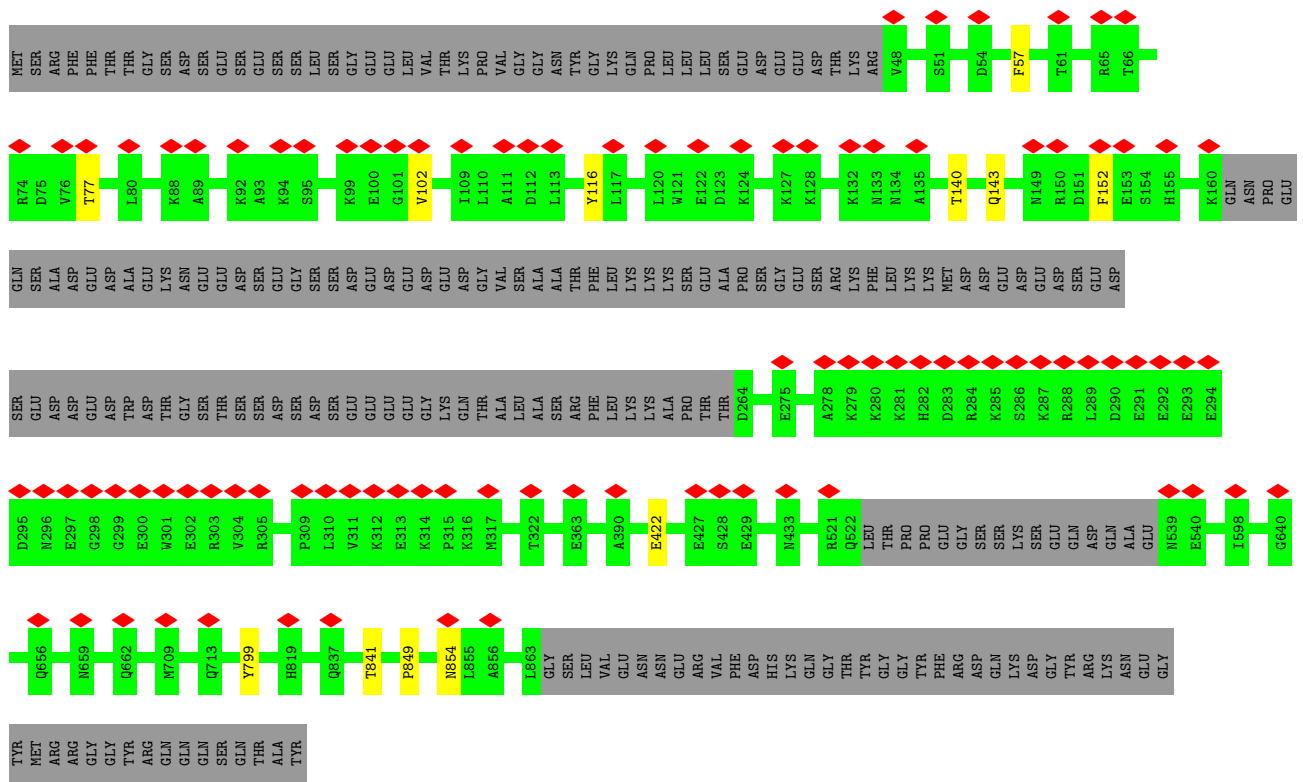
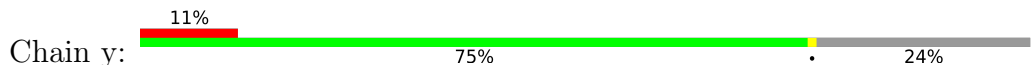
• Molecule 51: Initiator Met-tRNA-i



• Molecule 52: Eukaryotic translation initiation factor 3 subunit D



• Molecule 53: Eukaryotic translation initiation factor 3 subunit C



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: OMU, UR3, MG, A2M, 5MU, PSU, MA6, 5MC, ZN, OMC, OMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

All (3) bond length outliers are listed below:

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

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1304	U	C2'-C3'-O3'	11.53	134.87	109.50
9	A	1155	U	O5'-P-OP1	-11.51	95.34	105.70
9	A	1273	C	O5'-P-OP2	-9.28	97.34	105.70
9	A	392	A	C2'-C3'-O3'	8.64	128.51	109.50
9	A	367	U	C2'-C3'-O3'	8.50	128.21	109.50
9	A	501	C	C2-N1-C1'	8.15	127.76	118.80
9	A	396	U	C2'-C3'-O3'	8.04	127.18	109.50
9	A	365	C	C2'-C3'-O3'	7.74	126.53	109.50
9	A	996	A	O4'-C1'-N9	7.68	114.35	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1756	C	C2-N1-C1'	7.64	127.20	118.80
9	A	547	G	C4-N9-C1'	7.58	136.36	126.50
9	A	368	U	C2'-C3'-O3'	7.56	126.12	109.50
9	A	1115	U	C2-N1-C1'	7.51	126.71	117.70
9	A	547	G	C8-N9-C1'	-7.41	117.37	127.00
9	A	1752	C	C2-N1-C1'	7.39	126.93	118.80
9	A	366	U	C2'-C3'-O3'	7.32	125.61	109.50
9	A	1	U	P-O3'-C3'	7.10	128.22	119.70
9	A	201	C	C2'-C3'-O3'	7.06	125.04	109.50
9	A	501	C	C6-N1-C1'	-6.89	112.53	120.80
35	d	102	ARG	NE-CZ-NH1	-6.85	116.88	120.30
9	A	1	U	N1-C1'-C2'	6.84	122.89	114.00
9	A	372	U	C2'-C3'-O3'	6.83	124.63	113.70
9	A	1867	U	C2'-C3'-O3'	6.83	124.62	113.70
9	A	537	C	C2-N1-C1'	6.80	126.28	118.80
9	A	1139	C	C2-N1-C1'	6.78	126.25	118.80
1	1	599	LYS	CB-CA-C	-6.77	96.85	110.40
1	1	396	ASP	CB-CA-C	-6.77	96.87	110.40
9	A	1453	C	C2-N1-C1'	6.77	126.24	118.80
1	1	427	PRO	N-CA-CB	6.62	111.24	103.30
9	A	1422	G	C4-N9-C1'	6.60	135.08	126.50
9	A	1752	C	C6-N1-C1'	-6.59	112.89	120.80
9	A	393	U	N1-C1'-C2'	6.45	122.39	114.00
9	A	1422	G	C8-N9-C1'	-6.45	118.62	127.00
9	A	1520	G	C4-N9-C1'	6.39	134.81	126.50
24	P	138	ASP	N-CA-CB	-6.31	99.24	110.60
1	1	648	ILE	N-CA-CB	6.29	125.27	110.80
18	J	77	PRO	N-CA-C	-6.26	95.83	112.10
9	A	1756	C	C6-N1-C1'	-6.23	113.33	120.80
1	1	396	ASP	N-CA-C	-6.22	94.22	111.00
1	1	316	THR	CB-CA-C	-6.18	94.92	111.60
9	A	798	G	O5'-P-OP2	-6.14	100.17	105.70
24	P	138	ASP	CA-CB-CG	6.01	126.62	113.40
1	1	649	ALA	N-CA-CB	-5.99	101.71	110.10
9	A	1702	G	N9-C1'-C2'	-5.95	105.45	112.00
9	A	1308	U	C5'-C4'-C3'	5.93	125.50	116.00
9	A	1520	G	C8-N9-C1'	-5.90	119.33	127.00
40	k	106	TYR	CB-CG-CD1	5.88	124.53	121.00
9	A	547	G	O4'-C1'-N9	5.84	112.87	108.20
9	A	836	G	C4-N9-C1'	5.84	134.09	126.50
41	m	12	MET	N-CA-CB	5.81	121.06	110.60
9	A	130	G	C4-N9-C1'	5.79	134.03	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	659	G	C4-N9-C1'	5.76	133.99	126.50
51	w	34	A	O5'-P-OP1	5.76	117.62	110.70
51	w	35	U	C2'-C3'-O3'	5.76	122.92	113.70
13	E	71	ARG	NE-CZ-NH2	5.72	123.16	120.30
9	A	1139	C	C6-N1-C1'	-5.68	113.98	120.80
9	A	1307	U	N1-C1'-C2'	5.67	121.37	114.00
9	A	902	G	C4-N9-C1'	-5.65	119.15	126.50
9	A	1867	U	C4'-C3'-O3'	5.65	124.29	113.00
39	i	46	TYR	CB-CA-C	5.64	121.68	110.40
9	A	1359	U	O4'-C1'-N1	5.62	112.70	108.20
10	B	99	TYR	CB-CA-C	5.61	121.62	110.40
9	A	1115	U	C6-N1-C1'	-5.61	113.35	121.20
9	A	996	A	C4-N9-C1'	5.60	136.38	126.30
9	A	882	U	C2-N1-C1'	5.60	124.42	117.70
9	A	1453	C	C6-N1-C1'	-5.59	114.09	120.80
9	A	370	G	C5'-C4'-O4'	5.58	115.80	109.10
9	A	1418	C	O4'-C1'-N1	5.58	112.66	108.20
9	A	996	A	C8-N9-C1'	-5.54	117.72	127.70
9	A	537	C	N1-C2-O2	5.53	122.22	118.90
9	A	203	G	C5'-C4'-O4'	5.52	115.72	109.10
9	A	1752	C	O4'-C1'-N1	5.51	112.61	108.20
1	1	427	PRO	N-CA-C	-5.51	97.78	112.10
9	A	373	G	C4'-C3'-O3'	5.50	123.99	113.00
9	A	838	G	C5'-C4'-C3'	5.47	124.76	116.00
9	A	200	G	C5'-C4'-O4'	5.44	115.63	109.10
9	A	659	G	C8-N9-C1'	-5.41	119.96	127.00
1	1	316	THR	N-CA-C	-5.39	96.43	111.00
9	A	1757	G	C4-N9-C1'	5.39	133.51	126.50
9	A	1631	U	C5'-C4'-C3'	-5.38	107.39	116.00
25	Q	15	ARG	CG-CD-NE	5.38	123.10	111.80
9	A	537	C	C6-N1-C1'	-5.37	114.35	120.80
9	A	983	A	O4'-C1'-N9	-5.37	103.90	108.20
9	A	1022	U	C2-N1-C1'	5.36	124.13	117.70
9	A	836	G	C8-N9-C1'	-5.35	120.04	127.00
9	A	1204	A	N9-C1'-C2'	-5.35	106.12	112.00
9	A	370	G	C5'-C4'-C3'	5.34	124.54	116.00
9	A	556	U	C2-N1-C1'	5.33	124.09	117.70
9	A	130	G	C8-N9-C1'	-5.33	120.08	127.00
9	A	902	G	C8-N9-C1'	5.31	133.91	127.00
9	A	1600	G	P-O3'-C3'	5.31	126.08	119.70
9	A	1078	C	C2-N1-C1'	5.29	124.62	118.80
9	A	12	U	O4'-C1'-N1	5.28	112.42	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	374	G	C2'-C3'-O3'	5.28	122.15	113.70
24	P	101	GLY	C-N-CA	-5.28	111.21	122.30
9	A	1139	C	O4'-C1'-N1	5.24	112.39	108.20
9	A	1709	G	O4'-C1'-N9	5.23	112.39	108.20
9	A	1713	C	O4'-C1'-N1	5.23	112.38	108.20
9	A	1271	C	C2-N1-C1'	5.23	124.55	118.80
9	A	1776	G	C4-N9-C1'	5.22	133.29	126.50
9	A	1302	G	C5'-C4'-O4'	5.21	115.35	109.10
9	A	547	G	N9-C1'-C2'	-5.19	106.29	112.00
9	A	201	C	C4'-C3'-O3'	5.19	123.38	113.00
9	A	879	C	C2-N1-C1'	5.19	124.51	118.80
9	A	1261	C	C2-N1-C1'	5.18	124.50	118.80
5	6	227	LYS	N-CA-C	-5.18	97.02	111.00
41	m	12	MET	CA-CB-CG	-5.16	104.53	113.30
53	y	422	GLU	N-CA-C	-5.15	97.09	111.00
9	A	396	U	C5'-C4'-O4'	5.13	115.26	109.10
9	A	75	G	O4'-C1'-N9	-5.13	104.10	108.20
9	A	1498	A	C5'-C4'-O4'	5.11	115.23	109.10
9	A	200	G	C5'-C4'-C3'	5.11	124.17	116.00
20	L	194	ARG	CG-CD-NE	5.11	122.52	111.80
41	m	127	TYR	CB-CG-CD2	-5.07	117.96	121.00
9	A	392	A	C5'-C4'-O4'	5.07	115.18	109.10
9	A	1701	C	C2-N1-C1'	5.07	124.37	118.80
9	A	688	U	P-O3'-C3'	5.05	125.76	119.70

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	420/813 (52%)	394 (94%)	20 (5%)	6 (1%)	11	47
2	3	209/218 (96%)	205 (98%)	4 (2%)	0	100	100
3	4	251/357 (70%)	230 (92%)	18 (7%)	3 (1%)	13	50
4	5	307/564 (54%)	299 (97%)	8 (3%)	0	100	100
5	6	348/374 (93%)	320 (92%)	28 (8%)	0	100	100
7	8	313/352 (89%)	276 (88%)	36 (12%)	1 (0%)	41	76
8	9	22/25 (88%)	22 (100%)	0	0	100	100
10	B	138/158 (87%)	132 (96%)	6 (4%)	0	100	100
11	C	254/263 (97%)	246 (97%)	7 (3%)	1 (0%)	34	72
12	D	175/194 (90%)	175 (100%)	0	0	100	100
13	E	138/143 (96%)	136 (99%)	1 (1%)	1 (1%)	22	62
14	F	38/59 (64%)	37 (97%)	1 (3%)	0	100	100
15	G	171/194 (88%)	163 (95%)	8 (5%)	0	100	100
16	H	79/84 (94%)	77 (98%)	2 (2%)	0	100	100
17	I	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
18	J	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
19	K	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
20	L	218/293 (74%)	210 (96%)	8 (4%)	0	100	100
21	M	129/135 (96%)	123 (95%)	5 (4%)	1 (1%)	19	60
22	N	205/295 (70%)	196 (96%)	9 (4%)	0	100	100
23	O	209/264 (79%)	198 (95%)	10 (5%)	1 (0%)	29	68
24	P	131/151 (87%)	120 (92%)	11 (8%)	0	100	100
25	Q	97/115 (84%)	94 (97%)	2 (2%)	1 (1%)	15	54
26	R	194/208 (93%)	192 (99%)	2 (1%)	0	100	100
27	S	228/249 (92%)	225 (99%)	3 (1%)	0	100	100
28	T	123/133 (92%)	123 (100%)	0	0	100	100
29	V	180/204 (88%)	173 (96%)	6 (3%)	1 (1%)	25	65
30	Y	139/146 (95%)	137 (99%)	2 (1%)	0	100	100
31	Z	225/243 (93%)	221 (98%)	4 (2%)	0	100	100
32	a	97/165 (59%)	94 (97%)	3 (3%)	0	100	100
33	b	108/145 (74%)	104 (96%)	4 (4%)	0	100	100
34	c	311/317 (98%)	304 (98%)	7 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	d	140/145 (97%)	135 (96%)	5 (4%)	0	100	100
36	e	64/125 (51%)	62 (97%)	2 (3%)	0	100	100
37	f	140/152 (92%)	136 (97%)	4 (3%)	0	100	100
38	h	101/119 (85%)	98 (97%)	3 (3%)	0	100	100
39	i	48/56 (86%)	45 (94%)	2 (4%)	1 (2%)	7	38
40	k	49/156 (31%)	46 (94%)	2 (4%)	1 (2%)	7	40
41	m	120/132 (91%)	114 (95%)	5 (4%)	1 (1%)	19	60
42	n	61/69 (88%)	59 (97%)	2 (3%)	0	100	100
43	o	75/320 (23%)	74 (99%)	1 (1%)	0	100	100
44	p	83/113 (74%)	81 (98%)	1 (1%)	1 (1%)	13	50
45	q	86/144 (60%)	75 (87%)	9 (10%)	2 (2%)	6	36
46	r	273/315 (87%)	249 (91%)	23 (8%)	1 (0%)	34	72
47	s	136/333 (41%)	120 (88%)	15 (11%)	1 (1%)	22	62
48	t	346/472 (73%)	329 (95%)	11 (3%)	6 (2%)	9	43
49	u	705/1382 (51%)	676 (96%)	28 (4%)	1 (0%)	51	85
50	v	380/445 (85%)	349 (92%)	31 (8%)	0	100	100
52	x	415/548 (76%)	385 (93%)	30 (7%)	0	100	100
53	y	691/913 (76%)	661 (96%)	29 (4%)	1 (0%)	51	85
All	All	9724/13164 (74%)	9264 (95%)	428 (4%)	32 (0%)	44	76

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	282	PRO
1	1	427	PRO
1	1	648	ILE
3	4	264	GLY
23	O	117	TRP
29	V	203	ASN
39	i	8	TRP
41	m	92	CYS
48	t	167	GLN
48	t	168	PRO
48	t	224	ILE
1	1	647	ASN
7	8	154	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	k	102	VAL
44	p	40	GLY
45	q	86	ASP
46	r	195	ILE
48	t	247	PRO
48	t	248	ARG
1	1	286	PRO
1	1	499	PRO
3	4	263	ILE
11	C	24	THR
45	q	87	ASN
47	s	190	LYS
48	t	222	ILE
53	y	849	PRO
3	4	320	PRO
13	E	137	LYS
21	M	92	ASP
25	Q	96	THR
49	u	539	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%)	96 (99%)	1 (1%)	76 86
5	6	49/335 (15%)	48 (98%)	1 (2%)	55 73
8	9	23/24 (96%)	22 (96%)	1 (4%)	29 54
10	B	129/142 (91%)	112 (87%)	17 (13%)	4 20
11	C	220/225 (98%)	190 (86%)	30 (14%)	3 19
12	D	158/168 (94%)	156 (99%)	2 (1%)	69 82
13	E	112/115 (97%)	107 (96%)	5 (4%)	27 53
14	F	33/48 (69%)	26 (79%)	7 (21%)	1 7
15	G	159/174 (91%)	154 (97%)	5 (3%)	40 62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	H	73/76 (96%)	73 (100%)	0	100	100
17	I	130/131 (99%)	129 (99%)	1 (1%)	81	89
18	J	112/113 (99%)	107 (96%)	5 (4%)	27	53
19	K	65/67 (97%)	65 (100%)	0	100	100
20	L	186/225 (83%)	179 (96%)	7 (4%)	33	58
21	M	119/122 (98%)	108 (91%)	11 (9%)	9	31
22	N	173/243 (71%)	172 (99%)	1 (1%)	86	92
23	O	192/231 (83%)	189 (98%)	3 (2%)	62	79
24	P	104/119 (87%)	98 (94%)	6 (6%)	20	47
25	Q	86/98 (88%)	83 (96%)	3 (4%)	36	60
26	R	172/180 (96%)	166 (96%)	6 (4%)	36	60
27	S	200/218 (92%)	192 (96%)	8 (4%)	31	56
28	T	107/115 (93%)	101 (94%)	6 (6%)	21	48
29	V	156/170 (92%)	149 (96%)	7 (4%)	27	53
30	Y	117/121 (97%)	105 (90%)	12 (10%)	7	27
31	Z	190/202 (94%)	182 (96%)	8 (4%)	30	55
32	a	90/136 (66%)	81 (90%)	9 (10%)	7	28
33	b	100/130 (77%)	100 (100%)	0	100	100
34	c	272/275 (99%)	264 (97%)	8 (3%)	42	64
35	d	112/115 (97%)	109 (97%)	3 (3%)	44	66
36	e	58/103 (56%)	55 (95%)	3 (5%)	23	50
37	f	123/132 (93%)	119 (97%)	4 (3%)	38	61
38	h	94/107 (88%)	94 (100%)	0	100	100
39	i	44/49 (90%)	34 (77%)	10 (23%)	1	6
40	k	47/140 (34%)	30 (64%)	17 (36%)	0	1
41	m	104/108 (96%)	87 (84%)	17 (16%)	2	14
42	n	56/62 (90%)	55 (98%)	1 (2%)	59	77
43	o	64/277 (23%)	60 (94%)	4 (6%)	18	44
44	p	74/96 (77%)	63 (85%)	11 (15%)	3	16
45	q	75/123 (61%)	51 (68%)	24 (32%)	0	2
46	r	247/280 (88%)	226 (92%)	21 (8%)	10	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	s	128/304 (42%)	111 (87%)	17 (13%)	4	20
49	u	528/1259 (42%)	519 (98%)	9 (2%)	60	78
50	v	206/406 (51%)	197 (96%)	9 (4%)	28	54
52	x	206/494 (42%)	197 (96%)	9 (4%)	28	54
53	y	564/811 (70%)	554 (98%)	10 (2%)	59	77
All	All	6354/9770 (65%)	6015 (95%)	339 (5%)	26	49

All (339) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	566	ILE
5	6	333	VAL
8	9	23	ARG
10	B	11	GLN
10	B	15	THR
10	B	33	LEU
10	B	35	ARG
10	B	37	TYR
10	B	46	THR
10	B	48	LYS
10	B	65	ASN
10	B	69	ARG
10	B	74	SER
10	B	89	ARG
10	B	91	ASP
10	B	106	HIS
10	B	111	VAL
10	B	135	SER
10	B	139	ARG
10	B	151	THR
11	C	17	HIS
11	C	21	ASP
11	C	26	VAL
11	C	30	ARG
11	C	45	ILE
11	C	54	TYR
11	C	57	THR
11	C	79	ASP
11	C	87	MET
11	C	102	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	C	105	THR
11	C	109	PHE
11	C	111	VAL
11	C	113	ARG
11	C	122	LYS
11	C	129	ILE
11	C	143	ASP
11	C	154	ILE
11	C	166	THR
11	C	170	THR
11	C	173	ILE
11	C	182	MET
11	C	194	VAL
11	C	196	THR
11	C	210	VAL
11	C	216	ASN
11	C	220	THR
11	C	225	ILE
11	C	240	ARG
11	C	248	ILE
12	D	3	VAL
12	D	155	LYS
13	E	67	ARG
13	E	105	PHE
13	E	110	HIS
13	E	139	GLU
13	E	140	ARG
14	F	80	LEU
14	F	82	ARG
14	F	93	VAL
14	F	96	GLN
14	F	98	LYS
14	F	99	LYS
14	F	103	THR
15	G	98	ARG
15	G	99	ARG
15	G	100	ILE
15	G	121	THR
15	G	123	THR
17	I	20	ARG
18	J	2	VAL
18	J	30	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	J	54	ASP
18	J	79	PHE
18	J	80	ASP
20	L	115	GLN
20	L	116	THR
20	L	120	GLN
20	L	167	ARG
20	L	227	ARG
20	L	230	THR
20	L	248	TYR
21	M	16	ILE
21	M	47	ARG
21	M	61	ILE
21	M	66	VAL
21	M	75	GLU
21	M	79	GLU
21	M	81	ARG
21	M	82	ASP
21	M	85	VAL
21	M	128	PHE
21	M	132	ARG
22	N	33	GLN
23	O	77	ASP
23	O	82	ARG
23	O	111	CYS
24	P	52	THR
24	P	67	ASP
24	P	103	ASN
24	P	143	LYS
24	P	150	ARG
24	P	151	LEU
25	Q	12	LYS
25	Q	15	ARG
25	Q	86	ASN
26	R	6	ASP
26	R	72	CYS
26	R	135	GLU
26	R	142	SER
26	R	143	LYS
26	R	182	CYS
27	S	15	LEU
27	S	28	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	S	32	MET
27	S	43	GLU
27	S	98	ARG
27	S	120	ASP
27	S	181	THR
27	S	221	LYS
28	T	9	THR
28	T	50	THR
28	T	80	ASP
28	T	100	LYS
28	T	102	THR
28	T	113	ARG
29	V	41	VAL
29	V	79	HIS
29	V	119	SER
29	V	149	GLN
29	V	187	SER
29	V	193	LYS
29	V	195	GLU
30	Y	11	GLN
30	Y	20	THR
30	Y	25	CYS
30	Y	43	GLU
30	Y	47	LEU
30	Y	57	LEU
30	Y	67	ASP
30	Y	81	ILE
30	Y	100	VAL
30	Y	105	LYS
30	Y	123	ASP
30	Y	143	LYS
31	Z	42	THR
31	Z	44	THR
31	Z	86	LEU
31	Z	134	CYS
31	Z	139	SER
31	Z	162	ASP
31	Z	163	PRO
31	Z	209	SER
32	a	6	LYS
32	a	29	MET
32	a	44	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	53	LYS
32	a	66	HIS
32	a	67	PHE
32	a	74	GLU
32	a	93	THR
32	a	98	ARG
34	c	33	SER
34	c	107	ASP
34	c	113	PHE
34	c	116	ASP
34	c	134	THR
34	c	246	TYR
34	c	265	ILE
34	c	277	THR
35	d	34	VAL
35	d	96	SER
35	d	130	ASP
36	e	51	ASP
36	e	58	LEU
36	e	76	ARG
37	f	7	GLU
37	f	60	THR
37	f	83	PHE
37	f	112	GLU
39	i	8	TRP
39	i	9	SER
39	i	12	ARG
39	i	16	GLN
39	i	19	ARG
39	i	27	ARG
39	i	30	LEU
39	i	36	LEU
39	i	39	CYS
39	i	40	ARG
40	k	94	LYS
40	k	96	LYS
40	k	100	LEU
40	k	104	LYS
40	k	106	TYR
40	k	114	ILE
40	k	119	ARG
40	k	120	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	k	125	GLU
40	k	126	CYS
40	k	132	MET
40	k	136	PHE
40	k	137	ASP
40	k	138	ARG
40	k	140	TYR
40	k	141	CYS
40	k	143	LYS
41	m	12	MET
41	m	51	VAL
41	m	52	LEU
41	m	58	GLU
41	m	62	VAL
41	m	66	GLU
41	m	74	ILE
41	m	83	LYS
41	m	91	LEU
41	m	95	ASP
41	m	96	ARG
41	m	103	VAL
41	m	109	VAL
41	m	112	LYS
41	m	117	GLU
41	m	124	ILE
41	m	127	TYR
42	n	46	VAL
43	o	240	THR
43	o	286	SER
43	o	305	TYR
43	o	310	LEU
44	p	43	THR
44	p	48	GLN
44	p	50	ILE
44	p	58	LYS
44	p	59	LEU
44	p	60	VAL
44	p	65	LYS
44	p	98	VAL
44	p	102	LEU
44	p	108	LEU
44	p	113	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	q	22	GLU
45	q	24	ARG
45	q	25	GLU
45	q	26	LEU
45	q	28	PHE
45	q	33	GLN
45	q	35	TYR
45	q	39	ILE
45	q	47	LEU
45	q	51	CYS
45	q	53	ASP
45	q	55	VAL
45	q	62	ARG
45	q	64	LYS
45	q	66	ARG
45	q	73	THR
45	q	81	LEU
45	q	83	ASP
45	q	86	ASP
45	q	99	GLU
45	q	101	ARG
45	q	103	LEU
45	q	108	GLU
45	q	109	LEU
46	r	33	TYR
46	r	34	VAL
46	r	47	LEU
46	r	48	LEU
46	r	72	VAL
46	r	76	VAL
46	r	88	ARG
46	r	89	ARG
46	r	106	LYS
46	r	121	TYR
46	r	155	HIS
46	r	179	ASN
46	r	183	ARG
46	r	194	ASP
46	r	229	LEU
46	r	240	THR
46	r	248	LEU
46	r	263	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	r	270	ASN
46	r	271	VAL
46	r	278	VAL
47	s	182	ARG
47	s	187	MET
47	s	188	ARG
47	s	190	LYS
47	s	195	VAL
47	s	200	ARG
47	s	219	PHE
47	s	227	LYS
47	s	228	LEU
47	s	234	LYS
47	s	244	LEU
47	s	266	GLN
47	s	285	ARG
47	s	290	ILE
47	s	292	GLN
47	s	304	THR
47	s	306	HIS
49	u	62	ARG
49	u	109	GLN
49	u	337	ASP
49	u	340	ARG
49	u	351	LYS
49	u	448	GLN
49	u	459	VAL
49	u	562	ARG
49	u	572	ARG
50	v	203	SER
50	v	205	LEU
50	v	226	PRO
50	v	242	TYR
50	v	243	LEU
50	v	246	ILE
50	v	268	ARG
50	v	273	VAL
50	v	377	ASN
52	x	54	ARG
52	x	87	ARG
52	x	288	LEU
52	x	368	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	x	385	ASN
52	x	400	ASP
52	x	401	SER
52	x	466	LEU
52	x	471	PHE
53	y	57	PHE
53	y	77	THR
53	y	102	VAL
53	y	116	TYR
53	y	140	THR
53	y	143	GLN
53	y	152	PHE
53	y	799	TYR
53	y	841	THR
53	y	854	ASN

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

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

5.3.3 RNA [i](#)

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

All (498) RNA backbone outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	7	14	A
6	7	15	A
6	7	16	A
6	7	18	A
6	7	19	A
6	7	20	A
6	7	22	A
6	7	24	A
6	7	25	A
6	7	26	A
6	7	28	A
9	A	2	A
9	A	4	C
9	A	10	G
9	A	11	A
9	A	12	U
9	A	17	C
9	A	23	G
9	A	33	G
9	A	41	G
9	A	42	A
9	A	44	U
9	A	46	A
9	A	56	G
9	A	58	C
9	A	59	U
9	A	62	G
9	A	64	A
9	A	65	C
9	A	67	C
9	A	68	A
9	A	72	C
9	A	73	C
9	A	74	G
9	A	78	C
9	A	82	G
9	A	103	A
9	A	110	U
9	A	114	G
9	A	115	U
9	A	126	G
9	A	129	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	130	G
9	A	140	U
9	A	142	C
9	A	143	U
9	A	147	A
9	A	155	G
9	A	158	A
9	A	160	U
9	A	163	U
9	A	168	C
9	A	173	A
9	A	180	G
9	A	182	C
9	A	184	G
9	A	190	G
9	A	196	C
9	A	197	U
9	A	198	U
9	A	199	C
9	A	200	G
9	A	201	C
9	A	203	G
9	A	204	G
9	A	206	G
9	A	208	G
9	A	288	G
9	A	291	G
9	A	292	A
9	A	293	C
9	A	294	U
9	A	295	C
9	A	306	C
9	A	307	G
9	A	308	G
9	A	309	G
9	A	314	U
9	A	318	A
9	A	319	C
9	A	320	G
9	A	321	C
9	A	323	C
9	A	324	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	325	C
9	A	326	C
9	A	327	G
9	A	328	U
9	A	329	G
9	A	332	G
9	A	347	G
9	A	362	C
9	A	363	A
9	A	364	A
9	A	366	U
9	A	367	U
9	A	368	U
9	A	369	C
9	A	370	G
9	A	371	A
9	A	372	U
9	A	373	G
9	A	374	G
9	A	382	C
9	A	385	G
9	A	386	C
9	A	392	A
9	A	393	U
9	A	394	G
9	A	396	U
9	A	397	G
9	A	409	C
9	A	418	A
9	A	421	G
9	A	447	A
9	A	448	A
9	A	449	A
9	A	450	C
9	A	452	G
9	A	465	A
9	A	471	G
9	A	472	C
9	A	473	A
9	A	474	G
9	A	476	A
9	A	482	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	487	U
9	A	492	C
9	A	496	C
9	A	497	C
9	A	508	A
9	A	512	A
9	A	516	A
9	A	525	A
9	A	533	A
9	A	534	G
9	A	536	A
9	A	537	C
9	A	538	U
9	A	539	C
9	A	540	U
9	A	541	U
9	A	542	U
9	A	543	C
9	A	544	G
9	A	545	A
9	A	546	G
9	A	547	G
9	A	550	C
9	A	553	U
9	A	554	A
9	A	556	U
9	A	557	U
9	A	558	G
9	A	559	G
9	A	563	G
9	A	564	A
9	A	566	U
9	A	568	C
9	A	576	A
9	A	583	A
9	A	589	G
9	A	590	A
9	A	591	U
9	A	598	G
9	A	604	A
9	A	606	G
9	A	607	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	614	C
9	A	617	G
9	A	624	C
9	A	626	G
9	A	627	U
9	A	628	A
9	A	629	A
9	A	631	U
9	A	643	A
9	A	655	A
9	A	659	G
9	A	660	C
9	A	662	G
9	A	664	A
9	A	668	A2M
9	A	669	A
9	A	671	A
9	A	672	A
9	A	673	G
9	A	687	C
9	A	688	U
9	A	689	U
9	A	690	G
9	A	693	A
9	A	694	G
9	A	734	C
9	A	736	C
9	A	748	C
9	A	749	U
9	A	751	G
9	A	752	G
9	A	753	C
9	A	790	C
9	A	791	C
9	A	797	C
9	A	798	G
9	A	799	U
9	A	801	U
9	A	810	A
9	A	811	A
9	A	821	G
9	A	822	PSU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	827	A
9	A	830	A
9	A	836	G
9	A	837	A
9	A	838	G
9	A	839	C
9	A	840	C
9	A	841	G
9	A	845	G
9	A	869	A
9	A	870	A
9	A	872	A
9	A	873	G
9	A	878	G
9	A	880	G
9	A	886	A
9	A	888	U
9	A	889	U
9	A	890	U
9	A	891	G
9	A	892	U
9	A	894	G
9	A	895	G
9	A	896	U
9	A	897	U
9	A	898	U
9	A	899	U
9	A	900	C
9	A	903	A
9	A	909	G
9	A	912	C
9	A	913	A
9	A	920	A
9	A	922	A
9	A	930	C
9	A	933	G
9	A	943	U
9	A	950	C
9	A	963	A
9	A	965	U
9	A	969	U
9	A	970	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	989	C
9	A	990	A
9	A	992	A
9	A	999	G
9	A	1002	U
9	A	1017	U
9	A	1023	A
9	A	1061	U
9	A	1062	A
9	A	1083	A
9	A	1085	C
9	A	1096	G
9	A	1109	C
9	A	1112	U
9	A	1113	A
9	A	1114	U
9	A	1115	U
9	A	1117	C
9	A	1120	U
9	A	1134	G
9	A	1135	C
9	A	1136	U
9	A	1138	C
9	A	1153	C
9	A	1154	U
9	A	1170	A
9	A	1195	A
9	A	1204	A
9	A	1207	G
9	A	1208	A
9	A	1209	A
9	A	1215	C
9	A	1216	C
9	A	1217	A
9	A	1220	A
9	A	1224	G
9	A	1225	U
9	A	1226	G
9	A	1227	G
9	A	1242	U
9	A	1243	PSU
9	A	1245	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1250	A
9	A	1251	A
9	A	1253	A
9	A	1256	G
9	A	1257	G
9	A	1259	A
9	A	1274	G
9	A	1275	G
9	A	1284	A
9	A	1285	G
9	A	1286	G
9	A	1288	U
9	A	1292	C
9	A	1295	A
9	A	1301	A
9	A	1302	G
9	A	1303	C
9	A	1304	U
9	A	1308	U
9	A	1309	C
9	A	1310	U
9	A	1311	C
9	A	1312	G
9	A	1313	A
9	A	1314	U
9	A	1318	G
9	A	1322	G
9	A	1326	U
9	A	1342	U
9	A	1356	G
9	A	1357	A
9	A	1358	U
9	A	1371	U
9	A	1372	U
9	A	1378	A
9	A	1397	U
9	A	1402	A
9	A	1406	G
9	A	1417	C
9	A	1418	C
9	A	1419	C
9	A	1420	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1421	A
9	A	1422	G
9	A	1423	C
9	A	1424	G
9	A	1433	C
9	A	1435	C
9	A	1436	C
9	A	1437	C
9	A	1438	A
9	A	1454	A
9	A	1455	A
9	A	1463	U
9	A	1489	A
9	A	1490	G
9	A	1496	U
9	A	1498	A
9	A	1519	U
9	A	1520	G
9	A	1521	C
9	A	1522	A
9	A	1533	A
9	A	1534	C
9	A	1544	C
9	A	1556	A
9	A	1570	G
9	A	1580	A
9	A	1587	G
9	A	1588	A
9	A	1594	A
9	A	1598	G
9	A	1599	U
9	A	1600	G
9	A	1601	A
9	A	1602	U
9	A	1603	G
9	A	1604	G
9	A	1619	A
9	A	1621	U
9	A	1623	A
9	A	1624	U
9	A	1638	G
9	A	1639	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1644	C
9	A	1648	G
9	A	1654	G
9	A	1663	A
9	A	1665	G
9	A	1671	G
9	A	1686	G
9	A	1687	C
9	A	1695	A
9	A	1699	A
9	A	1700	C
9	A	1701	C
9	A	1702	G
9	A	1711	U
9	A	1712	A
9	A	1715	A
9	A	1719	A
9	A	1721	U
9	A	1722	G
9	A	1733	U
9	A	1744	G
9	A	1745	A
9	A	1749	G
9	A	1750	C
9	A	1752	C
9	A	1753	C
9	A	1754	G
9	A	1755	C
9	A	1756	C
9	A	1757	G
9	A	1758	G
9	A	1759	G
9	A	1760	G
9	A	1772	C
9	A	1773	C
9	A	1774	C
9	A	1775	U
9	A	1776	G
9	A	1777	G
9	A	1778	C
9	A	1779	G
9	A	1780	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1781	A
9	A	1782	G
9	A	1783	C
9	A	1784	G
9	A	1800	A
9	A	1804	U
9	A	1805	G
9	A	1808	U
9	A	1809	A
9	A	1813	A
9	A	1819	A
9	A	1822	A
9	A	1823	A
9	A	1824	A
9	A	1825	A
9	A	1829	G
9	A	1834	A
9	A	1835	A
9	A	1837	G
9	A	1838	U
9	A	1839	U
9	A	1841	C
9	A	1849	G
9	A	1853	C
9	A	1860	A
9	A	1861	G
9	A	1862	G
9	A	1863	A
9	A	1864	U
9	A	1865	C
9	A	1867	U
9	A	1868	U
9	A	1869	A
51	w	2	G
51	w	3	C
51	w	6	A
51	w	7	G
51	w	8	U
51	w	9	G
51	w	10	G
51	w	14	A
51	w	15	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	w	16	C
51	w	17	G
51	w	18	G
51	w	19	A
51	w	20	A
51	w	28	G
51	w	29	G
51	w	34	A
51	w	36	A
51	w	38	C
51	w	39	C
51	w	40	C
51	w	42	G
51	w	43	A
51	w	44	G
51	w	45	G
51	w	46	U
51	w	51	G
51	w	52	G
51	w	54	U
51	w	55	C
51	w	56	G
51	w	57	A
51	w	58	A
51	w	60	C
51	w	63	U
51	w	64	C
51	w	70	C
51	w	71	U
51	w	73	C
51	w	74	C
51	w	75	A

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	1	U
9	A	9	U
9	A	196	C
9	A	197	U
9	A	201	C
9	A	203	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	291	G
9	A	293	C
9	A	366	U
9	A	368	U
9	A	370	G
9	A	371	A
9	A	392	A
9	A	393	U
9	A	396	U
9	A	686	U
9	A	687	C
9	A	688	U
9	A	797	C
9	A	798	G
9	A	838	G
9	A	839	C
9	A	989	C
9	A	1250	A
9	A	1286	G
9	A	1301	A
9	A	1304	U
9	A	1312	G
9	A	1313	A
9	A	1434	C
9	A	1519	U
9	A	1520	G
9	A	1521	C
9	A	1598	G
9	A	1599	U
9	A	1600	G
9	A	1601	A
9	A	1603	G
9	A	1699	A
9	A	1700	C
9	A	1701	C
9	A	1744	G
9	A	1753	C
9	A	1759	G
9	A	1775	U
9	A	1781	A
9	A	1824	A
9	A	1834	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1862	G
9	A	1863	A
9	A	1867	U
9	A	1868	U

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

26 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	A2M	A	27	9	18,25,26	0.72	0	18,36,39	0.69	0
9	PSU	A	823	9	18,21,22	1.15	2 (11%)	22,30,33	1.14	2 (9%)
9	OMU	A	116	9	19,22,23	0.72	0	26,31,34	0.77	0
9	UR3	A	1830	9	19,22,23	0.98	1 (5%)	26,32,35	1.84	5 (19%)
9	A2M	A	1031	9	18,25,26	0.74	0	18,36,39	0.72	0

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

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1243	PSU	C6-C5	3.36	1.39	1.35
9	A	822	PSU	C6-C5	3.32	1.39	1.35
9	A	119	PSU	C6-C5	3.25	1.39	1.35
9	A	509	OMG	C6-N1	-3.06	1.33	1.37
9	A	823	PSU	C6-C5	2.86	1.38	1.35
9	A	1081	PSU	C6-C5	2.58	1.38	1.35
9	A	1243	PSU	C2'-C1'	-2.39	1.50	1.53
9	A	612	PSU	C6-C5	2.34	1.38	1.35
9	A	119	PSU	C4-N3	-2.16	1.34	1.38
9	A	814	5MU	C4-N3	-2.16	1.34	1.38
9	A	823	PSU	C4-N3	-2.14	1.34	1.38
9	A	644	OMG	C5-C6	-2.09	1.43	1.47
9	A	683	OMG	C6-N1	-2.07	1.34	1.37
9	A	1703	OMC	C5-C4	-2.04	1.38	1.42
9	A	1830	UR3	C5-C4	-2.02	1.38	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1830	UR3	C4-N3-C2	-5.57	119.32	124.56
9	A	1850	MA6	N1-C6-N6	4.21	121.49	117.06
9	A	1830	UR3	C1'-N1-C2	3.51	122.91	116.99
9	A	1830	UR3	O4'-C1'-N1	3.17	115.60	108.36
9	A	1081	PSU	C6-C5-C4	-3.06	116.06	118.20
9	A	1830	UR3	O3'-C3'-C2'	-3.03	102.02	111.82
9	A	823	PSU	N1-C2-N3	2.92	118.44	115.13
9	A	119	PSU	C6-C5-C4	-2.82	116.23	118.20
9	A	119	PSU	N1-C2-N3	2.56	118.03	115.13
9	A	1243	PSU	N1-C2-N3	2.55	118.02	115.13
9	A	1081	PSU	C3'-C2'-C1'	2.38	104.41	101.64
9	A	814	5MU	O4-C4-C5	-2.28	122.26	124.90
9	A	823	PSU	C6-C5-C4	-2.23	116.64	118.20
9	A	509	OMG	C5-C6-N1	2.20	117.84	113.95
9	A	822	PSU	N1-C2-N3	2.14	117.56	115.13
9	A	822	PSU	O2'-C2'-C1'	-2.13	106.17	111.23
9	A	1243	PSU	O2-C2-N1	-2.02	120.57	122.79
9	A	1830	UR3	C3U-N3-C2	2.01	120.83	117.31
9	A	121	OMU	N3-C2-N1	2.01	117.55	114.89
9	A	612	PSU	N1-C2-N3	2.00	117.40	115.13

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	509	OMG	C1'-C2'-O2'-CM2
9	A	1830	UR3	O4'-C1'-N1-C6
9	A	1830	UR3	O4'-C1'-N1-C2
9	A	1850	MA6	C5-C6-N6-C10
9	A	1851	MA6	O4'-C4'-C5'-O5'
9	A	1851	MA6	C5-C6-N6-C10
9	A	668	A2M	O4'-C4'-C5'-O5'
9	A	1851	MA6	C3'-C4'-C5'-O5'
9	A	668	A2M	C3'-C4'-C5'-O5'
9	A	1850	MA6	N1-C6-N6-C10
9	A	1851	MA6	N1-C6-N6-C10
9	A	1851	MA6	C5-C6-N6-C9
9	A	159	A2M	C3'-C4'-C5'-O5'
9	A	159	A2M	O4'-C4'-C5'-O5'
9	A	116	OMU	C1'-C2'-O2'-CM2
9	A	1850	MA6	C5-C6-N6-C9
9	A	1081	PSU	C4'-C5'-O5'-P
9	A	644	OMG	C4'-C5'-O5'-P
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 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.

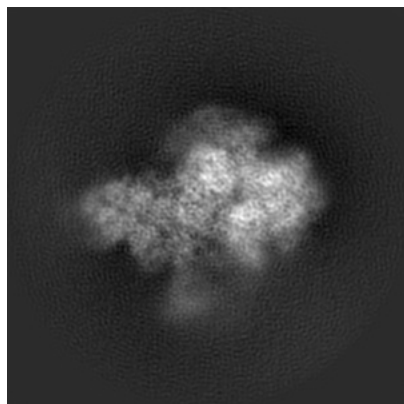
6 Map visualisation [i](#)

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.

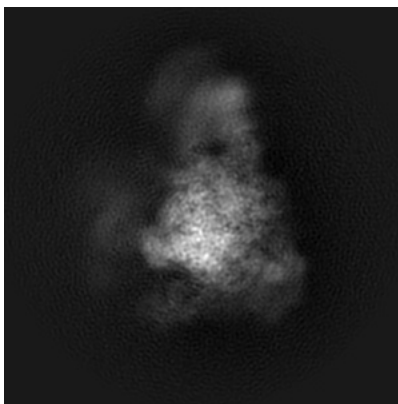
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

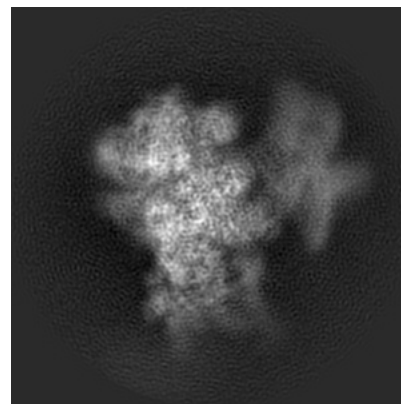
6.1.1 Primary map



X

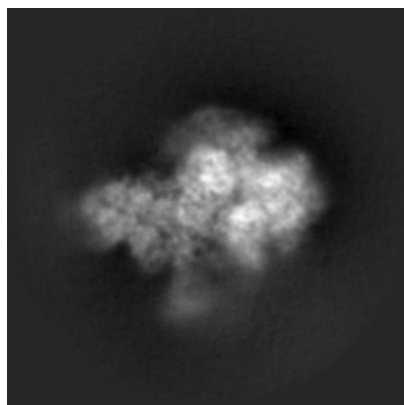


Y

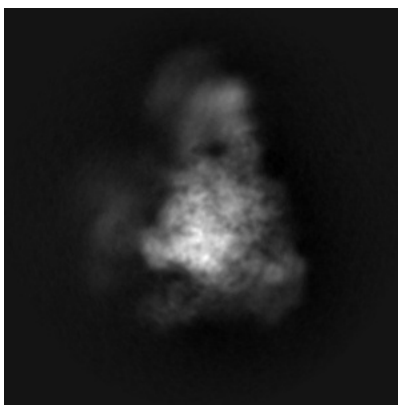


Z

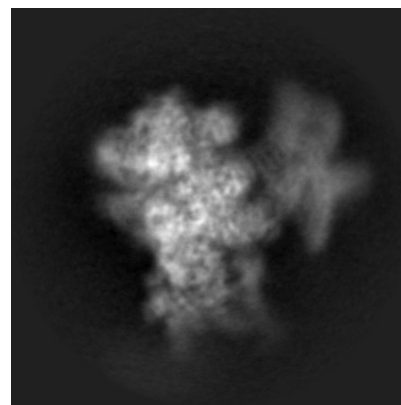
6.1.2 Raw map



X



Y

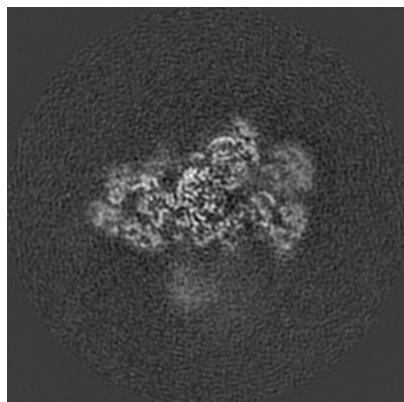


Z

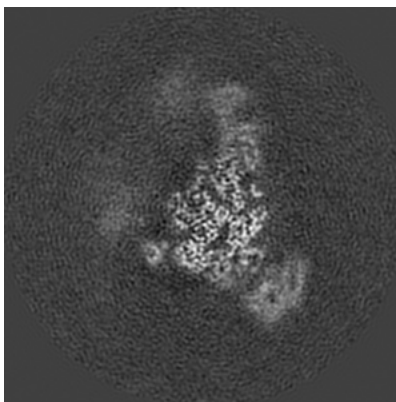
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

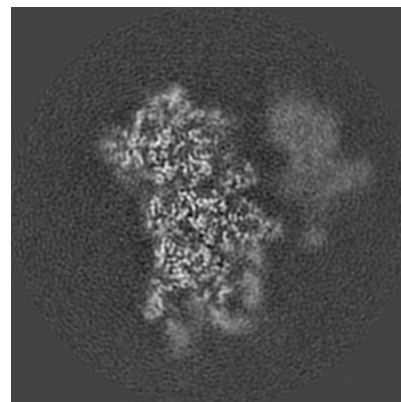
6.2.1 Primary map



X Index: 180

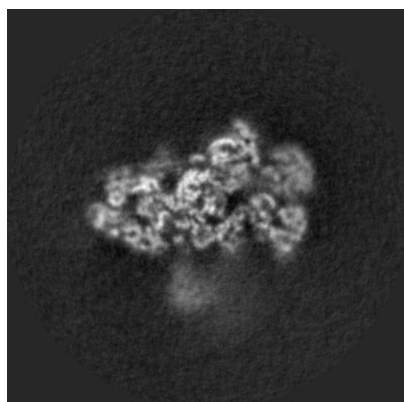


Y Index: 180

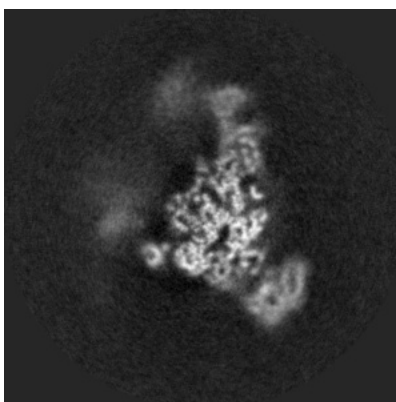


Z Index: 180

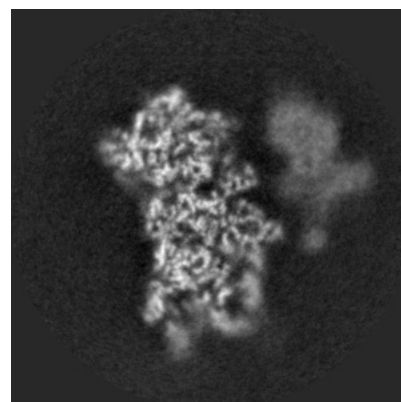
6.2.2 Raw map



X Index: 180



Y Index: 180

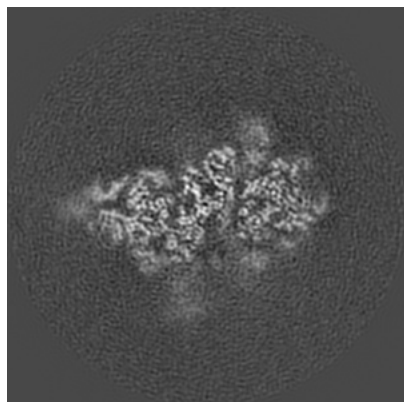


Z Index: 180

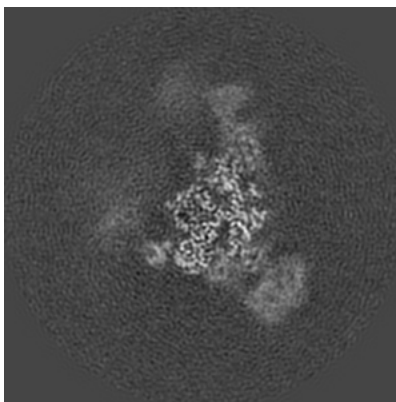
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

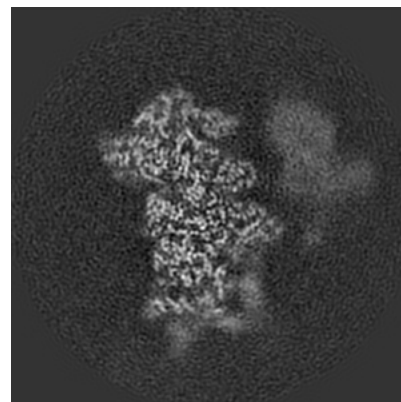
6.3.1 Primary map



X Index: 152

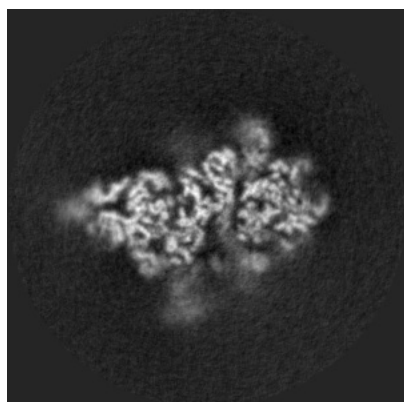


Y Index: 178

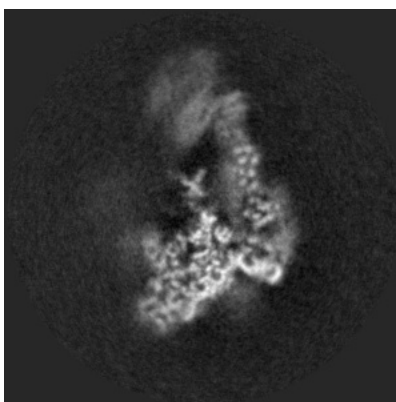


Z Index: 176

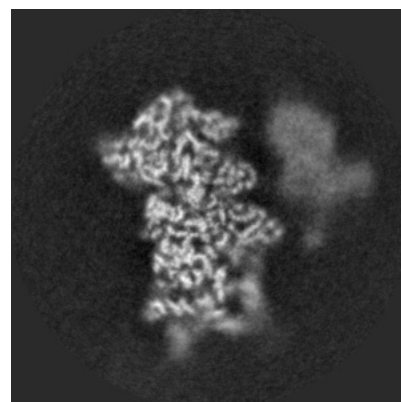
6.3.2 Raw map



X Index: 152



Y Index: 219

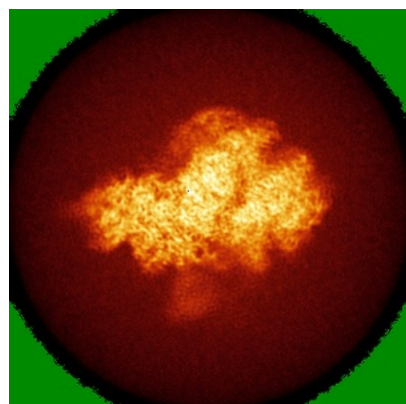


Z Index: 176

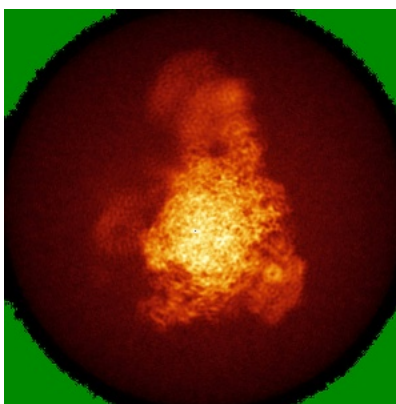
The images above show the largest variance slices of the map in three orthogonal directions.

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

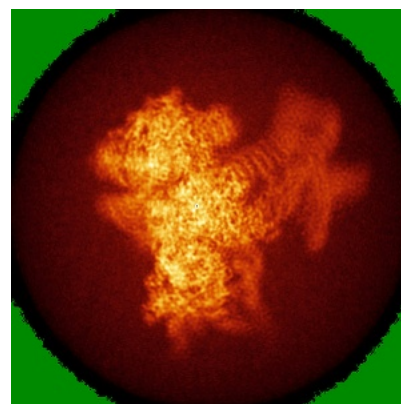
6.4.1 Primary map



X

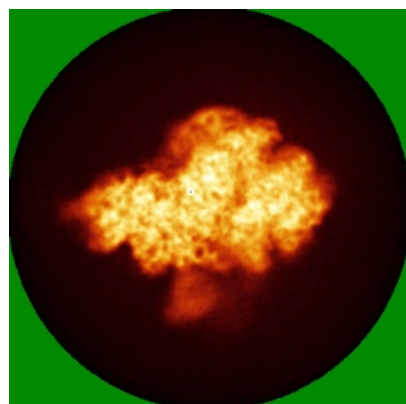


Y

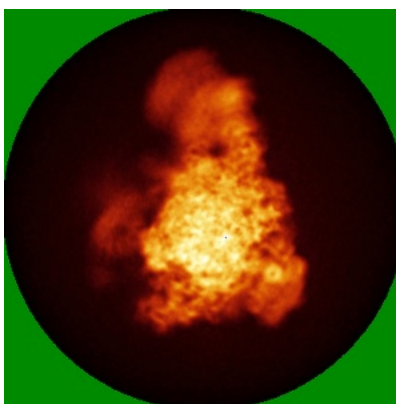


Z

6.4.2 Raw map



X



Y

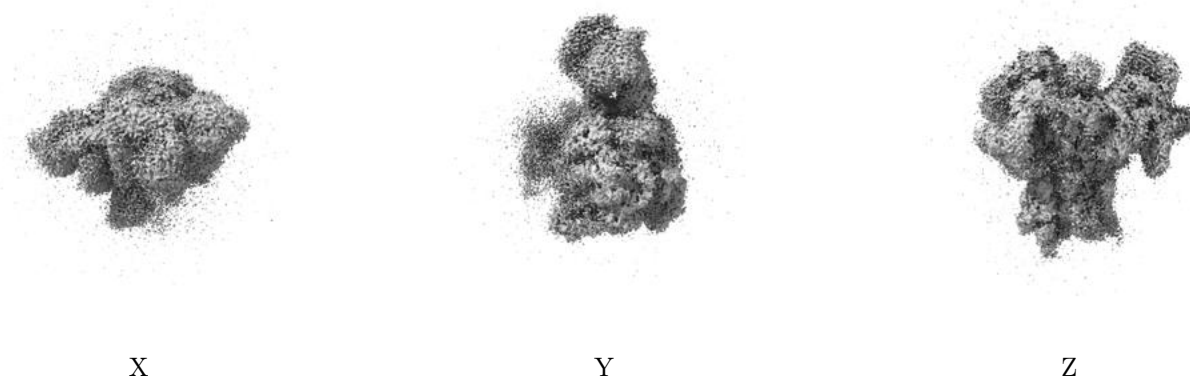


Z

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.

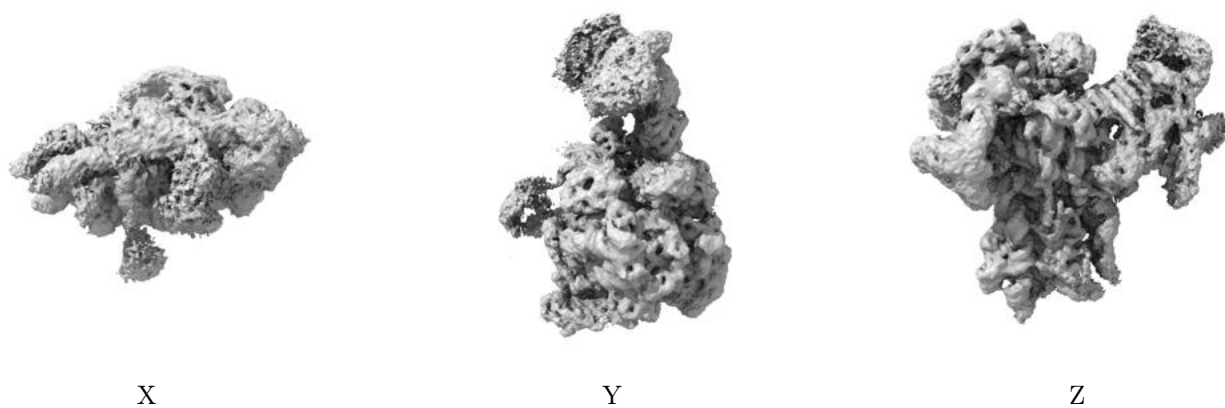
6.5 Orthogonal surface views [i](#)

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.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation [i](#)

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

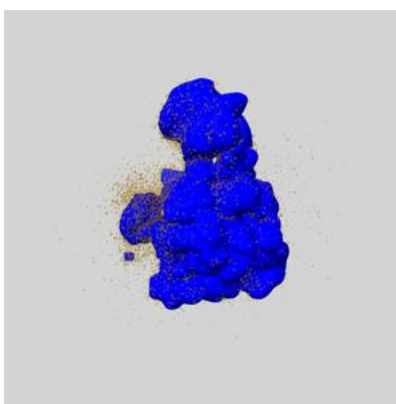
A mask typically either:

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

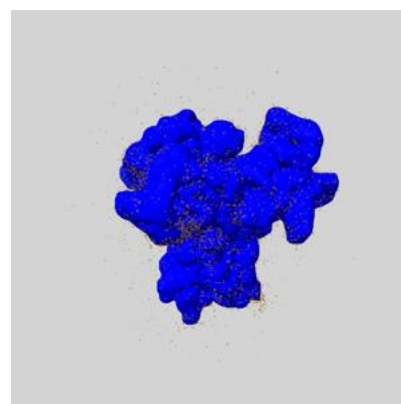
6.6.1 emd_14113_msk_1.map [i](#)



X



Y

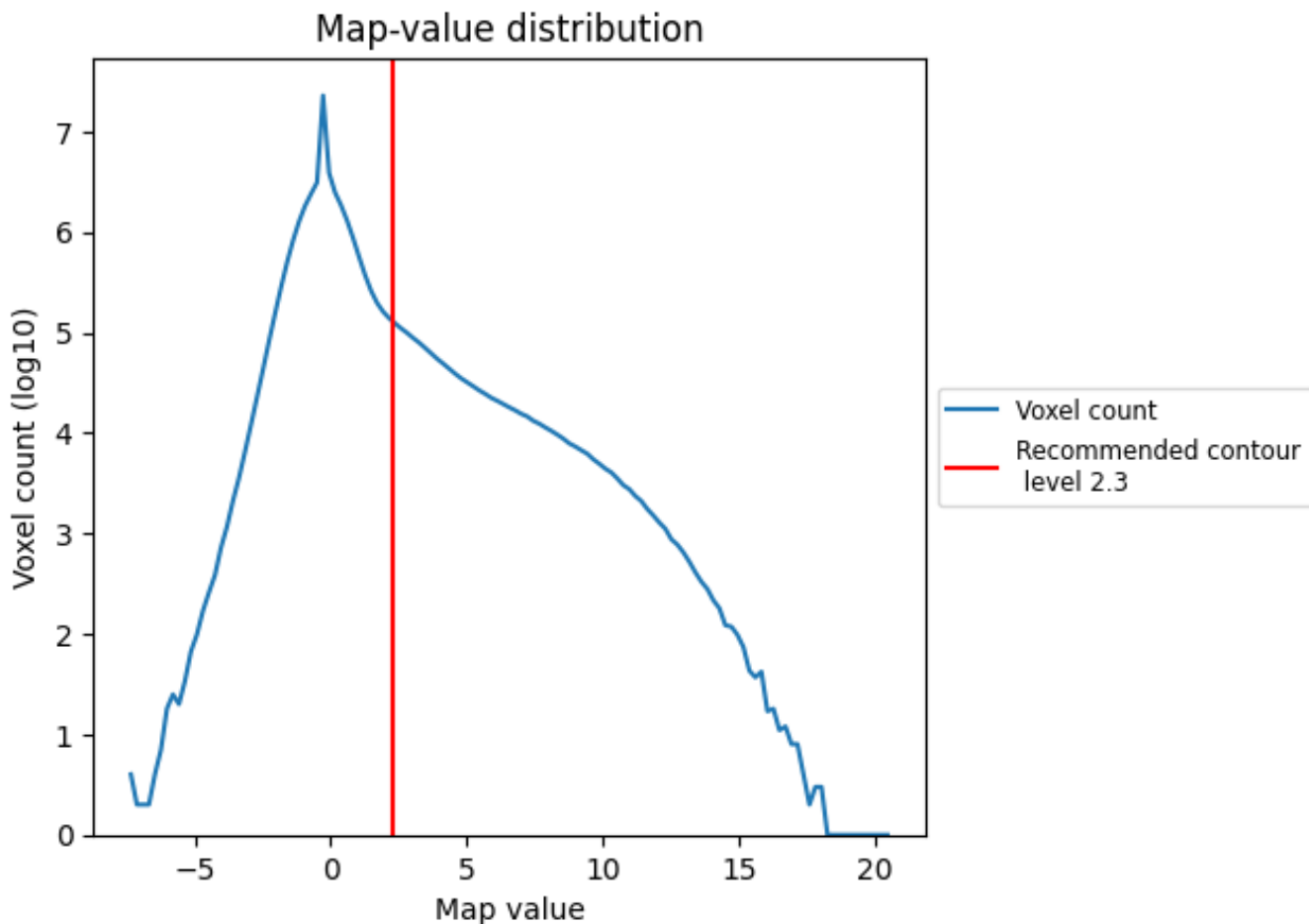


Z

7 Map analysis [i](#)

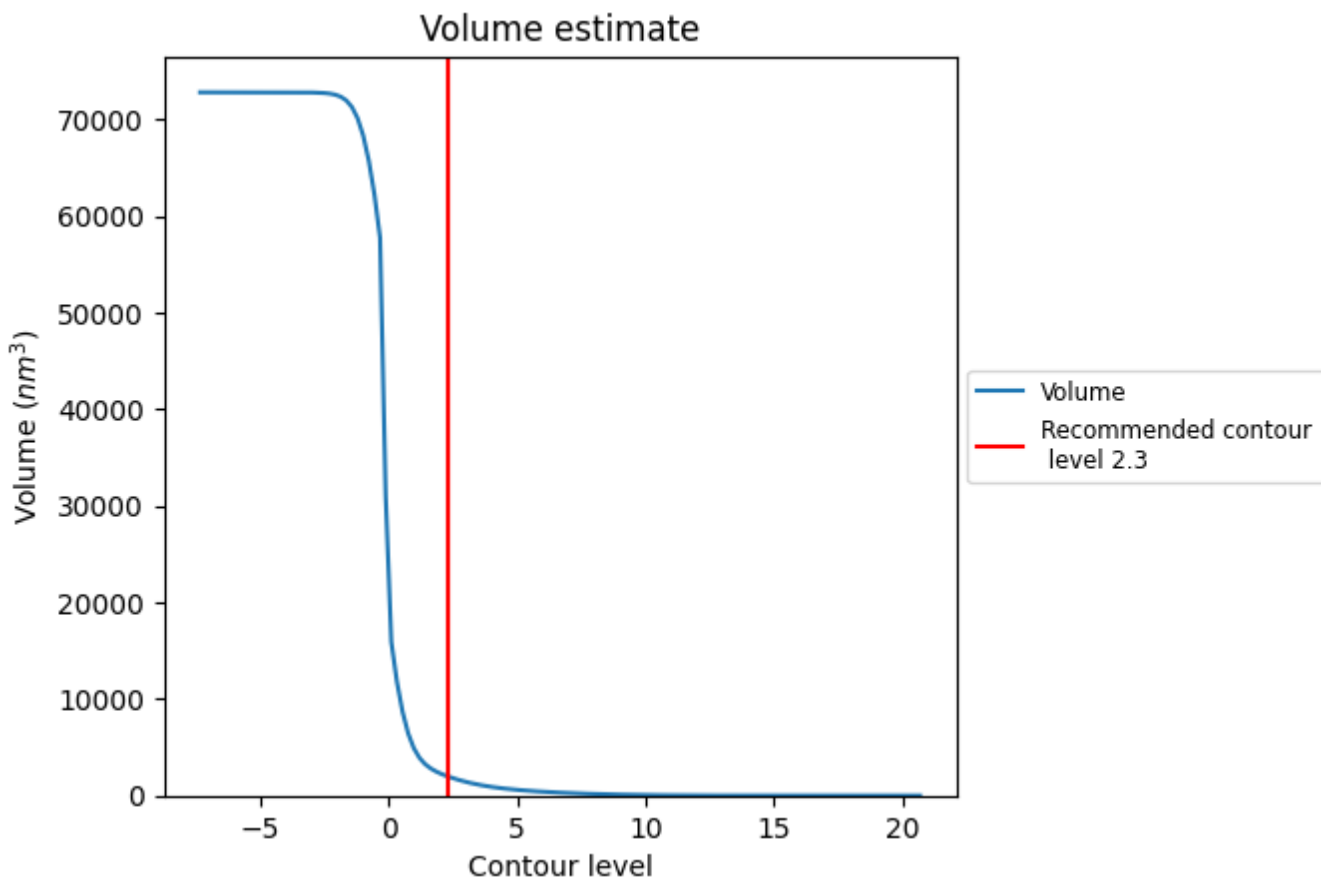
This section contains the results of statistical analysis of the map.

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.

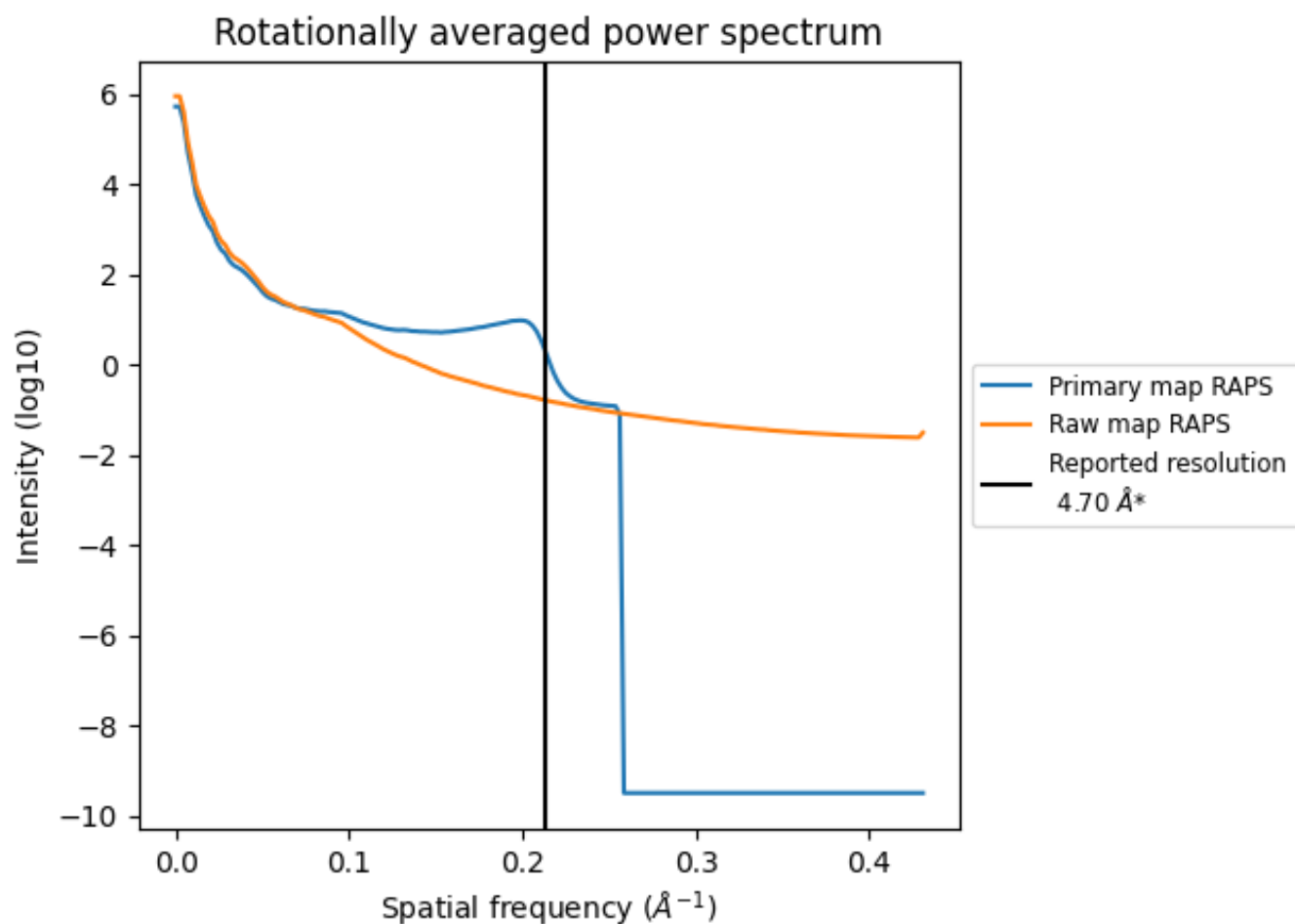
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum i

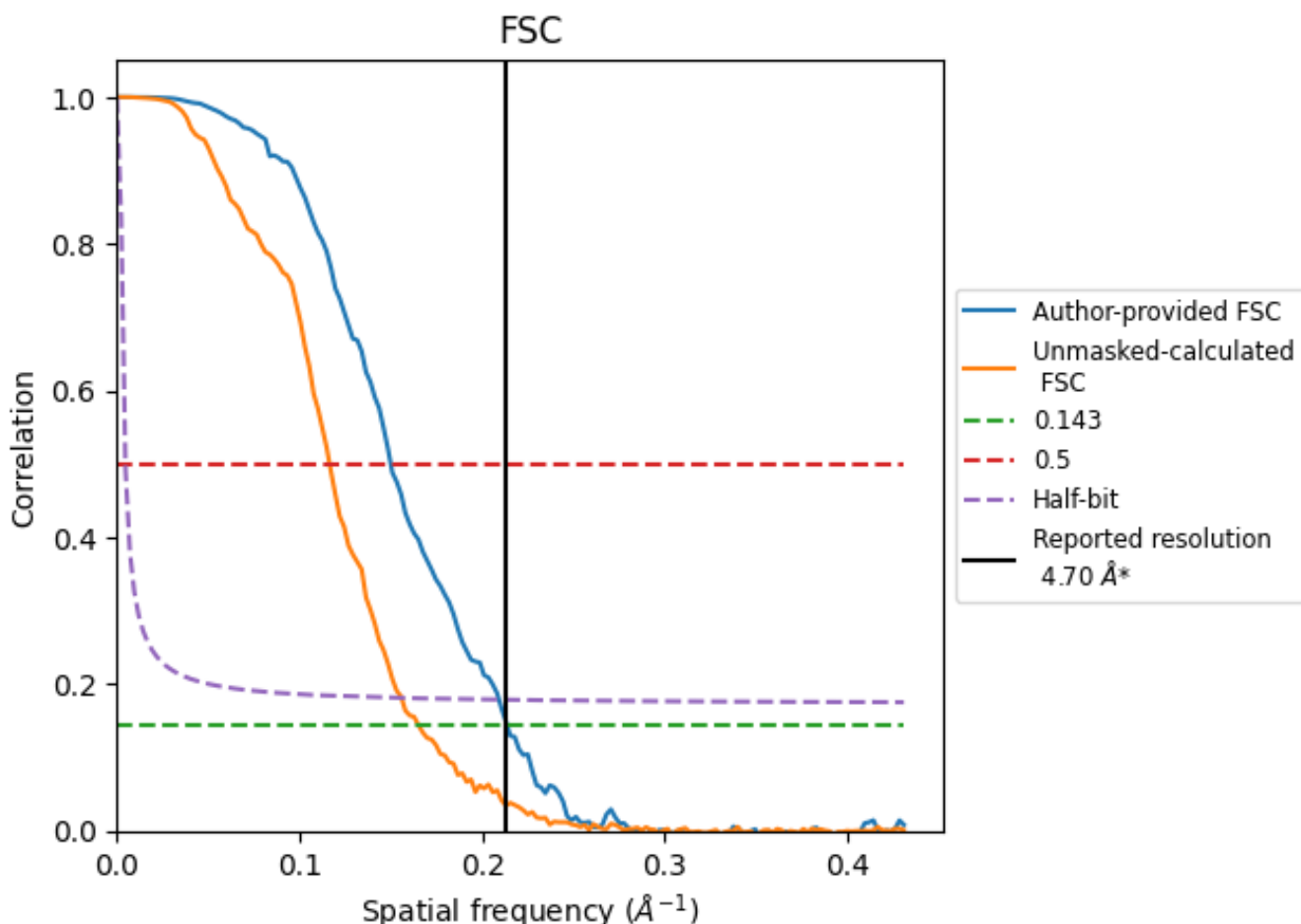


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

8 Fourier-Shell correlation [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 Å⁻¹

8.2 Resolution estimates [i](#)

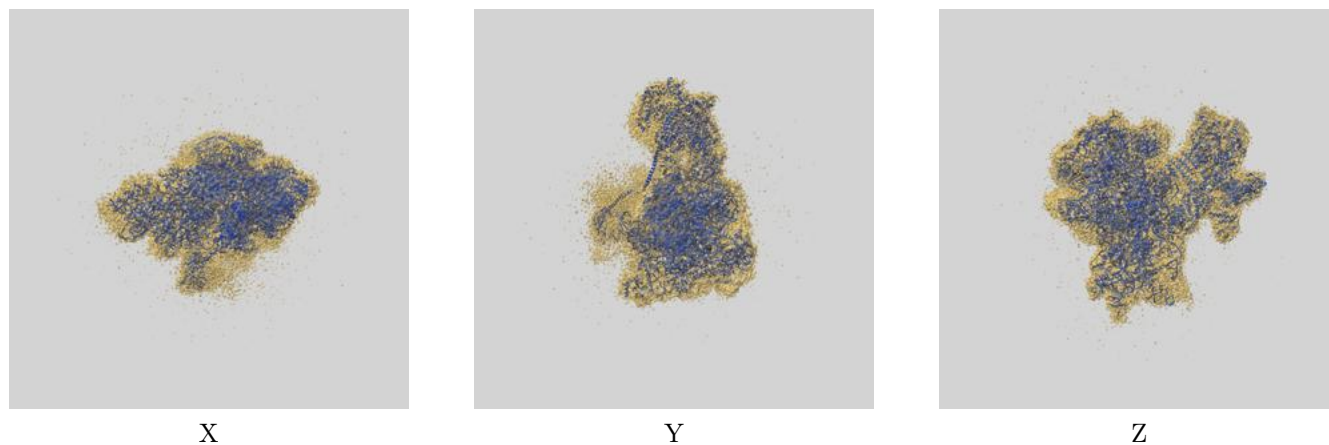
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.68	6.67	4.78
Unmasked-calculated*	6.05	8.58	6.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.05 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

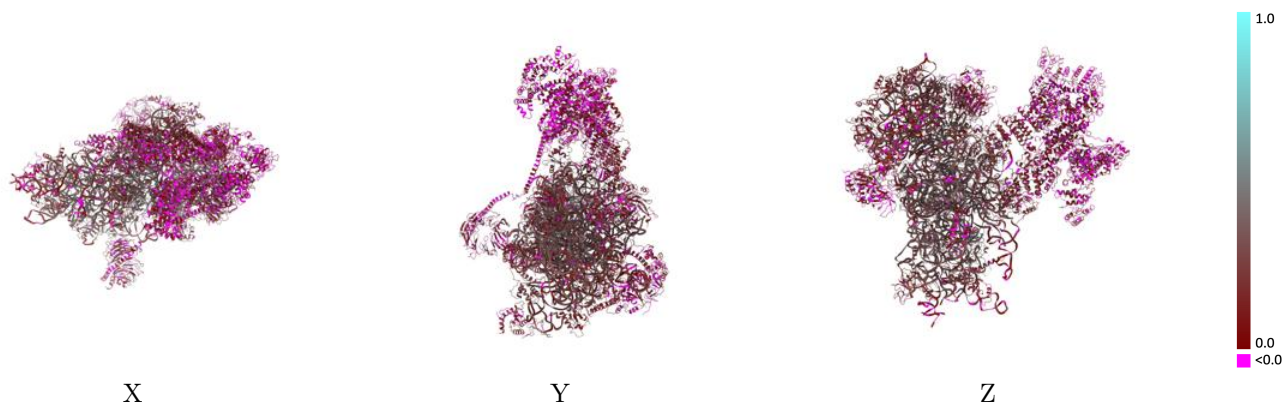
This section contains information regarding the fit between EMDB map EMD-14113 and PDB model 7QP6. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



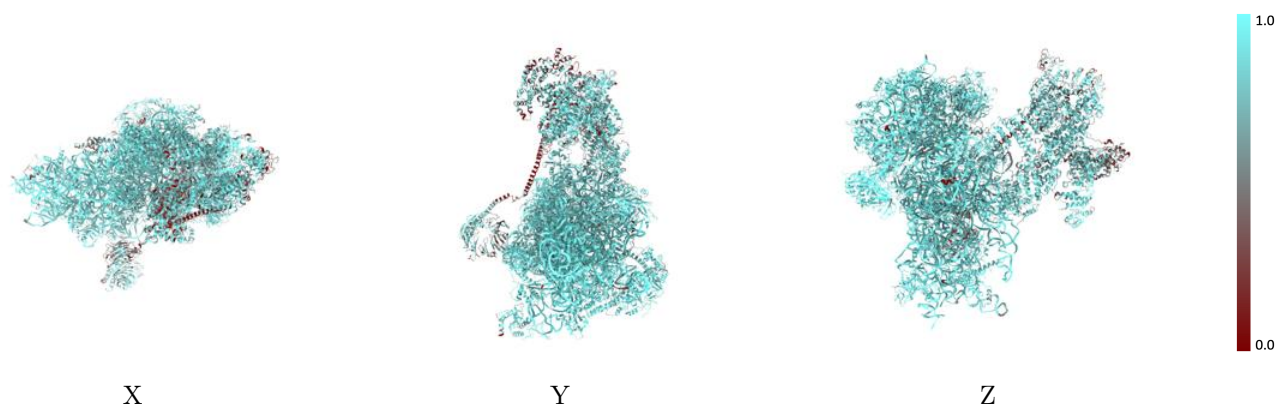
The images above show the 3D surface view of the map at the recommended contour level 2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



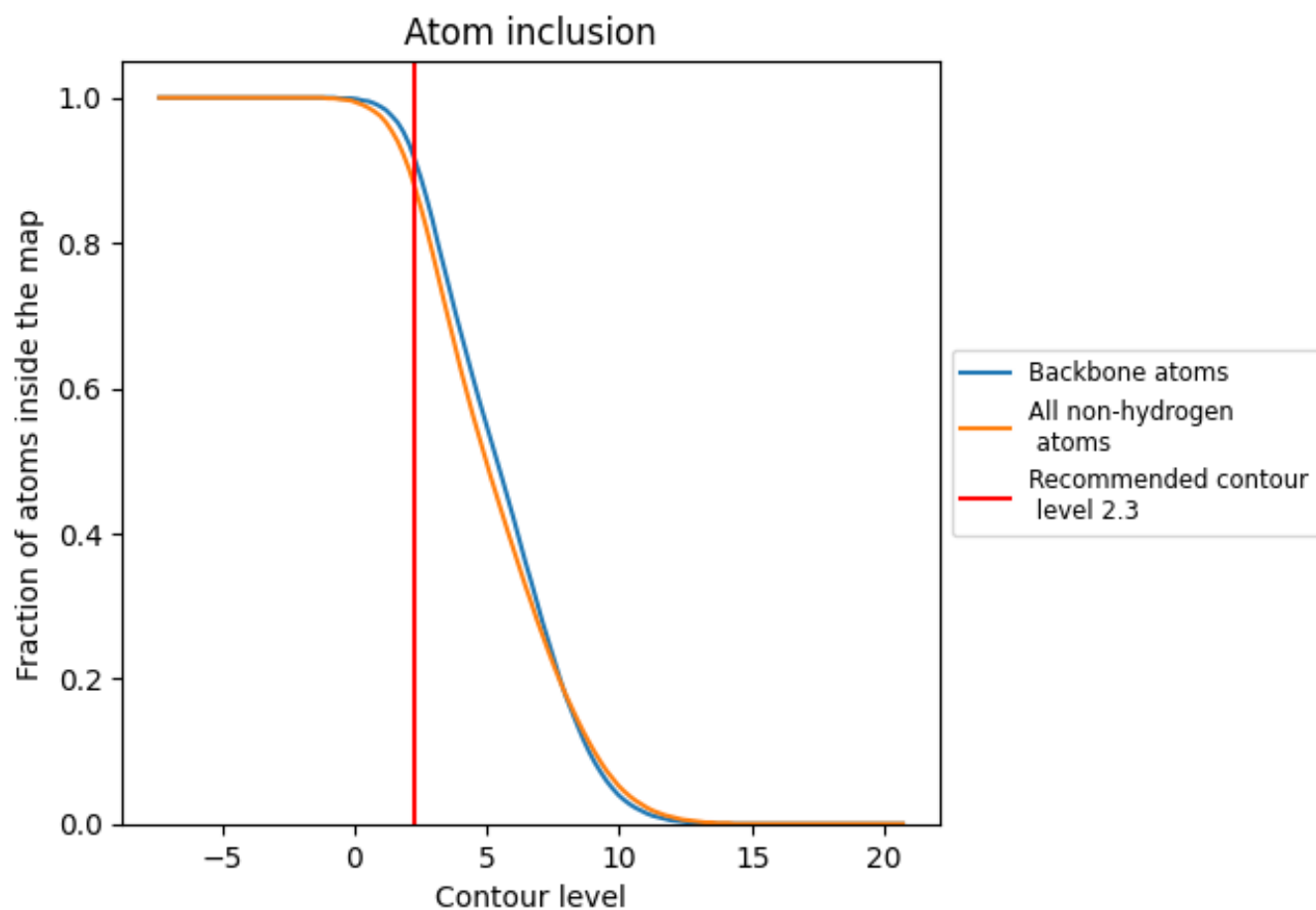
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 91% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary







































The table lists the average atom inclusion at the recommended contour level (2.3) and Q-score for the entire model and for each chain.

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



Continued on next page...

Continued from previous page...

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