



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 01:24 AM EST

PDB ID : 6MTB
EMDB ID : EMD-9237
Title : Rabbit 80S ribosome with P- and Z-site tRNAs (unrotated state)
Authors : Brown, A.; Baird, M.R.; Yip, M.C.J.; Murray, J.; Shao, S.
Deposited on : 2018-10-19
Resolution : 3.60 Å (reported)
Based on initial model : 5LZV

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:

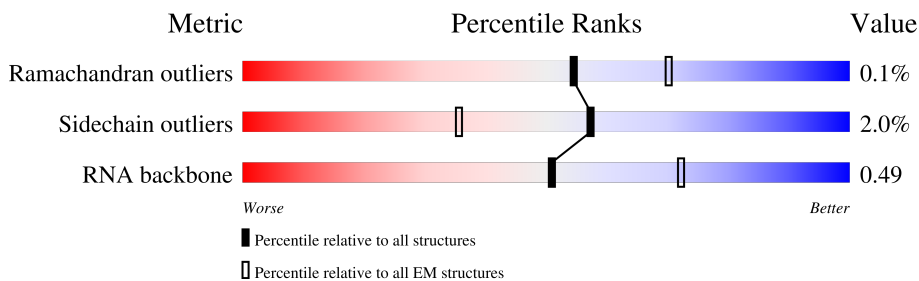
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 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.



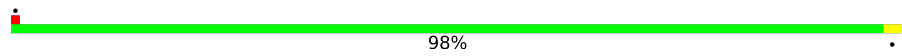
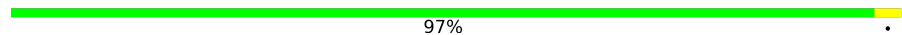
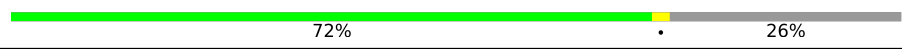
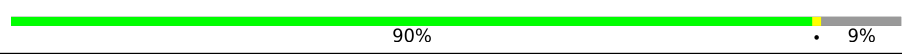

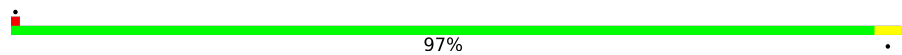
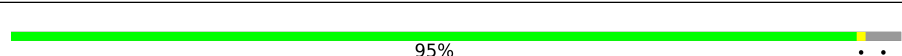
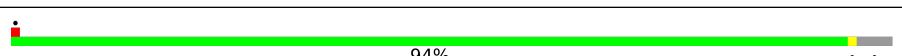
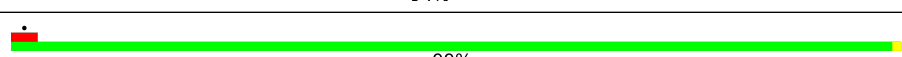
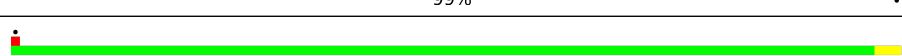
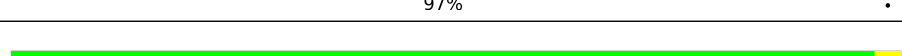
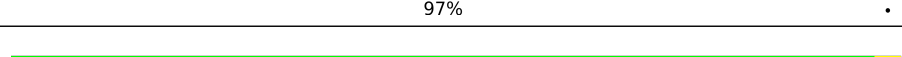
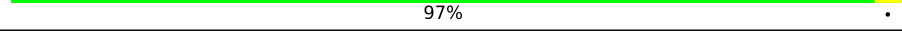
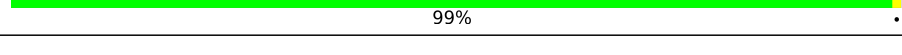
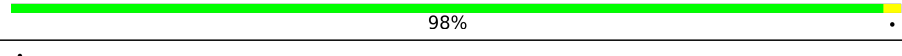
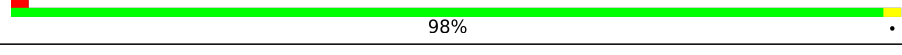
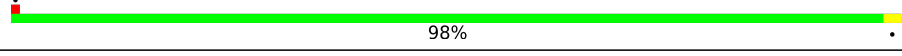
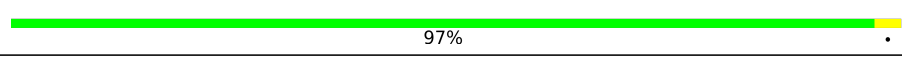
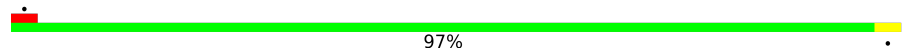
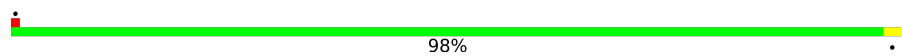
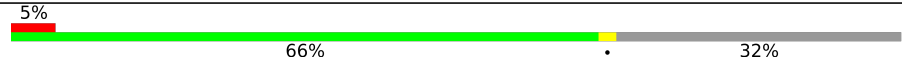

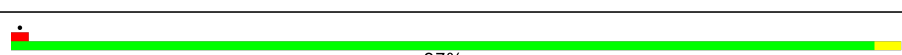
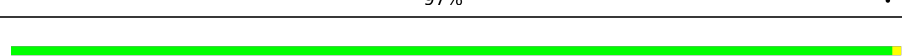
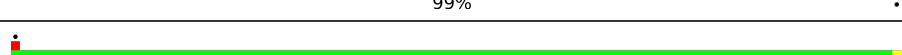
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	7	
2	2	76	
3	4	75	
4	5	3597	
5	7	120	
6	8	151	
7	A	248	
8	B	394	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	C	362	 98%
10	D	293	 97%
11	E	291	 72% 26%
12	F	247	 90% 9%
13	G	319	 70% 27%
14	H	190	 97%
15	I	214	 95%
16	J	178	 94%
17	L	210	 99%
18	M	138	 97%
19	N	203	 97%
20	O	199	 97%
21	P	153	 99%
22	Q	187	 98%
23	R	180	 98%
24	S	176	 98%
25	T	159	 97%
26	U	99	 97%
27	V	131	 98%
28	W	157	 5% 66% 32%
29	X	118	 100%
30	Y	134	 97%
31	Z	135	 99%
32	a	147	 99%
33	b	245	 40% 58%

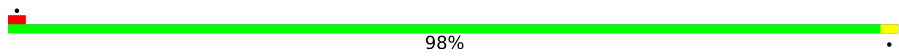
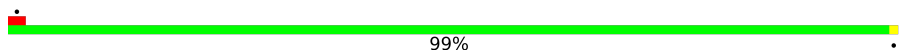
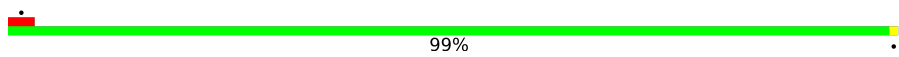

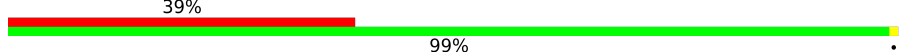
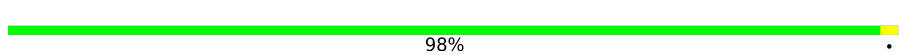
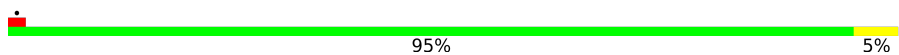
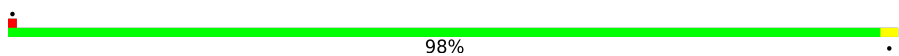
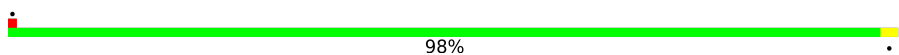
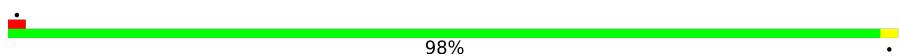
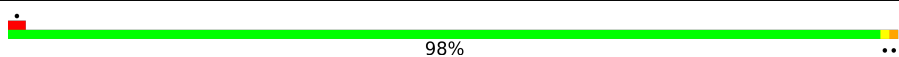
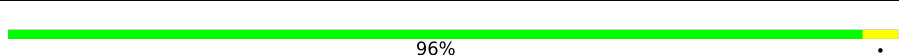
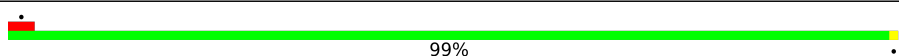
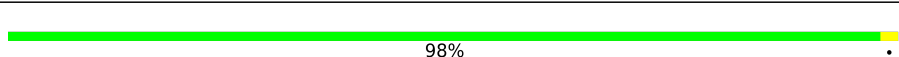
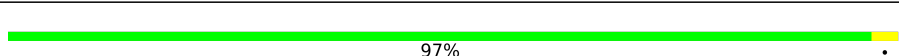
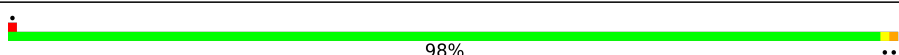
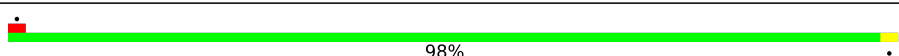
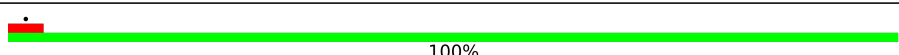
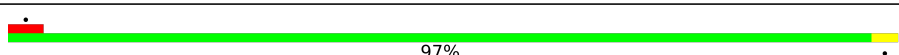
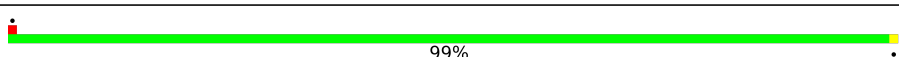
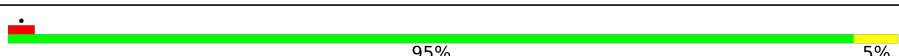
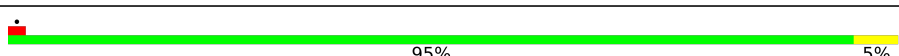
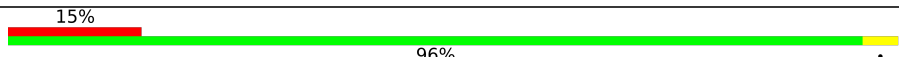

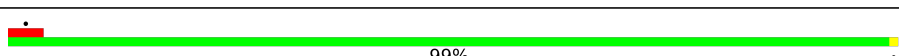
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	c	98	97%
35	d	107	98%
36	e	128	98%
37	f	109	97%
38	g	114	96%
39	h	122	98%
40	i	102	98%
41	j	86	99%
42	k	69	99%
43	l	50	96%
44	m	52	94% 6%
45	n	25	96%
46	o	103	98%
47	p	91	100%
48	r	124	96%
49	u	206	45% 93% 7%
50	9	1698	67% 29% 5%
51	AA	217	98%
52	BB	213	98%
53	CC	221	98%
54	DD	228	96%
55	EE	262	98%
56	FF	204	88% 9%
57	GG	237	99%
58	HH	194	94% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	II	206	 98%
60	JJ	185	 99%
61	KK	96	 99%
62	LL	158	 89% 9%
63	MM	117	 39% 99%
64	NN	149	 98%
65	OO	136	 95% 5%
66	PP	120	 98%
67	QQ	142	 98%
68	RR	132	 98%
69	SS	144	 98%
70	TT	141	 96%
71	UU	100	 99%
72	VV	83	 98%
73	WW	129	 97%
74	XX	141	 98%
75	YY	124	 98%
76	ZZ	75	 100%
77	aa	101	 97%
78	bb	83	 99%
79	cc	62	 95% 5%
80	dd	55	 95% 5%
81	ee	55	 15% 96%
82	ff	68	 38% 79% 18%
83	gg	313	 99%

2 Entry composition [i](#)

There are 85 unique types of molecules in this entry. The entry contains 216003 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 RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	7	149	67	27	48	7	0	0

- Molecule 2 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	76	1616	723	291	527	75	0	0

- Molecule 3 is a RNA chain called Z-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	75	1593	712	281	526	74	0	0

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	5	3597	77254	34469	14127	25061	3597	0	0

- Molecule 5 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	7	120	2558	1141	456	842	119	0	0

- Molecule 6 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	8	151	3209	1433	564	1062	150	0	0

- Molecule 7 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	A	248	1898	1189	389	314	6	0	0

- Molecule 8 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	B	394	3172	2020	597	542	13	0	0

- Molecule 9 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C	362	2884	1813	577	480	14	0	0

- Molecule 10 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D	293	2391	1512	438	427	14	0	0

- Molecule 11 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	E	216	1729	1115	329	282	3	0	0

- Molecule 12 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	F	225	1875	1205	358	303	9	0	0

- Molecule 13 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	G	233	1879	1199	361	315	4	0	0

- Molecule 14 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 15 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 16 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 17 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 18 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 19 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 20 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 21 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	P	153	1242	777	241	215	9	0	0

- Molecule 22 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Q	187	1515	946	315	250	4	0	0

- Molecule 23 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	R	180	1508	933	328	238	9	0	0

- Molecule 24 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	S	176	1462	930	285	236	11	0	0

- Molecule 25 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	T	159	1298	823	252	217	6	0	0

- Molecule 26 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	U	99	809	519	141	147	2	0	0

- Molecule 27 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	V	131	979	618	184	172	5	0	0

- Molecule 28 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	W	106	860	538	174	144	4	0	0

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	X	118	967	618	181	167	1	0	0

- Molecule 30 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Y	134	1115	700	226	186	3	0	0

- Molecule 31 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Z	135	1107	714	208	182	3	0	0

- Molecule 32 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	a	147	1162	734	239	185	4	0	0

- Molecule 33 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	b	104	848	527	189	129	3	0	0

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	c	98	761	481	134	140	6	0	0

- Molecule 35 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 36 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 37 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 38 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 39 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 40 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 41 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 42 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	k	69	569	366	103	99	1	0	0

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	l	50	447	286	96	64	1	0	0

- Molecule 44 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	m	52	430	267	90	67	6	0	0

- Molecule 45 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	n	25	239	145	64	27	3	0	0

- Molecule 46 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	o	103	842	528	172	136	6	0	0

- Molecule 47 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	p	91	708	445	136	120	7	0	0

- Molecule 48 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	r	124	994	616	205	167	6	0	0

- Molecule 49 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	206	Total	C	N	O	S	0	0
			1654	1058	297	291	8		

- Molecule 50 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	9	1698	Total	C	N	O	P	0	0
			36291	16217	6509	11868	1697		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AA	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 52 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 53 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	CC	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 54 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	DD	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 55 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	EE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 56 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	FF	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 57 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	GG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 58 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	HH	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 59 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	II	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 60 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	JJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 61 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	KK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 62 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LL	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 63 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	MM	117	908	570	161	169	8	0	0

- Molecule 64 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	NN	149	1202	770	228	203	1	0	0

- Molecule 65 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	OO	136	1016	621	199	190	6	0	0

- Molecule 66 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	PP	120	997	635	187	168	7	0	0

- Molecule 67 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	QQ	142	1128	717	213	195	3	0	0

- Molecule 68 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	RR	132	1068	670	199	195	4	0	0

- Molecule 69 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	SS	144	1190	746	241	202	1	0	0

- Molecule 70 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	TT	141	1097	688	211	195	3	0	0

- Molecule 71 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	UU	100	795	498	152	141	4	0	0

- Molecule 72 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	VV	83	636	393	117	121	5	0	0

- Molecule 73 is a protein called 40S ribosomal protein S15a.

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

- Molecule 74 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	XX	141	1098	693	219	183	3	0	0

- Molecule 75 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	YY	124	1011	640	198	168	5	0	0

- Molecule 76 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	ZZ	75	598	382	111	104	1	0	0

- Molecule 77 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	aa	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 78 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	bb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 79 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	cc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 80 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	dd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 81 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	ee	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 82 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	ff	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 83 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	5	199	Total 199	Mg 199	0
84	7	7	Total 7	Mg 7	0
84	8	7	Total 7	Mg 7	0
84	A	1	Total 1	Mg 1	0
84	P	1	Total 1	Mg 1	0
84	Q	1	Total 1	Mg 1	0
84	V	1	Total 1	Mg 1	0
84	a	1	Total 1	Mg 1	0
84	9	78	Total 78	Mg 78	0
84	aa	1	Total 1	Mg 1	0

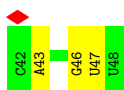
- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	g	1	Total 1	Zn 1	0
85	j	1	Total 1	Zn 1	0
85	m	1	Total 1	Zn 1	0
85	o	1	Total 1	Zn 1	0
85	p	1	Total 1	Zn 1	0
85	aa	1	Total 1	Zn 1	0
85	dd	1	Total 1	Zn 1	0
85	ff	1	Total 1	Zn 1	0

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.

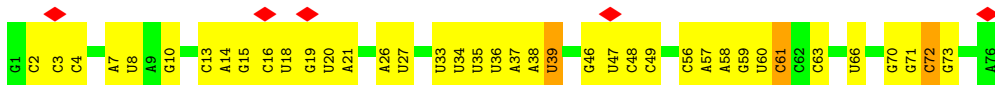
- Molecule 1: mRNA



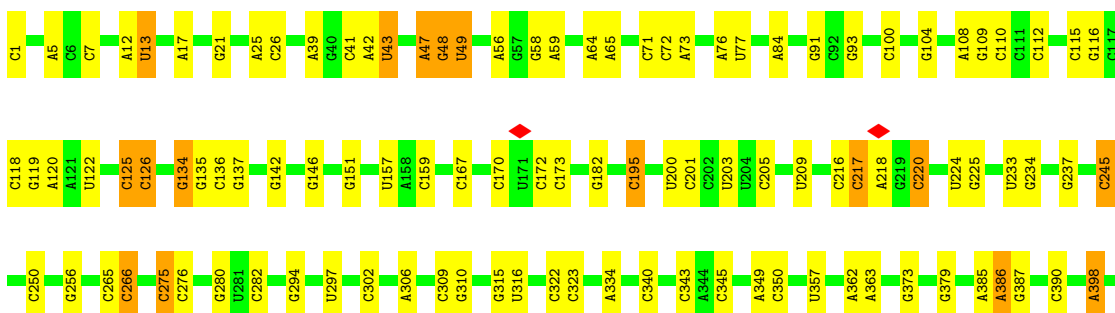
- Molecule 2: P-site tRNA

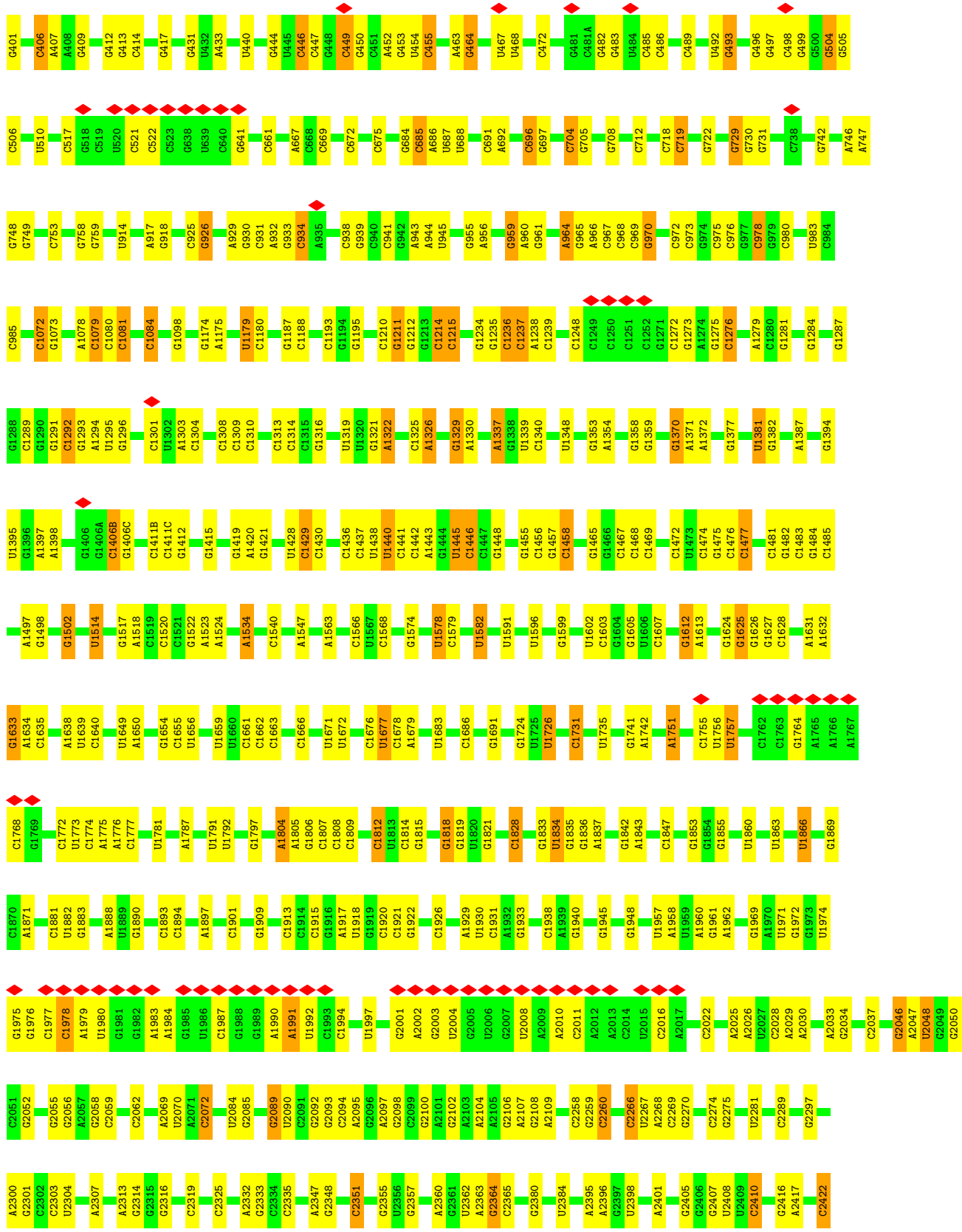


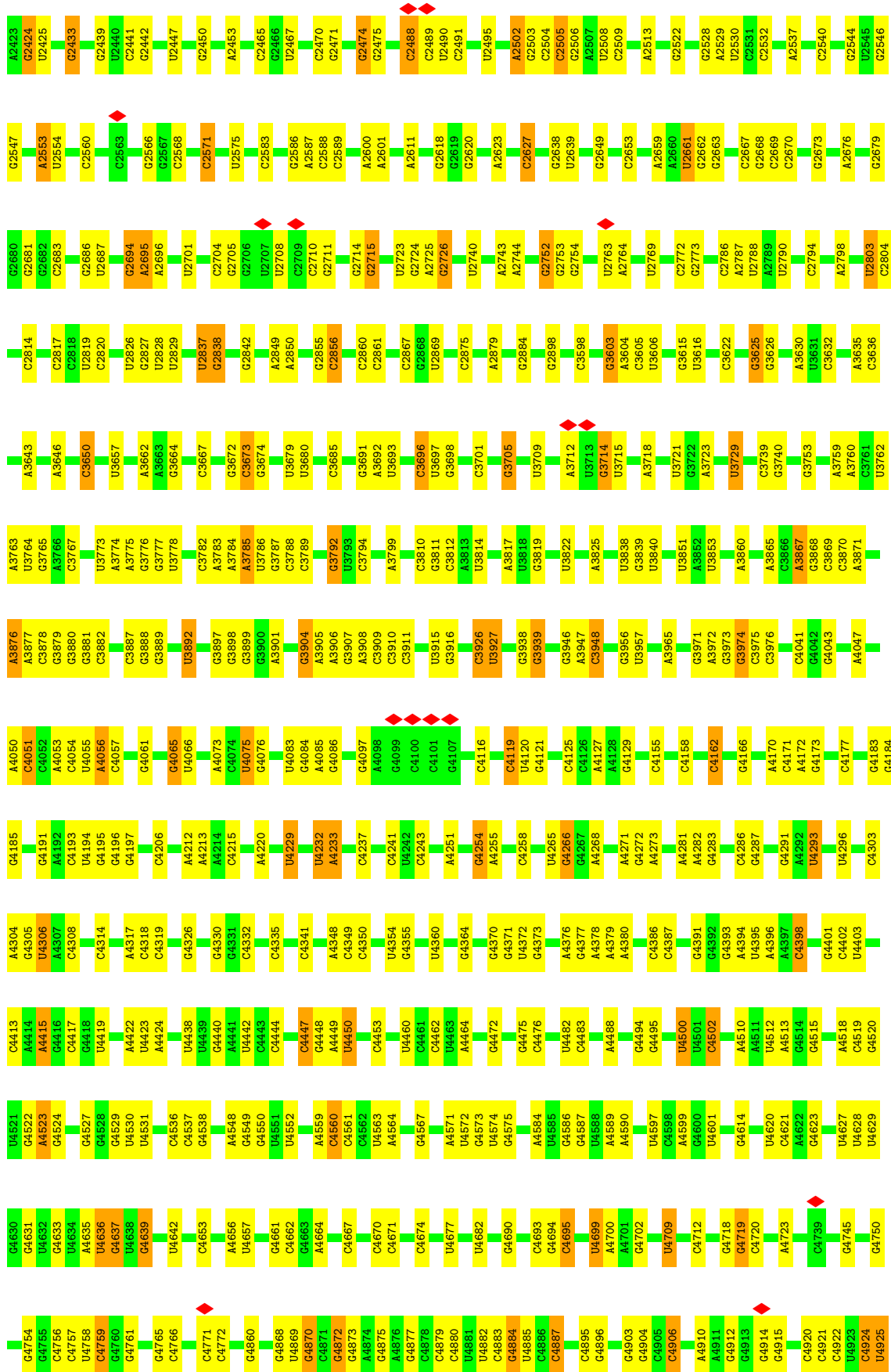
- Molecule 3: Z-site tRNA

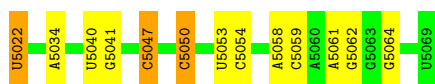
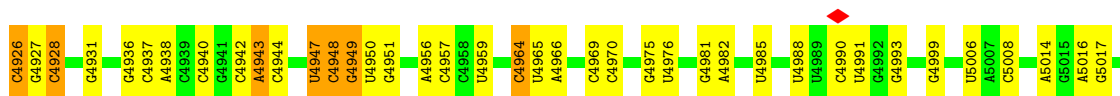


- Molecule 4: 28S rRNA

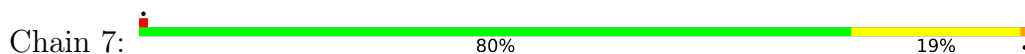




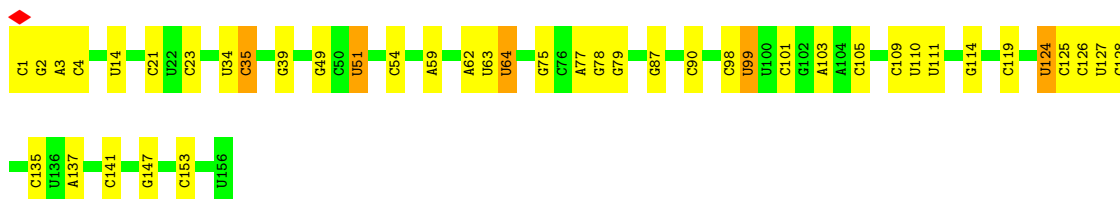




• Molecule 5: 5S rRNA



• Molecule 6: 5.8S rRNA



• Molecule 7: 60S ribosomal protein L8



• Molecule 8: 60S ribosomal protein L3



• Molecule 9: 60S ribosomal protein L4

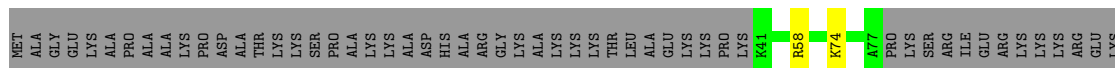


• Molecule 10: 60S ribosomal protein L5

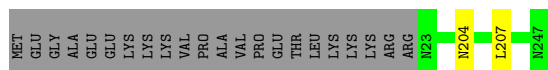
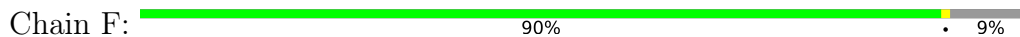




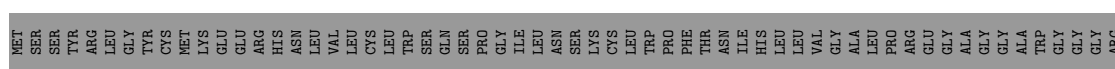
• Molecule 11: 60S ribosomal protein L6



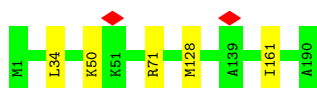
• Molecule 12: 60S ribosomal protein L7



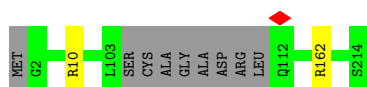
• Molecule 13: 60S ribosomal protein L7a



• Molecule 14: 60S ribosomal protein L9

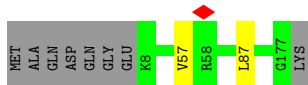


• Molecule 15: 60S ribosomal protein L10



• Molecule 16: 60S ribosomal protein L11

Chain J:  94%



- Molecule 17: 60S ribosomal protein L13

Chain L:  99%



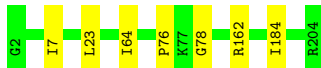
- Molecule 18: 60S ribosomal protein L14

Chain M:  97%



- Molecule 19: 60S ribosomal protein L15

Chain N:  97%



- Molecule 20: 60S ribosomal protein L13a

Chain O:  97%



- Molecule 21: 60S ribosomal protein L17

Chain P:  99%

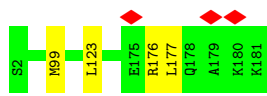


- Molecule 22: 60S ribosomal protein L18

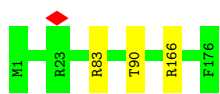
Chain Q:  98%



- Molecule 23: 60S ribosomal protein L19



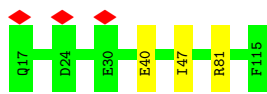
• Molecule 24: 60S ribosomal protein L18a



• Molecule 25: 60S ribosomal protein L21



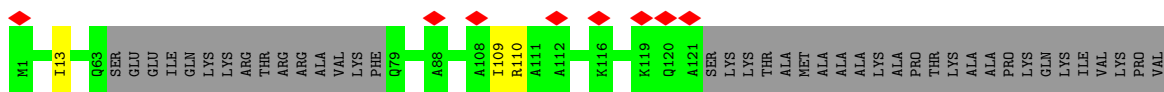
• Molecule 26: 60S ribosomal protein L22



• Molecule 27: 60S ribosomal protein L23



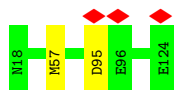
• Molecule 28: 60S ribosomal protein L24



LYS
VAL
SER
ALA
PRO
ARG
VAL
GLY
GLY
LYS
ARG

• Molecule 29: 60S ribosomal protein L23a





- Molecule 36: 60S ribosomal protein L32

Chain e: 98%



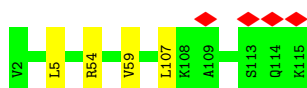
- Molecule 37: 60S ribosomal protein L35a

Chain f: 97%



- Molecule 38: 60S ribosomal protein L34

Chain g: 96%



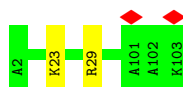
- Molecule 39: 60S ribosomal protein L35

Chain h: 98%



- Molecule 40: 60S ribosomal protein L36

Chain i: 98%



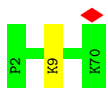
- Molecule 41: 60S ribosomal protein L37

Chain j: 99%



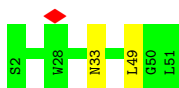
- Molecule 42: 60S ribosomal protein L38

Chain k:  99%



- Molecule 43: 60S ribosomal protein L39

Chain l:  96%



- Molecule 44: 60S ribosomal protein L40

Chain m:  94% 6%



- Molecule 45: 60S ribosomal protein L41

Chain n:  96%



- Molecule 46: 60S ribosomal protein L36a

Chain o:  98%



- Molecule 47: 60S ribosomal protein L37a

Chain p:  100%

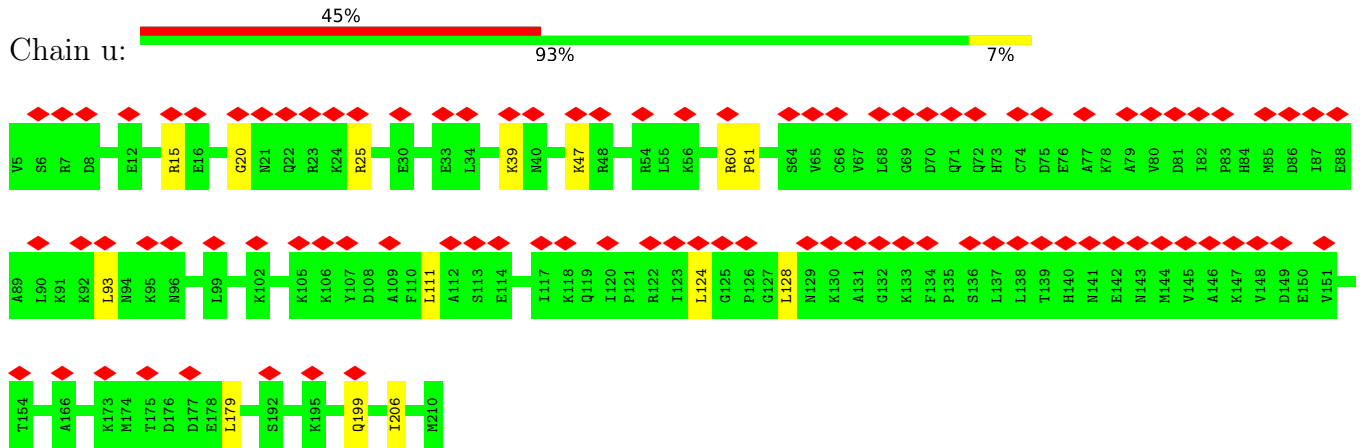


- Molecule 48: 60S ribosomal protein L28

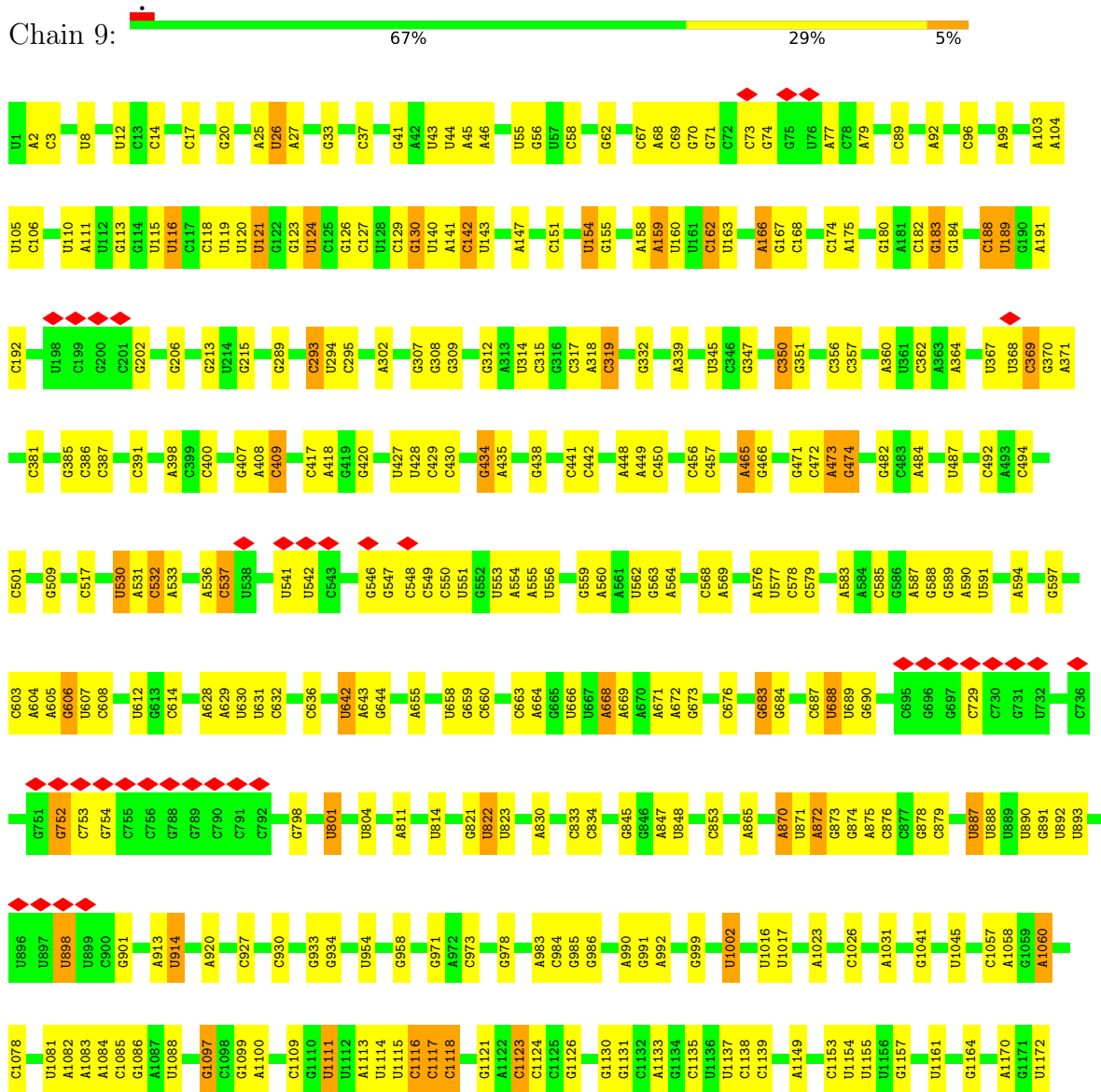
Chain r:  96%



• Molecule 49: 60S ribosomal protein L10a



• Molecule 50: 18S rRNA

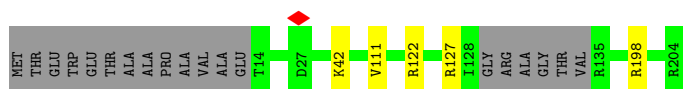




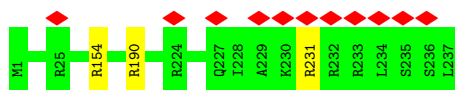
- Molecule 55: 40S ribosomal protein S4, X isoform



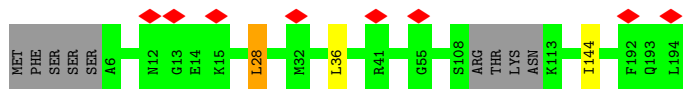
- Molecule 56: 40S ribosomal protein S5



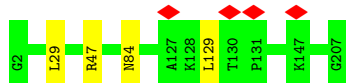
- Molecule 57: 40S ribosomal protein S6



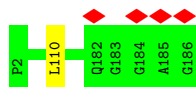
- Molecule 58: 40S ribosomal protein S7



- Molecule 59: 40S ribosomal protein S8

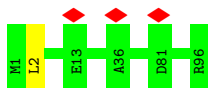


- Molecule 60: 40S ribosomal protein S9

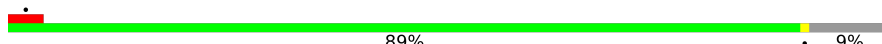


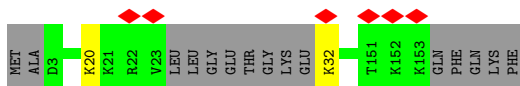
- Molecule 61: 40S ribosomal protein S10

Chain KK:  99%




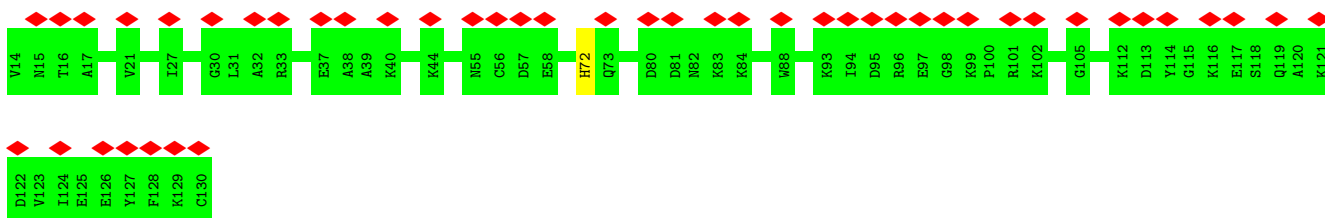
- Molecule 62: 40S ribosomal protein S11

Chain LL:  89%



- Molecule 63: 40S ribosomal protein S12

Chain MM:  39%



- Molecule 64: 40S ribosomal protein S13

Chain NN:  98%



- Molecule 65: 40S ribosomal protein S14

Chain OO:  95%



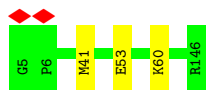
- Molecule 66: 40S ribosomal protein S15

Chain PP:  98%

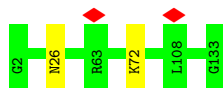


- Molecule 67: 40S ribosomal protein S16

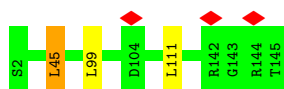
Chain QQ:  98%



- Molecule 68: 40S ribosomal protein S17



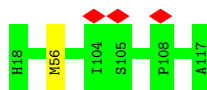
- Molecule 69: 40S ribosomal protein S18



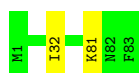
- Molecule 70: 40S ribosomal protein S19



- Molecule 71: 40S ribosomal protein S20



- Molecule 72: 40S ribosomal protein S21



- Molecule 73: 40S ribosomal protein S15a



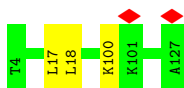
- Molecule 74: 40S ribosomal protein S23

Chain XX:  98%



- Molecule 75: 40S ribosomal protein S24

Chain YY:  98%



- Molecule 76: 40S ribosomal protein S25

Chain ZZ:  100%



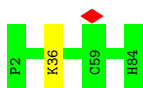
- Molecule 77: 40S ribosomal protein S26

Chain aa:  97%



- Molecule 78: 40S ribosomal protein S27

Chain bb:  99%



- Molecule 79: 40S ribosomal protein S28

Chain cc:  95%

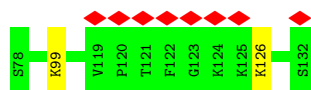


- Molecule 80: 40S ribosomal protein S29

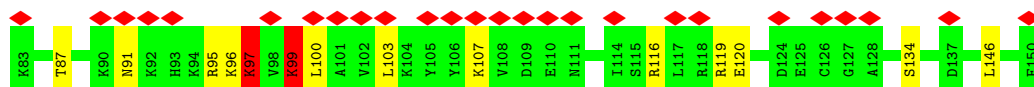
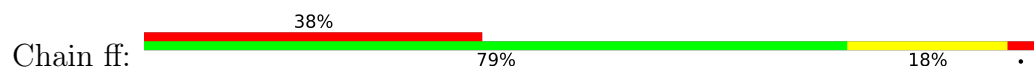
Chain dd:  95%



- Molecule 81: 40S ribosomal protein S30



- Molecule 82: 40S ribosomal protein S27a



- Molecule 83: Receptor of activated protein C kinase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62560	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.797	Depositor
Minimum map value	-0.567	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: B8W, 5MC, 1MA, I4U, B9B, A2M, P4U, E6G, B9H, OMG, P7G, B8N, PSU, MHG, 5MU, B8H, B8Q, 2MG, MLZ, M7A, MA6, ZN, OMC, BGH, UR3, 7MG, E3C, B8K, MG, B8T, 4AC, E7G, OMU, 6MZ

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	0.66	0/166	1.02	0/256
2	2	0.58	0/1805	1.19	19/2809 (0.7%)
3	4	0.42	0/1779	1.11	11/2771 (0.4%)
4	5	1.03	6/83825 (0.0%)	1.23	727/130614 (0.6%)
5	7	1.03	0/2858	1.19	17/4455 (0.4%)
6	8	1.01	0/3559	1.22	27/5543 (0.5%)
7	A	0.62	0/1936	0.69	0/2596
8	B	0.65	0/3240	0.70	0/4339
9	C	0.56	0/2927	0.67	1/3932 (0.0%)
10	D	0.55	0/2437	0.61	0/3264
11	E	0.51	0/1762	0.71	3/2362 (0.1%)
12	F	0.61	0/1911	0.68	1/2549 (0.0%)
13	G	0.49	0/1910	0.66	1/2569 (0.0%)
14	H	0.56	0/1535	0.69	1/2063 (0.0%)
15	I	0.55	0/1702	0.61	0/2272
16	J	0.52	0/1385	0.71	1/1852 (0.1%)
17	L	0.47	0/1733	0.64	0/2316
18	M	0.58	0/1158	0.68	0/1547
19	N	0.61	0/1746	0.68	0/2338
20	O	0.63	1/1662 (0.1%)	0.73	2/2222 (0.1%)
21	P	0.64	0/1268	0.69	0/1700
22	Q	0.56	0/1539	0.72	2/2054 (0.1%)
23	R	0.47	0/1524	0.70	2/2013 (0.1%)
24	S	0.60	0/1501	0.65	0/2012
25	T	0.58	0/1326	0.62	0/1770
26	U	0.45	0/823	0.67	0/1104
27	V	0.62	0/993	0.70	1/1332 (0.1%)
28	W	0.59	1/873 (0.1%)	0.64	0/1158
29	X	0.51	0/984	0.62	0/1323
30	Y	0.59	0/1132	0.66	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Z	0.57	0/1130	0.61	0/1507
32	a	0.61	0/1191	0.65	1/1590 (0.1%)
33	b	0.39	0/861	0.60	0/1138
34	c	0.56	0/771	0.65	0/1034
35	d	0.54	0/903	0.69	0/1216
36	e	0.60	0/1071	0.62	0/1429
37	f	0.69	0/895	0.71	0/1198
38	g	0.54	0/916	0.67	0/1220
39	h	0.48	0/1021	0.66	0/1348
40	i	0.44	0/841	0.59	0/1112
41	j	0.59	0/720	0.67	0/952
42	k	0.44	0/575	0.63	0/761
43	l	0.55	0/459	0.69	1/608 (0.2%)
44	m	0.55	0/425	0.77	0/561
45	n	0.48	0/240	0.77	0/305
46	o	0.50	0/855	0.59	0/1128
47	p	0.59	0/718	0.65	0/953
48	r	0.60	0/1010	0.72	0/1354
49	u	0.35	0/1680	0.76	3/2255 (0.1%)
50	9	0.96	32/39723 (0.1%)	1.33	508/61870 (0.8%)
51	AA	0.55	1/1747 (0.1%)	0.68	0/2374
52	BB	0.47	0/1756	0.66	0/2350
53	CC	0.59	0/1753	0.73	1/2369 (0.0%)
54	DD	0.46	0/1796	0.73	3/2417 (0.1%)
55	EE	0.50	0/2118	0.69	1/2849 (0.0%)
56	FF	0.47	0/1492	0.66	0/2005
57	GG	0.42	0/1946	0.63	0/2590
58	HH	0.44	0/1510	0.69	1/2022 (0.0%)
59	II	0.51	0/1715	0.68	2/2287 (0.1%)
60	JJ	0.47	0/1550	0.67	1/2069 (0.0%)
61	KK	0.46	0/834	0.70	1/1125 (0.1%)
62	LL	0.56	0/1195	0.65	0/1597
63	MM	0.35	0/918	0.71	0/1233
64	NN	0.49	0/1226	0.70	2/1649 (0.1%)
65	OO	0.48	0/1029	0.69	0/1380
66	PP	0.43	0/1017	0.63	0/1358
67	QQ	0.48	0/1146	0.68	0/1534
68	RR	0.44	0/1082	0.64	0/1452
69	SS	0.43	0/1208	0.71	2/1618 (0.1%)
70	TT	0.42	0/1115	0.66	1/1493 (0.1%)
71	UU	0.39	0/805	0.64	0/1081
72	VV	0.55	0/643	0.64	0/860
73	WW	0.57	0/1051	0.69	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	XX	0.54	0/1116	0.64	0/1490
75	YY	0.42	0/1028	0.64	0/1366
76	ZZ	0.42	0/604	0.69	0/810
77	aa	0.53	0/828	0.63	0/1109
78	bb	0.43	0/665	0.67	0/891
79	cc	0.46	0/490	0.68	0/656
80	dd	0.53	0/470	0.68	1/623 (0.2%)
81	ee	0.43	0/447	0.59	0/587
82	ff	0.88	3/567 (0.5%)	1.35	8/753 (1.1%)
83	gg	0.38	0/2493	0.68	1/3394 (0.0%)
All	All	0.84	44/228364 (0.0%)	1.08	1354/334975 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	B	0	1
9	C	0	2
10	D	0	1
13	G	0	1
14	H	0	1
19	N	0	3
25	T	0	1
30	Y	0	1
33	b	0	1
35	d	0	1
46	o	0	1
49	u	0	3
51	AA	0	2
63	MM	0	1
65	OO	0	1
69	SS	0	1
70	TT	0	1
71	UU	0	1
72	VV	0	1
73	WW	0	1
74	XX	0	1
82	ff	0	6
All	All	0	33

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	1287	A	N9-C4	12.29	1.45	1.37
50	9	1287	A	N7-C5	-10.18	1.33	1.39
50	9	1286	G	C5'-C4'	9.64	1.62	1.51
50	9	1287	A	P-O5'	8.68	1.68	1.59
50	9	1286	G	C3'-O3'	8.59	1.54	1.42

The worst 5 of 1354 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1287	A	N7-C8-N9	38.37	132.99	113.80
50	9	1287	A	C8-N9-C4	-37.37	90.85	105.80
50	9	1307	U	C5-C6-N1	32.51	138.95	122.70
50	9	1307	U	C6-N1-C2	-22.81	107.32	121.00
50	9	1504	U	C5-C4-O4	-20.00	113.90	125.90

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	B	16	PHE	Peptide
9	C	69	THR	Peptide
9	C	73	VAL	Peptide
10	D	235	MET	Peptide
13	G	215	ASP	Peptide

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	
7	A	246/248 (99%)	225 (92%)	21 (8%)	0	100	100
8	B	392/394 (100%)	366 (93%)	26 (7%)	0	100	100
9	C	359/362 (99%)	340 (95%)	19 (5%)	0	100	100
10	D	291/293 (99%)	275 (94%)	16 (6%)	0	100	100
11	E	208/291 (72%)	198 (95%)	10 (5%)	0	100	100
12	F	223/247 (90%)	212 (95%)	11 (5%)	0	100	100
13	G	229/319 (72%)	221 (96%)	8 (4%)	0	100	100
14	H	188/190 (99%)	175 (93%)	13 (7%)	0	100	100
15	I	201/214 (94%)	186 (92%)	15 (8%)	0	100	100
16	J	168/178 (94%)	160 (95%)	8 (5%)	0	100	100
17	L	208/210 (99%)	198 (95%)	9 (4%)	1 (0%)	29	68
18	M	136/138 (99%)	122 (90%)	14 (10%)	0	100	100
19	N	201/203 (99%)	187 (93%)	14 (7%)	0	100	100
20	O	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
21	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
22	Q	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
23	R	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
24	S	174/176 (99%)	159 (91%)	14 (8%)	1 (1%)	25	64
25	T	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
26	U	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
27	V	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
28	W	102/157 (65%)	97 (95%)	5 (5%)	0	100	100
29	X	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
30	Y	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
31	Z	133/135 (98%)	125 (94%)	7 (5%)	1 (1%)	19	59
32	a	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
33	b	100/245 (41%)	93 (93%)	7 (7%)	0	100	100
34	c	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
35	d	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
36	e	126/128 (98%)	114 (90%)	12 (10%)	0	100	100
37	f	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
38	g	112/114 (98%)	107 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	h	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
40	i	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
41	j	84/86 (98%)	77 (92%)	7 (8%)	0	100	100
42	k	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
43	l	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
44	m	49/52 (94%)	44 (90%)	4 (8%)	1 (2%)	7	41
45	n	23/25 (92%)	23 (100%)	0	0	100	100
46	o	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
47	p	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
48	r	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
49	u	204/206 (99%)	171 (84%)	32 (16%)	1 (0%)	29	68
51	AA	215/217 (99%)	203 (94%)	12 (6%)	0	100	100
52	BB	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
53	CC	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
54	DD	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
55	EE	260/262 (99%)	241 (93%)	19 (7%)	0	100	100
56	FF	181/204 (89%)	169 (93%)	12 (7%)	0	100	100
57	GG	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
58	HH	181/194 (93%)	169 (93%)	12 (7%)	0	100	100
59	II	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
60	JJ	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
61	KK	94/96 (98%)	86 (92%)	8 (8%)	0	100	100
62	LL	139/158 (88%)	128 (92%)	11 (8%)	0	100	100
63	MM	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
64	NN	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
65	OO	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
66	PP	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
67	QQ	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
68	RR	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
69	SS	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
70	TT	139/141 (99%)	134 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	UU	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
72	VV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
73	WW	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
74	XX	139/141 (99%)	128 (92%)	8 (6%)	3 (2%)	6	39
75	YY	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
76	ZZ	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
77	aa	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
78	bb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
79	cc	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
80	dd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
81	ee	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
82	ff	66/68 (97%)	49 (74%)	17 (26%)	0	100	100
83	gg	311/313 (99%)	279 (90%)	32 (10%)	0	100	100
All	All	11375/11984 (95%)	10695 (94%)	672 (6%)	8 (0%)	54	83

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	m	73	CYS
24	S	166	ARG
49	u	61	PRO
74	XX	62	PRO
31	Z	90	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	
7	A	190/190 (100%)	186 (98%)	4 (2%)	53	78
8	B	342/342 (100%)	336 (98%)	6 (2%)	59	81
9	C	301/301 (100%)	295 (98%)	6 (2%)	55	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	D	247/247 (100%)	240 (97%)	7 (3%)	43	72
11	E	190/251 (76%)	186 (98%)	4 (2%)	53	78
12	F	196/215 (91%)	195 (100%)	1 (0%)	88	95
13	G	200/272 (74%)	190 (95%)	10 (5%)	24	59
14	H	169/169 (100%)	166 (98%)	3 (2%)	59	81
15	I	175/181 (97%)	173 (99%)	2 (1%)	73	88
16	J	143/149 (96%)	142 (99%)	1 (1%)	84	93
17	L	175/175 (100%)	174 (99%)	1 (1%)	86	94
18	M	117/117 (100%)	113 (97%)	4 (3%)	37	69
19	N	171/171 (100%)	167 (98%)	4 (2%)	50	76
20	O	171/171 (100%)	168 (98%)	3 (2%)	59	81
21	P	134/134 (100%)	133 (99%)	1 (1%)	84	93
22	Q	164/164 (100%)	162 (99%)	2 (1%)	71	87
23	R	159/159 (100%)	156 (98%)	3 (2%)	57	80
24	S	157/157 (100%)	155 (99%)	2 (1%)	69	86
25	T	139/139 (100%)	136 (98%)	3 (2%)	52	77
26	U	89/89 (100%)	86 (97%)	3 (3%)	37	69
27	V	101/101 (100%)	99 (98%)	2 (2%)	55	79
28	W	86/126 (68%)	84 (98%)	2 (2%)	50	76
29	X	106/106 (100%)	106 (100%)	0	100	100
30	Y	124/124 (100%)	121 (98%)	3 (2%)	49	75
31	Z	117/117 (100%)	116 (99%)	1 (1%)	78	90
32	a	119/119 (100%)	118 (99%)	1 (1%)	81	91
33	b	84/184 (46%)	80 (95%)	4 (5%)	25	60
34	c	84/84 (100%)	81 (96%)	3 (4%)	35	67
35	d	98/98 (100%)	97 (99%)	1 (1%)	76	88
36	e	114/114 (100%)	111 (97%)	3 (3%)	46	74
37	f	88/88 (100%)	85 (97%)	3 (3%)	37	69
38	g	98/98 (100%)	94 (96%)	4 (4%)	30	64
39	h	109/109 (100%)	107 (98%)	2 (2%)	59	81
40	i	86/86 (100%)	84 (98%)	2 (2%)	50	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	j	73/73 (100%)	72 (99%)	1 (1%)	67	85
42	k	64/64 (100%)	63 (98%)	1 (2%)	62	83
43	l	47/47 (100%)	46 (98%)	1 (2%)	53	78
44	m	47/47 (100%)	45 (96%)	2 (4%)	29	63
45	n	24/24 (100%)	23 (96%)	1 (4%)	30	63
46	o	91/91 (100%)	90 (99%)	1 (1%)	73	88
47	p	74/74 (100%)	74 (100%)	0	100	100
48	r	108/108 (100%)	103 (95%)	5 (5%)	27	61
49	u	186/186 (100%)	179 (96%)	7 (4%)	33	66
51	AA	180/181 (99%)	178 (99%)	2 (1%)	73	88
52	BB	194/194 (100%)	190 (98%)	4 (2%)	53	78
53	CC	187/187 (100%)	184 (98%)	3 (2%)	62	83
54	DD	190/190 (100%)	184 (97%)	6 (3%)	39	70
55	EE	224/224 (100%)	220 (98%)	4 (2%)	59	81
56	FF	158/170 (93%)	153 (97%)	5 (3%)	39	70
57	GG	207/207 (100%)	204 (99%)	3 (1%)	67	85
58	HH	165/174 (95%)	162 (98%)	3 (2%)	59	81
59	II	178/178 (100%)	176 (99%)	2 (1%)	73	88
60	JJ	161/161 (100%)	161 (100%)	0	100	100
61	KK	87/87 (100%)	87 (100%)	0	100	100
62	LL	130/142 (92%)	128 (98%)	2 (2%)	65	84
63	MM	99/99 (100%)	99 (100%)	0	100	100
64	NN	130/130 (100%)	129 (99%)	1 (1%)	81	91
65	OO	106/106 (100%)	100 (94%)	6 (6%)	20	55
66	PP	109/109 (100%)	107 (98%)	2 (2%)	59	81
67	QQ	117/117 (100%)	114 (97%)	3 (3%)	46	74
68	RR	119/119 (100%)	117 (98%)	2 (2%)	60	82
69	SS	125/125 (100%)	124 (99%)	1 (1%)	81	91
70	TT	111/111 (100%)	108 (97%)	3 (3%)	44	73
71	UU	92/92 (100%)	92 (100%)	0	100	100
72	VV	67/67 (100%)	66 (98%)	1 (2%)	65	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	WW	112/112 (100%)	109 (97%)	3 (3%)	44	73
74	XX	113/113 (100%)	113 (100%)	0	100	100
75	YY	107/107 (100%)	104 (97%)	3 (3%)	43	72
76	ZZ	66/66 (100%)	66 (100%)	0	100	100
77	aa	88/88 (100%)	85 (97%)	3 (3%)	37	69
78	bb	75/75 (100%)	74 (99%)	1 (1%)	69	86
79	cc	55/55 (100%)	52 (94%)	3 (6%)	21	57
80	dd	48/48 (100%)	46 (96%)	2 (4%)	30	63
81	ee	46/46 (100%)	44 (96%)	2 (4%)	29	63
82	ff	61/61 (100%)	54 (88%)	7 (12%)	5	29
83	gg	272/272 (100%)	271 (100%)	1 (0%)	91	97
All	All	9936/10274 (97%)	9738 (98%)	198 (2%)	57	79

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	u	39	LYS
56	FF	198	ARG
49	u	206	ILE
54	DD	65	ARG
59	II	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
33	b	60	ASN
49	u	44	GLN
53	CC	267	GLN
52	BB	179	ASN
18	M	48	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	6/7 (85%)	3 (50%)	0
2	2	74/76 (97%)	21 (28%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	4	74/75 (98%)	37 (50%)	1 (1%)
4	5	3526/3597 (98%)	859 (24%)	67 (1%)
5	7	119/120 (99%)	16 (13%)	0
50	9	1671/1698 (98%)	413 (24%)	26 (1%)
6	8	149/151 (98%)	30 (20%)	1 (0%)
All	All	5619/5724 (98%)	1379 (24%)	95 (1%)

5 of 1379 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	43	A
1	1	46	G
1	1	47	U
2	2	7	G
2	2	8	U

5 of 95 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	5	4232	U
50	9	369	C
4	5	4447	5MC
4	5	4925	U
50	9	553	U

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

137 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
50	OMG	9	509	84,50	18,26,27	2.39	8 (44%)	19,38,41	1.58	4 (21%)
4	PSU	5	4450	4,84	18,21,22	1.14	2 (11%)	22,30,33	2.00	5 (22%)
4	2MG	5	4872	4,18	18,26,27	2.61	7 (38%)	16,38,41	1.63	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2M	5	2363	4,84	18,25,26	4.72	10 (55%)	18,36,39	2.76	4 (22%)
4	7MG	5	2522	4	22,26,27	3.38	10 (45%)	29,39,42	2.08	8 (27%)
4	PSU	5	4531	4	18,21,22	1.10	2 (11%)	22,30,33	1.69	4 (18%)
4	OMG	5	2050	4	18,26,27	2.34	8 (44%)	19,38,41	1.56	4 (21%)
4	7MG	5	1605	4	22,26,27	3.32	10 (45%)	29,39,42	2.09	8 (27%)
4	A2M	5	1871	4,84	18,25,26	4.64	10 (55%)	18,36,39	2.72	4 (22%)
4	OMU	5	4306	4	19,22,23	2.71	8 (42%)	26,31,34	1.74	5 (19%)
4	P4U	5	1348	4,84	21,24,25	3.44	8 (38%)	27,33,36	1.59	3 (11%)
4	OMC	5	2861	4	19,22,23	2.84	7 (36%)	26,31,34	1.05	2 (7%)
4	OMG	5	4623	4	18,26,27	2.39	8 (44%)	19,38,41	1.62	4 (21%)
50	A2M	9	668	84,50	18,25,26	4.58	9 (50%)	18,36,39	2.59	5 (27%)
4	5MC	5	3782	4	18,22,23	3.46	7 (38%)	26,32,35	1.42	5 (19%)
50	A2M	9	166	50	18,25,26	4.88	9 (50%)	18,36,39	2.89	5 (27%)
4	B8Q	5	1456	4	17,22,23	2.64	5 (29%)	22,32,35	2.02	5 (22%)
50	6MZ	9	1832	84,50	18,25,26	2.26	4 (22%)	16,36,39	1.70	2 (12%)
4	OMG	5	1522	4	18,26,27	2.40	8 (44%)	19,38,41	1.65	4 (21%)
50	4AC	9	1337	50	21,24,25	3.14	9 (42%)	29,34,37	1.16	4 (13%)
4	OMG	5	1883	4	18,26,27	2.49	8 (44%)	19,38,41	1.77	4 (21%)
50	OMC	9	1703	50	19,22,23	2.86	7 (36%)	26,31,34	0.70	0
4	OMU	5	4620	4	19,22,23	2.61	6 (31%)	26,31,34	1.76	5 (19%)
4	A2M	5	398	4	18,25,26	4.70	8 (44%)	18,36,39	2.57	3 (16%)
4	P7G	5	1909	4	24,28,29	3.90	10 (41%)	27,41,44	1.91	3 (11%)
50	OMG	9	683	50	18,26,27	2.49	8 (44%)	19,38,41	1.59	5 (26%)
4	UR3	5	4597	4	19,22,23	2.58	6 (31%)	26,32,35	1.25	4 (15%)
50	5MU	9	814	50	19,22,23	4.77	7 (36%)	28,32,35	3.39	13 (46%)
4	B9B	5	2754	4,84	21,28,29	6.32	8 (38%)	23,40,43	2.02	6 (26%)
50	A2M	9	1031	50	18,25,26	4.82	9 (50%)	18,36,39	2.42	3 (16%)
50	A2M	9	1678	50	18,25,26	4.71	9 (50%)	18,36,39	2.92	3 (16%)
4	A2M	5	3723	4	18,25,26	4.77	9 (50%)	18,36,39	2.57	3 (16%)
4	PSU	5	3729	4	18,21,22	1.09	1 (5%)	22,30,33	1.84	4 (18%)
4	PSU	5	2508	4	18,21,22	0.98	1 (5%)	22,30,33	1.64	4 (18%)
4	7MG	5	4550	4	22,26,27	3.28	10 (45%)	29,39,42	1.92	9 (31%)
50	PSU	9	1243	50	18,21,22	1.28	1 (5%)	22,30,33	1.47	4 (18%)
9	MLZ	C	333	9	8,9,10	0.96	0	4,9,11	0.99	0
4	B8T	5	4483	4	19,22,23	3.00	8 (42%)	26,31,34	1.09	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	MA6	9	1851	50	19,26,27	1.09	1 (5%)	18,38,41	2.77	2 (11%)
50	M7A	9	1806	50	20,25,26	2.02	3 (15%)	28,37,40	3.72	8 (28%)
4	B8W	5	4529	4,84	18,26,27	5.33	8 (44%)	21,38,41	6.53	9 (42%)
50	OMU	9	121	50	19,22,23	2.83	7 (36%)	26,31,34	1.83	5 (19%)
50	OMC	9	1710	50	19,22,23	2.88	7 (36%)	26,31,34	1.03	1 (3%)
50	A2M	9	484	50	18,25,26	4.65	8 (44%)	18,36,39	2.70	4 (22%)
4	E7G	5	1797	4	24,27,28	3.43	11 (45%)	30,40,43	2.18	9 (30%)
4	PSU	5	4403	4	18,21,22	1.06	2 (11%)	22,30,33	1.82	5 (22%)
4	OMG	5	4494	4	18,26,27	2.45	8 (44%)	19,38,41	1.73	5 (26%)
4	B8W	5	4129	4	18,26,27	5.31	8 (44%)	21,38,41	6.22	12 (57%)
4	I4U	5	4194	4	21,24,25	4.92	16 (76%)	27,34,37	1.34	4 (14%)
4	PSU	5	4636	4	18,21,22	1.08	2 (11%)	22,30,33	2.05	5 (22%)
4	2MG	5	1517	4	18,26,27	2.48	7 (38%)	16,38,41	1.69	4 (25%)
50	A2M	9	27	84,50	18,25,26	4.71	9 (50%)	18,36,39	2.70	3 (16%)
4	OMC	5	2422	4,84	19,22,23	2.83	7 (36%)	26,31,34	0.82	1 (3%)
4	PSU	5	3764	4	18,21,22	1.01	1 (5%)	22,30,33	1.62	4 (18%)
4	PSU	5	4293	4	18,21,22	1.09	3 (16%)	22,30,33	1.80	4 (18%)
4	A2M	5	4523	4,84	18,25,26	4.73	9 (50%)	18,36,39	2.89	5 (27%)
4	B8W	5	4472	4	18,26,27	5.25	9 (50%)	21,38,41	5.81	9 (42%)
4	MHG	5	4371	4	29,32,33	3.92	11 (37%)	34,46,49	2.26	8 (23%)
4	UR3	5	4530	4	19,22,23	2.51	6 (31%)	26,32,35	1.41	3 (11%)
4	A2M	5	3718	4	18,25,26	4.77	12 (66%)	18,36,39	2.44	3 (16%)
4	E7G	5	2297	4	24,27,28	3.32	11 (45%)	30,40,43	2.14	9 (30%)
4	B8H	5	4296	4	19,22,23	6.89	7 (36%)	22,32,35	2.59	5 (22%)
50	5MC	9	1374	50	18,22,23	3.66	7 (38%)	26,32,35	1.10	1 (3%)
50	OMU	9	116	50	19,22,23	2.74	7 (36%)	26,31,34	1.84	5 (19%)
4	UR3	5	1866	4	19,22,23	2.37	6 (31%)	26,32,35	1.17	2 (7%)
4	B8K	5	4690	4,14	24,28,29	4.94	16 (66%)	30,42,45	2.80	12 (40%)
50	4AC	9	1842	50	21,24,25	3.06	10 (47%)	29,34,37	1.49	7 (24%)
4	OMG	5	2364	4	18,26,27	2.35	7 (38%)	19,38,41	1.56	4 (21%)
4	A2M	5	2401	4,84	18,25,26	4.70	8 (44%)	18,36,39	2.61	3 (16%)
6	OMU	8	14	4,6	19,22,23	2.64	6 (31%)	26,31,34	1.85	5 (19%)
50	PSU	9	823	50	18,21,22	1.09	3 (16%)	22,30,33	1.67	4 (18%)
4	OMG	5	3792	4	18,26,27	2.45	8 (44%)	19,38,41	1.66	4 (21%)
4	OMG	5	1316	4	18,26,27	2.42	7 (38%)	19,38,41	1.61	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	B8Q	9	1219	84,50	17,22,23	2.89	5 (29%)	22,32,35	2.62	7 (31%)
50	MA6	9	1850	50	19,26,27	1.09	1 (5%)	18,38,41	2.84	2 (11%)
4	OMG	5	4637	4	18,26,27	2.32	8 (44%)	19,38,41	1.63	4 (21%)
4	OMG	5	373	4	18,26,27	2.42	8 (44%)	19,38,41	1.56	5 (26%)
4	OMC	5	3869	4	19,22,23	2.69	7 (36%)	26,31,34	0.90	0
4	6MZ	5	4220	4	18,25,26	2.16	4 (22%)	16,36,39	1.96	4 (25%)
4	OMC	5	3887	4	19,22,23	2.84	7 (36%)	26,31,34	0.88	0
4	OMG	5	2424	4	18,26,27	2.52	8 (44%)	19,38,41	1.60	4 (21%)
4	A2M	5	1534	4,84	18,25,26	4.73	9 (50%)	18,36,39	2.66	3 (16%)
4	PSU	5	1582	4	18,21,22	1.13	2 (11%)	22,30,33	1.77	4 (18%)
4	A2M	5	3825	4	18,25,26	4.71	8 (44%)	18,36,39	2.66	3 (16%)
4	OMC	5	3909	4	19,22,23	2.68	7 (36%)	26,31,34	0.94	1 (3%)
50	PSU	9	822	50	18,21,22	1.08	2 (11%)	22,30,33	2.02	6 (27%)
4	B8H	5	1860	4	19,22,23	6.81	6 (31%)	22,32,35	2.36	5 (22%)
4	OMG	5	4870	4	18,26,27	2.47	8 (44%)	19,38,41	1.60	4 (21%)
4	B9H	5	2786	4	20,25,26	2.95	3 (15%)	22,35,38	1.94	3 (13%)
4	P7G	5	3880	4	24,28,29	3.74	10 (41%)	27,41,44	1.69	4 (14%)
4	I4U	5	1659	4	21,24,25	4.86	15 (71%)	27,34,37	1.53	2 (7%)
50	PSU	9	119	50	18,21,22	0.87	1 (5%)	22,30,33	1.66	3 (13%)
4	OMG	5	4196	4,2	18,26,27	2.41	8 (44%)	19,38,41	1.50	4 (21%)
50	PSU	9	612	50	18,21,22	1.03	3 (16%)	22,30,33	1.59	3 (13%)
4	PSU	5	3715	4	18,21,22	0.95	1 (5%)	22,30,33	1.68	4 (18%)
50	UR3	9	1830	50	19,22,23	2.52	6 (31%)	26,32,35	1.76	4 (15%)
4	1MA	5	1322	4,84	16,25,26	3.74	5 (31%)	18,37,40	1.93	3 (16%)
4	A2M	5	1326	4	18,25,26	4.72	9 (50%)	18,36,39	2.78	3 (16%)
4	PSU	5	1683	4	18,21,22	1.18	2 (11%)	22,30,33	1.85	4 (18%)
4	OMG	5	2773	4	18,26,27	2.41	8 (44%)	19,38,41	1.49	4 (21%)
4	B8H	5	3762	4	19,22,23	6.82	6 (31%)	22,32,35	2.45	5 (22%)
4	A2M	5	4571	4	18,25,26	4.63	8 (44%)	18,36,39	2.69	3 (16%)
4	5MC	5	4447	4	18,22,23	3.60	7 (38%)	26,32,35	1.08	1 (3%)
4	A2M	5	3867	4	18,25,26	4.67	8 (44%)	18,36,39	2.81	6 (33%)
4	OMG	5	4370	4	18,26,27	2.40	8 (44%)	19,38,41	1.52	4 (21%)
4	OMC	5	3701	4,84	19,22,23	2.72	7 (36%)	26,31,34	0.82	0
4	2MG	5	729	4	18,26,27	2.43	5 (27%)	16,38,41	1.37	3 (18%)
4	PSU	5	1677	4	18,21,22	1.14	3 (16%)	22,30,33	1.87	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	OMG	9	644	50	18,26,27	2.42	8 (44%)	19,38,41	1.56	4 (21%)
50	A2M	9	159	50	18,25,26	4.79	8 (44%)	18,36,39	2.80	4 (22%)
4	M7A	5	4564	4	20,25,26	1.99	4 (20%)	28,37,40	3.78	7 (25%)
4	B8W	5	2380	4	18,26,27	5.24	8 (44%)	21,38,41	6.18	8 (38%)
50	E3C	9	568	50	18,23,24	3.38	6 (33%)	21,33,36	2.40	6 (28%)
4	B8K	5	3897	4	24,28,29	4.78	16 (66%)	30,42,45	2.57	12 (40%)
44	MLZ	m	72	44	8,9,10	0.82	0	4,9,11	1.09	0
4	PSU	5	4500	4	18,21,22	1.05	3 (16%)	22,30,33	2.05	4 (18%)
4	E6G	5	4355	4	20,27,28	5.75	9 (45%)	22,39,42	2.17	7 (31%)
4	PSU	5	4628	4	18,21,22	1.10	2 (11%)	22,30,33	1.96	4 (18%)
50	B8N	9	1248	50	24,29,30	2.78	7 (29%)	29,42,45	1.84	6 (20%)
4	OMC	5	4536	4	19,22,23	2.69	7 (36%)	26,31,34	1.08	2 (7%)
4	A2M	5	1524	4	18,25,26	4.70	9 (50%)	18,36,39	2.74	3 (16%)
4	B9B	5	1574	4	21,28,29	6.27	9 (42%)	23,40,43	2.16	6 (26%)
4	B8T	5	4671	4	19,22,23	2.91	8 (42%)	26,31,34	0.94	1 (3%)
50	OMC	9	517	50	19,22,23	2.82	7 (36%)	26,31,34	1.01	1 (3%)
4	OMC	5	2365	4	19,22,23	2.78	7 (36%)	26,31,34	0.75	0
4	B8W	5	4185	4	18,26,27	5.17	8 (44%)	21,38,41	5.98	12 (57%)
4	1MA	5	4415	4	16,25,26	4.01	4 (25%)	18,37,40	1.72	3 (16%)
50	PSU	9	1081	50	18,21,22	1.13	3 (16%)	22,30,33	1.78	4 (18%)
4	5MU	5	4083	4	19,22,23	4.65	7 (36%)	28,32,35	3.61	11 (39%)
4	A2M	5	3785	4	18,25,26	4.48	10 (55%)	18,36,39	2.62	4 (22%)
4	OMC	5	2804	4	19,22,23	2.82	7 (36%)	26,31,34	0.88	0
4	B9B	5	237	4	21,28,29	6.30	9 (42%)	23,40,43	2.29	7 (30%)
4	BGH	5	3899	4,84	25,29,30	4.11	16 (64%)	31,43,46	2.66	14 (45%)
4	PSU	5	4442	4	18,21,22	1.08	3 (16%)	22,30,33	2.07	4 (18%)
4	5MC	5	4335	4	18,22,23	3.51	7 (38%)	26,32,35	1.35	3 (11%)
4	OMG	5	1625	4,84	18,26,27	2.39	8 (44%)	19,38,41	1.55	4 (21%)
50	OMC	9	174	50	19,22,23	2.87	7 (36%)	26,31,34	0.84	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
50	OMG	9	509	84,50	-	0/5/27/28	0/3/3/3
4	PSU	5	4450	4,84	-	4/7/25/26	0/2/2/2
4	2MG	5	4872	4,18	-	2/5/27/28	0/3/3/3
4	A2M	5	2363	4,84	-	1/5/27/28	0/3/3/3
4	7MG	5	2522	4	-	0/7/37/38	0/3/3/3
4	PSU	5	4531	4	-	0/7/25/26	0/2/2/2
4	OMG	5	2050	4	-	0/5/27/28	0/3/3/3
4	7MG	5	1605	4	-	0/7/37/38	0/3/3/3
4	A2M	5	1871	4,84	-	0/5/27/28	0/3/3/3
4	OMU	5	4306	4	-	1/9/27/28	0/2/2/2
4	P4U	5	1348	4,84	-	5/10/29/30	0/2/2/2
4	OMC	5	2861	4	-	1/9/27/28	0/2/2/2
4	OMG	5	4623	4	-	0/5/27/28	0/3/3/3
50	A2M	9	668	84,50	-	3/5/27/28	0/3/3/3
4	5MC	5	3782	4	-	0/7/25/26	0/2/2/2
50	A2M	9	166	50	-	2/5/27/28	0/3/3/3
4	B8Q	5	1456	4	-	0/7/42/43	0/2/2/2
50	6MZ	9	1832	84,50	-	2/5/27/28	0/3/3/3
4	OMG	5	1522	4	-	0/5/27/28	0/3/3/3
50	4AC	9	1337	50	-	2/11/29/30	0/2/2/2
4	OMG	5	1883	4	-	2/5/27/28	0/3/3/3
50	OMC	9	1703	50	-	2/9/27/28	0/2/2/2
4	OMU	5	4620	4	-	1/9/27/28	0/2/2/2
4	A2M	5	398	4	-	2/5/27/28	0/3/3/3
4	P7G	5	1909	4	-	2/10/40/41	0/3/3/3
50	OMG	9	683	50	-	2/5/27/28	0/3/3/3
4	UR3	5	4597	4	-	0/7/25/26	0/2/2/2
50	5MU	9	814	50	-	1/7/25/26	0/2/2/2
4	B9B	5	2754	4,84	-	3/7/29/30	0/3/3/3
50	A2M	9	1031	50	-	0/5/27/28	0/3/3/3
50	A2M	9	1678	50	-	0/5/27/28	0/3/3/3
4	A2M	5	3723	4	-	0/5/27/28	0/3/3/3
4	PSU	5	3729	4	-	2/7/25/26	0/2/2/2
4	PSU	5	2508	4	-	0/7/25/26	0/2/2/2
4	7MG	5	4550	4	-	0/7/37/38	0/3/3/3
50	PSU	9	1243	50	-	2/7/25/26	0/2/2/2
9	MLZ	C	333	9	-	3/7/8/10	-
4	B8T	5	4483	4	-	0/7/27/28	0/2/2/2
50	MA6	9	1851	50	-	4/7/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	M7A	9	1806	50	-	0/7/37/38	0/3/3/3
4	B8W	5	4529	4,84	-	4/5/27/28	0/3/3/3
50	OMU	9	121	50	-	2/9/27/28	0/2/2/2
50	OMC	9	1710	50	-	1/9/27/28	0/2/2/2
50	A2M	9	484	50	-	0/5/27/28	0/3/3/3
4	E7G	5	1797	4	-	2/9/39/40	0/3/3/3
4	PSU	5	4403	4	-	3/7/25/26	0/2/2/2
4	OMG	5	4494	4	-	0/5/27/28	0/3/3/3
4	B8W	5	4129	4	-	3/5/27/28	0/3/3/3
4	I4U	5	4194	4	-	4/9/29/30	0/2/2/2
4	PSU	5	4636	4	-	3/7/25/26	0/2/2/2
4	2MG	5	1517	4	-	0/5/27/28	0/3/3/3
50	A2M	9	27	84,50	-	0/5/27/28	0/3/3/3
4	OMC	5	2422	4,84	-	1/9/27/28	0/2/2/2
4	PSU	5	3764	4	-	0/7/25/26	0/2/2/2
4	PSU	5	4293	4	-	2/7/25/26	0/2/2/2
4	A2M	5	4523	4,84	-	3/5/27/28	0/3/3/3
4	B8W	5	4472	4	-	3/5/27/28	0/3/3/3
4	MHG	5	4371	4	-	6/16/46/47	0/3/3/3
4	UR3	5	4530	4	-	1/7/25/26	0/2/2/2
4	A2M	5	3718	4	-	0/5/27/28	0/3/3/3
4	E7G	5	2297	4	-	1/9/39/40	0/3/3/3
4	B8H	5	4296	4	-	0/7/25/26	0/2/2/2
50	5MC	9	1374	50	-	0/7/25/26	0/2/2/2
50	OMU	9	116	50	-	3/9/27/28	0/2/2/2
4	UR3	5	1866	4	-	2/7/25/26	0/2/2/2
4	B8K	5	4690	4,14	-	0/11/41/42	0/3/3/3
50	4AC	9	1842	50	-	0/11/29/30	0/2/2/2
4	OMG	5	2364	4	-	2/5/27/28	0/3/3/3
4	A2M	5	2401	4,84	-	1/5/27/28	0/3/3/3
6	OMU	8	14	4,6	-	1/9/27/28	0/2/2/2
50	PSU	9	823	50	-	0/7/25/26	0/2/2/2
4	OMG	5	3792	4	-	2/5/27/28	0/3/3/3
4	OMG	5	1316	4	-	1/5/27/28	0/3/3/3
50	B8Q	9	1219	84,50	-	1/7/42/43	0/2/2/2
50	MA6	9	1850	50	-	1/7/29/30	0/3/3/3
4	OMG	5	4637	4	-	2/5/27/28	0/3/3/3
4	OMG	5	373	4	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMC	5	3869	4	-	0/9/27/28	0/2/2/2
4	6MZ	5	4220	4	-	1/5/27/28	0/3/3/3
4	OMC	5	3887	4	-	1/9/27/28	0/2/2/2
4	OMG	5	2424	4	-	2/5/27/28	0/3/3/3
4	A2M	5	1534	4,84	-	2/5/27/28	0/3/3/3
4	PSU	5	1582	4	-	2/7/25/26	0/2/2/2
4	A2M	5	3825	4	-	0/5/27/28	0/3/3/3
4	OMC	5	3909	4	-	0/9/27/28	0/2/2/2
50	PSU	9	822	50	-	0/7/25/26	0/2/2/2
4	B8H	5	1860	4	-	0/7/25/26	0/2/2/2
4	OMG	5	4870	4	-	4/5/27/28	0/3/3/3
4	B9H	5	2786	4	-	2/12/47/48	0/2/2/2
4	P7G	5	3880	4	-	2/10/40/41	0/3/3/3
4	I4U	5	1659	4	-	1/9/29/30	0/2/2/2
50	PSU	9	119	50	-	0/7/25/26	0/2/2/2
4	OMG	5	4196	4,2	-	0/5/27/28	0/3/3/3
50	PSU	9	612	50	-	0/7/25/26	0/2/2/2
4	PSU	5	3715	4	-	0/7/25/26	0/2/2/2
50	UR3	9	1830	50	-	2/7/25/26	0/2/2/2
4	1MA	5	1322	4,84	-	0/3/25/26	0/3/3/3
4	A2M	5	1326	4	-	1/5/27/28	0/3/3/3
4	PSU	5	1683	4	-	0/7/25/26	0/2/2/2
4	OMG	5	2773	4	-	0/5/27/28	0/3/3/3
4	B8H	5	3762	4	-	2/7/25/26	0/2/2/2
4	A2M	5	4571	4	-	0/5/27/28	0/3/3/3
4	5MC	5	4447	4	-	4/7/25/26	0/2/2/2
4	A2M	5	3867	4	-	2/5/27/28	0/3/3/3
4	OMG	5	4370	4	-	0/5/27/28	0/3/3/3
4	OMC	5	3701	4,84	-	6/9/27/28	0/2/2/2
4	2MG	5	729	4	-	2/5/27/28	0/3/3/3
4	PSU	5	1677	4	-	1/7/25/26	0/2/2/2
50	OMG	9	644	50	-	2/5/27/28	0/3/3/3
50	A2M	9	159	50	-	3/5/27/28	0/3/3/3
4	M7A	5	4564	4	-	0/7/37/38	0/3/3/3
4	B8W	5	2380	4	-	4/5/27/28	0/3/3/3
50	E3C	9	568	50	-	4/9/44/45	0/2/2/2
4	B8K	5	3897	4	-	3/11/41/42	0/3/3/3
44	MLZ	m	72	44	-	1/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	5	4500	4	-	3/7/25/26	0/2/2/2
4	E6G	5	4355	4	-	5/6/28/29	0/3/3/3
4	PSU	5	4628	4	-	0/7/25/26	0/2/2/2
50	B8N	9	1248	50	-	2/16/34/35	0/2/2/2
4	OMC	5	4536	4	-	0/9/27/28	0/2/2/2
4	A2M	5	1524	4	-	0/5/27/28	0/3/3/3
4	B9B	5	1574	4	-	3/7/29/30	0/3/3/3
4	B8T	5	4671	4	-	0/7/27/28	0/2/2/2
50	OMC	9	517	50	-	0/9/27/28	0/2/2/2
4	OMC	5	2365	4	-	0/9/27/28	0/2/2/2
4	B8W	5	4185	4	-	3/5/27/28	0/3/3/3
4	1MA	5	4415	4	-	2/3/25/26	0/3/3/3
50	PSU	9	1081	50	-	1/7/25/26	0/2/2/2
4	5MU	5	4083	4	-	0/7/25/26	0/2/2/2
4	A2M	5	3785	4	-	4/5/27/28	0/3/3/3
4	OMC	5	2804	4	-	0/9/27/28	0/2/2/2
4	B9B	5	237	4	-	4/7/29/30	0/3/3/3
4	BGH	5	3899	4,84	-	3/13/43/44	0/3/3/3
4	PSU	5	4442	4	-	0/7/25/26	0/2/2/2
4	5MC	5	4335	4	-	0/7/25/26	0/2/2/2
4	OMG	5	1625	4,84	-	1/5/27/28	0/3/3/3
50	OMC	9	174	50	-	0/9/27/28	0/2/2/2

The worst 5 of 943 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	2754	B9B	C2'-C1'	-18.26	1.26	1.53
4	5	1574	B9B	C2'-C1'	-17.78	1.26	1.53
4	5	237	B9B	C2'-C1'	-17.62	1.27	1.53
4	5	237	B9B	O4'-C1'	17.17	1.65	1.41
50	9	166	A2M	O4'-C1'	16.78	1.64	1.41

The worst 5 of 601 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4529	B8W	N2-C2-N3	17.65	146.56	117.79
4	5	2380	B8W	N2-C2-N3	17.41	146.16	117.79
4	5	4185	B8W	N2-C2-N3	16.41	144.54	117.79
4	5	4129	B8W	N2-C2-N3	16.31	144.38	117.79
4	5	4472	B8W	N2-C2-N3	16.08	143.99	117.79

There are no chirality outliers.

5 of 189 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	333	MLZ	N-CA-CB-CG
9	C	333	MLZ	C-CA-CB-CG
4	5	237	B9B	C5-C6-O6-C61
4	5	237	B9B	N1-C6-O6-C61
4	5	237	B9B	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	5	43
50	9	18

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
6	8	1
2	2	1
28	W	1

The worst 5 of 64 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	40.26
1	5	1252:C	O3'	1271:G	P	35.28
1	5	1405:C	O3'	1406:G	P	20.05
1	5	1219:G	O3'	1233:G	P	19.96
1	5	1406(C):G	O3'	1411:C	P	18.99

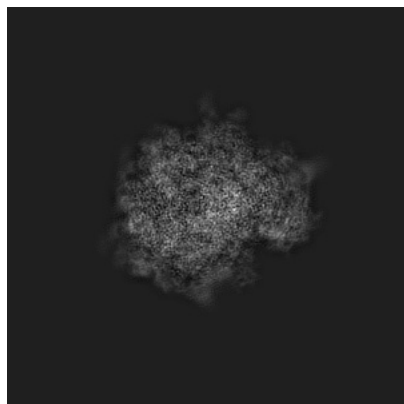
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9237. These allow visual inspection of the internal detail of the map and identification of artifacts.

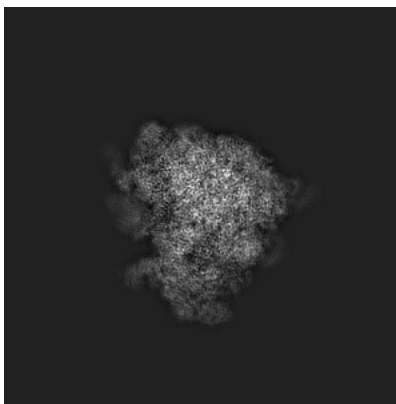
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

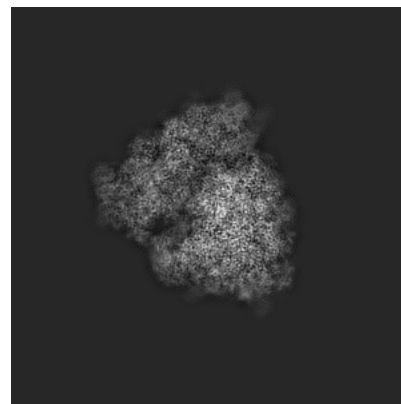
6.1.1 Primary map



X

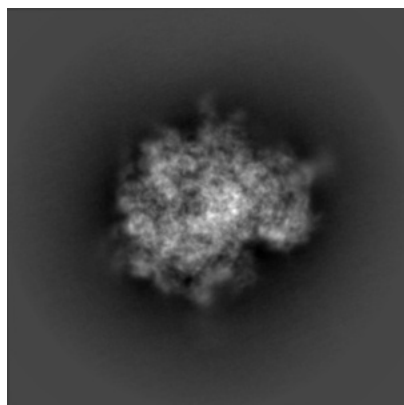


Y

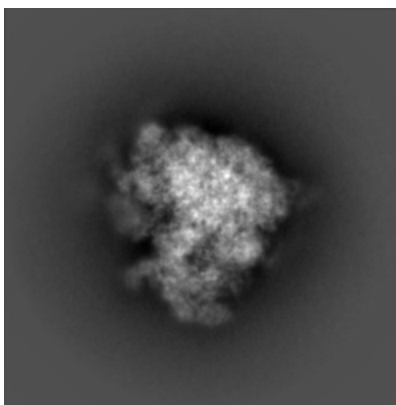


Z

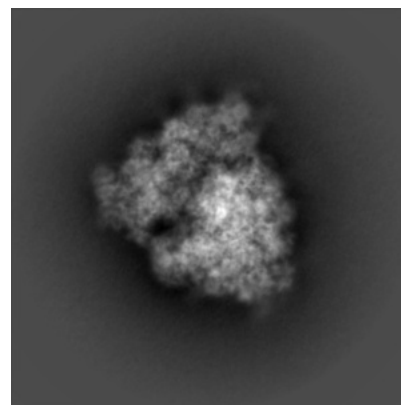
6.1.2 Raw map



X



Y

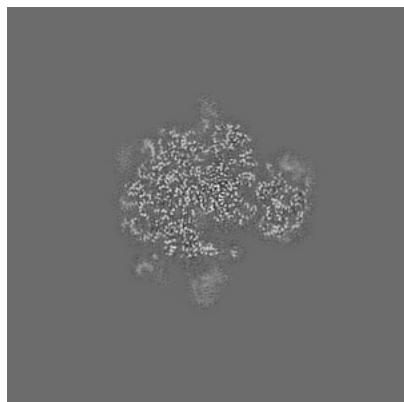


Z

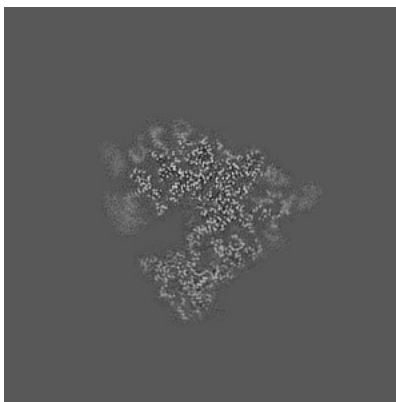
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

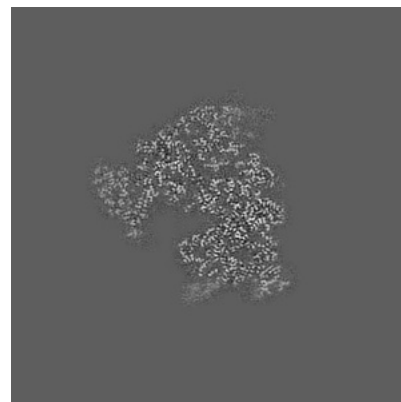
6.2.1 Primary map



X Index: 200

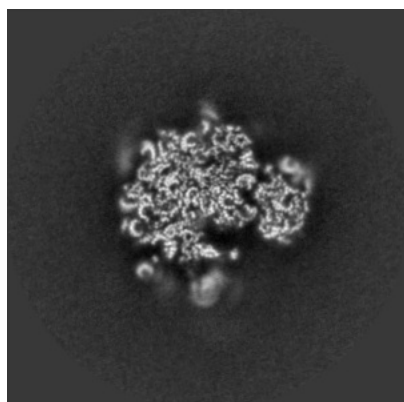


Y Index: 200

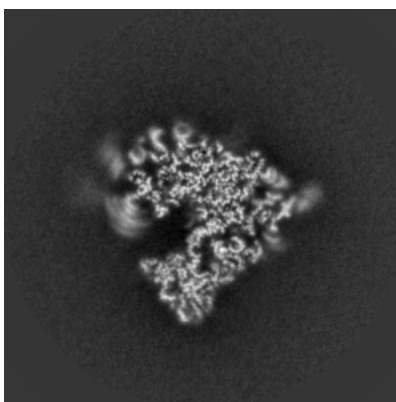


Z Index: 200

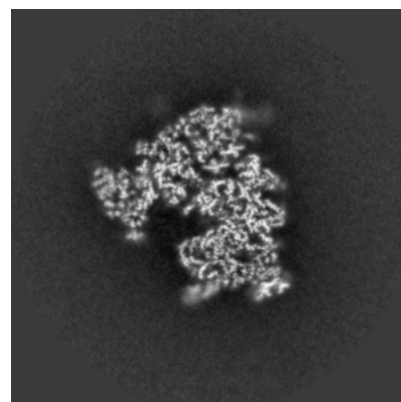
6.2.2 Raw map



X Index: 200



Y Index: 200

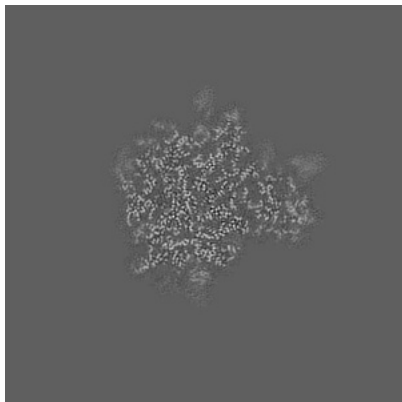


Z Index: 200

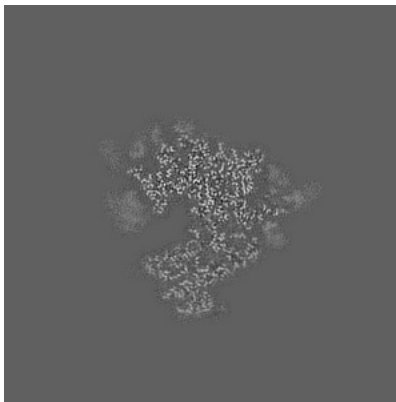
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

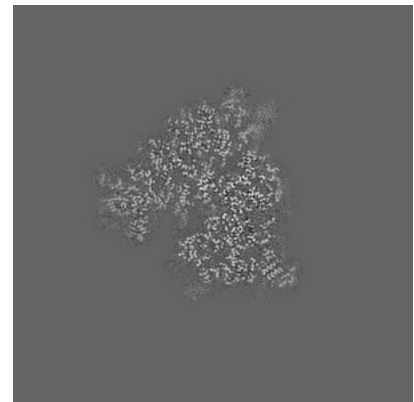
6.3.1 Primary map



X Index: 213

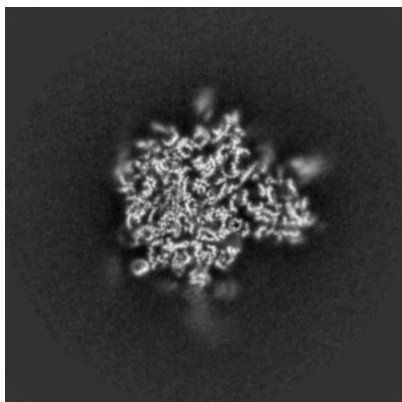


Y Index: 204

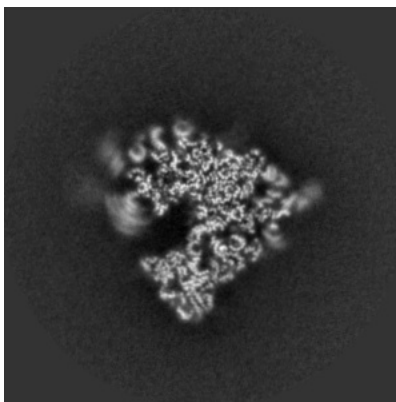


Z Index: 193

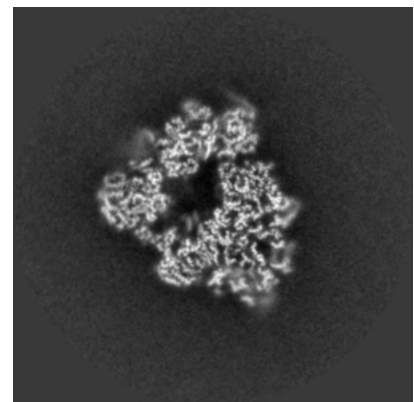
6.3.2 Raw map



X Index: 213



Y Index: 201

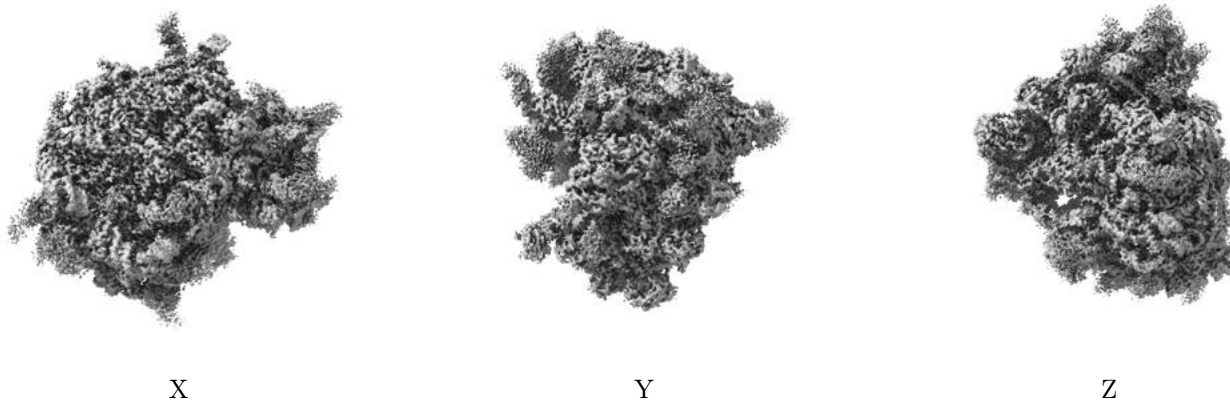


Z Index: 176

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

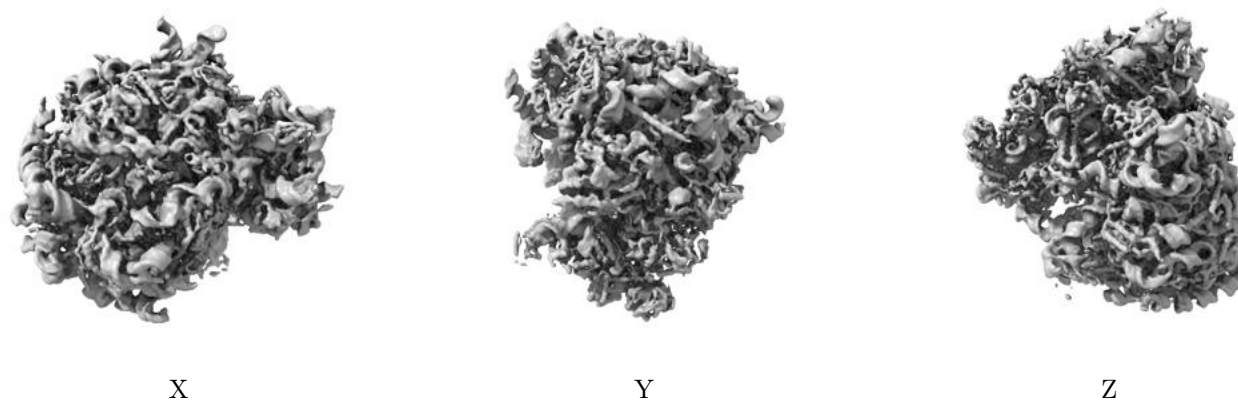
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

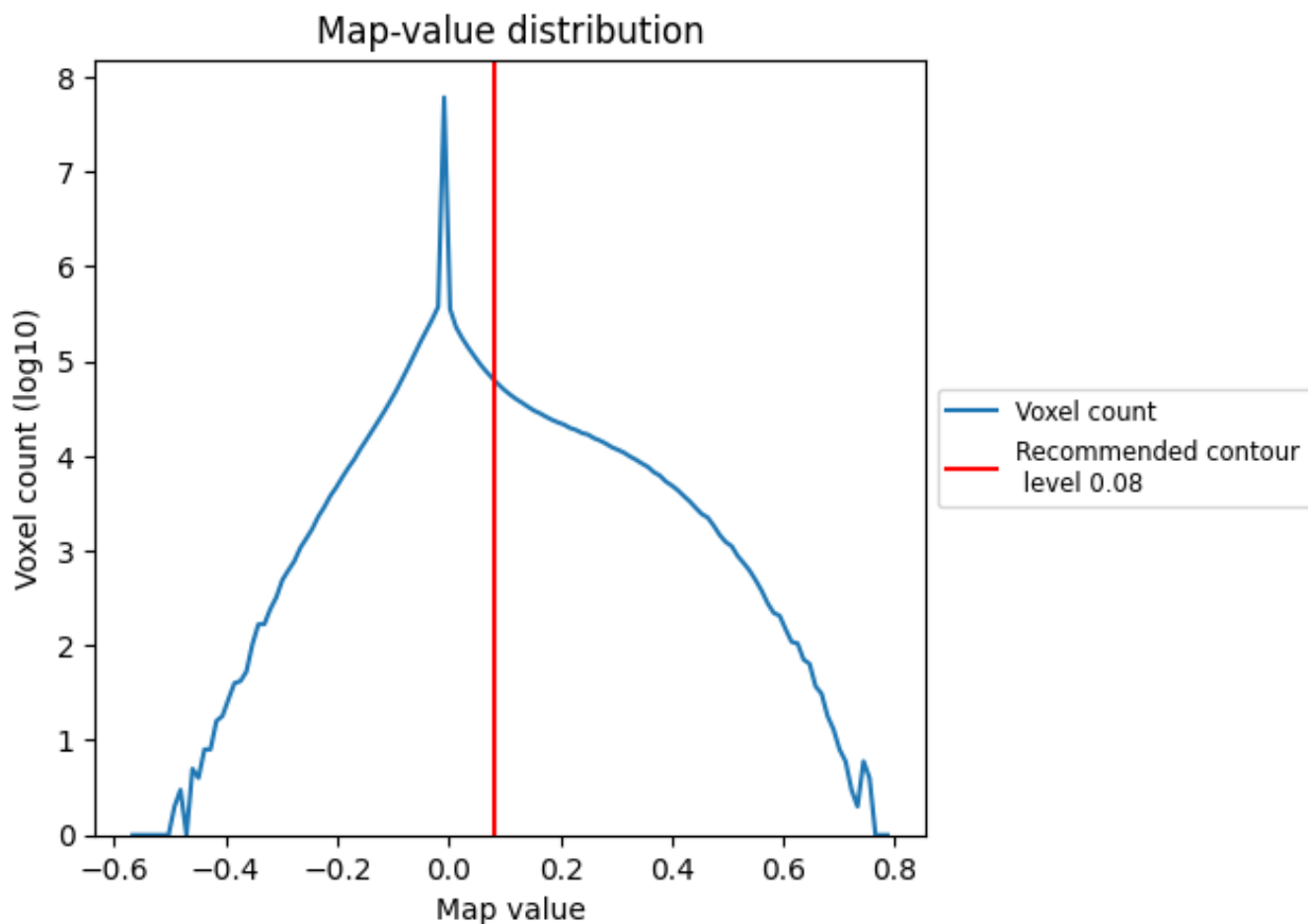
6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

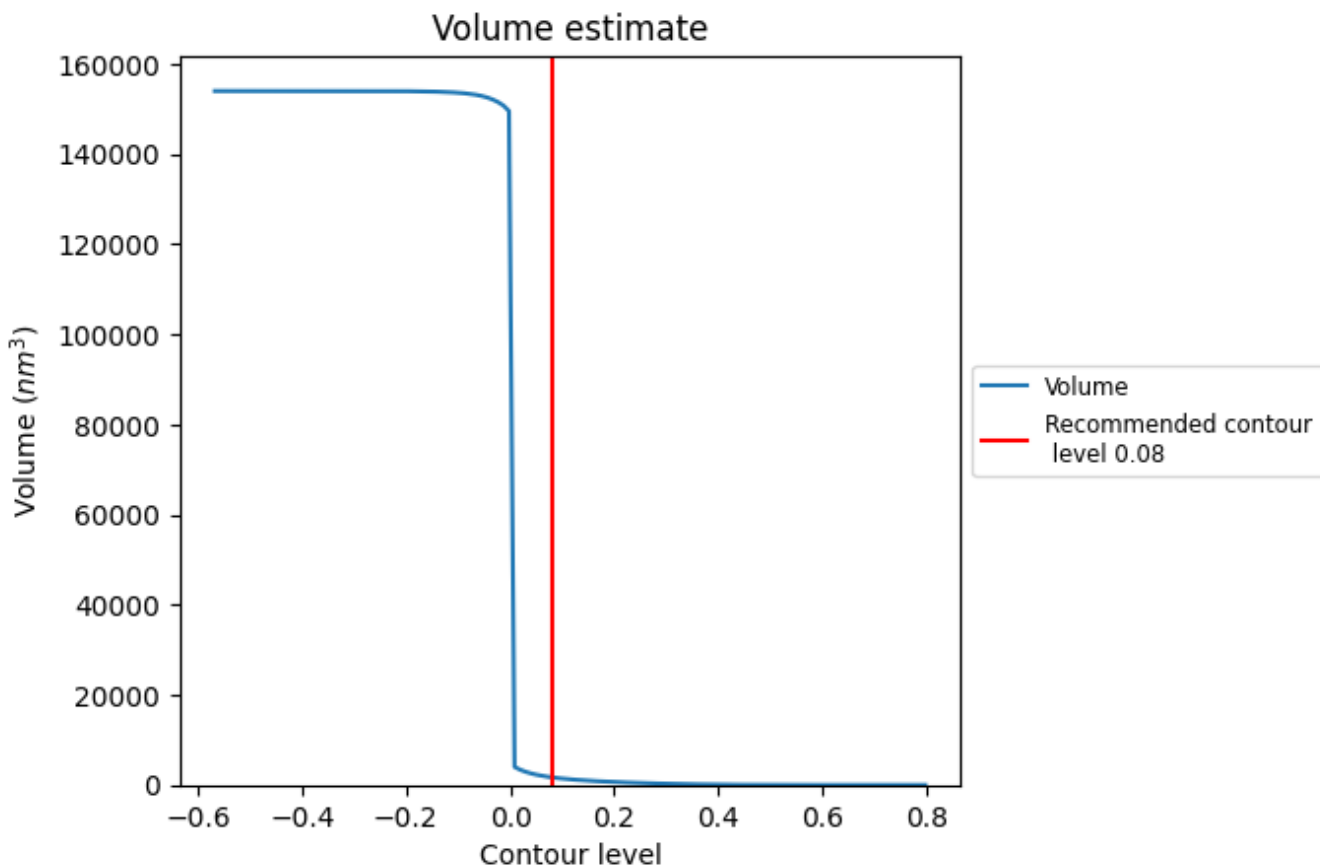
This section contains the results of statistical analysis of the map.

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.

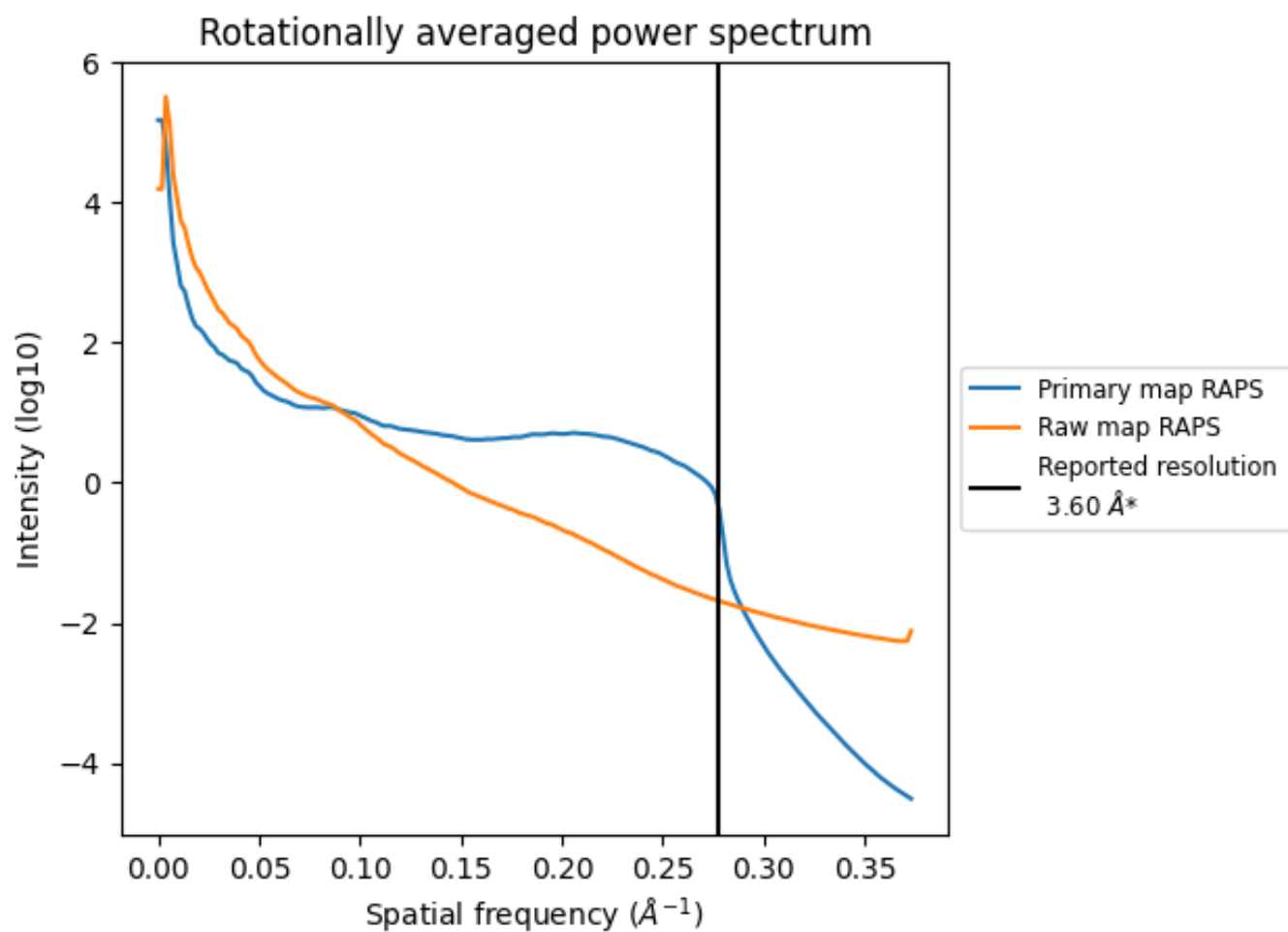
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1689 nm³; this corresponds to an approximate mass of 1525 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](#)

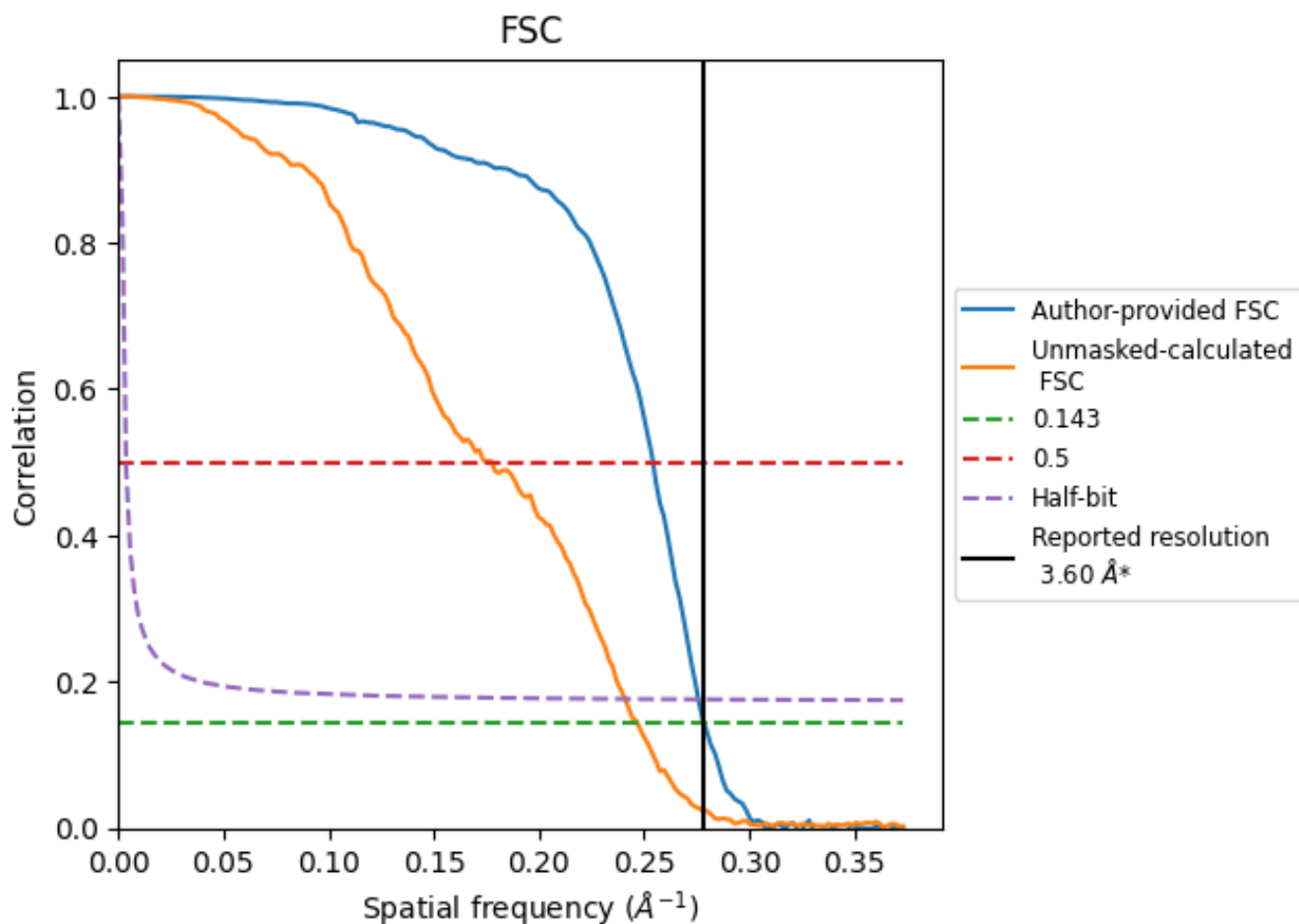


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

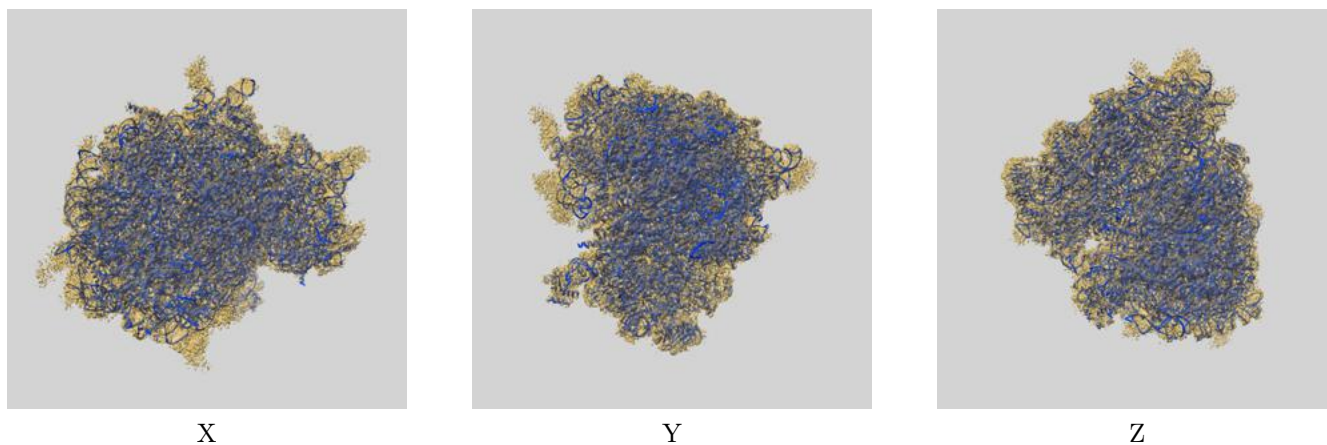
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	3.93	3.63
Unmasked-calculated*	4.05	5.64	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9237 and PDB model 6MTB. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



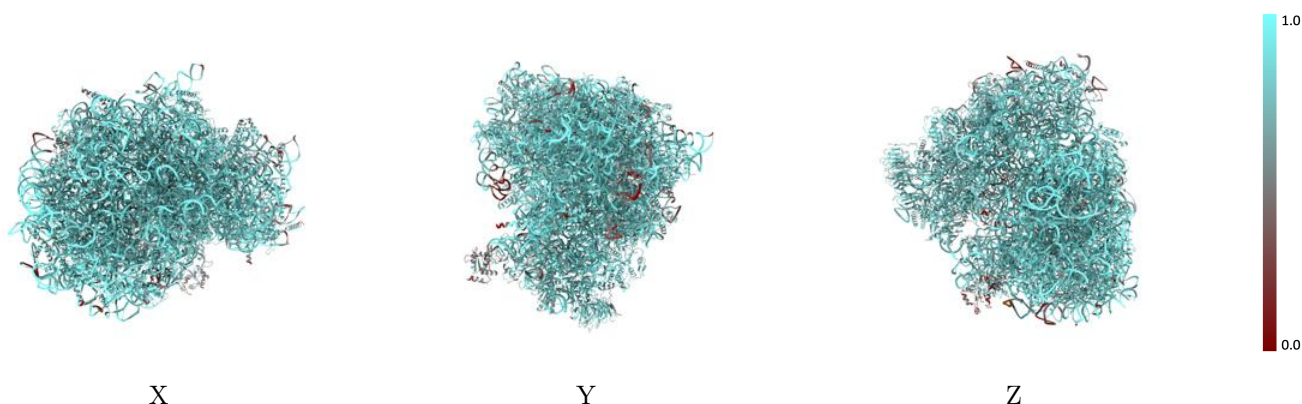
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



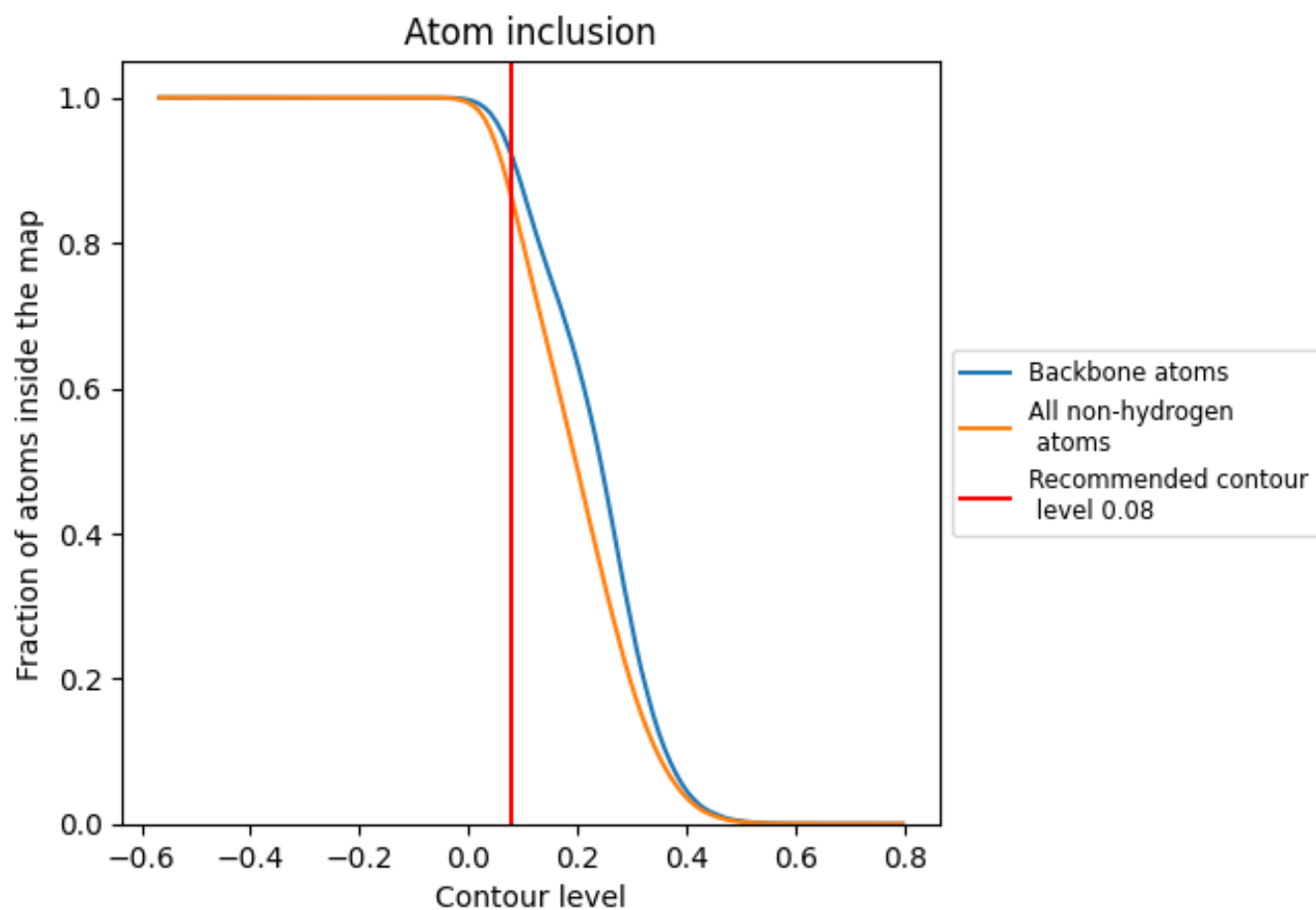
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8604	 0.4680
1	 0.7919	 0.4930
2	 0.6473	 0.3510
4	 0.7520	 0.2920
5	 0.8980	 0.4560
7	 0.9423	 0.4880
8	 0.9173	 0.4670
9	 0.8913	 0.4460
A	 0.8671	 0.5320
AA	 0.8418	 0.4980
B	 0.8876	 0.5300
BB	 0.8040	 0.4950
C	 0.8585	 0.5210
CC	 0.8468	 0.5130
D	 0.8676	 0.5000
DD	 0.7606	 0.4620
E	 0.8731	 0.5070
EE	 0.8370	 0.5010
F	 0.8484	 0.5150
FF	 0.8149	 0.4790
G	 0.8027	 0.4790
GG	 0.7827	 0.4510
H	 0.8444	 0.5170
HH	 0.7420	 0.4480
I	 0.8501	 0.5210
II	 0.8033	 0.4860
J	 0.8365	 0.4920
JJ	 0.8205	 0.4880
KK	 0.7570	 0.4400
L	 0.8182	 0.4970
LL	 0.8149	 0.5110
M	 0.8644	 0.5060
MM	 0.4519	 0.2670
N	 0.8636	 0.5280
NN	 0.8199	 0.4970

















Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
O	 0.8732	 0.5230
OO	 0.8004	 0.4920
P	 0.8807	 0.5300
PP	 0.7720	 0.4510
Q	 0.8663	 0.5280
QQ	 0.8086	 0.4800
R	 0.8223	 0.4840
RR	 0.7929	 0.4730
S	 0.8665	 0.5230
SS	 0.7921	 0.4650
T	 0.8496	 0.5180
TT	 0.8276	 0.4690
U	 0.7737	 0.4490
UU	 0.7390	 0.4520
V	 0.8612	 0.5280
VV	 0.8408	 0.5060
W	 0.7593	 0.4570
WW	 0.8525	 0.5180
X	 0.8372	 0.5100
XX	 0.8422	 0.5170
Y	 0.8349	 0.5040
YY	 0.8084	 0.4700
Z	 0.8667	 0.5110
ZZ	 0.7942	 0.4610
a	 0.8733	 0.5260
aa	 0.8352	 0.5200
b	 0.7669	 0.4620
bb	 0.7950	 0.4950
c	 0.8347	 0.5000
cc	 0.7638	 0.5000
d	 0.8436	 0.5110
dd	 0.8484	 0.4810
e	 0.8859	 0.5370
ee	 0.7488	 0.4780
f	 0.9050	 0.5410
ff	 0.4584	 0.1230
g	 0.8448	 0.5140
gg	 0.7357	 0.4260
h	 0.8223	 0.5000
i	 0.8354	 0.4940
j	 0.8782	 0.5240
k	 0.7612	 0.4700

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
l	 0.8759	 0.5230
m	 0.8801	 0.5120
n	 0.8119	 0.5060
o	 0.8409	 0.5270
p	 0.8229	 0.5200
r	 0.8736	 0.5220
u	 0.4502	 0.2750