



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2024 – 04:25 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

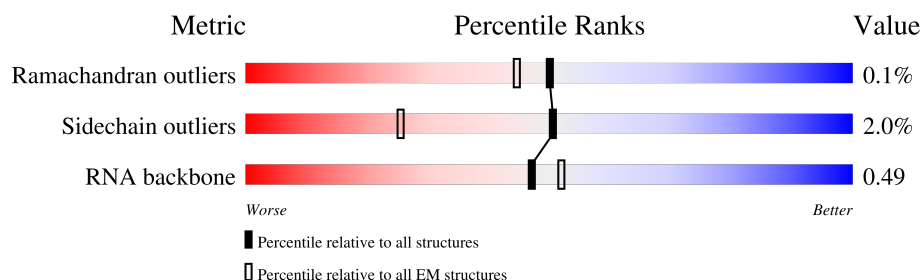
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



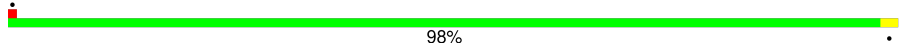
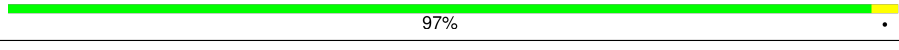
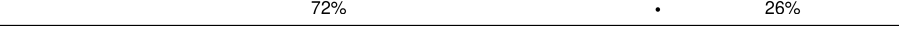
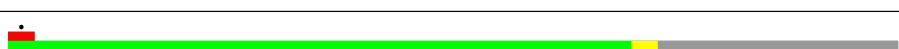

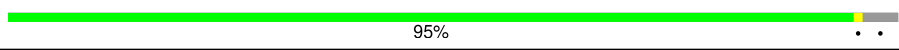
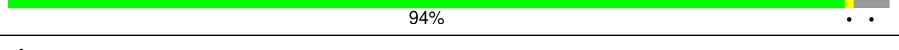
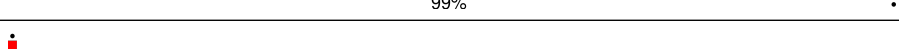
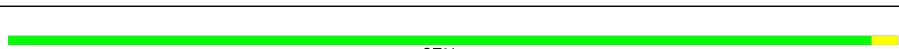
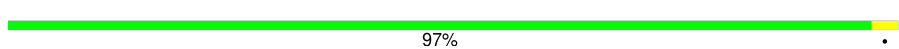
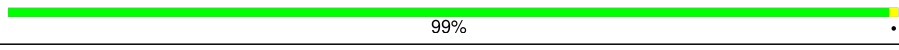
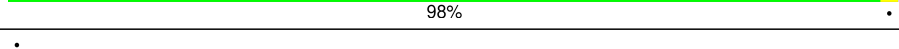
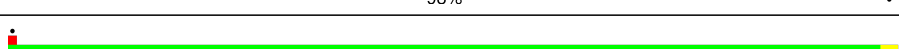
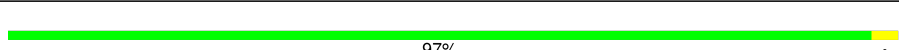
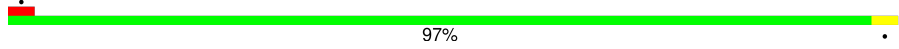
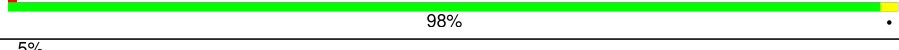
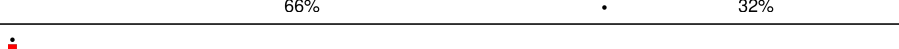

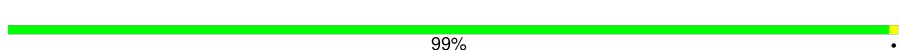
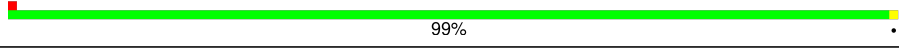




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	

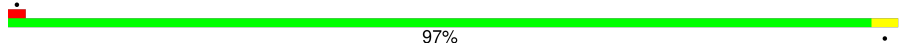
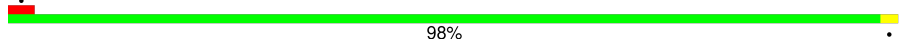
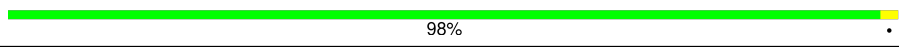
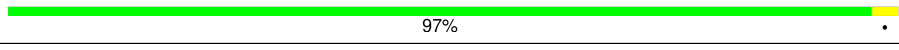
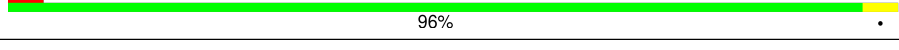
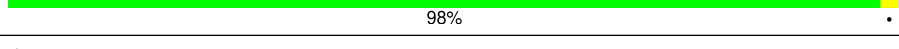
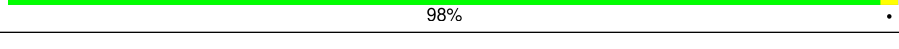
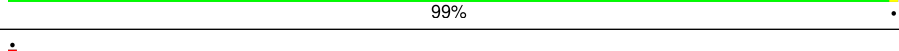
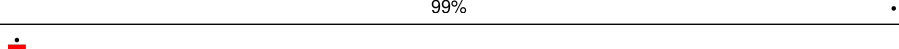
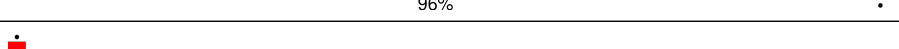
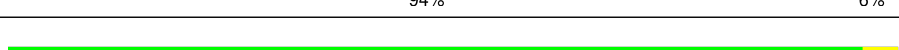
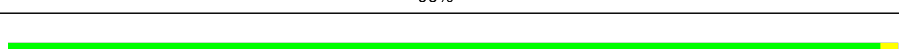
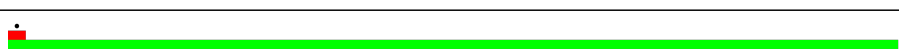
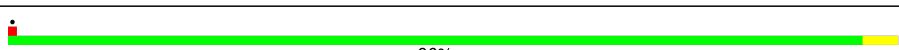
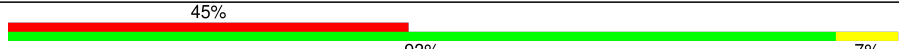

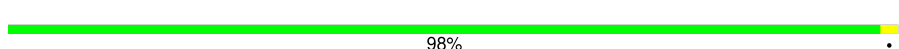
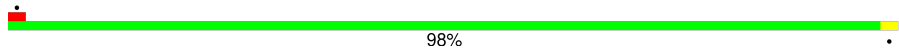
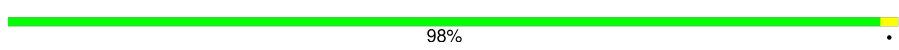
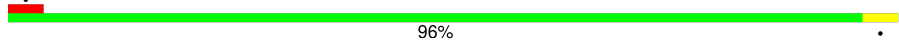
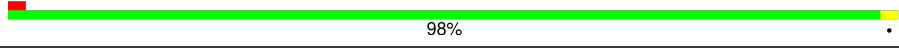
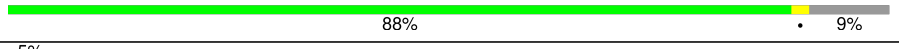
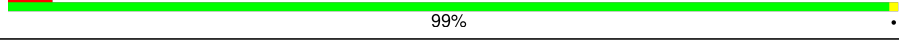
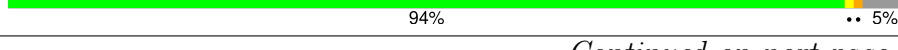

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Mol	Chain	Length	Quality of chain
9	C	362	
10	D	293	
11	E	291	
12	F	247	
13	G	319	
14	H	190	
15	I	214	
16	J	178	
17	L	210	
18	M	138	
19	N	203	
20	O	199	
21	P	153	
22	Q	187	
23	R	180	
24	S	176	
25	T	159	
26	U	99	
27	V	131	
28	W	157	
29	X	118	
30	Y	134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

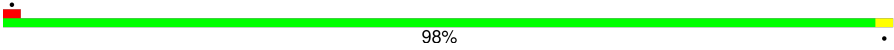
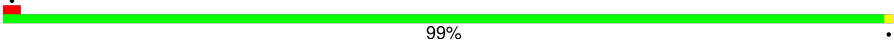
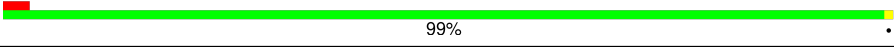

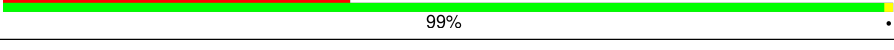
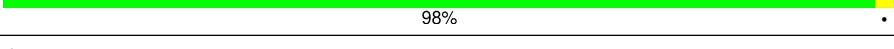
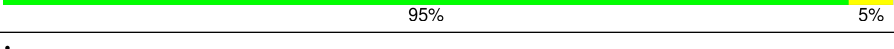
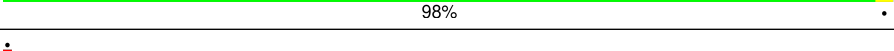
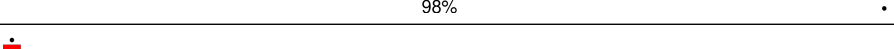
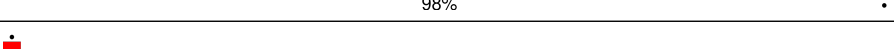
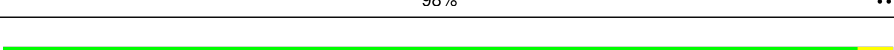
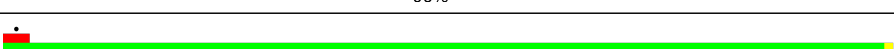
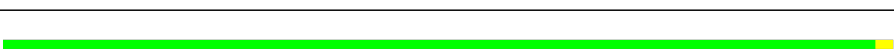
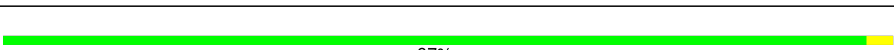
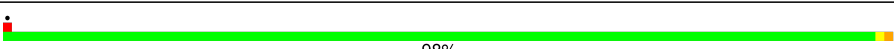
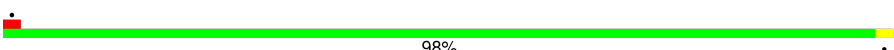

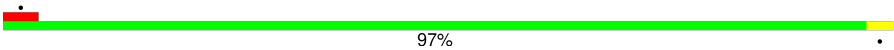
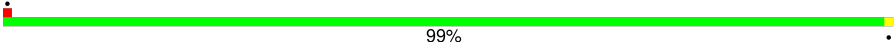
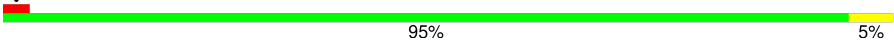
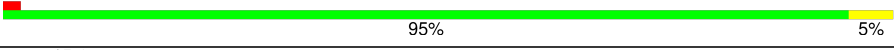
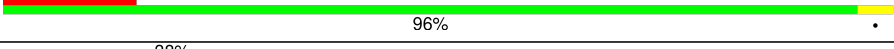

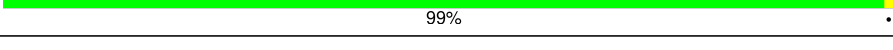

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Mol	Chain	Length	Quality of chain
34	c	98	
35	d	107	
36	e	128	
37	f	109	
38	g	114	
39	h	122	
40	i	102	
41	j	86	
42	k	69	
43	l	50	
44	m	52	
45	n	25	
46	o	103	
47	p	91	
48	r	124	
49	u	206	
50	9	1698	
51	AA	217	
52	BB	213	
53	CC	221	
54	DD	228	
55	EE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

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

2 Entry composition

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
1	1	7	Total	C	N	O	P	0	0
			149	67	27	48	7		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
21	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
42	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

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

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

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

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

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

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

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

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

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

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

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

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

- 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
63	MM	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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).

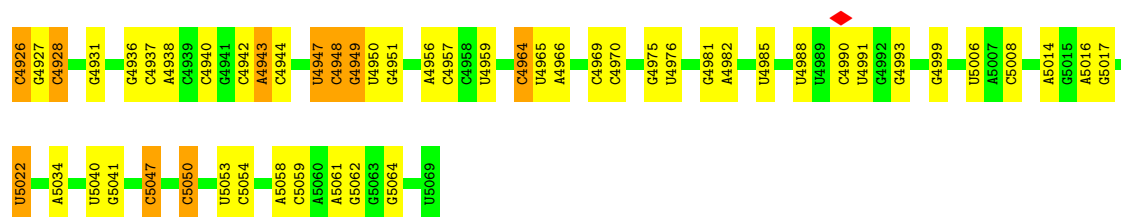
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84	7	7	Total 7	Mg 7	0
84	8	8	Total 8	Mg 8	0
84	A	1	Total 1	Mg 1	0
84	P	1	Total 1	Mg 1	0
84	V	1	Total 1	Mg 1	0
84	a	1	Total 1	Mg 1	0
84	j	1	Total 1	Mg 1	0
84	9	78	Total 78	Mg 78	0
84	TT	1	Total 1	Mg 1	0

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

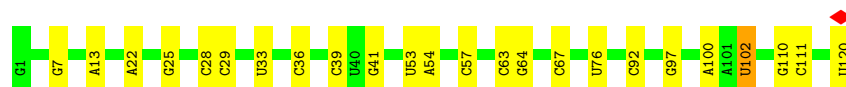
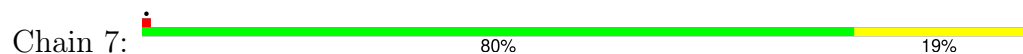
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85	j	1	Total 1	Zn 1	0
85	m	1	Total 1	Zn 1	0
85	o	1	Total 1	Zn 1	0
85	p	1	Total 1	Zn 1	0
85	aa	1	Total 1	Zn 1	0
85	dd	1	Total 1	Zn 1	0
85	ff	1	Total 1	Zn 1	0

A2300	G2051	C1768	G1633	G1497	U1395	G1288	C985	G748	C506	G401
G2301	G2052	G1769	A1634	A1498	G1396	C1289	C1072	G749	U510	C406
C2302	G2053	C1770	C1635	G1499	A1397	G1290	G1073	A407	C517	A408
U2304	G2054	C1771	A1638	G1502	A1398	G1291	A1078	G409	G518	G409
A2307	A2057	U1772	C1639	U1514	G1406	G1292	C1079	G758	G519	G412
A2313	G2058	C1773	C1640	U1517	G1406A	G1293	C1080	G759	U520	G413
G2314	C2059	A1774	U1649	G1518	G1406C	U1295	C1081	U914	C521	C414
G2315	G2062	C1777	A1650	A1519	C1411B	G1296	C1084	A917	C522	C417
G2316	A2069	U1781	G1654	C1520	C1411C	U1302	G1088	G918	C523	G417
G2319	U2070	A1787	U1655	C1521	G1412	A1303	G1175	C925	G638	G431
C2319	C2072	U1791	U1656	G1522	G1415	C1304	A1174	G926	U639	U432
C2325	U2084	U1792	C1663	A1524	G1421	C1308	U1179	A929	C640	U440
A2332	G2085	G1797	C1666	U1534	G1428	C1309	C1180	C930	G641	G444
G2333	G2089	A1804	U1672	C1540	C1429	C1310	G1187	C931	C661	U445
G2334	U2090	A1805	U1671	A1547	U1437	C1313	C1188	G934	A667	U446
C2335	C2091	G1806	U1672	C1563	C1430	G1314	G1193	C934	C688	C447
A2347	G2092	G1807	U1672	A1563	C1436	G1315	G1194	C935	C689	G448
G2348	C2093	C1808	U1672	C1566	C1437	G1316	G1195	C938	C672	C449
C2348	C2094	C1809	U1672	U1567	U1438	U1319	G1199	C939	C675	G450
C2351	A2095	C1812	C1676	C1568	U1440	U1320	C1210	C940	C451	A452
G2355	G2096	U1813	U1677	U1568	C1441	A1322	G1211	C941	A453	G453
U2356	C2097	G1814	C1679	G1574	C1442	C1325	G1212	G942	U454	U454
C2357	G2100	G1815	U1683	U1578	A1443	A1326	G1213	A943	C455	C455
A2360	A2101	G1818	U1686	C1579	G1444	G1329	C1214	A944	A686	A686
G2361	C2102	U1819	C1686	U1582	U1445	A1330	C1215	U945	U687	U687
U2362	A2103	U1820	U1691	U1591	C1446	U1337	G1234	G955	A463	A463
A2363	G2104	G1821	G1724	U1596	G1447	G1338	G1235	A956	C464	C464
G2364	A2105	G1822	U1725	U1599	C1448	U1339	G1236	C691	U467	U468
C2365	G2106	C1828	U1726	G1599	G1455	C1340	C1237	A960	C472	C472
A2107	A2107	G1833	U1731	U1602	C1456	U1348	G1248	C696	G704	G481
G2380	G2108	U1834	U1735	C1603	G1466	G1353	C1249	A964	G705	C481A
U2384	A2109	G1835	U1735	G1604	C1467	A1354	C1250	A966	G708	G482
A2395	C2258	G1836	U1741	G1606	C1468	G1358	C1251	C967	G708	C483
A2396	G2259	U1837	A1742	U1607	C1469	G1359	C1252	C968	U484	U484
G2397	C2260	G1842	U1751	C1607	C1472	G1370	G1271	C969	C485	C485
U2398	C2261	A1843	U1756	G1612	C1473	A1371	G1272	C972	C489	C489
A2401	A2268	C1847	U1757	A1613	U1474	A1372	G1273	C973	U492	U492
G2405	C2270	G1853	U1757	G1624	G1475	G1377	C1276	G722	G493	G493
G2406	C2271	G1854	C1762	G1625	C1477	U1381	A1279	G729	G730	G496
G2407	G2275	G1855	C1763	U1626	C1481	G1382	G1280	C978	G731	C497
U2408	U2281	U1860	C1764	G1627	G1482	G1387	G1281	C979	G736	C498
C2410	C2289	U1863	A1765	C1628	G1483	A1387	G1284	C980	G742	G500
G2416	G2297	U1866	A1766	U1631	G1484	G1394	G1287	U933	A746	A746
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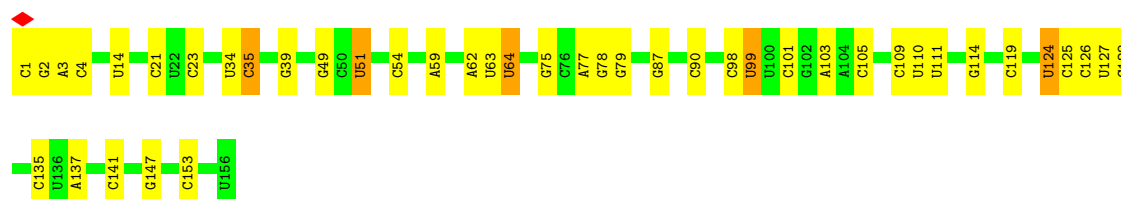
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• Molecule 5: 5S rRNA



• Molecule 6: 5.8S rRNA



• Molecule 7: 60S ribosomal protein L8



• Molecule 8: 60S ribosomal protein L3



• Molecule 9: 60S ribosomal protein L4

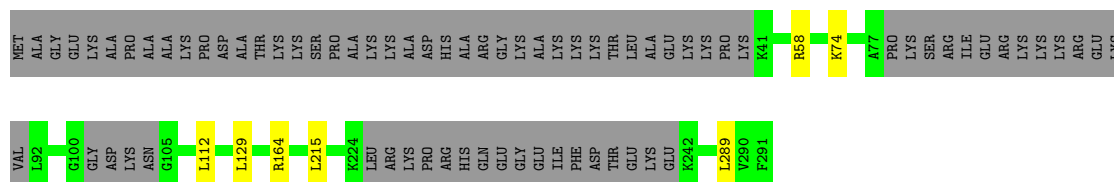


• Molecule 10: 60S ribosomal protein L5



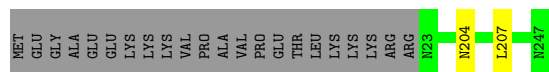
- Molecule 11: 60S ribosomal protein L6

Chain E:  72% . 26%



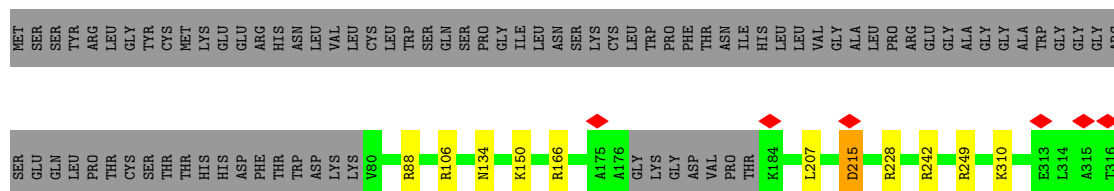
- Molecule 12: 60S ribosomal protein L7

Chain F: 90% 9%



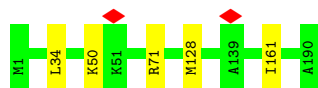
- Molecule 13: 60S ribosomal protein L7a

Chain G:  70% 27%



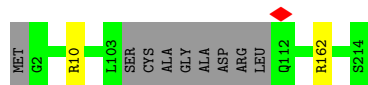
- Molecule 14: 60S ribosomal protein L9

Chain H: 97%



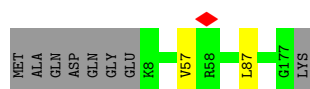
- Molecule 15: 60S ribosomal protein L10

Chain I:  95% ..



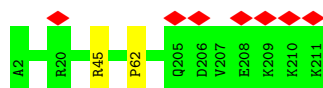
- Molecule 16: 60S ribosomal protein L11

Chain J:  94%



- Molecule 17: 60S ribosomal protein L13

Chain L:  99%



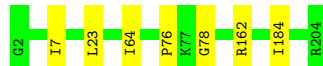
- Molecule 18: 60S ribosomal protein L14

Chain M:  97%



- Molecule 19: 60S ribosomal protein L15

Chain N:  97%



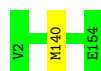
- Molecule 20: 60S ribosomal protein L13a

Chain O:  97%



- Molecule 21: 60S ribosomal protein L17

Chain P:  99%



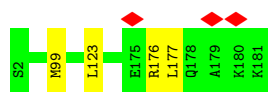
- Molecule 22: 60S ribosomal protein L18

Chain Q:  98%



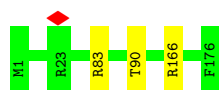
- Molecule 23: 60S ribosomal protein L19

Chain R:  98%



- Molecule 24: 60S ribosomal protein L18a

Chain S:  98%



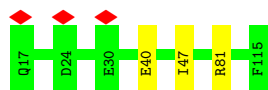
- Molecule 25: 60S ribosomal protein L21

Chain T:  97%



- Molecule 26: 60S ribosomal protein L22

Chain U:  97%



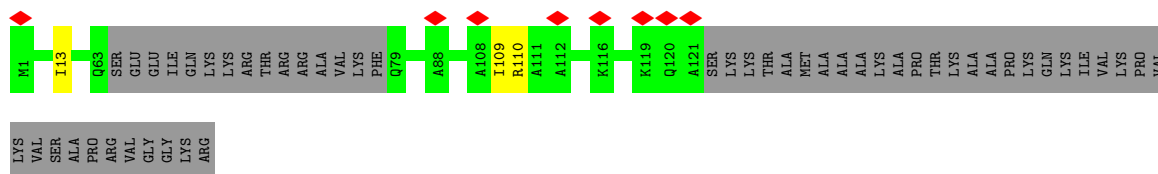
- Molecule 27: 60S ribosomal protein L23

Chain V:  98%



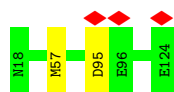
- Molecule 28: 60S ribosomal protein L24

Chain W:  5%  66%  32%



- Molecule 29: 60S ribosomal protein L23a

Chain X:  100%



- Molecule 36: 60S ribosomal protein L32

Chain e: 98%



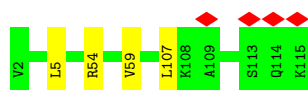
- Molecule 37: 60S ribosomal protein L35a

Chain f: 97%



- Molecule 38: 60S ribosomal protein L34

Chain g: 96%



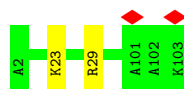
- Molecule 39: 60S ribosomal protein L35

Chain h: 98%



- Molecule 40: 60S ribosomal protein L36

Chain i: 98%



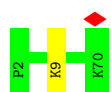
- Molecule 41: 60S ribosomal protein L37

Chain j: 99%



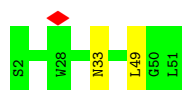
- Molecule 42: 60S ribosomal protein L38

Chain k:  99%



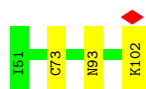
- Molecule 43: 60S ribosomal protein L39

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%

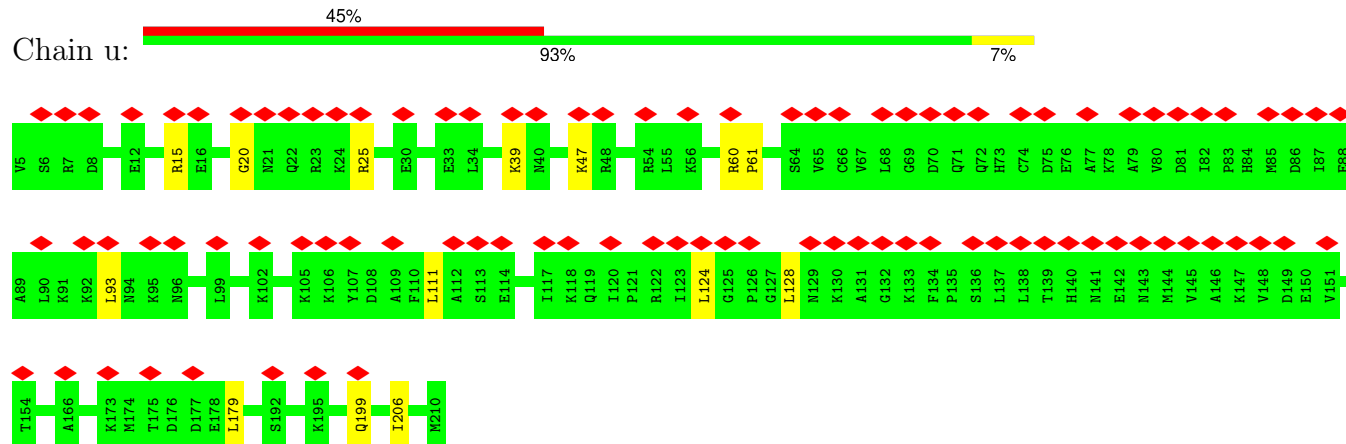


- Molecule 48: 60S ribosomal protein L28

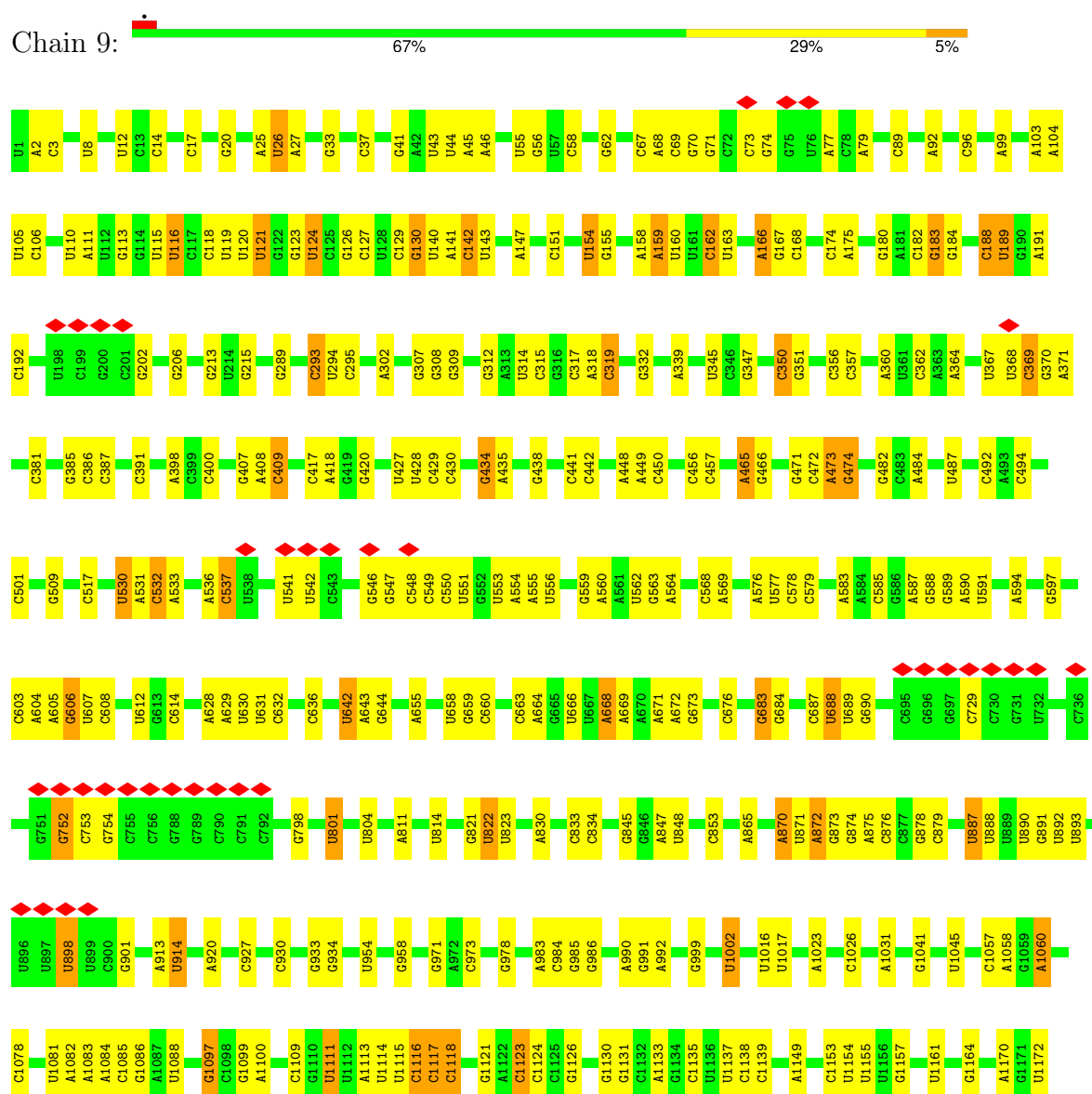
Chain r:  96%

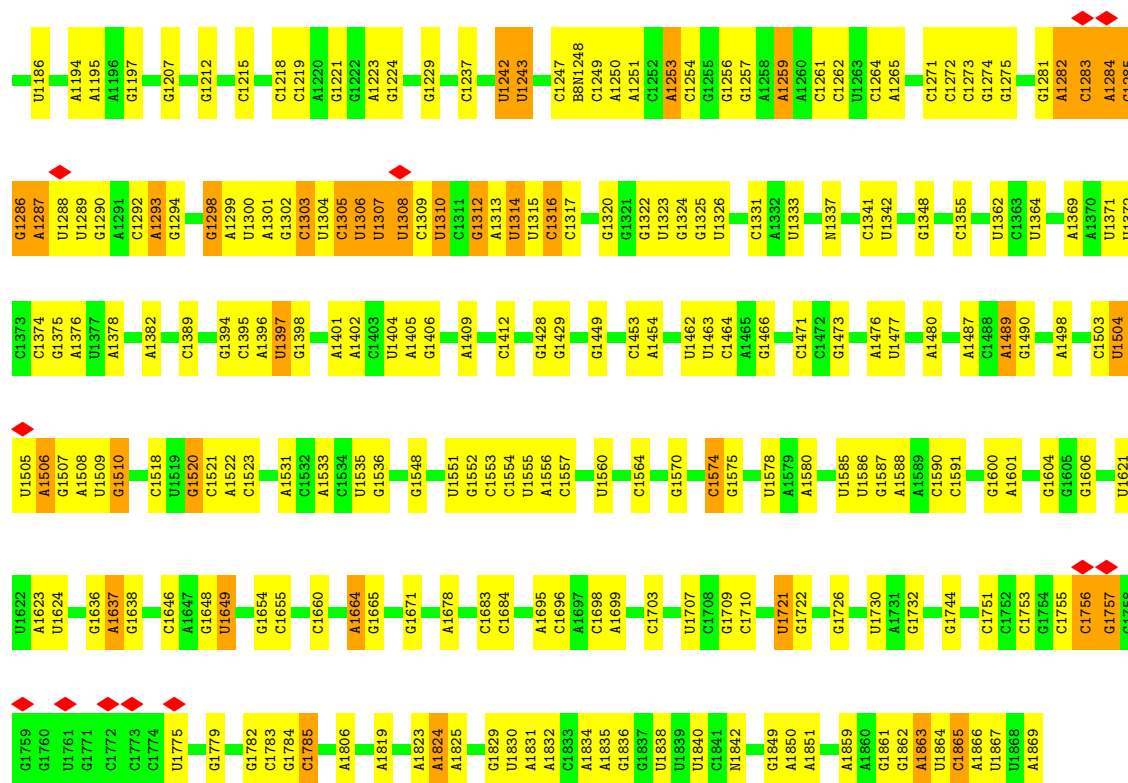


• Molecule 49: 60S ribosomal protein L10a



• Molecule 50: 18S rRNA





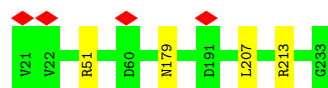
• Molecule 51: 40S ribosomal protein SA

Chain AA:  98%



• Molecule 52: 40S ribosomal protein S3a

Chain BB:  98%



• Molecule 53: 40S ribosomal protein S2

Chain CC:  98%

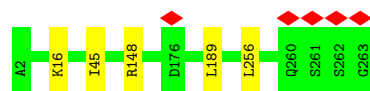


• Molecule 54: 40S ribosomal protein S3

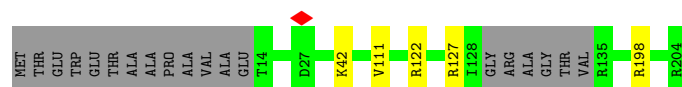
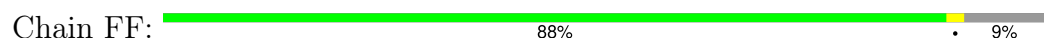
Chain DD:  96%



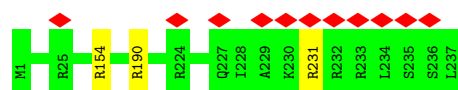
- Molecule 55: 40S ribosomal protein S4, X isoform



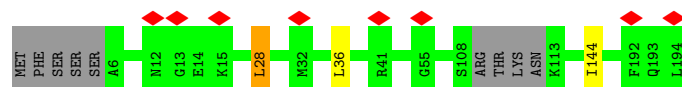
- Molecule 56: 40S ribosomal protein S5



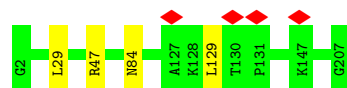
- Molecule 57: 40S ribosomal protein S6



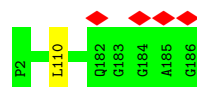
- Molecule 58: 40S ribosomal protein S7



- Molecule 59: 40S ribosomal protein S8

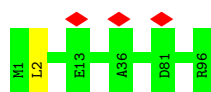


- Molecule 60: 40S ribosomal protein S9



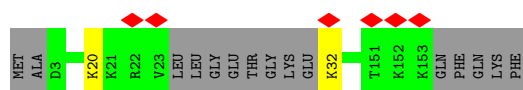
- Molecule 61: 40S ribosomal protein S10

Chain KK:  99%



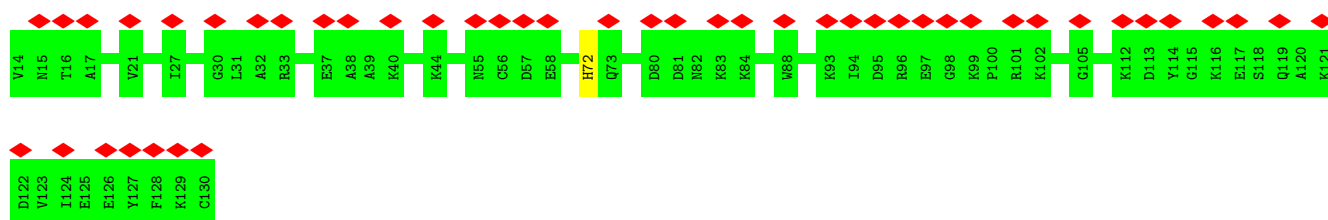
- Molecule 62: 40S ribosomal protein S11

Chain LL:  89%



- Molecule 63: 40S ribosomal protein S12

Chain MM:  39%



- Molecule 64: 40S ribosomal protein S13

Chain NN:  98%



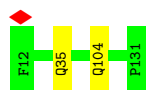
- Molecule 65: 40S ribosomal protein S14

Chain OO:  95%



- Molecule 66: 40S ribosomal protein S15

Chain PP:  98%



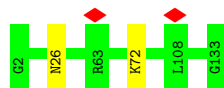
- Molecule 67: 40S ribosomal protein S16

Chain QQ:  98%



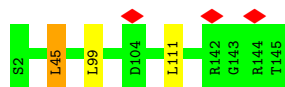
- Molecule 68: 40S ribosomal protein S17

Chain RR: 98%



- Molecule 69: 40S ribosomal protein S18

Chain SS: 98%



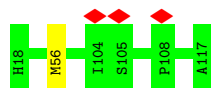
- Molecule 70: 40S ribosomal protein S19

Chain TT: 96%



- Molecule 71: 40S ribosomal protein S20

Chain UU: 99%



- Molecule 72: 40S ribosomal protein S21

Chain VV: 98%



- Molecule 73: 40S ribosomal protein S15a

Chain WW: 97%



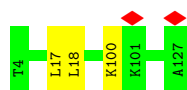
- Molecule 74: 40S ribosomal protein S23

Chain XX:  98% ..



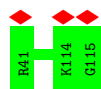
- Molecule 75: 40S ribosomal protein S24

Chain YY:  98% .



- Molecule 76: 40S ribosomal protein S25

Chain ZZ:  100%



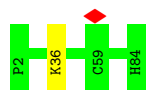
- Molecule 77: 40S ribosomal protein S26

Chain aa:  97% .



- Molecule 78: 40S ribosomal protein S27

Chain bb:  99% .



- Molecule 79: 40S ribosomal protein S28

Chain cc:  95% 5%

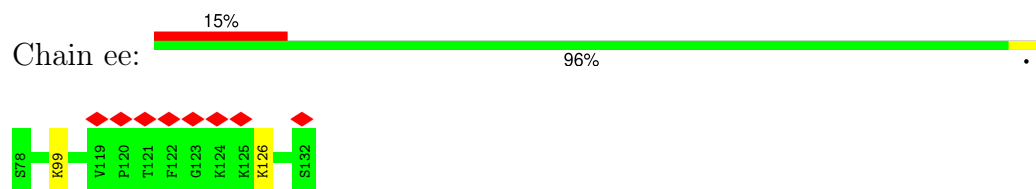


- Molecule 80: 40S ribosomal protein S29

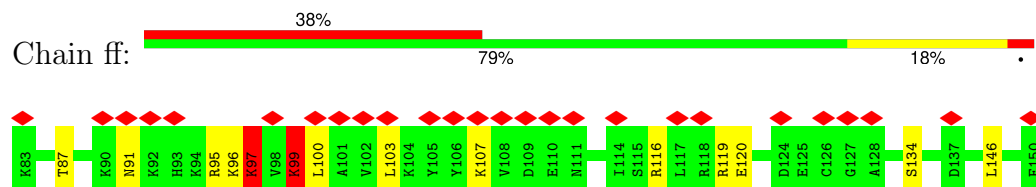
Chain dd:  95% 5%



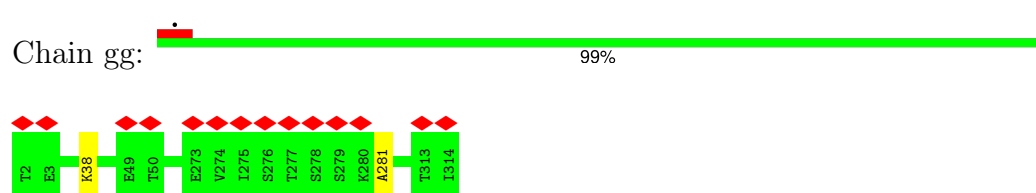
• Molecule 81: 40S ribosomal protein S30



• 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

5.1 Standard geometry

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

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%)	25	59
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%)	22	55
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%)	16	51
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

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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%)	6	34
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%)	25	59
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

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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%)	5	32
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%)	50	79

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 ⓘ

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%)	48	71
8	B	342/342 (100%)	336 (98%)	6 (2%)	54	74
9	C	301/301 (100%)	295 (98%)	6 (2%)	50	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	D	247/247 (100%)	240 (97%)	7 (3%)	38	64
11	E	190/251 (76%)	186 (98%)	4 (2%)	48	71
12	F	196/215 (91%)	195 (100%)	1 (0%)	86	93
13	G	200/272 (74%)	190 (95%)	10 (5%)	20	49
14	H	169/169 (100%)	166 (98%)	3 (2%)	54	74
15	I	175/181 (97%)	173 (99%)	2 (1%)	70	83
16	J	143/149 (96%)	142 (99%)	1 (1%)	81	90
17	L	175/175 (100%)	174 (99%)	1 (1%)	84	92
18	M	117/117 (100%)	113 (97%)	4 (3%)	32	60
19	N	171/171 (100%)	167 (98%)	4 (2%)	45	68
20	O	171/171 (100%)	168 (98%)	3 (2%)	54	74
21	P	134/134 (100%)	133 (99%)	1 (1%)	81	90
22	Q	164/164 (100%)	162 (99%)	2 (1%)	67	82
23	R	159/159 (100%)	156 (98%)	3 (2%)	52	73
24	S	157/157 (100%)	155 (99%)	2 (1%)	65	81
25	T	139/139 (100%)	136 (98%)	3 (2%)	47	69
26	U	89/89 (100%)	86 (97%)	3 (3%)	32	60
27	V	101/101 (100%)	99 (98%)	2 (2%)	50	72
28	W	86/126 (68%)	84 (98%)	2 (2%)	45	68
29	X	106/106 (100%)	106 (100%)	0	100	100
30	Y	124/124 (100%)	121 (98%)	3 (2%)	44	67
31	Z	117/117 (100%)	116 (99%)	1 (1%)	75	87
32	a	119/119 (100%)	118 (99%)	1 (1%)	79	88
33	b	84/184 (46%)	80 (95%)	4 (5%)	21	51
34	c	84/84 (100%)	81 (96%)	3 (4%)	30	59
35	d	98/98 (100%)	97 (99%)	1 (1%)	73	85
36	e	114/114 (100%)	111 (97%)	3 (3%)	41	65
37	f	88/88 (100%)	85 (97%)	3 (3%)	32	60
38	g	98/98 (100%)	94 (96%)	4 (4%)	26	55
39	h	109/109 (100%)	107 (98%)	2 (2%)	54	74
40	i	86/86 (100%)	84 (98%)	2 (2%)	45	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	j	73/73 (100%)	72 (99%)	1 (1%)	62	79
42	k	64/64 (100%)	63 (98%)	1 (2%)	58	76
43	l	47/47 (100%)	46 (98%)	1 (2%)	48	71
44	m	47/47 (100%)	45 (96%)	2 (4%)	25	54
45	n	24/24 (100%)	23 (96%)	1 (4%)	25	54
46	o	91/91 (100%)	90 (99%)	1 (1%)	70	83
47	p	74/74 (100%)	74 (100%)	0	100	100
48	r	108/108 (100%)	103 (95%)	5 (5%)	23	52
49	u	186/186 (100%)	179 (96%)	7 (4%)	28	57
51	AA	180/181 (99%)	178 (99%)	2 (1%)	70	83
52	BB	194/194 (100%)	190 (98%)	4 (2%)	48	71
53	CC	187/187 (100%)	184 (98%)	3 (2%)	58	76
54	DD	190/190 (100%)	184 (97%)	6 (3%)	34	61
55	EE	224/224 (100%)	220 (98%)	4 (2%)	54	74
56	FF	158/170 (93%)	153 (97%)	5 (3%)	34	61
57	GG	207/207 (100%)	204 (99%)	3 (1%)	62	79
58	HH	165/174 (95%)	162 (98%)	3 (2%)	54	74
59	II	178/178 (100%)	176 (99%)	2 (1%)	70	83
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%)	60	78
63	MM	99/99 (100%)	99 (100%)	0	100	100
64	NN	130/130 (100%)	129 (99%)	1 (1%)	79	88
65	OO	106/106 (100%)	100 (94%)	6 (6%)	17	46
66	PP	109/109 (100%)	107 (98%)	2 (2%)	54	74
67	QQ	117/117 (100%)	114 (97%)	3 (3%)	41	65
68	RR	119/119 (100%)	117 (98%)	2 (2%)	56	75
69	SS	125/125 (100%)	124 (99%)	1 (1%)	79	88
70	TT	111/111 (100%)	108 (97%)	3 (3%)	40	65
71	UU	92/92 (100%)	92 (100%)	0	100	100
72	VV	67/67 (100%)	66 (98%)	1 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	WW	112/112 (100%)	109 (97%)	3 (3%)	40	65
74	XX	113/113 (100%)	113 (100%)	0	100	100
75	YY	107/107 (100%)	104 (97%)	3 (3%)	38	64
76	ZZ	66/66 (100%)	66 (100%)	0	100	100
77	aa	88/88 (100%)	85 (97%)	3 (3%)	32	60
78	bb	75/75 (100%)	74 (99%)	1 (1%)	65	81
79	cc	55/55 (100%)	52 (94%)	3 (6%)	18	47
80	dd	48/48 (100%)	46 (96%)	2 (4%)	25	54
81	ee	46/46 (100%)	44 (96%)	2 (4%)	25	54
82	ff	61/61 (100%)	54 (88%)	7 (12%)	4	23
83	gg	272/272 (100%)	271 (100%)	1 (0%)	89	95
All	All	9936/10274 (97%)	9738 (98%)	198 (2%)	50	72

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 ⓘ

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

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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 ⓘ

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	5MC	9	1374	50	19,22,23	3.81	8 (42%)	26,32,35	1.12	2 (7%)
4	A2M	5	1871	4,84	18,25,26	4.86	9 (50%)	20,36,39	2.82	6 (30%)
4	B8W	5	4472	4	18,26,27	4.23	7 (38%)	17,38,41	6.68	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMC	5	2861	4	19,22,23	2.85	7 (36%)	25,31,34	1.08	2 (8%)
4	PSU	5	3729	4	18,21,22	1.11	2 (11%)	21,30,33	2.00	4 (19%)
4	PSU	5	3764	4	18,21,22	1.02	1 (5%)	21,30,33	1.73	4 (19%)
50	A2M	9	668	84,50	18,25,26	4.79	8 (44%)	20,36,39	3.33	7 (35%)
4	B8H	5	1860	4	19,22,23	6.85	6 (31%)	21,32,35	2.51	5 (23%)
50	PSU	9	823	50	18,21,22	1.11	3 (16%)	21,30,33	1.81	4 (19%)
50	OMC	9	1703	50	19,22,23	2.88	7 (36%)	25,31,34	0.71	0
4	B9H	5	2786	4	21,25,26	2.96	3 (14%)	22,35,38	2.11	4 (18%)
50	5MU	9	814	50	19,22,23	4.82	7 (36%)	27,32,35	3.39	13 (48%)
50	PSU	9	1081	50	18,21,22	1.14	3 (16%)	21,30,33	1.91	5 (23%)
50	MA6	9	1850	50	19,26,27	1.76	2 (10%)	18,38,41	2.94	3 (16%)
50	B8Q	9	1219	84,50	18,22,23	2.88	5 (27%)	21,32,35	2.64	7 (33%)
4	OMC	5	3909	4	19,22,23	2.69	7 (36%)	25,31,34	0.97	1 (4%)
4	5MC	5	4447	4	19,22,23	3.69	8 (42%)	26,32,35	1.17	2 (7%)
4	PSU	5	4628	4	18,21,22	1.11	3 (16%)	21,30,33	2.13	4 (19%)
50	6MZ	9	1832	84,50	17,25,26	1.59	3 (17%)	15,36,39	1.95	3 (20%)
50	PSU	9	1243	50	18,21,22	1.31	1 (5%)	21,30,33	1.60	4 (19%)
50	OMU	9	116	50	19,22,23	2.78	7 (36%)	25,31,34	1.95	5 (20%)
50	UR3	9	1830	50	19,22,23	2.54	6 (31%)	26,32,35	1.96	5 (19%)
4	PSU	5	3715	4	18,21,22	0.97	1 (5%)	21,30,33	1.82	4 (19%)
4	OMC	5	2804	4	19,22,23	2.83	7 (36%)	25,31,34	0.90	0
4	BGH	5	3899	4,84	25,29,30	4.08	15 (60%)	30,43,46	2.77	14 (46%)
4	OMG	5	1883	4	19,26,27	2.43	8 (42%)	21,38,41	1.67	4 (19%)
4	MHG	5	4371	4	29,32,33	3.63	11 (37%)	34,46,49	2.35	12 (35%)
4	B9B	5	237	4	20,28,29	5.11	8 (40%)	19,40,43	2.52	7 (36%)
4	OMG	5	1316	4	19,26,27	2.37	7 (36%)	21,38,41	1.54	5 (23%)
4	OMC	5	3701	4,84	19,22,23	2.74	7 (36%)	25,31,34	0.82	0
4	1MA	5	1322	4,84	17,25,26	3.67	5 (29%)	17,37,40	1.98	3 (17%)
4	PSU	5	4500	4	18,21,22	1.08	3 (16%)	21,30,33	2.21	5 (23%)
4	B8W	5	4529	4,84	18,26,27	4.18	7 (38%)	17,38,41	7.47	9 (52%)
4	I4U	5	1659	4	20,24,25	4.92	13 (65%)	27,34,37	2.13	3 (11%)
4	1MA	5	4415	4	17,25,26	3.91	4 (23%)	17,37,40	1.79	3 (17%)
4	OMG	5	4870	4	19,26,27	2.43	8 (42%)	21,38,41	1.56	4 (19%)
4	OMC	5	4536	4	19,22,23	2.70	7 (36%)	25,31,34	1.10	2 (8%)
4	B8W	5	4185	4	18,26,27	4.17	7 (38%)	17,38,41	7.14	11 (64%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	5MU	5	4083	4	19,22,23	4.69	7 (36%)	27,32,35	3.62	11 (40%)
4	6MZ	5	4220	4	17,25,26	1.92	3 (17%)	15,36,39	2.21	4 (26%)
4	OMG	5	1522	4	19,26,27	2.35	8 (42%)	21,38,41	1.58	4 (19%)
4	A2M	5	2363	4,84	18,25,26	4.93	9 (50%)	20,36,39	2.79	5 (25%)
4	A2M	5	2401	4,84	18,25,26	4.92	9 (50%)	20,36,39	2.62	4 (20%)
4	OMG	5	4196	4,2	19,26,27	2.36	7 (36%)	21,38,41	1.46	4 (19%)
4	PSU	5	1677	4	18,21,22	1.15	3 (16%)	21,30,33	2.01	6 (28%)
4	OMC	5	3869	4	19,22,23	2.69	7 (36%)	25,31,34	0.92	0
4	P7G	5	3880	4	24,28,29	3.40	10 (41%)	25,41,44	1.44	3 (12%)
4	B8W	5	4129	4	18,26,27	4.26	7 (38%)	17,38,41	7.26	11 (64%)
50	A2M	9	159	50	18,25,26	5.01	8 (44%)	20,36,39	2.89	5 (25%)
4	A2M	5	398	4	18,25,26	4.92	8 (44%)	20,36,39	2.58	3 (15%)
4	B8T	5	4671	4	19,22,23	2.93	8 (42%)	25,31,34	0.92	1 (4%)
4	OMG	5	373	4	19,26,27	2.38	8 (42%)	21,38,41	1.51	5 (23%)
4	A2M	5	4523	4,84	18,25,26	4.92	9 (50%)	20,36,39	3.07	7 (35%)
50	OMC	9	174	50	19,22,23	2.89	7 (36%)	25,31,34	0.85	0
4	A2M	5	3785	4	18,25,26	4.68	10 (55%)	20,36,39	3.02	6 (30%)
4	B8H	5	3762	4	19,22,23	6.86	6 (31%)	21,32,35	2.61	5 (23%)
50	A2M	9	27	84,50	18,25,26	4.91	9 (50%)	20,36,39	2.70	3 (15%)
44	MLZ	m	72	44	8,9,10	0.80	0	4,9,11	1.04	0
4	B8W	5	2380	4	18,26,27	4.25	6 (33%)	17,38,41	7.33	9 (52%)
4	E7G	5	1797	4	24,27,28	3.09	11 (45%)	28,40,43	2.31	10 (35%)
50	OMC	9	517	50	19,22,23	2.83	7 (36%)	25,31,34	1.05	1 (4%)
4	OMC	5	3887	4	19,22,23	2.85	7 (36%)	25,31,34	0.90	1 (4%)
4	B8K	5	4690	4	24,28,29	4.85	17 (70%)	29,42,45	2.94	12 (41%)
4	OMG	5	4370	4	19,26,27	2.35	8 (42%)	21,38,41	1.45	4 (19%)
4	B8H	5	4296	4	19,22,23	6.93	8 (42%)	21,32,35	2.76	6 (28%)
4	OMC	5	2422	4,84	19,22,23	2.84	7 (36%)	25,31,34	0.83	1 (4%)
4	B8K	5	3897	4	24,28,29	4.72	17 (70%)	29,42,45	2.70	12 (41%)
50	PSU	9	822	50	18,21,22	1.10	2 (11%)	21,30,33	2.18	6 (28%)
4	PSU	5	2508	4	18,21,22	1.00	1 (5%)	21,30,33	1.77	4 (19%)
4	OMG	5	3792	4	19,26,27	2.39	8 (42%)	21,38,41	1.60	4 (19%)
50	A2M	9	1031	50	18,25,26	5.04	10 (55%)	20,36,39	2.55	4 (20%)
4	PSU	5	4403	4	18,21,22	1.08	2 (11%)	21,30,33	1.97	6 (28%)
4	I4U	5	4194	4	20,24,25	4.99	13 (65%)	27,34,37	2.04	5 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	B9B	5	1574	4	20,28,29	5.01	8 (40%)	19,40,43	2.40	5 (26%)
4	OMC	5	2365	4	19,22,23	2.79	7 (36%)	25,31,34	0.76	0
4	B8T	5	4483	4	19,22,23	3.02	8 (42%)	25,31,34	1.11	2 (8%)
50	M7A	9	1806	50	19,25,26	1.59	3 (15%)	25,37,40	3.91	8 (32%)
4	P4U	5	1348	4,84	21,24,25	3.36	7 (33%)	28,33,36	2.00	5 (17%)
4	PSU	5	4636	4	18,21,22	1.10	3 (16%)	21,30,33	2.21	6 (28%)
4	7MG	5	4550	4	23,26,27	3.09	10 (43%)	27,39,42	2.06	10 (37%)
4	UR3	5	4530	4	19,22,23	2.54	7 (36%)	26,32,35	1.74	4 (15%)
4	E6G	5	4355	4	19,27,28	4.69	7 (36%)	18,39,42	2.20	6 (33%)
50	OMG	9	644	50	19,26,27	2.37	8 (42%)	21,38,41	1.50	4 (19%)
50	OMC	9	1710	50	19,22,23	2.89	7 (36%)	25,31,34	1.05	1 (4%)
4	5MC	5	3782	4	19,22,23	3.51	8 (42%)	26,32,35	1.44	5 (19%)
50	E3C	9	568	50	19,23,24	3.38	6 (31%)	21,33,36	2.72	7 (33%)
4	M7A	5	4564	4	19,25,26	1.58	3 (15%)	25,37,40	3.99	7 (28%)
4	E7G	5	2297	4	24,27,28	3.00	11 (45%)	28,40,43	2.27	9 (32%)
50	4AC	9	1337	50	21,24,25	3.12	10 (47%)	28,34,37	1.21	4 (14%)
4	OMG	5	2424	4	19,26,27	2.47	8 (42%)	21,38,41	1.52	4 (19%)
4	PSU	5	4450	4,84	18,21,22	1.14	3 (16%)	21,30,33	2.16	5 (23%)
4	PSU	5	4531	4	18,21,22	1.12	3 (16%)	21,30,33	1.82	4 (19%)
4	A2M	5	3723	4	18,25,26	4.99	9 (50%)	20,36,39	2.63	4 (20%)
4	P7G	5	1909	4	24,28,29	3.54	10 (41%)	25,41,44	1.59	2 (8%)
50	PSU	9	119	50	18,21,22	0.88	1 (5%)	21,30,33	1.78	4 (19%)
50	4AC	9	1842	50	21,24,25	3.03	10 (47%)	28,34,37	1.56	7 (25%)
4	2MG	5	729	4	18,26,27	2.47	5 (27%)	16,38,41	1.55	4 (25%)
50	A2M	9	484	50	18,25,26	4.84	9 (50%)	20,36,39	2.86	5 (25%)
4	OMG	5	4623	4	19,26,27	2.34	8 (42%)	21,38,41	1.54	4 (19%)
4	OMG	5	4494	4	19,26,27	2.41	8 (42%)	21,38,41	1.68	5 (23%)
4	2MG	5	4872	4	18,26,27	2.66	7 (38%)	16,38,41	2.80	6 (37%)
4	OMG	5	2364	4	19,26,27	2.30	8 (42%)	21,38,41	1.49	4 (19%)
4	OMG	5	2773	4	19,26,27	2.36	8 (42%)	21,38,41	1.43	4 (19%)
50	B8N	9	1248	50	25,29,30	3.07	8 (32%)	28,42,45	2.15	8 (28%)
4	A2M	5	3867	4	18,25,26	4.88	8 (44%)	20,36,39	2.76	6 (30%)
4	B8Q	5	1456	4	18,22,23	2.65	5 (27%)	21,32,35	1.89	5 (23%)
4	OMG	5	2050	4	19,26,27	2.30	8 (42%)	21,38,41	1.52	4 (19%)
50	PSU	9	612	50	18,21,22	1.04	3 (16%)	21,30,33	1.71	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	5	1582	4	18,21,22	1.14	3 (16%)	21,30,33	1.92	4 (19%)
4	A2M	5	1534	4,84	18,25,26	4.94	8 (44%)	20,36,39	2.67	4 (20%)
4	OMG	5	4637	4	19,26,27	2.27	8 (42%)	21,38,41	1.57	4 (19%)
50	OMU	9	121	50	19,22,23	2.87	7 (36%)	25,31,34	1.94	5 (20%)
6	OMU	8	14	4,6	19,22,23	2.67	6 (31%)	25,31,34	1.97	5 (20%)
9	MLZ	C	333	9	8,9,10	0.93	0	4,9,11	0.93	0
50	A2M	9	166	50	18,25,26	5.09	9 (50%)	20,36,39	2.88	6 (30%)
4	7MG	5	1605	4	23,26,27	3.14	10 (43%)	27,39,42	2.22	10 (37%)
4	PSU	5	1683	4	18,21,22	1.20	2 (11%)	21,30,33	2.00	4 (19%)
4	7MG	5	2522	4	23,26,27	3.18	10 (43%)	27,39,42	2.22	8 (29%)
4	OMU	5	4306	4	19,22,23	2.75	8 (42%)	25,31,34	1.86	5 (20%)
50	A2M	9	1678	50	18,25,26	4.92	9 (50%)	20,36,39	3.11	6 (30%)
50	MA6	9	1851	50	19,26,27	1.73	2 (10%)	18,38,41	2.78	3 (16%)
4	A2M	5	4571	4	18,25,26	4.84	8 (44%)	20,36,39	2.67	4 (20%)
4	OMG	5	1625	4,84	19,26,27	2.35	8 (42%)	21,38,41	1.54	4 (19%)
4	PSU	5	4293	4	18,21,22	1.11	3 (16%)	21,30,33	1.94	4 (19%)
50	OMG	9	509	84,50	19,26,27	2.34	8 (42%)	21,38,41	1.52	4 (19%)
4	PSU	5	4442	4	18,21,22	1.10	3 (16%)	21,30,33	2.24	6 (28%)
50	OMG	9	683	50	19,26,27	2.43	8 (42%)	21,38,41	1.53	4 (19%)
4	2MG	5	1517	4	18,26,27	2.53	7 (38%)	16,38,41	2.13	5 (31%)
4	UR3	5	1866	4	19,22,23	2.39	6 (31%)	26,32,35	1.39	4 (15%)
4	UR3	5	4597	4	19,22,23	2.61	6 (31%)	26,32,35	1.50	5 (19%)
4	A2M	5	3718	4	18,25,26	4.99	11 (61%)	20,36,39	2.43	4 (20%)
4	A2M	5	1326	4	18,25,26	4.93	9 (50%)	20,36,39	2.74	3 (15%)
4	B9B	5	2754	4,84	20,28,29	5.00	7 (35%)	19,40,43	2.28	6 (31%)
4	OMU	5	4620	4	19,22,23	2.64	6 (31%)	25,31,34	1.87	5 (20%)
4	5MC	5	4335	4	19,22,23	3.78	8 (42%)	26,32,35	1.32	3 (11%)
4	A2M	5	3825	4	18,25,26	4.93	8 (44%)	20,36,39	2.71	4 (20%)
4	A2M	5	1524	4	18,25,26	4.91	9 (50%)	20,36,39	3.39	4 (20%)

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	5MC	9	1374	50	-	0/7/25/26	0/2/2/2
4	A2M	5	1871	4,84	-	0/5/27/28	0/3/3/3
4	B8W	5	4472	4	-	3/5/27/28	0/3/3/3
4	OMC	5	2861	4	-	1/9/27/28	0/2/2/2
4	PSU	5	3729	4	-	2/7/25/26	0/2/2/2
4	PSU	5	3764	4	-	0/7/25/26	0/2/2/2
50	A2M	9	668	84,50	-	3/5/27/28	0/3/3/3
4	B8H	5	1860	4	-	0/7/25/26	0/2/2/2
50	PSU	9	823	50	-	0/7/25/26	0/2/2/2
50	OMC	9	1703	50	-	2/9/27/28	0/2/2/2
4	B9H	5	2786	4	-	2/12/47/48	0/2/2/2
50	5MU	9	814	50	-	1/7/25/26	0/2/2/2
50	PSU	9	1081	50	-	1/7/25/26	0/2/2/2
50	MA6	9	1850	50	-	2/7/29/30	0/3/3/3
50	B8Q	9	1219	84,50	-	1/7/42/43	0/2/2/2
4	OMC	5	3909	4	-	0/9/27/28	0/2/2/2
4	5MC	5	4447	4	-	4/7/25/26	0/2/2/2
4	PSU	5	4628	4	-	0/7/25/26	0/2/2/2
50	6MZ	9	1832	84,50	-	2/5/27/28	0/3/3/3
50	PSU	9	1243	50	-	2/7/25/26	0/2/2/2
50	OMU	9	116	50	-	3/9/27/28	0/2/2/2
50	UR3	9	1830	50	-	2/7/25/26	0/2/2/2
4	PSU	5	3715	4	-	0/7/25/26	0/2/2/2
4	OMC	5	2804	4	-	0/9/27/28	0/2/2/2
4	BGH	5	3899	4,84	-	3/13/43/44	0/3/3/3
4	OMG	5	1883	4	-	2/5/27/28	0/3/3/3
4	MHG	5	4371	4	-	6/16/46/47	0/3/3/3
4	B9B	5	237	4	-	4/7/29/30	0/3/3/3
4	OMG	5	1316	4	-	1/5/27/28	0/3/3/3
4	OMC	5	3701	4,84	-	6/9/27/28	0/2/2/2
4	1MA	5	1322	4,84	-	0/3/25/26	0/3/3/3
4	PSU	5	4500	4	-	3/7/25/26	0/2/2/2
4	B8W	5	4529	4,84	-	4/5/27/28	0/3/3/3
4	I4U	5	1659	4	-	1/9/29/30	0/2/2/2
4	1MA	5	4415	4	-	2/3/25/26	0/3/3/3
4	OMG	5	4870	4	-	4/5/27/28	0/3/3/3
4	OMC	5	4536	4	-	0/9/27/28	0/2/2/2
4	B8W	5	4185	4	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5MU	5	4083	4	-	0/7/25/26	0/2/2/2
4	6MZ	5	4220	4	-	2/5/27/28	0/3/3/3
4	OMG	5	1522	4	-	0/5/27/28	0/3/3/3
4	A2M	5	2363	4,84	-	1/5/27/28	0/3/3/3
4	A2M	5	2401	4,84	-	1/5/27/28	0/3/3/3
4	OMG	5	4196	4,2	-	0/5/27/28	0/3/3/3
4	PSU	5	1677	4	-	1/7/25/26	0/2/2/2
4	OMC	5	3869	4	-	0/9/27/28	0/2/2/2
4	P7G	5	3880	4	-	2/10/40/41	0/3/3/3
4	B8W	5	4129	4	-	3/5/27/28	0/3/3/3
50	A2M	9	159	50	-	3/5/27/28	0/3/3/3
4	A2M	5	398	4	-	2/5/27/28	0/3/3/3
4	B8T	5	4671	4	-	0/7/27/28	0/2/2/2
4	OMG	5	373	4	-	0/5/27/28	0/3/3/3
4	A2M	5	4523	4,84	-	3/5/27/28	0/3/3/3
50	OMC	9	174	50	-	0/9/27/28	0/2/2/2
4	A2M	5	3785	4	-	3/5/27/28	0/3/3/3
4	B8H	5	3762	4	-	2/7/25/26	0/2/2/2
50	A2M	9	27	84,50	-	0/5/27/28	0/3/3/3
44	MLZ	m	72	44	-	1/7/8/10	-
4	B8W	5	2380	4	-	4/5/27/28	0/3/3/3
4	E7G	5	1797	4	-	2/9/39/40	0/3/3/3
50	OMC	9	517	50	-	0/9/27/28	0/2/2/2
4	OMC	5	3887	4	-	1/9/27/28	0/2/2/2
4	B8K	5	4690	4	-	0/11/41/42	0/3/3/3
4	OMG	5	4370	4	-	0/5/27/28	0/3/3/3
4	B8H	5	4296	4	-	0/7/25/26	0/2/2/2
4	OMC	5	2422	4,84	-	0/9/27/28	0/2/2/2
4	B8K	5	3897	4	-	3/11/41/42	0/3/3/3
50	PSU	9	822	50	-	0/7/25/26	0/2/2/2
4	PSU	5	2508	4	-	0/7/25/26	0/2/2/2
4	OMG	5	3792	4	-	2/5/27/28	0/3/3/3
50	A2M	9	1031	50	-	0/5/27/28	0/3/3/3
4	PSU	5	4403	4	-	3/7/25/26	0/2/2/2
4	I4U	5	4194	4	-	4/9/29/30	0/2/2/2
4	B9B	5	1574	4	-	2/7/29/30	0/3/3/3
4	OMC	5	2365	4	-	0/9/27/28	0/2/2/2
4	B8T	5	4483	4	-	0/7/27/28	0/2/2/2
50	M7A	9	1806	50	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	P4U	5	1348	4,84	-	5/10/29/30	0/2/2/2
4	PSU	5	4636	4	-	3/7/25/26	0/2/2/2
4	7MG	5	4550	4	-	0/7/37/38	0/3/3/3
4	UR3	5	4530	4	-	1/7/25/26	0/2/2/2
4	E6G	5	4355	4	-	5/6/28/29	0/3/3/3
50	OMG	9	644	50	-	2/5/27/28	0/3/3/3
50	OMC	9	1710	50	-	1/9/27/28	0/2/2/2
4	5MC	5	3782	4	-	0/7/25/26	0/2/2/2
50	E3C	9	568	50	-	4/9/44/45	0/2/2/2
4	M7A	5	4564	4	-	0/7/37/38	0/3/3/3
4	E7G	5	2297	4	-	1/9/39/40	0/3/3/3
50	4AC	9	1337	50	-	2/11/29/30	0/2/2/2
4	OMG	5	2424	4	-	2/5/27/28	0/3/3/3
4	PSU	5	4450	4,84	-	4/7/25/26	0/2/2/2
4	PSU	5	4531	4	-	0/7/25/26	0/2/2/2
4	A2M	5	3723	4	-	0/5/27/28	0/3/3/3
4	P7G	5	1909	4	-	3/10/40/41	0/3/3/3
50	PSU	9	119	50	-	0/7/25/26	0/2/2/2
50	4AC	9	1842	50	-	0/11/29/30	0/2/2/2
4	2MG	5	729	4	-	2/5/27/28	0/3/3/3
50	A2M	9	484	50	-	0/5/27/28	0/3/3/3
4	OMG	5	4623	4	-	0/5/27/28	0/3/3/3
4	OMG	5	4494	4	-	0/5/27/28	0/3/3/3
4	2MG	5	4872	4	-	2/5/27/28	0/3/3/3
4	OMG	5	2364	4	-	2/5/27/28	0/3/3/3
4	OMG	5	2773	4	-	0/5/27/28	0/3/3/3
50	B8N	9	1248	50	-	2/16/34/35	0/2/2/2
4	A2M	5	3867	4	-	2/5/27/28	0/3/3/3
4	B8Q	5	1456	4	-	0/7/42/43	0/2/2/2
4	OMG	5	2050	4	-	0/5/27/28	0/3/3/3
50	PSU	9	612	50	-	0/7/25/26	0/2/2/2
4	PSU	5	1582	4	-	2/7/25/26	0/2/2/2
4	A2M	5	1534	4,84	-	2/5/27/28	0/3/3/3
4	OMG	5	4637	4	-	2/5/27/28	0/3/3/3
50	OMU	9	121	50	-	2/9/27/28	0/2/2/2
6	OMU	8	14	4,6	-	1/9/27/28	0/2/2/2
9	MLZ	C	333	9	-	3/7/8/10	-
50	A2M	9	166	50	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	7MG	5	1605	4	-	0/7/37/38	0/3/3/3
4	PSU	5	1683	4	-	0/7/25/26	0/2/2/2
4	7MG	5	2522	4	-	0/7/37/38	0/3/3/3
4	OMU	5	4306	4	-	1/9/27/28	0/2/2/2
50	A2M	9	1678	50	-	0/5/27/28	0/3/3/3
50	MA6	9	1851	50	-	4/7/29/30	0/3/3/3
4	A2M	5	4571	4	-	0/5/27/28	0/3/3/3
4	OMG	5	1625	4,84	-	1/5/27/28	0/3/3/3
4	PSU	5	4293	4	-	2/7/25/26	0/2/2/2
50	OMG	9	509	84,50	-	0/5/27/28	0/3/3/3
4	PSU	5	4442	4	-	0/7/25/26	0/2/2/2
50	OMG	9	683	50	-	2/5/27/28	0/3/3/3
4	2MG	5	1517	4	-	0/5/27/28	0/3/3/3
4	UR3	5	1866	4	-	2/7/25/26	0/2/2/2
4	UR3	5	4597	4	-	0/7/25/26	0/2/2/2
4	A2M	5	3718	4	-	0/5/27/28	0/3/3/3
4	A2M	5	1326	4	-	1/5/27/28	0/3/3/3
4	B9B	5	2754	4,84	-	4/7/29/30	0/3/3/3
4	OMU	5	4620	4	-	1/9/27/28	0/2/2/2
4	5MC	5	4335	4	-	0/7/25/26	0/2/2/2
4	A2M	5	3825	4	-	0/5/27/28	0/3/3/3
4	A2M	5	1524	4	-	0/5/27/28	0/3/3/3

The worst 5 of 937 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	237	B9B	O4'-C1'	18.39	1.65	1.40
50	9	166	A2M	O4'-C1'	17.98	1.64	1.40
4	5	1574	B9B	O4'-C1'	17.67	1.64	1.40
4	5	2754	B9B	O4'-C1'	17.50	1.63	1.40
50	9	1031	A2M	O4'-C1'	17.41	1.63	1.40

The worst 5 of 661 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4529	B8W	N2-C2-N3	18.43	146.56	117.79
4	5	2380	B8W	N2-C2-N3	18.17	146.16	117.79
4	5	4185	B8W	N2-C2-N3	17.14	144.54	117.79
4	5	4129	B8W	N2-C2-N3	17.03	144.38	117.79
4	5	4472	B8W	N2-C2-N3	16.78	143.99	117.79

There are no chirality outliers.

5 of 190 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
9	C	333	MLZ	CD-CE-NZ-CM
4	5	237	B9B	C5-C6-O6-C61
4	5	237	B9B	N1-C6-O6-C61

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

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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

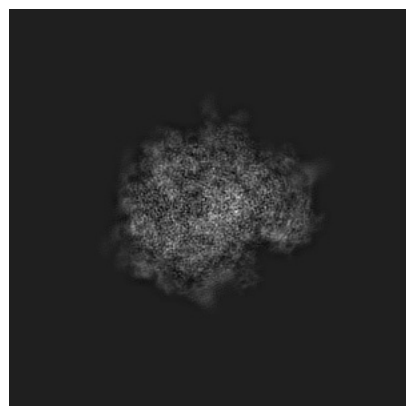
6 Map visualisation [i](#)

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.

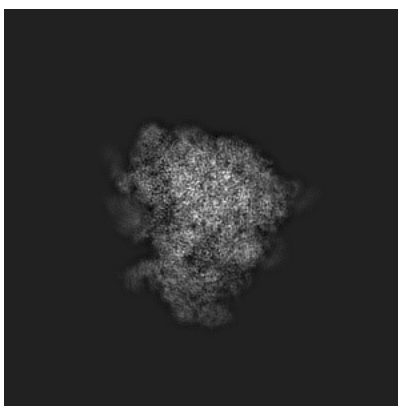
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

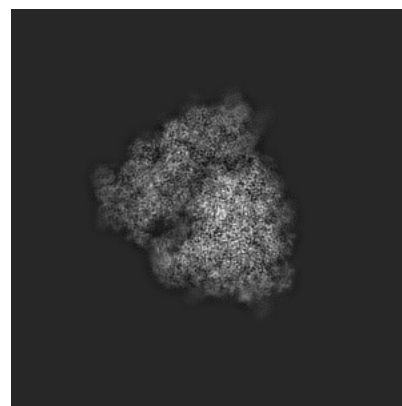
6.1.1 Primary map



X

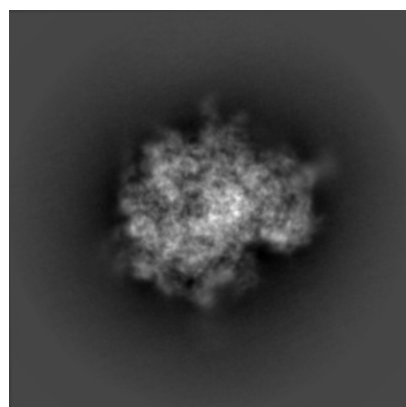


Y

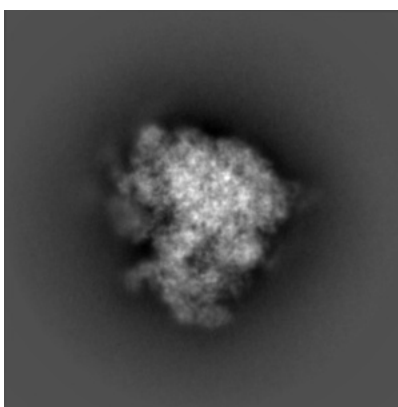


Z

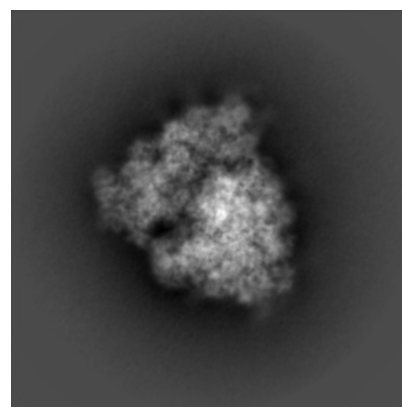
6.1.2 Raw map



X



Y



Z

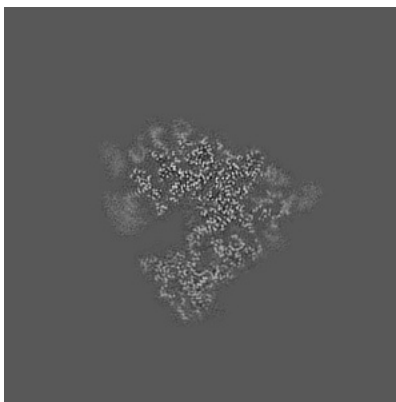
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

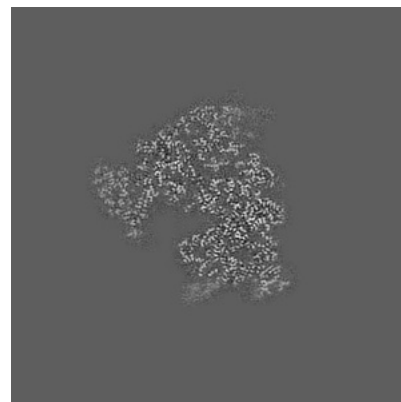
6.2.1 Primary map



X Index: 200

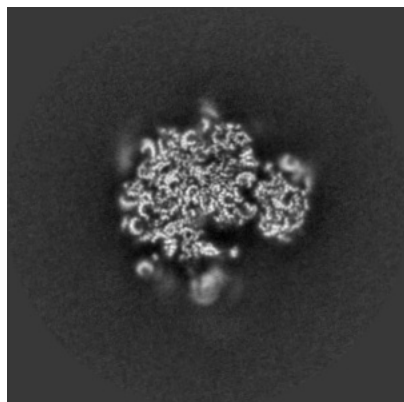


Y Index: 200

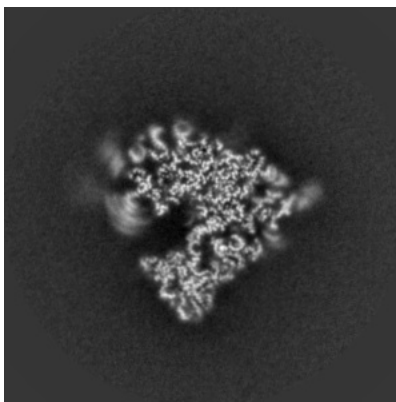


Z Index: 200

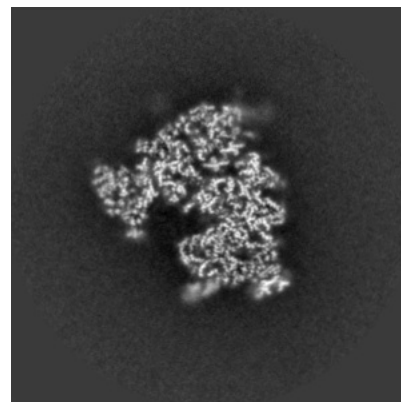
6.2.2 Raw map



X Index: 200



Y Index: 200

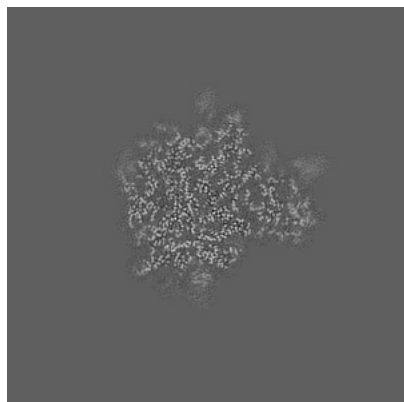


Z Index: 200

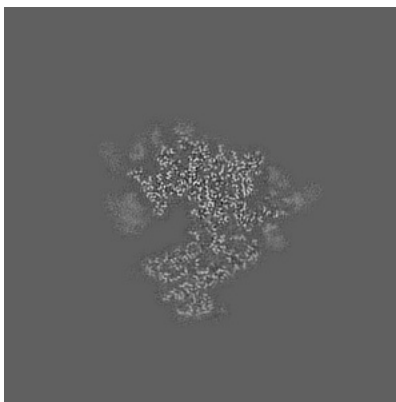
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

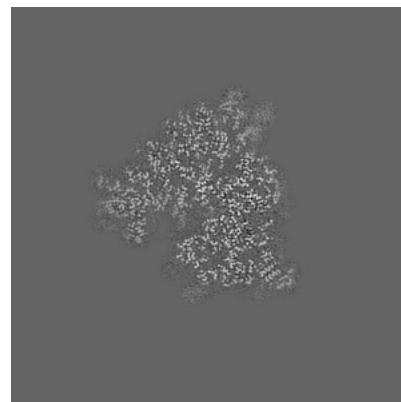
6.3.1 Primary map



X Index: 213

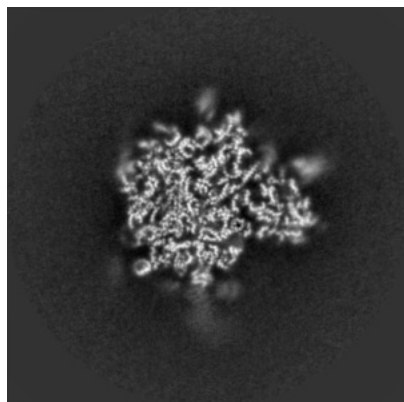


Y Index: 204

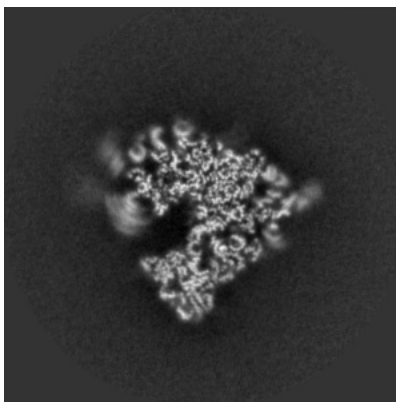


Z Index: 193

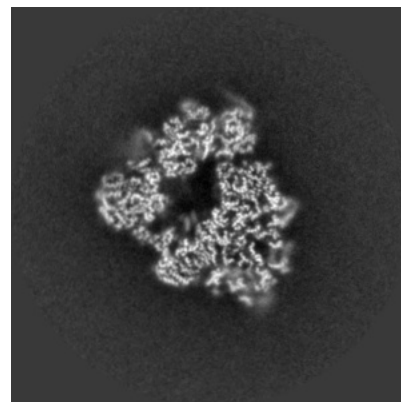
6.3.2 Raw map



X Index: 213



Y Index: 201

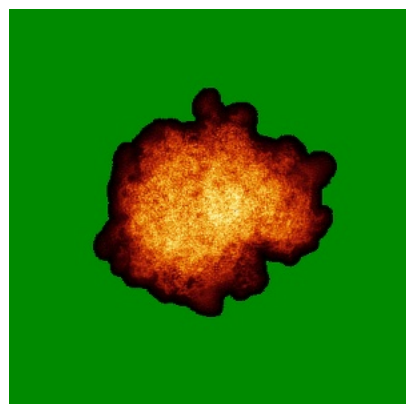


Z Index: 176

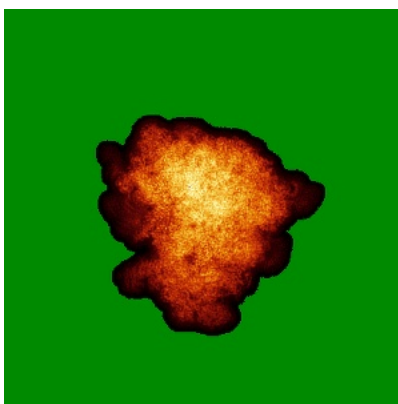
The images above show the largest variance slices of the map in three orthogonal directions.

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

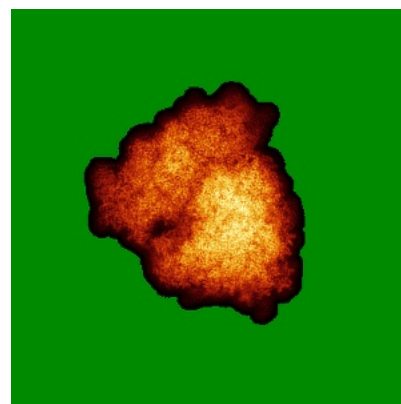
6.4.1 Primary map



X

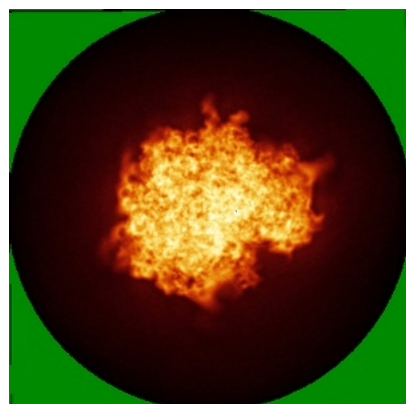


Y

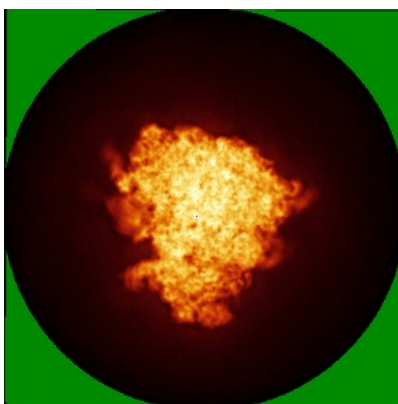


Z

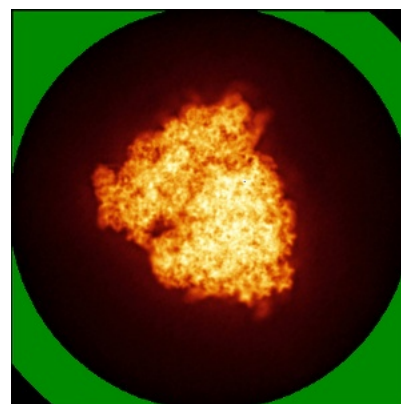
6.4.2 Raw map



X



Y

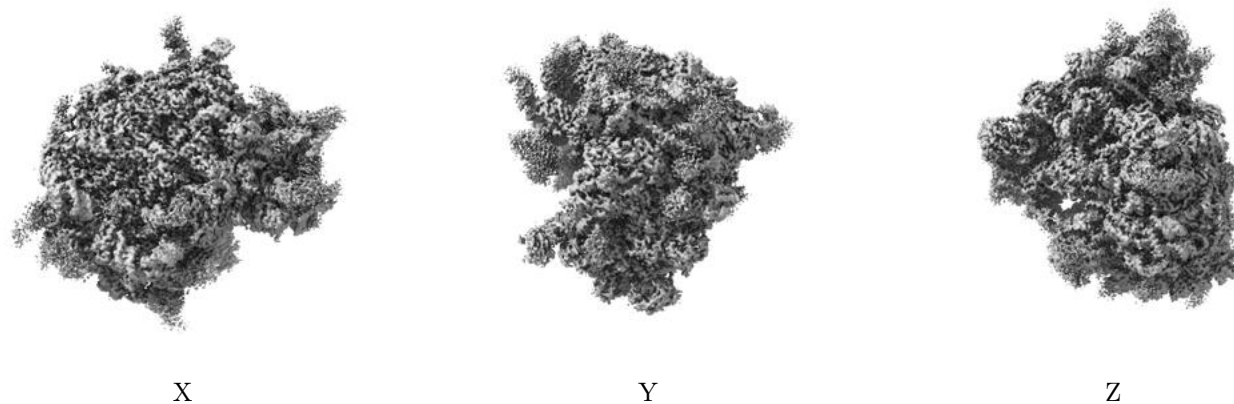


Z

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.

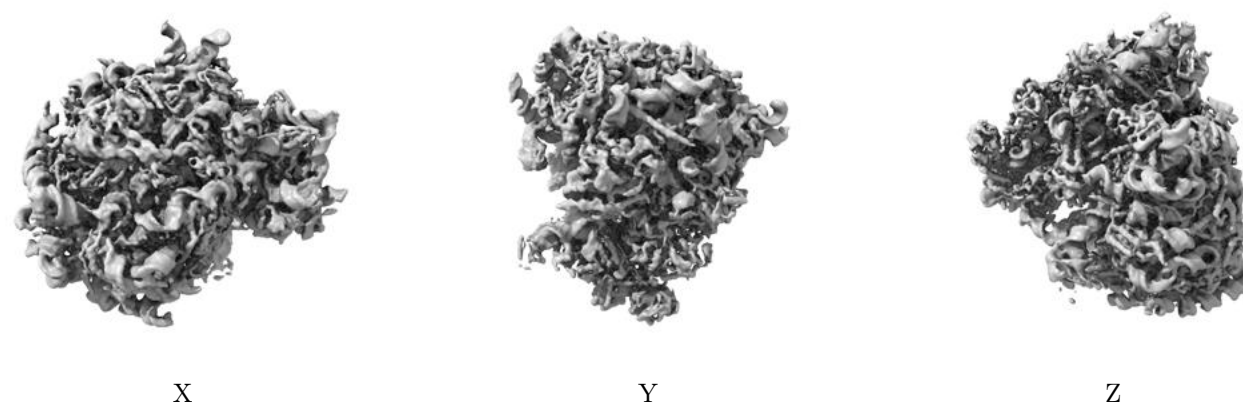
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

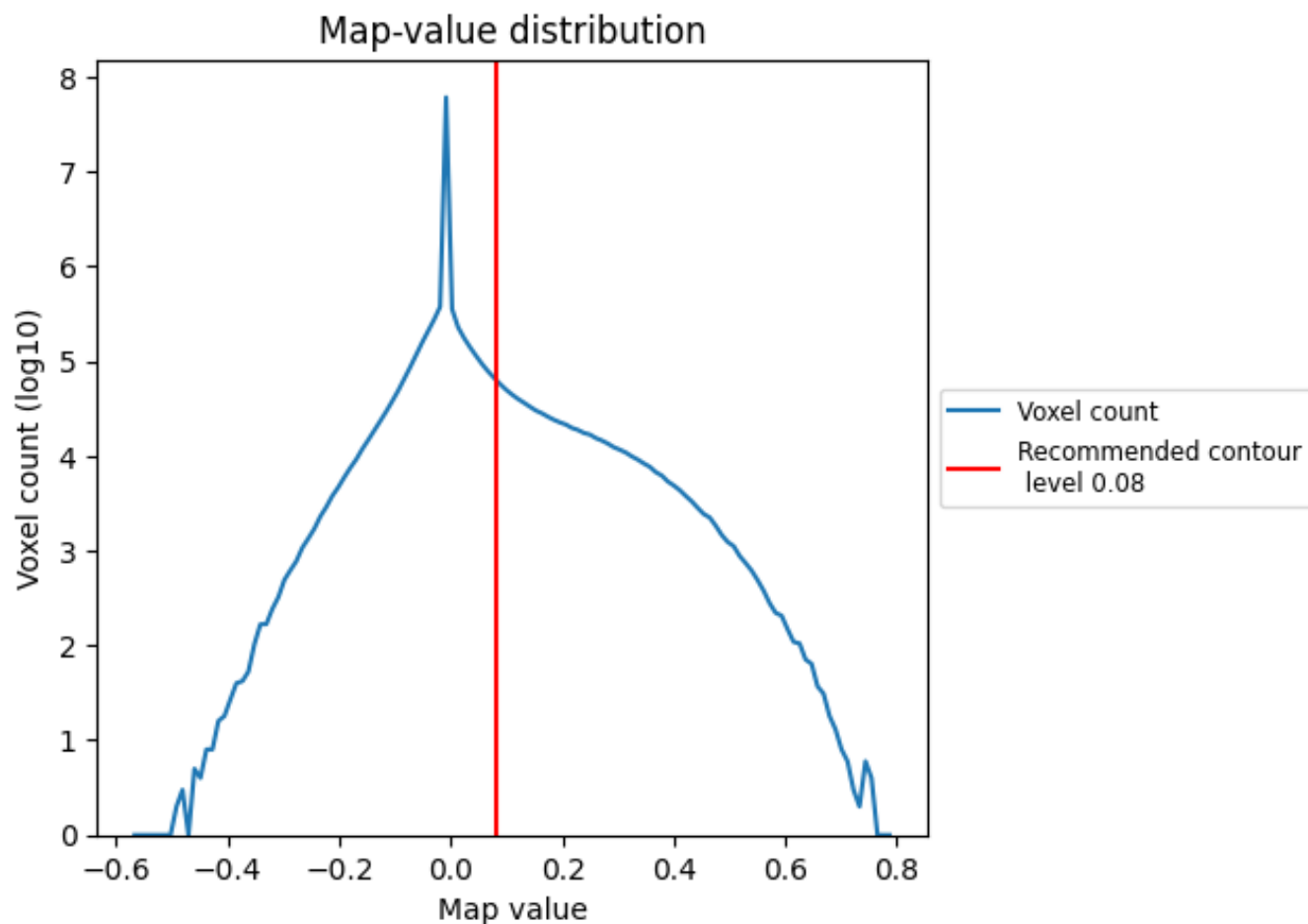
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

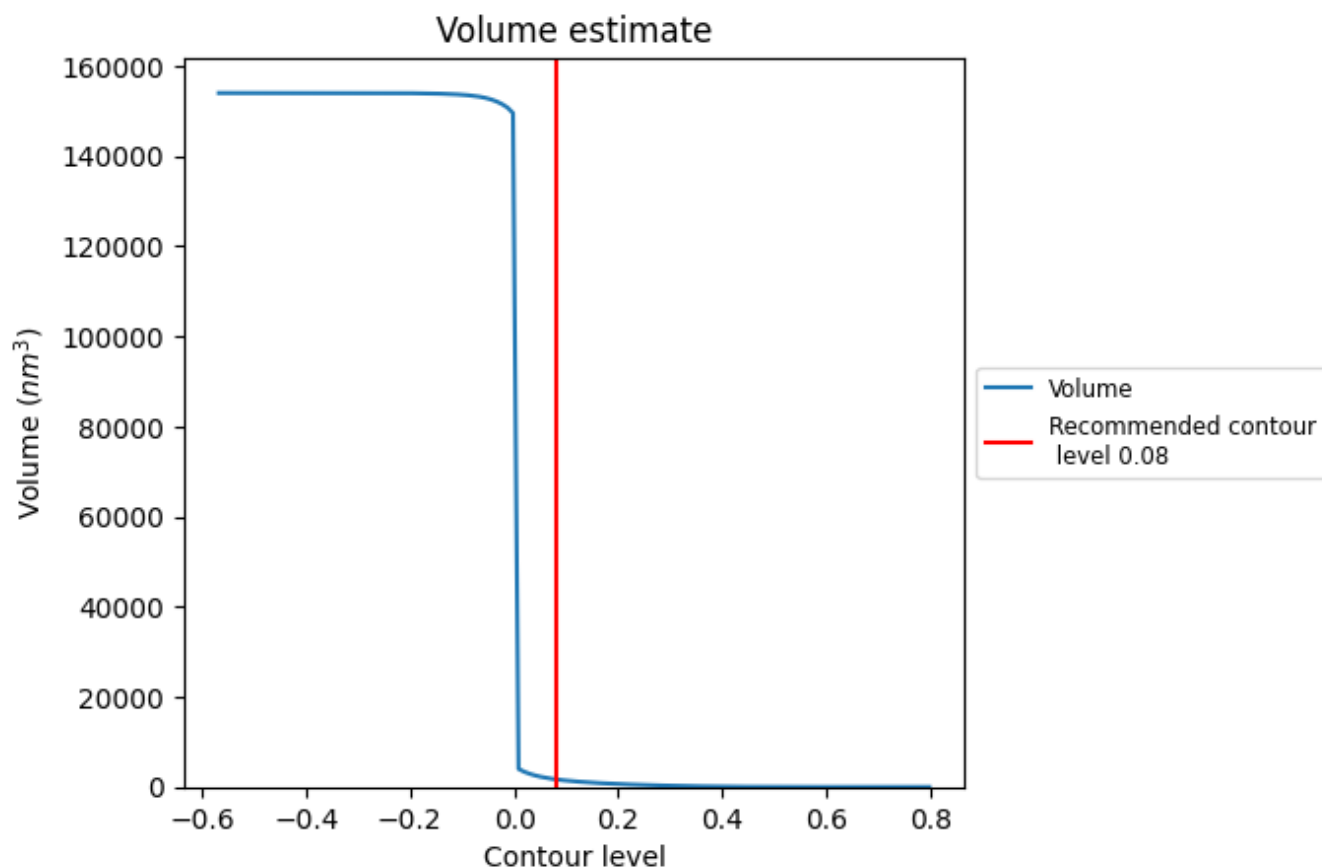
This section contains the results of statistical analysis of the map.

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.

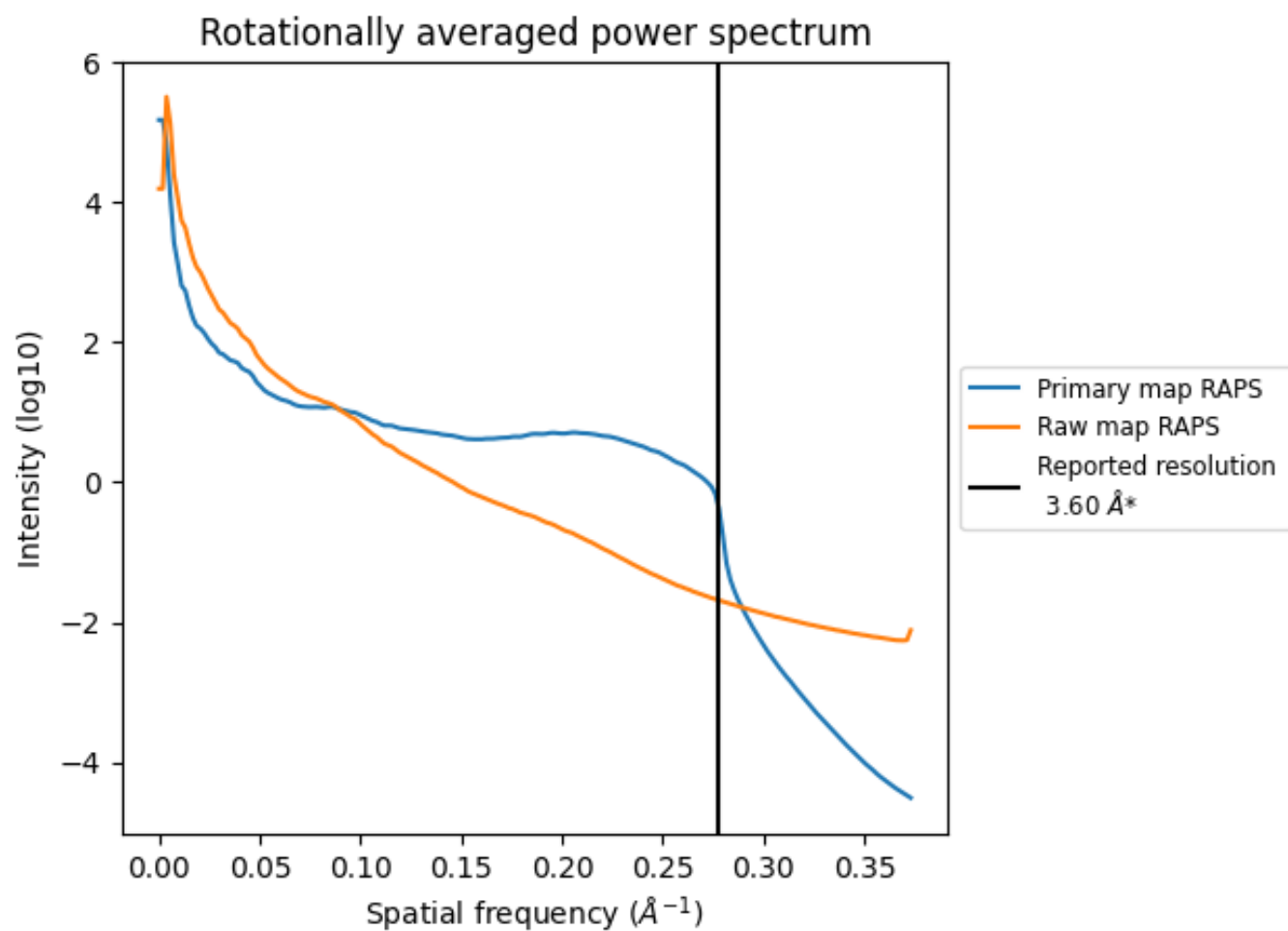
7.2 Volume estimate [i](#)



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](#)

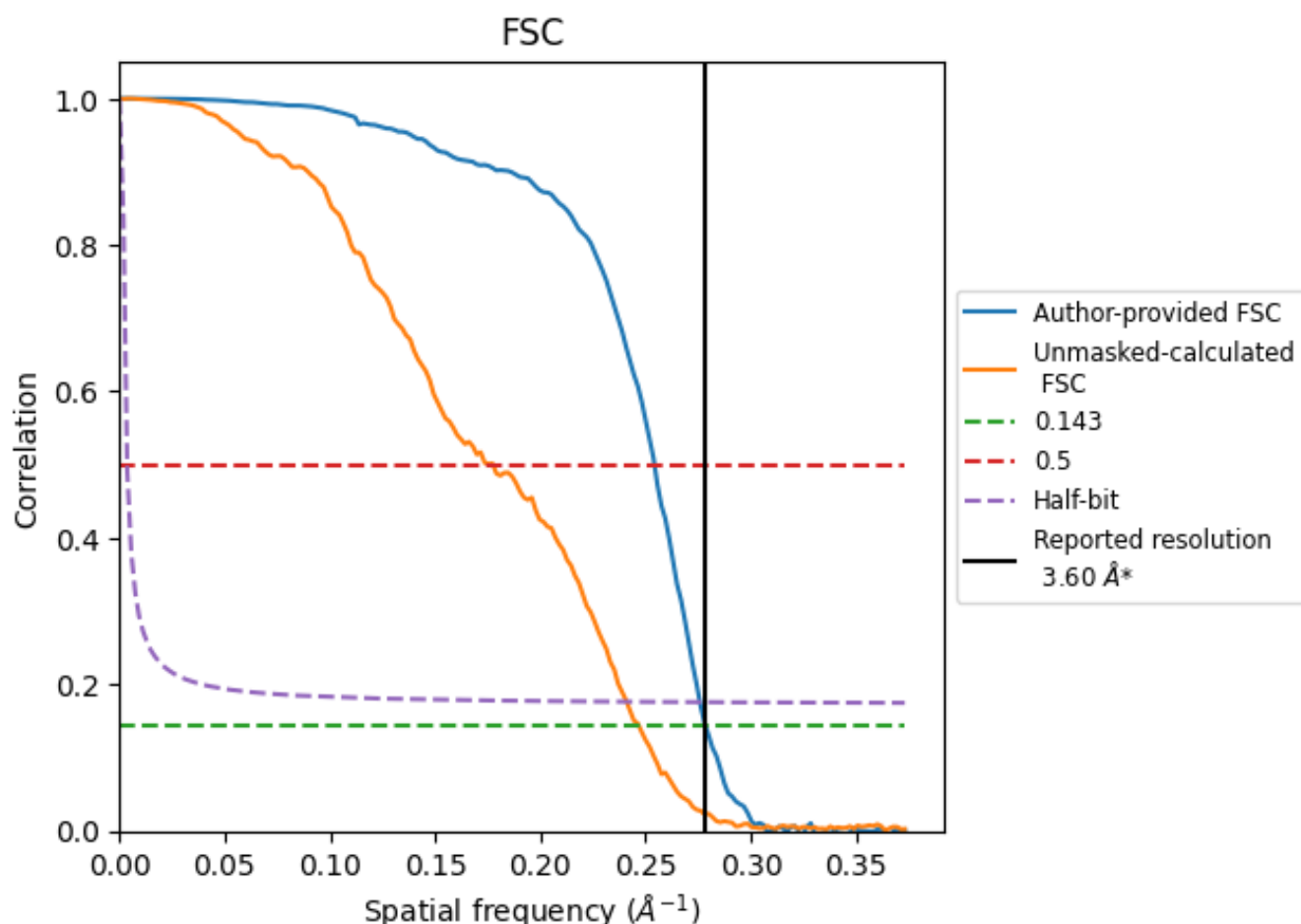


*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

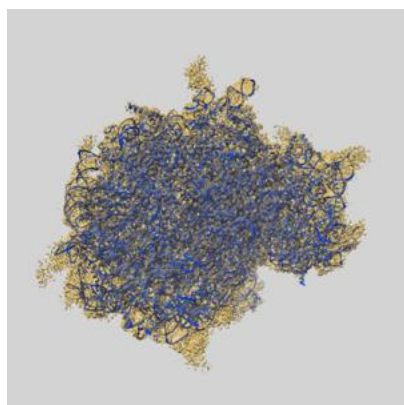
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	3.93	3.63
Unmasked-calculated*	4.05	5.64	4.15

*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 %

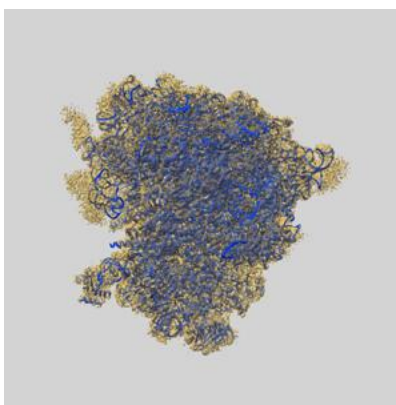
9 Map-model fit [i](#)

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](#).

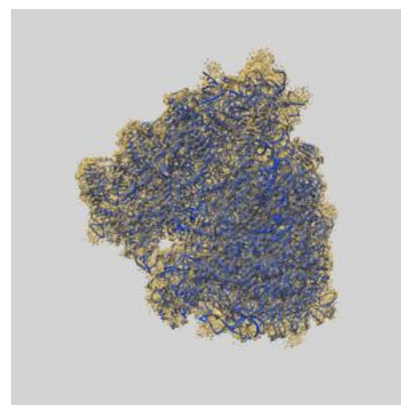
9.1 Map-model overlay [i](#)



X



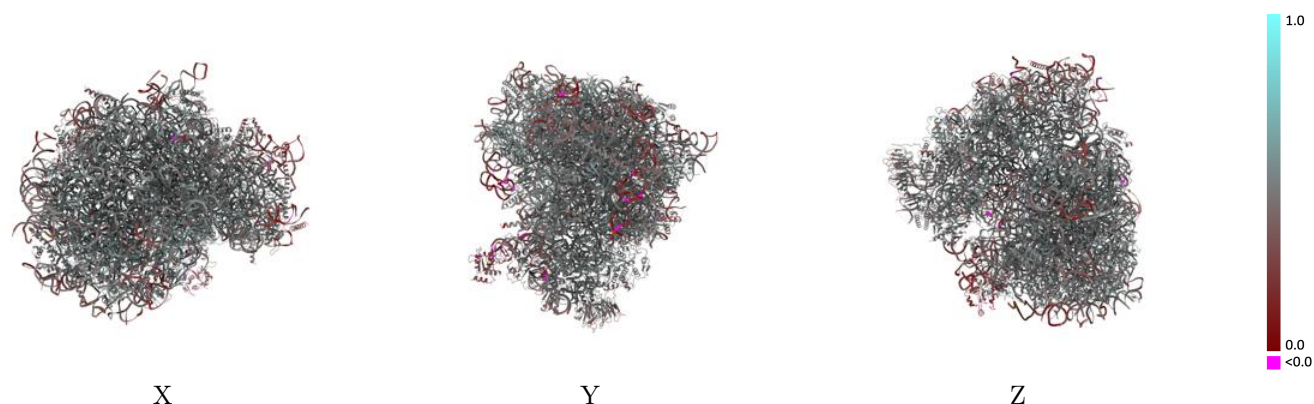
Y



Z

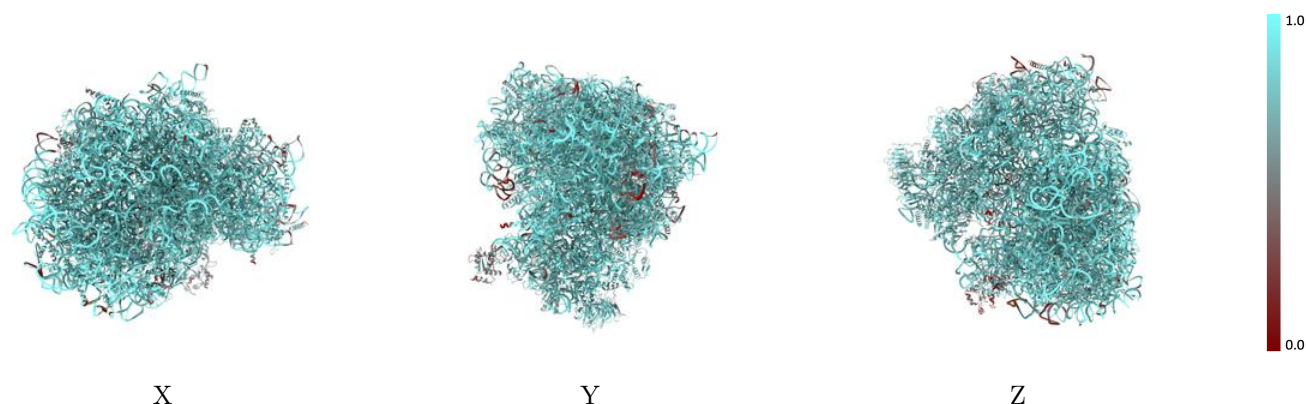
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



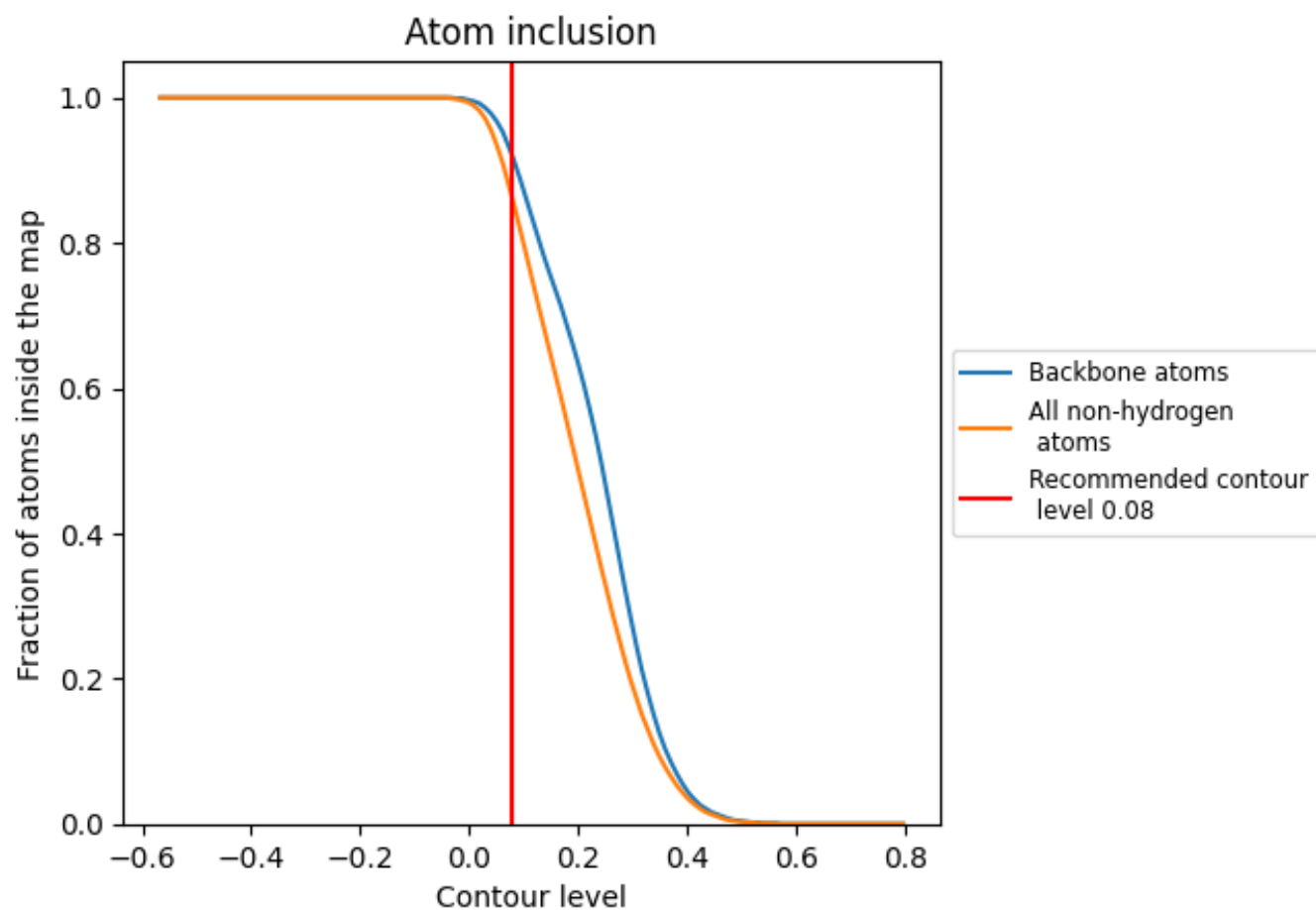
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.8600	 0.4680
1	 0.7920	 0.4930
2	 0.6470	 0.3510
4	 0.7520	 0.2920
5	 0.8980	 0.4560
7	 0.9420	 0.4880
8	 0.9170	 0.4670
9	 0.8910	 0.4460
A	 0.8670	 0.5320
AA	 0.8420	 0.4980
B	 0.8880	 0.5300
BB	 0.8040	 0.4950
C	 0.8590	 0.5210
CC	 0.8470	 0.5130
D	 0.8680	 0.5000
DD	 0.7610	 0.4620
E	 0.8730	 0.5080
EE	 0.8370	 0.5010
F	 0.8480	 0.5150
FF	 0.8150	 0.4790
G	 0.8030	 0.4790
GG	 0.7830	 0.4510
H	 0.8440	 0.5170
HH	 0.7420	 0.4480
I	 0.8500	 0.5210
II	 0.8030	 0.4860
J	 0.8370	 0.4920
JJ	 0.8210	 0.4880
KK	 0.7570	 0.4400
L	 0.8180	 0.4970
LL	 0.8150	 0.5110
M	 0.8640	 0.5060
MM	 0.4520	 0.2670
N	 0.8640	 0.5280
NN	 0.8200	 0.4970

















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Chain	Atom inclusion	Q-score
O	 0.8730	 0.5230
OO	 0.8000	 0.4920
P	 0.8810	 0.5300
PP	 0.7720	 0.4510
Q	 0.8660	 0.5280
QQ	 0.8090	 0.4810
R	 0.8220	 0.4840
RR	 0.7930	 0.4730
S	 0.8670	 0.5230
SS	 0.7920	 0.4650
T	 0.8500	 0.5180
TT	 0.8280	 0.4690
U	 0.7740	 0.4490
UU	 0.7390	 0.4520
V	 0.8610	 0.5280
VV	 0.8410	 0.5060
W	 0.7590	 0.4570
WW	 0.8530	 0.5180
X	 0.8370	 0.5100
XX	 0.8420	 0.5170
Y	 0.8350	 0.5040
YY	 0.8080	 0.4700
Z	 0.8670	 0.5110
ZZ	 0.7940	 0.4610
a	 0.8730	 0.5260
aa	 0.8350	 0.5190
b	 0.7670	 0.4620
bb	 0.7950	 0.4950
c	 0.8350	 0.5000
cc	 0.7640	 0.5000
d	 0.8440	 0.5110
dd	 0.8480	 0.4810
e	 0.8860	 0.5370
ee	 0.7490	 0.4780
f	 0.9050	 0.5410
ff	 0.4580	 0.1230
g	 0.8450	 0.5140
gg	 0.7360	 0.4260
h	 0.8220	 0.5000
i	 0.8350	 0.4940
j	 0.8780	 0.5240
k	 0.7610	 0.4700

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Chain	Atom inclusion	Q-score
l	 0.8760	 0.5230
m	 0.8800	 0.5120
n	 0.8120	 0.5060
o	 0.8410	 0.5270
p	 0.8230	 0.5200
r	 0.8740	 0.5220
u	 0.4500	 0.2750