



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:56 AM UTC

PDB ID : 8OVJ / pdb_00008ovj
EMDB ID : EMD-17216
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :
PARENTAL STRAIN
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2023-04-26
Resolution : 2.40 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

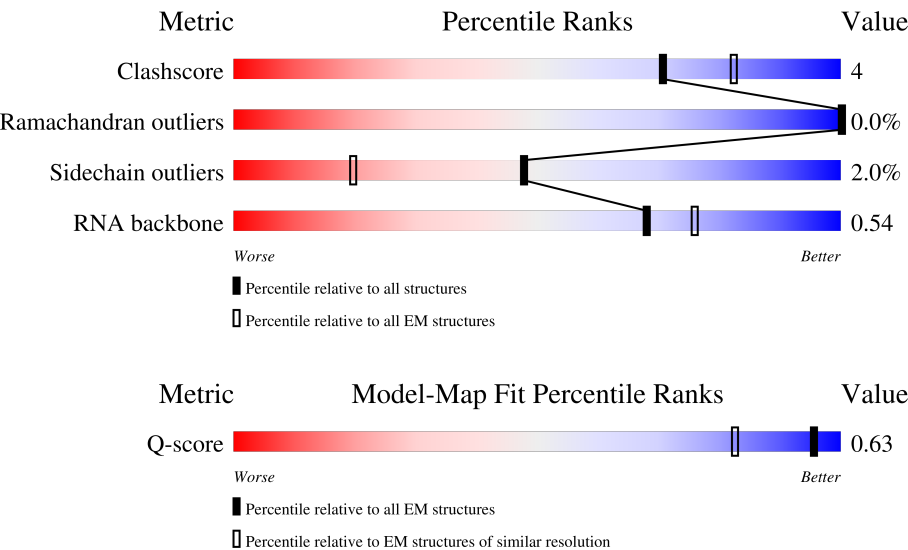
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 Å.

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



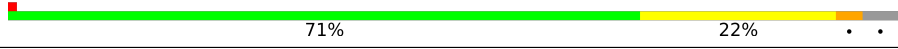
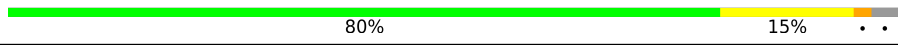
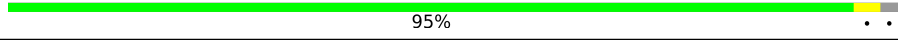
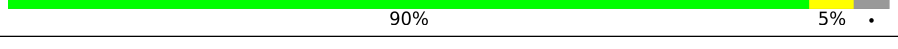
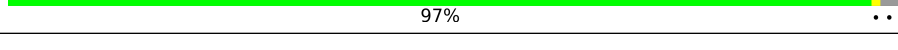
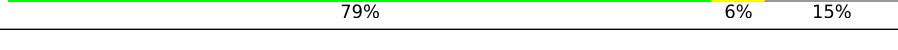
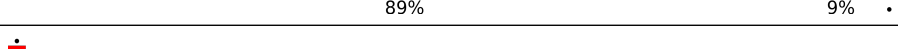
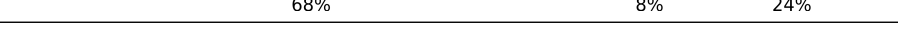
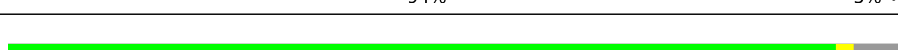
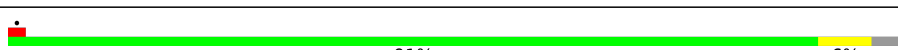
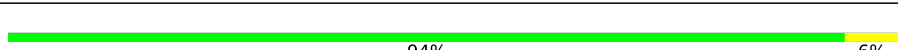
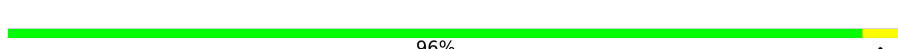
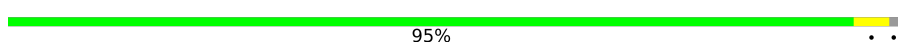
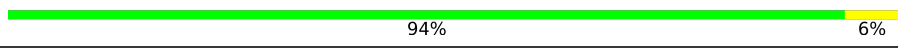
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	1782	63%22%5%10%
2	3	216	47%18%7%28%
3	4	183	74%20%5%

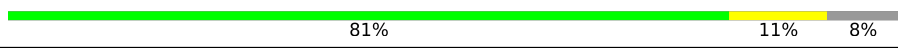
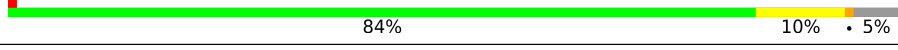
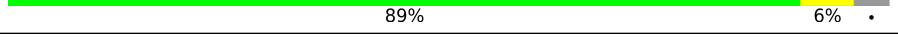
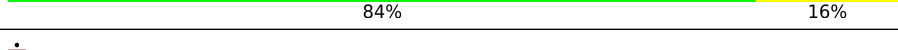
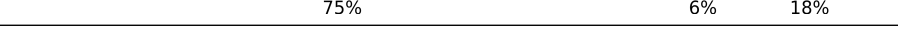
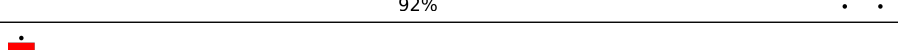
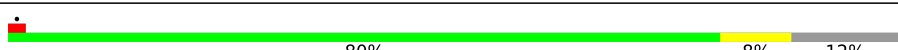
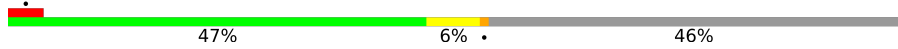
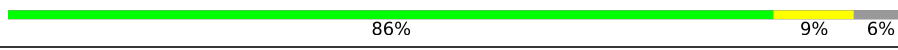
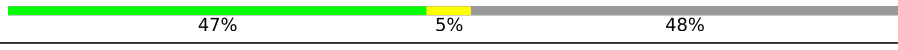
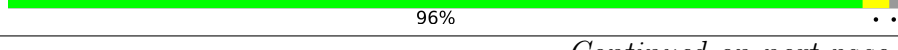
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Mol	Chain	Length	Quality of chain
4	5	135	
5	6	73	
6	7	171	
7	8	123	
8	A	260	
9	B	419	
10	C	373	
11	D	188	
12	E	190	
13	F	195	
14	G	264	
15	H	222	
16	I	220	
17	J	139	
18	K	175	
19	L	145	
20	M	204	
21	N	213	
22	O	305	
23	P	198	
24	Q	254	
25	R	179	
26	S1	2204	
27	S4	20	
28	SA	264	

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Mol	Chain	Length	Quality of chain
29	SB	246	
30	SC	219	
31	SD	190	
32	SE	273	
33	SF	265	
34	SG	249	
35	SH	190	
36	SI	200	
37	SK	220	
38	SL	149	
39	SM	116	
40	SN	168	
41	SO	144	
42	SP	143	
43	SQ	141	
44	SR	153	
45	SS	57	
46	ST	151	
47	SU	173	
48	SV	143	
49	SW	152	
50	SX	161	
51	SY	164	
52	SZ	137	
53	S	159	

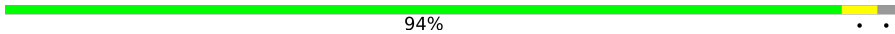
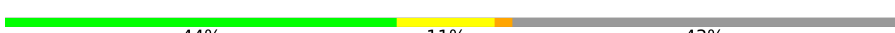
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Mol	Chain	Length	Quality of chain
54	Sa	120	
55	Sc	86	
56	Sb	112	
57	Sd	87	
58	Se	66	
59	Sg	312	
60	Sh	235	
61	SJ	130	
62	T	166	
63	U	129	
64	V	145	
65	W	143	
66	X	124	
67	Y	134	
68	Z	147	
69	a	127	
70	b	70	
71	c	252	
72	d	104	
73	e	188	
74	f	133	
75	g	144	
76	h	168	
77	i	105	
78	j	83	

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Mol	Chain	Length	Quality of chain
79	k	83	
80	l	51	
81	m	128	
82	n	34	
83	o	92	
84	p	106	
85	2	478	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 200822 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 LSUa_rRNA_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1611	Total	C	N	O	P	1	0
			34587	15461	6344	11171	1611		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	164	G	U	conflict	GB 321438308
1	165	U	C	conflict	GB 321438308
1	198	A	C	conflict	GB 321438308
1	523	A	G	conflict	GB 321438308
1	588	U	A	conflict	GB 321438308
1	593	C	U	conflict	GB 321438308
1	1428	A	C	conflict	GB 321438308

- Molecule 2 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	156	Total	C	N	O	P	0	0
			3312	1481	577	1098	156		

- Molecule 3 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	183	Total	C	N	O	P	0	0
			3917	1747	710	1277	183		

- Molecule 4 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	115	Total	C	N	O	P	0	0
			2456	1095	445	801	115		

- Molecule 5 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	71	Total	C	N	O	P	0	0
			1506	675	271	489	71		

- Molecule 6 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	164	Total	C	N	O	P	0	0
			3485	1561	618	1143	163		

- Molecule 7 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	119	Total	C	N	O	P	0	0
			2531	1132	452	828	119		

- Molecule 8 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	255	Total	C	N	O	S	1	0
			1893	1179	387	317	10		

- Molecule 9 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	401	Total	C	N	O	S	3	0
			3035	1923	595	504	13		

- Molecule 10 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	366	Total	C	N	O	S	0	0
			2664	1671	527	451	15		

- Molecule 11 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	160	Total	C	N	O	S	0	0
			1025	641	205	173	6		

- Molecule 12 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	186	Total	C	N	O	S	0	0
			1337	851	254	228	4		

- Molecule 13 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	148	Total	C	N	O	S	0	0
			1049	671	200	176	2		

- Molecule 14 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	226	Total	C	N	O	S	0	0
			1672	1061	328	276	7		

- Molecule 15 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	220	Total	C	N	O	S	0	0
			1652	1048	332	265	7		

- Molecule 16 is a protein called Putative 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	208	Total	C	N	O	S	0	0
			1539	959	315	258	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	203	ARG	ASN	conflict	UNP E9AEA8

- Molecule 17 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	137	Total	C	N	O	S	0	0
			979	616	185	172	6		

- Molecule 18 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	170	Total	C	N	O	S	0	0
			1229	771	244	207	7		

- Molecule 19 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	144	Total	C	N	O	S	0	0
			1102	696	225	175	6		

- Molecule 20 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	203	Total	C	N	O	S	0	0
			1688	1065	359	256	8		

- Molecule 21 is a protein called Putative 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	199	Total	C	N	O	S	0	0
			1615	1019	322	260	14		

- Molecule 22 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	276	Total	C	N	O	S	0	0
			1926	1226	370	327	3		

- Molecule 23 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	197	Total	C	N	O	S	0	0
			1500	943	300	251	6		

- Molecule 24 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	190	Total	C	N	O	S	0	0
			1427	884	313	224	6		

- Molecule 25 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	178	Total	C	N	O	S	0	0
			1405	898	271	231	5		

- Molecule 26 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S1	1755	Total	C	N	O	P	0	0
			37536	16792	6770	12219	1755		

- Molecule 27 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S4	20	Total	C	N	O	P	0	0
			427	191	81	136	19		

- Molecule 28 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SA	225	Total	C	N	O	S	2	0
			1828	1146	349	321	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SB	208	Total	C	N	O	S	0	0
			1590	1011	285	282	12		

- Molecule 30 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SC	212	Total	C	N	O	S	1	0
			1609	1018	295	283	13		

- Molecule 31 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SD	175	Total	C	N	O	S	0	0
			1422	897	283	234	8		

- Molecule 32 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SE	260	Total	C	N	O	S	0	0
			2050	1299	393	349	9		

- Molecule 33 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SF	218	Total	C	N	O	S	0	0
			1662	1063	297	293	9		

- Molecule 34 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SG	233	Total	C	N	O	S	0	0
			1826	1139	371	313	3		

- Molecule 35 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SH	182	Total	C	N	O	S	0	0
			1430	889	275	259	7		

- Molecule 36 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SI	199	Total	C	N	O	S	0	0
			1609	1024	311	267	7		

- Molecule 37 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SK	180	Total	C	N	O	S	0	0
			1430	898	303	227	2		

- Molecule 38 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SL	143	Total	C	N	O	S	0	0
			1118	721	203	191	3		

- Molecule 39 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SM	102	Total	C	N	O	S	0	0
			788	493	144	149	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SN	100	Total	C	N	O	S	0	0
			807	518	142	140	7		

- Molecule 41 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SO	136	Total	C	N	O	S	0	0
			995	615	195	178	7		

- Molecule 42 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SP	142	Total	C	N	O	S	2	0
			1117	704	223	187	3		

- Molecule 43 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SQ	100	Total	C	N	O	S	0	0
			672	413	122	132	5		

- Molecule 44 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SR	135	Total	C	N	O	S	1	0
			1081	684	213	180	4		

- Molecule 45 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SS	54	Total	C	N	O	S	0	0
			434	268	89	71	6		

- Molecule 46 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	ST	143	Total	C	N	O	S	0	0
			1163	733	230	191	9		

- Molecule 47 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SU	158	Total	C	N	O	S	0	0
			1260	799	248	208	5		

- Molecule 48 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SV	77	Total	C	N	O	S	0	0
			636	403	121	110	2		

- Molecule 49 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SW	115	Total	C	N	O	S	0	0
			909	578	172	155	4		

- Molecule 50 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SX	152	Total	C	N	O	S	0	0
			1202	764	237	197	4		

- Molecule 51 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SY	85	Total	C	N	O	S	0	0
			621	383	116	118	4		

- Molecule 52 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SZ	127	Total	C	N	O	S	0	0
			1021	656	196	166	3		

- Molecule 53 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S	157	Total	C	N	O	S	0	0
			1194	760	232	199	3		

- Molecule 54 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Sa	71	Total	C	N	O	S	0	0
			558	356	99	100	3		

- Molecule 55 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Sc	76	Total	C	N	O	S	0	0
			586	366	110	106	4		

- Molecule 56 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Sb	103	Total	C	N	O	S	0	0
			820	508	176	129	7		

- Molecule 57 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Sd	65	Total	C	N	O	S	0	0
			466	286	94	82	4		

- Molecule 58 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Se	54	Total	C	N	O	S	0	0
			430	270	91	68	1		

- Molecule 59 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Sg	306	Total	C	N	O	S	0	0
			2313	1453	411	437	12		

- Molecule 60 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Sh	157	Total	C	N	O	S	0	0
			1094	698	200	194	2		

- Molecule 61 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SJ	129	Total	C	N	O	S	0	0
			1021	646	188	179	8		

- Molecule 62 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	T	152	Total	C	N	O	S	0	0
			1209	756	240	202	11		

- Molecule 63 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	U	107	Total	C	N	O	S	0	0
			688	440	126	120	2		

- Molecule 64 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	V	118	Total	C	N	O	S	0	0
			915	581	177	155	2		

- Molecule 65 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	W	118	Total	C	N	O	S	0	0
			925	579	194	148	4		

- Molecule 66 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	X	64	Total	C	N	O	S	0	0
			539	354	102	80	3		

- Molecule 67 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Y	132	Total	C	N	O	S	0	0
			997	641	197	157	2		

- Molecule 68 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Z	145	Total	C	N	O	S	0	0
			1068	653	225	185	5		

- Molecule 69 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	a	123	Total	C	N	O	S	0	0
			995	623	210	159	3		

- Molecule 70 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	b	68	Total	C	N	O	S	0	0
			546	335	125	86			

- Molecule 71 is a protein called Putative 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	c	229	Total	C	N	O	S	0	0
			1866	1188	359	308	11		

- Molecule 72 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	d	93	Total	C	N	O	S	0	0
			713	444	130	134	5		

- Molecule 73 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	e	180	Total	C	N	O	S	0	0
			1414	889	287	234	4		

- Molecule 74 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	f	125	Total	C	N	O	S	0	0
			1011	636	201	170	4		

- Molecule 75 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	g	142	Total	C	N	O	S	0	0
			1142	710	239	188	5		

- Molecule 76 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	h	127	Total	C	N	O	S	0	0
			1038	639	226	167	6		

- Molecule 77 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	i	86	Total	C	N	O	S	0	0
			660	421	133	104	2		

- Molecule 78 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	j	81	Total	C	N	O	S	0	0
			668	407	154	101	6		

- Molecule 79 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	k	72	Total	C	N	O	S	0	0
			534	338	105	88	3		

- Molecule 80 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	l	50	Total	C	N	O	S	0	0
			450	291	95	63	1		

- Molecule 81 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	m	51	Total	C	N	O	S	0	0
			375	236	74	59	6		

- Molecule 82 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	n	33	Total	C	N	O	S	0	0
			292	178	75	37	2		

- Molecule 83 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	o	88	Total	C	N	O	S	0	0
			686	427	142	111	6		

- Molecule 84 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	p	97	Total	C	N	O	S	0	0
			780	494	158	123	5		

- Molecule 85 is a RNA chain called LSUb_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	2	1105	Total	C	N	O	P	0	0
			23639	10583	4263	7688	1105		

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	1	106	Total	Mg	0
			106	106	
86	3	1	Total	Mg	0
			1	1	
86	4	8	Total	Mg	0
			8	8	
86	5	1	Total	Mg	0
			1	1	
86	6	2	Total	Mg	0
			2	2	
86	7	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
86	8	2	Total 2	Mg 2	0
86	I	1	Total 1	Mg 1	0
86	J	1	Total 1	Mg 1	0
86	M	1	Total 1	Mg 1	0
86	S1	107	Total 107	Mg 107	0
86	SH	1	Total 1	Mg 1	0
86	SS	1	Total 1	Mg 1	0
86	SX	1	Total 1	Mg 1	0
86	T	1	Total 1	Mg 1	0
86	2	66	Total 66	Mg 66	0

- Molecule 87 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
87	1	3	Total 3	K 3	0
87	5	2	Total 2	K 2	0
87	7	2	Total 2	K 2	0
87	A	2	Total 2	K 2	0
87	B	1	Total 1	K 1	0
87	H	1	Total 1	K 1	0
87	M	1	Total 1	K 1	0
87	S1	25	Total 25	K 25	0
87	SG	1	Total 1	K 1	0

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Mol	Chain	Residues	Atoms		AltConf
87	2	5	Total 5	K 5	0

- Molecule 88 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
88	1	5	Total 5	Na 5	0
88	4	1	Total 1	Na 1	0
88	A	1	Total 1	Na 1	0
88	M	1	Total 1	Na 1	0
88	S1	4	Total 4	Na 4	0
88	Sb	1	Total 1	Na 1	0
88	2	4	Total 4	Na 4	0

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	SS	1	Total 1	Zn 1	0
89	Sb	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	p	1	Total 1	Zn 1	0

- Molecule 90 is water.

Mol	Chain	Residues	Atoms		AltConf
90	1	9	Total 9	O 9	0
90	5	1	Total 1	O 1	0

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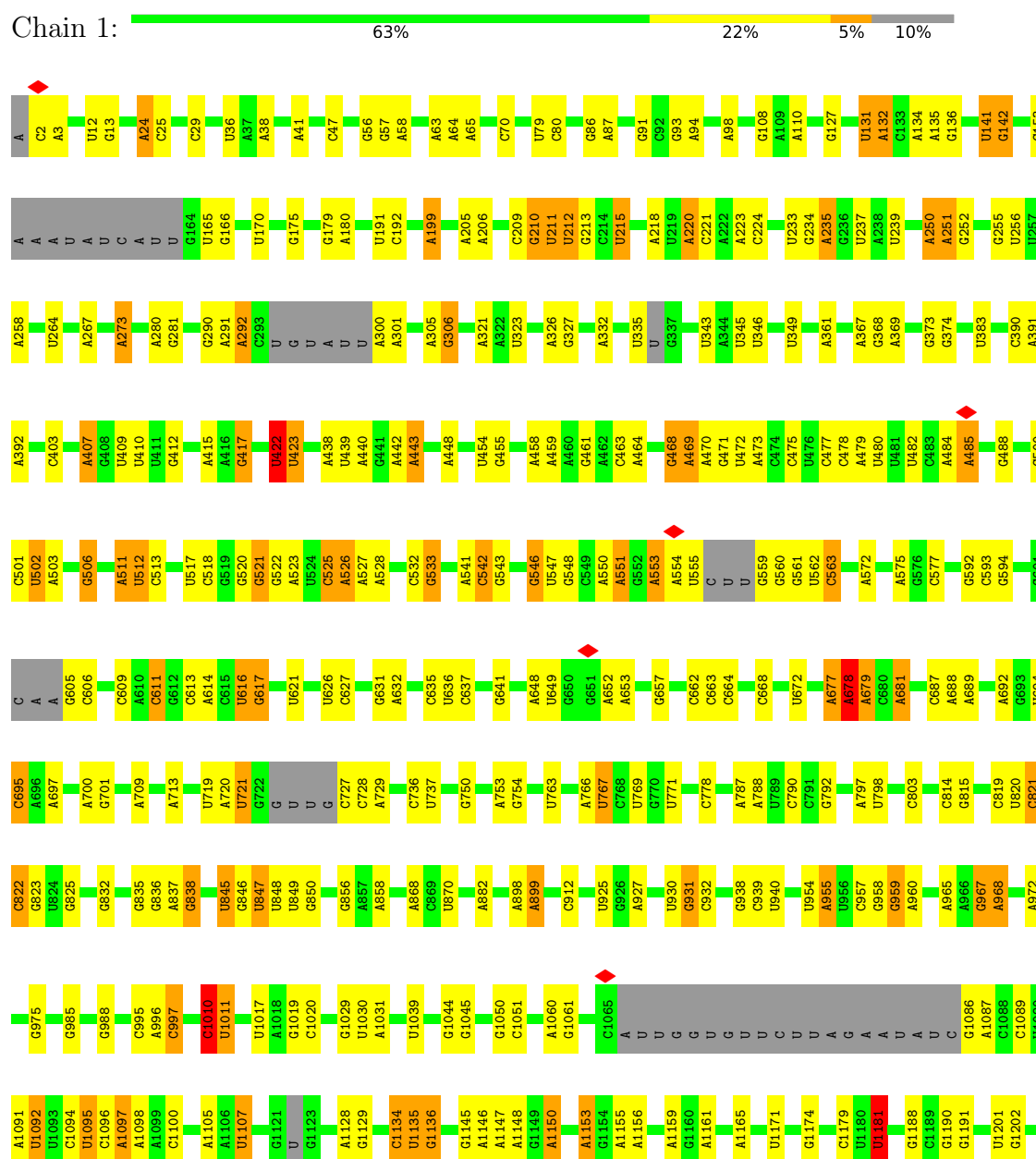
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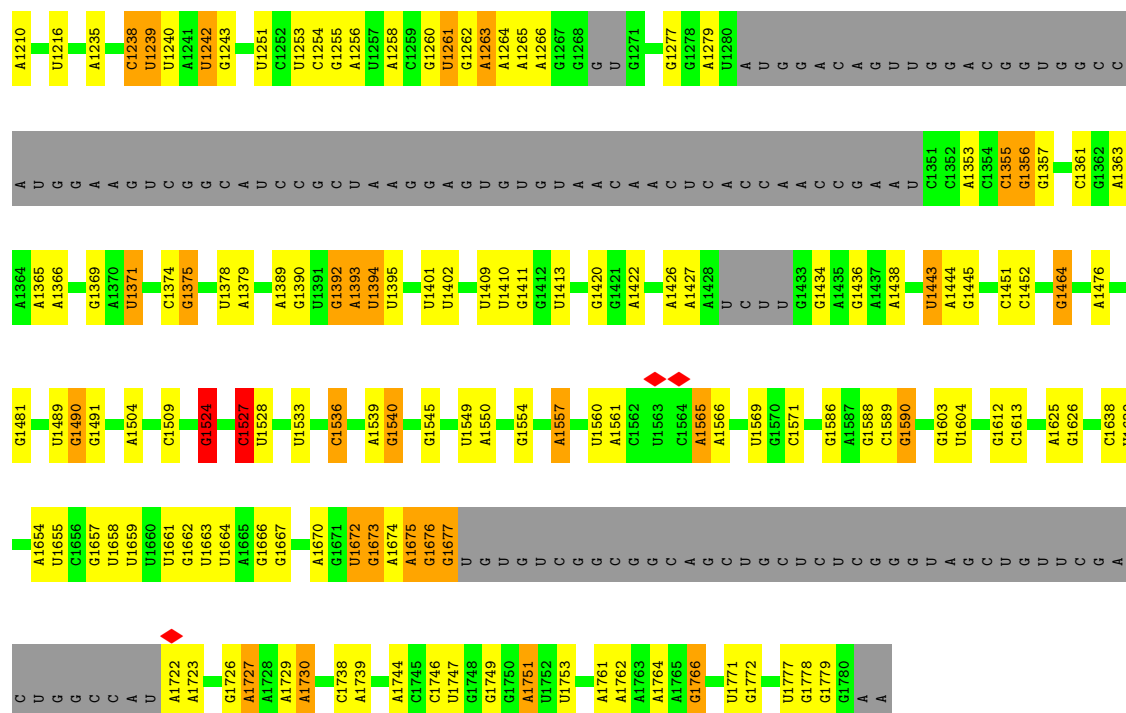
Mol	Chain	Residues	Atoms		AltConf
90	7	1	Total 1	O 1	0
90	A	1	Total 1	O 1	0
90	B	1	Total 1	O 1	0
90	H	1	Total 1	O 1	0
90	I	1	Total 1	O 1	0
90	M	4	Total 4	O 4	0
90	P	2	Total 2	O 2	0
90	S1	7	Total 7	O 7	0
90	SA	1	Total 1	O 1	0
90	S	1	Total 1	O 1	0
90	T	2	Total 2	O 2	0
90	2	17	Total 17	O 17	0

3 Residue-property plots

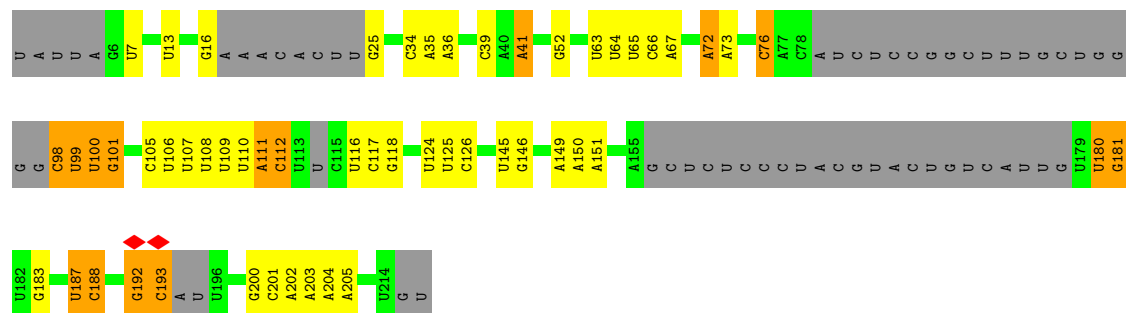
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: LSUa_rRNA_chain_1

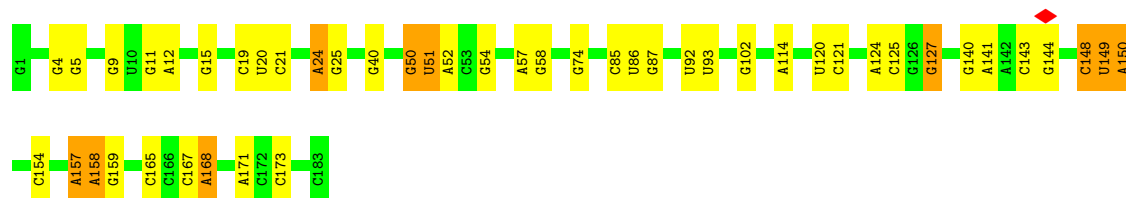
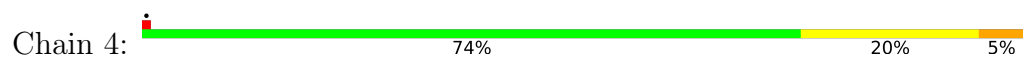




• Molecule 2: SR1_chain_3

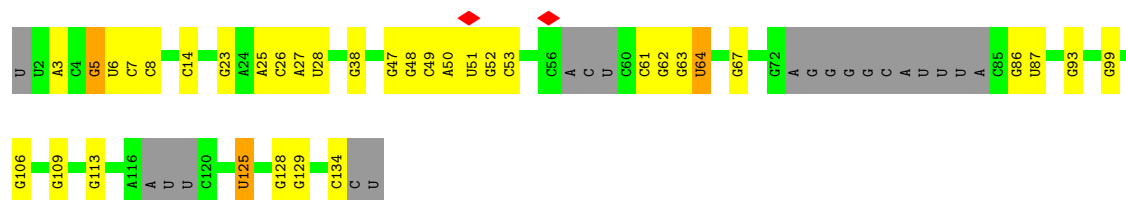


• Molecule 3: SR2_chain_4

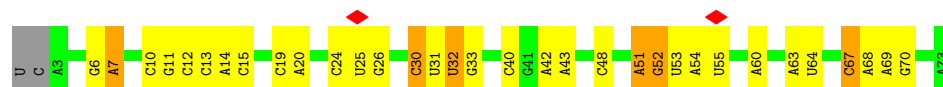


• Molecule 4: SR4_chain_5

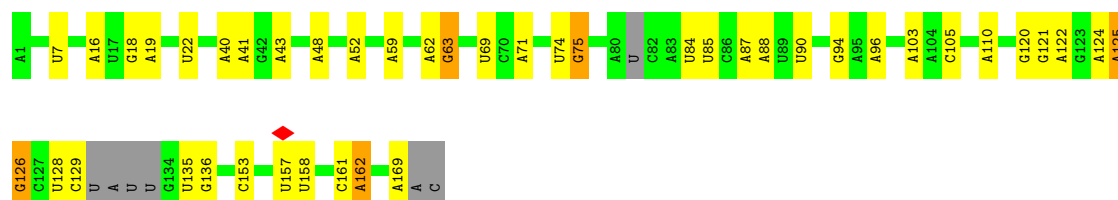




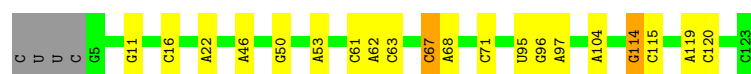
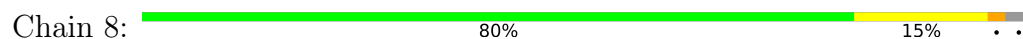
• Molecule 5: SR6_chain_6



• Molecule 6: 5.8S_rRNA_chain_7



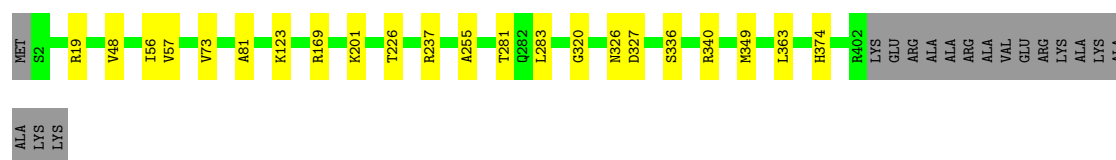
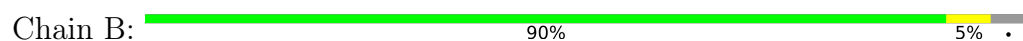
• Molecule 7: 5S_rRNA_chain_8



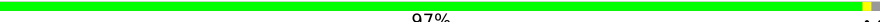
• Molecule 8: Putative 60S ribosomal protein L2



• Molecule 9: Putative ribosomal protein L3



• Molecule 10: Putative ribosomal protein L1a

Chain C:  97% ..



- Molecule 11: 60S ribosomal protein L11

Chain D:  79% 6% 15%



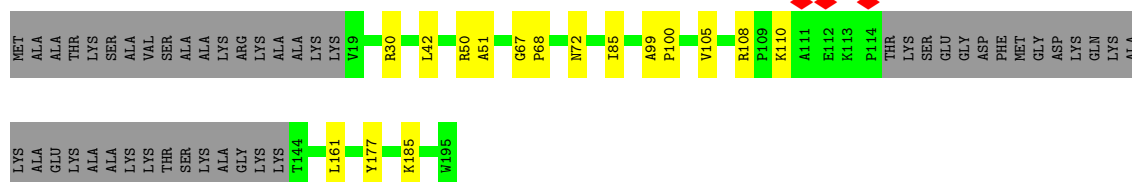
- Molecule 12: Putative 60S ribosomal protein L9

Chain E:  89% 9% .



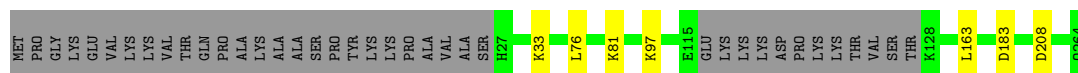
- Molecule 13: Putative 60S ribosomal protein L6

Chain F:  68% 8% 24%



- Molecule 14: 60S ribosomal protein L7a

Chain G:  83% 14%



- Molecule 15: Putative 60S ribosomal protein L13a

Chain H:  94% 5% .

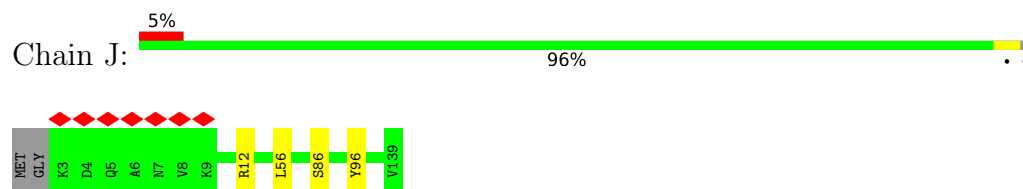


- Molecule 16: Putative 60S ribosomal protein L13

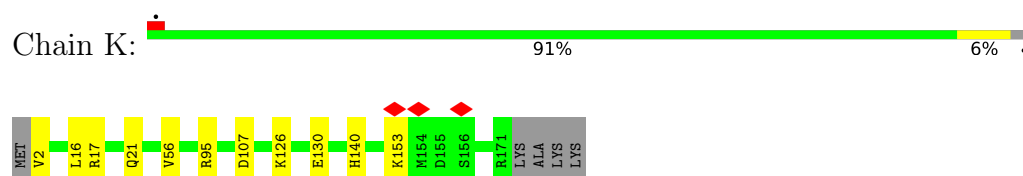
Chain I:  93% 5% .



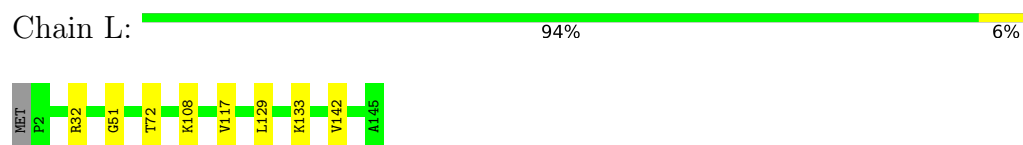
- Molecule 17: Putative 60S ribosomal protein L23



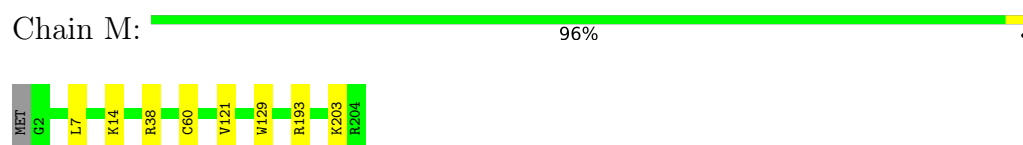
- Molecule 18: Putative 40S ribosomal protein L14



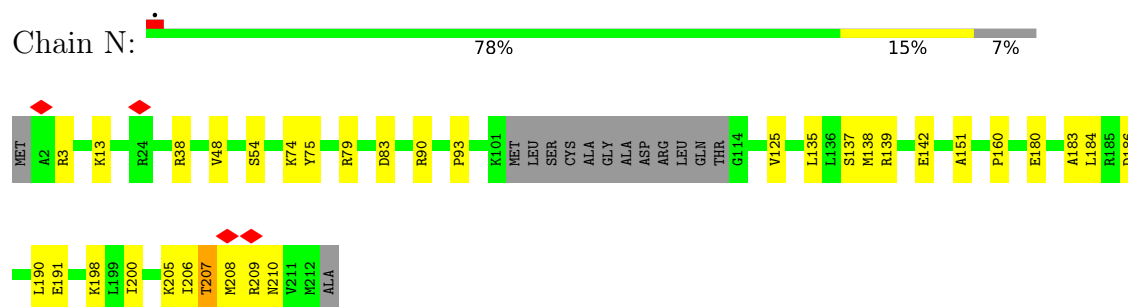
- Molecule 19: Putative 60S ribosomal protein L27A/L29



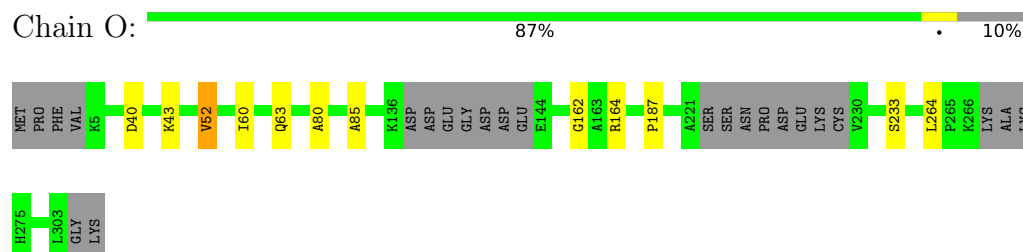
- Molecule 20: Ribosomal protein L15



- Molecule 21: Putative 60S ribosomal protein L10



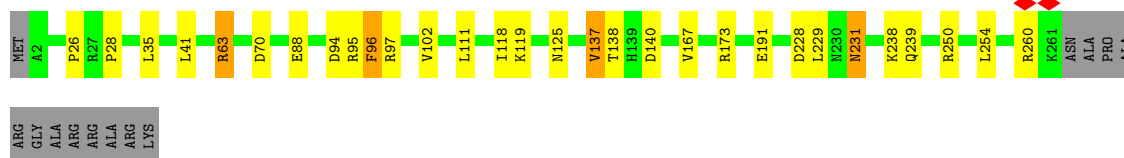
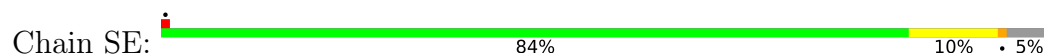
- Molecule 22: Putative 60S ribosomal protein L5



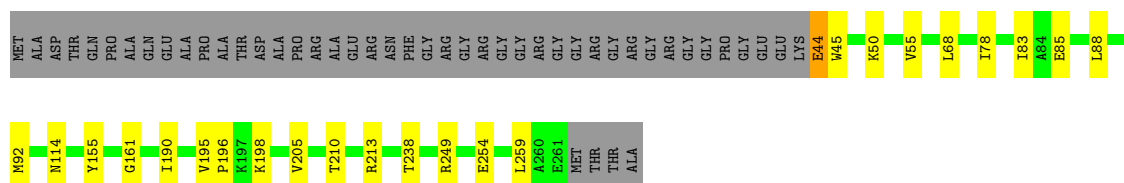
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G1940	G1866	G1766	C1693	U1583	A1459	G	A1187	A	G965	U	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
C1944	A1870	C	A1699	A1594	G1459	G	U1192	A	G966	U	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
U1948	A1871	G1770	A1701	U1596	G1466	U	A1199	A	G967	U	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
A1949	A1872	U1773	A1702	U1598	G1478	U	A1202	C1093	U971	U886	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
G1950	G1875	U1774	U1703	U1598	G1478	A	A1206	G1094	A972	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
A1955	C1877	G1782	C1705	U1601	A1490	C	C1207	C1095	U973	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
C1956	A1878	U1788	U1706	U1603	U1496	G	A1213	U1098	U975	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
A1966	U1880	U1789	G1707	A1608	U1497	C	A1235	C1099	G977	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
G1967	A1881	U1792	G1712	C1612	G1502	C	A1235	C1099	G977	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
G1968	A1882	U1793	C1713	C1613	A1503	A	U1192	U1100	U979	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
A1969	G1883	U1794	C1713	U1614	A1503	C	U1239	G1102	U980	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
U1970	U1890	U1795	A1718	G1615	C1511	C	A1245	A1105	U981	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
G1972	A1891	U1796	G1719	A1616	C1512	A	U1246	A1108	U982	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
A	A	A1797	C1725	A1617	A1514	C	A1252	A1109	U983	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
A1974	A	U	A	U1618	A1514	C	A1252	A1109	U983	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
A1975	A	U	A	U1619	A1514	C	A1252	A1109	U983	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
U1976	C	U	A	U1620	A1523	G	A1273	G1113	U984	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
U1977	G	U	A	U1621	G1524	A	A1274	G1114	U985	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
A1978	A	C	A	G1622	G1524	C	C1275	G1115	U986	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
U1979	U	U	U	G1623	C1533	C	A1276	U1116	U987	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
G1982	U	U	U	U1624	U1533	C	A1277	U1117	U988	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
U1983	U	U	U	G1625	U1537	C	U1278	U1118	U989	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
C1988	U	U	U	A1637	U1538	C	U1288	U1120	U990	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
A1989	U	U	U	U1638	U1539	C	A1289	G1121	U991	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
G1995	C	U	G	G1643	C1542	C	U1290	G1122	U992	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
G2004	A	U	G	U1644	C1543	C	U1291	G1123	U993	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
U2005	C	U	G	U1645	A1544	C	U1292	G1130	U994	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
G2010	C1910	C1827	U1911	G1651	A1548	A	U1297	G1138	U995	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
A2012	A1912	U1828	A1912	U1652	G1550	C	U1298	G1139	U996	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
G2013	U1915	G1830	U1915	U1653	G1551	C	U1299	G1140	U997	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
A2021	A1917	G1831	U1917	G1656	G1552	C	U1299	G1141	U998	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
U2026	U1918	U1833	U1918	U1657	G1553	C	U1299	G1142	U999	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
G2027	A1920	G1836	A1920	U1658	A1554	C	U1299	G1143	U1000	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
U2037	A1921	U1841	A1921	U1666	U1566	C	U1299	G1144	U1001	U887	U	U963	G876	U793	G792	G786	G785	C784	A780	A779	A774	A773	A772	A771	A770	A762	A761	U759	U758	U757	U756	U755	U754	A753	C752	C811	U750	C747	C746	G	G
C2038	G1924	U1846	G1924	U1667	G1569	C	U1299	G1145	U1002	U887	U	U963	G876	U793	G792	G786	G785	C784	A780																						



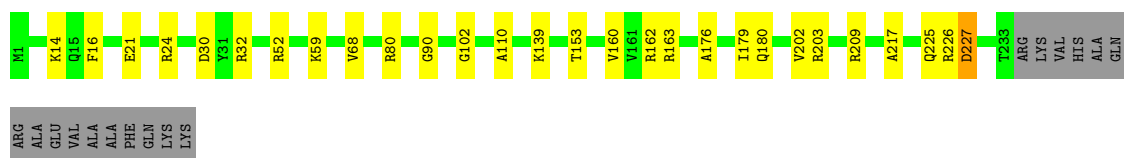
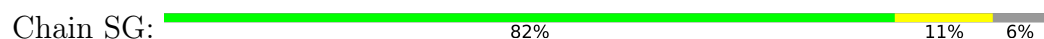
- Molecule 32: 40S ribosomal protein S4



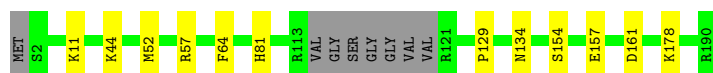
- Molecule 33: 40S ribosomal protein S2



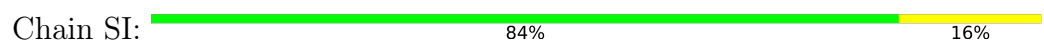
- Molecule 34: 40S ribosomal protein S6



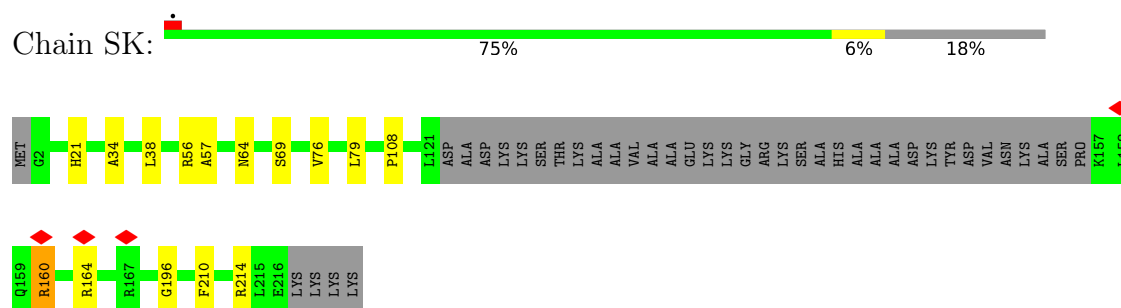
- Molecule 35: 40S ribosomal protein S5



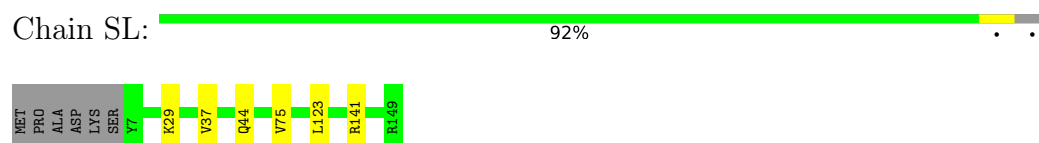
- Molecule 36: 40S ribosomal protein S7



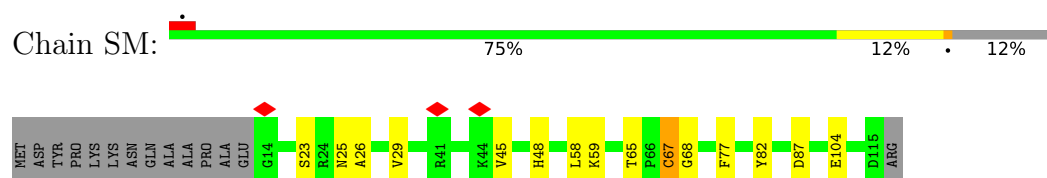
- Molecule 37: 40S ribosomal protein S8



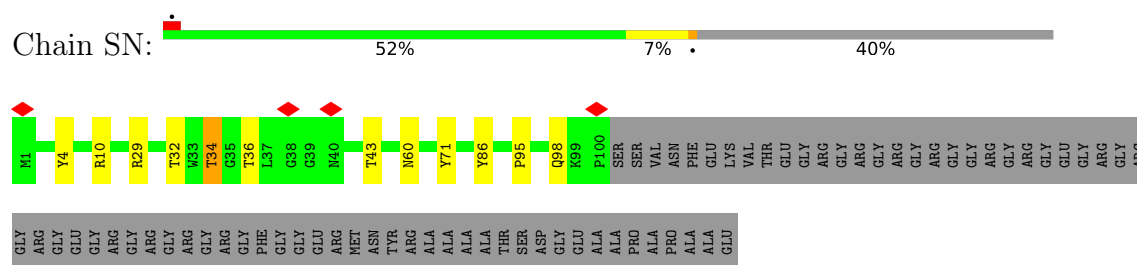
- Molecule 38: Putative 40S ribosomal protein S16



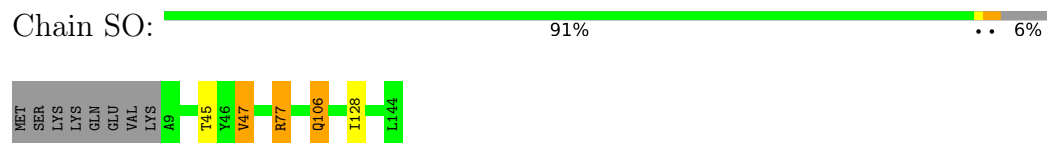
- Molecule 39: Putative ribosomal protein S20



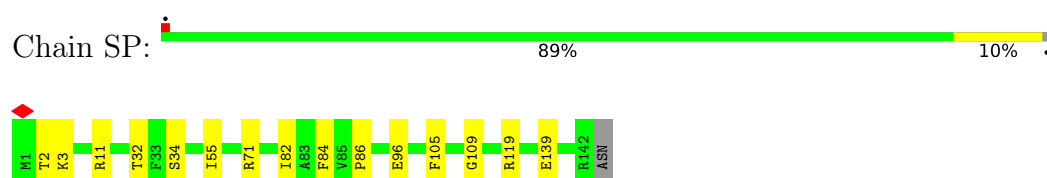
- Molecule 40: Putative 40S ribosomal protein S10



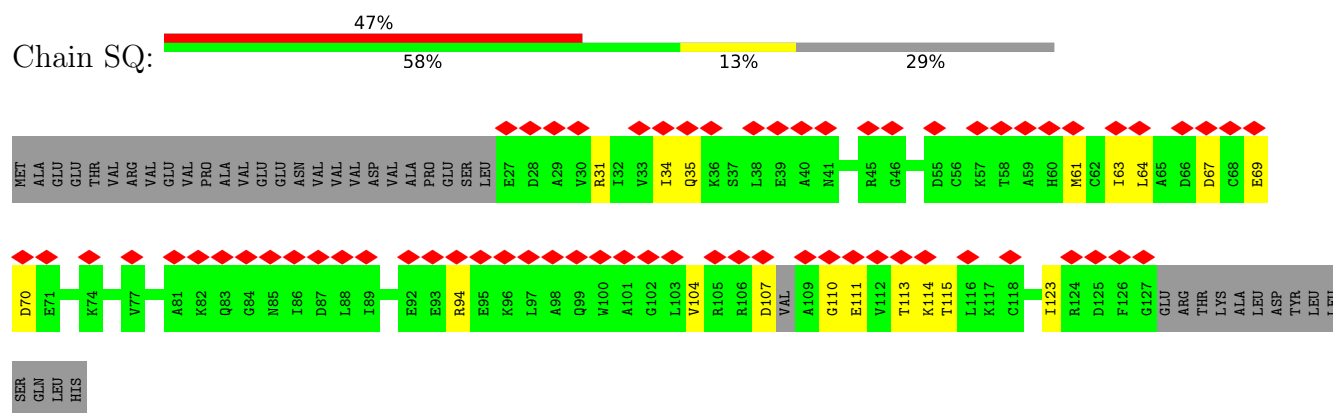
- Molecule 41: 40S ribosomal protein S14



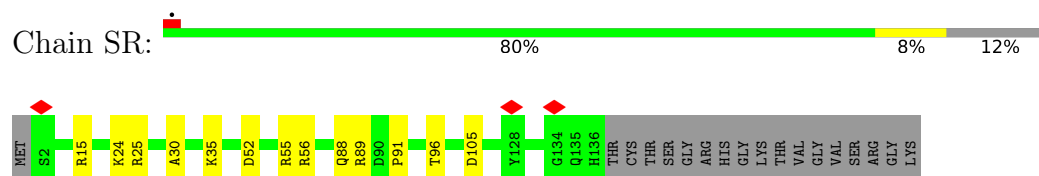
- Molecule 42: Putative 40S ribosomal protein S23



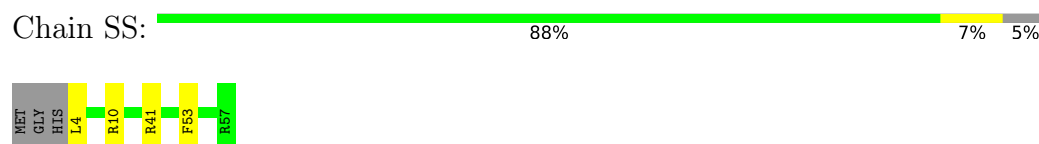
• Molecule 43: 40S ribosomal protein S12



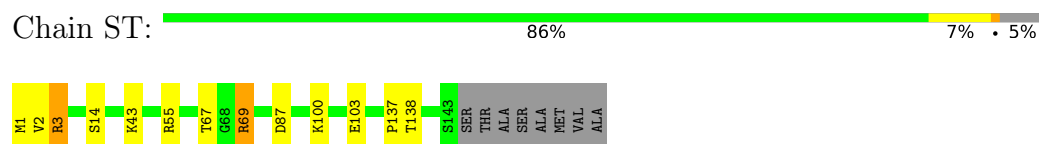
• Molecule 44: Putative 40S ribosomal protein S18



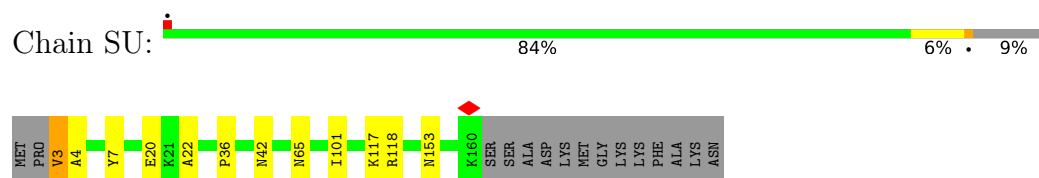
• Molecule 45: Putative ribosomal protein S29



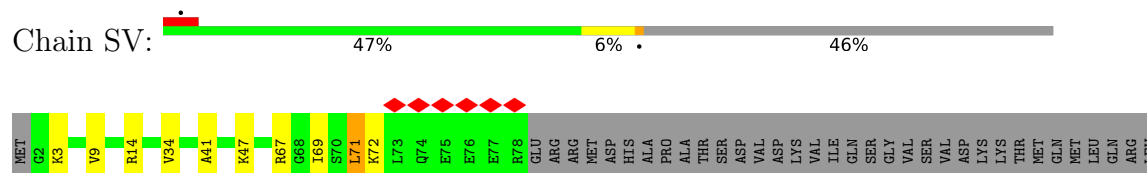
• Molecule 46: Putative 40S ribosomal protein S13



• Molecule 47: Putative 40S ribosomal protein S11



• Molecule 48: Putative 40S ribosomal protein S17



ARG
ALA
GLU
VAL
ALA
GLU
ARG
LYS
ALA
LYS
LYS
LYS

- Molecule 67: 60S ribosomal protein L27

Chain Y:  91% 7% .

MET THR K3 A23 G45 I46 K47 Q67 N76 H77 V99 Q117 M126 Q130 F134

- Molecule 68: Putative 60S ribosomal protein L28

Chain Z:  93% 5% ..

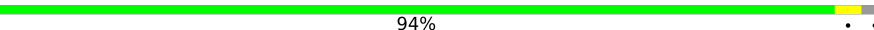
MET S2 K21 R22 R26 T81 V99 R109 R120 R143 A144 K145 R146 ASN

- Molecule 69: Putative 60S ribosomal protein L35

Chain a:  91% 5% . .

MET SER HIS H4 K26 K53 R77 R80 T92 R93 R94 R95 M112 K126 ILE

- Molecule 70: 60S ribosomal protein L29

Chain b:  94% . .

MET A2 K5 T8 K69 ASN

- Molecule 71: Putative 60S ribosomal protein L7

Chain c:  87% . 9%

MET ALA THR HIS SER VAL TYR GLY ASN ALA SER ASP MET PRO VAL VAL PRO ALA PRO GLU SER ALA ILE K24 R25 K29 Q30 Q31 Q32 T33 E34 R43 L87 Q109 V140 I152

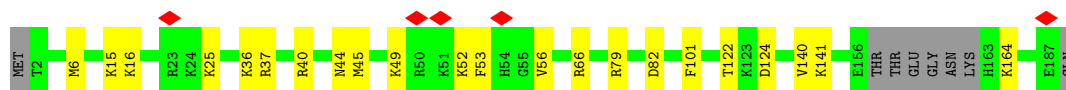
- Molecule 72: 60S ribosomal protein L30

Chain d:  75% 13% . 11%

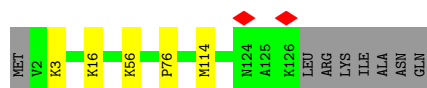
MET ALA LYS LYS THR LYS SER LYS VAL D10 T11 K24 Q38 G39 R40 N49 C50 P51 P52 L77 T89 C90 V94 T95 N96 V97 S100 D101 I102 ALA ALA

- Molecule 73: Putative 60S ribosomal subunit protein L31

Chain e:  84% 12% .



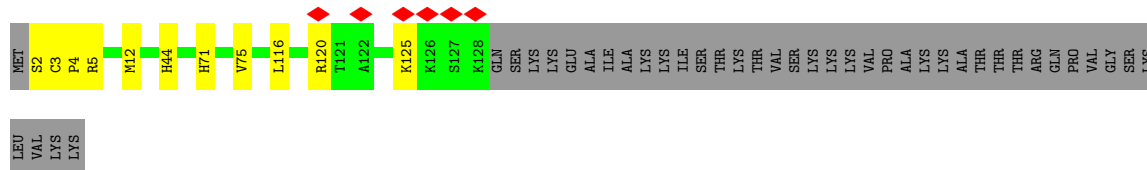
- Molecule 74: 60S ribosomal protein L32



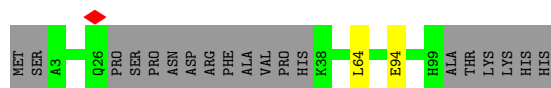
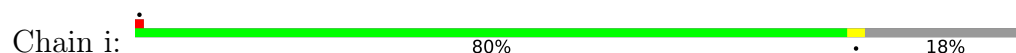
- Molecule 75: Putative ribosomal protein l35a



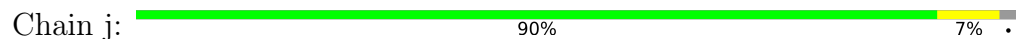
- Molecule 76: Putative 60S ribosomal protein L34



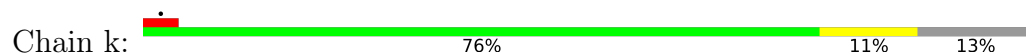
- Molecule 77: Putative 60S Ribosomal protein L36



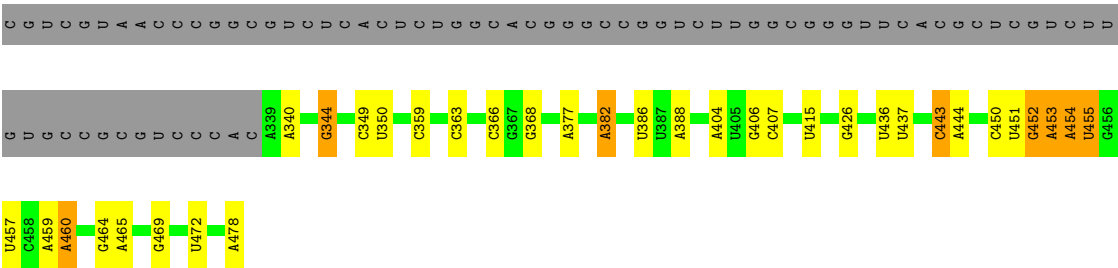
- Molecule 78: Ribosomal protein L37



- Molecule 79: Putative ribosomal protein L38



- [illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	212912	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 ($e^-/\text{\AA}^2$)	0.83	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, OMG, C4J, OMU, 1MA, OMC, MG, 7MG, MA6, ZN, NA, A2M, 5MC, K

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	0.21	3/37759 (0.0%)	0.31	0/58867
2	3	0.19	0/3671	0.32	0/5704
3	4	0.18	0/4354	0.29	0/6788
4	5	0.18	0/2742	0.30	0/4266
5	6	0.17	0/1683	0.34	0/2618
6	7	0.23	2/3748 (0.1%)	0.27	0/5834
7	8	0.16	0/2829	0.27	0/4405
8	A	0.16	0/1935	0.32	0/2606
9	B	0.15	0/3109	0.29	0/4214
10	C	0.15	0/2714	0.28	0/3679
11	D	0.10	0/1045	0.30	0/1423
12	E	0.13	0/1357	0.30	0/1850
13	F	0.14	0/1071	0.27	0/1466
14	G	0.15	0/1696	0.29	0/2303
15	H	0.15	0/1687	0.30	0/2291
16	I	0.15	0/1572	0.28	0/2129
17	J	0.15	0/996	0.30	0/1355
18	K	0.12	0/1248	0.23	0/1695
19	L	0.16	0/1129	0.34	0/1511
20	M	0.17	0/1728	0.33	0/2312
21	N	0.13	0/1647	0.27	0/2202
22	O	0.12	0/1963	0.26	0/2665
23	P	0.16	0/1524	0.29	0/2045
24	Q	0.17	0/1446	0.27	0/1940
25	R	0.14	0/1439	0.28	0/1949
26	S1	0.28	4/40844 (0.0%)	0.32	0/63606
27	S4	0.15	0/476	0.28	0/739
28	SA	0.22	0/1859	0.30	0/2501
29	SB	0.18	0/1623	0.29	0/2204
30	SC	0.13	0/1636	0.22	0/2192
31	SD	0.20	0/1447	0.28	0/1942
32	SE	0.21	0/2088	0.28	0/2814

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SF	0.23	0/1698	0.28	0/2301
34	SG	0.18	0/1849	0.23	0/2477
35	SH	0.16	0/1452	0.26	0/1948
36	SI	0.20	0/1639	0.27	0/2209
37	SK	0.22	0/1451	0.28	0/1944
38	SL	0.15	0/1139	0.25	0/1533
39	SM	0.14	0/798	0.22	0/1084
40	SN	0.12	0/830	0.22	0/1126
41	SO	0.23	0/1010	0.31	0/1362
42	SP	0.23	0/1143	0.29	0/1531
43	SQ	0.09	0/674	0.27	0/916
44	SR	0.14	0/1103	0.24	0/1481
45	SS	0.15	0/439	0.26	0/583
46	ST	0.25	0/1186	0.28	0/1590
47	SU	0.24	0/1290	0.29	0/1740
48	SV	0.17	0/643	0.25	0/854
49	SW	0.12	0/929	0.23	0/1255
50	SX	0.15	0/1233	0.24	0/1656
51	SY	0.15	0/630	0.24	0/858
52	SZ	0.18	0/1041	0.28	0/1388
53	S	0.14	0/1222	0.24	0/1656
54	Sa	0.14	0/563	0.25	0/757
55	Sc	0.21	0/596	0.28	0/801
56	Sb	0.28	0/837	0.27	0/1120
57	Sd	0.16	0/468	0.26	0/630
58	Se	0.19	0/436	0.24	0/577
59	Sg	0.11	0/2371	0.27	0/3233
60	Sh	0.09	0/1113	0.25	0/1514
61	SJ	0.25	0/1038	0.30	0/1391
62	T	0.16	0/1233	0.29	0/1656
63	U	0.09	0/695	0.23	0/939
64	V	0.14	0/930	0.24	0/1256
65	W	0.13	0/938	0.26	0/1254
66	X	0.14	0/560	0.25	0/757
67	Y	0.12	0/1018	0.22	0/1376
68	Z	0.13	0/1083	0.22	0/1461
69	a	0.13	0/1005	0.21	0/1339
70	b	0.14	0/557	0.25	0/743
71	c	0.15	0/1900	0.27	0/2544
72	d	0.15	0/723	0.24	0/979
73	e	0.13	0/1432	0.26	0/1904
74	f	0.15	0/1031	0.27	0/1380
75	g	0.15	0/1165	0.27	0/1563

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	h	0.13	0/1054	0.25	0/1399
77	i	0.12	0/668	0.27	0/889
78	j	0.16	0/682	0.31	0/910
79	k	0.09	0/542	0.21	0/733
80	l	0.16	0/463	0.29	0/617
81	m	0.12	0/381	0.29	0/515
82	n	0.23	0/296	0.32	0/386
83	o	0.18	0/698	0.35	0/930
84	p	0.14	0/793	0.26	0/1048
85	2	0.23	8/25035 (0.0%)	0.32	0/39014
All	All	0.21	17/211768 (0.0%)	0.30	0/311222

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S1	668	A2M	O3'-P	5.77	1.62	1.56
85	2	1372	A2M	O3'-P	5.62	1.61	1.56
85	2	527	A2M	O3'-P	5.35	1.61	1.56
85	2	570	A2M	O3'-P	5.30	1.61	1.56
85	2	1384	A2M	O3'-P	5.28	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	34587	0	17450	214	0
2	3	3312	0	1681	28	0
3	4	3917	0	1979	19	0
4	5	2456	0	1247	14	0
5	6	1506	0	768	12	0
6	7	3485	0	1770	13	0
7	8	2531	0	1283	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1893	0	1905	6	0
9	B	3035	0	3004	16	0
10	C	2664	0	2626	4	0
11	D	1025	0	787	6	0
12	E	1337	0	1269	8	0
13	F	1049	0	1025	11	0
14	G	1672	0	1696	4	0
15	H	1652	0	1644	7	0
16	I	1539	0	1491	2	0
17	J	979	0	968	2	0
18	K	1229	0	1194	7	0
19	L	1102	0	1124	4	0
20	M	1688	0	1748	5	0
21	N	1615	0	1685	23	0
22	O	1926	0	1761	8	0
23	P	1500	0	1568	4	0
24	Q	1427	0	1383	4	0
25	R	1405	0	1411	7	0
26	S1	37536	0	18968	359	0
27	S4	427	0	222	6	0
28	SA	1828	0	1917	12	0
29	SB	1590	0	1570	17	0
30	SC	1609	0	1655	16	0
31	SD	1422	0	1467	15	0
32	SE	2050	0	2144	20	0
33	SF	1662	0	1708	13	0
34	SG	1826	0	1914	23	0
35	SH	1430	0	1456	9	0
36	SI	1609	0	1668	21	0
37	SK	1430	0	1512	7	0
38	SL	1118	0	1168	1	0
39	SM	788	0	823	9	0
40	SN	807	0	782	6	0
41	SO	995	0	997	4	0
42	SP	1117	0	1166	8	0
43	SQ	672	0	602	11	0
44	SR	1081	0	1126	8	0
45	SS	434	0	438	5	0
46	ST	1163	0	1232	10	0
47	SU	1260	0	1277	6	0
48	SV	636	0	687	8	0
49	SW	909	0	909	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	SX	1202	0	1227	16	0
51	SY	621	0	601	6	0
52	SZ	1021	0	1083	12	0
53	S	1194	0	1184	3	0
54	Sa	558	0	606	7	0
55	Sc	586	0	570	4	0
56	Sb	820	0	854	5	0
57	Sd	466	0	476	2	0
58	Se	430	0	473	2	0
59	Sg	2313	0	2189	16	0
60	Sh	1094	0	1005	11	0
61	SJ	1021	0	1050	0	0
62	T	1209	0	1236	8	0
63	U	688	0	536	3	0
64	V	915	0	956	6	0
65	W	925	0	991	8	0
66	X	539	0	535	2	0
67	Y	997	0	988	5	0
68	Z	1068	0	1057	6	0
69	a	995	0	1076	5	0
70	b	546	0	575	1	0
71	c	1866	0	1970	7	0
72	d	713	0	730	5	0
73	e	1414	0	1532	14	0
74	f	1011	0	1054	4	0
75	g	1142	0	1196	11	0
76	h	1038	0	1109	6	0
77	i	660	0	714	1	0
78	j	668	0	680	4	0
79	k	534	0	534	4	0
80	l	450	0	483	1	0
81	m	375	0	370	4	0
82	n	292	0	331	5	0
83	o	686	0	702	8	0
84	p	780	0	838	4	0
85	2	23639	0	11982	156	0
86	1	106	0	0	0	0
86	2	66	0	0	0	0
86	3	1	0	0	0	0
86	4	8	0	0	0	0
86	5	1	0	0	0	0
86	6	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	7	2	0	0	0	0
86	8	2	0	0	0	0
86	I	1	0	0	0	0
86	J	1	0	0	0	0
86	M	1	0	0	0	0
86	S1	107	0	0	0	0
86	SH	1	0	0	0	0
86	SS	1	0	0	0	0
86	SX	1	0	0	0	0
86	T	1	0	0	0	0
87	1	3	0	0	0	0
87	2	5	0	0	0	0
87	5	2	0	0	0	0
87	7	2	0	0	0	0
87	A	2	0	0	0	0
87	B	1	0	0	0	0
87	H	1	0	0	0	0
87	M	1	0	0	0	0
87	S1	25	0	0	0	0
87	SG	1	0	0	0	0
88	1	5	0	0	0	0
88	2	4	0	0	0	0
88	4	1	0	0	0	0
88	A	1	0	0	0	0
88	M	1	0	0	0	0
88	S1	4	0	0	0	0
88	Sb	1	0	0	0	0
89	SS	1	0	0	0	0
89	Sb	1	0	0	0	0
89	j	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	1	9	0	0	0	0
90	2	17	0	0	0	0
90	5	1	0	0	0	0
90	7	1	0	0	0	0
90	A	1	0	0	0	0
90	B	1	0	0	0	0
90	H	1	0	0	0	0
90	I	1	0	0	0	0
90	M	4	0	0	0	0
90	P	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	S	1	0	0	0	0
90	S1	7	0	0	0	0
90	SA	1	0	0	0	0
90	T	2	0	0	0	0
All	All	200822	0	145368	1194	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 1194 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S1:955:A:N6	26:S1:980:G:H1	1.53	1.06
26:S1:1366:A:N1	26:S1:1416:G:N2	2.05	1.04
26:S1:781:A:H2	26:S1:839:G:H1	1.03	0.97
85:2:984:G:H1	85:2:1000:U:H3	0.92	0.92
1:1:520:G:HO2'	1:1:521:G:H8	0.95	0.92

There are no symmetry-related clashes.

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	
8	A	254/260 (98%)	248 (98%)	6 (2%)	0	100	100
9	B	402/419 (96%)	397 (99%)	5 (1%)	0	100	100
10	C	364/373 (98%)	353 (97%)	11 (3%)	0	100	100
11	D	156/188 (83%)	145 (93%)	11 (7%)	0	100	100
12	E	184/190 (97%)	176 (96%)	8 (4%)	0	100	100
13	F	144/195 (74%)	135 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	G	222/264 (84%)	218 (98%)	3 (1%)	1 (0%)	24	37
15	H	218/222 (98%)	218 (100%)	0	0	100	100
16	I	206/220 (94%)	202 (98%)	4 (2%)	0	100	100
17	J	135/139 (97%)	135 (100%)	0	0	100	100
18	K	168/175 (96%)	165 (98%)	3 (2%)	0	100	100
19	L	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
20	M	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
21	N	195/213 (92%)	193 (99%)	2 (1%)	0	100	100
22	O	268/305 (88%)	260 (97%)	8 (3%)	0	100	100
23	P	195/198 (98%)	188 (96%)	7 (4%)	0	100	100
24	Q	188/254 (74%)	185 (98%)	3 (2%)	0	100	100
25	R	176/179 (98%)	175 (99%)	1 (1%)	0	100	100
28	SA	225/264 (85%)	215 (96%)	10 (4%)	0	100	100
29	SB	206/246 (84%)	199 (97%)	7 (3%)	0	100	100
30	SC	211/219 (96%)	208 (99%)	3 (1%)	0	100	100
31	SD	169/190 (89%)	167 (99%)	2 (1%)	0	100	100
32	SE	258/273 (94%)	254 (98%)	4 (2%)	0	100	100
33	SF	216/265 (82%)	214 (99%)	2 (1%)	0	100	100
34	SG	231/249 (93%)	228 (99%)	3 (1%)	0	100	100
35	SH	178/190 (94%)	175 (98%)	3 (2%)	0	100	100
36	SI	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
37	SK	176/220 (80%)	174 (99%)	2 (1%)	0	100	100
38	SL	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
39	SM	100/116 (86%)	96 (96%)	4 (4%)	0	100	100
40	SN	98/168 (58%)	98 (100%)	0	0	100	100
41	SO	134/144 (93%)	131 (98%)	3 (2%)	0	100	100
42	SP	142/143 (99%)	139 (98%)	3 (2%)	0	100	100
43	SQ	96/141 (68%)	85 (88%)	11 (12%)	0	100	100
44	SR	134/153 (88%)	131 (98%)	3 (2%)	0	100	100
45	SS	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
46	ST	141/151 (93%)	139 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	SU	156/173 (90%)	151 (97%)	5 (3%)	0	100	100
48	SV	75/143 (52%)	73 (97%)	2 (3%)	0	100	100
49	SW	113/152 (74%)	109 (96%)	4 (4%)	0	100	100
50	SX	150/161 (93%)	143 (95%)	7 (5%)	0	100	100
51	SY	83/164 (51%)	81 (98%)	2 (2%)	0	100	100
52	SZ	125/137 (91%)	124 (99%)	1 (1%)	0	100	100
53	S	155/159 (98%)	154 (99%)	1 (1%)	0	100	100
54	Sa	69/120 (58%)	68 (99%)	1 (1%)	0	100	100
55	Sc	70/86 (81%)	70 (100%)	0	0	100	100
56	Sb	101/112 (90%)	99 (98%)	2 (2%)	0	100	100
57	Sd	63/87 (72%)	62 (98%)	1 (2%)	0	100	100
58	Se	50/66 (76%)	48 (96%)	2 (4%)	0	100	100
59	Sg	302/312 (97%)	290 (96%)	12 (4%)	0	100	100
60	Sh	153/235 (65%)	146 (95%)	7 (5%)	0	100	100
61	SJ	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
62	T	150/166 (90%)	148 (99%)	2 (1%)	0	100	100
63	U	99/129 (77%)	98 (99%)	1 (1%)	0	100	100
64	V	116/145 (80%)	115 (99%)	1 (1%)	0	100	100
65	W	116/143 (81%)	114 (98%)	2 (2%)	0	100	100
66	X	62/124 (50%)	61 (98%)	1 (2%)	0	100	100
67	Y	130/134 (97%)	129 (99%)	1 (1%)	0	100	100
68	Z	143/147 (97%)	140 (98%)	3 (2%)	0	100	100
69	a	121/127 (95%)	119 (98%)	2 (2%)	0	100	100
70	b	66/70 (94%)	66 (100%)	0	0	100	100
71	c	227/252 (90%)	220 (97%)	7 (3%)	0	100	100
72	d	91/104 (88%)	90 (99%)	1 (1%)	0	100	100
73	e	176/188 (94%)	172 (98%)	4 (2%)	0	100	100
74	f	123/133 (92%)	117 (95%)	6 (5%)	0	100	100
75	g	140/144 (97%)	138 (99%)	2 (1%)	0	100	100
76	h	125/168 (74%)	122 (98%)	3 (2%)	0	100	100
77	i	82/105 (78%)	81 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	j	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
79	k	70/83 (84%)	70 (100%)	0	0	100	100
80	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
81	m	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
82	n	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
83	o	86/92 (94%)	80 (93%)	6 (7%)	0	100	100
84	p	95/106 (90%)	93 (98%)	2 (2%)	0	100	100
All	All	11140/12774 (87%)	10878 (98%)	261 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	G	183	ASP

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	
8	A	186/204 (91%)	186 (100%)	0	100	100
9	B	294/351 (84%)	293 (100%)	1 (0%)	86	93
10	C	250/301 (83%)	249 (100%)	1 (0%)	84	92
11	D	62/162 (38%)	60 (97%)	2 (3%)	34	56
12	E	122/172 (71%)	116 (95%)	6 (5%)	22	39
13	F	94/153 (61%)	93 (99%)	1 (1%)	65	82
14	G	156/221 (71%)	155 (99%)	1 (1%)	78	89
15	H	155/188 (82%)	154 (99%)	1 (1%)	78	89
16	I	145/183 (79%)	143 (99%)	2 (1%)	59	79
17	J	95/111 (86%)	95 (100%)	0	100	100
18	K	109/145 (75%)	107 (98%)	2 (2%)	51	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	L	107/114 (94%)	105 (98%)	2 (2%)	50	71
20	M	172/180 (96%)	170 (99%)	2 (1%)	63	81
21	N	168/179 (94%)	165 (98%)	3 (2%)	51	73
22	O	148/242 (61%)	147 (99%)	1 (1%)	76	88
23	P	152/164 (93%)	151 (99%)	1 (1%)	76	88
24	Q	120/198 (61%)	117 (98%)	3 (2%)	42	64
25	R	144/159 (91%)	144 (100%)	0	100	100
28	SA	198/222 (89%)	191 (96%)	7 (4%)	32	53
29	SB	165/202 (82%)	157 (95%)	8 (5%)	23	40
30	SC	167/184 (91%)	164 (98%)	3 (2%)	51	73
31	SD	148/164 (90%)	145 (98%)	3 (2%)	48	70
32	SE	215/225 (96%)	210 (98%)	5 (2%)	44	66
33	SF	174/208 (84%)	168 (97%)	6 (3%)	32	54
34	SG	186/208 (89%)	180 (97%)	6 (3%)	34	56
35	SH	150/159 (94%)	148 (99%)	2 (1%)	61	80
36	SI	172/186 (92%)	169 (98%)	3 (2%)	53	74
37	SK	139/176 (79%)	135 (97%)	4 (3%)	37	60
38	SL	112/120 (93%)	107 (96%)	5 (4%)	24	42
39	SM	90/104 (86%)	87 (97%)	3 (3%)	33	55
40	SN	84/128 (66%)	79 (94%)	5 (6%)	17	31
41	SO	97/113 (86%)	94 (97%)	3 (3%)	35	57
42	SP	115/117 (98%)	112 (97%)	3 (3%)	40	63
43	SQ	57/120 (48%)	54 (95%)	3 (5%)	20	36
44	SR	112/130 (86%)	112 (100%)	0	100	100
45	SS	45/49 (92%)	44 (98%)	1 (2%)	45	67
46	ST	125/132 (95%)	123 (98%)	2 (2%)	55	76
47	SU	132/152 (87%)	129 (98%)	3 (2%)	44	66
48	SV	69/126 (55%)	65 (94%)	4 (6%)	18	32
49	SW	93/130 (72%)	92 (99%)	1 (1%)	65	82
50	SX	121/131 (92%)	120 (99%)	1 (1%)	73	86
51	SY	64/116 (55%)	63 (98%)	1 (2%)	55	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	SZ	107/118 (91%)	102 (95%)	5 (5%)	23	41
53	S	116/134 (87%)	116 (100%)	0	100	100
54	Sa	63/95 (66%)	62 (98%)	1 (2%)	55	76
55	Sc	62/76 (82%)	61 (98%)	1 (2%)	55	76
56	Sb	85/93 (91%)	83 (98%)	2 (2%)	43	65
57	Sd	46/75 (61%)	44 (96%)	2 (4%)	26	44
58	Se	45/54 (83%)	44 (98%)	1 (2%)	45	67
59	Sg	246/265 (93%)	239 (97%)	7 (3%)	38	60
60	Sh	91/177 (51%)	85 (93%)	6 (7%)	15	26
61	SJ	110/111 (99%)	108 (98%)	2 (2%)	51	73
62	T	125/143 (87%)	123 (98%)	2 (2%)	55	76
63	U	41/114 (36%)	41 (100%)	0	100	100
64	V	93/124 (75%)	91 (98%)	2 (2%)	45	67
65	W	96/122 (79%)	96 (100%)	0	100	100
66	X	56/104 (54%)	54 (96%)	2 (4%)	31	52
67	Y	93/116 (80%)	92 (99%)	1 (1%)	65	82
68	Z	102/118 (86%)	100 (98%)	2 (2%)	48	70
69	a	103/118 (87%)	100 (97%)	3 (3%)	37	60
70	b	56/58 (97%)	56 (100%)	0	100	100
71	c	192/209 (92%)	192 (100%)	0	100	100
72	d	81/89 (91%)	74 (91%)	7 (9%)	10	16
73	e	146/158 (92%)	144 (99%)	2 (1%)	59	79
74	f	106/115 (92%)	105 (99%)	1 (1%)	70	85
75	g	119/121 (98%)	118 (99%)	1 (1%)	73	86
76	h	110/146 (75%)	106 (96%)	4 (4%)	31	52
77	i	64/88 (73%)	64 (100%)	0	100	100
78	j	67/70 (96%)	67 (100%)	0	100	100
79	k	52/74 (70%)	50 (96%)	2 (4%)	29	49
80	l	46/47 (98%)	46 (100%)	0	100	100
81	m	36/113 (32%)	36 (100%)	0	100	100
82	n	30/32 (94%)	29 (97%)	1 (3%)	33	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
83	o	68/74 (92%)	66 (97%)	2 (3%)	37	60
84	p	82/92 (89%)	81 (99%)	1 (1%)	63	81
All	All	8644/10672 (81%)	8473 (98%)	171 (2%)	48	70

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	SZ	60	SER
66	X	29	THR
56	Sb	42	VAL
60	Sh	84	GLN
72	d	11	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
59	Sg	180	ASN
74	f	21	HIS
60	Sh	170	GLN
67	Y	86	ASN
75	g	113	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1598/1782 (89%)	281 (17%)	16 (1%)
2	3	151/216 (69%)	32 (21%)	4 (2%)
26	S1	1729/2204 (78%)	314 (18%)	12 (0%)
27	S4	18/20 (90%)	6 (33%)	0
3	4	182/183 (99%)	31 (17%)	3 (1%)
4	5	111/135 (82%)	21 (18%)	0
5	6	70/73 (95%)	22 (31%)	2 (2%)
6	7	161/171 (94%)	24 (14%)	0
7	8	118/123 (95%)	8 (6%)	0
85	2	1097/478 (229%)	208 (18%)	13 (1%)
All	All	5235/5385 (97%)	947 (18%)	50 (0%)

5 of 947 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	24	A
1	1	29	C
1	1	38	A
1	1	41	A
1	1	47	C

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	S1	277	U
26	S1	995	U
85	2	1452	U
26	S1	494	A
26	S1	790	U

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

105 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	$\# Z > 2$
85	OMC	2	359	85	19,22,23	3.00	8 (42%)	25,31,34	0.70	0
1	PSU	1	1011	1	18,21,22	4.61	9 (50%)	21,30,33	1.91	6 (28%)
6	PSU	7	74	6	18,21,22	4.62	7 (38%)	21,30,33	1.95	5 (23%)
26	PSU	S1	1533	26	18,21,22	4.59	7 (38%)	21,30,33	1.89	5 (23%)
1	A2M	1	305	1	22,25,26	3.51	9 (40%)	30,36,39	2.45	11 (36%)
26	PSU	S1	1192	26	18,21,22	4.50	8 (44%)	21,30,33	1.86	5 (23%)
1	OMC	1	1010	86,1,88	19,22,23	2.96	8 (42%)	25,31,34	0.85	0
1	A2M	1	1539	86,85,1	22,25,26	3.55	9 (40%)	30,36,39	2.26	11 (36%)
26	PSU	S1	104	26	18,21,22	4.53	7 (38%)	21,30,33	1.89	5 (23%)
1	PSU	1	239	1	18,21,22	4.63	7 (38%)	21,30,33	1.95	5 (23%)
26	MA6	S1	2184	26	23,26,27	1.54	5 (21%)	33,38,41	2.89	12 (36%)
26	PSU	S1	33	26	18,21,22	4.59	8 (44%)	21,30,33	1.90	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	1	845	1	19,22,23	3.01	8 (42%)	25,31,34	2.16	6 (24%)
6	A2M	7	162	1,6	22,25,26	3.55	9 (40%)	30,36,39	2.38	11 (36%)
26	OMG	S1	1829	86,26	23,26,27	2.40	9 (39%)	32,38,41	2.60	10 (31%)
1	PSU	1	940	1	18,21,22	4.61	7 (38%)	21,30,33	1.97	5 (23%)
1	PSU	1	422	1	18,21,22	4.64	7 (38%)	21,30,33	1.99	5 (23%)
26	PSU	S1	1156	26	18,21,22	4.51	7 (38%)	21,30,33	2.00	5 (23%)
26	OMG	S1	1623	26	23,26,27	2.41	9 (39%)	32,38,41	2.66	10 (31%)
85	OMU	2	56	85,1	19,22,23	3.03	8 (42%)	25,31,34	1.87	4 (16%)
26	OMU	S1	8	26	19,22,23	2.91	8 (42%)	25,31,34	1.94	5 (20%)
1	OMG	1	959[B]	1	23,26,27	2.44	8 (34%)	32,38,41	2.41	9 (28%)
85	OMG	2	71	86,85	23,26,27	2.42	9 (39%)	32,38,41	2.53	11 (34%)
26	PSU	S1	1539	26	18,21,22	4.57	7 (38%)	21,30,33	1.93	5 (23%)
26	C4J	S1	1543	26	25,29,30	2.87	9 (36%)	28,42,45	1.46	4 (14%)
1	PSU	1	1039	1	18,21,22	4.61	7 (38%)	21,30,33	2.01	5 (23%)
26	5MC	S1	1544	26	19,22,23	3.70	8 (42%)	26,32,35	1.05	1 (3%)
85	A2M	2	95	85	22,25,26	3.53	9 (40%)	30,36,39	2.31	11 (36%)
26	OMU	S1	1621	86,26	19,22,23	3.04	8 (42%)	25,31,34	1.83	5 (20%)
26	MA6	S1	2185	26	23,26,27	1.56	5 (21%)	33,38,41	2.91	13 (39%)
1	PSU	1	1528	1	18,21,22	4.61	7 (38%)	21,30,33	1.97	6 (28%)
1	A2M	1	955	1	22,25,26	3.56	9 (40%)	30,36,39	2.31	11 (36%)
85	A2M	2	382	85	22,25,26	3.52	9 (40%)	30,36,39	2.33	11 (36%)
26	OMC	S1	18	26	19,22,23	2.82	8 (42%)	25,31,34	0.78	0
6	PSU	7	69	6	18,21,22	4.61	9 (50%)	21,30,33	1.89	5 (23%)
1	A2M	1	858	1	22,25,26	3.46	9 (40%)	30,36,39	2.45	12 (40%)
1	A2M	1	407	1	22,25,26	3.57	9 (40%)	30,36,39	2.41	13 (43%)
2	OMU	3	13	2	19,22,23	3.04	8 (42%)	25,31,34	1.84	5 (20%)
26	OMG	S1	1478	26	23,26,27	2.36	9 (39%)	32,38,41	2.48	11 (34%)
26	OMC	S1	2140	26	19,22,23	2.95	8 (42%)	25,31,34	0.87	1 (4%)
85	OMU	2	73	85	19,22,23	3.01	8 (42%)	25,31,34	1.80	5 (20%)
85	PSU	2	78	85	18,21,22	4.58	7 (38%)	21,30,33	1.99	5 (23%)
85	PSU	2	472	85	18,21,22	4.62	7 (38%)	21,30,33	2.01	5 (23%)
1	A2M	1	235	1	22,25,26	3.54	9 (40%)	30,36,39	2.32	10 (33%)
26	OMG	S1	2151	26	23,26,27	2.40	9 (39%)	32,38,41	2.57	10 (31%)
1	A2M	1	681	1	22,25,26	3.50	9 (40%)	30,36,39	2.39	11 (36%)
6	OMG	7	75	6	23,26,27	2.42	9 (39%)	32,38,41	2.56	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	A2M	S1	2021	26	22,25,26	3.44	9 (40%)	30,36,39	2.42	11 (36%)
1	OMG	1	959[A]	1	23,26,27	2.45	9 (39%)	32,38,41	2.63	12 (37%)
26	PSU	S1	609	26	18,21,22	4.59	7 (38%)	21,30,33	2.04	5 (23%)
26	PSU	S1	2202	26	18,21,22	4.44	8 (44%)	21,30,33	1.79	4 (19%)
26	OMU	S1	1979	26	19,22,23	3.03	8 (42%)	25,31,34	1.84	5 (20%)
1	PSU	1	1017	86,1	18,21,22	4.53	7 (38%)	21,30,33	1.98	5 (23%)
26	PSU	S1	12	26	18,21,22	4.41	7 (38%)	21,30,33	1.97	5 (23%)
3	OMG	4	74	3	23,26,27	2.39	9 (39%)	32,38,41	2.53	11 (34%)
26	OMU	S1	29	86,26	19,22,23	2.98	8 (42%)	25,31,34	1.90	5 (20%)
1	A2M	1	697	1	22,25,26	3.50	9 (40%)	30,36,39	2.33	12 (40%)
26	OMU	S1	661	26	19,22,23	2.93	8 (42%)	25,31,34	1.89	5 (20%)
26	OMC	S1	38	26	19,22,23	2.89	8 (42%)	25,31,34	0.80	0
1	OMG	1	1524	1	23,26,27	2.42	9 (39%)	32,38,41	2.58	10 (31%)
26	PSU	S1	1246	86,26	18,21,22	4.49	7 (38%)	21,30,33	2.07	5 (23%)
1	OMC	1	695	1	19,22,23	2.95	8 (42%)	25,31,34	0.71	0
26	A2M	S1	479	26	22,25,26	3.51	9 (40%)	30,36,39	2.33	13 (43%)
1	OMU	1	1371	1	19,22,23	3.09	8 (42%)	25,31,34	1.98	6 (24%)
26	OMG	S1	600	26	23,26,27	2.40	9 (39%)	32,38,41	2.63	10 (31%)
26	PSU	S1	455	26	18,21,22	4.55	7 (38%)	21,30,33	2.05	5 (23%)
6	A2M	7	43	6	22,25,26	3.53	9 (40%)	30,36,39	2.33	12 (40%)
85	OMC	2	443	85,87	19,22,23	2.95	8 (42%)	25,31,34	0.83	0
26	PSU	S1	2048	26	18,21,22	4.40	7 (38%)	21,30,33	2.00	5 (23%)
1	PSU	1	1664	1	18,21,22	4.61	7 (38%)	21,30,33	1.99	6 (28%)
26	7MG	S1	1995	26	23,26,27	3.81	10 (43%)	27,39,42	2.19	9 (33%)
1	PSU	1	1402	1	18,21,22	4.57	7 (38%)	21,30,33	1.82	4 (19%)
1	OMU	1	1107	1	19,22,23	3.03	8 (42%)	25,31,34	1.87	5 (20%)
1	PSU	1	672	86,1	18,21,22	4.56	7 (38%)	21,30,33	2.00	6 (28%)
1	OMG	1	1626	1	23,26,27	2.42	9 (39%)	32,38,41	2.54	11 (34%)
1	1MA	1	677	86,1	21,25,26	2.96	5 (23%)	30,37,40	3.01	7 (23%)
26	PSU	S1	2046	26	18,21,22	4.46	7 (38%)	21,30,33	2.06	5 (23%)
1	PSU	1	1171	86,1	18,21,22	4.60	7 (38%)	21,30,33	1.98	6 (28%)
26	A2M	S1	98	86,26	22,25,26	3.56	9 (40%)	30,36,39	2.29	11 (36%)
85	PSU	2	437	85	18,21,22	4.55	7 (38%)	21,30,33	1.98	5 (23%)
26	OMG	S1	1550	26	23,26,27	2.42	9 (39%)	32,38,41	2.64	10 (31%)
26	PSU	S1	1657	26	18,21,22	4.49	7 (38%)	21,30,33	1.95	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1	870	1	18,21,22	4.58	7 (38%)	21,30,33	2.00	5 (23%)
1	OMG	1	1190	86,1	23,26,27	2.39	9 (39%)	32,38,41	2.48	13 (40%)
26	OMU	S1	1833	86,26	19,22,23	3.04	8 (42%)	25,31,34	1.88	5 (20%)
1	A2M	1	927	1	22,25,26	3.51	9 (40%)	30,36,39	2.36	11 (36%)
26	PSU	S1	1841	87,26	18,21,22	4.53	7 (38%)	21,30,33	2.09	5 (23%)
26	A2M	S1	668	86,26	22,25,26	3.48	9 (40%)	30,36,39	2.45	12 (40%)
1	OMU	1	1659	86,1	19,22,23	3.02	8 (42%)	25,31,34	1.84	5 (20%)
26	A2M	S1	512	86,26	22,25,26	3.55	9 (40%)	30,36,39	2.33	12 (40%)
26	OMG	S1	1647	26	23,26,27	2.37	8 (34%)	32,38,41	2.57	11 (34%)
1	PSU	1	1181	1	18,21,22	4.60	8 (44%)	21,30,33	1.87	5 (23%)
1	OMG	1	1540	85,1	23,26,27	2.37	9 (39%)	32,38,41	2.51	11 (34%)
6	OMU	7	7	1,6	19,22,23	3.02	8 (42%)	25,31,34	1.82	5 (20%)
26	PSU	S1	607	26	18,21,22	4.71	7 (38%)	21,30,33	1.88	6 (28%)
26	5MC	S1	2061	26	19,22,23	3.57	8 (42%)	26,32,35	0.98	2 (7%)
1	OMU	1	847	1	19,22,23	2.99	8 (42%)	25,31,34	1.87	5 (20%)
26	PSU	S1	1566	86,26	18,21,22	4.60	8 (44%)	21,30,33	1.85	4 (19%)
1	PSU	1	1533	85,1	18,21,22	4.60	7 (38%)	21,30,33	2.07	6 (28%)
26	OMC	S1	1866	26	19,22,23	2.91	8 (42%)	25,31,34	0.75	0
1	A2M	1	678	85,1	22,25,26	3.43	9 (40%)	30,36,39	3.11	16 (53%)
1	OMC	1	1527	1	19,22,23	2.95	8 (42%)	25,31,34	1.02	2 (8%)
1	OMG	1	856	1	23,26,27	2.39	9 (39%)	32,38,41	2.54	10 (31%)
26	OMG	S1	1865	26	23,26,27	2.39	9 (39%)	32,38,41	2.53	10 (31%)
26	OMG	S1	1879	26	23,26,27	2.41	9 (39%)	32,38,41	2.62	10 (31%)

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
85	OMC	2	359	85	-	0/9/27/28	0/2/2/2
1	PSU	1	1011	1	-	0/7/25/26	0/2/2/2
6	PSU	7	74	6	-	2/7/25/26	0/2/2/2
26	PSU	S1	1533	26	-	2/7/25/26	0/2/2/2
1	A2M	1	305	1	-	2/9/27/28	0/3/3/3
26	PSU	S1	1192	26	-	0/7/25/26	0/2/2/2
1	OMC	1	1010	86,1,88	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	1	1539	86,85,1	-	0/9/27/28	0/3/3/3
26	PSU	S1	104	26	-	2/7/25/26	0/2/2/2
1	PSU	1	239	1	-	0/7/25/26	0/2/2/2
26	MA6	S1	2184	26	-	0/11/29/30	0/3/3/3
26	PSU	S1	33	26	-	2/7/25/26	0/2/2/2
1	OMU	1	845	1	-	3/9/27/28	0/2/2/2
6	A2M	7	162	1,6	-	1/9/27/28	0/3/3/3
26	OMG	S1	1829	86,26	-	0/9/27/28	0/3/3/3
1	PSU	1	940	1	-	0/7/25/26	0/2/2/2
1	PSU	1	422	1	-	0/7/25/26	0/2/2/2
26	PSU	S1	1156	26	-	0/7/25/26	0/2/2/2
26	OMG	S1	1623	26	-	2/9/27/28	0/3/3/3
85	OMU	2	56	85,1	-	0/9/27/28	0/2/2/2
26	OMU	S1	8	26	-	5/9/27/28	0/2/2/2
1	OMG	1	959[B]	1	-	0/9/27/28	0/3/3/3
85	OMG	2	71	86,85	-	0/9/27/28	0/3/3/3
26	PSU	S1	1539	26	-	2/7/25/26	0/2/2/2
26	C4J	S1	1543	26	-	5/16/34/35	0/2/2/2
1	PSU	1	1039	1	-	0/7/25/26	0/2/2/2
26	5MC	S1	1544	26	-	0/7/25/26	0/2/2/2
85	A2M	2	95	85	-	0/9/27/28	0/3/3/3
26	OMU	S1	1621	86,26	-	0/9/27/28	0/2/2/2
26	MA6	S1	2185	26	-	1/11/29/30	0/3/3/3
1	PSU	1	1528	1	-	0/7/25/26	0/2/2/2
1	A2M	1	955	1	-	0/9/27/28	0/3/3/3
85	A2M	2	382	85	-	1/9/27/28	0/3/3/3
26	OMC	S1	18	26	-	0/9/27/28	0/2/2/2
6	PSU	7	69	6	-	3/7/25/26	0/2/2/2
1	A2M	1	858	1	-	1/9/27/28	0/3/3/3
1	A2M	1	407	1	-	3/9/27/28	0/3/3/3
2	OMU	3	13	2	-	0/9/27/28	0/2/2/2
26	OMG	S1	1478	26	-	0/9/27/28	0/3/3/3
26	OMC	S1	2140	26	-	2/9/27/28	0/2/2/2
85	OMU	2	73	85	-	0/9/27/28	0/2/2/2
85	PSU	2	78	85	-	0/7/25/26	0/2/2/2
85	PSU	2	472	85	-	0/7/25/26	0/2/2/2
1	A2M	1	235	1	-	0/9/27/28	0/3/3/3
26	OMG	S1	2151	26	-	0/9/27/28	0/3/3/3
1	A2M	1	681	1	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMG	7	75	6	-	2/9/27/28	0/3/3/3
26	A2M	S1	2021	26	-	2/9/27/28	0/3/3/3
1	OMG	1	959[A]	1	-	2/9/27/28	0/3/3/3
26	PSU	S1	609	26	-	0/7/25/26	0/2/2/2
26	PSU	S1	2202	26	-	1/7/25/26	0/2/2/2
26	OMU	S1	1979	26	-	0/9/27/28	0/2/2/2
1	PSU	1	1017	86,1	-	0/7/25/26	0/2/2/2
26	PSU	S1	12	26	-	0/7/25/26	0/2/2/2
3	OMG	4	74	3	-	0/9/27/28	0/3/3/3
26	OMU	S1	29	86,26	-	0/9/27/28	0/2/2/2
1	A2M	1	697	1	-	0/9/27/28	0/3/3/3
26	OMU	S1	661	26	-	0/9/27/28	0/2/2/2
26	OMC	S1	38	26	-	0/9/27/28	0/2/2/2
1	OMG	1	1524	1	-	1/9/27/28	0/3/3/3
26	PSU	S1	1246	86,26	-	0/7/25/26	0/2/2/2
1	OMC	1	695	1	-	0/9/27/28	0/2/2/2
26	A2M	S1	479	26	-	2/9/27/28	0/3/3/3
1	OMU	1	1371	1	-	4/9/27/28	0/2/2/2
26	OMG	S1	600	26	-	2/9/27/28	0/3/3/3
26	PSU	S1	455	26	-	0/7/25/26	0/2/2/2
6	A2M	7	43	6	-	0/9/27/28	0/3/3/3
85	OMC	2	443	85,87	-	4/9/27/28	0/2/2/2
26	PSU	S1	2048	26	-	0/7/25/26	0/2/2/2
1	PSU	1	1664	1	-	0/7/25/26	0/2/2/2
26	7MG	S1	1995	26	-	2/7/37/38	0/3/3/3
1	PSU	1	1402	1	-	2/7/25/26	0/2/2/2
1	OMU	1	1107	1	-	3/9/27/28	0/2/2/2
1	PSU	1	672	86,1	-	0/7/25/26	0/2/2/2
1	OMG	1	1626	1	-	0/9/27/28	0/3/3/3
1	1MA	1	677	86,1	-	0/7/25/26	0/3/3/3
26	PSU	S1	2046	26	-	0/7/25/26	0/2/2/2
1	PSU	1	1171	86,1	-	0/7/25/26	0/2/2/2
26	A2M	S1	98	86,26	-	2/9/27/28	0/3/3/3
85	PSU	2	437	85	-	0/7/25/26	0/2/2/2
26	OMG	S1	1550	26	-	3/9/27/28	0/3/3/3
26	PSU	S1	1657	26	-	2/7/25/26	0/2/2/2
1	PSU	1	870	1	-	0/7/25/26	0/2/2/2
1	OMG	1	1190	86,1	-	0/9/27/28	0/3/3/3
26	OMU	S1	1833	86,26	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	1	927	1	-	1/9/27/28	0/3/3/3
26	PSU	S1	1841	87,26	-	1/7/25/26	0/2/2/2
26	A2M	S1	668	86,26	-	4/9/27/28	0/3/3/3
1	OMU	1	1659	86,1	-	0/9/27/28	0/2/2/2
26	A2M	S1	512	86,26	-	2/9/27/28	0/3/3/3
26	OMG	S1	1647	26	-	0/9/27/28	0/3/3/3
1	PSU	1	1181	1	-	4/7/25/26	0/2/2/2
1	OMG	1	1540	85,1	-	2/9/27/28	0/3/3/3
6	OMU	7	7	1,6	-	1/9/27/28	0/2/2/2
26	PSU	S1	607	26	-	2/7/25/26	0/2/2/2
26	5MC	S1	2061	26	-	0/7/25/26	0/2/2/2
1	OMU	1	847	1	-	0/9/27/28	0/2/2/2
26	PSU	S1	1566	86,26	-	2/7/25/26	0/2/2/2
1	PSU	1	1533	85,1	-	0/7/25/26	0/2/2/2
26	OMC	S1	1866	26	-	0/9/27/28	0/2/2/2
1	A2M	1	678	85,1	-	3/9/27/28	0/3/3/3
1	OMC	1	1527	1	-	1/9/27/28	0/2/2/2
1	OMG	1	856	1	-	0/9/27/28	0/3/3/3
26	OMG	S1	1865	26	-	0/9/27/28	0/3/3/3
26	OMG	S1	1879	26	-	1/9/27/28	0/3/3/3

The worst 5 of 843 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	422	PSU	C6-C5	12.54	1.49	1.35
26	S1	607	PSU	C6-C5	12.36	1.49	1.35
26	S1	33	PSU	C6-C5	12.16	1.48	1.35
6	7	69	PSU	C6-C5	12.15	1.48	1.35
26	S1	1566	PSU	C6-C5	12.15	1.48	1.35

The worst 5 of 732 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S1	2185	MA6	N1-C6-N6	-9.89	104.81	116.86
26	S1	2184	MA6	N1-C6-N6	-9.67	105.07	116.86
1	1	677	1MA	C1'-N9-C8	-9.42	99.97	126.73
1	1	677	1MA	C1'-N9-C4	9.19	153.63	126.49
26	S1	1623	OMG	C1'-N9-C8	-8.15	103.59	126.73

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	407	A2M	O4'-C4'-C5'-O5'
1	1	678	A2M	O4'-C4'-C5'-O5'
1	1	681	A2M	O4'-C4'-C5'-O5'
1	1	845	OMU	O4'-C1'-N1-C2
1	1	845	OMU	O4'-C1'-N1-C6

There are no ring outliers.

26 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1010	OMC	1	0
1	1	845	OMU	3	0
6	7	162	A2M	1	0
1	1	422	PSU	1	0
26	S1	1539	PSU	1	0
85	2	95	A2M	2	0
26	S1	2185	MA6	1	0
1	1	955	A2M	2	0
85	2	382	A2M	1	0
1	1	235	A2M	1	0
26	S1	2021	A2M	1	0
1	1	959[A]	OMG	1	0
26	S1	2202	PSU	1	0
26	S1	29	OMU	1	0
26	S1	661	OMU	1	0
1	1	1524	OMG	1	0
1	1	695	OMC	1	0
26	S1	479	A2M	1	0
1	1	677	1MA	1	0
26	S1	1550	OMG	1	0
26	S1	668	A2M	1	0
1	1	1181	PSU	1	0
1	1	847	OMU	1	0
1	1	678	A2M	1	0
1	1	1527	OMC	1	0
26	S1	1879	OMG	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 367 ligands modelled in this entry, 367 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
27	S4	1
31	SD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S4	6:G	O3'	63:G	P	19.63
1	SD	163:PHE	C	164:GLY	N	4.10

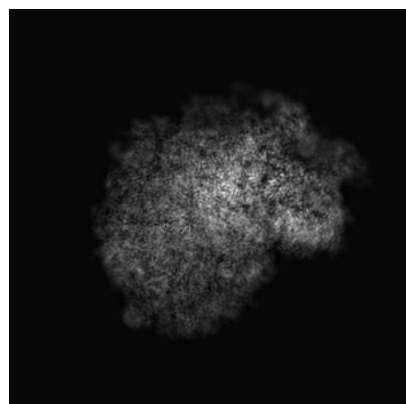
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17216. These allow visual inspection of the internal detail of the map and identification of artifacts.

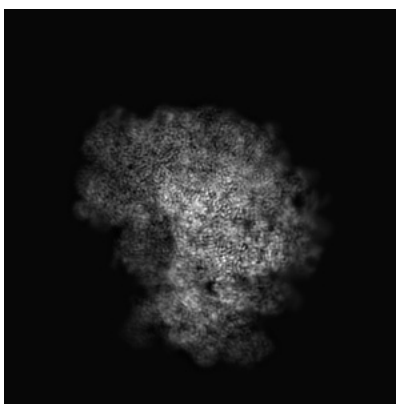
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

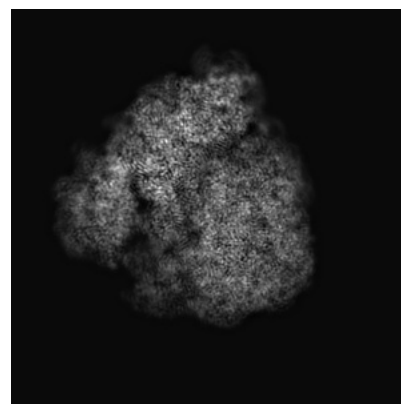
6.1.1 Primary map



X

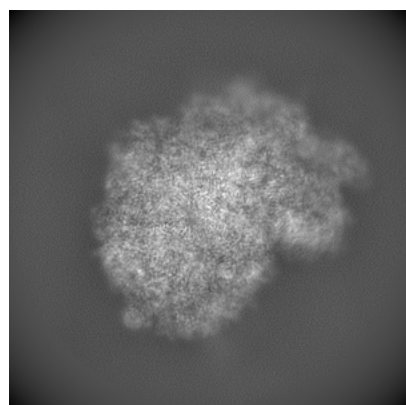


Y

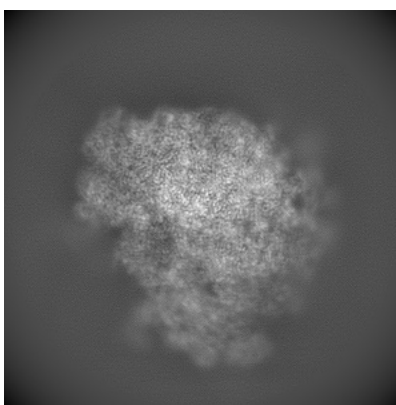


Z

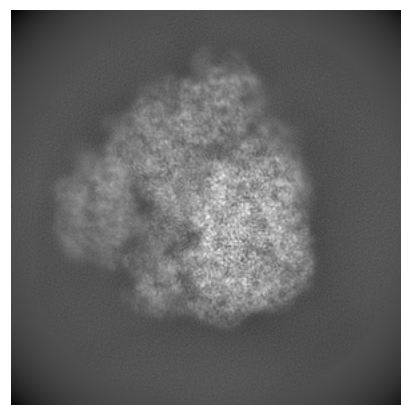
6.1.2 Raw map



X



Y

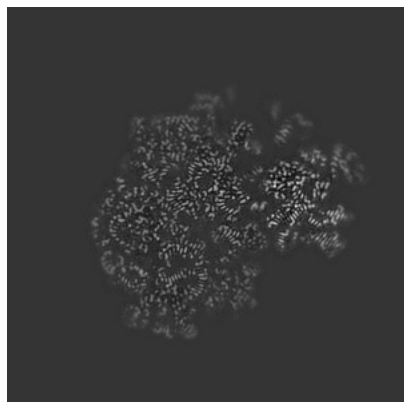


Z

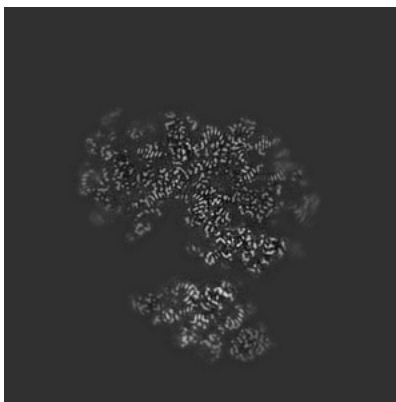
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

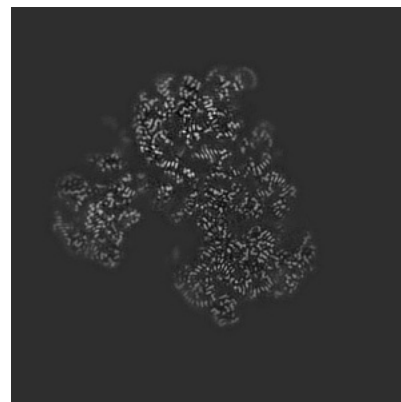
6.2.1 Primary map



X Index: 240

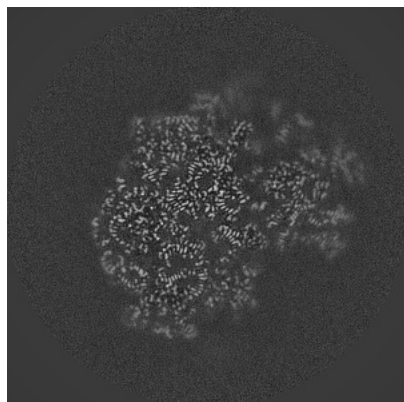


Y Index: 240

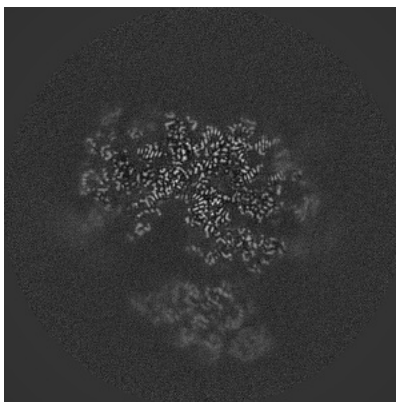


Z Index: 240

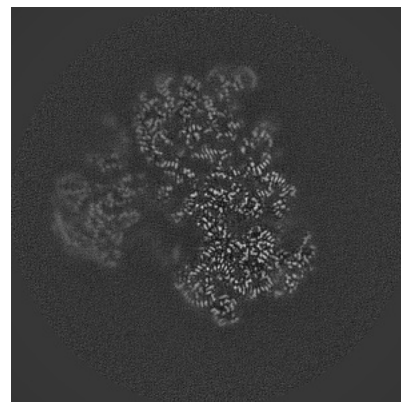
6.2.2 Raw map



X Index: 240



Y Index: 240

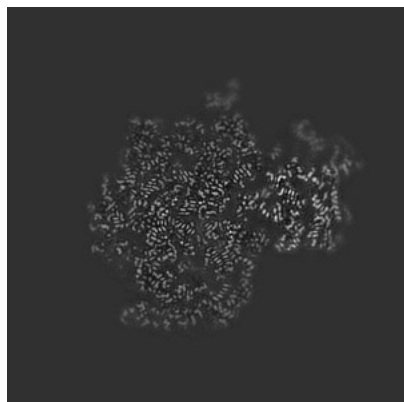


Z Index: 240

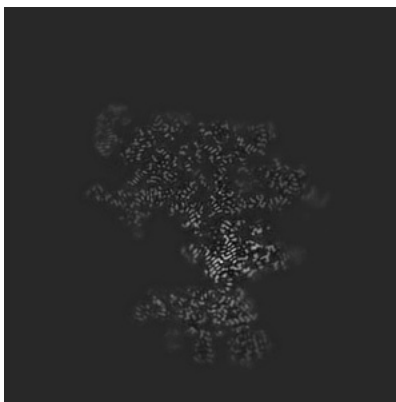
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

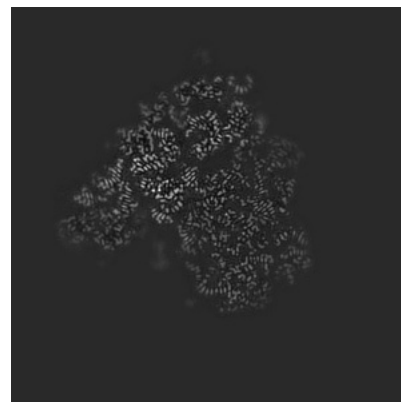
6.3.1 Primary map



X Index: 252

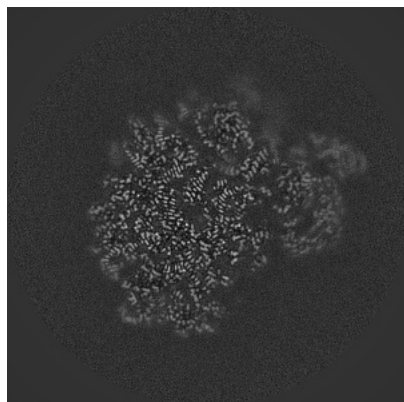


Y Index: 265

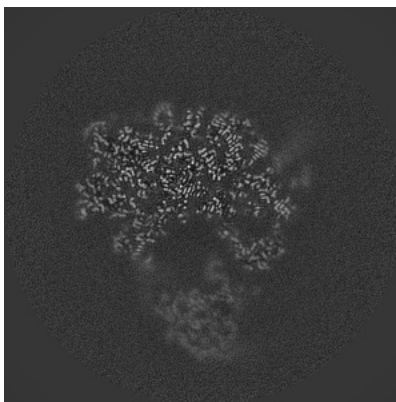


Z Index: 264

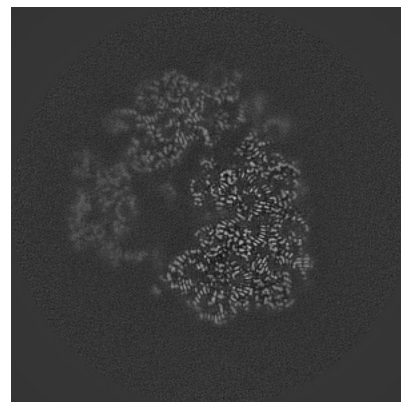
6.3.2 Raw map



X Index: 267



Y Index: 207

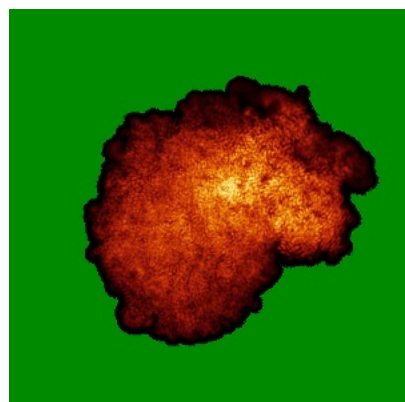


Z Index: 216

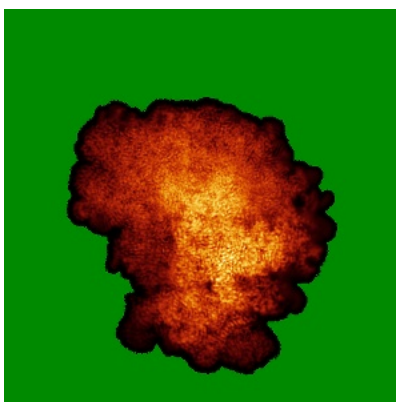
The images above show the largest variance slices of the map in three orthogonal directions.

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

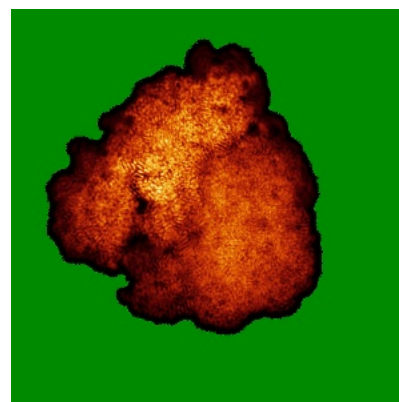
6.4.1 Primary map



X

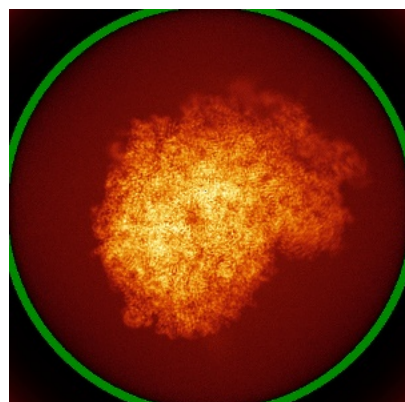


Y

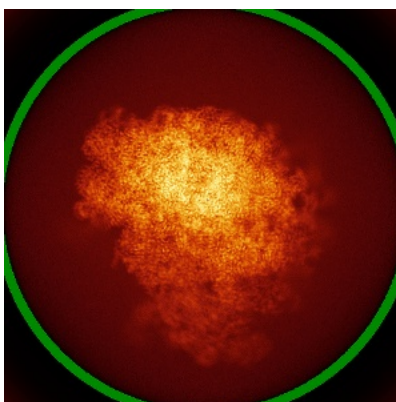


Z

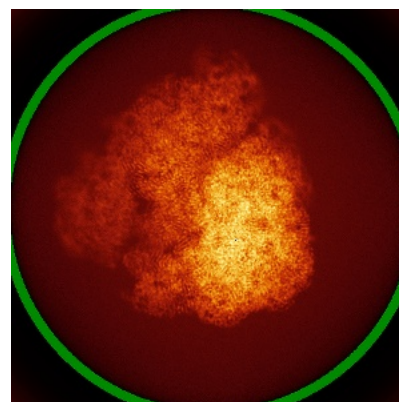
6.4.2 Raw map



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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

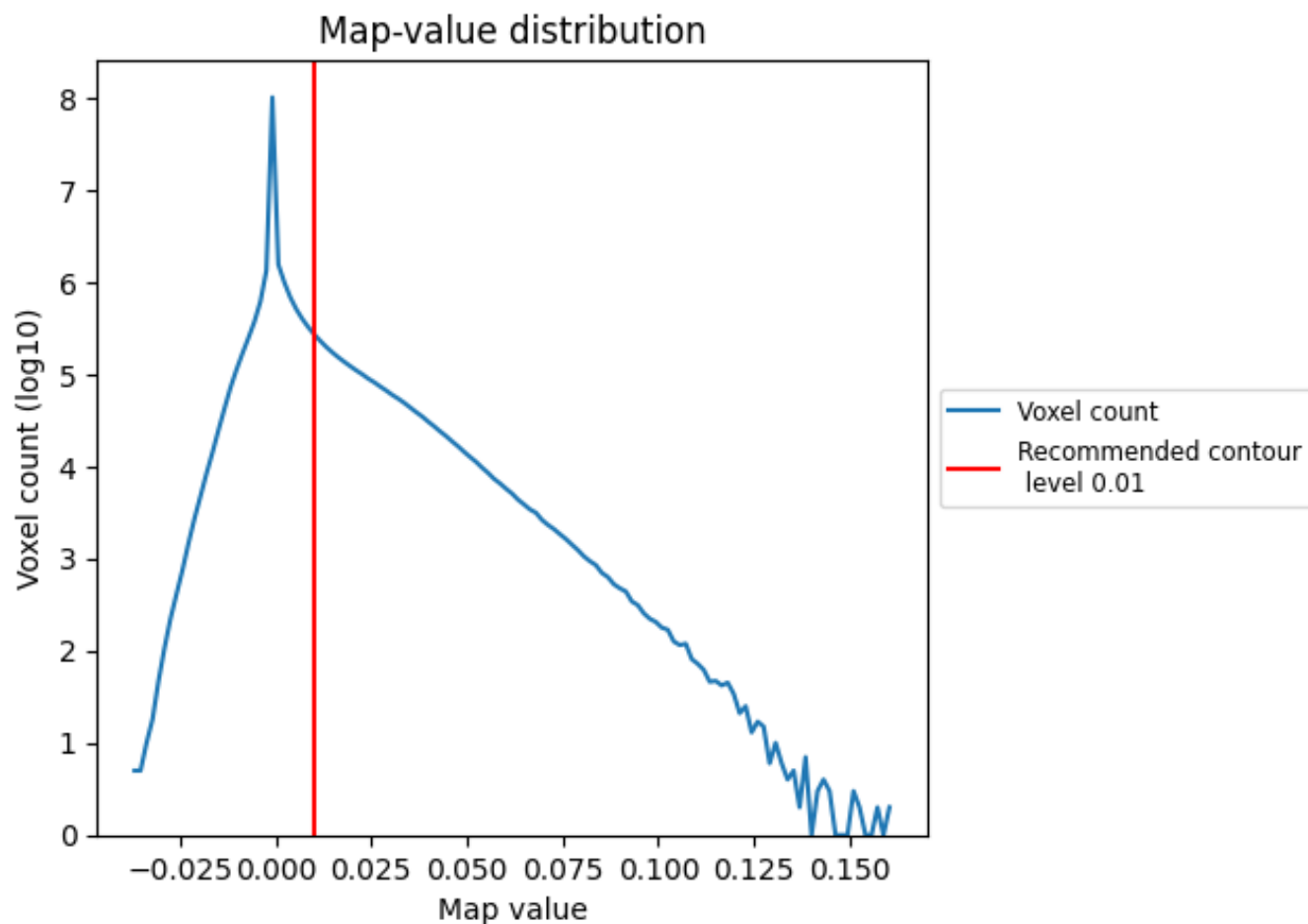
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

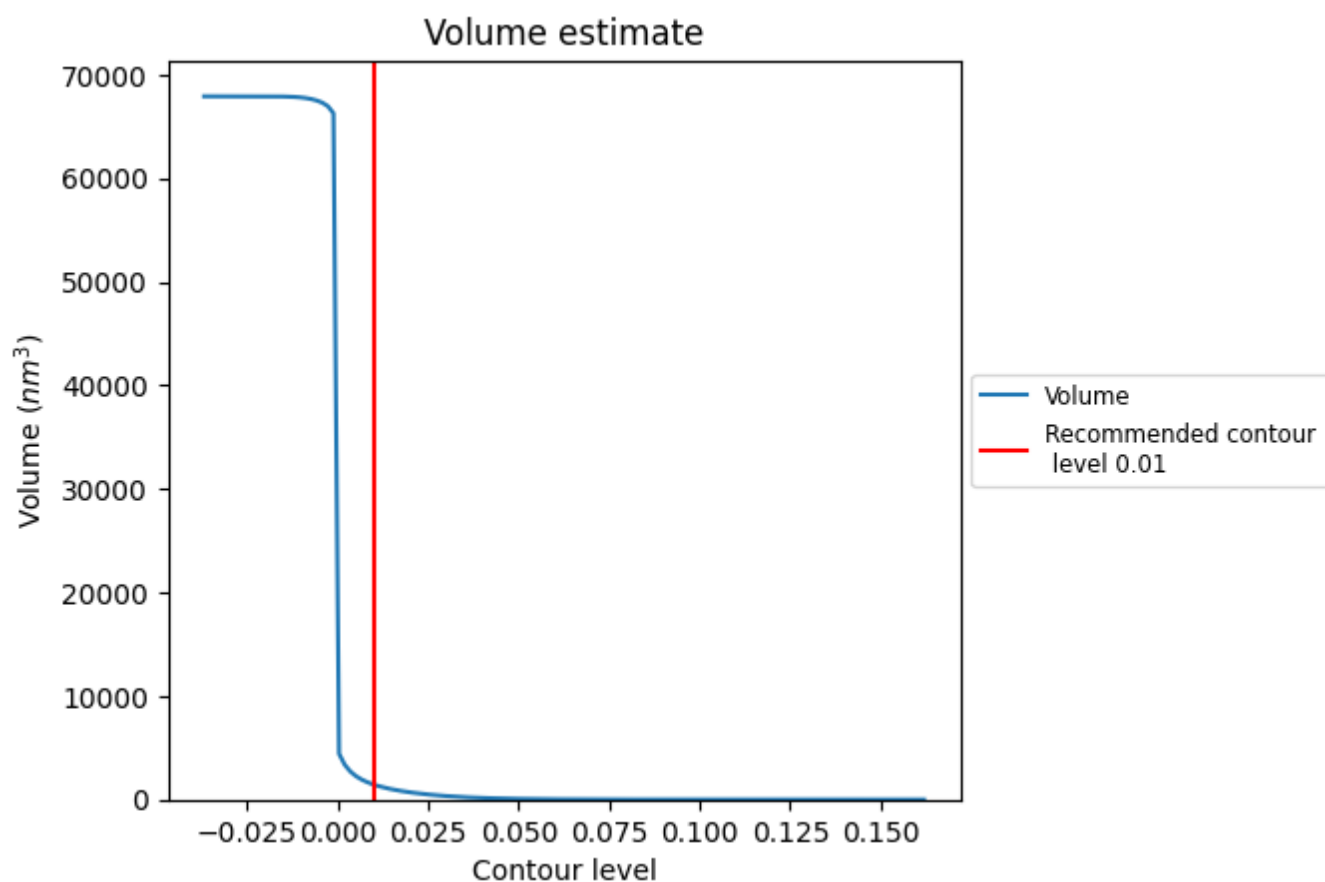
This section contains the results of statistical analysis of the map.

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.

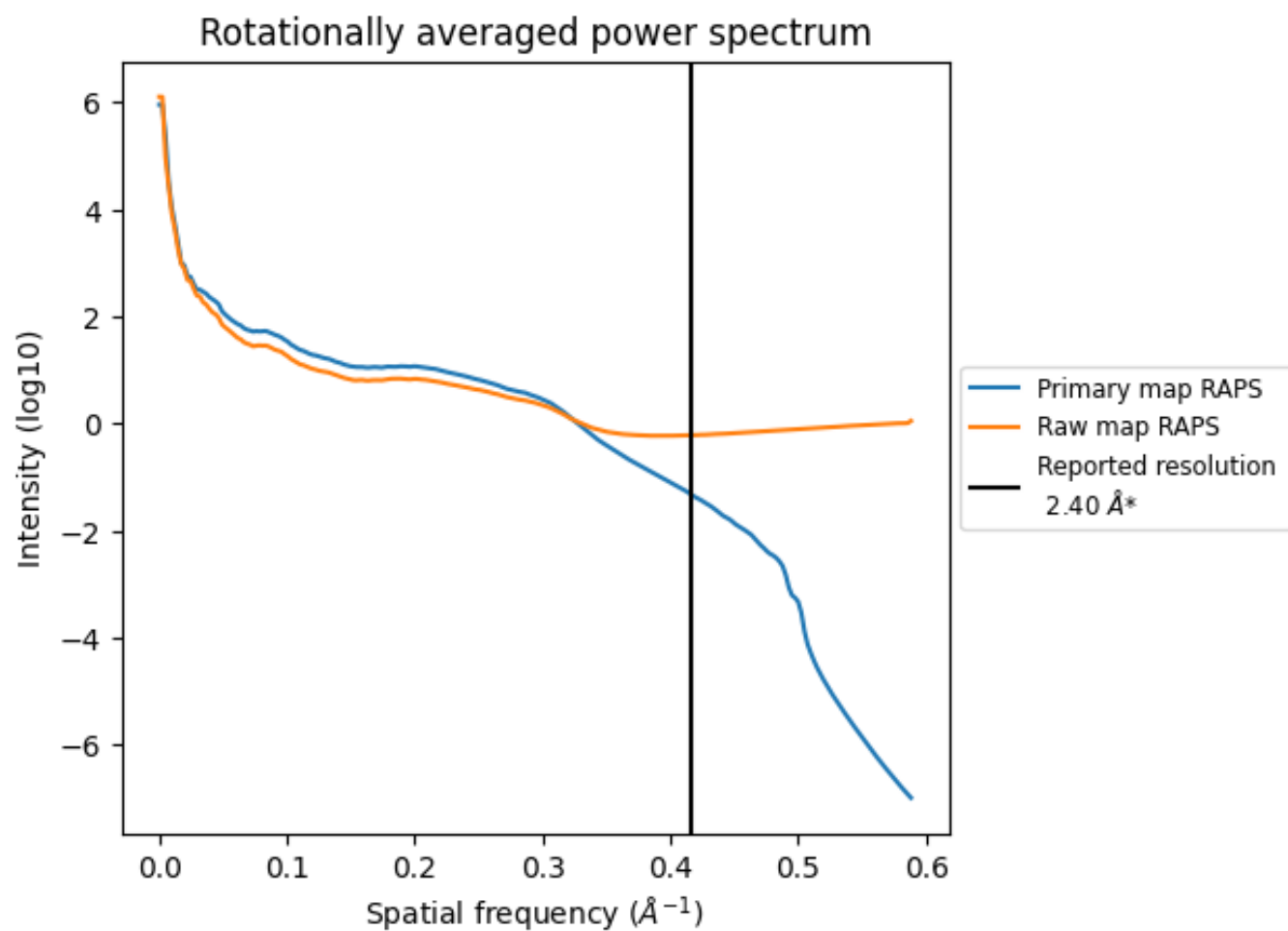
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1449 nm^3 ; this corresponds to an approximate mass of 1309 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

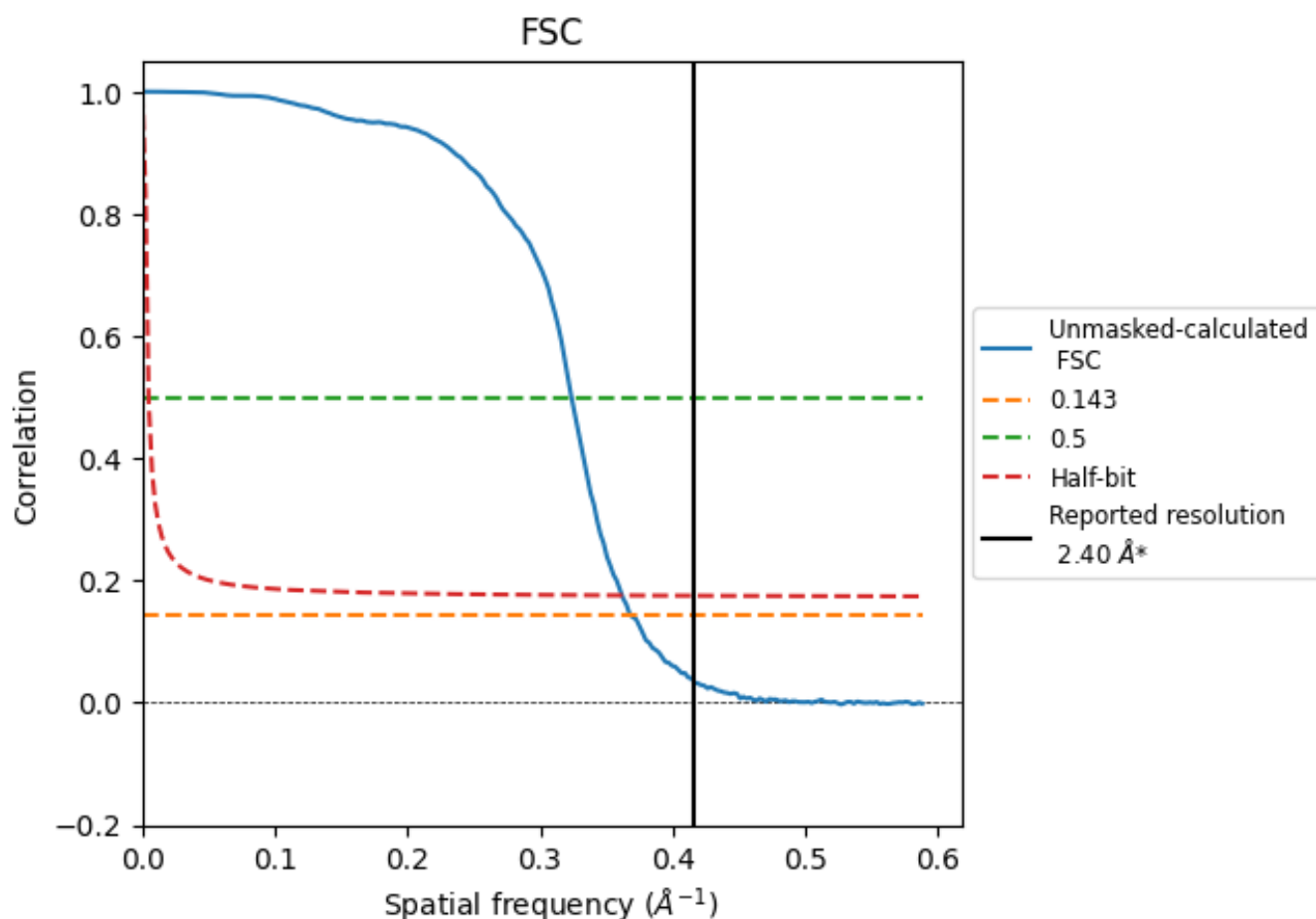


*Reported resolution corresponds to spatial frequency of $0.417 \text{ \AA}^{-1}$

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 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.71	3.09	2.76

*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 2.71 differs from the reported value 2.4 by more than 10 %

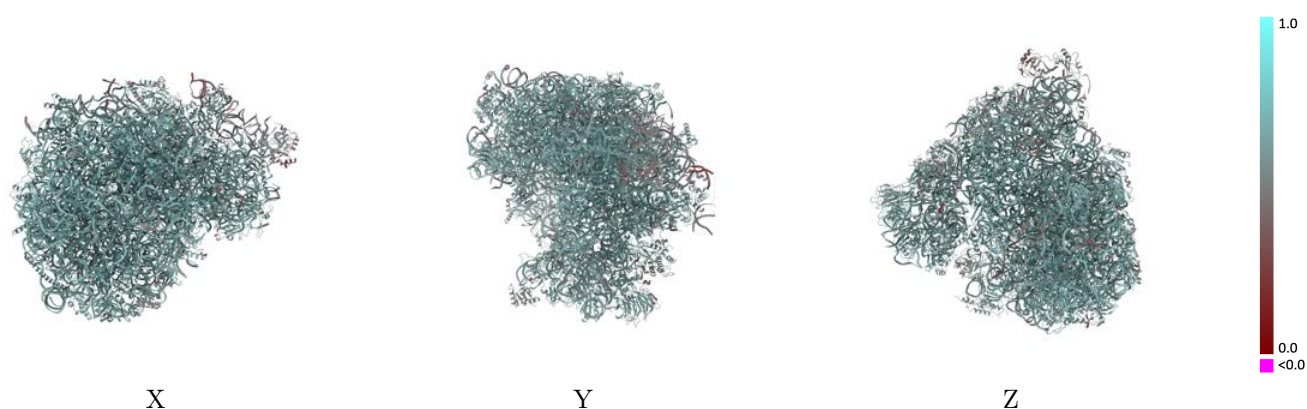
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17216 and PDB model 8OVJ. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)

This section was not generated.

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

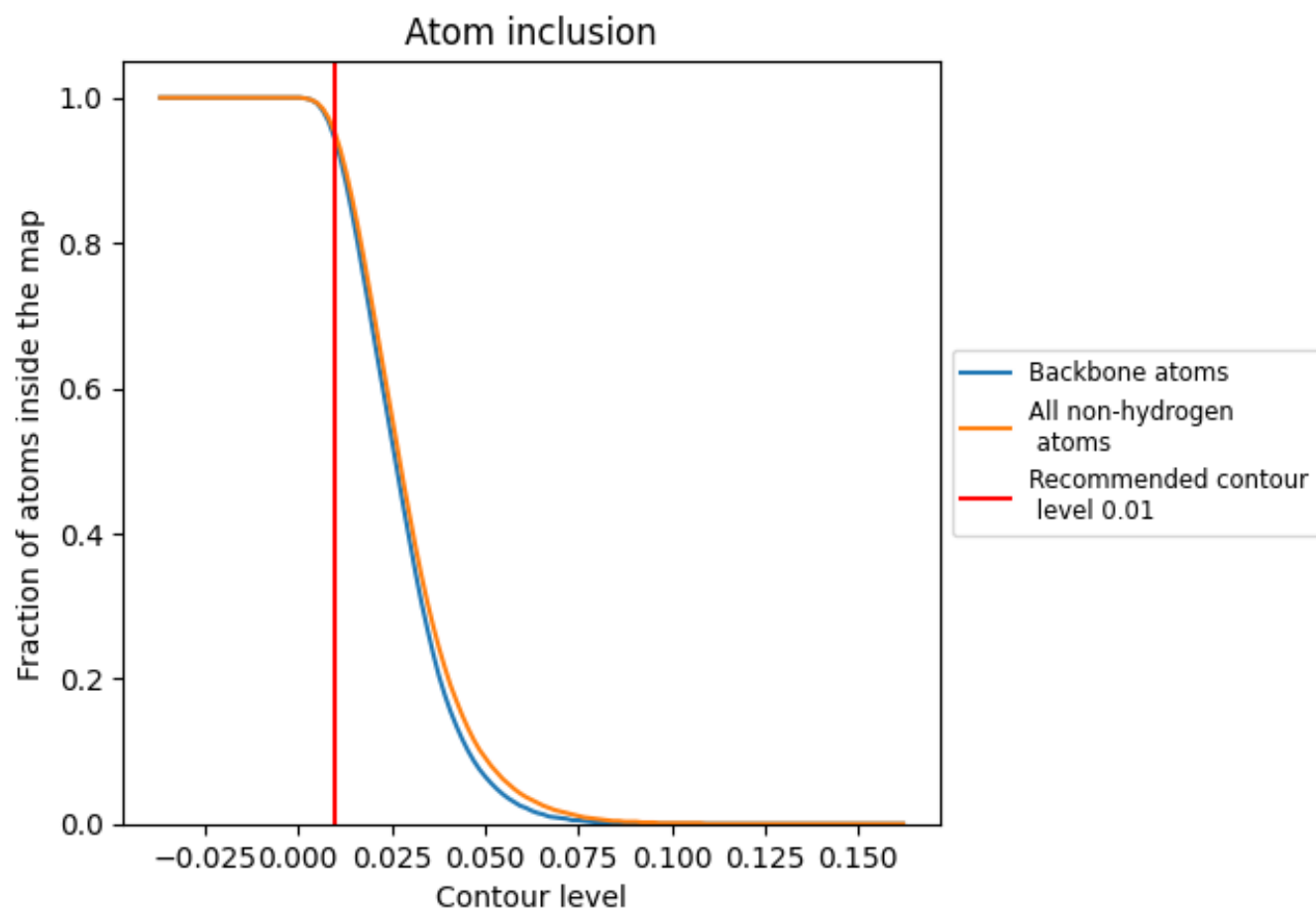


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.6300
1	 0.9760	 0.6460
2	 0.9730	 0.6410
3	 0.9530	 0.6210
4	 0.9780	 0.6420
5	 0.9610	 0.6280
6	 0.9320	 0.5920
7	 0.9750	 0.6410
8	 0.9880	 0.6130
A	 0.9740	 0.6870
B	 0.9720	 0.6620
C	 0.9710	 0.6600
D	 0.8890	 0.5650
E	 0.9170	 0.6220
F	 0.9300	 0.6190
G	 0.9510	 0.6370
H	 0.9740	 0.6590
I	 0.9360	 0.6530
J	 0.9310	 0.6600
K	 0.9080	 0.6100
L	 0.9720	 0.6820
M	 0.9870	 0.6890
N	 0.8480	 0.6160
O	 0.9190	 0.6020
P	 0.9680	 0.6760
Q	 0.9550	 0.6320
R	 0.9640	 0.6550
S	 0.9290	 0.6460
S1	 0.9800	 0.6180
S4	 0.7190	 0.5120
SA	 0.9690	 0.6230
SB	 0.9180	 0.5410
SC	 0.8590	 0.5970
SD	 0.9630	 0.6070
SE	 0.9530	 0.6210



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Chain	Atom inclusion	Q-score
SF	 0.9700	 0.6120
SG	 0.9400	 0.5980
SH	 0.9370	 0.6230
SI	 0.9780	 0.5940
SJ	 0.9780	 0.6440
SK	 0.9520	 0.6260
SL	 0.9500	 0.6350
SM	 0.8380	 0.6040
SN	 0.8430	 0.6080
SO	 0.9830	 0.6400
SP	 0.9720	 0.6380
SQ	 0.3390	 0.4980
SR	 0.8580	 0.6170
SS	 0.9690	 0.6400
ST	 0.9710	 0.6440
SU	 0.9630	 0.6440
SV	 0.8560	 0.5720
SW	 0.8410	 0.6140
SX	 0.9520	 0.6330
SY	 0.9430	 0.5800
SZ	 0.9670	 0.6030
Sa	 0.9190	 0.6070
Sb	 0.9900	 0.6450
Sc	 0.9450	 0.6090
Sd	 0.9380	 0.6000
Se	 0.9470	 0.5860
Sg	 0.8060	 0.5900
Sh	 0.5700	 0.4520
T	 0.9670	 0.6780
U	 0.6730	 0.5720
V	 0.9380	 0.6530
W	 0.9390	 0.6420
X	 0.9400	 0.6510
Y	 0.9190	 0.6200
Z	 0.9370	 0.6470
a	 0.9160	 0.6270
b	 0.9320	 0.6620
c	 0.9450	 0.6620
d	 0.8940	 0.6260
e	 0.8630	 0.6180
f	 0.9530	 0.6730
g	 0.9270	 0.6550

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Chain	Atom inclusion	Q-score
h	 0.8590	 0.6190
i	 0.8860	 0.6240
j	 0.9890	 0.6850
k	 0.8240	 0.6040
l	 0.9580	 0.6720
m	 0.8210	 0.6060
n	 0.9630	 0.6610
o	 0.9470	 0.6630
p	 0.9050	 0.6450