



wwPDB EM Validation Summary Report ⓘ

Feb 20, 2025 – 04:00 PM EST

PDB ID : 7XNY
EMDB ID : EMD-33330
Title : High resolution cry-EM structure of the human 80S ribosome from
SNORD127+/- Kasumi-1 cells
Authors : Cheng, J.; Beckmann, R.
Deposited on : 2022-04-30
Resolution : 2.50 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:

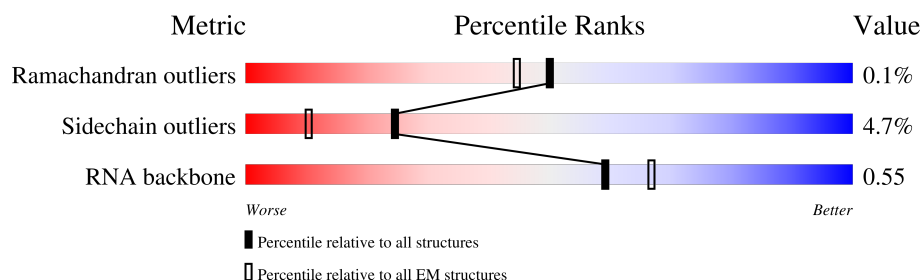
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

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 2.50 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.



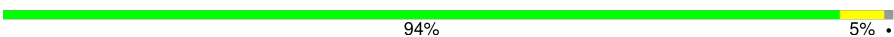
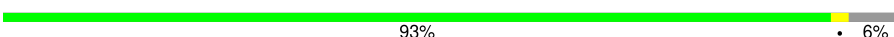

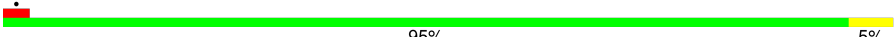




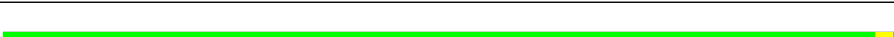


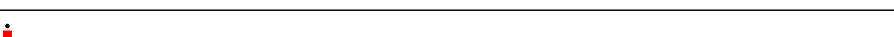
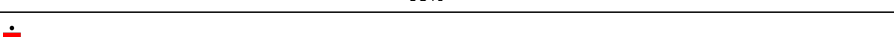
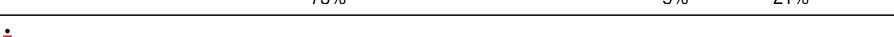



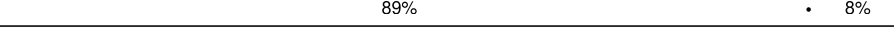
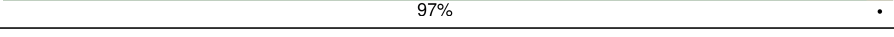
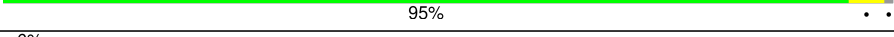





The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment 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	L1	5070	
2	L2	120	
3	L3	156	
4	LA	257	
5	LB	403	
6	LC	427	
7	LD	297	
8	LE	288	

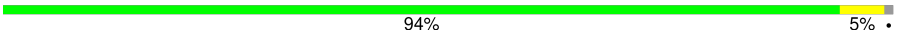

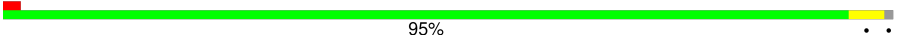
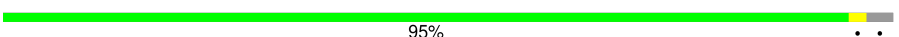






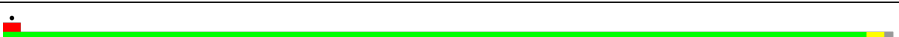


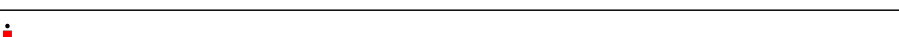
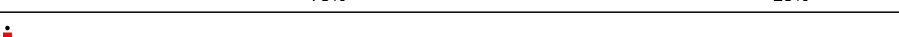
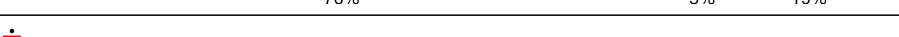

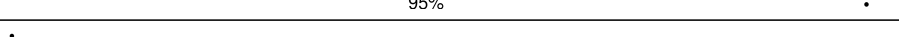

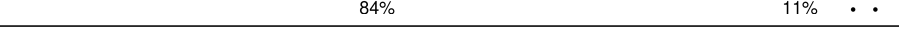
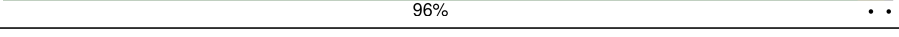




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Mol	Chain	Length	Quality of chain
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	135	
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	


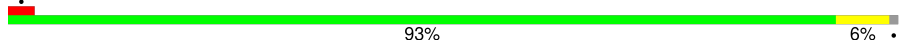
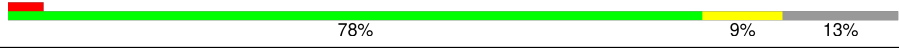
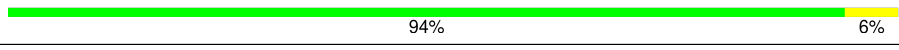
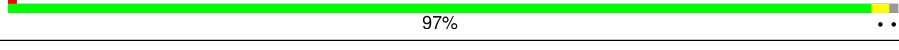


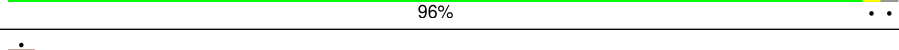
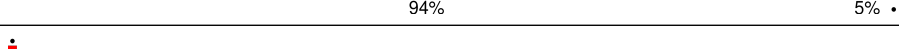
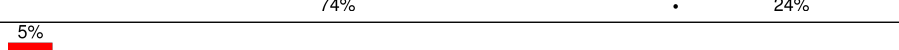

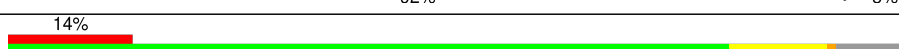


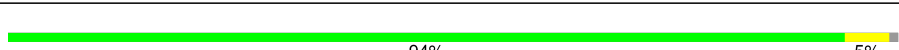


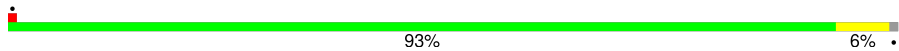
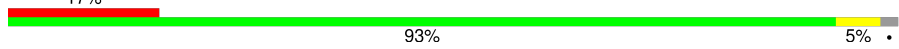


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Mol	Chain	Length	Quality of chain
34	Lf	110	
35	Lg	117	
36	Lh	123	
37	Li	105	
38	Lj	97	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	
46	S2	1869	
47	SA	295	
48	SB	264	
49	SD	243	
50	SE	263	
51	SF	204	
52	SH	194	
53	SI	208	
54	SK	165	
55	SL	158	
56	SP	145	
57	SQ	146	
58	SR	135	

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Mol	Chain	Length	Quality of chain
59	SS	152	
60	ST	145	
61	SU	119	
62	SV	83	
63	SX	143	
64	Sa	115	
65	Sc	69	
66	Sd	56	
67	Sg	317	
68	SC	293	
69	SG	249	
70	SJ	194	
71	SM	132	
72	SN	151	
73	SO	151	
74	SW	130	
75	SY	133	
76	SZ	125	
77	Sb	84	
78	Se	59	
79	Sf	156	

2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 216242 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 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	3773	Total	C	N	O	P	0	0
			80211	35727	14590	26122	3772		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	156	Total	C	N	O	P	0	0
			3316	1482	585	1094	155		

- Molecule 4 is a protein called 60S ribosomal protein L8.

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

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	365	Total	C	N	O	S	0	0
			2908	1829	580	486	13		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	220	Total	C	N	O	S	0	0
			1765	1136	334	291	4		

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	227	Total	C	N	O	S	0	0
			1835	1171	353	307	4		

- Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 12 is a protein called Ribosomal protein L10 isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	202	Total	C	N	O	S	0	0
			1639	1041	316	269	13		

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	169	Total	C	N	O	S	0	0
			1353	856	253	238	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 18 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 22 is a protein called 60S ribosomal protein L21.

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

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 24 is a protein called 60S ribosomal protein L23.

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

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	124	Total	C	N	O	S	0	0
			1015	634	207	170	4		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

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

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 32 is a protein called 60S ribosomal protein L31.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 35 is a protein called 60S ribosomal protein L34.

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

- Molecule 36 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	103	Total	C	N	O	S	0	0
			843	529	172	136	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 46 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S2	1740	Total	C	N	O	P	0	0
			36958	16514	6600	12105	1739		

- Molecule 47 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SA	222	Total	C	N	O	S	0	0
			1747	1109	306	324	8		

- Molecule 48 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 49 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 50 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 51 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SF	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 52 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 53 is a protein called 40S ribosomal protein S8.

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

- Molecule 54 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 55 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SL	144	Total	C	N	O	S	0	0
			1182	752	224	200	6		

- Molecule 56 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SP	127	Total	C	N	O	S	0	0
			1045	663	198	177	7		

- Molecule 57 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 58 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 59 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 60 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 61 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 62 is a protein called 40S ribosomal protein S21.

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

- Molecule 63 is a protein called 40S ribosomal protein S23.

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

- Molecule 64 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 65 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 66 is a protein called 40S ribosomal protein S29.

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

- Molecule 67 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 68 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 69 is a protein called 40S ribosomal protein S6.

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

- Molecule 70 is a protein called 40S ribosomal protein S9.

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

- Molecule 71 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 72 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 73 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 74 is a protein called 40S ribosomal protein S15a.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SY	125	Total	C	N	O	S	0	0
			1022	645	200	172	5		

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

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

- Molecule 77 is a protein called 40S ribosomal protein S27.

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

- Molecule 78 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 79 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sf	61	Total	C	N	O	S	0	0
			497	312	94	84	7		

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	L1	264	Total	Mg	0
			264	264	
80	L2	3	Total	Mg	0
			3	3	
80	L3	5	Total	Mg	0
			5	5	
80	LA	1	Total	Mg	0
			1	1	
80	LC	2	Total	Mg	0
			2	2	
80	LN	1	Total	Mg	0
			1	1	
80	LP	1	Total	Mg	0
			1	1	
80	LV	1	Total	Mg	0
			1	1	
80	Le	2	Total	Mg	0
			2	2	
80	Lf	1	Total	Mg	0
			1	1	
80	Lg	1	Total	Mg	0
			1	1	
80	Lo	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
80	S2	134	Total 134	Mg 134	0
80	ST	1	Total 1	Mg 1	0
80	Sd	1	Total 1	Mg 1	0
80	SG	1	Total 1	Mg 1	0
80	SJ	1	Total 1	Mg 1	0

- Molecule 81 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
81	L1	12	Total 12	K 12	0

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	Lg	1	Total 1	Zn 1	0
82	Lj	1	Total 1	Zn 1	0
82	Lm	1	Total 1	Zn 1	0
82	Lo	1	Total 1	Zn 1	0
82	Lp	1	Total 1	Zn 1	0
82	Sa	1	Total 1	Zn 1	0
82	Sd	1	Total 1	Zn 1	0
82	Sb	1	Total 1	Zn 1	0
82	Sf	1	Total 1	Zn 1	0

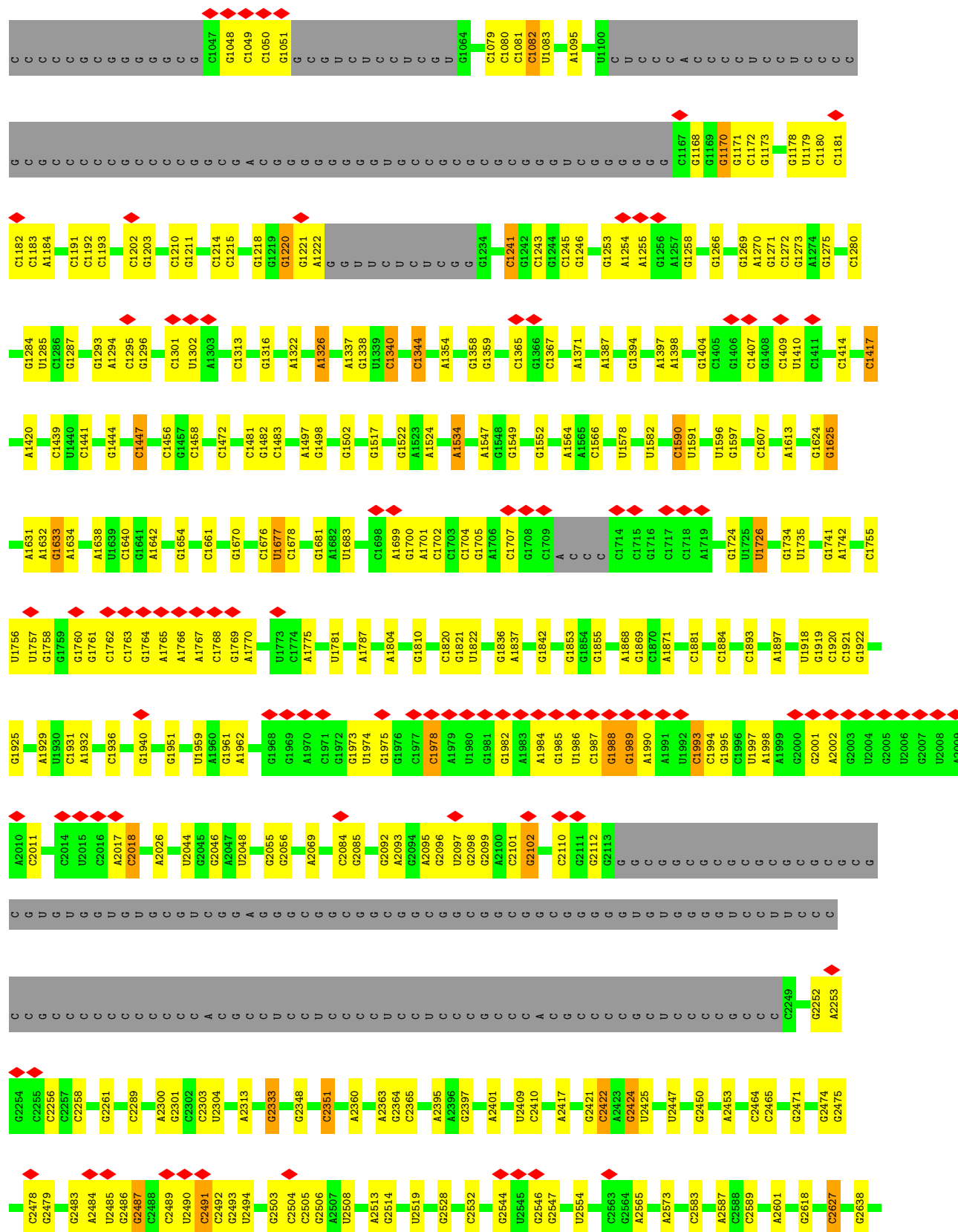
- Molecule 83 is water.

Mol	Chain	Residues	Atoms	AltConf
83	L1	767	Total O 767 767	0
83	L2	3	Total O 3 3	0
83	L3	6	Total O 6 6	0
83	LA	8	Total O 8 8	0
83	LB	2	Total O 2 2	0
83	LC	8	Total O 8 8	0
83	LD	1	Total O 1 1	0
83	LF	2	Total O 2 2	0
83	LI	1	Total O 1 1	0
83	LL	1	Total O 1 1	0
83	LN	2	Total O 2 2	0
83	LP	1	Total O 1 1	0
83	LR	1	Total O 1 1	0
83	LX	1	Total O 1 1	0
83	LY	1	Total O 1 1	0
83	La	5	Total O 5 5	0
83	Lb	1	Total O 1 1	0
83	Le	4	Total O 4 4	0
83	Lg	1	Total O 1 1	0
83	Lj	4	Total O 4 4	0
83	Ll	1	Total O 1 1	0
83	Lo	3	Total O 3 3	0

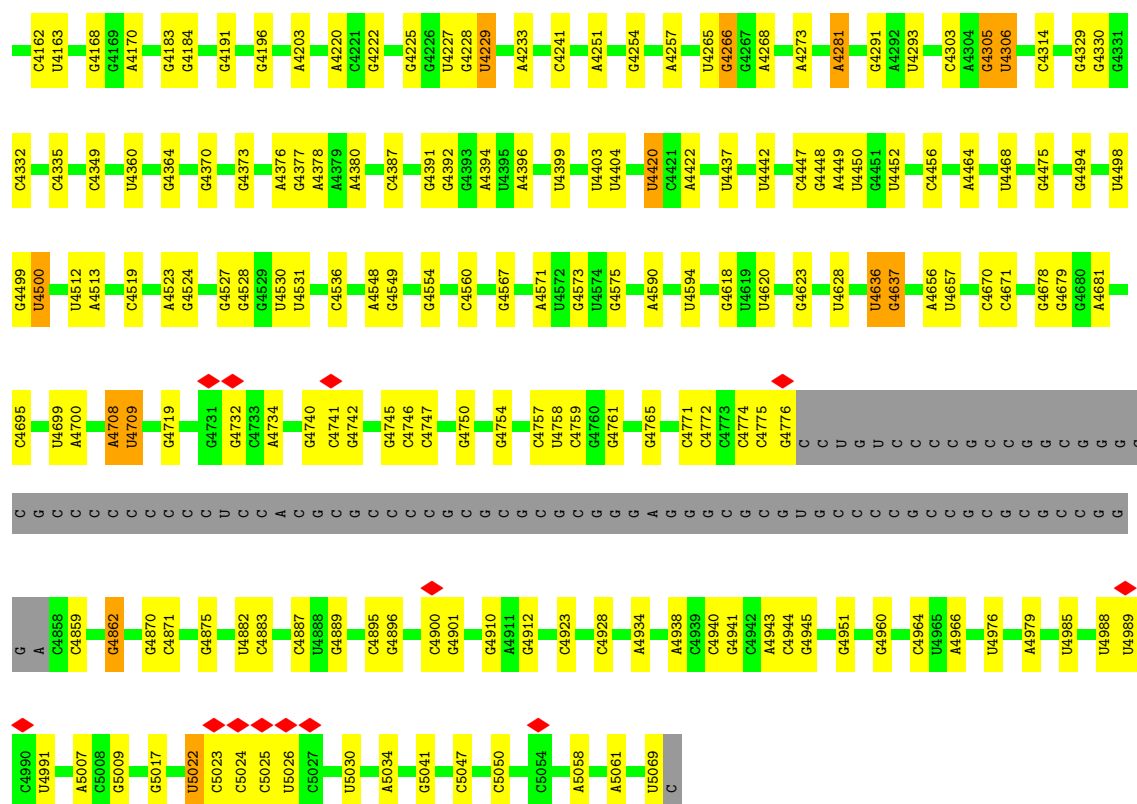
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Mol	Chain	Residues	Atoms		AltConf
83	S2	9	Total 9	O 9	0
83	SQ	1	Total 1	O 1	0
83	SX	1	Total 1	O 1	0
83	Sd	1	Total 1	O 1	0



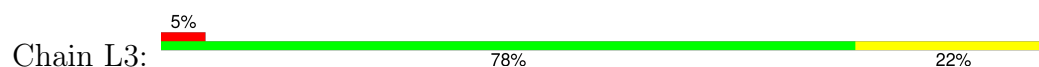




- Molecule 2: 5S rRNA



- Molecule 3: 5.8S rRNA



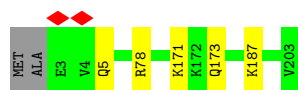
- Molecule 4: 60S ribosomal protein L8



- Molecule 5: 60S ribosomal protein L3

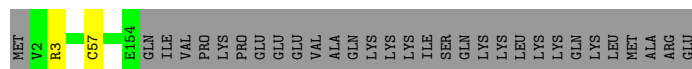


- Chain LO:  97%



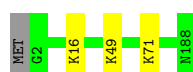
- Molecule 18: 60S ribosomal protein L17

Chain LP: 82% 17%



- Molecule 19: 60S ribosomal protein L18

Chain LQ: 98% ..



- Molecule 20: 60S ribosomal protein L19

Chain LR: 91% 5%



- Molecule 21: 60S ribosomal protein L18a

Chain LS: 97% .



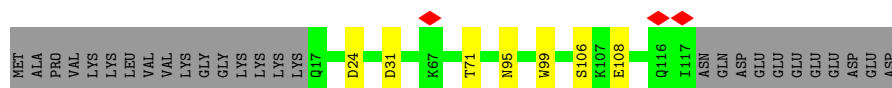
- Molecule 22: 60S ribosomal protein L21

Chain LT: 95% ..

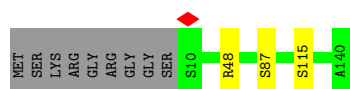


- Molecule 23: 60S ribosomal protein L22

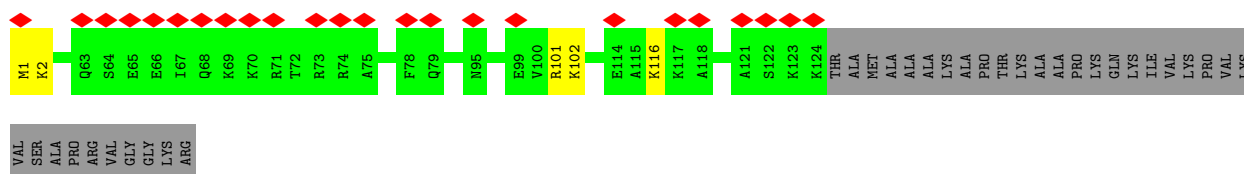
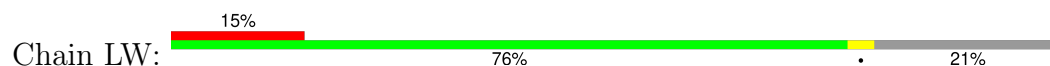
Chain LU: 73% 5% 21%



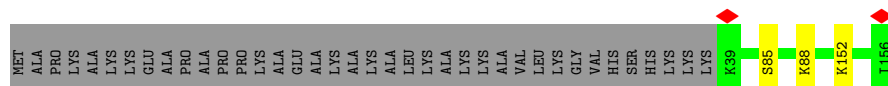
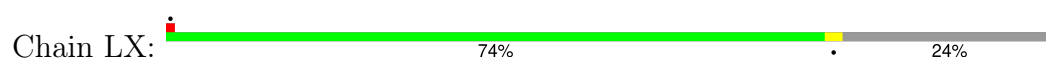
- Molecule 24: 60S ribosomal protein L23



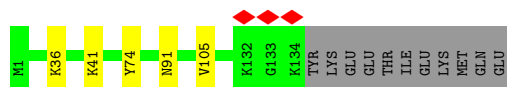
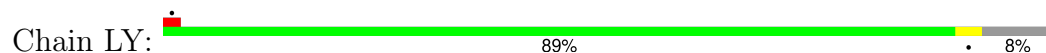
- Molecule 25: 60S ribosomal protein L24



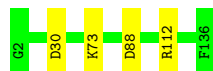
- Molecule 26: 60S ribosomal protein L23a



- Molecule 27: 60S ribosomal protein L26



- Molecule 28: 60S ribosomal protein L27

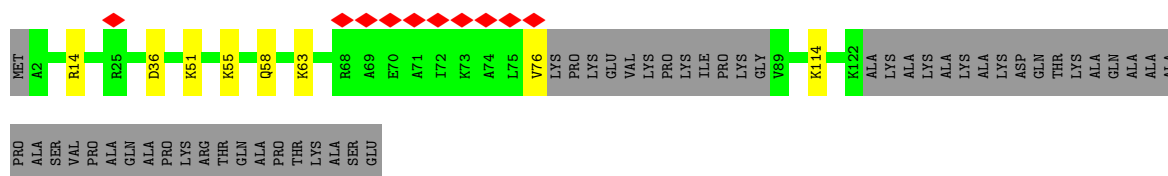


- Molecule 29: 60S ribosomal protein L27a

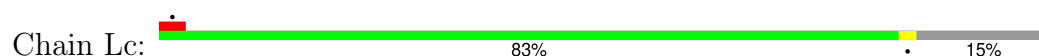


- Molecule 30: 60S ribosomal protein L29

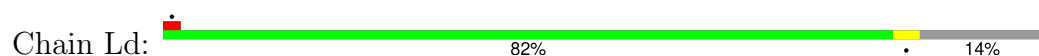




- Molecule 31: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L31



- Molecule 33: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L35a



- Molecule 35: 60S ribosomal protein L34



- Molecule 36: 60S ribosomal protein L35




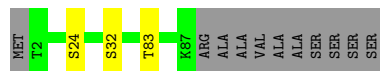
- Molecule 37: 60S ribosomal protein L36

Chain Li:  95%



- Molecule 38: 60S ribosomal protein L37

Chain Lj:  86% 11%



- Molecule 39: 60S ribosomal protein L38

Chain Lk:  90% 9%



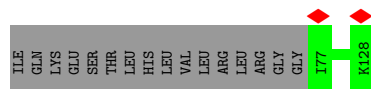
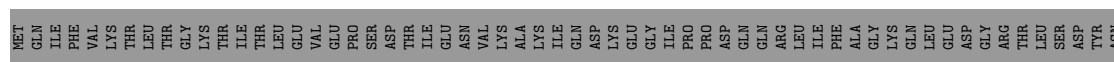
- Molecule 40: 60S ribosomal protein L39

Chain Ll:  92% 6%



- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Lm:  41% 59%



- Molecule 42: 60S ribosomal protein L41

Chain Ln:  88% 8%



- Molecule 43: 60S ribosomal protein L36a


Chain Lo:  93%

- Molecule 50: 40S ribosomal protein S4, X isoform

Chain SE:  95%




- Molecule 51: 40S ribosomal protein S5

Chain SF:  86% 10%



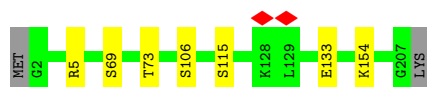
- Molecule 52: 40S ribosomal protein S7

Chain SH:  84% 11%



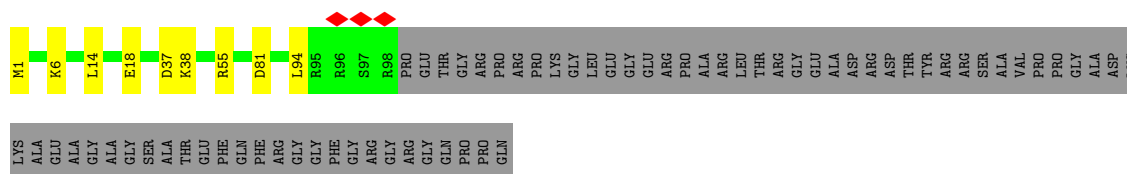
- Molecule 53: 40S ribosomal protein S8

Chain SI:  96%




- Molecule 54: 40S ribosomal protein S10

Chain SK:  54% 5% 41%

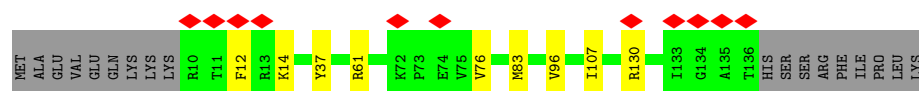
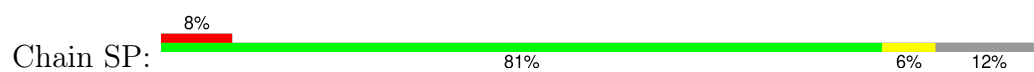


- Molecule 55: 40S ribosomal protein S11

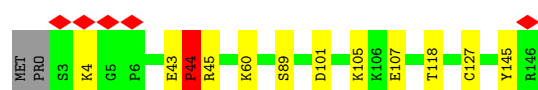
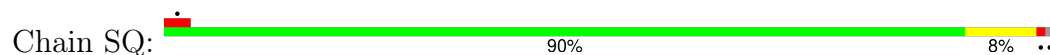
Chain SL:  86% 5% 9%



- Molecule 56: 40S ribosomal protein S15



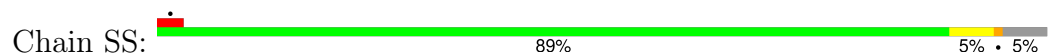
- Molecule 57: 40S ribosomal protein S16



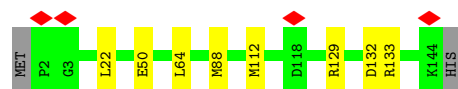
- Molecule 58: 40S ribosomal protein S17



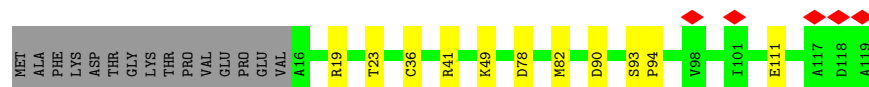
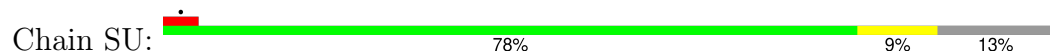
- Molecule 59: 40S ribosomal protein S18



- Molecule 60: 40S ribosomal protein S19




- Molecule 61: 40S ribosomal protein S20

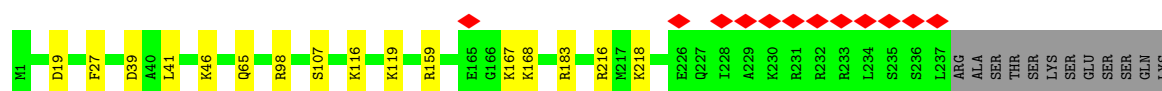


- Molecule 62: 40S ribosomal protein S21



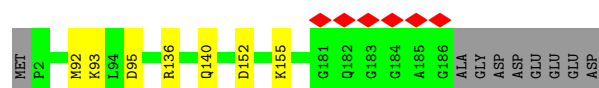
- Molecule 69: 40S ribosomal protein S6

Chain SG:  5% 89% 6% 5%




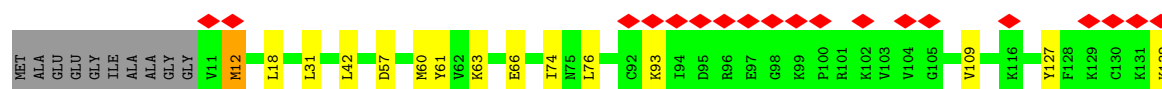
- Molecule 70: 40S ribosomal protein S9

Chain SJ:  92% 5%



- Molecule 71: 40S ribosomal protein S12

Chain SM:  14% 81% 11% 8%




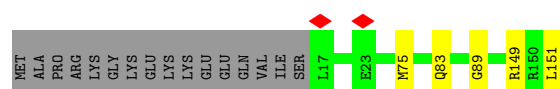
- Molecule 72: 40S ribosomal protein S13

Chain SN:  95%



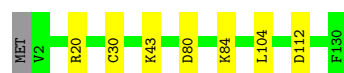
- Molecule 73: 40S ribosomal protein S14

Chain SO:  86% 11%



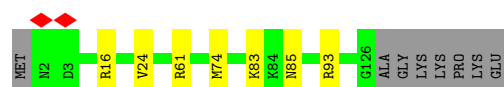
- Molecule 74: 40S ribosomal protein S15a

Chain SW:  94% 5%

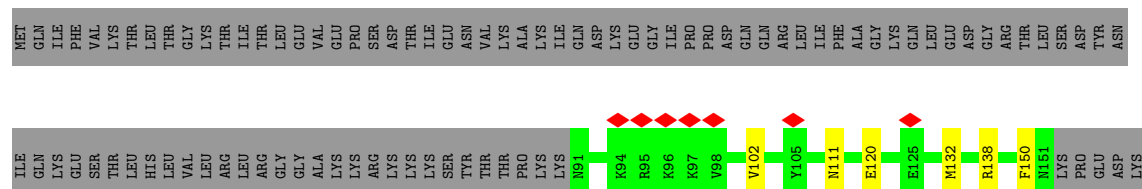


- Molecule 75: 40S ribosomal protein S24

Chain SY:  89% 5% 6%



- Chain SZ: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114446	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.785	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	444.78, 444.78, 444.78	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.059, 1.059, 1.059	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, 5MU, M7A, UY1, 4AC, MA6, B8H, 1MA, OMU, K, PSU, 6MZ, ZN, B8T, 5MC, MLZ, UR3, OMG, JMH, MG, OMC, 2MG, A2M

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	L1	0.52	1/87525 (0.0%)	1.01	275/136449 (0.2%)
2	L2	0.46	0/2858	0.92	2/4455 (0.0%)
3	L3	0.50	0/3653	0.93	1/5691 (0.0%)
4	LA	0.37	0/1936	0.69	0/2596
5	LB	0.32	0/3306	0.60	0/4424
6	LC	0.31	0/2962	0.63	2/3977 (0.1%)
7	LD	0.30	0/2428	0.56	0/3252
8	LE	0.30	0/1799	0.64	0/2414
9	LF	0.33	0/1905	0.60	0/2539
10	LG	0.29	0/1866	0.58	0/2511
11	LH	0.31	0/1537	0.59	1/2066 (0.0%)
12	LI	0.33	0/1677	0.60	0/2237
13	LJ	0.30	0/1376	0.61	0/1840
14	LL	0.30	0/1732	0.62	0/2315
15	LM	0.31	0/1161	0.58	0/1554
16	LN	0.34	0/1746	0.68	2/2338 (0.1%)
17	LO	0.32	0/1682	0.59	0/2250
18	LP	0.30	0/1268	0.59	0/1701
19	LQ	0.32	0/1537	0.65	0/2052
20	LR	0.30	0/1582	0.61	1/2091 (0.0%)
21	LS	0.33	0/1501	0.59	0/2013
22	LT	0.31	0/1326	0.56	0/1770
23	LU	0.36	0/839	0.70	1/1126 (0.1%)
24	LV	0.32	0/993	0.60	0/1332
25	LW	0.31	0/1030	0.60	0/1364
26	LX	0.28	0/984	0.56	0/1323
27	LY	0.30	0/1132	0.61	0/1504
28	LZ	0.33	0/1130	0.63	2/1507 (0.1%)
29	La	0.31	0/1191	0.61	0/1591
30	Lb	0.29	0/889	0.64	1/1175 (0.1%)
31	Lc	0.33	0/774	0.55	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.30	0/903	0.61	0/1216
33	Le	0.32	0/1071	0.65	0/1429
34	Lf	0.35	0/895	0.67	0/1198
35	Lg	0.32	0/916	0.63	0/1220
36	Lh	0.30	0/1023	0.58	0/1351
37	Li	0.28	0/843	0.61	0/1115
38	Lj	0.34	0/720	0.68	0/952
39	Lk	0.29	0/575	0.59	0/761
40	Ll	0.31	0/454	0.69	0/599
41	Lm	0.27	0/435	0.60	0/575
42	Ln	0.31	0/231	0.74	0/294
43	Lo	0.28	0/845	0.59	0/1113
44	Lp	0.32	0/718	0.58	0/953
45	Lr	0.31	0/1017	0.64	1/1364 (0.1%)
46	S2	0.42	0/39987	0.97	102/62288 (0.2%)
47	SA	0.30	0/1784	0.56	1/2424 (0.0%)
48	SB	0.28	0/1765	0.58	1/2362 (0.0%)
49	SD	0.32	0/1793	0.64	3/2414 (0.1%)
50	SE	0.29	0/2118	0.59	0/2849
51	SF	0.30	0/1481	0.56	0/1988
52	SH	0.37	0/1519	0.63	1/2033 (0.0%)
53	SI	0.31	0/1715	0.62	0/2287
54	SK	0.35	0/851	0.65	0/1147
55	SL	0.31	0/1202	0.60	0/1606
56	SP	0.30	0/1065	0.67	1/1423 (0.1%)
57	SQ	0.31	0/1160	0.72	3/1553 (0.2%)
58	SR	0.30	0/1105	0.72	2/1484 (0.1%)
59	SS	0.28	0/1216	0.73	5/1628 (0.3%)
60	ST	0.29	0/1131	0.62	1/1515 (0.1%)
61	SU	0.31	0/831	0.67	0/1115
62	SV	0.28	0/643	0.52	0/860
63	SX	0.30	0/1116	0.59	0/1490
64	Sa	0.30	0/836	0.61	0/1121
65	Sc	0.28	0/508	0.66	0/680
66	Sd	0.31	0/470	0.75	0/623
67	Sg	0.27	0/2493	0.61	1/3394 (0.0%)
68	SC	0.31	0/1762	0.57	1/2381 (0.0%)
69	SG	0.30	0/1946	0.62	1/2590 (0.0%)
70	SJ	0.32	0/1550	0.63	0/2069
71	SM	0.32	0/950	0.77	5/1275 (0.4%)
72	SN	0.31	0/1232	0.56	0/1656
73	SO	0.29	0/1023	0.65	0/1372
74	SW	0.31	0/1051	0.60	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SY	0.31	0/1039	0.58	0/1381
76	SZ	0.26	0/604	0.60	0/810
77	Sb	0.29	0/665	0.59	0/891
78	Se	0.28	0/465	0.61	0/612
79	Sf	0.27	0/507	0.61	0/673
All	All	0.42	1/227554 (0.0%)	0.87	417/334035 (0.1%)

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
61	SU	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	3646	A	N7-C5	-5.42	1.36	1.39

The worst 5 of 417 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1772	C	N1-C2-O2	13.79	127.17	118.90
46	S2	501	C	N1-C2-O2	13.05	126.73	118.90
46	S2	1772	C	N3-C2-O2	-12.99	112.81	121.90
46	S2	501	C	C2-N1-C1'	12.71	132.78	118.80
1	L1	906	C	N3-C2-O2	-12.46	113.18	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
61	SU	93	SER	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/257 (96%)	233 (95%)	13 (5%)	0	100	100
5	LB	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
6	LC	363/427 (85%)	355 (98%)	8 (2%)	0	100	100
7	LD	291/297 (98%)	284 (98%)	7 (2%)	0	100	100
8	LE	214/288 (74%)	208 (97%)	6 (3%)	0	100	100
9	LF	223/248 (90%)	215 (96%)	8 (4%)	0	100	100
10	LG	223/266 (84%)	220 (99%)	3 (1%)	0	100	100
11	LH	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
12	LI	198/214 (92%)	192 (97%)	6 (3%)	0	100	100
13	LJ	167/178 (94%)	163 (98%)	4 (2%)	0	100	100
14	LL	208/211 (99%)	198 (95%)	10 (5%)	0	100	100
15	LM	137/215 (64%)	133 (97%)	4 (3%)	0	100	100
16	LN	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
17	LO	199/203 (98%)	199 (100%)	0	0	100	100
18	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
19	LQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
20	LR	185/196 (94%)	184 (100%)	1 (0%)	0	100	100
21	LS	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
22	LT	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
23	LU	99/128 (77%)	95 (96%)	4 (4%)	0	100	100
24	LV	129/140 (92%)	122 (95%)	7 (5%)	0	100	100
25	LW	122/157 (78%)	117 (96%)	5 (4%)	0	100	100
26	LX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
27	LY	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
28	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	La	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
30	Lb	105/159 (66%)	99 (94%)	6 (6%)	0	100	100
31	Lc	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
32	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
33	Le	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
34	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
35	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
36	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
38	Lj	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
39	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
40	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
41	Lm	50/128 (39%)	50 (100%)	0	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	100/106 (94%)	96 (96%)	4 (4%)	0	100	100
44	Lp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	Lr	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
47	SA	220/295 (75%)	216 (98%)	4 (2%)	0	100	100
48	SB	212/264 (80%)	207 (98%)	5 (2%)	0	100	100
49	SD	225/243 (93%)	218 (97%)	7 (3%)	0	100	100
50	SE	260/263 (99%)	255 (98%)	5 (2%)	0	100	100
51	SF	180/204 (88%)	173 (96%)	7 (4%)	0	100	100
52	SH	182/194 (94%)	162 (89%)	16 (9%)	4 (2%)	5	9
53	SI	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
54	SK	96/165 (58%)	92 (96%)	4 (4%)	0	100	100
55	SL	140/158 (89%)	132 (94%)	8 (6%)	0	100	100
56	SP	125/145 (86%)	124 (99%)	1 (1%)	0	100	100
57	SQ	142/146 (97%)	130 (92%)	11 (8%)	1 (1%)	19	35
58	SR	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
59	SS	143/152 (94%)	137 (96%)	6 (4%)	0	100	100
60	ST	141/145 (97%)	136 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	SU	102/119 (86%)	96 (94%)	5 (5%)	1 (1%)	13	25
62	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
63	SX	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
64	Sa	100/115 (87%)	97 (97%)	2 (2%)	1 (1%)	13	25
65	Sc	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
66	Sd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
67	Sg	311/317 (98%)	294 (94%)	17 (6%)	0	100	100
68	SC	220/293 (75%)	216 (98%)	4 (2%)	0	100	100
69	SG	235/249 (94%)	228 (97%)	7 (3%)	0	100	100
70	SJ	183/194 (94%)	176 (96%)	7 (4%)	0	100	100
71	SM	120/132 (91%)	111 (92%)	9 (8%)	0	100	100
72	SN	148/151 (98%)	148 (100%)	0	0	100	100
73	SO	133/151 (88%)	124 (93%)	8 (6%)	1 (1%)	16	31
74	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
75	SY	123/133 (92%)	121 (98%)	2 (2%)	0	100	100
76	SZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
77	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
78	Se	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
79	Sf	59/156 (38%)	55 (93%)	4 (7%)	0	100	100
All	All	11249/12687 (89%)	10882 (97%)	359 (3%)	8 (0%)	50	69

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	SH	34	SER
57	SQ	44	PRO
52	SH	11	PRO
52	SH	40	LEU
61	SU	94	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	
4	LA	190/199 (96%)	185 (97%)	5 (3%)	41	68
5	LB	348/349 (100%)	325 (93%)	23 (7%)	14	28
6	LC	304/348 (87%)	294 (97%)	10 (3%)	33	59
7	LD	246/250 (98%)	239 (97%)	7 (3%)	38	65
8	LE	194/252 (77%)	190 (98%)	4 (2%)	48	74
9	LF	194/215 (90%)	190 (98%)	4 (2%)	48	74
10	LG	196/223 (88%)	190 (97%)	6 (3%)	35	62
11	LH	169/171 (99%)	161 (95%)	8 (5%)	22	44
12	LI	172/181 (95%)	168 (98%)	4 (2%)	45	72
13	LJ	142/149 (95%)	136 (96%)	6 (4%)	25	49
14	LL	176/177 (99%)	166 (94%)	10 (6%)	17	35
15	LM	118/161 (73%)	112 (95%)	6 (5%)	20	40
16	LN	171/172 (99%)	167 (98%)	4 (2%)	45	72
17	LO	173/174 (99%)	168 (97%)	5 (3%)	37	64
18	LP	134/163 (82%)	132 (98%)	2 (2%)	60	82
19	LQ	164/165 (99%)	161 (98%)	3 (2%)	54	78
20	LR	166/175 (95%)	159 (96%)	7 (4%)	25	49
21	LS	157/157 (100%)	152 (97%)	5 (3%)	34	60
22	LT	139/140 (99%)	132 (95%)	7 (5%)	20	41
23	LU	91/115 (79%)	85 (93%)	6 (7%)	14	28
24	LV	101/107 (94%)	98 (97%)	3 (3%)	36	63
25	LW	103/126 (82%)	98 (95%)	5 (5%)	21	42
26	LX	106/133 (80%)	103 (97%)	3 (3%)	38	65
27	LY	124/135 (92%)	119 (96%)	5 (4%)	27	51
28	LZ	117/117 (100%)	115 (98%)	2 (2%)	56	79
29	La	120/121 (99%)	114 (95%)	6 (5%)	20	41
30	Lb	88/126 (70%)	81 (92%)	7 (8%)	10	20
31	Lc	83/97 (86%)	81 (98%)	2 (2%)	44	70
32	Ld	98/110 (89%)	94 (96%)	4 (4%)	26	50
33	Le	114/121 (94%)	113 (99%)	1 (1%)	75	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	Lf	88/89 (99%)	82 (93%)	6 (7%)	13	27
35	Lg	98/100 (98%)	93 (95%)	5 (5%)	20	40
36	Lh	109/110 (99%)	104 (95%)	5 (5%)	23	45
37	Li	86/89 (97%)	84 (98%)	2 (2%)	45	72
38	Lj	73/80 (91%)	70 (96%)	3 (4%)	26	50
39	Lk	64/65 (98%)	58 (91%)	6 (9%)	7	15
40	Ll	47/48 (98%)	44 (94%)	3 (6%)	14	30
41	Lm	48/116 (41%)	48 (100%)	0	100	100
42	Ln	23/24 (96%)	21 (91%)	2 (9%)	8	17
43	Lo	90/93 (97%)	86 (96%)	4 (4%)	24	47
44	Lp	74/75 (99%)	72 (97%)	2 (3%)	40	67
45	Lr	109/121 (90%)	103 (94%)	6 (6%)	18	37
47	SA	184/243 (76%)	177 (96%)	7 (4%)	28	53
48	SB	195/231 (84%)	183 (94%)	12 (6%)	15	31
49	SD	190/202 (94%)	180 (95%)	10 (5%)	19	38
50	SE	224/225 (100%)	213 (95%)	11 (5%)	21	42
51	SF	156/170 (92%)	147 (94%)	9 (6%)	17	34
52	SH	166/174 (95%)	146 (88%)	20 (12%)	4	8
53	SI	178/180 (99%)	171 (96%)	7 (4%)	27	52
54	SK	89/136 (65%)	80 (90%)	9 (10%)	6	12
55	SL	130/142 (92%)	122 (94%)	8 (6%)	15	31
56	SP	113/130 (87%)	105 (93%)	8 (7%)	12	25
57	SQ	119/121 (98%)	108 (91%)	11 (9%)	7	15
58	SR	122/122 (100%)	119 (98%)	3 (2%)	42	69
59	SS	126/132 (96%)	120 (95%)	6 (5%)	21	43
60	ST	113/115 (98%)	106 (94%)	7 (6%)	15	31
61	SU	94/107 (88%)	85 (90%)	9 (10%)	7	14
62	SV	67/67 (100%)	62 (92%)	5 (8%)	11	23
63	SX	113/115 (98%)	110 (97%)	3 (3%)	40	67
64	Sa	89/98 (91%)	88 (99%)	1 (1%)	70	87
65	Sc	57/62 (92%)	54 (95%)	3 (5%)	19	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	Sd	48/49 (98%)	47 (98%)	1 (2%)	48	74
67	Sg	272/275 (99%)	258 (95%)	14 (5%)	20	40
68	SC	188/225 (84%)	182 (97%)	6 (3%)	34	60
69	SG	207/218 (95%)	192 (93%)	15 (7%)	12	24
70	SJ	161/168 (96%)	154 (96%)	7 (4%)	25	48
71	SM	102/108 (94%)	91 (89%)	11 (11%)	5	11
72	SN	130/131 (99%)	124 (95%)	6 (5%)	23	45
73	SO	105/119 (88%)	101 (96%)	4 (4%)	28	53
74	SW	112/113 (99%)	105 (94%)	7 (6%)	15	30
75	SY	109/115 (95%)	102 (94%)	7 (6%)	14	30
76	SZ	66/103 (64%)	62 (94%)	4 (6%)	15	32
77	Sb	75/76 (99%)	70 (93%)	5 (7%)	13	28
78	Se	47/48 (98%)	44 (94%)	3 (6%)	14	30
79	Sf	54/140 (39%)	48 (89%)	6 (11%)	5	10
All	All	9808/10799 (91%)	9349 (95%)	459 (5%)	24	44

5 of 459 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	SB	224	GLU
76	SZ	64	ASN
53	SI	106	SER
75	SY	83	LYS
70	SJ	92	MET

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

Mol	Chain	Res	Type
52	SH	12	ASN
57	SQ	77	HIS
59	SS	76	GLN
57	SQ	114	GLN
17	LO	63	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	3701/5070 (72%)	720 (19%)	11 (0%)
2	L2	119/120 (99%)	11 (9%)	0
3	L3	155/156 (99%)	31 (20%)	0
46	S2	1708/1869 (91%)	328 (19%)	9 (0%)
All	All	5683/7215 (78%)	1090 (19%)	20 (0%)

5 of 1090 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	15	A
1	L1	39	A
1	L1	42	A
1	L1	48	G
1	L1	56	A

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	S2	688	U
46	S2	1434	C
46	S2	1520	G
46	S2	1497	G
1	L1	2760	G

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

143 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	$\# Z > 2$
1	OMG	L1	4499	1	19,26,27	2.50	8 (42%)	21,38,41	1.43	4 (19%)
43	MLZ	Lo	53	43	8,9,10	0.73	0	4,9,11	0.66	0
1	5MC	L1	4335	1	19,22,23	3.78	8 (42%)	26,32,35	1.04	2 (7%)
46	PSU	S2	119	46	18,21,22	1.04	1 (5%)	21,30,33	1.78	4 (19%)
1	OMU	L1	4227	1	19,22,23	2.94	7 (36%)	25,31,34	1.85	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	A2M	S2	159	46	18,25,26	4.45	7 (38%)	20,36,39	3.33	3 (15%)
1	OMG	L1	2424	1	19,26,27	2.49	8 (42%)	21,38,41	1.42	4 (19%)
1	OMG	L1	4637	1	19,26,27	2.41	8 (42%)	21,38,41	1.37	3 (14%)
46	OMU	S2	172	46	19,22,23	2.94	6 (31%)	25,31,34	1.87	5 (20%)
1	OMC	L1	2351	1,80	19,22,23	2.97	8 (42%)	25,31,34	1.20	3 (12%)
46	M7A	S2	1806	46	19,25,26	1.83	4 (21%)	25,37,40	4.09	8 (32%)
1	5MC	L1	3782	1,80	19,22,23	3.69	8 (42%)	26,32,35	1.09	2 (7%)
3	OMU	L3	14	1,3	19,22,23	2.90	7 (36%)	25,31,34	1.91	4 (16%)
46	PSU	S2	823	46	18,21,22	1.76	6 (33%)	21,30,33	2.22	4 (19%)
1	OMC	L1	2824	1	19,22,23	2.97	8 (42%)	25,31,34	1.00	2 (8%)
1	PSU	L1	4531	1	18,21,22	1.17	1 (5%)	21,30,33	1.93	5 (23%)
1	OMC	L1	2861	1	19,22,23	2.98	8 (42%)	25,31,34	0.75	0
1	PSU	L1	4293	1	18,21,22	1.06	1 (5%)	21,30,33	1.87	4 (19%)
1	A2M	L1	3830	1	18,25,26	4.38	5 (27%)	20,36,39	3.35	4 (20%)
1	2MG	L1	1517	1	18,26,27	2.22	8 (44%)	16,38,41	2.11	5 (31%)
1	OMC	L1	2804	1	19,22,23	2.93	8 (42%)	25,31,34	0.83	0
1	A2M	L1	400	1	18,25,26	4.42	7 (38%)	20,36,39	3.26	4 (20%)
1	PSU	L1	1582	1	18,21,22	1.10	1 (5%)	21,30,33	1.71	4 (19%)
1	OMG	L1	3744	1	19,26,27	2.50	8 (42%)	21,38,41	1.44	4 (19%)
46	OMG	S2	601	46	19,26,27	2.46	8 (42%)	21,38,41	1.38	3 (14%)
1	OMU	L1	4306	1	19,22,23	2.86	6 (31%)	25,31,34	1.82	5 (20%)
1	B8T	L1	4671	1	19,22,23	3.22	8 (42%)	25,31,34	0.91	1 (4%)
1	PSU	L1	3715	1	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
1	OMG	L1	4228	1	19,26,27	2.50	8 (42%)	21,38,41	1.48	4 (19%)
1	OMC	L1	3701	1,80	19,22,23	2.88	8 (42%)	25,31,34	0.88	0
46	PSU	S2	822	46	18,21,22	1.10	1 (5%)	21,30,33	1.96	5 (23%)
1	OMC	L1	2422	1,80	19,22,23	2.90	8 (42%)	25,31,34	0.78	1 (4%)
46	OMU	S2	354	46	19,22,23	2.86	6 (31%)	25,31,34	1.84	5 (20%)
1	OMG	L1	1625	1	19,26,27	2.48	8 (42%)	21,38,41	1.49	4 (19%)
1	PSU	L1	4636	1	18,21,22	1.14	1 (5%)	21,30,33	2.11	5 (23%)
46	OMG	S2	1490	80,46	19,26,27	2.44	8 (42%)	21,38,41	1.35	4 (19%)
1	A2M	L1	4523	1,80	18,25,26	4.42	5 (27%)	20,36,39	3.49	5 (25%)
1	A2M	L1	3867	1	18,25,26	4.35	7 (38%)	20,36,39	3.42	5 (25%)
46	MA6	S2	1851	46	19,26,27	1.52	2 (10%)	18,38,41	4.60	5 (27%)
1	PSU	L1	2508	1	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UR3	L1	4530	1	19,22,23	2.75	8 (42%)	26,32,35	1.61	4 (15%)
46	OMG	S2	683	46	19,26,27	2.48	8 (42%)	21,38,41	1.48	4 (19%)
46	5MU	S2	814	46	19,22,23	7.32	8 (42%)	27,32,35	3.32	12 (44%)
1	A2M	L1	2401	1	18,25,26	4.38	6 (33%)	20,36,39	3.43	4 (20%)
1	A2M	L1	3718	1	18,25,26	4.42	6 (33%)	20,36,39	3.29	4 (20%)
1	PSU	L1	1677	1,81	18,21,22	1.14	2 (11%)	21,30,33	1.83	4 (19%)
1	UY1	L1	3818	1,81,80	19,22,23	4.45	12 (63%)	21,31,34	2.08	4 (19%)
46	A2M	S2	1031	46	18,25,26	4.38	5 (27%)	20,36,39	3.39	4 (20%)
1	OMC	L1	3887	1	19,22,23	2.94	8 (42%)	25,31,34	0.82	0
1	PSU	L1	3764	1	18,21,22	1.08	1 (5%)	21,30,33	1.76	4 (19%)
1	A2M	L1	2363	1,80	18,25,26	4.40	7 (38%)	20,36,39	3.15	4 (20%)
1	OMC	L1	3841	1	19,22,23	3.00	8 (42%)	25,31,34	0.96	1 (4%)
46	A2M	S2	484	46	18,25,26	4.39	6 (33%)	20,36,39	3.40	4 (20%)
1	OMG	L1	2364	1,80	19,26,27	2.44	8 (42%)	21,38,41	1.53	4 (19%)
1	PSU	L1	1683	1,81	18,21,22	1.15	1 (5%)	21,30,33	2.07	5 (23%)
46	OMG	S2	644	46	19,26,27	2.45	8 (42%)	21,38,41	1.39	4 (19%)
1	2MG	L1	978	1	18,26,27	2.30	8 (44%)	16,38,41	2.09	6 (37%)
1	OMU	L1	2837	1	19,22,23	2.88	6 (31%)	25,31,34	1.83	6 (24%)
1	OMC	L1	1881	1,80	19,22,23	2.94	8 (42%)	25,31,34	0.92	0
1	A2M	L1	398	1	18,25,26	4.43	7 (38%)	20,36,39	3.23	3 (15%)
46	OMC	S2	1391	46	19,22,23	3.00	8 (42%)	25,31,34	0.91	1 (4%)
1	2MG	L1	729	1	18,26,27	2.20	8 (44%)	16,38,41	1.56	3 (18%)
46	A2M	S2	1678	46	18,25,26	4.47	7 (38%)	20,36,39	3.41	4 (20%)
1	PSU	L1	3729	1	18,21,22	1.07	1 (5%)	21,30,33	1.84	4 (19%)
1	A2M	L1	1326	1	18,25,26	4.36	7 (38%)	20,36,39	3.37	3 (15%)
1	PSU	L1	4628	1	18,21,22	1.02	1 (5%)	21,30,33	1.92	5 (23%)
1	OMG	L1	4618	1	19,26,27	2.49	8 (42%)	21,38,41	1.45	5 (23%)
1	A2M	L1	3723	1	18,25,26	4.46	6 (33%)	20,36,39	3.29	4 (20%)
1	6MZ	L1	4220	1	17,25,26	1.31	2 (11%)	15,36,39	2.56	4 (26%)
46	OMC	S2	517	46	19,22,23	2.98	8 (42%)	25,31,34	0.81	1 (4%)
46	A2M	S2	590	46	18,25,26	4.43	6 (33%)	20,36,39	3.58	4 (20%)
46	OMG	S2	1328	46	19,26,27	2.52	7 (36%)	21,38,41	1.45	4 (19%)
1	OMG	L1	3792	1	19,26,27	2.42	8 (42%)	21,38,41	1.42	4 (19%)
46	5MC	S2	1374	46	19,22,23	3.82	8 (42%)	26,32,35	1.04	2 (7%)
1	A2M	L1	1524	1	18,25,26	4.31	7 (38%)	20,36,39	3.78	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	OMC	S2	174	80,46	19,22,23	3.01	8 (42%)	25,31,34	0.76	0
1	OMU	L1	4620	1	19,22,23	2.87	7 (36%)	25,31,34	1.80	5 (20%)
1	A2M	L1	2815	1	18,25,26	4.44	6 (33%)	20,36,39	3.30	4 (20%)
46	A2M	S2	576	46	18,25,26	4.42	6 (33%)	20,36,39	3.35	4 (20%)
1	OMU	L1	3925	1	19,22,23	2.97	7 (36%)	25,31,34	1.88	4 (16%)
46	OMU	S2	1288	46	19,22,23	3.03	8 (42%)	25,31,34	1.79	5 (20%)
1	OMC	L1	1340	1	19,22,23	2.84	8 (42%)	25,31,34	0.84	0
46	6MZ	S2	1832	80,46	17,25,26	1.19	2 (11%)	15,36,39	2.74	4 (26%)
46	UR3	S2	1830	46	19,22,23	2.82	7 (36%)	26,32,35	1.80	5 (19%)
1	A2M	L1	4571	1	18,25,26	4.47	7 (38%)	20,36,39	3.41	3 (15%)
1	A2M	L1	1871	1,80	18,25,26	4.42	7 (38%)	20,36,39	3.44	5 (25%)
1	OMG	L1	4623	1	19,26,27	2.43	8 (42%)	21,38,41	1.41	3 (14%)
46	PSU	S2	1243	80,46	18,21,22	1.11	1 (5%)	21,30,33	1.80	4 (19%)
1	5MC	L1	4447	1,80	19,22,23	3.78	8 (42%)	26,32,35	1.27	3 (11%)
3	OMG	L3	75	3	19,26,27	2.49	8 (42%)	21,38,41	1.47	4 (19%)
46	JMH	S2	1219	80,46	18,22,23	2.82	5 (27%)	23,32,35	1.65	4 (17%)
1	OMG	L1	4196	1	19,26,27	2.46	8 (42%)	21,38,41	1.46	4 (19%)
46	A2M	S2	512	46	18,25,26	4.42	6 (33%)	20,36,39	3.38	3 (15%)
1	PSU	L1	4500	1	18,21,22	0.97	1 (5%)	21,30,33	1.90	5 (23%)
46	OMU	S2	428	46	19,22,23	2.93	6 (31%)	25,31,34	1.79	5 (20%)
46	4AC	S2	1842	46	21,24,25	3.29	10 (47%)	28,34,37	1.10	3 (10%)
46	OMU	S2	121	46	19,22,23	2.91	6 (31%)	25,31,34	1.86	5 (20%)
46	OMG	S2	509	46	19,26,27	2.41	8 (42%)	21,38,41	1.38	4 (19%)
1	OMG	L1	3627	1	19,26,27	2.44	8 (42%)	21,38,41	1.47	3 (14%)
1	A2M	L1	2787	1	18,25,26	4.38	7 (38%)	20,36,39	3.32	4 (20%)
1	OMC	L1	4456	1	19,22,23	2.88	8 (42%)	25,31,34	0.85	1 (4%)
1	JMH	L1	1456	1	18,22,23	2.67	5 (27%)	23,32,35	0.99	1 (4%)
1	OMG	L1	4494	1	19,26,27	2.46	8 (42%)	21,38,41	1.45	4 (19%)
46	A2M	S2	27	80,46	18,25,26	4.41	6 (33%)	20,36,39	3.34	4 (20%)
1	A2M	L1	3825	1	18,25,26	4.43	7 (38%)	20,36,39	3.30	4 (20%)
46	OMG	S2	867	46	19,26,27	2.52	7 (36%)	21,38,41	1.46	4 (19%)
1	OMG	L1	2876	1	19,26,27	2.47	8 (42%)	21,38,41	1.48	4 (19%)
1	OMC	L1	3808	1	19,22,23	2.95	8 (42%)	25,31,34	0.98	1 (4%)
46	B8N	S2	1248	46	25,29,30	3.46	6 (24%)	28,42,45	2.00	8 (28%)
1	PSU	L1	4450	1,80	18,21,22	1.08	1 (5%)	21,30,33	1.92	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	B8H	L1	3762	1	19,22,23	6.76	6 (31%)	21,32,35	2.50	5 (23%)
1	OMG	L1	1316	1,80	19,26,27	2.50	8 (42%)	21,38,41	1.55	3 (14%)
46	A2M	S2	468	46	18,25,26	4.44	7 (38%)	20,36,39	3.40	4 (20%)
46	OMG	S2	436	46	19,26,27	2.47	8 (42%)	21,38,41	1.46	4 (19%)
46	A2M	S2	1383	46	18,25,26	4.46	5 (27%)	20,36,39	3.50	4 (20%)
1	OMC	L1	3869	1	19,22,23	2.97	8 (42%)	25,31,34	0.96	1 (4%)
1	OMG	L1	4370	1	19,26,27	2.47	8 (42%)	21,38,41	1.42	3 (14%)
46	OMU	S2	116	46	19,22,23	2.90	6 (31%)	25,31,34	1.79	5 (20%)
46	OMU	S2	1442	80,46	19,22,23	2.95	8 (42%)	25,31,34	1.78	5 (20%)
46	MA6	S2	1850	46	19,26,27	1.71	3 (15%)	18,38,41	4.36	4 (22%)
1	OMU	L1	4498	1	19,22,23	2.91	6 (31%)	25,31,34	1.88	4 (16%)
1	OMC	L1	2365	1,80	19,22,23	2.86	8 (42%)	25,31,34	0.71	0
46	4AC	S2	1337	46	21,24,25	3.41	10 (47%)	28,34,37	1.10	2 (7%)
46	PSU	S2	612	46	18,21,22	1.09	1 (5%)	21,30,33	1.93	5 (23%)
1	PSU	L1	4403	1	18,21,22	1.08	1 (5%)	21,30,33	1.78	4 (19%)
1	A2M	L1	1534	1,80	18,25,26	4.49	6 (33%)	20,36,39	3.50	3 (15%)
46	OMC	S2	462	46	19,22,23	3.01	8 (42%)	25,31,34	0.76	0
46	OMC	S2	1703	46	19,22,23	2.98	8 (42%)	25,31,34	0.73	0
1	OMG	L1	3899	1,80	19,26,27	2.46	8 (42%)	21,38,41	1.52	5 (23%)
46	OMC	S2	1272	46	19,22,23	3.07	8 (42%)	25,31,34	0.84	0
1	OMG	L1	4392	1	19,26,27	2.45	8 (42%)	21,38,41	1.41	3 (14%)
46	A2M	S2	668	80,46	18,25,26	4.32	6 (33%)	20,36,39	3.65	4 (20%)
1	OMC	L1	4536	1	19,22,23	2.86	8 (42%)	25,31,34	0.79	0
1	OMG	L1	1522	1	19,26,27	2.48	8 (42%)	21,38,41	1.59	4 (19%)
46	A2M	S2	99	80,46	18,25,26	4.43	7 (38%)	20,36,39	3.26	4 (20%)
1	A2M	L1	3785	1	18,25,26	4.11	7 (38%)	20,36,39	4.02	6 (30%)
46	PSU	S2	1081	46	18,21,22	1.11	1 (5%)	21,30,33	1.88	5 (23%)
46	UY1	S2	1326	80,46	19,22,23	4.36	11 (57%)	21,31,34	2.01	4 (19%)
46	OMC	S2	1710	46	19,22,23	3.01	8 (42%)	25,31,34	0.89	1 (4%)
46	A2M	S2	166	46	18,25,26	4.49	7 (38%)	20,36,39	3.49	4 (20%)
1	PSU	L1	4442	1	18,21,22	1.06	1 (5%)	21,30,33	1.91	4 (19%)
1	OMG	L1	3944	1	19,26,27	2.51	7 (36%)	21,38,41	1.45	4 (19%)
1	1MA	L1	1322	1,80	17,25,26	3.51	5 (29%)	17,37,40	2.10	4 (23%)

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
1	OMG	L1	4499	1	-	2/5/27/28	0/3/3/3
43	MLZ	Lo	53	43	-	3/7/8/10	-
1	5MC	L1	4335	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	119	46	-	0/7/25/26	0/2/2/2
1	OMU	L1	4227	1	-	0/9/27/28	0/2/2/2
46	A2M	S2	159	46	-	2/5/27/28	0/3/3/3
1	OMG	L1	2424	1	-	2/5/27/28	0/3/3/3
1	OMG	L1	4637	1	-	1/5/27/28	0/3/3/3
46	OMU	S2	172	46	-	0/9/27/28	0/2/2/2
1	OMC	L1	2351	1,80	-	1/9/27/28	0/2/2/2
46	M7A	S2	1806	46	-	0/7/37/38	0/3/3/3
1	5MC	L1	3782	1,80	-	0/7/25/26	0/2/2/2
3	OMU	L3	14	1,3	-	1/9/27/28	0/2/2/2
46	PSU	S2	823	46	-	2/7/25/26	0/2/2/2
1	OMC	L1	2824	1	-	1/9/27/28	0/2/2/2
1	PSU	L1	4531	1	-	0/7/25/26	0/2/2/2
1	OMC	L1	2861	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	4293	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	3830	1	-	0/5/27/28	0/3/3/3
1	2MG	L1	1517	1	-	0/5/27/28	0/3/3/3
1	OMC	L1	2804	1	-	0/9/27/28	0/2/2/2
1	A2M	L1	400	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	1582	1	-	1/7/25/26	0/2/2/2
1	OMG	L1	3744	1	-	1/5/27/28	0/3/3/3
46	OMG	S2	601	46	-	1/5/27/28	0/3/3/3
1	OMU	L1	4306	1	-	0/9/27/28	0/2/2/2
1	B8T	L1	4671	1	-	0/7/27/28	0/2/2/2
1	PSU	L1	3715	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	4228	1	-	0/5/27/28	0/3/3/3
1	OMC	L1	3701	1,80	-	4/9/27/28	0/2/2/2
46	PSU	S2	822	46	-	1/7/25/26	0/2/2/2
1	OMC	L1	2422	1,80	-	1/9/27/28	0/2/2/2
46	OMU	S2	354	46	-	0/9/27/28	0/2/2/2
1	OMG	L1	1625	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	4636	1	-	3/7/25/26	0/2/2/2
46	OMG	S2	1490	80,46	-	1/5/27/28	0/3/3/3
1	A2M	L1	4523	1,80	-	0/5/27/28	0/3/3/3
1	A2M	L1	3867	1	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	MA6	S2	1851	46	-	2/7/29/30	0/3/3/3
1	PSU	L1	2508	1	-	0/7/25/26	0/2/2/2
1	UR3	L1	4530	1	-	0/7/25/26	0/2/2/2
46	OMG	S2	683	46	-	1/5/27/28	0/3/3/3
46	5MU	S2	814	46	-	0/7/25/26	0/2/2/2
1	A2M	L1	2401	1	-	1/5/27/28	0/3/3/3
1	A2M	L1	3718	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	1677	1,81	-	3/7/25/26	0/2/2/2
1	UY1	L1	3818	1,81,80	-	5/9/27/28	0/2/2/2
46	A2M	S2	1031	46	-	0/5/27/28	0/3/3/3
1	OMC	L1	3887	1	-	1/9/27/28	0/2/2/2
1	PSU	L1	3764	1	-	2/7/25/26	0/2/2/2
1	A2M	L1	2363	1,80	-	1/5/27/28	0/3/3/3
1	OMC	L1	3841	1	-	2/9/27/28	0/2/2/2
46	A2M	S2	484	46	-	0/5/27/28	0/3/3/3
1	OMG	L1	2364	1,80	-	2/5/27/28	0/3/3/3
1	PSU	L1	1683	1,81	-	0/7/25/26	0/2/2/2
46	OMG	S2	644	46	-	1/5/27/28	0/3/3/3
1	2MG	L1	978	1	-	0/5/27/28	0/3/3/3
1	OMU	L1	2837	1	-	0/9/27/28	0/2/2/2
1	OMC	L1	1881	1,80	-	0/9/27/28	0/2/2/2
1	A2M	L1	398	1	-	2/5/27/28	0/3/3/3
46	OMC	S2	1391	46	-	2/9/27/28	0/2/2/2
1	2MG	L1	729	1	-	1/5/27/28	0/3/3/3
46	A2M	S2	1678	46	-	1/5/27/28	0/3/3/3
1	PSU	L1	3729	1	-	2/7/25/26	0/2/2/2
1	A2M	L1	1326	1	-	1/5/27/28	0/3/3/3
1	PSU	L1	4628	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	4618	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	3723	1	-	0/5/27/28	0/3/3/3
1	6MZ	L1	4220	1	-	0/5/27/28	0/3/3/3
46	OMC	S2	517	46	-	0/9/27/28	0/2/2/2
46	A2M	S2	590	46	-	3/5/27/28	0/3/3/3
46	OMG	S2	1328	46	-	1/5/27/28	0/3/3/3
1	OMG	L1	3792	1	-	3/5/27/28	0/3/3/3
46	5MC	S2	1374	46	-	0/7/25/26	0/2/2/2
1	A2M	L1	1524	1	-	0/5/27/28	0/3/3/3
46	OMC	S2	174	80,46	-	0/9/27/28	0/2/2/2
1	OMU	L1	4620	1	-	0/9/27/28	0/2/2/2
1	A2M	L1	2815	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	A2M	S2	576	46	-	2/5/27/28	0/3/3/3
1	OMU	L1	3925	1	-	0/9/27/28	0/2/2/2
46	OMU	S2	1288	46	-	1/9/27/28	0/2/2/2
1	OMC	L1	1340	1	-	2/9/27/28	0/2/2/2
46	6MZ	S2	1832	80,46	-	2/5/27/28	0/3/3/3
46	UR3	S2	1830	46	-	2/7/25/26	0/2/2/2
1	A2M	L1	4571	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	1871	1,80	-	0/5/27/28	0/3/3/3
1	OMG	L1	4623	1	-	0/5/27/28	0/3/3/3
46	PSU	S2	1243	80,46	-	2/7/25/26	0/2/2/2
1	5MC	L1	4447	1,80	-	4/7/25/26	0/2/2/2
3	OMG	L3	75	3	-	1/5/27/28	0/3/3/3
46	JMH	S2	1219	80,46	-	1/7/25/26	0/2/2/2
1	OMG	L1	4196	1	-	1/5/27/28	0/3/3/3
46	A2M	S2	512	46	-	2/5/27/28	0/3/3/3
1	PSU	L1	4500	1	-	3/7/25/26	0/2/2/2
46	OMU	S2	428	46	-	6/9/27/28	0/2/2/2
46	4AC	S2	1842	46	-	0/11/29/30	0/2/2/2
46	OMU	S2	121	46	-	0/9/27/28	0/2/2/2
46	OMG	S2	509	46	-	0/5/27/28	0/3/3/3
1	OMG	L1	3627	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	2787	1	-	2/5/27/28	0/3/3/3
1	OMC	L1	4456	1	-	0/9/27/28	0/2/2/2
1	JMH	L1	1456	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	4494	1	-	0/5/27/28	0/3/3/3
46	A2M	S2	27	80,46	-	0/5/27/28	0/3/3/3
1	A2M	L1	3825	1	-	0/5/27/28	0/3/3/3
46	OMG	S2	867	46	-	3/5/27/28	0/3/3/3
1	OMG	L1	2876	1	-	1/5/27/28	0/3/3/3
1	OMC	L1	3808	1	-	2/9/27/28	0/2/2/2
46	B8N	S2	1248	46	-	2/16/34/35	0/2/2/2
1	PSU	L1	4450	1,80	-	2/7/25/26	0/2/2/2
1	B8H	L1	3762	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	1316	1,80	-	0/5/27/28	0/3/3/3
46	A2M	S2	468	46	-	0/5/27/28	0/3/3/3
46	OMG	S2	436	46	-	0/5/27/28	0/3/3/3
46	A2M	S2	1383	46	-	0/5/27/28	0/3/3/3
1	OMC	L1	3869	1	-	1/9/27/28	0/2/2/2
1	OMG	L1	4370	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	OMU	S2	116	46	-	1/9/27/28	0/2/2/2
46	OMU	S2	1442	80,46	-	3/9/27/28	0/2/2/2
46	MA6	S2	1850	46	-	1/7/29/30	0/3/3/3
1	OMU	L1	4498	1	-	0/9/27/28	0/2/2/2
1	OMC	L1	2365	1,80	-	0/9/27/28	0/2/2/2
46	4AC	S2	1337	46	-	0/11/29/30	0/2/2/2
46	PSU	S2	612	46	-	0/7/25/26	0/2/2/2
1	PSU	L1	4403	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	1534	1,80	-	2/5/27/28	0/3/3/3
46	OMC	S2	462	46	-	0/9/27/28	0/2/2/2
46	OMC	S2	1703	46	-	0/9/27/28	0/2/2/2
1	OMG	L1	3899	1,80	-	0/5/27/28	0/3/3/3
46	OMC	S2	1272	46	-	0/9/27/28	0/2/2/2
1	OMG	L1	4392	1	-	0/5/27/28	0/3/3/3
46	A2M	S2	668	80,46	-	2/5/27/28	0/3/3/3
1	OMC	L1	4536	1	-	0/9/27/28	0/2/2/2
1	OMG	L1	1522	1	-	0/5/27/28	0/3/3/3
46	A2M	S2	99	80,46	-	2/5/27/28	0/3/3/3
1	A2M	L1	3785	1	-	2/5/27/28	0/3/3/3
46	PSU	S2	1081	46	-	1/7/25/26	0/2/2/2
46	UY1	S2	1326	80,46	-	2/9/27/28	0/2/2/2
46	OMC	S2	1710	46	-	0/9/27/28	0/2/2/2
46	A2M	S2	166	46	-	0/5/27/28	0/3/3/3
1	PSU	L1	4442	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	3944	1	-	2/5/27/28	0/3/3/3
1	1MA	L1	1322	1,80	-	0/3/25/26	0/3/3/3

The worst 5 of 892 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	814	5MU	C4-C5	21.06	1.79	1.44
46	S2	166	A2M	O4'-C1'	16.63	1.62	1.40
46	S2	1383	A2M	O4'-C1'	16.60	1.62	1.40
1	L1	1534	A2M	O4'-C1'	16.52	1.62	1.40
1	L1	4571	A2M	O4'-C1'	16.48	1.62	1.40

The worst 5 of 512 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1851	MA6	N1-C6-N6	-15.80	98.57	116.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1850	MA6	N1-C6-N6	-14.06	100.58	116.83
46	S2	1806	M7A	C5-C6-N6	13.70	147.03	123.75
1	L1	1534	A2M	C5-C6-N6	11.37	137.63	120.31
46	S2	1806	M7A	N6-C6-N1	-11.32	93.16	118.38

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	Lo	53	MLZ	CD-CE-NZ-CM
1	L1	1340	OMC	O4'-C4'-C5'-O5'
1	L1	1534	A2M	C3'-C2'-O2'-CM'
1	L1	2424	OMG	O4'-C4'-C5'-O5'
1	L1	2424	OMG	C3'-C4'-C5'-O5'

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 442 ligands modelled in this entry, 442 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 ⓘ

There are no chain breaks in this entry.

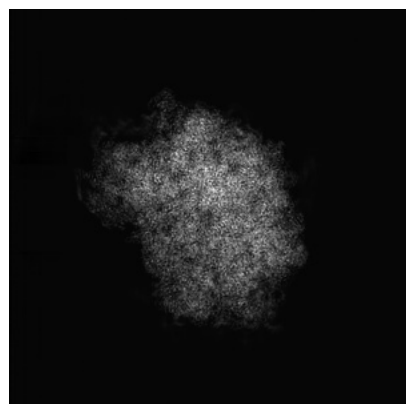
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33330. These allow visual inspection of the internal detail of the map and identification of artifacts.

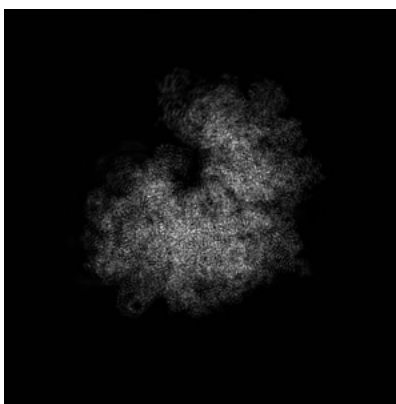
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

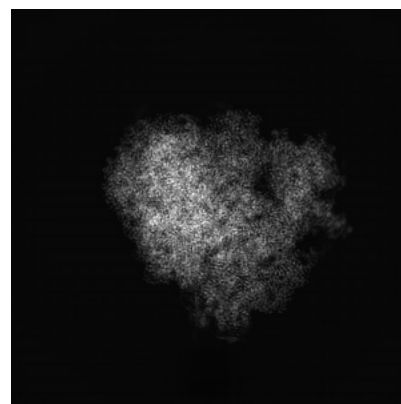
6.1.1 Primary map



X

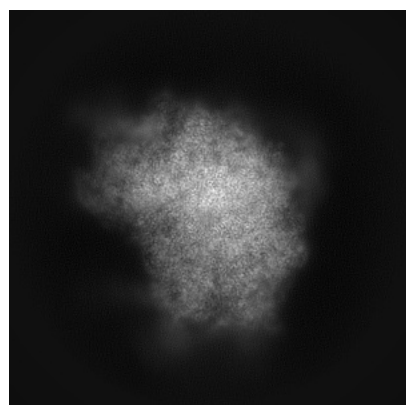


Y

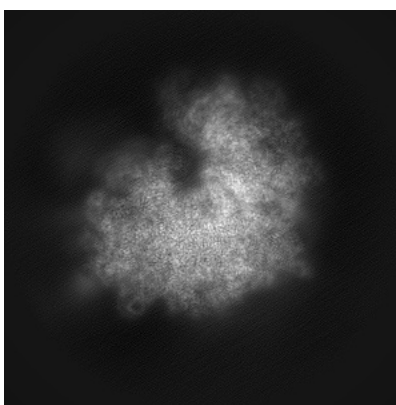


Z

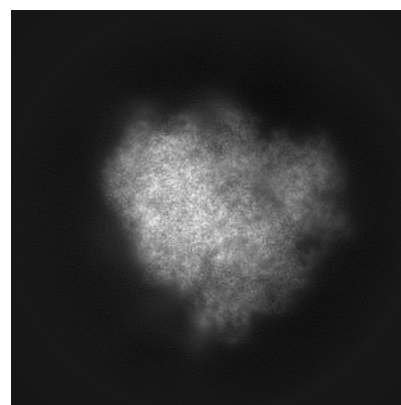
6.1.2 Raw map



X



Y

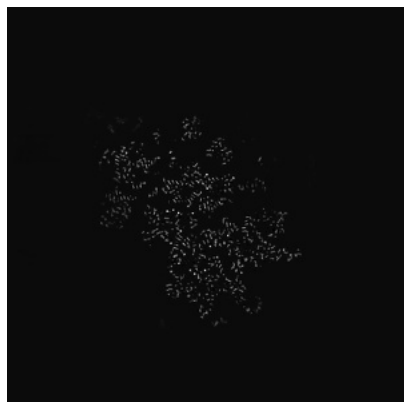


Z

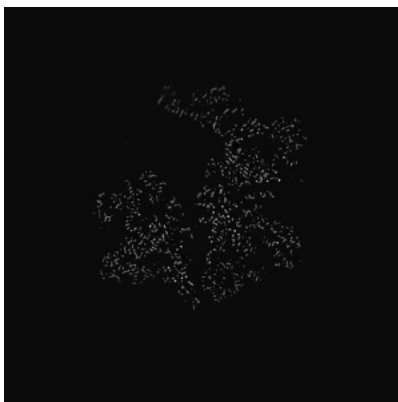
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210

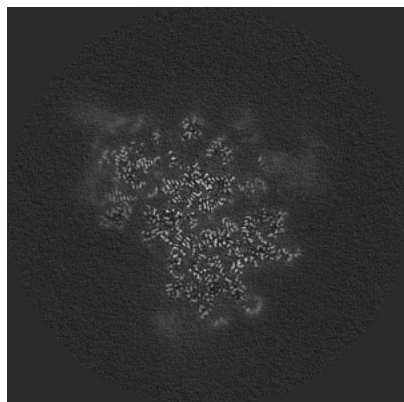


Y Index: 210

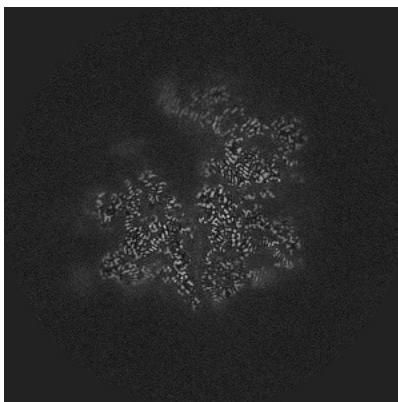


Z Index: 210

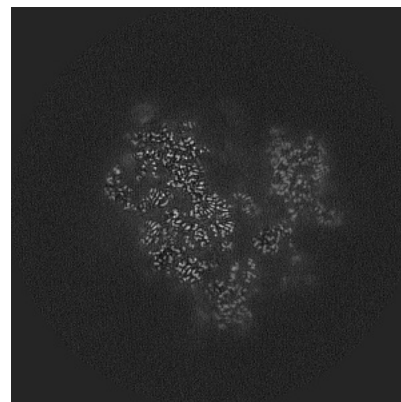
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

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: 170

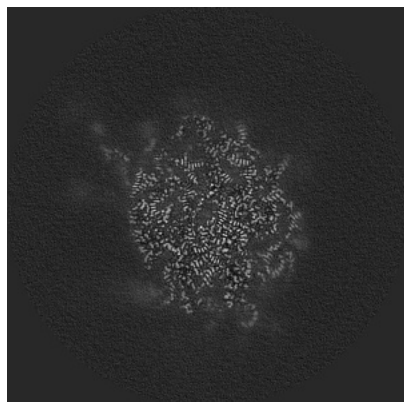


Y Index: 203

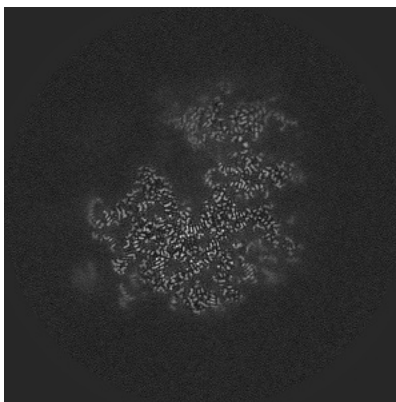


Z Index: 232

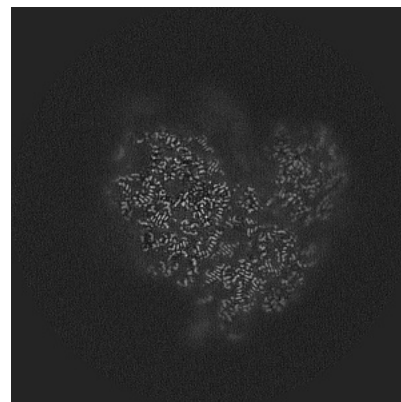
6.3.2 Raw map



X Index: 187



Y Index: 224

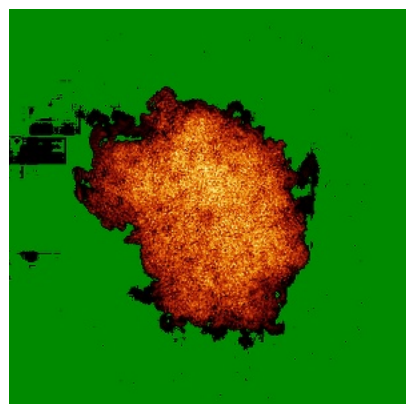


Z Index: 230

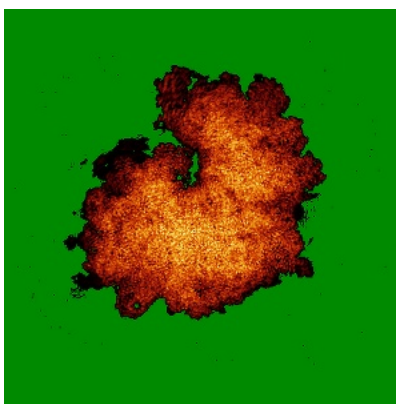
The images above show the largest variance slices of the map in three orthogonal directions.

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

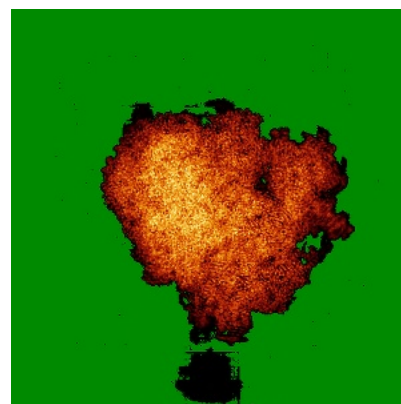
6.4.1 Primary map



X

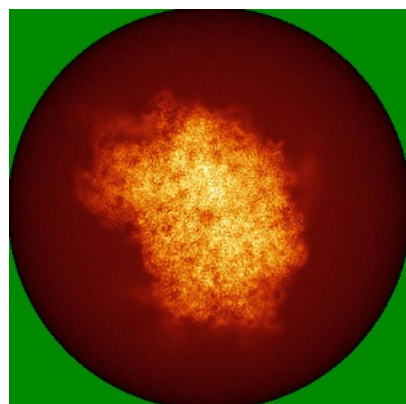


Y

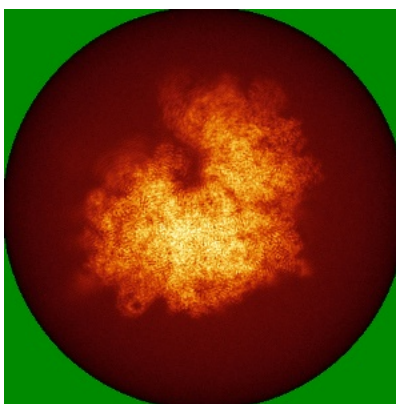


Z

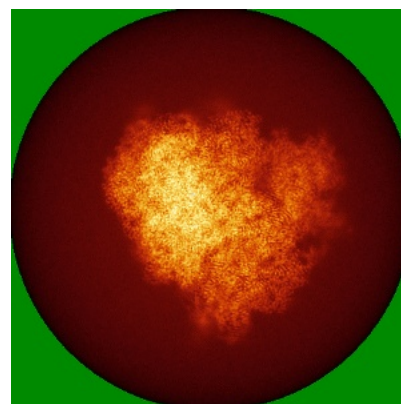
6.4.2 Raw map



X



Y



Z

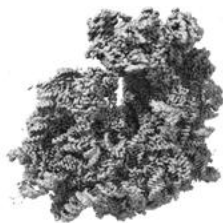
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



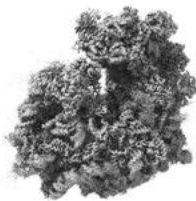
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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



X



Y



Z

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.

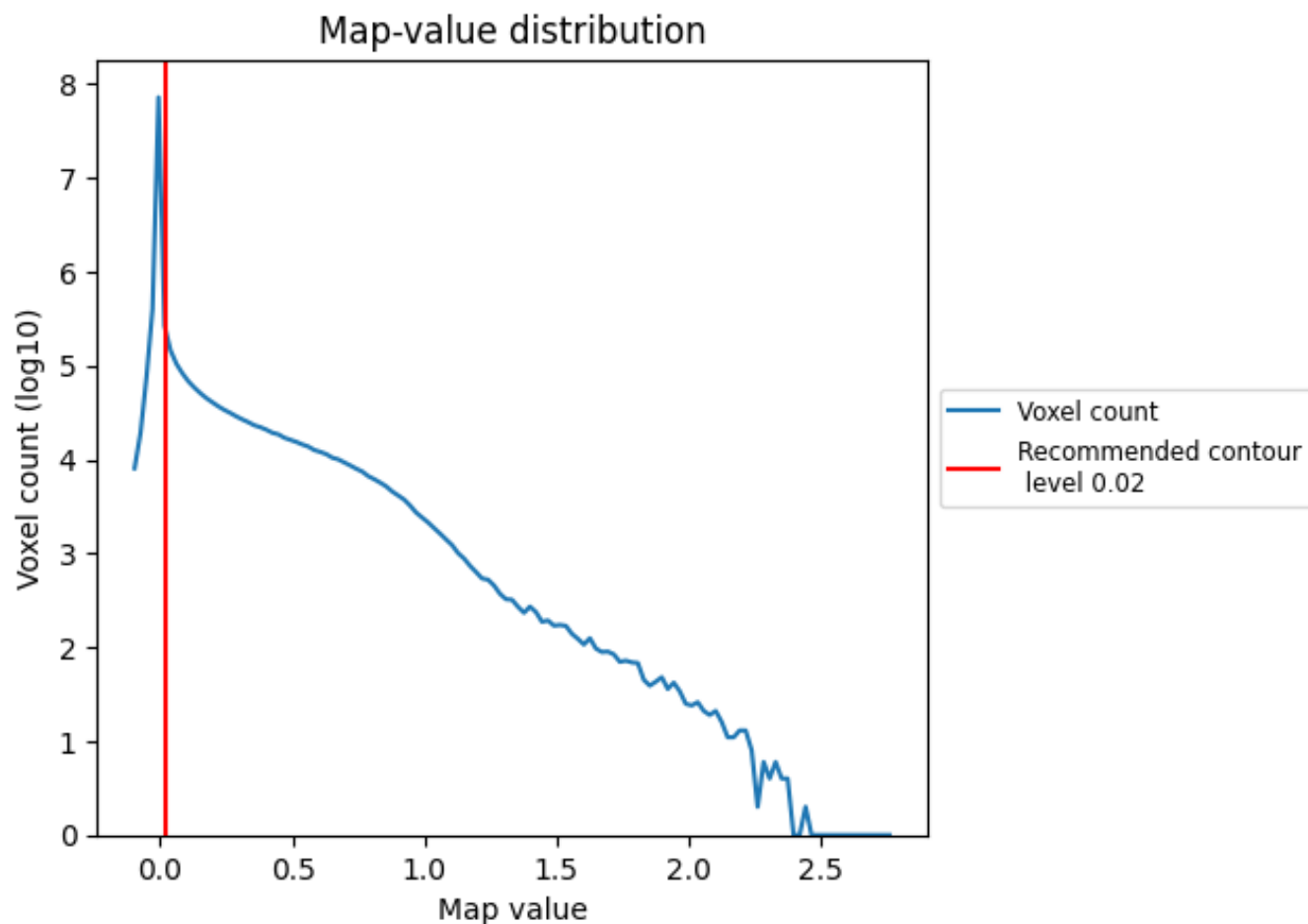
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

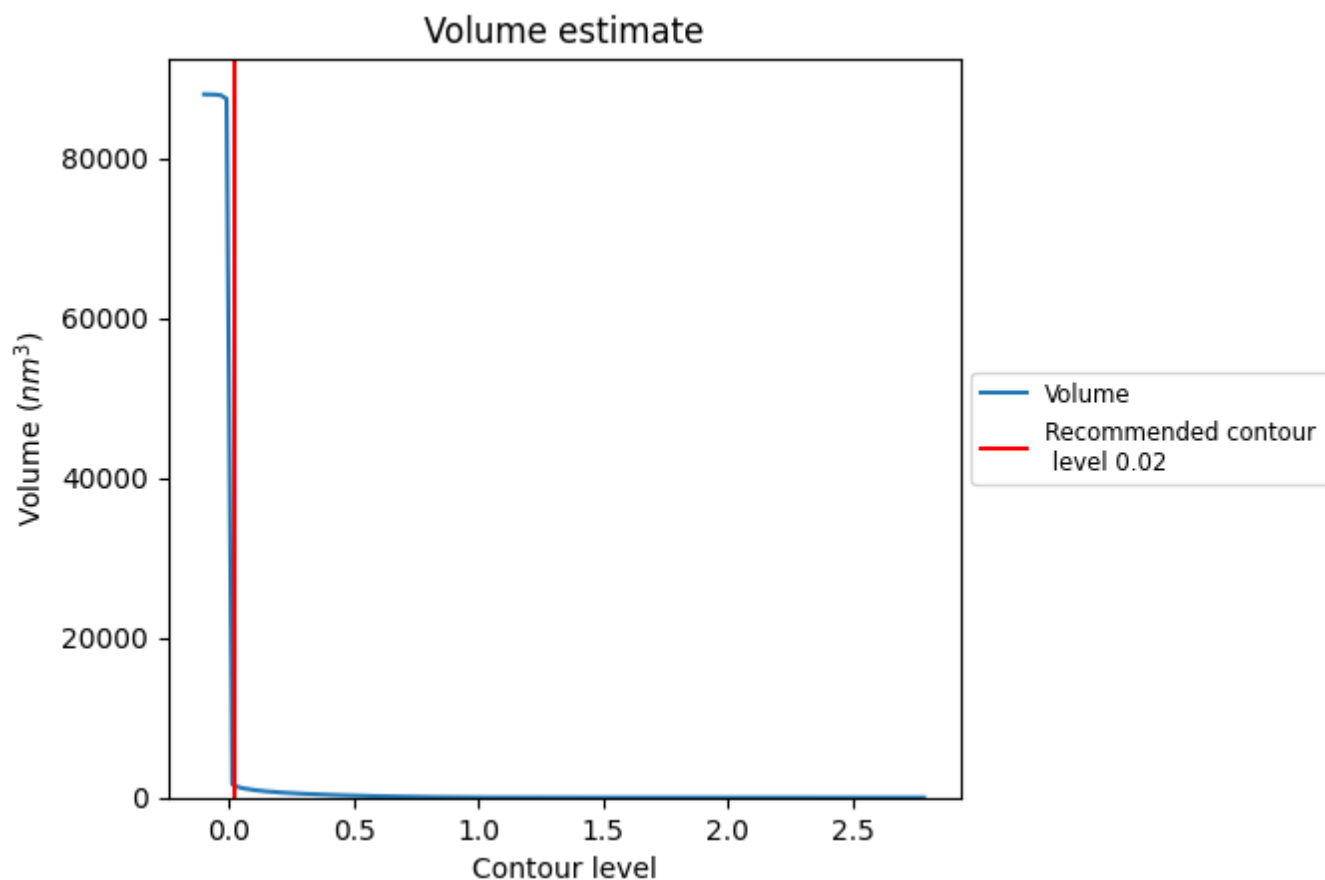
This section contains the results of statistical analysis of the map.

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.

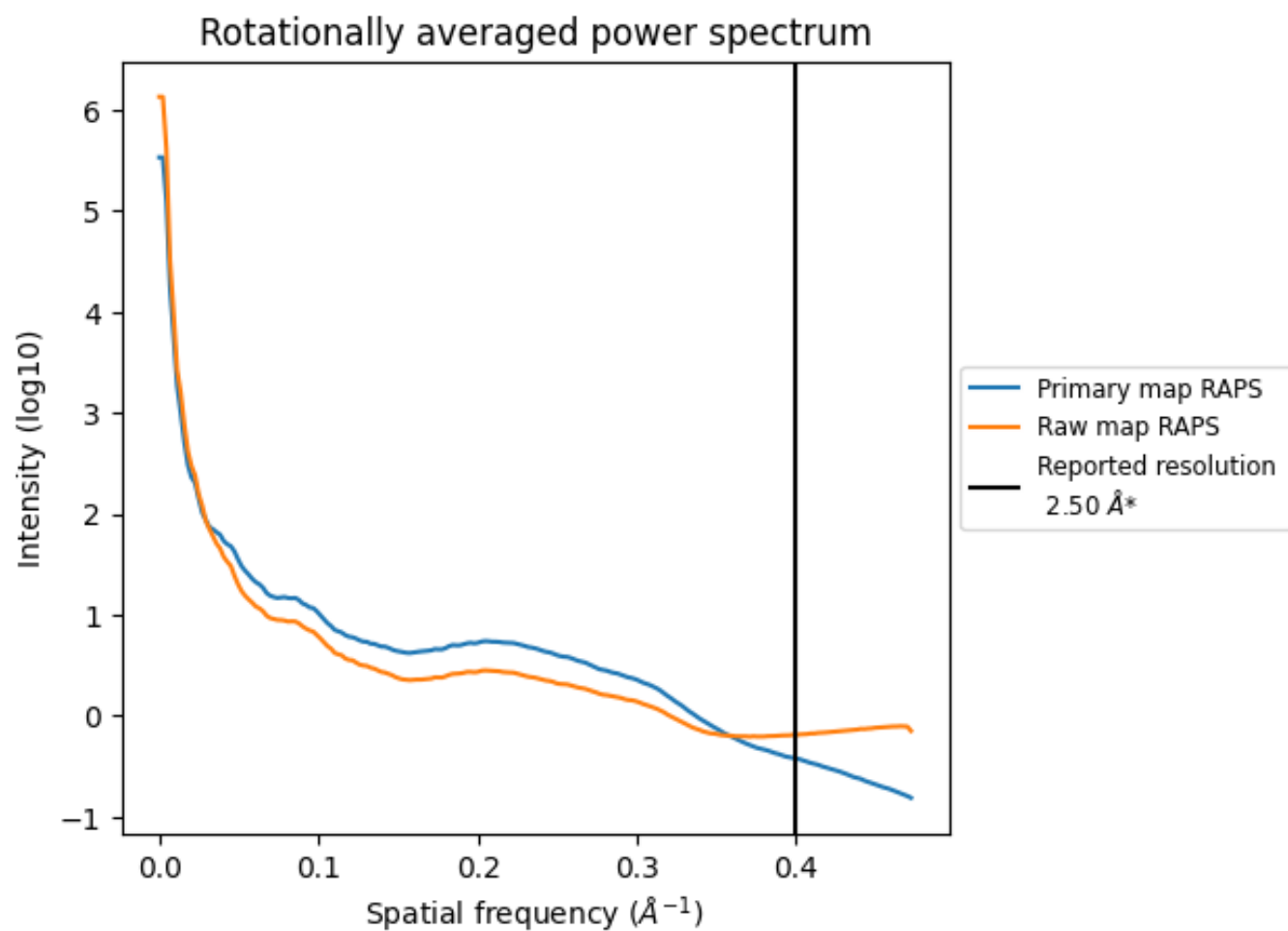
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1583 nm³; this corresponds to an approximate mass of 1430 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 ⓘ

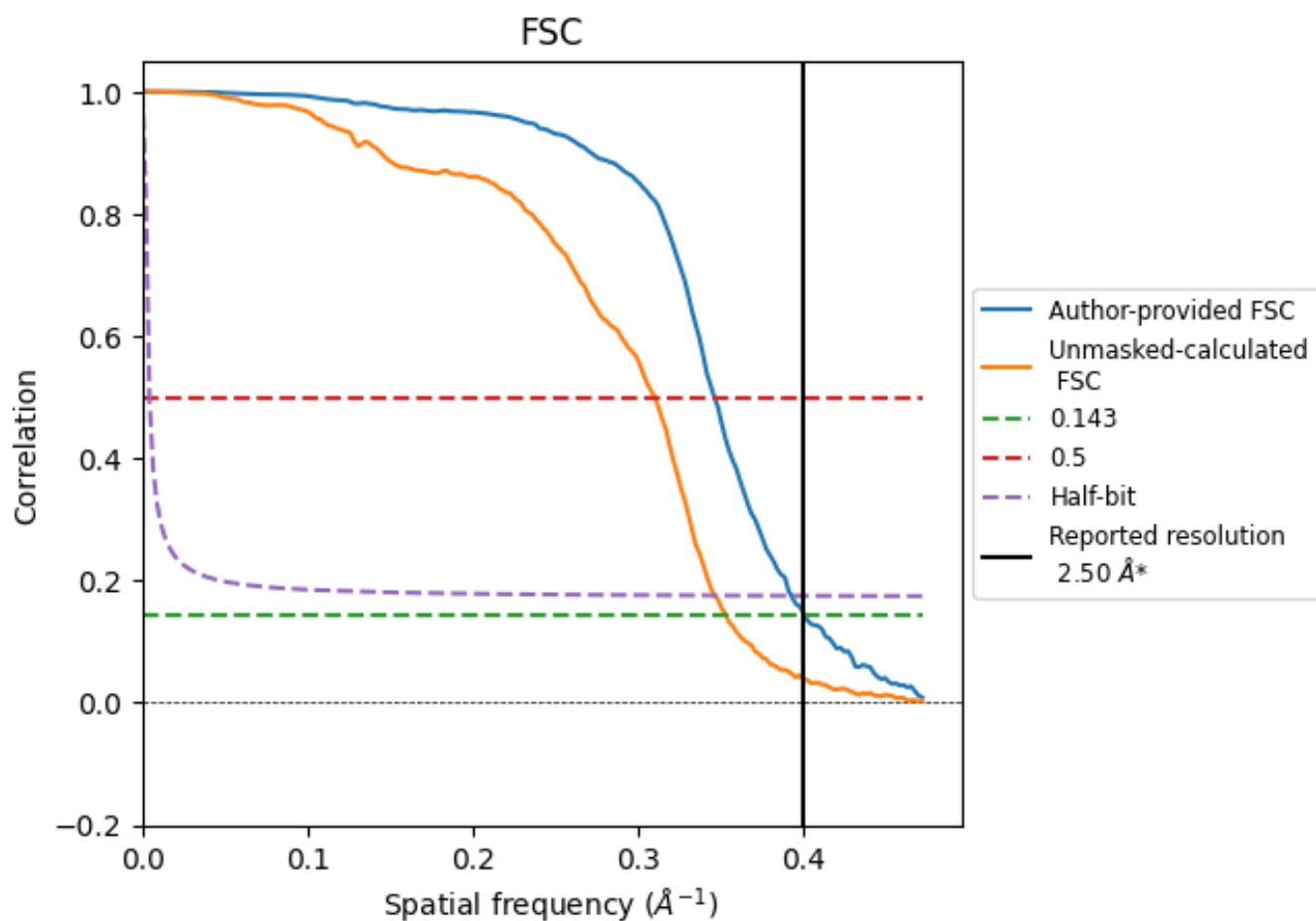


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 \AA^{-1}

8.2 Resolution estimates [i](#)

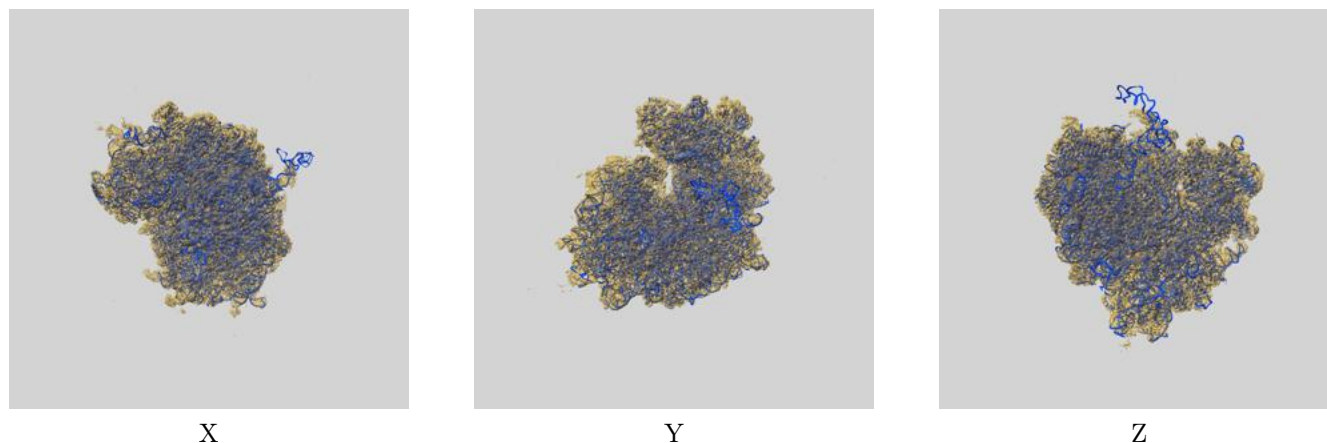
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.89	2.55
Unmasked-calculated*	2.83	3.22	2.89

*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 2.83 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

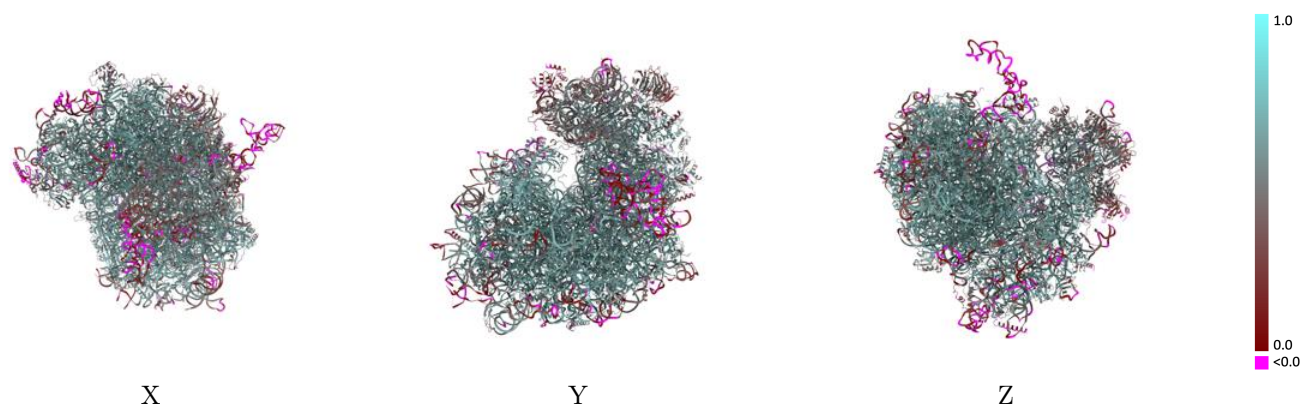
This section contains information regarding the fit between EMDB map EMD-33330 and PDB model 7XNY. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

9.1 Map-model overlay [i](#)



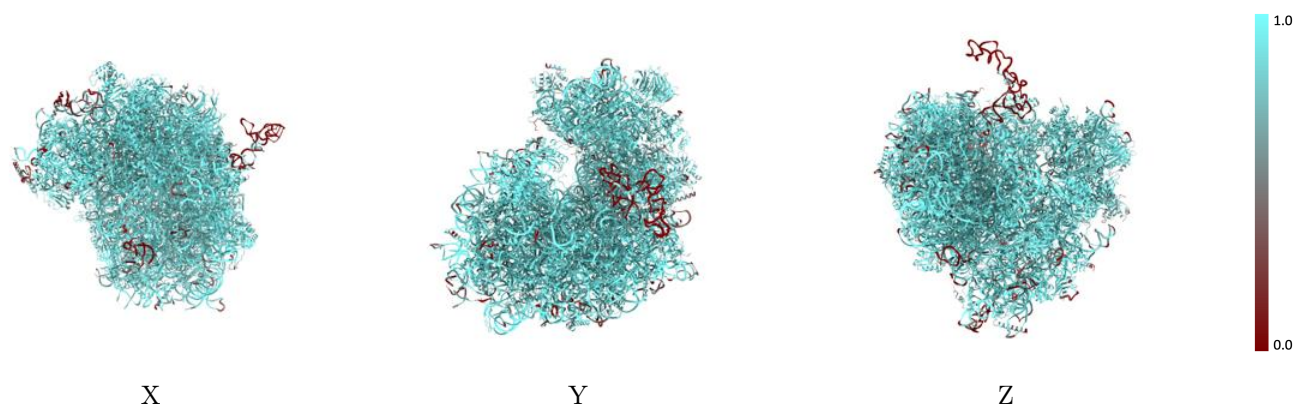
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



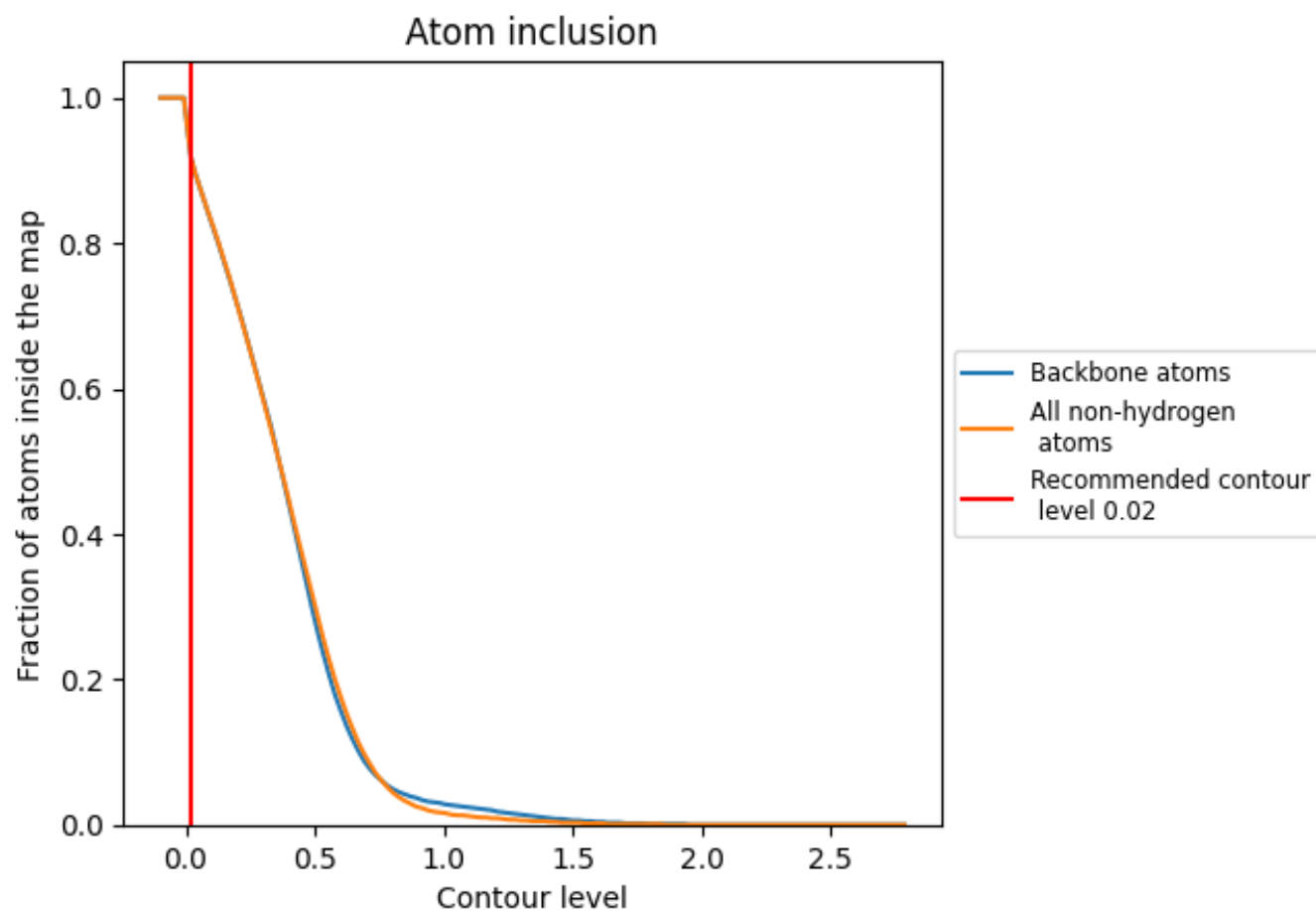
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.5600
L1	 0.9070	 0.5570
L2	 0.9920	 0.6420
L3	 0.9310	 0.5930
LA	 0.9800	 0.6660
LB	 0.9490	 0.6340
LC	 0.9560	 0.6380
LD	 0.9370	 0.5890
LE	 0.9480	 0.5930
LF	 0.9620	 0.6540
LG	 0.9210	 0.5740
LH	 0.9450	 0.6000
LI	 0.9560	 0.6220
LJ	 0.9160	 0.5370
LL	 0.9180	 0.5870
LM	 0.9490	 0.6120
LN	 0.9820	 0.6700
LO	 0.9520	 0.6360
LP	 0.9490	 0.6450
LQ	 0.9660	 0.6550
LR	 0.9090	 0.5840
LS	 0.9790	 0.6550
LT	 0.9380	 0.6080
LU	 0.8760	 0.4830
LV	 0.9560	 0.6440
LW	 0.7220	 0.3800
LX	 0.9370	 0.6200
LY	 0.9310	 0.6040
LZ	 0.9550	 0.6050
La	 0.9690	 0.6530
Lb	 0.8680	 0.5420
Lc	 0.9370	 0.6280
Ld	 0.9320	 0.6100
Le	 0.9670	 0.6480
Lf	 0.9750	 0.6590









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Chain	Atom inclusion	Q-score
Lg	 0.9450	 0.6200
Lh	 0.9220	 0.5900
Li	 0.9390	 0.5890
Lj	 0.9720	 0.6370
Lk	 0.8890	 0.5310
Ll	 0.9360	 0.6000
Lm	 0.9420	 0.6180
Ln	 0.9380	 0.6130
Lo	 0.9390	 0.6240
Lp	 0.9350	 0.6340
Lr	 0.9670	 0.6430
S2	 0.9320	 0.5450
SA	 0.9460	 0.5840
SB	 0.9410	 0.5860
SC	 0.9530	 0.6080
SD	 0.8840	 0.4580
SE	 0.9500	 0.5920
SF	 0.9170	 0.4870
SG	 0.8720	 0.4700
SH	 0.8820	 0.4870
SI	 0.9210	 0.5630
SJ	 0.9190	 0.5490
SK	 0.8600	 0.3830
SL	 0.9390	 0.6210
SM	 0.6410	 0.1100
SN	 0.9620	 0.6210
SO	 0.9470	 0.5980
SP	 0.7840	 0.3350
SQ	 0.8900	 0.4770
SR	 0.8900	 0.4920
SS	 0.8610	 0.3910
ST	 0.8780	 0.4270
SU	 0.8750	 0.4150
SV	 0.9570	 0.5940
SW	 0.9680	 0.6410
SX	 0.9490	 0.6160
SY	 0.9190	 0.5260
SZ	 0.7940	 0.3540
Sa	 0.9300	 0.5740
Sb	 0.9170	 0.5400
Sc	 0.8520	 0.4740
Sd	 0.9190	 0.5200

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Chain	Atom inclusion	Q-score
Se	 0.7720	 0.4650
Sf	 0.7400	 0.1880
Sg	 0.8670	 0.3790