



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 02:59 AM UTC

PDB ID : 8A3W / pdb_00008a3w
EMDB ID : EMD-15124
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :
WILD TYPE
Authors : Rajan, K.S.; Yonath, A.; Bashan, A.
Deposited on : 2022-06-09
Resolution : 2.89 Å (reported)
Based on initial models : 6AZ1, 6AZ3, 5T2A

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:

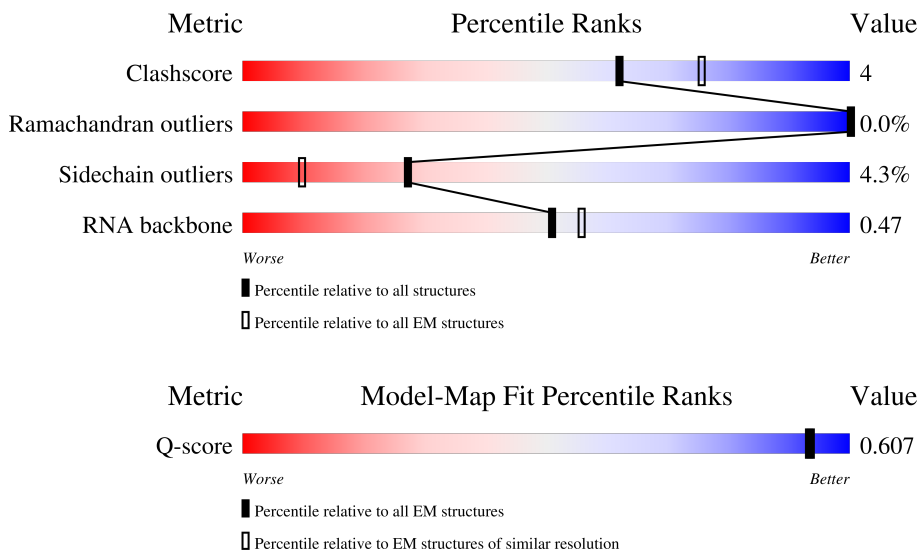
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

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

The reported resolution of this entry is 2.89 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	12148 (2.39 - 3.39)

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	SD	190	 14% 69% 15% 1% 1%
2	SE	273	 14% 81% 13% 5% 1%
3	SF	265	 14% 66% 12% 8% 1%

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Mol	Chain	Length	Quality of chain
4	SG	249	85% 8% 6%
5	SH	190	80% 15% . .
6	SI	200	84% 15%
7	SJ	130	91% 8% .
8	SK	220	5% 71% 12% 16%
9	SL	149	89% 6% 5%
10	SM	116	62% 24% . 12%
11	SN	168	45% 12% . 42%
12	SO	144	79% 11% . 7%
13	SP	143	87% 11% ..
14	SR	153	73% 15% . 12%
15	SS	57	74% 21% 5%
16	ST	151	81% 12% 7%
17	SU	173	6% 83% 6% 11%
18	SV	143	41% 8% 50%
19	SW	152	60% 12% . 27%
20	SX	161	74% 12% . 13%
21	SY	164	26% 44% 9% . 46%
22	SZ	137	75% 13% . 11%
23	Sa	120	50% 8% 42%
24	Sb	112	62% 6% 6% 25%
25	Sc	86	5% 85% 13% .
26	Sd	87	5% 51% 11% 38%
27	Se	66	8% 62% 8% 30%
28	Sg	312	78% 13% . 7%

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Mol	Chain	Length	Quality of chain
29	S1	2204	46% 23% 6% 25%
30	SA	264	66% 10% 23%
31	SB	246	27% 60% 23% 15%
32	SC	219	78% 14% 8%
33	Sh	235	18% 30% 11% 60%
34	S4	20	35% 40% 10% 15%
35	8	123	72% 20% 8% 2%
36	6	73	37% 30% 19% 14%
37	2	1522	40% 16% 5% 38%
38	7	171	68% 19% 8% 5%
39	5	135	53% 17% 27%
40	4	183	61% 21% 14%
41	3	216	47% 18% 6% 29%
42	1	1782	56% 20% 6% 18%
43	B	419	86% 8% 6%
44	C	373	81% 6% 13%
45	A	260	91% 6% 3%
46	c	252	83% 7% 10%
47	O	305	74% 6% 20%
48	M	204	93% 6%
49	H	222	91% 8% 1%
50	G	264	73% 6% 20%
51	P	198	92% 7% 1%
52	R	179	86% 13% 1%
53	I	220	69% 7% 23%





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Mol	Chain	Length	Quality of chain
54	Q	254	61% 5% 34%
55	T	166	81% 10% 8%
56	S	159	85% 9% 5%
57	L	145	94% 6%
58	F	195	66% 7% 27%
59	E	190	69% 9% 22%
60	Y	134	87% 11%
61	f	133	87% 5% 8%
62	g	144	71% 14% 14%
63	a	127	86% 10% 4%
64	J	139	86% 7% 7%
65	W	143	72% 10% 18%
66	V	145	73% 8% 19%
67	h	168	58% 8% 33%
68	Z	147	72% 9% 18%
69	K	175	61% 7% 32%
70	j	83	81% 16%
71	i	105	69% 12% 18%
72	U	129	78% 10% 12%
73	p	106	66% 12% 22%
74	o	92	78% 16% 6%
75	D	188	46% 6% 47%
76	d	104	69% 14% 15%
77	X	124	49% 48%
78	b	70	84% 10% 6%

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Mol	Chain	Length	Quality of chain
79	k	83	 72% 13% 14%
80	l	51	 86% 12%
81	n	34	 44% 74% 26%
82	e	188	 73% 7% 20%

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 183881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	SD	163	1347	852	266	221	8	1	0

- Molecule 2 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SE	260	2060	1307	397	347	9	2	0

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SF	205	1555	1000	279	267	9	0	0

- Molecule 4 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SG	233	1810	1132	370	305	3	1	0

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SH	183	1404	876	263	258	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SI	199	1583	1010	301	265	7	0	0

- Molecule 7 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SJ	129	1017	644	188	177	8	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SK	184	1453	912	307	232	2	0	0

- Molecule 9 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SL	142	1112	715	205	189	3	0	0

- Molecule 10 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SM	102	807	503	150	152	2	2	0

- Molecule 11 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SN	98	791	507	139	138	7	0	0

- Molecule 12 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SO	134	975	602	192	174	7	0	0

- Molecule 13 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SP	142	1119	706	223	187	3	3	0

- Molecule 14 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	SR	135	1077	681	212	180	4	1	0

- Molecule 15 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	SS	54	417	257	84	71	5	0	0

- Molecule 16 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	ST	140	1140	720	227	185	8	0	0

- Molecule 17 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	SU	154	1218	771	241	201	5	0	0

- Molecule 18 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	SV	71	577	368	110	97	2	0	0

- Molecule 19 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	SW	111	866	553	164	145	4	0	0

- Molecule 20 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	SX	140	1092	694	211	183	4	0	0

- Molecule 21 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SY	88	Total	C	N	O	S	0	0
			622	382	116	121	3		

- Molecule 22 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SZ	122	Total	C	N	O	S	0	0
			972	623	187	160	2		

- Molecule 23 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Sa	70	Total	C	N	O	S	0	0
			549	351	97	98	3		

- Molecule 24 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Sb	84	Total	C	N	O	S	0	0
			661	410	138	106	7		

- Molecule 25 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Sc	84	Total	C	N	O	S	0	0
			624	390	118	112	4		

- Molecule 26 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Sd	54	Total	C	N	O	S	0	0
			390	240	80	66	4		

- Molecule 27 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Se	46	Total	C	N	O	S	0	0
			350	221	71	57	1		

- Molecule 28 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Sg	290	Total	C	N	O	S	1	0
			2173	1369	381	411	12		

- Molecule 29 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S1	1663	Total	C	N	O	P	0	0
			35569	15906	6433	11567	1663		

- Molecule 30 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SA	204	Total	C	N	O	S	1	0
			1653	1043	314	287	9		

- Molecule 31 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SB	210	Total	C	N	O	S	0	0
			1595	1015	281	287	12		

- Molecule 32 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SC	202	Total	C	N	O	S	1	0
			1525	974	272	266	13		

- Molecule 33 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sh	95	Total	C	N	O	S	0	0
			668	413	128	125	2		

- Molecule 34 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S4	17	Total	C	N	O	P	0	0
			359	161	66	116	16		

- Molecule 35 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
35	8	119	2531	1132	452	828	119	0	0

- Molecule 36 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
36	6	63	1329	595	238	433	63	0	0

- Molecule 37 is a RNA chain called LSub_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
37	2	947	20228	9057	3635	6589	947	0	0

- Molecule 38 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	7	163	3463	1551	613	1137	162	0	0

- Molecule 39 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	5	98	2096	934	381	683	98	0	0

- Molecule 40 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
40	4	158	3378	1507	611	1102	158	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	4	G	A	conflict	GB 321438308

- Molecule 41 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3	153	Total	C	N	O	P	0	0
			3252	1454	570	1075	153		

- Molecule 42 is a RNA chain called LSUa_rRNA_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1	1467	Total	C	N	O	P	1	0
			31495	14076	5781	10171	1467		

- Molecule 43 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	B	395	Total	C	N	O	S	4	0
			2955	1874	575	494	12		

- Molecule 44 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	C	325	Total	C	N	O	S	0	0
			2343	1481	447	401	14		

- Molecule 45 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	A	254	Total	C	N	O	S	1	0
			1852	1153	375	314	10		

- Molecule 46 is a protein called uL30_chain_c.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	c	227	Total	C	N	O	S	0	0
			1779	1134	340	294	11		

- Molecule 47 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	O	243	Total	C	N	O	S	1	0
			1764	1130	333	298	3		

- Molecule 48 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	M	203	1692	1068	360	256	8	0	0

- Molecule 49 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	H	220	1690	1071	340	272	7	0	0

- Molecule 50 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	G	212	1635	1036	324	268	7	0	0

- Molecule 51 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	P	196	1513	952	303	252	6	0	0

- Molecule 52 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	R	178	1399	894	267	233	5	0	0

- Molecule 53 is a protein called eL13_chain_I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	I	169	1299	822	262	208	7	0	0

- Molecule 54 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	Q	168	1290	802	276	206	6	0	0

- Molecule 55 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	T	152	1217	761	241	204	11	0	0

- Molecule 56 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	S	151	1164	738	228	195	3	0	0

- Molecule 57 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	L	144	1114	703	226	179	6	0	0

- Molecule 58 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	F	142	1032	658	191	181	2	0	0

- Molecule 59 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	E	148	1032	659	191	179	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	Y	132	1008	649	198	159	2	0	0

- Molecule 61 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	f	123	993	624	197	168	4	0	0

- Molecule 62 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	g	124	989	618	207	159	5	0	0

- Molecule 63 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	a	123	955	597	199	157	2	0	0

- Molecule 64 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	J	129	933	590	174	163	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	W	117	928	580	193	151	4	0	0

- Molecule 66 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	V	118	917	582	174	159	2	0	0

- Molecule 67 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	h	112	889	548	195	142	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	Z	120	892	548	182	157	5	0	0

- Molecule 69 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	K	119	Total	C	N	O	S	0	0
			883	557	176	146	4		

- Molecule 70 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	j	80	Total	C	N	O	S	0	0
			659	401	152	100	6		

- Molecule 71 is a protein called Putative 60S Ribosomal protein L36.

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

- Molecule 72 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	U	114	Total	C	N	O	S	0	0
			795	508	147	138	2		

- Molecule 73 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	p	83	Total	C	N	O	S	0	0
			640	410	126	102	2		

- Molecule 74 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	o	88	Total	C	N	O	S	0	0
			659	410	135	108	6		

- Molecule 75 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	D	100	Total	C	N	O	S	0	0
			649	406	129	109	5		

- Molecule 76 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	d	88	Total	C	N	O	S	0	0
			607	379	109	114	5		

- Molecule 77 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	X	64	Total	C	N	O	S	0	0
			548	359	105	80	4		

- Molecule 78 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	b	66	Total	C	N	O	0	0
			520	318	120	82		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
79	k	71	Total	C	N	O	S	0	0
			508	323	96	86	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
			440	285	91	63	1		

- Molecule 81 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms				AltConf	Trace
81	n	25	Total	C	N	O	0	0
			159	97	36	26		

- Molecule 82 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	e	151	Total	C	N	O	S	0	0
			1103	698	210	193	2		

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
83	SD	1	Total 1	Mg 1	0
83	S1	30	Total 30	Mg 30	0
83	2	25	Total 25	Mg 25	0
83	7	2	Total 2	Mg 2	0
83	5	1	Total 1	Mg 1	0
83	3	1	Total 1	Mg 1	0
83	1	52	Total 52	Mg 52	0
83	C	1	Total 1	Mg 1	0
83	T	1	Total 1	Mg 1	0

- Molecule 84 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
84	SO	1	Total 1	Na 1	0
84	S1	23	Total 23	Na 23	0
84	2	9	Total 9	Na 9	0
84	4	1	Total 1	Na 1	0
84	1	22	Total 22	Na 22	0
84	J	1	Total 1	Na 1	0

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	SS	1	Total 1	Zn 1	0
85	Sb	1	Total 1	Zn 1	0
85	j	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
85	o	1	Total 1	Zn 1	0

- Molecule 86 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
86	Sb	1	Total 1	K 1	0
86	S1	4	Total 4	K 4	0
86	8	1	Total 1	K 1	0
86	2	3	Total 3	K 3	0
86	4	1	Total 1	K 1	0
86	1	3	Total 3	K 3	0

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
87	SH	1	Total 1	O 1	0
87	SN	2	Total 2	O 2	0
87	SR	1	Total 1	O 1	0
87	ST	1	Total 1	O 1	0
87	SX	1	Total 1	O 1	0
87	S1	36	Total 36	O 36	0
87	8	5	Total 5	O 5	0
87	6	1	Total 1	O 1	0
87	2	148	Total 148	O 148	0
87	7	40	Total 40	O 40	0

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Mol	Chain	Residues	Atoms		AltConf
87	5	19	Total 19	O 19	0
87	4	29	Total 29	O 29	0
87	3	17	Total 17	O 17	0
87	1	283	Total 283	O 283	0
87	B	9	Total 9	O 9	0
87	C	11	Total 11	O 11	0
87	A	10	Total 10	O 10	0
87	c	3	Total 3	O 3	0
87	M	9	Total 9	O 9	0
87	H	3	Total 3	O 3	0
87	G	3	Total 3	O 3	0
87	P	8	Total 8	O 8	0
87	R	1	Total 1	O 1	0
87	I	4	Total 4	O 4	0
87	Q	4	Total 4	O 4	0
87	T	7	Total 7	O 7	0
87	S	1	Total 1	O 1	0
87	L	3	Total 3	O 3	0
87	f	2	Total 2	O 2	0
87	g	1	Total 1	O 1	0
87	a	1	Total 1	O 1	0

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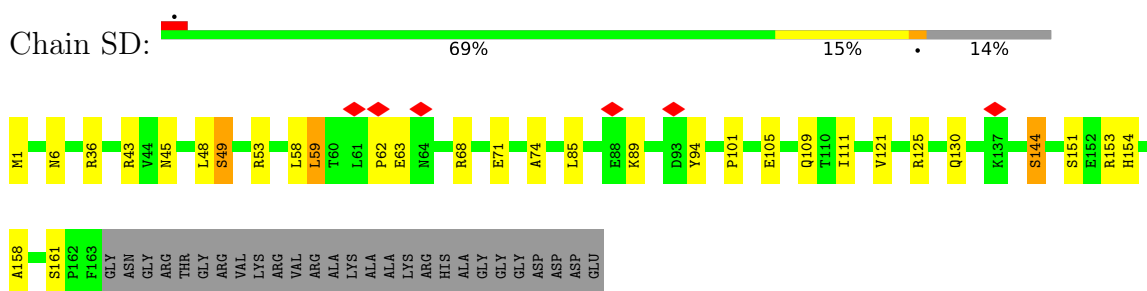
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
87	J	1	Total 1	O 1	0
87	W	1	Total 1	O 1	0
87	V	2	Total 2	O 2	0
87	h	3	Total 3	O 3	0
87	j	7	Total 7	O 7	0
87	d	1	Total 1	O 1	0
87	X	1	Total 1	O 1	0
87	l	4	Total 4	O 4	0
87	e	3	Total 3	O 3	0

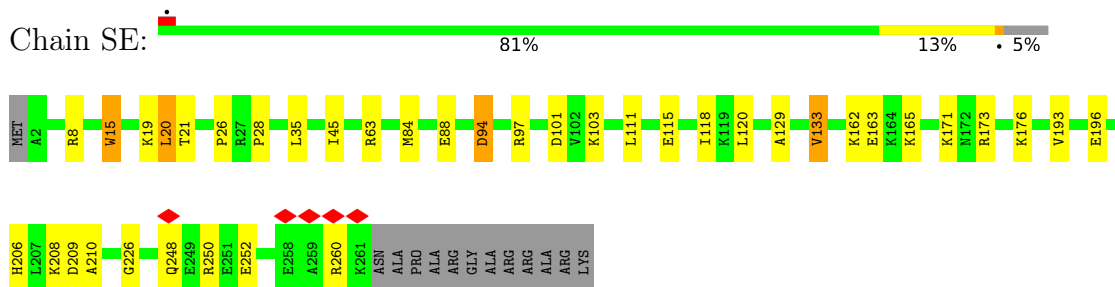
3 Residue-property plots

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.

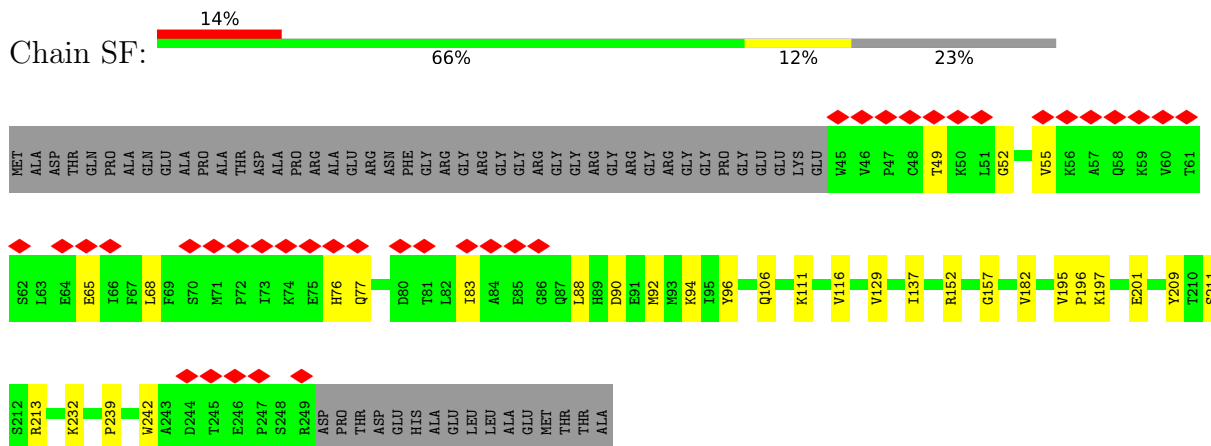
- Molecule 1: Putative 40S ribosomal protein S9



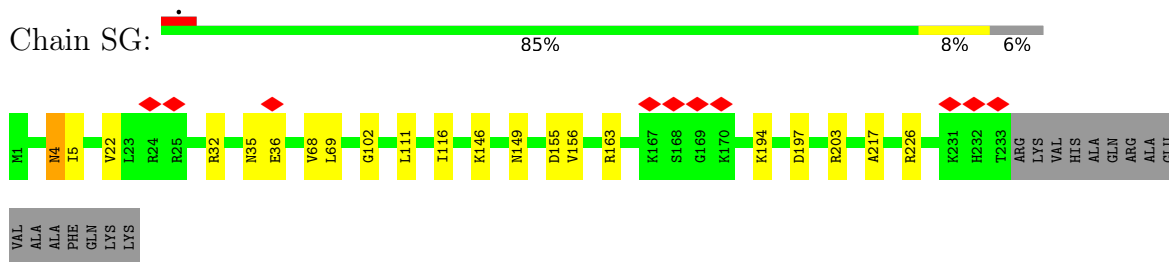
- Molecule 2: 40S ribosomal protein S4



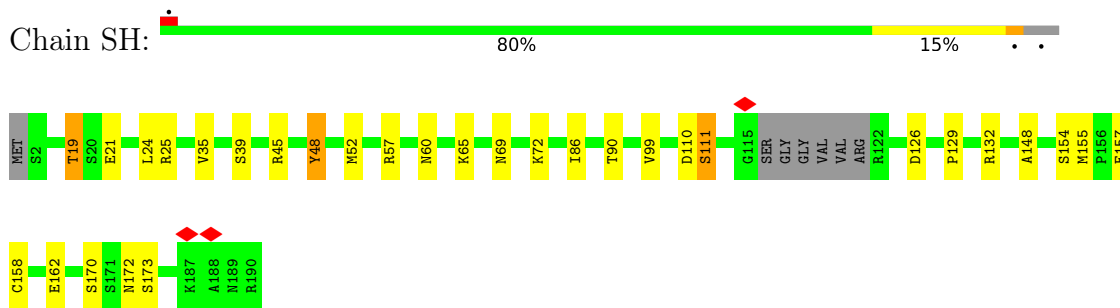
- Molecule 3: 40S ribosomal protein S2



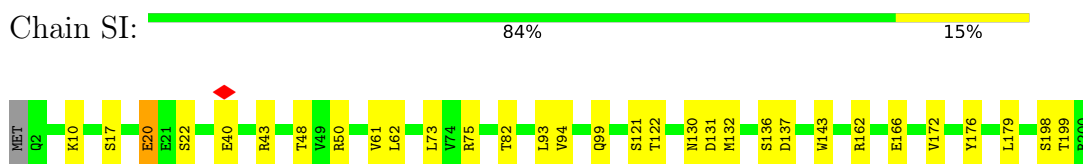
- Molecule 4: 40S ribosomal protein S6



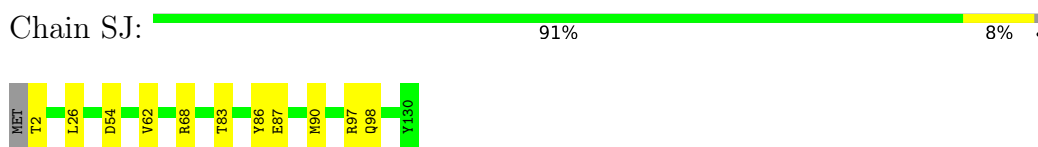
• Molecule 5: 40S ribosomal protein S5



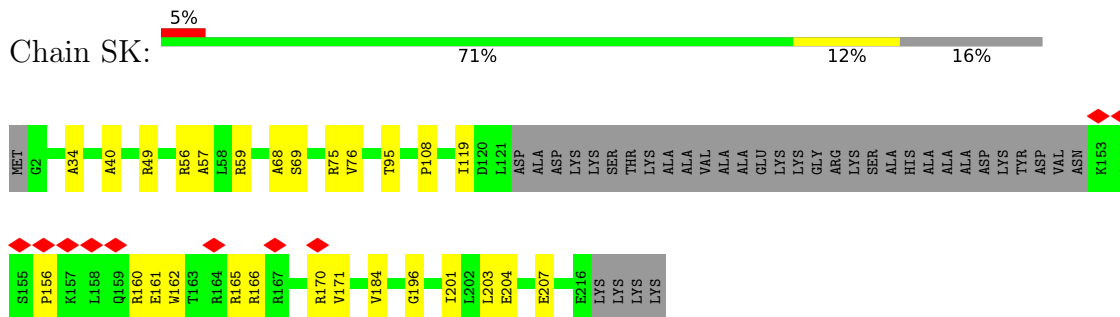
• Molecule 6: 40S ribosomal protein S7



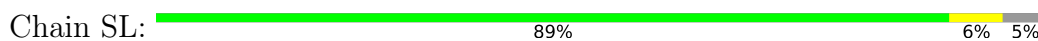
• Molecule 7: Putative 40S ribosomal protein S15A



• Molecule 8: 40S ribosomal protein S8



• Molecule 9: Putative 40S ribosomal protein S16





- Molecule 16: Putative 40S ribosomal protein S13

Chain ST: 81% 12% 7%



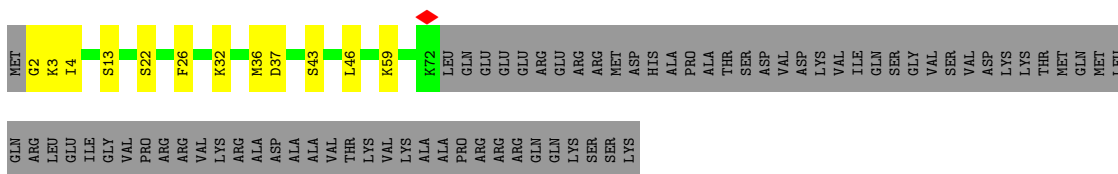
- Molecule 17: Putative 40S ribosomal protein S11

Chain SU: 6% 83% 6% 11%



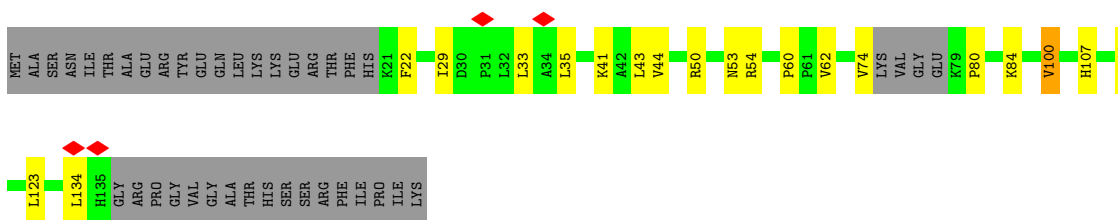
- Molecule 18: Putative 40S ribosomal protein S17

Chain SV: 41% 8% 50%



- Molecule 19: Putative 40S ribosomal protein S15

Chain SW: 60% 12% 27%

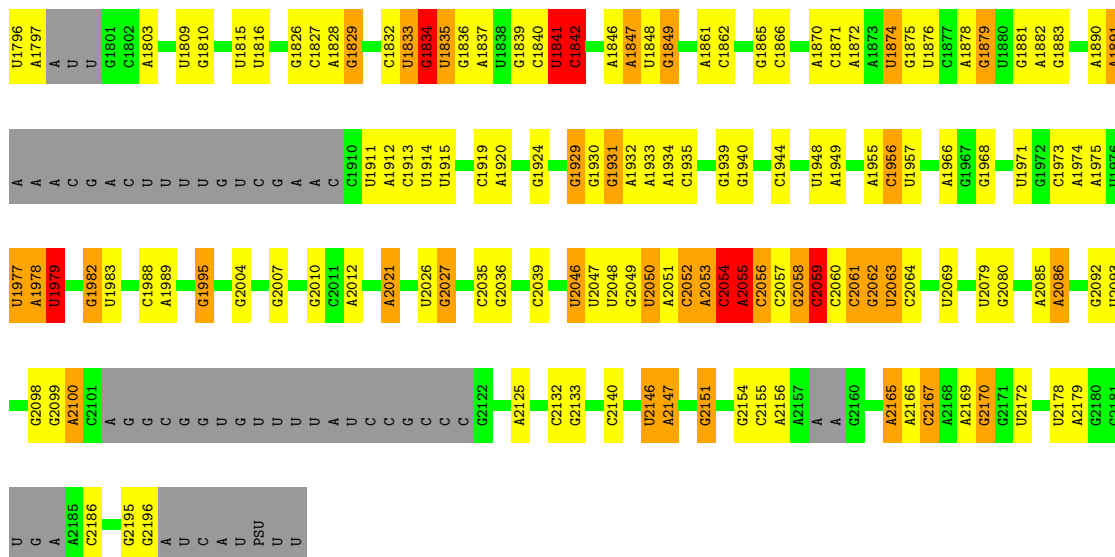


- Molecule 20: 40S ribosomal protein S19-like protein

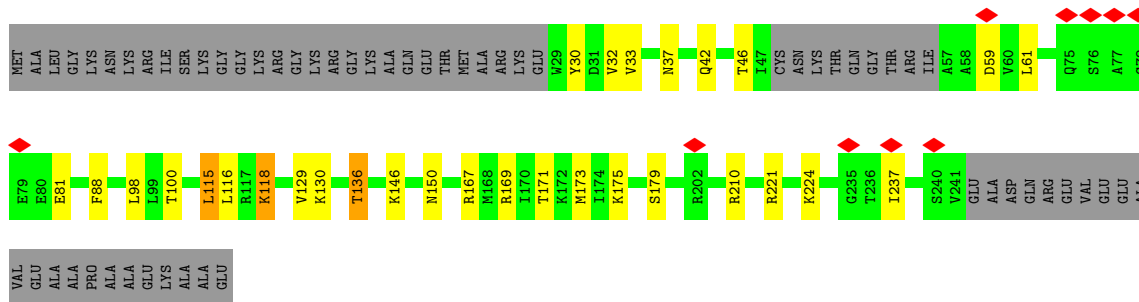
Chain SX: 74% 12% 13%



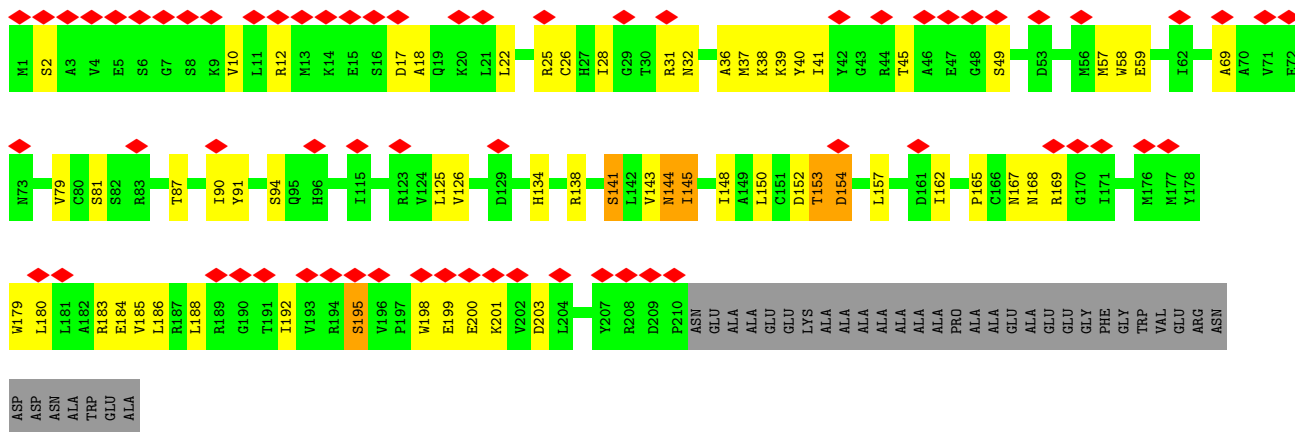
- Molecule 21: Putative 40S ribosomal protein S21



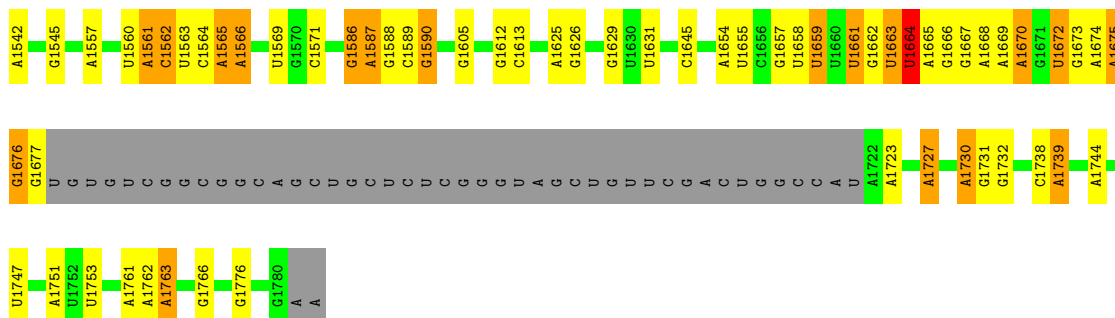
• Molecule 30: 40S ribosomal protein S3a



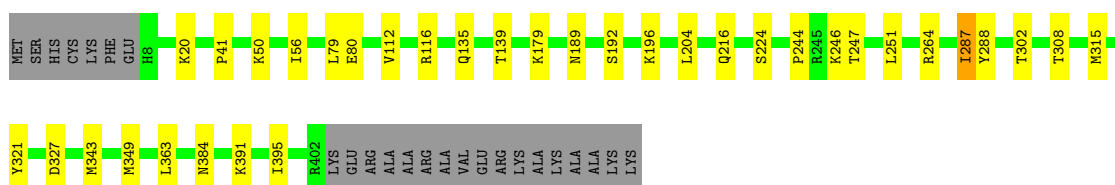
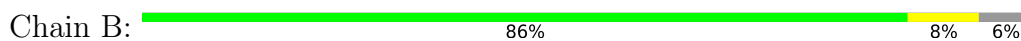
• Molecule 31: 40S ribosomal protein SA



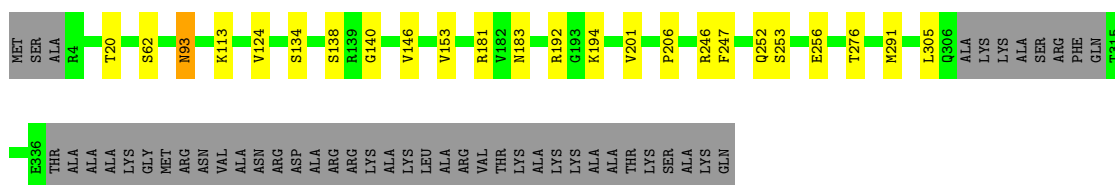
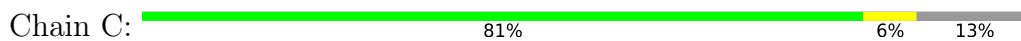
• Molecule 32: Putative 40S ribosomal protein S3



• Molecule 43: Putative ribosomal protein L3



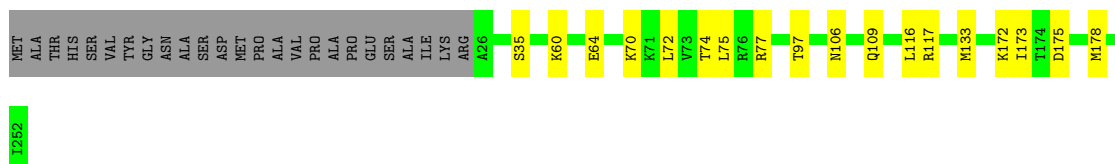
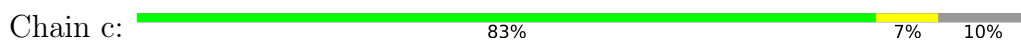
• Molecule 44: Putative ribosomal protein L1a



• Molecule 45: Putative 60S ribosomal protein L2

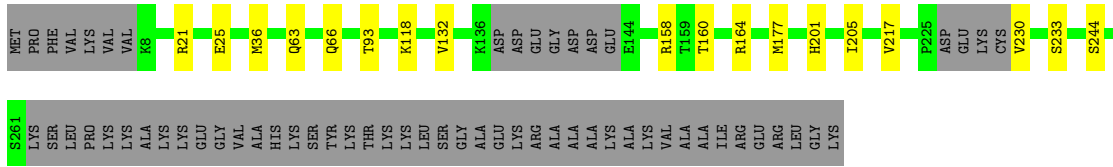


• Molecule 46: uL30_chain_c

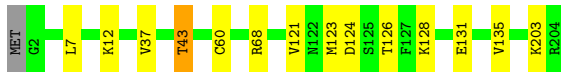


• Molecule 47: Putative 60S ribosomal protein L5

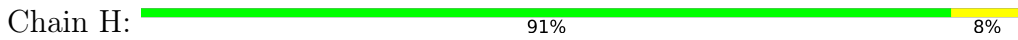




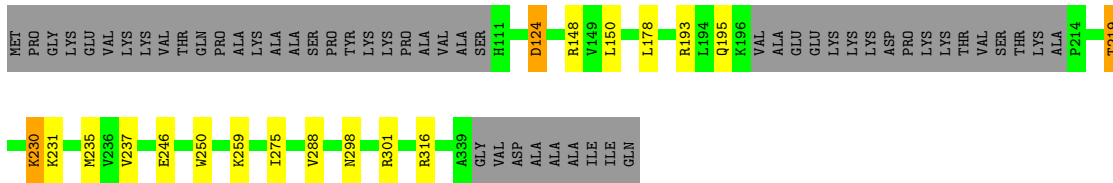
• Molecule 48: Ribosomal protein L15



• Molecule 49: Putative 60S ribosomal protein L13a



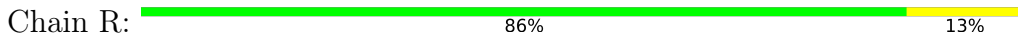
• Molecule 50: 60S ribosomal protein L7a



• Molecule 51: 60S ribosomal protein L18



• Molecule 52: 60S ribosomal protein L18a

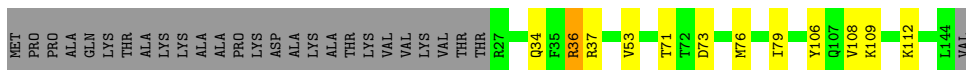


• Molecule 53: eL13_chain_I

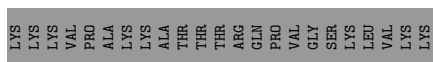
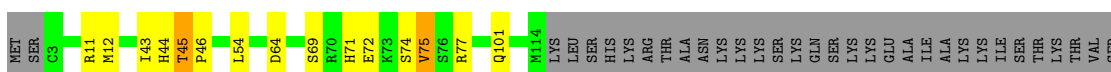




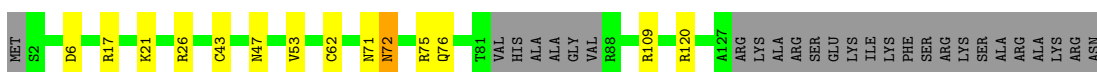
• Molecule 66: Putative 60S ribosomal protein L23a



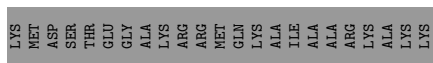
• Molecule 67: Putative 60S ribosomal protein L34



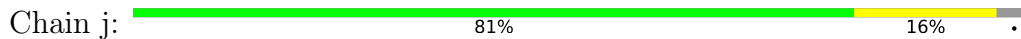
• Molecule 68: Putative 60S ribosomal protein L28



• Molecule 69: Putative 40S ribosomal protein L14

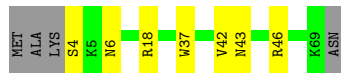
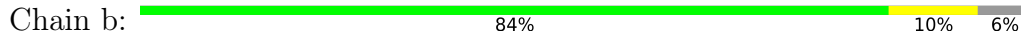


• Molecule 70: Ribosomal protein L37



• Molecule 71: Putative 60S Ribosomal protein L36

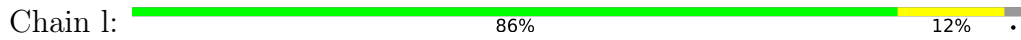




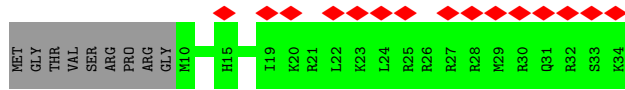
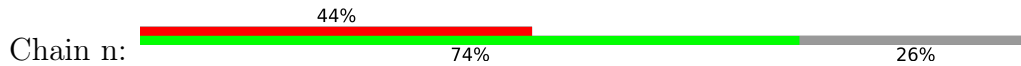
• Molecule 79: Putative ribosomal protein L38



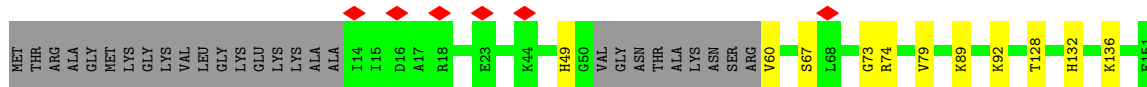
• Molecule 80: Putative 60S ribosomal protein L39



• Molecule 81: 60S ribosomal protein L41



• Molecule 82: Putative 60S ribosomal subunit protein L31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	742580	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.292	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	374.0, 374.0, 374.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, OMU, ZN, G7M, PSU, 5MC, C4J, K, OMG, NA, MG, 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	SD	0.14	0/1374	0.28	0/1850
2	SE	0.16	0/2104	0.30	0/2834
3	SF	0.14	0/1589	0.25	0/2152
4	SG	0.12	0/1836	0.22	0/2462
5	SH	0.29	0/1426	0.30	0/1919
6	SI	0.13	0/1613	0.24	0/2179
7	SJ	0.17	0/1034	0.23	0/1386
8	SK	0.17	0/1475	0.26	0/1978
9	SL	0.25	0/1132	0.28	0/1522
10	SM	0.21	0/817	0.30	0/1109
11	SN	0.54	2/813 (0.2%)	0.90	4/1103 (0.4%)
12	SO	0.31	0/989	0.41	0/1333
13	SP	0.15	0/1148	0.26	0/1538
14	SR	0.28	0/1099	0.33	0/1477
15	SS	0.22	0/422	0.32	0/565
16	ST	0.19	0/1163	0.28	0/1560
17	SU	0.17	0/1245	0.24	0/1677
18	SV	0.23	0/584	0.28	0/777
19	SW	0.23	0/885	0.29	0/1197
20	SX	0.26	0/1121	0.30	0/1512
21	SY	0.60	2/631 (0.3%)	0.81	3/863 (0.3%)
22	SZ	0.32	1/991 (0.1%)	0.53	3/1324 (0.2%)
23	Sa	0.26	0/554	0.34	0/745
24	Sb	0.36	0/676	0.53	0/906
25	Sc	0.14	0/637	0.26	0/862
26	Sd	0.25	0/388	0.27	0/517
27	Se	0.11	0/355	0.22	0/474
28	Sg	0.22	0/2225	0.33	0/3035
29	S1	0.29	0/38833	0.46	82/60463 (0.1%)
30	SA	0.24	0/1677	0.33	0/2260
31	SB	0.10	0/1629	0.27	0/2215
32	SC	0.18	0/1551	0.31	0/2080

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Sh	0.13	0/676	0.34	0/920
34	S4	0.24	0/399	0.33	0/618
35	8	0.29	0/2829	0.32	0/4405
36	6	0.36	0/1484	0.44	0/2306
37	2	0.50	1/21251 (0.0%)	0.49	25/33095 (0.1%)
38	7	0.51	0/3723	0.45	4/5795 (0.1%)
39	5	0.46	0/2340	0.42	0/3640
40	4	0.45	0/3746	0.38	0/5829
41	3	0.41	0/3605	0.39	0/5602
42	1	0.52	0/34332	0.47	31/53510 (0.1%)
43	B	0.40	0/3026	0.41	0/4105
44	C	0.40	0/2391	0.38	0/3249
45	A	0.40	0/1893	0.40	0/2556
46	c	0.38	0/1812	0.37	0/2440
47	O	0.24	0/1798	0.31	0/2435
48	M	0.46	0/1732	0.41	0/2316
49	H	0.37	0/1724	0.39	0/2330
50	G	0.35	0/1660	0.39	0/2241
51	P	0.41	0/1537	0.40	0/2057
52	R	0.34	0/1433	0.35	0/1943
53	I	0.37	0/1328	0.41	0/1792
54	Q	0.34	0/1307	0.35	0/1751
55	T	0.46	0/1241	0.46	0/1665
56	S	0.32	0/1190	0.31	0/1609
57	L	0.42	0/1141	0.42	0/1525
58	F	0.31	0/1051	0.34	0/1434
59	E	0.15	0/1042	0.29	0/1418
60	Y	0.30	0/1029	0.32	0/1389
61	f	0.48	0/1013	0.46	0/1358
62	g	0.44	0/1010	0.46	0/1360
63	a	0.33	0/965	0.31	0/1295
64	J	0.36	0/950	0.36	0/1291
65	W	0.35	0/941	0.47	2/1257 (0.2%)
66	V	0.40	0/932	0.40	0/1259
67	h	0.37	0/903	0.39	0/1207
68	Z	0.32	0/905	0.39	0/1221
69	K	0.25	0/897	0.29	0/1220
70	j	0.49	0/673	0.44	0/899
71	i	0.27	0/668	0.32	0/889
72	U	0.22	0/803	0.36	0/1082
73	p	0.34	0/649	0.37	0/864
74	o	0.36	0/670	0.47	0/897
75	D	0.15	0/658	0.27	0/889

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	d	0.26	0/617	0.28	0/848
77	X	0.36	0/569	0.36	0/767
78	b	0.34	0/531	0.35	0/712
79	k	0.24	0/515	0.26	0/699
80	l	0.47	0/453	0.41	0/606
81	n	0.12	0/159	0.20	0/215
82	e	0.36	0/1117	0.39	1/1505 (0.1%)
All	All	0.39	6/193334 (0.0%)	0.43	155/284189 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	SY	46	PRO	CG-CD	-13.62	1.04	1.50
11	SN	95	PRO	CG-CD	-12.32	1.08	1.50
22	SZ	35	PRO	CG-CD	-7.16	1.26	1.50
11	SN	95	PRO	N-CD	5.72	1.55	1.47
21	SY	46	PRO	N-CD	5.52	1.55	1.47

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1264	PSU	O3'-P-O5'	18.48	131.71	104.00
11	SN	95	PRO	N-CD-CG	-18.11	76.04	103.20
21	SY	46	PRO	N-CD-CG	-17.03	77.65	103.20
11	SN	95	PRO	CA-N-CD	-13.86	92.60	112.00
11	SN	95	PRO	CA-CB-CG	-12.10	81.50	104.50

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	SD	1347	0	1385	19	0
2	SE	2060	0	2166	27	0
3	SF	1555	0	1614	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	SG	1810	0	1893	14	0
5	SH	1404	0	1407	16	0
6	SI	1583	0	1620	18	0
7	SJ	1017	0	1046	7	0
8	SK	1453	0	1531	15	0
9	SL	1112	0	1170	4	0
10	SM	807	0	840	17	0
11	SN	791	0	762	15	0
12	SO	975	0	979	19	0
13	SP	1119	0	1168	9	0
14	SR	1077	0	1115	15	0
15	SS	417	0	398	8	0
16	ST	1140	0	1209	15	0
17	SU	1218	0	1231	6	0
18	SV	577	0	626	7	0
19	SW	866	0	858	11	0
20	SX	1092	0	1095	13	0
21	SY	622	0	588	8	0
22	SZ	972	0	1022	12	0
23	Sa	549	0	595	6	0
24	Sb	661	0	675	11	0
25	Sc	624	0	592	11	0
26	Sd	390	0	413	6	0
27	Se	350	0	369	3	0
28	Sg	2173	0	2023	25	0
29	S1	35569	0	17959	313	0
30	SA	1653	0	1727	22	0
31	SB	1595	0	1560	38	0
32	SC	1525	0	1557	19	0
33	Sh	668	0	624	15	0
34	S4	359	0	189	7	0
35	8	2531	0	1283	13	0
36	6	1329	0	678	17	0
37	2	20228	0	10271	132	0
38	7	3463	0	1758	14	0
39	5	2096	0	1065	10	0
40	4	3378	0	1714	26	0
41	3	3252	0	1650	32	0
42	1	31495	0	15888	188	0
43	B	2955	0	2926	20	0
44	C	2343	0	2272	11	0
45	A	1852	0	1830	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	c	1779	0	1822	9	0
47	O	1764	0	1693	8	0
48	M	1692	0	1759	6	0
49	H	1690	0	1732	12	0
50	G	1635	0	1702	10	0
51	P	1513	0	1610	6	0
52	R	1399	0	1393	17	0
53	I	1299	0	1317	12	0
54	Q	1290	0	1288	6	0
55	T	1217	0	1251	11	0
56	S	1164	0	1172	5	0
57	L	1114	0	1143	2	0
58	F	1032	0	1031	7	0
59	E	1032	0	966	8	0
60	Y	1008	0	1012	5	0
61	f	993	0	1025	3	0
62	g	989	0	1028	17	0
63	a	955	0	983	9	0
64	J	933	0	937	6	0
65	W	928	0	997	10	0
66	V	917	0	953	7	0
67	h	889	0	912	13	0
68	Z	892	0	885	9	0
69	K	883	0	855	7	0
70	j	659	0	667	7	0
71	i	660	0	714	7	0
72	U	795	0	734	8	0
73	p	640	0	657	6	0
74	o	659	0	656	10	0
75	D	649	0	516	7	0
76	d	607	0	549	8	0
77	X	548	0	553	1	0
78	b	520	0	531	4	0
79	k	508	0	493	6	0
80	l	440	0	461	4	0
81	n	159	0	122	0	0
82	e	1103	0	1097	8	0
83	1	52	0	0	0	0
83	2	25	0	0	0	0
83	3	1	0	0	0	0
83	5	1	0	0	0	0
83	7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	C	1	0	0	0	0
83	S1	30	0	0	0	0
83	SD	1	0	0	0	0
83	T	1	0	0	0	0
84	1	22	0	0	0	0
84	2	9	0	0	0	0
84	4	1	0	0	0	0
84	J	1	0	0	0	0
84	S1	23	0	0	0	0
84	SO	1	0	0	0	0
85	SS	1	0	0	0	0
85	Sb	1	0	0	0	0
85	j	1	0	0	0	0
85	o	1	0	0	0	0
86	1	3	0	0	0	0
86	2	3	0	0	0	0
86	4	1	0	0	0	0
86	8	1	0	0	0	0
86	S1	4	0	0	0	0
86	Sb	1	0	0	0	0
87	1	283	0	0	2	0
87	2	148	0	0	0	0
87	3	17	0	0	0	0
87	4	29	0	0	2	0
87	5	19	0	0	0	0
87	6	1	0	0	0	0
87	7	40	0	0	1	0
87	8	5	0	0	0	0
87	A	10	0	0	0	0
87	B	9	0	0	0	0
87	C	11	0	0	0	0
87	G	3	0	0	0	0
87	H	3	0	0	0	0
87	I	4	0	0	0	0
87	J	1	0	0	2	0
87	L	3	0	0	0	0
87	M	9	0	0	0	0
87	P	8	0	0	0	0
87	Q	4	0	0	0	0
87	R	1	0	0	0	0
87	S	1	0	0	0	0
87	S1	36	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	SH	1	0	0	0	0
87	SN	2	0	0	2	0
87	SR	1	0	0	0	0
87	ST	1	0	0	0	0
87	SX	1	0	0	0	0
87	T	7	0	0	0	0
87	V	2	0	0	0	0
87	W	1	0	0	0	0
87	X	1	0	0	0	0
87	a	1	0	0	0	0
87	c	3	0	0	0	0
87	d	1	0	0	1	0
87	e	3	0	0	1	0
87	f	2	0	0	0	0
87	g	1	0	0	0	0
87	h	3	0	0	0	0
87	j	7	0	0	0	0
87	l	4	0	0	0	0
All	All	183881	0	132557	1323	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 1323 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)
41:3:41:A:H62	41:3:188:C:N4	1.27	1.32
41:3:41:A:N6	41:3:188:C:H42	1.32	1.26
22:SZ:35:PRO:HD2	22:SZ:36:HIS:H	1.27	0.98
37:2:814:A:H62	37:2:964:G:H1	1.03	0.97
37:2:514:U:H3	37:2:518:G:H1	0.99	0.94

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	
1	SD	162/190 (85%)	154 (95%)	8 (5%)	0	100	100
2	SE	260/273 (95%)	254 (98%)	6 (2%)	0	100	100
3	SF	203/265 (77%)	198 (98%)	5 (2%)	0	100	100
4	SG	232/249 (93%)	231 (100%)	1 (0%)	0	100	100
5	SH	179/190 (94%)	171 (96%)	8 (4%)	0	100	100
6	SI	197/200 (98%)	191 (97%)	6 (3%)	0	100	100
7	SJ	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
8	SK	180/220 (82%)	178 (99%)	2 (1%)	0	100	100
9	SL	140/149 (94%)	132 (94%)	8 (6%)	0	100	100
10	SM	102/116 (88%)	99 (97%)	3 (3%)	0	100	100
11	SN	96/168 (57%)	88 (92%)	7 (7%)	1 (1%)	12	39
12	SO	132/144 (92%)	126 (96%)	6 (4%)	0	100	100
13	SP	143/143 (100%)	140 (98%)	3 (2%)	0	100	100
14	SR	134/153 (88%)	131 (98%)	3 (2%)	0	100	100
15	SS	52/57 (91%)	50 (96%)	2 (4%)	0	100	100
16	ST	138/151 (91%)	137 (99%)	1 (1%)	0	100	100
17	SU	152/173 (88%)	148 (97%)	4 (3%)	0	100	100
18	SV	69/143 (48%)	67 (97%)	2 (3%)	0	100	100
19	SW	107/152 (70%)	102 (95%)	5 (5%)	0	100	100
20	SX	138/161 (86%)	131 (95%)	7 (5%)	0	100	100
21	SY	86/164 (52%)	84 (98%)	2 (2%)	0	100	100
22	SZ	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
23	Sa	68/120 (57%)	65 (96%)	3 (4%)	0	100	100
24	Sb	82/112 (73%)	77 (94%)	5 (6%)	0	100	100
25	Sc	82/86 (95%)	75 (92%)	7 (8%)	0	100	100
26	Sd	48/87 (55%)	45 (94%)	3 (6%)	0	100	100
27	Se	42/66 (64%)	40 (95%)	2 (5%)	0	100	100
28	Sg	281/312 (90%)	265 (94%)	16 (6%)	0	100	100
30	SA	201/264 (76%)	197 (98%)	4 (2%)	0	100	100
31	SB	208/246 (85%)	204 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	SC	199/219 (91%)	195 (98%)	4 (2%)	0	100	100
33	Sh	93/235 (40%)	84 (90%)	9 (10%)	0	100	100
43	B	397/419 (95%)	381 (96%)	16 (4%)	0	100	100
44	C	321/373 (86%)	308 (96%)	13 (4%)	0	100	100
45	A	253/260 (97%)	245 (97%)	8 (3%)	0	100	100
46	c	225/252 (89%)	215 (96%)	10 (4%)	0	100	100
47	O	238/305 (78%)	225 (94%)	13 (6%)	0	100	100
48	M	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
49	H	218/222 (98%)	215 (99%)	3 (1%)	0	100	100
50	G	208/264 (79%)	199 (96%)	9 (4%)	0	100	100
51	P	194/198 (98%)	187 (96%)	7 (4%)	0	100	100
52	R	176/179 (98%)	173 (98%)	3 (2%)	0	100	100
53	I	165/220 (75%)	157 (95%)	8 (5%)	0	100	100
54	Q	166/254 (65%)	163 (98%)	3 (2%)	0	100	100
55	T	150/166 (90%)	140 (93%)	10 (7%)	0	100	100
56	S	149/159 (94%)	145 (97%)	4 (3%)	0	100	100
57	L	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
58	F	138/195 (71%)	131 (95%)	7 (5%)	0	100	100
59	E	140/190 (74%)	134 (96%)	6 (4%)	0	100	100
60	Y	130/134 (97%)	127 (98%)	3 (2%)	0	100	100
61	f	121/133 (91%)	116 (96%)	5 (4%)	0	100	100
62	g	122/144 (85%)	114 (93%)	8 (7%)	0	100	100
63	a	121/127 (95%)	120 (99%)	1 (1%)	0	100	100
64	J	127/139 (91%)	124 (98%)	3 (2%)	0	100	100
65	W	115/143 (80%)	113 (98%)	2 (2%)	0	100	100
66	V	116/145 (80%)	113 (97%)	3 (3%)	0	100	100
67	h	110/168 (66%)	105 (96%)	5 (4%)	0	100	100
68	Z	116/147 (79%)	114 (98%)	2 (2%)	0	100	100
69	K	115/175 (66%)	113 (98%)	2 (2%)	0	100	100
70	j	78/83 (94%)	75 (96%)	3 (4%)	0	100	100
71	i	82/105 (78%)	81 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	U	110/129 (85%)	106 (96%)	4 (4%)	0	100	100
73	p	79/106 (74%)	74 (94%)	5 (6%)	0	100	100
74	o	86/92 (94%)	78 (91%)	8 (9%)	0	100	100
75	D	94/188 (50%)	91 (97%)	3 (3%)	0	100	100
76	d	86/104 (83%)	85 (99%)	1 (1%)	0	100	100
77	X	62/124 (50%)	60 (97%)	2 (3%)	0	100	100
78	b	64/70 (91%)	64 (100%)	0	0	100	100
79	k	69/83 (83%)	67 (97%)	2 (3%)	0	100	100
80	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
81	n	23/34 (68%)	23 (100%)	0	0	100	100
82	e	145/188 (77%)	134 (92%)	11 (8%)	0	100	100
All	All	10153/12292 (83%)	9786 (96%)	366 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	SN	94	MET

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	SD	142/164 (87%)	134 (94%)	8 (6%)	19	50
2	SE	216/225 (96%)	211 (98%)	5 (2%)	44	76
3	SF	162/208 (78%)	158 (98%)	4 (2%)	42	74
4	SG	181/208 (87%)	177 (98%)	4 (2%)	45	77
5	SH	145/159 (91%)	139 (96%)	6 (4%)	27	61
6	SI	167/186 (90%)	159 (95%)	8 (5%)	23	55
7	SJ	109/111 (98%)	108 (99%)	1 (1%)	70	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	SK	141/176 (80%)	138 (98%)	3 (2%)	47	77
9	SL	112/120 (93%)	109 (97%)	3 (3%)	39	73
10	SM	92/104 (88%)	84 (91%)	8 (9%)	9	30
11	SN	82/128 (64%)	77 (94%)	5 (6%)	17	46
12	SO	95/113 (84%)	91 (96%)	4 (4%)	26	60
13	SP	115/117 (98%)	110 (96%)	5 (4%)	26	60
14	SR	111/130 (85%)	106 (96%)	5 (4%)	24	58
15	SS	41/49 (84%)	40 (98%)	1 (2%)	43	75
16	ST	122/132 (92%)	121 (99%)	1 (1%)	73	90
17	SU	126/152 (83%)	122 (97%)	4 (3%)	34	68
18	SV	62/126 (49%)	59 (95%)	3 (5%)	23	55
19	SW	87/130 (67%)	80 (92%)	7 (8%)	11	34
20	SX	109/131 (83%)	103 (94%)	6 (6%)	19	50
21	SY	62/116 (53%)	58 (94%)	4 (6%)	15	44
22	SZ	101/118 (86%)	98 (97%)	3 (3%)	36	70
23	Sa	62/95 (65%)	60 (97%)	2 (3%)	34	68
24	Sb	69/93 (74%)	60 (87%)	9 (13%)	4	13
25	Sc	62/76 (82%)	61 (98%)	1 (2%)	55	83
26	Sd	40/75 (53%)	37 (92%)	3 (8%)	12	37
27	Se	35/54 (65%)	33 (94%)	2 (6%)	18	49
28	Sg	226/265 (85%)	213 (94%)	13 (6%)	18	49
30	SA	178/222 (80%)	172 (97%)	6 (3%)	32	66
31	SB	165/202 (82%)	152 (92%)	13 (8%)	11	34
32	SC	156/184 (85%)	149 (96%)	7 (4%)	24	58
33	Sh	60/177 (34%)	55 (92%)	5 (8%)	10	32
43	B	283/351 (81%)	279 (99%)	4 (1%)	59	85
44	C	222/301 (74%)	209 (94%)	13 (6%)	18	48
45	A	178/204 (87%)	175 (98%)	3 (2%)	53	82
46	c	174/209 (83%)	171 (98%)	3 (2%)	53	82
47	O	150/242 (62%)	143 (95%)	7 (5%)	23	56
48	M	173/180 (96%)	167 (96%)	6 (4%)	32	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	H	165/188 (88%)	161 (98%)	4 (2%)	43	75
50	G	162/221 (73%)	154 (95%)	8 (5%)	22	54
51	P	157/164 (96%)	153 (98%)	4 (2%)	42	74
52	R	143/159 (90%)	135 (94%)	8 (6%)	19	50
53	I	130/183 (71%)	123 (95%)	7 (5%)	20	51
54	Q	117/198 (59%)	114 (97%)	3 (3%)	40	73
55	T	127/143 (89%)	122 (96%)	5 (4%)	28	63
56	S	117/134 (87%)	105 (90%)	12 (10%)	7	23
57	L	110/114 (96%)	105 (96%)	5 (4%)	24	58
58	F	99/153 (65%)	92 (93%)	7 (7%)	13	40
59	E	92/172 (54%)	87 (95%)	5 (5%)	20	51
60	Y	96/116 (83%)	90 (94%)	6 (6%)	16	45
61	f	104/115 (90%)	101 (97%)	3 (3%)	37	71
62	g	100/121 (83%)	96 (96%)	4 (4%)	28	62
63	a	93/118 (79%)	90 (97%)	3 (3%)	34	68
64	J	93/111 (84%)	91 (98%)	2 (2%)	45	77
65	W	98/122 (80%)	96 (98%)	2 (2%)	48	78
66	V	94/124 (76%)	89 (95%)	5 (5%)	20	52
67	h	87/146 (60%)	84 (97%)	3 (3%)	32	66
68	Z	89/118 (75%)	86 (97%)	3 (3%)	32	66
69	K	80/145 (55%)	76 (95%)	4 (5%)	22	53
70	j	66/70 (94%)	64 (97%)	2 (3%)	36	70
71	i	64/88 (73%)	60 (94%)	4 (6%)	16	45
72	U	64/114 (56%)	60 (94%)	4 (6%)	16	45
73	p	61/92 (66%)	59 (97%)	2 (3%)	33	67
74	o	62/74 (84%)	59 (95%)	3 (5%)	23	55
75	D	42/162 (26%)	34 (81%)	8 (19%)	1	5
76	d	58/89 (65%)	53 (91%)	5 (9%)	10	30
77	X	58/104 (56%)	57 (98%)	1 (2%)	53	82
78	b	52/58 (90%)	50 (96%)	2 (4%)	29	64
79	k	47/74 (64%)	46 (98%)	1 (2%)	47	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
80	l	44/47 (94%)	43 (98%)	1 (2%)	44	76
81	n	8/32 (25%)	8 (100%)	0	100	100
82	e	104/158 (66%)	99 (95%)	5 (5%)	23	55
All	All	7896/10260 (77%)	7560 (96%)	336 (4%)	27	60

5 of 336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	T	22	LEU
66	V	79	ILE
56	S	46	SER
59	E	91	VAL
71	i	5	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
54	Q	141	HIS
65	W	16	HIS
55	T	78	GLN
59	E	77	GLN
67	h	101	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	S1	1627/2204 (73%)	312 (19%)	19 (1%)
34	S4	15/20 (75%)	6 (40%)	0
35	8	118/123 (95%)	18 (15%)	0
36	6	61/73 (83%)	30 (49%)	2 (3%)
37	2	933/1522 (61%)	186 (19%)	12 (1%)
38	7	160/171 (93%)	32 (20%)	1 (0%)
39	5	94/135 (69%)	18 (19%)	0
40	4	153/183 (83%)	23 (15%)	1 (0%)
41	3	148/216 (68%)	29 (19%)	6 (4%)
42	1	1445/1782 (81%)	308 (21%)	20 (1%)
All	All	4754/6429 (73%)	962 (20%)	61 (1%)

5 of 962 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	S1	3	U
29	S1	17	C
29	S1	25	C
29	S1	26	A
29	S1	33	PSU

5 of 61 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
37	2	1052	C
42	1	1269	G
41	3	98	C
42	1	1135	U
42	1	1586	G

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

142 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
42	PSU	1	1181	42	18,21,22	1.40	2 (11%)	21,30,33	2.22	5 (23%)
37	A2M	2	604	37,42	22,25,26	3.31	9 (40%)	30,36,39	2.94	12 (40%)
42	PSU	1	1017	83,42	18,21,22	1.50	4 (22%)	21,30,33	2.26	4 (19%)
37	OMG	2	641	37	23,26,27	2.32	8 (34%)	32,38,41	2.49	13 (40%)
37	OMG	2	1078	37	23,26,27	2.30	8 (34%)	32,38,41	2.46	12 (37%)
37	PSU	2	472	37	18,21,22	1.42	3 (16%)	21,30,33	2.23	5 (23%)
29	PSU	S1	1156	29	18,21,22	1.39	3 (16%)	21,30,33	2.24	5 (23%)
29	PSU	S1	12	29	18,21,22	4.56	7 (38%)	21,30,33	1.97	5 (23%)
42	OMG	1	1524	42	23,26,27	2.34	9 (39%)	32,38,41	2.52	11 (34%)
37	PSU	2	510	37	18,21,22	4.76	9 (50%)	21,30,33	1.75	4 (19%)
29	OMC	S1	2140	29	19,22,23	2.96	8 (42%)	25,31,34	0.85	0
42	OMC	1	695	42	19,22,23	2.62	7 (36%)	25,31,34	0.88	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	A2M	2	1372	37	22,25,26	3.31	10 (45%)	30,36,39	3.21	12 (40%)
37	PSU	2	1354	37	18,21,22	4.36	7 (38%)	21,30,33	2.04	5 (23%)
29	PSU	S1	2046	29	18,21,22	1.46	3 (16%)	21,30,33	2.13	5 (23%)
37	PSU	2	1303	37	18,21,22	1.37	2 (11%)	21,30,33	2.20	5 (23%)
37	OMG	2	1360	37	23,26,27	2.39	8 (34%)	32,38,41	2.53	11 (34%)
42	OMU	1	845	42	19,22,23	2.73	6 (31%)	25,31,34	2.58	9 (36%)
29	OMG	S1	600	29	23,26,27	2.42	9 (39%)	32,38,41	2.65	10 (31%)
42	OMG	1	856	42	23,26,27	2.30	8 (34%)	32,38,41	2.42	13 (40%)
29	PSU	S1	1539	29	18,21,22	1.44	3 (16%)	21,30,33	2.21	5 (23%)
29	PSU	S1	1657	29	18,21,22	1.43	3 (16%)	21,30,33	2.25	4 (19%)
29	OMU	S1	1979	29	19,22,23	2.96	8 (42%)	25,31,34	1.84	5 (20%)
29	OMU	S1	661	29	19,22,23	3.00	8 (42%)	25,31,34	1.83	5 (20%)
29	PSU	S1	1533	29	18,21,22	1.45	3 (16%)	21,30,33	2.16	5 (23%)
37	PSU	2	1413	37	18,21,22	4.23	8 (44%)	21,30,33	2.05	4 (19%)
42	OMG	1	959[A]	42	23,26,27	2.41	9 (39%)	32,38,41	2.68	11 (34%)
37	PSU	2	78	37	18,21,22	1.47	4 (22%)	21,30,33	2.19	5 (23%)
37	OMU	2	667	37	19,22,23	2.76	7 (36%)	25,31,34	2.03	5 (20%)
37	A2M	2	382	37	22,25,26	3.35	10 (45%)	30,36,39	2.98	11 (36%)
29	PSU	S1	1192	29	18,21,22	1.39	3 (16%)	21,30,33	2.29	5 (23%)
38	PSU	7	69	38	18,21,22	1.40	3 (16%)	21,30,33	2.32	5 (23%)
42	OMU	1	1659	42	19,22,23	2.77	7 (36%)	25,31,34	1.86	5 (20%)
42	PSU	1	1533	37,42	18,21,22	1.45	3 (16%)	21,30,33	2.32	5 (23%)
42	PSU	1	870	83,42	18,21,22	4.27	8 (44%)	21,30,33	2.01	5 (23%)
29	PSU	S1	104	29	18,21,22	4.61	7 (38%)	21,30,33	1.94	5 (23%)
42	PSU	1	940	42	18,21,22	4.10	8 (44%)	21,30,33	2.18	4 (19%)
37	OMU	2	1359	37	19,22,23	2.85	8 (42%)	25,31,34	1.94	5 (20%)
38	A2M	7	162	38,42	22,25,26	3.27	10 (45%)	30,36,39	3.07	12 (40%)
37	A2M	2	527	37	22,25,26	3.35	10 (45%)	30,36,39	3.34	15 (50%)
38	OMG	7	75	38	23,26,27	1.23	3 (13%)	32,38,41	2.13	7 (21%)
37	A2M	2	1185	37	22,25,26	3.30	9 (40%)	30,36,39	3.00	13 (43%)
40	OMG	4	74	40	23,26,27	2.29	8 (34%)	32,38,41	2.58	13 (40%)
37	A2M	2	628	37	22,25,26	3.34	10 (45%)	30,36,39	3.19	12 (40%)
38	A2M	7	43	38	22,25,26	3.32	10 (45%)	30,36,39	3.12	11 (36%)
29	OMG	S1	2151	29	23,26,27	2.41	9 (39%)	32,38,41	2.63	10 (31%)
37	OMU	2	1077	37	19,22,23	2.88	8 (42%)	25,31,34	1.93	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	OMG	2	1231	37	23,26,27	2.32	8 (34%)	32,38,41	2.51	13 (40%)
37	PSU	2	593	37	18,21,22	1.50	3 (16%)	21,30,33	2.27	6 (28%)
42	PSU	1	1011	42	18,21,22	4.47	9 (50%)	21,30,33	2.11	6 (28%)
37	A2M	2	95	37	22,25,26	3.30	10 (45%)	30,36,39	2.99	13 (43%)
37	OMG	2	1253	37	23,26,27	2.28	8 (34%)	32,38,41	2.44	9 (28%)
42	A2M	1	235	42	22,25,26	3.31	10 (45%)	30,36,39	3.04	11 (36%)
42	OMG	1	959[B]	42	23,26,27	2.36	9 (39%)	32,38,41	2.21	9 (28%)
29	OMG	S1	1550	29	23,26,27	2.42	9 (39%)	32,38,41	2.55	10 (31%)
29	OMG	S1	1829	84,83,29	23,26,27	2.40	9 (39%)	32,38,41	2.57	10 (31%)
37	PSU	2	1060	37	18,21,22	1.45	3 (16%)	21,30,33	2.25	5 (23%)
37	OMG	2	71	37	23,26,27	1.25	3 (13%)	32,38,41	2.17	8 (25%)
29	OMC	S1	18	29	19,22,23	2.91	8 (42%)	25,31,34	0.76	0
29	PSU	S1	33	29	18,21,22	1.40	3 (16%)	21,30,33	2.14	4 (19%)
42	OMU	1	1107	42	19,22,23	2.87	8 (42%)	25,31,34	1.98	5 (20%)
37	PSU	2	1144	37	18,21,22	1.43	3 (16%)	21,30,33	2.25	5 (23%)
38	PSU	7	74	38	18,21,22	1.43	3 (16%)	21,30,33	2.15	5 (23%)
29	PSU	S1	609	29	18,21,22	1.40	3 (16%)	21,30,33	2.19	5 (23%)
42	A2M	1	407	42	22,25,26	3.36	10 (45%)	30,36,39	3.12	13 (43%)
42	A2M	1	1539	37,83,42	22,25,26	3.33	10 (45%)	30,36,39	3.04	13 (43%)
37	A2M	2	1384	37	22,25,26	3.32	10 (45%)	30,36,39	3.06	11 (36%)
37	OMU	2	73	37	19,22,23	1.36	3 (15%)	25,31,34	1.95	5 (20%)
42	PSU	1	422	42	18,21,22	1.51	5 (27%)	21,30,33	2.38	5 (23%)
42	OMU	1	847	42	19,22,23	2.78	7 (36%)	25,31,34	1.98	5 (20%)
37	OMC	2	583	37	19,22,23	2.67	7 (36%)	25,31,34	0.76	0
29	OMG	S1	1478	29	23,26,27	2.37	9 (39%)	32,38,41	2.52	10 (31%)
41	OMU	3	13	41	19,22,23	2.87	7 (36%)	25,31,34	2.36	7 (28%)
37	OMG	2	1046	37	23,26,27	2.40	9 (39%)	32,38,41	2.55	11 (34%)
29	OMG	S1	1647	29	23,26,27	2.43	9 (39%)	32,38,41	2.58	10 (31%)
29	OMC	S1	1866	29	19,22,23	2.82	8 (42%)	25,31,34	0.71	0
29	5MC	S1	2061	29	19,22,23	1.46	3 (15%)	26,32,35	1.23	4 (15%)
29	PSU	S1	455	29	18,21,22	4.61	7 (38%)	21,30,33	1.91	5 (23%)
42	PSU	1	672	84,83,42	18,21,22	1.46	3 (16%)	21,30,33	2.28	5 (23%)
42	PSU	1	1528	42	18,21,22	1.46	3 (16%)	21,30,33	2.25	5 (23%)
42	A2M	1	697	42	22,25,26	3.39	10 (45%)	30,36,39	3.06	11 (36%)
37	PSU	2	1194	37	18,21,22	4.37	7 (38%)	21,30,33	1.95	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	A2M	1	858	42	22,25,26	3.26	10 (45%)	30,36,39	3.17	14 (46%)
42	PSU	1	1171	42	18,21,22	4.34	9 (50%)	21,30,33	2.21	8 (38%)
42	PSU	1	1664	42	18,21,22	1.47	4 (22%)	21,30,33	2.27	4 (19%)
29	C4J	S1	1543	29	25,29,30	2.90	9 (36%)	28,42,45	1.47	3 (10%)
29	A2M	S1	2021	29	22,25,26	3.25	10 (45%)	30,36,39	3.18	13 (43%)
42	PSU	1	239	42	18,21,22	1.41	3 (16%)	21,30,33	2.25	5 (23%)
37	OMC	2	1159	37	19,22,23	2.70	7 (36%)	25,31,34	0.80	0
29	5MC	S1	1544	29	19,22,23	3.78	8 (42%)	26,32,35	0.99	2 (7%)
37	PSU	2	1058	37	18,21,22	1.43	3 (16%)	21,30,33	2.17	5 (23%)
29	OMG	S1	1865	29	23,26,27	2.41	9 (39%)	32,38,41	2.56	12 (37%)
37	OMC	2	1397	37	19,22,23	2.64	7 (36%)	25,31,34	0.81	0
37	PSU	2	1382	37,86	18,21,22	4.35	9 (50%)	21,30,33	1.99	5 (23%)
29	OMG	S1	1879	29	23,26,27	2.38	9 (39%)	32,38,41	2.63	10 (31%)
42	OMC	1	1527	42	19,22,23	0.87	0	25,31,34	0.94	1 (4%)
37	OMU	2	1152	37	19,22,23	2.82	7 (36%)	25,31,34	1.92	5 (20%)
38	OMU	7	7	38,42	19,22,23	2.87	7 (36%)	25,31,34	1.83	5 (20%)
37	OMC	2	1317	37	19,22,23	2.70	7 (36%)	25,31,34	0.80	1 (4%)
37	PSU	2	1264	37	18,21,22	1.49	3 (16%)	21,30,33	2.14	4 (19%)
37	5MC	2	1308	37	19,22,23	4.63	13 (68%)	26,32,35	1.37	2 (7%)
42	A2M	1	955	42	22,25,26	3.33	10 (45%)	30,36,39	3.11	13 (43%)
37	OMC	2	443	37,86	19,22,23	2.83	8 (42%)	25,31,34	0.91	0
42	OMG	1	1540	37,42	23,26,27	2.30	8 (34%)	32,38,41	2.38	13 (40%)
42	A2M	1	678	37,42	22,25,26	3.26	10 (45%)	30,36,39	3.03	13 (43%)
29	OMC	S1	38	29	19,22,23	2.95	8 (42%)	25,31,34	0.76	0
37	A2M	2	591	37	22,25,26	1.45	5 (22%)	30,36,39	2.12	10 (33%)
42	OMG	1	1190	42	23,26,27	2.40	9 (39%)	32,38,41	2.52	11 (34%)
37	PSU	2	597	37	18,21,22	1.46	3 (16%)	21,30,33	2.23	5 (23%)
42	OMC	1	1010	42	19,22,23	2.85	8 (42%)	25,31,34	0.88	1 (4%)
42	OMG	1	1626	42	23,26,27	2.26	8 (34%)	32,38,41	2.48	12 (37%)
42	PSU	1	1402	42	18,21,22	4.33	7 (38%)	21,30,33	1.90	5 (23%)
29	OMU	S1	8	29	19,22,23	2.98	8 (42%)	25,31,34	1.86	5 (20%)
29	OMG	S1	1623	29	23,26,27	1.21	3 (13%)	32,38,41	2.09	7 (21%)
29	A2M	S1	668	83,29	22,25,26	3.24	9 (40%)	30,36,39	3.12	11 (36%)
37	OMG	2	534	37	23,26,27	2.34	8 (34%)	32,38,41	2.57	10 (31%)
37	PSU	2	437	37	18,21,22	4.34	8 (44%)	21,30,33	2.05	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PSU	S1	1566	29	18,21,22	4.57	8 (44%)	21,30,33	1.82	3 (14%)
37	PSU	2	1361	37	18,21,22	4.49	8 (44%)	21,30,33	1.99	4 (19%)
42	A2M	1	681	42	22,25,26	3.28	10 (45%)	30,36,39	2.97	11 (36%)
29	PSU	S1	607	29	18,21,22	1.36	2 (11%)	21,30,33	2.25	6 (28%)
37	OMU	2	560	84,37	19,22,23	2.83	7 (36%)	25,31,34	1.88	4 (16%)
37	PSU	2	662	84,37	18,21,22	4.22	8 (44%)	21,30,33	1.93	4 (19%)
42	OMU	1	1371	42	19,22,23	2.91	8 (42%)	25,31,34	2.13	7 (28%)
37	PSU	2	512	37	18,21,22	4.64	7 (38%)	21,30,33	1.99	5 (23%)
37	PSU	2	626	37	18,21,22	4.25	8 (44%)	21,30,33	2.02	4 (19%)
42	A2M	1	927	42	22,25,26	3.32	10 (45%)	30,36,39	3.10	12 (40%)
37	A2M	2	572	37	22,25,26	3.33	10 (45%)	30,36,39	3.14	12 (40%)
37	OMG	2	1229	37	23,26,27	2.33	9 (39%)	32,38,41	2.53	13 (40%)
29	A2M	S1	512	84,29	22,25,26	1.49	5 (22%)	30,36,39	2.18	10 (33%)
29	PSU	S1	1246	29	18,21,22	1.41	2 (11%)	21,30,33	2.16	4 (19%)
37	PSU	2	1403	37	18,21,22	1.44	3 (16%)	21,30,33	2.29	5 (23%)
42	A2M	1	305	42	22,25,26	3.34	10 (45%)	30,36,39	3.08	15 (50%)
37	A2M	2	570	37,42	22,25,26	3.34	10 (45%)	30,36,39	3.22	15 (50%)
37	OMG	2	655	37	23,26,27	2.31	8 (34%)	32,38,41	2.50	12 (37%)
29	G7M	S1	1995	29	23,26,27	3.76	11 (47%)	34,39,42	1.74	8 (23%)
37	OMU	2	1419	37	19,22,23	2.81	7 (36%)	25,31,34	1.91	5 (20%)
29	PSU	S1	2048	29	18,21,22	1.43	3 (16%)	21,30,33	2.27	5 (23%)
29	PSU	S1	1841	29	18,21,22	1.45	3 (16%)	21,30,33	2.22	5 (23%)
37	OMC	2	1248	37	19,22,23	2.73	7 (36%)	25,31,34	1.00	1 (4%)
37	OMC	2	359	37	19,22,23	2.83	8 (42%)	25,31,34	0.71	0
37	PSU	2	1318	37	18,21,22	4.24	8 (44%)	21,30,33	2.02	4 (19%)

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
42	PSU	1	1181	42	-	3/7/25/26	0/2/2/2
37	A2M	2	604	37,42	-	1/9/27/28	0/3/3/3
42	PSU	1	1017	83,42	-	0/7/25/26	0/2/2/2
37	OMG	2	641	37	-	0/9/27/28	0/3/3/3
37	OMG	2	1078	37	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PSU	2	472	37	-	0/7/25/26	0/2/2/2
29	PSU	S1	1156	29	-	0/7/25/26	0/2/2/2
29	PSU	S1	12	29	-	0/7/25/26	0/2/2/2
42	OMG	1	1524	42	-	1/9/27/28	0/3/3/3
37	PSU	2	510	37	-	5/7/25/26	0/2/2/2
29	OMC	S1	2140	29	-	2/9/27/28	0/2/2/2
42	OMC	1	695	42	-	2/9/27/28	0/2/2/2
37	A2M	2	1372	37	-	0/9/27/28	0/3/3/3
37	PSU	2	1354	37	-	0/7/25/26	0/2/2/2
29	PSU	S1	2046	29	-	2/7/25/26	0/2/2/2
37	PSU	2	1303	37	-	0/7/25/26	0/2/2/2
37	OMG	2	1360	37	-	0/9/27/28	0/3/3/3
42	OMU	1	845	42	-	2/9/27/28	0/2/2/2
29	OMG	S1	600	29	-	2/9/27/28	0/3/3/3
42	OMG	1	856	42	-	0/9/27/28	0/3/3/3
29	PSU	S1	1539	29	-	0/7/25/26	0/2/2/2
29	PSU	S1	1657	29	-	2/7/25/26	0/2/2/2
29	OMU	S1	1979	29	-	1/9/27/28	0/2/2/2
29	OMU	S1	661	29	-	0/9/27/28	0/2/2/2
29	PSU	S1	1533	29	-	0/7/25/26	0/2/2/2
37	PSU	2	1413	37	-	0/7/25/26	0/2/2/2
42	OMG	1	959[A]	42	-	2/9/27/28	0/3/3/3
37	PSU	2	78	37	-	2/7/25/26	0/2/2/2
37	OMU	2	667	37	-	1/9/27/28	0/2/2/2
37	A2M	2	382	37	-	0/9/27/28	0/3/3/3
29	PSU	S1	1192	29	-	0/7/25/26	0/2/2/2
38	PSU	7	69	38	-	0/7/25/26	0/2/2/2
42	OMU	1	1659	42	-	0/9/27/28	0/2/2/2
42	PSU	1	1533	37,42	-	1/7/25/26	0/2/2/2
42	PSU	1	870	83,42	-	1/7/25/26	0/2/2/2
29	PSU	S1	104	29	-	2/7/25/26	0/2/2/2
42	PSU	1	940	42	-	0/7/25/26	0/2/2/2
37	OMU	2	1359	37	-	0/9/27/28	0/2/2/2
38	A2M	7	162	38,42	-	1/9/27/28	0/3/3/3
37	A2M	2	527	37	-	0/9/27/28	0/3/3/3
38	OMG	7	75	38	-	3/9/27/28	0/3/3/3
37	A2M	2	1185	37	-	2/9/27/28	0/3/3/3
40	OMG	4	74	40	-	0/9/27/28	0/3/3/3
37	A2M	2	628	37	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	A2M	7	43	38	-	0/9/27/28	0/3/3/3
29	OMG	S1	2151	29	-	2/9/27/28	0/3/3/3
37	OMU	2	1077	37	-	1/9/27/28	0/2/2/2
37	OMG	2	1231	37	-	0/9/27/28	0/3/3/3
37	PSU	2	593	37	-	0/7/25/26	0/2/2/2
42	PSU	1	1011	42	-	2/7/25/26	0/2/2/2
37	A2M	2	95	37	-	0/9/27/28	0/3/3/3
37	OMG	2	1253	37	-	0/9/27/28	0/3/3/3
42	A2M	1	235	42	-	1/9/27/28	0/3/3/3
42	OMG	1	959[B]	42	-	0/9/27/28	0/3/3/3
29	OMG	S1	1550	29	-	2/9/27/28	0/3/3/3
29	OMG	S1	1829	84,83,29	-	1/9/27/28	0/3/3/3
37	PSU	2	1060	37	-	2/7/25/26	0/2/2/2
37	OMG	2	71	37	-	2/9/27/28	0/3/3/3
29	OMC	S1	18	29	-	1/9/27/28	0/2/2/2
29	PSU	S1	33	29	-	4/7/25/26	0/2/2/2
42	OMU	1	1107	42	-	2/9/27/28	0/2/2/2
37	PSU	2	1144	37	-	1/7/25/26	0/2/2/2
38	PSU	7	74	38	-	2/7/25/26	0/2/2/2
29	PSU	S1	609	29	-	0/7/25/26	0/2/2/2
42	A2M	1	407	42	-	2/9/27/28	0/3/3/3
42	A2M	1	1539	37,83,42	-	1/9/27/28	0/3/3/3
37	A2M	2	1384	37	-	0/9/27/28	0/3/3/3
37	OMU	2	73	37	-	1/9/27/28	0/2/2/2
42	PSU	1	422	42	-	2/7/25/26	0/2/2/2
42	OMU	1	847	42	-	0/9/27/28	0/2/2/2
37	OMC	2	583	37	-	1/9/27/28	0/2/2/2
29	OMG	S1	1478	29	-	0/9/27/28	0/3/3/3
41	OMU	3	13	41	-	3/9/27/28	0/2/2/2
37	OMG	2	1046	37	-	3/9/27/28	0/3/3/3
29	OMG	S1	1647	29	-	0/9/27/28	0/3/3/3
29	OMC	S1	1866	29	-	0/9/27/28	0/2/2/2
29	5MC	S1	2061	29	-	0/7/25/26	0/2/2/2
29	PSU	S1	455	29	-	3/7/25/26	0/2/2/2
42	PSU	1	672	84,83,42	-	2/7/25/26	0/2/2/2
42	PSU	1	1528	42	-	2/7/25/26	0/2/2/2
42	A2M	1	697	42	-	0/9/27/28	0/3/3/3
37	PSU	2	1194	37	-	0/7/25/26	0/2/2/2
42	A2M	1	858	42	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	PSU	1	1171	42	-	2/7/25/26	0/2/2/2
42	PSU	1	1664	42	-	2/7/25/26	0/2/2/2
29	C4J	S1	1543	29	-	8/16/34/35	0/2/2/2
29	A2M	S1	2021	29	-	2/9/27/28	0/3/3/3
42	PSU	1	239	42	-	0/7/25/26	0/2/2/2
37	OMC	2	1159	37	-	0/9/27/28	0/2/2/2
29	5MC	S1	1544	29	-	2/7/25/26	0/2/2/2
37	PSU	2	1058	37	-	1/7/25/26	0/2/2/2
29	OMG	S1	1865	29	-	1/9/27/28	0/3/3/3
37	OMC	2	1397	37	-	0/9/27/28	0/2/2/2
37	PSU	2	1382	37,86	-	0/7/25/26	0/2/2/2
29	OMG	S1	1879	29	-	0/9/27/28	0/3/3/3
42	OMC	1	1527	42	-	2/9/27/28	0/2/2/2
37	OMU	2	1152	37	-	0/9/27/28	0/2/2/2
38	OMU	7	7	38,42	-	0/9/27/28	0/2/2/2
37	OMC	2	1317	37	-	0/9/27/28	0/2/2/2
37	PSU	2	1264	37	-	0/7/25/26	0/2/2/2
37	5MC	2	1308	37	-	4/7/25/26	0/2/2/2
42	A2M	1	955	42	-	0/9/27/28	0/3/3/3
37	OMC	2	443	37,86	-	5/9/27/28	0/2/2/2
42	OMG	1	1540	37,42	-	2/9/27/28	0/3/3/3
42	A2M	1	678	37,42	-	0/9/27/28	0/3/3/3
29	OMC	S1	38	29	-	0/9/27/28	0/2/2/2
37	A2M	2	591	37	-	1/9/27/28	0/3/3/3
42	OMG	1	1190	42	-	0/9/27/28	0/3/3/3
37	PSU	2	597	37	-	2/7/25/26	0/2/2/2
42	OMC	1	1010	42	-	1/9/27/28	0/2/2/2
42	OMG	1	1626	42	-	1/9/27/28	0/3/3/3
42	PSU	1	1402	42	-	5/7/25/26	0/2/2/2
29	OMU	S1	8	29	-	6/9/27/28	0/2/2/2
29	OMG	S1	1623	29	-	1/9/27/28	0/3/3/3
29	A2M	S1	668	83,29	-	4/9/27/28	0/3/3/3
37	OMG	2	534	37	-	2/9/27/28	0/3/3/3
37	PSU	2	437	37	-	2/7/25/26	0/2/2/2
29	PSU	S1	1566	29	-	2/7/25/26	0/2/2/2
37	PSU	2	1361	37	-	4/7/25/26	0/2/2/2
42	A2M	1	681	42	-	2/9/27/28	0/3/3/3
29	PSU	S1	607	29	-	5/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	OMU	2	560	84,37	-	1/9/27/28	0/2/2/2
37	PSU	2	662	84,37	-	0/7/25/26	0/2/2/2
42	OMU	1	1371	42	-	4/9/27/28	0/2/2/2
37	PSU	2	512	37	-	2/7/25/26	0/2/2/2
37	PSU	2	626	37	-	0/7/25/26	0/2/2/2
42	A2M	1	927	42	-	0/9/27/28	0/3/3/3
37	A2M	2	572	37	-	0/9/27/28	0/3/3/3
37	OMG	2	1229	37	-	0/9/27/28	0/3/3/3
29	A2M	S1	512	84,29	-	3/9/27/28	0/3/3/3
29	PSU	S1	1246	29	-	0/7/25/26	0/2/2/2
37	PSU	2	1403	37	-	0/7/25/26	0/2/2/2
42	A2M	1	305	42	-	2/9/27/28	0/3/3/3
37	A2M	2	570	37,42	-	6/9/27/28	0/3/3/3
37	OMG	2	655	37	-	0/9/27/28	0/3/3/3
29	G7M	S1	1995	29	-	2/7/25/26	0/3/3/3
37	OMU	2	1419	37	-	0/9/27/28	0/2/2/2
29	PSU	S1	2048	29	-	0/7/25/26	0/2/2/2
29	PSU	S1	1841	29	-	2/7/25/26	0/2/2/2
37	OMC	2	1248	37	-	1/9/27/28	0/2/2/2
37	OMC	2	359	37	-	0/9/27/28	0/2/2/2
37	PSU	2	1318	37	-	0/7/25/26	0/2/2/2

The worst 5 of 987 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	510	PSU	C6-C5	12.70	1.49	1.35
37	2	512	PSU	C6-C5	12.24	1.48	1.35
29	S1	455	PSU	C6-C5	12.18	1.48	1.35
29	S1	1566	PSU	C6-C5	12.00	1.48	1.35
29	S1	104	PSU	C6-C5	11.98	1.48	1.35

The worst 5 of 986 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1	959[A]	OMG	C1'-N9-C8	-8.28	103.20	126.73
29	S1	600	OMG	C1'-N9-C8	-8.13	103.63	126.73
29	S1	2151	OMG	C1'-N9-C8	-8.04	103.88	126.73
29	S1	1879	OMG	C1'-N9-C8	-8.00	104.00	126.73
29	S1	1829	OMG	C1'-N9-C8	-7.95	104.14	126.73

There are no chirality outliers.

5 of 173 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	2	71	OMG	C1'-C2'-O2'-CM2
37	2	73	OMU	C1'-C2'-O2'-CM2
37	2	78	PSU	O4'-C4'-C5'-O5'
37	2	437	PSU	C3'-C4'-C5'-O5'
37	2	437	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

54 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	1	1181	PSU	1	0
37	2	604	A2M	3	0
37	2	472	PSU	1	0
29	S1	1156	PSU	2	0
42	1	695	OMC	1	0
37	2	1372	A2M	1	0
29	S1	2046	PSU	2	0
37	2	1303	PSU	1	0
42	1	845	OMU	2	0
29	S1	600	OMG	1	0
29	S1	1657	PSU	1	0
29	S1	1979	OMU	2	0
29	S1	661	OMU	2	0
42	1	959[A]	OMG	1	0
37	2	667	OMU	1	0
29	S1	1192	PSU	1	0
38	7	69	PSU	1	0
42	1	1659	OMU	1	0
40	4	74	OMG	1	0
42	1	959[B]	OMG	3	0
37	2	71	OMG	1	0
38	7	74	PSU	1	0
29	S1	609	PSU	2	0
42	1	407	A2M	1	0
42	1	1539	A2M	1	0
37	2	73	OMU	1	0
42	1	422	PSU	1	0
42	1	847	OMU	1	0
41	3	13	OMU	2	0
37	2	1046	OMG	1	0
29	S1	2061	5MC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	1	672	PSU	1	0
42	1	1664	PSU	2	0
42	1	239	PSU	1	0
37	2	1058	PSU	1	0
29	S1	1879	OMG	1	0
38	7	7	OMU	1	0
37	2	1264	PSU	2	0
37	2	1308	5MC	1	0
42	1	955	A2M	1	0
37	2	591	A2M	2	0
42	1	1010	OMC	1	0
29	S1	1623	OMG	1	0
42	1	681	A2M	1	0
29	S1	607	PSU	1	0
37	2	560	OMU	1	0
37	2	512	PSU	2	0
29	S1	512	A2M	2	0
29	S1	1246	PSU	1	0
42	1	305	A2M	5	0
37	2	570	A2M	1	0
37	2	655	OMG	1	0
29	S1	1995	G7M	1	0
29	S1	1841	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 188 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

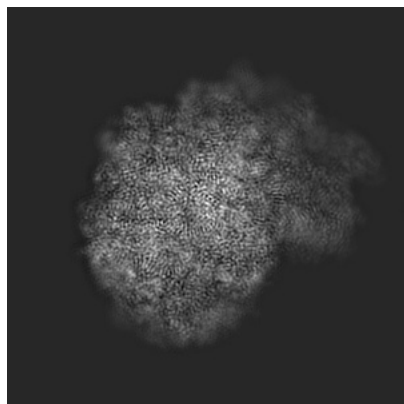
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15124. These allow visual inspection of the internal detail of the map and identification of artifacts.

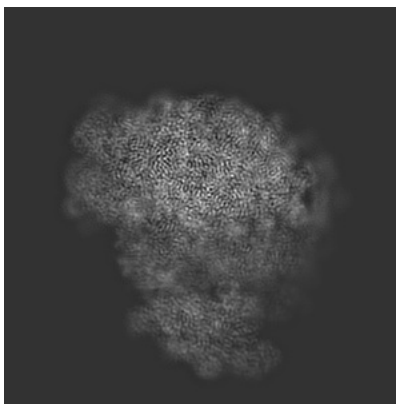
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

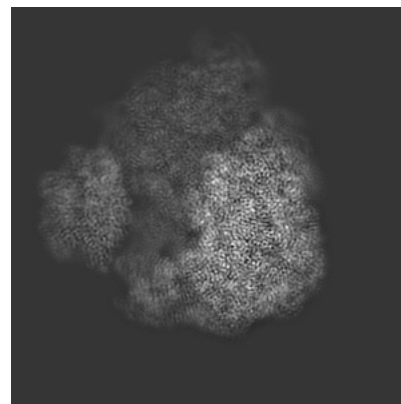
6.1.1 Primary map



X

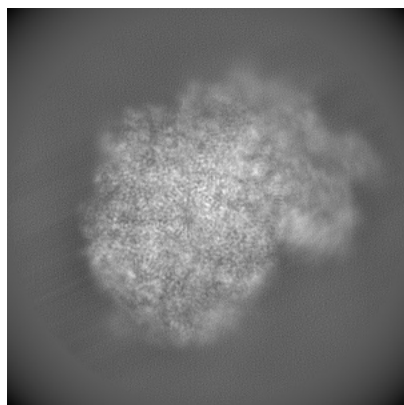


Y

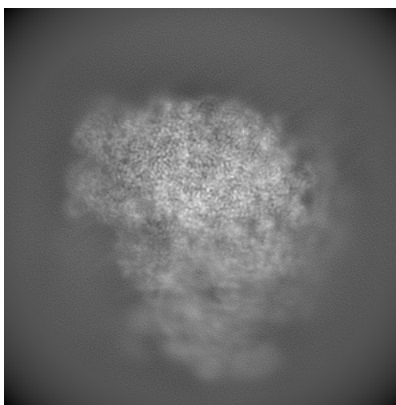


Z

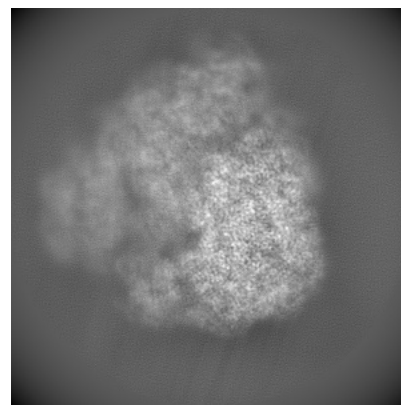
6.1.2 Raw map



X



Y

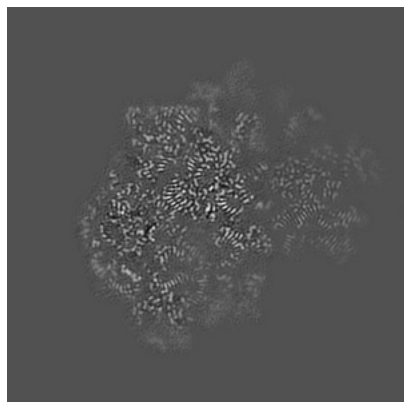


Z

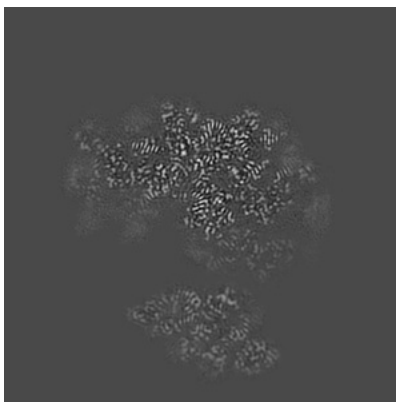
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

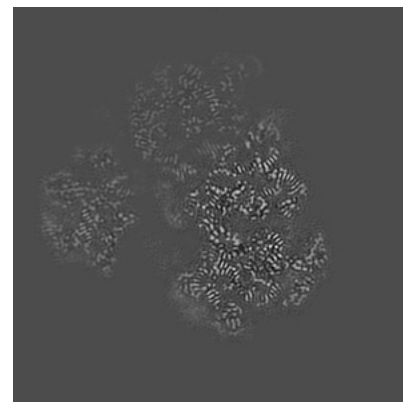
6.2.1 Primary map



X Index: 220

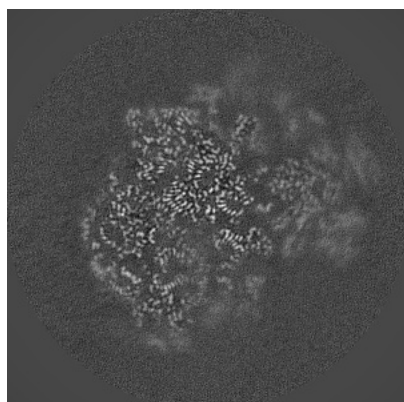


Y Index: 220

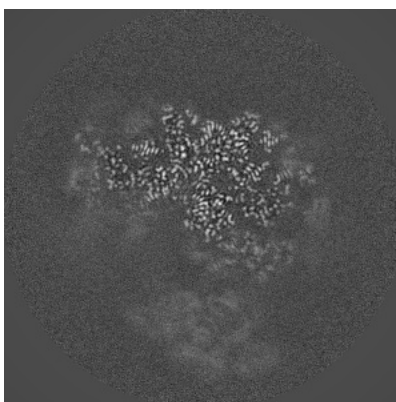


Z Index: 220

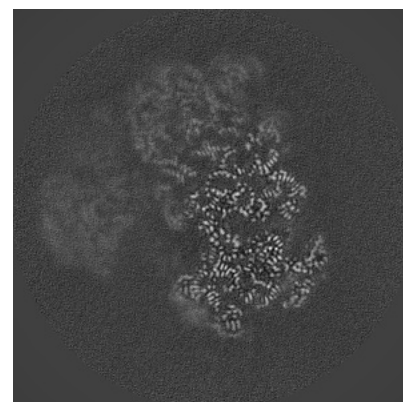
6.2.2 Raw map



X Index: 220



Y Index: 220

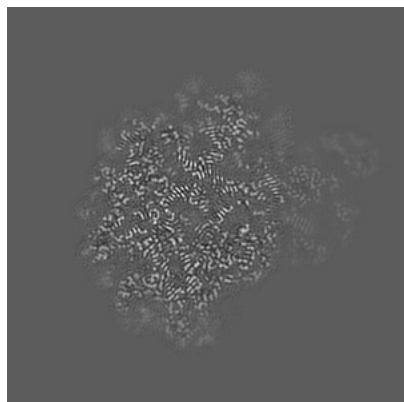


Z Index: 220

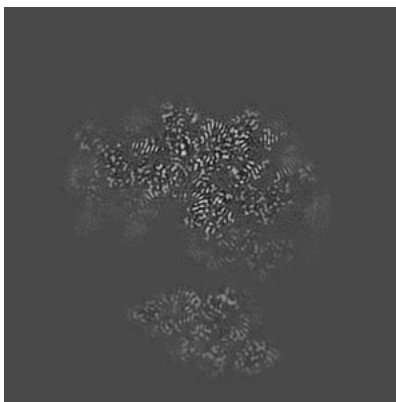
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

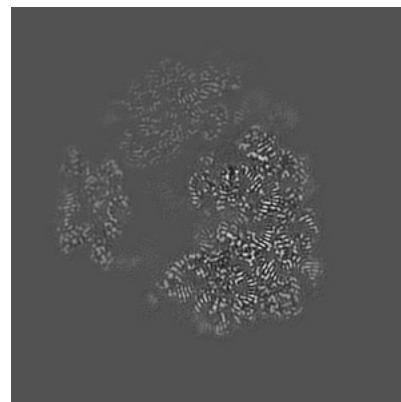
6.3.1 Primary map



X Index: 255

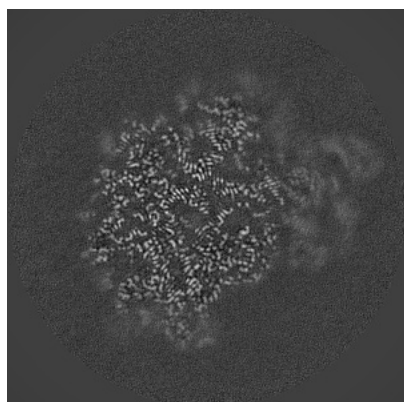


Y Index: 220

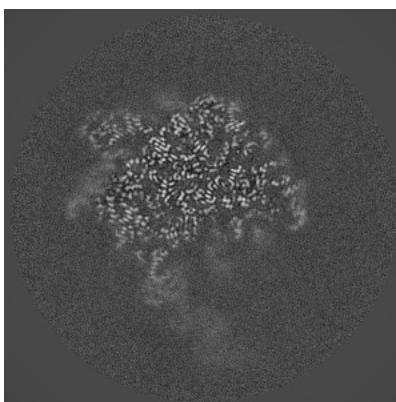


Z Index: 198

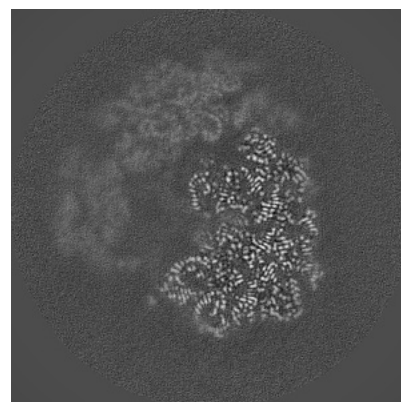
6.3.2 Raw map



X Index: 255



Y Index: 162

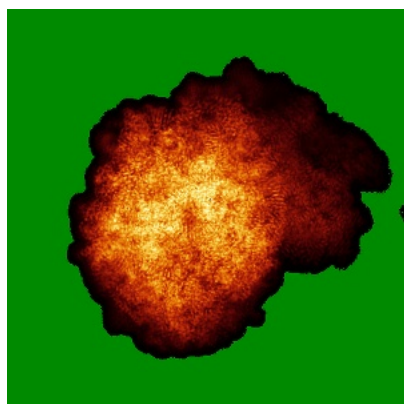


Z Index: 199

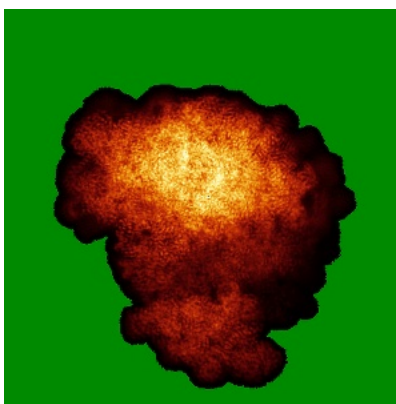
The images above show the largest variance slices of the map in three orthogonal directions.

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

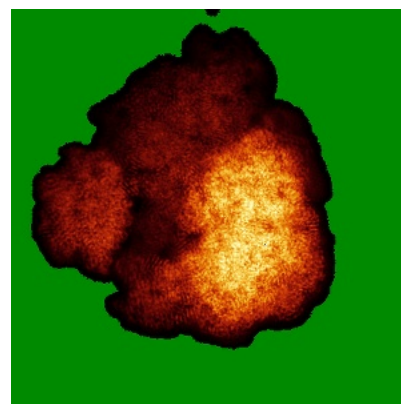
6.4.1 Primary map



X

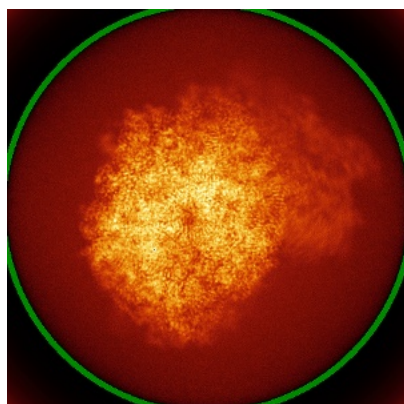


Y

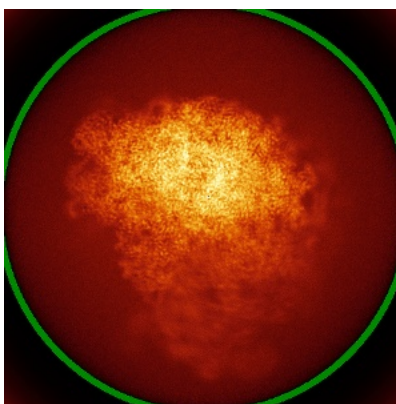


Z

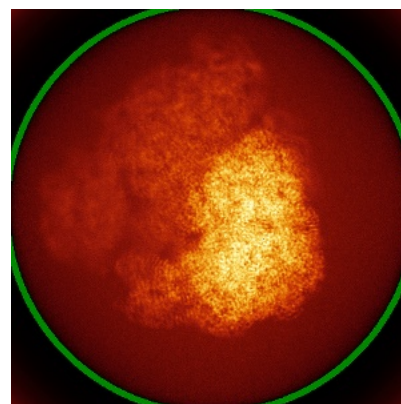
6.4.2 Raw map



X



Y

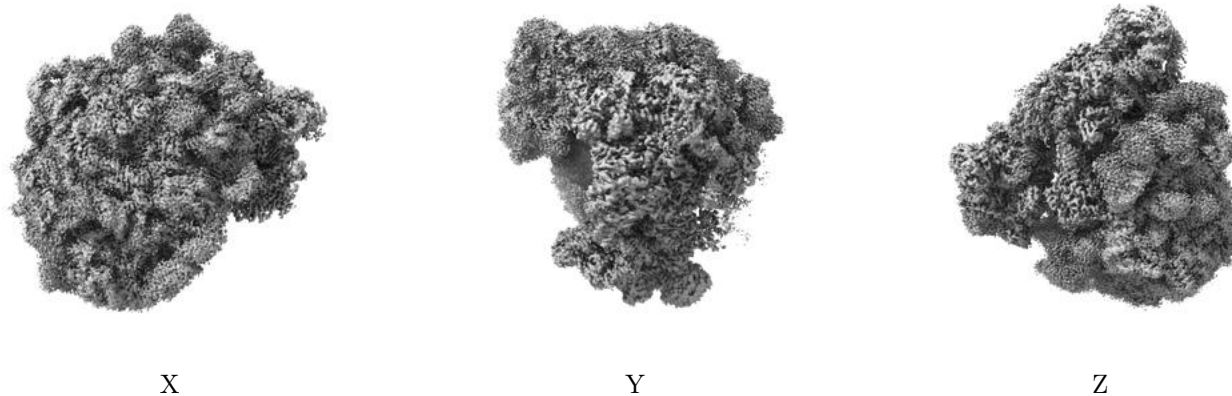


Z

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.

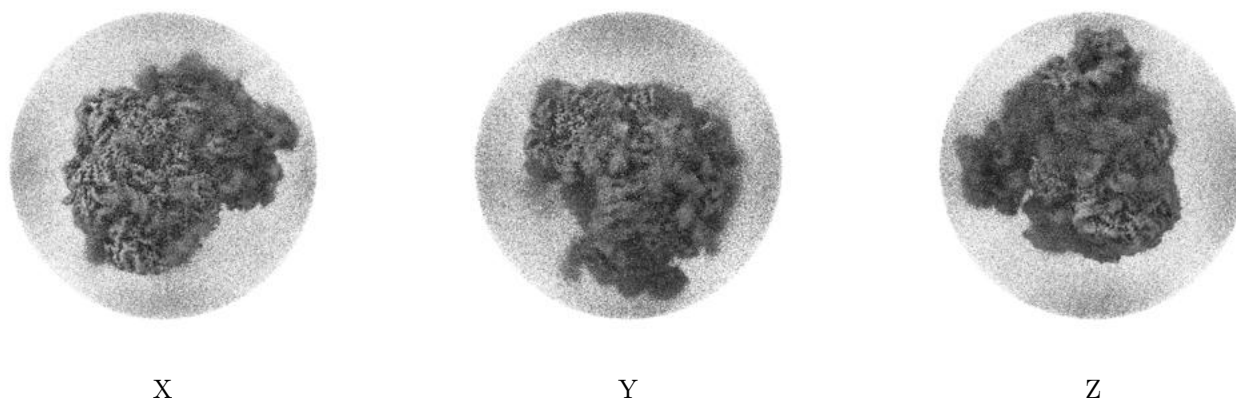
6.5 Orthogonal surface views [i](#)

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.

6.5.2 Raw map



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

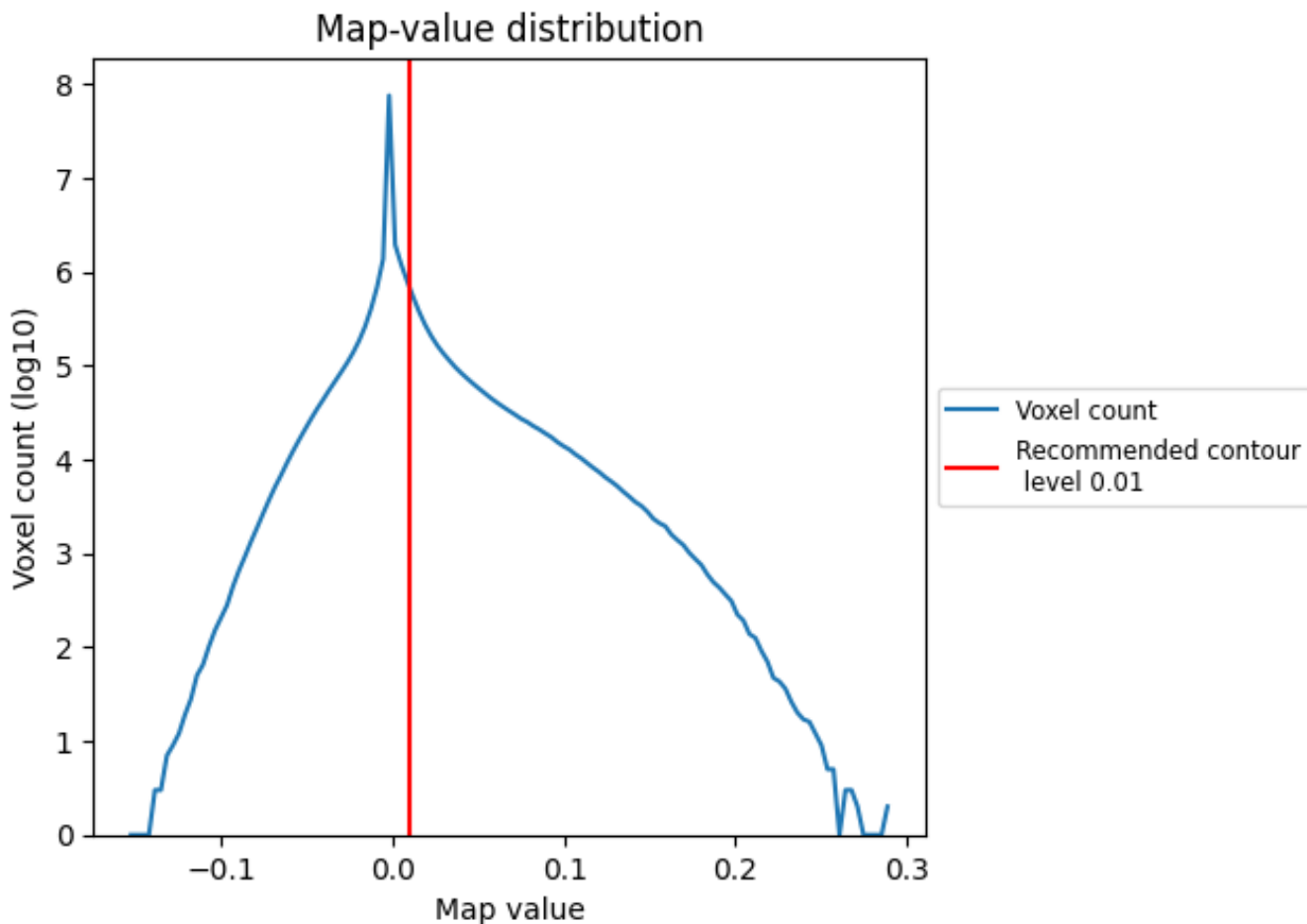
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

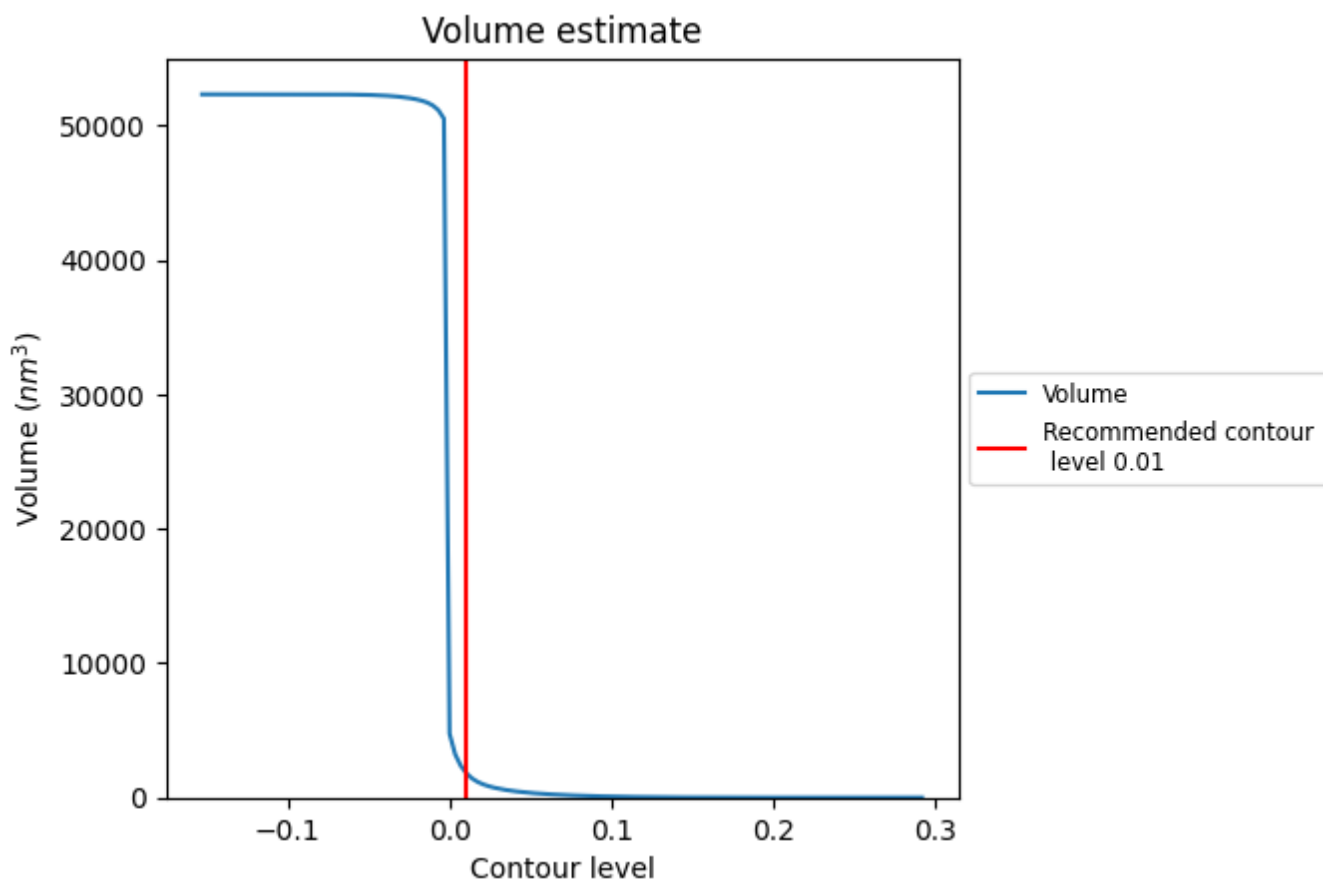
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

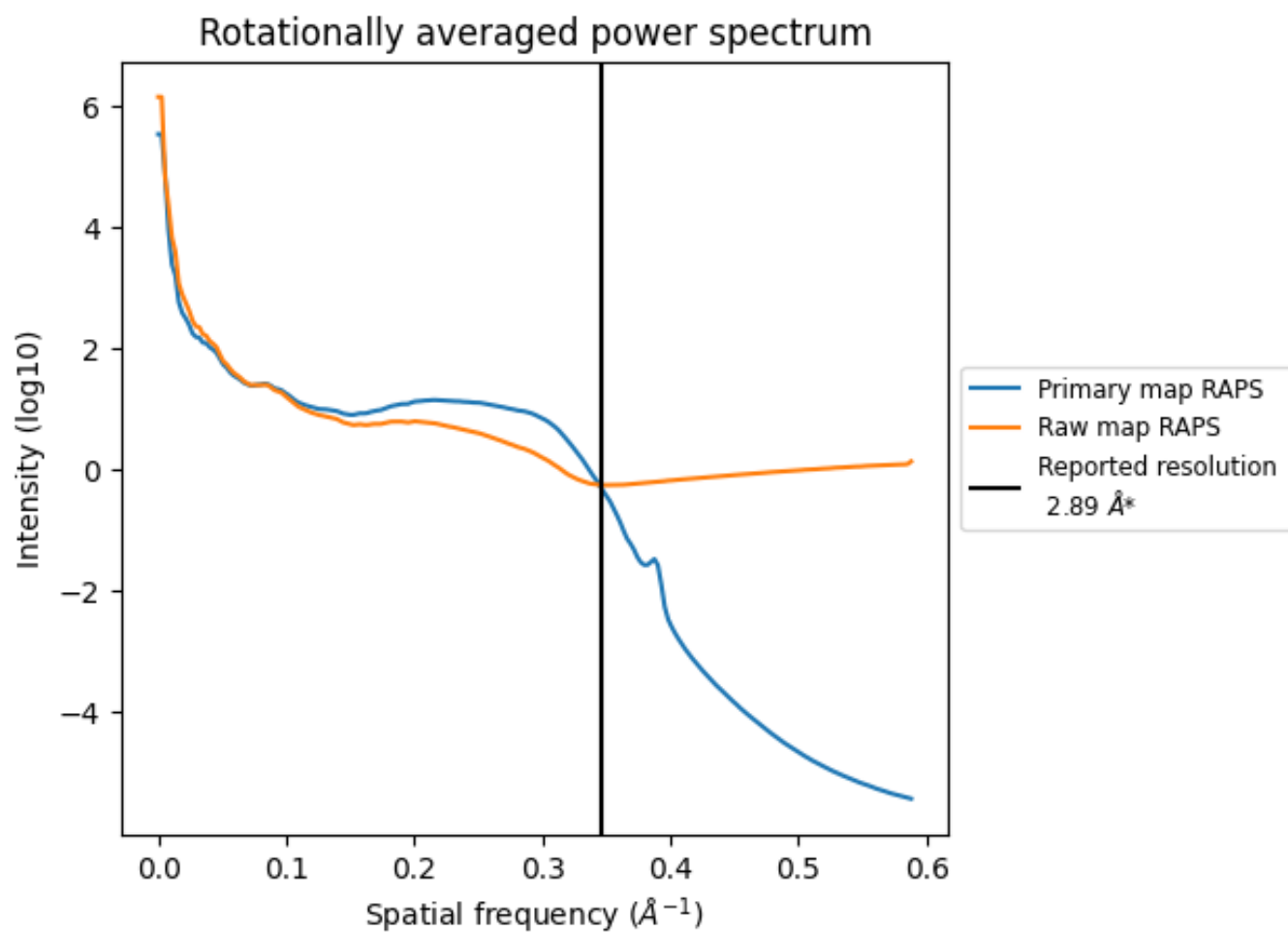
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1903 nm³; this corresponds to an approximate mass of 1719 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

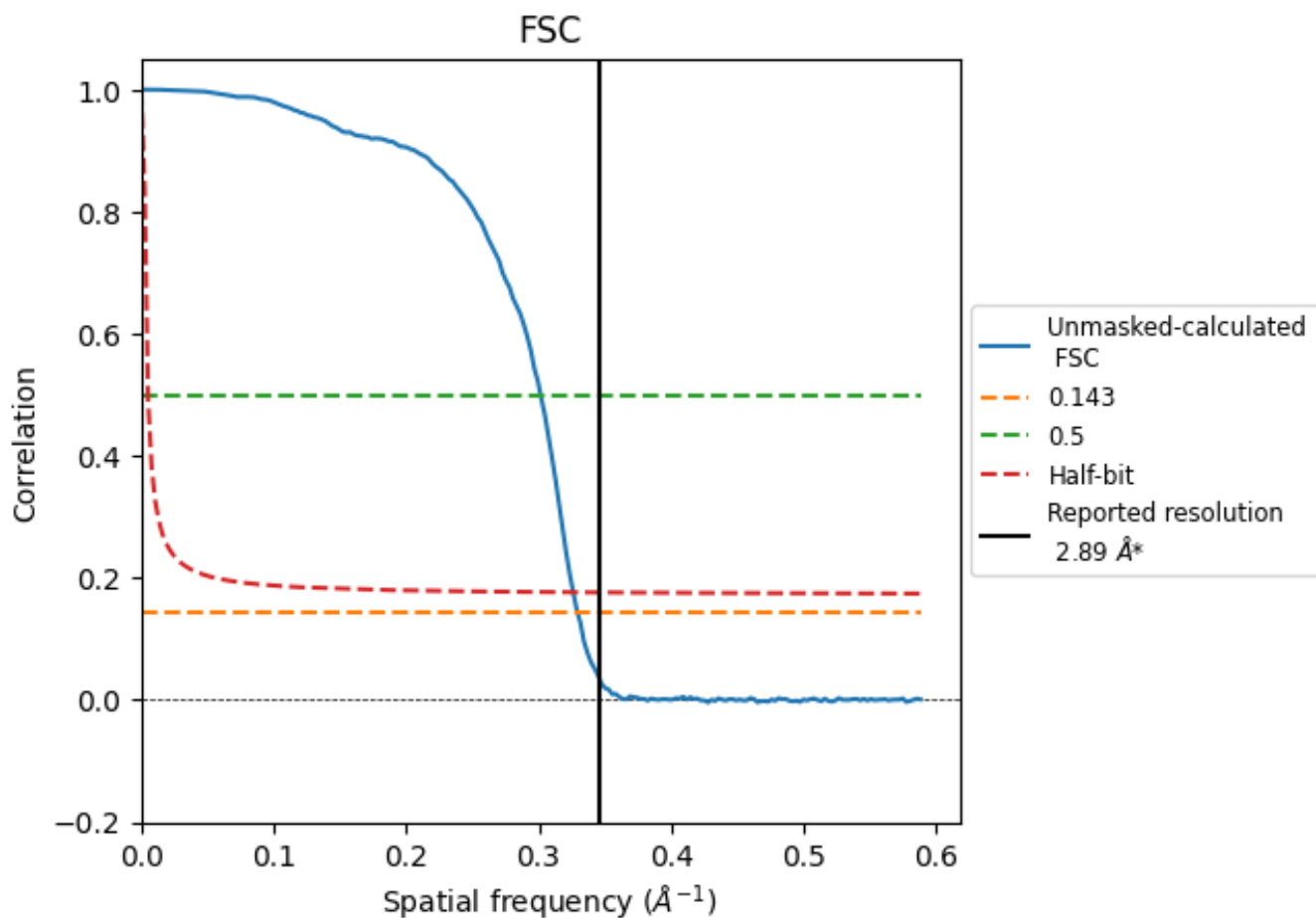


*Reported resolution corresponds to spatial frequency of 0.346 Å⁻¹

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 0.346 \AA^{-1}

8.2 Resolution estimates [i](#)

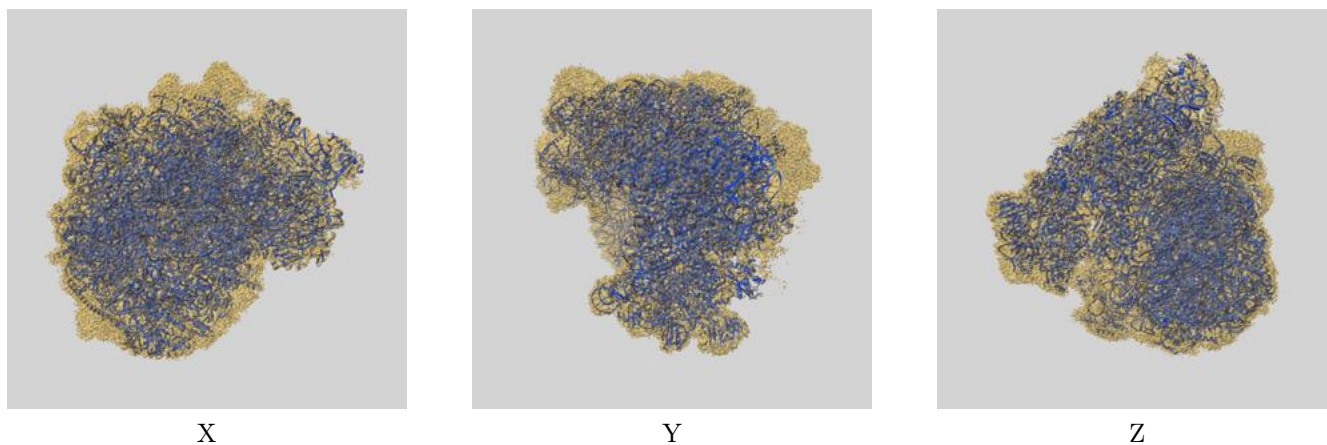
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.04	3.32	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

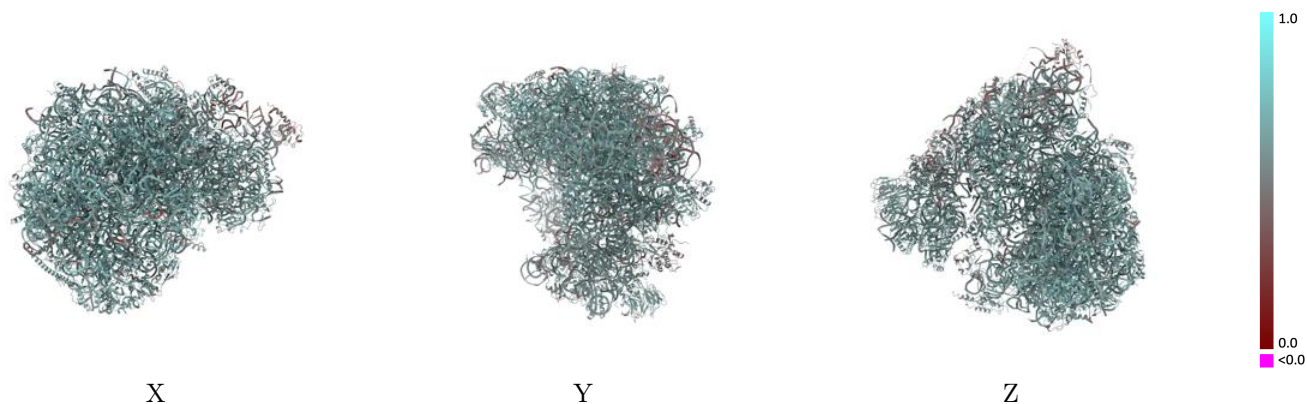
This section contains information regarding the fit between EMDB map EMD-15124 and PDB model 8A3W. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



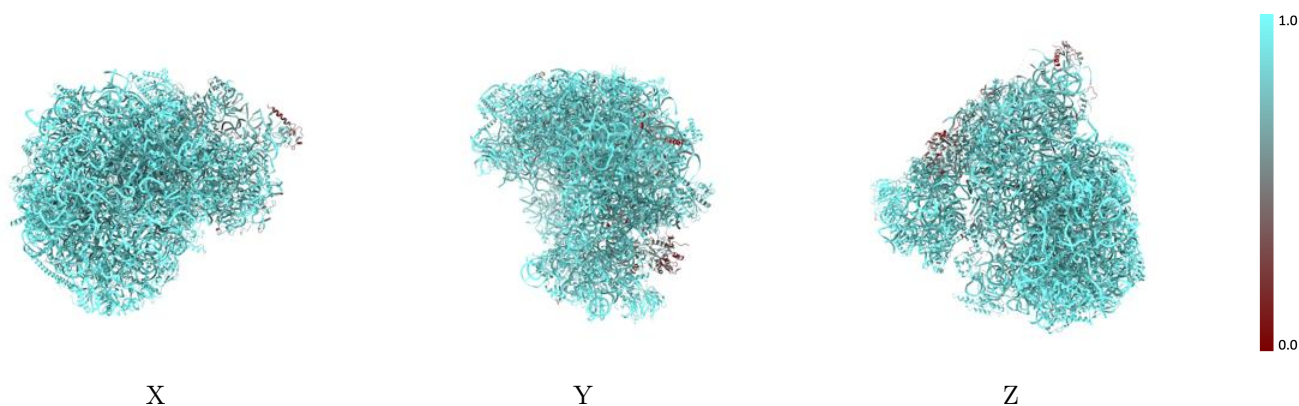
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



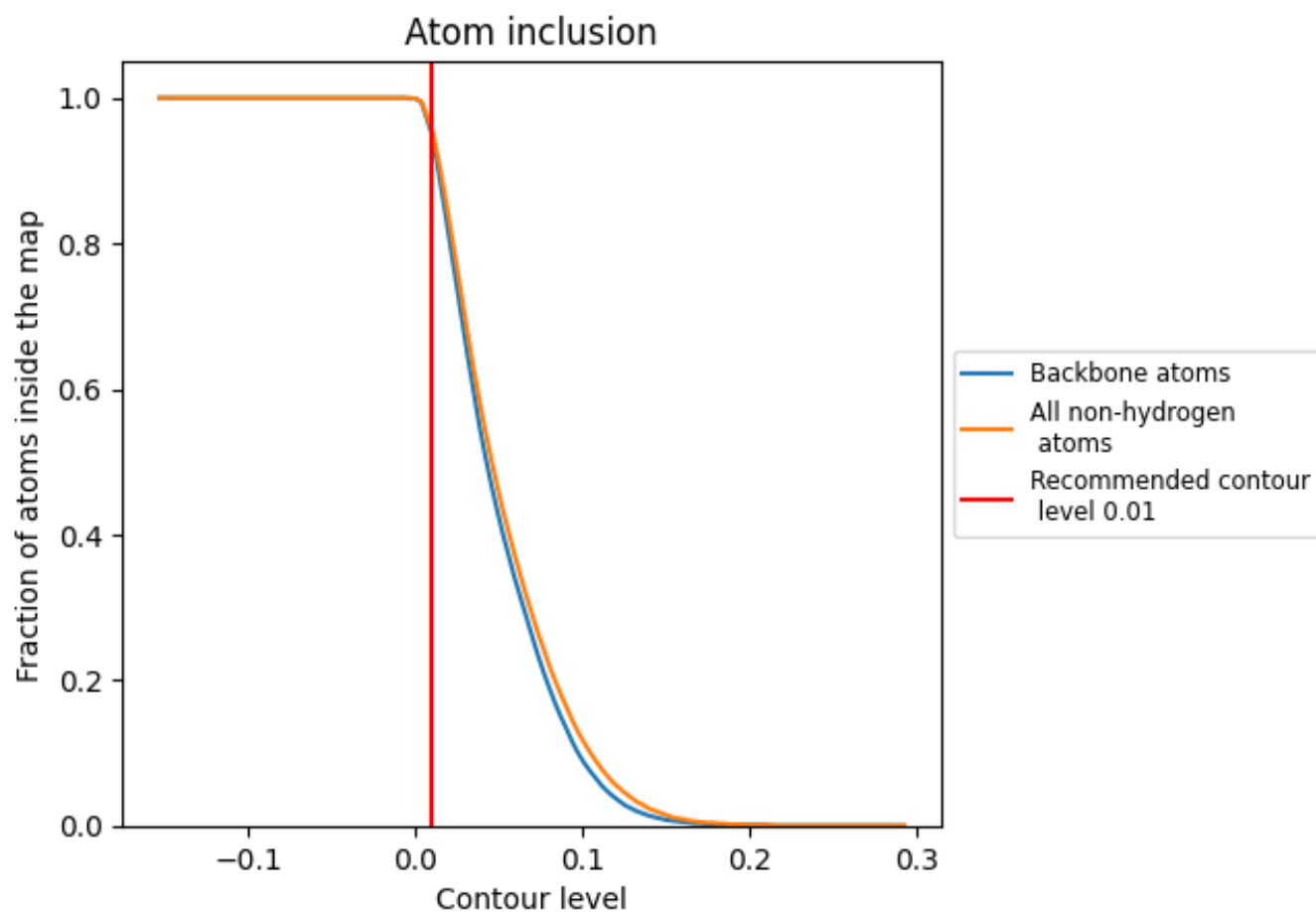
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).







































































9.4 Atom inclusion [i](#)

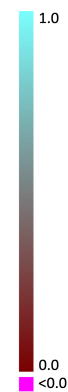


At the recommended contour level, 95% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

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	 0.9570	 0.6070
1	 0.9940	 0.6260
2	 0.9950	 0.6320
3	 0.9930	 0.6170
4	 0.9940	 0.6100
5	 0.9980	 0.6360
6	 0.9860	 0.5860
7	 0.9950	 0.6330
8	 0.9950	 0.5830
A	 0.9960	 0.6570
B	 0.9980	 0.6500
C	 0.9980	 0.6510
D	 0.9890	 0.5400
E	 0.9550	 0.5610
F	 0.9930	 0.6110
G	 0.9940	 0.6280
H	 0.9900	 0.6350
I	 0.9900	 0.6360
J	 0.9980	 0.6450
K	 0.9920	 0.6130
L	 0.9940	 0.6520
M	 0.9970	 0.6620
O	 0.9930	 0.5900
P	 0.9970	 0.6510
Q	 0.9930	 0.6160
R	 0.9890	 0.6310
S	 0.9910	 0.6290
S1	 0.9470	 0.5790
S4	 0.8940	 0.5140
SA	 0.8050	 0.5800
SB	 0.5340	 0.4940
SC	 0.9190	 0.5400
SD	 0.8200	 0.5450
SE	 0.8660	 0.6010
SF	 0.7520	 0.5740















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Chain	Atom inclusion	Q-score
SG	0.7990	0.5780
SH	0.9550	0.5990
SI	0.8500	0.5790
SJ	0.9300	0.6260
SK	0.8990	0.6070
SL	0.9820	0.6110
SM	0.9530	0.5660
SN	0.9320	0.5410
SO	0.8740	0.5890
SP	0.8650	0.5990
SR	0.9680	0.5970
SS	0.9630	0.5810
ST	0.9320	0.6130
SU	0.8760	0.6190
SV	0.9610	0.5870
SW	0.9510	0.5870
SX	0.9930	0.6120
SY	0.4200	0.5030
SZ	0.8380	0.5770
Sa	0.9790	0.5880
Sb	0.8120	0.5750
Sc	0.8300	0.5680
Sd	0.9420	0.5800
Se	0.7240	0.5690
Sg	0.9640	0.5670
Sh	0.4360	0.4140
T	0.9940	0.6550
U	0.9850	0.5590
V	0.9960	0.6420
W	0.9920	0.6350
X	0.9940	0.6410
Y	0.9950	0.6130
Z	0.9880	0.6210
a	0.9960	0.6250
b	0.9920	0.6350
c	0.9940	0.6340
d	0.9880	0.5800
e	0.9350	0.5920
f	0.9960	0.6480
g	0.9890	0.6490
h	0.9880	0.6330
i	0.9830	0.6180

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Chain	Atom inclusion	Q-score
j	 1.0000	 0.6630
k	 0.9900	 0.5940
l	 0.9930	 0.6550
n	 0.3860	 0.4500
o	 0.9910	 0.6240
p	 0.9940	 0.6330