



wwPDB EM Validation Summary Report ⓘ

Oct 12, 2026 – 04:18 pm BST

PDB ID : 9SYG / pdb_00009syg
EMDB ID : EMD-55348
Title : CRYO-EM STRUCTURE OF TRYPA NOSOMA BRUCEI BLOODSTREAM
FORM 80S RIBOSOME : NATIVE VACANT
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2025-10-12
Resolution : 2.68 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:

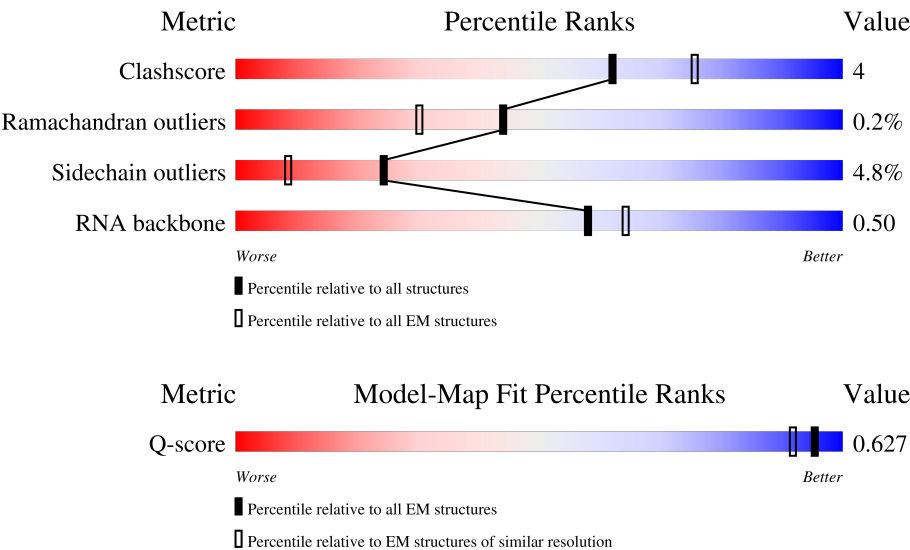
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.68 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	9255 (2.18 - 3.18)

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	A0	256	71% 14% • 13%
2	A1	273	85% 11% •
3	A2	190	88% 8% •

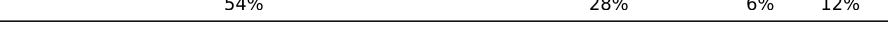
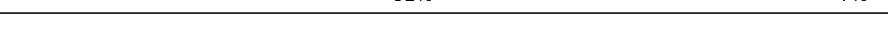
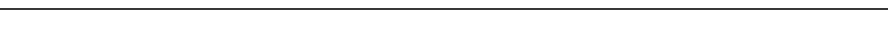
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	A3	250	
5	A4	202	
6	A5	220	
7	A6	190	
8	A7	318	
9	A8	57	
10	AA	2280	
11	AB	76	
12	AC	277	
13	AD	172	
14	AE	174	
15	AG	151	
16	AH	144	
17	AI	152	
18	AJ	130	
19	AK	149	
20	AL	142	
21	AM	153	
22	AO	167	
23	AP	266	
24	AQ	117	
25	AR	194	
26	AS	143	
27	AT	137	
28	AU	113	

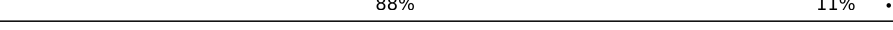
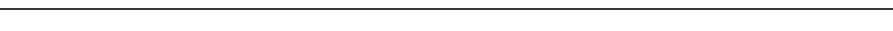
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	AV	111	 77% 15% 6%
30	AW	86	 77% 21% ..
31	AX	214	 75% 20% ..
32	AY	66	 79% 11% 11%
33	AZ	103	 50% 7% 43%
34	Az	279	 17% 12% 70%
35	BA	1866	 61% 21% 14%
36	BB	1544	 49% 20% 27%
37	BC	209	 52% 22% 23%
38	BD	120	 82% 15% ..
39	BE	216	 54% 20% 6% 19%
40	BF	78	 53% 27% 9% 12%
41	BG	183	 74% 20% 7%
42	BH	136	 54% 28% 6% 12%
43	BI	193	 91% 8% ..
44	BK	213	 79% 16% ..
45	BL	194	 72% 19% 8%
46	BN	218	 87% 11% .
47	BO	222	 92% 7%
48	BP	189	 79% 13% 6%
49	BQ	221	 84% 8% 8%
50	BR	166	 86% 5% 8%
51	BS	179	 85% 13% ..
52	BT	260	 65% 10% 24%
53	BU	159	 82% 15% ..

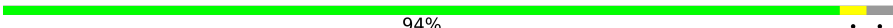
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	BV	130	 72%19%6%
55	BW	139	 87%6%6%
56	BX	164	 67%5%28%
57	BY	125	 46%49%
58	BZ	143	 72%13%15%
59	Ba	133	 82%17%
60	Bb	145	 89%10%
61	Bc	146	 82%17%
62	Bd	71	 92%6%
63	Be	260	 92%7%
64	Bf	429	 82%9%8%
65	Bg	105	 76%11%12%
66	Bh	188	 65%11%21%
67	Bi	132	 88%11%
68	Bj	170	 71%5%23%
69	Bk	127	 83%13%
70	Bl	149	 82%13%
71	Bm	109	 82%8%10%
72	Bn	84	 86%12%
73	Bo	93	 84%12%
74	Bp	82	 68%21%9%
75	Bq	51	 88%10%
76	Br	374	 90%8%
77	Bs	128	 36%61%
78	Bt	106	 87%5%8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	Bu	308	 83% 15% .
80	Bv	192	 59% 17% 24%
81	Bw	257	 78% 11% 11%
82	Bx	276	 76% 8% . 15%
83	By	189	 71% 26% ..
84	Bz	34	 94% . .

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 207369 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 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	222	Total	C	N	O	S	0	0
			1801	1136	339	318	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	262	Total	C	N	O	S	0	0
			2062	1306	388	359	9		

- Molecule 3 is a protein called 40S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	183	Total	C	N	O	S	0	0
			1463	915	282	261	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A3	238	Total	C	N	O	S	0	0
			1885	1170	388	323	4		

- Molecule 5 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A4	198	Total	C	N	O	S	0	0
			1606	1026	309	266	5		

- Molecule 6 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A5	190	Total	C	N	O	S	0	0
			1521	959	303	257	2		

- Molecule 7 is a protein called Probable 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A6	179	Total	C	N	O	S	0	0
			1477	929	297	243	8		

- Molecule 8 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A7	305	Total	C	N	O	S	0	0
			2315	1450	412	442	11		

- Molecule 9 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A8	57	Total	C	N	O	S	0	0
			461	284	96	76	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A8	5	HIS	ASP	conflict	UNP G0UD55
A8	19	SER	ALA	conflict	UNP G0UD55
A8	50	ASN	HIS	conflict	UNP G0UD55

- Molecule 10 is a RNA chain called SSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AA	1829	Total	C	N	O	P	0	0
			39092	17480	7034	12749	1829		

- Molecule 11 is a RNA chain called E-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AB	10	Total	C	N	O	P	0	0
			210	95	40	66	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AC	208	Total	C	N	O	S	0	0
			1647	1049	297	291	10		

- Molecule 13 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AD	99	Total	C	N	O	S	0	0
			814	531	140	139	4		

- Molecule 14 is a protein called 40S ribosomal proteins S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AE	153	Total	C	N	O	S	0	0
			1251	783	253	210	5		

- Molecule 15 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AG	150	Total	C	N	O	S	0	0
			1198	753	234	203	8		

- Molecule 16 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AH	136	Total	C	N	O	S	0	0
			1011	622	195	186	8		

- Molecule 17 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AI	121	Total	C	N	O	S	0	0
			975	619	190	163	3		

- Molecule 18 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AJ	129	Total	C	N	O	S	0	0
			1018	645	191	174	8		

- Molecule 19 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AK	143	Total	C	N	O	S	0	0
			1143	731	214	195	3		

- Molecule 20 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AL	122	Total	C	N	O	S	0	0
			969	613	192	159	5		

- Molecule 21 is a protein called 40S ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AM	135	Total	C	N	O	S	0	0
			1098	689	215	190	4		

- Molecule 22 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AO	154	Total	C	N	O	S	0	0
			1220	770	242	199	9		

- Molecule 23 is a protein called 40S ribosomal protein S2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AP	218	Total	C	N	O	S	0	0
			1688	1078	298	303	9		

- Molecule 24 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AQ	100	Total	C	N	O	S	0	0
			800	501	152	144	3		

- Molecule 25 is a protein called 40S ribosomal protein S21, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AR	89	Total	C	N	O	S	0	0
			666	415	119	129	3		

- Molecule 26 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AS	139	Total	C	N	O	S	0	0
			1089	692	212	183	2		

- Molecule 27 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AT	130	Total	C	N	O	S	0	0
			1043	665	204	171	3		

- Molecule 28 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AU	74	Total	C	N	O	S	0	0
			582	369	106	102	5		

- Molecule 29 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AV	104	Total	C	N	O	S	0	0
			835	515	176	136	8		

- Molecule 30 is a protein called 40S ribosomal protein S27, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AW	85	Total	C	N	O	S	0	0
			660	411	124	116	9		

- Molecule 31 is a protein called 40S ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AX	208	Total	C	N	O	S	0	0
			1652	1036	310	294	12		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AY	59	Total	C	N	O	S	0	0
			474	298	98	77	1		

- Molecule 33 is a protein called 40S ribosomal protein S33, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AZ	59	Total	C	N	O	S	0	0
			454	274	95	81	4		

- Molecule 34 is a protein called RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Az	84	Total	C	N	O	S	0	0
			673	427	124	121	1		

- Molecule 35 is a RNA chain called LSUa rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	1614	Total	C	N	O	P	1	0
			34591	15454	6264	11258	1615		

- Molecule 36 is a RNA chain called LSUb rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BB	1126	Total	C	N	O	P	0	0
			24057	10763	4299	7869	1126		

- Molecule 37 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	160	Total	C	N	O	P	0	0
			3412	1530	610	1113	159		

- Molecule 38 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BD	120	Total	C	N	O	P	0	0
			2553	1140	452	842	119		

- Molecule 39 is a RNA chain called SrRNA-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BE	174	Total	C	N	O	P	0	0
			3691	1649	644	1224	174		

- Molecule 40 is a RNA chain called SrRNA-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BF	69	Total	C	N	O	P	0	0
			1444	646	239	490	69		

- Molecule 41 is a RNA chain called SrRNA-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BG	183	Total	C	N	O	P	0	0
			3919	1746	708	1282	183		

- Molecule 42 is a RNA chain called SrRNA-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BH	119	Total	C	N	O	P	0	0
			2540	1132	453	836	119		

- Molecule 43 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BI	192	Total	C	N	O	S	0	0
			1526	956	315	247	8		

- Molecule 44 is a protein called 60S ribosomal protein L10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BK	204	Total	C	N	O	S	0	0
			1668	1055	327	273	13		

- Molecule 45 is a protein called 60S ribosomal protein L11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BL	178	Total	C	N	O	S	0	0
			1408	889	263	249	7		

- Molecule 46 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BN	215	Total	C	N	O	S	0	0
			1762	1097	365	294	6		

- Molecule 47 is a protein called 60S ribosomal protein L13a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BO	221	Total	C	N	O	S	0	0
			1801	1141	364	289	7		

- Molecule 48 is a protein called 40S ribosomal protein L14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BP	177	Total	C	N	O	S	0	0
			1414	892	278	240	4		

- Molecule 49 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BQ	203	Total	C	N	O	S	0	0
			1716	1077	370	264	5		

- Molecule 50 is a protein called 60S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BR	152	Total	C	N	O	S	0	0
			1228	772	244	204	8		

- Molecule 51 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BS	178	Total	C	N	O	S	0	0
			1465	926	289	243	7		

- Molecule 52 is a protein called 60S ribosomal protein L19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BT	197	Total	C	N	O	S	0	0
			1597	979	350	260	8		

- Molecule 53 is a protein called 60S ribosomal protein L21E, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BU	158	Total	C	N	O	S	0	0
			1253	799	243	205	6		

- Molecule 54 is a protein called 60S ribosomal protein L22, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BV	122	Total	C	N	O	S	0	0
			979	629	179	168	3		

- Molecule 55 is a protein called 60S ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BW	130	Total	C	N	O	S	0	0
			983	623	186	169	5		

- Molecule 56 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BX	118	Total	C	N	O	S	0	0
			966	614	182	168	2		

- Molecule 57 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BY	64	Total	C	N	O	S	0	0
			547	356	108	79	4		

- Molecule 58 is a protein called 60S ribosomal protein L26, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BZ	122	Total	C	N	O	S	0	0
			993	614	210	164	5		

- Molecule 59 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Ba	133	Total	C	N	O	S	0	0
			1090	691	220	176	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Bb	144	Total	C	N	O	S	0	0
			1137	717	228	186	6		

- Molecule 61 is a protein called 60S ribosomal protein L28, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bc	144	Total	C	N	O	S	0	0
			1162	723	234	197	8		

- Molecule 62 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bd	69	Total	C	N	O	S	0	0
			561	343	126	91	1		

- Molecule 63 is a protein called 60S ribosomal protein L2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Be	257	Total	C	N	O	S	1	0
			1962	1223	401	325	13		

- Molecule 64 is a protein called Ribosomal protein L3, mitochondrial, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bf	396	Total	C	N	O	S	0	0
			3174	2001	626	534	13		

- Molecule 65 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Bg	92	Total	C	N	O	S	0	0
			708	441	128	134	5		

- Molecule 66 is a protein called 60S ribosomal subunit protein L31, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Bh	148	Total	C	N	O	S	0	0
			1160	735	231	190	4		

- Molecule 67 is a protein called 60S ribosomal protein L32, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bi	131	Total	C	N	O	S	0	0
			1075	678	217	176	4		

- Molecule 68 is a protein called 60S ribosomal protein L34, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bj	131	Total	C	N	O	S	0	0
			1035	638	229	164	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bk	123	Total	C	N	O	S	0	0
			1018	639	218	158	3		

- Molecule 70 is a protein called 60S ribosomal protein L35A, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bl	144	Total	C	N	O	S	0	0
			1163	728	239	193	3		

- Molecule 71 is a protein called Ribosomal protein L36, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bm	98	Total	C	N	O	S	0	0
			786	493	164	127	2		

- Molecule 72 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bn	82	Total	C	N	O	S	0	0
			693	422	160	105	6		

- Molecule 73 is a protein called 60S ribosomal protein L37a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bo	89	Total	C	N	O	S	0	0
			699	434	144	115	6		

- Molecule 74 is a protein called 60S ribosomal protein L38, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bp	75	Total	C	N	O	S	0	0
			609	383	121	101	4		

- Molecule 75 is a protein called 60S ribosomal protein L39, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
75	Bq	50	Total	C	N	O	0	0
			457	297	98	62		

- Molecule 76 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Br	367	Total	C	N	O	S	0	0
			2882	1802	575	488	17		

- Molecule 77 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bs	50	Total	C	N	O	S	0	0
			400	250	83	60	7		

- Molecule 78 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bt	97	Total	C	N	O	S	0	0
			801	507	159	130	5		

- Molecule 79 is a protein called 60S ribosomal protein L5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bu	303	Total	C	N	O	S	0	0
			2388	1503	458	421	6		

- Molecule 80 is a protein called 60S ribosomal protein L6, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bv	146	Total	C	N	O	S	0	0
			1121	712	206	200	3		

- Molecule 81 is a protein called 60S ribosomal protein L7, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bw	230	Total	C	N	O	S	0	0
			1872	1190	362	312	8		

- Molecule 82 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Bx	235	Total	C	N	O	S	0	0
			1874	1178	369	321	6		

- Molecule 83 is a protein called 60S ribosomal protein L9, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	By	186	Total	C	N	O	S	0	0
			1515	961	281	269	4		

- Molecule 84 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bz	33	Total	C	N	O	S	0	0
			289	175	75	37	2		

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	A0	1	Total	Mg	0
			1	1	
85	A3	1	Total	Mg	0
			1	1	
85	AA	50	Total	Mg	0
			50	50	
85	BA	69	Total	Mg	0
			69	69	
85	BB	61	Total	Mg	0
			61	61	
85	BC	4	Total	Mg	0
			4	4	
85	BD	3	Total	Mg	0
			3	3	
85	BE	3	Total	Mg	0
			3	3	
85	BF	1	Total	Mg	0
			1	1	
85	BG	1	Total	Mg	0
			1	1	
85	BH	1	Total	Mg	0
			1	1	
85	BW	1	Total	Mg	0
			1	1	
85	Bn	1	Total	Mg	0
			1	1	

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
86	A8	1	Total 1	Zn 1	0
86	AV	1	Total 1	Zn 1	0
86	Bn	1	Total 1	Zn 1	0
86	Bo	1	Total 1	Zn 1	0
86	Bs	1	Total 1	Zn 1	0
86	Bt	1	Total 1	Zn 1	0

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

Mol	Chain	Residues	Atoms		AltConf
87	AA	25	Total 25	K 25	0
87	BA	22	Total 22	K 22	0
87	BB	22	Total 22	K 22	0
87	BC	1	Total 1	K 1	0
87	BE	1	Total 1	K 1	0
87	BG	6	Total 6	K 6	0
87	BH	1	Total 1	K 1	0
87	Be	1	Total 1	K 1	0
87	Bn	1	Total 1	K 1	0

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

Mol	Chain	Residues	Atoms		AltConf
88	AA	5	Total 5	Na 5	0
88	BA	8	Total 8	Na 8	0
88	BB	9	Total 9	Na 9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
88	BR	1	Total 1	Na 1	0
88	BU	1	Total 1	Na 1	0

- Molecule 89 is water.

Mol	Chain	Residues	Atoms		AltConf
89	A1	1	Total 1	O 1	0
89	A2	1	Total 1	O 1	0
89	A5	6	Total 6	O 6	0
89	AA	264	Total 264	O 264	0
89	AC	1	Total 1	O 1	0
89	AE	5	Total 5	O 5	0
89	AG	10	Total 10	O 10	0
89	AH	3	Total 3	O 3	0
89	AO	1	Total 1	O 1	0
89	AP	2	Total 2	O 2	0
89	AV	7	Total 7	O 7	0
89	AX	1	Total 1	O 1	0
89	BA	239	Total 239	O 239	0
89	BB	353	Total 353	O 353	0
89	BC	8	Total 8	O 8	0
89	BE	13	Total 13	O 13	0
89	BG	40	Total 40	O 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
89	BH	9	Total 9	O 9	0
89	BI	2	Total 2	O 2	0
89	BK	2	Total 2	O 2	0
89	BQ	4	Total 4	O 4	0
89	BR	6	Total 6	O 6	0
89	BT	4	Total 4	O 4	0
89	BU	1	Total 1	O 1	0
89	BV	3	Total 3	O 3	0
89	BW	11	Total 11	O 11	0
89	BY	2	Total 2	O 2	0
89	Bb	3	Total 3	O 3	0
89	Be	6	Total 6	O 6	0
89	Bf	25	Total 25	O 25	0
89	Bi	3	Total 3	O 3	0
89	Bj	1	Total 1	O 1	0
89	Bl	2	Total 2	O 2	0
89	Bn	9	Total 9	O 9	0
89	Bo	6	Total 6	O 6	0
89	Br	4	Total 4	O 4	0
89	Bt	1	Total 1	O 1	0
89	Bx	1	Total 1	O 1	0

Continued on next page...

Continued from previous page...

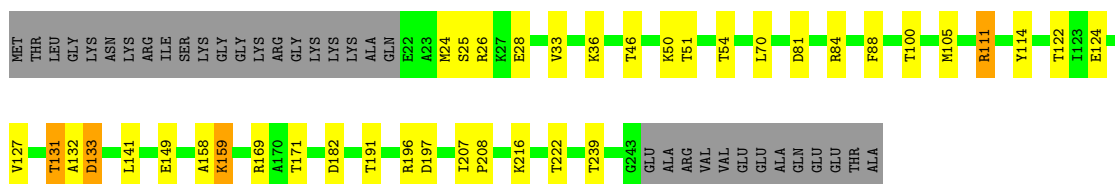
Mol	Chain	Residues	Atoms		AltConf
89	Bz	5	Total	O	0
			5	5	

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.

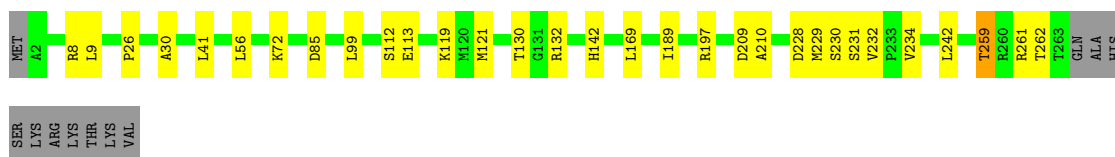
- Molecule 1: 40S ribosomal protein S3a

Chain A0: 



- Molecule 2: 40S ribosomal protein S4

Chain A1: 



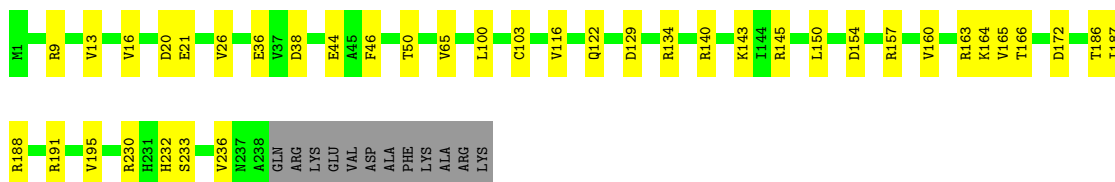
- Molecule 3: 40S ribosomal protein S5, putative

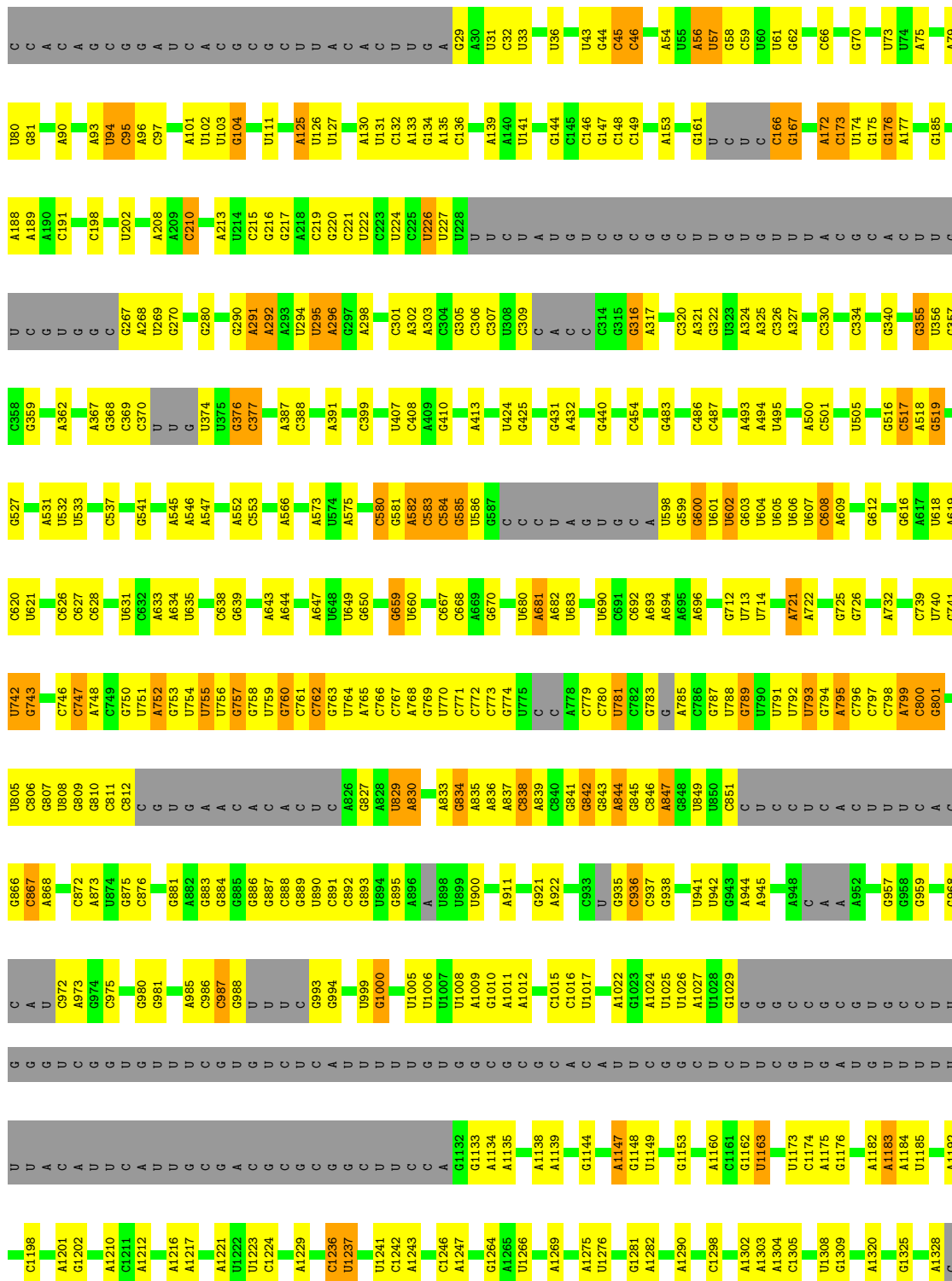
Chain A2: 

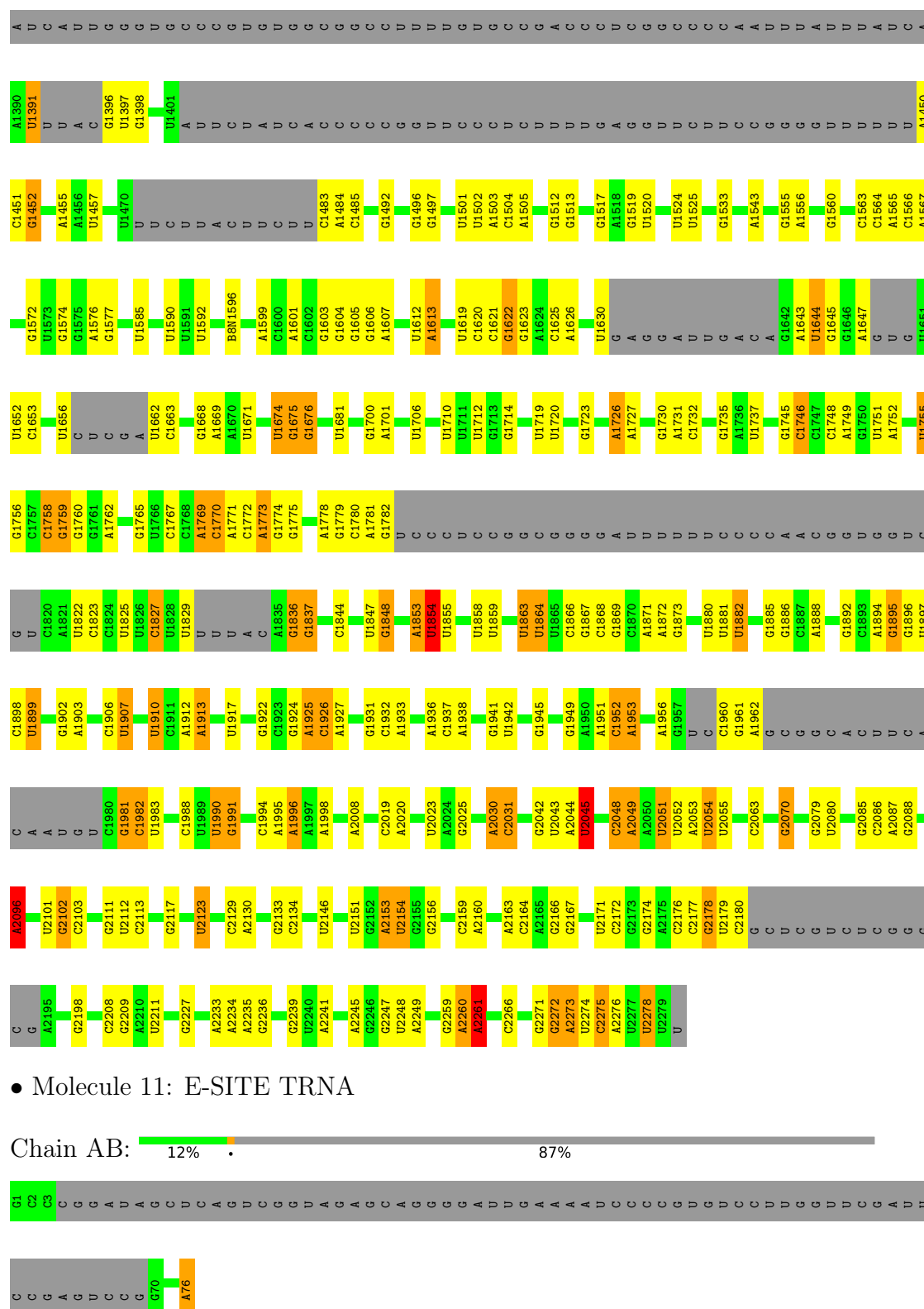


- Molecule 4: 40S ribosomal protein S6

Chain A3: 

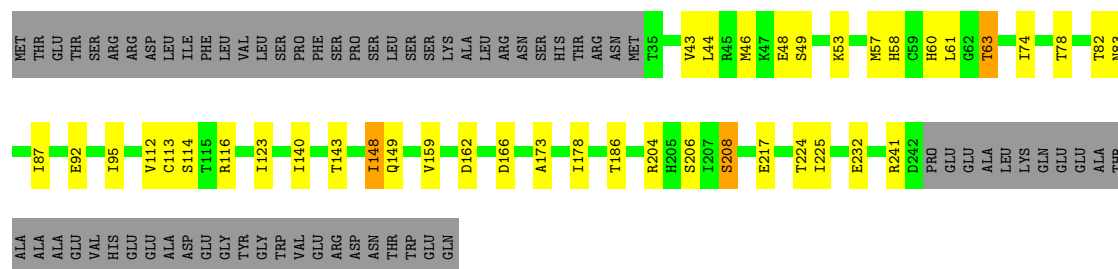






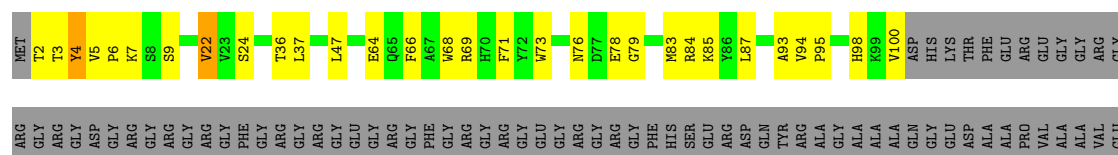
• Molecule 11: E-SITE TRNA

• Molecule 12: 40S ribosomal protein SA



- Molecule 13: 40S ribosomal protein S10, putative

Chain AD: 40% 16% 42%



- Molecule 14: 40S ribosomal proteins S11, putative

Chain AE: 82% 5% 12%



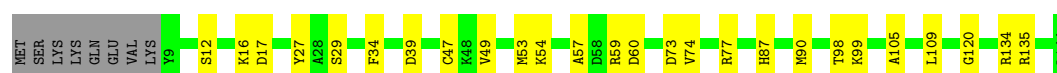
- Molecule 15: 40S ribosomal protein S13, putative

Chain AG: 85% 13% 2%



- Molecule 16: 40S ribosomal protein S14

Chain AH: 76% 18% 6%



- Molecule 17: 40S ribosomal protein S15, putative

Chain AI: 61% 18% 20%



- Molecule 18: 40S ribosomal protein S15a, putative

ME1	T2	R23	L26	S30	S31	G59	K60	I61	V62	L104	T105	T106	S107	E114	R117	A118	R119	N120	Y130
-----	----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|
| ME7 | SER | GLY | GLU | LYS | THR | H7 | V12 | C33 | R36 | G39 | I42 | I45 | L46 | P47 | E48 | E56 | L69 | G76 | G77 | S78 | V87 | R88 | I91 | K101 | I102 | H103 | N104 | E107 | D119 | S147 | I148 | R149 |
|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ALA | ARG | ARG | GLY | PRO | ALA | ARG | LYS | MET | G2 | T8 | K19 | K23 | L24 | N25 | K26 | K36 | M58 | R63 | R67 | K72 | L73 | E77 | R80 | R81 | M82 | V85 | P86 | E87 | V88 | R100 | V101 | D102 | K103 | Q104 | T105 | L106 | A107 | K110 | R111 | M112 | L121 | P122 | N123 | VAL | VAL | ALA | ALA | PRO | ASN | VAL | SER | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|

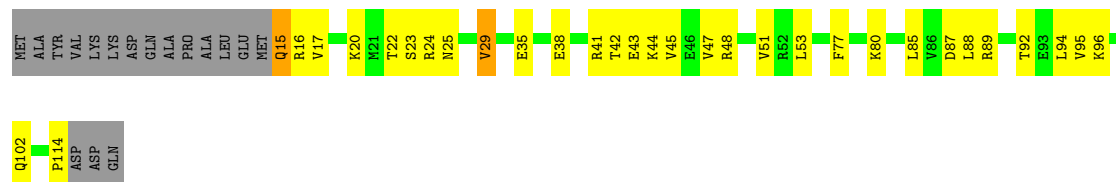
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLY | VAL | SER | ARG | THR | LYS | MET | L3 | R15 | T19 | G23 | K33 | T34 | K35 | N44 | A57 | L60 | K67 | L85 | Q88 | R89 | K92 | T93 | T96 | M103 | V104 | D105 | T106 | R107 | D111 | R114 | K117 | R125 | L130 | H136 | T137 | CYS | THR | SER | GLY | ARG | ARG | GLY | LYS | THR |
|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|
| MET | ALA | VAL | ALA | ARG | THR | LYS | ASP | T22 | H27 | R30 | H38 | E42 | G43 | K44 | C50 | E51 | E52 | F53 | K54 | R55 | T56 | S57 | A112 | L127 | C133 | A136 | K142 | D149 | M160 | G161 | ALA | GLU | THR | LYS | ALA | VAL |
|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|

- [illegible]

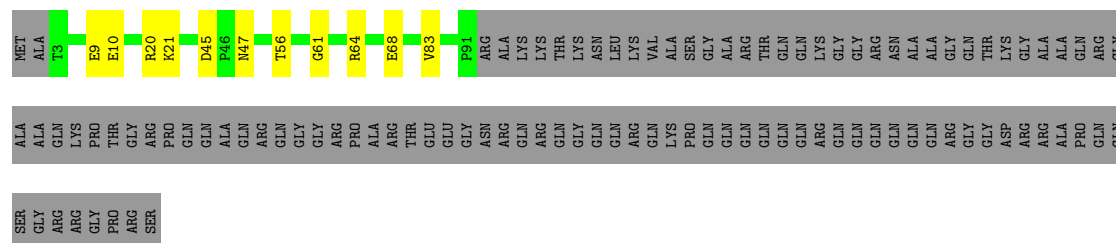
- 

Chain AQ:  58% 26% 15%



- Molecule 25: 40S ribosomal protein S21, putative

Chain AR:  40% 6% 54%



- Molecule 26: 40S ribosomal protein S23, putative

Chain AS:  83% 13% 2%



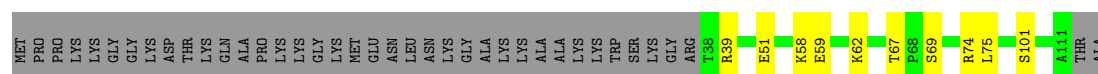
- Molecule 27: 40S ribosomal protein S24

Chain AT:  82% 11% 5%



- Molecule 28: 40S ribosomal protein S25

Chain AU:  57% 9% 35%



- Molecule 29: 40S ribosomal protein S26

Chain AV:  77% 15% 6%



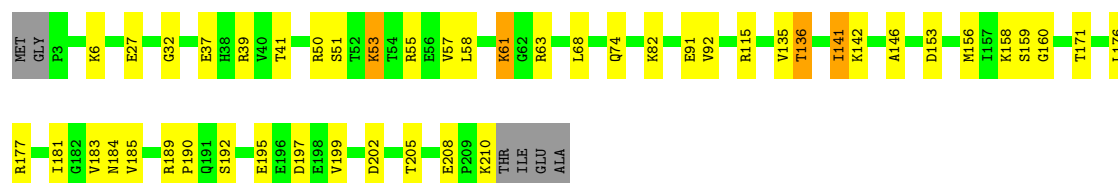
- Molecule 30: 40S ribosomal protein S27, putative

Chain AW:  77% 21% ..



- Molecule 31: 40S ribosomal protein S3, putative

Chain AX:  75% 20% ..



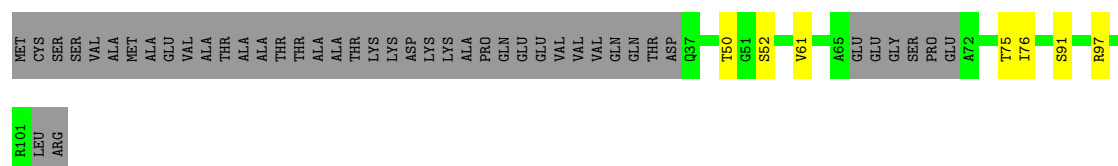
- Molecule 32: 40S ribosomal protein S30

Chain AY:  79% 11% 11%



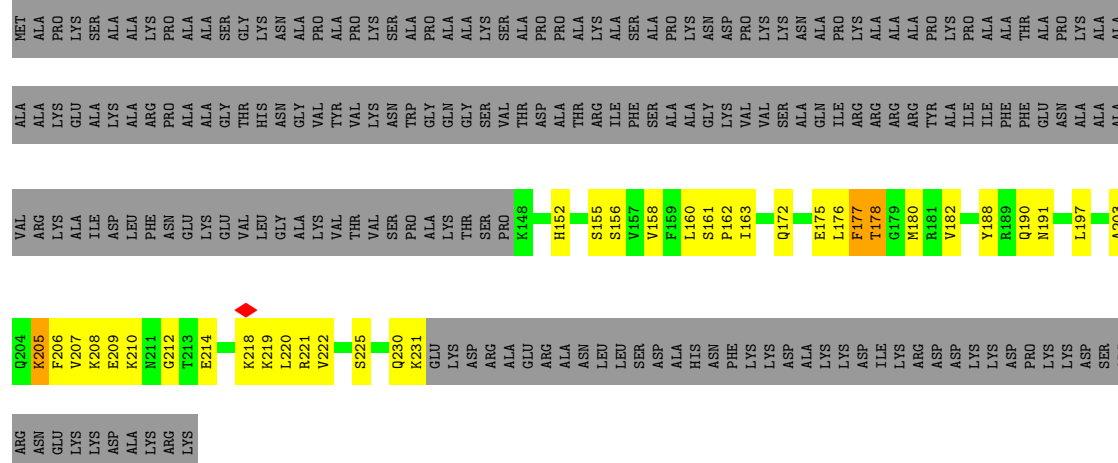
- Molecule 33: 40S ribosomal protein S33, putative

Chain AZ:  50% 7% 43%

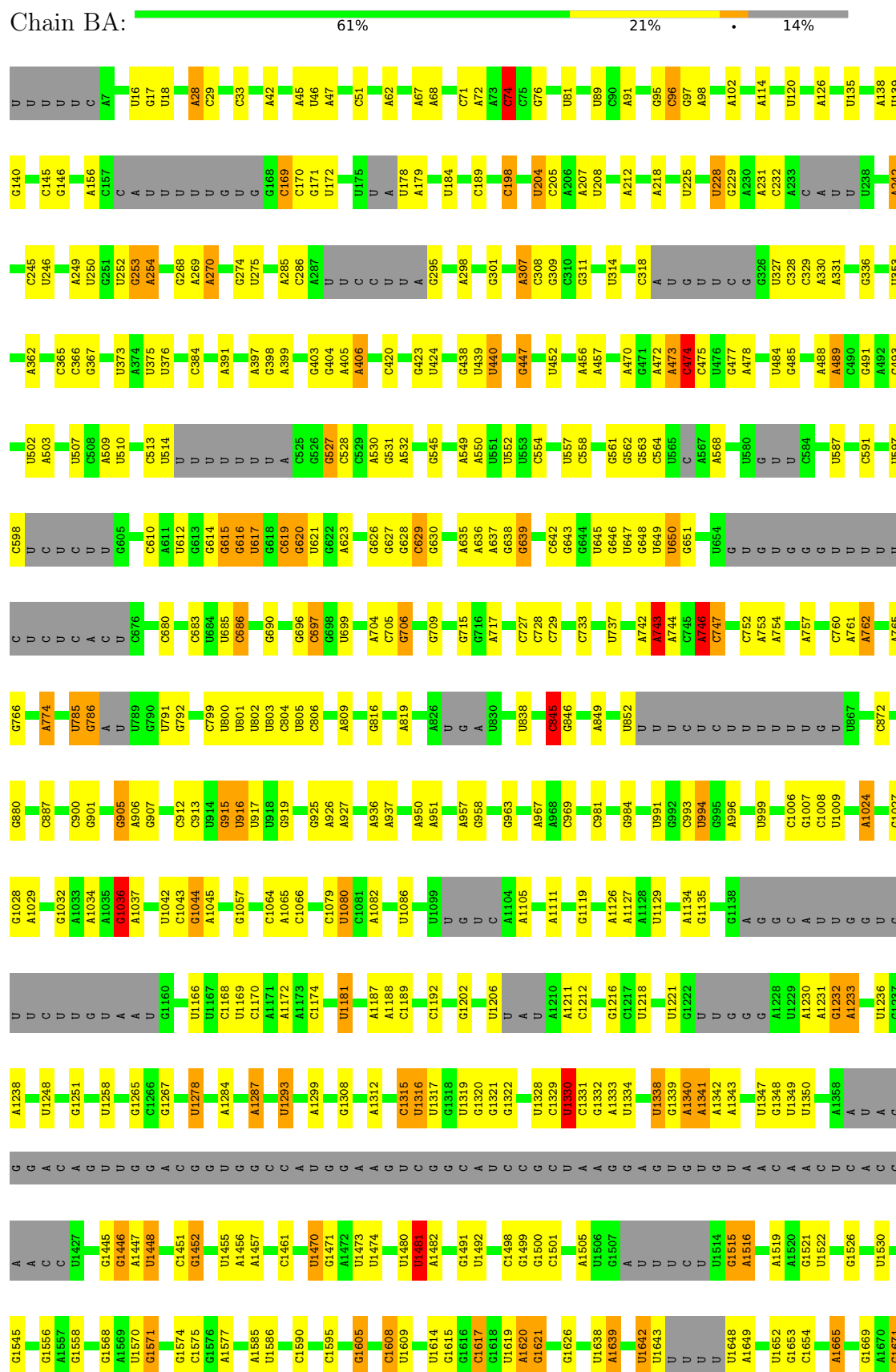


- Molecule 34: RNA-binding protein

Chain Az:  17% 12% 70%



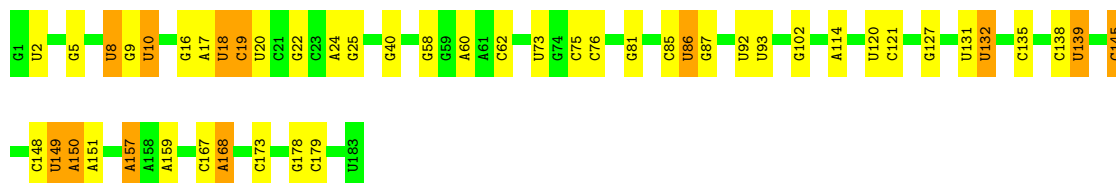
● Molecule 35: LSUa rRNA





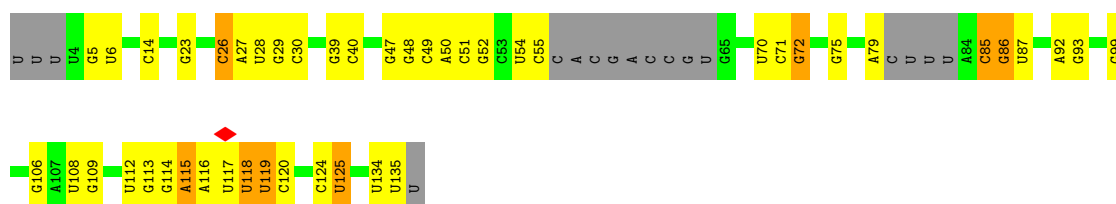
- Molecule 41: SrRNA-2

Chain BG: 74% 20% 7%



- Molecule 42: SrRNA-4

Chain BH: 54% 28% 6% 12%



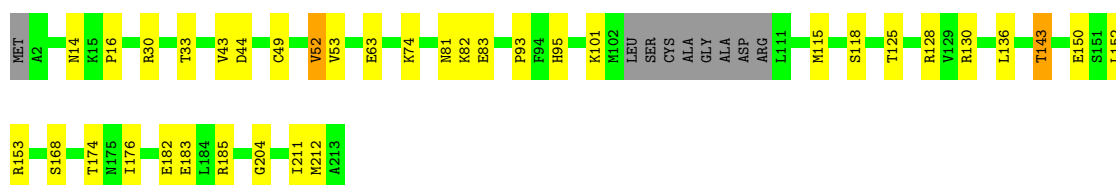
- Molecule 43: 60S ribosomal protein L18

Chain BI: 91% 8% ..



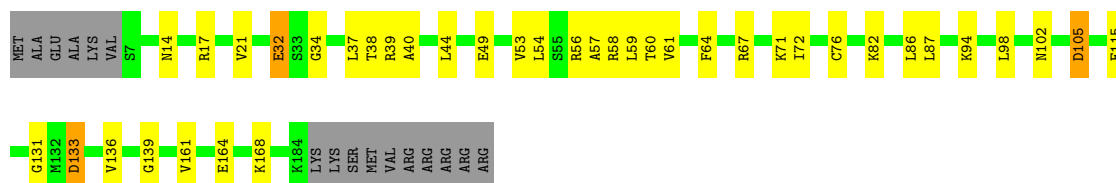
- Molecule 44: 60S ribosomal protein L10, putative

Chain BK: 79% 16% . .



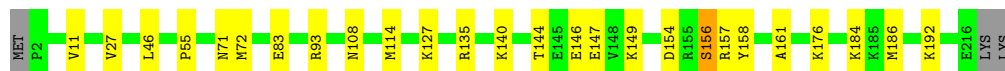
- Molecule 45: 60S ribosomal protein L11, putative

Chain BL: 72% 19% . 8%

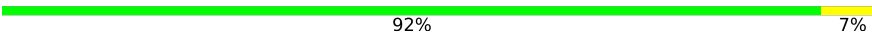


- Molecule 46: 60S ribosomal protein L13

Chain BN:  87% 11%



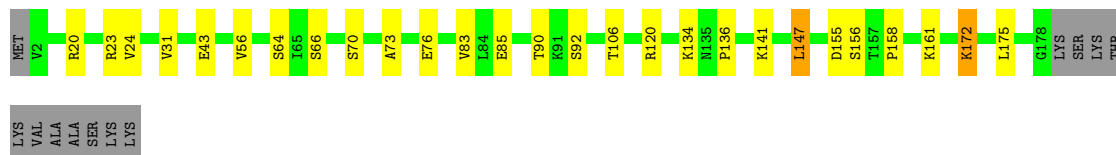
- Molecule 47: 60S ribosomal protein L13a, putative

Chain BO:  92% 7%



- Molecule 48: 40S ribosomal protein L14, putative

Chain BP:  79% 13% 6%



- Molecule 49: Ribosomal protein L15

Chain BQ:  84% 8% 8%



- Molecule 50: 60S ribosomal protein L17, putative

Chain BR:  86% 5% 8%



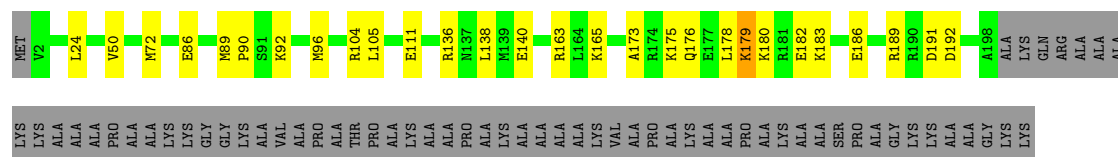
- Molecule 51: 60S ribosomal protein L18a

Chain BS:  85% 13%



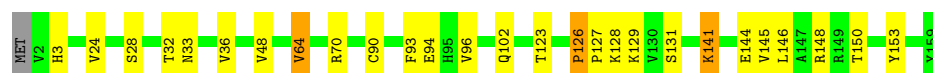
- Molecule 52: 60S ribosomal protein L19, putative

Chain BT:  65% 10% 24%



- Molecule 53: 60S ribosomal protein L21E, putative

Chain BU: 82% 15% ..



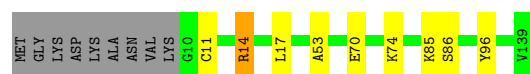
- Molecule 54: 60S ribosomal protein L22, putative

Chain BV: 72% 19% • 6%



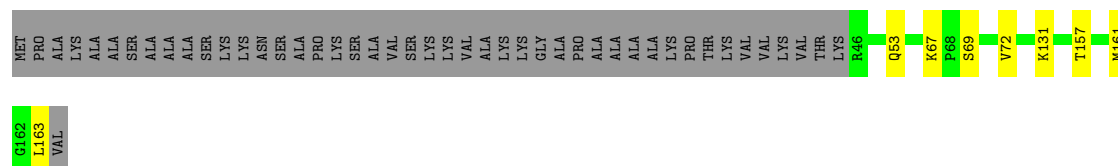
- Molecule 55: 60S ribosomal protein L23, putative

Chain BW: 87% 6% • 6%



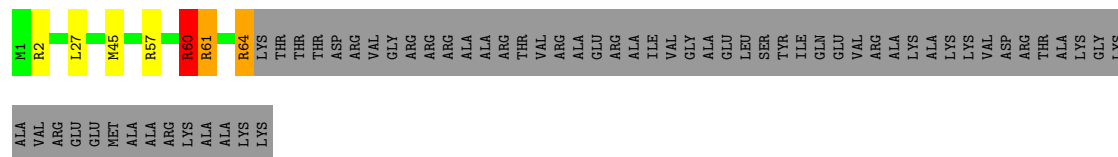
- Molecule 56: 60S ribosomal protein L23a

Chain BX: 67% 5% 28%



- Molecule 57: Ribosomal protein L24

Chain BY: 46% 49% • •



- Molecule 58: 60S ribosomal protein L26, putative

Chain BZ: 72% 13% 15%



- Molecule 59: 60S ribosomal protein L27

Chain Ba: 82% 17% .



- Molecule 60: 60S ribosomal protein L27a

Chain Bb: 89% 10% ..



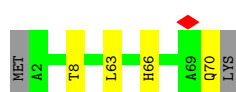
- Molecule 61: 60S ribosomal protein L28, putative

Chain Bc: 82% 17% .



- Molecule 62: 60S ribosomal protein L29

Chain Bd: 92% 6% .



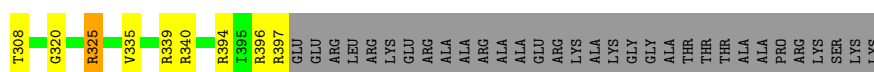
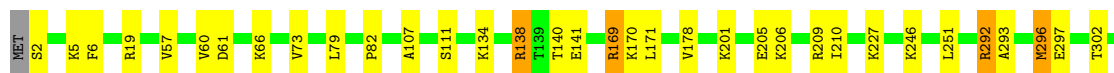
- Molecule 63: 60S ribosomal protein L2, putative

Chain Be: 92% 7% .



- Molecule 64: Ribosomal protein L3, mitochondrial, putative

Chain Bf: 82% 9% 8%



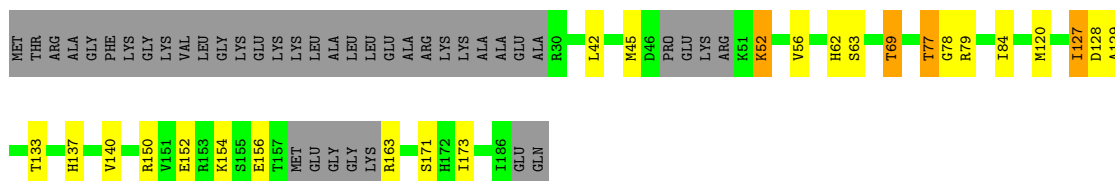
- Molecule 65: 60S ribosomal protein L30

Chain Bg:  76% 11% 12%



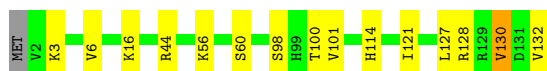
- Molecule 66: 60S ribosomal subunit protein L31, putative

Chain Bh:  65% 11% 21%



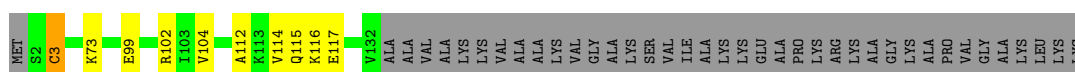
- Molecule 67: 60S ribosomal protein L32, putative

Chain Bi:  88% 11% ..



- Molecule 68: 60S ribosomal protein L34, putative

Chain Bj:  71% 5% 23%



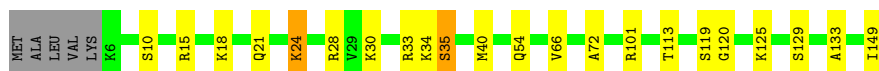
- Molecule 69: 60S ribosomal protein L35, putative

Chain Bk:  83% 13% ..



- Molecule 70: 60S ribosomal protein L35A, putative

Chain Bl:  82% 13% ..



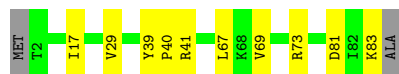
- Molecule 71: Ribosomal protein L36, putative

Chain Bm:  82% 8% 10%



- Molecule 72: Ribosomal protein L37

Chain Bn:  86% 12%



- Molecule 73: 60S ribosomal protein L37a, putative

Chain Bo:  84% 12%



- Molecule 74: 60S ribosomal protein L38, putative

Chain Bp:  68% 21% 9%



- Molecule 75: 60S ribosomal protein L39, putative

Chain Bq:  88% 10%



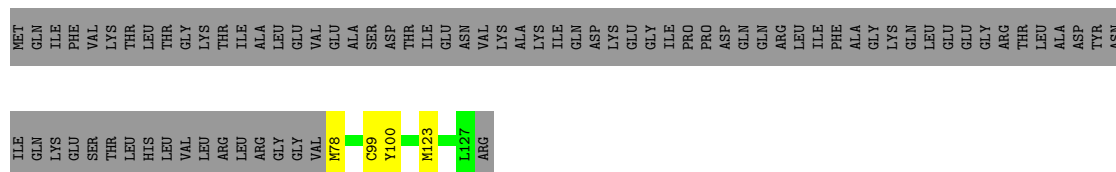
- Molecule 76: 60S ribosomal protein L4

Chain Br:  90% 8%



- Molecule 77: Ubiquitin-60S ribosomal protein L40

Chain Bs:  36% 61%



- Molecule 78: 60S ribosomal protein L44

MET	V2	K6	K9	N94	D95	K96	K97	K98	THR	GLY	ASN	LYS	ASP	PRO	THR	TRP
-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

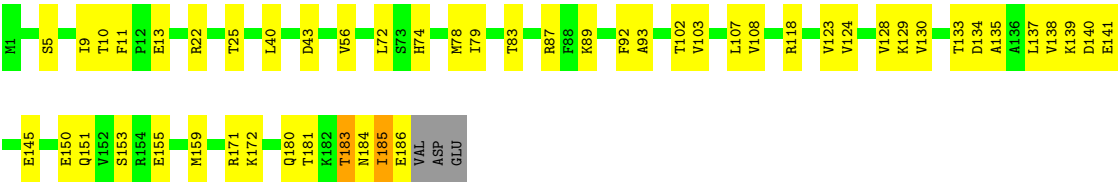
- [illegible]

- [illegible]

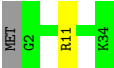
- | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| W218 | P219 | G228 | M229 | R233 | R234 | D241 | D246 | T247 | R251 | R255 | M256 | I257 | Met | Phe | Thr | Gly | Leu | Ile | Leu | Gly | Lys | Gly | Arg | Glu | Val | Met | Pro | Ala | Lys | Ala | Val | Pro | Ala | Pro | Glu | Ser | Ala | T28 | K29 | R30 | A31 | Q35 | S61 | R71 | K75 | K76 | L77 | L80 | R81 | H87 | Y91 | L92 | E93 | R122 | V176 | D180 | H189 | W200 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

- [illegible]

- WORLDWIDE
PDB
PROTEIN DATA BANK



• Molecule 84: 60S ribosomal protein L41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	212263	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.309	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	0.261	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SNC, PSU, OMG, 5MC, ZN, 1MA, NA, A2M, B8N, K, MA6, MG, OMC, G7M, OMU

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	A0	0.23	0/1828	0.38	0/2460
2	A1	0.22	0/2096	0.38	0/2819
3	A2	0.21	0/1485	0.32	0/1997
4	A3	0.21	0/1907	0.36	0/2548
5	A4	0.20	0/1638	0.35	0/2212
6	A5	0.26	0/1545	0.39	0/2067
7	A6	0.21	0/1507	0.32	0/2023
8	A7	1.02	0/2360	1.14	0/3216
9	A8	0.40	0/467	0.53	0/618
10	AA	0.67	8/42683 (0.0%)	1.29	45/66469 (0.1%)
11	AB	0.50	0/233	0.85	0/359
12	AC	0.23	0/1681	0.39	0/2274
13	AD	0.20	0/837	0.45	0/1129
14	AE	0.25	0/1276	0.33	0/1717
15	AG	0.33	0/1219	0.42	0/1634
16	AH	0.28	0/1026	0.48	0/1377
17	AI	0.19	0/996	0.35	0/1336
18	AJ	0.25	0/1035	0.41	0/1386
19	AK	0.23	0/1163	0.43	0/1564
20	AL	0.19	0/981	0.36	0/1310
21	AM	0.20	0/1116	0.30	0/1495
22	AO	0.20	0/1245	0.36	0/1665
23	AP	0.24	0/1723	0.35	0/2328
24	AQ	0.23	0/809	0.50	0/1091
25	AR	0.19	0/676	0.36	0/919
26	AS	0.24	0/1110	0.39	0/1485
27	AT	0.21	0/1059	0.44	0/1406
28	AU	0.20	0/588	0.41	0/786
29	AV	0.31	0/851	0.39	0/1139
30	AW	0.21	0/674	0.45	0/904
31	AX	0.19	0/1674	0.36	0/2236
32	AY	0.21	0/480	0.35	0/634

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AZ	0.17	0/453	0.29	0/602
34	Az	0.19	0/685	0.57	0/920
35	BA	0.66	0/37724	0.84	39/58780 (0.1%)
36	BB	0.71	3/25581 (0.0%)	0.85	16/39866 (0.0%)
37	BC	0.61	0/3640	0.75	0/5666
38	BD	0.56	0/2852	0.75	1/4444 (0.0%)
39	BE	0.58	0/4116	0.87	12/6397 (0.2%)
40	BF	0.47	0/1604	0.90	2/2487 (0.1%)
41	BG	0.63	0/4383	0.82	1/6835 (0.0%)
42	BH	0.59	0/2836	0.82	1/4415 (0.0%)
43	BI	0.30	0/1552	0.43	0/2070
44	BK	0.21	0/1702	0.35	0/2281
45	BL	0.22	0/1430	0.41	0/1911
46	BN	0.22	0/1793	0.37	0/2391
47	BO	0.24	0/1832	0.37	0/2446
48	BP	0.26	0/1434	0.42	0/1921
49	BQ	0.27	0/1755	0.36	0/2346
50	BR	0.24	0/1253	0.36	0/1681
51	BS	0.23	0/1500	0.36	0/2018
52	BT	0.24	0/1614	0.37	0/2140
53	BU	0.25	0/1283	0.42	1/1727 (0.1%)
54	BV	0.16	0/995	0.44	0/1329
55	BW	0.32	0/1000	0.43	0/1347
56	BX	0.22	0/983	0.33	0/1322
57	BY	0.37	0/567	0.53	0/763
58	BZ	0.20	0/1006	0.33	0/1340
59	Ba	0.26	0/1110	0.39	0/1479
60	Bb	0.25	0/1165	0.35	0/1554
61	Bc	0.22	0/1179	0.35	0/1573
62	Bd	0.45	0/572	0.66	0/766
63	Be	0.28	0/2007	0.39	0/2700
64	Bf	0.39	0/3244	0.51	0/4360
65	Bg	0.33	0/718	0.44	0/969
66	Bh	0.34	0/1179	0.49	0/1577
67	Bi	0.24	0/1097	0.31	0/1468
68	Bj	0.22	0/1053	0.35	0/1410
69	Bk	0.22	0/1026	0.41	0/1355
70	Bl	0.40	0/1187	0.57	0/1592
71	Bm	0.21	0/796	0.40	0/1057
72	Bn	0.29	0/707	0.40	0/942
73	Bo	0.38	0/711	0.49	0/946
74	Bp	0.20	0/618	0.48	0/822
75	Bq	0.24	0/471	0.31	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Br	0.32	0/2936	0.45	0/3941
77	Bs	0.14	0/406	0.34	0/538
78	Bt	0.25	0/815	0.38	0/1077
79	Bu	0.20	0/2428	0.37	0/3254
80	Bv	0.21	0/1141	0.35	0/1538
81	Bw	0.29	0/1907	0.39	0/2556
82	Bx	0.28	0/1901	0.44	0/2557
83	By	0.19	0/1536	0.36	0/2065
84	Bz	0.39	0/293	0.34	0/381
All	All	0.54	11/217744 (0.0%)	0.84	118/319151 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	A7	0	13
9	A8	0	1
43	BI	0	2
55	BW	0	1
57	BY	0	3
59	Ba	0	1
64	Bf	0	4
70	Bl	0	1
73	Bo	0	1
76	Br	0	1
82	Bx	0	1
All	All	0	29

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AA	1613	A	N9-C4	24.33	1.52	1.37
10	AA	1613	A	N9-C8	-19.16	1.22	1.37
10	AA	1613	A	C8-N7	14.92	1.42	1.31
10	AA	1613	A	C5-C4	-13.90	1.29	1.38
10	AA	1613	A	N3-C4	5.59	1.38	1.34

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	1613	A	N7-C8-N9	-158.07	34.76	113.80
10	AA	1613	A	C4-C5-N7	-148.03	36.68	110.70
10	AA	1613	A	C8-N9-C4	-109.12	62.15	105.80
10	AA	1613	A	C5-N7-C8	70.12	138.96	103.90
10	AA	1613	A	C6-C5-N7	25.34	150.04	132.30

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	A7	122	ARG	Sidechain
8	A7	36	ARG	Sidechain
8	A7	61	ARG	Sidechain
8	A7	62	ARG	Sidechain
8	A7	92	ARG	Sidechain

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	A0	1801	0	1871	24	0
2	A1	2062	0	2181	17	0
3	A2	1463	0	1524	9	0
4	A3	1885	0	1994	23	0
5	A4	1606	0	1675	21	0
6	A5	1521	0	1604	14	0
7	A6	1477	0	1536	12	0
8	A7	2315	0	2212	32	0
9	A8	461	0	467	3	0
10	AA	39092	0	19779	285	0
11	AB	210	0	113	1	0
12	AC	1647	0	1684	25	0
13	AD	814	0	819	19	0
14	AE	1251	0	1301	9	0
15	AG	1198	0	1276	11	0
16	AH	1011	0	1021	20	0
17	AI	975	0	1008	22	0
18	AJ	1018	0	1050	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AK	1143	0	1204	13	0
20	AL	969	0	1039	21	0
21	AM	1098	0	1146	14	0
22	AO	1220	0	1286	15	0
23	AP	1688	0	1734	19	0
24	AQ	800	0	856	21	0
25	AR	666	0	670	9	0
26	AS	1089	0	1144	9	0
27	AT	1043	0	1130	10	0
28	AU	582	0	629	5	0
29	AV	835	0	869	13	0
30	AW	660	0	664	11	0
31	AX	1652	0	1721	31	0
32	AY	474	0	519	7	0
33	AZ	454	0	488	1	0
34	Az	673	0	689	30	0
35	BA	34591	0	17479	170	0
36	BB	24057	0	12189	140	0
37	BC	3412	0	1738	19	0
38	BD	2553	0	1294	9	0
39	BE	3691	0	1875	22	0
40	BF	1444	0	744	19	0
41	BG	3919	0	1975	25	0
42	BH	2540	0	1286	22	0
43	BI	1526	0	1646	8	0
44	BK	1668	0	1743	22	0
45	BL	1408	0	1440	24	0
46	BN	1762	0	1864	16	0
47	BO	1801	0	1952	9	0
48	BP	1414	0	1514	14	0
49	BQ	1716	0	1795	10	0
50	BR	1228	0	1286	2	0
51	BS	1465	0	1500	14	0
52	BT	1597	0	1671	19	0
53	BU	1253	0	1304	15	0
54	BV	979	0	1002	17	0
55	BW	983	0	1040	7	0
56	BX	966	0	1030	6	0
57	BY	547	0	551	4	0
58	BZ	993	0	1072	12	0
59	Ba	1090	0	1156	16	0
60	Bb	1137	0	1174	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	Bc	1162	0	1246	18	0
62	Bd	561	0	583	2	0
63	Be	1962	0	2024	13	0
64	Bf	3174	0	3300	18	0
65	Bg	708	0	726	6	0
66	Bh	1160	0	1207	18	0
67	Bi	1075	0	1135	11	0
68	Bj	1035	0	1065	6	0
69	Bk	1018	0	1141	13	0
70	Bl	1163	0	1221	15	0
71	Bm	786	0	865	7	0
72	Bn	693	0	708	6	0
73	Bo	699	0	726	6	0
74	Bp	609	0	666	14	0
75	Bq	457	0	495	4	0
76	Br	2882	0	3011	16	0
77	Bs	400	0	428	3	0
78	Bt	801	0	861	5	0
79	Bu	2388	0	2455	33	0
80	Bv	1121	0	1182	19	0
81	Bw	1872	0	1966	16	0
82	Bx	1874	0	2008	12	0
83	By	1515	0	1589	30	0
84	Bz	289	0	325	0	0
85	A0	1	0	0	0	0
85	A3	1	0	0	0	0
85	AA	50	0	0	0	0
85	BA	69	0	0	0	0
85	BB	61	0	0	0	0
85	BC	4	0	0	0	0
85	BD	3	0	0	0	0
85	BE	3	0	0	0	0
85	BF	1	0	0	0	0
85	BG	1	0	0	0	0
85	BH	1	0	0	0	0
85	BW	1	0	0	0	0
85	Bn	1	0	0	0	0
86	A8	1	0	0	0	0
86	AV	1	0	0	0	0
86	Bn	1	0	0	0	0
86	Bo	1	0	0	0	0
86	Bs	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	Bt	1	0	0	0	0
87	AA	25	0	0	0	0
87	BA	22	0	0	0	0
87	BB	22	0	0	0	0
87	BC	1	0	0	0	0
87	BE	1	0	0	0	0
87	BG	6	0	0	0	0
87	BH	1	0	0	0	0
87	Be	1	0	0	0	0
87	Bn	1	0	0	0	0
88	AA	5	0	0	0	0
88	BA	8	0	0	0	0
88	BB	9	0	0	0	0
88	BR	1	0	0	0	0
88	BU	1	0	0	0	0
89	A1	1	0	0	0	0
89	A2	1	0	0	0	0
89	A5	6	0	0	0	0
89	AA	264	0	0	2	0
89	AC	1	0	0	0	0
89	AE	5	0	0	1	0
89	AG	10	0	0	1	0
89	AH	3	0	0	0	0
89	AO	1	0	0	0	0
89	AP	2	0	0	0	0
89	AV	7	0	0	0	0
89	AX	1	0	0	0	0
89	BA	239	0	0	1	0
89	BB	353	0	0	2	0
89	BC	8	0	0	0	0
89	BE	13	0	0	0	0
89	BG	40	0	0	1	0
89	BH	9	0	0	0	0
89	BI	2	0	0	0	0
89	BK	2	0	0	0	0
89	BQ	4	0	0	0	0
89	BR	6	0	0	0	0
89	BT	4	0	0	0	0
89	BU	1	0	0	0	0
89	BV	3	0	0	0	0
89	BW	11	0	0	1	0
89	BY	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	Bb	3	0	0	0	0
89	Be	6	0	0	1	0
89	Bf	25	0	0	1	0
89	Bi	3	0	0	0	0
89	Bj	1	0	0	0	0
89	Bl	2	0	0	0	0
89	Bn	9	0	0	0	0
89	Bo	6	0	0	0	0
89	Br	4	0	0	0	0
89	Bt	1	0	0	0	0
89	Bx	1	0	0	0	0
89	Bz	5	0	0	0	0
All	All	207369	0	153156	1510	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 1510 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)
36:BB:1424:C:H4'	36:BB:1425:A:C6	1.88	1.07
10:AA:837:A:H2	10:AA:893:G:N1	1.58	1.01
10:AA:837:A:C2	10:AA:893:G:N1	2.30	0.99
35:BA:1864:G:H1	36:BB:6:A:H61	1.10	0.97
36:BB:1424:C:H4'	36:BB:1425:A:C5	1.99	0.97

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	A0	220/256 (86%)	209 (95%)	9 (4%)	2 (1%)	14	31
2	A1	260/273 (95%)	241 (93%)	19 (7%)	0	100	100
3	A2	179/190 (94%)	177 (99%)	2 (1%)	0	100	100
4	A3	236/250 (94%)	231 (98%)	5 (2%)	0	100	100
5	A4	196/202 (97%)	190 (97%)	6 (3%)	0	100	100
6	A5	186/220 (84%)	178 (96%)	8 (4%)	0	100	100
7	A6	177/190 (93%)	171 (97%)	6 (3%)	0	100	100
8	A7	298/318 (94%)	257 (86%)	33 (11%)	8 (3%)	4	9
9	A8	55/57 (96%)	52 (94%)	3 (6%)	0	100	100
12	AC	206/277 (74%)	196 (95%)	10 (5%)	0	100	100
13	AD	97/172 (56%)	95 (98%)	2 (2%)	0	100	100
14	AE	151/174 (87%)	146 (97%)	5 (3%)	0	100	100
15	AG	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
16	AH	134/144 (93%)	123 (92%)	11 (8%)	0	100	100
17	AI	119/152 (78%)	114 (96%)	5 (4%)	0	100	100
18	AJ	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
19	AK	141/149 (95%)	131 (93%)	9 (6%)	1 (1%)	18	37
20	AL	120/142 (84%)	115 (96%)	5 (4%)	0	100	100
21	AM	133/153 (87%)	131 (98%)	2 (2%)	0	100	100
22	AO	152/167 (91%)	150 (99%)	2 (1%)	0	100	100
23	AP	216/266 (81%)	208 (96%)	7 (3%)	1 (0%)	24	45
24	AQ	98/117 (84%)	97 (99%)	1 (1%)	0	100	100
25	AR	87/194 (45%)	84 (97%)	3 (3%)	0	100	100
26	AS	137/143 (96%)	125 (91%)	12 (9%)	0	100	100
27	AT	128/137 (93%)	120 (94%)	7 (6%)	1 (1%)	16	34
28	AU	72/113 (64%)	68 (94%)	4 (6%)	0	100	100
29	AV	102/111 (92%)	94 (92%)	8 (8%)	0	100	100
30	AW	83/86 (96%)	75 (90%)	8 (10%)	0	100	100
31	AX	206/214 (96%)	198 (96%)	7 (3%)	1 (0%)	24	45
32	AY	55/66 (83%)	52 (94%)	3 (6%)	0	100	100
33	AZ	55/103 (53%)	54 (98%)	1 (2%)	0	100	100
34	Az	82/279 (29%)	70 (85%)	11 (13%)	1 (1%)	10	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BI	190/193 (98%)	181 (95%)	9 (5%)	0	100	100
44	BK	200/213 (94%)	193 (96%)	7 (4%)	0	100	100
45	BL	176/194 (91%)	170 (97%)	6 (3%)	0	100	100
46	BN	213/218 (98%)	204 (96%)	9 (4%)	0	100	100
47	BO	219/222 (99%)	215 (98%)	4 (2%)	0	100	100
48	BP	175/189 (93%)	170 (97%)	5 (3%)	0	100	100
49	BQ	201/221 (91%)	198 (98%)	3 (2%)	0	100	100
50	BR	150/166 (90%)	145 (97%)	5 (3%)	0	100	100
51	BS	176/179 (98%)	170 (97%)	6 (3%)	0	100	100
52	BT	195/260 (75%)	191 (98%)	4 (2%)	0	100	100
53	BU	156/159 (98%)	145 (93%)	11 (7%)	0	100	100
54	BV	120/130 (92%)	112 (93%)	8 (7%)	0	100	100
55	BW	128/139 (92%)	126 (98%)	2 (2%)	0	100	100
56	BX	116/164 (71%)	112 (97%)	4 (3%)	0	100	100
57	BY	62/125 (50%)	61 (98%)	1 (2%)	0	100	100
58	BZ	120/143 (84%)	116 (97%)	4 (3%)	0	100	100
59	Ba	131/133 (98%)	128 (98%)	3 (2%)	0	100	100
60	Bb	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
61	Bc	142/146 (97%)	138 (97%)	4 (3%)	0	100	100
62	Bd	67/71 (94%)	64 (96%)	3 (4%)	0	100	100
63	Be	256/260 (98%)	250 (98%)	6 (2%)	0	100	100
64	Bf	394/429 (92%)	381 (97%)	13 (3%)	0	100	100
65	Bg	90/105 (86%)	87 (97%)	3 (3%)	0	100	100
66	Bh	142/188 (76%)	134 (94%)	8 (6%)	0	100	100
67	Bi	129/132 (98%)	127 (98%)	2 (2%)	0	100	100
68	Bj	129/170 (76%)	125 (97%)	4 (3%)	0	100	100
69	Bk	121/127 (95%)	116 (96%)	4 (3%)	1 (1%)	16	34
70	Bl	142/149 (95%)	138 (97%)	4 (3%)	0	100	100
71	Bm	96/109 (88%)	94 (98%)	2 (2%)	0	100	100
72	Bn	80/84 (95%)	76 (95%)	4 (5%)	0	100	100
73	Bo	87/93 (94%)	84 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	Bp	73/82 (89%)	70 (96%)	3 (4%)	0	100	100
75	Bq	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
76	Br	365/374 (98%)	358 (98%)	7 (2%)	0	100	100
77	Bs	48/128 (38%)	47 (98%)	1 (2%)	0	100	100
78	Bt	95/106 (90%)	89 (94%)	6 (6%)	0	100	100
79	Bu	299/308 (97%)	288 (96%)	11 (4%)	0	100	100
80	Bv	142/192 (74%)	134 (94%)	8 (6%)	0	100	100
81	Bw	228/257 (89%)	218 (96%)	10 (4%)	0	100	100
82	Bx	231/276 (84%)	221 (96%)	9 (4%)	1 (0%)	30	51
83	By	184/189 (97%)	173 (94%)	11 (6%)	0	100	100
84	Bz	31/34 (91%)	31 (100%)	0	0	100	100
All	All	11145/12849 (87%)	10678 (96%)	450 (4%)	17 (0%)	44	65

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A0	159	LYS
8	A7	284	ILE
19	AK	46	LEU
34	Az	177	PHE
8	A7	165	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	191/218 (88%)	181 (95%)	10 (5%)	21	43
2	A1	221/231 (96%)	214 (97%)	7 (3%)	34	61
3	A2	157/160 (98%)	153 (98%)	4 (2%)	42	69
4	A3	194/207 (94%)	184 (95%)	10 (5%)	21	43
5	A4	174/187 (93%)	165 (95%)	9 (5%)	21	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	A5	154/180 (86%)	150 (97%)	4 (3%)	40	68
7	A6	159/166 (96%)	156 (98%)	3 (2%)	50	75
8	A7	247/266 (93%)	164 (66%)	83 (34%)	0	0
9	A8	48/50 (96%)	45 (94%)	3 (6%)	16	35
12	AC	182/243 (75%)	175 (96%)	7 (4%)	29	55
13	AD	87/131 (66%)	82 (94%)	5 (6%)	18	40
14	AE	138/156 (88%)	134 (97%)	4 (3%)	37	64
15	AG	129/131 (98%)	121 (94%)	8 (6%)	16	36
16	AH	102/112 (91%)	99 (97%)	3 (3%)	37	64
17	AI	100/128 (78%)	98 (98%)	2 (2%)	48	74
18	AJ	108/109 (99%)	106 (98%)	2 (2%)	50	75
19	AK	117/124 (94%)	113 (97%)	4 (3%)	32	59
20	AL	101/122 (83%)	95 (94%)	6 (6%)	18	38
21	AM	118/133 (89%)	112 (95%)	6 (5%)	21	44
22	AO	127/137 (93%)	122 (96%)	5 (4%)	28	54
23	AP	181/204 (89%)	174 (96%)	7 (4%)	28	54
24	AQ	90/104 (86%)	84 (93%)	6 (7%)	15	32
25	AR	73/150 (49%)	73 (100%)	0	100	100
26	AS	114/118 (97%)	106 (93%)	8 (7%)	14	31
27	AT	109/116 (94%)	104 (95%)	5 (5%)	24	48
28	AU	65/94 (69%)	61 (94%)	4 (6%)	16	36
29	AV	90/97 (93%)	86 (96%)	4 (4%)	25	50
30	AW	74/75 (99%)	69 (93%)	5 (7%)	14	32
31	AX	176/180 (98%)	167 (95%)	9 (5%)	21	44
32	AY	49/53 (92%)	48 (98%)	1 (2%)	48	74
33	AZ	49/84 (58%)	43 (88%)	6 (12%)	5	10
34	Az	72/216 (33%)	66 (92%)	6 (8%)	10	24
43	BI	164/165 (99%)	159 (97%)	5 (3%)	36	63
44	BK	178/185 (96%)	172 (97%)	6 (3%)	32	59
45	BL	148/167 (89%)	142 (96%)	6 (4%)	27	52
46	BN	185/188 (98%)	179 (97%)	6 (3%)	34	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	BO	194/195 (100%)	191 (98%)	3 (2%)	57	79
48	BP	147/158 (93%)	136 (92%)	11 (8%)	12	28
49	BQ	176/193 (91%)	172 (98%)	4 (2%)	44	71
50	BR	130/144 (90%)	124 (95%)	6 (5%)	24	48
51	BS	159/160 (99%)	153 (96%)	6 (4%)	29	55
52	BT	154/198 (78%)	151 (98%)	3 (2%)	50	75
53	BU	132/134 (98%)	121 (92%)	11 (8%)	10	24
54	BV	100/116 (86%)	89 (89%)	11 (11%)	6	13
55	BW	101/108 (94%)	100 (99%)	1 (1%)	68	84
56	BX	105/136 (77%)	104 (99%)	1 (1%)	68	84
57	BY	56/102 (55%)	53 (95%)	3 (5%)	20	42
58	BZ	108/125 (86%)	105 (97%)	3 (3%)	38	65
59	Ba	115/117 (98%)	112 (97%)	3 (3%)	40	68
60	Bb	115/116 (99%)	113 (98%)	2 (2%)	53	77
61	Bc	128/130 (98%)	123 (96%)	5 (4%)	28	54
62	Bd	57/59 (97%)	55 (96%)	2 (4%)	32	58
63	Be	201/204 (98%)	199 (99%)	2 (1%)	68	84
64	Bf	337/360 (94%)	318 (94%)	19 (6%)	19	40
65	Bg	81/92 (88%)	78 (96%)	3 (4%)	30	56
66	Bh	121/162 (75%)	112 (93%)	9 (7%)	13	28
67	Bi	116/117 (99%)	111 (96%)	5 (4%)	26	51
68	Bj	100/137 (73%)	98 (98%)	2 (2%)	48	74
69	Bk	106/114 (93%)	103 (97%)	3 (3%)	38	65
70	Bl	122/126 (97%)	114 (93%)	8 (7%)	15	33
71	Bm	81/90 (90%)	80 (99%)	1 (1%)	63	82
72	Bn	70/71 (99%)	69 (99%)	1 (1%)	59	80
73	Bo	72/76 (95%)	69 (96%)	3 (4%)	26	52
74	Bp	70/77 (91%)	64 (91%)	6 (9%)	10	22
75	Bq	46/47 (98%)	46 (100%)	0	100	100
76	Br	304/310 (98%)	296 (97%)	8 (3%)	40	68
77	Bs	42/111 (38%)	41 (98%)	1 (2%)	43	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	Bt	87/95 (92%)	87 (100%)	0	100	100
79	Bu	239/247 (97%)	232 (97%)	7 (3%)	37	64
80	Bv	121/160 (76%)	115 (95%)	6 (5%)	22	45
81	Bw	193/213 (91%)	188 (97%)	5 (3%)	40	68
82	Bx	199/229 (87%)	190 (96%)	9 (4%)	24	49
83	By	169/172 (98%)	158 (94%)	11 (6%)	15	34
84	Bz	29/31 (94%)	28 (97%)	1 (3%)	32	59
All	All	9554/10819 (88%)	9100 (95%)	454 (5%)	24	46

5 of 454 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	AX	199	VAL
83	By	10	THR
49	BQ	219	ARG
82	Bx	139	THR
73	Bo	88	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
58	BZ	78	HIS
66	Bh	83	ASN
59	Ba	85	ASN
62	Bd	6	ASN
69	Bk	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	AA	1803/2280 (79%)	406 (22%)	14 (0%)
11	AB	8/76 (10%)	1 (12%)	0
35	BA	1591/1866 (85%)	294 (18%)	13 (0%)
36	BB	1120/1544 (72%)	208 (18%)	13 (1%)
37	BC	157/209 (75%)	24 (15%)	0
38	BD	119/120 (99%)	11 (9%)	1 (0%)
39	BE	168/216 (77%)	36 (21%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
40	BF	66/78 (84%)	13 (19%)	1 (1%)
41	BG	182/183 (99%)	26 (14%)	2 (1%)
42	BH	116/136 (85%)	28 (24%)	1 (0%)
All	All	5330/6708 (79%)	1047 (19%)	45 (0%)

5 of 1047 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	AA	32	C
10	AA	33	U
10	AA	45	C
10	AA	54	A
10	AA	62	G

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BB	636	A
36	BB	1172	G
36	BB	817	C
36	BB	982	U
36	BB	1524	U

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

145 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	$\# Z > 2$
36	PSU	BB	1403	85,36	18,21,22	4.27	8 (44%)	22,30,33	1.92	6 (27%)
36	OMG	BB	673	36	23,26,27	2.36	9 (39%)	33,38,41	2.56	10 (30%)
10	A2M	AA	125	85,10	22,25,26	3.48	10 (45%)	31,36,39	2.41	10 (32%)
10	MA6	AA	2261	10	23,26,27	1.60	5 (21%)	34,38,41	3.02	11 (32%)
36	PSU	BB	1229	36	18,21,22	4.34	7 (38%)	22,30,33	1.83	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	PSU	BA	1609	35	18,21,22	4.32	7 (38%)	22,30,33	1.77	5 (22%)
36	PSU	BB	518	36	18,21,22	4.42	8 (44%)	22,30,33	1.74	4 (18%)
10	OMG	AA	1676	10	23,26,27	2.37	9 (39%)	33,38,41	2.61	10 (30%)
35	A2M	BA	996	35	22,25,26	3.46	10 (45%)	31,36,39	2.40	10 (32%)
10	B8N	AA	1596	10	24,29,30	3.01	6 (25%)	29,42,45	1.72	5 (17%)
10	PSU	AA	1592	10	18,21,22	4.39	7 (38%)	22,30,33	1.82	5 (22%)
36	PSU	BB	680	85,36	18,21,22	0.87	1 (5%)	22,30,33	0.63	0
10	A2M	AA	2153	10	22,25,26	3.50	11 (50%)	31,36,39	2.44	11 (35%)
36	PSU	BB	1210	36	18,21,22	4.33	7 (38%)	22,30,33	1.82	5 (22%)
35	PSU	BA	1169	35	18,21,22	4.36	7 (38%)	22,30,33	1.88	5 (22%)
35	PSU	BA	1086	35,87	18,21,22	4.29	7 (38%)	22,30,33	1.82	5 (22%)
8	SNC	A7	157	8	4,7,8	0.71	0	1,7,9	0.33	0
36	PSU	BB	1434	36	18,21,22	4.35	7 (38%)	22,30,33	1.77	5 (22%)
10	PSU	AA	2045	10	18,21,22	4.35	7 (38%)	22,30,33	1.75	4 (18%)
10	OMG	AA	1517	10	23,26,27	2.39	9 (39%)	33,38,41	2.57	10 (30%)
36	OMU	BB	1435	36	19,22,23	2.87	8 (42%)	26,31,34	1.73	4 (15%)
36	PSU	BB	1409	36	18,21,22	4.39	7 (38%)	22,30,33	1.74	5 (22%)
35	PSU	BA	1129	35,87	18,21,22	4.33	7 (38%)	22,30,33	1.81	5 (22%)
36	OMC	BB	1264	36	19,22,23	2.88	8 (42%)	26,31,34	0.82	0
35	OMG	BA	1709	35	23,26,27	2.36	9 (39%)	33,38,41	2.43	11 (33%)
10	OMC	AA	66	10	19,22,23	2.90	8 (42%)	26,31,34	0.76	0
36	OMG	BB	1245	36	23,26,27	2.35	9 (39%)	33,38,41	2.52	10 (30%)
10	OMC	AA	1844	10	19,22,23	2.91	8 (42%)	26,31,34	0.69	0
36	PSU	BB	1419	36	18,21,22	4.35	8 (44%)	22,30,33	1.91	6 (27%)
35	OMU	BA	1742	85,35	19,22,23	2.88	8 (42%)	26,31,34	1.78	5 (19%)
10	PSU	AA	1907	10	18,21,22	4.38	8 (44%)	22,30,33	1.78	5 (22%)
36	A2M	BB	646	36	22,25,26	3.47	10 (45%)	31,36,39	2.40	9 (29%)
35	A2M	BA	1620	85,35,36	22,25,26	3.49	10 (45%)	31,36,39	2.37	9 (29%)
36	OMU	BB	1093	36	19,22,23	2.94	8 (42%)	26,31,34	1.77	5 (19%)
36	OMG	BB	1269	36	23,26,27	2.33	8 (34%)	33,38,41	2.53	10 (30%)
36	A2M	BB	545	85,36	22,25,26	3.40	10 (45%)	31,36,39	2.56	14 (45%)
36	OMU	BB	1375	36	19,22,23	0.21	0	26,31,34	0.47	0
10	OMC	AA	2134	10	19,22,23	0.27	0	26,31,34	0.46	0
10	PSU	AA	131	10	18,21,22	4.41	7 (38%)	22,30,33	1.86	5 (22%)
36	PSU	BB	644	36	18,21,22	4.30	7 (38%)	22,30,33	1.82	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	A2M	BC	43	37	22,25,26	3.46	10 (45%)	31,36,39	2.39	9 (29%)
36	A2M	BB	588	35,36	22,25,26	0.19	0	31,36,39	0.31	0
35	A2M	BA	1665	35,36	22,25,26	3.44	10 (45%)	31,36,39	2.43	10 (32%)
36	PSU	BB	455	36,87	18,21,22	0.88	1 (5%)	22,30,33	0.63	0
35	OMC	BA	1329	35	19,22,23	2.97	8 (42%)	26,31,34	0.70	0
35	OMG	BA	1621	85,35,36	23,26,27	2.34	9 (39%)	33,38,41	2.49	11 (33%)
37	PSU	BC	74	37	18,21,22	4.42	7 (38%)	22,30,33	1.86	5 (22%)
10	PSU	AA	1710	10	18,21,22	4.33	7 (38%)	22,30,33	1.74	4 (18%)
35	A2M	BA	927	35	22,25,26	3.45	10 (45%)	31,36,39	2.41	10 (32%)
36	OMG	BB	1094	36	23,26,27	2.34	9 (39%)	33,38,41	2.44	12 (36%)
35	OMU	BA	916	35	19,22,23	2.89	8 (42%)	26,31,34	1.79	5 (19%)
36	PSU	BB	1334	36	18,21,22	4.31	7 (38%)	22,30,33	1.88	5 (22%)
35	OMG	BA	1605	35	23,26,27	2.36	9 (39%)	33,38,41	2.57	10 (30%)
10	OMG	AA	1931	10	23,26,27	2.38	9 (39%)	33,38,41	2.54	10 (30%)
35	A2M	BA	254	35	22,25,26	3.45	9 (40%)	31,36,39	2.38	11 (35%)
36	OMU	BB	685	36	19,22,23	2.91	8 (42%)	26,31,34	1.78	5 (19%)
36	A2M	BB	590	36	22,25,26	3.45	10 (45%)	31,36,39	2.37	10 (32%)
35	OMG	BA	915	35	23,26,27	2.39	9 (39%)	33,38,41	2.52	10 (30%)
37	OMU	BC	7	37,35	19,22,23	2.90	8 (42%)	26,31,34	1.74	5 (19%)
10	OMG	AA	1603	10	23,26,27	2.40	9 (39%)	33,38,41	2.51	10 (30%)
36	OMG	BB	72	36	23,26,27	2.34	8 (34%)	33,38,41	2.50	10 (30%)
10	OMU	AA	714	10	19,22,23	2.89	8 (42%)	26,31,34	1.78	5 (19%)
36	PSU	BB	1429	36,87	18,21,22	4.24	7 (38%)	22,30,33	1.78	5 (22%)
35	PSU	BA	1614	35,36	18,21,22	4.33	7 (38%)	22,30,33	1.85	5 (22%)
36	OMC	BB	377	36	19,22,23	2.95	8 (42%)	26,31,34	0.72	0
35	OMG	BA	1267	35	23,26,27	2.35	9 (39%)	33,38,41	2.43	12 (36%)
10	OMU	AA	2123	10	19,22,23	2.73	7 (36%)	26,31,34	1.81	5 (19%)
36	OMU	BB	578	36,87	19,22,23	2.89	8 (42%)	26,31,34	1.73	4 (15%)
35	A2M	BA	762	35	22,25,26	3.52	11 (50%)	31,36,39	2.37	10 (32%)
36	A2M	BB	95	36	22,25,26	3.51	10 (45%)	31,36,39	2.40	11 (35%)
10	PSU	AA	1276	10	18,21,22	4.35	7 (38%)	22,30,33	1.83	5 (22%)
36	A2M	BB	1388	36	22,25,26	3.48	9 (40%)	31,36,39	2.39	11 (35%)
10	A2M	AA	2096	10	22,25,26	3.44	9 (40%)	31,36,39	2.40	11 (35%)
10	A2M	AA	721	85,10	22,25,26	3.43	10 (45%)	31,36,39	2.45	11 (35%)
10	OMU	AA	1899	10	19,22,23	2.98	8 (42%)	26,31,34	1.78	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	PSU	BA	1080	35,36	18,21,22	4.43	7 (38%)	22,30,33	1.88	6 (27%)
36	PSU	BB	490	36	18,21,22	4.45	7 (38%)	22,30,33	1.89	5 (22%)
35	1MA	BA	742	85,35	21,25,26	2.83	6 (28%)	31,37,40	2.94	8 (25%)
10	OMU	AA	36	10	19,22,23	0.22	0	26,31,34	0.50	0
36	OMC	BB	601	36	19,22,23	2.76	7 (36%)	26,31,34	0.70	0
35	PSU	BA	737	85,35	18,21,22	4.31	7 (38%)	22,30,33	1.76	6 (27%)
10	MA6	AA	2260	10	23,26,27	1.50	5 (21%)	34,38,41	3.01	12 (35%)
36	OMG	BB	1247	36	23,26,27	2.37	9 (39%)	33,38,41	2.52	10 (30%)
36	PSU	BB	611	36	18,21,22	4.32	7 (38%)	22,30,33	1.65	4 (18%)
36	5MC	BB	1324	36,87	18,22,23	3.41	7 (38%)	26,32,35	1.18	1 (3%)
37	OMG	BC	75	37	23,26,27	2.38	9 (39%)	33,38,41	2.50	10 (30%)
36	OMC	BB	1413	36	19,22,23	2.80	8 (42%)	26,31,34	0.78	0
10	OMU	AA	57	10	19,22,23	2.91	8 (42%)	26,31,34	1.71	5 (19%)
10	PSU	AA	505	10	18,21,22	4.31	7 (38%)	22,30,33	1.94	5 (22%)
36	OMG	BB	552	36	23,26,27	2.34	9 (39%)	33,38,41	2.49	10 (30%)
37	A2M	BC	41	37	22,25,26	3.47	10 (45%)	31,36,39	2.40	10 (32%)
10	OMG	AA	1895	85,10	23,26,27	2.36	9 (39%)	33,38,41	2.51	10 (30%)
36	A2M	BB	609	36	22,25,26	3.48	10 (45%)	31,36,39	2.36	11 (35%)
35	PSU	BA	1248	35,87	18,21,22	4.30	8 (44%)	22,30,33	1.86	6 (27%)
36	PSU	BB	629	36	18,21,22	4.31	7 (38%)	22,30,33	1.77	5 (22%)
10	OMU	AA	2154	10	19,22,23	2.93	8 (42%)	26,31,34	1.80	5 (19%)
35	OMC	BA	1006	35	19,22,23	2.83	8 (42%)	26,31,34	0.75	0
36	PSU	BB	1160	36	18,21,22	4.36	7 (38%)	22,30,33	1.85	5 (22%)
35	PSU	BA	1009	35	18,21,22	4.28	7 (38%)	22,30,33	1.83	4 (18%)
10	OMG	AA	1531	10	23,26,27	0.30	0	33,38,41	0.36	0
35	OMU	BA	46	35	19,22,23	2.92	8 (42%)	26,31,34	1.83	5 (19%)
10	G7M	AA	2070	10	23,26,27	3.70	11 (47%)	35,39,42	1.68	7 (20%)
36	5MC	BB	542	85,36	18,22,23	3.34	7 (38%)	26,32,35	1.08	2 (7%)
37	OMU	BC	167	37,35	19,22,23	2.94	8 (42%)	26,31,34	1.78	5 (19%)
36	OMG	BB	659	85,36	23,26,27	2.31	9 (39%)	33,38,41	2.38	12 (36%)
35	OMU	BA	1181	35	19,22,23	2.90	8 (42%)	26,31,34	1.82	5 (19%)
36	OMU	BB	73	36	19,22,23	2.90	8 (42%)	26,31,34	1.76	5 (19%)
35	OMG	BA	1028	85,35	23,26,27	2.35	9 (39%)	33,38,41	2.29	9 (27%)
10	OMC	AA	1932	10	19,22,23	2.89	8 (42%)	26,31,34	0.75	0
10	PSU	AA	2146	10	18,21,22	4.21	7 (38%)	22,30,33	1.83	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PSU	AA	61	10	18,21,22	4.42	7 (38%)	22,30,33	1.87	5 (22%)
35	PSU	BA	1258	35	18,21,22	4.37	7 (38%)	22,30,33	1.85	5 (22%)
36	OMG	BB	71	36	23,26,27	2.37	8 (34%)	33,38,41	2.44	12 (36%)
36	A2M	BB	400	36	22,25,26	3.45	10 (45%)	31,36,39	2.33	9 (29%)
35	OMC	BA	1608	35	19,22,23	2.84	8 (42%)	26,31,34	0.82	1 (3%)
37	A2M	BC	163	37,35	22,25,26	3.47	10 (45%)	31,36,39	2.36	11 (35%)
10	OMU	AA	2054	10	19,22,23	2.92	8 (42%)	26,31,34	1.78	5 (19%)
36	PSU	BB	1076	36	18,21,22	4.34	7 (38%)	22,30,33	1.98	5 (22%)
10	OMG	AA	1700	10	23,26,27	2.32	9 (39%)	33,38,41	2.47	11 (33%)
35	A2M	BA	743	35,36	22,25,26	3.49	10 (45%)	31,36,39	2.48	12 (38%)
10	OMG	AA	2227	10	23,26,27	2.30	8 (34%)	33,38,41	2.45	10 (30%)
10	PSU	AA	1619	10	18,21,22	4.40	8 (44%)	22,30,33	1.67	4 (18%)
35	OMC	BA	747	85,35	19,22,23	2.82	7 (36%)	26,31,34	0.86	0
36	OMG	BB	1062	36	23,26,27	2.36	9 (39%)	33,38,41	2.54	10 (30%)
10	OMU	AA	1674	10	19,22,23	2.97	8 (42%)	26,31,34	1.71	5 (19%)
35	A2M	BA	746	35	22,25,26	3.41	9 (40%)	31,36,39	2.40	9 (29%)
10	PSU	AA	2278	10	18,21,22	4.37	7 (38%)	22,30,33	1.75	5 (22%)
36	PSU	BB	1280	36	18,21,22	4.29	8 (44%)	22,30,33	1.90	6 (27%)
35	PSU	BA	1166	35	18,21,22	4.37	7 (38%)	22,30,33	1.76	5 (22%)
36	A2M	BB	1400	88,36	22,25,26	0.17	0	31,36,39	0.55	0
35	OMU	BA	1448	35	19,22,23	2.92	8 (42%)	26,31,34	1.77	4 (15%)
10	A2M	AA	56	85,10	22,25,26	3.47	10 (45%)	31,36,39	2.39	9 (29%)
36	OMC	BB	1175	36	19,22,23	0.28	0	26,31,34	0.41	0
35	OMC	BA	760	35	19,22,23	2.86	8 (42%)	26,31,34	0.73	0
36	PSU	BB	1319	36	18,21,22	4.36	8 (44%)	22,30,33	1.90	6 (27%)
36	PSU	BB	615	36	18,21,22	4.30	7 (38%)	22,30,33	1.81	5 (22%)
36	A2M	BB	622	35,36	22,25,26	3.46	9 (40%)	31,36,39	2.38	10 (32%)
35	A2M	BA	1024	35	22,25,26	3.50	10 (45%)	31,36,39	2.42	10 (32%)
10	PSU	AA	1612	10	18,21,22	0.86	1 (5%)	22,30,33	0.64	0
35	OMG	BA	925	35	23,26,27	2.34	9 (39%)	33,38,41	2.44	10 (30%)
10	OMC	AA	46	10	19,22,23	2.85	8 (42%)	26,31,34	0.75	0
35	OMU	BA	1330	35	19,22,23	3.05	8 (42%)	26,31,34	1.84	5 (19%)
35	PSU	BA	452	35	18,21,22	4.37	7 (38%)	22,30,33	1.87	5 (22%)
36	PSU	BB	528	36	18,21,22	4.37	7 (38%)	22,30,33	1.84	5 (22%)
36	A2M	BB	1201	36	22,25,26	3.44	10 (45%)	31,36,39	2.48	12 (38%)

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
36	PSU	BB	1403	85,36	-	0/7/25/26	0/2/2/2
36	OMG	BB	673	36	-	0/9/27/28	0/3/3/3
10	A2M	AA	125	85,10	-	2/9/27/28	0/3/3/3
10	MA6	AA	2261	10	-	0/11/29/30	0/3/3/3
36	PSU	BB	1229	36	-	0/7/25/26	0/2/2/2
35	PSU	BA	1609	35	-	0/7/25/26	0/2/2/2
36	PSU	BB	518	36	-	2/7/25/26	0/2/2/2
10	OMG	AA	1676	10	-	1/9/27/28	0/3/3/3
35	A2M	BA	996	35	-	0/9/27/28	0/3/3/3
10	B8N	AA	1596	10	-	1/16/34/35	0/2/2/2
10	PSU	AA	1592	10	-	1/7/25/26	0/2/2/2
36	PSU	BB	680	85,36	-	0/7/25/26	0/2/2/2
10	A2M	AA	2153	10	-	1/9/27/28	0/3/3/3
36	PSU	BB	1210	36	-	0/7/25/26	0/2/2/2
35	PSU	BA	1169	35	-	0/7/25/26	0/2/2/2
35	PSU	BA	1086	35,87	-	0/7/25/26	0/2/2/2
8	SNC	A7	157	8	-	0/0/6/8	-
36	PSU	BB	1434	36	-	2/7/25/26	0/2/2/2
10	PSU	AA	2045	10	-	2/7/25/26	0/2/2/2
10	OMG	AA	1517	10	-	0/9/27/28	0/3/3/3
36	OMU	BB	1435	36	-	0/9/27/28	0/2/2/2
36	PSU	BB	1409	36	-	0/7/25/26	0/2/2/2
35	PSU	BA	1129	35,87	-	0/7/25/26	0/2/2/2
36	OMC	BB	1264	36	-	1/9/27/28	0/2/2/2
35	OMG	BA	1709	35	-	0/9/27/28	0/3/3/3
10	OMC	AA	66	10	-	0/9/27/28	0/2/2/2
36	OMG	BB	1245	36	-	0/9/27/28	0/3/3/3
10	OMC	AA	1844	10	-	0/9/27/28	0/2/2/2
36	PSU	BB	1419	36	-	0/7/25/26	0/2/2/2
35	OMU	BA	1742	85,35	-	0/9/27/28	0/2/2/2
10	PSU	AA	1907	10	-	1/7/25/26	0/2/2/2
36	A2M	BB	646	36	-	1/9/27/28	0/3/3/3
35	A2M	BA	1620	85,35,36	-	0/9/27/28	0/3/3/3
36	OMU	BB	1093	36	-	0/9/27/28	0/2/2/2
36	OMG	BB	1269	36	-	0/9/27/28	0/3/3/3
36	A2M	BB	545	85,36	-	2/9/27/28	0/3/3/3
36	OMU	BB	1375	36	-	0/9/27/28	0/2/2/2
10	OMC	AA	2134	10	-	2/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PSU	AA	131	10	-	0/7/25/26	0/2/2/2
36	PSU	BB	644	36	-	0/7/25/26	0/2/2/2
37	A2M	BC	43	37	-	0/9/27/28	0/3/3/3
36	A2M	BB	588	35,36	-	3/9/27/28	0/3/3/3
35	A2M	BA	1665	35,36	-	0/9/27/28	0/3/3/3
36	PSU	BB	455	36,87	-	0/7/25/26	0/2/2/2
35	OMC	BA	1329	35	-	3/9/27/28	0/2/2/2
35	OMG	BA	1621	85,35,36	-	1/9/27/28	0/3/3/3
37	PSU	BC	74	37	-	0/7/25/26	0/2/2/2
10	PSU	AA	1710	10	-	2/7/25/26	0/2/2/2
35	A2M	BA	927	35	-	0/9/27/28	0/3/3/3
36	OMG	BB	1094	36	-	0/9/27/28	0/3/3/3
35	OMU	BA	916	35	-	0/9/27/28	0/2/2/2
36	PSU	BB	1334	36	-	0/7/25/26	0/2/2/2
35	OMG	BA	1605	35	-	2/9/27/28	0/3/3/3
10	OMG	AA	1931	10	-	2/9/27/28	0/3/3/3
35	A2M	BA	254	35	-	0/9/27/28	0/3/3/3
36	OMU	BB	685	36	-	1/9/27/28	0/2/2/2
36	A2M	BB	590	36	-	0/9/27/28	0/3/3/3
35	OMG	BA	915	35	-	0/9/27/28	0/3/3/3
37	OMU	BC	7	37,35	-	1/9/27/28	0/2/2/2
10	OMG	AA	1603	10	-	2/9/27/28	0/3/3/3
36	OMG	BB	72	36	-	0/9/27/28	0/3/3/3
10	OMU	AA	714	10	-	0/9/27/28	0/2/2/2
36	PSU	BB	1429	36,87	-	0/7/25/26	0/2/2/2
35	PSU	BA	1614	35,36	-	2/7/25/26	0/2/2/2
36	OMC	BB	377	36	-	0/9/27/28	0/2/2/2
35	OMG	BA	1267	35	-	0/9/27/28	0/3/3/3
10	OMU	AA	2123	10	-	0/9/27/28	0/2/2/2
36	OMU	BB	578	36,87	-	4/9/27/28	0/2/2/2
35	A2M	BA	762	35	-	1/9/27/28	0/3/3/3
36	A2M	BB	95	36	-	1/9/27/28	0/3/3/3
10	PSU	AA	1276	10	-	0/7/25/26	0/2/2/2
36	A2M	BB	1388	36	-	0/9/27/28	0/3/3/3
10	A2M	AA	2096	10	-	1/9/27/28	0/3/3/3
10	A2M	AA	721	85,10	-	3/9/27/28	0/3/3/3
10	OMU	AA	1899	10	-	1/9/27/28	0/2/2/2
35	PSU	BA	1080	35,36	-	3/7/25/26	0/2/2/2
36	PSU	BB	490	36	-	0/7/25/26	0/2/2/2
35	1MA	BA	742	85,35	-	0/7/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	OMU	AA	36	10	-	5/9/27/28	0/2/2/2
36	OMC	BB	601	36	-	0/9/27/28	0/2/2/2
35	PSU	BA	737	85,35	-	0/7/25/26	0/2/2/2
10	MA6	AA	2260	10	-	0/11/29/30	0/3/3/3
36	OMG	BB	1247	36	-	0/9/27/28	0/3/3/3
36	PSU	BB	611	36	-	0/7/25/26	0/2/2/2
36	5MC	BB	1324	36,87	-	4/7/25/26	0/2/2/2
37	OMG	BC	75	37	-	0/9/27/28	0/3/3/3
36	OMC	BB	1413	36	-	0/9/27/28	0/2/2/2
10	OMU	AA	57	10	-	1/9/27/28	0/2/2/2
10	PSU	AA	505	10	-	0/7/25/26	0/2/2/2
36	OMG	BB	552	36	-	2/9/27/28	0/3/3/3
37	A2M	BC	41	37	-	0/9/27/28	0/3/3/3
10	OMG	AA	1895	85,10	-	1/9/27/28	0/3/3/3
36	A2M	BB	609	36	-	0/9/27/28	0/3/3/3
35	PSU	BA	1248	35,87	-	0/7/25/26	0/2/2/2
36	PSU	BB	629	36	-	2/7/25/26	0/2/2/2
10	OMU	AA	2154	10	-	1/9/27/28	0/2/2/2
35	OMC	BA	1006	35	-	1/9/27/28	0/2/2/2
36	PSU	BB	1160	36	-	0/7/25/26	0/2/2/2
35	PSU	BA	1009	35	-	0/7/25/26	0/2/2/2
10	OMG	AA	1531	10	-	2/9/27/28	0/3/3/3
35	OMU	BA	46	35	-	0/9/27/28	0/2/2/2
10	G7M	AA	2070	10	-	0/7/25/26	0/3/3/3
36	5MC	BB	542	85,36	-	1/7/25/26	0/2/2/2
37	OMU	BC	167	37,35	-	0/9/27/28	0/2/2/2
36	OMG	BB	659	85,36	-	1/9/27/28	0/3/3/3
35	OMU	BA	1181	35	-	0/9/27/28	0/2/2/2
36	OMU	BB	73	36	-	1/9/27/28	0/2/2/2
35	OMG	BA	1028	85,35	-	0/9/27/28	0/3/3/3
10	OMC	AA	1932	10	-	0/9/27/28	0/2/2/2
10	PSU	AA	2146	10	-	0/7/25/26	0/2/2/2
10	PSU	AA	61	10	-	0/7/25/26	0/2/2/2
35	PSU	BA	1258	35	-	2/7/25/26	0/2/2/2
36	OMG	BB	71	36	-	0/9/27/28	0/3/3/3
36	A2M	BB	400	36	-	0/9/27/28	0/3/3/3
35	OMC	BA	1608	35	-	4/9/27/28	0/2/2/2
37	A2M	BC	163	37,35	-	1/9/27/28	0/3/3/3
10	OMU	AA	2054	10	-	2/9/27/28	0/2/2/2
36	PSU	BB	1076	36	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	OMG	AA	1700	10	-	0/9/27/28	0/3/3/3
35	A2M	BA	743	35,36	-	1/9/27/28	0/3/3/3
10	OMG	AA	2227	10	-	0/9/27/28	0/3/3/3
10	PSU	AA	1619	10	-	4/7/25/26	0/2/2/2
35	OMC	BA	747	85,35	-	0/9/27/28	0/2/2/2
36	OMG	BB	1062	36	-	2/9/27/28	0/3/3/3
10	OMU	AA	1674	10	-	0/9/27/28	0/2/2/2
35	A2M	BA	746	35	-	1/9/27/28	0/3/3/3
10	PSU	AA	2278	10	-	1/7/25/26	0/2/2/2
36	PSU	BB	1280	36	-	0/7/25/26	0/2/2/2
35	PSU	BA	1166	35	-	0/7/25/26	0/2/2/2
36	A2M	BB	1400	88,36	-	1/9/27/28	0/3/3/3
35	OMU	BA	1448	35	-	2/9/27/28	0/2/2/2
10	A2M	AA	56	85,10	-	1/9/27/28	0/3/3/3
36	OMC	BB	1175	36	-	0/9/27/28	0/2/2/2
35	OMC	BA	760	35	-	0/9/27/28	0/2/2/2
36	PSU	BB	1319	36	-	0/7/25/26	0/2/2/2
36	PSU	BB	615	36	-	0/7/25/26	0/2/2/2
36	A2M	BB	622	35,36	-	0/9/27/28	0/3/3/3
35	A2M	BA	1024	35	-	1/9/27/28	0/3/3/3
10	PSU	AA	1612	10	-	1/7/25/26	0/2/2/2
35	OMG	BA	925	35	-	0/9/27/28	0/3/3/3
10	OMC	AA	46	10	-	0/9/27/28	0/2/2/2
35	OMU	BA	1330	35	-	3/9/27/28	0/2/2/2
35	PSU	BA	452	35	-	0/7/25/26	0/2/2/2
36	PSU	BB	528	36	-	0/7/25/26	0/2/2/2
36	A2M	BB	1201	36	-	1/9/27/28	0/3/3/3

The worst 5 of 1098 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1080	PSU	C6-C5	11.60	1.48	1.35
36	BB	1409	PSU	C6-C5	11.50	1.48	1.35
10	AA	1619	PSU	C6-C5	11.47	1.48	1.35
37	BC	74	PSU	C6-C5	11.44	1.48	1.35
36	BB	518	PSU	C6-C5	11.42	1.48	1.35

The worst 5 of 889 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	2261	MA6	N1-C6-N6	-11.57	104.44	117.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	2260	MA6	N1-C6-N6	-11.11	104.94	117.08
35	BA	742	1MA	C1'-N9-C8	-9.31	100.20	126.70
35	BA	742	1MA	C1'-N9-C4	8.91	152.98	126.50
10	AA	1676	OMG	C1'-N9-C8	-8.24	103.25	126.70

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	AA	56	A2M	C1'-C2'-O2'-CM'
10	AA	57	OMU	C1'-C2'-O2'-CM2
10	AA	721	A2M	C3'-C4'-C5'-O5'
10	AA	1619	PSU	C2'-C1'-C5-C4
10	AA	1676	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

39 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	AA	2261	MA6	1	0
10	AA	1676	OMG	1	0
10	AA	2153	A2M	1	0
10	AA	2045	PSU	2	0
36	BB	1245	OMG	1	0
36	BB	646	A2M	1	0
35	BA	1620	A2M	1	0
36	BB	545	A2M	1	0
36	BB	1375	OMU	1	0
36	BB	644	PSU	1	0
35	BA	1665	A2M	1	0
35	BA	916	OMU	1	0
35	BA	254	A2M	2	0
36	BB	685	OMU	1	0
35	BA	915	OMG	1	0
37	BC	7	OMU	2	0
36	BB	1429	PSU	1	0
10	AA	2123	OMU	1	0
36	BB	578	OMU	3	0
35	BA	762	A2M	3	0
36	BB	95	A2M	1	0
10	AA	2096	A2M	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	AA	2260	MA6	1	0
10	AA	57	OMU	1	0
36	BB	609	A2M	2	0
10	AA	2154	OMU	1	0
10	AA	2070	G7M	1	0
35	BA	1181	OMU	1	0
36	BB	400	A2M	1	0
37	BC	163	A2M	1	0
35	BA	743	A2M	3	0
35	BA	747	OMC	2	0
10	AA	1674	OMU	1	0
35	BA	746	A2M	1	0
36	BB	1400	A2M	1	0
10	AA	56	A2M	1	0
35	BA	1024	A2M	1	0
10	AA	46	OMC	1	0
35	BA	1330	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 307 ligands modelled in this entry, 307 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.

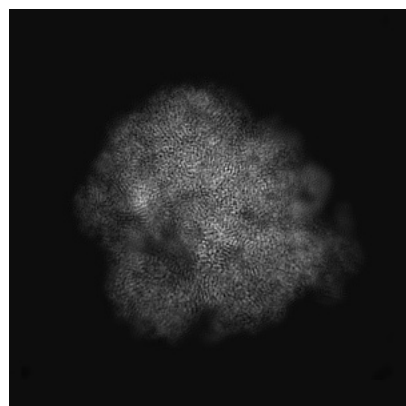
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55348. These allow visual inspection of the internal detail of the map and identification of artifacts.

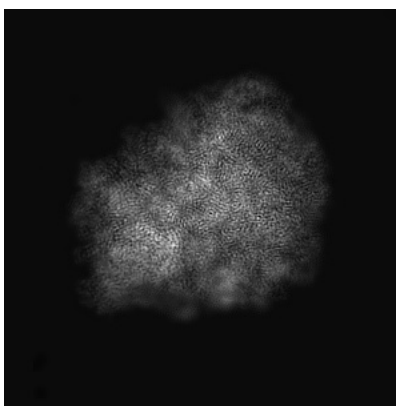
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

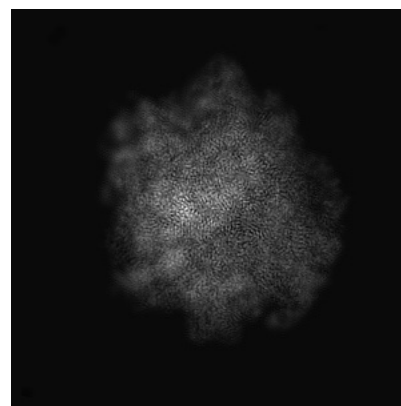
6.1.1 Primary map



X

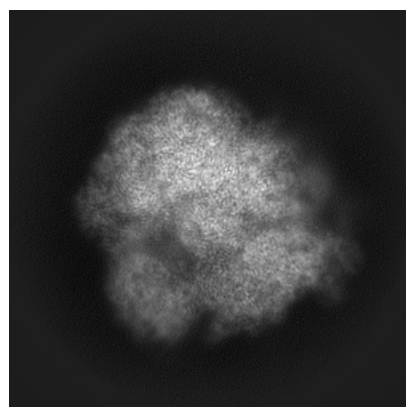


Y

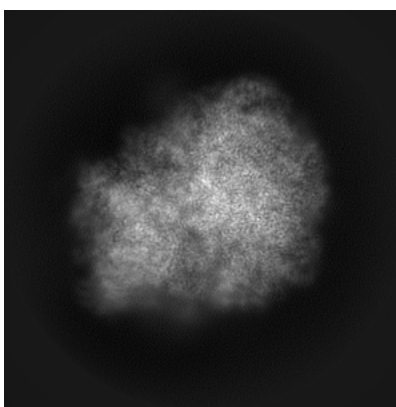


Z

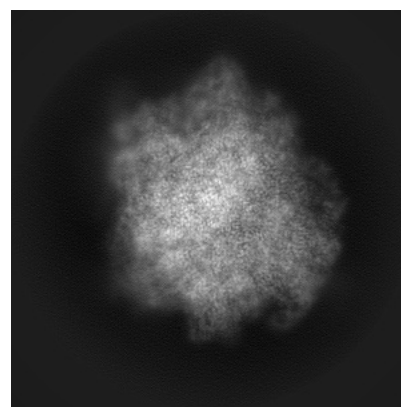
6.1.2 Raw map



X



Y

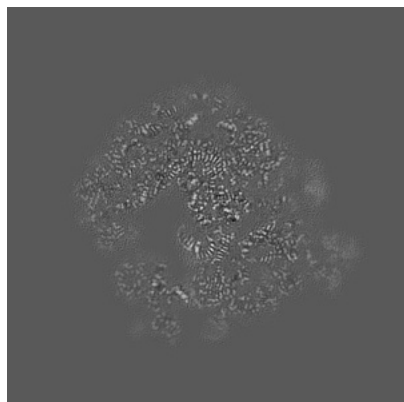


Z

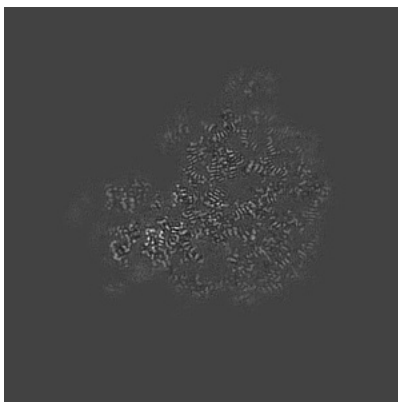
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

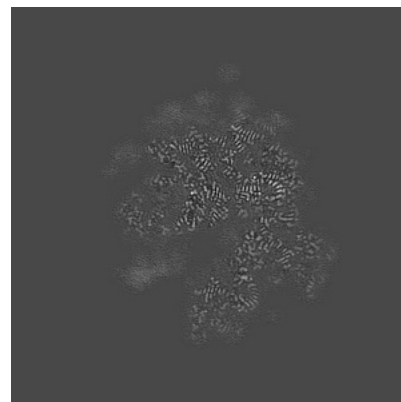
6.2.1 Primary map



X Index: 240

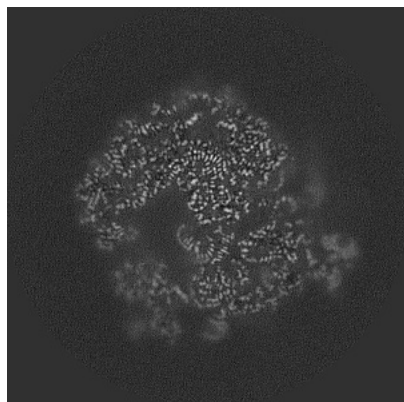


Y Index: 240

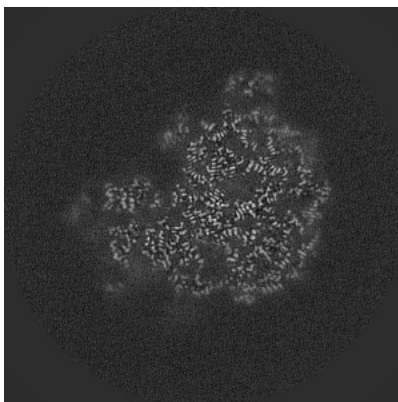


Z Index: 240

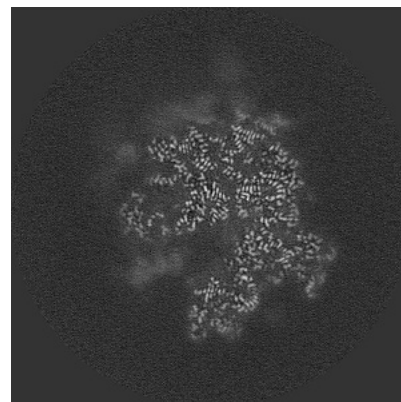
6.2.2 Raw map



X Index: 240



Y Index: 240

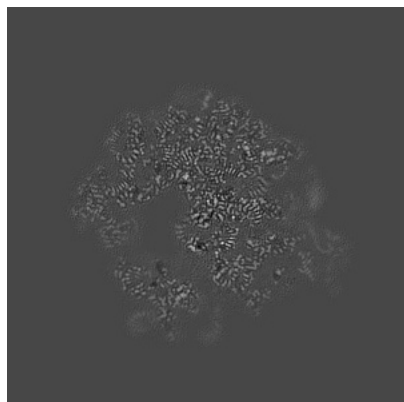


Z Index: 240

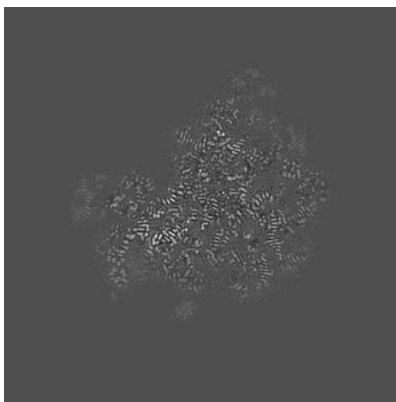
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

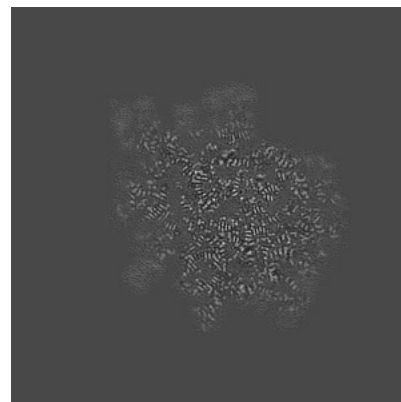
6.3.1 Primary map



X Index: 228

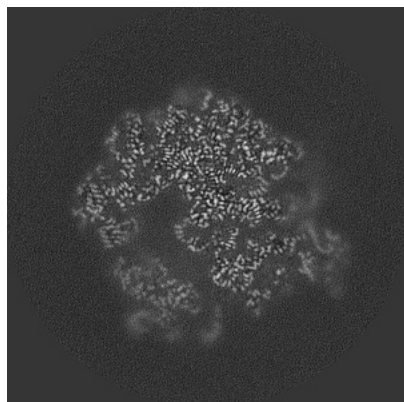


Y Index: 251

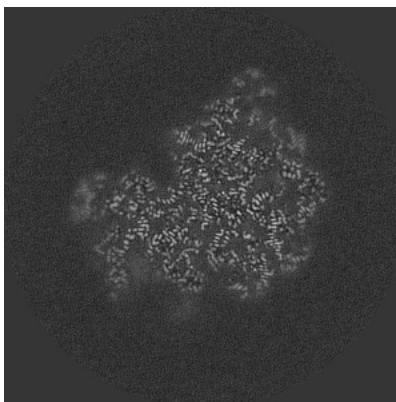


Z Index: 279

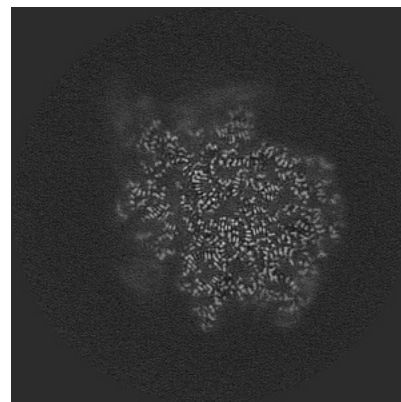
6.3.2 Raw map



X Index: 228



Y Index: 251

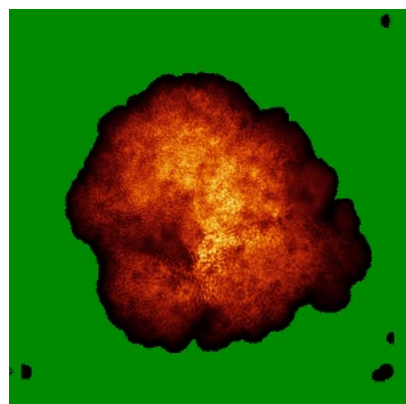


Z Index: 279

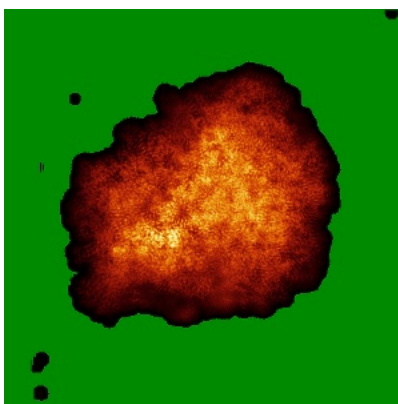
The images above show the largest variance slices of the map in three orthogonal directions.

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

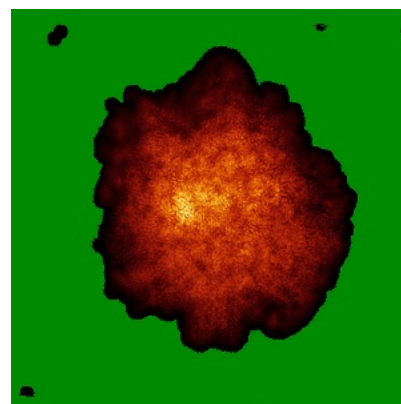
6.4.1 Primary map



X

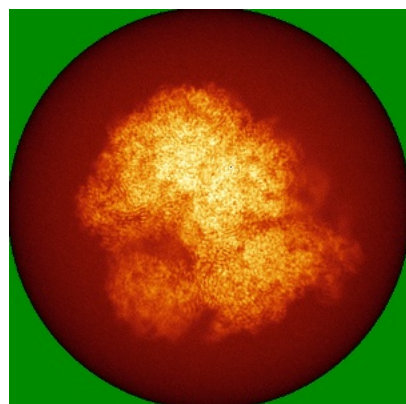


Y

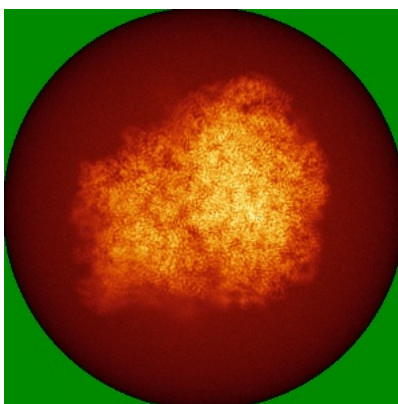


Z

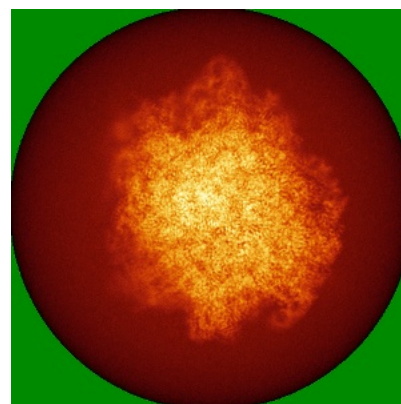
6.4.2 Raw map



X



Y

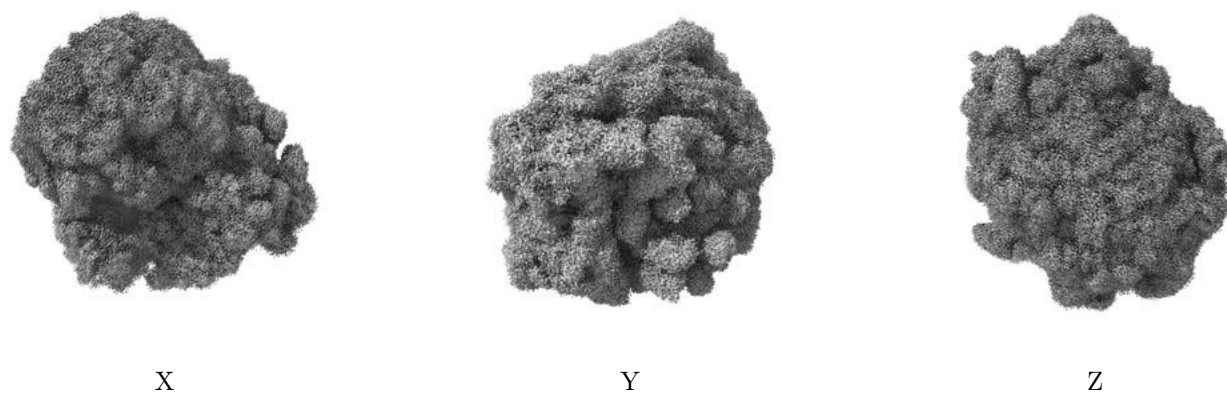


Z

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.

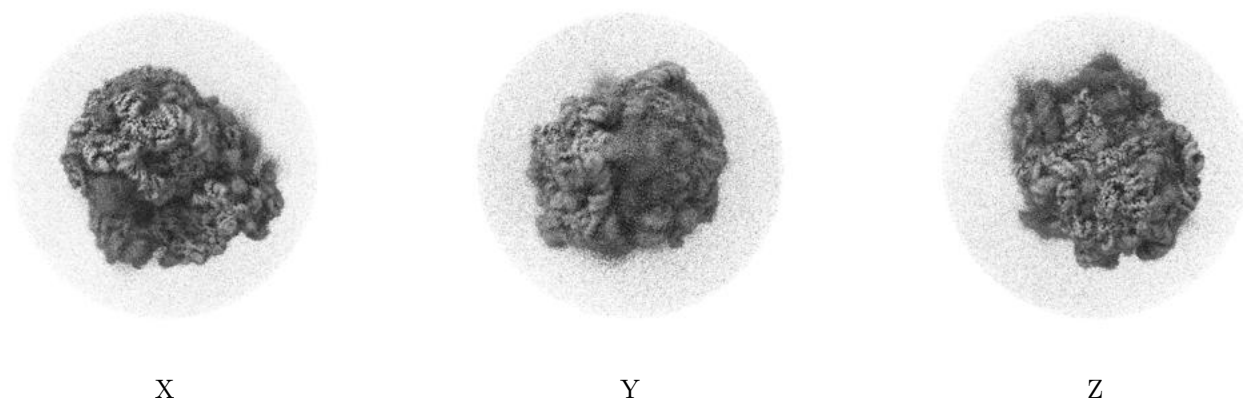
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

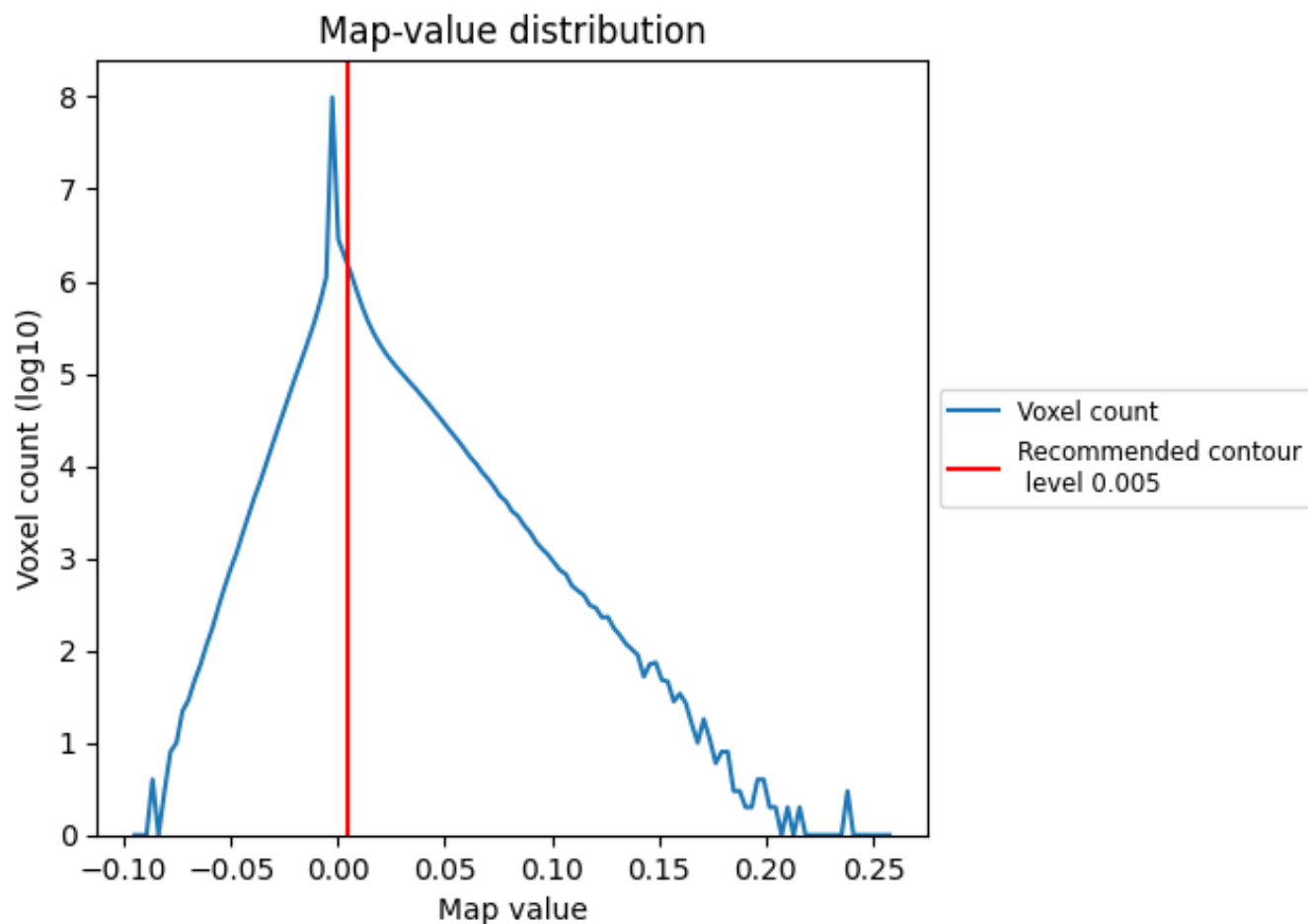
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

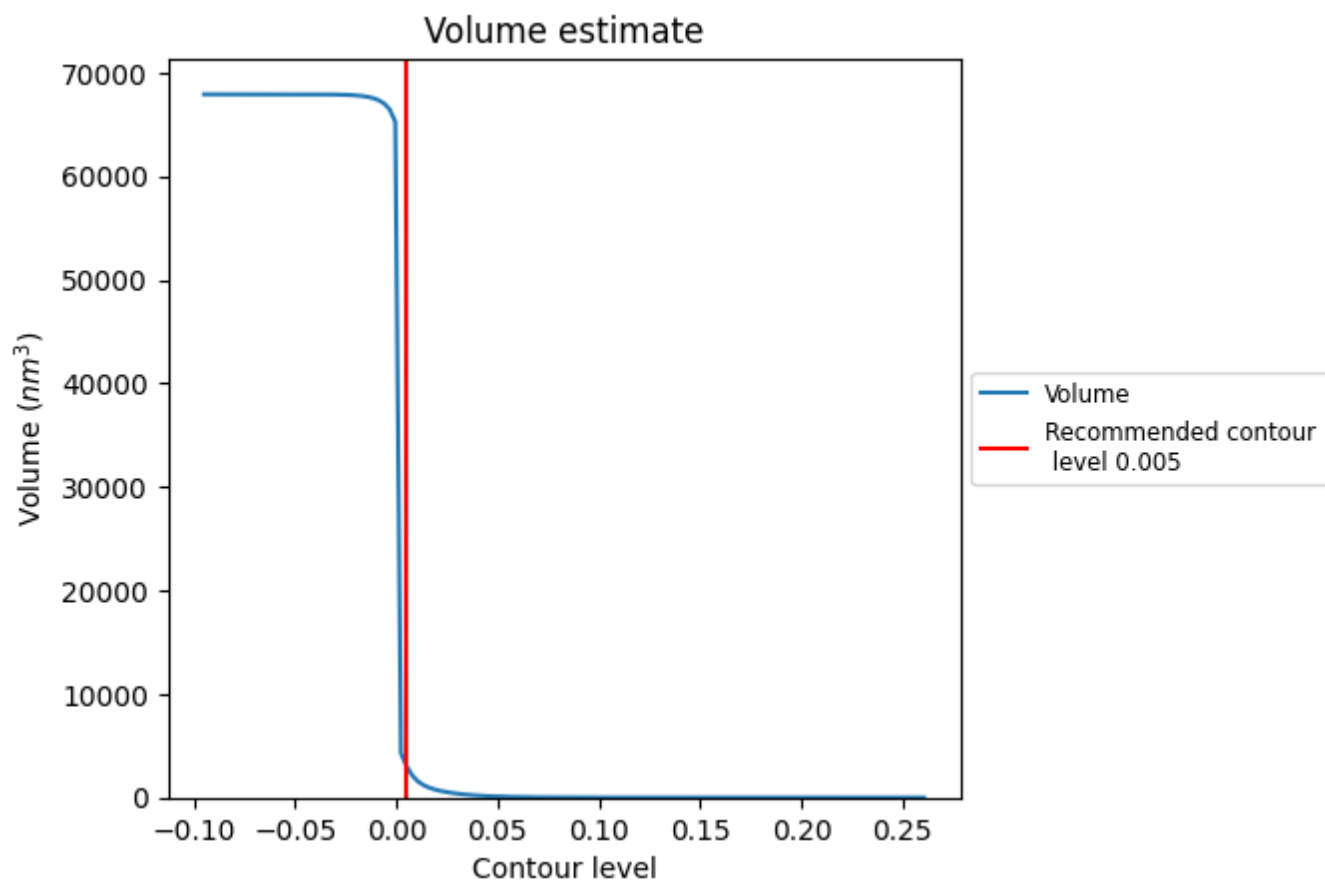
This section contains the results of statistical analysis of the map.

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.

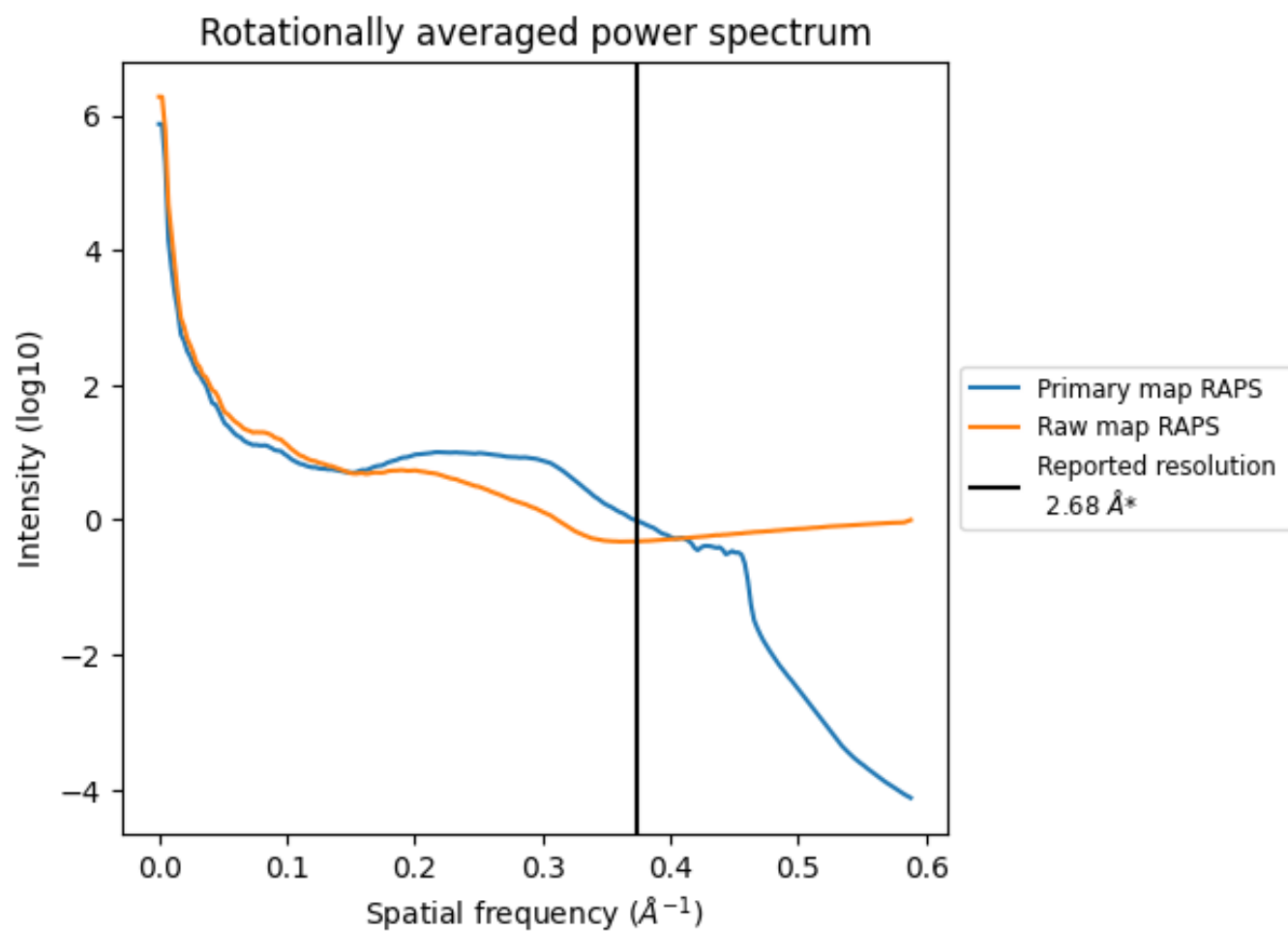
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3041 nm³; this corresponds to an approximate mass of 2747 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 ⓘ

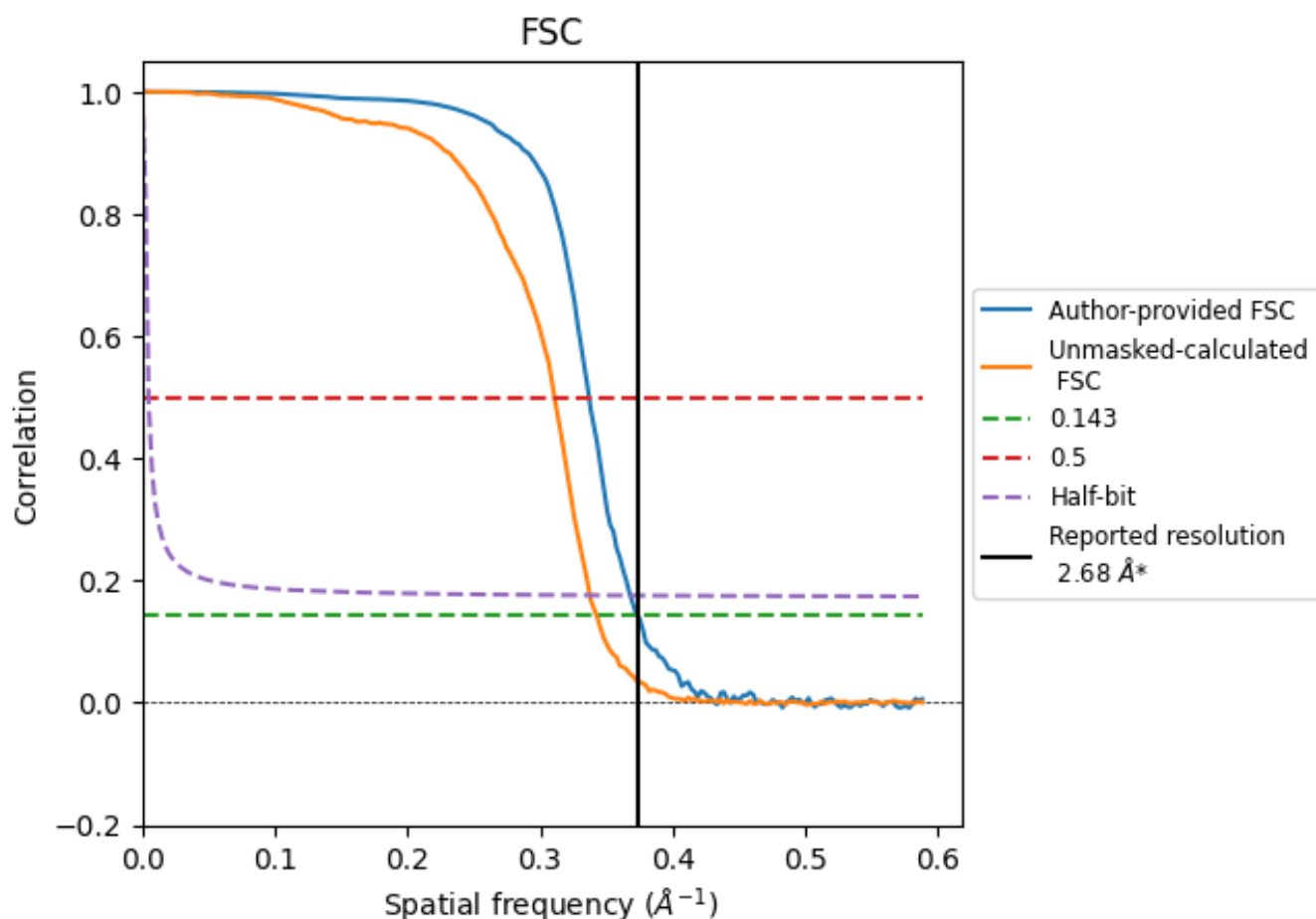


*Reported resolution corresponds to spatial frequency of $0.373 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.373 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

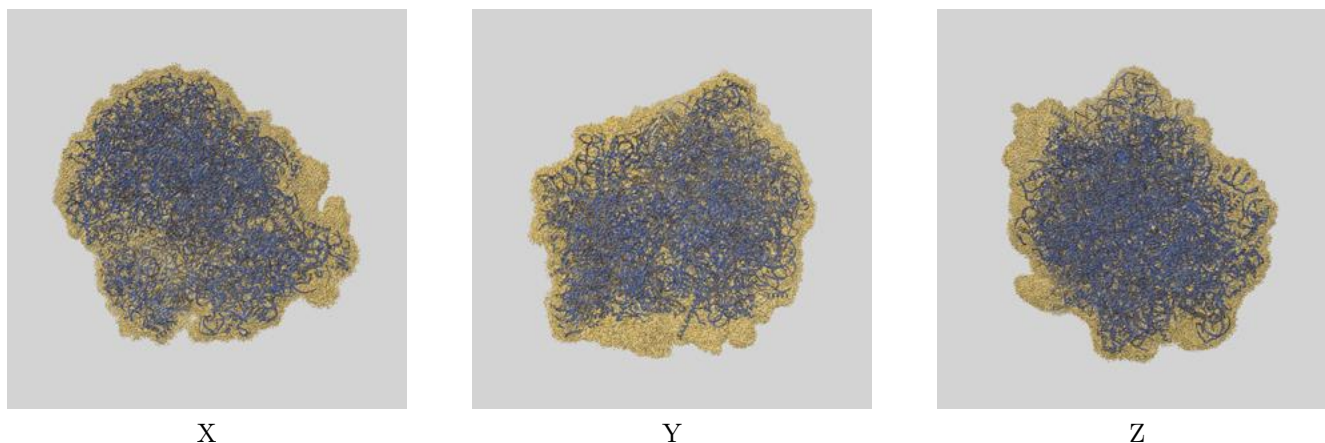
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	2.97	2.72
Unmasked-calculated*	2.92	3.22	2.96

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

9 Map-model fit [i](#)

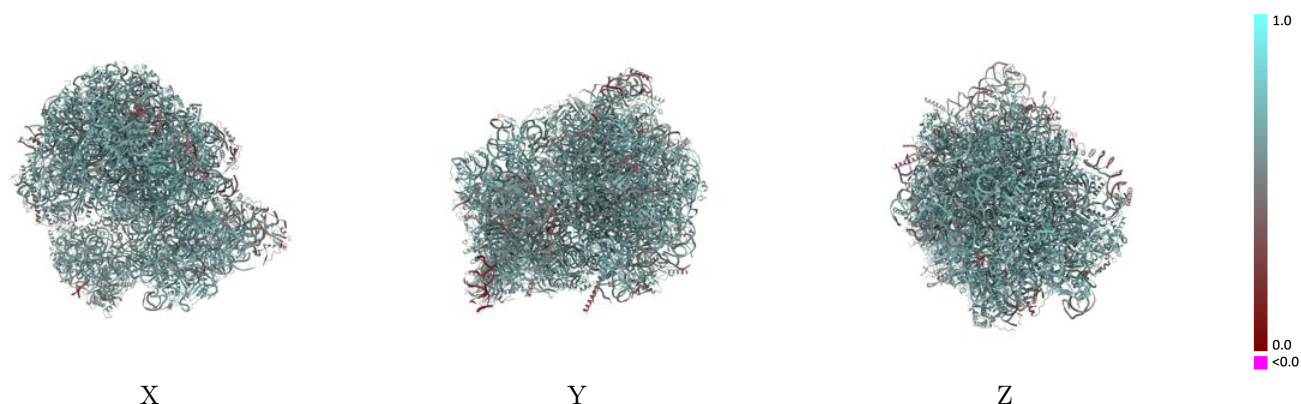
This section contains information regarding the fit between EMDB map EMD-55348 and PDB model 9SYG. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



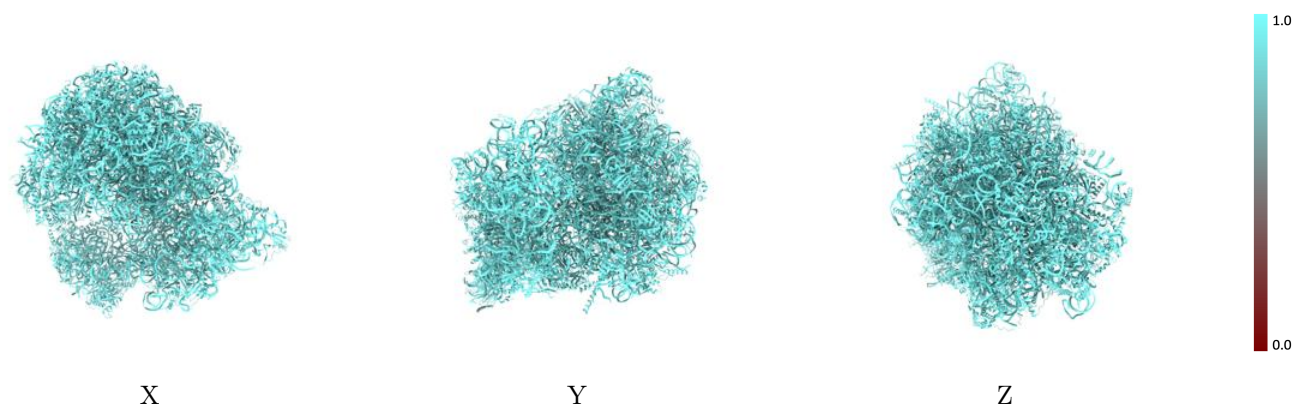
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



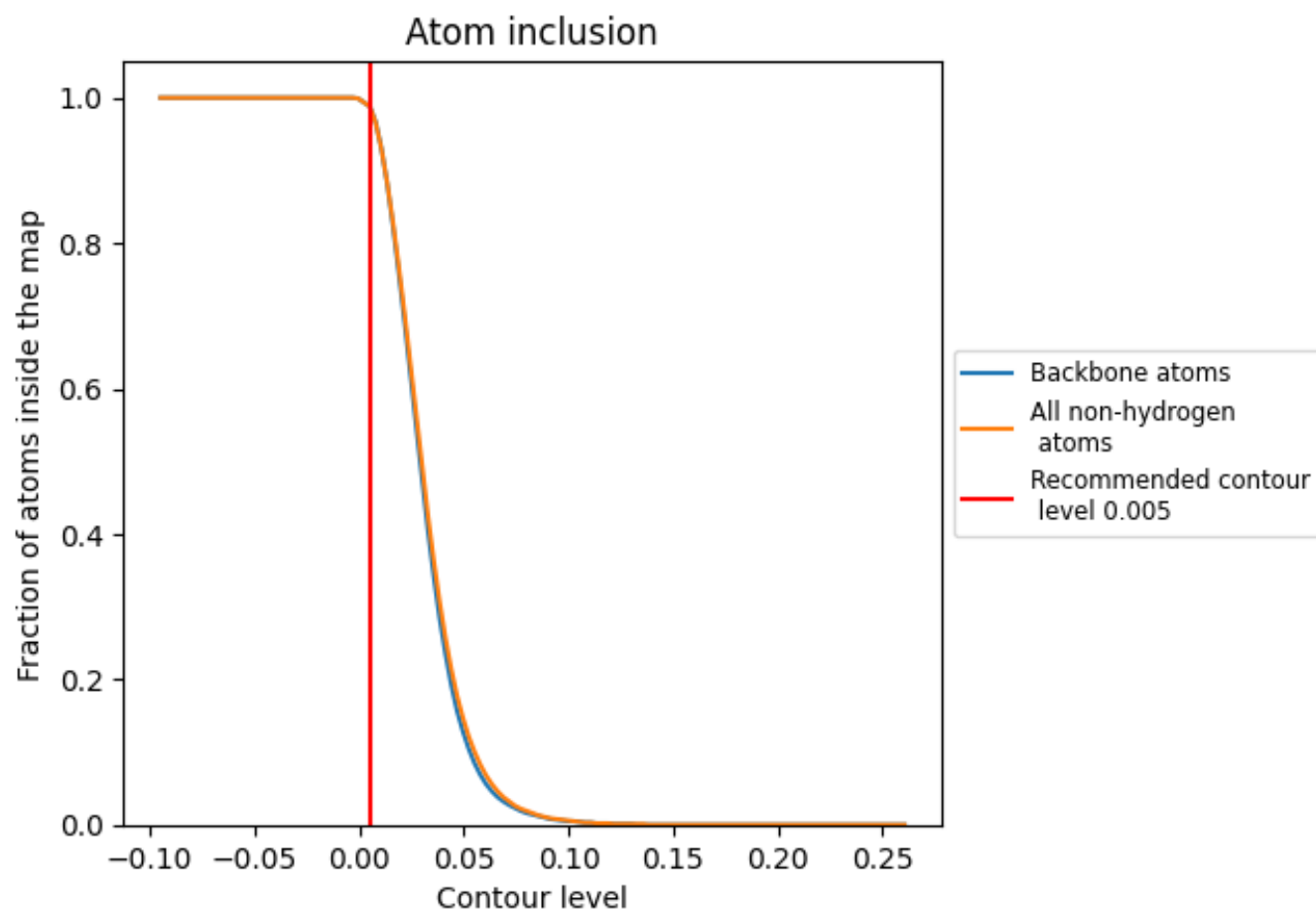
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9880	 0.6270
A0	 0.9910	 0.6360
A1	 0.9840	 0.6430
A2	 0.9900	 0.6300
A3	 0.9820	 0.6010
A4	 0.9860	 0.6190
A5	 0.9950	 0.6570
A6	 0.9890	 0.6480
A7	 0.9230	 0.5310
A8	 0.9780	 0.6360
AA	 0.9860	 0.6100
AB	 0.9910	 0.5860
AC	 0.9930	 0.6130
AD	 0.9620	 0.5630
AE	 0.9840	 0.6470
AG	 0.9950	 0.6460
AH	 0.9810	 0.6230
AI	 0.9690	 0.5800
AJ	 0.9960	 0.6650
AK	 0.9870	 0.6370
AL	 0.9890	 0.5710
AM	 0.9840	 0.6060
AO	 0.9890	 0.6270
AP	 0.9810	 0.6410
AQ	 0.9500	 0.5890
AR	 0.9790	 0.6070
AS	 0.9850	 0.6440
AT	 0.9790	 0.6310
AU	 0.9720	 0.5950
AV	 0.9940	 0.6430
AW	 0.9810	 0.6180
AX	 0.9740	 0.5990
AY	 0.9780	 0.6160
AZ	 0.9770	 0.5810
Az	 0.9170	 0.4520



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BA	 0.9940	 0.6410
BB	 0.9930	 0.6340
BC	 0.9970	 0.6470
BD	 1.0000	 0.6380
BE	 0.9880	 0.6100
BF	 0.9880	 0.6020
BG	 0.9960	 0.6400
BH	 0.9840	 0.6080
BI	 0.9900	 0.6500
BK	 0.9880	 0.6330
BL	 0.9800	 0.5550
BN	 0.9800	 0.6280
BO	 0.9930	 0.6640
BP	 0.9750	 0.5990
BQ	 0.9990	 0.6840
BR	 0.9970	 0.6820
BS	 0.9910	 0.6550
BT	 0.9920	 0.6240
BU	 0.9800	 0.6040
BV	 0.9500	 0.4940
BW	 0.9930	 0.6740
BX	 0.9940	 0.6590
BY	 0.9960	 0.6640
BZ	 0.9900	 0.6440
Ba	 0.9920	 0.6250
Bb	 0.9910	 0.6610
Bc	 0.9920	 0.6400
Bd	 0.9820	 0.6400
Be	 0.9970	 0.6810
Bf	 0.9930	 0.6710
Bg	 0.9930	 0.6530
Bh	 0.9830	 0.6240
Bi	 0.9950	 0.6590
Bj	 0.9770	 0.6090
Bk	 0.9920	 0.6160
Bl	 0.9990	 0.6710
Bm	 0.9930	 0.6240
Bn	 0.9970	 0.6830
Bo	 0.9970	 0.6720
Bp	 0.9760	 0.5900
Bq	 0.9910	 0.6630
Br	 0.9940	 0.6550

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Bs	 0.9790	 0.5740
Bt	 0.9900	 0.6530
Bu	 0.9780	 0.5830
Bv	 0.9810	 0.6020
Bw	 0.9950	 0.6570
Bx	 0.9820	 0.6170
By	 0.9870	 0.5990
Bz	 0.9960	 0.6650