wwPDB EM Validation Summary Report ⓘ

May 12, 2024 – 12:12 pm BST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

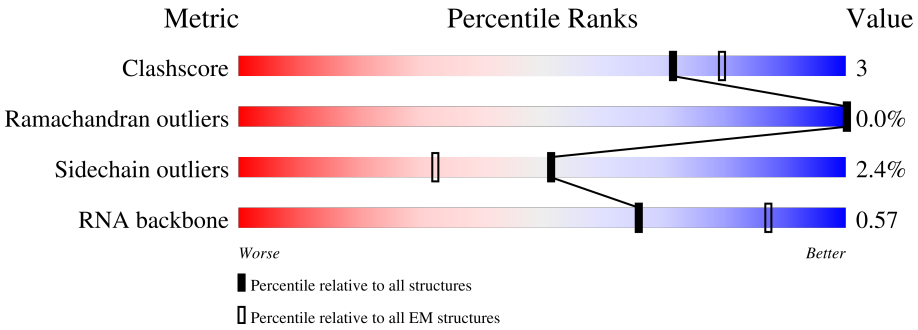
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	1782	63% 21% 5% • 10%
2	3	216	• 48% 17% 6% • 28%
3	4	183	• 74% 21% 5%
4	5	135	• 59% 24% • 15%
5	6	73	• 52% 36% 10% •
6	7	171	• 71% 22% • •
7	8	123	80% 15% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	A	260	94%
9	B	419	90% 5%
10	C	373	97%
11	D	188	81% 15%
12	E	190	89% 9%
13	F	195	68% 8% 24%
14	G	264	83% 14%
15	H	222	94% 5%
16	I	220	93% 5%
17	J	139	5% 96%
18	K	175	93% 5%
19	L	145	94% 5%
20	M	204	96%
21	N	213	77% 16% 7%
22	O	305	86% 10%
23	P	198	95%
24	Q	254	71% 25%
25	R	179	94% 5%
26	S1	2204	51% 23% 5% 20%
27	S4	20	5% 50% 35% 15%
28	SA	264	73% 11% 15%
29	SB	246	73% 11% 15%
30	SC	219	85% 11%
31	SD	190	81% 10% 8%
32	SE	273	84% 10% 5%

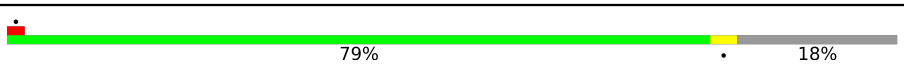
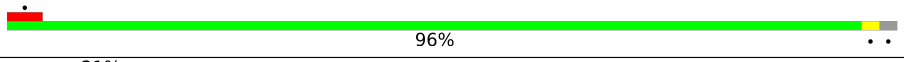
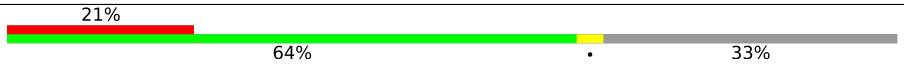
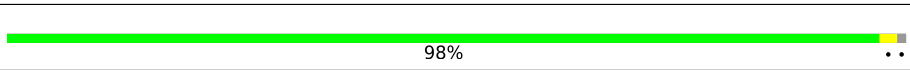
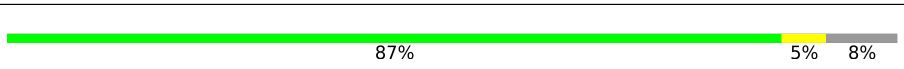
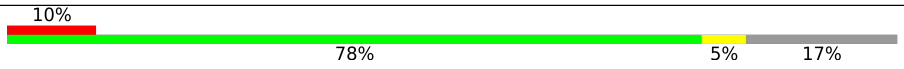
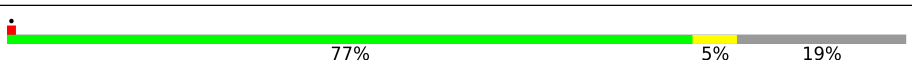
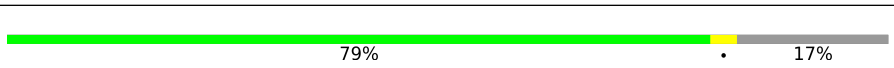
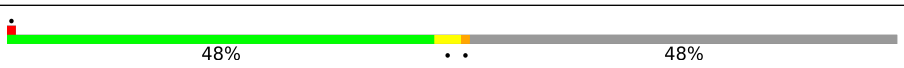
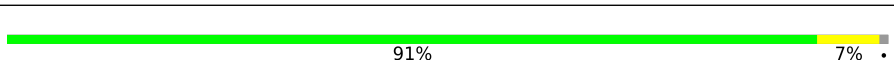
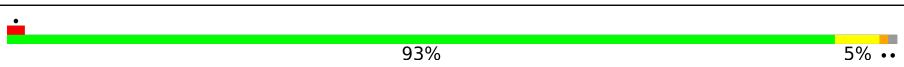
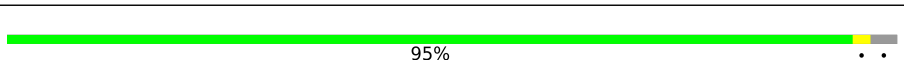
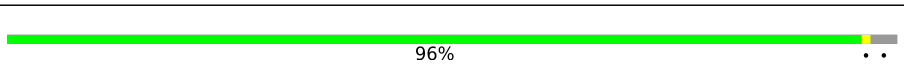
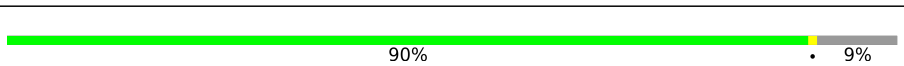
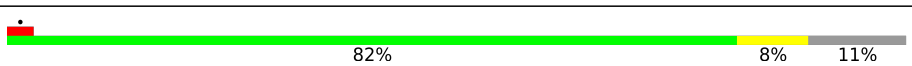
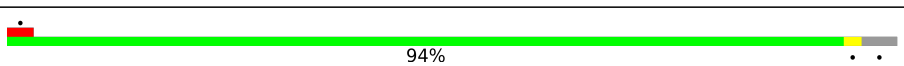
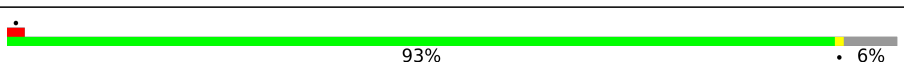
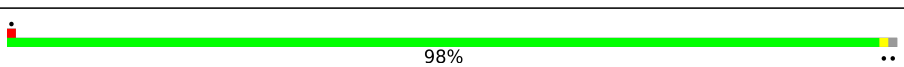
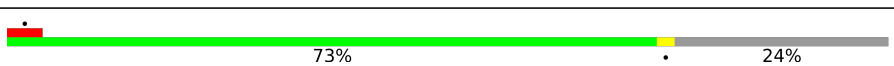
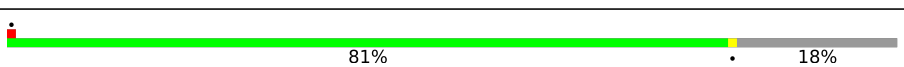
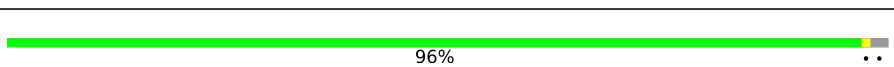
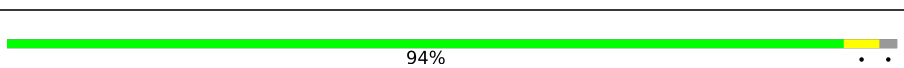
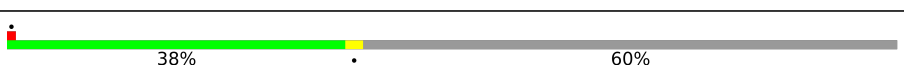
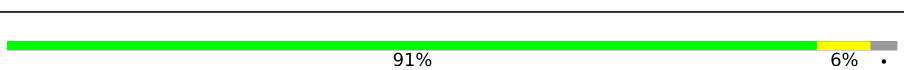
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	SF	265	75% 7% 18%
34	SG	249	83% 10% 6%
35	SH	190	91% 5%
36	SI	200	82% 17%
37	SK	220	75% 6% 18%
38	SL	149	93%
39	SM	116	77% 10% 12%
40	SN	168	51% 8% 40%
41	SO	144	90% 6%
42	SP	143	90% 9%
43	SQ	141	47% 60% 11% 29%
44	SR	153	79% 9% 12%
45	SS	57	86% 9% 5%
46	ST	151	86% 8% 5%
47	SU	173	86% 9%
48	SV	143	46% 7% 46%
49	SW	152	5% 66% 10% 24%
50	SX	161	86% 9% 6%
51	SY	164	48% 48%
52	SZ	137	77% 15% 7%
53	S	159	97%
54	Sa	120	59% 41%
55	Sc	86	86% 12%
56	Sb	112	90% 8%
57	Sd	87	71% 25%

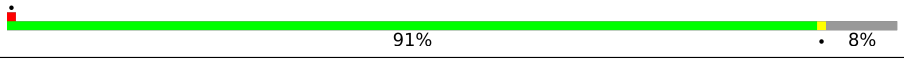
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
58	Se	66	
59	Sg	312	
60	Sh	235	
61	SJ	130	
62	T	166	
63	U	129	
64	V	145	
65	W	143	
66	X	124	
67	Y	134	
68	Z	147	
69	a	127	
70	b	70	
71	c	252	
72	d	104	
73	e	188	
74	f	133	
75	g	144	
76	h	168	
77	i	105	
78	j	83	
79	k	83	
80	l	51	
81	m	128	
82	n	34	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
83	o	92	
84	p	106	
85	2	1526	

2 Entry composition (i)

There are 90 unique types of molecules in this entry. The entry contains 200822 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called LSUa_rRNA_chain_1.

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

There are 7 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a RNA chain called SR1_chain_3.

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

- Molecule 3 is a RNA chain called SR2_chain_4.

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

- Molecule 4 is a RNA chain called SR4_chain_5.

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

- Molecule 5 is a RNA chain called SR6_chain_6.

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

- Molecule 6 is a RNA chain called 5.8S_rRNA_chain_7.

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

- Molecule 7 is a RNA chain called 5S_rRNA_chain_8.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

- Molecule 20 is a protein called Ribosomal protein L15.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 26 is a RNA chain called SSU_rRNA_chain_S1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 78 is a protein called Ribosomal protein L37.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 85 is a RNA chain called LSUb_rRNA_chain_2.

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

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

Continued on next page...

Continued from previous page...

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

- Molecule 87 is POTASSIUM ION (three-letter code: K) (formula: K).

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

Continued on next page...

Continued from previous page...

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

- Molecule 88 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 90 is water.

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

Continued on next page...

Continued from previous page...

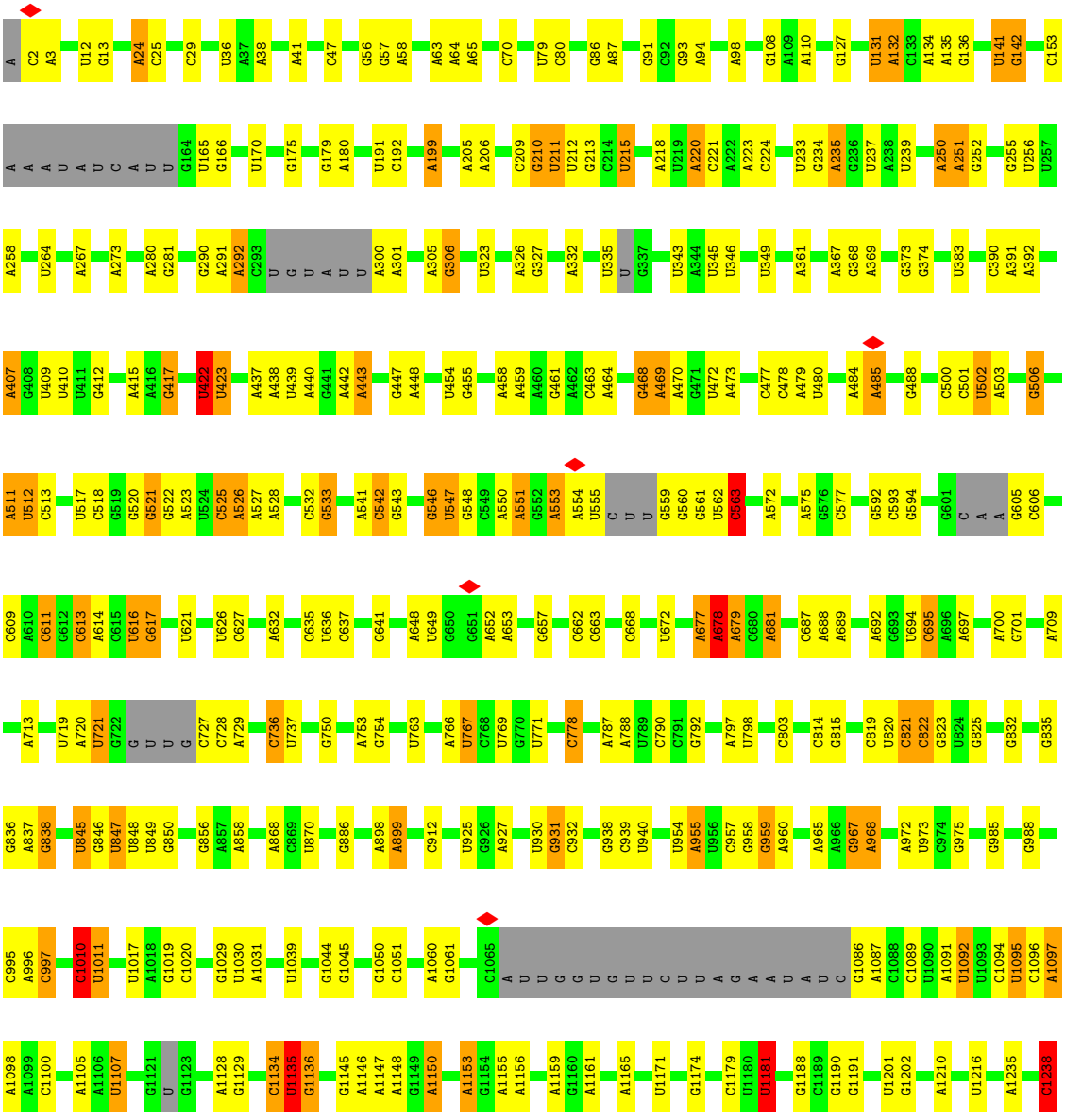
Mol	Chain	Residues	Atoms	AltConf
90	7	1	Total O 1 1	0
90	A	1	Total O 1 1	0
90	B	1	Total O 1 1	0
90	H	1	Total O 1 1	0
90	I	1	Total O 1 1	0
90	M	4	Total O 4 4	0
90	P	2	Total O 2 2	0
90	S1	7	Total O 7 7	0
90	SA	1	Total O 1 1	0
90	S	1	Total O 1 1	0
90	T	2	Total O 2 2	0
90	2	17	Total O 17 17	0

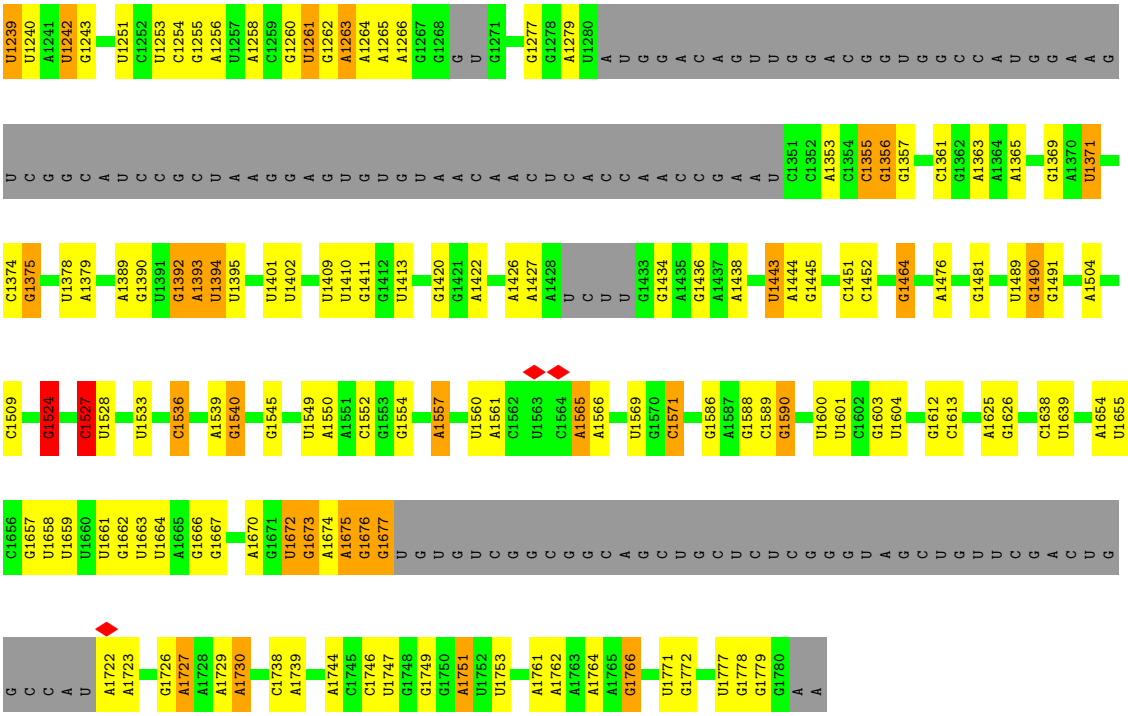
3 Residue-property plots (i)

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

- Molecule 1: LSUa_rRNA_chain_1

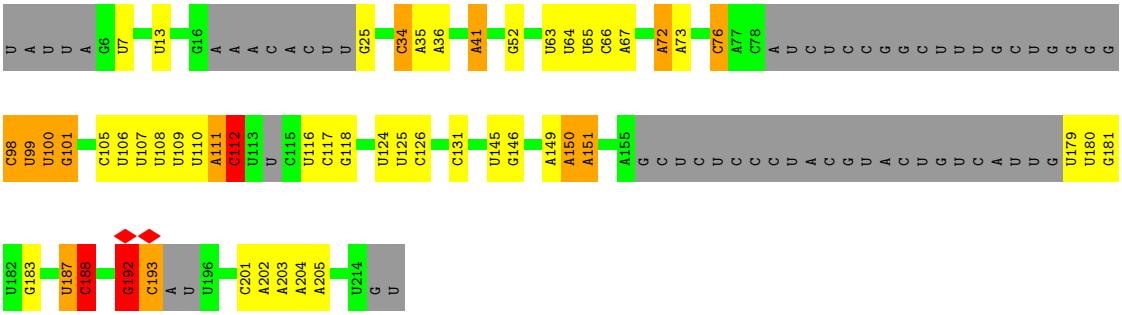
Chain 1:





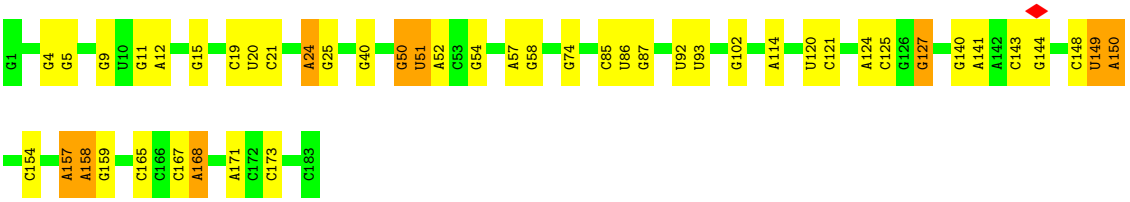
• Molecule 2: SR1_chain_3

Chain 3:



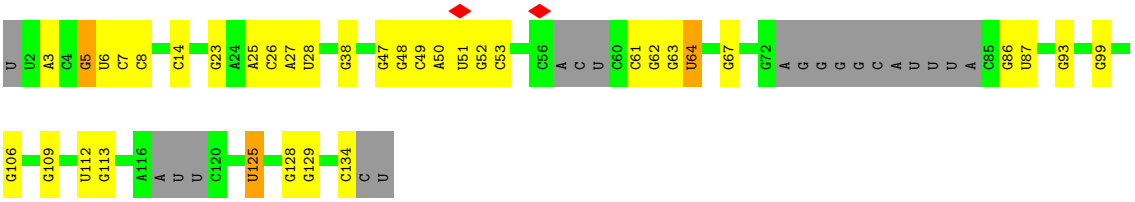
• Molecule 3: SR2_chain_4

Chain 4:



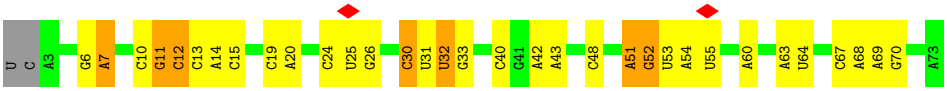
• Molecule 4: SR4_chain_5

Chain 5:



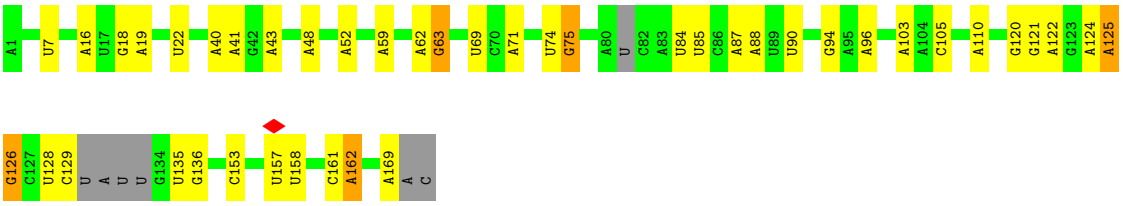
• Molecule 5: SR6_chain_6

Chain 6:



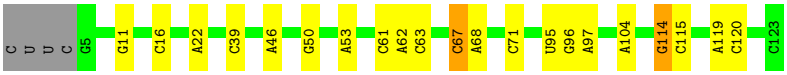
• Molecule 6: 5.8S_rRNA_chain_7

Chain 7:



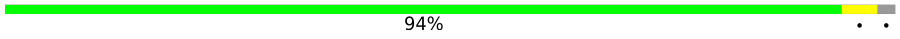
• Molecule 7: 5S_rRNA_chain_8

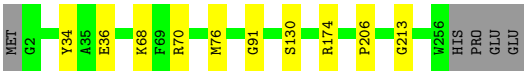
Chain 8:



• Molecule 8: Putative 60S ribosomal protein L2

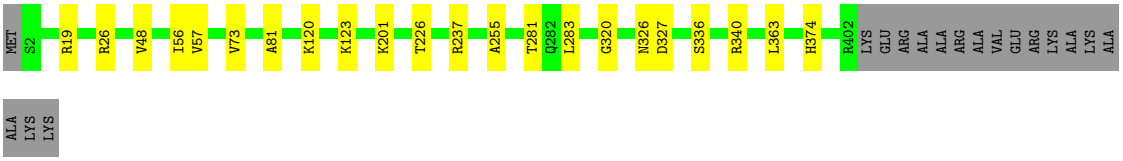
Chain A:





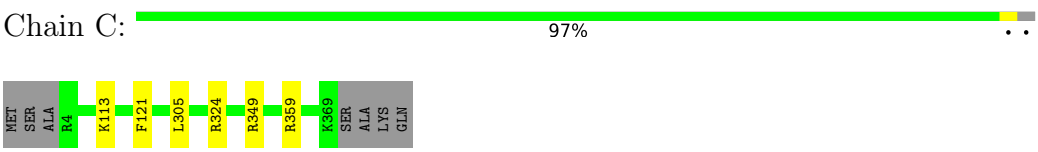
• Molecule 9: Putative ribosomal protein L3

Chain B:



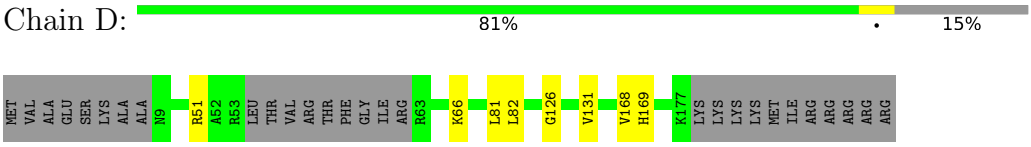
• Molecule 10: Putative ribosomal protein L1a

Chain C:



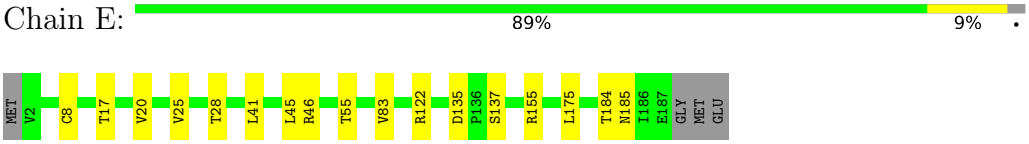
• Molecule 11: 60S ribosomal protein L11

Chain D:



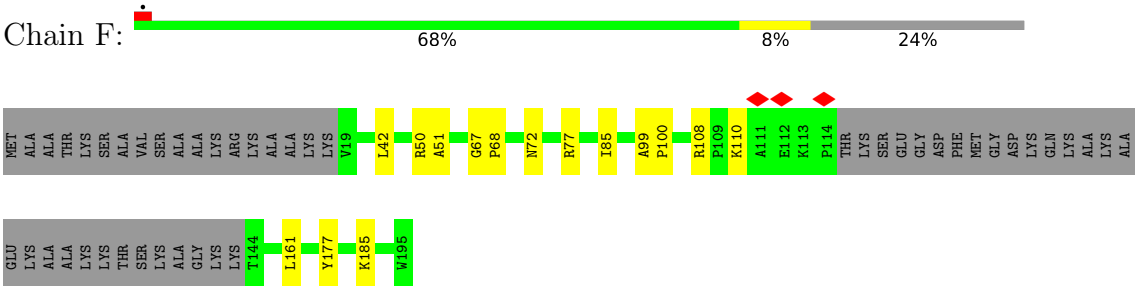
• Molecule 12: Putative 60S ribosomal protein L9

Chain E:



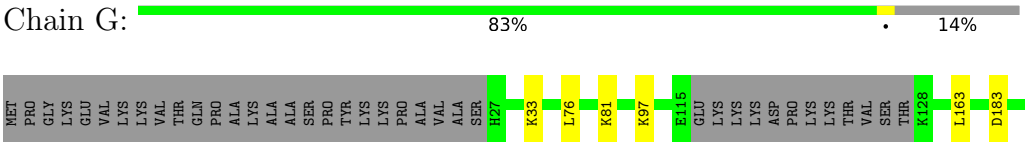
• Molecule 13: Putative 60S ribosomal protein L6

Chain F:



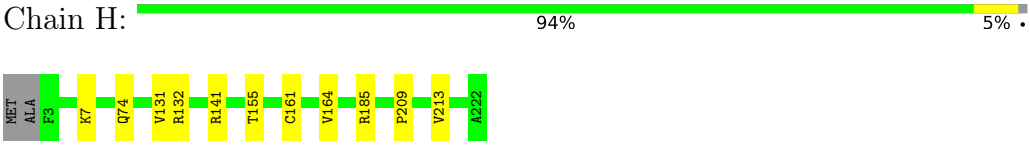
• Molecule 14: 60S ribosomal protein L7a

Chain G:



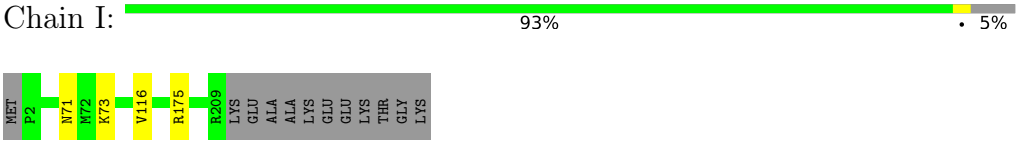
• Molecule 15: Putative 60S ribosomal protein L13a

Chain H:



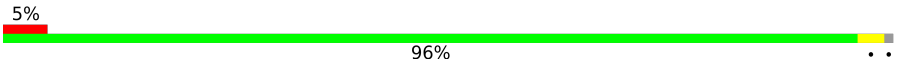
• Molecule 16: Putative 60S ribosomal protein L13

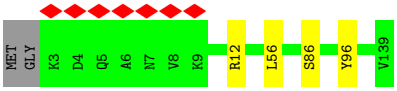
Chain I:



• Molecule 17: Putative 60S ribosomal protein L23

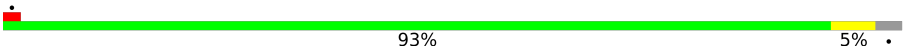
Chain J:





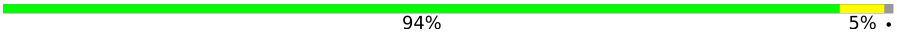
• Molecule 18: Putative 40S ribosomal protein L14

Chain K:



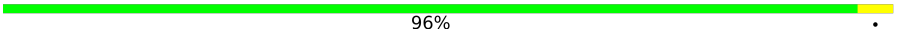
• Molecule 19: Putative 60S ribosomal protein L27A/L29

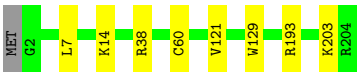
Chain L:



• Molecule 20: Ribosomal protein L15

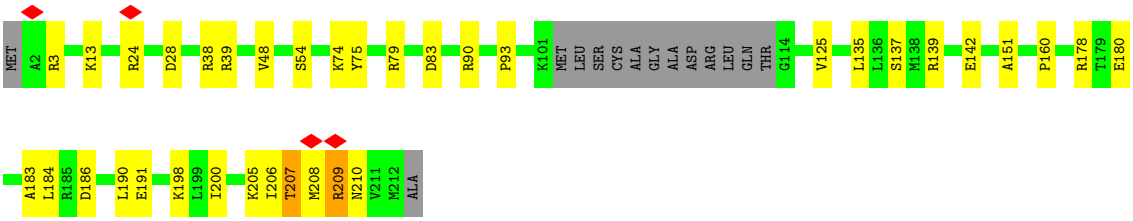
Chain M:





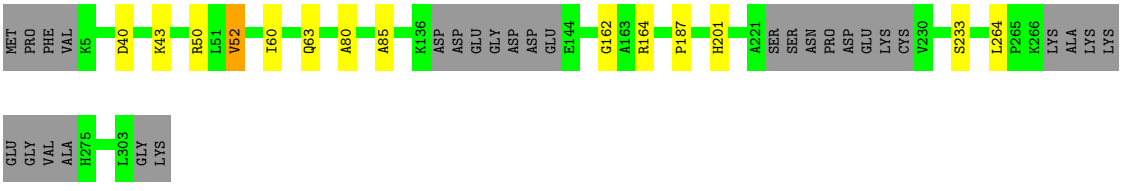
• Molecule 21: Putative 60S ribosomal protein L10

Chain N:



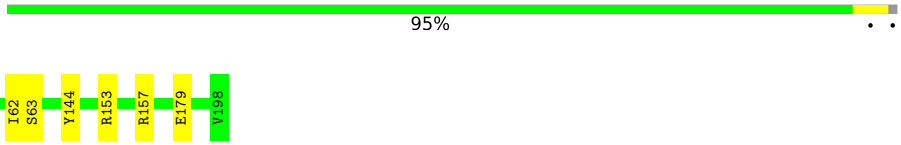
• Molecule 22: Putative 60S ribosomal protein L5

Chain O:



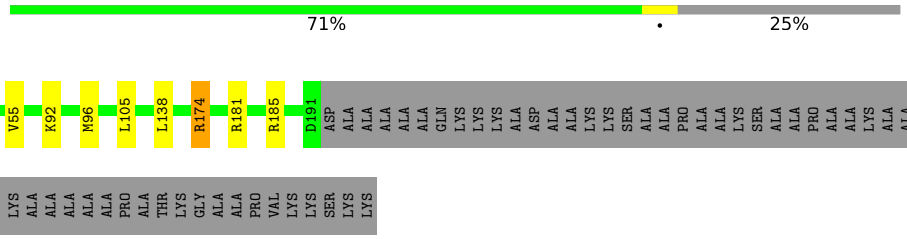
• Molecule 23: 60S ribosomal protein L18

Chain P:



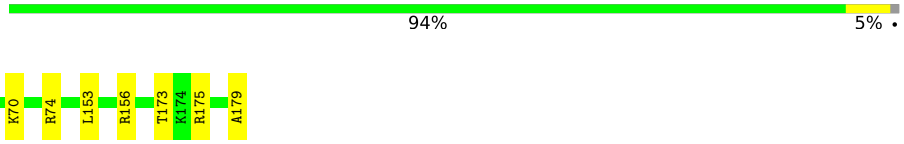
• Molecule 24: Putative 60S ribosomal protein L19

Chain Q:



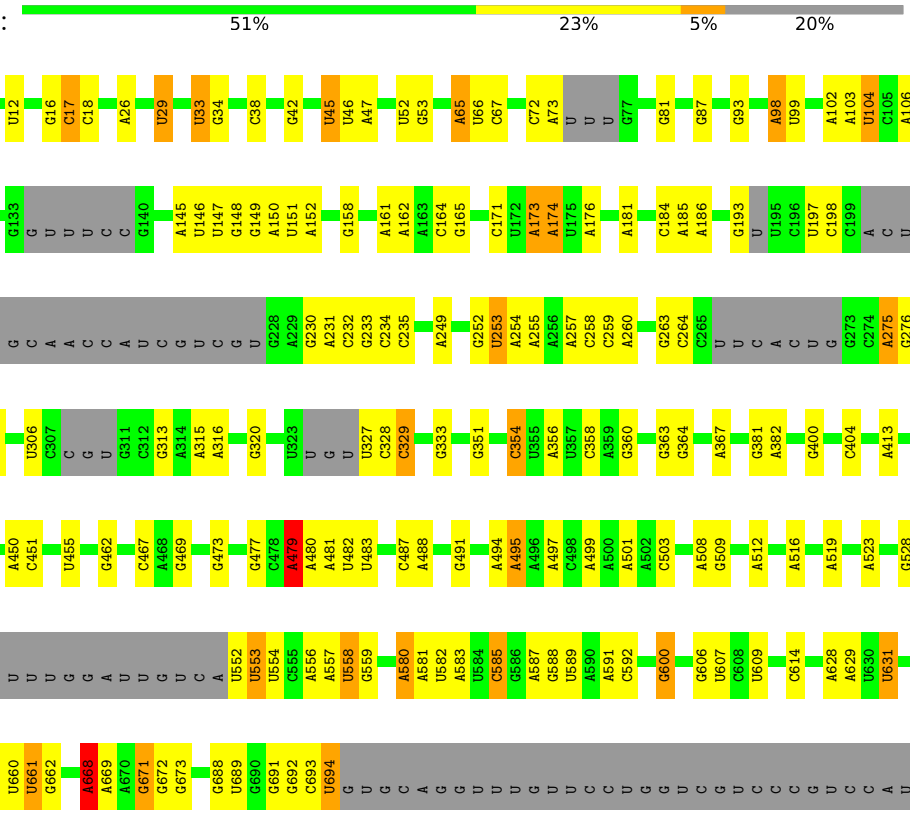
• Molecule 25: 60S ribosomal protein L18a

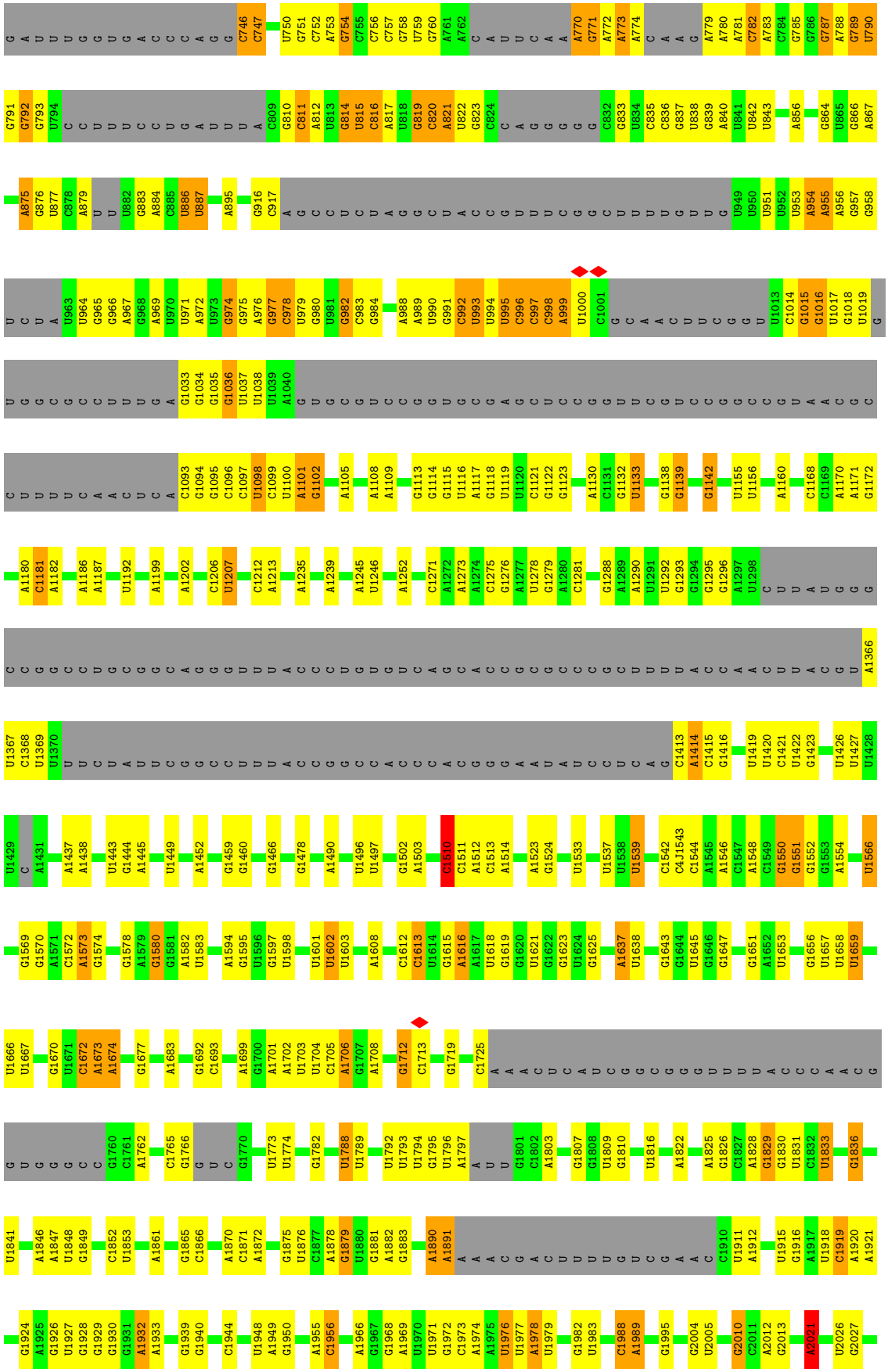
Chain R:

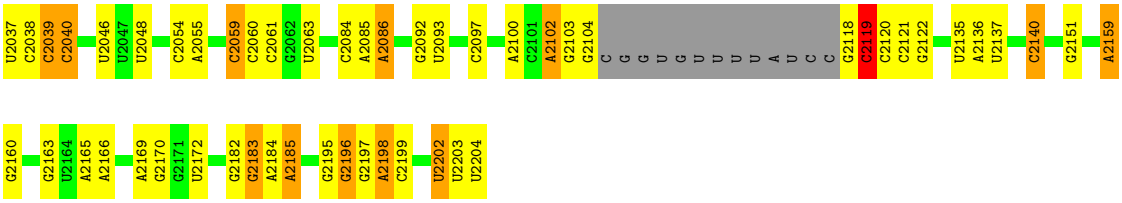


• Molecule 26: SSU_rRNA_chain_S1

Chain S1:

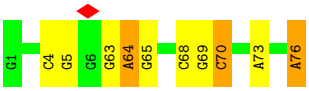






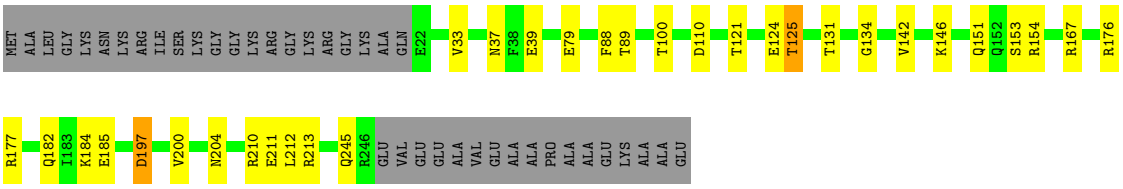
• Molecule 27: E-site_tRNA_chain_S4

Chain S4:



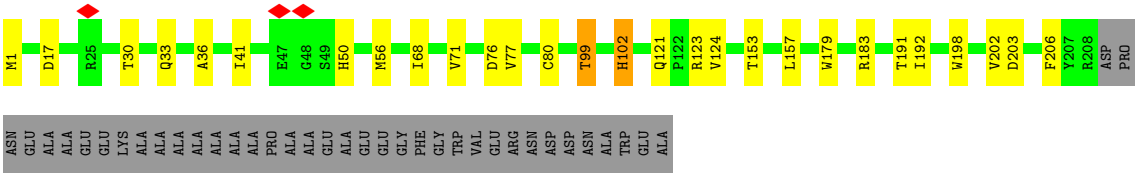
• Molecule 28: 40S ribosomal protein S3a

Chain SA:



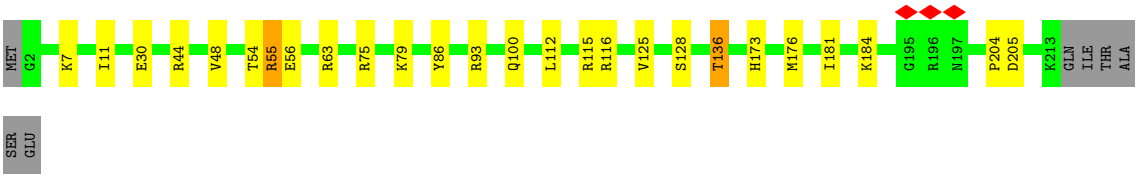
• Molecule 29: 40S ribosomal protein SA

Chain SB:



• Molecule 30: Putative 40S ribosomal protein S3

Chain SC:

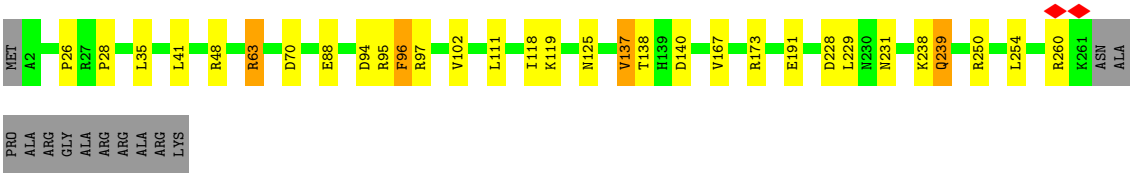


• Molecule 31: Putative 40S ribosomal protein S9

Chain SD:

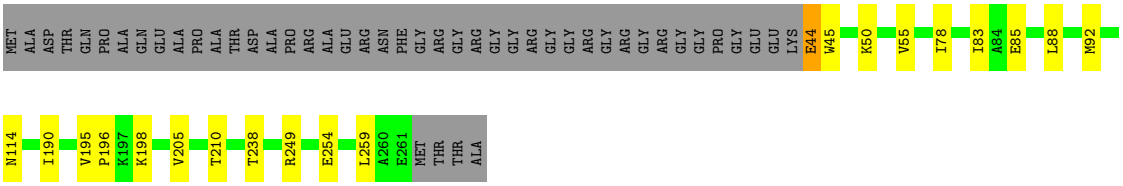
• Molecule 32: 40S ribosomal protein S4

Chain SE:



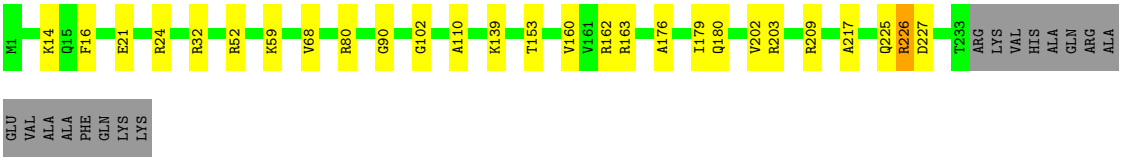
• Molecule 33: 40S ribosomal protein S2

Chain SF:



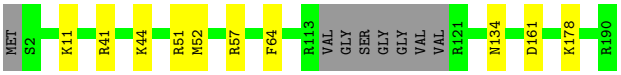
• Molecule 34: 40S ribosomal protein S6

Chain SG:



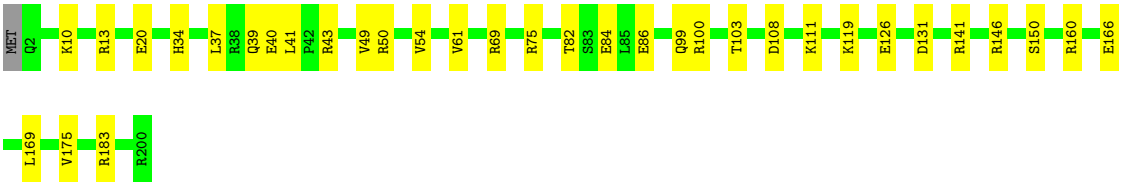
• Molecule 35: 40S ribosomal protein S5

Chain SH:



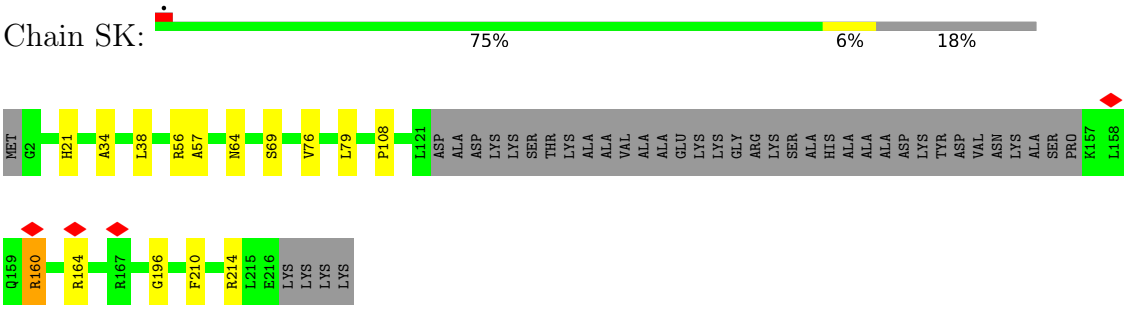
• Molecule 36: 40S ribosomal protein S7

Chain SI:



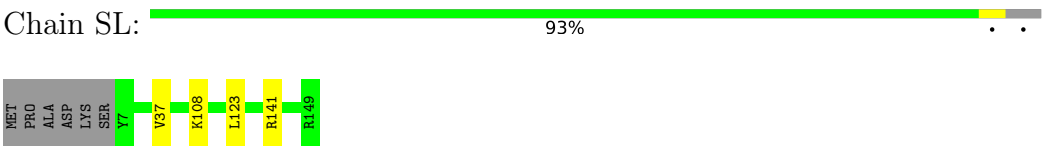
• Molecule 37: 40S ribosomal protein S8

Chain SK:



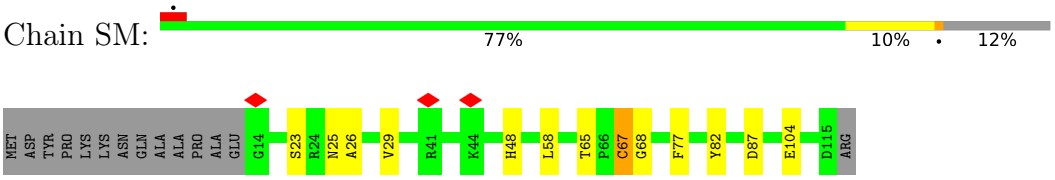
• Molecule 38: Putative 40S ribosomal protein S16

Chain SL:



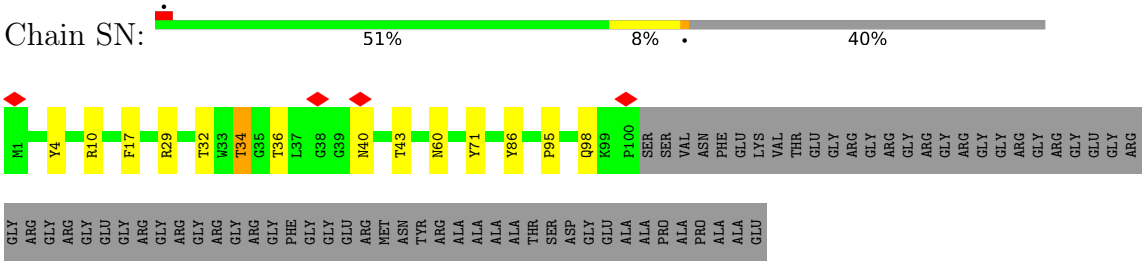
• Molecule 39: Putative ribosomal protein S20

Chain SM:



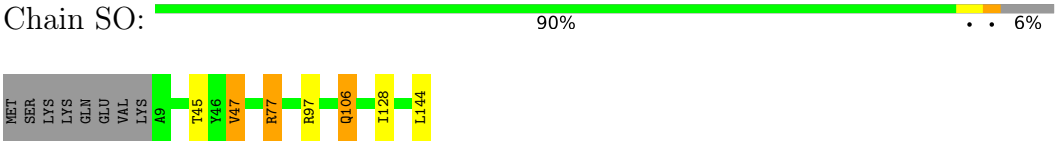
• Molecule 40: Putative 40S ribosomal protein S10

Chain SN:



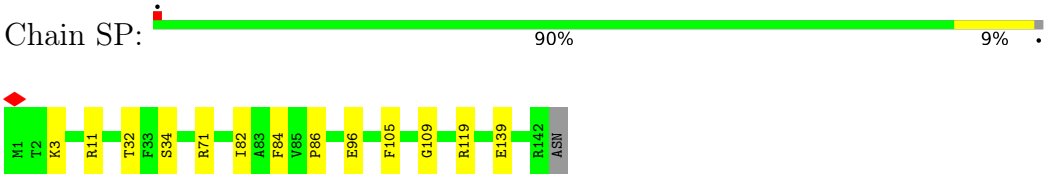
• Molecule 41: 40S ribosomal protein S14

Chain SO:



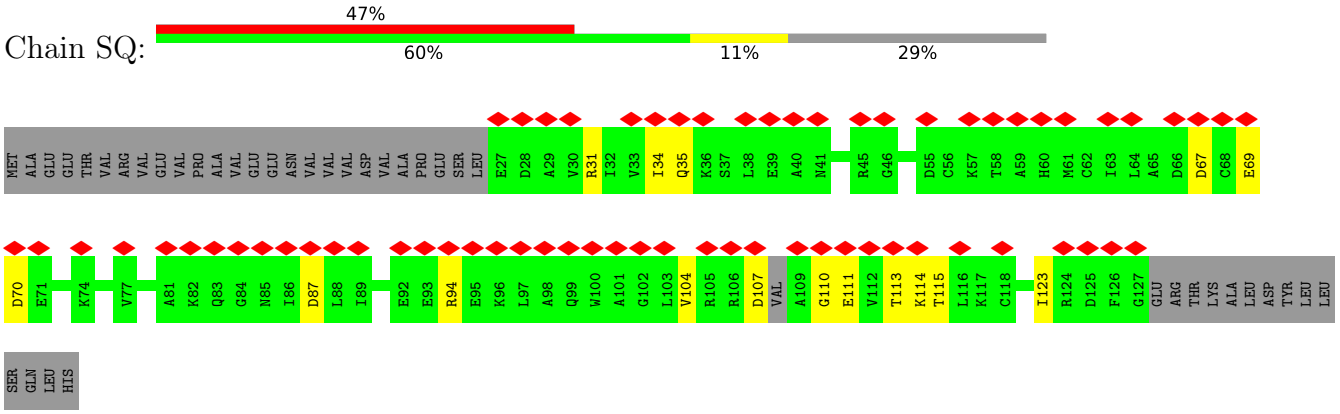
• Molecule 42: Putative 40S ribosomal protein S23

Chain SP:



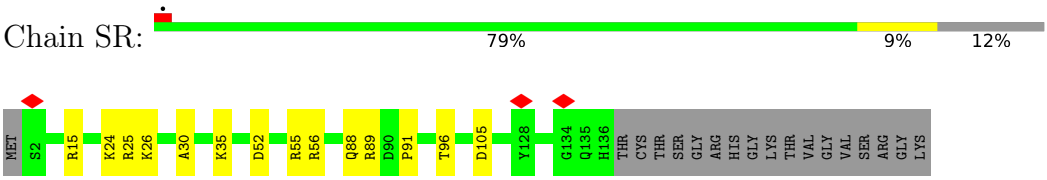
• Molecule 43: 40S ribosomal protein S12

Chain SQ:



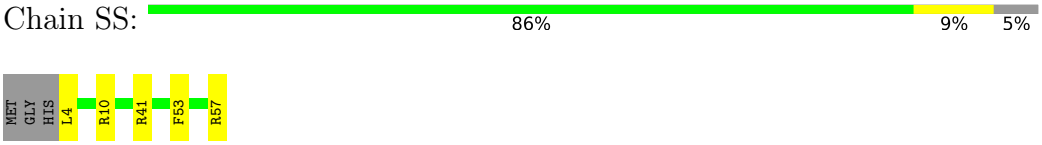
• Molecule 44: Putative 40S ribosomal protein S18

Chain SR:



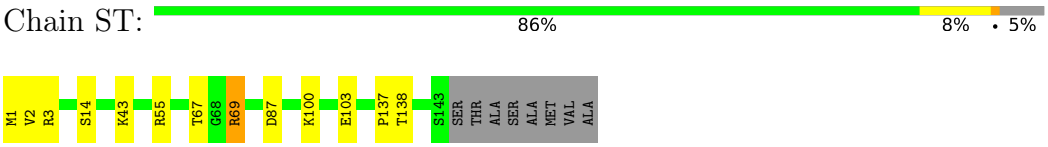
• Molecule 45: Putative ribosomal protein S29

Chain SS:



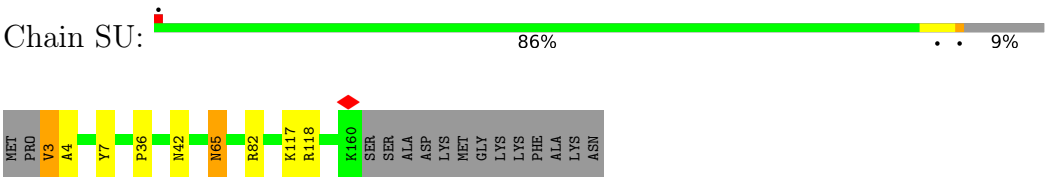
• Molecule 46: Putative 40S ribosomal protein S13

Chain ST:



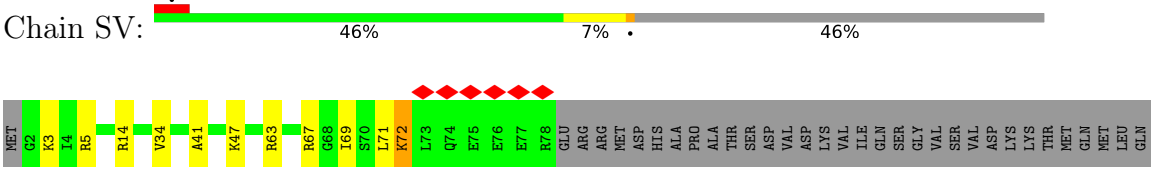
• Molecule 47: Putative 40S ribosomal protein S11

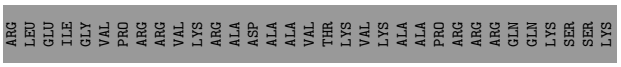
Chain SU:



• Molecule 48: Putative 40S ribosomal protein S17

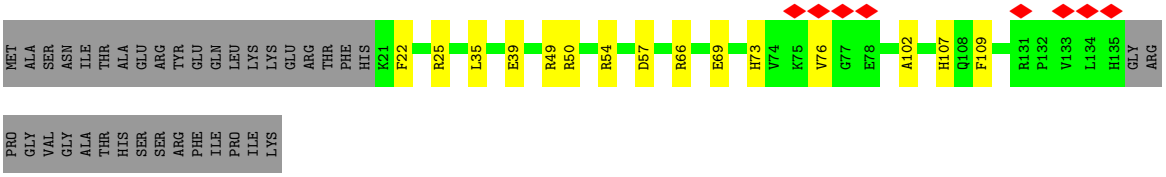
Chain SV:





• Molecule 49: Putative 40S ribosomal protein S15

Chain SW:

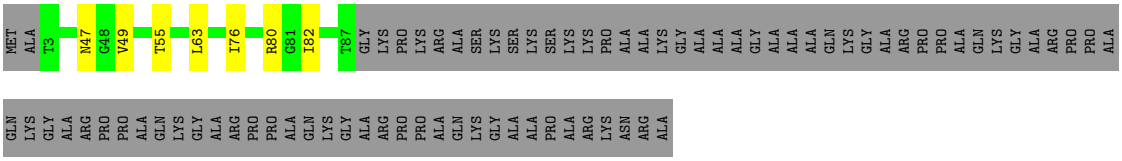


• Molecule 50: 40S ribosomal protein S19-like protein

Chain SX:

• Molecule 51: Putative 40S ribosomal protein S21

Chain SY:

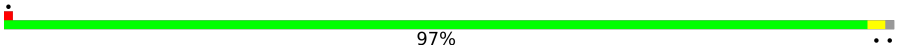


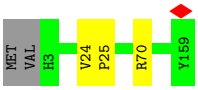
• Molecule 52: 40S ribosomal protein S24

Chain SZ:

• Molecule 53: Putative 60S ribosomal protein L21

Chain S:



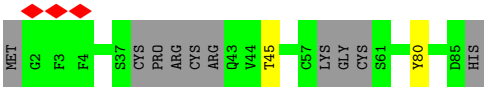


• Molecule 54: 40S ribosomal protein S25

Chain Sa:

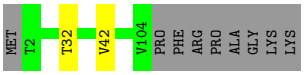
• Molecule 55: Putative 40S ribosomal protein S27-1

Chain Sc:



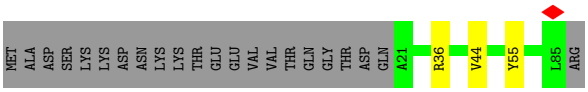
• Molecule 56: 40S ribosomal protein S26

Chain Sb:



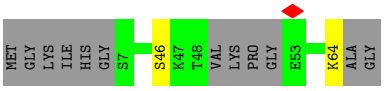
• Molecule 57: Putative 40S ribosomal protein S33

Chain Sd:



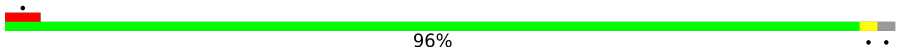
• Molecule 58: 40S ribosomal protein S30

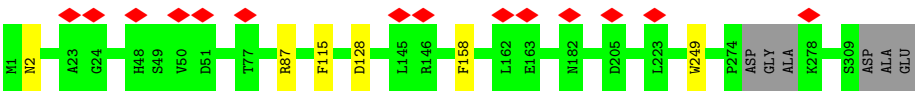
Chain Se:



• Molecule 59: Guanine nucleotide-binding protein subunit beta-like protein

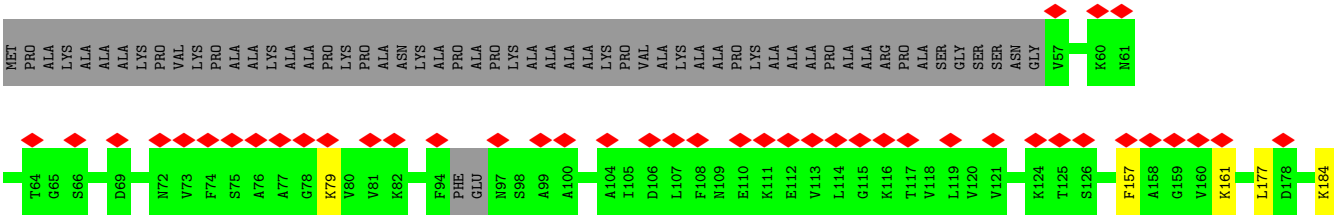
Chain Sg:

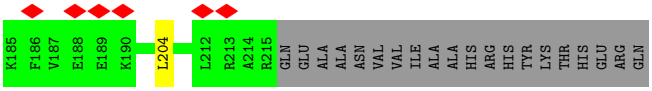




• Molecule 60: Putative RNA binding protein

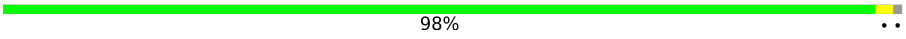
Chain Sh:

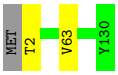




• Molecule 61: Putative 40S ribosomal protein S15A

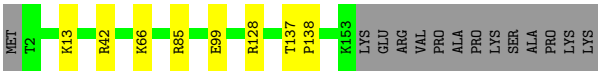
Chain SJ:





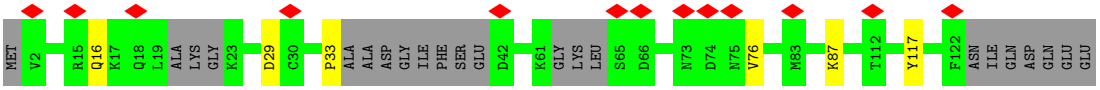
• Molecule 62: Putative 60S ribosomal protein L17

Chain T:



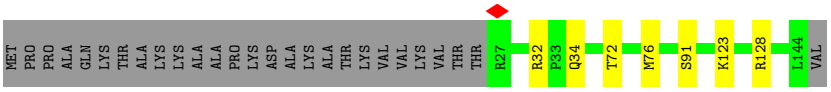
• Molecule 63: Putative 60S ribosomal protein L22

Chain U:



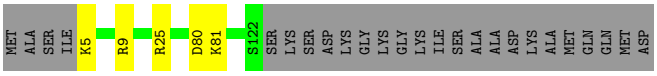
• Molecule 64: Putative 60S ribosomal protein L23a

Chain V:



• Molecule 65: Putative 60S ribosomal protein L26

Chain W:

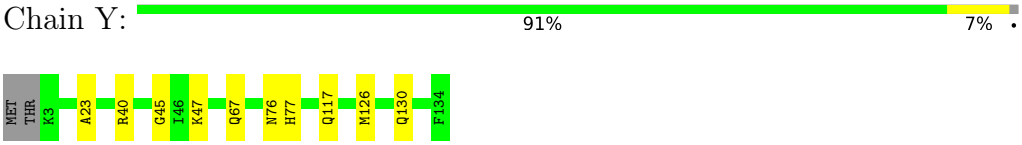


• Molecule 66: Putative ribosomal protein L24

Chain X:

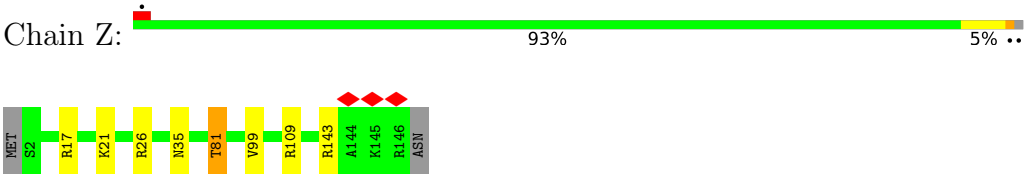
• Molecule 67: 60S ribosomal protein L27

Chain Y:



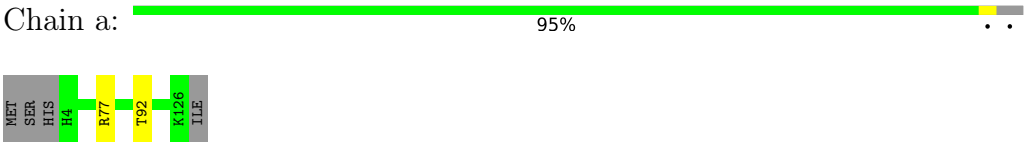
• Molecule 68: Putative 60S ribosomal protein L28

Chain Z:



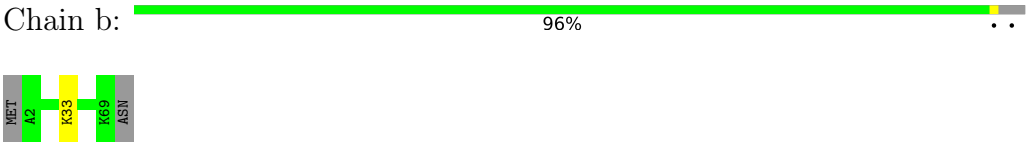
• Molecule 69: Putative 60S ribosomal protein L35

Chain a:



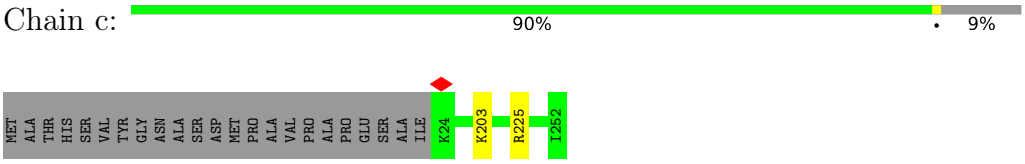
• Molecule 70: 60S ribosomal protein L29

Chain b:



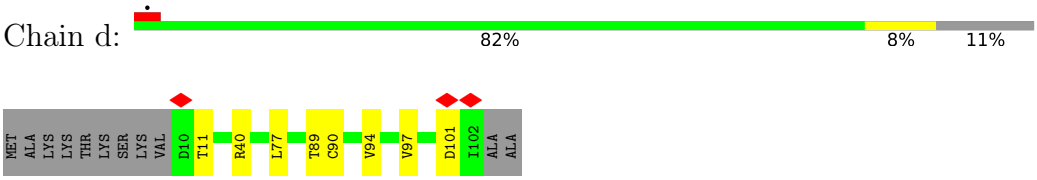
• Molecule 71: Putative 60S ribosomal protein L7

Chain c:



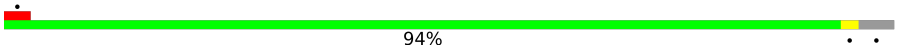
• Molecule 72: 60S ribosomal protein L30

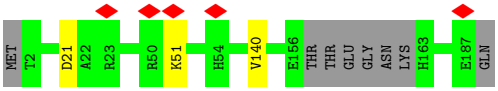
Chain d:



• Molecule 73: Putative 60S ribosomal subunit protein L31

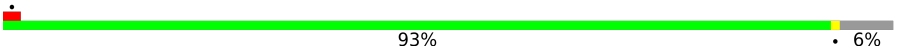
Chain e:

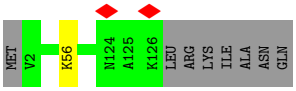




• Molecule 74: 60S ribosomal protein L32

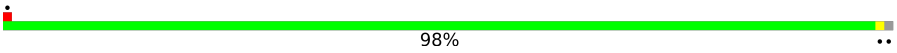
Chain f:

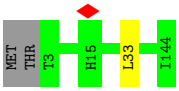




• Molecule 75: Putative ribosomal protein l35a

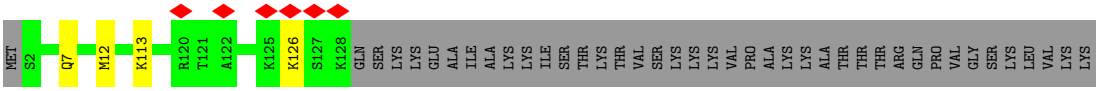
Chain g:





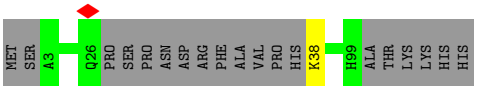
• Molecule 76: Putative 60S ribosomal protein L34

Chain h:



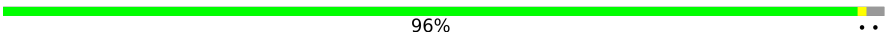
• Molecule 77: Putative 60S Ribosomal protein L36

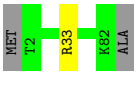
Chain i:



• Molecule 78: Ribosomal protein L37

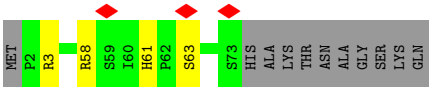
Chain j:





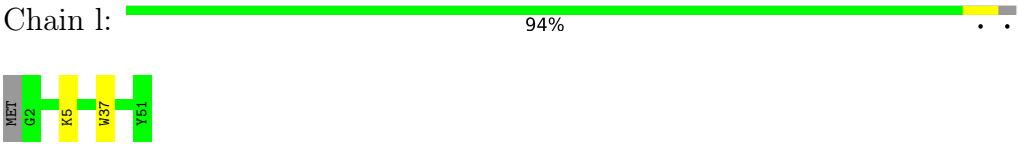
• Molecule 79: Putative ribosomal protein L38

Chain k:



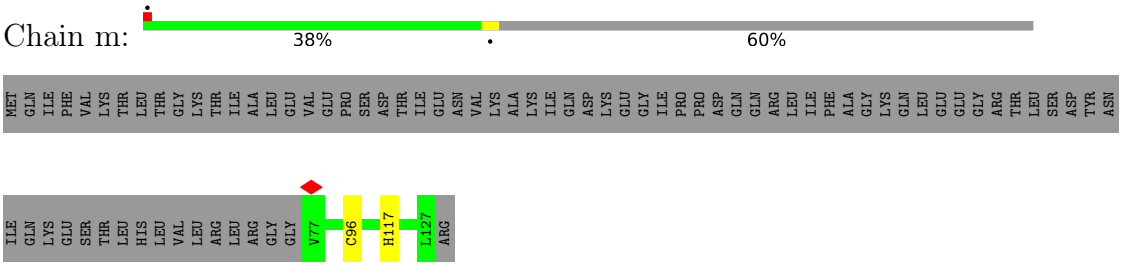
• Molecule 80: Putative 60S ribosomal protein L39

Chain l:



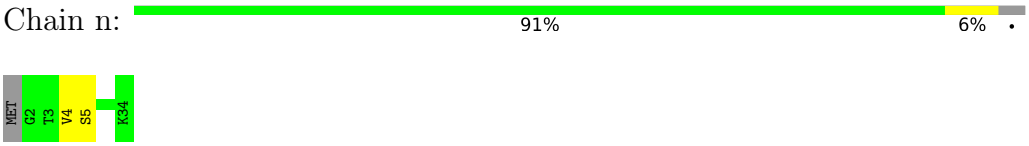
• Molecule 81: Ubiquitin-60S ribosomal protein L40

Chain m:



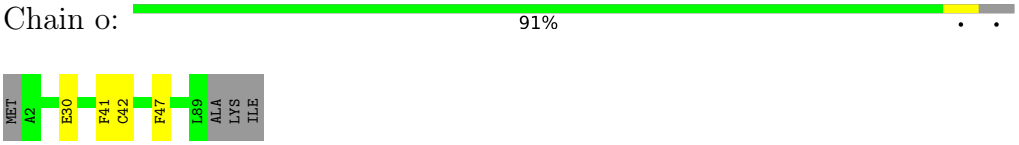
• Molecule 82: 60S ribosomal protein L41

Chain n:



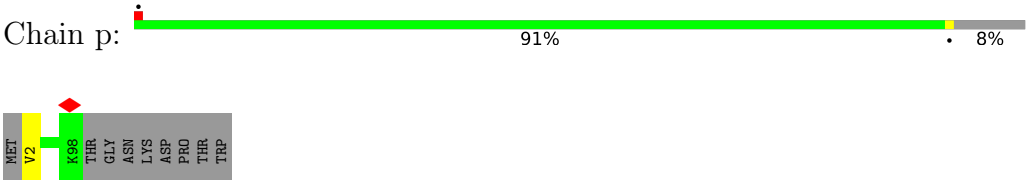
• Molecule 83: 60S ribosomal protein L37a

Chain o:



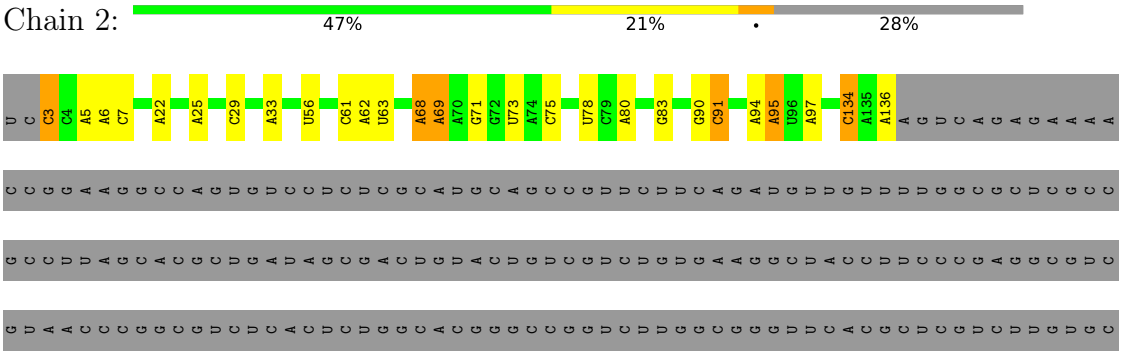
• Molecule 84: Putative 60S ribosomal protein L44

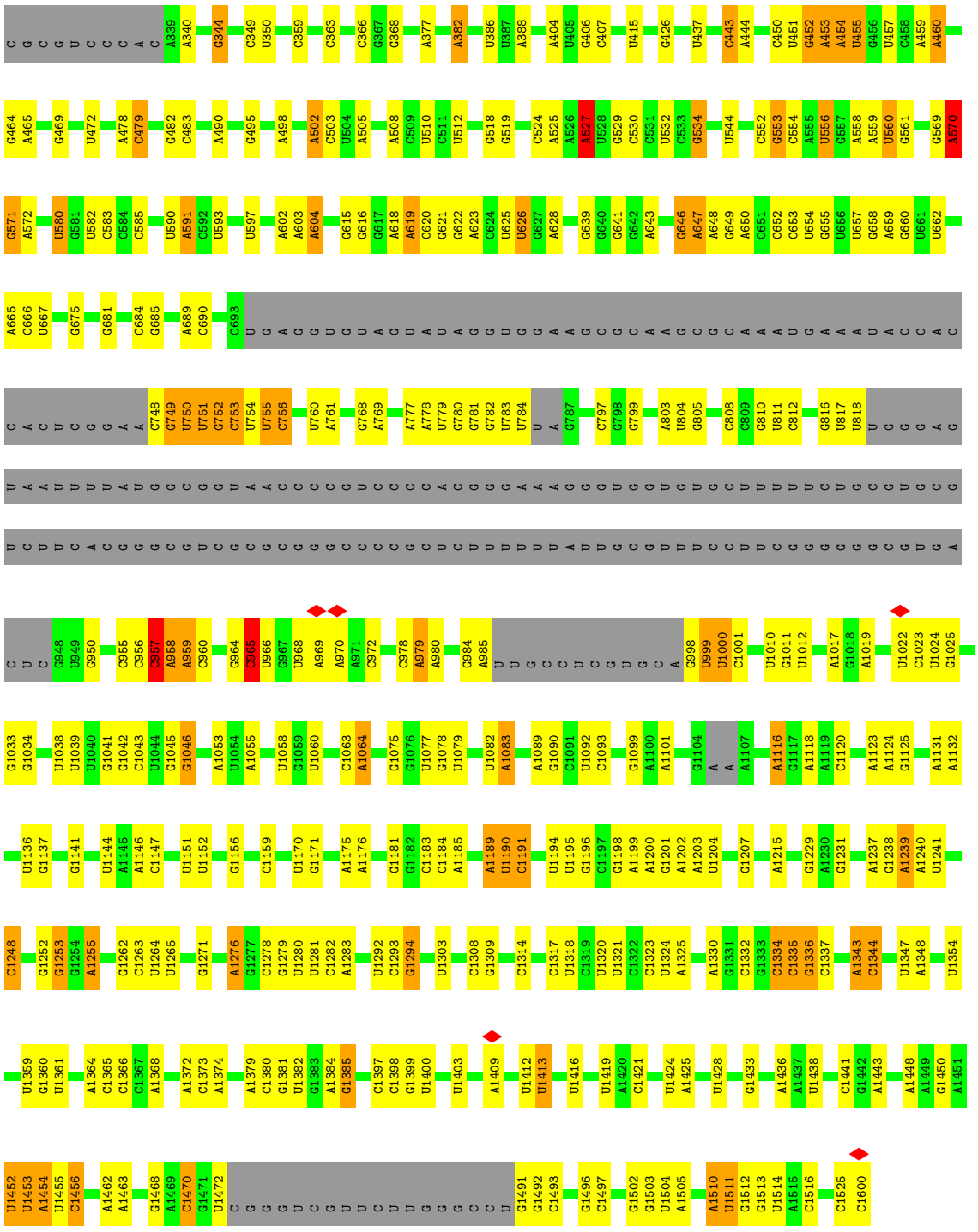
Chain p:



• Molecule 85: LSUb_rRNA_chain_2

Chain 2:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	212912	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	0.83	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NA, PSU, K, C4J, 5MC, MA6, OMC, OMG, 1MA, MG, 7MG, A2M, 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	1	0.41	0/37759	0.83	29/58867 (0.0%)
2	3	0.36	0/3671	0.86	12/5704 (0.2%)
3	4	0.37	0/4354	0.80	0/6788
4	5	0.38	0/2742	0.84	2/4266 (0.0%)
5	6	0.36	0/1683	0.86	0/2618
6	7	0.38	0/3748	0.80	0/5834
7	8	0.34	0/2829	0.82	1/4405 (0.0%)
8	A	0.28	0/1935	0.56	0/2606
9	B	0.27	0/3109	0.54	0/4214
10	C	0.26	0/2714	0.53	0/3679
11	D	0.25	0/1045	0.48	0/1423
12	E	0.25	0/1357	0.52	0/1850
13	F	0.27	0/1071	0.51	0/1466
14	G	0.26	0/1696	0.52	0/2303
15	H	0.28	0/1687	0.53	0/2291
16	I	0.26	0/1572	0.52	0/2129
17	J	0.28	0/996	0.53	0/1355
18	K	0.25	0/1248	0.49	0/1695
19	L	0.28	0/1129	0.53	0/1511
20	M	0.27	0/1728	0.58	0/2312
21	N	0.26	0/1647	0.55	0/2202
22	O	0.27	0/1963	0.49	0/2665
23	P	0.28	0/1524	0.55	0/2045
24	Q	0.27	0/1446	0.55	0/1940
25	R	0.27	0/1439	0.51	0/1949
26	S1	0.58	0/40844	0.85	37/63606 (0.1%)
27	S4	0.29	0/476	0.86	1/739 (0.1%)
28	SA	0.30	0/1859	0.55	0/2501
29	SB	0.29	0/1623	0.49	0/2204
30	SC	0.27	0/1636	0.50	0/2192
31	SD	0.30	0/1447	0.54	0/1942
32	SE	0.31	0/2088	0.53	0/2814

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	SF	0.32	0/1698	0.50	0/2301
34	SG	0.30	0/1849	0.56	0/2477
35	SH	0.27	0/1452	0.50	0/1948
36	SI	0.31	0/1639	0.53	0/2209
37	SK	0.30	0/1451	0.59	0/1944
38	SL	0.27	0/1139	0.47	0/1533
39	SM	0.25	0/798	0.51	0/1084
40	SN	0.26	0/830	0.47	0/1126
41	SO	0.33	0/1010	0.56	0/1362
42	SP	0.32	0/1143	0.53	0/1531
43	SQ	0.22	0/674	0.47	0/916
44	SR	0.27	0/1103	0.53	0/1481
45	SS	0.27	0/439	0.53	0/583
46	ST	0.34	0/1186	0.54	0/1590
47	SU	0.35	0/1290	0.52	0/1740
48	SV	0.28	0/643	0.50	0/854
49	SW	0.26	0/929	0.49	0/1255
50	SX	0.27	0/1233	0.49	0/1656
51	SY	0.27	0/630	0.51	0/858
52	SZ	0.30	0/1041	0.51	0/1388
53	S	0.27	0/1222	0.51	0/1656
54	Sa	0.27	0/563	0.50	0/757
55	Sc	0.32	0/596	0.55	0/801
56	Sb	0.36	0/837	0.58	0/1120
57	Sd	0.26	0/468	0.57	0/630
58	Se	0.29	0/436	0.53	0/577
59	Sg	0.25	0/2371	0.50	0/3233
60	Sh	0.24	0/1113	0.48	0/1514
61	SJ	0.34	0/1038	0.52	0/1391
62	T	0.26	0/1233	0.52	0/1656
63	U	0.26	0/695	0.45	0/939
64	V	0.26	0/930	0.51	0/1256
65	W	0.25	0/938	0.55	0/1254
66	X	0.28	0/560	0.52	0/757
67	Y	0.27	0/1018	0.52	0/1376
68	Z	0.25	0/1083	0.53	0/1461
69	a	0.25	0/1005	0.54	0/1339
70	b	0.25	0/557	0.50	0/743
71	c	0.27	0/1900	0.51	0/2544
72	d	0.28	0/723	0.47	0/979
73	e	0.25	0/1432	0.54	0/1904
74	f	0.27	0/1031	0.55	0/1380
75	g	0.28	0/1165	0.57	0/1563

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	h	0.25	0/1054	0.55	0/1399
77	i	0.25	0/668	0.51	0/889
78	j	0.27	0/682	0.62	0/910
79	k	0.25	0/542	0.51	0/733
80	l	0.27	0/463	0.54	0/617
81	m	0.24	0/381	0.53	0/515
82	n	0.28	0/296	0.66	0/386
83	o	0.29	0/698	0.57	0/930
84	p	0.27	0/793	0.50	0/1048
85	2	0.42	0/25035	0.84	27/39014 (0.1%)
All	All	0.40	0/211768	0.73	109/311222 (0.0%)

There are no bond length outliers.

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S1	2059	C	O4'-C1'-N1	8.29	114.83	108.20
1	1	1238	C	C2-N1-C1'	7.66	127.22	118.80
26	S1	2203	U	N1-C2-O2	7.66	128.16	122.80
85	2	1063	C	C2-N1-C1'	7.55	127.11	118.80
2	3	179	U	C2-N1-C1'	7.45	126.63	117.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	34587	0	17450	200	0
2	3	3312	0	1681	24	0
3	4	3917	0	1979	18	0
4	5	2456	0	1247	13	0
5	6	1506	0	768	12	0
6	7	3485	0	1770	13	0
7	8	2531	0	1283	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1893	0	1905	6	0
9	B	3035	0	3004	15	0
10	C	2664	0	2626	4	0
11	D	1025	0	787	4	0
12	E	1337	0	1269	8	0
13	F	1049	0	1025	10	0
14	G	1672	0	1696	4	0
15	H	1652	0	1644	7	0
16	I	1539	0	1491	2	0
17	J	979	0	968	2	0
18	K	1229	0	1194	6	0
19	L	1102	0	1124	4	0
20	M	1688	0	1748	5	0
21	N	1615	0	1685	22	0
22	O	1926	0	1761	8	0
23	P	1500	0	1568	4	0
24	Q	1427	0	1383	4	0
25	R	1405	0	1411	6	0
26	S1	37536	0	18968	352	0
27	S4	427	0	222	7	0
28	SA	1828	0	1917	13	0
29	SB	1590	0	1570	16	0
30	SC	1609	0	1655	13	0
31	SD	1422	0	1467	15	0
32	SE	2050	0	2144	20	0
33	SF	1662	0	1708	12	0
34	SG	1826	0	1914	23	0
35	SH	1430	0	1456	5	0
36	SI	1609	0	1668	21	0
37	SK	1430	0	1512	7	0
38	SL	1118	0	1168	1	0
39	SM	788	0	823	9	0
40	SN	807	0	782	6	0
41	SO	995	0	997	4	0
42	SP	1117	0	1166	8	0
43	SQ	672	0	602	10	0
44	SR	1081	0	1126	8	0
45	SS	434	0	438	5	0
46	ST	1163	0	1232	10	0
47	SU	1260	0	1277	5	0
48	SV	636	0	687	8	0
49	SW	909	0	909	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	SX	1202	0	1227	16	0
51	SY	621	0	601	5	0
52	SZ	1021	0	1083	12	0
53	S	1194	0	1184	2	0
54	Sa	558	0	606	0	0
55	Sc	586	0	570	0	0
56	Sb	820	0	854	0	0
57	Sd	466	0	476	0	0
58	Se	430	0	473	0	0
59	Sg	2313	0	2189	0	0
60	Sh	1094	0	1005	0	0
61	SJ	1021	0	1050	1	0
62	T	1209	0	1236	6	0
63	U	688	0	536	3	0
64	V	915	0	956	4	0
65	W	925	0	991	8	0
66	X	539	0	535	2	0
67	Y	997	0	988	5	0
68	Z	1068	0	1057	4	0
69	a	995	0	1076	0	0
70	b	546	0	575	0	0
71	c	1866	0	1970	0	0
72	d	713	0	730	0	0
73	e	1414	0	1532	0	0
74	f	1011	0	1054	0	0
75	g	1142	0	1196	0	0
76	h	1038	0	1109	0	0
77	i	660	0	714	0	0
78	j	668	0	680	0	0
79	k	534	0	534	0	0
80	l	450	0	483	0	0
81	m	375	0	370	0	0
82	n	292	0	331	0	0
83	o	686	0	702	0	0
84	p	780	0	838	0	0
85	2	23639	0	11982	148	0
86	1	106	0	0	0	0
86	2	66	0	0	0	0
86	3	1	0	0	0	0
86	4	8	0	0	0	0
86	5	1	0	0	0	0
86	6	2	0	0	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	S	1	0	0	0	0
90	S1	7	0	0	0	0
90	SA	1	0	0	0	0
90	T	2	0	0	0	0
All	All	200822	0	145368	1052	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 3.

The worst 5 of 1052 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	G	183	ASP

5.3.2 Protein sidechains (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	
8	A	186/204 (91%)	185 (100%)	1 (0%)	88	95
9	B	294/351 (84%)	292 (99%)	2 (1%)	84	92
10	C	250/301 (83%)	248 (99%)	2 (1%)	81	91
11	D	62/162 (38%)	61 (98%)	1 (2%)	62	79
12	E	122/172 (71%)	116 (95%)	6 (5%)	25	40
13	F	94/153 (61%)	93 (99%)	1 (1%)	73	87
14	G	156/221 (71%)	154 (99%)	2 (1%)	69	84
15	H	155/188 (82%)	154 (99%)	1 (1%)	86	94
16	I	145/183 (79%)	143 (99%)	2 (1%)	67	82
17	J	95/111 (86%)	95 (100%)	0	100	100
18	K	109/145 (75%)	109 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	L	107/114 (94%)	106 (99%)	1 (1%)	78 90
20	M	172/180 (96%)	170 (99%)	2 (1%)	71 85
21	N	168/179 (94%)	161 (96%)	7 (4%)	30 47
22	O	148/242 (61%)	145 (98%)	3 (2%)	55 74
23	P	152/164 (93%)	151 (99%)	1 (1%)	84 92
24	Q	120/198 (61%)	116 (97%)	4 (3%)	38 57
25	R	144/159 (91%)	144 (100%)	0	100 100
28	SA	198/222 (89%)	187 (94%)	11 (6%)	21 34
29	SB	165/202 (82%)	159 (96%)	6 (4%)	35 54
30	SC	167/184 (91%)	159 (95%)	8 (5%)	25 41
31	SD	148/164 (90%)	143 (97%)	5 (3%)	37 56
32	SE	215/225 (96%)	209 (97%)	6 (3%)	43 63
33	SF	174/208 (84%)	170 (98%)	4 (2%)	50 70
34	SG	186/208 (89%)	181 (97%)	5 (3%)	44 65
35	SH	150/159 (94%)	146 (97%)	4 (3%)	44 65
36	SI	172/186 (92%)	167 (97%)	5 (3%)	42 62
37	SK	139/176 (79%)	135 (97%)	4 (3%)	42 62
38	SL	112/120 (93%)	109 (97%)	3 (3%)	44 65
39	SM	90/104 (86%)	89 (99%)	1 (1%)	73 87
40	SN	84/128 (66%)	77 (92%)	7 (8%)	11 17
41	SO	97/113 (86%)	92 (95%)	5 (5%)	23 38
42	SP	115/117 (98%)	114 (99%)	1 (1%)	78 90
43	SQ	57/120 (48%)	55 (96%)	2 (4%)	36 55
44	SR	112/130 (86%)	111 (99%)	1 (1%)	78 90
45	SS	45/49 (92%)	43 (96%)	2 (4%)	28 45
46	ST	125/132 (95%)	124 (99%)	1 (1%)	81 91
47	SU	132/152 (87%)	129 (98%)	3 (2%)	50 70
48	SV	69/126 (55%)	64 (93%)	5 (7%)	14 23
49	SW	93/130 (72%)	90 (97%)	3 (3%)	39 59
50	SX	121/131 (92%)	120 (99%)	1 (1%)	81 91
51	SY	64/116 (55%)	63 (98%)	1 (2%)	62 79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	SZ	107/118 (91%)	102 (95%)	5 (5%)	26 42
53	S	116/134 (87%)	116 (100%)	0	100 100
54	Sa	63/95 (66%)	63 (100%)	0	100 100
55	Sc	62/76 (82%)	60 (97%)	2 (3%)	39 59
56	Sb	85/93 (91%)	83 (98%)	2 (2%)	49 68
57	Sd	46/75 (61%)	43 (94%)	3 (6%)	17 27
58	Se	45/54 (83%)	43 (96%)	2 (4%)	28 45
59	Sg	246/265 (93%)	240 (98%)	6 (2%)	49 68
60	Sh	91/177 (51%)	85 (93%)	6 (7%)	16 26
61	SJ	110/111 (99%)	109 (99%)	1 (1%)	78 90
62	T	125/143 (87%)	123 (98%)	2 (2%)	62 79
63	U	41/114 (36%)	40 (98%)	1 (2%)	49 68
64	V	93/124 (75%)	92 (99%)	1 (1%)	73 87
65	W	96/122 (79%)	96 (100%)	0	100 100
66	X	56/104 (54%)	53 (95%)	3 (5%)	22 36
67	Y	93/116 (80%)	92 (99%)	1 (1%)	73 87
68	Z	102/118 (86%)	98 (96%)	4 (4%)	32 50
69	a	103/118 (87%)	101 (98%)	2 (2%)	57 75
70	b	56/58 (97%)	55 (98%)	1 (2%)	59 76
71	c	192/209 (92%)	190 (99%)	2 (1%)	76 88
72	d	81/89 (91%)	73 (90%)	8 (10%)	8 11
73	e	146/158 (92%)	143 (98%)	3 (2%)	53 72
74	f	106/115 (92%)	105 (99%)	1 (1%)	78 90
75	g	119/121 (98%)	118 (99%)	1 (1%)	81 91
76	h	110/146 (75%)	106 (96%)	4 (4%)	35 54
77	i	64/88 (73%)	63 (98%)	1 (2%)	62 79
78	j	67/70 (96%)	66 (98%)	1 (2%)	65 80
79	k	52/74 (70%)	48 (92%)	4 (8%)	13 20
80	l	46/47 (98%)	44 (96%)	2 (4%)	29 46
81	m	36/113 (32%)	34 (94%)	2 (6%)	21 34
82	n	30/32 (94%)	28 (93%)	2 (7%)	16 26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
83	o	68/74 (92%)	64 (94%)	4 (6%)	19 32
84	p	82/92 (89%)	81 (99%)	1 (1%)	71 85
All	All	8644/10672 (81%)	8436 (98%)	208 (2%)	51 68

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	SS	57	ARG
58	Se	64	LYS
81	m	96	CYS
47	SU	82	ARG
52	SZ	32	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
71	c	30	GLN
74	f	50	GLN
76	h	101	GLN
76	h	7	GLN
66	X	63	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1598/1782 (89%)	281 (17%)	16 (1%)
2	3	151/216 (69%)	32 (21%)	4 (2%)
26	S1	1726/2204 (78%)	310 (17%)	12 (0%)
27	S4	18/20 (90%)	6 (33%)	0
3	4	182/183 (99%)	31 (17%)	3 (1%)
4	5	111/135 (82%)	21 (18%)	0
5	6	70/73 (95%)	22 (31%)	2 (2%)
6	7	161/171 (94%)	24 (14%)	0
7	8	118/123 (95%)	8 (6%)	0
85	2	1097/1526 (71%)	207 (18%)	13 (1%)
All	All	5232/6433 (81%)	942 (18%)	50 (0%)

5 of 942 RNA backbone outliers are listed below:

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

5 of 50 RNA pucker outliers are listed below:

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

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

154 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	PSU	2	1413	85	18,21,22	4.38	7 (38%)	22,30,33	1.79	5 (22%)
26	A2M	S1	98	86,26	18,25,26	4.26	7 (38%)	18,36,39	2.56	3 (16%)
1	PSU	1	940	1	18,21,22	4.44	7 (38%)	22,30,33	1.82	5 (22%)
85	PSU	2	626	85	18,21,22	4.40	7 (38%)	22,30,33	1.77	4 (18%)
85	PSU	2	1361	85	18,21,22	4.44	7 (38%)	22,30,33	1.80	5 (22%)
1	A2M	1	927	1	18,25,26	4.20	6 (33%)	18,36,39	2.74	3 (16%)
1	PSU	1	1181	1	18,21,22	4.43	8 (44%)	22,30,33	1.73	4 (18%)
85	PSU	2	593	85	18,21,22	4.38	7 (38%)	22,30,33	1.71	4 (18%)
26	PSU	S1	2048	26	18,21,22	4.25	8 (44%)	22,30,33	1.85	5 (22%)
1	OMU	1	1371	1	19,22,23	3.04	8 (42%)	26,31,34	1.88	5 (19%)
26	PSU	S1	1657	26	18,21,22	4.33	7 (38%)	22,30,33	1.81	5 (22%)
26	PSU	S1	1533	26	18,21,22	4.42	7 (38%)	22,30,33	1.75	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
85	PSU	2	437	85	18,21,22	4.38	7 (38%)	22,30,33	1.83	5 (22%)
1	A2M	1	678	85,1	18,25,26	4.24	6 (33%)	18,36,39	3.59	7 (38%)
85	PSU	2	597	85	18,21,22	4.42	7 (38%)	22,30,33	1.81	5 (22%)
85	5MC	2	524	85,86	18,22,23	3.44	7 (38%)	26,32,35	1.04	2 (7%)
1	OMC	1	695	1	19,22,23	2.94	8 (42%)	26,31,34	0.70	0
1	PSU	1	422	1	18,21,22	4.47	7 (38%)	22,30,33	1.86	4 (18%)
1	OMG	1	856	1	18,26,27	2.50	8 (44%)	19,38,41	1.55	4 (21%)
26	OMU	S1	29	86,26	19,22,23	2.93	8 (42%)	26,31,34	1.79	5 (19%)
26	OMC	S1	2140	26	19,22,23	2.94	8 (42%)	26,31,34	0.86	0
6	OMU	7	7	6,1	19,22,23	2.97	8 (42%)	26,31,34	1.72	5 (19%)
1	PSU	1	672	86,1	18,21,22	4.39	7 (38%)	22,30,33	1.85	6 (27%)
26	OMU	S1	8	26	19,22,23	2.86	8 (42%)	26,31,34	1.82	5 (19%)
26	PSU	S1	104	26	18,21,22	4.37	7 (38%)	22,30,33	1.75	5 (22%)
85	OMC	2	443	85,87	19,22,23	2.94	8 (42%)	26,31,34	0.80	0
1	OMG	1	1540	85,1	18,26,27	2.47	8 (44%)	19,38,41	1.54	5 (26%)
85	OMU	2	73	85	19,22,23	2.96	8 (42%)	26,31,34	1.69	5 (19%)
26	PSU	S1	1566	86,26	18,21,22	4.43	8 (44%)	22,30,33	1.72	4 (18%)
1	OMG	1	1190	86,1	18,26,27	2.50	8 (44%)	19,38,41	1.64	4 (21%)
1	PSU	1	1039	1	18,21,22	4.44	7 (38%)	22,30,33	1.87	5 (22%)
85	OMG	2	1229	85	18,26,27	2.52	8 (44%)	19,38,41	1.59	5 (26%)
26	OMU	S1	1833	86,26	19,22,23	2.99	8 (42%)	26,31,34	1.77	5 (19%)
6	A2M	7	43	6	18,25,26	4.25	6 (33%)	18,36,39	2.62	3 (16%)
26	OMG	S1	1550	26	18,26,27	2.53	8 (44%)	19,38,41	1.55	4 (21%)
85	OMG	2	1046	85	18,26,27	2.52	8 (44%)	19,38,41	1.54	4 (21%)
85	A2M	2	527	85	18,25,26	3.98	7 (38%)	18,36,39	2.69	3 (16%)
85	PSU	2	662	85,86	18,21,22	4.40	7 (38%)	22,30,33	1.82	5 (22%)
85	PSU	2	1058	85	18,21,22	4.45	7 (38%)	22,30,33	1.85	5 (22%)
26	PSU	S1	2046	26	18,21,22	4.30	7 (38%)	22,30,33	1.91	5 (22%)
1	PSU	1	1528	1	18,21,22	4.44	7 (38%)	22,30,33	1.82	5 (22%)
85	OMU	2	560	85	19,22,23	2.98	8 (42%)	26,31,34	1.76	5 (19%)
6	PSU	7	74	6	18,21,22	4.45	7 (38%)	22,30,33	1.81	5 (22%)
1	PSU	1	239	1	18,21,22	4.47	7 (38%)	22,30,33	1.81	5 (22%)
85	OMU	2	56	85,1	19,22,23	2.98	8 (42%)	26,31,34	1.76	4 (15%)
85	OMG	2	534	85	18,26,27	2.51	8 (44%)	19,38,41	1.56	4 (21%)
85	OMG	2	1253	85	18,26,27	2.47	8 (44%)	19,38,41	1.52	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
85	OMU	2	667	85	19,22,23	2.98	8 (42%)	26,31,34	1.71	4 (15%)
1	PSU	1	1664	1	18,21,22	4.44	7 (38%)	22,30,33	1.84	6 (27%)
26	PSU	S1	1539	26	18,21,22	4.41	7 (38%)	22,30,33	1.78	5 (22%)
1	A2M	1	858	1	18,25,26	4.15	7 (38%)	18,36,39	2.78	4 (22%)
85	A2M	2	604	85,1	18,25,26	4.22	6 (33%)	18,36,39	2.66	3 (16%)
85	OMU	2	1419	85	19,22,23	2.99	8 (42%)	26,31,34	1.72	4 (15%)
26	OMG	S1	1647	26	18,26,27	2.44	8 (44%)	19,38,41	1.66	4 (21%)
85	OMG	2	71	85,86	18,26,27	2.54	8 (44%)	19,38,41	1.58	4 (21%)
26	PSU	S1	33	26	18,21,22	4.42	8 (44%)	22,30,33	1.75	4 (18%)
26	PSU	S1	1156	26	18,21,22	4.35	7 (38%)	22,30,33	1.85	5 (22%)
85	A2M	2	591	85	18,25,26	4.23	6 (33%)	18,36,39	2.71	3 (16%)
26	A2M	S1	479	26	18,25,26	4.21	7 (38%)	18,36,39	2.68	5 (27%)
85	OMC	2	359	85	19,22,23	2.98	8 (42%)	26,31,34	0.69	0
85	A2M	2	570	85,1	18,25,26	4.15	7 (38%)	18,36,39	2.85	5 (27%)
6	OMG	7	75	6	18,26,27	2.54	8 (44%)	19,38,41	1.56	4 (21%)
1	OMG	1	959[A]	1	18,26,27	2.58	8 (44%)	19,38,41	1.65	5 (26%)
26	OMG	S1	600	26	18,26,27	2.48	8 (44%)	19,38,41	1.55	4 (21%)
1	OMG	1	1524	1	18,26,27	2.53	8 (44%)	19,38,41	1.65	4 (21%)
85	OMU	2	1359	85	19,22,23	2.98	8 (42%)	26,31,34	1.70	5 (19%)
85	PSU	2	1354	85	18,21,22	4.43	7 (38%)	22,30,33	1.84	5 (22%)
26	PSU	S1	1192	26	18,21,22	4.34	7 (38%)	22,30,33	1.72	4 (18%)
26	OMG	S1	1829	86,26	18,26,27	2.50	8 (44%)	19,38,41	1.53	4 (21%)
85	A2M	2	95	85	18,25,26	4.22	6 (33%)	18,36,39	2.68	3 (16%)
1	1MA	1	677	86,1	16,25,26	3.94	4 (25%)	18,37,40	1.83	3 (16%)
1	OMG	1	1626	1	18,26,27	2.53	8 (44%)	19,38,41	1.58	5 (26%)
1	OMU	1	1107	1	19,22,23	2.99	8 (42%)	26,31,34	1.76	5 (19%)
85	PSU	2	1303	85	18,21,22	4.42	8 (44%)	22,30,33	1.86	6 (27%)
85	PSU	2	1265	85,88	18,21,22	4.45	7 (38%)	22,30,33	1.91	5 (22%)
85	PSU	2	1144	85	18,21,22	4.43	7 (38%)	22,30,33	1.85	5 (22%)
85	A2M	2	1185	85	18,25,26	4.18	7 (38%)	18,36,39	2.63	4 (22%)
1	OMU	1	845	1	19,22,23	2.96	8 (42%)	26,31,34	2.05	6 (23%)
85	A2M	2	628	85	18,25,26	4.22	6 (33%)	18,36,39	2.60	3 (16%)
26	C4J	S1	1543	26	24,29,30	2.97	9 (37%)	29,42,45	1.37	3 (10%)
3	OMG	4	74	3	18,26,27	2.50	8 (44%)	19,38,41	1.52	5 (26%)
1	A2M	1	955	1	18,25,26	4.25	6 (33%)	18,36,39	2.67	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	5MC	S1	1544	26	18,22,23	3.47	7 (38%)	26,32,35	1.05	1 (3%)
1	A2M	1	407	1	18,25,26	4.37	7 (38%)	18,36,39	2.54	4 (22%)
85	A2M	2	572	85	18,25,26	4.22	6 (33%)	18,36,39	2.66	3 (16%)
85	A2M	2	382	85	18,25,26	4.28	6 (33%)	18,36,39	2.78	3 (16%)
1	PSU	1	1533	85,1	18,21,22	4.43	7 (38%)	22,30,33	1.92	6 (27%)
1	A2M	1	1539	85,86,1	18,25,26	4.24	6 (33%)	18,36,39	2.58	3 (16%)
85	OMC	2	1248	85	19,22,23	2.92	8 (42%)	26,31,34	0.82	0
26	OMC	S1	18	26	19,22,23	2.81	8 (42%)	26,31,34	0.78	0
85	A2M	2	1384	85,86	18,25,26	4.23	6 (33%)	18,36,39	2.60	3 (16%)
1	A2M	1	305	1	18,25,26	4.18	6 (33%)	18,36,39	2.73	3 (16%)
1	A2M	1	697	1	18,25,26	4.22	6 (33%)	18,36,39	2.65	3 (16%)
26	PSU	S1	1841	26,87	18,21,22	4.37	7 (38%)	22,30,33	1.93	5 (22%)
26	PSU	S1	455	26	18,21,22	4.38	7 (38%)	22,30,33	1.90	5 (22%)
1	PSU	1	1171	86,1	18,21,22	4.43	7 (38%)	22,30,33	1.83	6 (27%)
26	OMG	S1	2151	26	18,26,27	2.50	8 (44%)	19,38,41	1.61	4 (21%)
85	OMC	2	1317	85	19,22,23	2.92	8 (42%)	26,31,34	0.77	0
85	PSU	2	1318	85	18,21,22	4.40	7 (38%)	22,30,33	1.78	6 (27%)
26	PSU	S1	1246	86,26	18,21,22	4.33	7 (38%)	22,30,33	1.92	5 (22%)
6	PSU	7	69	6	18,21,22	4.44	9 (50%)	22,30,33	1.75	5 (22%)
1	PSU	1	1402	1	18,21,22	4.41	7 (38%)	22,30,33	1.68	4 (18%)
26	MA6	S1	2185	26	18,26,27	1.18	1 (5%)	19,38,41	3.00	2 (10%)
26	OMU	S1	1621	86,26	19,22,23	2.99	8 (42%)	26,31,34	1.72	4 (15%)
85	OMG	2	1231	85	18,26,27	2.52	8 (44%)	19,38,41	1.52	4 (21%)
85	PSU	2	1264	85,87	18,21,22	4.44	8 (44%)	22,30,33	1.88	6 (27%)
85	OMU	2	1077	85	19,22,23	3.00	8 (42%)	26,31,34	1.75	5 (19%)
26	PSU	S1	607	26	18,21,22	4.54	7 (38%)	22,30,33	1.74	6 (27%)
26	PSU	S1	12	26	18,21,22	4.26	8 (44%)	22,30,33	1.83	5 (22%)
26	OMU	S1	1979	26	19,22,23	2.98	8 (42%)	26,31,34	1.73	4 (15%)
85	OMC	2	1159	85	19,22,23	2.93	8 (42%)	26,31,34	0.79	0
85	OMG	2	655	85	18,26,27	2.50	8 (44%)	19,38,41	1.59	4 (21%)
1	PSU	1	1011	1	18,21,22	4.45	9 (50%)	22,30,33	1.77	5 (22%)
26	OMU	S1	661	26	19,22,23	2.88	8 (42%)	26,31,34	1.77	5 (19%)
1	PSU	1	870	1	18,21,22	4.41	7 (38%)	22,30,33	1.85	5 (22%)
1	A2M	1	235	1	18,25,26	4.33	7 (38%)	18,36,39	2.60	3 (16%)
26	MA6	S1	2184	26	18,26,27	1.18	1 (5%)	19,38,41	2.95	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
85	PSU	2	1194	85	18,21,22	4.45	7 (38%)	22,30,33	1.78	5 (22%)
26	PSU	S1	609	26	18,21,22	4.42	7 (38%)	22,30,33	1.89	5 (22%)
1	OMU	1	1659	86,1	19,22,23	2.98	8 (42%)	26,31,34	1.73	5 (19%)
6	A2M	7	162	6,1	18,25,26	4.22	6 (33%)	18,36,39	2.80	3 (16%)
85	PSU	2	510	85	18,21,22	4.47	7 (38%)	22,30,33	1.78	5 (22%)
85	5MC	2	1308	85,86	18,21,23	4.64	12 (66%)	25,30,35	1.30	2 (8%)
1	PSU	1	1017	86,1	18,21,22	4.36	7 (38%)	22,30,33	1.83	5 (22%)
26	7MG	S1	1995	26	22,26,27	4.13	10 (45%)	29,39,42	2.05	9 (31%)
1	A2M	1	681	1	18,25,26	4.19	6 (33%)	18,36,39	2.79	3 (16%)
85	OMG	2	1078	85	18,26,27	2.51	8 (44%)	19,38,41	1.65	5 (26%)
85	PSU	2	78	85	18,21,22	4.41	7 (38%)	22,30,33	1.84	5 (22%)
26	A2M	S1	2021	26	18,25,26	4.10	7 (38%)	18,36,39	2.77	3 (16%)
85	PSU	2	512	85	18,21,22	4.47	7 (38%)	22,30,33	1.83	5 (22%)
26	A2M	S1	512	86,26	18,25,26	4.24	7 (38%)	18,36,39	2.55	3 (16%)
85	PSU	2	472	85	18,21,22	4.45	7 (38%)	22,30,33	1.86	5 (22%)
85	OMC	2	583	85	19,22,23	2.92	8 (42%)	26,31,34	0.69	0
85	OMG	2	1360	85	18,26,27	2.52	8 (44%)	19,38,41	1.52	4 (21%)
85	OMC	2	1397	85	19,22,23	2.91	8 (42%)	26,31,34	0.77	0
2	OMU	3	13	2	19,22,23	2.99	8 (42%)	26,31,34	1.73	5 (19%)
26	OMG	S1	1623	26	18,26,27	2.51	8 (44%)	19,38,41	1.54	4 (21%)
1	OMC	1	1527	1	19,22,23	2.94	8 (42%)	26,31,34	0.99	2 (7%)
1	OMC	1	1010	86,1,88	19,22,23	2.94	8 (42%)	26,31,34	0.83	0
26	OMG	S1	1865	26	18,26,27	2.49	8 (44%)	19,38,41	1.57	4 (21%)
26	PSU	S1	2202	26	18,21,22	4.29	8 (44%)	22,30,33	1.65	4 (18%)
26	OMG	S1	1879	26	18,26,27	2.51	8 (44%)	19,38,41	1.56	4 (21%)
26	A2M	S1	668	86,26	18,25,26	4.04	7 (38%)	18,36,39	2.85	4 (22%)
26	5MC	S1	2061	26	18,22,23	3.35	7 (38%)	26,32,35	0.99	2 (7%)
85	PSU	2	1060	85	18,21,22	4.40	7 (38%)	22,30,33	1.91	5 (22%)
85	A2M	2	1372	85	18,25,26	4.15	6 (33%)	18,36,39	2.73	4 (22%)
85	PSU	2	1403	85	18,21,22	4.43	7 (38%)	22,30,33	1.86	6 (27%)
85	OMG	2	641	85	18,26,27	2.51	8 (44%)	19,38,41	1.59	5 (26%)
1	OMU	1	847	1	19,22,23	2.94	8 (42%)	26,31,34	1.76	5 (19%)
1	OMG	1	959[B]	1	18,26,27	2.56	8 (44%)	19,38,41	1.51	4 (21%)
26	OMC	S1	38	26	19,22,23	2.88	8 (42%)	26,31,34	0.79	0
26	OMG	S1	1478	26	18,26,27	2.43	8 (44%)	19,38,41	1.58	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
85	PSU	2	1382	85	18,21,22	4.42	7 (38%)	22,30,33	1.89	6 (27%)
26	OMC	S1	1866	26	19,22,23	2.90	8 (42%)	26,31,34	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	PSU	2	1413	85	-	0/7/25/26	0/2/2/2
26	A2M	S1	98	86,26	-	2/5/27/28	0/3/3/3
1	PSU	1	940	1	-	0/7/25/26	0/2/2/2
85	PSU	2	626	85	-	0/7/25/26	0/2/2/2
85	PSU	2	1361	85	-	1/7/25/26	0/2/2/2
1	A2M	1	927	1	-	1/5/27/28	0/3/3/3
1	PSU	1	1181	1	-	4/7/25/26	0/2/2/2
85	PSU	2	593	85	-	0/7/25/26	0/2/2/2
26	PSU	S1	2048	26	-	0/7/25/26	0/2/2/2
1	OMU	1	1371	1	-	4/9/27/28	0/2/2/2
26	PSU	S1	1657	26	-	2/7/25/26	0/2/2/2
26	PSU	S1	1533	26	-	2/7/25/26	0/2/2/2
85	PSU	2	437	85	-	0/7/25/26	0/2/2/2
1	A2M	1	678	85,1	-	3/5/27/28	0/3/3/3
85	PSU	2	597	85	-	0/7/25/26	0/2/2/2
85	5MC	2	524	85,86	-	0/7/25/26	0/2/2/2
1	OMC	1	695	1	-	0/9/27/28	0/2/2/2
1	PSU	1	422	1	-	0/7/25/26	0/2/2/2
1	OMG	1	856	1	-	0/5/27/28	0/3/3/3
26	OMU	S1	29	86,26	-	0/9/27/28	0/2/2/2
26	OMC	S1	2140	26	-	2/9/27/28	0/2/2/2
6	OMU	7	7	6,1	-	1/9/27/28	0/2/2/2
1	PSU	1	672	86,1	-	0/7/25/26	0/2/2/2
26	OMU	S1	8	26	-	6/9/27/28	0/2/2/2
26	PSU	S1	104	26	-	2/7/25/26	0/2/2/2
85	OMC	2	443	85,87	-	4/9/27/28	0/2/2/2
1	OMG	1	1540	85,1	-	2/5/27/28	0/3/3/3
85	OMU	2	73	85	-	0/9/27/28	0/2/2/2
26	PSU	S1	1566	86,26	-	2/7/25/26	0/2/2/2
1	OMG	1	1190	86,1	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	1039	1	-	0/7/25/26	0/2/2/2
85	OMG	2	1229	85	-	0/5/27/28	0/3/3/3
26	OMU	S1	1833	86,26	-	2/9/27/28	0/2/2/2
6	A2M	7	43	6	-	0/5/27/28	0/3/3/3
26	OMG	S1	1550	26	-	3/5/27/28	0/3/3/3
85	OMG	2	1046	85	-	2/5/27/28	0/3/3/3
85	A2M	2	527	85	-	2/5/27/28	0/3/3/3
85	PSU	2	662	85,86	-	0/7/25/26	0/2/2/2
85	PSU	2	1058	85	-	0/7/25/26	0/2/2/2
26	PSU	S1	2046	26	-	0/7/25/26	0/2/2/2
1	PSU	1	1528	1	-	0/7/25/26	0/2/2/2
85	OMU	2	560	85	-	1/9/27/28	0/2/2/2
6	PSU	7	74	6	-	2/7/25/26	0/2/2/2
1	PSU	1	239	1	-	0/7/25/26	0/2/2/2
85	OMU	2	56	85,1	-	0/9/27/28	0/2/2/2
85	OMG	2	534	85	-	2/5/27/28	0/3/3/3
85	OMG	2	1253	85	-	0/5/27/28	0/3/3/3
85	OMU	2	667	85	-	1/9/27/28	0/2/2/2
1	PSU	1	1664	1	-	0/7/25/26	0/2/2/2
26	PSU	S1	1539	26	-	2/7/25/26	0/2/2/2
1	A2M	1	858	1	-	0/5/27/28	0/3/3/3
85	A2M	2	604	85,1	-	0/5/27/28	0/3/3/3
85	OMU	2	1419	85	-	0/9/27/28	0/2/2/2
26	OMG	S1	1647	26	-	0/5/27/28	0/3/3/3
85	OMG	2	71	85,86	-	0/5/27/28	0/3/3/3
26	PSU	S1	33	26	-	2/7/25/26	0/2/2/2
26	PSU	S1	1156	26	-	0/7/25/26	0/2/2/2
85	A2M	2	591	85	-	1/5/27/28	0/3/3/3
26	A2M	S1	479	26	-	2/5/27/28	0/3/3/3
85	OMC	2	359	85	-	0/9/27/28	0/2/2/2
85	A2M	2	570	85,1	-	3/5/27/28	0/3/3/3
6	OMG	7	75	6	-	2/5/27/28	0/3/3/3
1	OMG	1	959[A]	1	-	2/5/27/28	0/3/3/3
26	OMG	S1	600	26	-	2/5/27/28	0/3/3/3
1	OMG	1	1524	1	-	1/5/27/28	0/3/3/3
85	OMU	2	1359	85	-	0/9/27/28	0/2/2/2
85	PSU	2	1354	85	-	0/7/25/26	0/2/2/2
26	PSU	S1	1192	26	-	0/7/25/26	0/2/2/2
26	OMG	S1	1829	86,26	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	A2M	2	95	85	-	0/5/27/28	0/3/3/3
1	1MA	1	677	86,1	-	0/3/25/26	0/3/3/3
1	OMG	1	1626	1	-	0/5/27/28	0/3/3/3
1	OMU	1	1107	1	-	3/9/27/28	0/2/2/2
85	PSU	2	1303	85	-	0/7/25/26	0/2/2/2
85	PSU	2	1265	85,88	-	1/7/25/26	0/2/2/2
85	PSU	2	1144	85	-	0/7/25/26	0/2/2/2
85	A2M	2	1185	85	-	2/5/27/28	0/3/3/3
1	OMU	1	845	1	-	3/9/27/28	0/2/2/2
85	A2M	2	628	85	-	0/5/27/28	0/3/3/3
26	C4J	S1	1543	26	-	6/16/34/35	0/2/2/2
3	OMG	4	74	3	-	0/5/27/28	0/3/3/3
1	A2M	1	955	1	-	0/5/27/28	0/3/3/3
26	5MC	S1	1544	26	-	0/7/25/26	0/2/2/2
1	A2M	1	407	1	-	4/5/27/28	0/3/3/3
85	A2M	2	572	85	-	0/5/27/28	0/3/3/3
85	A2M	2	382	85	-	1/5/27/28	0/3/3/3
1	PSU	1	1533	85,1	-	0/7/25/26	0/2/2/2
1	A2M	1	1539	85,86,1	-	0/5/27/28	0/3/3/3
85	OMC	2	1248	85	-	1/9/27/28	0/2/2/2
26	OMC	S1	18	26	-	0/9/27/28	0/2/2/2
85	A2M	2	1384	85,86	-	0/5/27/28	0/3/3/3
1	A2M	1	305	1	-	2/5/27/28	0/3/3/3
1	A2M	1	697	1	-	0/5/27/28	0/3/3/3
26	PSU	S1	1841	26,87	-	1/7/25/26	0/2/2/2
26	PSU	S1	455	26	-	0/7/25/26	0/2/2/2
1	PSU	1	1171	86,1	-	0/7/25/26	0/2/2/2
26	OMG	S1	2151	26	-	0/5/27/28	0/3/3/3
85	OMC	2	1317	85	-	0/9/27/28	0/2/2/2
85	PSU	2	1318	85	-	0/7/25/26	0/2/2/2
26	PSU	S1	1246	86,26	-	0/7/25/26	0/2/2/2
6	PSU	7	69	6	-	4/7/25/26	0/2/2/2
1	PSU	1	1402	1	-	2/7/25/26	0/2/2/2
26	MA6	S1	2185	26	-	1/7/29/30	0/3/3/3
26	OMU	S1	1621	86,26	-	0/9/27/28	0/2/2/2
85	OMG	2	1231	85	-	0/5/27/28	0/3/3/3
85	PSU	2	1264	85,87	-	0/7/25/26	0/2/2/2
85	OMU	2	1077	85	-	0/9/27/28	0/2/2/2
26	PSU	S1	607	26	-	2/7/25/26	0/2/2/2
26	PSU	S1	12	26	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	OMU	S1	1979	26	-	1/9/27/28	0/2/2/2
85	OMC	2	1159	85	-	0/9/27/28	0/2/2/2
85	OMG	2	655	85	-	1/5/27/28	0/3/3/3
1	PSU	1	1011	1	-	0/7/25/26	0/2/2/2
26	OMU	S1	661	26	-	0/9/27/28	0/2/2/2
1	PSU	1	870	1	-	0/7/25/26	0/2/2/2
1	A2M	1	235	1	-	0/5/27/28	0/3/3/3
26	MA6	S1	2184	26	-	0/7/29/30	0/3/3/3
85	PSU	2	1194	85	-	0/7/25/26	0/2/2/2
26	PSU	S1	609	26	-	0/7/25/26	0/2/2/2
1	OMU	1	1659	86,1	-	0/9/27/28	0/2/2/2
6	A2M	7	162	6,1	-	1/5/27/28	0/3/3/3
85	PSU	2	510	85	-	0/7/25/26	0/2/2/2
85	5MC	2	1308	85,86	-	4/6/24/26	0/2/2/2
1	PSU	1	1017	86,1	-	0/7/25/26	0/2/2/2
26	7MG	S1	1995	26	-	2/7/37/38	0/3/3/3
1	A2M	1	681	1	-	3/5/27/28	0/3/3/3
85	OMG	2	1078	85	-	0/5/27/28	0/3/3/3
85	PSU	2	78	85	-	0/7/25/26	0/2/2/2
26	A2M	S1	2021	26	-	2/5/27/28	0/3/3/3
85	PSU	2	512	85	-	0/7/25/26	0/2/2/2
26	A2M	S1	512	86,26	-	2/5/27/28	0/3/3/3
85	PSU	2	472	85	-	0/7/25/26	0/2/2/2
85	OMC	2	583	85	-	0/9/27/28	0/2/2/2
85	OMG	2	1360	85	-	0/5/27/28	0/3/3/3
85	OMC	2	1397	85	-	0/9/27/28	0/2/2/2
2	OMU	3	13	2	-	0/9/27/28	0/2/2/2
26	OMG	S1	1623	26	-	2/5/27/28	0/3/3/3
1	OMC	1	1527	1	-	3/9/27/28	0/2/2/2
1	OMC	1	1010	86,1,88	-	1/9/27/28	0/2/2/2
26	OMG	S1	1865	26	-	0/5/27/28	0/3/3/3
26	PSU	S1	2202	26	-	1/7/25/26	0/2/2/2
26	OMG	S1	1879	26	-	1/5/27/28	0/3/3/3
26	A2M	S1	668	86,26	-	2/5/27/28	0/3/3/3
26	5MC	S1	2061	26	-	0/7/25/26	0/2/2/2
85	PSU	2	1060	85	-	0/7/25/26	0/2/2/2
85	A2M	2	1372	85	-	0/5/27/28	0/3/3/3
85	PSU	2	1403	85	-	0/7/25/26	0/2/2/2
85	OMG	2	641	85	-	0/5/27/28	0/3/3/3
1	OMU	1	847	1	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1	959[B]	1	-	0/5/27/28	0/3/3/3
26	OMC	S1	38	26	-	0/9/27/28	0/2/2/2
26	OMG	S1	1478	26	-	0/5/27/28	0/3/3/3
85	PSU	2	1382	85	-	0/7/25/26	0/2/2/2
26	OMC	S1	1866	26	-	0/9/27/28	0/2/2/2

The worst 5 of 1130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	407	A2M	O4'-C1'	15.76	1.63	1.41
1	1	235	A2M	O4'-C1'	15.63	1.62	1.41
85	2	382	A2M	O4'-C1'	15.49	1.62	1.41
1	1	678	A2M	O4'-C1'	15.43	1.62	1.41
6	7	43	A2M	O4'-C1'	15.30	1.62	1.41

The worst 5 of 617 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S1	2185	MA6	N1-C6-N6	-11.63	104.81	117.06
26	S1	2184	MA6	N1-C6-N6	-11.39	105.07	117.06
1	1	681	A2M	C5-C6-N6	8.44	133.18	120.35
85	2	382	A2M	C5-C6-N6	8.37	133.08	120.35
26	S1	668	A2M	C5-C6-N6	8.33	133.01	120.35

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	407	A2M	O4'-C4'-C5'-O5'
1	1	407	A2M	C3'-C4'-C5'-O5'
1	1	678	A2M	O4'-C4'-C5'-O5'
1	1	681	A2M	O4'-C4'-C5'-O5'
1	1	845	OMU	O4'-C1'-N1-C2

There are no ring outliers.

33 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	2	1413	PSU	1	0
85	2	626	PSU	1	0
1	1	1181	PSU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	678	A2M	1	0
1	1	695	OMC	1	0
1	1	422	PSU	1	0
26	S1	29	OMU	1	0
26	S1	1550	OMG	1	0
85	2	527	A2M	1	0
85	2	560	OMU	1	0
85	2	1253	OMG	1	0
26	S1	1539	PSU	1	0
85	2	604	A2M	2	0
85	2	591	A2M	2	0
26	S1	479	A2M	1	0
85	2	570	A2M	1	0
1	1	959[A]	OMG	1	0
1	1	1524	OMG	1	0
85	2	95	A2M	2	0
1	1	677	1MA	1	0
1	1	845	OMU	3	0
1	1	955	A2M	2	0
85	2	382	A2M	1	0
26	S1	2185	MA6	1	0
26	S1	661	OMU	1	0
1	1	235	A2M	1	0
6	7	162	A2M	1	0
26	S1	2021	A2M	1	0
1	1	1527	OMC	1	0
1	1	1010	OMC	1	0
26	S1	1879	OMG	1	0
26	S1	668	A2M	1	0
1	1	847	OMU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 367 ligands modelled in this entry, 367 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
27	S4	1
31	SD	1

All chain breaks are listed below:

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

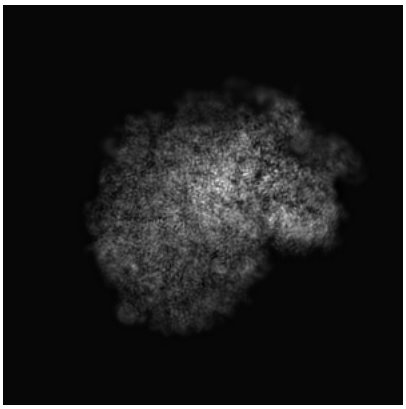
6 Map visualisation

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

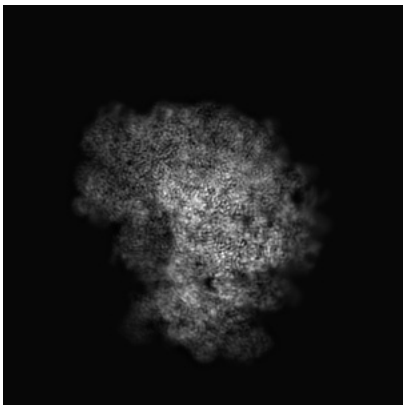
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

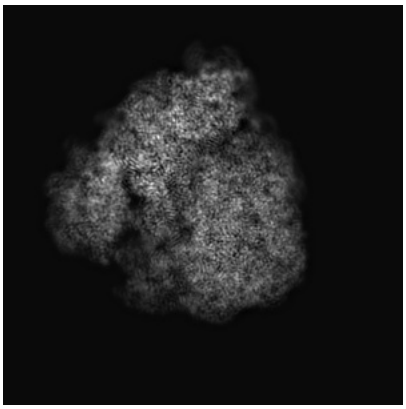
6.1.1 Primary map



X

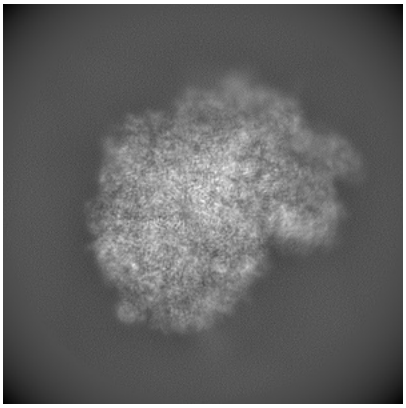


Y

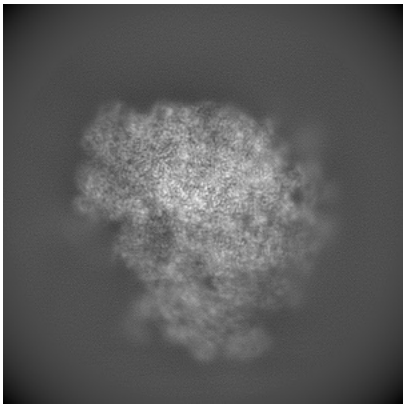


Z

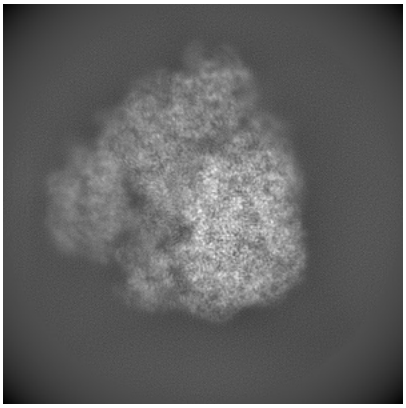
6.1.2 Raw map



X



Y

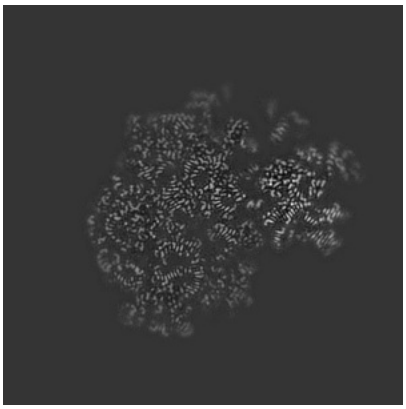


Z

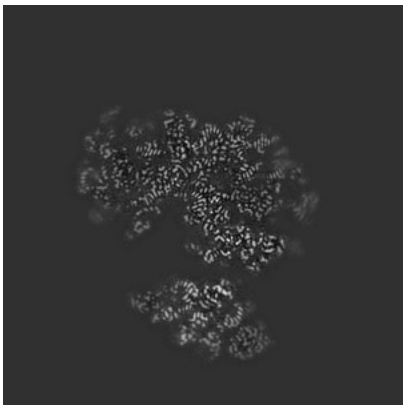
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

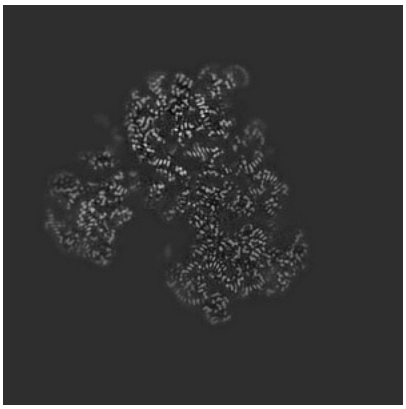
6.2.1 Primary map



X Index: 240

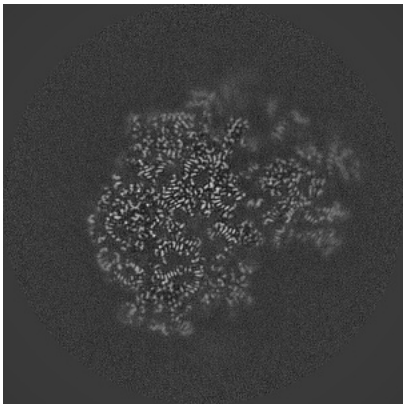


Y Index: 240

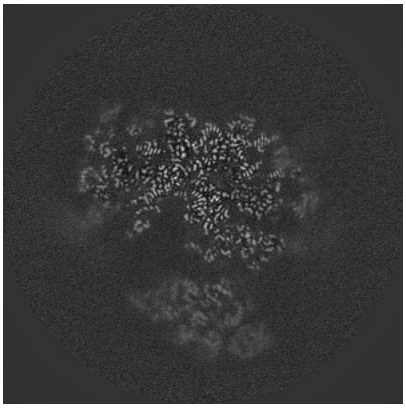


Z Index: 240

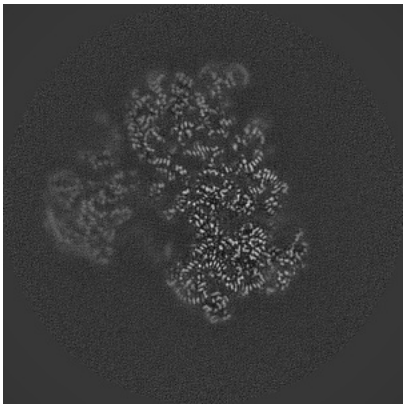
6.2.2 Raw map



X Index: 240



Y Index: 240

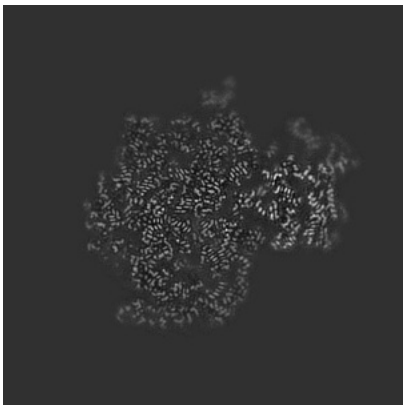


Z Index: 240

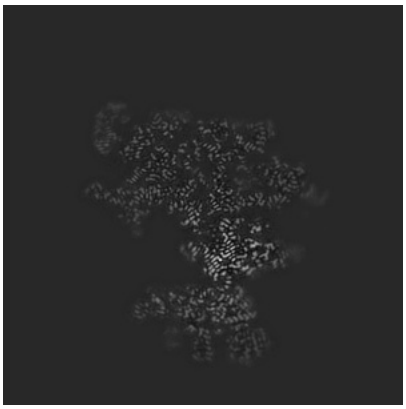
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

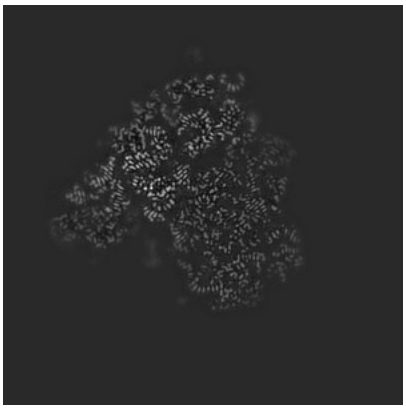
6.3.1 Primary map



X Index: 252

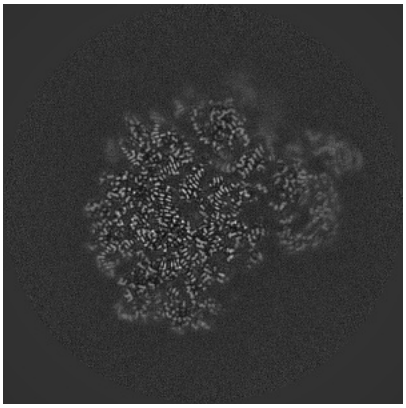


Y Index: 265

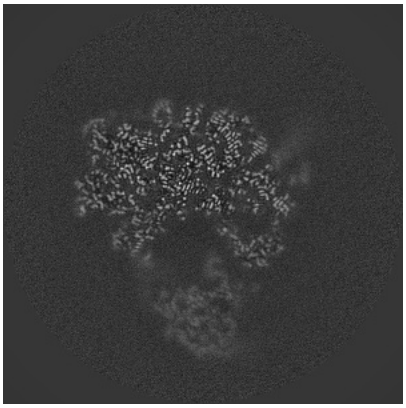


Z Index: 264

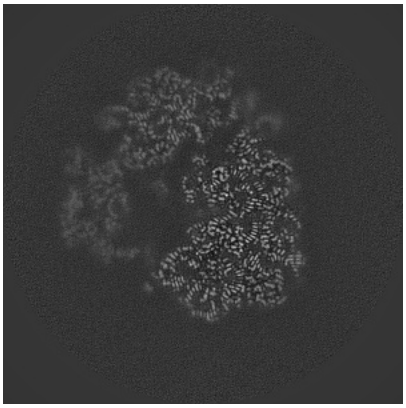
6.3.2 Raw map



X Index: 267



Y Index: 207

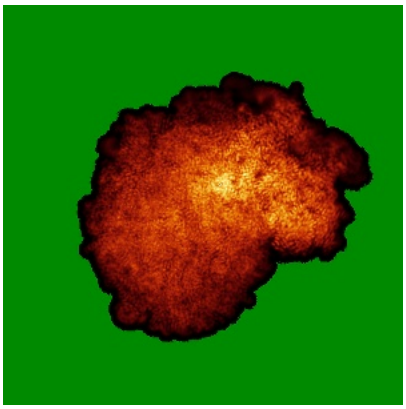


Z Index: 216

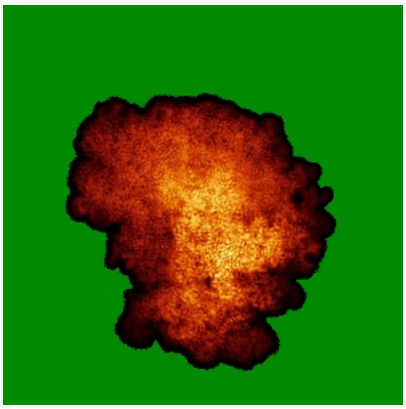
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

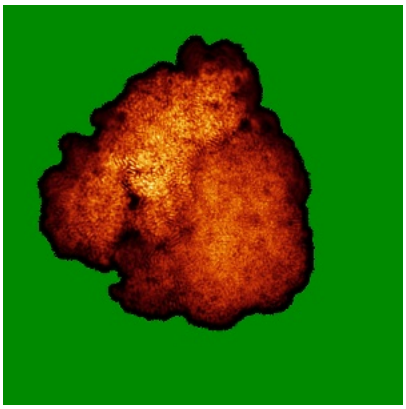
6.4.1 Primary map



X

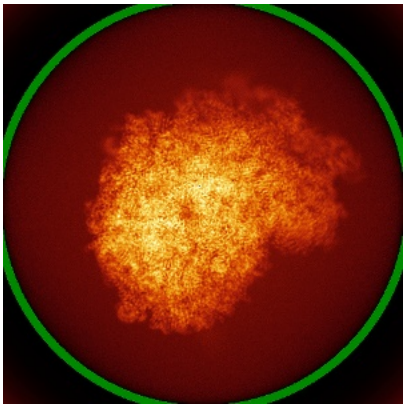


Y

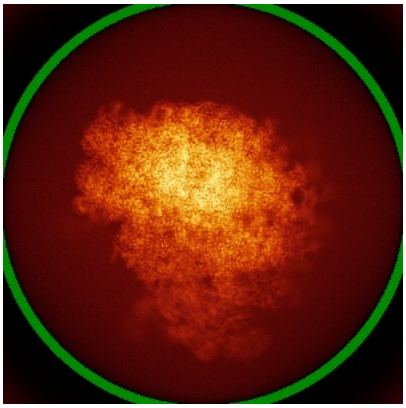


Z

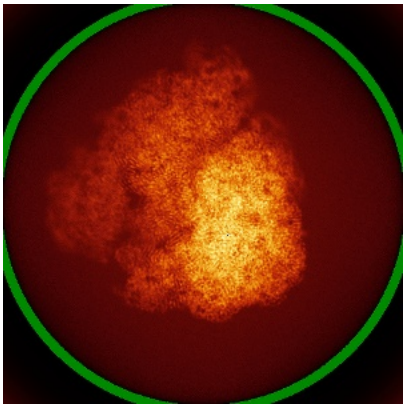
6.4.2 Raw map



X



Y

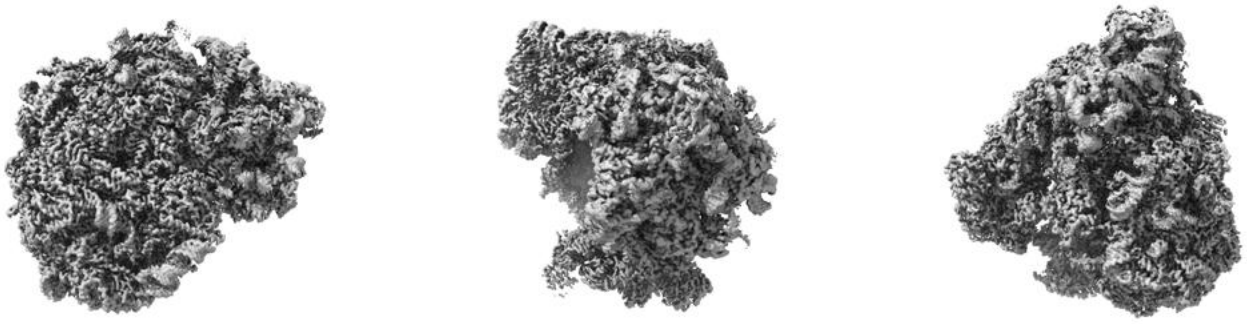


Z

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

6.5 Orthogonal surface views (i)

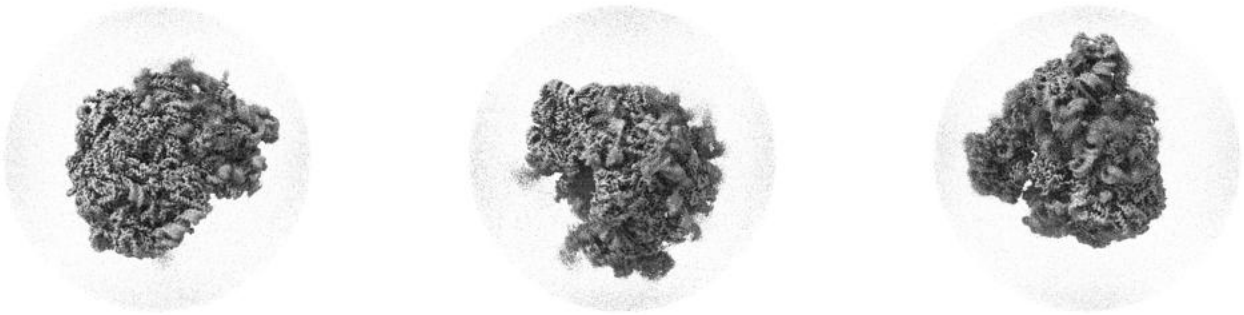
6.5.1 Primary map



X Y Z

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



X Y Z

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

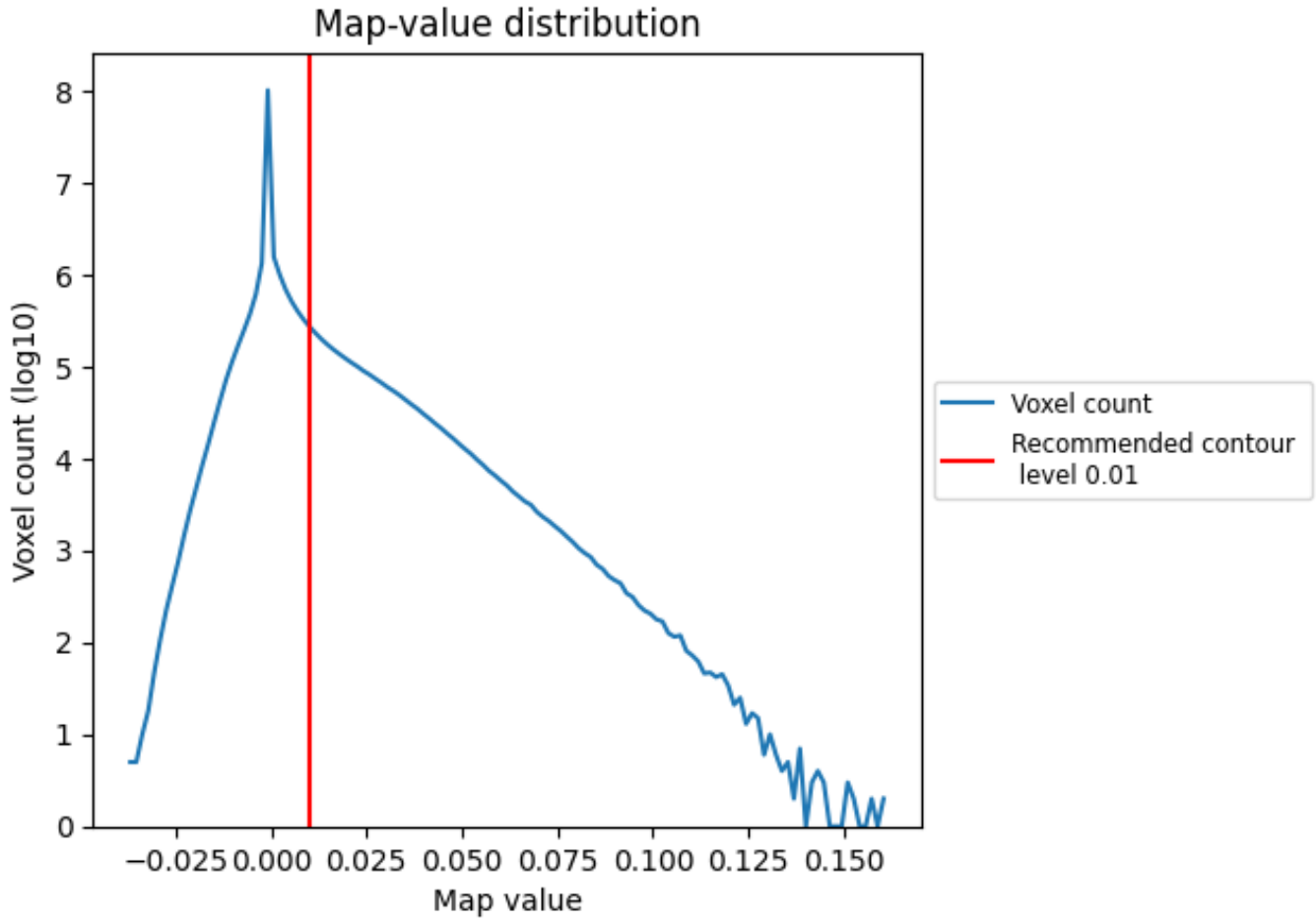
6.6 Mask visualisation (i)

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

7 Map analysis

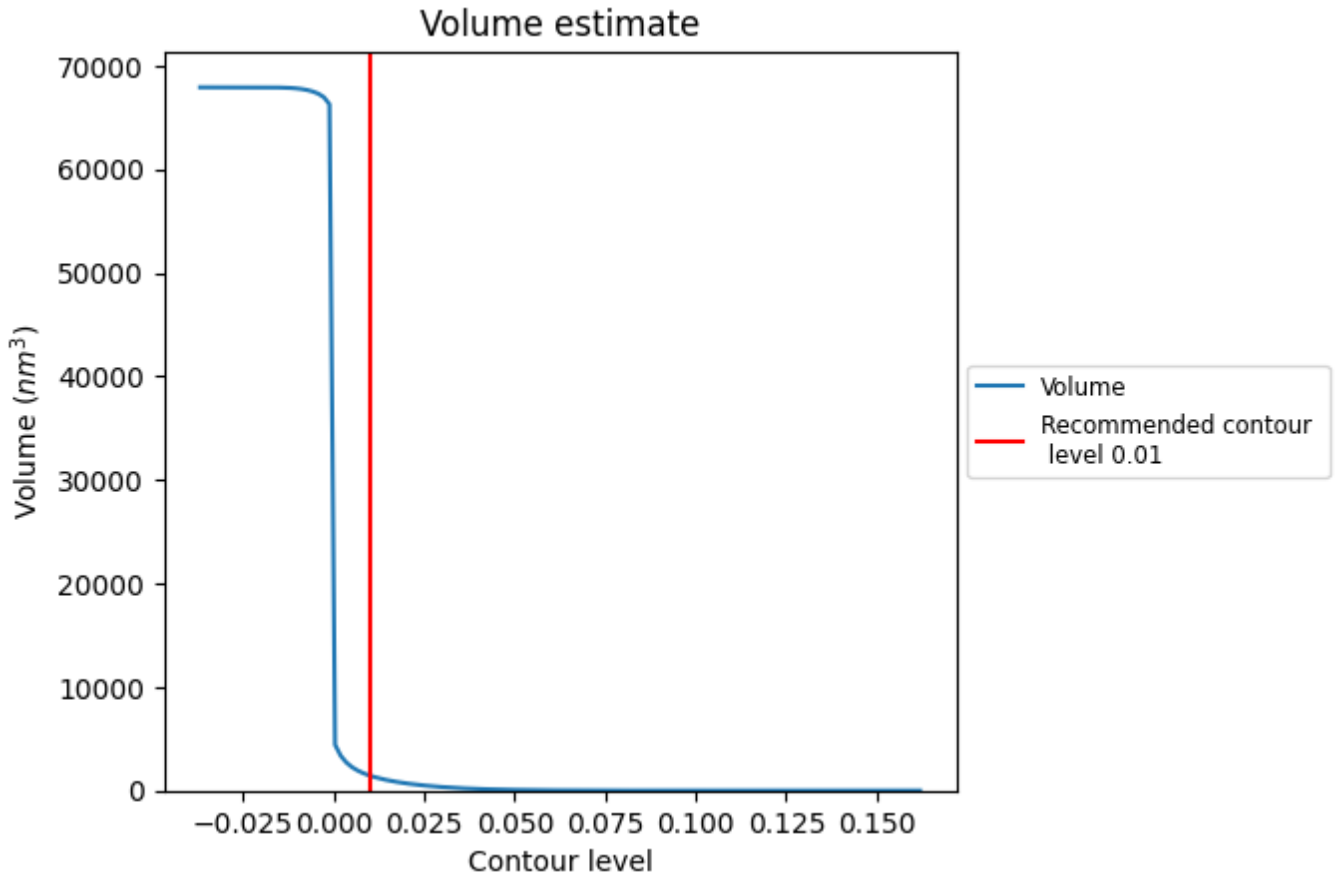
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

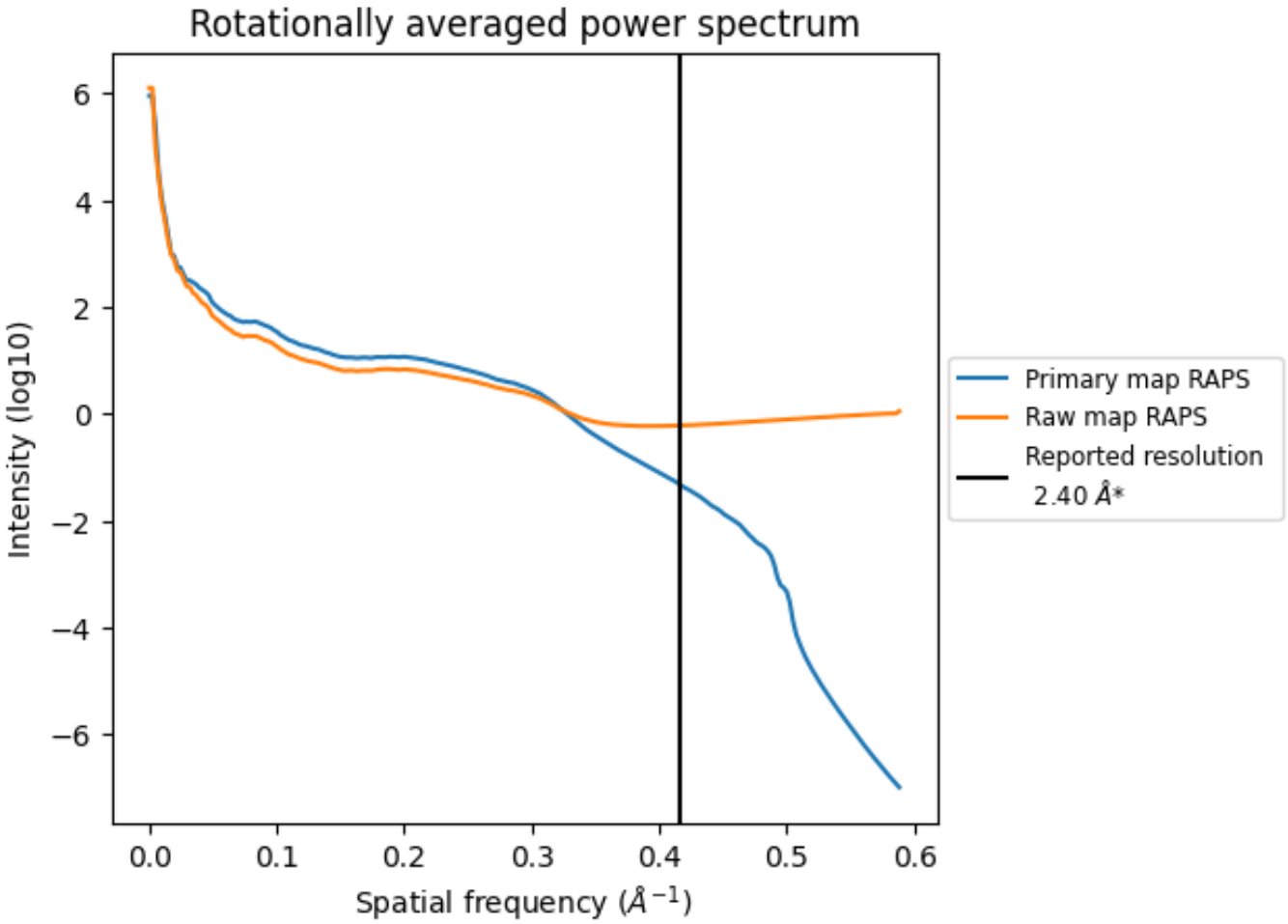
7.2 Volume estimate (i)



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

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

7.3 Rotationally averaged power spectrum (i)

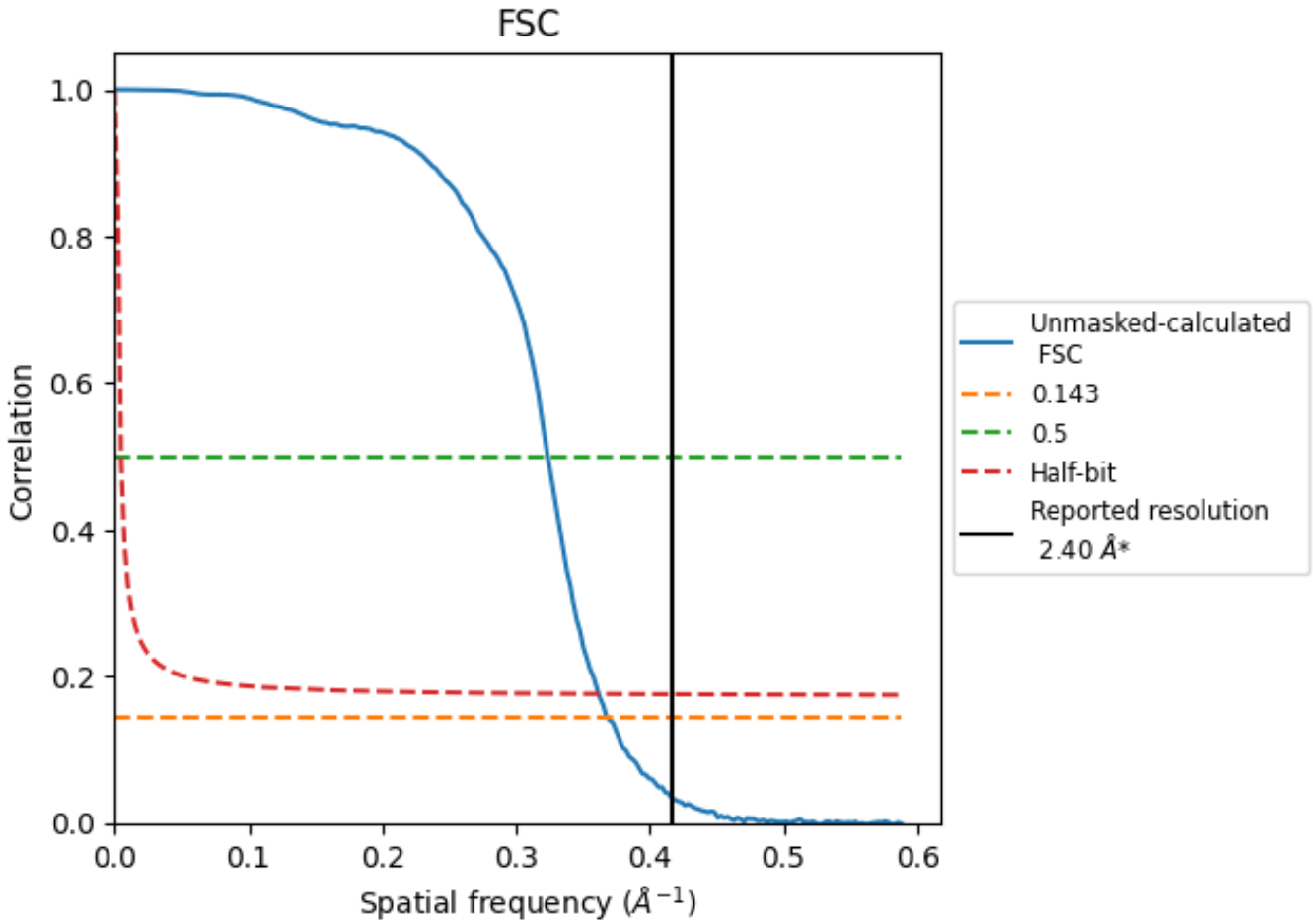


*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8.2 Resolution estimates (i)

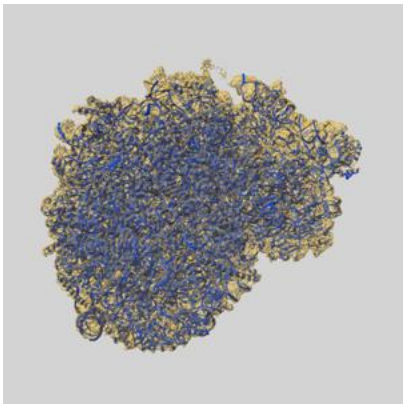
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.71	3.09	2.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.71 differs from the reported value 2.4 by more than 10 %

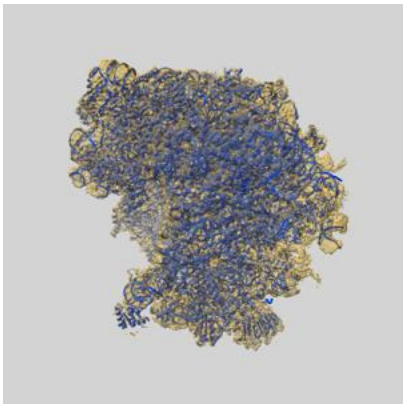
9 Map-model fit

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

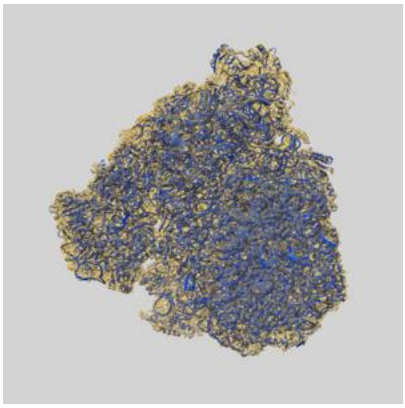
9.1 Map-model overlay



X



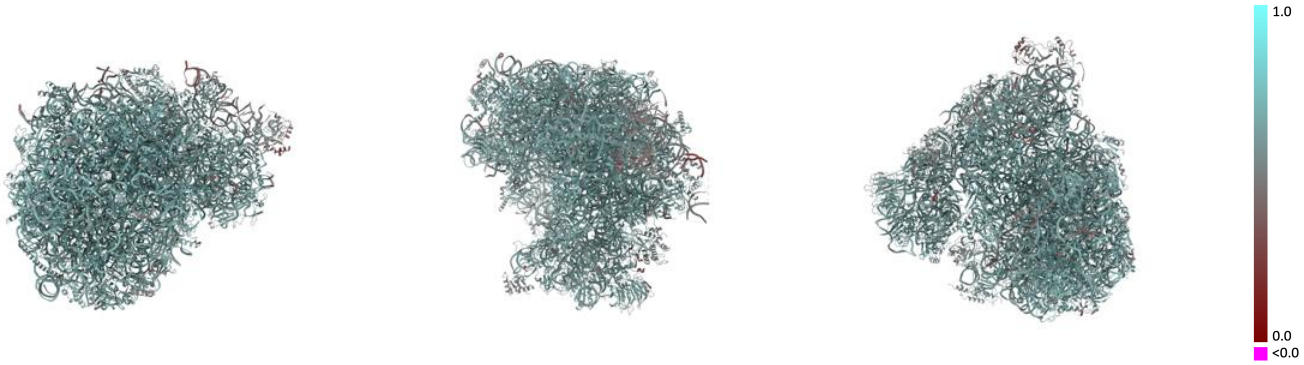
Y



Z

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.

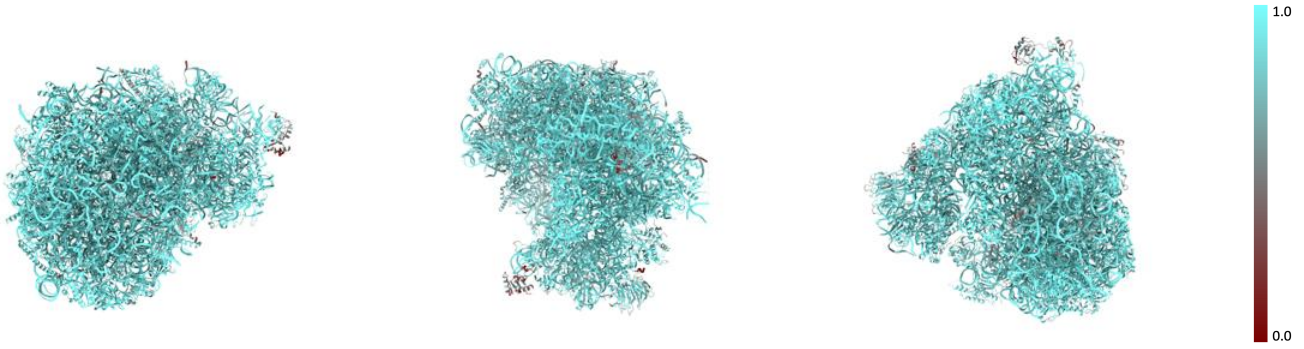
9.2 Q-score mapped to coordinate model



X Y Z

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

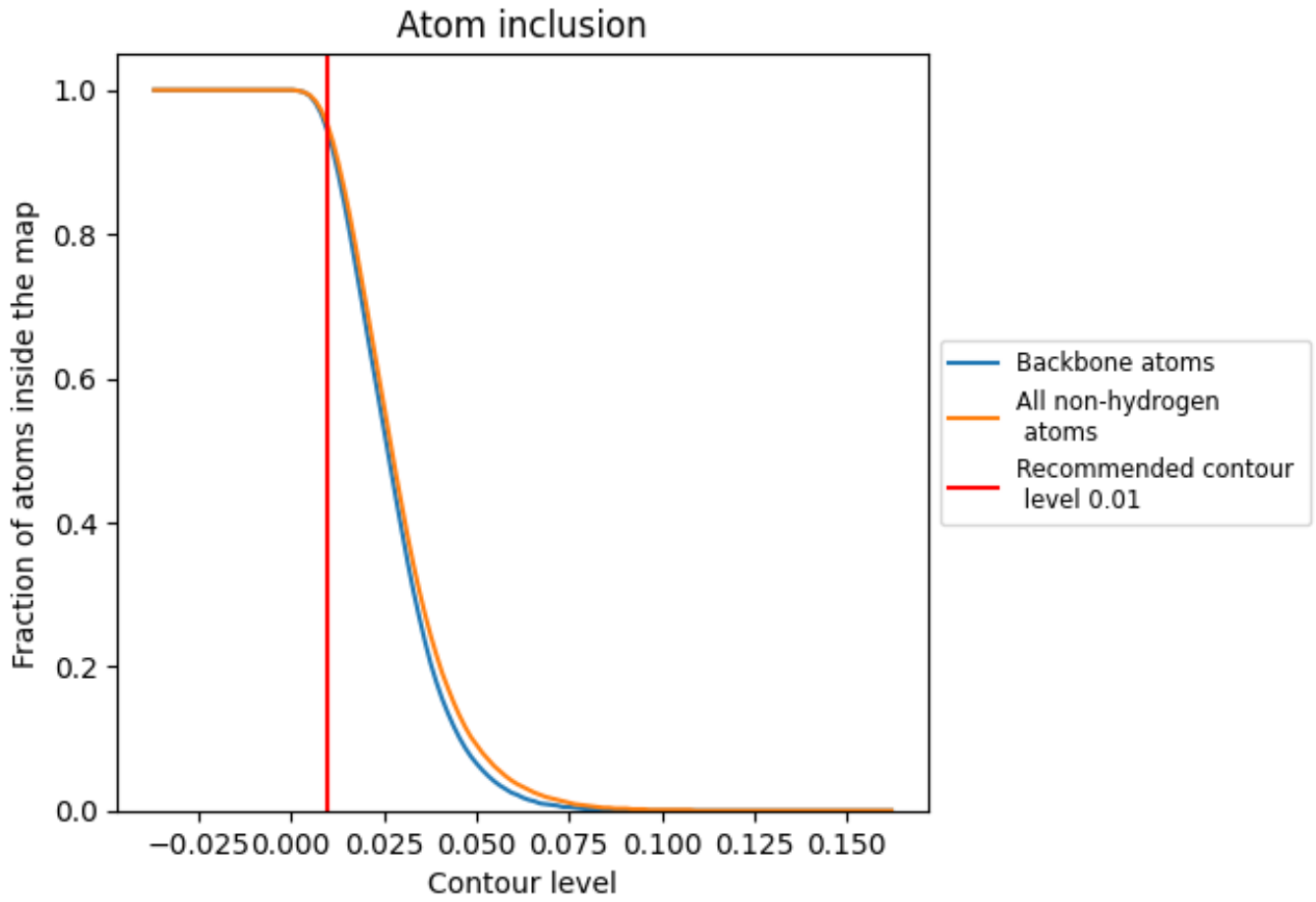
9.3 Atom inclusion mapped to coordinate model



X Y Z

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, 94% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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