



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2022 – 08:54 pm GMT

PDB ID : 6ZJ3
EMDB ID : EMD-11232
Title : Cryo-EM structure of the highly atypical cytoplasmic ribosome of *Euglena gracilis*
Authors : Matzov, D.; Halfon, H.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Gray, M.W.; Yonath, A.E.; Shalev-Benami, M.
Deposited on : 2020-06-27
Resolution : 3.15 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.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

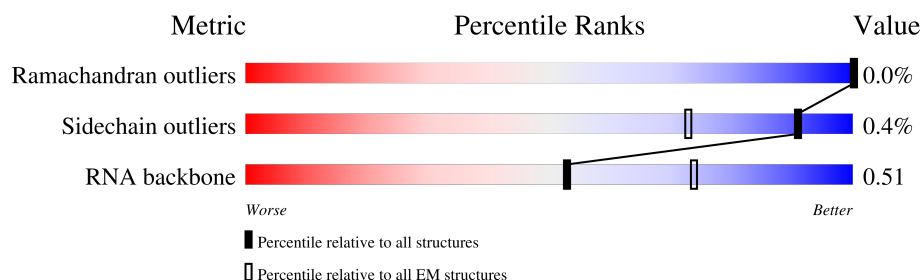
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 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.




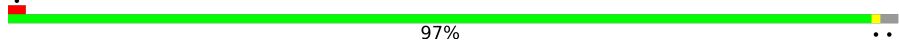


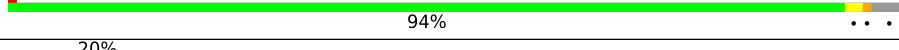
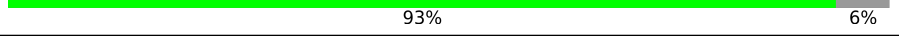
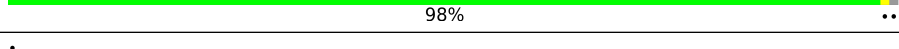
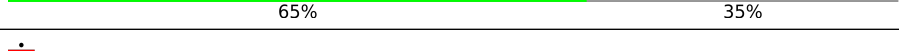
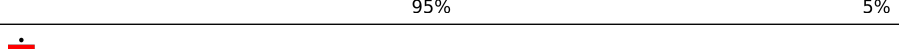
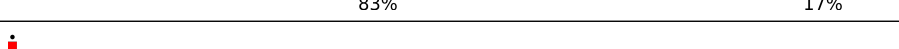
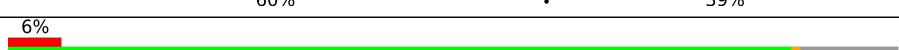

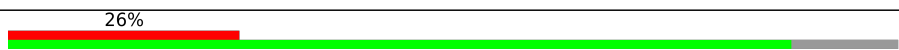
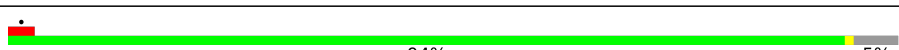
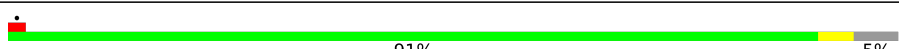

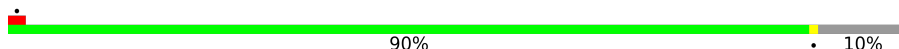


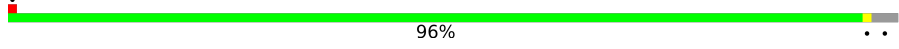
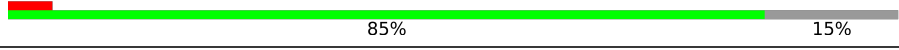
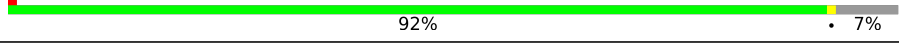



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	S1	2315	<div> <div>10%</div> <div>63%</div> <div>22%</div> <div>•</div> <div>13%</div> </div>
2	S2	76	<div> <div>74%</div> <div>43%</div> <div>53%</div> <div>•</div> </div>
3	S3	76	<div> <div>11%</div> <div>66%</div> <div>33%</div> <div>•</div> </div>
4	S4	76	<div> <div>41%</div> <div>41%</div> <div>55%</div> <div>•</div> </div>
5	S5	12	<div> <div>92%</div> <div>8%</div> </div>
6	SA	249	<div> <div>89%</div> <div>11%</div> </div>
7	SB	261	<div> <div>79%</div> <div>21%</div> </div>
8	SC	220	<div> <div>96%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
9	SD	196	
10	SE	271	
11	SF	257	
12	SG	283	
13	SH	190	
14	SI	200	
15	SJ	130	
16	SK	304	
17	SL	151	
18	SM	121	
19	SN	152	
20	SO	152	
21	SP	143	
22	SQ	139	
23	SR	153	
24	SS	55	
25	ST	151	
26	SU	164	
27	SV	145	
28	SW	150	
29	SX	148	
30	SY	96	
31	SZ	137	
32	Sa	119	
33	Sb	120	

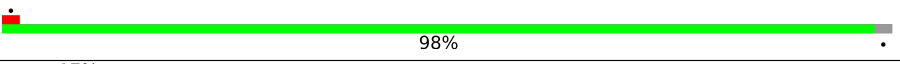
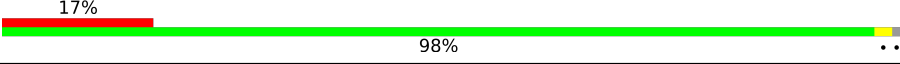

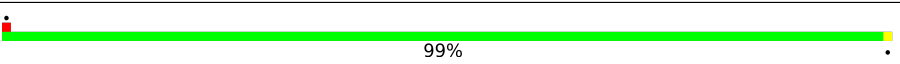
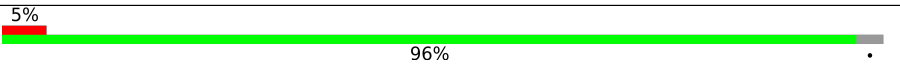
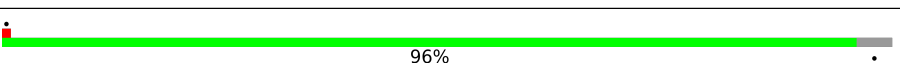
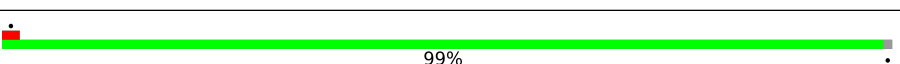
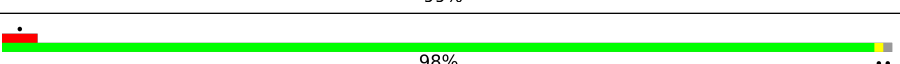
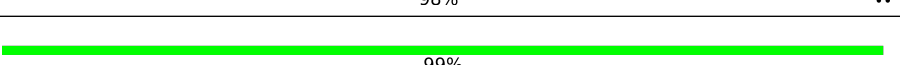
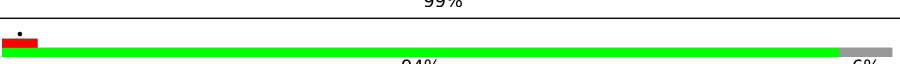
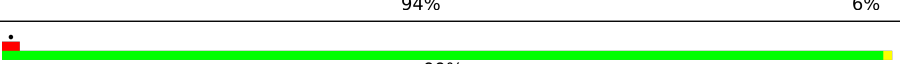
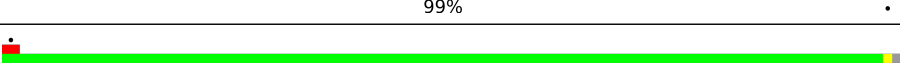
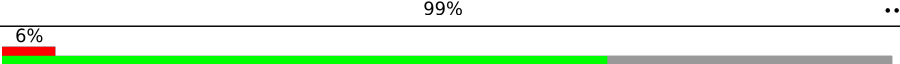
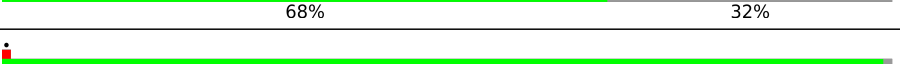
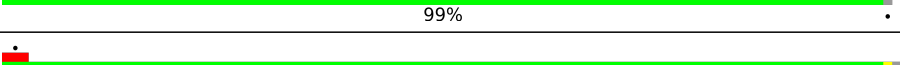
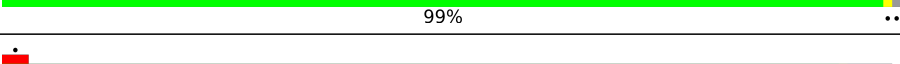
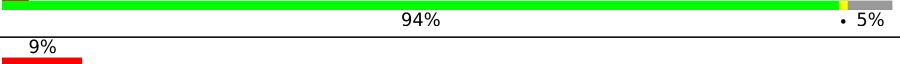
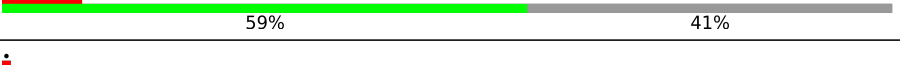



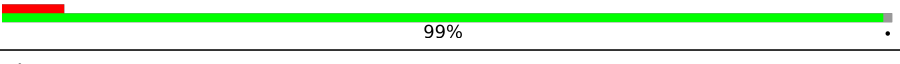

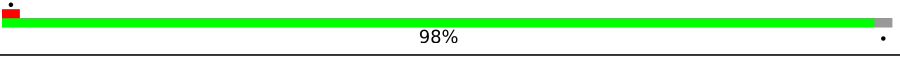

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Mol	Chain	Length	Quality of chain
34	Sc	86	
35	Sd	76	
36	Se	67	
37	Sf	157	
38	Sg	295	
39	Sh	317	
40	LA	163	
41	LB	133	
42	LC	350	
43	LD	116	
44	LE	698	
45	LF	527	
46	LG	234	
47	LH	744	
48	LI	617	
49	LJ	164	
50	LK	64	
51	LL	95	
52	LM	58	
53	LN	86	
54	LO	120	
55	LP	264	
56	LQ	410	
57	LR	375	
58	LS	191	



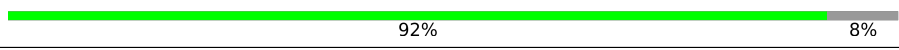
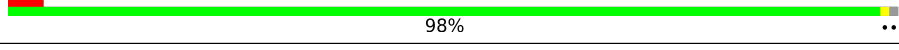

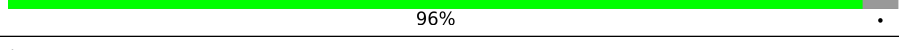
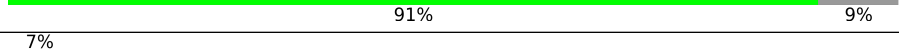
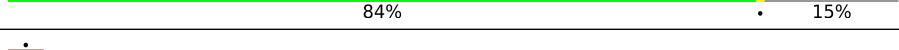
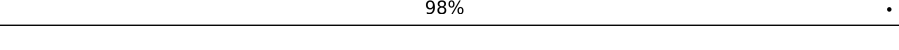
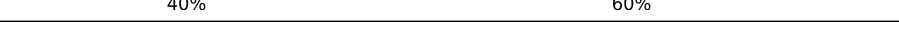
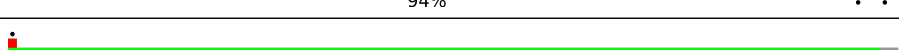
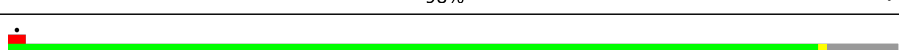


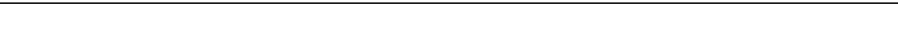
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Mol	Chain	Length	Quality of chain
59	LT	193	
60	LU	195	
61	LV	295	
62	LW	209	
63	LX	226	
64	LY	140	
65	LZ	219	
66	La	152	
67	Lb	204	
68	Lc	215	
69	Ld	260	
70	Le	193	
71	Lf	250	
72	Lg	182	
73	Lh	159	
74	Li	164	
75	Lj	170	
76	Lk	163	
77	Ll	146	
78	Lm	157	
79	Ln	134	
80	Lo	72	
81	Lp	123	
82	Lq	117	
83	Lr	242	

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Mol	Chain	Length	Quality of chain
84	Ls	109	
85	Lt	151	
86	Lu	139	
87	Lv	115	
88	Lw	128	
89	Lx	106	
90	Ly	117	
91	Lz	82	
92	L1	51	
93	L2	126	
94	L3	34	
95	L5	92	
96	L4	106	
97	L6	69	
98	L7	64	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	B8N	S1	1601	X	-	-	-

2 Entry composition

There are 100 unique types of molecules in this entry. The entry contains 223607 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S1	2024	Total	C	N	O	P	0	0
			43278	19338	7765	14151	2024		

- Molecule 2 is a RNA chain called A-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	S2	76	Total	C	N	O	P	S	0	0
			1626	729	290	531	75	1		

- Molecule 3 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S3	76	Total	C	N	O	P	0	0
			1614	721	285	533	75		

- Molecule 4 is a RNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S4	76	Total	C	N	O	P	0	0
			1621	724	292	530	75		

- Molecule 5 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S5	12	Total	C	N	O	P	0	0
			251	113	43	83	12		

- Molecule 6 is a protein called Ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SA	221	Total	C	N	O	S	0	0
			1797	1133	331	323	10		

- Molecule 7 is a protein called Ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SB	207	Total	C	N	O	S	0	0
			1657	1058	295	293	11		

- Molecule 8 is a protein called Ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SC	212	Total	C	N	O	S	0	0
			1675	1061	310	296	8		

- Molecule 9 is a protein called Ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SD	177	Total	C	N	O	S	0	0
			1436	913	277	240	6		

- Molecule 10 is a protein called Ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SE	265	Total	C	N	O	S	0	0
			2125	1366	394	357	8		

- Molecule 11 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SF	221	Total	C	N	O	S	0	0
			1713	1105	301	300	7		

- Molecule 12 is a protein called Ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SG	248	Total	C	N	O	S	0	0
			2016	1263	402	345	6		

- Molecule 13 is a protein called Ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SH	182	Total	C	N	O	S	0	0
			1450	908	271	266	5		

- Molecule 14 is a protein called Ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SI	187	Total	C	N	O	S	0	0
			1514	967	284	262	1		

- Molecule 15 is a protein called Ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SJ	129	Total	C	N	O	S	0	0
			1037	658	194	178	7		

- Molecule 16 is a protein called Ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SK	199	Total	C	N	O	S	0	0
			1644	1038	338	264	4		

- Molecule 17 is a protein called Ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SL	143	Total	C	N	O	S	0	0
			1144	725	220	194	5		

- Molecule 18 is a protein called Ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SM	101	Total	C	N	O	S	0	0
			796	501	150	142	3		

- Molecule 19 is a protein called Ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SN	92	Total	C	N	O	S	0	0
			775	509	130	133	3		

- Molecule 20 is a protein called Ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SO	135	Total	C	N	O	S	0	0
			1010	616	198	189	7		

- Molecule 21 is a protein called Ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SP	141	Total	C	N	O	S	0	0
			1101	692	216	188	5		

- Molecule 22 is a protein called Ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SQ	122	Total	C	N	O	S	0	0
			919	574	164	171	10		

- Molecule 23 is a protein called Ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SR	146	Total	C	N	O	S	0	0
			1181	737	234	204	6		

- Molecule 24 is a protein called Ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SS	52	Total	C	N	O	S	0	0
			433	267	95	68	3		

- Molecule 25 is a protein called Ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	ST	148	Total	C	N	O	S	0	0
			1180	746	228	202	4		

- Molecule 26 is a protein called Ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SU	148	Total	C	N	O	S	0	0
			1225	793	230	199	3		

- Molecule 27 is a protein called Ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SV	125	Total	C	N	O	S	0	0
			998	625	183	183	7		

- Molecule 28 is a protein called Ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SW	125	Total	C	N	O	S	0	0
			990	632	186	167	5		

- Molecule 29 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SX	143	Total	C	N	O	S	0	0
			1125	720	205	195	5		

- Molecule 30 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SY	82	Total	C	N	O	S	0	0
			624	391	111	119	3		

- Molecule 31 is a protein called Ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SZ	127	Total	C	N	O	S	0	0
			1052	668	205	174	5		

- Molecule 32 is a protein called Ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sa	78	Total	C	N	O	S	0	0
			633	405	118	108	2		

- Molecule 33 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sb	97	Total	C	N	O	S	0	0
			780	481	162	129	8		

- Molecule 34 is a protein called Ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sc	84	Total	C	N	O	S	0	0
			649	414	115	114	6		

- Molecule 35 is a protein called Ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sd	63	Total	C	N	O	S	0	0
			499	304	103	90	2		

- Molecule 36 is a protein called Ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Se	64	Total	C	N	O		0	0
			484	305	101	78			

- Molecule 37 is a protein called Ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Sf	64	Total	C	N	O	S	0	0
			508	322	95	85	6		

- Molecule 38 is a protein called Ribosomal protein eSEug1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Sg	199	Total	C	N	O	S	0	0
			1597	1022	301	267	7		

- Molecule 39 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Sh	311	Total	C	N	O	S	0	0
			2393	1516	407	454	16		

- Molecule 40 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LA	160	Total	C	N	O	P	0	0
			3423	1528	613	1122	160		

- Molecule 41 is a RNA chain called LSU rRNA chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LB	133	Total	C	N	O	P	0	0
			2847	1275	523	916	133		

- Molecule 42 is a RNA chain called LSU rRNA chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LC	350	Total	C	N	O	P	0	0
			7516	3355	1368	2443	350		

- Molecule 43 is a RNA chain called LSU rRNA chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LD	110	Total	C	N	O	P	0	0
			2342	1043	418	771	110		

- Molecule 44 is a RNA chain called LSU rRNA chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LE	652	Total	C	N	O	P	0	0
			13955	6233	2494	4576	652		

- Molecule 45 is a RNA chain called LSU rRNA chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LF	456	Total	C	N	O	P	0	0
			9702	4340	1740	3166	456		

- Molecule 46 is a RNA chain called LSU rRNA chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LG	207	Total	C	N	O	P	0	0
			4422	1975	789	1451	207		

- Molecule 47 is a RNA chain called LSU rRNA chain 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LH	559	Total	C	N	O	P	0	0
			11980	5366	2143	3912	559		

- Molecule 48 is a RNA chain called LSU rRNA chain 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LI	573	Total	C	N	O	P	0	0
			12233	5480	2170	4010	573		

- Molecule 49 is a RNA chain called LSU rRNA chain 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LJ	163	Total	C	N	O	P	0	0
			3486	1558	630	1135	163		

- Molecule 50 is a RNA chain called LSU rRNA chain 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LK	61	Total	C	N	O	P	0	0
			1301	581	237	422	61		

- Molecule 51 is a RNA chain called LSU rRNA chain 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LL	92	Total	C	N	O	P	0	0
			1983	882	366	643	92		

- Molecule 52 is a RNA chain called LSU rRNA chain 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LM	54	Total	C	N	O	P	0	0
			1158	517	214	373	54		

- Molecule 53 is a RNA chain called LSU rRNA chain 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LN	79	Total	C	N	O	P	0	0
			1696	753	307	557	79		

- Molecule 54 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LO	120	Total	C	N	O	P	0	0
			2559	1142	457	840	120		

- Molecule 55 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LP	249	Total	C	N	O	S	0	0
			1901	1193	380	317	11		

- Molecule 56 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LQ	392	Total	C	N	O	S	1	0
			3118	1987	592	521	18		

- Molecule 57 is a protein called Ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LR	365	Total	C	N	O	S	0	0
			2868	1807	572	482	7		

- Molecule 58 is a protein called Ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LS	178	Total	C	N	O	S	0	0
			1437	912	273	248	4		

- Molecule 59 is a protein called Ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LT	190	Total	C	N	O	S	0	0
			1521	959	283	269	10		

- Molecule 60 is a protein called Ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LU	194	Total	C	N	O	S	0	0
			1580	1010	297	269	4		

- Molecule 61 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LV	238	Total	C	N	O	S	0	0
			1926	1236	365	321	4		

- Molecule 62 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LW	208	Total	C	N	O	S	0	0
			1713	1086	346	270	11		

- Molecule 63 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LX	219	Total	C	N	O	S	0	0
			1769	1115	357	292	5		

- Molecule 64 is a protein called Ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LY	134	Total	C	N	O	S	0	0
			1001	634	187	173	7		

- Molecule 65 is a protein called Ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	LZ	217	Total	C	N	O	S	0	0
			1780	1126	357	293	4		

- Molecule 66 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	La	151	Total	C	N	O	S	0	0
			1210	759	254	193	4		

- Molecule 67 is a protein called Ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Lb	203	Total	C	N	O	S	0	0
			1711	1080	363	259	9		

- Molecule 68 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Lc	203	Total	C	N	O	S	0	0
			1643	1036	328	267	12		

- Molecule 69 is a protein called Ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ld	260	Total	C	N	O	S	0	0
			2074	1313	384	367	10		

- Molecule 70 is a protein called Ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Le	192	Total	C	N	O	S	0	0
			1526	963	313	241	9		

- Molecule 71 is a protein called Ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Lf	170	Total	C	N	O	S	0	0
			1392	874	291	219	8		

- Molecule 72 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Lg	181	Total	C	N	O	S	0	0
			1494	961	278	246	9		

- Molecule 73 is a protein called Ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Lh	158	Total	C	N	O	S	0	0
			1279	814	254	209	2		

- Molecule 74 is a protein called Ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Li	155	Total	C	N	O	S	0	0
			1255	785	250	213	7		

- Molecule 75 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Lj	101	Total	C	N	O	S	0	0
			827	540	140	146	1		

- Molecule 76 is a protein called Ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lk	131	Total	C	N	O	S	0	0
			1073	684	204	182	3		

- Molecule 77 is a protein called Ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ll	124	Total	C	N	O	S	0	0
			1008	629	206	171	2		

- Molecule 78 is a protein called Ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Lm	66	Total	C	N	O	S	0	0
			549	355	108	84	2		

- Molecule 79 is a protein called Ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ln	133	Total	C	N	O	S	0	0
			1084	695	213	172	4		

- Molecule 80 is a protein called Ribosomal protein eLEgr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Lo	58	Total	C	N	O	S	0	0
			459	291	86	80	2		

- Molecule 81 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Lp	121	Total	C	N	O	S	0	0
			1010	645	198	164	3		

- Molecule 82 is a protein called Ribosomal protein eL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	Lq	91	Total	C	N	O	0	0
			767	478	164	125		

- Molecule 83 is a protein called Ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Lr	218	Total	C	N	O	S	0	0
			1825	1184	346	285	10		

- Molecule 84 is a protein called Ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Ls	97	Total	C	N	O	S	0	0
			747	466	132	143	6		

- Molecule 85 is a protein called Ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Lt	111	Total	C	N	O	S	0	0
			923	589	182	150	2		

- Molecule 86 is a protein called Ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Lu	128	Total	C	N	O	S	0	0
			1068	680	219	167	2		

- Molecule 87 is a protein called Ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Lv	114	Total	C	N	O	S	0	0
			915	589	182	140	4		

- Molecule 88 is a protein called Ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Lw	114	Total	C	N	O	S	0	0
			922	577	197	147	1		

- Molecule 89 is a protein called Ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Lx	102	Total	C	N	O	S	0	0
			835	527	177	127	4		

- Molecule 90 is a protein called Ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	Ly	106	Total	C	N	O	S	0	0
			859	525	189	137	8		

- Molecule 91 is a protein called Ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	Lz	70	Total	C	N	O	S	0	0
			570	367	103	98	2		

- Molecule 92 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	L1	50	Total	C	N	O	S	0	0
			447	287	93	65	2		

- Molecule 93 is a protein called Ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	L2	51	Total	C	N	O	S	0	0
			415	255	83	67	10		

- Molecule 94 is a protein called Ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	L3	33	Total	C	N	O	S	0	0
			302	180	81	38	3		

- Molecule 95 is a protein called Ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
95	L5	90	Total	C	N	O	S	0	0
			719	449	147	117	6		

- Molecule 96 is a protein called Ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	L4	97	Total	C	N	O	S	0	0
			785	501	152	126	6		

- Molecule 97 is a protein called Ribosomal protein eLEgr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	L6	59	Total	C	N	O	S	0	0
			493	308	99	85	1		

- Molecule 98 is a protein called Ribosomal protein eLEgr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
98	L7	54	Total	C	N	O	S	0	0
			455	288	85	81	1		

- Molecule 99 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
99	Sb	1	Total	Zn	0
			1	1	
99	Ly	1	Total	Zn	0
			1	1	
99	L2	1	Total	Zn	0
			1	1	
99	L5	1	Total	Zn	0
			1	1	
99	L4	1	Total	Zn	0
			1	1	

- Molecule 100 is water.

Mol	Chain	Residues	Atoms		AltConf
100	S1	393	Total	O	0
			393	393	
100	S2	3	Total	O	0
			3	3	
100	S3	17	Total	O	0
			17	17	
100	S4	2	Total	O	0
			2	2	
100	S5	11	Total	O	0
			11	11	
100	SB	1	Total	O	0
			1	1	
100	SC	3	Total	O	0
			3	3	
100	SF	4	Total	O	0
			4	4	
100	SG	3	Total	O	0
			3	3	
100	SH	2	Total	O	0
			2	2	
100	SK	5	Total	O	0
			5	5	
100	SL	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
100	SM	1	Total 1	O 1	0
100	SO	1	Total 1	O 1	0
100	SP	4	Total 4	O 4	0
100	SR	1	Total 1	O 1	0
100	SS	2	Total 2	O 2	0
100	SU	1	Total 1	O 1	0
100	SX	2	Total 2	O 2	0
100	SZ	2	Total 2	O 2	0
100	Sb	1	Total 1	O 1	0
100	Sh	1	Total 1	O 1	0
100	LA	29	Total 29	O 29	0
100	LB	15	Total 15	O 15	0
100	LC	32	Total 32	O 32	0
100	LD	9	Total 9	O 9	0
100	LE	97	Total 97	O 97	0
100	LF	93	Total 93	O 93	0
100	LG	33	Total 33	O 33	0
100	LH	174	Total 174	O 174	0
100	LI	82	Total 82	O 82	0
100	LJ	46	Total 46	O 46	0
100	LK	3	Total 3	O 3	0

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Mol	Chain	Residues	Atoms		AltConf
100	LL	5	Total 5	O 5	0
100	LM	11	Total 11	O 11	0
100	LN	12	Total 12	O 12	0
100	LO	15	Total 15	O 15	0
100	LP	2	Total 2	O 2	0
100	LQ	8	Total 8	O 8	0
100	LR	8	Total 8	O 8	0
100	LU	2	Total 2	O 2	0
100	LW	7	Total 7	O 7	0
100	LY	3	Total 3	O 3	0
100	La	2	Total 2	O 2	0
100	Lb	2	Total 2	O 2	0
100	Lc	2	Total 2	O 2	0
100	Ld	1	Total 1	O 1	0
100	Lf	1	Total 1	O 1	0
100	Li	2	Total 2	O 2	0
100	Lk	1	Total 1	O 1	0
100	Ll	1	Total 1	O 1	0
100	Lm	3	Total 3	O 3	0
100	Lp	1	Total 1	O 1	0
100	Lq	3	Total 3	O 3	0

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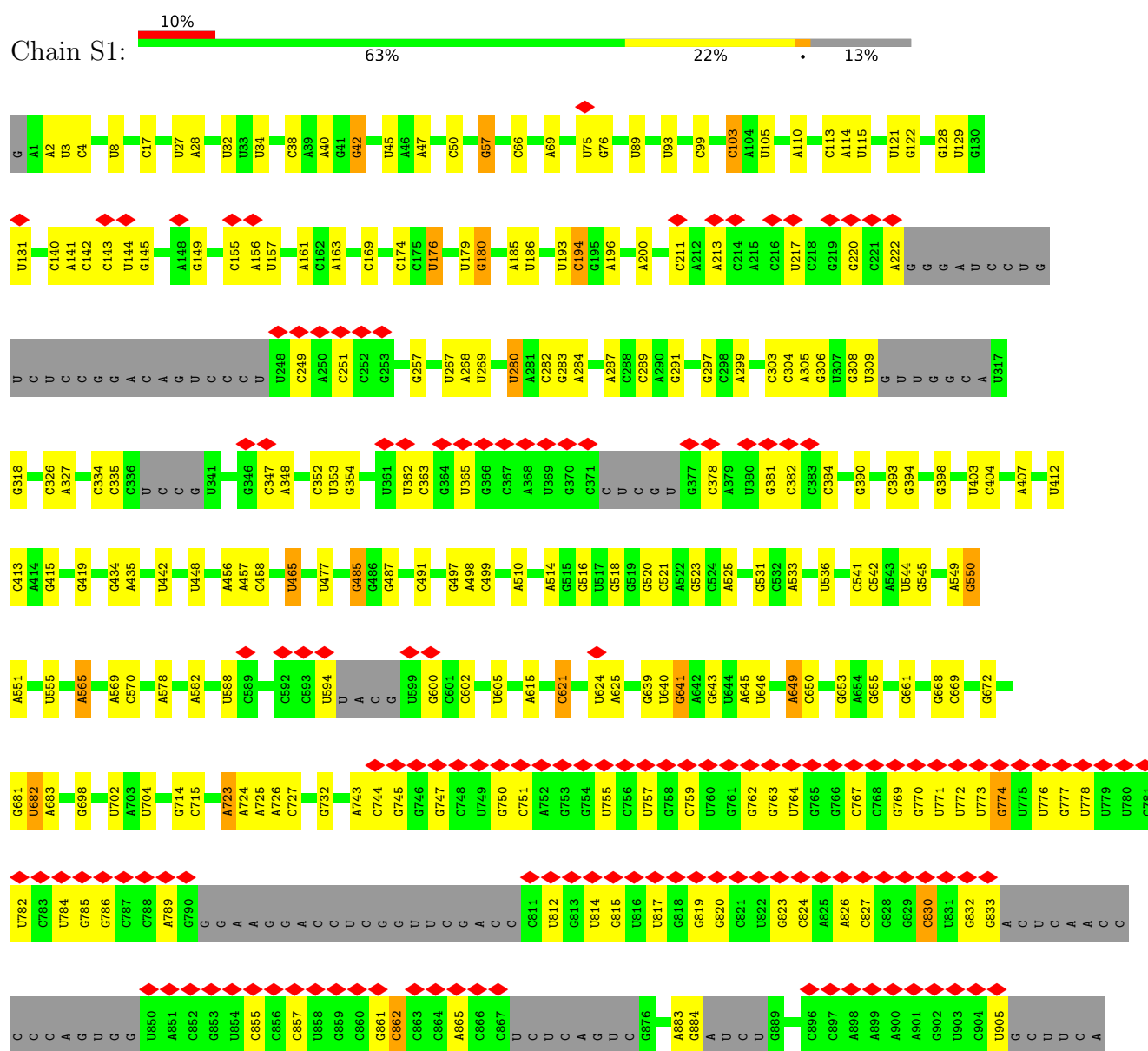
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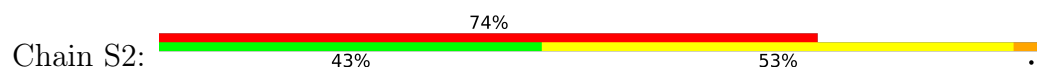
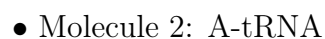
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100	Ls	1	Total 1	O 1	0
100	Lt	4	Total 4	O 4	0
100	Lu	1	Total 1	O 1	0
100	Lw	2	Total 2	O 2	0
100	Ly	2	Total 2	O 2	0
100	L2	3	Total 3	O 3	0
100	L3	10	Total 10	O 10	0
100	L5	2	Total 2	O 2	0
100	L4	1	Total 1	O 1	0
100	L7	1	Total 1	O 1	0

3 Residue-property plots

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

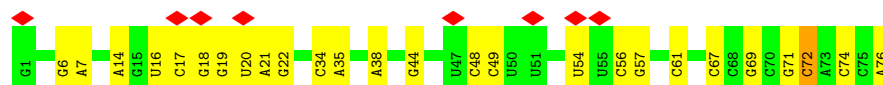
• Molecule 1: 18S rRNA



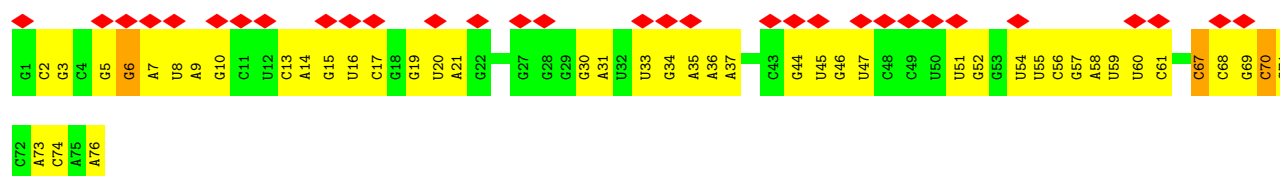




• Molecule 3: P-tRNA



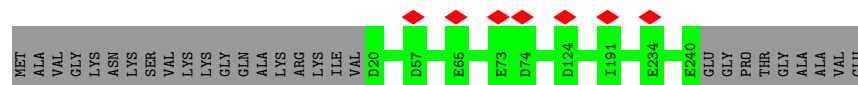
• Molecule 4: E-tRNA



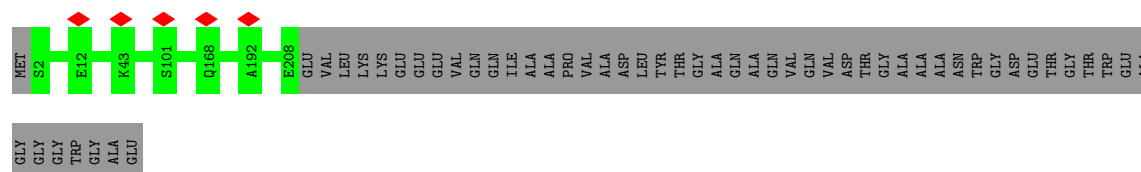
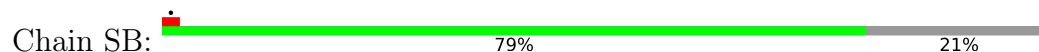
• Molecule 5: A-site tRNA



• Molecule 6: Ribosomal protein eS1



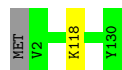
• Molecule 7: Ribosomal protein uS2



• Molecule 8: Ribosomal protein uS3

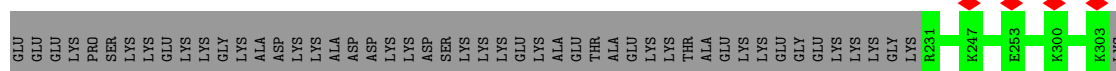
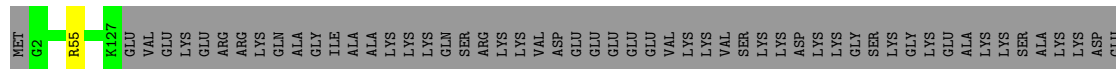
- Molecule 15: Ribosomal protein uS8

Chain SJ:  98%



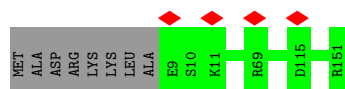
- Molecule 16: Ribosomal protein eS8

Chain SK:  65% 35%




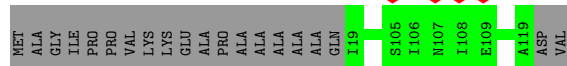
- Molecule 17: Ribosomal protein uS9

Chain SL: 95% 5%



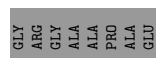
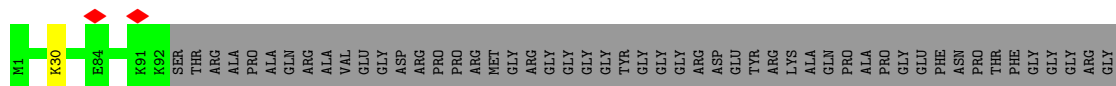
- Molecule 18: Ribosomal protein uS10

Chain SM:  83% 17%

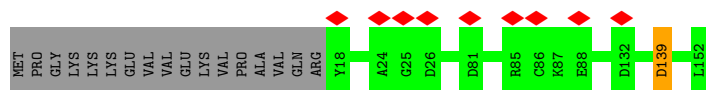


- Molecule 19: Ribosomal protein eS10

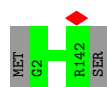
Chain SN: 



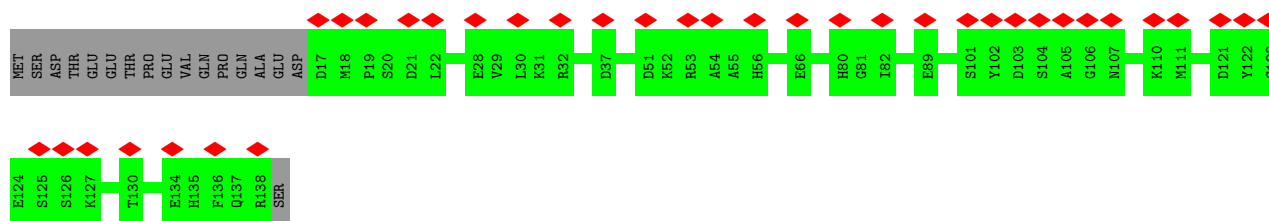
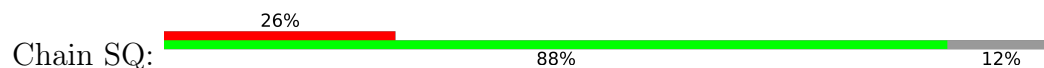
- Molecule 20: Ribosomal protein uS11



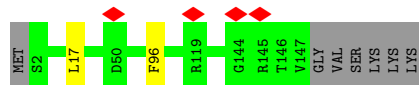
- Molecule 21: Ribosomal protein uS12



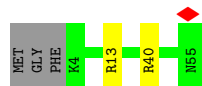
- Molecule 22: Ribosomal protein eS12



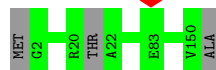
- Molecule 23: Ribosomal protein uS13



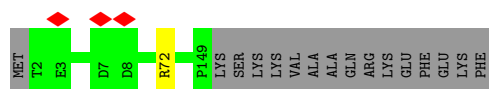
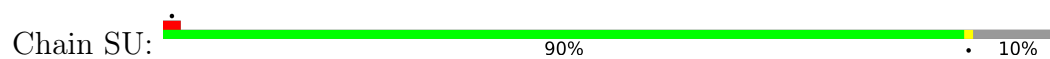
- Molecule 24: Ribosomal protein uS14



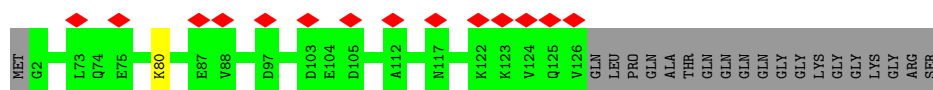
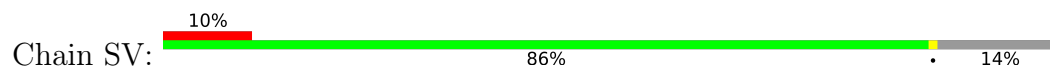
- Molecule 25: Ribosomal protein uS15



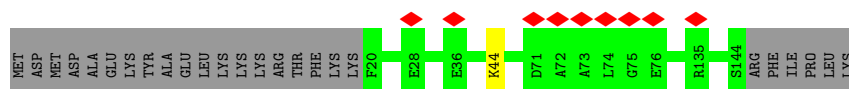
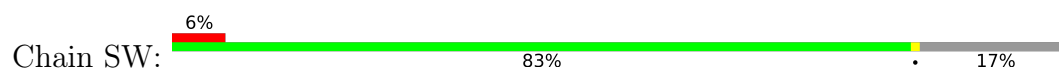
- Molecule 26: Ribosomal protein uS17



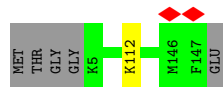
- Molecule 27: Ribosomal protein eS17



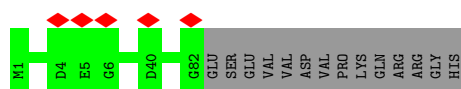
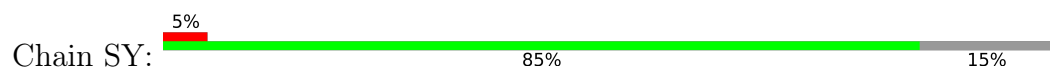
- Molecule 28: Ribosomal protein uS19



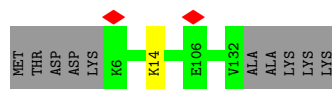
- Molecule 29: Ribosomal protein eS19



- Molecule 30: Ribosomal protein eS21



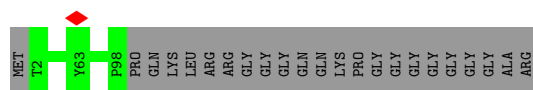
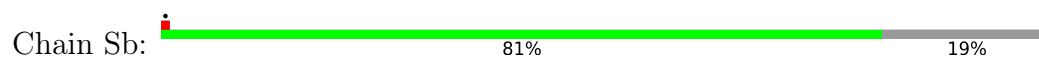
- Molecule 31: Ribosomal protein eS24



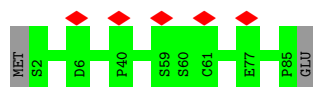
- Molecule 32: Ribosomal protein eS25



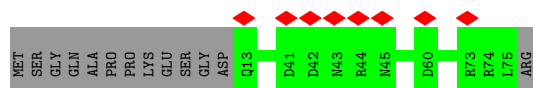
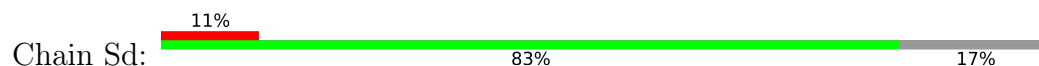
• Molecule 33: Ribosomal protein eS26



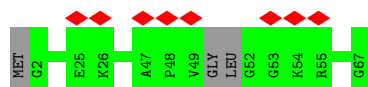
• Molecule 34: Ribosomal protein eS27



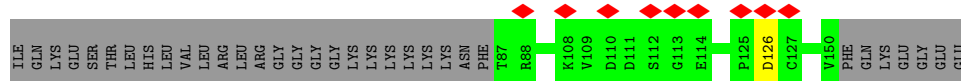
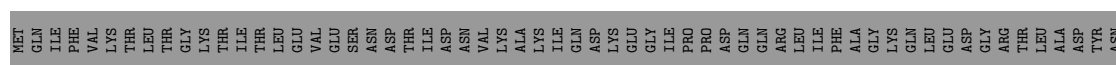
• Molecule 35: Ribosomal protein eS28



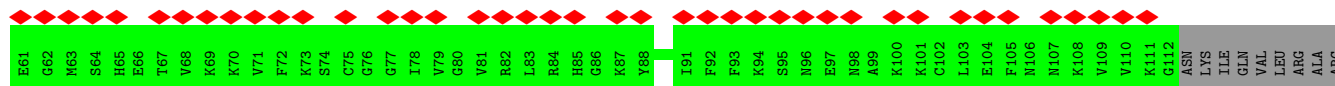
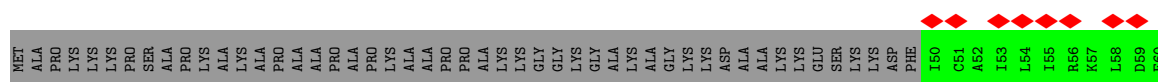
• Molecule 36: Ribosomal protein eS30

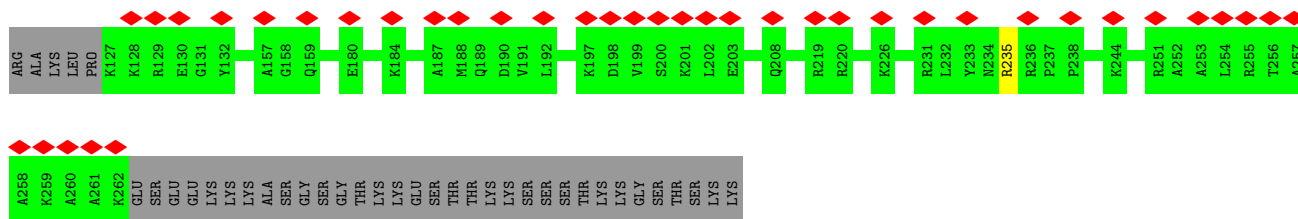


• Molecule 37: Ribosomal protein eS31

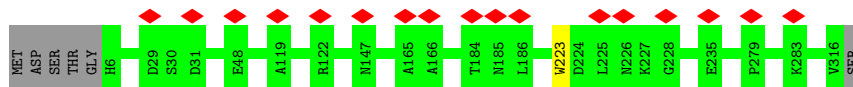


• Molecule 38: Ribosomal protein eSEug1

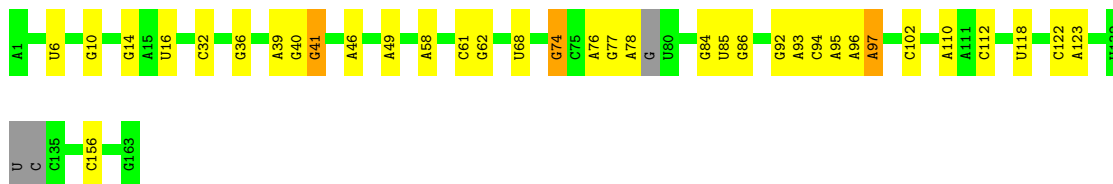
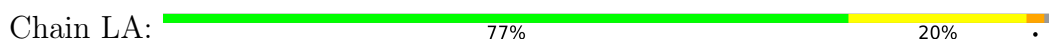




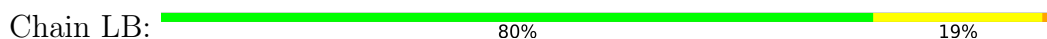
• Molecule 39: RACK1



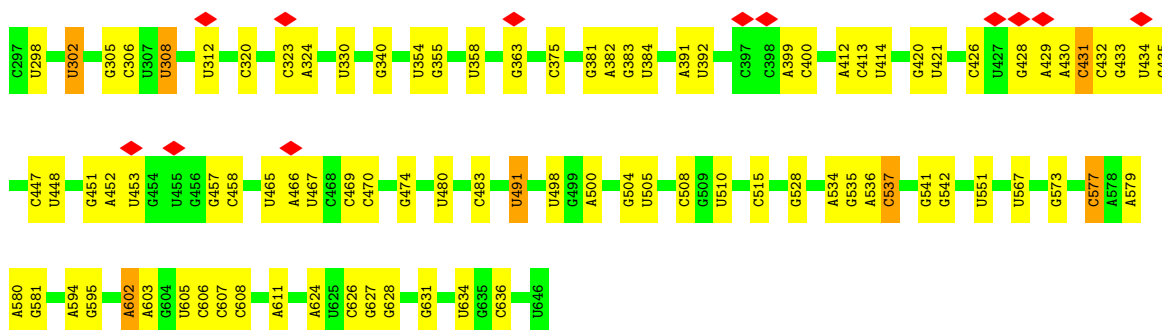
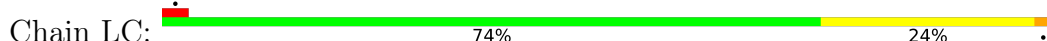
• Molecule 40: 5.8S rRNA



• Molecule 41: LSU rRNA chain 1



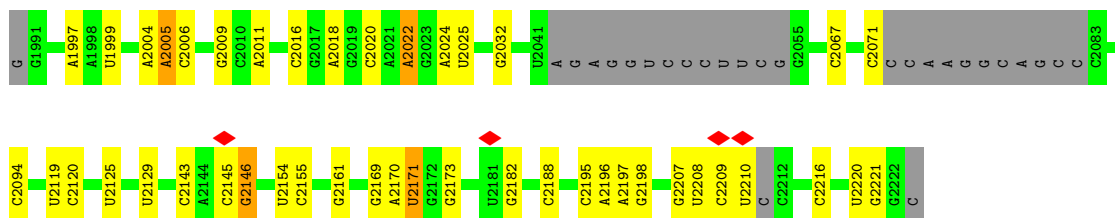
• Molecule 42: LSU rRNA chain 2



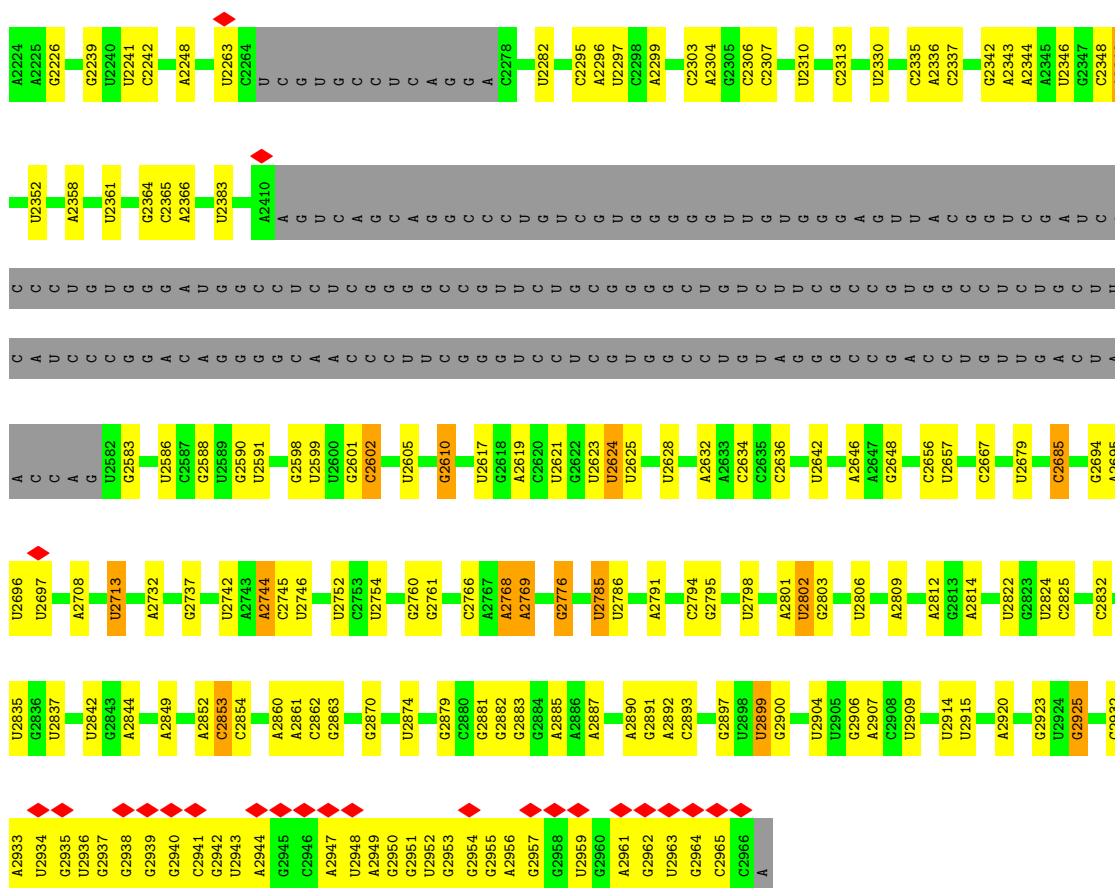
• Molecule 43: LSU rRNA chain 3



- Molecule 46: LSU rRNA chain 6



- Molecule 47: LSU rRNA chain 7

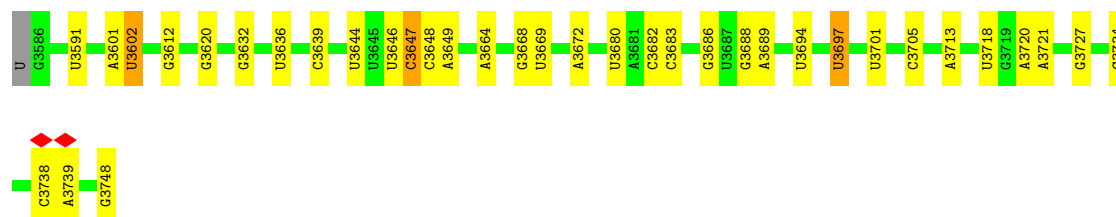
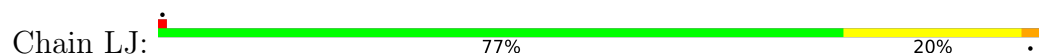


- Molecule 48: LSU rRNA chain 8

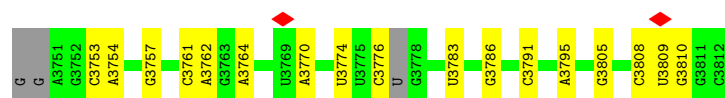




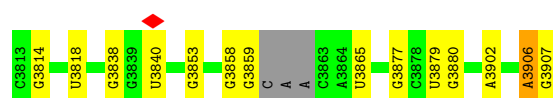
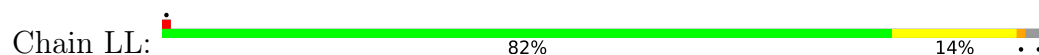
• Molecule 49: LSU rRNA chain 9



• Molecule 50: LSU rRNA chain 10

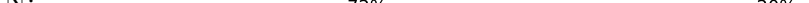


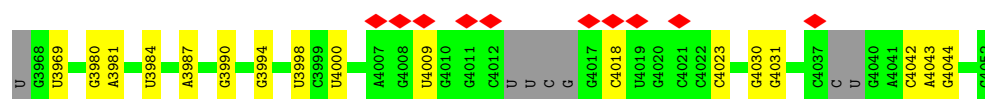
• Molecule 51: LSU rRNA chain 11



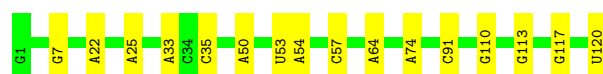
• Molecule 52: LSU rRNA chain 12

C C3910 A3911 C3921 C3922 C3927 G3944 A3951 G3952 U3953 G3954 U U C3957 G3961 G3962 U3963 A3964 A3965 U

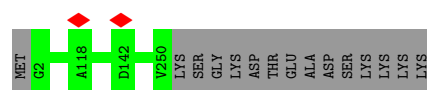
- Chain LN: 



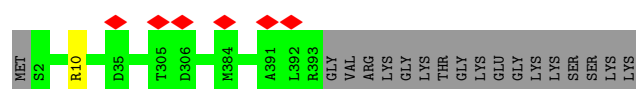
- Chain LO:  87% 13%



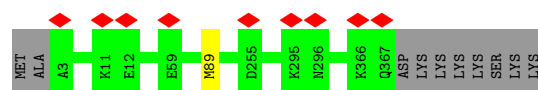
- Chain LP:  94% 6%



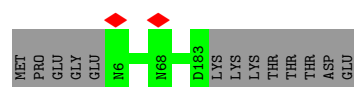
- Chain LQ: 95%



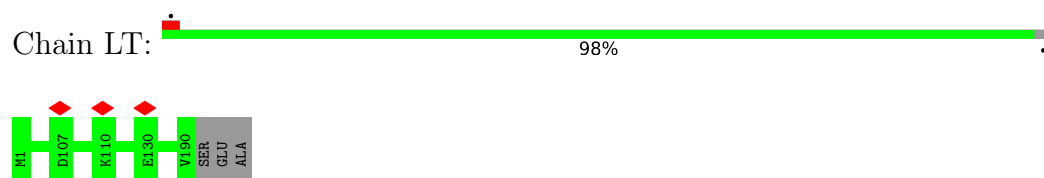
- Chain LR: 



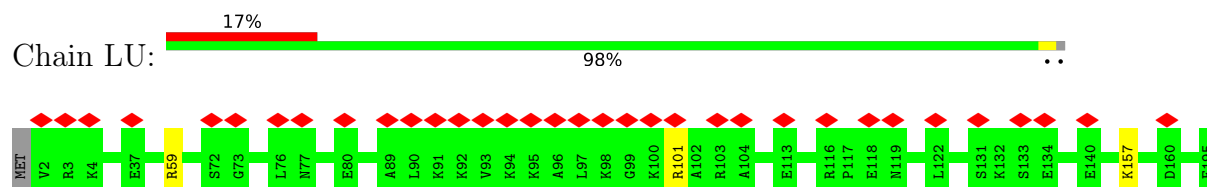
- Chain LS:  93% 7%



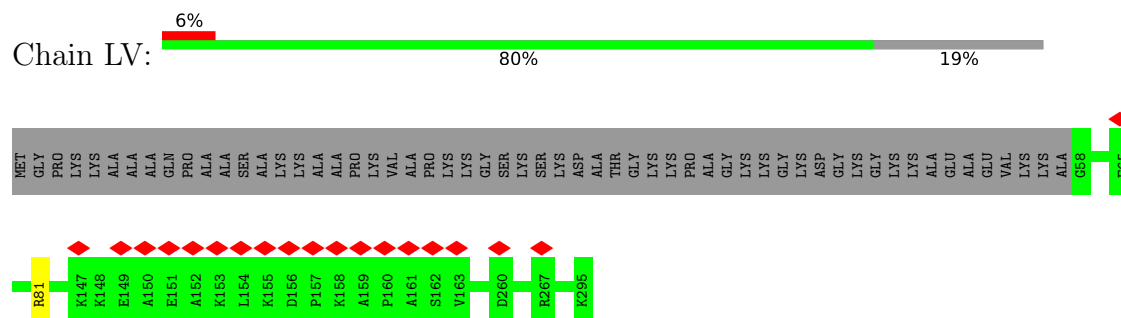
- Molecule 59: Ribosomal protein uL6



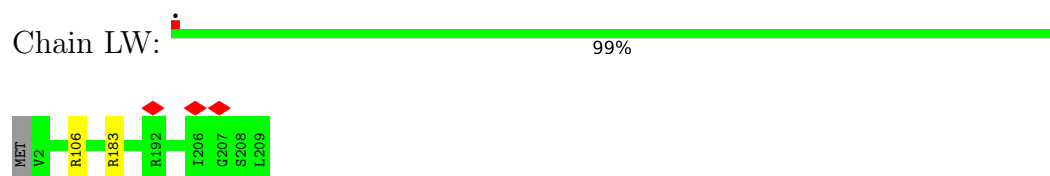
- Molecule 60: Ribosomal protein eL6



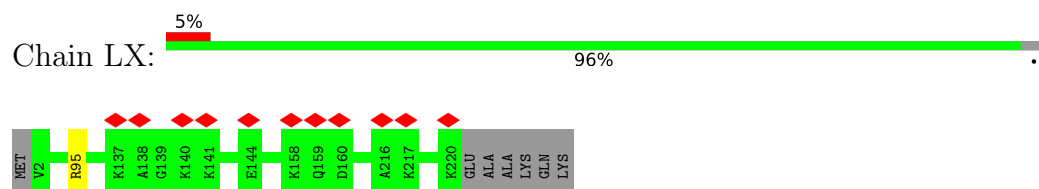
- Molecule 61: 60S ribosomal protein L7a



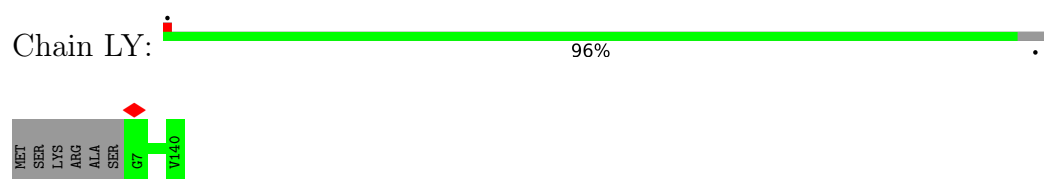
- Molecule 62: Ribosomal protein uL13



- Molecule 63: Ribosomal protein eL13



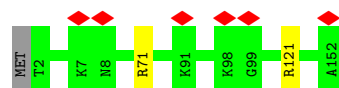
- Molecule 64: Ribosomal protein uL14



- Molecule 65: Ribosomal protein eL14



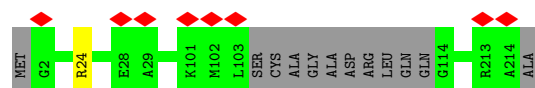
- Chain La:  98%



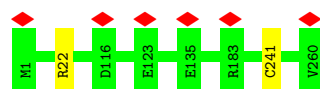
- Chain Lb:



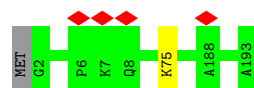
- Chain Lc:  94% 6%



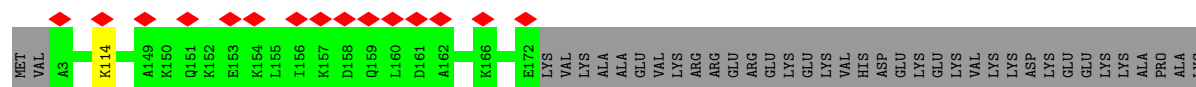
- Chain Ld: 99%



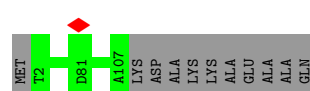
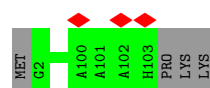
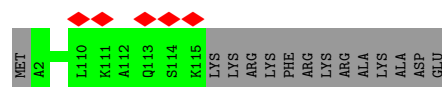
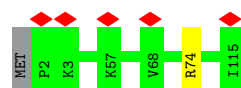
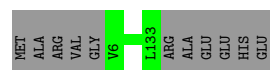
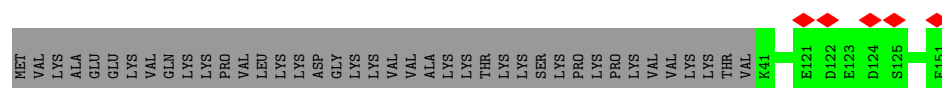
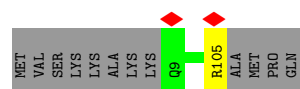
- Chain Le: 99%



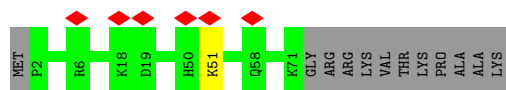
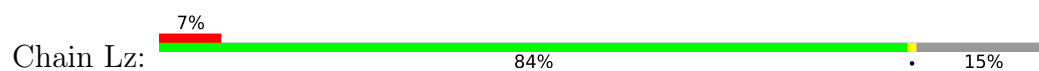
- Chain Lf: 



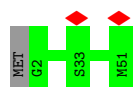
- Molecule 84: Ribosomal protein eL30



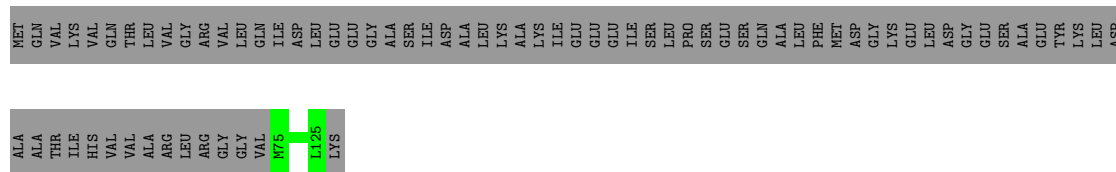
• Molecule 91: Ribosomal protein eL38



• Molecule 92: Ribosomal protein eL39



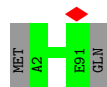
• Molecule 93: Ribosomal protein eL40



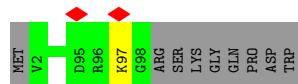
• Molecule 94: Ribosomal protein eL41



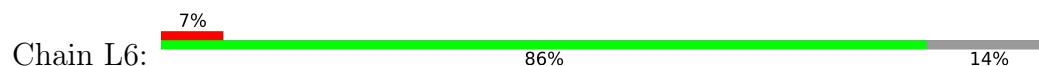
• Molecule 95: Ribosomal protein eL42

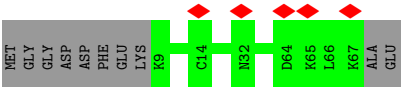


• Molecule 96: Ribosomal protein eL43

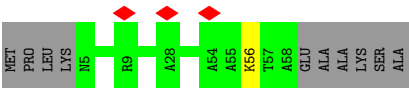
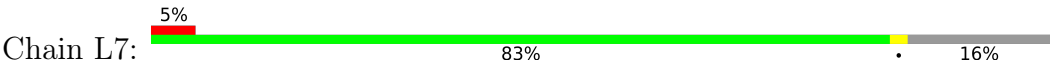


• Molecule 97: Ribosomal protein eLEgr2





• Molecule 98: Ribosomal protein eLEgr3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176308	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.408	Depositor
Minimum map value	-0.214	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, A2M, B8H, 6MZ, 5MC, PSU, B8N, MIA, JMC, JMH, ZN, 1MA, OMC, 7MG, OMU, UR3, OMG

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	S1	0.57	0/46353	0.85	43/72230 (0.1%)
2	S2	0.35	0/1783	0.91	5/2776 (0.2%)
3	S3	0.52	0/1802	0.96	1/2807 (0.0%)
4	S4	0.38	0/1812	1.07	11/2824 (0.4%)
5	S5	0.87	0/279	0.95	0/431
6	SA	0.31	0/1828	0.51	0/2458
7	SB	0.31	0/1694	0.48	0/2301
8	SC	0.35	0/1701	0.48	0/2281
9	SD	0.32	0/1461	0.47	0/1955
10	SE	0.35	0/2169	0.51	0/2909
11	SF	0.36	0/1752	0.49	0/2371
12	SG	0.31	0/2036	0.48	0/2709
13	SH	0.53	2/1472 (0.1%)	0.65	3/1982 (0.2%)
14	SI	0.31	0/1538	0.49	0/2060
15	SJ	0.35	0/1056	0.49	0/1415
16	SK	0.35	0/1678	0.51	0/2240
17	SL	0.35	0/1162	0.47	0/1554
18	SM	0.31	0/808	0.49	0/1089
19	SN	0.36	0/796	0.51	1/1072 (0.1%)
20	SO	0.35	0/1024	0.55	1/1375 (0.1%)
21	SP	0.36	0/1119	0.52	0/1493
22	SQ	0.29	0/931	0.54	0/1252
23	SR	0.34	0/1198	0.56	1/1603 (0.1%)
24	SS	0.36	0/441	0.50	0/583
25	ST	0.32	0/1201	0.50	0/1608
26	SU	0.38	0/1259	0.47	0/1695
27	SV	0.32	0/1006	0.47	0/1344
28	SW	0.35	0/1008	0.47	0/1346
29	SX	0.37	0/1148	0.48	0/1543
30	SY	0.32	0/631	0.48	0/849
31	SZ	0.35	0/1070	0.47	0/1412

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sa	0.35	0/642	0.50	0/862
33	Sb	0.36	0/791	0.51	0/1057
34	Sc	0.32	0/663	0.46	0/891
35	Sd	0.31	0/500	0.57	0/669
36	Se	0.32	0/490	0.51	0/646
37	Sf	0.33	0/519	0.54	1/691 (0.1%)
38	Sg	0.38	0/1623	0.56	0/2158
39	Sh	0.35	0/2454	0.56	0/3339
40	LA	0.59	0/3674	0.82	3/5722 (0.1%)
41	LB	0.61	0/3021	0.80	0/4708
42	LC	0.52	0/8081	0.81	4/12607 (0.0%)
43	LD	0.46	0/2613	0.83	2/4069 (0.0%)
44	LE	0.53	0/14709	0.79	3/22917 (0.0%)
45	LF	0.60	0/10013	0.83	9/15601 (0.1%)
46	LG	0.56	0/4698	0.83	0/7316
47	LH	0.64	0/12014	0.83	3/18729 (0.0%)
48	LI	0.55	0/12455	0.82	3/19402 (0.0%)
49	LJ	0.63	0/3692	0.86	6/5756 (0.1%)
50	LK	0.47	0/1453	0.82	1/2260 (0.0%)
51	LL	0.39	0/2170	0.79	0/3384
52	LM	0.60	0/1228	0.83	3/1914 (0.2%)
53	LN	0.45	0/1871	0.86	0/2914
54	LO	0.52	0/2860	0.78	1/4456 (0.0%)
55	LP	0.37	0/1941	0.49	0/2604
56	LQ	0.37	0/3177	0.49	0/4254
57	LR	0.34	0/2918	0.46	0/3918
58	LS	0.32	0/1456	0.50	0/1937
59	LT	0.33	0/1545	0.48	0/2068
60	LU	0.30	0/1606	0.48	0/2142
61	LV	0.31	0/1963	0.45	0/2627
62	LW	0.35	0/1745	0.49	0/2327
63	LX	0.33	0/1803	0.46	0/2404
64	LY	0.36	0/1017	0.50	0/1368
65	LZ	0.30	0/1809	0.45	0/2409
66	La	0.33	0/1238	0.47	0/1650
67	Lb	0.37	0/1757	0.49	1/2355 (0.0%)
68	Lc	0.33	0/1675	0.46	0/2237
69	Ld	0.33	0/2112	0.45	0/2838
70	Le	0.35	0/1554	0.49	0/2073
71	Lf	0.32	0/1410	0.45	0/1870
72	Lg	0.36	0/1532	0.49	0/2056
73	Lh	0.33	0/1306	0.47	0/1748
74	Li	0.39	0/1281	0.51	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lj	0.29	0/841	0.48	0/1125
76	Lk	0.34	0/1088	0.50	0/1455
77	Ll	0.31	0/1019	0.48	0/1350
78	Lm	0.33	0/562	0.49	0/756
79	Ln	0.32	0/1103	0.46	0/1470
80	Lo	0.34	0/470	0.45	0/631
81	Lp	0.31	0/1020	0.43	0/1352
82	Lq	0.29	0/780	0.41	0/1027
83	Lr	0.36	0/1867	0.46	0/2500
84	Ls	0.36	0/756	0.45	0/1014
85	Lt	0.36	0/941	0.50	0/1257
86	Lu	0.35	0/1093	0.45	0/1462
87	Lv	0.37	0/935	0.48	0/1247
88	Lw	0.34	0/937	0.50	0/1254
89	Lx	0.30	0/847	0.42	0/1122
90	Ly	0.35	0/872	0.52	0/1151
91	Lz	0.32	0/577	0.49	0/767
92	L1	0.32	0/457	0.46	0/603
93	L2	0.32	0/420	0.47	0/554
94	L3	0.50	0/304	0.63	0/390
95	L5	0.36	0/732	0.50	0/975
96	L4	0.36	0/798	0.46	0/1054
97	L6	0.29	0/500	0.45	0/665
98	L7	0.30	0/463	0.37	0/616
All	All	0.48	2/231677 (0.0%)	0.73	106/340038 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S1	1	0
45	LF	1	0
All	All	2	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	SH	60	ASN	C-O	9.43	1.41	1.23
13	SH	57	ARG	C-O	6.93	1.36	1.23

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	LI	3566	U	OP2-P-O3'	-11.41	80.11	105.20
13	SH	64	TYR	C-N-CA	9.75	146.07	121.70
4	S4	68	C	N3-C2-O2	-9.34	115.36	121.90
48	LI	3566	U	OP1-P-O3'	-8.56	86.36	105.20
45	LF	1704	C	N3-C2-O2	-8.25	116.12	121.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	S1	1601	B8N	C33
45	LF	1923	JMC	C4

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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	
6	SA	219/249 (88%)	197 (90%)	22 (10%)	0	100	100
7	SB	205/261 (78%)	186 (91%)	19 (9%)	0	100	100
8	SC	210/220 (96%)	196 (93%)	14 (7%)	0	100	100
9	SD	175/196 (89%)	166 (95%)	9 (5%)	0	100	100
10	SE	263/271 (97%)	243 (92%)	20 (8%)	0	100	100
11	SF	219/257 (85%)	207 (94%)	12 (6%)	0	100	100
12	SG	246/283 (87%)	227 (92%)	19 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	SH	178/190 (94%)	154 (86%)	23 (13%)	1 (1%)	25	62
14	SI	183/200 (92%)	168 (92%)	15 (8%)	0	100	100
15	SJ	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
16	SK	195/304 (64%)	182 (93%)	13 (7%)	0	100	100
17	SL	141/151 (93%)	132 (94%)	9 (6%)	0	100	100
18	SM	99/121 (82%)	96 (97%)	3 (3%)	0	100	100
19	SN	90/152 (59%)	86 (96%)	4 (4%)	0	100	100
20	SO	133/152 (88%)	125 (94%)	8 (6%)	0	100	100
21	SP	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
22	SQ	120/139 (86%)	100 (83%)	20 (17%)	0	100	100
23	SR	144/153 (94%)	132 (92%)	12 (8%)	0	100	100
24	SS	50/55 (91%)	44 (88%)	6 (12%)	0	100	100
25	ST	144/151 (95%)	129 (90%)	15 (10%)	0	100	100
26	SU	146/164 (89%)	135 (92%)	11 (8%)	0	100	100
27	SV	123/145 (85%)	113 (92%)	10 (8%)	0	100	100
28	SW	123/150 (82%)	117 (95%)	6 (5%)	0	100	100
29	SX	141/148 (95%)	130 (92%)	11 (8%)	0	100	100
30	SY	80/96 (83%)	72 (90%)	8 (10%)	0	100	100
31	SZ	125/137 (91%)	116 (93%)	9 (7%)	0	100	100
32	Sa	74/119 (62%)	69 (93%)	5 (7%)	0	100	100
33	Sb	95/120 (79%)	89 (94%)	6 (6%)	0	100	100
34	Sc	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
35	Sd	61/76 (80%)	50 (82%)	11 (18%)	0	100	100
36	Se	60/67 (90%)	53 (88%)	7 (12%)	0	100	100
37	Sf	62/157 (40%)	57 (92%)	5 (8%)	0	100	100
38	Sg	195/295 (66%)	164 (84%)	31 (16%)	0	100	100
39	Sh	309/317 (98%)	270 (87%)	39 (13%)	0	100	100
55	LP	247/264 (94%)	232 (94%)	15 (6%)	0	100	100
56	LQ	390/410 (95%)	365 (94%)	25 (6%)	0	100	100
57	LR	363/375 (97%)	338 (93%)	25 (7%)	0	100	100
58	LS	176/191 (92%)	166 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	LT	188/193 (97%)	177 (94%)	11 (6%)	0	100	100
60	LU	192/195 (98%)	171 (89%)	21 (11%)	0	100	100
61	LV	236/295 (80%)	228 (97%)	8 (3%)	0	100	100
62	LW	206/209 (99%)	194 (94%)	12 (6%)	0	100	100
63	LX	217/226 (96%)	196 (90%)	21 (10%)	0	100	100
64	LY	132/140 (94%)	120 (91%)	12 (9%)	0	100	100
65	LZ	215/219 (98%)	198 (92%)	17 (8%)	0	100	100
66	La	149/152 (98%)	138 (93%)	11 (7%)	0	100	100
67	Lb	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
68	Lc	199/215 (93%)	183 (92%)	16 (8%)	0	100	100
69	Ld	258/260 (99%)	242 (94%)	16 (6%)	0	100	100
70	Le	190/193 (98%)	176 (93%)	14 (7%)	0	100	100
71	Lf	168/250 (67%)	157 (94%)	11 (6%)	0	100	100
72	Lg	179/182 (98%)	160 (89%)	19 (11%)	0	100	100
73	Lh	156/159 (98%)	141 (90%)	15 (10%)	0	100	100
74	Li	153/164 (93%)	147 (96%)	6 (4%)	0	100	100
75	Lj	99/170 (58%)	94 (95%)	5 (5%)	0	100	100
76	Lk	129/163 (79%)	114 (88%)	15 (12%)	0	100	100
77	Ll	122/146 (84%)	112 (92%)	10 (8%)	0	100	100
78	Lm	64/157 (41%)	62 (97%)	2 (3%)	0	100	100
79	Ln	131/134 (98%)	122 (93%)	9 (7%)	0	100	100
80	Lo	54/72 (75%)	48 (89%)	6 (11%)	0	100	100
81	Lp	119/123 (97%)	115 (97%)	4 (3%)	0	100	100
82	Lq	89/117 (76%)	83 (93%)	6 (7%)	0	100	100
83	Lr	216/242 (89%)	208 (96%)	8 (4%)	0	100	100
84	Ls	95/109 (87%)	92 (97%)	3 (3%)	0	100	100
85	Lt	109/151 (72%)	98 (90%)	11 (10%)	0	100	100
86	Lu	126/139 (91%)	121 (96%)	5 (4%)	0	100	100
87	Lv	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
88	Lw	112/128 (88%)	99 (88%)	13 (12%)	0	100	100
89	Lx	100/106 (94%)	96 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
90	Ly	104/117 (89%)	95 (91%)	9 (9%)	0	100	100
91	Lz	68/82 (83%)	66 (97%)	2 (3%)	0	100	100
92	L1	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
93	L2	49/126 (39%)	48 (98%)	1 (2%)	0	100	100
94	L3	31/34 (91%)	27 (87%)	4 (13%)	0	100	100
95	L5	88/92 (96%)	82 (93%)	6 (7%)	0	100	100
96	L4	95/106 (90%)	87 (92%)	8 (8%)	0	100	100
97	L6	57/69 (83%)	53 (93%)	4 (7%)	0	100	100
98	L7	52/64 (81%)	51 (98%)	1 (2%)	0	100	100
All	All	11440/13164 (87%)	10574 (92%)	865 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	SH	64	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	SA	204/224 (91%)	204 (100%)	0	100	100
7	SB	179/215 (83%)	179 (100%)	0	100	100
8	SC	177/184 (96%)	177 (100%)	0	100	100
9	SD	155/169 (92%)	155 (100%)	0	100	100
10	SE	231/237 (98%)	229 (99%)	2 (1%)	78	91
11	SF	184/206 (89%)	184 (100%)	0	100	100
12	SG	217/231 (94%)	216 (100%)	1 (0%)	88	95
13	SH	160/166 (96%)	159 (99%)	1 (1%)	86	94
14	SI	165/176 (94%)	164 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	SJ	115/116 (99%)	114 (99%)	1 (1%)	78	91
16	SK	169/258 (66%)	168 (99%)	1 (1%)	86	94
17	SL	119/125 (95%)	119 (100%)	0	100	100
18	SM	91/104 (88%)	91 (100%)	0	100	100
19	SN	83/119 (70%)	83 (100%)	0	100	100
20	SO	104/119 (87%)	103 (99%)	1 (1%)	76	89
21	SP	118/120 (98%)	118 (100%)	0	100	100
22	SQ	97/113 (86%)	97 (100%)	0	100	100
23	SR	129/135 (96%)	128 (99%)	1 (1%)	81	92
24	SS	43/45 (96%)	41 (95%)	2 (5%)	26	60
25	ST	129/131 (98%)	129 (100%)	0	100	100
26	SU	132/146 (90%)	131 (99%)	1 (1%)	81	92
27	SV	111/125 (89%)	110 (99%)	1 (1%)	78	91
28	SW	104/127 (82%)	103 (99%)	1 (1%)	76	89
29	SX	114/117 (97%)	113 (99%)	1 (1%)	78	91
30	SY	63/76 (83%)	63 (100%)	0	100	100
31	SZ	113/121 (93%)	112 (99%)	1 (1%)	78	91
32	Sa	70/99 (71%)	70 (100%)	0	100	100
33	Sb	85/97 (88%)	85 (100%)	0	100	100
34	Sc	75/77 (97%)	75 (100%)	0	100	100
35	Sd	55/65 (85%)	55 (100%)	0	100	100
36	Se	48/50 (96%)	48 (100%)	0	100	100
37	Sf	55/136 (40%)	55 (100%)	0	100	100
38	Sg	169/241 (70%)	168 (99%)	1 (1%)	86	94
39	Sh	261/267 (98%)	260 (100%)	1 (0%)	91	96
55	LP	195/208 (94%)	195 (100%)	0	100	100
56	LQ	329/344 (96%)	328 (100%)	1 (0%)	92	97
57	LR	305/314 (97%)	304 (100%)	1 (0%)	92	97
58	LS	154/166 (93%)	154 (100%)	0	100	100
59	LT	166/168 (99%)	166 (100%)	0	100	100
60	LU	173/174 (99%)	170 (98%)	3 (2%)	60	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	LV	206/242 (85%)	205 (100%)	1 (0%)	88	95
62	LW	182/183 (100%)	180 (99%)	2 (1%)	73	88
63	LX	187/192 (97%)	186 (100%)	1 (0%)	88	95
64	LY	104/109 (95%)	104 (100%)	0	100	100
65	LZ	190/192 (99%)	190 (100%)	0	100	100
66	La	123/124 (99%)	121 (98%)	2 (2%)	62	83
67	Lb	174/175 (99%)	174 (100%)	0	100	100
68	Lc	167/175 (95%)	166 (99%)	1 (1%)	86	94
69	Ld	213/213 (100%)	211 (99%)	2 (1%)	78	91
70	Le	162/163 (99%)	161 (99%)	1 (1%)	86	94
71	Lf	142/208 (68%)	141 (99%)	1 (1%)	84	93
72	Lg	164/165 (99%)	164 (100%)	0	100	100
73	Lh	140/141 (99%)	139 (99%)	1 (1%)	84	93
74	Li	131/139 (94%)	130 (99%)	1 (1%)	81	92
75	Lj	90/144 (62%)	90 (100%)	0	100	100
76	Lk	117/139 (84%)	117 (100%)	0	100	100
77	Ll	110/129 (85%)	110 (100%)	0	100	100
78	Lm	62/135 (46%)	62 (100%)	0	100	100
79	Ln	116/117 (99%)	116 (100%)	0	100	100
80	Lo	48/59 (81%)	48 (100%)	0	100	100
81	Lp	111/113 (98%)	111 (100%)	0	100	100
82	Lq	81/102 (79%)	81 (100%)	0	100	100
83	Lr	193/215 (90%)	192 (100%)	1 (0%)	88	95
84	Ls	84/94 (89%)	83 (99%)	1 (1%)	71	87
85	Lt	101/138 (73%)	101 (100%)	0	100	100
86	Lu	113/121 (93%)	113 (100%)	0	100	100
87	Lv	97/98 (99%)	96 (99%)	1 (1%)	76	89
88	Lw	101/113 (89%)	101 (100%)	0	100	100
89	Lx	86/90 (96%)	86 (100%)	0	100	100
90	Ly	89/96 (93%)	89 (100%)	0	100	100
91	Lz	67/76 (88%)	66 (98%)	1 (2%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
92	L1	47/48 (98%)	47 (100%)	0	100	100
93	L2	47/108 (44%)	47 (100%)	0	100	100
94	L3	31/32 (97%)	30 (97%)	1 (3%)	39	70
95	L5	74/76 (97%)	74 (100%)	0	100	100
96	L4	86/94 (92%)	85 (99%)	1 (1%)	71	87
97	L6	54/61 (88%)	54 (100%)	0	100	100
98	L7	46/53 (87%)	45 (98%)	1 (2%)	52	77
All	All	9982/11183 (89%)	9939 (100%)	43 (0%)	91	96

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
66	La	121	ARG
74	Li	26	VAL
68	Lc	24	ARG
70	Le	75	LYS
84	Ls	105	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
85	Lt	45	ASN
86	Lu	130	ASN
29	SX	70	ASN
28	SW	87	ASN
88	Lw	46	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S1	2001/2315 (86%)	483 (24%)	16 (0%)
2	S2	74/76 (97%)	41 (55%)	2 (2%)
3	S3	75/76 (98%)	25 (33%)	2 (2%)
4	S4	75/76 (98%)	41 (54%)	3 (4%)
40	LA	157/163 (96%)	30 (19%)	0
41	LB	132/133 (99%)	22 (16%)	1 (0%)
42	LC	349/350 (99%)	79 (22%)	5 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
43	LD	108/116 (93%)	30 (27%)	1 (0%)
44	LE	641/698 (91%)	106 (16%)	4 (0%)
45	LF	447/527 (84%)	88 (19%)	1 (0%)
46	LG	203/234 (86%)	38 (18%)	0
47	LH	554/744 (74%)	119 (21%)	7 (1%)
48	LI	567/617 (91%)	136 (23%)	1 (0%)
49	LJ	162/164 (98%)	27 (16%)	0
5	S5	11/12 (91%)	1 (9%)	0
50	LK	59/64 (92%)	16 (27%)	0
51	LL	90/95 (94%)	13 (14%)	0
52	LM	52/58 (89%)	6 (11%)	0
53	LN	76/86 (88%)	16 (21%)	0
54	LO	119/120 (99%)	15 (12%)	0
All	All	5952/6724 (88%)	1332 (22%)	43 (0%)

5 of 1332 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S1	2	A
1	S1	3	U
1	S1	4	C
1	S1	17	C
1	S1	34	U

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
42	LC	602	A
47	LH	2342	G
43	LD	726	C
44	LE	1224	G
47	LH	2768	A2M

5.4 Non-standard residues in protein, DNA, RNA chains

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	OMG	S1	1901	1	18,26,27	1.31	2 (11%)	19,38,41	1.53	5 (26%)
47	PSU	LH	2842	45,47	18,21,22	4.02	8 (44%)	22,30,33	1.80	6 (27%)
1	OMC	S1	38	1	19,22,23	1.01	1 (5%)	26,31,34	1.13	3 (11%)
1	A2M	S1	407	1	18,25,26	4.24	8 (44%)	18,36,39	2.99	4 (22%)
47	PSU	LH	2621	44,47	18,21,22	4.15	7 (38%)	22,30,33	1.75	5 (22%)
47	PSU	LH	2914	48,47	18,21,22	4.15	7 (38%)	22,30,33	1.89	5 (22%)
47	OMU	LH	2346	47	19,22,23	0.63	0	26,31,34	1.06	2 (7%)
48	OMG	LI	3509	48,2	18,26,27	1.31	2 (11%)	19,38,41	1.49	3 (15%)
47	PSU	LH	2899	48,47	18,21,22	4.11	7 (38%)	22,30,33	1.86	5 (22%)
1	UR3	S1	1597	1	19,22,23	0.78	1 (5%)	26,32,35	0.58	0
47	PSU	LH	2754	47	18,21,22	4.05	7 (38%)	22,30,33	1.96	5 (22%)
48	UR3	LI	3540	48	19,22,23	0.73	0	26,32,35	0.60	0
47	A2M	LH	2349	47	18,25,26	4.23	7 (38%)	18,36,39	3.00	3 (16%)
1	PSU	S1	2116	1	18,21,22	4.10	7 (38%)	22,30,33	1.71	4 (18%)
44	OMU	LE	1081	44	19,22,23	0.51	0	26,31,34	0.88	2 (7%)
1	A2M	S1	40	1	18,25,26	4.17	7 (38%)	18,36,39	2.96	3 (16%)
44	PSU	LE	1171	44	18,21,22	4.15	7 (38%)	22,30,33	1.88	5 (22%)
47	A2M	LH	2744	47	18,25,26	4.13	7 (38%)	18,36,39	3.14	5 (27%)
1	PSU	S1	1068	1	18,21,22	4.20	7 (38%)	22,30,33	1.81	5 (22%)
48	OMU	LI	3508	48	19,22,23	0.56	0	26,31,34	0.95	2 (7%)
45	OMC	LF	1822	44,45	19,22,23	0.87	1 (5%)	26,31,34	1.06	2 (7%)
48	OMG	LI	3434	48	18,26,27	1.31	2 (11%)	19,38,41	1.54	6 (31%)
1	OMG	S1	1536	1,94	18,26,27	1.31	2 (11%)	19,38,41	1.63	4 (21%)
45	PSU	LF	1582	45	18,21,22	4.11	7 (38%)	22,30,33	1.89	5 (22%)
1	PSU	S1	1591	1	18,21,22	3.97	7 (38%)	22,30,33	1.83	6 (27%)
47	PSU	LH	2623	47	18,21,22	4.09	7 (38%)	22,30,33	1.95	5 (22%)
44	OMG	LE	1104	44	18,26,27	1.34	2 (11%)	19,38,41	1.54	4 (21%)
47	A2M	LH	2358	47	18,25,26	4.13	7 (38%)	18,36,39	3.16	4 (22%)
48	OMU	LI	3300	48	19,22,23	0.53	0	26,31,34	1.00	2 (7%)
1	PSU	S1	1711	1	18,21,22	4.00	7 (38%)	22,30,33	1.95	5 (22%)
1	OMU	S1	2041	1	19,22,23	0.55	0	26,31,34	0.76	1 (3%)
47	PSU	LH	2874	48,47	18,21,22	4.19	7 (38%)	22,30,33	1.98	5 (22%)
1	OMU	S1	1679	1	19,22,23	0.58	0	26,31,34	0.96	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMU	LF	1824	44,45,42	19,22,23	0.50	0	26,31,34	1.01	2 (7%)
1	PSU	S1	2305	1	18,21,22	4.15	7 (38%)	22,30,33	1.72	5 (22%)
47	OMU	LH	2713	47	19,22,23	0.68	0	26,31,34	0.88	2 (7%)
47	PSU	LH	2802	47	18,21,22	4.17	7 (38%)	22,30,33	1.81	5 (22%)
47	OMG	LH	2883	48,47	18,26,27	1.37	2 (11%)	19,38,41	1.50	4 (21%)
45	OMG	LF	1662	45	18,26,27	1.35	3 (16%)	19,38,41	1.50	5 (26%)
53	PSU	LN	3969	53,52	18,21,22	4.30	7 (38%)	22,30,33	1.73	5 (22%)
1	OMG	S1	57	1	18,26,27	1.27	2 (11%)	19,38,41	1.61	5 (26%)
1	PSU	S1	640	1	18,21,22	4.16	7 (38%)	22,30,33	1.67	4 (18%)
1	OMU	S1	1966	1,29	19,22,23	0.53	0	26,31,34	0.83	2 (7%)
1	PSU	S1	2131	1	18,21,22	4.14	7 (38%)	22,30,33	1.91	5 (22%)
52	OMC	LM	3957	53,52	19,22,23	0.95	2 (10%)	26,31,34	1.02	2 (7%)
49	PSU	LJ	3701	49	18,21,22	4.10	7 (38%)	22,30,33	1.90	5 (22%)
44	PSU	LE	1198	44	18,21,22	4.11	7 (38%)	22,30,33	1.92	5 (22%)
48	OMC	LI	3355	48,44	19,22,23	0.97	1 (5%)	26,31,34	1.08	3 (11%)
1	OMG	S1	42	1	18,26,27	1.36	3 (16%)	19,38,41	1.60	5 (26%)
47	A2M	LH	2887	48,47	18,25,26	4.26	7 (38%)	18,36,39	3.10	3 (16%)
52	PSU	LM	3953	53,52	18,21,22	4.18	7 (38%)	22,30,33	1.83	5 (22%)
1	PSU	S1	280	1	18,21,22	4.19	7 (38%)	22,30,33	1.90	5 (22%)
44	PSU	LE	1407	44	18,21,22	4.11	7 (38%)	22,30,33	1.87	5 (22%)
48	6MZ	LI	3214	48,45	18,25,26	0.83	1 (5%)	16,36,39	2.14	4 (25%)
1	PSU	S1	105	1	18,21,22	4.21	7 (38%)	22,30,33	1.85	5 (22%)
48	OMC	LI	3222	48	19,22,23	0.91	1 (5%)	26,31,34	1.17	4 (15%)
47	JMH	LH	2636	47	18,22,23	1.11	1 (5%)	21,32,35	1.51	5 (23%)
42	OMU	LC	491	42	19,22,23	0.66	0	26,31,34	0.94	2 (7%)
1	PSU	S1	32	1	18,21,22	4.12	7 (38%)	22,30,33	1.88	5 (22%)
1	PSU	S1	403	1	18,21,22	4.20	7 (38%)	22,30,33	1.69	4 (18%)
47	OMC	LH	2685	47	19,22,23	1.26	1 (5%)	26,31,34	1.42	4 (15%)
44	PSU	LE	1184	44	18,21,22	4.13	7 (38%)	22,30,33	1.79	5 (22%)
41	PSU	LB	234	41	18,21,22	4.15	7 (38%)	22,30,33	1.79	5 (22%)
1	A2M	S1	1096	1	18,25,26	4.24	7 (38%)	18,36,39	2.92	3 (16%)
48	PSU	LI	3568	48,47	18,21,22	4.05	7 (38%)	22,30,33	1.83	6 (27%)
1	PSU	S1	1715	1	18,21,22	4.14	7 (38%)	22,30,33	1.77	5 (22%)
42	PSU	LC	302	42	18,21,22	4.20	7 (38%)	22,30,33	1.92	5 (22%)
45	OMG	LF	1883	45	18,26,27	1.33	3 (16%)	19,38,41	1.48	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMU	LF	1828	45,47	19,22,23	0.50	0	26,31,34	0.87	0
48	PSU	LI	3562	48	18,21,22	4.05	7 (38%)	22,30,33	1.97	5 (22%)
45	OMG	LF	1956	45	18,26,27	1.33	2 (11%)	19,38,41	1.51	4 (21%)
47	PSU	LH	2586	47	18,21,22	4.21	7 (38%)	22,30,33	1.80	5 (22%)
44	OMC	LE	936	44	19,22,23	0.81	0	26,31,34	1.09	3 (11%)
1	PSU	S1	2065	1	18,21,22	4.16	7 (38%)	22,30,33	1.88	5 (22%)
47	PSU	LH	2915	48,47	18,21,22	4.13	7 (38%)	22,30,33	1.81	5 (22%)
1	MA6	S1	2288	1	19,26,27	1.08	1 (5%)	18,38,41	3.76	2 (11%)
42	PSU	LC	308	42	18,21,22	4.22	7 (38%)	22,30,33	1.89	5 (22%)
1	OMG	S1	390	1	18,26,27	1.36	2 (11%)	19,38,41	1.53	5 (26%)
1	A2M	S1	649	1	18,25,26	4.11	7 (38%)	18,36,39	3.05	3 (16%)
44	OMG	LE	1324	44	18,26,27	1.35	3 (16%)	19,38,41	1.45	3 (15%)
47	PSU	LH	2624	47	18,21,22	4.10	8 (44%)	22,30,33	1.75	4 (18%)
48	A2M	LI	3367	48,42	18,25,26	4.23	7 (38%)	18,36,39	2.99	3 (16%)
1	A2M	S1	565	1	18,25,26	4.21	7 (38%)	18,36,39	3.09	4 (22%)
48	A2M	LI	3348	48	18,25,26	4.21	7 (38%)	18,36,39	3.01	3 (16%)
47	OMG	LH	2870	47	18,26,27	1.30	2 (11%)	19,38,41	1.53	5 (26%)
40	PSU	LA	68	40	18,21,22	4.13	8 (44%)	22,30,33	2.07	6 (27%)
41	OMU	LB	247	41	19,22,23	0.70	0	26,31,34	0.92	2 (7%)
47	OMC	LH	2832	47	19,22,23	0.81	0	26,31,34	1.10	3 (11%)
49	OMU	LJ	3694	49	19,22,23	0.55	0	26,31,34	0.94	2 (7%)
45	OMG	LF	1667	45	18,26,27	1.32	2 (11%)	19,38,41	1.56	4 (21%)
48	PSU	LI	3204	48	18,21,22	4.09	7 (38%)	22,30,33	1.82	5 (22%)
1	PSU	S1	89	1	18,21,22	4.12	7 (38%)	22,30,33	1.87	5 (22%)
1	PSU	S1	544	1	18,21,22	4.09	7 (38%)	22,30,33	1.95	5 (22%)
1	A2M	S1	110	1	18,25,26	4.17	7 (38%)	18,36,39	3.08	3 (16%)
1	OMU	S1	682	1	19,22,23	0.48	0	26,31,34	1.06	2 (7%)
47	PSU	LH	2591	47	18,21,22	4.15	7 (38%)	22,30,33	1.82	5 (22%)
44	PSU	LE	1075	44,48	18,21,22	4.07	8 (44%)	22,30,33	1.79	5 (22%)
1	A2M	S1	645	1	18,25,26	4.16	7 (38%)	18,36,39	3.06	4 (22%)
46	PSU	LG	2171	46	18,21,22	4.23	8 (44%)	22,30,33	1.78	4 (18%)
46	A2M	LG	2005	45,46	18,25,26	4.15	7 (38%)	18,36,39	3.15	3 (16%)
47	OMC	LH	2853	47	19,22,23	0.88	1 (5%)	26,31,34	1.12	3 (11%)
48	OMU	LI	3171	48,47	19,22,23	0.58	0	26,31,34	0.90	2 (7%)
1	PSU	S1	27	1	18,21,22	4.08	7 (38%)	22,30,33	1.84	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMC	LF	1976	45	19,22,23	0.87	1 (5%)	26,31,34	1.16	3 (11%)
2	MIA	S2	37	2	24,31,32	2.48	4 (16%)	26,44,47	2.81	8 (30%)
48	5MC	LI	3518	48,64	18,22,23	1.53	4 (22%)	26,32,35	1.31	5 (19%)
1	OMC	S1	1625	1	19,22,23	0.77	0	26,31,34	0.98	3 (11%)
1	PSU	S1	2101	1	18,21,22	4.12	8 (44%)	22,30,33	1.75	4 (18%)
1	OMU	S1	1616	1	19,22,23	0.58	0	26,31,34	0.85	2 (7%)
44	OMG	LE	1201	44	18,26,27	1.34	2 (11%)	19,38,41	1.49	2 (10%)
48	PSU	LI	3503	48	18,21,22	4.10	7 (38%)	22,30,33	1.93	5 (22%)
1	A2M	S1	723	1	18,25,26	4.09	7 (38%)	18,36,39	3.04	4 (22%)
42	OMC	LC	483	42	19,22,23	0.93	1 (5%)	26,31,34	1.04	3 (11%)
47	OMU	LH	2605	47,49	19,22,23	0.56	0	26,31,34	0.82	1 (3%)
45	OMU	LF	1957	45	19,22,23	0.55	0	26,31,34	0.99	2 (7%)
1	PSU	S1	1396	1	18,21,22	4.17	7 (38%)	22,30,33	1.95	5 (22%)
44	OMG	LE	1208	44	18,26,27	1.04	1 (5%)	19,38,41	1.31	3 (15%)
47	OMC	LH	2825	47	19,22,23	0.79	0	26,31,34	1.07	4 (15%)
1	PSU	S1	1393	1	18,21,22	4.11	7 (38%)	22,30,33	1.94	5 (22%)
41	PSU	LB	280	41	18,21,22	4.15	7 (38%)	22,30,33	1.81	5 (22%)
40	OMG	LA	74	40	18,26,27	1.34	2 (11%)	19,38,41	1.43	3 (15%)
45	PSU	LF	1876	45	18,21,22	4.17	7 (38%)	22,30,33	1.88	5 (22%)
49	PSU	LJ	3644	49	18,21,22	3.97	7 (38%)	22,30,33	1.97	6 (27%)
45	PSU	LF	1859	45	18,21,22	4.13	7 (38%)	22,30,33	1.88	5 (22%)
42	OMG	LC	631	44,42	18,26,27	1.35	3 (16%)	19,38,41	1.53	4 (21%)
47	PSU	LH	2742	47	18,21,22	4.18	7 (38%)	22,30,33	1.79	4 (18%)
45	A2M	LF	1815	45	18,25,26	4.21	7 (38%)	18,36,39	2.96	3 (16%)
1	OMU	S1	1641	1	19,22,23	0.65	0	26,31,34	0.99	2 (7%)
45	OMU	LF	1504	45	19,22,23	0.57	0	26,31,34	0.98	2 (7%)
40	A2M	LA	39	40	18,25,26	4.27	7 (38%)	18,36,39	2.89	4 (22%)
44	PSU	LE	1363	44	18,21,22	4.14	7 (38%)	22,30,33	1.89	5 (22%)
44	A2M	LE	935	44	18,25,26	4.17	7 (38%)	18,36,39	3.02	3 (16%)
44	OMC	LE	1165	44	19,22,23	1.08	1 (5%)	26,31,34	1.28	4 (15%)
47	5MC	LH	2766	47	18,22,23	1.58	3 (16%)	26,32,35	1.21	3 (11%)
1	OMC	S1	2123	1	19,22,23	0.87	1 (5%)	26,31,34	1.01	3 (11%)
51	PSU	LL	3865	51	18,21,22	4.23	7 (38%)	22,30,33	1.93	5 (22%)
1	OMC	S1	1037	1	19,22,23	0.92	1 (5%)	26,31,34	1.14	3 (11%)
45	OMG	LF	1826	44,45	18,26,27	1.33	2 (11%)	19,38,41	1.51	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	A2M	LH	2708	47	18,25,26	4.27	7 (38%)	18,36,39	2.92	3 (16%)
1	PSU	S1	1624	1	18,21,22	4.14	7 (38%)	22,30,33	1.80	5 (22%)
48	PSU	LI	3185	48	18,21,22	4.11	7 (38%)	22,30,33	1.88	5 (22%)
48	OMC	LI	3546	48	19,22,23	0.82	0	26,31,34	1.21	4 (15%)
1	OMU	S1	8	1	19,22,23	0.43	0	26,31,34	1.02	2 (7%)
44	PSU	LE	1118	44	18,21,22	4.12	7 (38%)	22,30,33	1.86	4 (18%)
44	OMU	LE	1222	44	19,22,23	1.37	4 (21%)	26,31,34	1.93	7 (26%)
47	OMG	LH	2897	48,47	18,26,27	1.33	2 (11%)	19,38,41	1.61	5 (26%)
48	A2M	LI	3521	48	18,25,26	4.17	6 (33%)	18,36,39	3.06	3 (16%)
48	OMC	LI	3374	48	19,22,23	0.85	1 (5%)	26,31,34	1.09	3 (11%)
41	A2M	LB	183	41	18,25,26	4.15	7 (38%)	18,36,39	2.95	3 (16%)
49	PSU	LJ	3680	49	18,21,22	4.13	8 (44%)	22,30,33	2.11	6 (27%)
46	OMU	LG	2129	46	19,22,23	0.59	0	26,31,34	0.87	1 (3%)
47	OMC	LH	2313	45,47	19,22,23	0.83	1 (5%)	26,31,34	1.09	4 (15%)
42	OMC	LC	577	42	19,22,23	0.90	1 (5%)	26,31,34	1.00	2 (7%)
1	A2M	S1	1549	1	18,25,26	4.25	7 (38%)	18,36,39	3.13	4 (22%)
48	OMC	LI	3465	48	19,22,23	0.88	1 (5%)	26,31,34	1.04	3 (11%)
42	OMG	LC	541	40,42	18,26,27	1.30	2 (11%)	19,38,41	1.59	4 (21%)
46	PSU	LG	2119	46	18,21,22	4.20	7 (38%)	22,30,33	1.97	5 (22%)
44	A2M	LE	1121	44	18,25,26	4.25	8 (44%)	18,36,39	2.99	3 (16%)
42	OMC	LC	537	40,42	19,22,23	0.98	1 (5%)	26,31,34	1.11	4 (15%)
1	B8N	S1	1601	1	24,29,30	0.98	2 (8%)	29,42,45	2.20	8 (27%)
1	A2M	S1	1063	1	18,25,26	4.23	7 (38%)	18,36,39	2.94	3 (16%)
44	A2M	LE	1106	44	18,25,26	4.17	7 (38%)	18,36,39	3.01	4 (22%)
44	PSU	LE	1365	44	18,21,22	4.15	7 (38%)	22,30,33	1.88	5 (22%)
45	PSU	LF	1692	45	18,21,22	4.10	7 (38%)	22,30,33	1.89	5 (22%)
44	7MG	LE	938	44	22,26,27	1.71	2 (9%)	29,39,42	1.15	3 (10%)
1	OMC	S1	2142	1	19,22,23	0.78	0	26,31,34	1.06	3 (11%)
1	OMC	S1	99	1	19,22,23	0.85	1 (5%)	26,31,34	1.12	4 (15%)
47	OMG	LH	2610	47	18,26,27	1.33	2 (11%)	19,38,41	1.60	6 (31%)
45	A2M	LF	1888	45	18,25,26	4.25	7 (38%)	18,36,39	2.93	3 (16%)
48	PSU	LI	3206	48	18,21,22	4.11	7 (38%)	22,30,33	1.96	6 (27%)
48	OMG	LI	3191	48,3	18,26,27	1.32	2 (11%)	19,38,41	1.43	4 (21%)
1	PSU	S1	2129	1	18,21,22	4.10	7 (38%)	22,30,33	1.83	5 (22%)
1	OMG	S1	180	1	18,26,27	1.31	2 (11%)	19,38,41	1.47	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	OMC	LE	1312	44	19,22,23	0.84	1 (5%)	26,31,34	1.07	3 (11%)
1	OMG	S1	485	1	18,26,27	1.32	2 (11%)	19,38,41	1.44	3 (15%)
47	A2M	LH	2920	48,47	18,25,26	4.26	7 (38%)	18,36,39	2.93	3 (16%)
48	A2M	LI	3533	48,47	18,25,26	4.21	7 (38%)	18,36,39	2.95	3 (16%)
46	PSU	LG	2154	46	18,21,22	4.09	7 (38%)	22,30,33	1.85	6 (27%)
1	OMC	S1	393	1	19,22,23	0.86	0	26,31,34	1.05	2 (7%)
45	PSU	LF	1926	45	18,21,22	4.19	8 (44%)	22,30,33	1.72	4 (18%)
48	OMC	LI	3347	48	19,22,23	0.94	1 (5%)	26,31,34	1.03	3 (11%)
49	OMU	LJ	3718	49	19,22,23	0.59	0	26,31,34	0.75	1 (3%)
48	PSU	LI	3542	48,47	18,21,22	4.16	7 (38%)	22,30,33	1.88	5 (22%)
45	OMG	LF	1683	45	18,26,27	1.29	2 (11%)	19,38,41	1.48	4 (21%)
1	A2M	S1	28	1	18,25,26	4.22	7 (38%)	18,36,39	2.98	3 (16%)
47	OMU	LH	2909	48,47	19,22,23	0.56	0	26,31,34	0.95	2 (7%)
48	OMG	LI	3504	48	18,26,27	1.32	2 (11%)	19,38,41	1.47	4 (21%)
45	OMU	LF	1681	45	19,22,23	0.55	0	26,31,34	0.99	2 (7%)
48	OMC	LI	3535	48	19,22,23	0.91	1 (5%)	26,31,34	0.98	3 (11%)
1	OMG	S1	2075	1	18,26,27	1.36	2 (11%)	19,38,41	1.52	4 (21%)
1	OMG	S1	1705	1	18,26,27	1.34	2 (11%)	19,38,41	1.61	4 (21%)
48	PSU	LI	2999	48,47	18,21,22	4.33	7 (38%)	22,30,33	1.96	5 (22%)
45	PSU	LF	1568	45,54	18,21,22	4.34	7 (38%)	22,30,33	1.74	5 (22%)
47	A2M	LH	2812	47	18,25,26	4.22	7 (38%)	18,36,39	2.97	3 (16%)
47	B8H	LH	2904	48,47	19,22,23	1.35	3 (15%)	22,32,35	1.97	3 (13%)
44	PSU	LE	1266	44	18,21,22	4.07	7 (38%)	22,30,33	1.93	5 (22%)
48	OMG	LI	3401	48,47	18,26,27	1.24	2 (11%)	19,38,41	1.58	5 (26%)
44	OMC	LE	1218	44	19,22,23	0.84	0	26,31,34	1.15	4 (15%)
48	OMC	LI	3208	48	19,22,23	0.85	0	26,31,34	1.17	4 (15%)
48	PSU	LI	3444	48	18,21,22	4.14	8 (44%)	22,30,33	1.97	6 (27%)
44	A2M	LE	1204	44	18,25,26	4.27	7 (38%)	18,36,39	3.01	3 (16%)
47	PSU	LH	2837	47	18,21,22	4.16	7 (38%)	22,30,33	1.84	5 (22%)
44	PSU	LE	1235	44	18,21,22	4.15	7 (38%)	22,30,33	1.85	5 (22%)
47	OMU	LH	2806	47	19,22,23	0.63	0	26,31,34	0.89	2 (7%)
1	A2M	S1	1900	1,27	18,25,26	4.18	6 (33%)	18,36,39	2.91	3 (16%)
48	PSU	LI	3145	48	18,21,22	4.31	8 (44%)	22,30,33	1.95	5 (22%)
1	A2M	S1	1371	1	18,25,26	4.32	7 (38%)	18,36,39	3.11	3 (16%)
48	PSU	LI	3451	48	18,21,22	4.16	8 (44%)	22,30,33	1.96	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	PSU	LA	16	40,42	18,21,22	4.11	7 (38%)	22,30,33	1.86	5 (22%)
1	PSU	S1	1554	1	18,21,22	3.97	7 (38%)	22,30,33	1.76	4 (18%)
1	OMC	S1	621	1	19,22,23	0.90	1 (5%)	26,31,34	1.20	4 (15%)
49	PSU	LJ	3591	49	18,21,22	4.11	7 (38%)	22,30,33	1.90	5 (22%)
46	OMG	LG	2146	46	18,26,27	1.31	3 (16%)	19,38,41	1.49	3 (15%)
1	A2M	S1	2046	1	18,25,26	4.19	7 (38%)	18,36,39	3.10	3 (16%)
47	PSU	LH	2746	47	18,21,22	4.09	7 (38%)	22,30,33	2.14	5 (22%)
48	PSU	LI	3042	48	18,21,22	4.32	7 (38%)	22,30,33	1.83	5 (22%)
44	OMU	LE	1189	44	19,22,23	0.47	0	26,31,34	0.94	2 (7%)
44	PSU	LE	1023	44	18,21,22	4.15	7 (38%)	22,30,33	1.90	5 (22%)
47	OMU	LH	2835	47	19,22,23	0.69	1 (5%)	26,31,34	0.86	1 (3%)
1	PSU	S1	176	1	18,21,22	4.16	7 (38%)	22,30,33	1.87	5 (22%)
45	A2M	LF	1502	45	18,25,26	4.21	7 (38%)	18,36,39	3.08	3 (16%)
45	A2M	LF	1738	45	18,25,26	4.15	7 (38%)	18,36,39	3.02	3 (16%)
47	PSU	LH	2679	47	18,21,22	4.08	7 (38%)	22,30,33	1.83	5 (22%)
44	OMU	LE	1315	44	19,22,23	0.56	0	26,31,34	0.89	2 (7%)
1	PSU	S1	465	1	18,21,22	4.12	7 (38%)	22,30,33	1.94	5 (22%)
1	OMU	S1	179	1	19,22,23	0.64	0	26,31,34	0.93	2 (7%)
1	5MC	S1	2144	1	18,22,23	1.57	4 (22%)	26,32,35	1.20	4 (15%)
44	A2M	LE	1039	44	18,25,26	4.23	6 (33%)	18,36,39	2.96	3 (16%)
48	OMG	LI	3223	48	18,26,27	1.37	3 (16%)	19,38,41	1.46	4 (21%)
46	OMG	LG	2009	46	18,26,27	1.33	2 (11%)	19,38,41	1.49	5 (26%)
47	PSU	LH	2617	47	18,21,22	4.15	7 (38%)	22,30,33	1.95	5 (22%)
47	PSU	LH	2642	47	18,21,22	4.11	7 (38%)	22,30,33	1.88	5 (22%)
45	OMU	LF	1553	45	19,22,23	0.58	0	26,31,34	0.94	2 (7%)
1	OMC	S1	103	1	19,22,23	1.05	1 (5%)	26,31,34	1.13	3 (11%)
45	A2M	LF	1891	45,47	18,25,26	4.21	7 (38%)	18,36,39	2.96	3 (16%)
1	OMU	S1	1744	1	19,22,23	0.55	0	26,31,34	0.85	1 (3%)
44	1MA	LE	931	44	16,25,26	1.45	2 (12%)	18,37,40	1.05	3 (16%)
41	OMU	LB	206	41	19,22,23	0.57	0	26,31,34	0.83	1 (3%)
47	A2M	LH	2809	47	18,25,26	4.19	7 (38%)	18,36,39	3.10	3 (16%)
45	OMG	LF	1835	45,47	18,26,27	1.29	2 (11%)	19,38,41	1.57	4 (21%)
47	OMC	LH	2242	46,47	19,22,23	0.83	0	26,31,34	0.99	3 (11%)
1	PSU	S1	1660	1	18,21,22	4.25	7 (38%)	22,30,33	1.90	5 (22%)
48	OMG	LI	3377	48	18,26,27	1.29	2 (11%)	19,38,41	1.59	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	S1	2180	1	18,25,26	1.00	1 (5%)	18,36,39	1.21	2 (11%)
1	OMU	S1	186	1	19,22,23	0.52	0	26,31,34	1.08	2 (7%)
49	OMG	LJ	3688	49	18,26,27	1.34	2 (11%)	19,38,41	1.62	3 (15%)
49	PSU	LJ	3697	49	18,21,22	4.15	7 (38%)	22,30,33	1.90	5 (22%)
1	MA6	S1	2287	1	19,26,27	1.15	1 (5%)	18,38,41	3.55	2 (11%)
44	OMU	LE	1270	44,45	19,22,23	0.60	0	26,31,34	1.06	2 (7%)
44	PSU	LE	1126	44	18,21,22	4.09	7 (38%)	22,30,33	1.89	5 (22%)
48	PSU	LI	3531	48	18,21,22	4.19	7 (38%)	22,30,33	1.92	5 (22%)
48	PSU	LI	3440	48	18,21,22	4.12	7 (38%)	22,30,33	1.89	5 (22%)
41	PSU	LB	281	41	18,21,22	4.13	7 (38%)	22,30,33	1.72	4 (18%)
1	PSU	S1	121	1	18,21,22	1.41	4 (22%)	22,30,33	1.92	4 (18%)
42	PSU	LC	567	42	18,21,22	4.06	7 (38%)	22,30,33	1.86	5 (22%)
44	PSU	LE	1260	44,48	18,21,22	4.28	8 (44%)	22,30,33	2.09	6 (27%)
45	OMG	LF	1819	44,45	18,26,27	1.31	2 (11%)	19,38,41	1.58	5 (26%)
42	PSU	LC	498	42	18,21,22	4.14	7 (38%)	22,30,33	1.88	5 (22%)
1	PSU	S1	2081	1	18,21,22	4.17	7 (38%)	22,30,33	1.95	5 (22%)
44	OMU	LE	1185	44	19,22,23	0.58	0	26,31,34	0.83	1 (3%)
42	A2M	LC	594	42	18,25,26	4.23	7 (38%)	18,36,39	2.87	3 (16%)
46	PSU	LG	2125	46	18,21,22	4.12	7 (38%)	22,30,33	1.89	6 (27%)
48	OMG	LI	3379	48	18,26,27	1.31	2 (11%)	19,38,41	1.52	5 (26%)
52	PSU	LM	3963	53,52	18,21,22	4.24	7 (38%)	22,30,33	1.84	5 (22%)
1	PSU	S1	1592	1	18,21,22	4.11	7 (38%)	22,30,33	1.91	5 (22%)
48	OMG	LI	3187	48	18,26,27	1.33	2 (11%)	19,38,41	1.47	4 (21%)
40	A2M	LA	97	40	18,25,26	4.14	6 (33%)	18,36,39	3.12	4 (22%)
48	PSU	LI	3332	48	18,21,22	4.10	7 (38%)	22,30,33	1.91	5 (22%)
49	OMU	LJ	3636	49	19,22,23	0.56	0	26,31,34	0.87	1 (3%)
1	OMG	S1	1681	1	18,26,27	1.33	2 (11%)	19,38,41	1.46	4 (21%)
45	OMC	LF	1573	45	19,22,23	1.16	1 (5%)	26,31,34	1.21	4 (15%)
47	OMG	LH	2879	48,47	18,26,27	1.30	2 (11%)	19,38,41	1.48	5 (26%)
48	A2M	LI	3315	48	18,25,26	4.27	7 (38%)	18,36,39	3.01	4 (22%)
1	OMU	S1	702	1	19,22,23	0.57	0	26,31,34	0.91	2 (7%)
1	A2M	S1	533	1	18,25,26	4.21	7 (38%)	18,36,39	2.82	3 (16%)
47	A2M	LH	2769	47	18,25,26	4.06	7 (38%)	18,36,39	3.03	3 (16%)
44	OMG	LE	1217	44	18,26,27	1.31	2 (11%)	19,38,41	1.54	5 (26%)
45	OMC	LF	1836	45,47	19,22,23	0.82	1 (5%)	26,31,34	1.17	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	OMC	LE	949	44	19,22,23	0.78	0	26,31,34	1.02	2 (7%)
47	OMC	LH	2348	47	19,22,23	0.89	1 (5%)	26,31,34	1.06	3 (11%)
1	OMU	S1	704	1	19,22,23	0.52	0	26,31,34	0.93	2 (7%)
40	OMG	LA	41	40	18,26,27	1.34	2 (11%)	19,38,41	1.43	3 (15%)
46	A2M	LG	2022	45,46	18,25,26	4.23	7 (38%)	18,36,39	2.93	3 (16%)
42	PSU	LC	421	42	18,21,22	4.15	7 (38%)	22,30,33	1.76	4 (18%)
47	OMC	LH	2602	47	19,22,23	0.84	0	26,31,34	1.15	2 (7%)
45	PSU	LF	1586	45	18,21,22	4.17	7 (38%)	22,30,33	1.93	5 (22%)
47	A2M	LH	2768	47	18,25,26	4.18	8 (44%)	18,36,39	3.03	4 (22%)
45	A2M	LF	1929	45	18,25,26	4.17	7 (38%)	18,36,39	2.97	3 (16%)
41	OMG	LB	215	41	18,26,27	1.33	2 (11%)	19,38,41	1.54	3 (15%)
47	PSU	LH	2361	47	18,21,22	4.05	7 (38%)	22,30,33	1.87	5 (22%)
48	A2M	LI	3500	48	18,25,26	4.24	7 (38%)	18,36,39	2.92	3 (16%)
45	OMU	LF	1898	45,47	19,22,23	0.62	0	26,31,34	0.98	2 (7%)
51	A2M	LL	3906	60,51	18,25,26	4.25	7 (38%)	18,36,39	2.84	3 (16%)
47	PSU	LH	2330	45,47	18,21,22	4.05	7 (38%)	22,30,33	1.77	5 (22%)
48	PSU	LI	3175	48,47	18,21,22	4.15	7 (38%)	22,30,33	1.95	5 (22%)
47	A2M	LH	2814	47	18,25,26	4.23	7 (38%)	18,36,39	3.07	3 (16%)
47	OMG	LH	2925	48,47	18,26,27	1.34	2 (11%)	19,38,41	1.49	3 (15%)
47	OMG	LH	2776	47	18,26,27	1.32	3 (16%)	19,38,41	1.49	5 (26%)
42	PSU	LC	480	42	18,21,22	4.16	7 (38%)	22,30,33	1.97	5 (22%)
48	PSU	LI	3510	48,2	18,21,22	4.19	7 (38%)	22,30,33	1.92	5 (22%)
1	OMG	S1	641	1	18,26,27	1.35	3 (16%)	19,38,41	1.56	4 (21%)
1	PSU	S1	1378	1	18,21,22	4.04	7 (38%)	22,30,33	1.92	5 (22%)
48	PSU	LI	3446	48	18,21,22	4.27	7 (38%)	22,30,33	1.77	4 (18%)
42	OMG	LC	628	42	18,26,27	1.33	2 (11%)	19,38,41	1.49	5 (26%)
48	PSU	LI	3167	48	18,21,22	4.22	7 (38%)	22,30,33	1.84	5 (22%)
48	PSU	LI	3412	48	18,21,22	4.08	8 (44%)	22,30,33	1.99	6 (27%)
47	OMU	LH	2625	47	19,22,23	0.56	0	26,31,34	1.10	2 (7%)
47	A2M	LH	2849	47	18,25,26	4.18	7 (38%)	18,36,39	3.01	3 (16%)
1	7MG	S1	2078	3,1	22,26,27	1.73	2 (9%)	29,39,42	1.23	5 (17%)
44	OMU	LE	1452	44	19,22,23	0.65	0	26,31,34	0.88	2 (7%)
48	5MC	LI	3456	48,47	18,22,23	1.62	4 (22%)	26,32,35	1.23	3 (11%)
47	PSU	LH	2752	47	18,21,22	4.14	7 (38%)	22,30,33	1.89	5 (22%)
46	OMU	LG	1999	45,46	19,22,23	0.60	0	26,31,34	0.89	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMG	LF	1856	45	18,26,27	1.35	3 (16%)	19,38,41	1.52	3 (15%)
1	PSU	S1	1960	1	18,21,22	4.08	7 (38%)	22,30,33	1.86	5 (22%)
48	OMU	LI	3159	48	19,22,23	0.60	0	26,31,34	0.97	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	S1	1901	1	-	0/5/27/28	0/3/3/3
47	PSU	LH	2842	45,47	-	0/7/25/26	0/2/2/2
1	OMC	S1	38	1	-	0/9/27/28	0/2/2/2
1	A2M	S1	407	1	-	0/5/27/28	0/3/3/3
47	PSU	LH	2621	44,47	-	0/7/25/26	0/2/2/2
47	PSU	LH	2914	48,47	-	0/7/25/26	0/2/2/2
47	OMU	LH	2346	47	-	0/9/27/28	0/2/2/2
48	OMG	LI	3509	48,2	-	0/5/27/28	0/3/3/3
47	PSU	LH	2899	48,47	-	2/7/25/26	0/2/2/2
1	UR3	S1	1597	1	-	0/7/25/26	0/2/2/2
47	PSU	LH	2754	47	-	0/7/25/26	0/2/2/2
48	UR3	LI	3540	48	-	0/7/25/26	0/2/2/2
47	A2M	LH	2349	47	-	2/5/27/28	0/3/3/3
1	PSU	S1	2116	1	-	2/7/25/26	0/2/2/2
44	OMU	LE	1081	44	-	1/9/27/28	0/2/2/2
1	A2M	S1	40	1	-	0/5/27/28	0/3/3/3
44	PSU	LE	1171	44	-	0/7/25/26	0/2/2/2
47	A2M	LH	2744	47	-	2/5/27/28	0/3/3/3
1	PSU	S1	1068	1	-	3/7/25/26	0/2/2/2
48	OMU	LI	3508	48	-	0/9/27/28	0/2/2/2
45	OMC	LF	1822	44,45	-	2/9/27/28	0/2/2/2
48	OMG	LI	3434	48	-	0/5/27/28	0/3/3/3
1	OMG	S1	1536	1,94	-	2/5/27/28	0/3/3/3
45	PSU	LF	1582	45	-	0/7/25/26	0/2/2/2
1	PSU	S1	1591	1	-	0/7/25/26	0/2/2/2
47	PSU	LH	2623	47	-	0/7/25/26	0/2/2/2
44	OMG	LE	1104	44	-	0/5/27/28	0/3/3/3
47	A2M	LH	2358	47	-	1/5/27/28	0/3/3/3
48	OMU	LI	3300	48	-	0/9/27/28	0/2/2/2
1	PSU	S1	1711	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	S1	2041	1	-	1/9/27/28	0/2/2/2
47	PSU	LH	2874	48,47	-	0/7/25/26	0/2/2/2
1	OMU	S1	1679	1	-	0/9/27/28	0/2/2/2
45	OMU	LF	1824	44,45,42	-	0/9/27/28	0/2/2/2
1	PSU	S1	2305	1	-	3/7/25/26	0/2/2/2
47	OMU	LH	2713	47	-	3/9/27/28	0/2/2/2
47	PSU	LH	2802	47	-	4/7/25/26	0/2/2/2
47	OMG	LH	2883	48,47	-	0/5/27/28	0/3/3/3
45	OMG	LF	1662	45	-	2/5/27/28	0/3/3/3
53	PSU	LN	3969	53,52	-	0/7/25/26	0/2/2/2
1	OMG	S1	57	1	-	3/5/27/28	0/3/3/3
1	PSU	S1	640	1	-	3/7/25/26	0/2/2/2
1	OMU	S1	1966	1,29	-	1/9/27/28	0/2/2/2
1	PSU	S1	2131	1	-	0/7/25/26	0/2/2/2
52	OMC	LM	3957	53,52	-	2/9/27/28	0/2/2/2
49	PSU	LJ	3701	49	-	0/7/25/26	0/2/2/2
44	PSU	LE	1198	44	-	0/7/25/26	0/2/2/2
48	OMC	LI	3355	48,44	-	1/9/27/28	0/2/2/2
1	OMG	S1	42	1	-	0/5/27/28	0/3/3/3
47	A2M	LH	2887	48,47	-	1/5/27/28	0/3/3/3
52	PSU	LM	3953	53,52	-	0/7/25/26	0/2/2/2
1	PSU	S1	280	1	-	4/7/25/26	0/2/2/2
44	PSU	LE	1407	44	-	0/7/25/26	0/2/2/2
48	6MZ	LI	3214	48,45	-	4/5/27/28	0/3/3/3
1	PSU	S1	105	1	-	0/7/25/26	0/2/2/2
48	OMC	LI	3222	48	-	0/9/27/28	0/2/2/2
47	JMH	LH	2636	47	-	2/7/25/26	0/2/2/2
42	OMU	LC	491	42	-	2/9/27/28	0/2/2/2
1	PSU	S1	32	1	-	0/7/25/26	0/2/2/2
1	PSU	S1	403	1	-	3/7/25/26	0/2/2/2
47	OMC	LH	2685	47	-	5/9/27/28	0/2/2/2
44	PSU	LE	1184	44	-	0/7/25/26	0/2/2/2
41	PSU	LB	234	41	-	1/7/25/26	0/2/2/2
1	A2M	S1	1096	1	-	3/5/27/28	0/3/3/3
48	PSU	LI	3568	48,47	-	0/7/25/26	0/2/2/2
1	PSU	S1	1715	1	-	1/7/25/26	0/2/2/2
42	PSU	LC	302	42	-	2/7/25/26	0/2/2/2
45	OMG	LF	1883	45	-	0/5/27/28	0/3/3/3
45	OMU	LF	1828	45,47	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	LI	3562	48	-	0/7/25/26	0/2/2/2
45	OMG	LF	1956	45	-	0/5/27/28	0/3/3/3
47	PSU	LH	2586	47	-	1/7/25/26	0/2/2/2
44	OMC	LE	936	44	-	2/9/27/28	0/2/2/2
1	PSU	S1	2065	1	-	0/7/25/26	0/2/2/2
47	PSU	LH	2915	48,47	-	0/7/25/26	0/2/2/2
1	MA6	S1	2288	1	-	2/7/29/30	0/3/3/3
42	PSU	LC	308	42	-	2/7/25/26	0/2/2/2
1	OMG	S1	390	1	-	2/5/27/28	0/3/3/3
1	A2M	S1	649	1	-	2/5/27/28	0/3/3/3
44	OMG	LE	1324	44	-	0/5/27/28	0/3/3/3
47	PSU	LH	2624	47	-	0/7/25/26	0/2/2/2
48	A2M	LI	3367	48,42	-	1/5/27/28	0/3/3/3
1	A2M	S1	565	1	-	2/5/27/28	0/3/3/3
48	A2M	LI	3348	48	-	0/5/27/28	0/3/3/3
47	OMG	LH	2870	47	-	0/5/27/28	0/3/3/3
40	PSU	LA	68	40	-	0/7/25/26	0/2/2/2
41	OMU	LB	247	41	-	5/9/27/28	0/2/2/2
47	OMC	LH	2832	47	-	0/9/27/28	0/2/2/2
49	OMU	LJ	3694	49	-	2/9/27/28	0/2/2/2
45	OMG	LF	1667	45	-	3/5/27/28	0/3/3/3
48	PSU	LI	3204	48	-	0/7/25/26	0/2/2/2
1	PSU	S1	89	1	-	0/7/25/26	0/2/2/2
1	PSU	S1	544	1	-	0/7/25/26	0/2/2/2
1	A2M	S1	110	1	-	2/5/27/28	0/3/3/3
1	OMU	S1	682	1	-	2/9/27/28	0/2/2/2
47	PSU	LH	2591	47	-	0/7/25/26	0/2/2/2
44	PSU	LE	1075	44,48	-	4/7/25/26	0/2/2/2
1	A2M	S1	645	1	-	1/5/27/28	0/3/3/3
46	PSU	LG	2171	46	-	2/7/25/26	0/2/2/2
46	A2M	LG	2005	45,46	-	2/5/27/28	0/3/3/3
47	OMC	LH	2853	47	-	2/9/27/28	0/2/2/2
48	OMU	LI	3171	48,47	-	2/9/27/28	0/2/2/2
1	PSU	S1	27	1	-	0/7/25/26	0/2/2/2
45	OMC	LF	1976	45	-	2/9/27/28	0/2/2/2
2	MIA	S2	37	2	-	4/11/33/34	0/3/3/3
48	5MC	LI	3518	48,64	-	0/7/25/26	0/2/2/2
1	OMC	S1	1625	1	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S1	2101	1	-	2/7/25/26	0/2/2/2
1	OMU	S1	1616	1	-	0/9/27/28	0/2/2/2
44	OMG	LE	1201	44	-	0/5/27/28	0/3/3/3
48	PSU	LI	3503	48	-	0/7/25/26	0/2/2/2
1	A2M	S1	723	1	-	2/5/27/28	0/3/3/3
42	OMC	LC	483	42	-	3/9/27/28	0/2/2/2
47	OMU	LH	2605	47,49	-	0/9/27/28	0/2/2/2
45	OMU	LF	1957	45	-	2/9/27/28	0/2/2/2
1	PSU	S1	1396	1	-	0/7/25/26	0/2/2/2
44	OMG	LE	1208	44	-	0/5/27/28	0/3/3/3
47	OMC	LH	2825	47	-	0/9/27/28	0/2/2/2
1	PSU	S1	1393	1	-	0/7/25/26	0/2/2/2
41	PSU	LB	280	41	-	2/7/25/26	0/2/2/2
40	OMG	LA	74	40	-	3/5/27/28	0/3/3/3
45	PSU	LF	1876	45	-	0/7/25/26	0/2/2/2
49	PSU	LJ	3644	49	-	0/7/25/26	0/2/2/2
45	PSU	LF	1859	45	-	0/7/25/26	0/2/2/2
42	OMG	LC	631	44,42	-	0/5/27/28	0/3/3/3
47	PSU	LH	2742	47	-	2/7/25/26	0/2/2/2
45	A2M	LF	1815	45	-	0/5/27/28	0/3/3/3
1	OMU	S1	1641	1	-	0/9/27/28	0/2/2/2
45	OMU	LF	1504	45	-	2/9/27/28	0/2/2/2
40	A2M	LA	39	40	-	0/5/27/28	0/3/3/3
44	PSU	LE	1363	44	-	0/7/25/26	0/2/2/2
44	A2M	LE	935	44	-	2/5/27/28	0/3/3/3
44	OMC	LE	1165	44	-	2/9/27/28	0/2/2/2
47	5MC	LH	2766	47	-	1/7/25/26	0/2/2/2
1	OMC	S1	2123	1	-	0/9/27/28	0/2/2/2
51	PSU	LL	3865	51	-	0/7/25/26	0/2/2/2
1	OMC	S1	1037	1	-	0/9/27/28	0/2/2/2
45	OMG	LF	1826	44,45	-	0/5/27/28	0/3/3/3
47	A2M	LH	2708	47	-	0/5/27/28	0/3/3/3
1	PSU	S1	1624	1	-	2/7/25/26	0/2/2/2
48	PSU	LI	3185	48	-	0/7/25/26	0/2/2/2
48	OMC	LI	3546	48	-	0/9/27/28	0/2/2/2
1	OMU	S1	8	1	-	6/9/27/28	0/2/2/2
44	PSU	LE	1118	44	-	2/7/25/26	0/2/2/2
44	OMU	LE	1222	44	-	4/9/27/28	0/2/2/2
47	OMG	LH	2897	48,47	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A2M	LI	3521	48	-	0/5/27/28	0/3/3/3
48	OMC	LI	3374	48	-	0/9/27/28	0/2/2/2
41	A2M	LB	183	41	-	0/5/27/28	0/3/3/3
49	PSU	LJ	3680	49	-	1/7/25/26	0/2/2/2
46	OMU	LG	2129	46	-	1/9/27/28	0/2/2/2
47	OMC	LH	2313	45,47	-	0/9/27/28	0/2/2/2
42	OMC	LC	577	42	-	3/9/27/28	0/2/2/2
1	A2M	S1	1549	1	-	2/5/27/28	0/3/3/3
48	OMC	LI	3465	48	-	0/9/27/28	0/2/2/2
42	OMG	LC	541	40,42	-	1/5/27/28	0/3/3/3
46	PSU	LG	2119	46	-	0/7/25/26	0/2/2/2
44	A2M	LE	1121	44	-	0/5/27/28	0/3/3/3
42	OMC	LC	537	40,42	-	2/9/27/28	0/2/2/2
1	B8N	S1	1601	1	1/1/7/7	3/16/34/35	0/2/2/2
1	A2M	S1	1063	1	-	2/5/27/28	0/3/3/3
44	A2M	LE	1106	44	-	1/5/27/28	0/3/3/3
44	PSU	LE	1365	44	-	0/7/25/26	0/2/2/2
45	PSU	LF	1692	45	-	0/7/25/26	0/2/2/2
44	7MG	LE	938	44	-	0/7/37/38	0/3/3/3
1	OMC	S1	2142	1	-	2/9/27/28	0/2/2/2
1	OMC	S1	99	1	-	1/9/27/28	0/2/2/2
47	OMG	LH	2610	47	-	1/5/27/28	0/3/3/3
45	A2M	LF	1888	45	-	0/5/27/28	0/3/3/3
48	PSU	LI	3206	48	-	1/7/25/26	0/2/2/2
48	OMG	LI	3191	48,3	-	3/5/27/28	0/3/3/3
1	PSU	S1	2129	1	-	0/7/25/26	0/2/2/2
1	OMG	S1	180	1	-	3/5/27/28	0/3/3/3
44	OMC	LE	1312	44	-	0/9/27/28	0/2/2/2
1	OMG	S1	485	1	-	2/5/27/28	0/3/3/3
47	A2M	LH	2920	48,47	-	1/5/27/28	0/3/3/3
48	A2M	LI	3533	48,47	-	0/5/27/28	0/3/3/3
46	PSU	LG	2154	46	-	0/7/25/26	0/2/2/2
1	OMC	S1	393	1	-	0/9/27/28	0/2/2/2
45	PSU	LF	1926	45	-	2/7/25/26	0/2/2/2
48	OMC	LI	3347	48	-	0/9/27/28	0/2/2/2
49	OMU	LJ	3718	49	-	1/9/27/28	0/2/2/2
48	PSU	LI	3542	48,47	-	0/7/25/26	0/2/2/2
45	OMG	LF	1683	45	-	0/5/27/28	0/3/3/3
1	A2M	S1	28	1	-	0/5/27/28	0/3/3/3
47	OMU	LH	2909	48,47	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMG	LI	3504	48	-	1/5/27/28	0/3/3/3
45	OMU	LF	1681	45	-	2/9/27/28	0/2/2/2
48	OMC	LI	3535	48	-	0/9/27/28	0/2/2/2
1	OMG	S1	2075	1	-	2/5/27/28	0/3/3/3
1	OMG	S1	1705	1	-	2/5/27/28	0/3/3/3
48	PSU	LI	2999	48,47	-	1/7/25/26	0/2/2/2
45	PSU	LF	1568	45,54	-	1/7/25/26	0/2/2/2
47	A2M	LH	2812	47	-	1/5/27/28	0/3/3/3
47	B8H	LH	2904	48,47	-	0/7/25/26	0/2/2/2
44	PSU	LE	1266	44	-	0/7/25/26	0/2/2/2
48	OMG	LI	3401	48,47	-	0/5/27/28	0/3/3/3
44	OMC	LE	1218	44	-	0/9/27/28	0/2/2/2
48	OMC	LI	3208	48	-	4/9/27/28	0/2/2/2
48	PSU	LI	3444	48	-	0/7/25/26	0/2/2/2
44	A2M	LE	1204	44	-	0/5/27/28	0/3/3/3
47	PSU	LH	2837	47	-	0/7/25/26	0/2/2/2
44	PSU	LE	1235	44	-	0/7/25/26	0/2/2/2
47	OMU	LH	2806	47	-	0/9/27/28	0/2/2/2
1	A2M	S1	1900	1,27	-	2/5/27/28	0/3/3/3
48	PSU	LI	3145	48	-	0/7/25/26	0/2/2/2
1	A2M	S1	1371	1	-	3/5/27/28	0/3/3/3
48	PSU	LI	3451	48	-	0/7/25/26	0/2/2/2
40	PSU	LA	16	40,42	-	0/7/25/26	0/2/2/2
1	PSU	S1	1554	1	-	2/7/25/26	0/2/2/2
1	OMC	S1	621	1	-	2/9/27/28	0/2/2/2
49	PSU	LJ	3591	49	-	0/7/25/26	0/2/2/2
46	OMG	LG	2146	46	-	2/5/27/28	0/3/3/3
1	A2M	S1	2046	1	-	0/5/27/28	0/3/3/3
47	PSU	LH	2746	47	-	3/7/25/26	0/2/2/2
48	PSU	LI	3042	48	-	3/7/25/26	0/2/2/2
44	OMU	LE	1189	44	-	0/9/27/28	0/2/2/2
44	PSU	LE	1023	44	-	0/7/25/26	0/2/2/2
47	OMU	LH	2835	47	-	3/9/27/28	0/2/2/2
1	PSU	S1	176	1	-	2/7/25/26	0/2/2/2
45	A2M	LF	1502	45	-	0/5/27/28	0/3/3/3
45	A2M	LF	1738	45	-	0/5/27/28	0/3/3/3
47	PSU	LH	2679	47	-	0/7/25/26	0/2/2/2
44	OMU	LE	1315	44	-	0/9/27/28	0/2/2/2
1	PSU	S1	465	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	S1	179	1	-	0/9/27/28	0/2/2/2
1	5MC	S1	2144	1	-	0/7/25/26	0/2/2/2
44	A2M	LE	1039	44	-	0/5/27/28	0/3/3/3
48	OMG	LI	3223	48	-	1/5/27/28	0/3/3/3
46	OMG	LG	2009	46	-	1/5/27/28	0/3/3/3
47	PSU	LH	2617	47	-	0/7/25/26	0/2/2/2
47	PSU	LH	2642	47	-	0/7/25/26	0/2/2/2
45	OMU	LF	1553	45	-	0/9/27/28	0/2/2/2
1	OMC	S1	103	1	-	3/9/27/28	0/2/2/2
45	A2M	LF	1891	45,47	-	0/5/27/28	0/3/3/3
1	OMU	S1	1744	1	-	0/9/27/28	0/2/2/2
44	1MA	LE	931	44	-	0/3/25/26	0/3/3/3
41	OMU	LB	206	41	-	0/9/27/28	0/2/2/2
47	A2M	LH	2809	47	-	0/5/27/28	0/3/3/3
45	OMG	LF	1835	45,47	-	2/5/27/28	0/3/3/3
47	OMC	LH	2242	46,47	-	3/9/27/28	0/2/2/2
1	PSU	S1	1660	1	-	0/7/25/26	0/2/2/2
48	OMG	LI	3377	48	-	2/5/27/28	0/3/3/3
1	A2M	S1	2180	1	-	0/5/27/28	0/3/3/3
1	OMU	S1	186	1	-	1/9/27/28	0/2/2/2
49	OMG	LJ	3688	49	-	2/5/27/28	0/3/3/3
49	PSU	LJ	3697	49	-	2/7/25/26	0/2/2/2
1	MA6	S1	2287	1	-	0/7/29/30	0/3/3/3
44	OMU	LE	1270	44,45	-	0/9/27/28	0/2/2/2
44	PSU	LE	1126	44	-	3/7/25/26	0/2/2/2
48	PSU	LI	3531	48	-	1/7/25/26	0/2/2/2
48	PSU	LI	3440	48	-	0/7/25/26	0/2/2/2
41	PSU	LB	281	41	-	3/7/25/26	0/2/2/2
1	PSU	S1	121	1	-	0/7/25/26	0/2/2/2
42	PSU	LC	567	42	-	1/7/25/26	0/2/2/2
44	PSU	LE	1260	44,48	-	3/7/25/26	0/2/2/2
45	OMG	LF	1819	44,45	-	5/5/27/28	0/3/3/3
42	PSU	LC	498	42	-	0/7/25/26	0/2/2/2
1	PSU	S1	2081	1	-	0/7/25/26	0/2/2/2
44	OMU	LE	1185	44	-	1/9/27/28	0/2/2/2
42	A2M	LC	594	42	-	0/5/27/28	0/3/3/3
46	PSU	LG	2125	46	-	1/7/25/26	0/2/2/2
48	OMG	LI	3379	48	-	0/5/27/28	0/3/3/3
52	PSU	LM	3963	53,52	-	0/7/25/26	0/2/2/2
1	PSU	S1	1592	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMG	LI	3187	48	-	0/5/27/28	0/3/3/3
40	A2M	LA	97	40	-	2/5/27/28	0/3/3/3
48	PSU	LI	3332	48	-	0/7/25/26	0/2/2/2
49	OMU	LJ	3636	49	-	1/9/27/28	0/2/2/2
1	OMG	S1	1681	1	-	0/5/27/28	0/3/3/3
45	OMC	LF	1573	45	-	5/9/27/28	0/2/2/2
47	OMG	LH	2879	48,47	-	1/5/27/28	0/3/3/3
48	A2M	LI	3315	48	-	2/5/27/28	0/3/3/3
1	OMU	S1	702	1	-	0/9/27/28	0/2/2/2
1	A2M	S1	533	1	-	0/5/27/28	0/3/3/3
47	A2M	LH	2769	47	-	3/5/27/28	0/3/3/3
44	OMG	LE	1217	44	-	0/5/27/28	0/3/3/3
45	OMC	LF	1836	45,47	-	0/9/27/28	0/2/2/2
44	OMC	LE	949	44	-	1/9/27/28	0/2/2/2
47	OMC	LH	2348	47	-	0/9/27/28	0/2/2/2
1	OMU	S1	704	1	-	1/9/27/28	0/2/2/2
40	OMG	LA	41	40	-	0/5/27/28	0/3/3/3
46	A2M	LG	2022	45,46	-	3/5/27/28	0/3/3/3
42	PSU	LC	421	42	-	0/7/25/26	0/2/2/2
47	OMC	LH	2602	47	-	5/9/27/28	0/2/2/2
45	PSU	LF	1586	45	-	0/7/25/26	0/2/2/2
47	A2M	LH	2768	47	-	2/5/27/28	0/3/3/3
45	A2M	LF	1929	45	-	2/5/27/28	0/3/3/3
41	OMG	LB	215	41	-	1/5/27/28	0/3/3/3
47	PSU	LH	2361	47	-	0/7/25/26	0/2/2/2
48	A2M	LI	3500	48	-	2/5/27/28	0/3/3/3
45	OMU	LF	1898	45,47	-	0/9/27/28	0/2/2/2
51	A2M	LL	3906	60,51	-	2/5/27/28	0/3/3/3
47	PSU	LH	2330	45,47	-	0/7/25/26	0/2/2/2
48	PSU	LI	3175	48,47	-	0/7/25/26	0/2/2/2
47	A2M	LH	2814	47	-	0/5/27/28	0/3/3/3
47	OMG	LH	2925	48,47	-	3/5/27/28	0/3/3/3
47	OMG	LH	2776	47	-	3/5/27/28	0/3/3/3
42	PSU	LC	480	42	-	0/7/25/26	0/2/2/2
48	PSU	LI	3510	48,2	-	1/7/25/26	0/2/2/2
1	OMG	S1	641	1	-	2/5/27/28	0/3/3/3
1	PSU	S1	1378	1	-	0/7/25/26	0/2/2/2
48	PSU	LI	3446	48	-	3/7/25/26	0/2/2/2
42	OMG	LC	628	42	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	LI	3167	48	-	5/7/25/26	0/2/2/2
48	PSU	LI	3412	48	-	0/7/25/26	0/2/2/2
47	OMU	LH	2625	47	-	0/9/27/28	0/2/2/2
47	A2M	LH	2849	47	-	1/5/27/28	0/3/3/3
1	7MG	S1	2078	3,1	-	2/7/37/38	0/3/3/3
44	OMU	LE	1452	44	-	0/9/27/28	0/2/2/2
48	5MC	LI	3456	48,47	-	4/7/25/26	0/2/2/2
47	PSU	LH	2752	47	-	0/7/25/26	0/2/2/2
46	OMU	LG	1999	45,46	-	0/9/27/28	0/2/2/2
45	OMG	LF	1856	45	-	2/5/27/28	0/3/3/3
1	PSU	S1	1960	1	-	0/7/25/26	0/2/2/2
48	OMU	LI	3159	48	-	0/9/27/28	0/2/2/2

The worst 5 of 1348 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S1	1371	A2M	O4'-C1'	15.42	1.62	1.41
47	LH	2708	A2M	O4'-C1'	15.36	1.62	1.41
40	LA	39	A2M	O4'-C1'	15.36	1.62	1.41
51	LL	3906	A2M	O4'-C1'	15.29	1.62	1.41
48	LI	3315	A2M	O4'-C1'	15.29	1.62	1.41

The worst 5 of 1210 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S1	2288	MA6	N1-C6-N6	-14.51	101.79	117.06
1	S1	2287	MA6	N1-C6-N6	-13.76	102.57	117.06
1	S1	110	A2M	C5-C6-N6	9.57	134.90	120.35
1	S1	565	A2M	C5-C6-N6	9.45	134.72	120.35
47	LH	2809	A2M	C5-C6-N6	9.42	134.66	120.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	S1	1601	B8N	C33

5 of 318 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S1	57	OMG	O4'-C4'-C5'-O5'
1	S1	57	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	S1	110	A2M	C1'-C2'-O2'-CM'
1	S1	180	OMG	C1'-C2'-O2'-CM2
1	S1	280	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

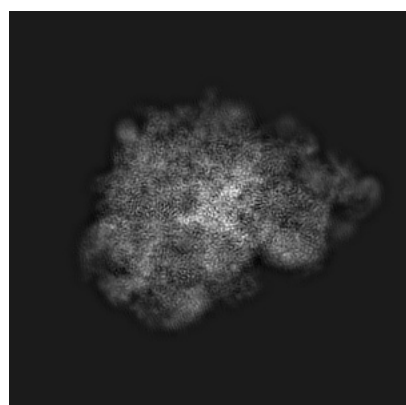
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11232. These allow visual inspection of the internal detail of the map and identification of artifacts.

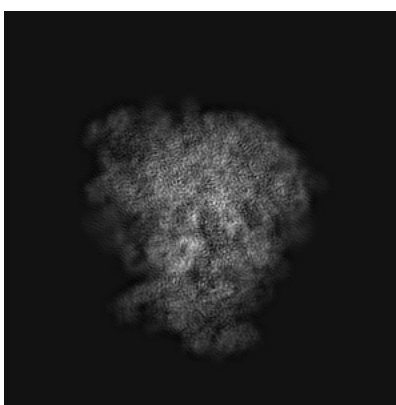
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

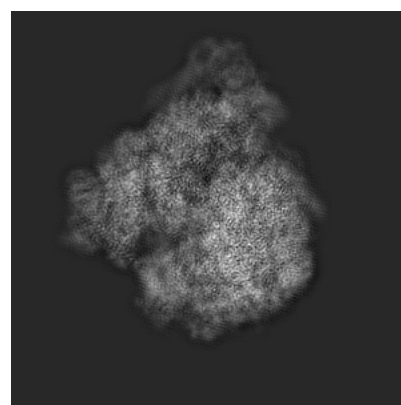
6.1.1 Primary map



X



Y

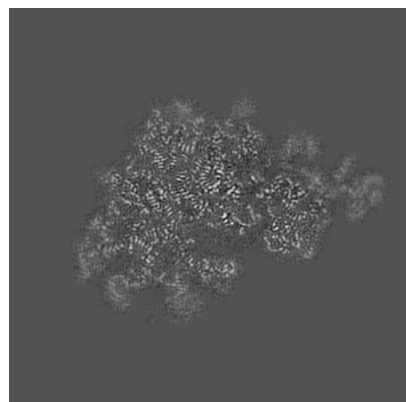


Z

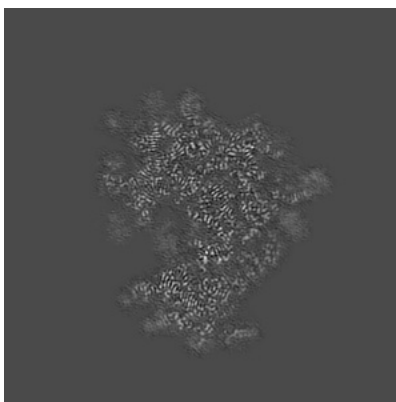
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

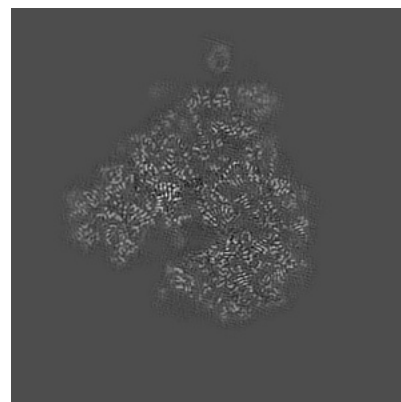
6.2.1 Primary map



X Index: 200



Y Index: 200

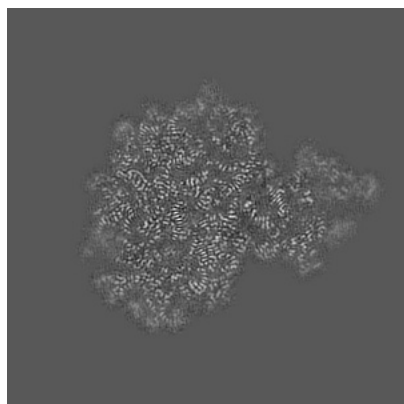


Z Index: 200

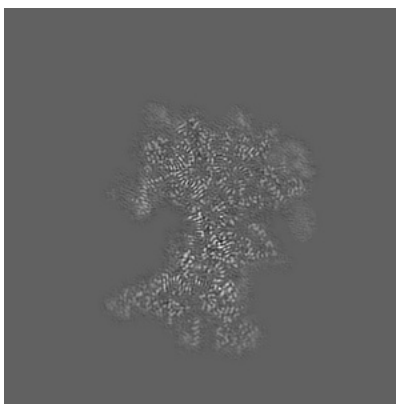
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

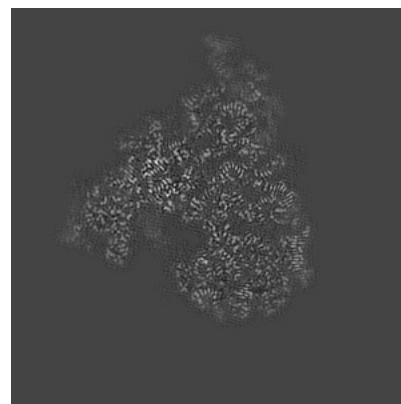
6.3.1 Primary map



X Index: 220



Y Index: 224

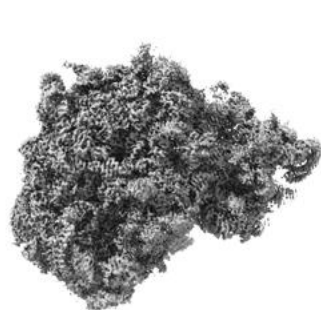


Z Index: 208

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

6.4 Orthogonal surface views [i](#)

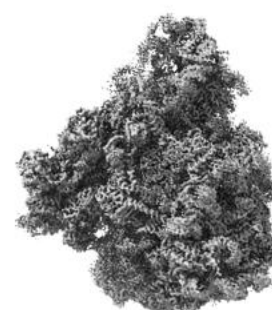
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

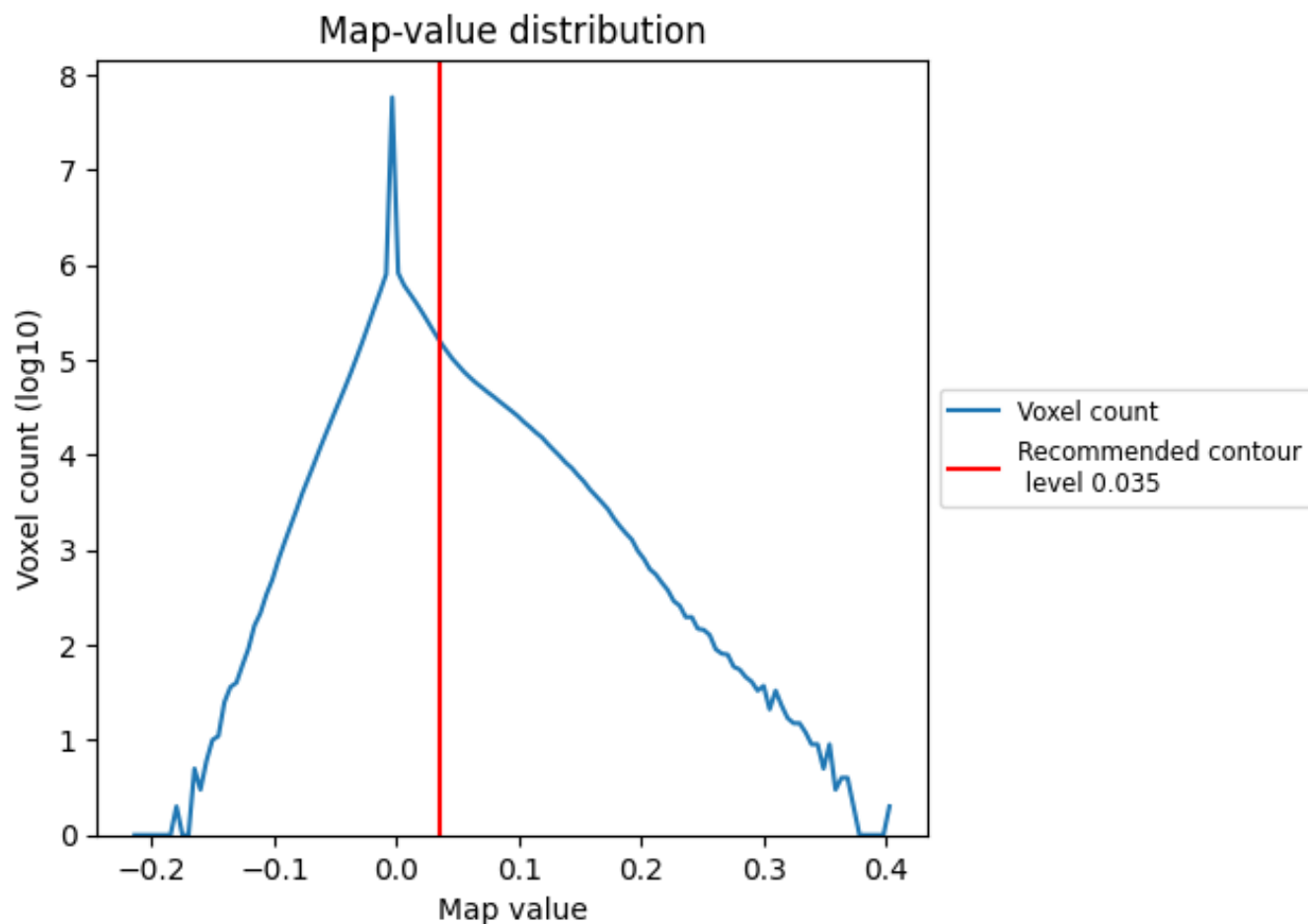
6.5 Mask visualisation

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

7 Map analysis [i](#)

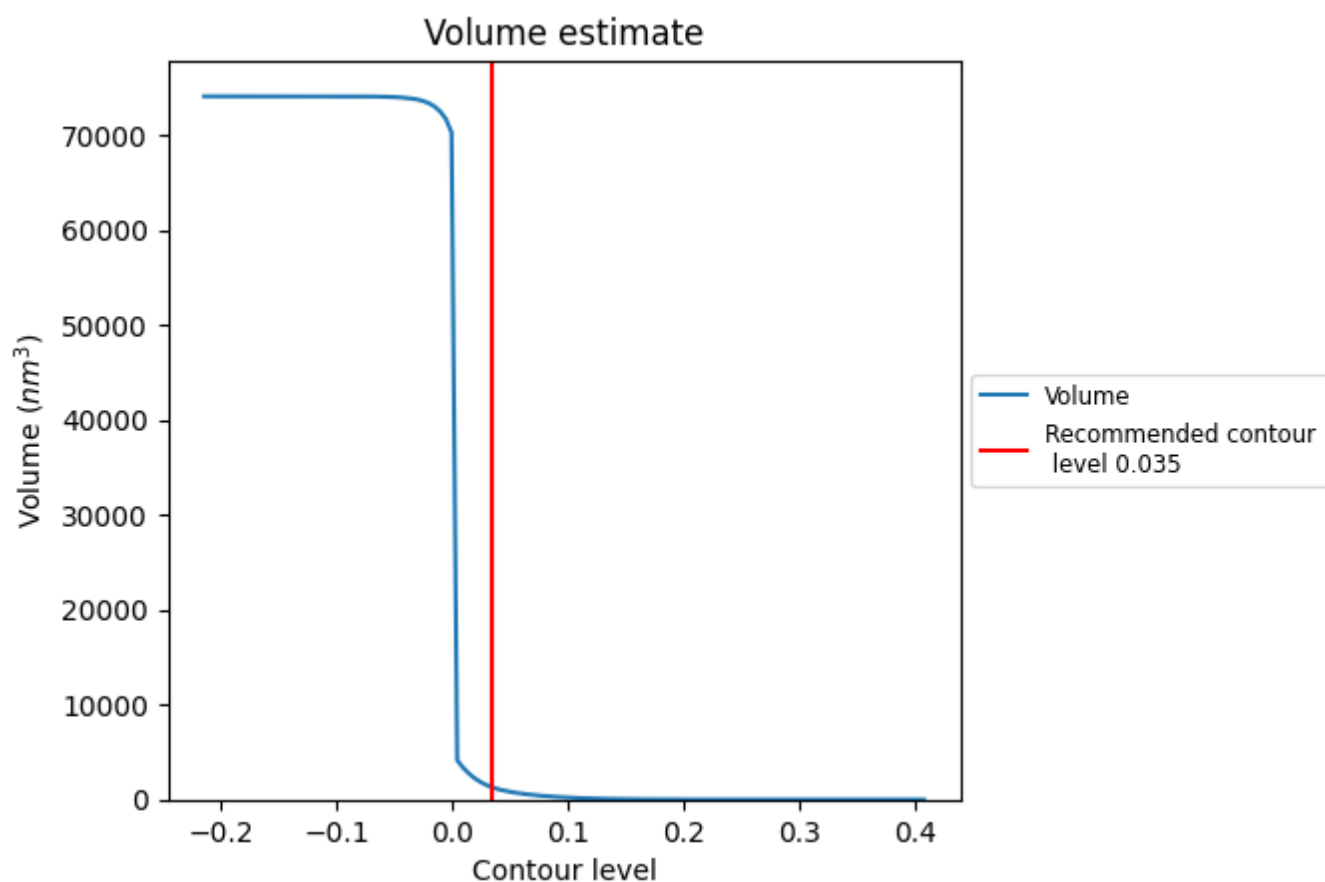
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

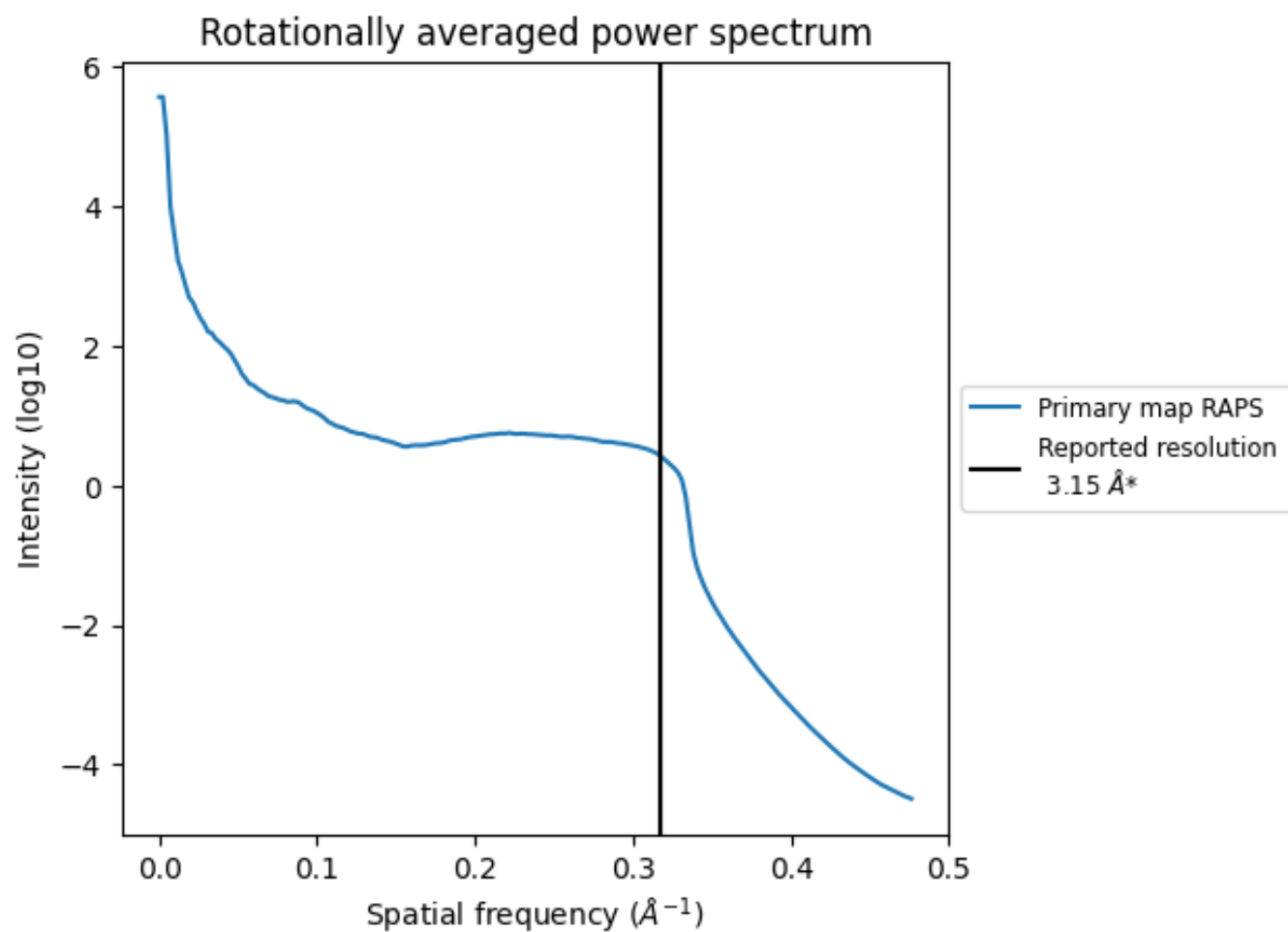
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1287 nm³; this corresponds to an approximate mass of 1163 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.317 Å⁻¹

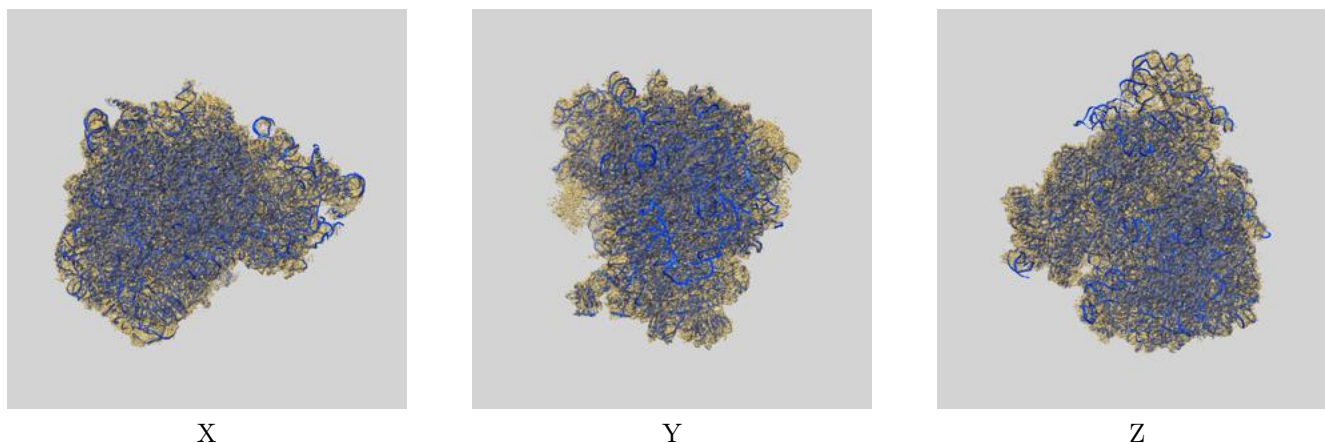
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

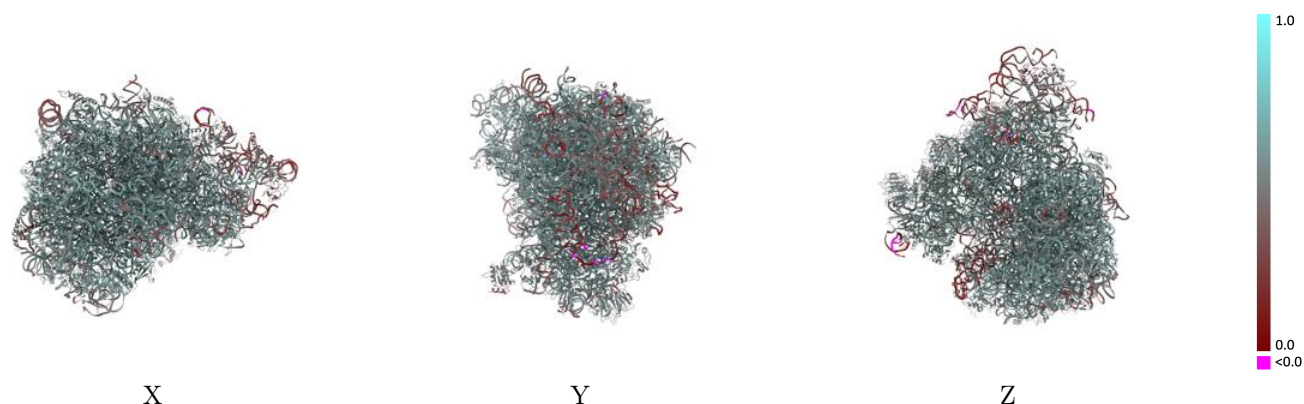
This section contains information regarding the fit between EMDB map EMD-11232 and PDB model 6ZJ3. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)



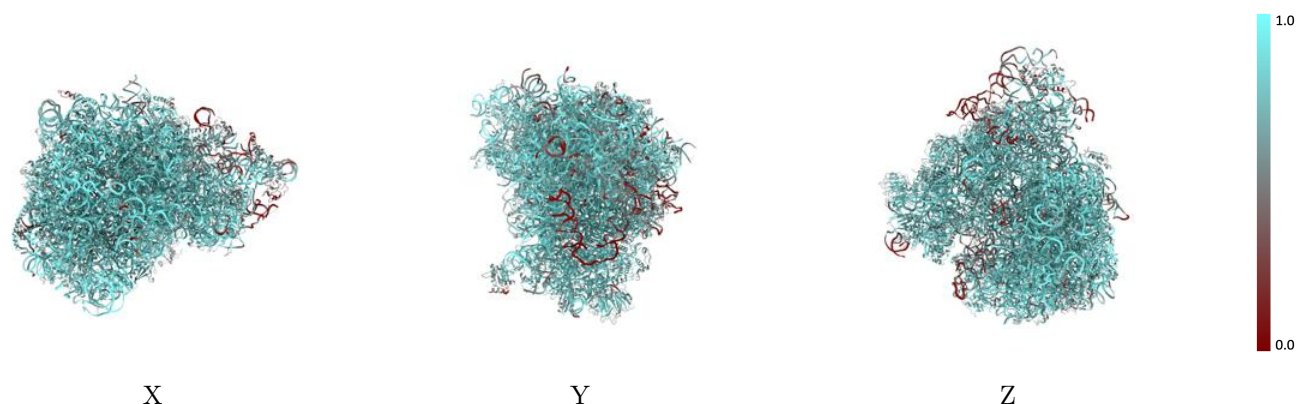
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



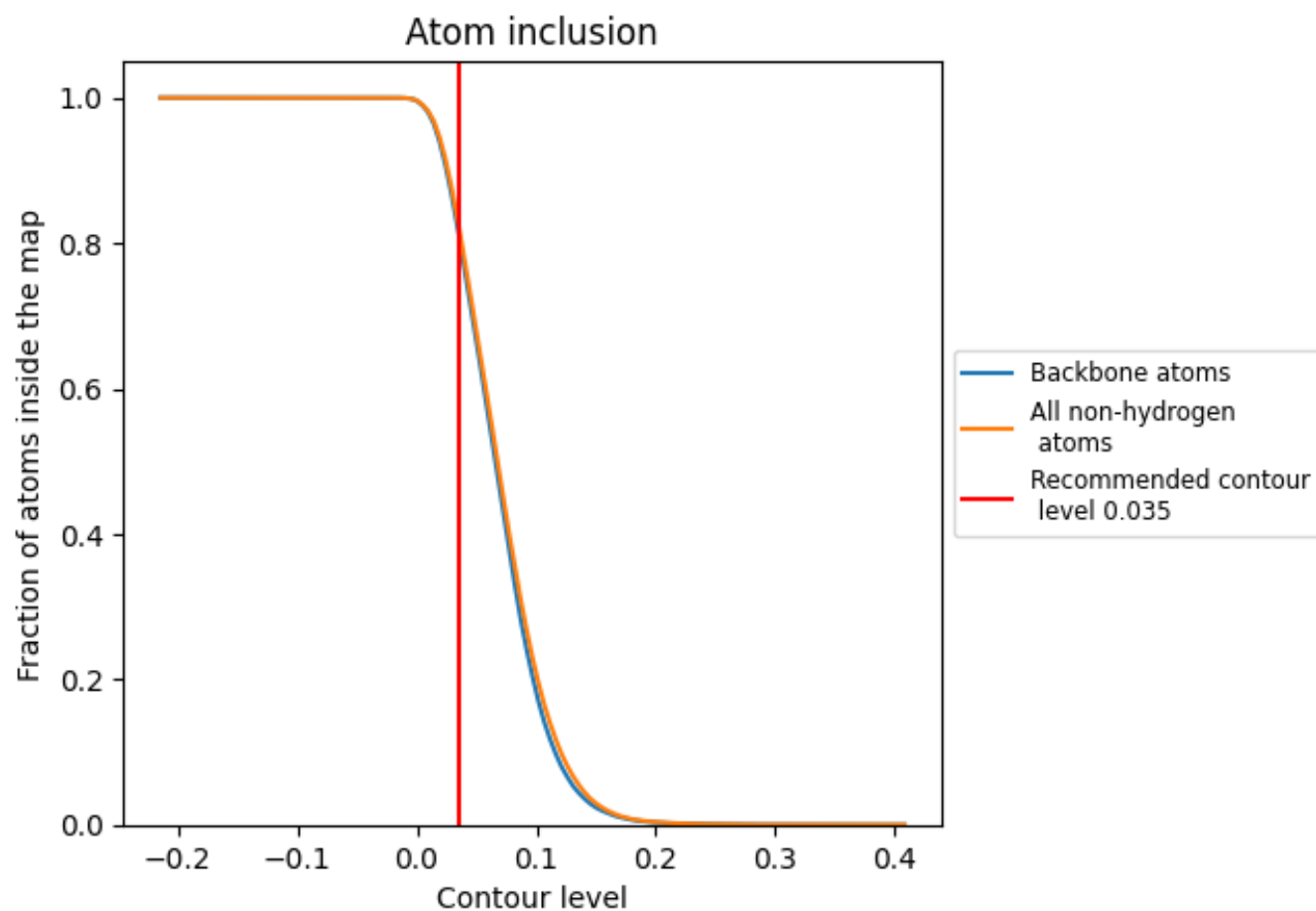
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 83% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8254	 0.5480
L1	 0.7850	 0.5730
L2	 0.8831	 0.5940
L3	 0.8982	 0.5890
L4	 0.8344	 0.6000
L5	 0.8543	 0.5980
L6	 0.6848	 0.5090
L7	 0.7020	 0.5340
LA	 0.9483	 0.5950
LB	 0.9540	 0.6010
LC	 0.8732	 0.5390
LD	 0.8813	 0.5420
LE	 0.8771	 0.5470
LF	 0.9334	 0.5980
LG	 0.9005	 0.5740
LH	 0.9033	 0.5750
LI	 0.8659	 0.5530
LJ	 0.9544	 0.6030
LK	 0.8832	 0.5600
LL	 0.8452	 0.5070
LM	 0.9465	 0.5950
LN	 0.7323	 0.4480
LO	 0.9601	 0.5900
LP	 0.8591	 0.6080
LQ	 0.8709	 0.6000
LR	 0.8075	 0.5750
LS	 0.7780	 0.5390
LT	 0.8395	 0.5800
LU	 0.6725	 0.5130
LV	 0.7457	 0.5500
LW	 0.8539	 0.5900
LX	 0.8020	 0.5650
LY	 0.8502	 0.5960
LZ	 0.8282	 0.5720
La	 0.8282	 0.5970















































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Chain	Atom inclusion	Q-score
Lb	 0.8881	 0.6130
Lc	 0.7555	 0.5610
Ld	 0.8312	 0.5660
Le	 0.8350	 0.5980
Lf	 0.7545	 0.5550
Lg	 0.8632	 0.5930
Lh	 0.8061	 0.5860
Li	 0.8697	 0.5970
Lj	 0.6440	 0.5160
Lk	 0.7921	 0.5670
Ll	 0.8214	 0.5720
Lm	 0.8264	 0.5920
Ln	 0.7600	 0.5530
Lo	 0.7611	 0.5570
Lp	 0.8018	 0.5710
Lq	 0.7702	 0.5490
Lr	 0.8384	 0.5860
Ls	 0.7943	 0.5590
Lt	 0.8635	 0.5800
Lu	 0.8429	 0.5960
Lv	 0.8360	 0.6090
Lw	 0.8369	 0.5830
Lx	 0.8095	 0.5780
Ly	 0.8343	 0.5860
Lz	 0.6993	 0.5420
S1	 0.8231	 0.5160
S2	 0.2835	 0.2810
S3	 0.7968	 0.4760
S4	 0.5102	 0.2660
S5	 0.9482	 0.5610
SA	 0.7138	 0.5350
SB	 0.8007	 0.5490
SC	 0.7951	 0.5440
SD	 0.7709	 0.5550
SE	 0.8011	 0.5790
SF	 0.8048	 0.5660
SG	 0.7118	 0.5330
SH	 0.8016	 0.5490
SI	 0.5892	 0.4930
SJ	 0.8289	 0.5840
SK	 0.8222	 0.5720
SL	 0.8070	 0.5640

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Chain	Atom inclusion	Q-score
SM	 0.7442	 0.5290
SN	 0.7952	 0.5540
SO	 0.7318	 0.5530
SP	 0.8332	 0.5900
SQ	 0.5150	 0.4050
SR	 0.7941	 0.5510
SS	 0.8995	 0.5890
ST	 0.7890	 0.5650
SU	 0.8529	 0.6060
SV	 0.7216	 0.5110
SW	 0.7832	 0.5500
SX	 0.7960	 0.5450
SY	 0.7243	 0.5490
SZ	 0.7994	 0.5560
Sa	 0.7614	 0.5440
Sb	 0.8275	 0.5730
Sc	 0.7477	 0.5580
Sd	 0.7098	 0.5040
Se	 0.7209	 0.5180
Sf	 0.6559	 0.4920
Sg	 0.4737	 0.3850
Sh	 0.7211	 0.5050