



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2023 – 10:25 PM EDT

PDB ID : 8GLP
EMDB ID : EMD-40205
Title : mRNA decoding in human is kinetically and structurally distinct from bacteria
(Consensus LSU focused refined structure)
Authors : Holm, M.; Natchiar, K.S.; Rundlet, E.J.; Myasnikov, A.G.; Watson, Z.L.;
Altman, R.B.; Blanchard, S.C.
Deposited on : 2023-03-22
Resolution : 1.67 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:

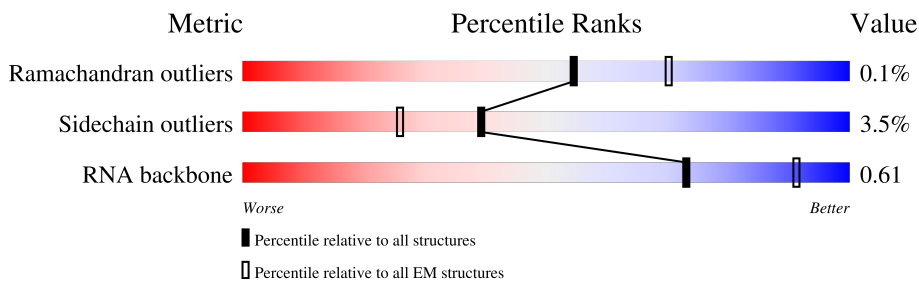
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.67 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	S2	1869	
2	L8	156	
3	L5	5069	
4	L7	120	
5	SB	264	
6	SA	295	
7	SD	243	
8	SJ	194	

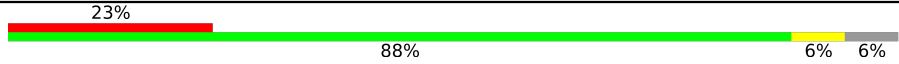

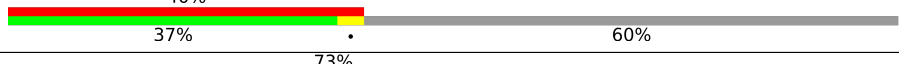
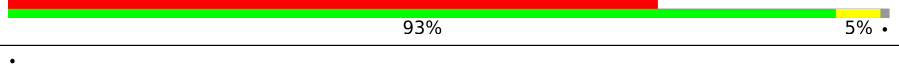
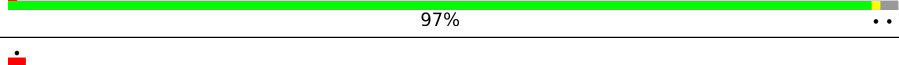
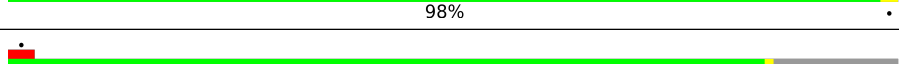
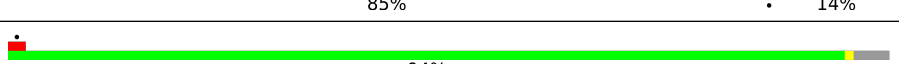
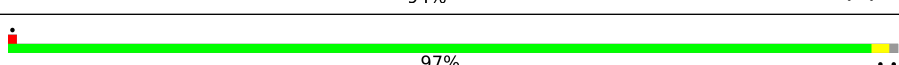
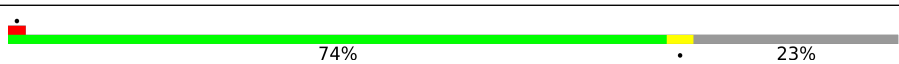

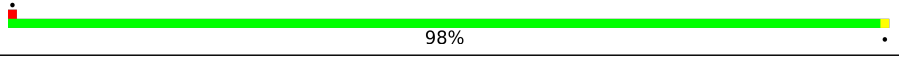
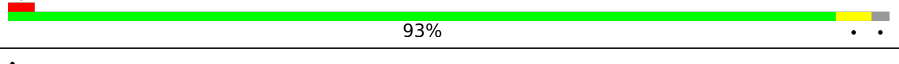
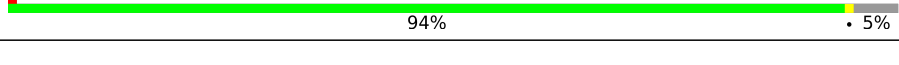

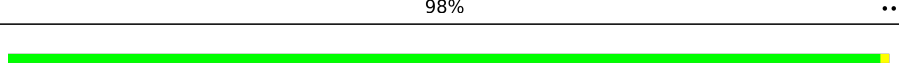
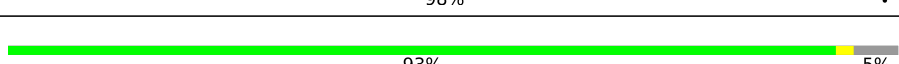
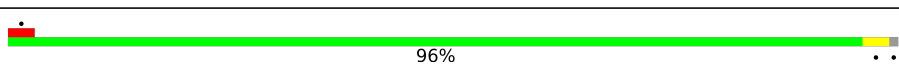
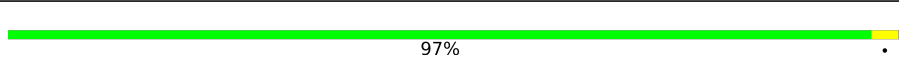
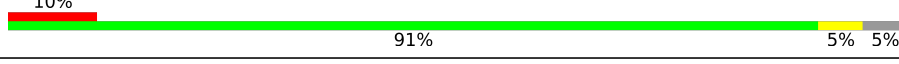
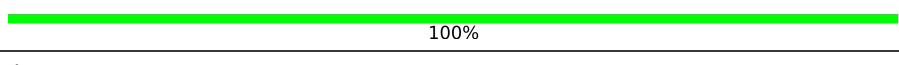
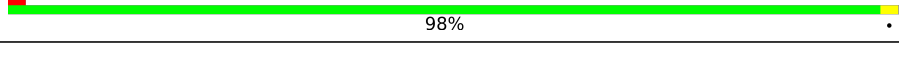




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Mol	Chain	Length	Quality of chain
9	SE	263	8% 98%
10	SC	293	73% 24%
11	SG	249	33% 92% 5%
12	SF	204	9% 88% 7%
13	SH	194	29% 91% 7%
14	SW	130	97%
15	SI	208	14% 92% 7%
16	SQ	146	12% 91% 5%
17	SU	119	33% 83% 15%
18	SK	165	30% 56% 42%
19	SO	151	5% 88% 11%
20	SX	143	93% 5%
21	SM	132	92% 80% 11% 8%
22	SS	152	11% 93% 5%
23	Sd	56	7% 93% 5%
24	SN	151	97%
25	SL	158	9% 89% 8%
26	SR	135	29% 93% 7%
27	SP	145	34% 85% 6% 10%
28	ST	145	16% 91% 7%
29	SV	83	7% 95% 5%
30	SY	133	20% 92% 7%
31	SZ	125	21% 62% 5% 33%
32	Sa	115	83% 14%
33	Sb	84	12% 93% 6%




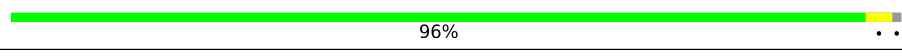
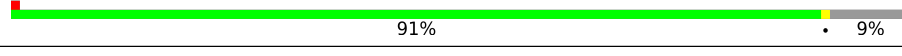
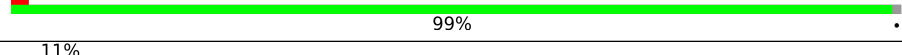

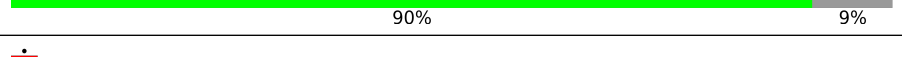
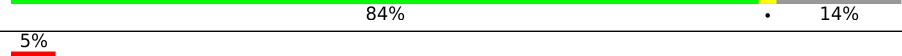
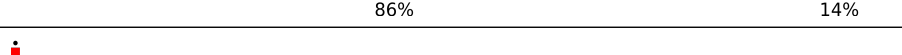
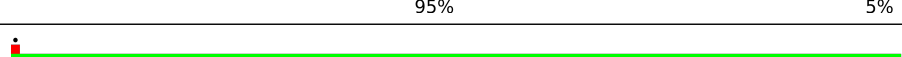
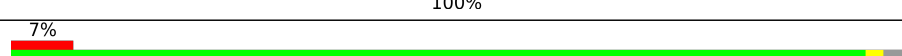
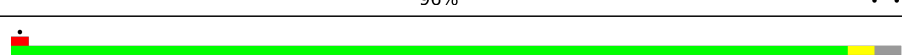
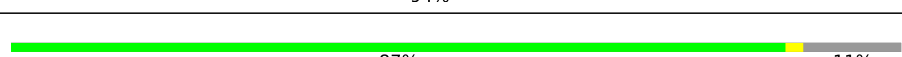
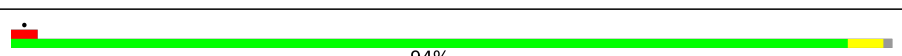
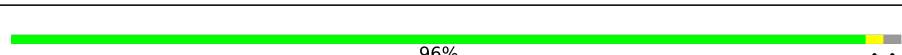
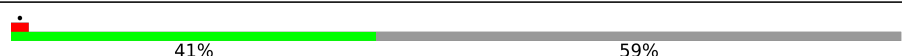
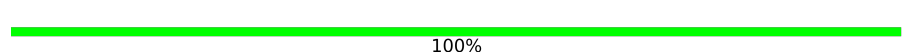
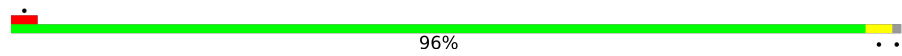
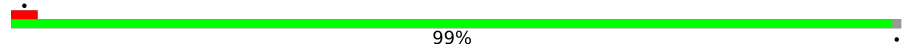

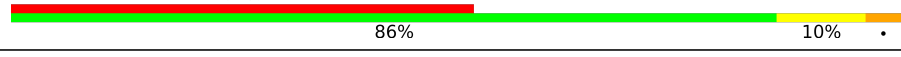
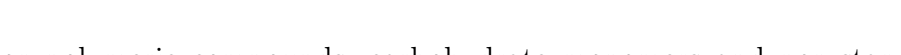
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Mol	Chain	Length	Quality of chain
34	Sc	69	
35	Se	133	
36	Sf	156	
37	Sg	317	
38	LA	257	
39	LB	403	
40	LC	427	
41	LJ	178	
42	LH	192	
43	LE	288	
44	LG	266	
45	LO	203	
46	LL	211	
47	LV	140	
48	LM	215	
49	La	148	
50	LN	204	
51	LI	214	
52	LD	297	
53	LQ	188	
54	LR	196	
55	LS	176	
56	LT	160	
57	LP	184	
58	LU	128	

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Mol	Chain	Length	Quality of chain
59	LX	156	 75% 24%
60	LY	145	 87% 6% 8%
61	LW	157	 34% 74% 25%
62	LZ	136	 96%
63	Lr	137	 91% 9%
64	Lh	123	 99%
65	Lb	159	 11% 68% 30%
66	LF	248	 90% 9%
67	Lc	115	 84% 14%
68	Ld	125	 5% 86% 14%
69	Le	135	 95% 5%
70	Lf	110	 100%
71	Lg	117	 7% 96%
72	Li	105	 94%
73	Lj	97	 87% 11%
74	Lk	70	 94%
75	Ll	51	 96%
76	Lm	128	 41% 59%
77	Ln	25	 100%
78	Lo	106	 96%
79	Lp	92	 99%
80	mR	60	 8% 8% 5% 87%
81	Pt	77	 52% 86% 10%

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
6	SAC	SA	2	-	X	-	-

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 220877 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
			Total	C	N	O	P		
1	S2	1672	35736	15981	6403	11681	1671	0	0

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L8	156	3316	1482	585	1094	155	0	0

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L5	3546	76116	33935	13923	24712	3546	1	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L7	120	2558	1141	456	842	119	0	0

- Molecule 5 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SB	223	1806	1145	325	322	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SA	222	1750	1111	306	325	8	0	0

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SD	226	1756	1119	315	314	8	0	0

- Molecule 8 is a protein called 40S ribosomal protein S9.

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

- Molecule 9 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 10 is a protein called 40S ribosomal protein S2.

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

- Molecule 11 is a protein called 40S ribosomal protein S6.

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

- Molecule 12 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SF	189	1494	934	284	269	7	0	0

- Molecule 13 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SH	189	1517	966	279	271	1	0	0

- Molecule 14 is a protein called 40S ribosomal protein S15a.

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

- Molecule 15 is a protein called 40S ribosomal protein S8.

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

- Molecule 16 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	SQ	141	1123	715	212	193	3	0	0

- Molecule 17 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	SU	101	803	504	153	142	4	0	0

- Molecule 18 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	SK	96	810	530	143	131	6	0	0

- Molecule 19 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	SO	135	1009	618	198	187	6	0	0

- Molecule 20 is a protein called 40S ribosomal protein S23 (uS12).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	SX	140	1088	687	215	183	3	0	0

- Molecule 21 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SM	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 22 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SS	148	Total	C	N	O	S	0	0
			1214	761	245	207	1		

- Molecule 23 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Sd	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 24 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SN	150	Total	C	N	O	S	1	0
			1214	778	231	204	1		

- Molecule 25 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SL	146	Total	C	N	O	S	0	0
			1200	766	226	202	6		

- Molecule 26 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SR	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		

- Molecule 27 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SP	131	Total	C	N	O	S	0	0
			1078	684	204	183	7		

- Molecule 28 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	ST	142	1121	707	212	199	3	1	0

- Molecule 29 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	SV	83	639	395	117	122	5	0	0

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	SY	131	1065	673	209	178	5	0	0

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	SZ	84	674	433	126	114	1	0	0

- Molecule 32 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Sa	99	800	497	168	130	5	1	0

- Molecule 33 is a protein called 40S ribosomal protein S27.

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

- Molecule 34 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Sc	65	512	311	103	96	2	0	0

- Molecule 35 is a protein called FAU ubiquitin-like and ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Se	50	Total	C	N	O	S	0	0
			394	241	88	64	1		

- Molecule 36 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sf	63	Total	C	N	O	S	0	0
			515	324	98	86	7		

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 38 is a protein called 60S ribosomal protein L8 (uL2).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LA	251	Total	C	N	O	S	1	0
			1930	1209	396	319	6		

- Molecule 39 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 40 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LC	366	Total	C	N	O	S	0	0
			2914	1832	581	487	14		

- Molecule 41 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 42 is a protein called 60S ribosomal protein L9.

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

- Molecule 43 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LE	223	Total	C	N	O	S	0	0
			1786	1150	339	293	4		

- Molecule 44 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LG	241	Total	C	N	O	S	0	0
			1926	1228	371	323	4		

- Molecule 45 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LO	202	Total	C	N	O	S	0	0
			1654	1066	322	261	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LL	206	Total	C	N	O	S	1	0
			1672	1046	348	274	4		

- Molecule 47 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LV	133	Total	C	N	O	S	0	0
			988	623	186	174	5		

- Molecule 48 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LM	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 49 is a protein called 60S ribosomal protein L27a.

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

- Molecule 50 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LN	203	Total	C	N	O	S	0	0
			1700	1072	359	265	4		

- Molecule 51 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LI	203	Total	C	N	O	S	0	0
			1645	1045	317	270	13		

- Molecule 52 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LD	294	Total	C	N	O	S	0	0
			2391	1513	436	428	14		

- Molecule 53 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LQ	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

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

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

- Molecule 55 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LS	176	Total	C	N	O	S	0	0
			1460	930	284	235	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	LT	159	1311	833	256	216	6	2	0

- Molecule 57 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	LP	153	1249	781	243	216	9	1	0

- Molecule 58 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	LU	99	808	518	141	147	2	0	0

- Molecule 59 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	LX	118	966	618	181	166	1	0	0

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

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

- Molecule 61 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	LW	118	950	595	192	159	4	0	0

- Molecule 62 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	LZ	135	1115	719	211	182	3	1	0

- Molecule 63 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	Lr	125	1011	629	208	169	5	1	0

- Molecule 64 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	Lh	122	1014	641	205	167	1	0	0

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	Lb	111	898	560	195	139	4	0	0

- Molecule 66 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	LF	225	1885	1212	364	300	9	2	0

- Molecule 67 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	Lc	99	770	488	136	140	6	0	0

- Molecule 68 is a protein called 60S ribosomal protein L31.

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

- Molecule 69 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	Le	128	1061	672	219	165	5	1	0

- Molecule 70 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Lf	110	Total	C	N	O	S	0	0
			883	560	175	144	4		

- Molecule 71 is a protein called 60S ribosomal protein L34.

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

- Molecule 72 is a protein called 60S ribosomal protein L36.

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

- Molecule 73 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Lj	86	Total	C	N	O	S	1	0
			712	439	157	111	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Lk	69	Total	C	N	O	S	0	0
			568	366	103	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Ll	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 76 is a protein called 60S ribosomal protein L40 (eL40).

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lm	52	Total	C	N	O	S	1	0
			436	272	91	67	6		

- Molecule 77 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ln	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 78 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Lo	105	Total	C	N	O	S	1	0
			870	548	177	139	6		

- Molecule 79 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Lp	91	Total	C	N	O	S	1	0
			715	450	139	119	7		

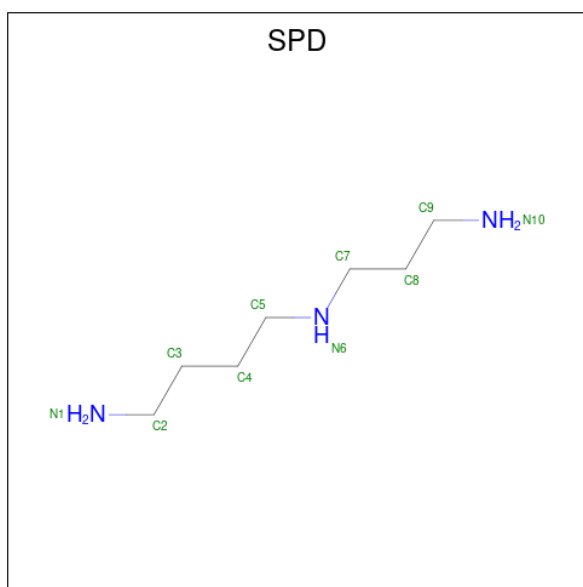
- Molecule 80 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	mR	8	Total	C	N	O	P	0	0
			172	77	32	55	8		

- Molecule 81 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
81	Pt	77	Total	C	N	O	P	S	0	0
			1645	734	298	535	77	1		

- Molecule 82 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



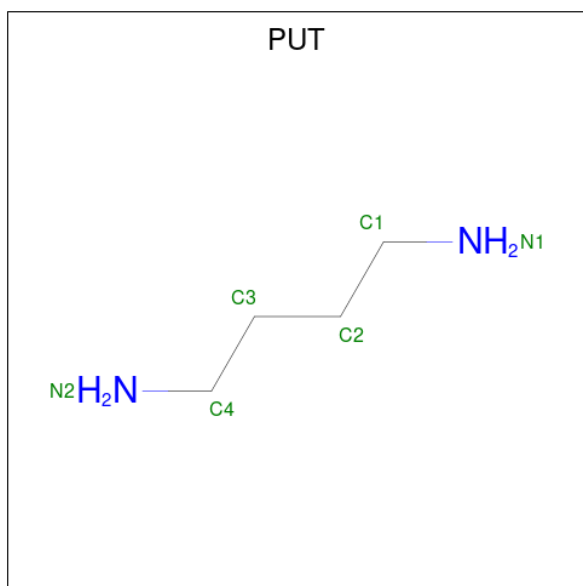
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
82	S2	1	10	7	3	0
82	S2	1	10	7	3	0
82	L5	1	10	7	3	0
82	L5	1	10	7	3	0
82	L5	1	10	7	3	0
82	L5	1	10	7	3	0
82	L5	1	10	7	3	0
82	L5	1	10	7	3	0
82	L5	1	10	7	3	0
82	L5	1	10	7	3	0
82	L5	1	10	7	3	0
82	L5	1	10	7	3	0
82	L5	1	10	7	3	0
82	L5	1	10	7	3	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
82	L5	1	10	7	3	0

- Molecule 83 is 1,4-DIAMINOBTUTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
83	S2	1	6	4	2	0
83	L5	1	6	4	2	0
83	L5	1	6	4	2	0
83	L5	1	6	4	2	0
83	L5	1	6	4	2	0
83	L5	1	6	4	2	0
83	L5	1	6	4	2	0
83	L5	1	6	4	2	0
83	L5	1	6	4	2	0

- Molecule 84 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
84	S2	12	Total 12	K 12	0
84	L8	4	Total 4	K 4	0
84	L5	117	Total 117	K 117	0
84	L7	4	Total 4	K 4	0
84	SO	1	Total 1	K 1	0
84	SL	1	Total 1	K 1	0
84	Sa	1	Total 1	K 1	0
84	LA	3	Total 3	K 3	0
84	LH	1	Total 1	K 1	0
84	LL	1	Total 1	K 1	0
84	LN	1	Total 1	K 1	0
84	LI	1	Total 1	K 1	0
84	LQ	1	Total 1	K 1	0
84	Lb	1	Total 1	K 1	0
84	Le	1	Total 1	K 1	0
84	Lf	1	Total 1	K 1	0
84	Ll	1	Total 1	K 1	0

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	S2	137	Total 137	Mg 137	0
85	L8	16	Total 16	Mg 16	0
85	L5	463	Total 463	Mg 463	0

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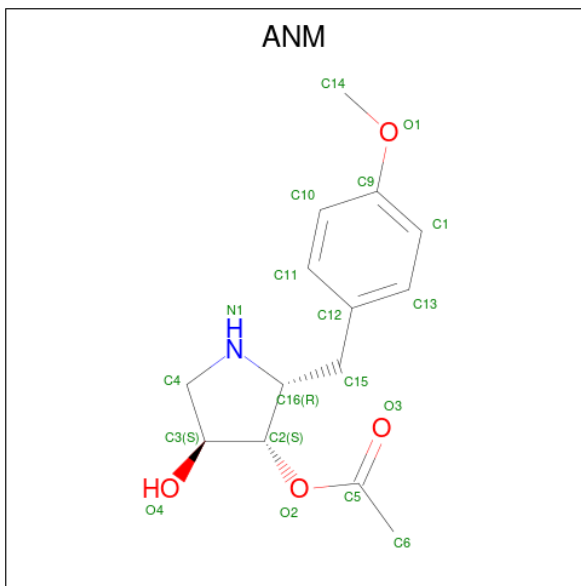
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
85	L7	15	15	15	0
85	SG	1	1	1	0
85	SX	1	1	1	0
85	SS	2	2	2	0
85	Sd	1	1	1	0
85	SN	1	1	1	0
85	ST	1	1	1	0
85	LB	1	1	1	0
85	LC	1	1	1	0
85	LH	1	1	1	0
85	LG	1	1	1	0
85	LO	2	2	2	0
85	LL	1	1	1	0
85	LV	1	1	1	0
85	La	1	1	1	0
85	LN	3	3	3	0
85	LD	1	1	1	0
85	LQ	2	2	2	0
85	LR	1	1	1	0
85	LS	1	1	1	0
85	LP	2	2	2	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
85	Lr	3	3	3	0
85	LF	1	1	1	0
85	Lc	1	1	1	0
85	Lf	1	1	1	0
85	Lg	1	1	1	0
85	Lj	2	2	2	0
85	Lo	1	1	1	0
85	Lp	2	2	2	0
85	Pt	2	2	2	0

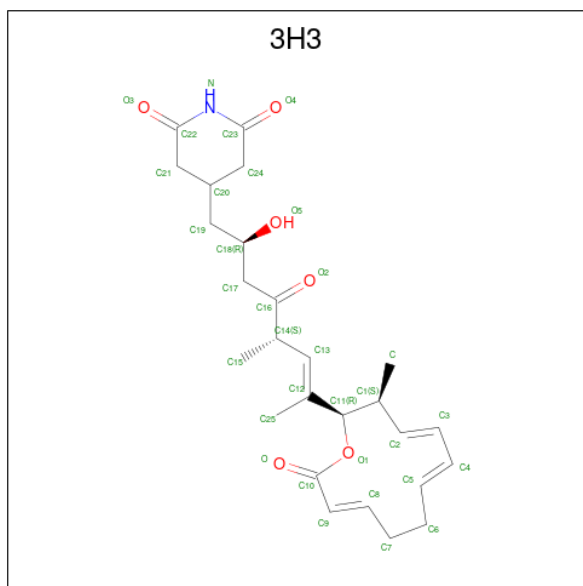
- Molecule 86 is ANISOMYCIN (three-letter code: ANM) (formula: C₁₄H₁₉NO₄).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
86	L5	1	19	14	1	4	0

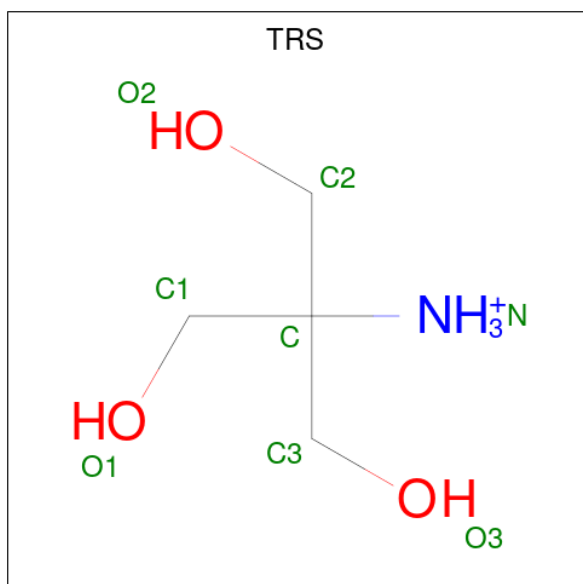
- Molecule 87 is 4-[(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxooxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl]piperidine-2,6-dione (three-letter code:

3H3) (formula: $C_{26}H_{35}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
87	L5	1	33	26	1	6	0

- Molecule 88 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
88	L5	1	8	4	1	3	0

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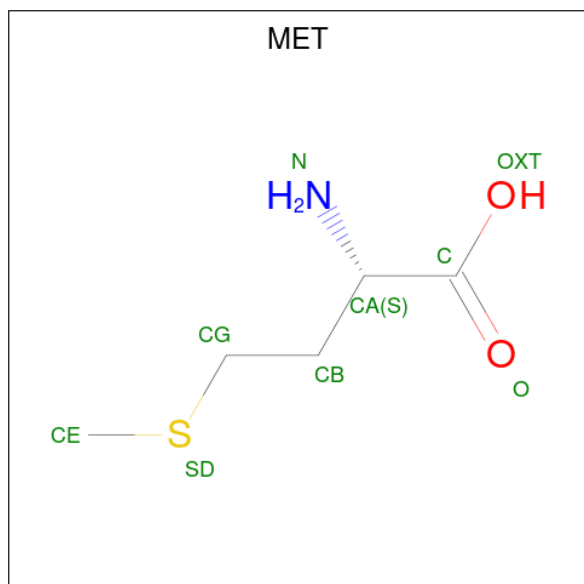
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
88	L5	1	8	4	1	3	0

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

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

- Molecule 90 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
90	Pt	1	8	5	1	1	1	0

- Molecule 91 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
91	S2	266	266	266	0
91	L8	189	189	189	0
91	L5	5661	5661	5661	0
91	L7	133	133	133	0
91	SA	1	1	1	0
91	SE	1	1	1	0
91	SF	1	1	1	0
91	SO	3	3	3	0
91	SN	3	3	3	0
91	SL	2	2	2	0
91	Sa	4	4	4	0
91	Sb	1	1	1	0
91	LA	93	93	93	0
91	LB	113	113	113	0
91	LC	137	137	137	0
91	LJ	4	4	4	0
91	LH	14	14	14	0
91	LE	28	28	28	0
91	LG	28	28	28	0

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Mol	Chain	Residues	Atoms		AltConf
91	LO	69	Total 69	O 69	0
91	LL	62	Total 62	O 62	0
91	LV	25	Total 25	O 25	0
91	LM	10	Total 10	O 10	0
91	La	71	Total 71	O 71	0
91	LN	112	Total 112	O 112	0
91	LI	33	Total 33	O 33	0
91	LD	37	Total 37	O 37	0
91	LQ	81	Total 81	O 81	0
91	LR	34	Total 34	O 34	0
91	LS	51	Total 51	O 51	0
91	LT	58	Total 58	O 58	0
91	LP	44	Total 44	O 44	0
91	LU	1	Total 1	O 1	0
91	LX	15	Total 15	O 15	0
91	LY	23	Total 23	O 23	0
91	LW	8	Total 8	O 8	0
91	LZ	7	Total 7	O 7	0
91	Lr	53	Total 53	O 53	0
91	Lh	10	Total 10	O 10	0
91	Lb	21	Total 21	O 21	0

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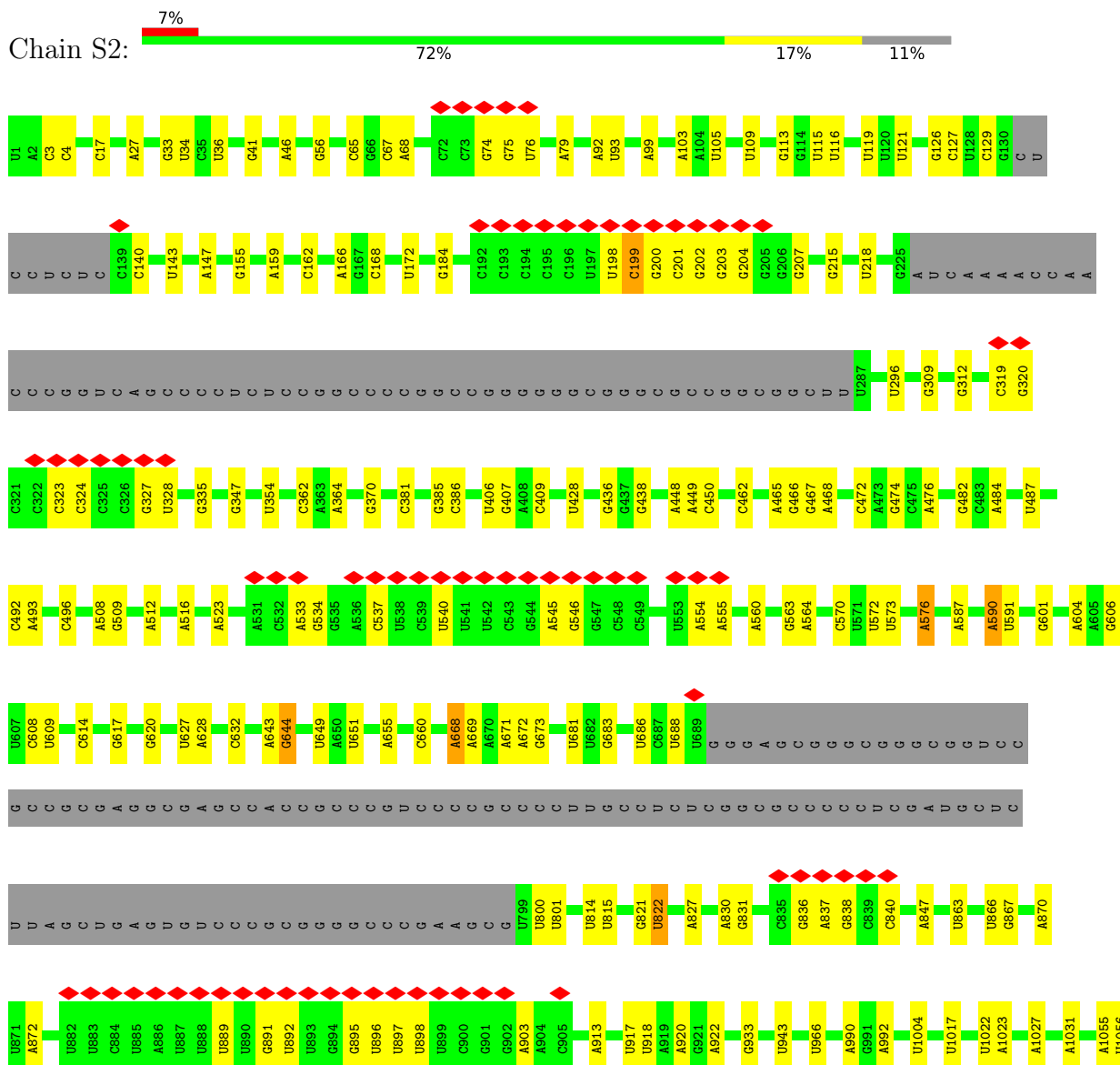
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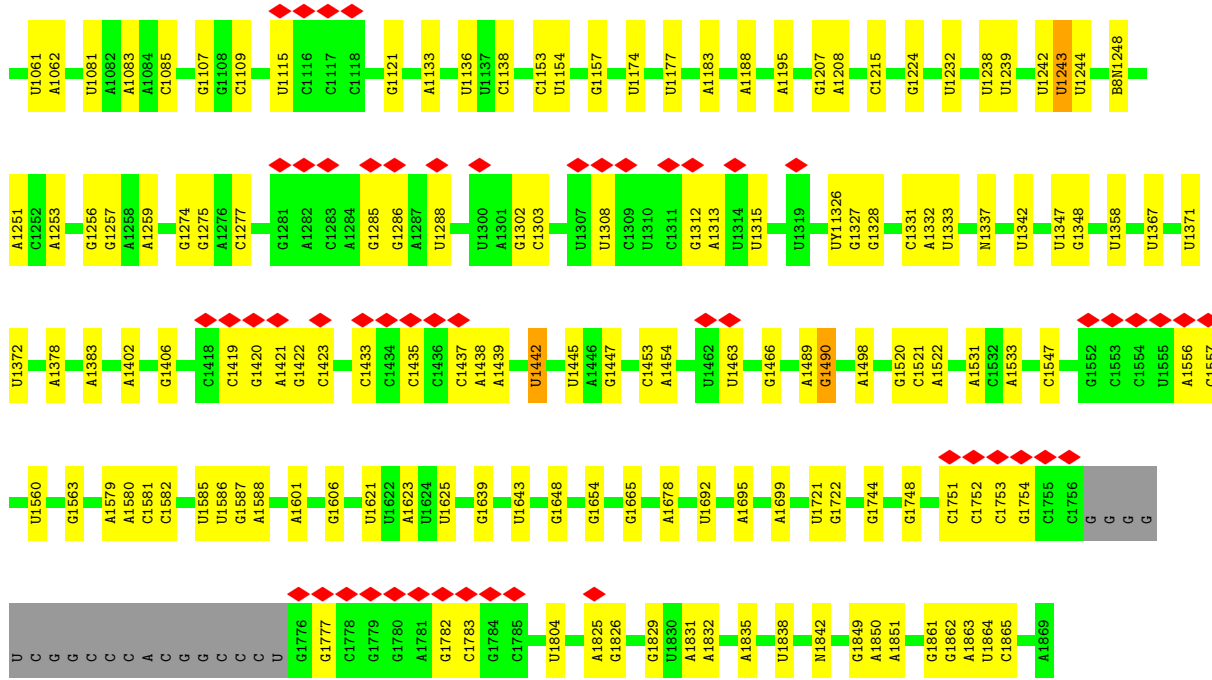
Mol	Chain	Residues	Atoms		AltConf
91	LF	77	Total 77	O 77	0
91	Lc	5	Total 5	O 5	0
91	Ld	20	Total 20	O 20	0
91	Le	71	Total 71	O 71	0
91	Lf	45	Total 45	O 45	0
91	Lg	39	Total 39	O 39	0
91	Li	15	Total 15	O 15	0
91	Lj	36	Total 36	O 36	0
91	Lk	2	Total 2	O 2	0
91	Ll	14	Total 14	O 14	0
91	Lm	8	Total 8	O 8	0
91	Ln	4	Total 4	O 4	0
91	Lo	37	Total 37	O 37	0
91	Lp	24	Total 24	O 24	0
91	Pt	1	Total 1	O 1	0

3 Residue-property plots [i](#)

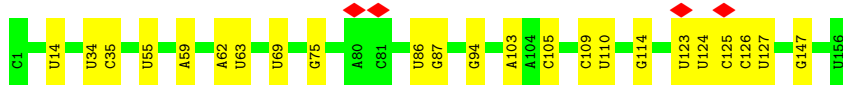
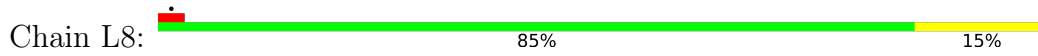
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 18S rRNA

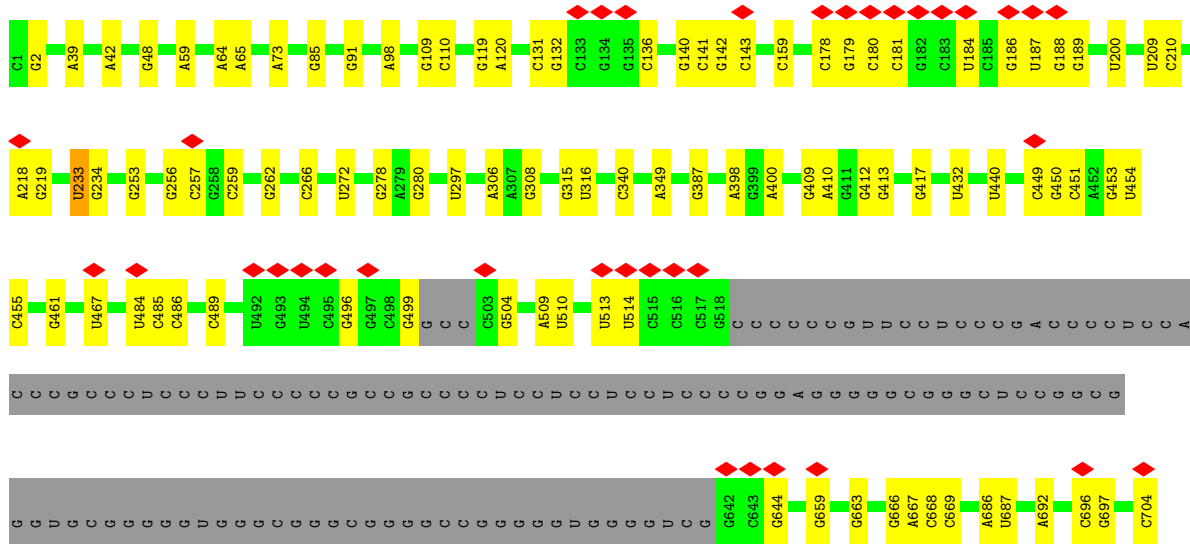


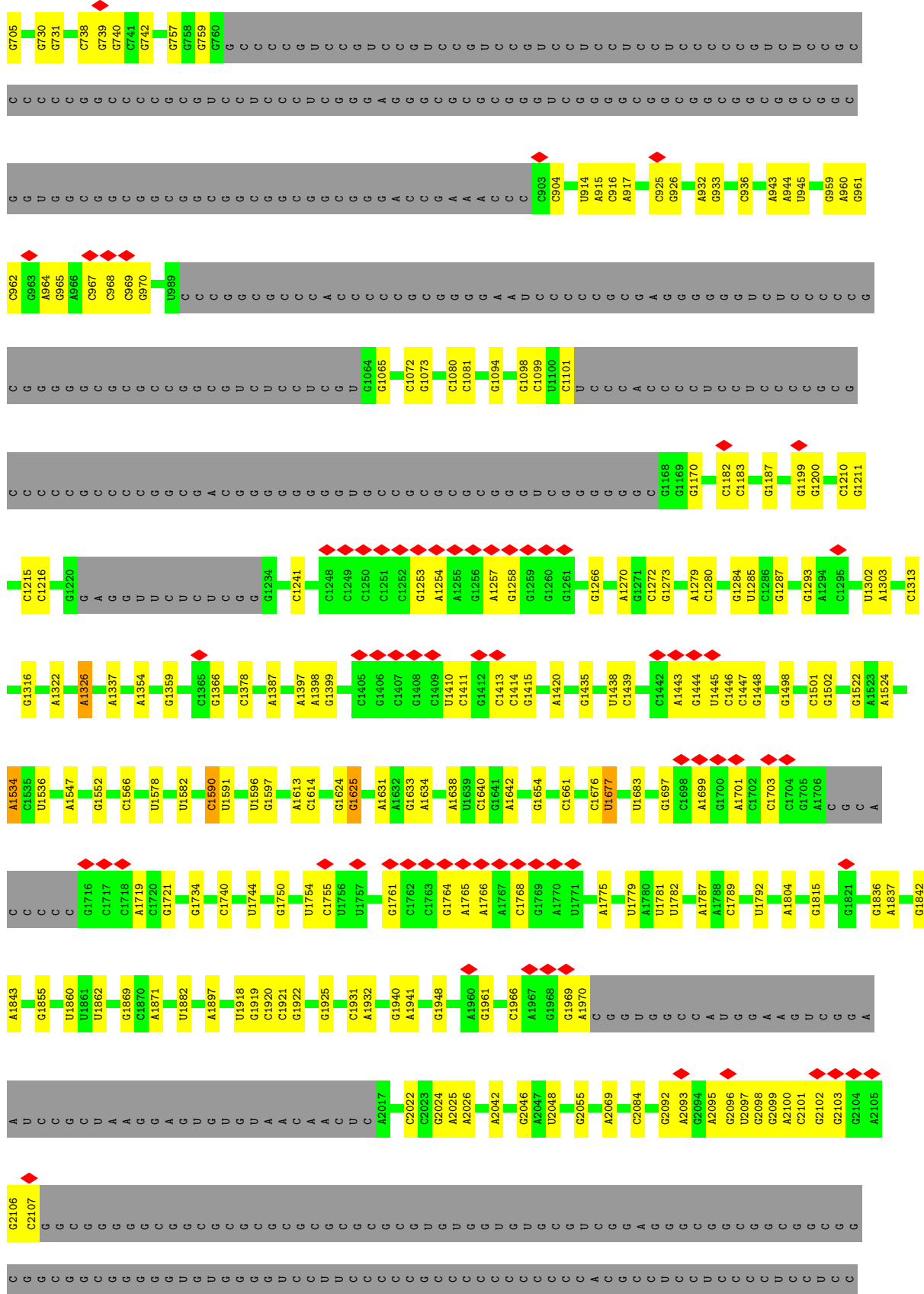


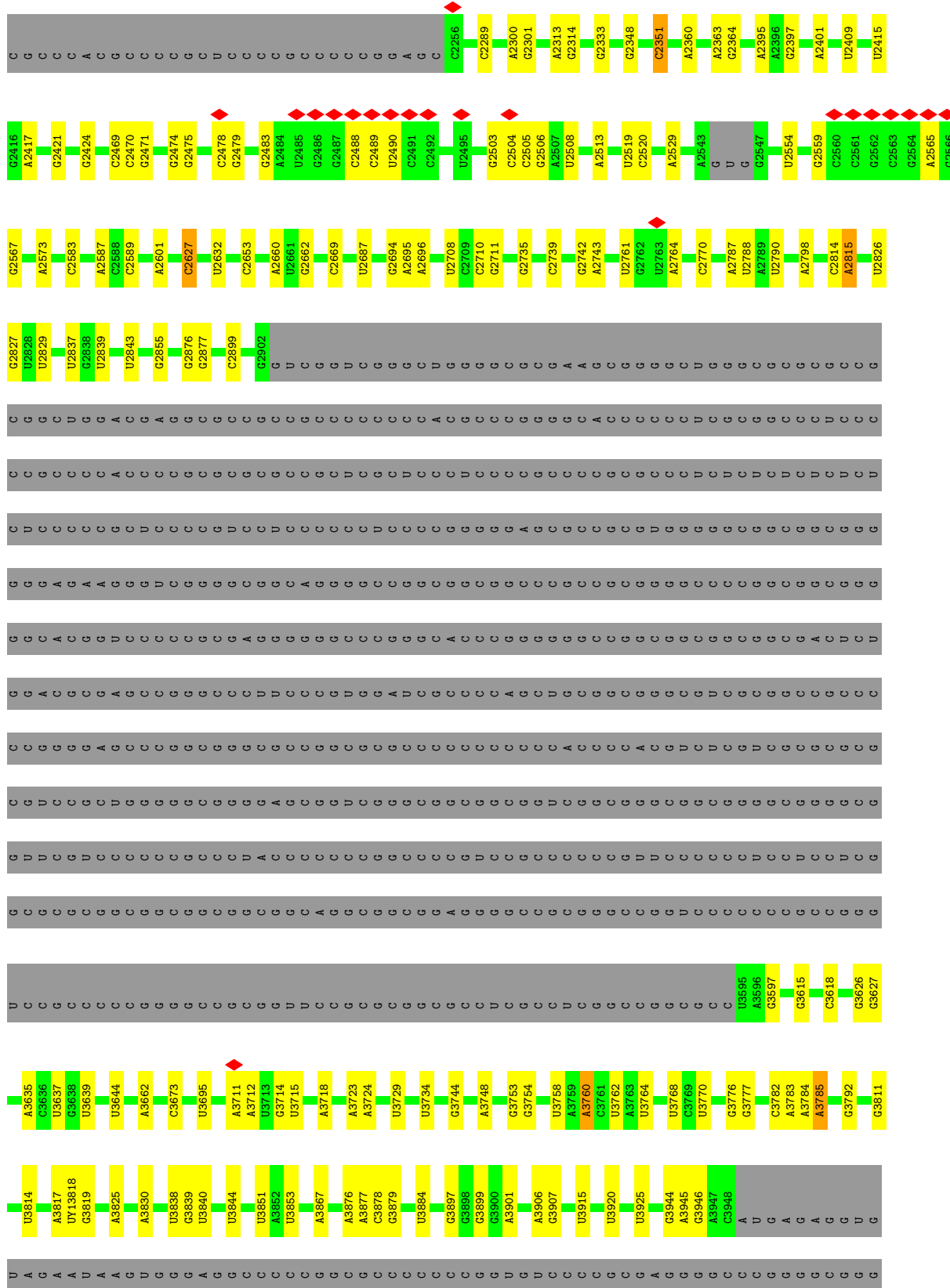
• Molecule 2: 5.8S rRNA

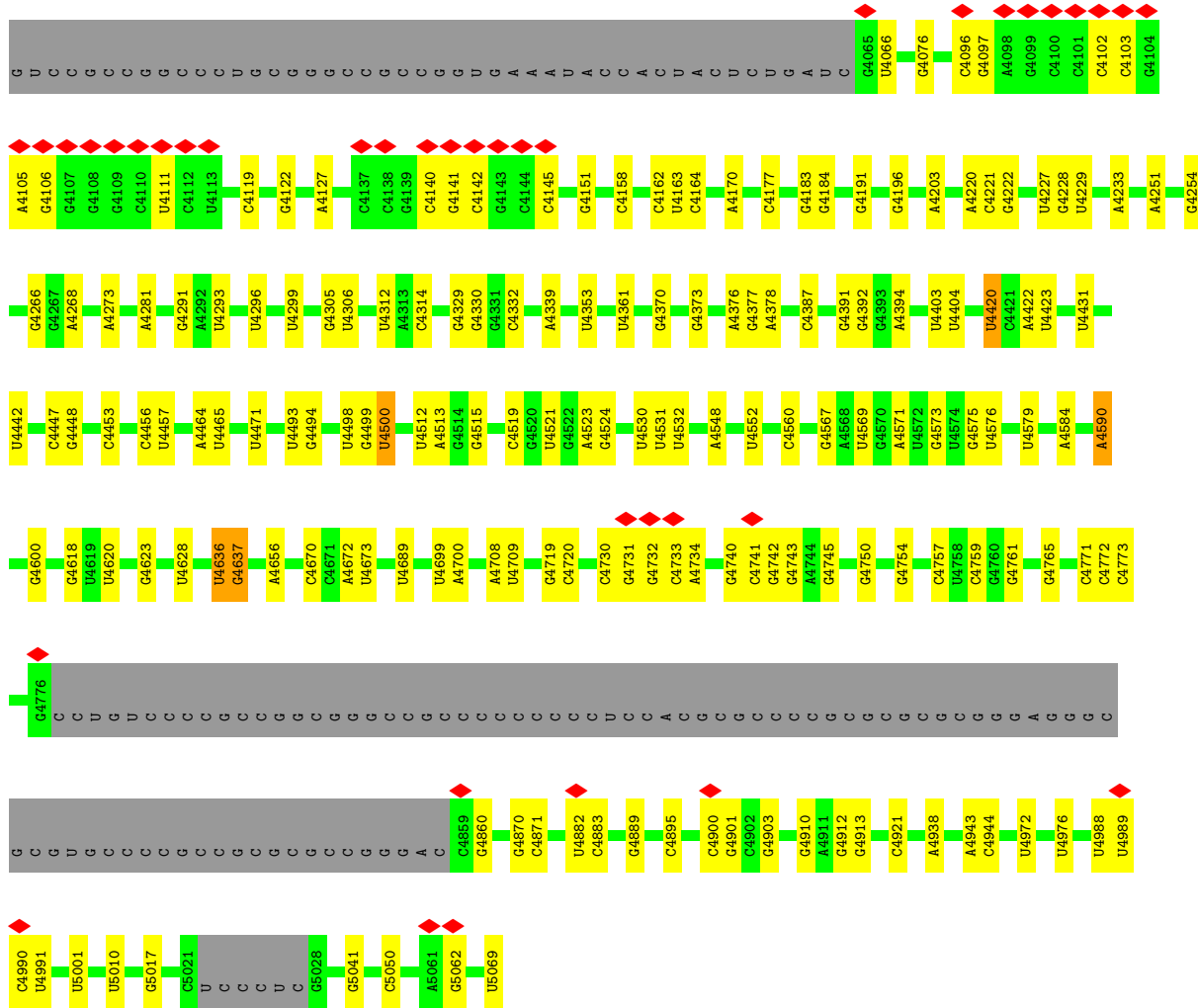


• Molecule 3: 28S rRNA

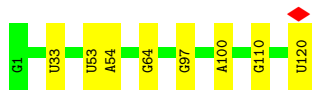
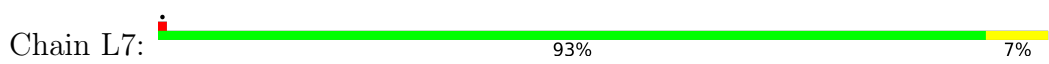




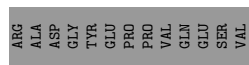
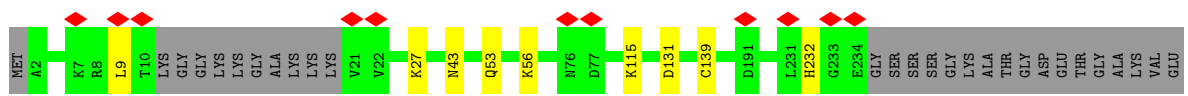
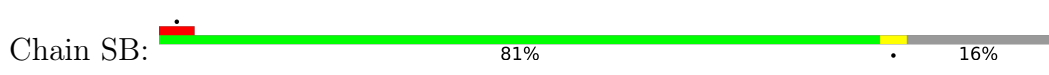




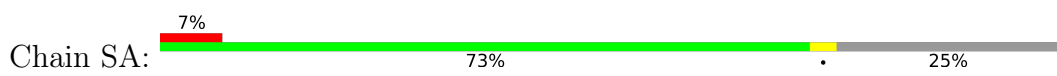
• Molecule 4: 5S rRNA

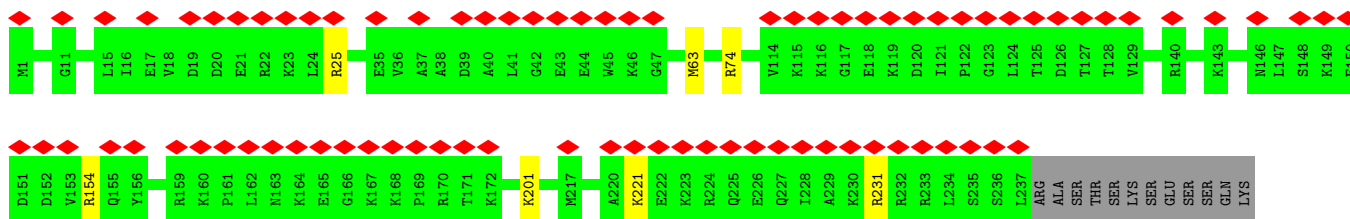


• Molecule 5: 40S ribosomal protein S3a

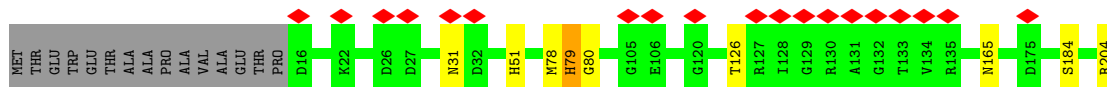
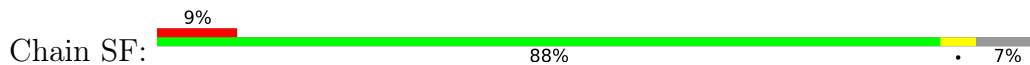


• Molecule 6: 40S ribosomal protein SA

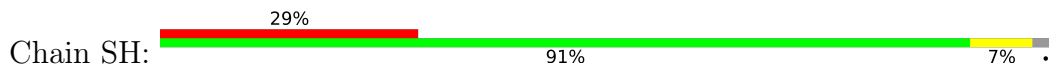




- Molecule 12: 40S ribosomal protein S5



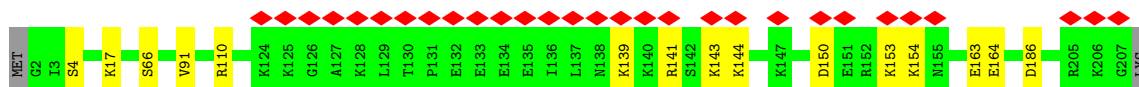
- Molecule 13: 40S ribosomal protein S7



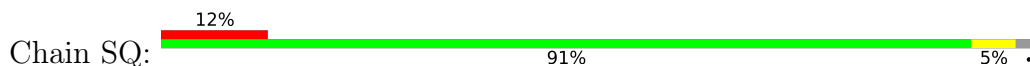
- Molecule 14: 40S ribosomal protein S15a



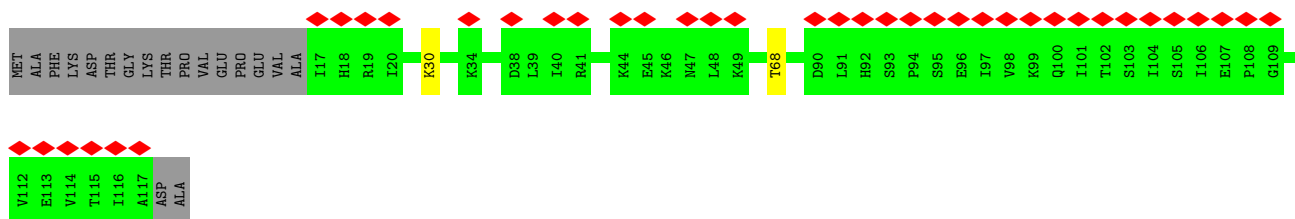
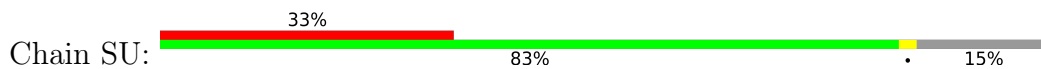
- Molecule 15: 40S ribosomal protein S8



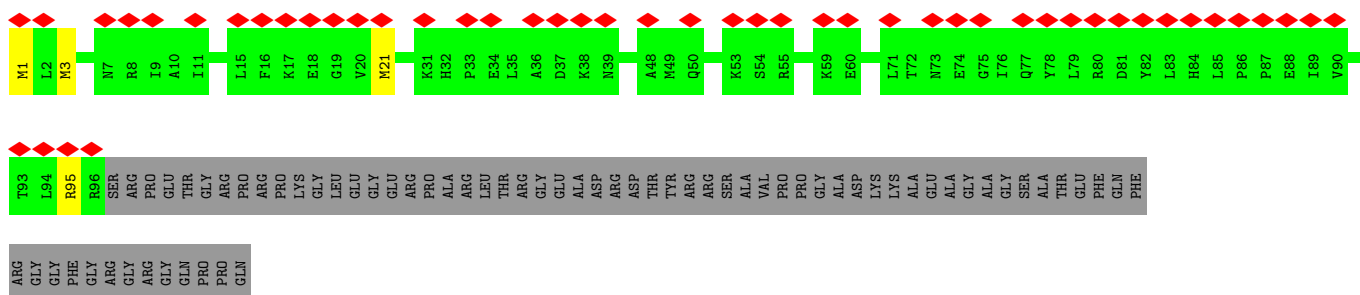
- Molecule 16: 40S ribosomal protein S16



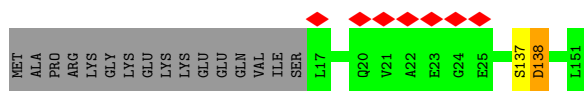
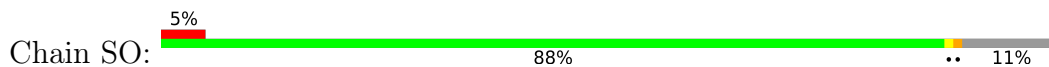
- Molecule 17: 40S ribosomal protein S20



• Molecule 18: 40S ribosomal protein S10



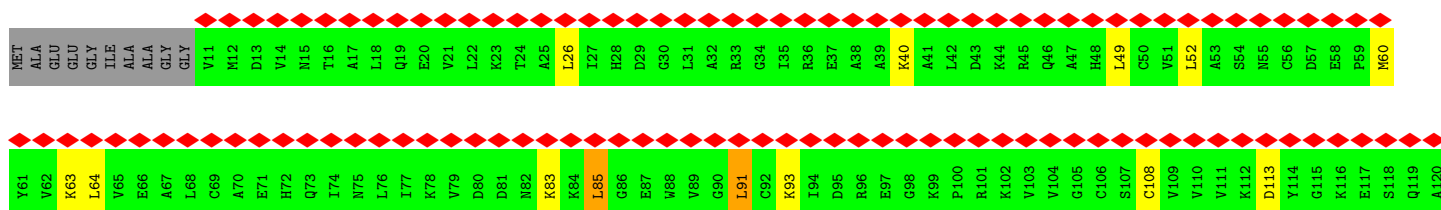
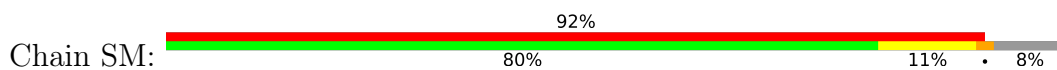
• Molecule 19: 40S ribosomal protein S14

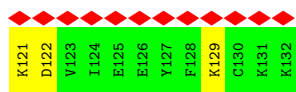


• Molecule 20: 40S ribosomal protein S23 (uS12)

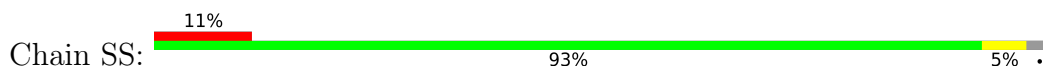


• Molecule 21: 40S ribosomal protein S12

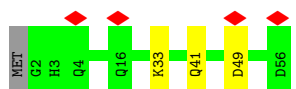




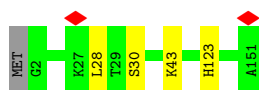
- Molecule 22: 40S ribosomal protein S18



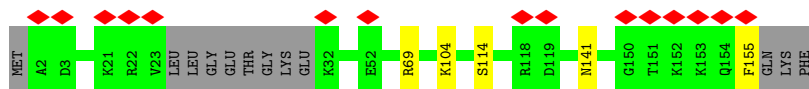
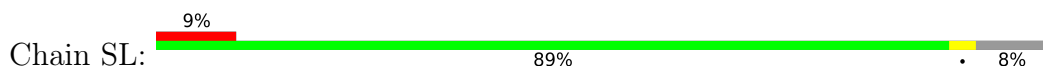
- Molecule 23: 40S ribosomal protein S29



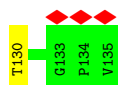
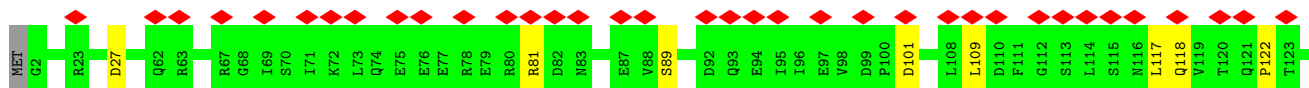
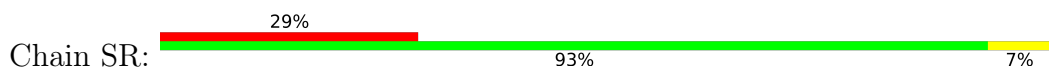
- Molecule 24: 40S ribosomal protein S13



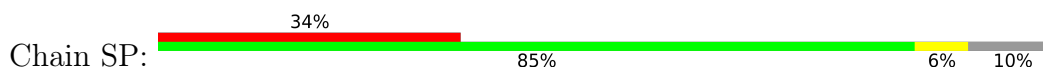
- Molecule 25: 40S ribosomal protein S11

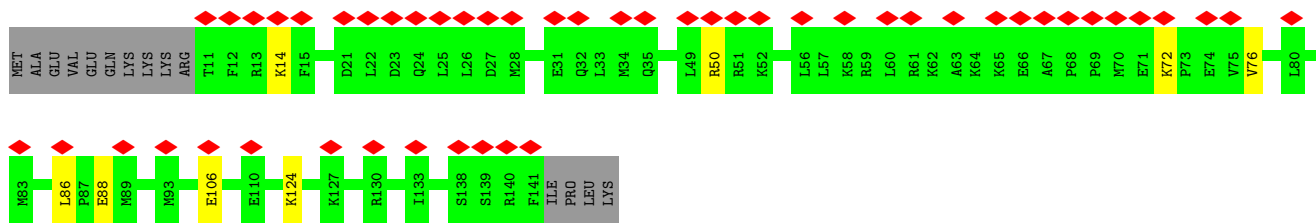


- Molecule 26: 40S ribosomal protein S17

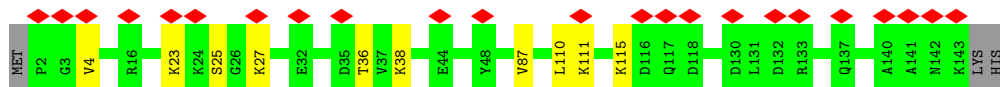
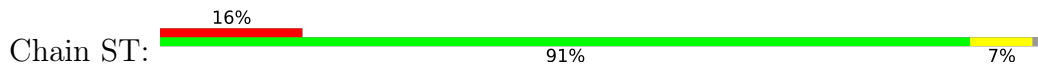


- Molecule 27: 40S ribosomal protein S15

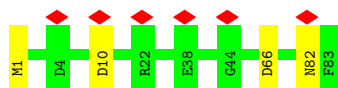




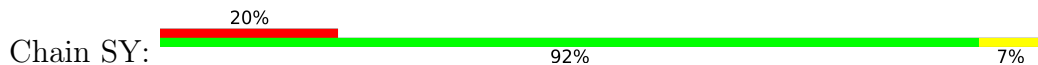
• Molecule 28: 40S ribosomal protein S19



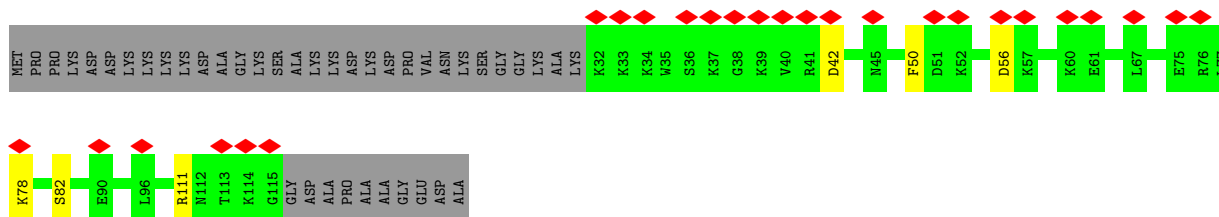
• Molecule 29: 40S ribosomal protein S21



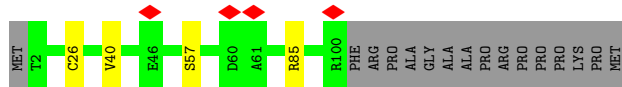
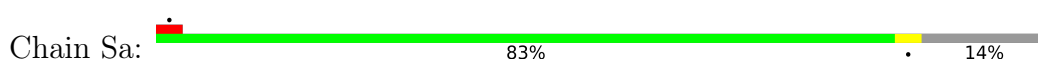
• Molecule 30: 40S ribosomal protein S24



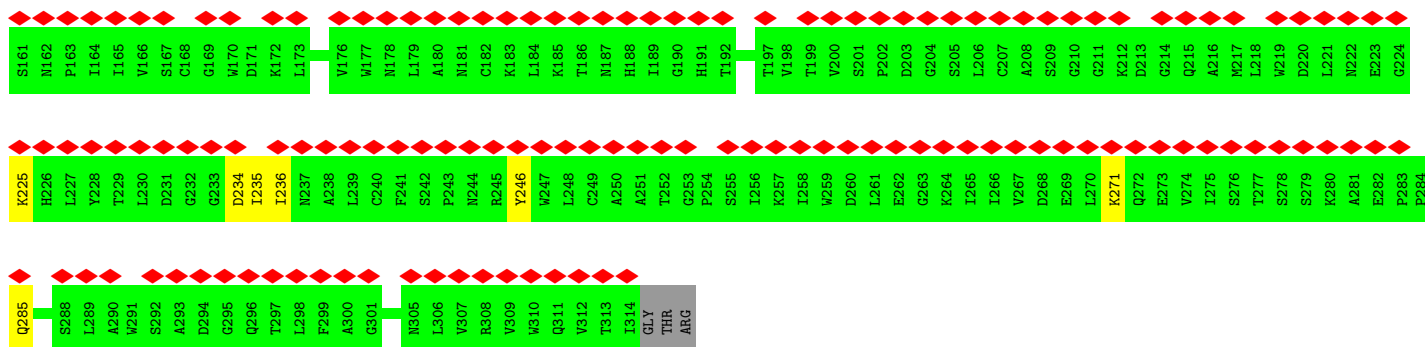
• Molecule 31: 40S ribosomal protein S25



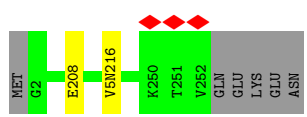
• Molecule 32: 40S ribosomal protein S26



• Molecule 33: 40S ribosomal protein S27



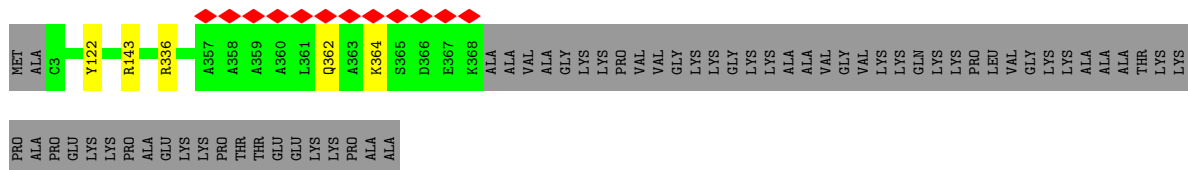
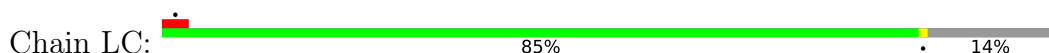
- Molecule 38: 60S ribosomal protein L8 (uL2)



- Molecule 39: 60S ribosomal protein L3



- Molecule 40: 60S ribosomal protein L4

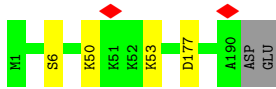


- Molecule 41: 60S ribosomal protein L11



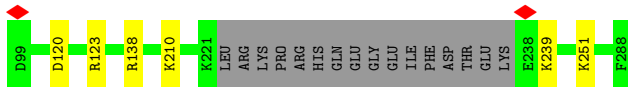
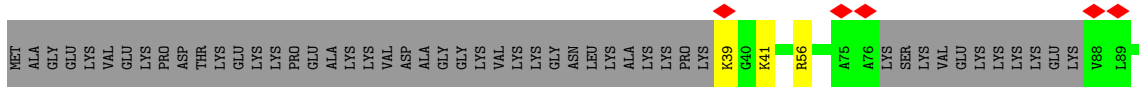
- Molecule 42: 60S ribosomal protein L9





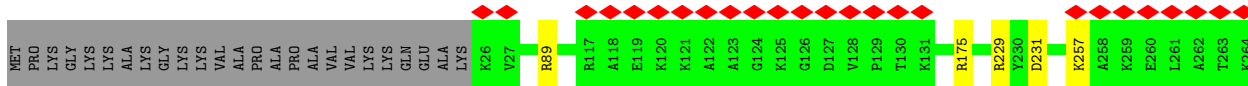
- Molecule 43: 60S ribosomal protein L6

Chain LE: 74% 23%



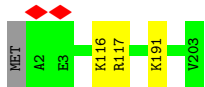
- Molecule 44: 60S ribosomal protein L7a

Chain LG: 10% 89% 9%



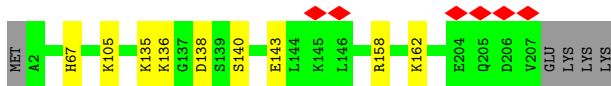
- Molecule 45: 60S ribosomal protein L13a

Chain LO: 98%



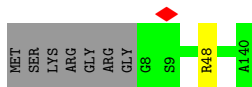
- Molecule 46: 60S ribosomal protein L13

Chain LL: 93%

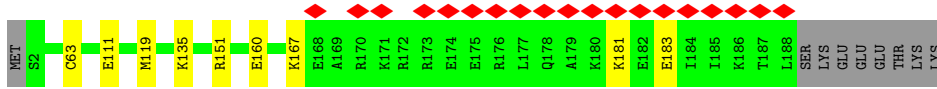


- Molecule 47: 60S ribosomal protein L23

Chain LV: 94% 5%



- Molecule 48: 60S ribosomal protein L14

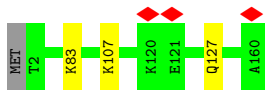


• Molecule 55: 60S ribosomal protein L18a

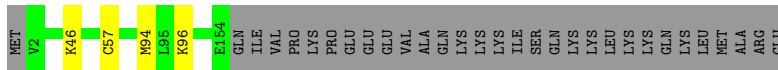
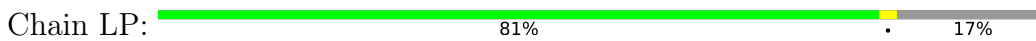


There are no outlier residues recorded for this chain.

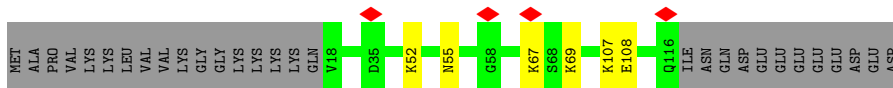
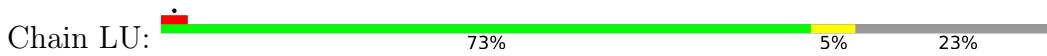
• Molecule 56: 60S ribosomal protein L21



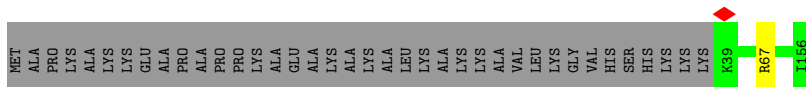
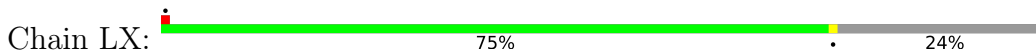
• Molecule 57: 60S ribosomal protein L17



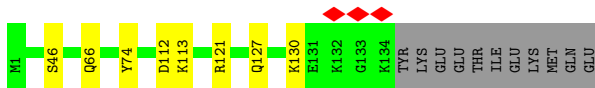
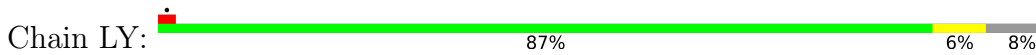
• Molecule 58: 60S ribosomal protein L22



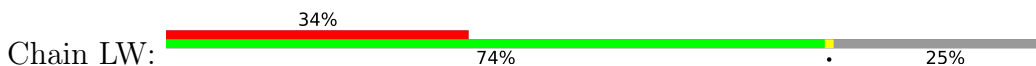
• Molecule 59: 60S ribosomal protein L23a

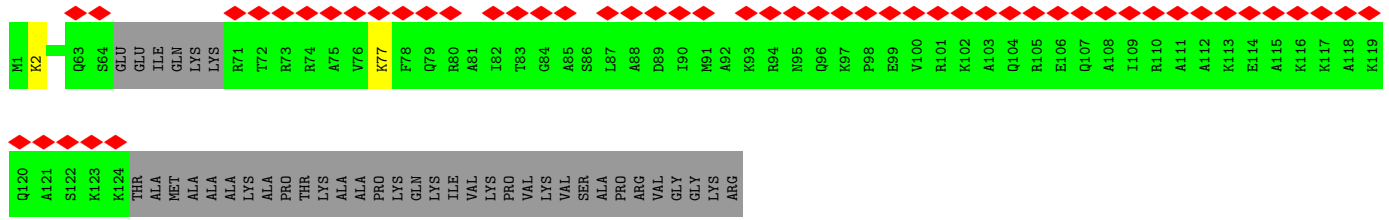


• Molecule 60: 60S ribosomal protein L26

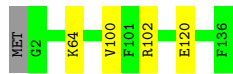


• Molecule 61: 60S ribosomal protein L24

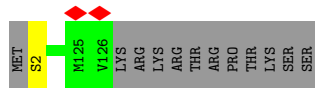




• Molecule 62: 60S ribosomal protein L27



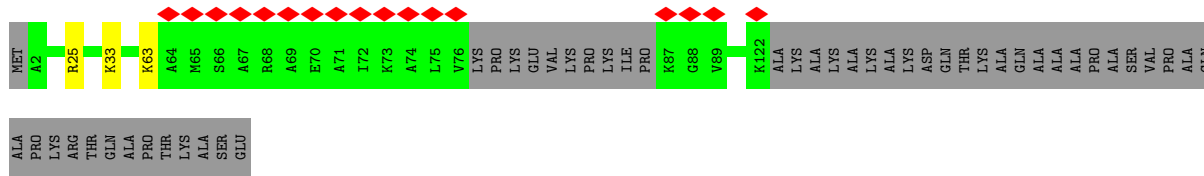
• Molecule 63: 60S ribosomal protein L28



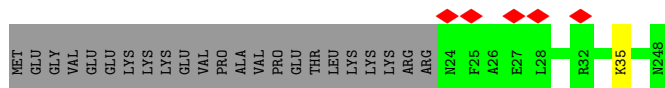
• Molecule 64: 60S ribosomal protein L35



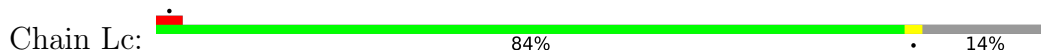
• Molecule 65: 60S ribosomal protein L29

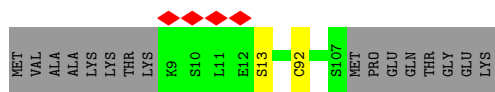


• Molecule 66: 60S ribosomal protein L7

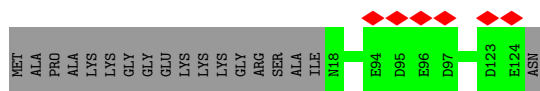
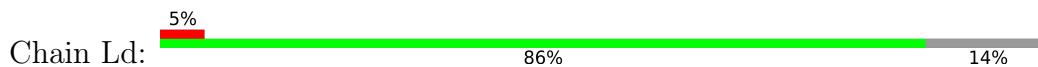


• Molecule 67: 60S ribosomal protein L30

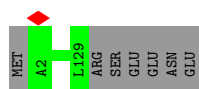




• Molecule 68: 60S ribosomal protein L31



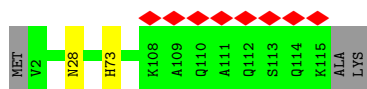
• Molecule 69: 60S ribosomal protein L32



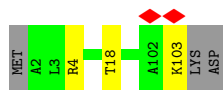
• Molecule 70: 60S ribosomal protein L35a



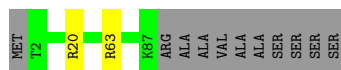
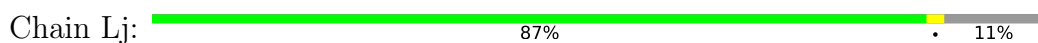
• Molecule 71: 60S ribosomal protein L34



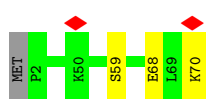
• Molecule 72: 60S ribosomal protein L36



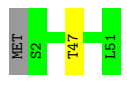
• Molecule 73: 60S ribosomal protein L37



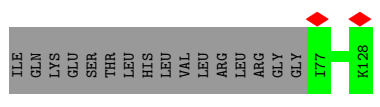
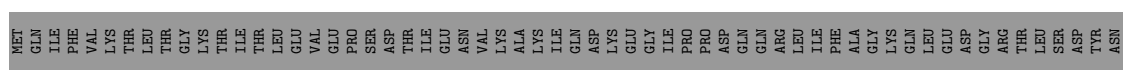
• Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39



- Molecule 76: 60S ribosomal protein L40 (eL40)

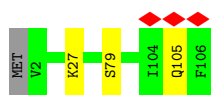


- Molecule 77: 60S ribosomal protein L41

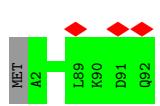


There are no outlier residues recorded for this chain.

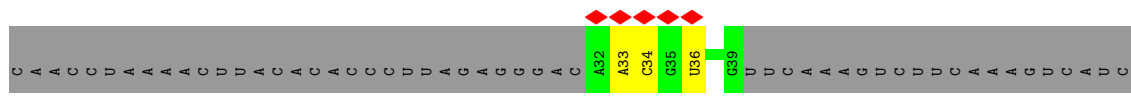
- Molecule 78: 60S ribosomal protein L36a



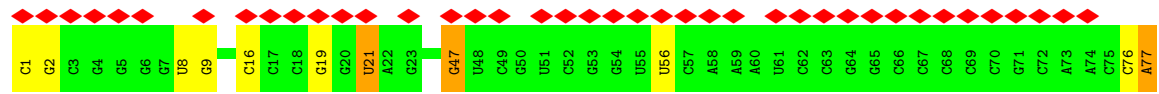
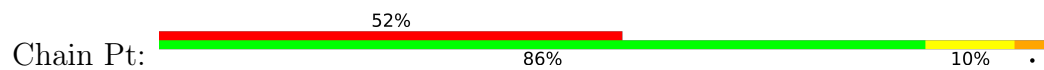
- Molecule 79: 60S ribosomal protein L37a



- Molecule 80: mRNA



• Molecule 81: P-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	845750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	79	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (\AA)	528.64, 528.64, 528.64	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82600003, 0.82600003, 0.82600003	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, MG, HY3, K, G7M, ANM, A2M, MA6, OMG, MLZ, SAC, B8N, TRS, SPD, HIC, M3L, 6MZ, ZN, 1MA, V5N, PSU, 4SU, AME, H2U, OMC, 5MC, PUT, 4AC, 3H3, UY1, OMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	S2	0.35	0/37935	0.77	11/59125 (0.0%)
2	L8	0.55	0/3609	0.78	0/5623
3	L5	0.55	0/82080	0.81	16/128048 (0.0%)
4	L7	0.56	0/2858	0.78	0/4455
5	SB	0.27	0/1832	0.50	0/2449
6	SA	0.26	0/1778	0.49	0/2416
7	SD	0.26	0/1784	0.52	0/2403
8	SJ	0.25	0/1550	0.54	0/2069
9	SE	0.26	0/2118	0.53	0/2849
10	SC	0.30	0/1762	0.52	0/2381
11	SG	0.26	0/1946	0.55	0/2590
12	SF	0.29	0/1515	0.55	1/2037 (0.0%)
13	SH	0.29	0/1540	0.53	0/2064
14	SW	0.28	0/1051	0.54	0/1406
15	SI	0.28	0/1715	0.55	0/2287
16	SQ	0.26	0/1141	0.52	0/1528
17	SU	0.27	0/813	0.60	0/1092
18	SK	0.26	0/834	0.49	0/1125
19	SO	0.28	0/1022	0.57	0/1372
20	SX	0.27	0/1096	0.50	0/1461
21	SM	0.26	0/960	0.69	4/1286 (0.3%)
22	SS	0.26	0/1232	0.55	0/1651
23	Sd	0.25	0/469	0.52	0/623
24	SN	0.27	0/1242	0.51	0/1671
25	SL	0.29	0/1221	0.53	0/1632
26	SR	0.27	0/1097	0.61	2/1474 (0.1%)
27	SP	0.28	0/1100	0.56	0/1470
28	ST	0.26	0/1148	0.56	1/1540 (0.1%)
29	SV	0.27	0/635	0.50	0/850
30	SY	0.25	0/1083	0.52	0/1438
31	SZ	0.24	0/682	0.50	0/911

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sa	0.28	0/816	0.58	0/1093
33	Sb	0.28	0/665	0.49	0/891
34	Sc	0.25	0/514	0.59	0/688
35	Se	0.25	0/396	0.55	0/519
36	Sf	0.25	0/525	0.54	0/695
37	Sg	0.24	0/2493	0.53	0/3394
38	LA	0.32	0/1958	0.59	0/2623
39	LB	0.32	0/3294	0.54	0/4406
40	LC	0.30	0/2968	0.55	0/3985
41	LJ	0.29	0/1385	0.53	0/1852
42	LH	0.30	0/1537	0.54	0/2066
43	LE	0.29	0/1820	0.53	0/2442
44	LG	0.29	0/1959	0.53	0/2637
45	LO	0.32	0/1686	0.53	0/2257
46	LL	0.29	0/1706	0.58	0/2284
47	LV	0.31	0/1002	0.55	0/1345
48	LM	0.31	0/1142	0.52	0/1527
49	La	0.33	0/1178	0.53	0/1573
50	LN	0.36	0/1745	0.61	1/2338 (0.0%)
51	LI	0.31	0/1683	0.54	0/2247
52	LD	0.31	0/2437	0.50	0/3263
53	LQ	0.32	0/1536	0.61	0/2052
54	LR	0.28	0/1582	0.59	0/2091
55	LS	0.34	0/1500	0.56	0/2013
56	LT	0.32	0/1345	0.54	0/1795
57	LP	0.34	0/1279	0.56	0/1716
58	LU	0.31	0/822	0.52	0/1103
59	LX	0.30	0/983	0.53	0/1323
60	LY	0.31	0/1132	0.56	0/1504
61	LW	0.29	0/964	0.54	0/1278
62	LZ	0.32	0/1141	0.53	0/1521
63	Lr	0.31	0/1020	0.58	0/1367
64	Lh	0.29	0/1022	0.52	0/1351
65	Lb	0.28	0/900	0.56	0/1187
66	LF	0.33	0/1926	0.55	0/2567
67	Lc	0.31	0/780	0.50	0/1046
68	Ld	0.30	0/903	0.57	0/1216
69	Le	0.32	0/1082	0.56	0/1443
70	Lf	0.35	0/902	0.58	0/1208
71	Lg	0.31	0/916	0.57	0/1220
72	Li	0.28	0/843	0.55	0/1115
73	Lj	0.33	0/731	0.60	0/967
74	Lk	0.30	0/574	0.50	0/761

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Ll	0.30	0/453	0.56	0/599
76	Lm	0.31	0/433	0.54	0/575
77	Ln	0.28	0/240	0.68	0/305
78	Lo	0.32	0/877	0.53	0/1156
79	Lp	0.31	0/728	0.55	0/967
80	mR	0.18	0/192	0.68	0/297
81	Pt	0.57	6/1721 (0.3%)	1.00	12/2679 (0.4%)
All	All	0.43	6/222284 (0.0%)	0.71	48/325873 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	Pt	77	A	C5-C4	11.31	1.46	1.38
81	Pt	1	C	OP3-P	-10.58	1.48	1.61
81	Pt	77	A	C5-C6	8.07	1.48	1.41
81	Pt	77	A	N7-C5	-7.33	1.34	1.39
81	Pt	77	A	C8-N7	7.02	1.36	1.31

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	Pt	77	A	C2-N3-C4	20.46	120.83	110.60
81	Pt	77	A	N3-C4-C5	-11.77	118.56	126.80
81	Pt	77	A	N1-C2-N3	-11.43	123.59	129.30
81	Pt	77	A	N3-C4-N9	9.67	135.13	127.40
81	Pt	77	A	O4'-C1'-N9	8.27	114.82	108.20

There are no chirality outliers.

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	
5	SB	219/264 (83%)	217 (99%)	2 (1%)	0	100	100
6	SA	220/295 (75%)	214 (97%)	6 (3%)	0	100	100
7	SD	224/243 (92%)	213 (95%)	11 (5%)	0	100	100
8	SJ	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
9	SE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
10	SC	220/293 (75%)	215 (98%)	5 (2%)	0	100	100
11	SG	235/249 (94%)	232 (99%)	3 (1%)	0	100	100
12	SF	187/204 (92%)	179 (96%)	6 (3%)	2 (1%)	14	3
13	SH	187/194 (96%)	176 (94%)	9 (5%)	2 (1%)	14	3
14	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
15	SI	204/208 (98%)	198 (97%)	6 (3%)	0	100	100
16	SQ	139/146 (95%)	134 (96%)	5 (4%)	0	100	100
17	SU	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
18	SK	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
19	SO	133/151 (88%)	128 (96%)	4 (3%)	1 (1%)	19	6
20	SX	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
21	SM	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
22	SS	146/152 (96%)	143 (98%)	3 (2%)	0	100	100
23	Sd	53/56 (95%)	53 (100%)	0	0	100	100
24	SN	149/151 (99%)	148 (99%)	1 (1%)	0	100	100
25	SL	142/158 (90%)	139 (98%)	3 (2%)	0	100	100
26	SR	132/135 (98%)	121 (92%)	11 (8%)	0	100	100
27	SP	129/145 (89%)	126 (98%)	3 (2%)	0	100	100
28	ST	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
29	SV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
30	SY	129/133 (97%)	126 (98%)	3 (2%)	0	100	100
31	SZ	82/125 (66%)	78 (95%)	4 (5%)	0	100	100
32	Sa	98/115 (85%)	98 (100%)	0	0	100	100
33	Sb	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
34	Sc	63/69 (91%)	60 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Se	46/133 (35%)	45 (98%)	0	1 (2%)	6	1
36	Sf	61/156 (39%)	53 (87%)	8 (13%)	0	100	100
37	Sg	311/317 (98%)	292 (94%)	19 (6%)	0	100	100
38	LA	249/257 (97%)	240 (96%)	9 (4%)	0	100	100
39	LB	399/403 (99%)	391 (98%)	8 (2%)	0	100	100
40	LC	364/427 (85%)	361 (99%)	3 (1%)	0	100	100
41	LJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
42	LH	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
43	LE	217/288 (75%)	212 (98%)	5 (2%)	0	100	100
44	LG	239/266 (90%)	230 (96%)	9 (4%)	0	100	100
45	LO	200/203 (98%)	199 (100%)	1 (0%)	0	100	100
46	LL	205/211 (97%)	198 (97%)	7 (3%)	0	100	100
47	LV	131/140 (94%)	130 (99%)	1 (1%)	0	100	100
48	LM	134/215 (62%)	132 (98%)	2 (2%)	0	100	100
49	La	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	22	8
50	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
51	LI	199/214 (93%)	198 (100%)	1 (0%)	0	100	100
52	LD	292/297 (98%)	288 (99%)	4 (1%)	0	100	100
53	LQ	185/188 (98%)	184 (100%)	1 (0%)	0	100	100
54	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
55	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
56	LT	159/160 (99%)	157 (99%)	2 (1%)	0	100	100
57	LP	152/184 (83%)	150 (99%)	2 (1%)	0	100	100
58	LU	97/128 (76%)	95 (98%)	1 (1%)	1 (1%)	15	3
59	LX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
60	LY	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
61	LW	114/157 (73%)	109 (96%)	5 (4%)	0	100	100
62	LZ	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
63	Lr	124/137 (90%)	124 (100%)	0	0	100	100
64	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
65	Lb	106/159 (67%)	103 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	LF	225/248 (91%)	219 (97%)	6 (3%)	0	100	100
67	Lc	97/115 (84%)	97 (100%)	0	0	100	100
68	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
69	Le	127/135 (94%)	127 (100%)	0	0	100	100
70	Lf	108/110 (98%)	108 (100%)	0	0	100	100
71	Lg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
72	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
73	Lj	85/97 (88%)	85 (100%)	0	0	100	100
74	Lk	67/70 (96%)	67 (100%)	0	0	100	100
75	Ll	48/51 (94%)	48 (100%)	0	0	100	100
76	Lm	50/128 (39%)	50 (100%)	0	0	100	100
77	Ln	23/25 (92%)	23 (100%)	0	0	100	100
78	Lo	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
79	Lp	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
All	All	11301/12762 (89%)	11033 (98%)	260 (2%)	8 (0%)	54	32

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	Se	119	VAL
19	SO	138	ASP
13	SH	18	GLU
12	SF	79	HIS
12	SF	80	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	SB	202/231 (87%)	193 (96%)	9 (4%)	27	9
6	SA	183/242 (76%)	176 (96%)	7 (4%)	33	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	SD	189/202 (94%)	178 (94%)	11 (6%)	20	5
8	SJ	161/168 (96%)	154 (96%)	7 (4%)	29	10
9	SE	224/225 (100%)	219 (98%)	5 (2%)	52	32
10	SC	188/225 (84%)	180 (96%)	8 (4%)	29	10
11	SG	207/218 (95%)	200 (97%)	7 (3%)	37	15
12	SF	159/170 (94%)	152 (96%)	7 (4%)	28	9
13	SH	168/174 (97%)	157 (94%)	11 (6%)	17	4
14	SW	112/113 (99%)	109 (97%)	3 (3%)	44	24
15	SI	178/180 (99%)	163 (92%)	15 (8%)	11	2
16	SQ	117/121 (97%)	109 (93%)	8 (7%)	16	3
17	SU	93/107 (87%)	91 (98%)	2 (2%)	52	32
18	SK	87/136 (64%)	83 (95%)	4 (5%)	27	9
19	SO	105/119 (88%)	103 (98%)	2 (2%)	57	38
20	SX	111/114 (97%)	105 (95%)	6 (5%)	22	6
21	SM	104/108 (96%)	89 (86%)	15 (14%)	3	0
22	SS	128/132 (97%)	121 (94%)	7 (6%)	21	6
23	Sd	48/49 (98%)	45 (94%)	3 (6%)	18	4
24	SN	131/131 (100%)	126 (96%)	5 (4%)	33	12
25	SL	132/142 (93%)	127 (96%)	5 (4%)	33	12
26	SR	121/122 (99%)	114 (94%)	7 (6%)	20	5
27	SP	117/130 (90%)	109 (93%)	8 (7%)	16	3
28	ST	114/115 (99%)	105 (92%)	9 (8%)	12	2
29	SV	66/66 (100%)	63 (96%)	3 (4%)	27	9
30	SY	113/115 (98%)	104 (92%)	9 (8%)	12	2
31	SZ	74/103 (72%)	68 (92%)	6 (8%)	11	2
32	Sa	87/98 (89%)	82 (94%)	5 (6%)	20	5
33	Sb	75/76 (99%)	70 (93%)	5 (7%)	16	3
34	Sc	58/62 (94%)	54 (93%)	4 (7%)	15	3
35	Se	40/104 (38%)	39 (98%)	1 (2%)	47	26
36	Sf	56/140 (40%)	51 (91%)	5 (9%)	9	2
37	Sg	272/275 (99%)	255 (94%)	17 (6%)	18	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	LA	193/198 (98%)	192 (100%)	1 (0%)	88	83
39	LB	347/348 (100%)	341 (98%)	6 (2%)	60	43
40	LC	305/348 (88%)	300 (98%)	5 (2%)	62	46
41	LJ	143/149 (96%)	141 (99%)	2 (1%)	67	51
42	LH	169/171 (99%)	165 (98%)	4 (2%)	49	28
43	LE	196/252 (78%)	187 (95%)	9 (5%)	27	9
44	LG	203/223 (91%)	198 (98%)	5 (2%)	47	26
45	LO	173/174 (99%)	170 (98%)	3 (2%)	60	43
46	LL	173/177 (98%)	164 (95%)	9 (5%)	23	7
47	LV	102/107 (95%)	101 (99%)	1 (1%)	76	65
48	LM	116/161 (72%)	115 (99%)	1 (1%)	78	69
49	La	119/120 (99%)	119 (100%)	0	100	100
50	LN	171/172 (99%)	169 (99%)	2 (1%)	71	57
51	LI	173/181 (96%)	168 (97%)	5 (3%)	42	21
52	LD	247/250 (99%)	238 (96%)	9 (4%)	35	14
53	LQ	164/165 (99%)	159 (97%)	5 (3%)	41	20
54	LR	166/175 (95%)	157 (95%)	9 (5%)	22	6
55	LS	157/157 (100%)	157 (100%)	0	100	100
56	LT	141/140 (101%)	138 (98%)	3 (2%)	53	33
57	LP	135/163 (83%)	131 (97%)	4 (3%)	41	20
58	LU	89/115 (77%)	84 (94%)	5 (6%)	21	6
59	LX	106/133 (80%)	105 (99%)	1 (1%)	78	69
60	LY	124/135 (92%)	116 (94%)	8 (6%)	17	4
61	LW	95/126 (75%)	93 (98%)	2 (2%)	53	33
62	LZ	118/118 (100%)	114 (97%)	4 (3%)	37	15
63	Lr	109/120 (91%)	109 (100%)	0	100	100
64	Lh	109/110 (99%)	109 (100%)	0	100	100
65	Lb	90/125 (72%)	87 (97%)	3 (3%)	38	16
66	LF	196/215 (91%)	195 (100%)	1 (0%)	88	83
67	Lc	84/97 (87%)	82 (98%)	2 (2%)	49	28
68	Ld	98/110 (89%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	Le	115/121 (95%)	115 (100%)	0	100	100
70	Lf	89/89 (100%)	89 (100%)	0	100	100
71	Lg	98/100 (98%)	96 (98%)	2 (2%)	55	36
72	Li	86/89 (97%)	83 (96%)	3 (4%)	36	15
73	Lj	74/80 (92%)	72 (97%)	2 (3%)	44	24
74	Lk	64/65 (98%)	61 (95%)	3 (5%)	26	8
75	Ll	47/48 (98%)	46 (98%)	1 (2%)	53	33
76	Lm	48/115 (42%)	48 (100%)	0	100	100
77	Ln	24/24 (100%)	24 (100%)	0	100	100
78	Lo	93/93 (100%)	90 (97%)	3 (3%)	39	17
79	Lp	75/75 (100%)	75 (100%)	0	100	100
All	All	9844/10847 (91%)	9495 (96%)	349 (4%)	39	15

5 of 349 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	LB	358	ARG
52	LD	259	LYS
41	LJ	85	LYS
45	LO	191	LYS
54	LR	181	LYS

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

Mol	Chain	Res	Type
31	SZ	106	GLN
57	LP	75	GLN
60	LY	66	GLN
60	LY	18	HIS
26	SR	48	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1660/1869 (88%)	255 (15%)	1 (0%)
2	L8	155/156 (99%)	19 (12%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3528/5069 (69%)	504 (14%)	15 (0%)
4	L7	119/120 (99%)	8 (6%)	0
80	mR	7/60 (11%)	3 (42%)	0
81	Pt	76/77 (98%)	8 (10%)	0
All	All	5545/7351 (75%)	797 (14%)	16 (0%)

5 of 797 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	3	C
1	S2	4	C
1	S2	17	C
1	S2	33	G
1	S2	41	G

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	4699	U
3	L5	3876	A
3	L5	1754	U
3	L5	2489	C
3	L5	1633	G

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

233 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
3	A2M	L5	398	3	18,25,26	1.02	1 (5%)	18,36,39	1.25	2 (11%)
3	PSU	L5	1536	3	18,21,22	1.42	3 (16%)	22,30,33	1.97	3 (13%)
1	PSU	S2	109	1	18,21,22	1.36	3 (16%)	22,30,33	1.89	3 (13%)
1	OMG	S2	601	1	18,26,27	0.92	1 (5%)	19,38,41	1.02	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	S2	644	1	18,26,27	0.94	1 (5%)	19,38,41	1.10	2 (10%)
3	OMG	L5	1625	3,84	18,26,27	0.96	1 (5%)	19,38,41	1.06	2 (10%)
3	PSU	L5	4423	3	18,21,22	1.39	3 (16%)	22,30,33	1.95	4 (18%)
3	PSU	L5	4431	3	18,21,22	1.42	3 (16%)	22,30,33	1.89	3 (13%)
1	PSU	S2	572	1	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
81	OMC	Pt	33	81	19,22,23	0.80	0	26,31,34	0.76	0
1	A2M	S2	668	85,1	18,25,26	0.93	1 (5%)	18,36,39	1.35	3 (16%)
1	PSU	S2	651	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
1	PSU	S2	866	1	18,21,22	1.35	2 (11%)	22,30,33	1.94	3 (13%)
1	PSU	S2	801	1	18,21,22	1.34	3 (16%)	22,30,33	1.90	4 (18%)
3	PSU	L5	4493	3,84	18,21,22	1.41	3 (16%)	22,30,33	1.91	3 (13%)
3	PSU	L5	4628	3	18,21,22	1.38	4 (22%)	22,30,33	1.84	3 (13%)
1	OMU	S2	1804	1	19,22,23	1.21	2 (10%)	26,31,34	1.75	5 (19%)
1	OMG	S2	683	1	18,26,27	0.93	1 (5%)	19,38,41	1.13	2 (10%)
3	A2M	L5	1524	3	18,25,26	0.95	1 (5%)	18,36,39	1.29	2 (11%)
3	UY1	L5	3818	3,84	19,22,23	1.38	3 (15%)	22,31,34	2.05	4 (18%)
3	PSU	L5	1779	3	18,21,22	1.37	3 (16%)	22,30,33	1.94	3 (13%)
3	OMC	L5	2351	3,85	19,22,23	0.81	0	26,31,34	0.96	1 (3%)
1	A2M	S2	1031	1	18,25,26	0.94	1 (5%)	18,36,39	1.34	3 (16%)
3	PSU	L5	3853	3,85,84	18,21,22	1.39	3 (16%)	22,30,33	1.93	3 (13%)
3	OMG	L5	3627	3	18,26,27	0.91	1 (5%)	19,38,41	1.22	3 (15%)
1	PSU	S2	815	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
29	AME	SV	1	29	9,10,11	3.34	2 (22%)	9,11,13	4.28	5 (55%)
3	A2M	L5	3760	3,85	18,25,26	1.04	1 (5%)	18,36,39	1.28	2 (11%)
3	OMU	L5	4227	3	19,22,23	1.24	3 (15%)	26,31,34	1.78	5 (19%)
3	A2M	L5	2787	3,85	18,25,26	1.01	1 (5%)	18,36,39	1.35	2 (11%)
1	OMU	S2	1288	1	19,22,23	1.25	4 (21%)	26,31,34	1.67	5 (19%)
1	PSU	S2	1136	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
3	PSU	L5	4579	3	18,21,22	1.38	3 (16%)	22,30,33	1.90	3 (13%)
1	OMU	S2	428	1	19,22,23	1.18	3 (15%)	26,31,34	1.72	5 (19%)
6	SAC	SA	2	6	7,8,9	3.78	2 (28%)	8,9,11	4.49	4 (50%)
3	A2M	L5	2363	3,85	18,25,26	0.93	1 (5%)	18,36,39	1.21	2 (11%)
3	PSU	L5	3762	3	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
3	PSU	L5	5001	3,85	18,21,22	1.42	3 (16%)	22,30,33	1.87	3 (13%)
1	OMG	S2	436	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	2508	3	18,21,22	1.35	3 (16%)	22,30,33	1.94	4 (18%)
3	PSU	L5	3770	3	18,21,22	1.53	5 (27%)	22,30,33	2.00	5 (22%)
3	OMC	L5	2861	3	19,22,23	0.79	0	26,31,34	0.68	0
3	PSU	L5	4420	3	18,21,22	1.45	3 (16%)	22,30,33	1.87	3 (13%)
3	OMC	L5	3869	3	19,22,23	0.81	0	26,31,34	0.75	0
3	OMC	L5	3701	3,84	19,22,23	0.80	0	26,31,34	0.86	0
1	4AC	S2	1337	1	21,24,25	1.08	2 (9%)	29,34,37	1.01	2 (6%)
3	PSU	L5	4972	3,84	18,21,22	1.39	3 (16%)	22,30,33	1.91	3 (13%)
1	OMU	S2	121	1	19,22,23	1.21	3 (15%)	26,31,34	1.72	5 (19%)
3	OMC	L5	2804	3	19,22,23	0.80	0	26,31,34	0.63	0
3	A2M	L5	3718	3	18,25,26	0.96	1 (5%)	18,36,39	1.10	2 (11%)
3	OMC	L5	2824	3	19,22,23	0.81	0	26,31,34	0.77	0
49	V5N	La	39	49	4,11,12	0.64	0	5,14,16	1.68	1 (20%)
3	PSU	L5	4552	3	18,21,22	1.39	3 (16%)	22,30,33	1.91	3 (13%)
3	PSU	L5	4636	3,85	18,21,22	1.41	3 (16%)	22,30,33	1.88	4 (18%)
1	PSU	S2	36	1	18,21,22	1.35	2 (11%)	22,30,33	1.93	3 (13%)
3	PSU	L5	3851	3	18,21,22	1.42	3 (16%)	22,30,33	1.90	3 (13%)
3	PSU	L5	1862	3	18,21,22	1.36	3 (16%)	22,30,33	1.98	4 (18%)
3	OMG	L5	2364	3	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
3	OMC	L5	3808	3	19,22,23	0.79	0	26,31,34	0.71	0
1	PSU	S2	1004	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
3	6MZ	L5	4220	3	18,25,26	0.82	1 (5%)	16,36,39	2.02	4 (25%)
1	PSU	S2	34	1	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
3	PSU	L5	3768	3	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
3	PSU	L5	1582	3	18,21,22	1.42	3 (16%)	22,30,33	1.92	3 (13%)
3	OMG	L5	4499	3	18,26,27	0.93	1 (5%)	19,38,41	1.04	2 (10%)
3	UR3	L5	4530	3	19,22,23	0.92	0	26,32,35	1.62	2 (7%)
76	M3L	Lm	98	76	10,11,12	0.50	0	9,14,16	0.46	0
1	PSU	S2	406	1	18,21,22	1.37	3 (16%)	22,30,33	1.93	3 (13%)
3	PSU	L5	3734	3	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	S2	822	1	18,21,22	1.37	3 (16%)	22,30,33	1.95	4 (18%)
81	PSU	Pt	56	81	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	S2	1703	85,1	19,22,23	0.79	0	26,31,34	0.70	0
3	PSU	L5	4293	3	18,21,22	1.35	3 (16%)	22,30,33	1.90	3 (13%)
65	MLZ	Lb	5	65,84	8,9,10	0.81	0	4,9,11	0.67	0
1	MA6	S2	1851	85,1	19,26,27	0.88	1 (5%)	18,38,41	1.42	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	S2	462	1	19,22,23	0.87	0	26,31,34	0.95	1 (3%)
3	A2M	L5	2815	3,85	18,25,26	0.95	1 (5%)	18,36,39	1.17	2 (11%)
1	A2M	S2	468	1	18,25,26	0.99	1 (5%)	18,36,39	1.22	2 (11%)
3	PSU	L5	4296	3	18,21,22	1.41	3 (16%)	22,30,33	1.98	3 (13%)
3	OMG	L5	2424	3	18,26,27	0.95	1 (5%)	19,38,41	1.02	2 (10%)
1	A2M	S2	159	1	18,25,26	1.01	1 (5%)	18,36,39	1.26	2 (11%)
3	A2M	L5	3785	3	18,25,26	0.89	0	18,36,39	1.54	3 (16%)
3	OMU	L5	2837	3	19,22,23	1.25	3 (15%)	26,31,34	1.79	5 (19%)
1	A2M	S2	590	1	18,25,26	1.03	1 (5%)	18,36,39	1.20	2 (11%)
3	OMC	L5	1340	3	19,22,23	0.79	0	26,31,34	0.72	0
3	PSU	L5	4353	3	18,21,22	1.39	3 (16%)	22,30,33	1.90	4 (18%)
3	PSU	L5	1744	3,84	18,21,22	1.39	3 (16%)	22,30,33	1.88	3 (13%)
3	PSU	L5	4403	3,84	18,21,22	1.39	3 (16%)	22,30,33	1.98	4 (18%)
3	PSU	L5	3920	3,85	18,21,22	1.37	3 (16%)	22,30,33	1.97	4 (18%)
1	OMU	S2	627	1	19,22,23	1.18	2 (10%)	26,31,34	1.73	5 (19%)
3	PSU	L5	4689	3	18,21,22	1.38	3 (16%)	22,30,33	1.91	3 (13%)
1	PSU	S2	1625	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
3	PSU	L5	4457	3	18,21,22	1.34	3 (16%)	22,30,33	2.00	3 (13%)
81	4SU	Pt	8	81	18,21,22	1.73	4 (22%)	26,30,33	2.18	4 (15%)
1	PSU	S2	1445	1	18,21,22	1.33	2 (11%)	22,30,33	1.94	4 (18%)
1	PSU	S2	296	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
3	OMC	L5	1881	3,85	19,22,23	0.80	0	26,31,34	0.93	0
3	PSU	L5	1860	3	18,21,22	1.41	3 (16%)	22,30,33	1.89	3 (13%)
3	1MA	L5	1322	3,85	16,25,26	1.35	2 (12%)	18,37,40	1.08	2 (11%)
1	PSU	S2	863	1	18,21,22	1.37	2 (11%)	22,30,33	1.93	3 (13%)
1	G7M	S2	1639	81,1	20,26,27	2.60	4 (20%)	17,39,42	0.93	1 (5%)
1	4AC	S2	1842	1	21,24,25	1.00	1 (4%)	29,34,37	1.11	3 (10%)
3	OMC	L5	2422	3,85	19,22,23	0.82	0	26,31,34	0.68	0
3	PSU	L5	4531	3	18,21,22	1.31	3 (16%)	22,30,33	1.99	5 (22%)
1	UY1	S2	1326	85,1	19,22,23	1.31	2 (10%)	22,31,34	1.89	4 (18%)
3	PSU	L5	5010	3	18,21,22	1.36	3 (16%)	22,30,33	1.90	3 (13%)
1	OMU	S2	116	1	19,22,23	1.18	3 (15%)	26,31,34	1.69	5 (19%)
1	PSU	S2	681	1	18,21,22	1.40	3 (16%)	22,30,33	1.92	4 (18%)
3	PSU	L5	3715	3	18,21,22	1.36	3 (16%)	22,30,33	1.92	3 (13%)
1	OMG	S2	867	1	18,26,27	0.91	1 (5%)	19,38,41	1.09	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	918	1	18,21,22	1.43	2 (11%)	22,30,33	1.86	3 (13%)
3	PSU	L5	4312	3,85	18,21,22	1.38	3 (16%)	22,30,33	1.89	3 (13%)
3	PSU	L5	3884	3	18,21,22	1.38	3 (16%)	22,30,33	1.78	4 (18%)
78	MLZ	Lo	53	78	8,9,10	0.74	0	4,9,11	0.61	0
3	PSU	L5	3758	3	18,21,22	1.36	3 (16%)	22,30,33	1.90	3 (13%)
3	OMU	L5	3925	3	19,22,23	1.27	3 (15%)	26,31,34	1.79	5 (19%)
3	5MC	L5	3782	3,85	18,22,23	0.96	2 (11%)	26,32,35	1.16	2 (7%)
3	OMU	L5	4306	3	19,22,23	1.26	3 (15%)	26,31,34	1.66	4 (15%)
3	PSU	L5	1792	3,84	18,21,22	1.34	3 (16%)	22,30,33	1.94	4 (18%)
3	OMG	L5	4637	3,84	18,26,27	0.95	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	S2	1177	1	18,21,22	1.37	3 (16%)	22,30,33	1.94	4 (18%)
1	A2M	S2	484	1	18,25,26	0.99	1 (5%)	18,36,39	1.23	2 (11%)
1	PSU	S2	1174	85,1	18,21,22	1.39	3 (16%)	22,30,33	1.89	3 (13%)
3	OMC	L5	4456	3	19,22,23	0.81	0	26,31,34	0.75	1 (3%)
81	H2U	Pt	21	81	18,21,22	0.95	2 (11%)	21,30,33	1.42	2 (9%)
38	V5N	LA	216	38	4,11,12	0.68	0	5,14,16	1.63	2 (40%)
1	OMU	S2	354	1	19,22,23	1.24	3 (15%)	26,31,34	1.75	5 (19%)
3	OMG	L5	1316	3	18,26,27	0.93	1 (5%)	19,38,41	1.07	1 (5%)
3	PSU	L5	1781	3	18,21,22	1.37	3 (16%)	22,30,33	1.88	3 (13%)
1	PSU	S2	814	1	18,21,22	1.35	3 (16%)	22,30,33	1.85	3 (13%)
3	PSU	L5	4673	3,85	18,21,22	1.39	3 (16%)	22,30,33	1.97	3 (13%)
1	PSU	S2	1056	1	18,21,22	1.34	2 (11%)	22,30,33	1.94	4 (18%)
1	A2M	S2	27	85,1	18,25,26	1.01	1 (5%)	18,36,39	1.16	2 (11%)
3	PSU	L5	4532	3	18,21,22	1.49	3 (16%)	22,30,33	2.20	4 (18%)
3	OMC	L5	2365	3,85	19,22,23	0.78	0	26,31,34	0.76	0
3	PSU	L5	4442	3	18,21,22	1.37	3 (16%)	22,30,33	1.96	5 (22%)
1	OMC	S2	517	1	19,22,23	0.80	0	26,31,34	0.77	0
3	OMU	L5	4498	3,84	19,22,23	1.24	3 (15%)	26,31,34	1.71	5 (19%)
3	OMC	L5	3841	3	19,22,23	0.79	0	26,31,34	0.66	0
3	PSU	L5	1677	3	18,21,22	1.43	4 (22%)	22,30,33	1.93	3 (13%)
3	PSU	L5	3729	3	18,21,22	1.37	3 (16%)	22,30,33	1.94	3 (13%)
1	PSU	S2	1239	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
81	G7M	Pt	47	81	20,26,27	2.42	3 (15%)	17,39,42	0.63	0
3	OMG	L5	4623	3	18,26,27	0.91	1 (5%)	19,38,41	1.16	2 (10%)
2	OMU	L8	14	3,2,84	19,22,23	1.25	2 (10%)	26,31,34	1.66	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3867	3	18,25,26	0.96	1 (5%)	18,36,39	1.30	3 (16%)
3	PSU	L5	4361	3	18,21,22	1.39	3 (16%)	22,30,33	1.88	3 (13%)
1	A2M	S2	99	85,1	18,25,26	1.01	1 (5%)	18,36,39	1.18	2 (11%)
1	PSU	S2	93	1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
3	OMU	L5	4620	3	19,22,23	1.26	3 (15%)	26,31,34	1.73	5 (19%)
1	PSU	S2	686	1	18,21,22	1.37	2 (11%)	22,30,33	1.93	3 (13%)
1	OMU	S2	1442	85,1	19,22,23	1.21	3 (15%)	26,31,34	1.70	4 (15%)
3	OMC	L5	4536	3	19,22,23	0.78	0	26,31,34	0.80	0
3	PSU	L5	3639	3	18,21,22	1.40	3 (16%)	22,30,33	1.89	3 (13%)
3	PSU	L5	4521	3,85,84	18,21,22	1.41	3 (16%)	22,30,33	1.93	5 (22%)
3	PSU	L5	4471	3,85	18,21,22	1.39	3 (16%)	22,30,33	1.94	4 (18%)
3	OMC	L5	3887	3,85	19,22,23	0.82	0	26,31,34	0.78	0
1	PSU	S2	1367	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	S2	649	1	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
3	OMG	L5	3792	3	18,26,27	0.93	1 (5%)	19,38,41	1.05	3 (15%)
1	PSU	S2	1232	1	18,21,22	1.38	2 (11%)	22,30,33	1.92	3 (13%)
3	PSU	L5	2839	3	18,21,22	1.42	3 (16%)	22,30,33	1.99	4 (18%)
3	A2M	L5	1534	3,85	18,25,26	0.98	1 (5%)	18,36,39	1.41	3 (16%)
3	PSU	L5	3695	3,84	18,21,22	1.38	3 (16%)	22,30,33	1.89	4 (18%)
3	OMG	L5	3744	3	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
3	A2M	L5	3830	3	18,25,26	0.98	1 (5%)	18,36,39	1.20	2 (11%)
3	OMG	L5	4196	3,81	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
3	A2M	L5	4590	3	18,25,26	0.98	1 (5%)	18,36,39	1.37	3 (16%)
1	A2M	S2	1678	1	18,25,26	1.03	1 (5%)	18,36,39	1.25	2 (11%)
1	PSU	S2	218	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	4 (18%)
3	A2M	L5	3825	3	18,25,26	0.92	1 (5%)	18,36,39	1.22	2 (11%)
1	PSU	S2	966	1	18,21,22	1.36	3 (16%)	22,30,33	1.87	3 (13%)
3	A2M	L5	4523	3,85	18,25,26	0.95	1 (5%)	18,36,39	1.29	2 (11%)
1	OMG	S2	1447	1	18,26,27	0.96	1 (5%)	19,38,41	1.09	2 (10%)
3	OMG	L5	3944	3	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
3	OMG	L5	4618	3,84	18,26,27	0.91	1 (5%)	19,38,41	1.12	2 (10%)
20	HY3	SX	62	20	6,8,9	1.35	1 (16%)	5,10,12	1.33	1 (20%)
1	A2M	S2	576	1	18,25,26	0.98	1 (5%)	18,36,39	1.26	2 (11%)
3	OMG	L5	2876	3	18,26,27	0.96	1 (5%)	19,38,41	1.03	2 (10%)
3	A2M	L5	1326	3	18,25,26	1.00	1 (5%)	18,36,39	1.18	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	4392	3	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
3	A2M	L5	2401	3,85	18,25,26	0.98	1 (5%)	18,36,39	1.19	2 (11%)
1	OMG	S2	509	85,1	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
1	PSU	S2	1081	1	18,21,22	1.44	4 (22%)	22,30,33	1.90	3 (13%)
3	A2M	L5	1871	3,85	18,25,26	0.96	1 (5%)	18,36,39	1.36	3 (16%)
1	B8N	S2	1248	1	24,29,30	0.94	1 (4%)	29,42,45	1.54	5 (17%)
3	PSU	L5	1782	3	18,21,22	1.38	3 (16%)	22,30,33	1.92	3 (13%)
1	PSU	S2	609	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
3	A2M	L5	3723	3	18,25,26	0.99	1 (5%)	18,36,39	1.21	2 (11%)
1	PSU	S2	573	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	S2	1692	1	18,21,22	1.38	3 (16%)	22,30,33	1.92	3 (13%)
1	A2M	S2	512	1	18,25,26	0.98	1 (5%)	18,36,39	1.25	2 (11%)
1	OMC	S2	174	85,1	19,22,23	0.80	0	26,31,34	0.81	0
3	OMG	L5	1522	3	18,26,27	0.91	1 (5%)	19,38,41	1.20	3 (15%)
3	PSU	L5	2632	3	18,21,22	1.40	4 (22%)	22,30,33	1.84	3 (13%)
3	A2M	L5	400	3	18,25,26	0.98	1 (5%)	18,36,39	1.21	2 (11%)
1	OMC	S2	1391	1	19,22,23	0.83	0	26,31,34	0.79	0
1	OMG	S2	1490	85,1	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
3	PSU	L5	4299	3	18,21,22	1.38	3 (16%)	22,30,33	1.95	3 (13%)
3	A2M	L5	4571	3	18,25,26	1.01	1 (5%)	18,36,39	1.20	2 (11%)
1	A2M	S2	166	1	18,25,26	1.01	1 (5%)	18,36,39	1.25	2 (11%)
1	PSU	S2	1244	1	18,21,22	1.35	2 (11%)	22,30,33	1.95	3 (13%)
1	OMG	S2	1328	1	18,26,27	0.94	1 (5%)	19,38,41	1.04	2 (10%)
3	PSU	L5	2843	3	18,21,22	1.37	3 (16%)	22,30,33	1.91	5 (22%)
3	A2M	L5	3724	3	18,25,26	0.99	1 (5%)	18,36,39	1.18	2 (11%)
3	PSU	L5	3764	3,85	18,21,22	1.37	3 (16%)	22,30,33	1.91	3 (13%)
3	OMG	L5	4228	3	18,26,27	0.87	1 (5%)	19,38,41	1.21	2 (10%)
1	PSU	S2	1238	1	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
39	HIC	LB	245	39	8,11,12	1.52	2 (25%)	6,14,16	1.06	0
1	A2M	S2	1383	1	18,25,26	1.00	1 (5%)	18,36,39	1.28	2 (11%)
3	PSU	L5	4500	3,85	18,21,22	1.37	2 (11%)	22,30,33	1.98	3 (13%)
3	PSU	L5	3844	3	18,21,22	1.45	3 (16%)	22,30,33	1.91	3 (13%)
3	PSU	L5	3637	3,84	18,21,22	1.42	3 (16%)	22,30,33	1.95	5 (22%)
3	OMG	L5	4370	3	18,26,27	0.95	1 (5%)	19,38,41	1.05	2 (10%)
3	PSU	L5	4569	3	18,21,22	1.40	3 (16%)	22,30,33	1.94	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4576	3	18,21,22	1.38	2 (11%)	22,30,33	1.93	3 (13%)
63	SAC	Lr	2	63	7,8,9	3.80	2 (28%)	8,9,11	4.29	4 (50%)
2	PSU	L8	69	85,2	18,21,22	1.38	3 (16%)	22,30,33	1.95	4 (18%)
1	6MZ	S2	1832	85,84,1	18,25,26	0.86	1 (5%)	16,36,39	2.13	3 (18%)
3	OMU	L5	2415	3	19,22,23	1.23	3 (15%)	26,31,34	1.71	4 (15%)
1	PSU	S2	1643	85,1	18,21,22	1.38	2 (11%)	22,30,33	1.90	5 (22%)
2	PSU	L8	55	2	18,21,22	1.37	3 (16%)	22,30,33	1.89	4 (18%)
1	PSU	S2	105	1	18,21,22	1.38	3 (16%)	22,30,33	1.92	4 (18%)
3	5MC	L5	4447	3,84	18,22,23	1.02	2 (11%)	26,32,35	1.27	2 (7%)
1	PSU	S2	1347	1	18,21,22	1.35	3 (16%)	22,30,33	1.89	3 (13%)
3	PSU	L5	1683	3,84	18,21,22	1.43	3 (16%)	22,30,33	1.99	3 (13%)
1	MA6	S2	1850	1	19,26,27	0.90	1 (5%)	18,38,41	1.32	3 (16%)
2	OMG	L8	75	2	18,26,27	0.89	1 (5%)	19,38,41	1.08	2 (10%)
3	OMG	L5	4494	3,85	18,26,27	0.95	1 (5%)	19,38,41	1.11	3 (15%)
1	OMU	S2	172	1	19,22,23	1.21	2 (10%)	26,31,34	1.77	5 (19%)
1	PSU	S2	119	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
3	OMG	L5	3899	3	18,26,27	0.91	1 (5%)	19,38,41	1.14	2 (10%)
1	PSU	S2	1243	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)

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
3	A2M	L5	398	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	601	1	-	1/5/27/28	0/3/3/3
1	OMG	S2	644	1	-	4/5/27/28	0/3/3/3
3	OMG	L5	1625	3,84	-	1/5/27/28	0/3/3/3
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
81	OMC	Pt	33	81	-	0/9/27/28	0/2/2/2
1	A2M	S2	668	85,1	-	2/5/27/28	0/3/3/3
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3,84	-	0/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	1804	1	-	1/9/27/28	0/2/2/2
1	OMG	S2	683	1	-	0/5/27/28	0/3/3/3
3	A2M	L5	1524	3	-	1/5/27/28	0/3/3/3
3	UY1	L5	3818	3,84	-	2/9/27/28	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	3,85	-	2/9/27/28	0/2/2/2
1	A2M	S2	1031	1	-	0/5/27/28	0/3/3/3
3	PSU	L5	3853	3,85,84	-	0/7/25/26	0/2/2/2
3	OMG	L5	3627	3	-	0/5/27/28	0/3/3/3
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
29	AME	SV	1	29	-	1/9/10/12	-
3	A2M	L5	3760	3,85	-	1/5/27/28	0/3/3/3
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2787	3,85	-	0/5/27/28	0/3/3/3
1	OMU	S2	1288	1	-	3/9/27/28	0/2/2/2
1	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	428	1	-	4/9/27/28	0/2/2/2
6	SAC	SA	2	6	-	5/7/8/10	-
3	A2M	L5	2363	3,85	-	1/5/27/28	0/3/3/3
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	3,85	-	0/7/25/26	0/2/2/2
1	OMG	S2	436	1	-	0/5/27/28	0/3/3/3
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4420	3	-	3/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3701	3,84	-	4/9/27/28	0/2/2/2
1	4AC	S2	1337	1	-	2/11/29/30	0/2/2/2
3	PSU	L5	4972	3,84	-	0/7/25/26	0/2/2/2
1	OMU	S2	121	1	-	0/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3718	3	-	1/5/27/28	0/3/3/3
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
49	V5N	La	39	49	-	0/5/10/12	0/1/1/1
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4636	3,85	-	2/7/25/26	0/2/2/2
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2364	3	-	0/5/27/28	0/3/3/3
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
3	6MZ	L5	4220	3	-	0/5/27/28	0/3/3/3
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	0/5/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
76	M3L	Lm	98	76	-	0/9/10/12	-
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	2/7/25/26	0/2/2/2
81	PSU	Pt	56	81	-	0/7/25/26	0/2/2/2
1	OMC	S2	1703	85,1	-	0/9/27/28	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
65	MLZ	Lb	5	65,84	-	1/7/8/10	-
1	MA6	S2	1851	85,1	-	3/7/29/30	0/3/3/3
1	OMC	S2	462	1	-	1/9/27/28	0/2/2/2
3	A2M	L5	2815	3,85	-	3/5/27/28	0/3/3/3
1	A2M	S2	468	1	-	1/5/27/28	0/3/3/3
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	0/5/27/28	0/3/3/3
1	A2M	S2	159	1	-	1/5/27/28	0/3/3/3
3	A2M	L5	3785	3	-	2/5/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
1	A2M	S2	590	1	-	2/5/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1744	3,84	-	0/7/25/26	0/2/2/2
3	PSU	L5	4403	3,84	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	3,85	-	0/7/25/26	0/2/2/2
1	OMU	S2	627	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
81	4SU	Pt	8	81	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	1881	3,85	-	0/9/27/28	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	1MA	L5	1322	3,85	-	0/3/25/26	0/3/3/3
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
1	G7M	S2	1639	81,1	-	0/3/25/26	0/3/3/3
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
3	OMC	L5	2422	3,85	-	2/9/27/28	0/2/2/2
3	PSU	L5	4531	3	-	1/7/25/26	0/2/2/2
1	UY1	S2	1326	85,1	-	2/9/27/28	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	116	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	867	1	-	1/5/27/28	0/3/3/3
1	PSU	S2	918	1	-	3/7/25/26	0/2/2/2
3	PSU	L5	4312	3,85	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
78	MLZ	Lo	53	78	-	1/7/8/10	-
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
3	5MC	L5	3782	3,85	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1792	3,84	-	0/7/25/26	0/2/2/2
3	OMG	L5	4637	3,84	-	1/5/27/28	0/3/3/3
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	1/5/27/28	0/3/3/3
1	PSU	S2	1174	85,1	-	0/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
81	H2U	Pt	21	81	-	2/7/38/39	0/2/2/2
38	V5N	LA	216	38	-	1/5/10/12	0/1/1/1
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2
3	OMG	L5	1316	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	1781	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3,85	-	0/7/25/26	0/2/2/2
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	27	85,1	-	1/5/27/28	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2365	3,85	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
3	OMU	L5	4498	3,84	-	0/9/27/28	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1677	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3729	3	-	1/7/25/26	0/2/2/2
1	PSU	S2	1239	1	-	0/7/25/26	0/2/2/2
81	G7M	Pt	47	81	-	0/3/25/26	0/3/3/3
3	OMG	L5	4623	3	-	0/5/27/28	0/3/3/3
2	OMU	L8	14	3,2,84	-	1/9/27/28	0/2/2/2
3	A2M	L5	3867	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	99	85,1	-	0/5/27/28	0/3/3/3
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1442	85,1	-	2/9/27/28	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	3,85,84	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3,85	-	0/7/25/26	0/2/2/2
3	OMC	L5	3887	3,85	-	0/9/27/28	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/5/27/28	0/3/3/3
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1534	3,85	-	2/5/27/28	0/3/3/3
3	PSU	L5	3695	3,84	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	3830	3	-	0/5/27/28	0/3/3/3
3	OMG	L5	4196	3,81	-	1/5/27/28	0/3/3/3
3	A2M	L5	4590	3	-	1/5/27/28	0/3/3/3
1	A2M	S2	1678	1	-	1/5/27/28	0/3/3/3
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	0/5/27/28	0/3/3/3
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	3,85	-	0/5/27/28	0/3/3/3
1	OMG	S2	1447	1	-	2/5/27/28	0/3/3/3
3	OMG	L5	3944	3	-	1/5/27/28	0/3/3/3
3	OMG	L5	4618	3,84	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	HY3	SX	62	20	-	1/1/12/14	0/1/1/1
1	A2M	S2	576	1	-	2/5/27/28	0/3/3/3
3	OMG	L5	2876	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	1326	3	-	1/5/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	2401	3,85	-	0/5/27/28	0/3/3/3
1	OMG	S2	509	85,1	-	0/5/27/28	0/3/3/3
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
3	A2M	L5	1871	3,85	-	0/5/27/28	0/3/3/3
1	B8N	S2	1248	1	-	1/16/34/35	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	3723	3	-	1/5/27/28	0/3/3/3
1	PSU	S2	573	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	512	1	-	1/5/27/28	0/3/3/3
1	OMC	S2	174	85,1	-	0/9/27/28	0/2/2/2
3	OMG	L5	1522	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	0/5/27/28	0/3/3/3
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
1	OMG	S2	1490	85,1	-	3/5/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4571	3	-	1/5/27/28	0/3/3/3
1	A2M	S2	166	1	-	0/5/27/28	0/3/3/3
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1328	1	-	1/5/27/28	0/3/3/3
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3724	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	3764	3,85	-	0/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	0/5/27/28	0/3/3/3
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
39	HIC	LB	245	39	-	1/5/6/8	0/1/1/1
1	A2M	S2	1383	1	-	1/5/27/28	0/3/3/3
3	PSU	L5	4500	3,85	-	1/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	3637	3,84	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4569	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
63	SAC	Lr	2	63	-	2/7/8/10	-
2	PSU	L8	69	85,2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	S2	1832	85,84,1	-	0/5/27/28	0/3/3/3
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
1	PSU	S2	1643	85,1	-	0/7/25/26	0/2/2/2
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	3,84	-	4/7/25/26	0/2/2/2
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	3,84	-	0/7/25/26	0/2/2/2
1	MA6	S2	1850	1	-	0/7/29/30	0/3/3/3
2	OMG	L8	75	2	-	0/5/27/28	0/3/3/3
3	OMG	L5	4494	3,85	-	1/5/27/28	0/3/3/3
1	OMU	S2	172	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	0/5/27/28	0/3/3/3
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2

The worst 5 of 436 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	Lr	2	SAC	OAC-C1A	8.97	1.43	1.23
6	SA	2	SAC	OAC-C1A	8.96	1.43	1.23
29	SV	1	AME	OT-CT1	8.92	1.43	1.23
1	S2	1639	G7M	C8-N9	7.50	1.46	1.33
81	Pt	47	G7M	C8-N9	7.34	1.46	1.33

The worst 5 of 640 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	SA	2	SAC	OAC-C1A-C2A	-7.63	107.89	122.06
1	S2	1832	6MZ	C2-N1-C6	7.17	122.74	116.59
29	SV	1	AME	CA-N-CT1	-7.11	110.04	123.15
3	L5	4532	PSU	N1-C2-N3	7.10	123.17	115.13
63	Lr	2	SAC	OAC-C1A-N	-6.90	109.27	121.95

There are no chirality outliers.

5 of 119 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L8	14	OMU	C1'-C2'-O2'-CM2
6	SA	2	SAC	OAC-C1A-N-CA
6	SA	2	SAC	CB-CA-N-C1A

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Mol	Chain	Res	Type	Atoms
6	SA	2	SAC	O-C-CA-CB
29	SV	1	AME	OT-CT1-N-CA

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 860 ligands modelled in this entry, 831 are monoatomic - leaving 29 for Mogul analysis.

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	$\# Z > 2$
83	PUT	L5	5122	-	5,5,5	0.12	0	4,4,4	0.16	0
83	PUT	L5	5116	-	5,5,5	0.09	0	4,4,4	0.17	0
87	3H3	L5	5102	-	33,34,34	3.52	11 (33%)	34,45,45	3.93	19 (55%)
82	SPD	L5	5113	-	9,9,9	0.15	0	8,8,8	0.21	0
82	SPD	L5	5106	-	9,9,9	0.20	0	8,8,8	0.24	0
83	PUT	L5	5118	-	5,5,5	0.09	0	4,4,4	0.18	0
82	SPD	S2	1902	-	9,9,9	0.33	0	8,8,8	0.77	0
83	PUT	L5	5123	-	5,5,5	0.14	0	4,4,4	0.15	0
88	TRS	L5	5125	-	7,7,7	0.08	0	9,9,9	0.24	0
82	SPD	L5	5109	-	9,9,9	0.15	0	8,8,8	0.24	0
90	MET	Pt	78	81	6,7,8	0.68	0	2,7,9	2.86	1 (50%)
83	PUT	L5	5117	-	5,5,5	0.10	0	4,4,4	0.15	0
82	SPD	L5	5107	-	9,9,9	0.31	0	8,8,8	0.92	0
82	SPD	L5	5110	-	9,9,9	0.32	0	8,8,8	0.97	0
82	SPD	S2	1901	-	9,9,9	0.32	0	8,8,8	0.75	0
82	SPD	L5	5111	-	9,9,9	0.14	0	8,8,8	0.21	0
82	SPD	L5	5114	-	9,9,9	0.16	0	8,8,8	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	SPD	L5	5115	-	9,9,9	0.18	0	8,8,8	0.27	0
82	SPD	L5	5112	-	9,9,9	0.18	0	8,8,8	0.28	0
82	SPD	L5	5104	-	9,9,9	0.15	0	8,8,8	0.30	0
83	PUT	L5	5121	-	5,5,5	0.16	0	4,4,4	0.21	0
83	PUT	L5	5119	-	5,5,5	0.10	0	4,4,4	0.16	0
82	SPD	L5	5103	-	9,9,9	0.31	0	8,8,8	0.83	0
82	SPD	L5	5108	-	9,9,9	0.32	0	8,8,8	1.00	0
86	ANM	L5	5101	84	20,20,20	1.15	1 (5%)	22,27,27	1.35	2 (9%)
88	TRS	L5	5124	-	7,7,7	0.38	0	9,9,9	0.56	0
82	SPD	L5	5105	-	9,9,9	0.17	0	8,8,8	0.27	0
83	PUT	S2	1903	-	5,5,5	0.11	0	4,4,4	0.15	0
83	PUT	L5	5120	-	5,5,5	0.11	0	4,4,4	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	PUT	L5	5122	-	-	0/3/3/3	-
83	PUT	L5	5116	-	-	0/3/3/3	-
87	3H3	L5	5102	-	-	14/39/51/51	0/1/2/2
82	SPD	L5	5113	-	-	6/7/7/7	-
82	SPD	L5	5106	-	-	3/7/7/7	-
83	PUT	L5	5118	-	-	0/3/3/3	-
82	SPD	S2	1902	-	-	5/7/7/7	-
83	PUT	L5	5123	-	-	0/3/3/3	-
88	TRS	L5	5125	-	-	6/9/9/9	-
82	SPD	L5	5109	-	-	4/7/7/7	-
90	MET	Pt	78	81	-	4/5/6/8	-
83	PUT	L5	5117	-	-	1/3/3/3	-
82	SPD	L5	5107	-	-	3/7/7/7	-
82	SPD	L5	5110	-	-	3/7/7/7	-
82	SPD	S2	1901	-	-	2/7/7/7	-
82	SPD	L5	5111	-	-	3/7/7/7	-
82	SPD	L5	5114	-	-	5/7/7/7	-
82	SPD	L5	5115	-	-	1/7/7/7	-
82	SPD	L5	5112	-	-	5/7/7/7	-
82	SPD	L5	5104	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	PUT	L5	5121	-	-	1/3/3/3	-
83	PUT	L5	5119	-	-	1/3/3/3	-
82	SPD	L5	5103	-	-	0/7/7/7	-
82	SPD	L5	5108	-	-	4/7/7/7	-
86	ANM	L5	5101	84	-	0/10/23/23	0/2/2/2
88	TRS	L5	5124	-	-	0/9/9/9	-
82	SPD	L5	5105	-	-	5/7/7/7	-
83	PUT	S2	1903	-	-	0/3/3/3	-
83	PUT	L5	5120	-	-	1/3/3/3	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	L5	5102	3H3	C13-C12	9.62	1.53	1.33
87	L5	5102	3H3	O3-C22	7.90	1.39	1.23
87	L5	5102	3H3	O4-C23	7.55	1.38	1.23
87	L5	5102	3H3	C23-N	7.33	1.50	1.37
87	L5	5102	3H3	C22-N	6.46	1.48	1.37

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	L5	5102	3H3	C22-N-C23	-12.58	110.52	125.78
87	L5	5102	3H3	O3-C22-N	-7.67	108.12	120.28
87	L5	5102	3H3	O4-C23-N	-7.50	108.39	120.28
87	L5	5102	3H3	O4-C23-C24	-6.93	109.12	122.62
87	L5	5102	3H3	O3-C22-C21	-6.73	109.51	122.62

There are no chirality outliers.

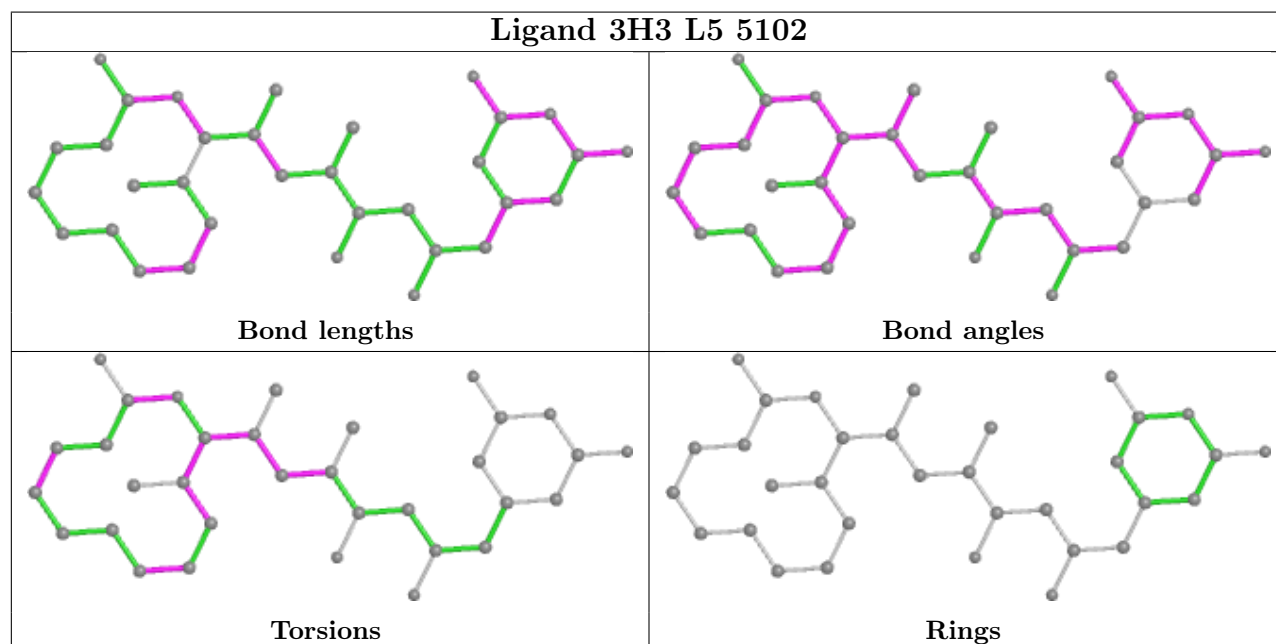
5 of 81 torsion outliers are listed below:

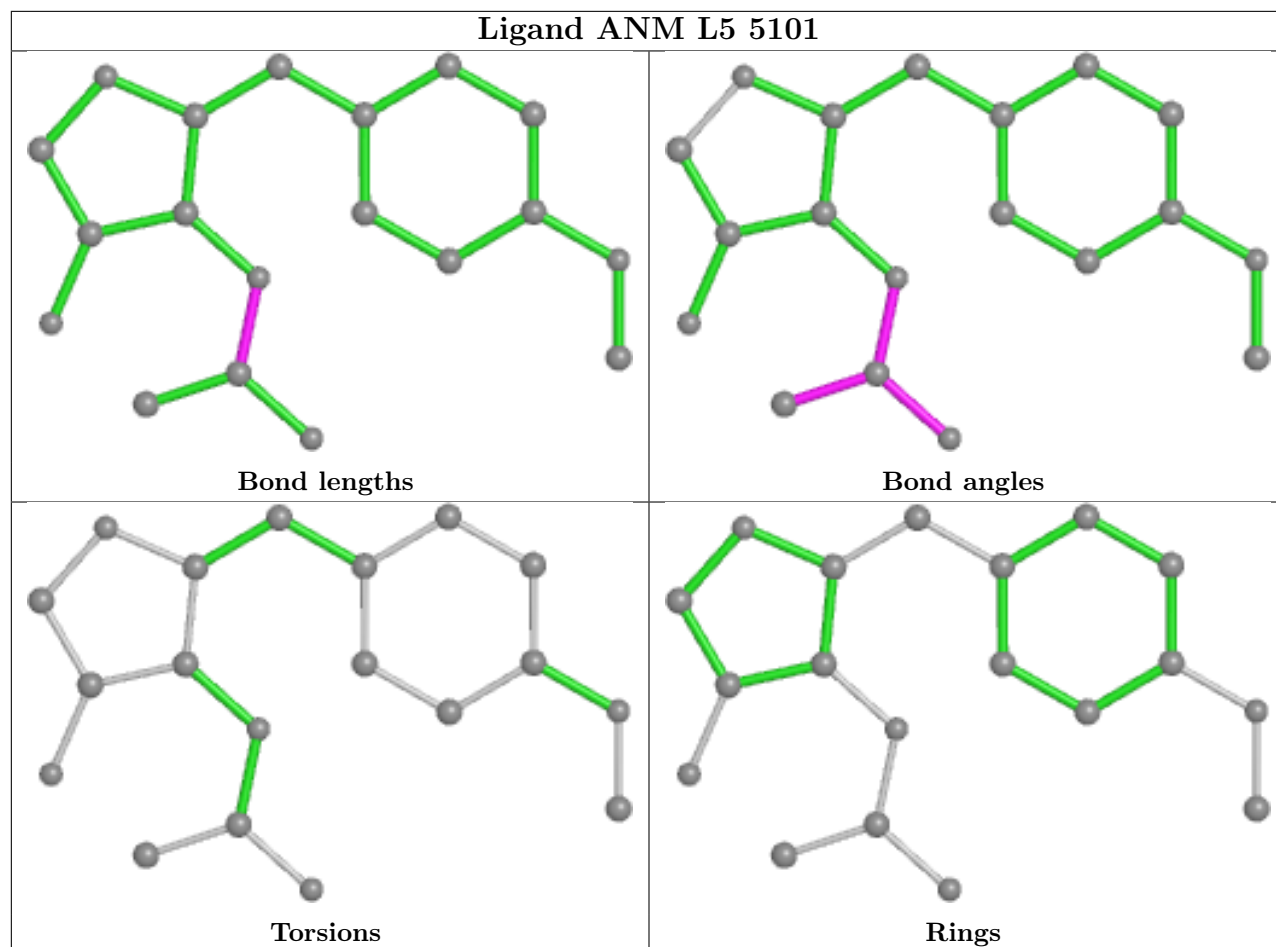
Mol	Chain	Res	Type	Atoms
82	L5	5108	SPD	C7-C8-C9-N10
82	L5	5114	SPD	C4-C5-N6-C7
87	L5	5102	3H3	C2-C1-C11-O1
87	L5	5102	3H3	C2-C1-C11-C12
87	L5	5102	3H3	C-C1-C11-O1

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

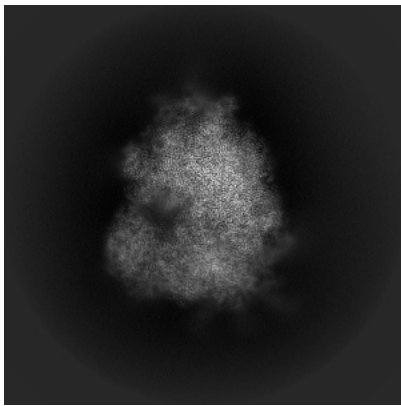
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40205. These allow visual inspection of the internal detail of the map and identification of artifacts.

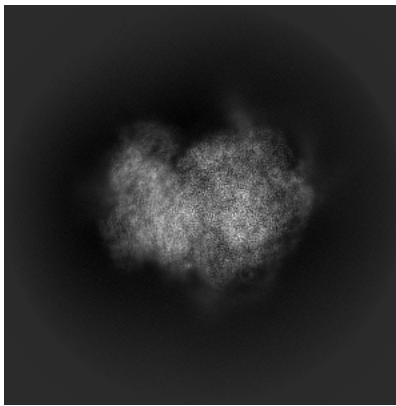
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

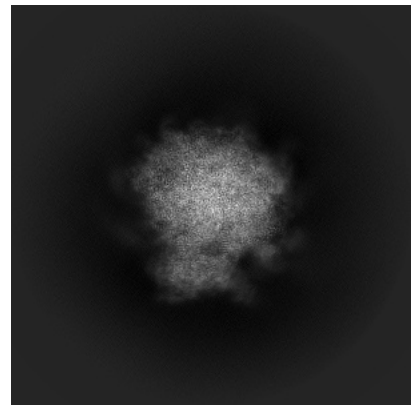
6.1.1 Primary map



X

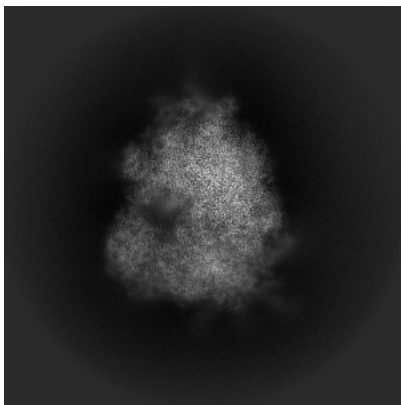


Y

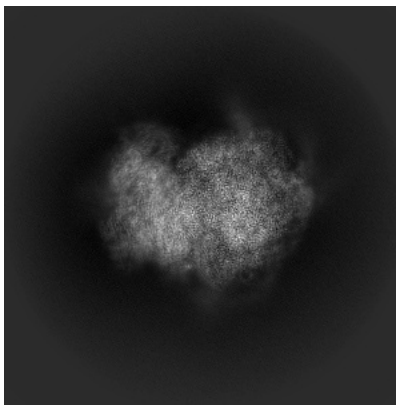


Z

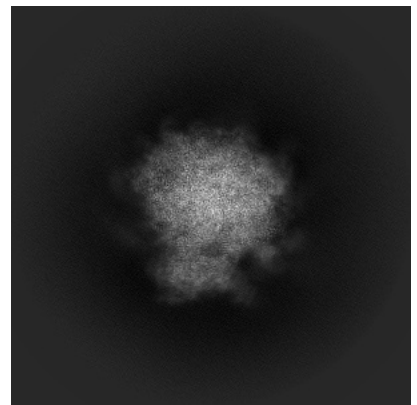
6.1.2 Raw map



X



Y

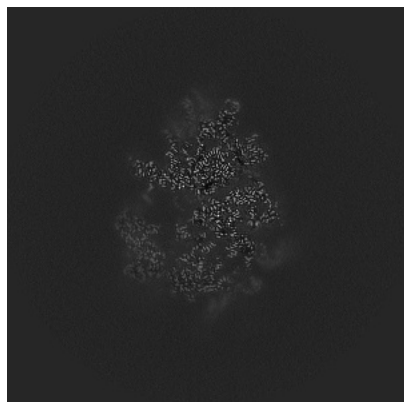


Z

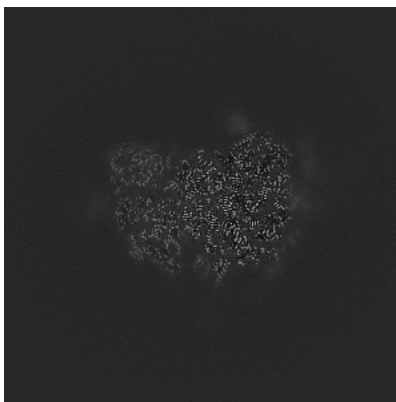
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

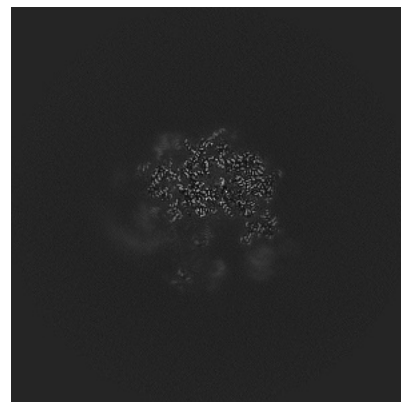
6.2.1 Primary map



X Index: 320

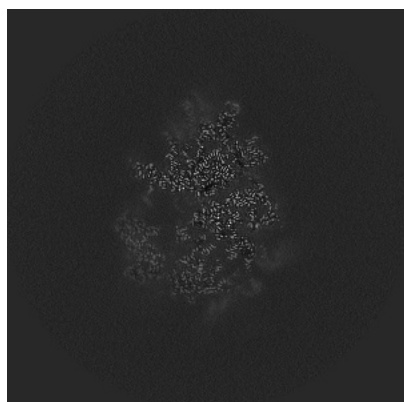


Y Index: 320

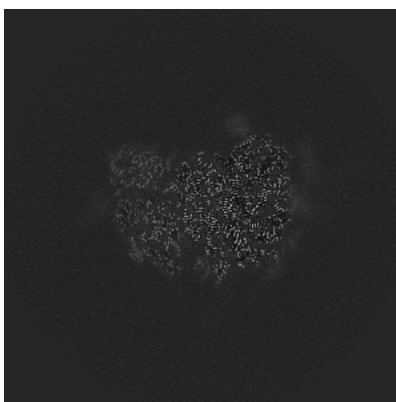


Z Index: 320

6.2.2 Raw map



X Index: 320



Y Index: 320

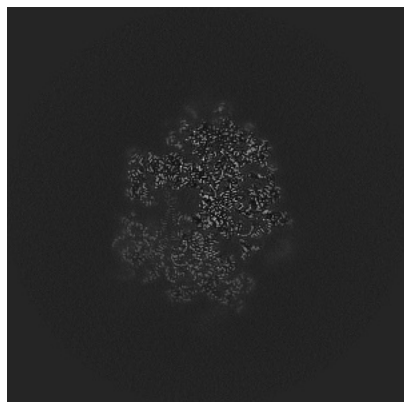


Z Index: 320

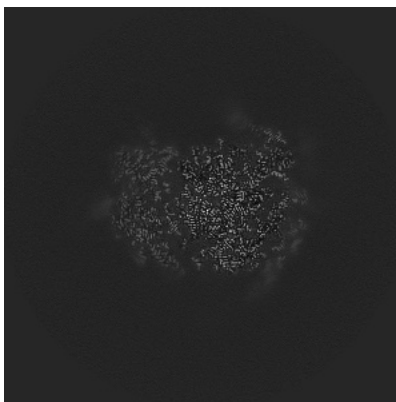
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 299

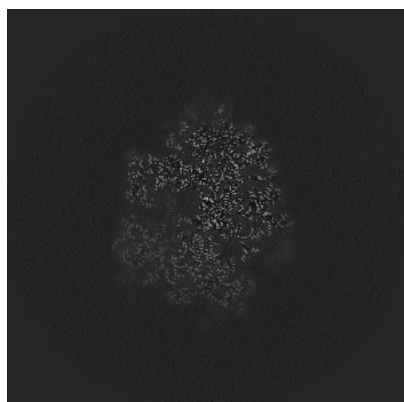


Y Index: 332

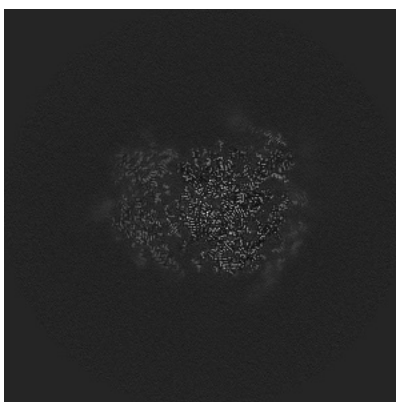


Z Index: 362

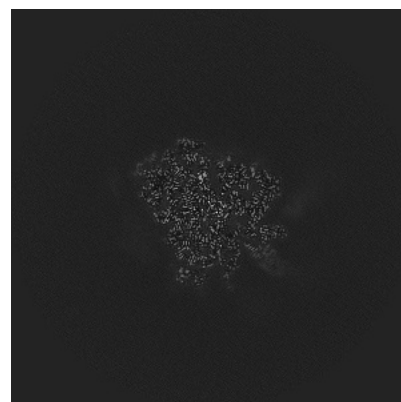
6.3.2 Raw map



X Index: 299



Y Index: 332

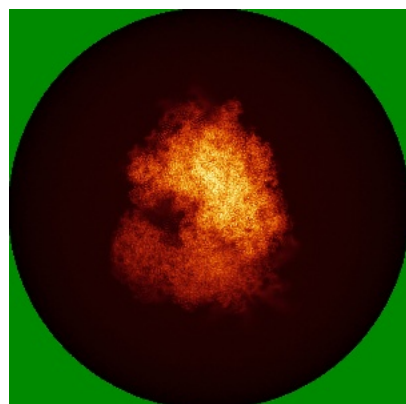


Z Index: 362

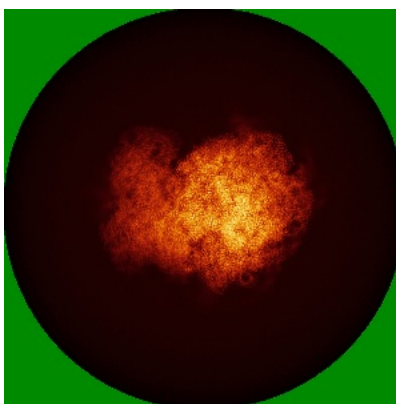
The images above show the largest variance slices of the map in three orthogonal directions.

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

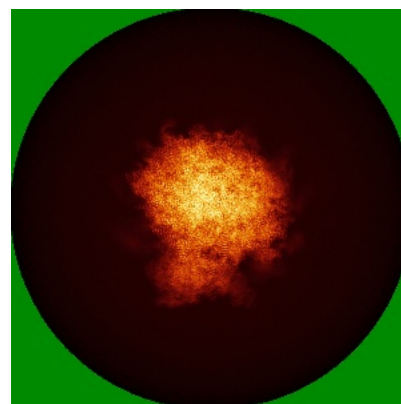
6.4.1 Primary map



X

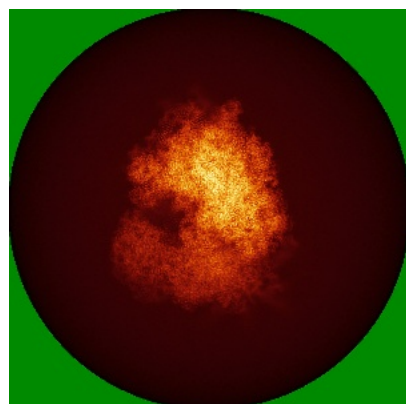


Y

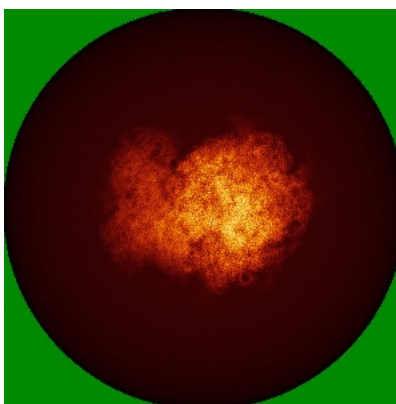


Z

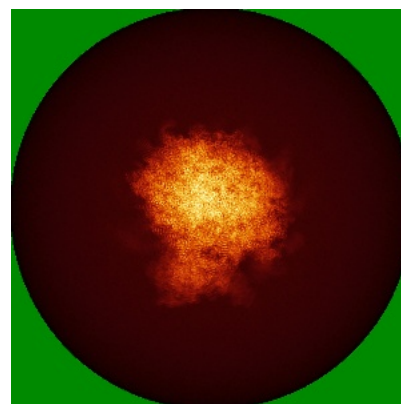
6.4.2 Raw map



X



Y

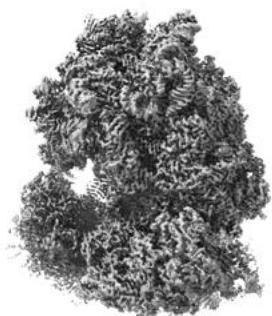


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

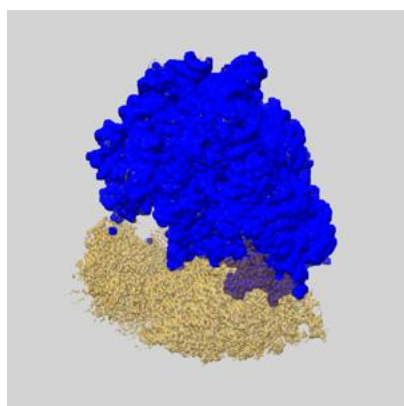
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

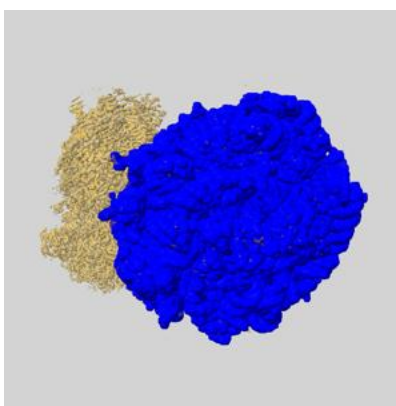
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

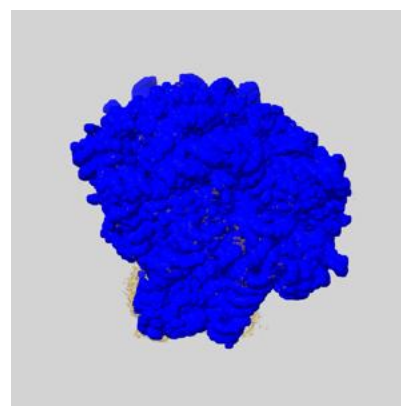
6.6.1 emd_40205_msk_1.map [i](#)



X



Y

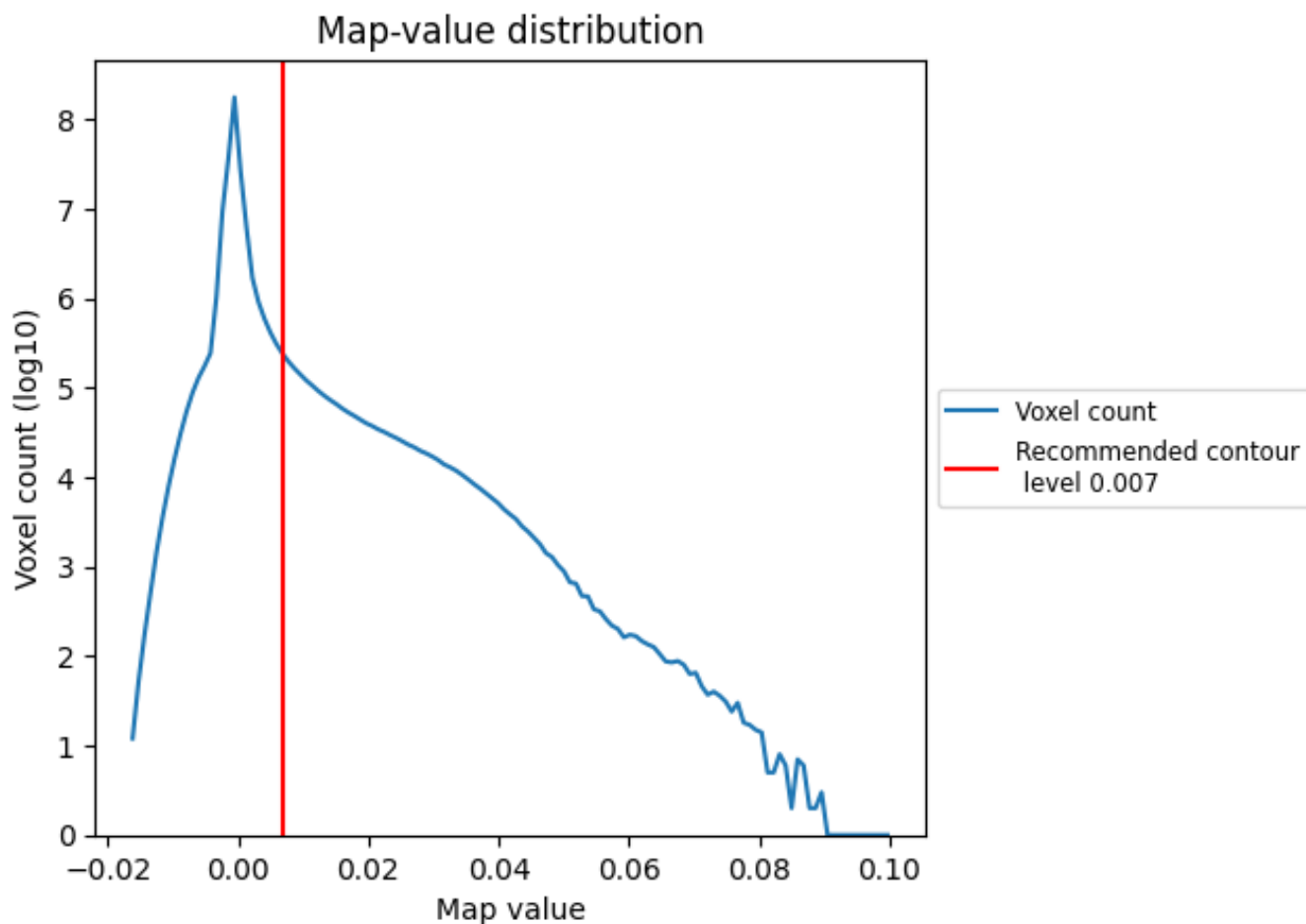


Z

7 Map analysis [i](#)

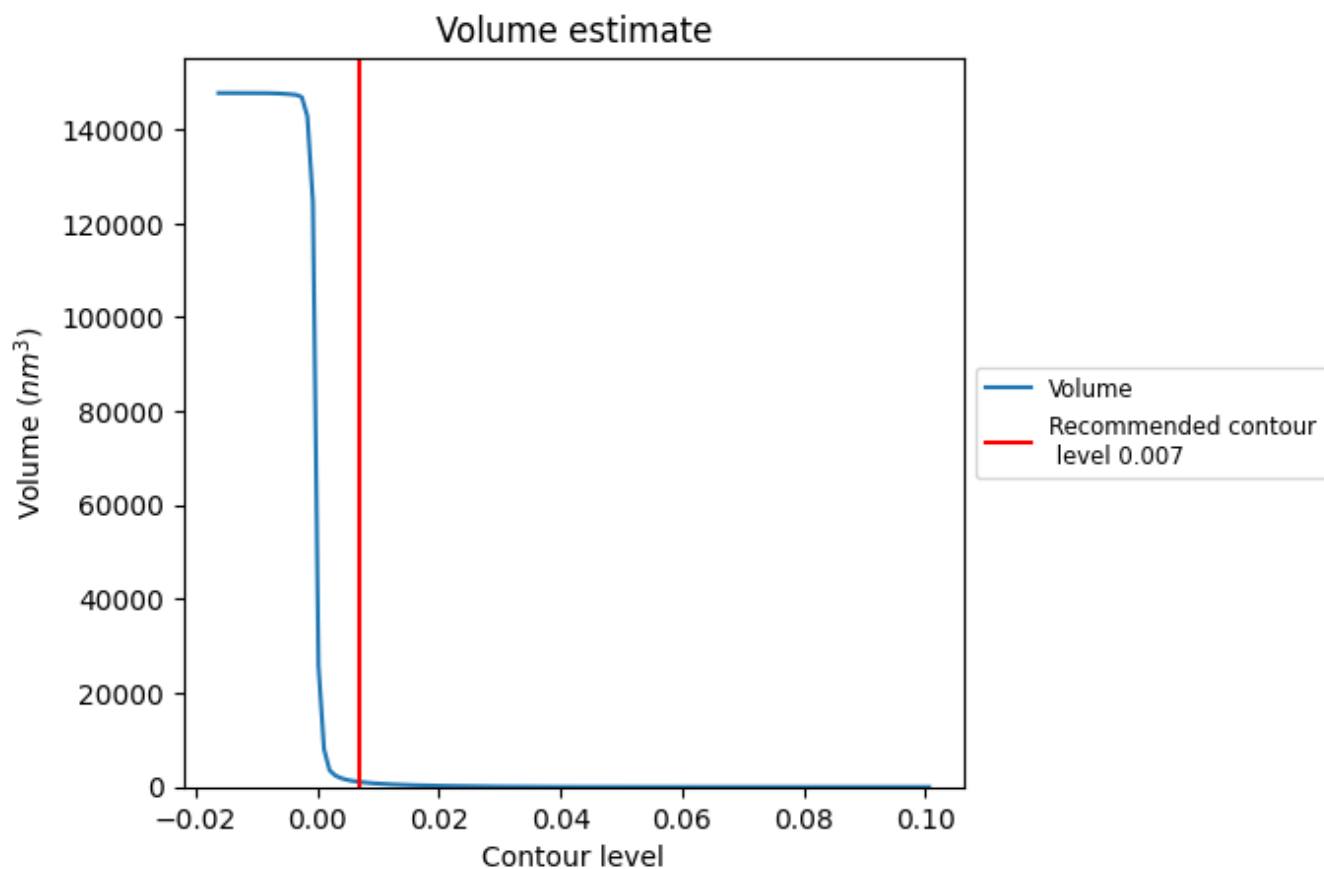
This section contains the results of statistical analysis of the map.

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.

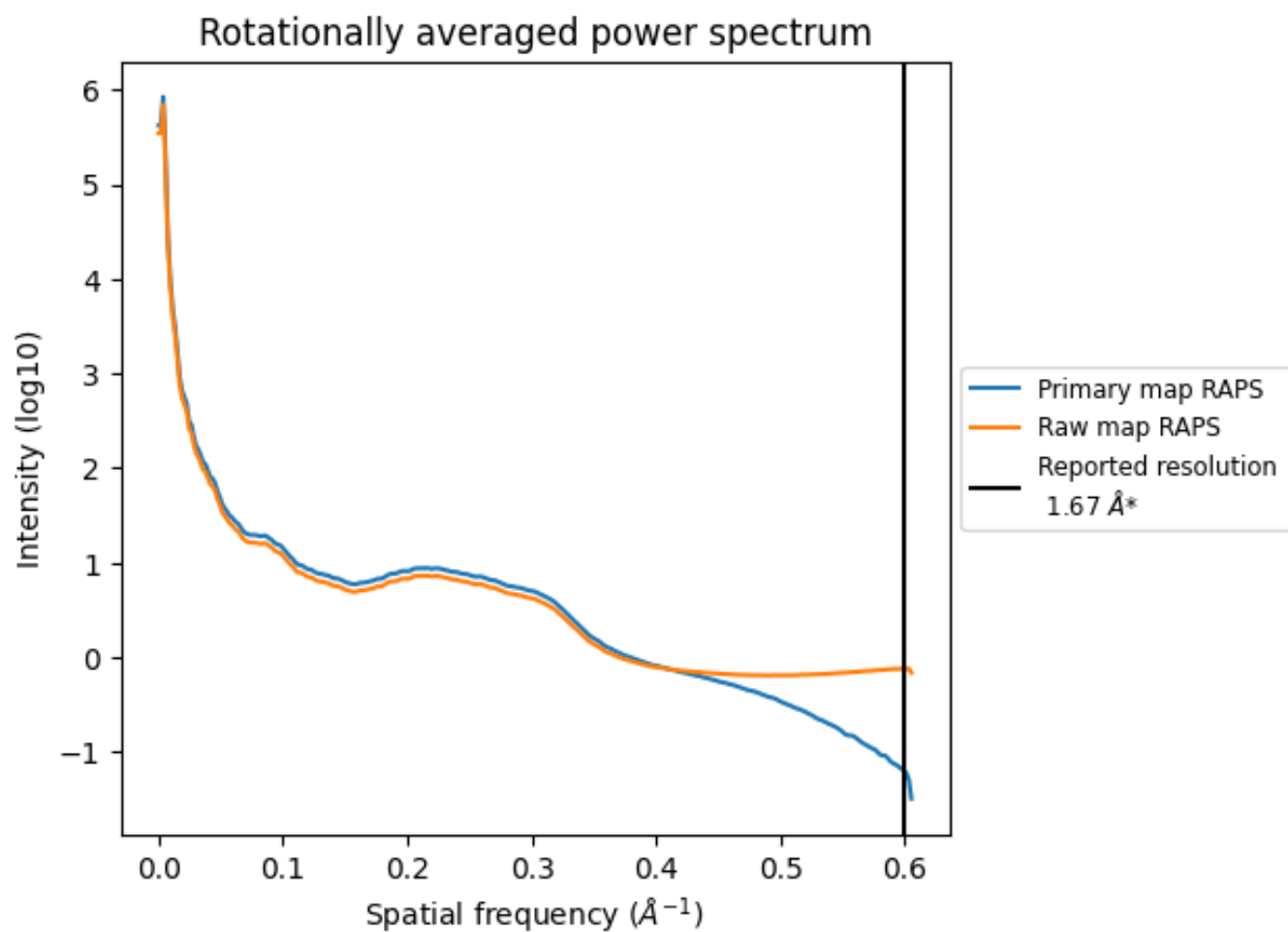
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1063 nm^3 ; this corresponds to an approximate mass of 960 kDa.

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

7.3 Rotationally averaged power spectrum i

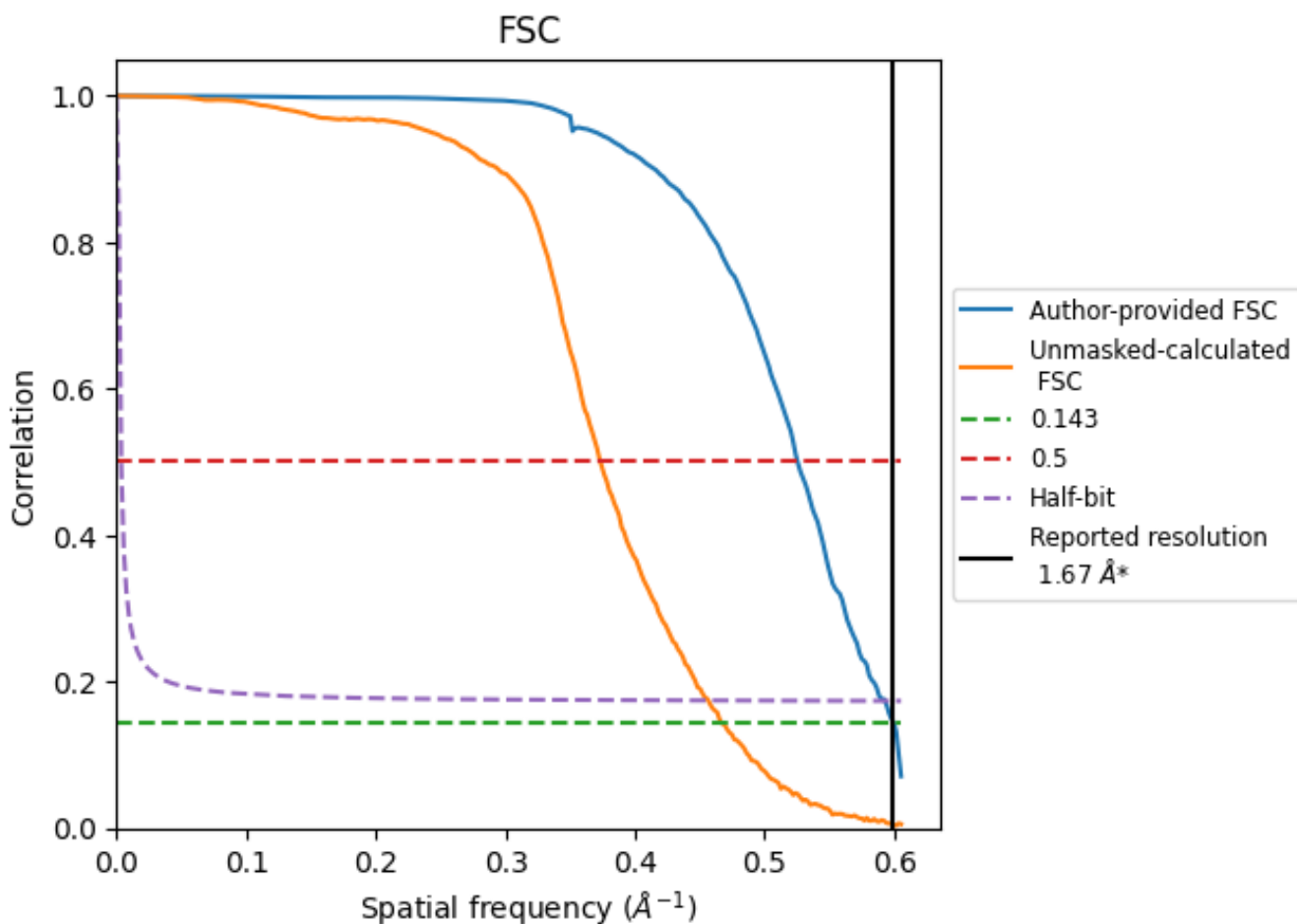


*Reported resolution corresponds to spatial frequency of 0.599 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.599 Å⁻¹

8.2 Resolution estimates [i](#)

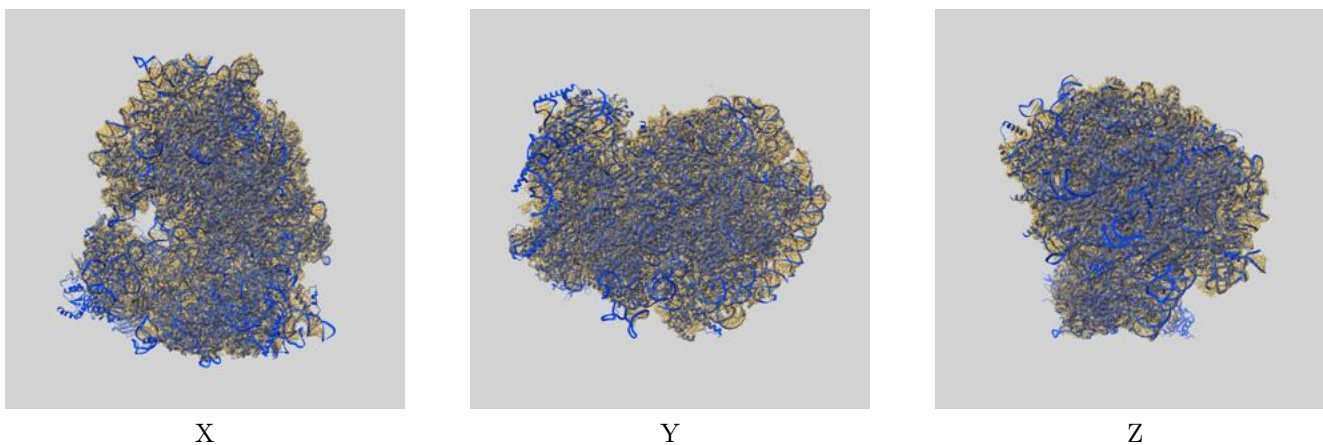
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.67	-	-
Author-provided FSC curve	1.67	1.90	1.69
Unmasked-calculated*	2.14	2.68	2.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.14 differs from the reported value 1.67 by more than 10 %

9 Map-model fit [i](#)

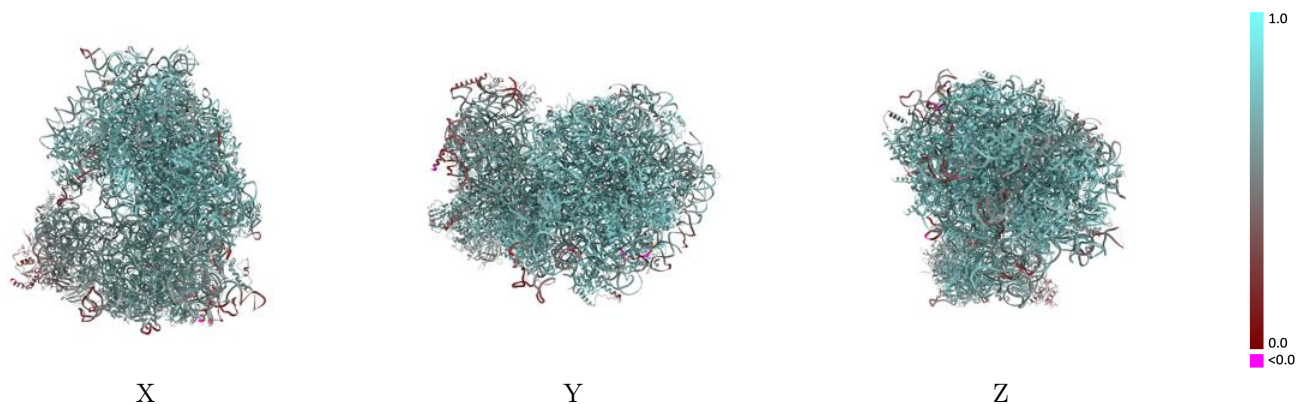
This section contains information regarding the fit between EMDB map EMD-40205 and PDB model 8GLP. Per-residue inclusion information can be found in section 3 on page 29.

9.1 Map-model overlay [i](#)



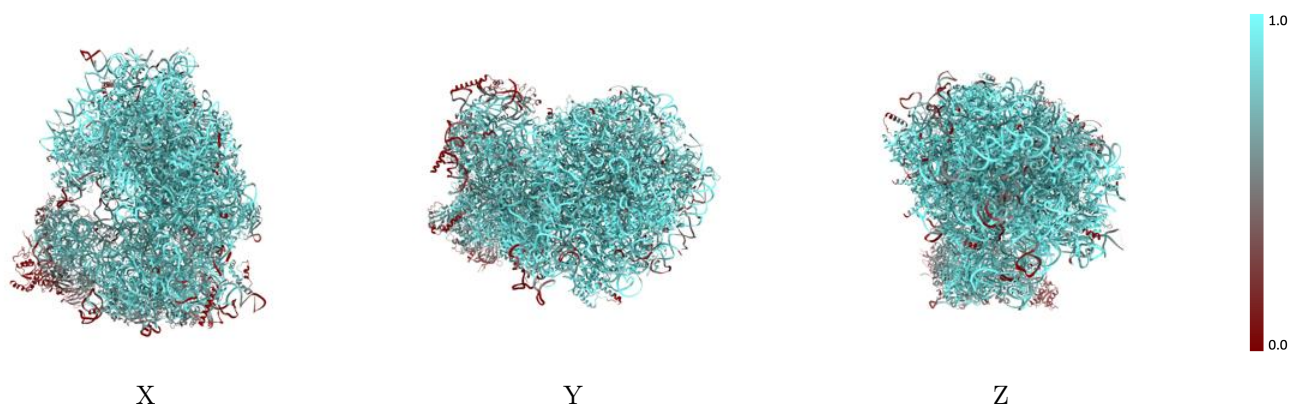
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



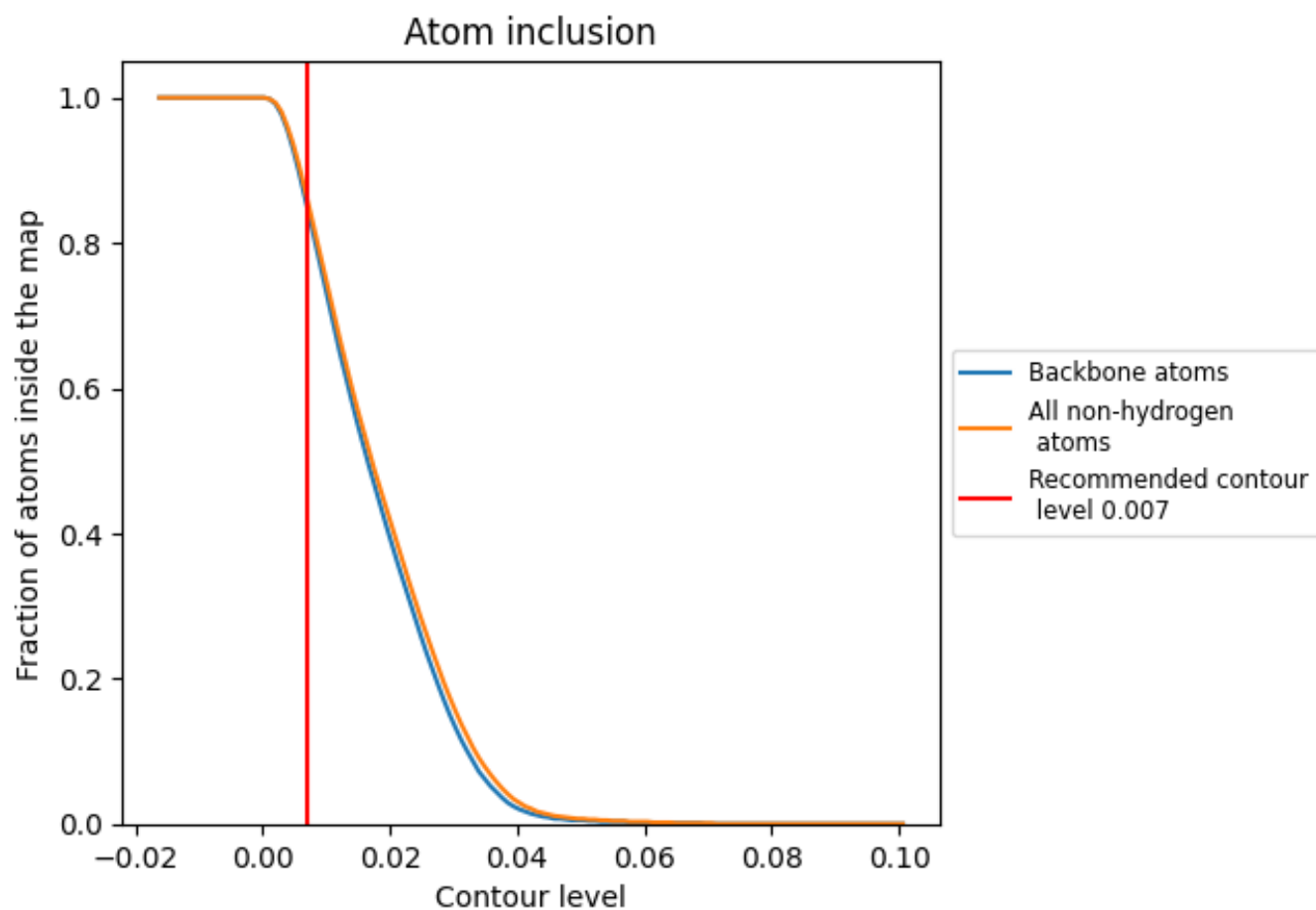
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 86% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8610	 0.6730
L5	 0.9260	 0.6950
L7	 0.9930	 0.7260
L8	 0.9600	 0.7170
LA	 0.9760	 0.7710
LB	 0.9450	 0.7530
LC	 0.9500	 0.7580
LD	 0.9200	 0.7160
LE	 0.9070	 0.7160
LF	 0.9550	 0.7620
LG	 0.8390	 0.6800
LH	 0.9350	 0.7190
LI	 0.9560	 0.7390
LJ	 0.8800	 0.6850
LL	 0.9100	 0.7240
LM	 0.9490	 0.7300
LN	 0.9980	 0.7780
LO	 0.9540	 0.7570
LP	 0.9600	 0.7640
LQ	 0.9810	 0.7820
LR	 0.8490	 0.6920
LS	 0.9790	 0.7560
LT	 0.9250	 0.7400
LU	 0.8200	 0.6540
LV	 0.9650	 0.7600
LW	 0.5570	 0.5540
LX	 0.9400	 0.7380
LY	 0.9280	 0.7400
LZ	 0.9330	 0.7200
La	 0.9770	 0.7730
Lb	 0.8050	 0.6790
Lc	 0.9110	 0.7260
Ld	 0.9050	 0.7250
Le	 0.9790	 0.7790
Lf	 0.9750	 0.7730













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Chain	Atom inclusion	Q-score
Lg	 0.9050	 0.7370
Lh	 0.9260	 0.7320
Li	 0.9070	 0.7210
Lj	 0.9910	 0.7740
Lk	 0.8270	 0.6840
Ll	 0.9760	 0.7540
Lm	 0.9380	 0.7330
Ln	 0.9500	 0.7320
Lo	 0.9260	 0.7470
Lp	 0.9360	 0.7510
Lr	 0.9660	 0.7620
Pt	 0.4250	 0.6000
S2	 0.8740	 0.6160
SA	 0.7440	 0.6310
SB	 0.7980	 0.6670
SC	 0.8050	 0.6500
SD	 0.5010	 0.5400
SE	 0.7260	 0.6250
SF	 0.6950	 0.6120
SG	 0.5300	 0.5400
SH	 0.5660	 0.5770
SI	 0.7920	 0.6540
SJ	 0.7020	 0.6010
SK	 0.4230	 0.5040
SL	 0.8390	 0.6890
SM	 0.0070	 0.2880
SN	 0.8960	 0.7060
SO	 0.8720	 0.6880
SP	 0.5240	 0.5520
SQ	 0.6820	 0.5980
SR	 0.5890	 0.5660
SS	 0.6750	 0.6080
ST	 0.6510	 0.5890
SU	 0.4910	 0.5240
SV	 0.7630	 0.6480
SW	 0.9200	 0.6950
SX	 0.8780	 0.6760
SY	 0.5720	 0.5590
SZ	 0.5120	 0.5690
Sa	 0.8900	 0.6910
Sb	 0.7210	 0.6440
Sc	 0.5630	 0.5770

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Chain	Atom inclusion	Q-score
Sd	 0.7960	 0.6090
Se	 0.6200	 0.5770
Sf	 0.0620	 0.3100
Sg	 0.2780	 0.4970
mR	 0.2500	 0.4990