



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2026 – 12:51 AM EDT

PDB ID : 8G61 / pdb_00008g61
EMDB ID : EMD-29760
Title : mRNA decoding in human is kinetically and structurally distinct from bacteria (AC state)
Authors : Holm, M.; Natchiar, K.S.; Rundlet, E.J.; Myasnikov, A.G.; Altman, R.B.; Blanchard, S.C.
Deposited on : 2023-02-14
Resolution : 2.94 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:

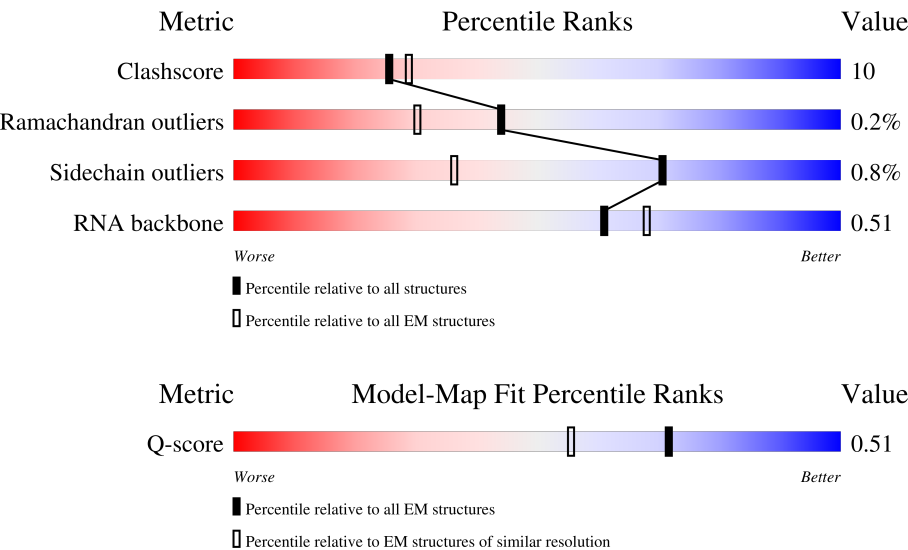
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.94 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13068 (2.44 - 3.44)

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	39%40%10%10%
2	L8	156	42%53%6%
3	L5	5069	37%28%6%28%

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Mol	Chain	Length	Quality of chain
4	L7	120	
5	SB	264	
6	SA	295	
7	SD	243	
8	SJ	194	
9	SE	263	
10	SC	293	
11	SG	249	
12	SF	204	
13	SH	194	
14	SW	130	
15	SI	208	
16	SQ	146	
17	SU	119	
18	SK	165	
19	SO	151	
20	SX	143	
21	SM	132	
22	SS	152	
23	Sd	56	
24	SN	151	
25	SL	158	
26	SR	135	
27	SP	145	
28	ST	145	

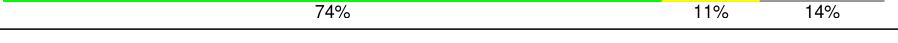
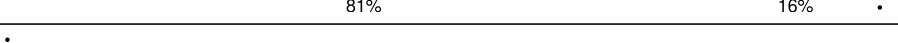
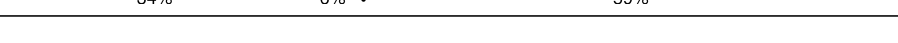
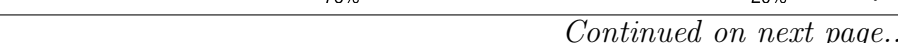
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Mol	Chain	Length	Quality of chain
29	SV	83	
30	SY	133	
31	SZ	125	
32	Sa	115	
33	Sb	84	
34	Sc	69	
35	Se	133	
36	Sf	156	
37	Sg	317	
38	Lz	217	
39	LA	257	
40	LB	403	
41	LC	427	
42	LJ	178	
43	LH	192	
44	LE	288	
45	LG	266	
46	LO	203	
47	LL	211	
48	LV	140	
49	LM	215	
50	La	148	
51	LN	204	
52	LI	214	
53	LD	297	

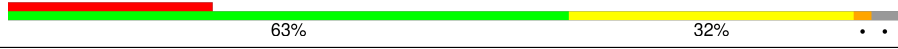
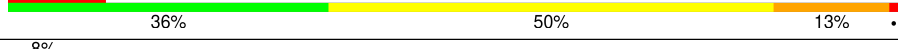
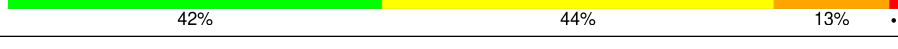
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Mol	Chain	Length	Quality of chain
54	LQ	188	
55	LR	196	
56	LS	176	
57	LT	160	
58	LP	184	
59	LU	128	
60	LX	156	
61	LY	145	
62	LW	157	
63	LZ	136	
64	Lr	137	
65	Lh	123	
66	Lb	159	
67	LF	248	
68	Lc	115	
69	Ld	125	
70	Le	135	
71	Lf	110	
72	Lg	117	
73	Li	105	
74	Lj	97	
75	Lk	70	
76	Ll	51	
77	Lm	128	
78	Ln	25	

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Mol	Chain	Length	Quality of chain
79	Lo	106	
80	Lp	92	
81	5A	154	
82	mR	60	
83	At	76	
84	Pt	77	

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 [i](#)

There are 92 unique types of molecules in this entry. The entry contains 219329 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1682	Total	C	N	O	P	1	0
			35978	16086	6447	11762	1683		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L8	156	Total	C	N	O	P	0	0
			3320	1482	585	1097	156		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3657	Total	C	N	O	P	0	0
			78479	34987	14355	25480	3657		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2562	1141	456	845	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 20 is a protein called uS12.

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

- 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
			940	590	164	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	54	Total	C	N	O	S	0	0
			454	284	93	72	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	145	Total	C	N	O	S	0	0
			1189	757	225	201	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
			1083	680	201	198	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SP	135	Total	C	N	O	S	0	0
			1110	707	209	187	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SZ	86	Total	C	N	O	S	0	0
			688	442	129	116	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sa	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sb	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sc	65	Total	C	N	O	S	0	0
			517	314	106	95	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Se	57	Total	C	N	O	S	0	0
			452	281	99	71	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 L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lz	213	Total	C	N	O	S	0	0
			1714	1097	309	300	8		

- Molecule 39 is a protein called uL2.

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

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LB	402	Total	C	N	O	S	0	0
			3240	2061	608	557	14		

- Molecule 41 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 42 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LJ	169	Total	C	N	O	S	0	0
			1358	859	253	240	6		

- Molecule 43 is a protein called 60S ribosomal protein L9.

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

- Molecule 44 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LE	223	Total	C	N	O	S	0	0
			1787	1150	339	294	4		

- Molecule 45 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LG	239	Total	C	N	O	S	0	0
			1913	1218	368	323	4		

- Molecule 46 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LO	200	Total	C	N	O	S	0	0
			1641	1058	320	258	5		

- Molecule 47 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LL	206	Total	C	N	O	S	0	0
			1664	1041	345	274	4		

- Molecule 48 is a protein called 60S ribosomal protein L23.

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

- Molecule 49 is a protein called 60S ribosomal protein L14.

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

- Molecule 50 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	La	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 51 is a protein called 60S ribosomal protein L15.

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

- Molecule 52 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LI	203	Total	C	N	O	S	0	0
			1646	1045	317	271	13		

- Molecule 53 is a protein called 60S ribosomal protein L5.

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

- Molecule 54 is a protein called 60S ribosomal protein L18.

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

- Molecule 55 is a protein called 60S ribosomal protein L19.

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

- Molecule 56 is a protein called 60S ribosomal protein L18a.

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

- Molecule 57 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LT	159	Total	C	N	O	S	0	0
			1297	823	252	216	6		

- Molecule 58 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 59 is a protein called 60S ribosomal protein L22.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 61 is a protein called 60S ribosomal protein L26.

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

- Molecule 62 is a protein called 60S ribosomal protein L24.

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

- Molecule 63 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LZ	135	Total	C	N	O	S	0	0
			1106	714	208	181	3		

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Lr	125	Total	C	N	O	S	0	0
			1005	624	207	169	5		

- Molecule 65 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 66 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Lb	109	Total	C	N	O	S	0	0
			885	552	192	137	4		

- Molecule 67 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 68 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 69 is a protein called 60S ribosomal protein L31.

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

- Molecule 70 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 71 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 72 is a protein called 60S ribosomal protein L34.

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

- Molecule 73 is a protein called 60S ribosomal protein L36.

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

- Molecule 74 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 75 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 76 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 77 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Lm	52	Total	C	N	O	S	0	0
			431	269	90	66	6		

- Molecule 78 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 79 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Lo	104	Total	C	N	O	S	0	0
			852	534	174	138	6		

- Molecule 80 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 81 is a protein called eIF5A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	5A	150	Total	C	N	O	S	0	0
			1144	716	194	225	9		

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	mR	10	Total	C	N	O	P	0	0
			210	94	34	72	10		

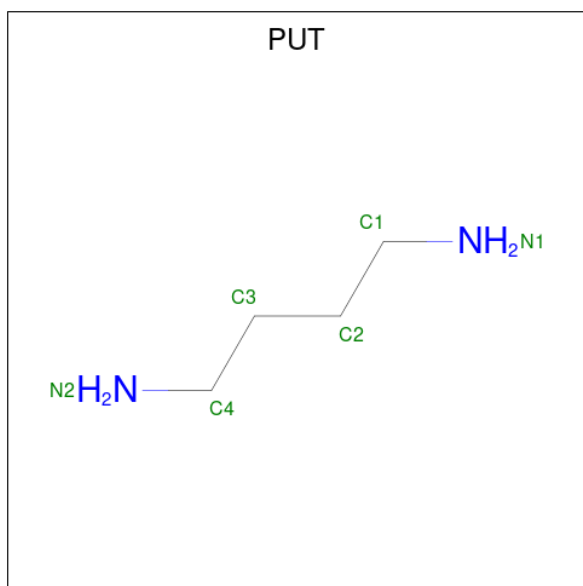
- Molecule 83 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	At	76	Total	C	N	O	P	S	0	0
			1624	724	290	533	76	1		

- Molecule 84 is a RNA chain called RNA (77-MER).

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

- Molecule 85 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



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

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

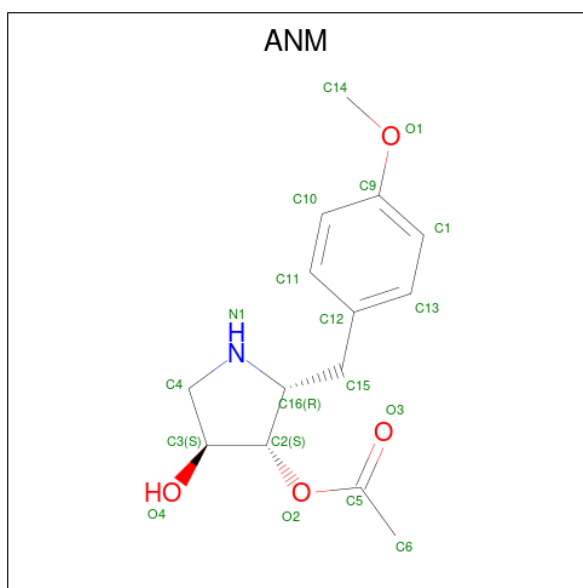
Mol	Chain	Residues	Atoms		AltConf
86	S2	1	Total	K	0
			1	1	
86	L5	13	Total	K	0
			13	13	
86	LA	1	Total	K	0
			1	1	
86	Lf	1	Total	K	0
			1	1	

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	S2	67	Total 67	Mg 67	0
87	L8	6	Total 6	Mg 6	0
87	L5	231	Total 231	Mg 231	0
87	L7	4	Total 4	Mg 4	0
87	SC	1	Total 1	Mg 1	0
87	SS	1	Total 1	Mg 1	0
87	SN	1	Total 1	Mg 1	0
87	Sa	1	Total 1	Mg 1	0
87	LA	1	Total 1	Mg 1	0
87	LB	1	Total 1	Mg 1	0
87	LV	1	Total 1	Mg 1	0
87	LN	2	Total 2	Mg 2	0
87	LP	1	Total 1	Mg 1	0
87	Le	1	Total 1	Mg 1	0
87	Lg	1	Total 1	Mg 1	0
87	Ln	1	Total 1	Mg 1	0
87	Lo	1	Total 1	Mg 1	0
87	5A	1	Total 1	Mg 1	0
87	At	1	Total 1	Mg 1	0
87	Pt	2	Total 2	Mg 2	0

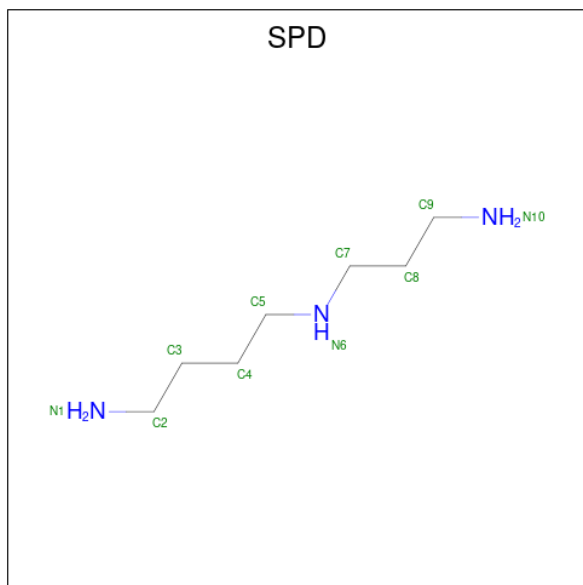
- Molecule 88 is ANISOMYCIN (CCD ID: ANM) (formula: C₁₄H₁₉NO₄) (labeled as "Ligand

of Interest" by depositor).



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

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



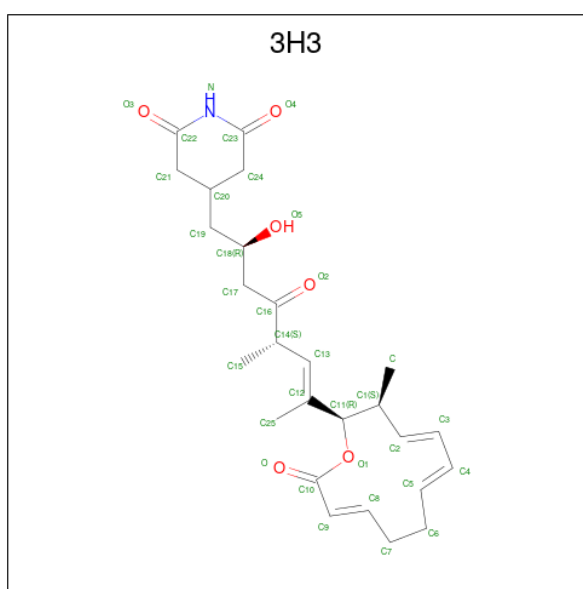
Mol	Chain	Residues	Atoms			AltConf
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	

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

- Molecule 90 is 4-[(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxo oxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl]piperidine-2,6-dione (CCD ID: 3H3) (formula: C₂₆H₃₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn).

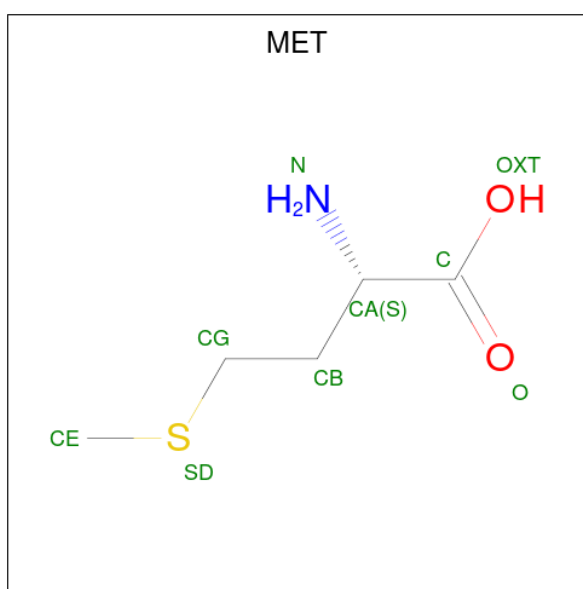
Mol	Chain	Residues	Atoms		AltConf
91	Sd	1	Total	Zn	0
			1	1	
91	Sa	1	Total	Zn	0
			1	1	
91	Sf	1	Total	Zn	0
			1	1	
91	Lg	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
91	Lj	1	Total	Zn	0
			1	1	
91	Lm	1	Total	Zn	0
			1	1	
91	Lo	1	Total	Zn	0
			1	1	
91	Lp	1	Total	Zn	0
			1	1	

- Molecule 92 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



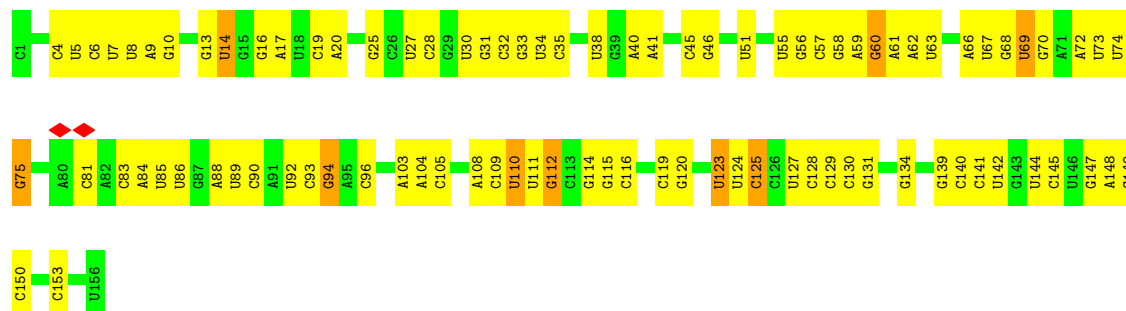
Mol	Chain	Residues	Atoms					AltConf
92	Pt	1	Total	C	N	O	S	0
			8	5	1	1	1	



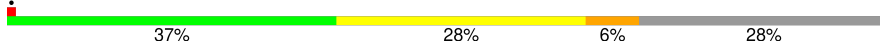
G1862
A1863
U1864
C1865
A1866
A1869

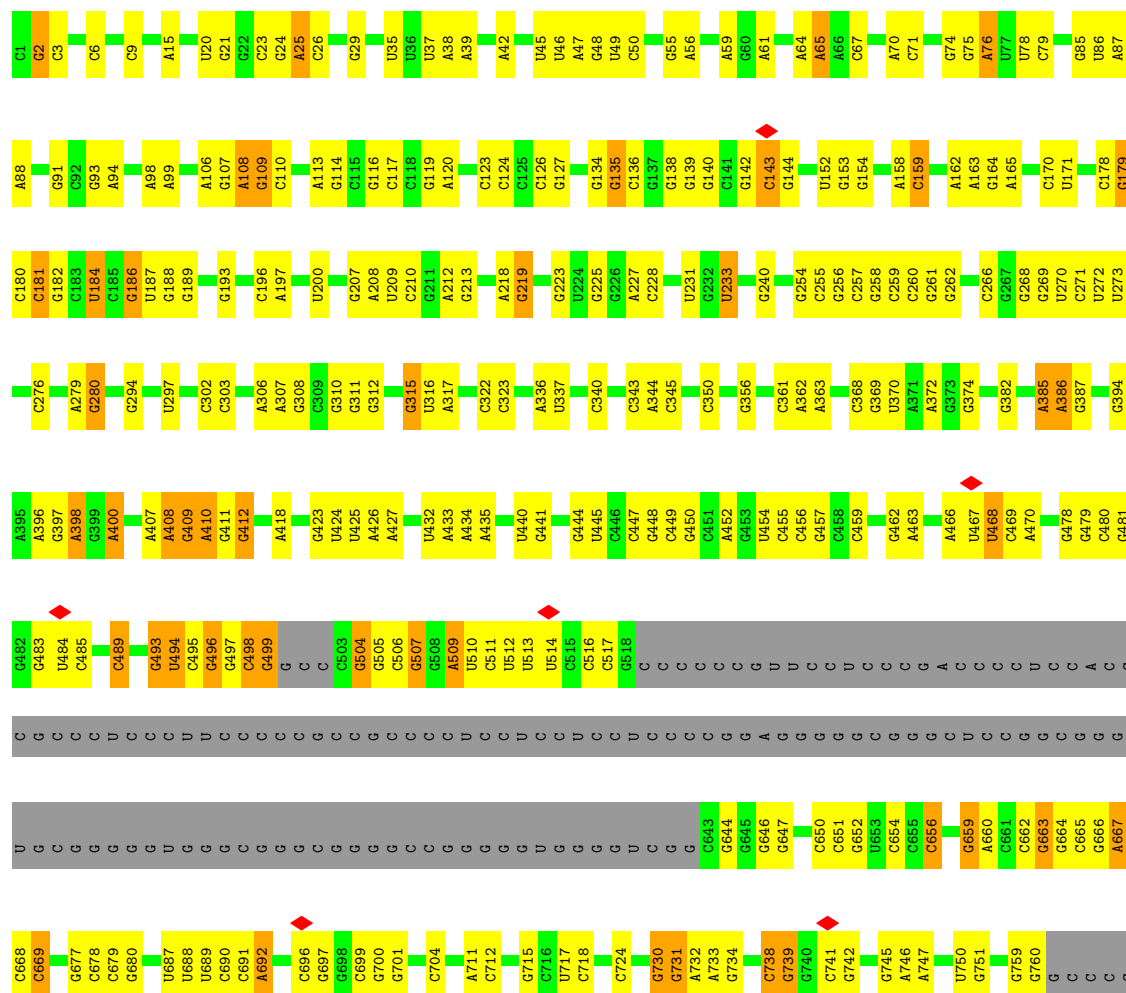
• Molecule 2: 5.8S rRNA

Chain L8:  42% 53% 6%



• Molecule 3: 28S rRNA

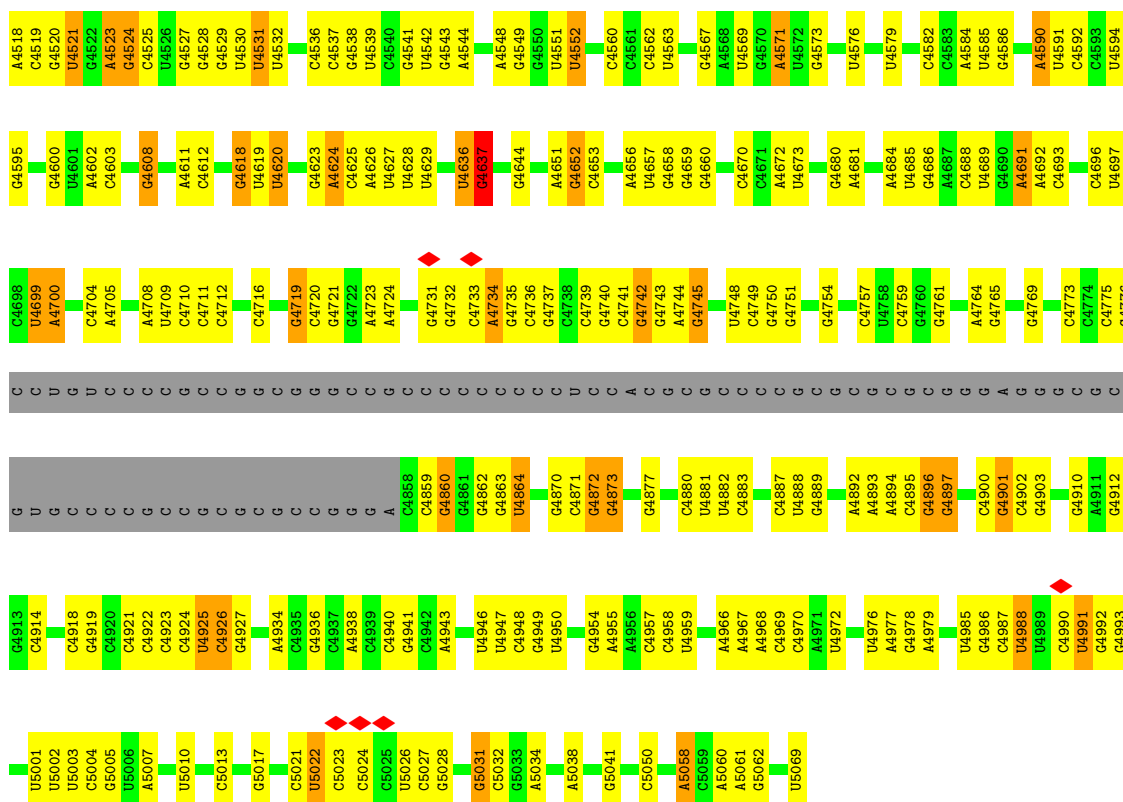
Chain L5:  37% 28% 6% 28%



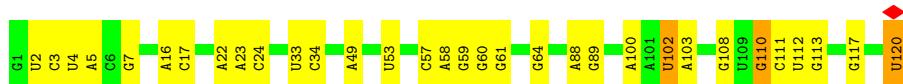
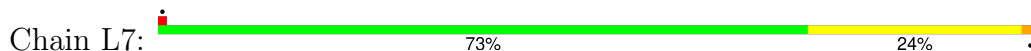




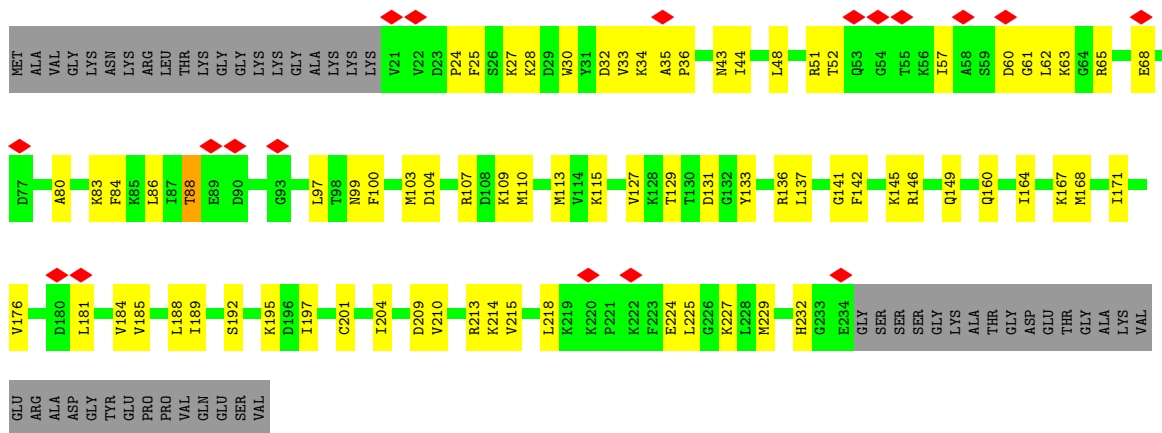




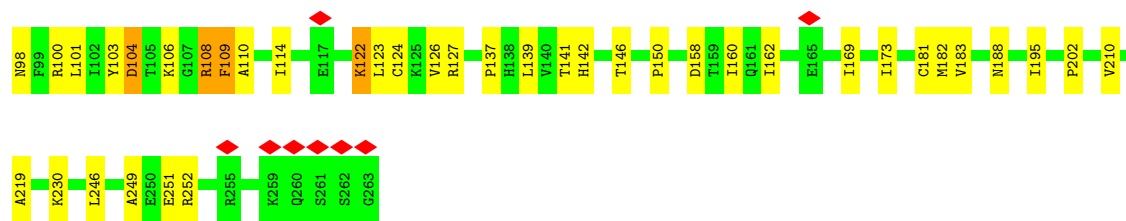
• Molecule 4: 5S rRNA



• Molecule 5: 40S ribosomal protein S3a

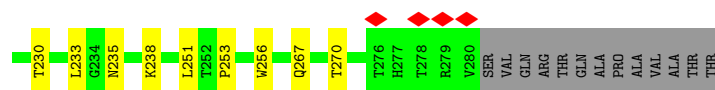
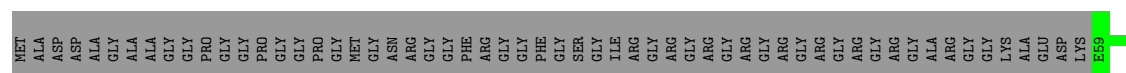


• Molecule 6: 40S ribosomal protein SA



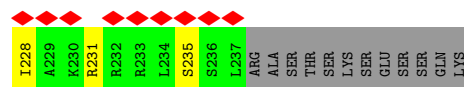
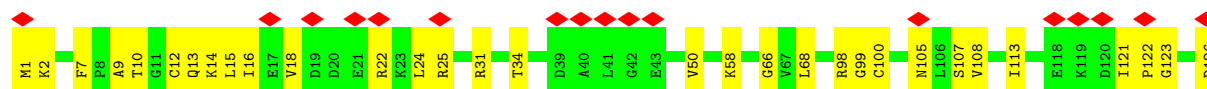
- Molecule 10: 40S ribosomal protein S2

Chain SC: 60% 15% 24%



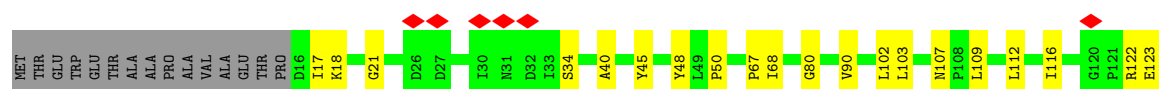
- Molecule 11: 40S ribosomal protein S6

Chain SG: 14% 68% 27% 5%



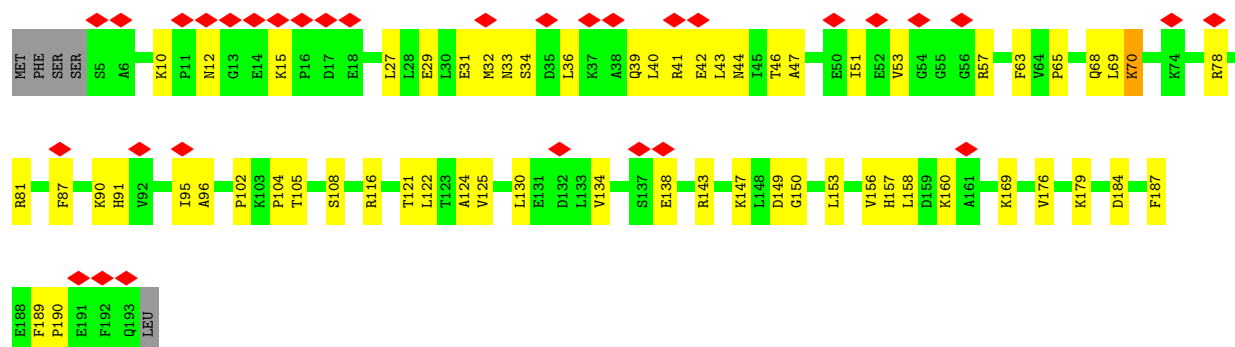
- Molecule 12: 40S ribosomal protein S5

Chain SF: 5% 72% 21% 7%



- Molecule 13: 40S ribosomal protein S7

Chain SH: 16% 66% 31% 2%



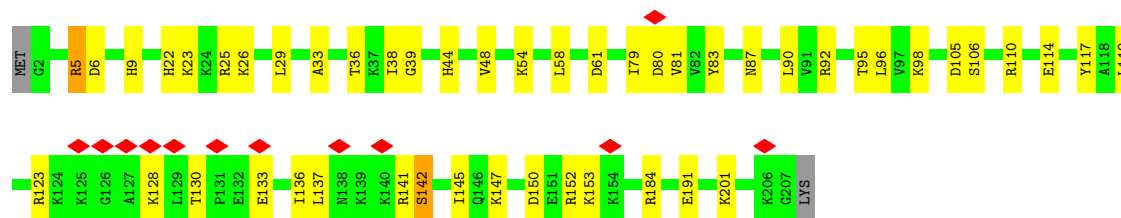
- Molecule 14: 40S ribosomal protein S15a

Chain SW: 75% 24% ..



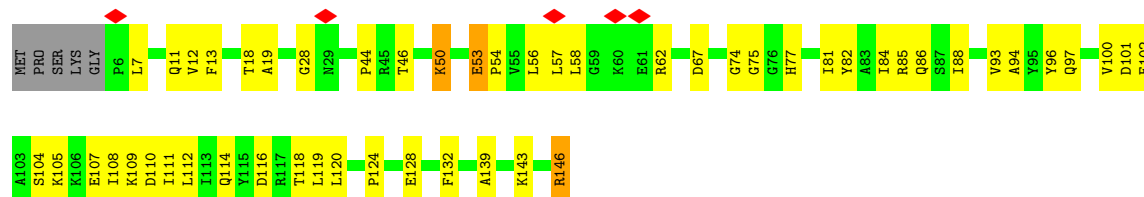
- Molecule 15: 40S ribosomal protein S8

Chain SI: 6% 75% 23% ..



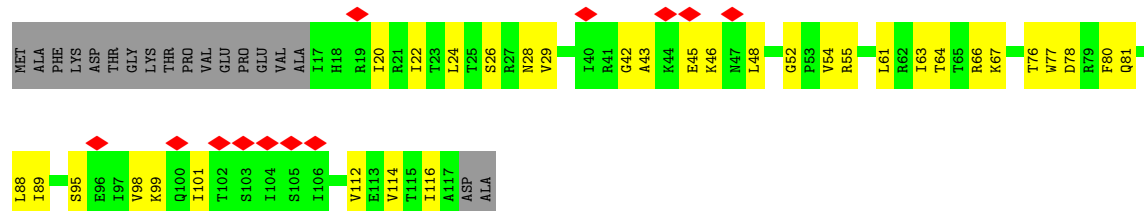
- Molecule 16: 40S ribosomal protein S16

Chain SQ: 61% 34% ..

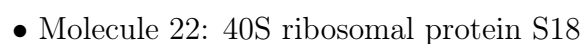
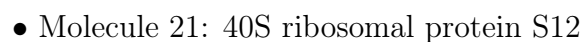
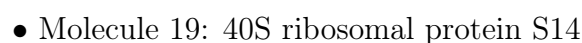


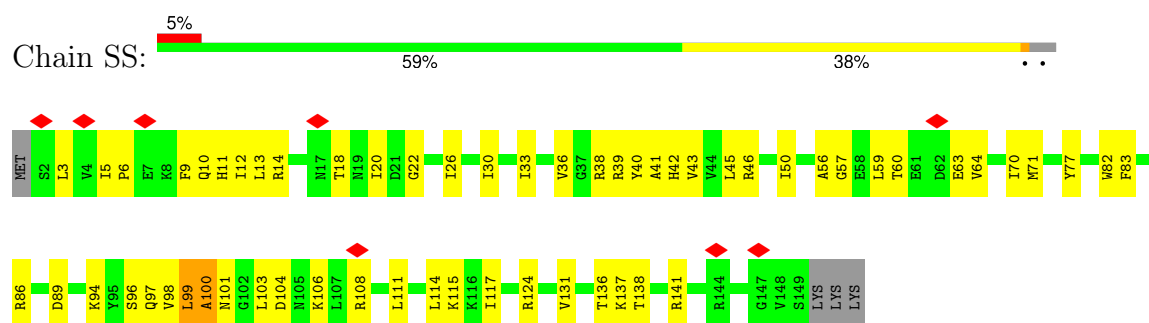
- Molecule 17: 40S ribosomal protein S20

Chain SU: 10% 57% 28% 15%

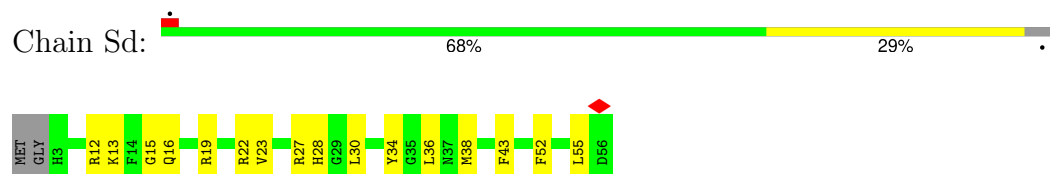


- Chain SK:

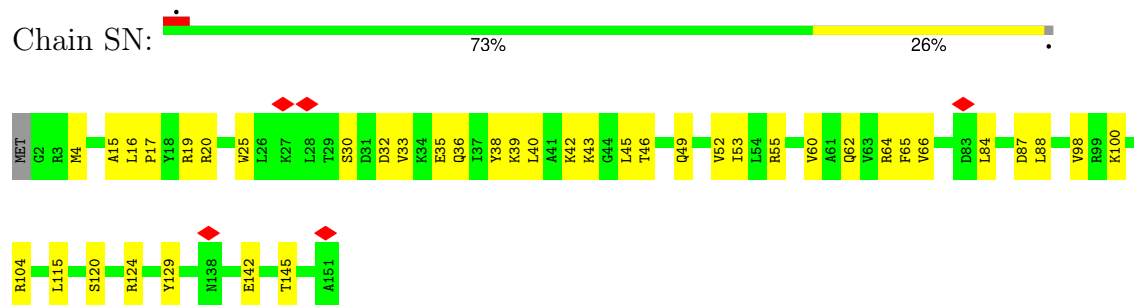




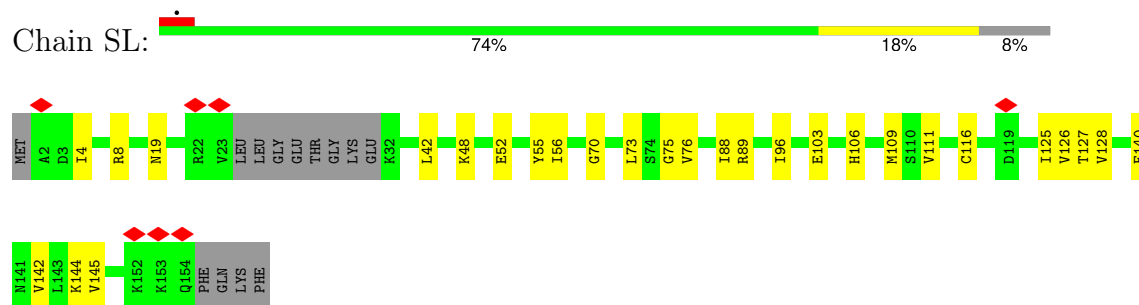
- Molecule 23: 40S ribosomal protein S29



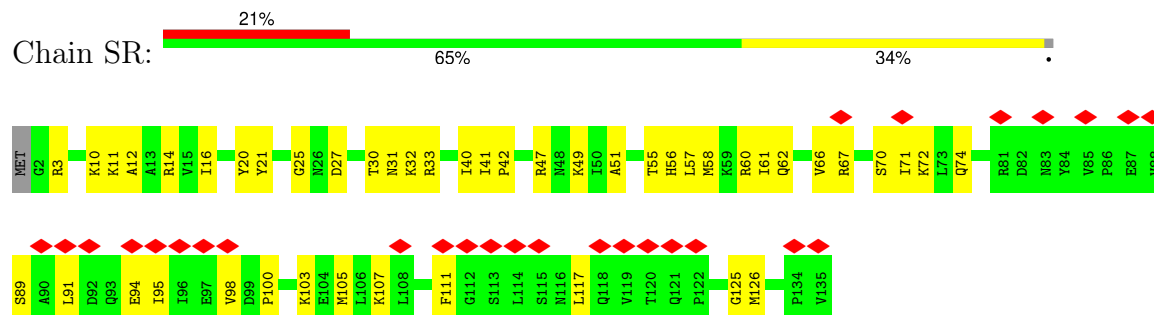
- Molecule 24: 40S ribosomal protein S13



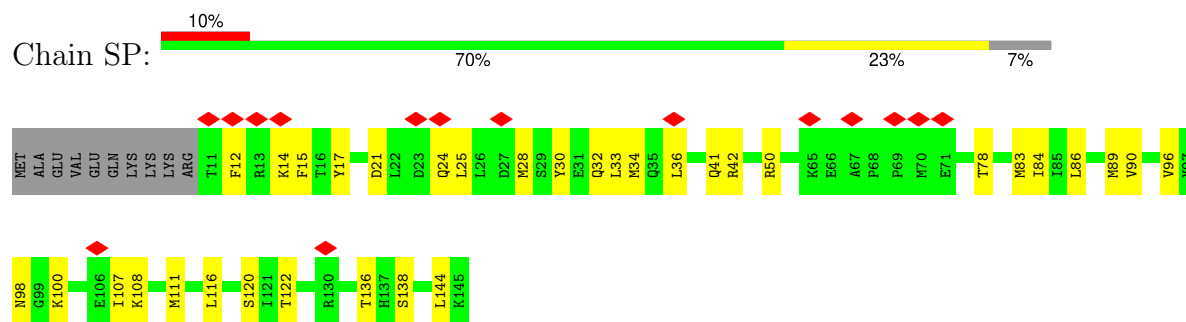
- Molecule 25: 40S ribosomal protein S11



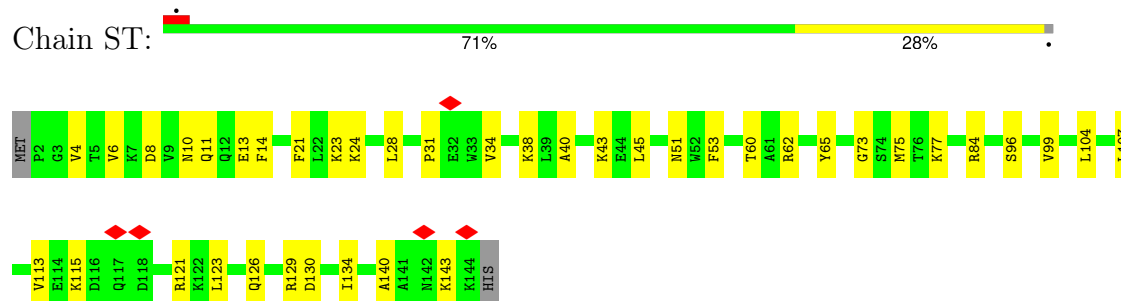
- Molecule 26: 40S ribosomal protein S17



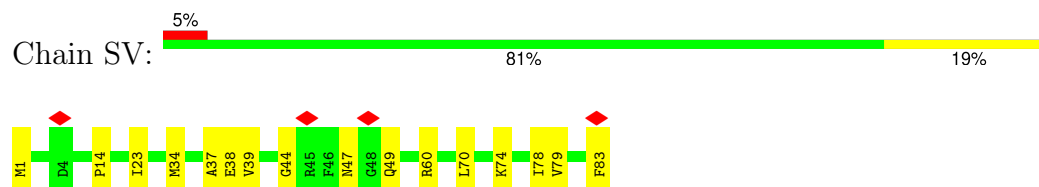
- Molecule 27: 40S ribosomal protein S15



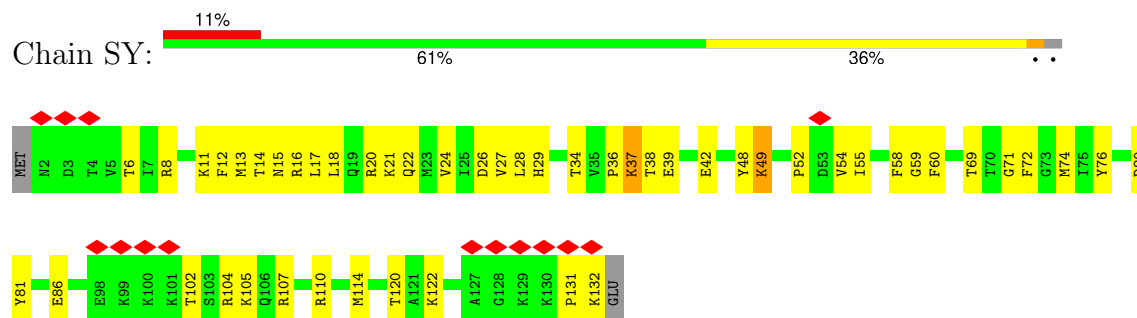
- Molecule 28: 40S ribosomal protein S19



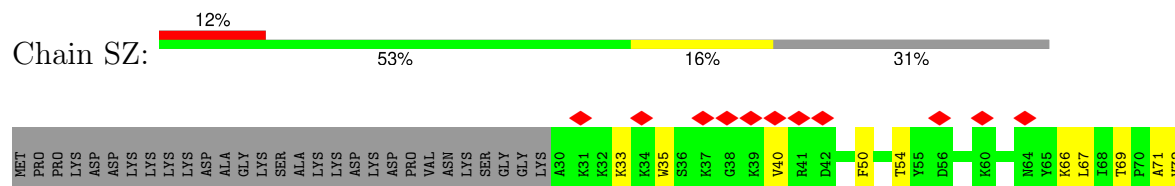
- Molecule 29: 40S ribosomal protein S21

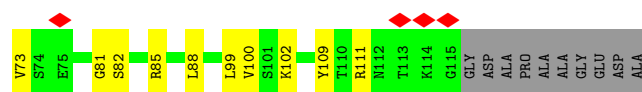


- Molecule 30: 40S ribosomal protein S24

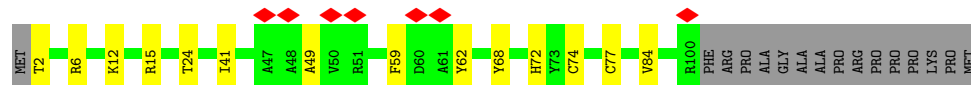
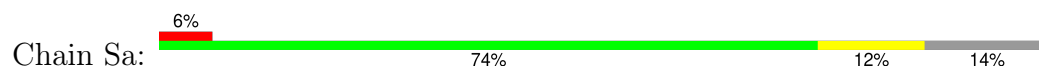


- Molecule 31: 40S ribosomal protein S25

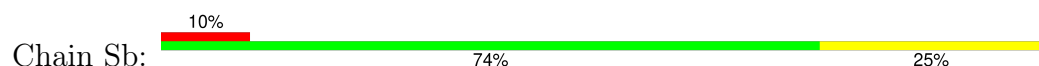




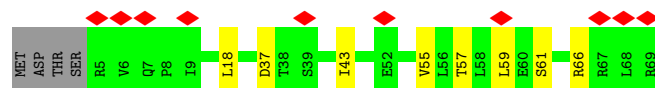
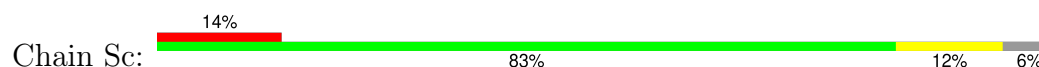
- Molecule 32: 40S ribosomal protein S26



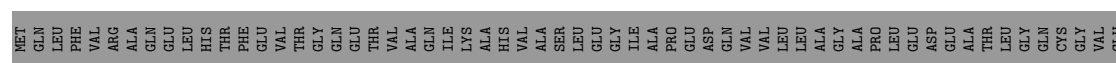
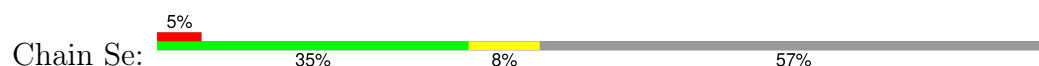
- Molecule 33: 40S ribosomal protein S27



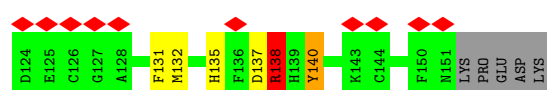
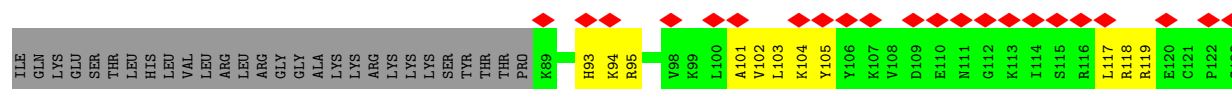
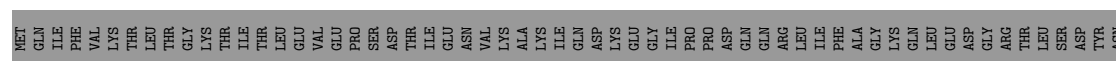
- Molecule 34: 40S ribosomal protein S28



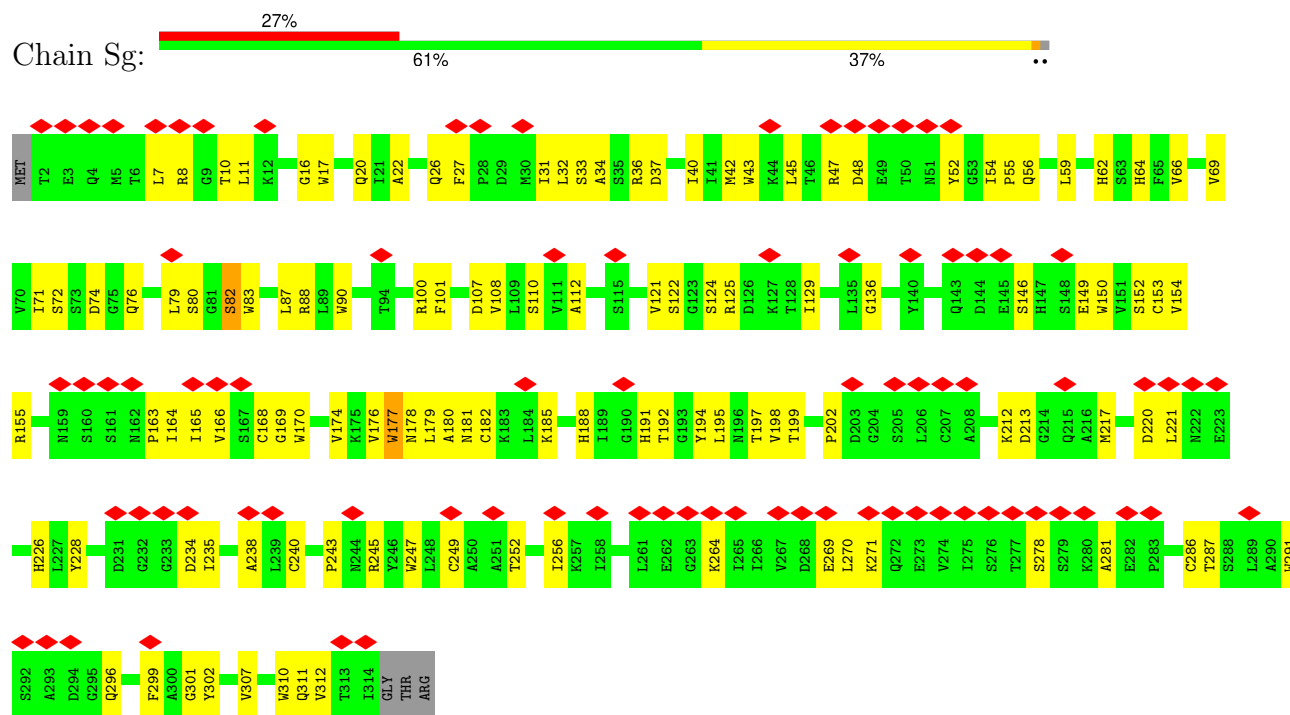
- Molecule 35: FAU ubiquitin-like and ribosomal protein S30



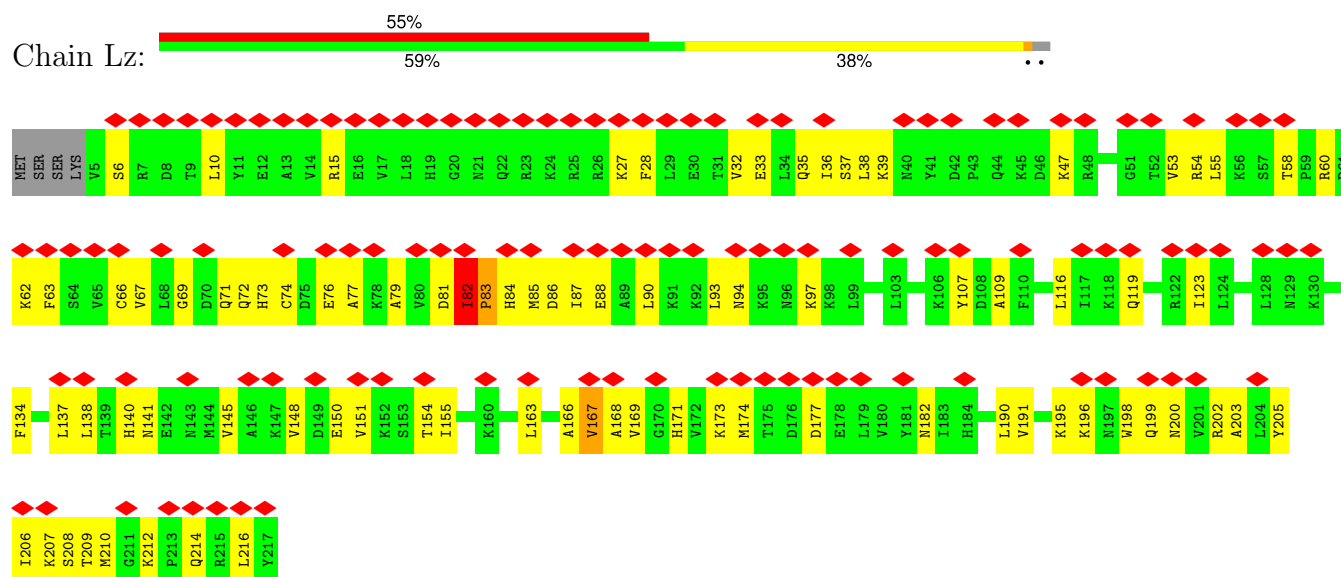
- Molecule 36: Ubiquitin-40S ribosomal protein S27a



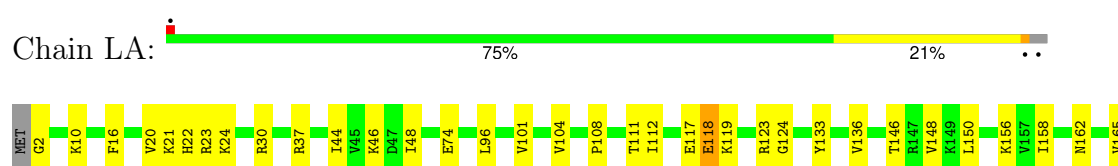
- Molecule 37: Receptor of activated protein C kinase 1



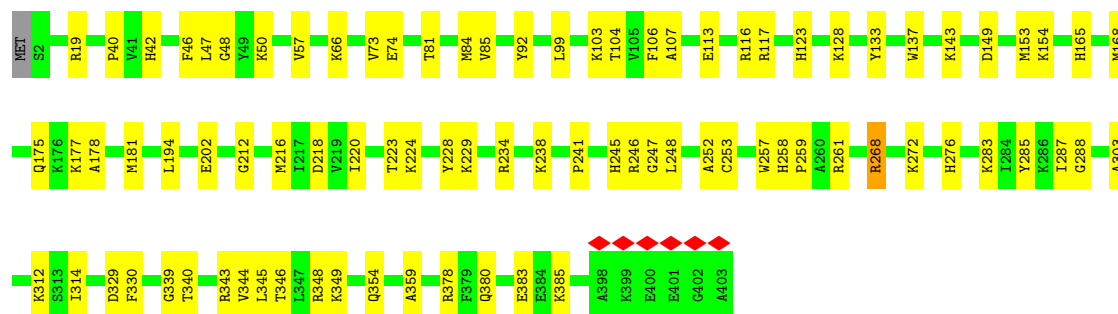
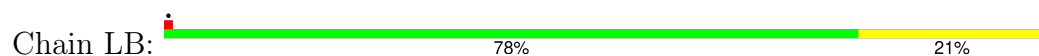
- Molecule 38: 60S ribosomal protein L10a



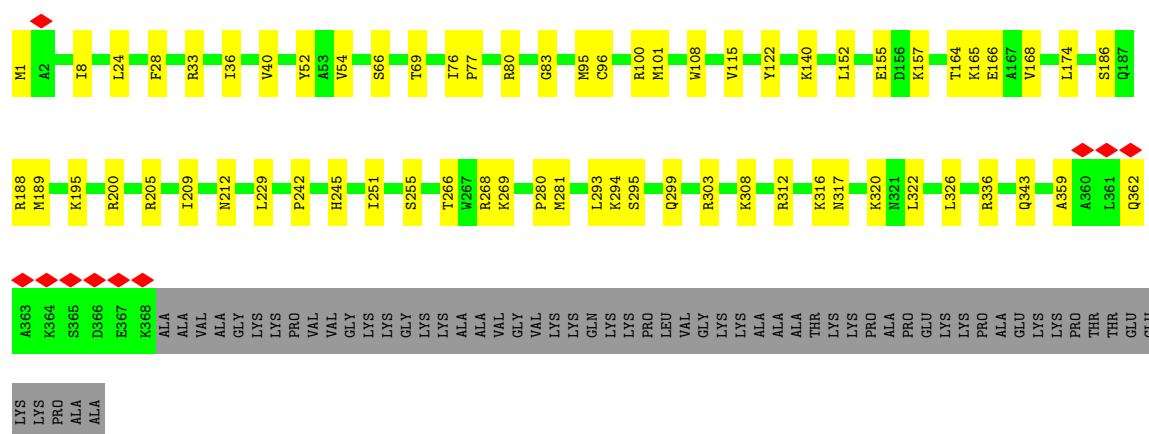
- Molecule 39: uL2



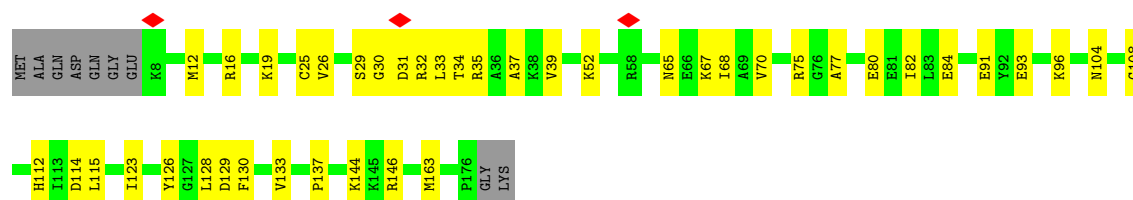
- Molecule 40: 60S ribosomal protein L3



- Molecule 41: 60S ribosomal protein L4

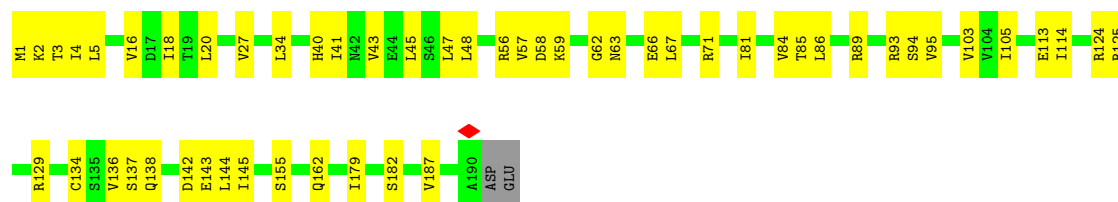


- Molecule 42: 60S ribosomal protein L11

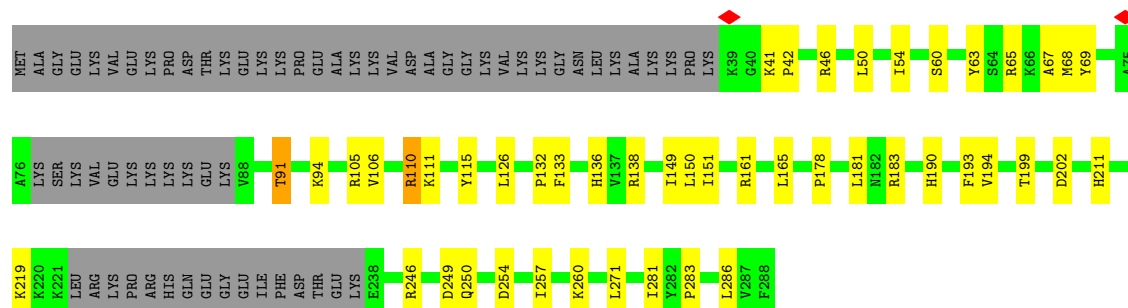


- Molecule 43: 60S ribosomal protein L9

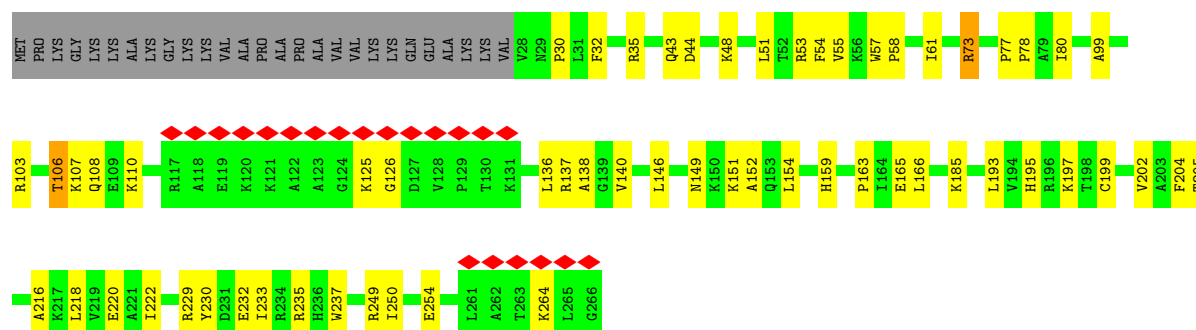




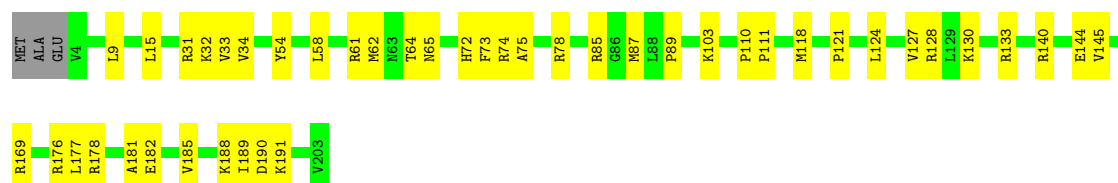
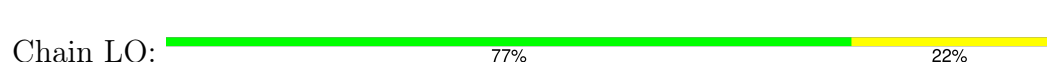
• Molecule 44: 60S ribosomal protein L6



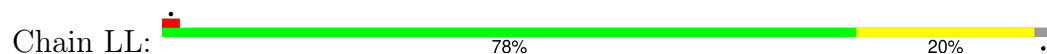
• Molecule 45: 60S ribosomal protein L7a

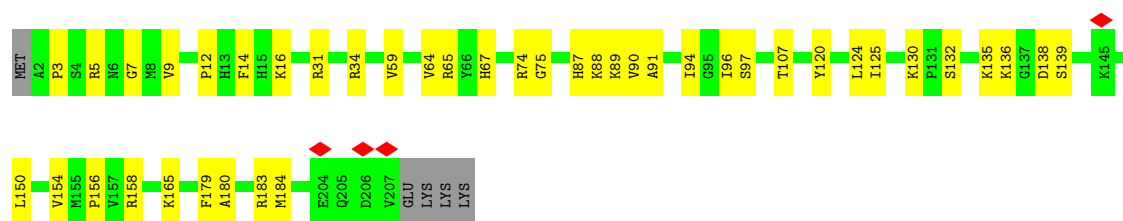


• Molecule 46: 60S ribosomal protein L13a

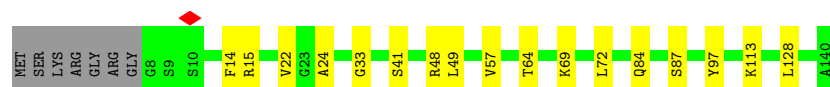
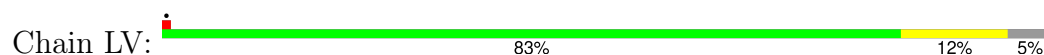


• Molecule 47: 60S ribosomal protein L13

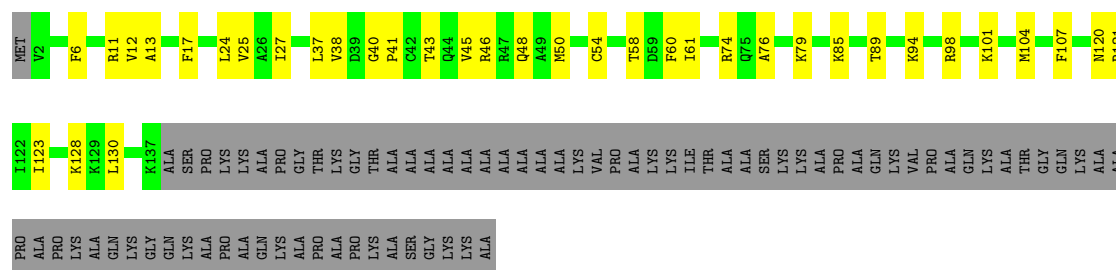




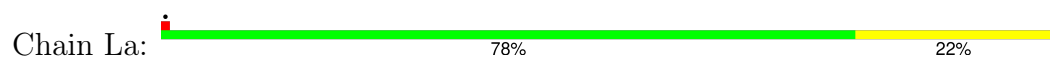
- Molecule 48: 60S ribosomal protein L23



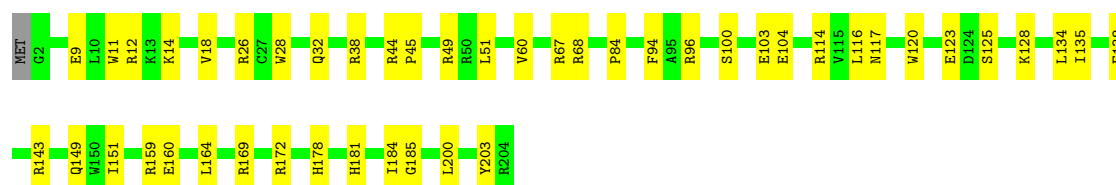
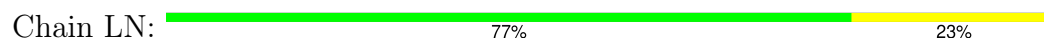
- Molecule 49: 60S ribosomal protein L14



- Molecule 50: 60S ribosomal protein L27a

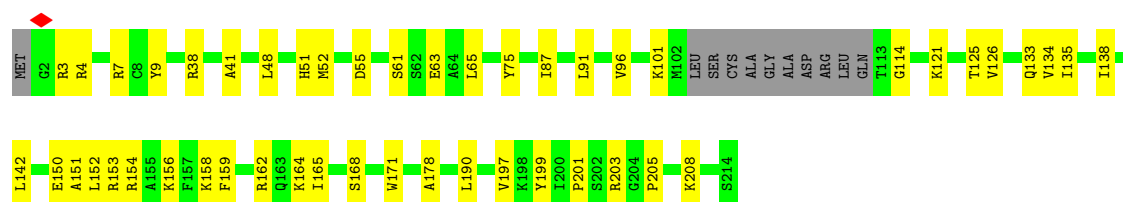


- Molecule 51: 60S ribosomal protein L15

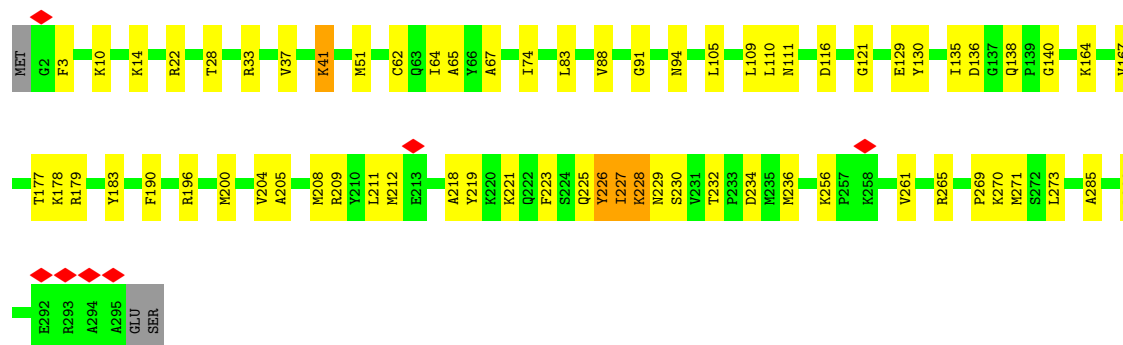
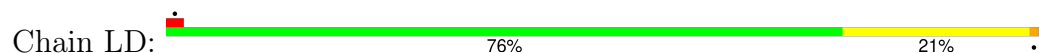


- Molecule 52: 60S ribosomal protein L10

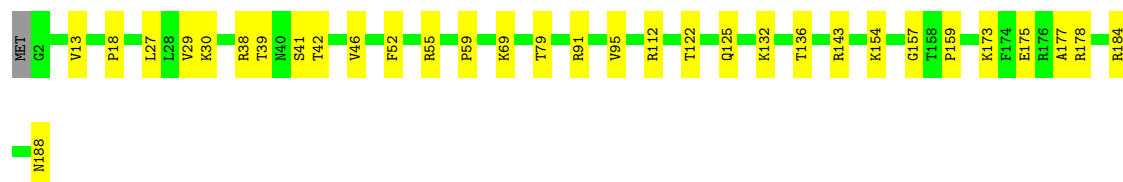
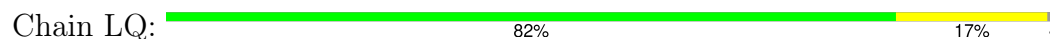




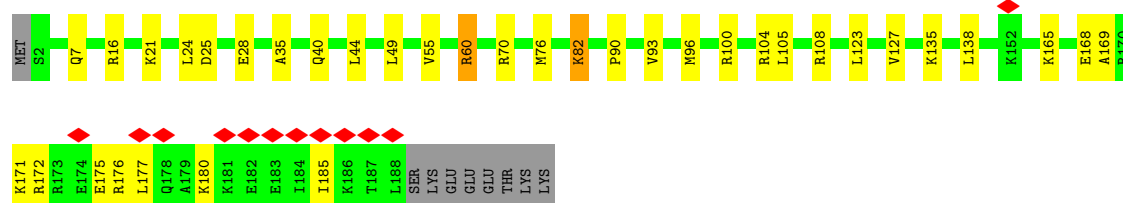
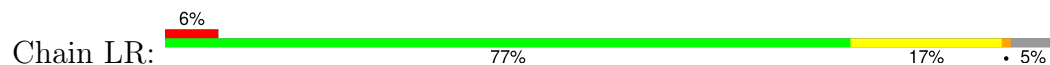
- Molecule 53: 60S ribosomal protein L5



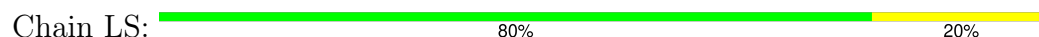
- Molecule 54: 60S ribosomal protein L18

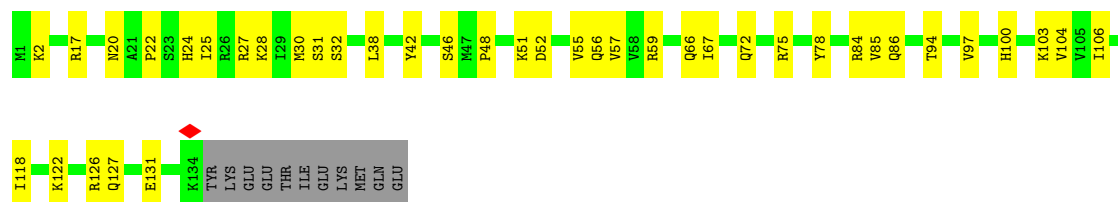


- Molecule 55: 60S ribosomal protein L19

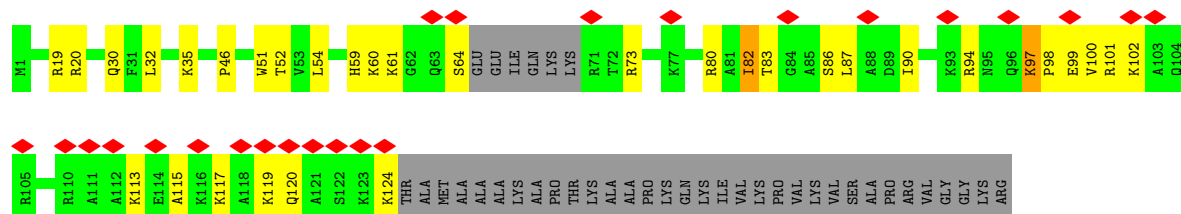


- Molecule 56: 60S ribosomal protein L18a

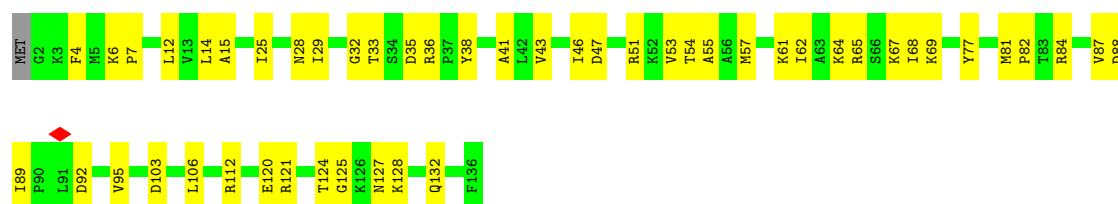




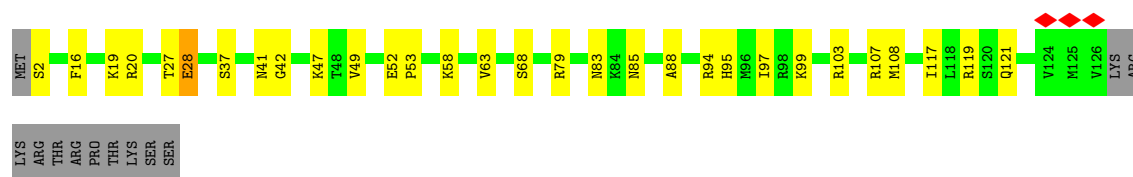
- Molecule 62: 60S ribosomal protein L24



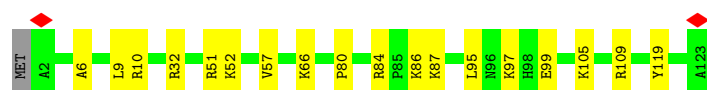
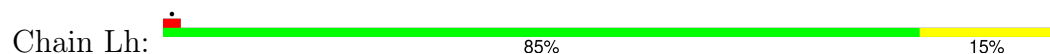
- Molecule 63: 60S ribosomal protein L27



- Molecule 64: 60S ribosomal protein L28

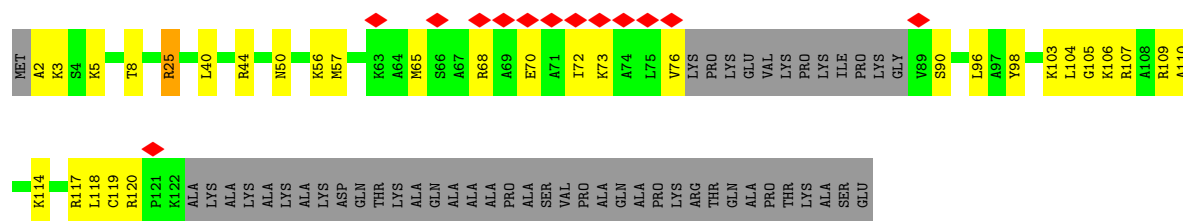


- Molecule 65: 60S ribosomal protein L35



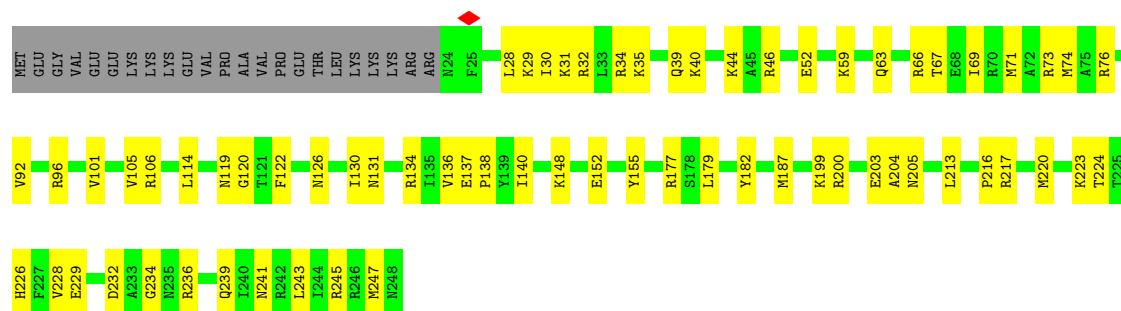
- Molecule 66: 60S ribosomal protein L29





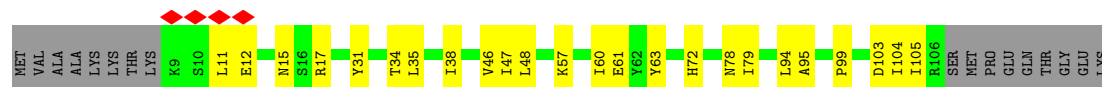
- Molecule 67: 60S ribosomal protein L7

Chain LF: 64% 27% 9%



- Molecule 68: 60S ribosomal protein L30

Chain Lc: 64% 21% 15%



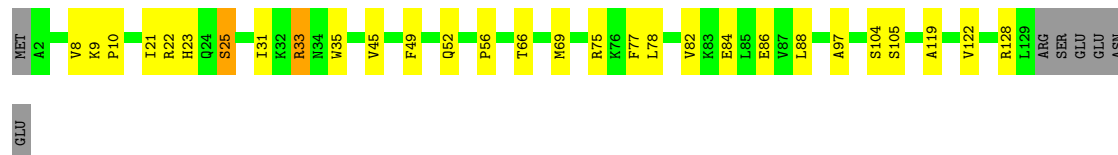
- Molecule 69: 60S ribosomal protein L31

Chain Ld: 74% 11% 14%



- Molecule 70: 60S ribosomal protein L32

Chain Le: 73% 20% 5%

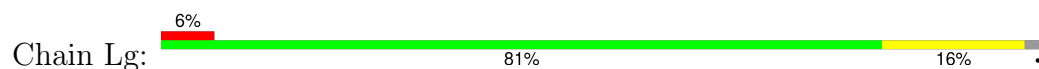


- Molecule 71: 60S ribosomal protein L35a

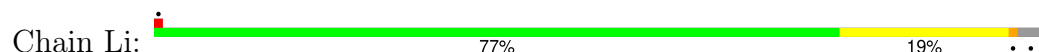
Chain Lf: 84% 15% 1%



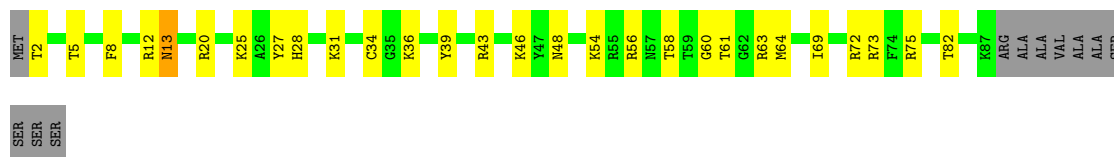
- Molecule 72: 60S ribosomal protein L34



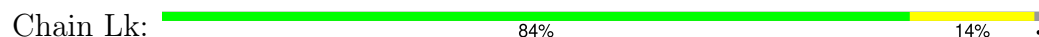
- Molecule 73: 60S ribosomal protein L36



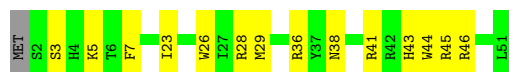
- Molecule 74: 60S ribosomal protein L37



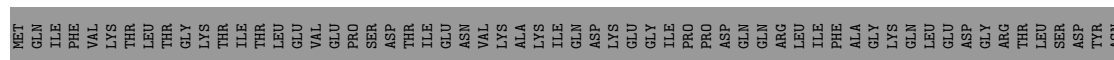
- Molecule 75: 60S ribosomal protein L38

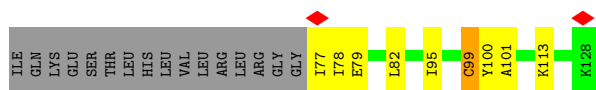


- Molecule 76: 60S ribosomal protein L39



- Molecule 77: eL40





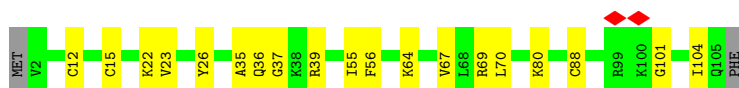
- Molecule 78: 60S ribosomal protein L41

Chain Ln: 76% 20% .



- Molecule 79: 60S ribosomal protein L36a

Chain Lo: 80% 18% .



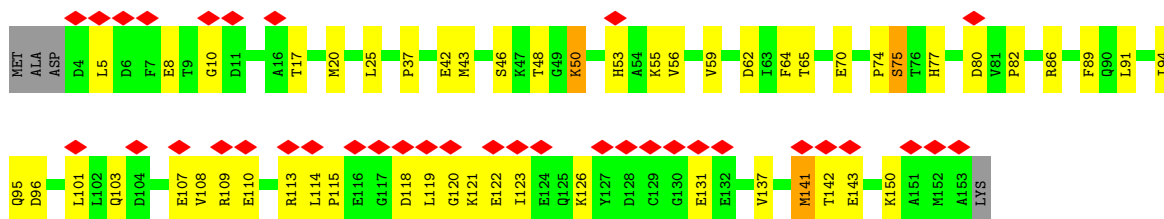
- Molecule 80: 60S ribosomal protein L37a

Chain Lp: 79% 18% ..



- Molecule 81: eIF5A1

Chain 5A: 23% 63% 32% . .



- Molecule 82: mRNA

Chain mR: 13% . 83%



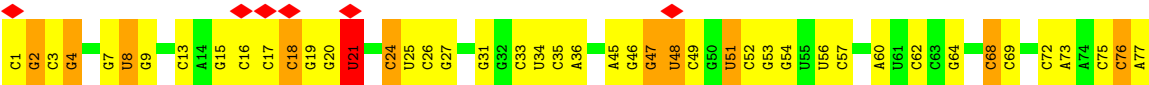
- Molecule 83: A-site tRNA

Chain At: 11% 36% 50% 13% .



A76

● Molecule 84: RNA (77-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9750	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	0.030	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	0.82600003, 0.82600003, 0.82600003	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, 1MA, 5MC, K, PSU, MLZ, MG, G7M, A2M, 6MZ, B8N, 5CT, 4AC, HY3, SPD, OMC, AME, 4SU, 7MG, OMU, UY1, 3H3, SAC, OMG, ZN, PUT, ANM, HIC, MA6, M3L, H2U, V5N

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	0.23	1/38205 (0.0%)	0.32	0/59545
2	L8	0.25	0/3613	0.31	0/5627
3	L5	0.27	0/84727	0.34	0/132180
4	L7	0.22	0/2862	0.29	0/4459
5	SB	0.22	0/1765	0.45	0/2362
6	SA	0.21	0/1778	0.44	0/2416
7	SD	0.21	0/1784	0.40	0/2403
8	SJ	0.23	0/1550	0.44	0/2069
9	SE	0.27	0/2118	0.45	0/2849
10	SC	0.23	0/1762	0.44	0/2381
11	SG	0.29	0/1946	0.57	0/2590
12	SF	0.19	0/1515	0.41	0/2037
13	SH	0.19	0/1540	0.45	0/2064
14	SW	0.26	0/1051	0.45	0/1406
15	SI	0.27	0/1715	0.49	0/2287
16	SQ	0.28	0/1141	0.55	0/1528
17	SU	0.14	0/813	0.34	0/1092
18	SK	0.51	0/834	0.77	0/1125
19	SO	0.38	0/1022	0.59	0/1372
20	SX	0.19	0/1096	0.37	0/1461
21	SM	0.20	0/950	0.48	0/1275
22	SS	0.27	0/1232	0.57	0/1651
23	Sd	0.27	0/465	0.50	0/618
24	SN	0.17	0/1242	0.35	0/1671
25	SL	0.19	0/1209	0.32	0/1616
26	SR	0.22	0/1098	0.52	0/1474
27	SP	0.21	0/1133	0.44	0/1515
28	ST	0.24	0/1131	0.40	0/1515
29	SV	0.16	0/635	0.38	0/850
30	SY	0.27	0/1083	0.55	0/1438
31	SZ	0.19	0/696	0.50	0/929

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sa	0.18	0/805	0.34	0/1079
33	Sb	0.14	0/664	0.34	0/891
34	Sc	0.18	0/519	0.38	0/694
35	Se	0.26	0/458	0.47	0/604
36	Sf	0.40	0/525	0.58	0/695
37	Sg	0.26	0/2493	0.44	0/3394
38	Lz	0.28	0/1742	0.55	0/2338
39	LA	0.35	0/1958	0.53	2/2623 (0.1%)
40	LB	0.28	0/3295	0.43	0/4406
41	LC	0.27	0/2981	0.45	0/4002
42	LJ	0.21	0/1381	0.40	0/1847
43	LH	0.23	0/1537	0.44	0/2066
44	LE	0.25	0/1821	0.40	0/2442
45	LG	0.19	0/1946	0.38	0/2620
46	LO	0.32	0/1673	0.51	0/2238
47	LL	0.27	0/1695	0.47	0/2270
48	LV	0.23	0/1002	0.39	0/1345
49	LM	0.23	0/1142	0.40	0/1527
50	La	0.28	0/1179	0.44	0/1573
51	LN	0.30	0/1745	0.50	0/2338
52	LI	0.24	0/1684	0.42	0/2247
53	LD	0.22	0/2437	0.42	2/3263 (0.1%)
54	LQ	0.30	0/1536	0.47	0/2052
55	LR	0.26	0/1582	0.45	0/2091
56	LS	0.27	0/1500	0.43	0/2013
57	LT	0.25	0/1325	0.40	0/1770
58	LP	0.24	0/1268	0.40	0/1701
59	LU	0.23	0/822	0.46	0/1103
60	LX	0.25	0/984	0.38	0/1323
61	LY	0.28	0/1132	0.50	0/1504
62	LW	0.32	0/964	0.48	0/1278
63	LZ	0.25	0/1129	0.48	0/1507
64	Lr	0.33	0/1011	0.51	0/1356
65	Lh	0.24	0/1023	0.40	0/1351
66	Lb	0.24	0/887	0.44	0/1171
67	LF	0.24	0/1905	0.43	0/2539
68	Lc	0.21	0/774	0.39	0/1038
69	Ld	0.21	0/903	0.36	0/1216
70	Le	0.32	0/1071	0.49	0/1429
71	Lf	0.25	0/895	0.40	0/1198
72	Lg	0.25	0/916	0.43	0/1220
73	Li	0.21	0/843	0.42	0/1115
74	Lj	0.37	0/720	0.61	0/952

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lk	0.18	0/575	0.35	0/761
76	Ll	0.32	0/454	0.56	0/599
77	Lm	0.33	0/425	0.51	0/564
78	Ln	0.37	0/231	0.59	0/294
79	Lo	0.31	0/854	0.49	0/1125
80	Lp	0.26	0/718	0.44	0/953
81	5A	0.29	0/1144	0.55	0/1539
82	mR	0.28	0/233	0.42	0/360
83	At	0.17	0/1677	0.29	0/2612
84	Pt	0.29	0/1721	0.33	0/2679
All	All	0.26	1/229615 (0.0%)	0.39	4/336720 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	172	OMU	O3'-P	5.07	1.61	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	LA	245[A]	ARG	CA-C-O	5.93	127.67	121.15
39	LA	245[B]	ARG	CA-C-O	5.93	127.67	121.15
53	LD	227	ILE	N-CA-C	-5.56	107.22	111.62
53	LD	226	TYR	N-CA-C	-5.45	106.61	113.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	35978	0	18210	723	0
2	L8	3320	0	1686	60	0
3	L5	78479	0	39731	1198	0
4	L7	2562	0	1295	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	SB	1738	0	1809	52	0
6	SA	1750	0	1755	78	0
7	SD	1756	0	1852	43	0
8	SJ	1525	0	1640	40	0
9	SE	2076	0	2177	53	0
10	SC	1725	0	1813	34	0
11	SG	1923	0	2089	64	0
12	SF	1494	0	1549	33	0
13	SH	1517	0	1605	40	0
14	SW	1034	0	1080	25	0
15	SI	1686	0	1772	38	0
16	SQ	1123	0	1192	47	0
17	SU	803	0	873	27	0
18	SK	810	0	836	49	0
19	SO	1009	0	1034	40	0
20	SX	1088	0	1149	30	0
21	SM	940	0	965	28	0
22	SS	1214	0	1275	47	0
23	Sd	454	0	447	21	0
24	SN	1214	0	1301	36	0
25	SL	1189	0	1262	20	0
26	SR	1083	0	1137	36	0
27	SP	1110	0	1163	30	0
28	ST	1112	0	1146	36	0
29	SV	639	0	638	12	0
30	SY	1065	0	1142	49	0
31	SZ	688	0	766	17	0
32	Sa	792	0	842	11	0
33	Sb	650	0	672	17	0
34	Sc	517	0	549	7	0
35	Se	452	0	498	10	0
36	Sf	515	0	521	14	0
37	Sg	2436	0	2393	91	0
38	Lz	1714	0	1824	75	0
39	LA	1930	0	2028	44	0
40	LB	3240	0	3377	64	0
41	LC	2927	0	3104	49	0
42	LJ	1358	0	1396	30	0
43	LH	1518	0	1601	34	0
44	LE	1787	0	1945	38	0
45	LG	1913	0	2054	42	0
46	LO	1641	0	1788	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	LL	1664	0	1773	33	0
48	LV	988	0	1047	13	0
49	LM	1120	0	1187	25	0
50	La	1163	0	1206	27	0
51	LN	1700	0	1749	37	0
52	LI	1646	0	1694	33	0
53	LD	2391	0	2426	53	0
54	LQ	1512	0	1628	26	0
55	LR	1566	0	1729	26	0
56	LS	1460	0	1502	28	0
57	LT	1297	0	1366	26	0
58	LP	1242	0	1269	26	0
59	LU	808	0	831	15	0
60	LX	967	0	1040	19	0
61	LY	1115	0	1205	32	0
62	LW	950	0	999	26	0
63	LZ	1106	0	1182	31	0
64	Lr	1005	0	1072	22	0
65	Lh	1015	0	1148	12	0
66	Lb	885	0	967	24	0
67	LF	1870	0	1996	61	0
68	Lc	764	0	804	15	0
69	Ld	888	0	930	8	0
70	Le	1053	0	1147	21	0
71	Lf	876	0	911	14	0
72	Lg	906	0	998	14	0
73	Li	832	0	917	14	0
74	Lj	705	0	737	22	0
75	Lk	569	0	637	7	0
76	Ll	444	0	483	14	0
77	Lm	431	0	471	8	0
78	Ln	230	0	276	6	0
79	Lo	852	0	921	14	0
80	Lp	708	0	757	15	0
81	5A	1144	0	1141	45	0
82	mR	210	0	107	2	0
83	At	1624	0	829	37	0
84	Pt	1645	0	843	29	0
85	L5	18	0	36	0	0
85	S2	6	0	12	0	0
86	L5	13	0	0	0	0
86	LA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	Lf	1	0	0	0	0
86	S2	1	0	0	0	0
87	5A	1	0	0	0	0
87	At	1	0	0	0	0
87	L5	231	0	0	0	0
87	L7	4	0	0	0	0
87	L8	6	0	0	0	0
87	LA	1	0	0	0	0
87	LB	1	0	0	0	0
87	LN	2	0	0	0	0
87	LP	1	0	0	0	0
87	LV	1	0	0	0	0
87	Le	1	0	0	0	0
87	Lg	1	0	0	0	0
87	Ln	1	0	0	0	0
87	Lo	1	0	0	0	0
87	Pt	2	0	0	0	0
87	S2	67	0	0	0	0
87	SC	1	0	0	0	0
87	SN	1	0	0	0	0
87	SS	1	0	0	0	0
87	Sa	1	0	0	0	0
88	L5	19	0	19	1	0
89	L5	50	0	95	2	0
90	L5	33	0	35	3	0
91	Lg	1	0	0	0	0
91	Lj	1	0	0	0	0
91	Lm	1	0	0	0	0
91	Lo	1	0	0	0	0
91	Lp	1	0	0	0	0
91	Sa	1	0	0	0	0
91	Sd	1	0	0	0	0
91	Sf	1	0	0	0	0
92	Pt	8	0	8	0	0
All	All	219329	0	163111	3901	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 3901 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SG:161:PRO:HA	11:SG:171:THR:HA	1.43	1.01
6:SA:159:ILE:HD11	29:SV:34:MET:HE1	1.50	0.93
16:SQ:86:GLN:HE21	16:SQ:118:THR:HG22	1.31	0.92
17:SU:46:LYS:HE3	17:SU:101:ILE:HD13	1.52	0.91
3:L5:3710:G:H1'	3:L5:3711:A:H2	1.33	0.91

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	SB	212/264 (80%)	204 (96%)	8 (4%)	0	100	100
6	SA	220/295 (75%)	213 (97%)	7 (3%)	0	100	100
7	SD	224/243 (92%)	221 (99%)	3 (1%)	0	100	100
8	SJ	183/194 (94%)	174 (95%)	9 (5%)	0	100	100
9	SE	260/263 (99%)	251 (96%)	8 (3%)	1 (0%)	30	54
10	SC	220/293 (75%)	215 (98%)	4 (2%)	1 (0%)	24	49
11	SG	235/249 (94%)	221 (94%)	13 (6%)	1 (0%)	30	54
12	SF	187/204 (92%)	169 (90%)	18 (10%)	0	100	100
13	SH	187/194 (96%)	178 (95%)	8 (4%)	1 (0%)	24	49
14	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
15	SI	204/208 (98%)	194 (95%)	9 (4%)	1 (0%)	24	49
16	SQ	139/146 (95%)	135 (97%)	4 (3%)	0	100	100
17	SU	99/119 (83%)	97 (98%)	2 (2%)	0	100	100
18	SK	94/165 (57%)	82 (87%)	8 (8%)	4 (4%)	2	4
19	SO	133/151 (88%)	122 (92%)	9 (7%)	2 (2%)	8	23
20	SX	137/143 (96%)	131 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	SM	120/132 (91%)	113 (94%)	5 (4%)	2 (2%)	7	20
22	SS	146/152 (96%)	136 (93%)	9 (6%)	1 (1%)	18	40
23	Sd	52/56 (93%)	49 (94%)	3 (6%)	0	100	100
24	SN	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
25	SL	141/158 (89%)	134 (95%)	7 (5%)	0	100	100
26	SR	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
27	SP	133/145 (92%)	125 (94%)	8 (6%)	0	100	100
28	ST	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
29	SV	81/83 (98%)	81 (100%)	0	0	100	100
30	SY	129/133 (97%)	123 (95%)	6 (5%)	0	100	100
31	SZ	84/125 (67%)	79 (94%)	5 (6%)	0	100	100
32	Sa	97/115 (84%)	93 (96%)	4 (4%)	0	100	100
33	Sb	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
34	Sc	63/69 (91%)	60 (95%)	3 (5%)	0	100	100
35	Se	55/133 (41%)	51 (93%)	4 (7%)	0	100	100
36	Sf	61/156 (39%)	53 (87%)	7 (12%)	1 (2%)	7	21
37	Sg	311/317 (98%)	285 (92%)	25 (8%)	1 (0%)	36	59
38	Lz	211/217 (97%)	170 (81%)	36 (17%)	5 (2%)	4	13
39	LA	249/257 (97%)	240 (96%)	8 (3%)	1 (0%)	30	54
40	LB	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
41	LC	366/427 (86%)	358 (98%)	8 (2%)	0	100	100
42	LJ	167/178 (94%)	163 (98%)	4 (2%)	0	100	100
43	LH	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
44	LE	217/288 (75%)	207 (95%)	10 (5%)	0	100	100
45	LG	237/266 (89%)	223 (94%)	13 (6%)	1 (0%)	30	54
46	LO	198/203 (98%)	192 (97%)	6 (3%)	0	100	100
47	LL	204/211 (97%)	192 (94%)	12 (6%)	0	100	100
48	LV	131/140 (94%)	125 (95%)	6 (5%)	0	100	100
49	LM	134/215 (62%)	131 (98%)	3 (2%)	0	100	100
50	La	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	18	40
51	LN	201/204 (98%)	193 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	LI	199/214 (93%)	192 (96%)	7 (4%)	0	100	100
53	LD	292/297 (98%)	285 (98%)	7 (2%)	0	100	100
54	LQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
55	LR	185/196 (94%)	184 (100%)	1 (0%)	0	100	100
56	LS	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
57	LT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
58	LP	151/184 (82%)	149 (99%)	2 (1%)	0	100	100
59	LU	97/128 (76%)	91 (94%)	6 (6%)	0	100	100
60	LX	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
61	LY	132/145 (91%)	127 (96%)	5 (4%)	0	100	100
62	LW	114/157 (73%)	107 (94%)	6 (5%)	1 (1%)	14	34
63	LZ	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
64	Lr	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
65	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
66	Lb	104/159 (65%)	100 (96%)	4 (4%)	0	100	100
67	LF	223/248 (90%)	212 (95%)	11 (5%)	0	100	100
68	Lc	96/115 (84%)	92 (96%)	4 (4%)	0	100	100
69	Ld	105/125 (84%)	101 (96%)	4 (4%)	0	100	100
70	Le	126/135 (93%)	121 (96%)	5 (4%)	0	100	100
71	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
72	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
73	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
74	Lj	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
75	Lk	67/70 (96%)	67 (100%)	0	0	100	100
76	Ll	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
77	Lm	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
78	Ln	22/25 (88%)	21 (96%)	1 (4%)	0	100	100
79	Lo	101/106 (95%)	96 (95%)	5 (5%)	0	100	100
80	Lp	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
81	5A	147/154 (96%)	130 (88%)	14 (10%)	3 (2%)	6	17
All	All	11641/13133 (89%)	11127 (96%)	486 (4%)	28 (0%)	44	65

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	SM	82	ASN
38	Lz	82	ILE
38	Lz	86	ASP
81	5A	75	SER
81	5A	131	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	SB	195/231 (84%)	194 (100%)	1 (0%)	81	90
6	SA	183/242 (76%)	183 (100%)	0	100	100
7	SD	189/202 (94%)	189 (100%)	0	100	100
8	SJ	161/168 (96%)	161 (100%)	0	100	100
9	SE	224/225 (100%)	221 (99%)	3 (1%)	61	77
10	SC	188/225 (84%)	185 (98%)	3 (2%)	55	74
11	SG	207/218 (95%)	204 (99%)	3 (1%)	59	76
12	SF	159/170 (94%)	159 (100%)	0	100	100
13	SH	168/174 (97%)	166 (99%)	2 (1%)	63	78
14	SW	112/113 (99%)	110 (98%)	2 (2%)	51	72
15	SI	178/180 (99%)	177 (99%)	1 (1%)	78	89
16	SQ	117/121 (97%)	113 (97%)	4 (3%)	32	58
17	SU	93/107 (87%)	93 (100%)	0	100	100
18	SK	87/136 (64%)	81 (93%)	6 (7%)	14	33
19	SO	105/119 (88%)	104 (99%)	1 (1%)	68	81
20	SX	111/114 (97%)	110 (99%)	1 (1%)	70	82
21	SM	102/108 (94%)	101 (99%)	1 (1%)	68	81
22	SS	128/132 (97%)	127 (99%)	1 (1%)	73	84
23	Sd	48/49 (98%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	SN	131/131 (100%)	131 (100%)	0	100	100
25	SL	131/142 (92%)	131 (100%)	0	100	100
26	SR	121/122 (99%)	121 (100%)	0	100	100
27	SP	121/130 (93%)	121 (100%)	0	100	100
28	ST	113/115 (98%)	113 (100%)	0	100	100
29	SV	66/66 (100%)	66 (100%)	0	100	100
30	SY	113/115 (98%)	110 (97%)	3 (3%)	39	64
31	SZ	75/103 (73%)	75 (100%)	0	100	100
32	Sa	86/98 (88%)	86 (100%)	0	100	100
33	Sb	75/76 (99%)	75 (100%)	0	100	100
34	Sc	58/62 (94%)	58 (100%)	0	100	100
35	Se	46/104 (44%)	46 (100%)	0	100	100
36	Sf	56/140 (40%)	54 (96%)	2 (4%)	31	56
37	Sg	272/275 (99%)	270 (99%)	2 (1%)	76	86
38	Lz	192/196 (98%)	191 (100%)	1 (0%)	81	90
39	LA	193/198 (98%)	190 (98%)	3 (2%)	55	74
40	LB	347/348 (100%)	345 (99%)	2 (1%)	78	89
41	LC	306/348 (88%)	306 (100%)	0	100	100
42	LJ	143/149 (96%)	142 (99%)	1 (1%)	76	86
43	LH	169/171 (99%)	169 (100%)	0	100	100
44	LE	196/252 (78%)	192 (98%)	4 (2%)	48	70
45	LG	202/223 (91%)	201 (100%)	1 (0%)	81	90
46	LO	172/174 (99%)	171 (99%)	1 (1%)	78	89
47	LL	172/177 (97%)	170 (99%)	2 (1%)	63	78
48	LV	102/107 (95%)	102 (100%)	0	100	100
49	LM	116/161 (72%)	116 (100%)	0	100	100
50	La	119/120 (99%)	119 (100%)	0	100	100
51	LN	171/172 (99%)	169 (99%)	2 (1%)	63	78
52	LI	173/181 (96%)	173 (100%)	0	100	100
53	LD	247/250 (99%)	245 (99%)	2 (1%)	73	84
54	LQ	164/165 (99%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	LR	166/175 (95%)	164 (99%)	2 (1%)	63	78
56	LS	157/157 (100%)	157 (100%)	0	100	100
57	LT	139/140 (99%)	138 (99%)	1 (1%)	76	86
58	LP	134/163 (82%)	134 (100%)	0	100	100
59	LU	89/115 (77%)	89 (100%)	0	100	100
60	LX	106/133 (80%)	106 (100%)	0	100	100
61	LY	124/135 (92%)	124 (100%)	0	100	100
62	LW	95/126 (75%)	90 (95%)	5 (5%)	20	43
63	LZ	117/118 (99%)	116 (99%)	1 (1%)	70	82
64	Lr	108/120 (90%)	107 (99%)	1 (1%)	70	82
65	Lh	109/110 (99%)	109 (100%)	0	100	100
66	Lb	89/125 (71%)	88 (99%)	1 (1%)	65	80
67	LF	194/215 (90%)	194 (100%)	0	100	100
68	Lc	83/97 (86%)	83 (100%)	0	100	100
69	Ld	98/110 (89%)	98 (100%)	0	100	100
70	Le	114/121 (94%)	110 (96%)	4 (4%)	32	56
71	Lf	88/89 (99%)	88 (100%)	0	100	100
72	Lg	98/100 (98%)	96 (98%)	2 (2%)	48	70
73	Li	86/89 (97%)	84 (98%)	2 (2%)	44	68
74	Lj	73/80 (91%)	71 (97%)	2 (3%)	39	64
75	Lk	64/65 (98%)	64 (100%)	0	100	100
76	Ll	47/48 (98%)	45 (96%)	2 (4%)	26	51
77	Lm	47/115 (41%)	46 (98%)	1 (2%)	47	70
78	Ln	23/24 (96%)	23 (100%)	0	100	100
79	Lo	91/93 (98%)	90 (99%)	1 (1%)	65	80
80	Lp	74/75 (99%)	73 (99%)	1 (1%)	59	76
81	5A	122/127 (96%)	119 (98%)	3 (2%)	42	66
All	All	10138/11170 (91%)	10054 (99%)	84 (1%)	70	84

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	LT	55	LYS

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Mol	Chain	Res	Type
72	Lg	52	ARG
62	LW	82	ILE
66	Lb	25	ARG
74	Lj	13	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
70	Le	52	GLN
73	Li	36	HIS
33	Sb	84	HIS
33	Sb	26	GLN
74	Lj	66	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1676/1869 (89%)	327 (19%)	11 (0%)
2	L8	155/156 (99%)	27 (17%)	0
3	L5	3644/5069 (71%)	678 (18%)	21 (0%)
4	L7	119/120 (99%)	7 (5%)	0
82	mR	9/60 (15%)	0	0
83	At	75/76 (98%)	15 (20%)	0
84	Pt	76/77 (98%)	21 (27%)	0
All	All	5754/7427 (77%)	1075 (18%)	32 (0%)

5 of 1075 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	4	C
1	S2	26	U
1	S2	33	G
1	S2	41	G
1	S2	44	U

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	4872	G
3	L5	4925	U

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Mol	Chain	Res	Type
3	L5	408	A
3	L5	385	A
3	L5	5027	C

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

240 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	$\# Z > 2$
2	OMG	L8	75	2	23,26,27	1.17	3 (13%)	32,38,41	2.02	7 (21%)
3	OMG	L5	3627	3	23,26,27	1.18	3 (13%)	32,38,41	2.08	6 (18%)
3	PSU	L5	3768	3	18,21,22	1.50	3 (16%)	21,30,33	2.24	6 (28%)
1	PSU	S2	866	1	18,21,22	1.37	2 (11%)	21,30,33	2.08	4 (19%)
3	PSU	L5	4521	3,87	18,21,22	1.46	3 (16%)	21,30,33	2.09	5 (23%)
1	A2M	S2	668	1,87	22,25,26	1.47	4 (18%)	30,36,39	2.03	9 (30%)
3	OMC	L5	3869	3	19,22,23	0.81	0	25,31,34	0.84	0
3	PSU	L5	4420	3	18,21,22	1.41	4 (22%)	21,30,33	1.96	5 (23%)
1	A2M	S2	484	1	22,25,26	1.47	4 (18%)	30,36,39	2.11	9 (30%)
3	OMC	L5	3701	86,3	19,22,23	0.77	0	25,31,34	0.75	0
1	PSU	S2	966	1	18,21,22	1.37	2 (11%)	21,30,33	2.11	4 (19%)
3	PSU	L5	2508	3	18,21,22	1.44	3 (16%)	21,30,33	2.12	4 (19%)
3	PSU	L5	4689	3	18,21,22	1.43	4 (22%)	21,30,33	2.09	3 (14%)
1	OMG	S2	1490	1,87	23,26,27	1.20	3 (13%)	32,38,41	1.99	6 (18%)
3	OMG	L5	4618	3	23,26,27	1.26	4 (17%)	32,38,41	2.14	8 (25%)
3	A2M	L5	3724	3	22,25,26	1.48	4 (18%)	30,36,39	2.05	8 (26%)
2	PSU	L8	55	2	18,21,22	1.42	3 (16%)	21,30,33	2.06	4 (19%)
3	A2M	L5	1524	3	22,25,26	1.54	4 (18%)	30,36,39	1.92	9 (30%)
1	PSU	S2	814	1	18,21,22	1.39	3 (16%)	21,30,33	2.04	4 (19%)
1	PSU	S2	1081	1	18,21,22	1.49	5 (27%)	21,30,33	2.23	5 (23%)
1	PSU	S2	109	1	18,21,22	1.55	5 (27%)	21,30,33	2.29	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	1004	1	18,21,22	1.47	3 (16%)	21,30,33	2.22	5 (23%)
1	A2M	S2	1031	1	22,25,26	1.47	5 (22%)	30,36,39	2.09	9 (30%)
3	PSU	L5	4576	3	18,21,22	1.42	3 (16%)	21,30,33	2.02	3 (14%)
3	PSU	L5	4500	83,3	18,21,22	1.39	2 (11%)	21,30,33	2.10	4 (19%)
1	PSU	S2	1445	1	18,21,22	1.33	2 (11%)	21,30,33	2.04	4 (19%)
1	OMU	S2	121	1	19,22,23	1.25	3 (15%)	25,31,34	1.76	4 (16%)
3	OMG	L5	3744	3	23,26,27	1.19	3 (13%)	32,38,41	2.01	6 (18%)
3	A2M	L5	4571	3	22,25,26	1.50	4 (18%)	30,36,39	2.04	7 (23%)
3	PSU	L5	4312	3	18,21,22	1.40	4 (22%)	21,30,33	2.12	4 (19%)
3	PSU	L5	4579	3	18,21,22	1.39	3 (16%)	21,30,33	2.13	4 (19%)
3	OMU	L5	4498	3	19,22,23	1.23	3 (15%)	25,31,34	1.88	5 (20%)
3	OMG	L5	4637	3	23,26,27	1.24	3 (13%)	32,38,41	2.17	8 (25%)
3	OMG	L5	2364	3	23,26,27	1.18	4 (17%)	32,38,41	1.97	6 (18%)
3	PSU	L5	1792	3	18,21,22	1.43	3 (16%)	21,30,33	2.04	4 (19%)
84	OMC	Pt	33	84	19,22,23	0.82	0	25,31,34	1.05	2 (8%)
1	PSU	S2	1692	1	18,21,22	1.54	5 (27%)	21,30,33	2.23	4 (19%)
83	4SU	At	8	83	18,21,22	1.88	4 (22%)	25,30,33	2.31	5 (20%)
3	A2M	L5	1871	3	22,25,26	1.47	5 (22%)	30,36,39	2.19	9 (30%)
1	OMC	S2	462	1	19,22,23	0.78	0	25,31,34	0.83	0
3	PSU	L5	3851	3	18,21,22	1.42	4 (22%)	21,30,33	2.05	5 (23%)
3	UR3	L5	4530	3	19,22,23	0.94	1 (5%)	26,32,35	1.74	3 (11%)
1	PSU	S2	918	1	18,21,22	1.39	2 (11%)	21,30,33	2.34	5 (23%)
3	OMG	L5	4494	3	23,26,27	1.22	3 (13%)	32,38,41	2.01	6 (18%)
1	OMC	S2	174	1	19,22,23	0.78	0	25,31,34	0.79	0
3	A2M	L5	398	3	22,25,26	1.48	5 (22%)	30,36,39	2.10	8 (26%)
1	PSU	S2	119	1	18,21,22	1.34	2 (11%)	21,30,33	1.90	4 (19%)
84	PSU	Pt	56	84	18,21,22	1.36	2 (11%)	21,30,33	2.02	3 (14%)
1	A2M	S2	590	1	22,25,26	1.50	4 (18%)	30,36,39	2.07	8 (26%)
83	H2U	At	16	83	18,21,22	1.02	2 (11%)	19,30,33	0.98	2 (10%)
1	OMG	S2	683	1	23,26,27	1.19	3 (13%)	32,38,41	1.98	5 (15%)
64	SAC	Lr	2	64	7,8,9	3.81	2 (28%)	7,9,11	4.15	3 (42%)
1	PSU	S2	1244	1	18,21,22	1.37	3 (16%)	21,30,33	2.08	4 (19%)
3	PSU	L5	2839	3	18,21,22	1.32	2 (11%)	21,30,33	2.13	3 (14%)
3	PSU	L5	3764	3	18,21,22	1.49	4 (22%)	21,30,33	2.34	5 (23%)
3	OMG	L5	4370	3	23,26,27	1.22	3 (13%)	32,38,41	1.96	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMU	L5	4306	3	19,22,23	1.29	3 (15%)	25,31,34	1.80	5 (20%)
1	OMU	S2	172	1	19,22,23	1.37	4 (21%)	25,31,34	1.98	6 (24%)
2	PSU	L8	69	2	18,21,22	1.42	3 (16%)	21,30,33	2.11	4 (19%)
3	A2M	L5	4590	3	22,25,26	1.47	4 (18%)	30,36,39	2.12	9 (30%)
3	6MZ	L5	4220	3	22,25,26	1.45	4 (18%)	29,36,39	2.15	10 (34%)
83	H2U	At	20	83	18,21,22	0.96	2 (11%)	19,30,33	1.02	1 (5%)
1	OMU	S2	1804	1	19,22,23	1.29	3 (15%)	25,31,34	1.78	4 (16%)
3	OMG	L5	4196	3,84	23,26,27	1.26	4 (17%)	32,38,41	2.01	8 (25%)
3	A2M	L5	400	3	22,25,26	1.49	4 (18%)	30,36,39	2.03	9 (30%)
1	A2M	S2	159	1	22,25,26	1.51	4 (18%)	30,36,39	2.09	7 (23%)
3	PSU	L5	4403	3	18,21,22	1.47	4 (22%)	21,30,33	2.15	4 (19%)
3	PSU	L5	5010	3	18,21,22	1.39	2 (11%)	21,30,33	2.07	3 (14%)
1	A2M	S2	166	1	22,25,26	1.47	5 (22%)	30,36,39	2.22	10 (33%)
3	PSU	L5	1744	86,3	18,21,22	1.41	3 (16%)	21,30,33	2.08	4 (19%)
3	OMC	L5	2824	3	19,22,23	0.76	0	25,31,34	0.79	0
1	A2M	S2	512	1	22,25,26	1.49	4 (18%)	30,36,39	2.22	10 (33%)
3	PSU	L5	3770	3	18,21,22	1.35	2 (11%)	21,30,33	2.01	4 (19%)
3	OMG	L5	4228	3	23,26,27	1.18	4 (17%)	32,38,41	1.91	6 (18%)
3	OMC	L5	3808	3	19,22,23	0.80	0	25,31,34	0.91	1 (4%)
1	PSU	S2	34	1	18,21,22	1.36	2 (11%)	21,30,33	2.10	4 (19%)
1	A2M	S2	468	1	22,25,26	1.48	4 (18%)	30,36,39	2.05	9 (30%)
3	A2M	L5	3723	3	22,25,26	1.51	4 (18%)	30,36,39	2.03	7 (23%)
3	OMC	L5	2422	3,87	19,22,23	0.80	0	25,31,34	0.86	1 (4%)
1	OMU	S2	428	1	19,22,23	1.22	3 (15%)	25,31,34	1.86	5 (20%)
3	OMU	L5	3925	3	19,22,23	1.24	3 (15%)	25,31,34	1.93	5 (20%)
40	HIC	LB	245	40	10,11,12	1.43	1 (10%)	9,14,16	1.39	2 (22%)
3	PSU	L5	4442	3	18,21,22	1.51	4 (22%)	21,30,33	2.34	5 (23%)
1	PSU	S2	649	1	18,21,22	1.40	3 (16%)	21,30,33	2.08	3 (14%)
39	V5N	LA	216	39	8,11,12	1.54	1 (12%)	8,14,16	1.93	2 (25%)
3	A2M	L5	3825	3	22,25,26	1.45	4 (18%)	30,36,39	2.08	8 (26%)
3	OMC	L5	4456	3	19,22,23	0.80	0	25,31,34	0.84	1 (4%)
1	OMU	S2	1288	1	19,22,23	1.21	3 (15%)	25,31,34	1.76	4 (16%)
1	PSU	S2	1232	1	18,21,22	1.37	2 (11%)	21,30,33	2.12	4 (19%)
3	A2M	L5	2787	3	22,25,26	1.45	4 (18%)	30,36,39	2.10	9 (30%)
3	PSU	L5	1860	3	18,21,22	1.45	4 (22%)	21,30,33	2.10	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	H2U	Pt	21	84	18,21,22	0.97	2 (11%)	19,30,33	1.05	1 (5%)
3	PSU	L5	2632	3	18,21,22	1.42	4 (22%)	21,30,33	1.94	3 (14%)
3	PSU	L5	1782	3	18,21,22	1.41	3 (16%)	21,30,33	2.08	3 (14%)
3	OMC	L5	3841	3	19,22,23	0.80	0	25,31,34	0.84	1 (4%)
3	OMC	L5	1340	3	19,22,23	0.86	1 (5%)	25,31,34	0.81	0
3	PSU	L5	4628	3	18,21,22	1.43	3 (16%)	21,30,33	2.08	3 (14%)
1	A2M	S2	27	1	22,25,26	1.48	4 (18%)	30,36,39	2.10	10 (33%)
1	PSU	S2	93	1	18,21,22	1.38	2 (11%)	21,30,33	2.04	3 (14%)
3	PSU	L5	1677	3	18,21,22	1.53	4 (22%)	21,30,33	2.12	4 (19%)
3	PSU	L5	4493	3	18,21,22	1.42	3 (16%)	21,30,33	1.98	4 (19%)
3	A2M	L5	4523	3,87	22,25,26	1.45	5 (22%)	30,36,39	2.38	10 (33%)
1	OMU	S2	354	1	19,22,23	1.29	3 (15%)	25,31,34	1.89	5 (20%)
79	MLZ	Lo	53	79	8,9,10	0.80	0	4,9,11	0.62	0
1	G7M	S2	1639	1,84	23,26,27	2.40	5 (21%)	34,39,42	3.10	11 (32%)
3	PSU	L5	4423	3,87	18,21,22	1.40	3 (16%)	21,30,33	2.09	4 (19%)
3	PSU	L5	4299	3	18,21,22	1.46	3 (16%)	21,30,33	2.08	5 (23%)
1	PSU	S2	1238	1	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
1	PSU	S2	1177	1	18,21,22	1.42	3 (16%)	21,30,33	2.07	3 (14%)
1	MA6	S2	1850	1	23,26,27	1.50	5 (21%)	33,38,41	2.02	9 (27%)
3	PSU	L5	1781	3	18,21,22	1.46	3 (16%)	21,30,33	2.03	3 (14%)
3	OMG	L5	3899	3	23,26,27	1.22	4 (17%)	32,38,41	2.06	7 (21%)
3	A2M	L5	1534	3,87	22,25,26	1.51	5 (22%)	30,36,39	2.15	10 (33%)
1	PSU	S2	1243	1	18,21,22	1.39	2 (11%)	21,30,33	2.03	3 (14%)
1	6MZ	S2	1832	1,87	22,25,26	1.48	5 (22%)	29,36,39	2.06	9 (31%)
3	PSU	L5	3639	3	18,21,22	1.48	4 (22%)	21,30,33	2.10	5 (23%)
1	OMG	S2	867	1	23,26,27	1.22	3 (13%)	32,38,41	2.12	7 (21%)
3	OMG	L5	3792	3	23,26,27	1.20	3 (13%)	32,38,41	1.96	6 (18%)
1	OMG	S2	1328	1	23,26,27	1.20	3 (13%)	32,38,41	2.00	6 (18%)
1	PSU	S2	1174	1,87	18,21,22	1.39	4 (22%)	21,30,33	2.02	3 (14%)
3	A2M	L5	3785	3,87	22,25,26	1.46	5 (22%)	30,36,39	2.46	12 (40%)
3	A2M	L5	3867	3	22,25,26	1.51	4 (18%)	30,36,39	2.01	7 (23%)
1	A2M	S2	99	1,87	22,25,26	1.49	4 (18%)	30,36,39	2.17	10 (33%)
3	A2M	L5	2363	3,87	22,25,26	1.46	3 (13%)	30,36,39	2.03	7 (23%)
1	OMG	S2	509	1,87	23,26,27	1.19	3 (13%)	32,38,41	1.97	6 (18%)
1	OMG	S2	1447	1	23,26,27	1.19	3 (13%)	32,38,41	1.98	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	1316	3	23,26,27	1.25	4 (17%)	32,38,41	1.93	6 (18%)
3	OMG	L5	1522	3	23,26,27	1.23	4 (17%)	32,38,41	2.04	7 (21%)
3	PSU	L5	4353	3	18,21,22	1.42	3 (16%)	21,30,33	2.09	5 (23%)
3	UY1	L5	3818	3,87	19,22,23	1.43	4 (21%)	21,31,34	2.12	4 (19%)
3	OMU	L5	4620	3	19,22,23	1.33	3 (15%)	25,31,34	1.90	5 (20%)
83	7MG	At	46	83	23,26,27	1.34	3 (13%)	27,39,42	2.79	9 (33%)
1	PSU	S2	1367	1	18,21,22	1.37	2 (11%)	21,30,33	2.07	3 (14%)
3	PSU	L5	4293	3	18,21,22	1.45	4 (22%)	21,30,33	2.00	3 (14%)
1	OMG	S2	436	1	23,26,27	1.19	3 (13%)	32,38,41	1.98	6 (18%)
1	PSU	S2	822	1	18,21,22	1.35	2 (11%)	21,30,33	2.23	5 (23%)
3	OMC	L5	1881	3,87	19,22,23	0.78	0	25,31,34	0.78	0
1	PSU	S2	686	1	18,21,22	1.41	2 (11%)	21,30,33	2.03	3 (14%)
3	A2M	L5	2815	3,87	22,25,26	1.47	4 (18%)	30,36,39	2.06	8 (26%)
1	PSU	S2	218	1	18,21,22	1.35	3 (16%)	21,30,33	2.00	4 (19%)
3	PSU	L5	4552	3	18,21,22	1.44	4 (22%)	21,30,33	2.16	4 (19%)
3	PSU	L5	4296	3	18,21,22	1.40	3 (16%)	21,30,33	2.11	4 (19%)
3	PSU	L5	3853	3,87	18,21,22	1.43	4 (22%)	21,30,33	2.12	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.44	4 (22%)	21,30,33	2.23	4 (19%)
81	5CT	5A	50	81	13,14,15	0.69	1 (7%)	8,15,17	2.25	3 (37%)
1	PSU	S2	296	1	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
3	OMG	L5	3944	3	23,26,27	1.17	2 (8%)	32,38,41	2.00	6 (18%)
1	PSU	S2	105	1	18,21,22	1.36	3 (16%)	21,30,33	2.06	4 (19%)
3	PSU	L5	3884	3	18,21,22	1.46	4 (22%)	21,30,33	2.11	3 (14%)
3	OMC	L5	2365	3	19,22,23	0.79	0	25,31,34	0.77	0
3	PSU	L5	4457	3	18,21,22	1.43	3 (16%)	21,30,33	2.09	6 (28%)
1	PSU	S2	863	1	18,21,22	1.41	2 (11%)	21,30,33	2.04	3 (14%)
3	PSU	L5	3758	3	18,21,22	1.57	5 (27%)	21,30,33	2.16	4 (19%)
1	OMU	S2	627	1	19,22,23	1.22	3 (15%)	25,31,34	1.79	5 (20%)
1	UY1	S2	1326	1,87	19,22,23	1.33	3 (15%)	21,31,34	2.08	4 (19%)
6	SAC	SA	2	6	7,8,9	3.81	2 (28%)	7,9,11	4.26	4 (57%)
3	PSU	L5	1779	3	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
1	OMC	S2	1391	1	19,22,23	0.80	0	25,31,34	0.84	1 (4%)
1	PSU	S2	1136	1	18,21,22	1.36	2 (11%)	21,30,33	2.05	3 (14%)
3	PSU	L5	3734	3	18,21,22	1.35	2 (11%)	21,30,33	2.07	4 (19%)
1	PSU	S2	1625	1	18,21,22	1.36	2 (11%)	21,30,33	2.01	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4361	3	18,21,22	1.43	3 (16%)	21,30,33	2.08	4 (19%)
1	OMG	S2	601	1	23,26,27	1.19	3 (13%)	32,38,41	2.00	6 (18%)
1	PSU	S2	651	1	18,21,22	1.40	2 (11%)	21,30,33	2.12	4 (19%)
3	OMC	L5	2861	3	19,22,23	0.77	0	25,31,34	0.71	0
3	PSU	L5	4471	3	18,21,22	1.38	3 (16%)	21,30,33	2.01	4 (19%)
1	PSU	S2	1347	1	18,21,22	1.36	3 (16%)	21,30,33	2.01	4 (19%)
3	PSU	L5	3637	3	18,21,22	1.47	3 (16%)	21,30,33	2.08	5 (23%)
3	5MC	L5	3782	3,87	19,22,23	1.45	3 (15%)	26,32,35	1.16	3 (11%)
1	OMC	S2	517	1	19,22,23	0.79	0	25,31,34	0.84	0
3	PSU	L5	3695	3	18,21,22	1.42	3 (16%)	21,30,33	2.08	4 (19%)
3	5MC	L5	4447	86,3	19,22,23	1.62	3 (15%)	26,32,35	1.35	4 (15%)
3	PSU	L5	4532	3	18,21,22	1.51	3 (16%)	21,30,33	2.07	4 (19%)
3	PSU	L5	1582	3	18,21,22	1.48	3 (16%)	21,30,33	2.22	6 (28%)
3	PSU	L5	4673	3	18,21,22	1.57	4 (22%)	21,30,33	2.18	5 (23%)
3	PSU	L5	1536	3	18,21,22	1.50	3 (16%)	21,30,33	2.00	4 (19%)
1	PSU	S2	572	1	18,21,22	1.43	3 (16%)	21,30,33	2.18	5 (23%)
3	OMG	L5	2424	3	23,26,27	1.23	3 (13%)	32,38,41	1.91	6 (18%)
3	OMG	L5	2876	3	23,26,27	1.21	3 (13%)	32,38,41	2.12	7 (21%)
1	PSU	S2	609	1	18,21,22	1.38	2 (11%)	21,30,33	2.05	3 (14%)
3	OMG	L5	4392	3	23,26,27	1.21	4 (17%)	32,38,41	1.91	5 (15%)
3	OMG	L5	4499	83,3	23,26,27	1.18	3 (13%)	32,38,41	2.00	6 (18%)
3	OMG	L5	4623	3	23,26,27	1.22	4 (17%)	32,38,41	1.98	6 (18%)
77	M3L	Lm	98	77	10,11,12	0.48	0	9,14,16	0.11	0
1	A2M	S2	1678	1	22,25,26	1.45	4 (18%)	30,36,39	2.15	7 (23%)
3	OMU	L5	4227	3	19,22,23	1.28	3 (15%)	25,31,34	1.82	5 (20%)
83	PSU	At	32	83	18,21,22	1.36	2 (11%)	21,30,33	1.98	3 (14%)
3	OMC	L5	2804	3	19,22,23	0.78	0	25,31,34	0.87	0
1	A2M	S2	576	1	22,25,26	1.49	5 (22%)	30,36,39	2.12	9 (30%)
3	PSU	L5	1683	3	18,21,22	1.52	4 (22%)	21,30,33	1.99	4 (19%)
1	PSU	S2	1239	1	18,21,22	1.39	2 (11%)	21,30,33	2.04	3 (14%)
1	OMU	S2	1442	1,87	19,22,23	1.23	3 (15%)	25,31,34	1.81	4 (16%)
3	A2M	L5	3830	3	22,25,26	1.43	3 (13%)	30,36,39	2.20	9 (30%)
3	PSU	L5	5001	3	18,21,22	1.41	3 (16%)	21,30,33	2.11	4 (19%)
3	1MA	L5	1322	3,87	21,25,26	1.36	3 (14%)	30,37,40	1.73	5 (16%)
1	OMU	S2	116	1	19,22,23	1.25	3 (15%)	25,31,34	1.78	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	801	1	18,21,22	1.37	3 (16%)	21,30,33	2.08	4 (19%)
3	PSU	L5	4569	3	18,21,22	1.44	3 (16%)	21,30,33	2.11	3 (14%)
66	MLZ	Lb	5	66	8,9,10	0.81	0	4,9,11	0.71	0
1	4AC	S2	1842	1	21,24,25	1.00	1 (4%)	28,34,37	1.13	4 (14%)
3	A2M	L5	3718	3	22,25,26	1.50	4 (18%)	30,36,39	2.00	8 (26%)
1	PSU	S2	681	1	18,21,22	1.44	3 (16%)	21,30,33	2.12	4 (19%)
1	PSU	S2	1056	1	18,21,22	1.35	2 (11%)	21,30,33	2.06	4 (19%)
3	PSU	L5	3715	3	18,21,22	1.39	3 (16%)	21,30,33	2.03	4 (19%)
1	4AC	S2	1337	1	21,24,25	1.18	2 (9%)	28,34,37	1.15	3 (10%)
1	OMG	S2	644	1	23,26,27	1.20	3 (13%)	32,38,41	2.03	6 (18%)
3	A2M	L5	2401	3	22,25,26	1.47	5 (22%)	30,36,39	2.21	10 (33%)
83	PSU	At	39	83	18,21,22	1.36	3 (16%)	21,30,33	2.08	4 (19%)
2	OMU	L8	14	2,3	19,22,23	1.29	3 (15%)	25,31,34	1.81	4 (16%)
3	OMC	L5	2351	3	19,22,23	0.82	0	25,31,34	0.76	0
50	V5N	La	39	50	8,11,12	1.34	1 (12%)	8,14,16	1.88	2 (25%)
3	PSU	L5	4431	3	18,21,22	1.35	2 (11%)	21,30,33	2.10	4 (19%)
1	OMC	S2	1703	1	19,22,23	0.79	0	25,31,34	0.70	0
3	PSU	L5	4636	3	18,21,22	1.51	4 (22%)	21,30,33	2.38	6 (28%)
3	PSU	L5	3729	3	18,21,22	1.37	2 (11%)	21,30,33	2.04	4 (19%)
3	OMG	L5	1625	3,87	23,26,27	1.23	3 (13%)	32,38,41	2.06	6 (18%)
29	AME	SV	1	29	9,10,11	3.41	2 (22%)	9,11,13	3.78	3 (33%)
3	A2M	L5	3760	3,87	22,25,26	1.51	5 (22%)	30,36,39	2.09	10 (33%)
3	PSU	L5	4972	3	18,21,22	1.36	3 (16%)	21,30,33	1.98	5 (23%)
3	OMC	L5	4536	3	19,22,23	0.83	0	25,31,34	0.81	1 (4%)
1	PSU	S2	406	1	18,21,22	1.37	3 (16%)	21,30,33	2.04	3 (14%)
1	PSU	S2	1643	1,87	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
3	A2M	L5	1326	3	22,25,26	1.51	5 (22%)	30,36,39	2.08	8 (26%)
3	PSU	L5	3762	3	18,21,22	1.38	2 (11%)	21,30,33	2.07	3 (14%)
1	PSU	S2	573	1	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
3	PSU	L5	2843	3	18,21,22	1.44	3 (16%)	21,30,33	2.14	4 (19%)
20	HY3	SX	62	20	7,8,9	1.45	1 (14%)	7,10,12	1.34	0
3	PSU	L5	3844	3	18,21,22	1.47	3 (16%)	21,30,33	2.02	4 (19%)
1	PSU	S2	815	1	18,21,22	1.38	3 (16%)	21,30,33	2.07	4 (19%)
3	OMU	L5	2415	3	19,22,23	1.33	4 (21%)	25,31,34	1.91	5 (20%)
3	PSU	L5	3920	3,87	18,21,22	1.43	3 (16%)	21,30,33	2.16	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	36	1	18,21,22	1.38	3 (16%)	21,30,33	2.01	3 (14%)
84	4SU	Pt	8	84	18,21,22	1.82	4 (22%)	25,30,33	2.26	5 (20%)
1	A2M	S2	1383	1	22,25,26	1.49	4 (18%)	30,36,39	2.22	9 (30%)
3	OMU	L5	2837	3	19,22,23	1.29	2 (10%)	25,31,34	1.89	4 (16%)
84	G7M	Pt	47	84	23,26,27	1.88	3 (13%)	34,39,42	1.11	1 (2%)
1	MA6	S2	1851	1	23,26,27	1.47	5 (21%)	33,38,41	2.02	9 (27%)
1	B8N	S2	1248	1	25,29,30	0.99	2 (8%)	28,42,45	1.72	5 (17%)
3	OMC	L5	3887	3	19,22,23	0.75	0	25,31,34	0.83	0
3	PSU	L5	4531	3	18,21,22	1.47	2 (11%)	21,30,33	2.27	5 (23%)

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
2	OMG	L8	75	2	-	0/9/27/28	0/3/3/3
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	3,87	-	0/7/25/26	0/2/2/2
1	A2M	S2	668	1,87	-	4/9/27/28	0/3/3/3
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4420	3	-	4/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	0/9/27/28	0/3/3/3
3	OMC	L5	3701	86,3	-	4/9/27/28	0/2/2/2
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	1490	1,87	-	1/9/27/28	0/3/3/3
3	OMG	L5	4618	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	1/9/27/28	0/3/3/3
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1031	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4500	83,3	-	1/7/25/26	0/2/2/2
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	121	1	-	1/9/27/28	0/2/2/2
3	OMG	L5	3744	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	4571	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4637	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	2364	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
84	OMC	Pt	33	84	-	2/9/27/28	0/2/2/2
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
83	4SU	At	8	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	3	-	0/9/27/28	0/3/3/3
1	OMC	S2	462	1	-	1/9/27/28	0/2/2/2
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	918	1	-	2/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
84	PSU	Pt	56	84	-	0/7/25/26	0/2/2/2
1	A2M	S2	590	1	-	1/9/27/28	0/3/3/3
83	H2U	At	16	83	-	1/7/38/39	0/2/2/2
1	OMG	S2	683	1	-	2/9/27/28	0/3/3/3
64	SAC	Lr	2	64	-	1/7/8/10	-
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3764	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
1	OMU	S2	172	1	-	0/9/27/28	0/2/2/2
2	PSU	L8	69	2	-	0/7/25/26	0/2/2/2
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
83	H2U	At	20	83	-	0/7/38/39	0/2/2/2
1	OMU	S2	1804	1	-	1/9/27/28	0/2/2/2
3	OMG	L5	4196	3,84	-	1/9/27/28	0/3/3/3
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	S2	159	1	-	3/9/27/28	0/3/3/3
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	166	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	1744	86,3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
1	A2M	S2	512	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	1/9/27/28	0/3/3/3
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	2422	3,87	-	3/9/27/28	0/2/2/2
1	OMU	S2	428	1	-	6/9/27/28	0/2/2/2
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
40	HIC	LB	245	40	-	3/5/6/8	0/1/1/1
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
39	V5N	LA	216	39	-	2/9/10/12	0/1/1/1
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
1	OMU	S2	1288	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
84	H2U	Pt	21	84	-	6/7/38/39	0/2/2/2
3	PSU	L5	2632	3	-	4/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	27	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	3,87	-	1/9/27/28	0/3/3/3
1	OMU	S2	354	1	-	2/9/27/28	0/2/2/2
79	MLZ	Lo	53	79	-	1/7/8/10	-
1	G7M	S2	1639	1,84	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4423	3,87	-	0/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
3	PSU	L5	1781	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1534	3,87	-	2/9/27/28	0/3/3/3
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
1	6MZ	S2	1832	1,87	-	2/9/27/28	0/3/3/3
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	867	1	-	3/9/27/28	0/3/3/3
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
1	OMG	S2	1328	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1174	1,87	-	0/7/25/26	0/2/2/2
3	A2M	L5	3785	3,87	-	3/9/27/28	0/3/3/3
3	A2M	L5	3867	3	-	3/9/27/28	0/3/3/3
1	A2M	S2	99	1,87	-	0/9/27/28	0/3/3/3
3	A2M	L5	2363	3,87	-	0/9/27/28	0/3/3/3
1	OMG	S2	509	1,87	-	0/9/27/28	0/3/3/3
1	OMG	S2	1447	1	-	2/9/27/28	0/3/3/3
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	UY1	L5	3818	3,87	-	2/9/27/28	0/2/2/2
3	OMU	L5	4620	3	-	1/9/27/28	0/2/2/2
83	7MG	At	46	83	-	3/7/37/38	0/3/3/3
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	822	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	1881	3,87	-	0/9/27/28	0/2/2/2
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	2815	3,87	-	1/9/27/28	0/3/3/3
1	PSU	S2	218	1	-	3/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	3,87	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	5CT	5A	50	81	-	8/13/14/16	-
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	3944	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	863	1	-	2/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	627	1	-	1/9/27/28	0/2/2/2
1	UY1	S2	1326	1,87	-	1/9/27/28	0/2/2/2
6	SAC	SA	2	6	-	5/7/8/10	-
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
1	OMC	S2	1391	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	1136	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	1625	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4471	3	-	2/7/25/26	0/2/2/2
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	3,87	-	2/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	86,3	-	4/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	3/9/27/28	0/3/3/3
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4499	83,3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
77	M3L	Lm	98	77	-	4/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	S2	1678	1	-	3/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	1/9/27/28	0/2/2/2
83	PSU	At	32	83	-	0/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
1	A2M	S2	576	1	-	2/9/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1239	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1442	1,87	-	1/9/27/28	0/2/2/2
3	A2M	L5	3830	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	1MA	L5	1322	3,87	-	2/7/25/26	0/3/3/3
1	OMU	S2	116	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4569	3	-	0/7/25/26	0/2/2/2
66	MLZ	Lb	5	66	-	3/7/8/10	-
1	4AC	S2	1842	1	-	2/11/29/30	0/2/2/2
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	2/11/29/30	0/2/2/2
1	OMG	S2	644	1	-	4/9/27/28	0/3/3/3
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
83	PSU	At	39	83	-	0/7/25/26	0/2/2/2
2	OMU	L8	14	2,3	-	1/9/27/28	0/2/2/2
3	OMC	L5	2351	3	-	0/9/27/28	0/2/2/2
50	V5N	La	39	50	-	0/9/10/12	0/1/1/1
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
1	OMC	S2	1703	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	4636	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3729	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	1625	3,87	-	1/9/27/28	0/3/3/3
29	AME	SV	1	29	-	2/9/10/12	-
3	A2M	L5	3760	3,87	-	0/9/27/28	0/3/3/3
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1643	1,87	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	573	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
20	HY3	SX	62	20	-	1/1/12/14	0/1/1/1
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	3920	3,87	-	0/7/25/26	0/2/2/2
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
84	4SU	Pt	8	84	-	0/7/25/26	0/2/2/2
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
84	G7M	Pt	47	84	-	2/7/25/26	0/3/3/3
1	MA6	S2	1851	1	-	2/11/29/30	0/3/3/3
1	B8N	S2	1248	1	-	4/16/34/35	0/2/2/2
3	OMC	L5	3887	3	-	2/9/27/28	0/2/2/2
3	PSU	L5	4531	3	-	2/7/25/26	0/2/2/2

The worst 5 of 684 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	SV	1	AME	OT-CT1	9.11	1.43	1.23
6	SA	2	SAC	OAC-C1A	9.02	1.43	1.23
64	Lr	2	SAC	OAC-C1A	8.99	1.43	1.23
84	Pt	47	G7M	C8-N7	7.41	1.45	1.33
1	S2	1639	G7M	C8-N7	7.36	1.45	1.33

The worst 5 of 1121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	At	46	7MG	N9-C4-N3	9.21	138.95	125.46
1	S2	1639	G7M	CN7-N7-C8	-7.75	113.06	124.79
6	SA	2	SAC	OAC-C1A-C2A	-7.41	108.86	122.05
29	SV	1	AME	OT-CT1-N	-7.35	108.98	121.98
3	L5	4636	PSU	N1-C2-N3	7.29	122.86	115.17

There are no chirality outliers.

5 of 199 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L8	14	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
6	SA	2	SAC	C-CA-N-C1A
6	SA	2	SAC	C-CA-CB-OG
29	SV	1	AME	OT-CT1-N-CA
66	Lb	5	MLZ	N-CA-CB-CG

There are no ring outliers.

118 monomers are involved in 204 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L8	75	OMG	1	0
3	L5	3768	PSU	2	0
1	S2	866	PSU	1	0
3	L5	4521	PSU	1	0
1	S2	484	A2M	1	0
1	S2	1490	OMG	2	0
3	L5	4618	OMG	2	0
3	L5	3724	A2M	2	0
1	S2	121	OMU	2	0
3	L5	4571	A2M	2	0
3	L5	4637	OMG	1	0
3	L5	2364	OMG	1	0
3	L5	1871	A2M	1	0
1	S2	918	PSU	2	0
1	S2	174	OMC	1	0
3	L5	398	A2M	2	0
1	S2	683	OMG	2	0
1	S2	1244	PSU	1	0
3	L5	3764	PSU	2	0
3	L5	4370	OMG	2	0
3	L5	4306	OMU	2	0
1	S2	172	OMU	2	0
2	L8	69	PSU	1	0
3	L5	4220	6MZ	2	0
1	S2	1804	OMU	2	0
3	L5	4196	OMG	1	0
3	L5	400	A2M	1	0
1	S2	159	A2M	3	0
1	S2	166	A2M	2	0
3	L5	2824	OMC	1	0
1	S2	512	A2M	5	0
3	L5	3770	PSU	2	0
3	L5	4228	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3808	OMC	1	0
1	S2	34	PSU	2	0
1	S2	468	A2M	2	0
3	L5	3723	A2M	5	0
3	L5	2422	OMC	1	0
3	L5	4456	OMC	1	0
1	S2	1288	OMU	2	0
3	L5	2787	A2M	1	0
84	Pt	21	H2U	1	0
3	L5	2632	PSU	2	0
3	L5	1340	OMC	2	0
1	S2	27	A2M	3	0
1	S2	93	PSU	1	0
3	L5	1677	PSU	1	0
3	L5	4493	PSU	1	0
3	L5	4523	A2M	1	0
1	S2	1639	G7M	1	0
1	S2	1850	MA6	2	0
3	L5	1781	PSU	1	0
3	L5	3899	OMG	1	0
3	L5	1534	A2M	2	0
1	S2	1832	6MZ	1	0
1	S2	867	OMG	3	0
3	L5	3792	OMG	1	0
1	S2	1174	PSU	2	0
3	L5	3785	A2M	2	0
3	L5	3867	A2M	4	0
3	L5	2363	A2M	3	0
1	S2	509	OMG	4	0
1	S2	1447	OMG	3	0
3	L5	3818	UY1	1	0
3	L5	4620	OMU	2	0
83	At	46	7MG	3	0
1	S2	822	PSU	1	0
3	L5	1881	OMC	1	0
3	L5	2815	A2M	2	0
1	S2	218	PSU	1	0
3	L5	4552	PSU	1	0
3	L5	4296	PSU	1	0
81	5A	50	5CT	5	0
3	L5	3944	OMG	2	0
3	L5	3884	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4457	PSU	1	0
1	S2	863	PSU	1	0
3	L5	3758	PSU	2	0
6	SA	2	SAC	3	0
3	L5	1779	PSU	1	0
1	S2	1391	OMC	3	0
1	S2	1136	PSU	3	0
3	L5	3734	PSU	1	0
3	L5	4361	PSU	1	0
1	S2	601	OMG	3	0
1	S2	651	PSU	1	0
3	L5	2861	OMC	1	0
3	L5	4447	5MC	2	0
3	L5	1536	PSU	1	0
1	S2	572	PSU	1	0
3	L5	2424	OMG	3	0
3	L5	2876	OMG	3	0
1	S2	609	PSU	1	0
3	L5	4392	OMG	2	0
1	S2	1678	A2M	2	0
3	L5	4227	OMU	2	0
3	L5	2804	OMC	1	0
1	S2	576	A2M	4	0
3	L5	1683	PSU	1	0
1	S2	1442	OMU	2	0
1	S2	116	OMU	3	0
66	Lb	5	MLZ	1	0
1	S2	1842	4AC	2	0
3	L5	3718	A2M	4	0
1	S2	681	PSU	2	0
3	L5	3715	PSU	1	0
1	S2	1337	4AC	5	0
1	S2	644	OMG	1	0
2	L8	14	OMU	1	0
3	L5	2351	OMC	2	0
1	S2	1703	OMC	1	0
1	S2	1643	PSU	1	0
1	S2	573	PSU	2	0
3	L5	2415	OMU	2	0
3	L5	3920	PSU	1	0
1	S2	36	PSU	2	0
1	S2	1383	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	1851	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 362 ligands modelled in this entry, 350 are monoatomic - leaving 12 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
89	SPD	L5	5304	-	9,9,9	0.20	0	8,8,8	0.21	0
89	SPD	L5	5307	-	9,9,9	0.32	0	8,8,8	0.65	0
88	ANM	L5	5301	86	20,20,20	1.17	1 (5%)	24,27,27	1.47	4 (16%)
85	PUT	S2	1901	-	5,5,5	0.10	0	4,4,4	0.11	0
89	SPD	L5	5303	-	9,9,9	0.39	0	8,8,8	0.87	0
89	SPD	L5	5302	-	9,9,9	0.37	0	8,8,8	0.89	0
89	SPD	L5	5306	-	9,9,9	0.16	0	8,8,8	0.23	0
85	PUT	L5	5305	-	5,5,5	0.11	0	4,4,4	0.12	0
85	PUT	L5	5309	-	5,5,5	0.15	0	4,4,4	0.23	0
92	MET	Pt	78	84	6,7,8	0.55	0	2,7,9	1.50	1 (50%)
90	3H3	L5	5310	-	34,34,34	3.40	12 (35%)	36,45,45	3.94	16 (44%)
85	PUT	L5	5308	-	5,5,5	0.14	0	4,4,4	0.24	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
89	SPD	L5	5304	-	-	5/7/7/7	-
89	SPD	L5	5307	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	ANM	L5	5301	86	-	4/10/23/23	0/2/2/2
85	PUT	S2	1901	-	-	1/3/3/3	-
89	SPD	L5	5303	-	-	3/7/7/7	-
89	SPD	L5	5302	-	-	0/7/7/7	-
89	SPD	L5	5306	-	-	1/7/7/7	-
85	PUT	L5	5305	-	-	1/3/3/3	-
85	PUT	L5	5309	-	-	3/3/3/3	-
92	MET	Pt	78	84	-	1/5/6/8	-
90	3H3	L5	5310	-	-	17/39/51/51	0/1/2/2
85	PUT	L5	5308	-	-	1/3/3/3	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	L5	5310	3H3	C13-C12	9.03	1.53	1.33
90	L5	5310	3H3	O3-C22	8.19	1.39	1.23
90	L5	5310	3H3	O4-C23	7.70	1.38	1.23
90	L5	5310	3H3	C23-N	6.77	1.48	1.37
90	L5	5310	3H3	C22-N	6.54	1.48	1.37

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	L5	5310	3H3	C22-N-C23	-11.65	111.83	125.87
90	L5	5310	3H3	O4-C23-N	-8.79	106.75	120.30
90	L5	5310	3H3	O3-C22-N	-7.83	108.22	120.30
90	L5	5310	3H3	O3-C22-C21	-7.16	108.95	122.62
90	L5	5310	3H3	O4-C23-C24	-7.00	109.26	122.62

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

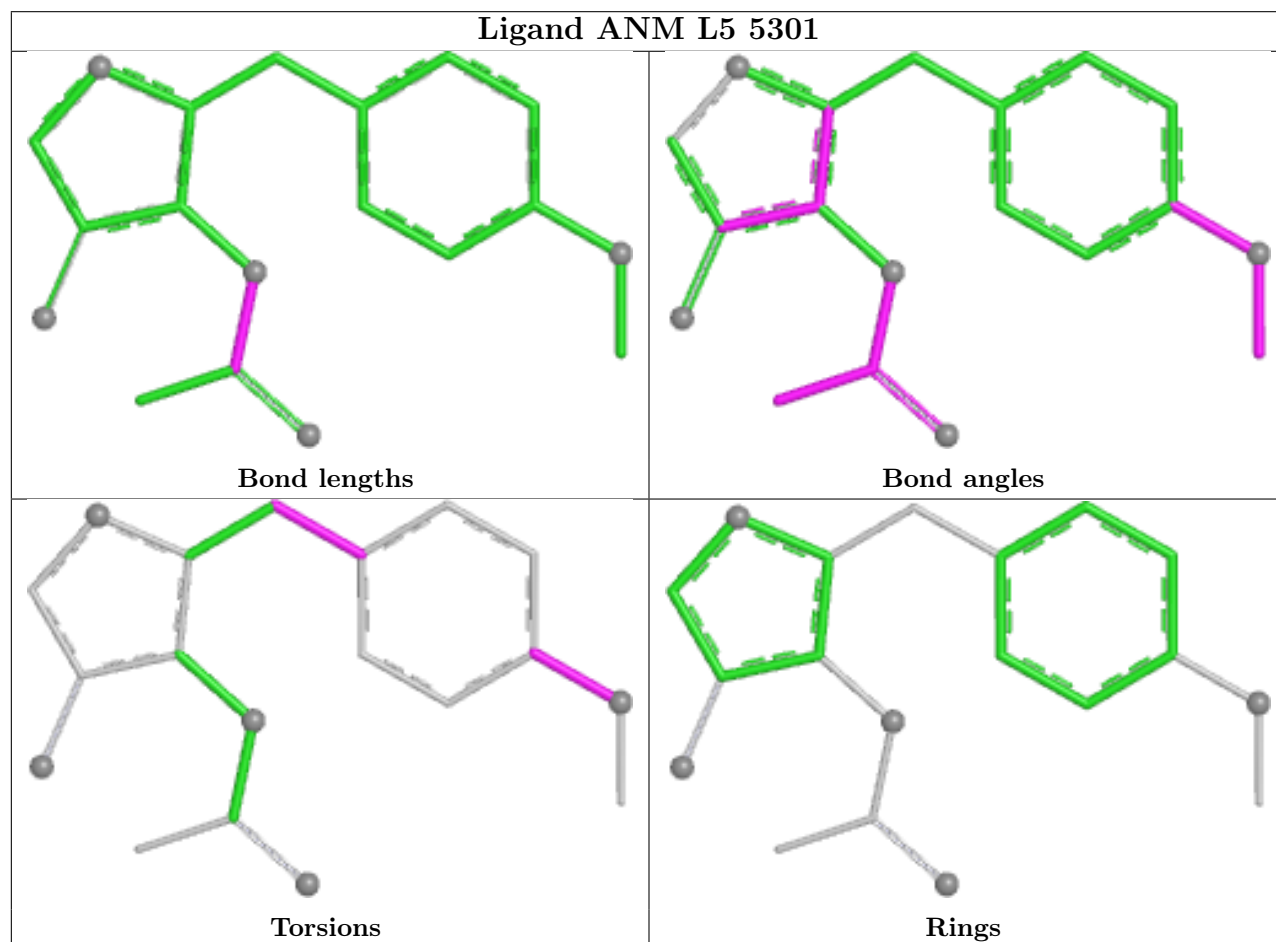
Mol	Chain	Res	Type	Atoms
90	L5	5310	3H3	C2-C1-C11-O1
90	L5	5310	3H3	C2-C1-C11-C12
90	L5	5310	3H3	C-C1-C11-O1
90	L5	5310	3H3	C-C1-C11-C12
90	L5	5310	3H3	C9-C10-O1-C11

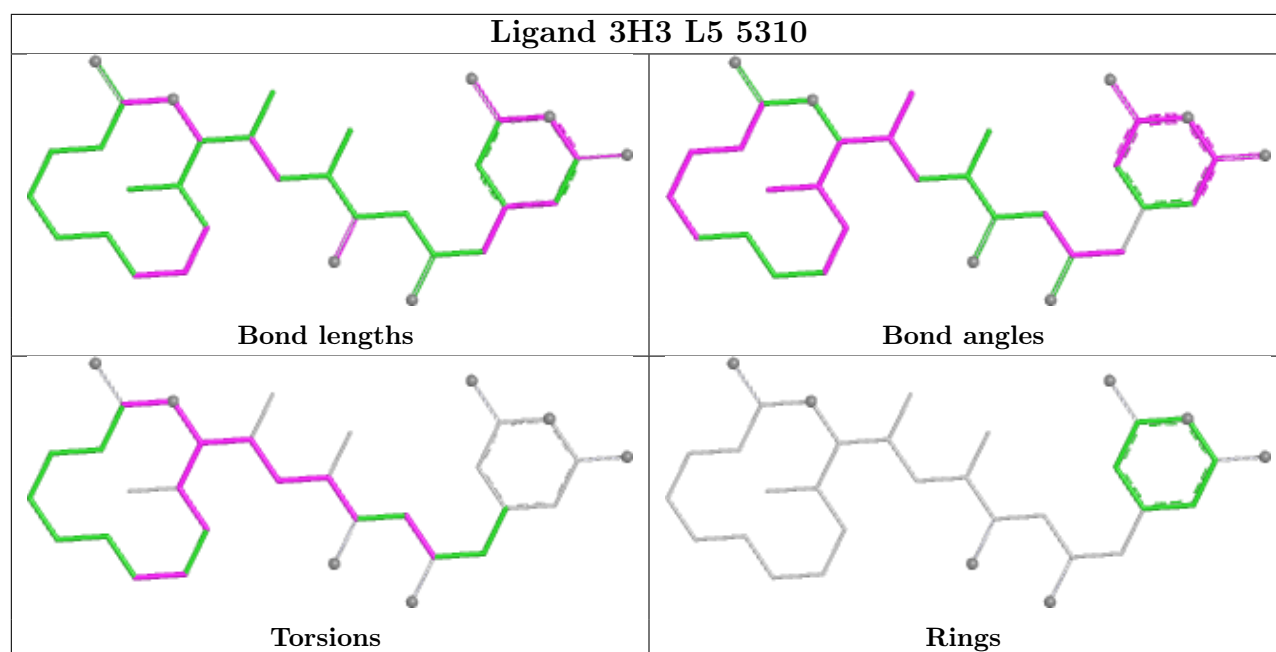
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5304	SPD	1	0
88	L5	5301	ANM	1	0
89	L5	5302	SPD	1	0
90	L5	5310	3H3	3	0

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.

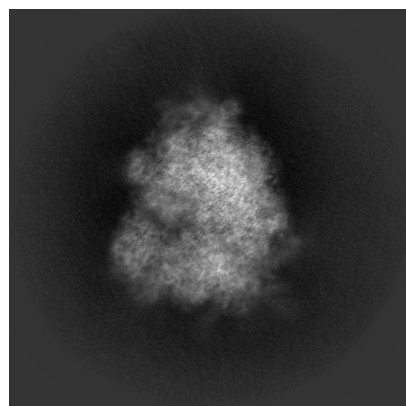
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29760. These allow visual inspection of the internal detail of the map and identification of artifacts.

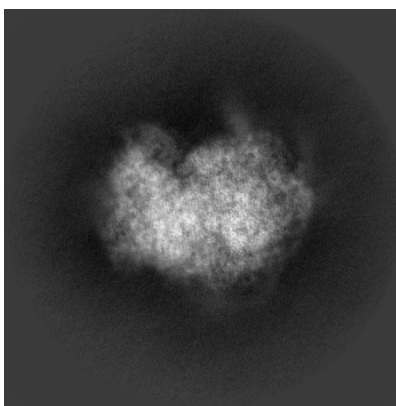
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

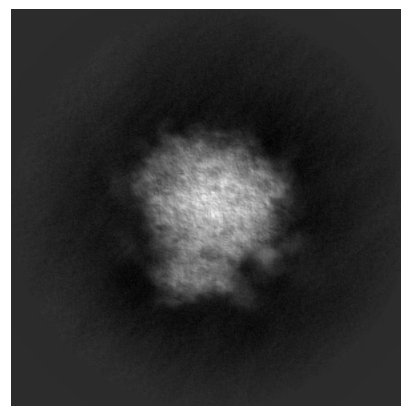
6.1.1 Primary map



X

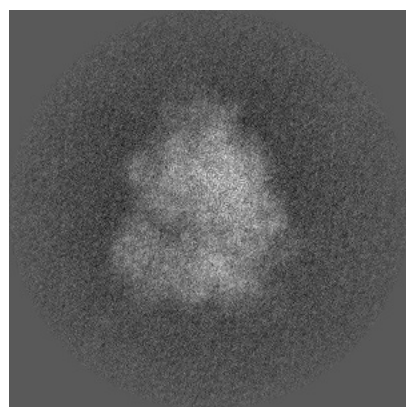


Y

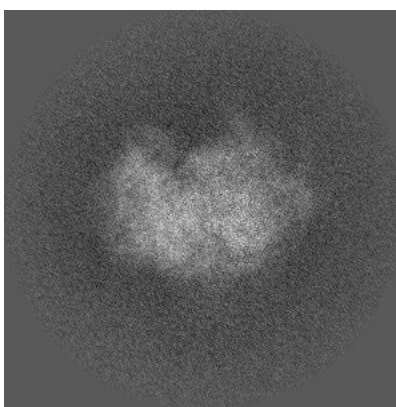


Z

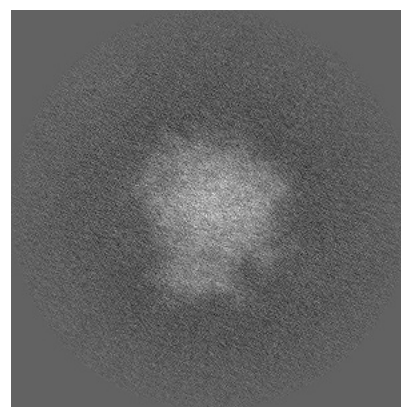
6.1.2 Raw map



X



Y

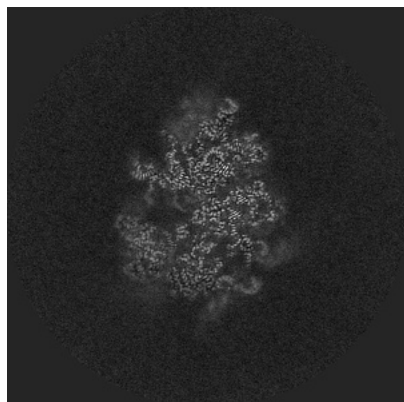


Z

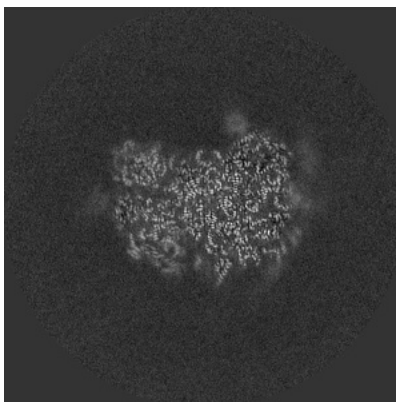
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

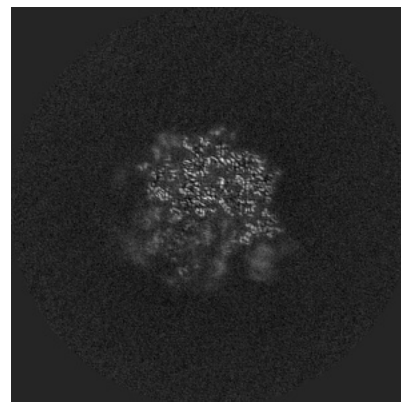
6.2.1 Primary map



X Index: 320

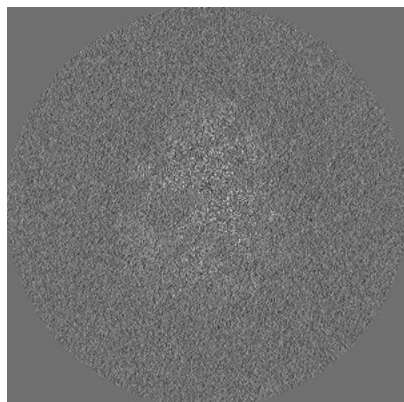


Y Index: 320

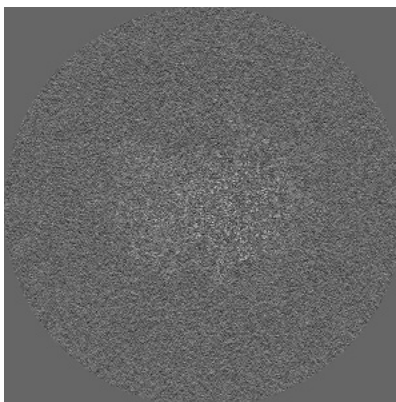


Z Index: 320

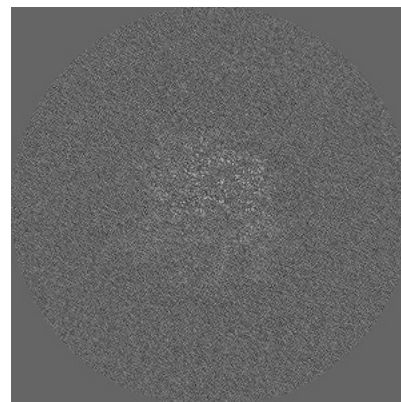
6.2.2 Raw map



X Index: 320



Y Index: 320

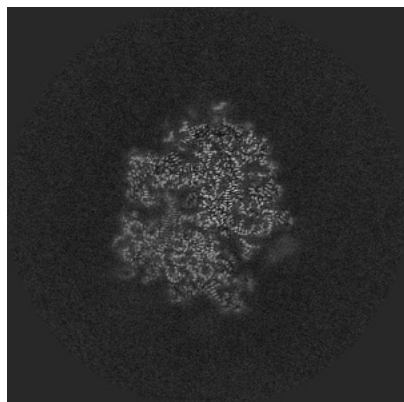


Z Index: 320

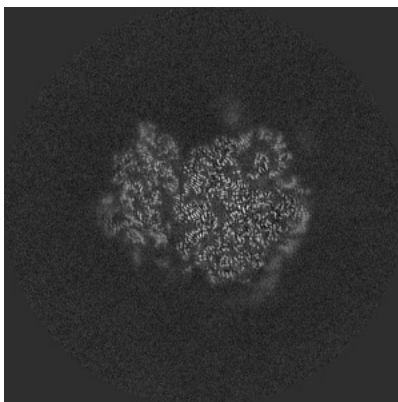
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

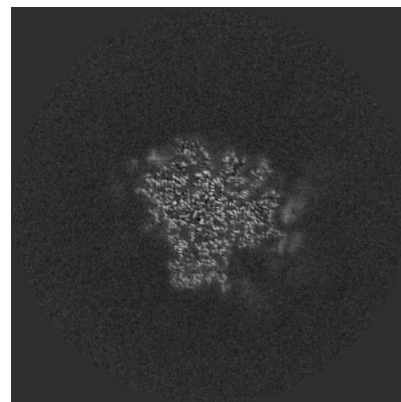
6.3.1 Primary map



X Index: 298

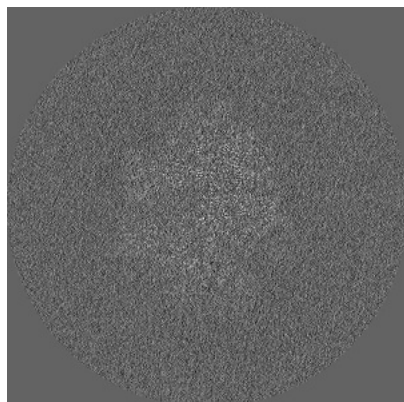


Y Index: 341

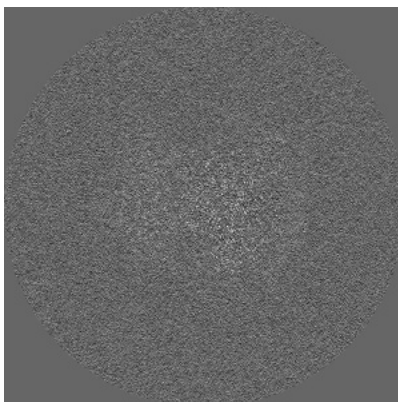


Z Index: 376

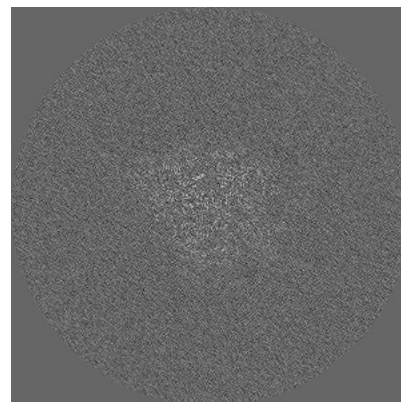
6.3.2 Raw map



X Index: 304



Y Index: 332

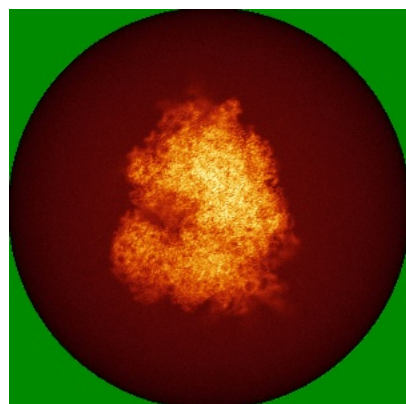


Z Index: 355

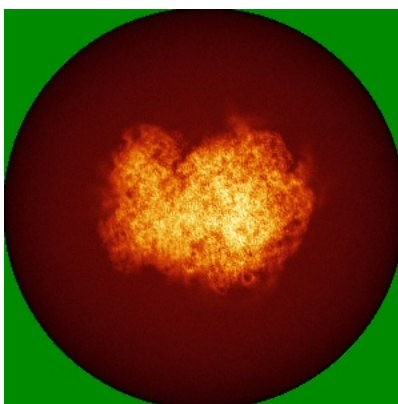
The images above show the largest variance slices of the map in three orthogonal directions.

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

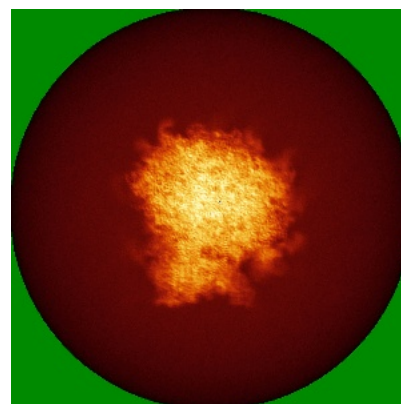
6.4.1 Primary map



X

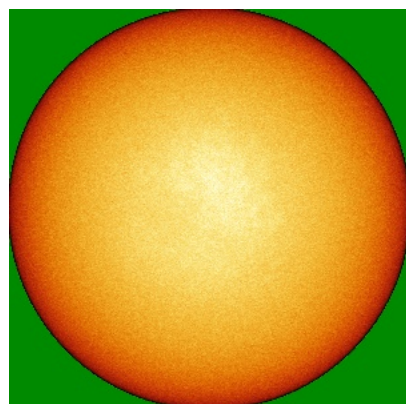


Y

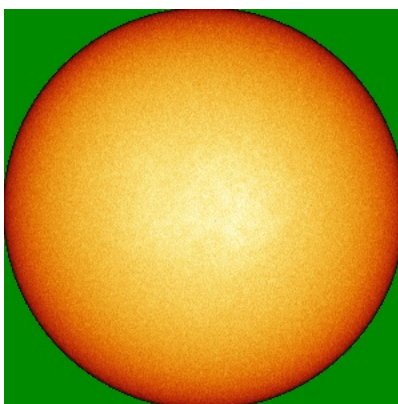


Z

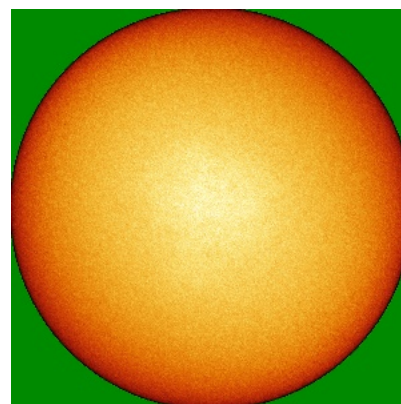
6.4.2 Raw map



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



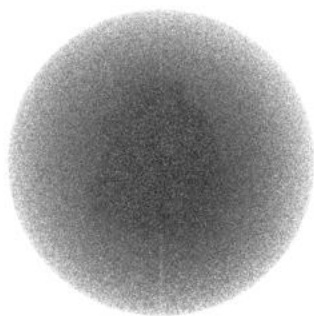
Y



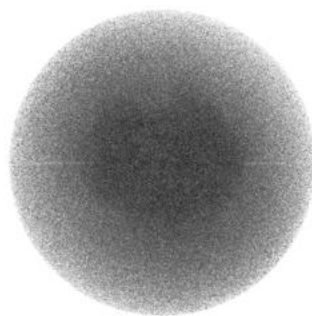
Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

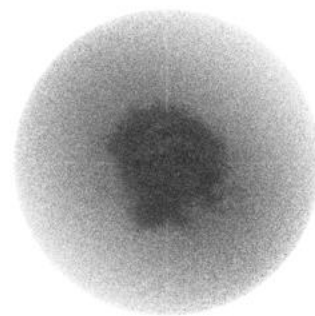
6.5.2 Raw map



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.

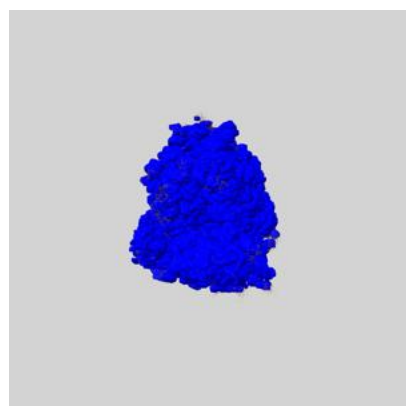
6.6 Mask visualisation [i](#)

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

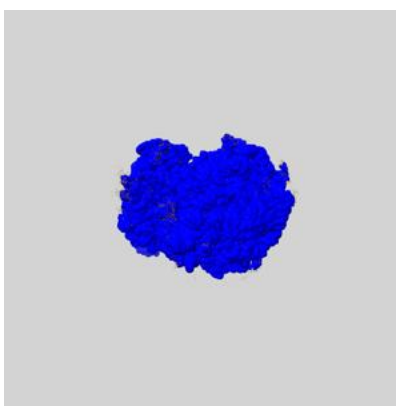
A mask typically either:

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

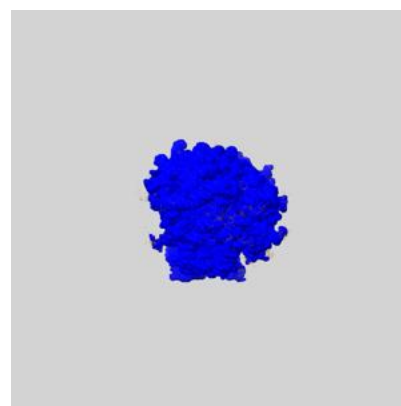
6.6.1 emd_29760_msk_1.map [i](#)



X



Y

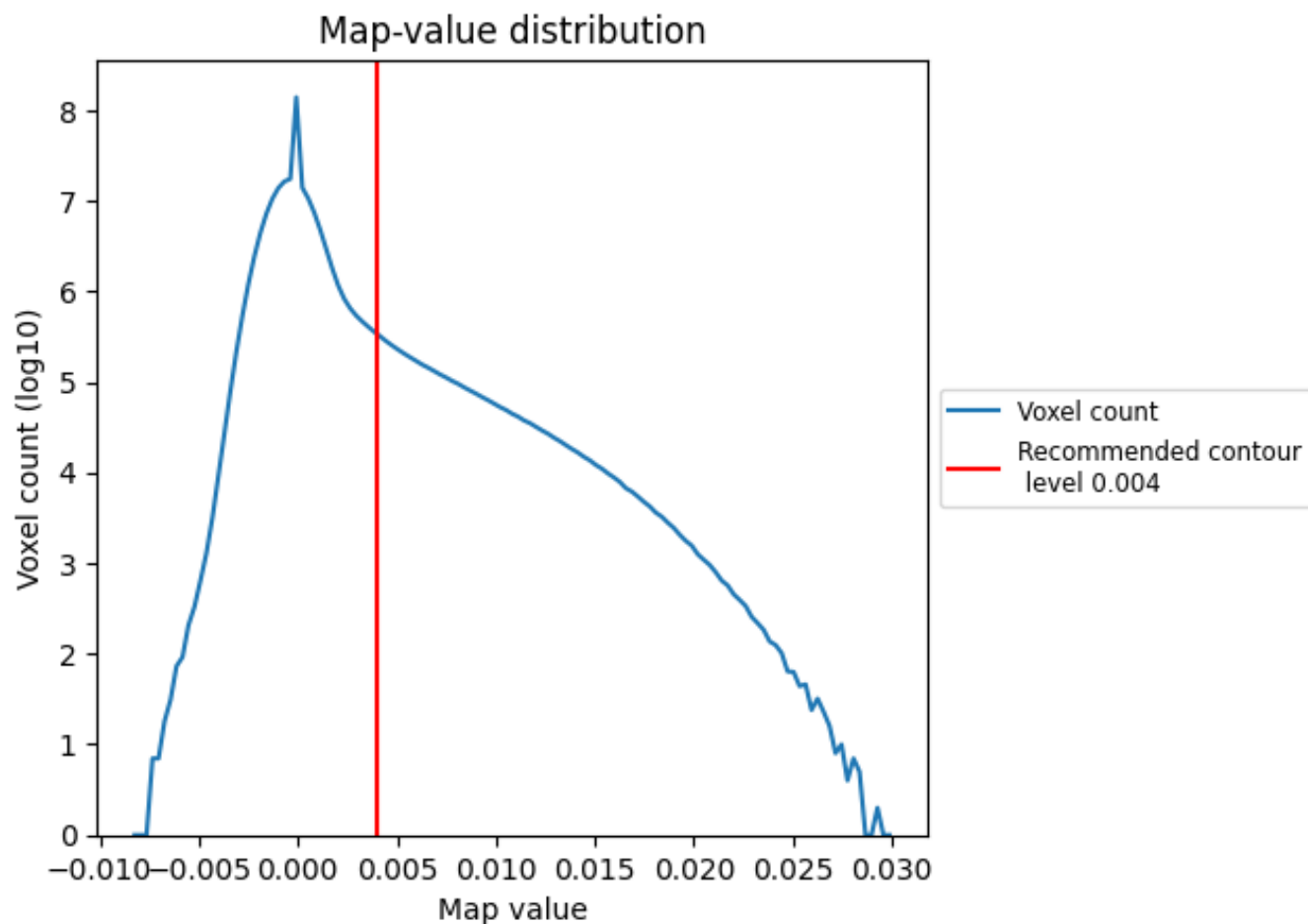


Z

7 Map analysis [i](#)

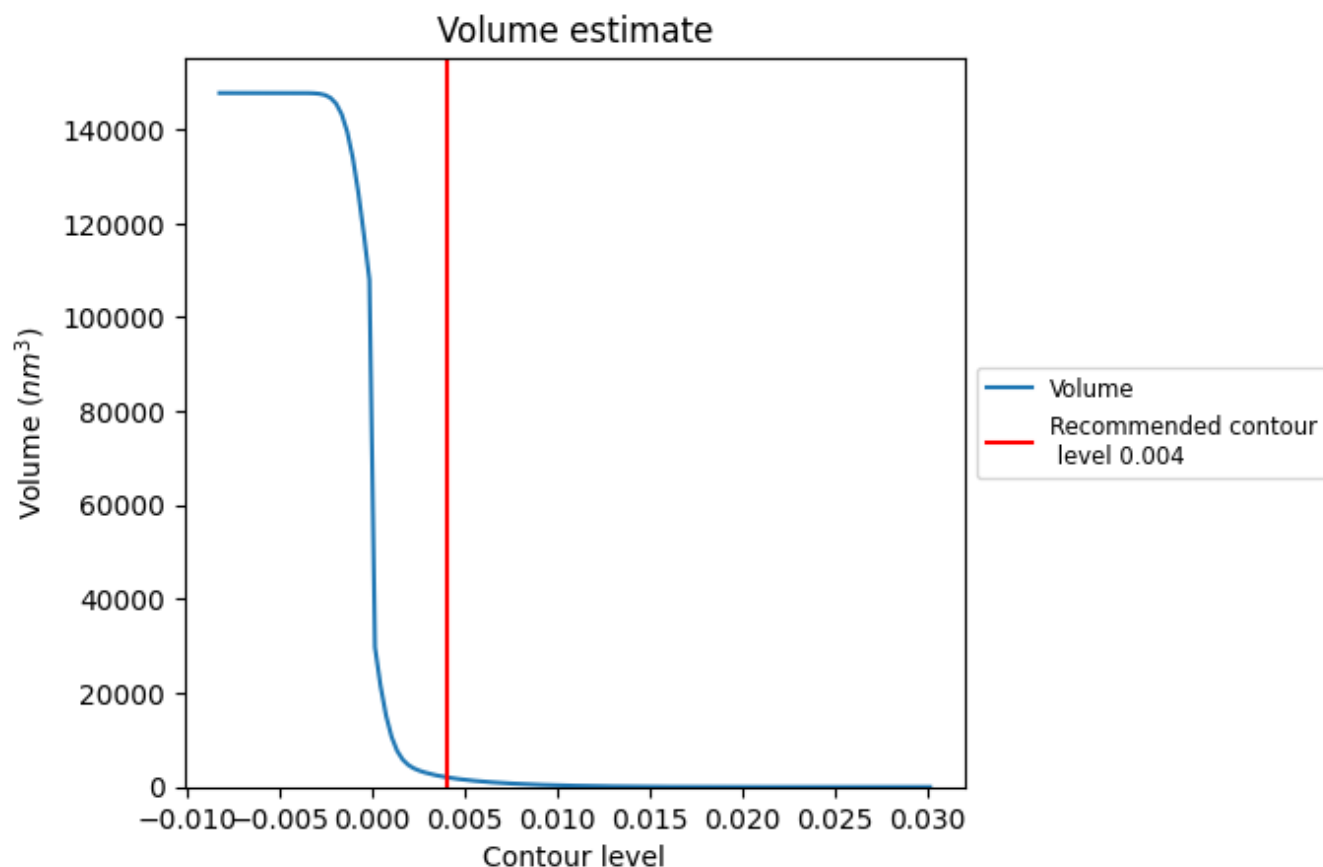
This section contains the results of statistical analysis of the map.

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.

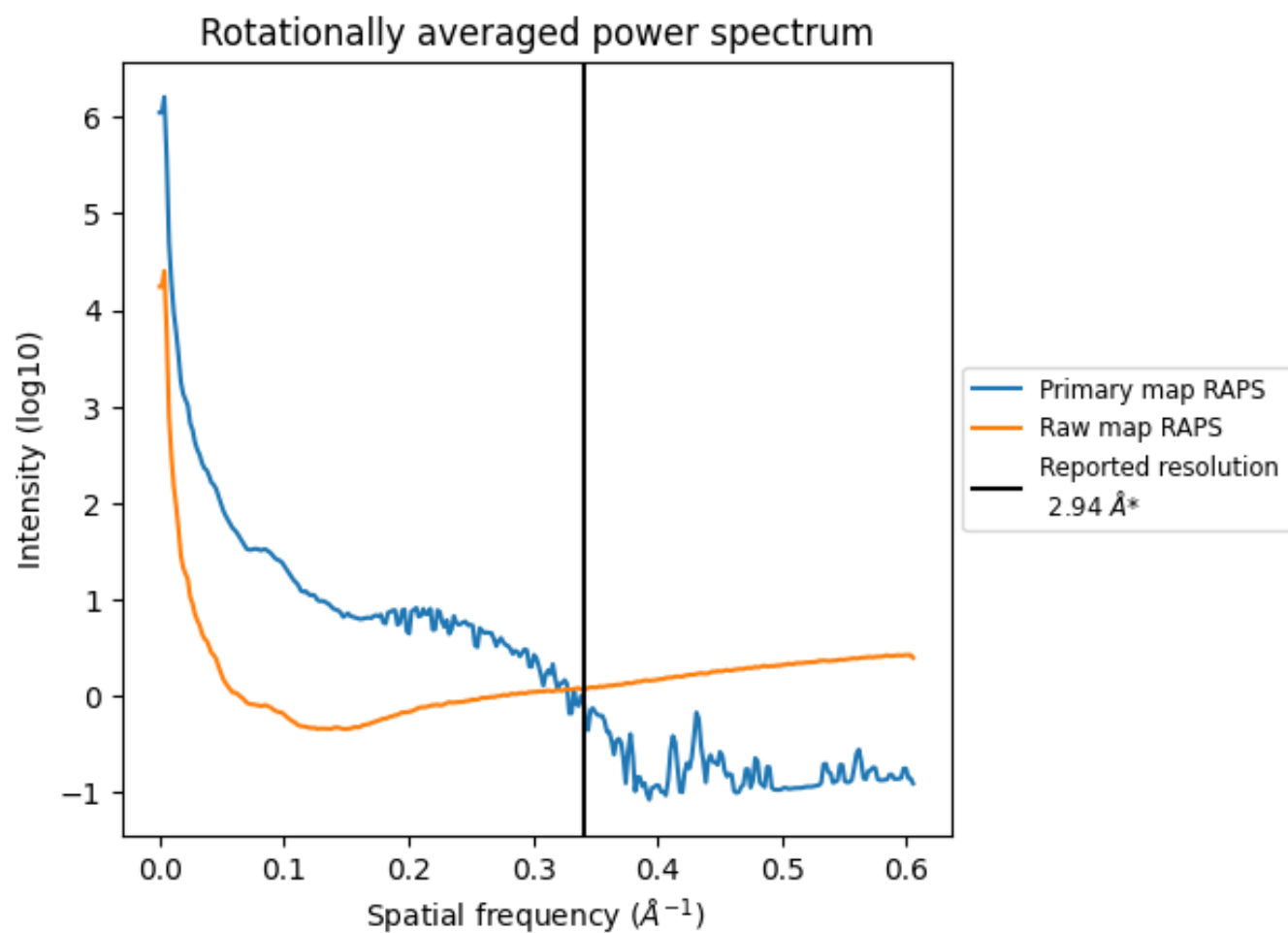
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2088 nm^3 ; this corresponds to an approximate mass of 1886 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

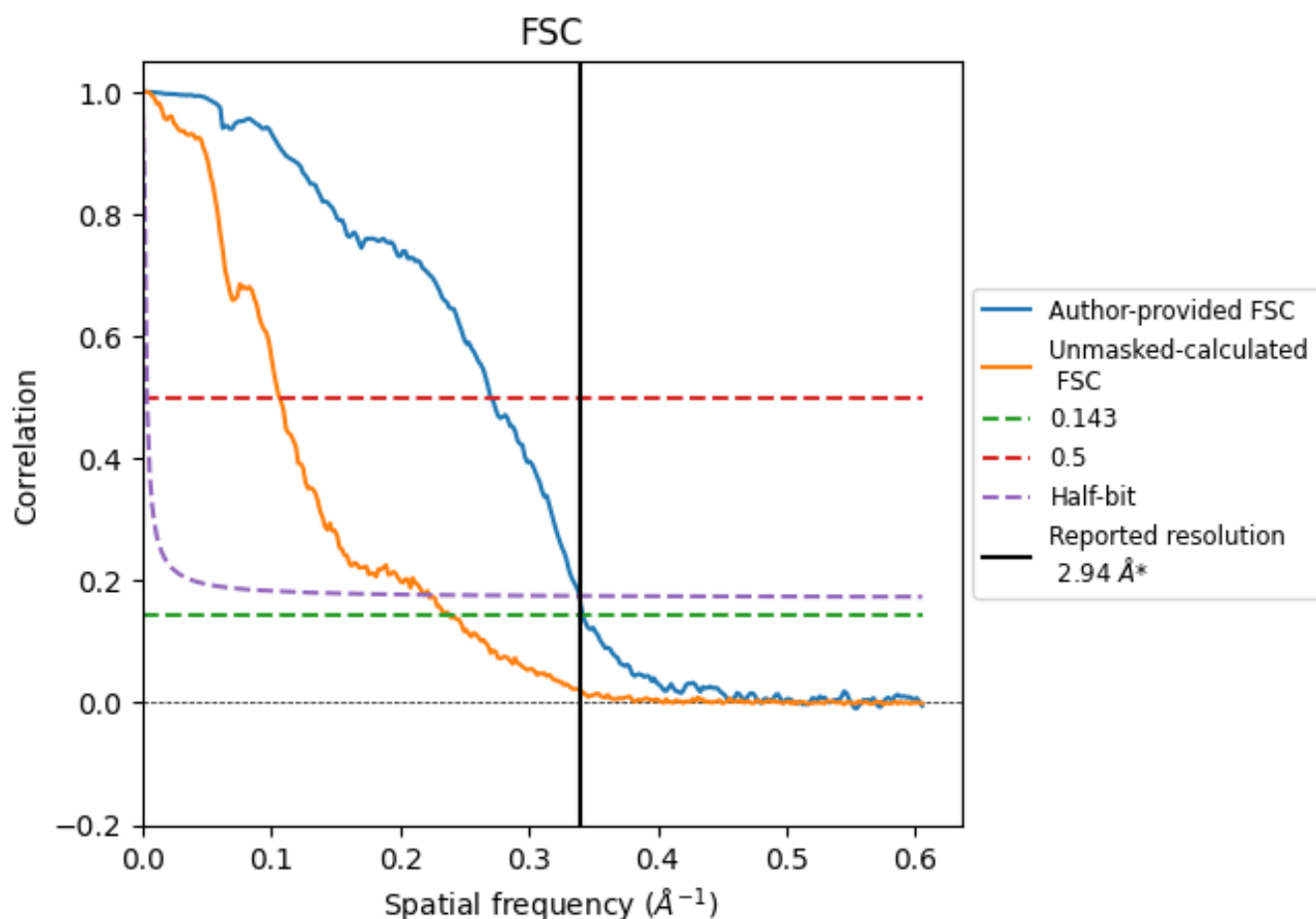


*Reported resolution corresponds to spatial frequency of 0.340 Å⁻¹

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 0.340 Å⁻¹

8.2 Resolution estimates [i](#)

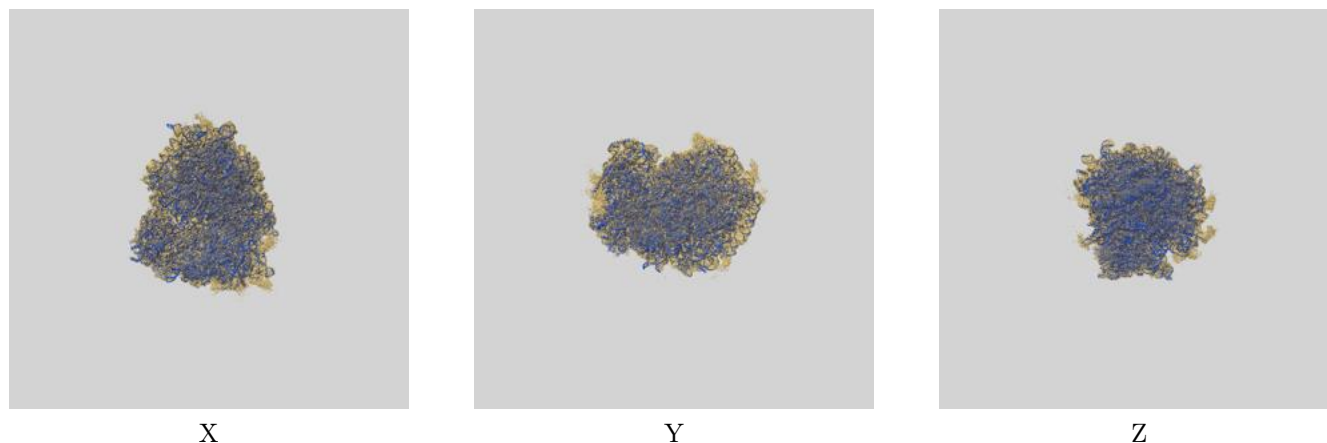
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.92	3.70	2.95
Unmasked-calculated*	4.19	9.40	4.56

*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 4.19 differs from the reported value 2.94 by more than 10 %

9 Map-model fit [i](#)

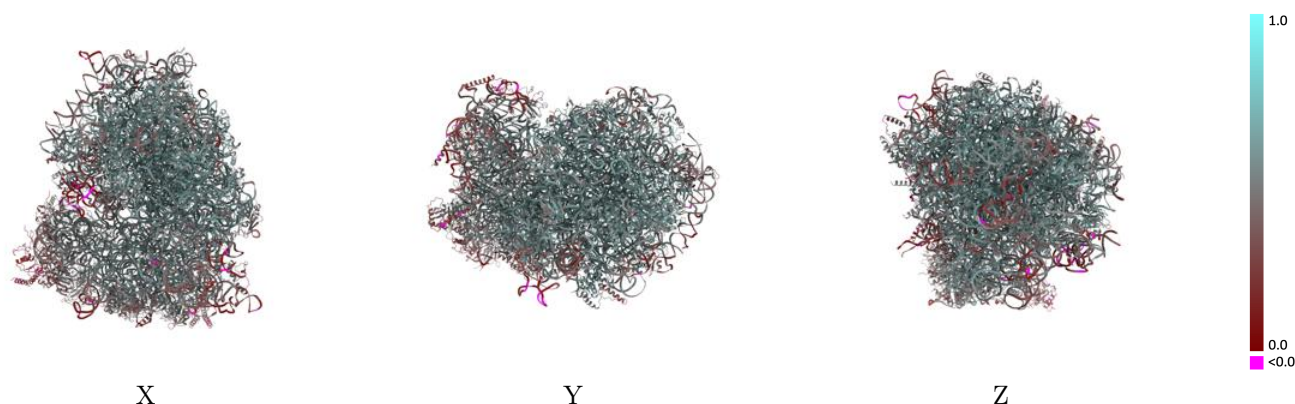
This section contains information regarding the fit between EMDB map EMD-29760 and PDB model 8G61. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



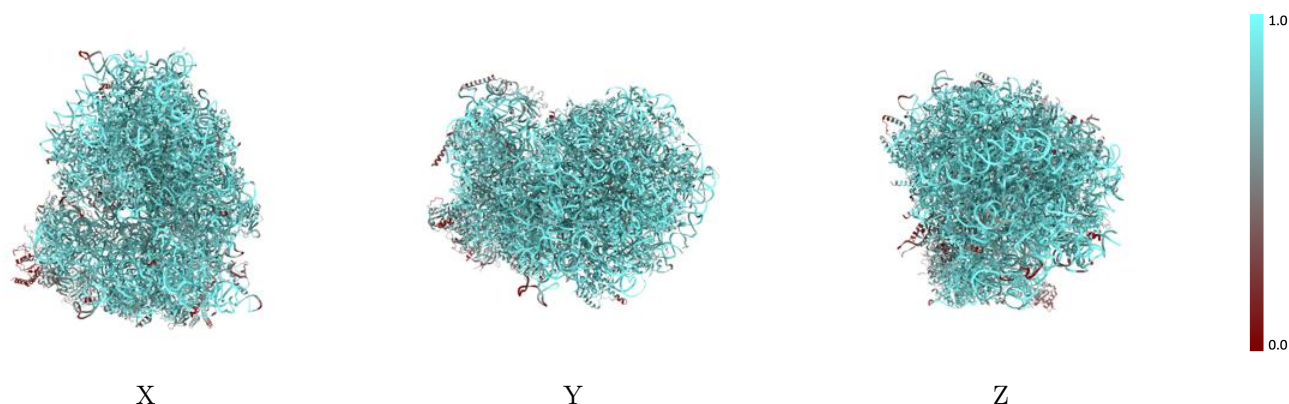
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



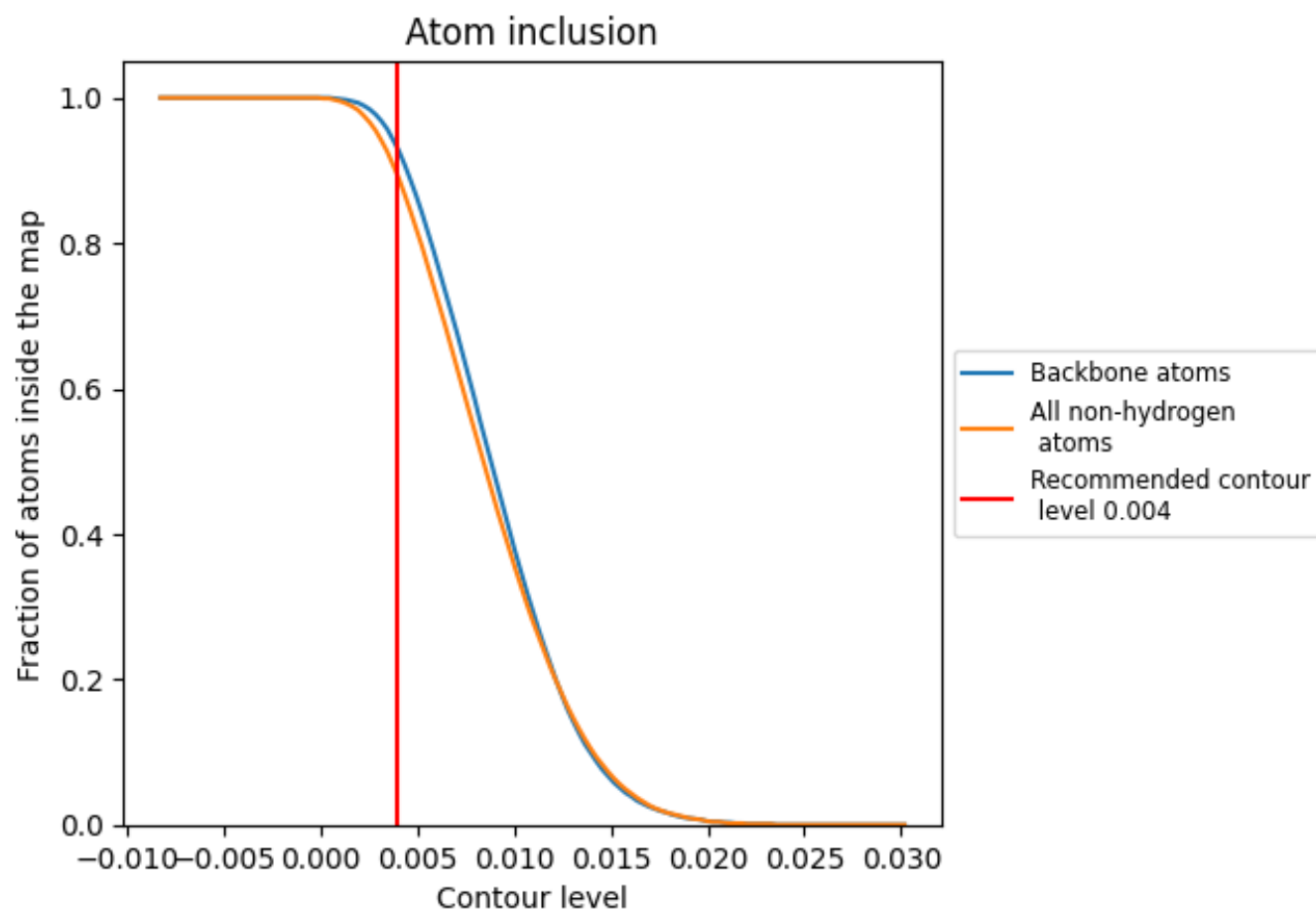
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.5100
5A	 0.5460	 0.4450
At	 0.7180	 0.4270
L5	 0.9520	 0.5290
L7	 0.9880	 0.5760
L8	 0.9810	 0.5630
LA	 0.9410	 0.6010
LB	 0.9020	 0.5770
LC	 0.9140	 0.5770
LD	 0.8790	 0.5230
LE	 0.8720	 0.5410
LF	 0.9250	 0.5730
LG	 0.8020	 0.5020
LH	 0.8690	 0.5390
LI	 0.9030	 0.5570
LJ	 0.8250	 0.4720
LL	 0.8800	 0.5470
LM	 0.9020	 0.5500
LN	 0.9780	 0.6100
LO	 0.9230	 0.5770
LP	 0.9300	 0.5920
LQ	 0.9490	 0.6050
LR	 0.8470	 0.5160
LS	 0.9470	 0.5870
LT	 0.9130	 0.5760
LU	 0.8020	 0.4820
LV	 0.9250	 0.5810
LW	 0.6940	 0.4220
LX	 0.9190	 0.5650
LY	 0.9030	 0.5590
LZ	 0.8770	 0.5350
La	 0.9510	 0.6000
Lb	 0.8060	 0.4950
Lc	 0.8410	 0.5400
Ld	 0.8890	 0.5550



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Chain	Atom inclusion	Q-score
Le	 0.9630	 0.6070
Lf	 0.9530	 0.6030
Lg	 0.8900	 0.5680
Lh	 0.8860	 0.5450
Li	 0.8860	 0.5270
Lj	 0.9670	 0.6080
Lk	 0.8060	 0.5110
Ll	 0.9310	 0.5630
Lm	 0.8990	 0.5580
Ln	 0.9380	 0.5690
Lo	 0.9010	 0.5670
Lp	 0.9000	 0.5740
Lr	 0.9190	 0.5810
Lz	 0.3610	 0.3050
Pt	 0.8110	 0.4480
S2	 0.9560	 0.4870
SA	 0.7540	 0.4380
SB	 0.7030	 0.3990
SC	 0.8190	 0.4990
SD	 0.7200	 0.4450
SE	 0.8250	 0.4810
SF	 0.7770	 0.4490
SG	 0.7270	 0.4140
SH	 0.6270	 0.3820
SI	 0.8160	 0.4800
SJ	 0.7940	 0.4410
SK	 0.7110	 0.4050
SL	 0.8550	 0.5270
SM	 0.1570	 0.1880
SN	 0.8120	 0.4880
SO	 0.7690	 0.4310
SP	 0.7300	 0.3990
SQ	 0.8200	 0.4540
SR	 0.6540	 0.3790
SS	 0.7660	 0.4380
ST	 0.8360	 0.4680
SU	 0.7440	 0.4190
SV	 0.7760	 0.4720
SW	 0.8770	 0.5250
SX	 0.9010	 0.5380
SY	 0.7510	 0.4040
SZ	 0.6240	 0.4100

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Chain	Atom inclusion	Q-score
Sa	 0.8520	 0.4810
Sb	 0.7210	 0.4450
Sc	 0.7030	 0.4220
Sd	 0.9220	 0.5000
Se	 0.7780	 0.4480
Sf	 0.4000	 0.2380
Sg	 0.5670	 0.3550
mR	 0.9710	 0.5440