wwPDB EM Validation Summary Report (i)

Jul 2, 2024 – 04:00 PM JST

PDB ID	:	8XSZ
EMDB ID	:	EMD-38631
Title	:	Cryo-EM structure of the human 80S ribosome with Tigecycline, E-tRNA and P-tRNA
Authors	:	Li, X.; Wang, M.; Cheng, J.
Deposited on	:	2024-01-10
Resolution	:	3.20 Å(reported)
Based on initial model	:	6Z6M

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 (i) 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 (i)) were used in the production of this report:

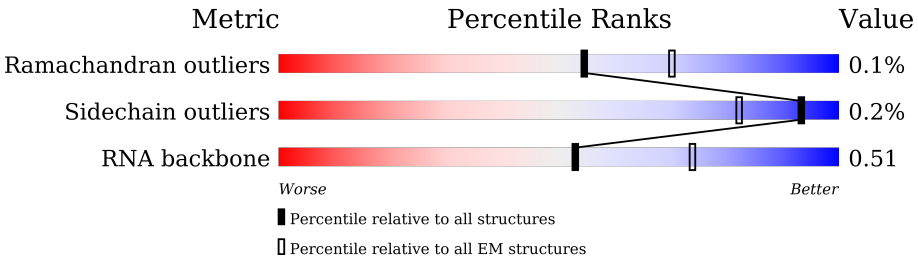
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	L5	5070	55% 17% 28%
2	L7	121	87% 12%
3	L8	157	83% 16%
4	LA	257	96%
5	LB	403	98%
6	LC	427	86% 14%
7	LD	297	99%
8	LE	288	77% 23%

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Mol	Chain	Length	Quality of chain
9	LF	248	90% 9%
10	LG	266	8% 90% 9%
11	LH	192	98%
12	LI	214	93% 6%
13	LJ	178	6% 99%
14	LL	211	99%
15	LM	215	63% 35%
16	LN	204	99%
17	LO	203	98%
18	LP	184	82% 17%
19	LQ	188	99%
20	LR	196	9% 95% 5%
21	LS	176	99%
22	LT	160	99%
23	LU	128	77% 22%
24	LV	140	94% 6%
25	LW	157	25% 75% 25%
26	LX	156	76% 23%
27	LY	145	92% 8%
28	LZ	136	99%
29	La	148	99%
30	Lb	159	8% 68% 31%
31	Lc	115	5% 85% 15%
32	Ld	125	86% 14%
33	Le	135	95% 5%

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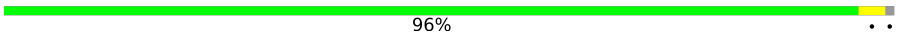
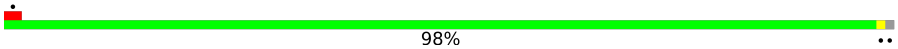
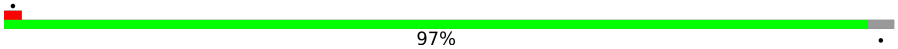
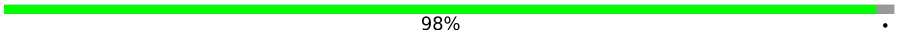
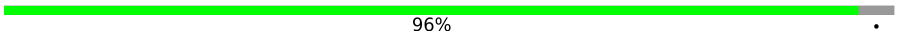
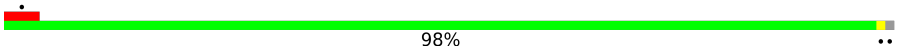
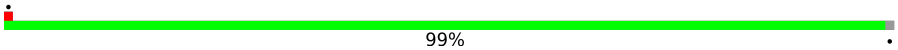
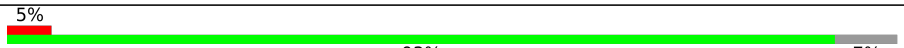
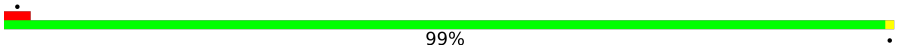
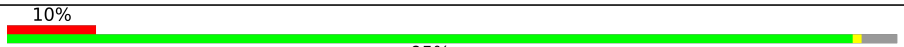
Mol	Chain	Length	Quality of chain
34	Lf	110	
35	Lg	117	
36	Lh	123	
37	Li	105	
38	Lj	97	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	
46	Ls	317	
47	Lt	165	
48	S2	1869	
49	SA	295	
50	SB	264	
51	SD	243	
52	SE	263	
53	SF	204	
54	SH	194	
55	SI	208	
56	SK	165	
57	SL	158	
58	SP	145	

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Mol	Chain	Length	Quality of chain
59	SQ	146	6% 98%
60	SR	135	100%
61	SS	152	93% 5%
62	ST	145	98%
63	SU	119	8% 86% 13%
64	SV	83	99%
65	SX	143	97%
66	Sa	115	5% 88% 11%
67	Sc	69	14% 93% 7%
68	Sd	56	98%
69	Sg	317	9% 97%
70	SC	293	75% 24%
71	SG	249	12% 95% 5%
72	SJ	194	7% 92% 5%
73	SM	132	37% 89% 8%
74	SN	151	99%
75	SO	151	89% 11%
76	SW	130	99%
77	SY	133	9% 93% 5%
78	SZ	125	6% 58% 40%
79	Sb	84	5% 98%
80	Se	59	20% 97%
81	Sf	156	12% 40% 57%
82	CA	394	90% 90% 10%
83	CB	408	96%

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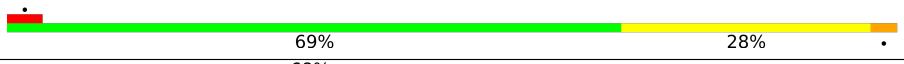
Mol	Chain	Length	Quality of chain
84	CC	75	
84	CD	75	
85	CE	11	

2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 222841 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 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L5	3668	78633	35016	14390	25560	3667	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L5	2113	C	G	conflict	GB 86475748

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L7	120	2561	1141	456	844	120	0	0

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L8	156	3314	1480	585	1094	155	0	0

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	LA	248	1898	1189	389	314	6	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	LB	402	3238	2060	608	556	14	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4.

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

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	221	Total	C	N	O	S	0	0
			1774	1142	336	292	4		

- Molecule 9 is a protein called 60S ribosomal protein L7.

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

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	202	Total	C	N	O	S	0	0
			1639	1041	316	269	13		

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 16 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 18 is a protein called 60S ribosomal protein L17.

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

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called 60S ribosomal protein L19.

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

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 22 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	100	Total	C	N	O	S	0	0
			816	524	142	148	2		

- Molecule 24 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	118	Total	C	N	O	S	0	0
			965	604	199	158	4		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 27 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LY	133	Total	C	N	O	S	0	0
			1106	694	224	185	3		

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 29 is a protein called 60S ribosomal protein L27a.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

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

- Molecule 35 is a protein called 60S ribosomal protein L34.

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

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

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

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

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

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 46 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ls	196	Total	C	N	O	S	0	0
			1496	952	259	276	9		

- Molecule 47 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lt	141	Total	C	N	O	S	0	0
			1046	652	191	199	4		

- Molecule 48 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S2	1740	Total	C	N	O	P	0	0
			36896	16458	6597	12102	1739		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	582	C	U	conflict	GB 36162
S2	583	C	A	conflict	GB 36162
S2	584	G	A	conflict	GB 36162
S2	798	A	G	conflict	GB 36162
S2	1095	U	C	conflict	GB 36162

- Molecule 49 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 50 is a protein called 40S ribosomal protein S3a.

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

- Molecule 51 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 52 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SF	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 54 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 55 is a protein called 40S ribosomal protein S8.

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

- Molecule 56 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SK	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

- Molecule 57 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SL	144	Total	C	N	O	S	0	0
			1182	752	224	200	6		

- Molecule 58 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SP	129	Total	C	N	O	S	0	0
			1061	672	202	180	7		

- Molecule 59 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 60 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 61 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 62 is a protein called 40S ribosomal protein S19.

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

- Molecule 63 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 64 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 65 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 66 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 67 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 68 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 69 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 70 is a protein called 40S ribosomal protein S2.

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

- Molecule 71 is a protein called 40S ribosomal protein S6.

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

- Molecule 72 is a protein called 40S ribosomal protein S9.

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

- Molecule 73 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SM	122	Total	C	N	O	S	0	0
			942	590	165	179	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	52	GLN	LEU	conflict	UNP P25398
SM	69	LEU	CYS	conflict	UNP P25398
SM	99	ASN	LYS	conflict	UNP P25398

- Molecule 74 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 75 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 76 is a protein called 40S ribosomal protein S15a.

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

- Molecule 77 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SY	126	Total	C	N	O	S	0	0
			1027	648	201	173	5		

- Molecule 78 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 79 is a protein called 40S ribosomal protein S27.

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

- Molecule 80 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 82 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	CA	354	Total	C	N	O	S	4	0
			2764	1744	475	528	17		

- Molecule 83 is a protein called SERPINE1 mRNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	CB	16	Total	C	N	O	S	0	0
			127	80	22	24	1		

- Molecule 84 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	CC	75	Total	C	N	O	P	0	0
			1607	717	298	517	75		
84	CD	75	Total	C	N	O	P	0	0
			1607	717	298	517	75		

- Molecule 85 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	CE	11	Total	C	N	O	P	0	0
			232	104	37	80	11		

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

Mol	Chain	Residues	Atoms		AltConf
86	L5	212	Total	Mg	0
			212	212	
86	L7	3	Total	Mg	0
			3	3	
86	L8	5	Total	Mg	0
			5	5	
86	LA	1	Total	Mg	0
			1	1	
86	LI	1	Total	Mg	0
			1	1	

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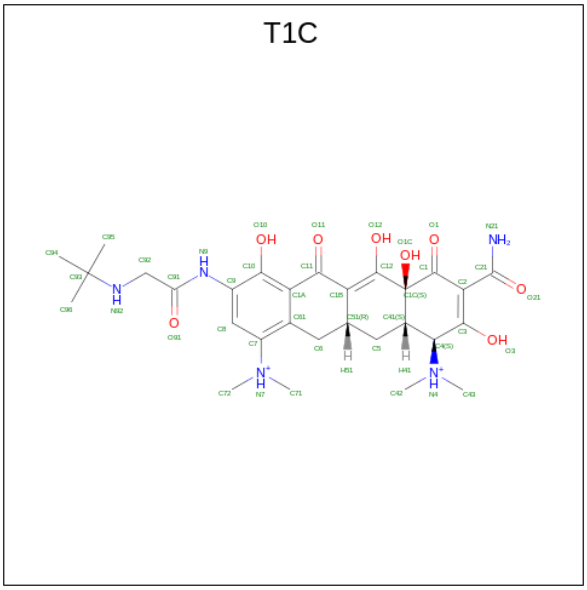
Mol	Chain	Residues	Atoms	AltConf
86	LP	1	Total Mg 1 1	0
86	LV	1	Total Mg 1 1	0
86	Le	1	Total Mg 1 1	0
86	Lg	1	Total Mg 1 1	0
86	Lj	1	Total Mg 1 1	0
86	S2	19	Total Mg 19 19	0
86	SI	1	Total Mg 1 1	0
86	SQ	1	Total Mg 1 1	0

- Molecule 87 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
87	L5	1	Total C N O 42 29 5 8	0
87	L5	1	Total C N O 42 29 5 8	0
87	L5	1	Total C N O 42 29 5 8	0

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Mol	Chain	Residues	Atoms				AltConf
87	L5	1	Total	C	N	O	0
			42	29	5	8	
87	L5	1	Total	C	N	O	0
			42	29	5	8	

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

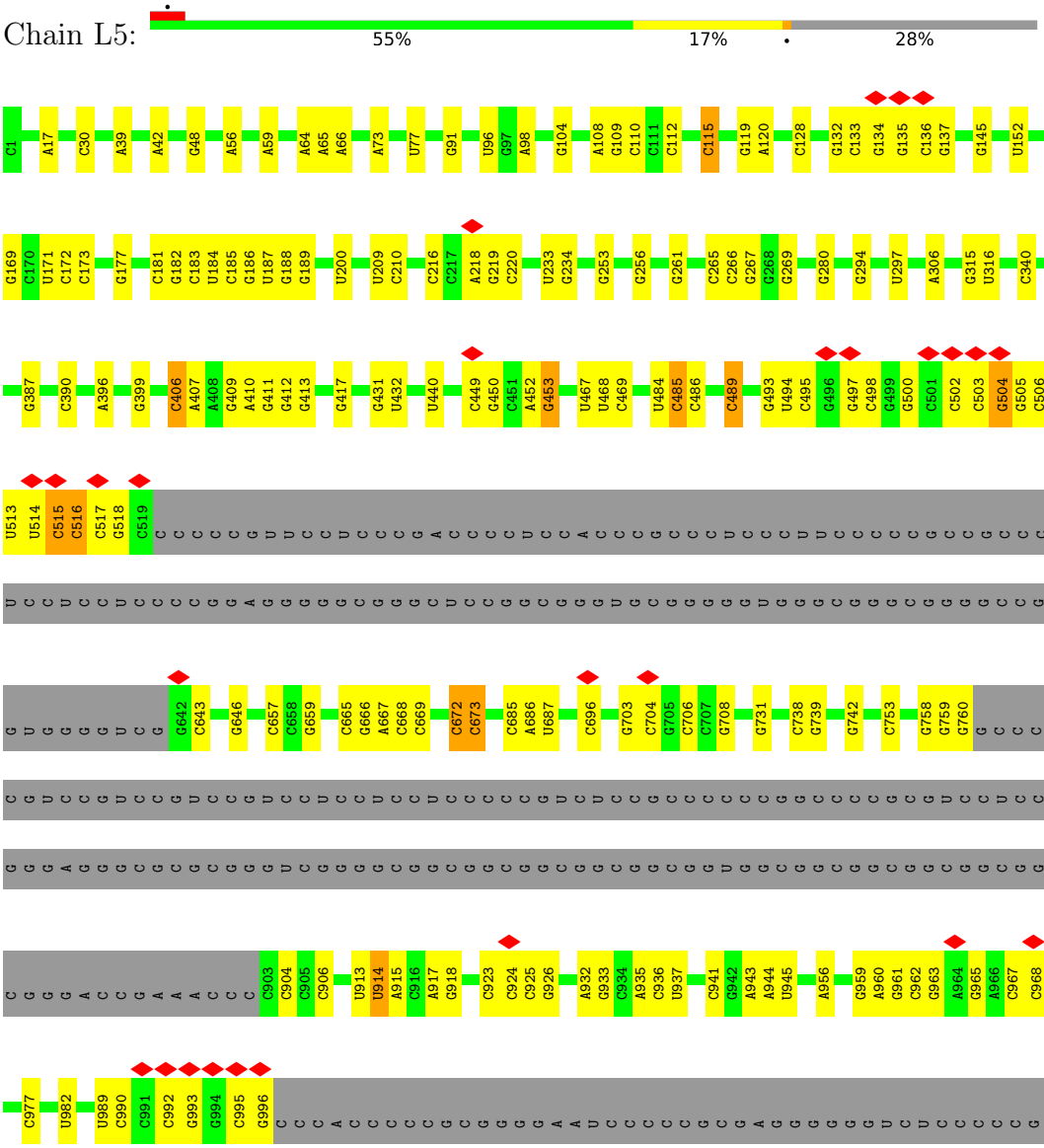
Mol	Chain	Residues	Atoms		AltConf
88	Lg	1	Total	Zn	0
			1	1	
88	Lj	1	Total	Zn	0
			1	1	
88	Lm	1	Total	Zn	0
			1	1	
88	Lo	1	Total	Zn	0
			1	1	
88	Lp	1	Total	Zn	0
			1	1	
88	S2	2	Total	Zn	0
			2	2	
88	SM	1	Total	Zn	0
			1	1	

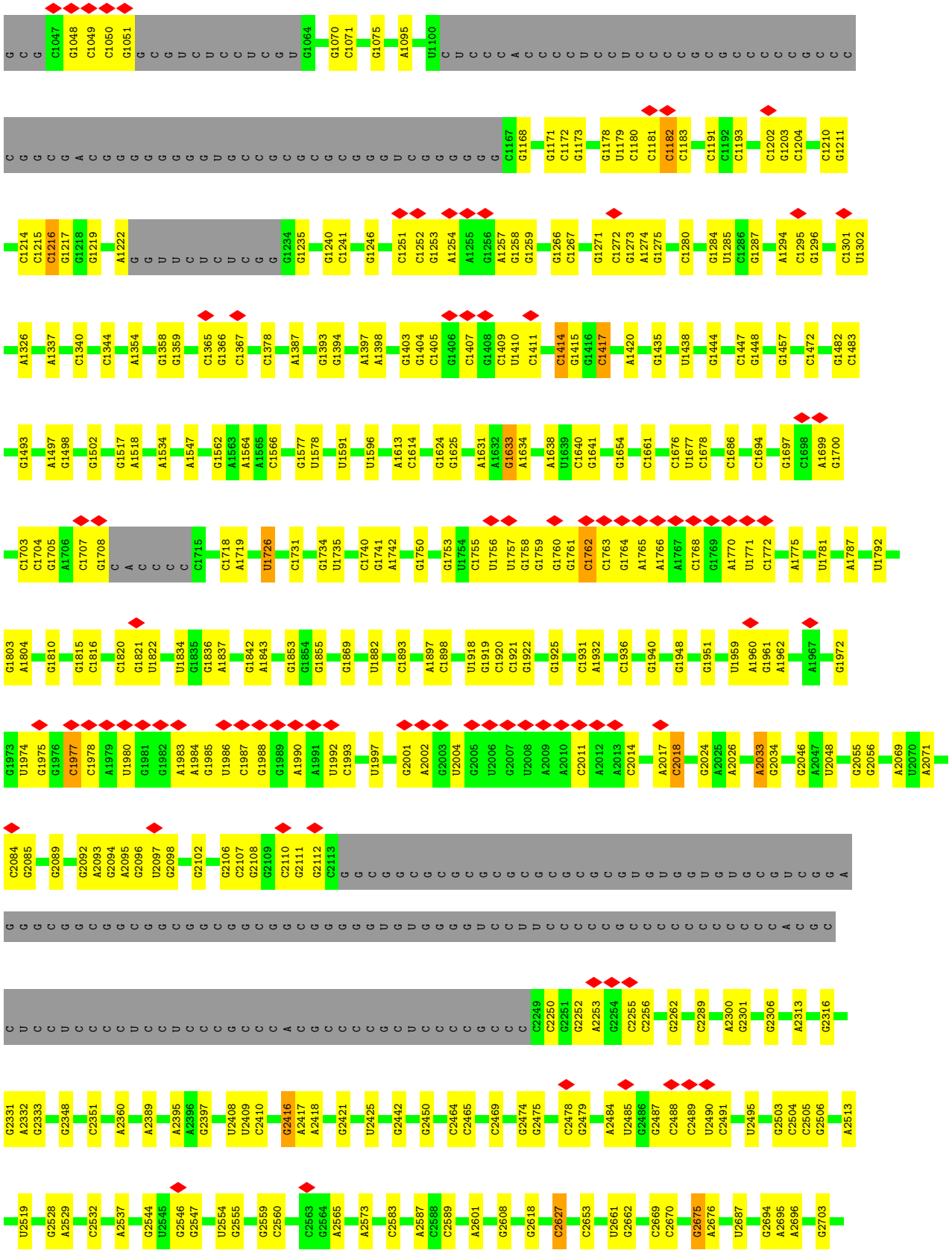
3 Residue-property plots (i)

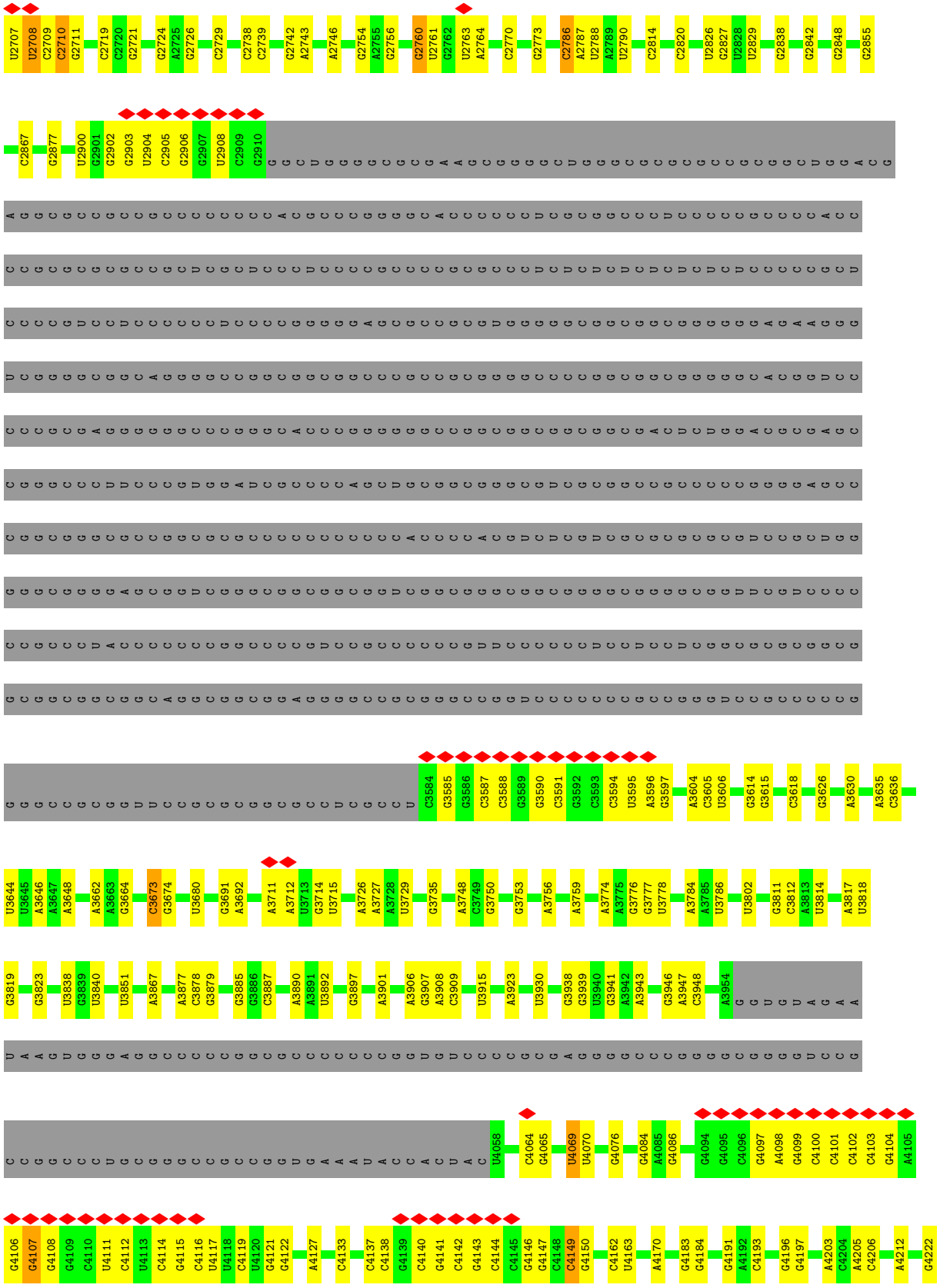
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

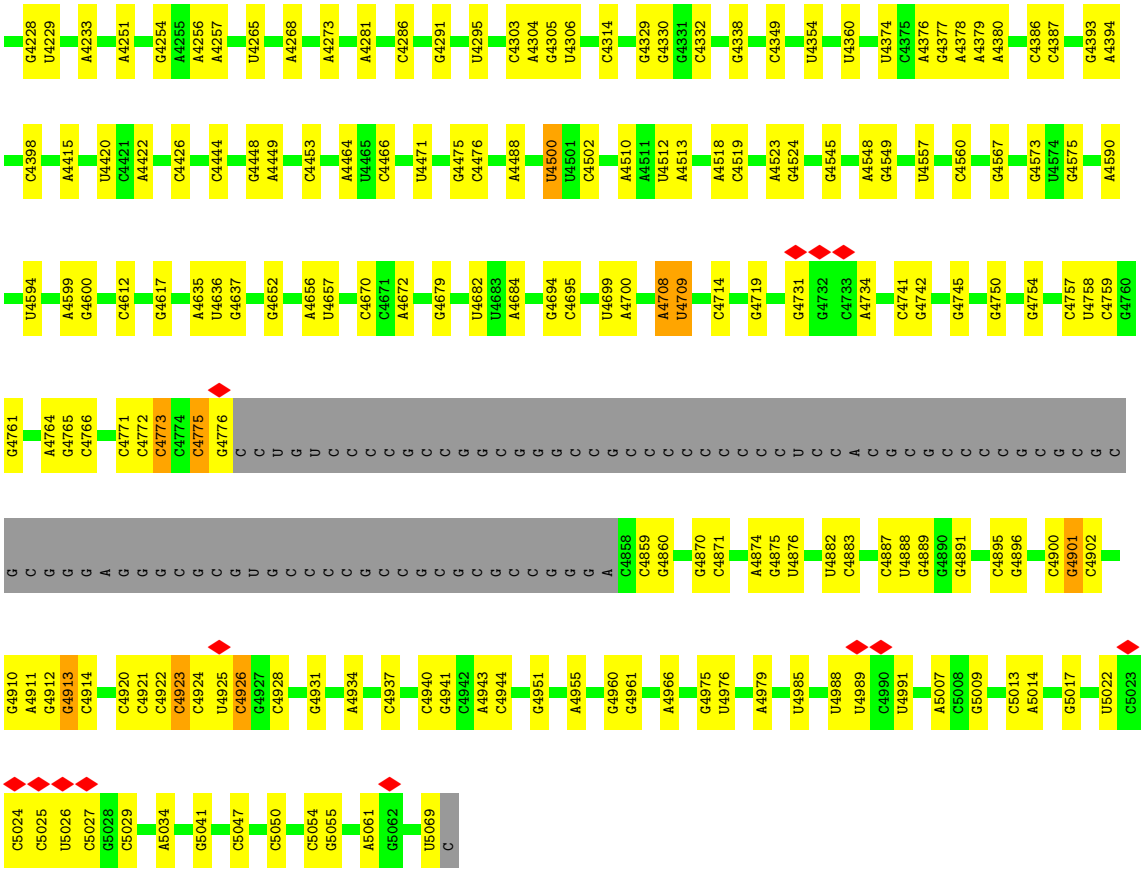
- Molecule 1: 28S rRNA

Chain L5:



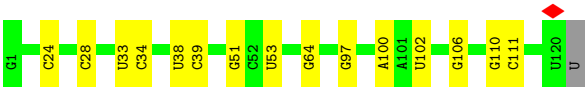






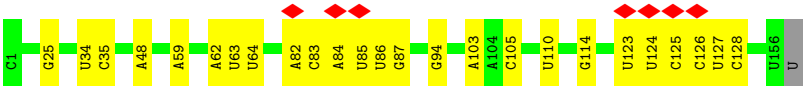
• Molecule 2: 5S rRNA

Chain L7:



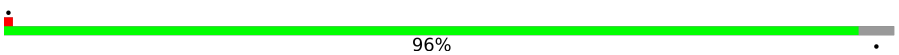
• Molecule 3: 5.8S rRNA

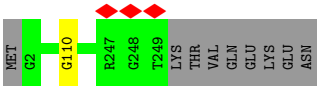
Chain L8:



• Molecule 4: 60S ribosomal protein L8

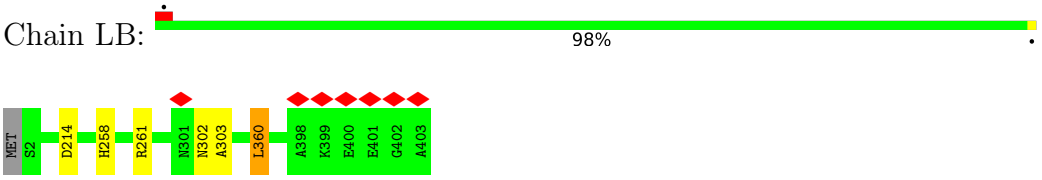
Chain LA:





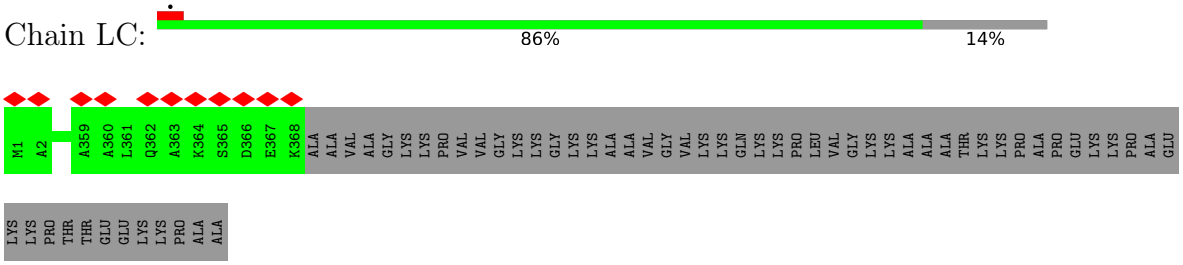
• Molecule 5: 60S ribosomal protein L3

Chain LB:



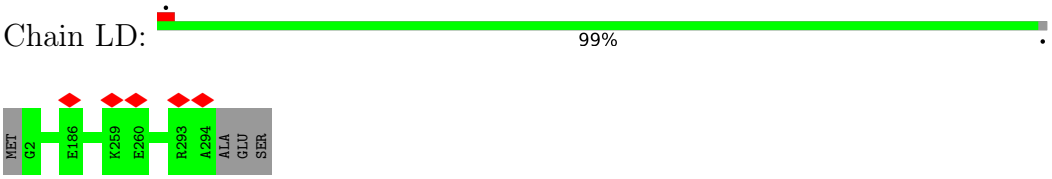
• Molecule 6: 60S ribosomal protein L4

Chain LC:



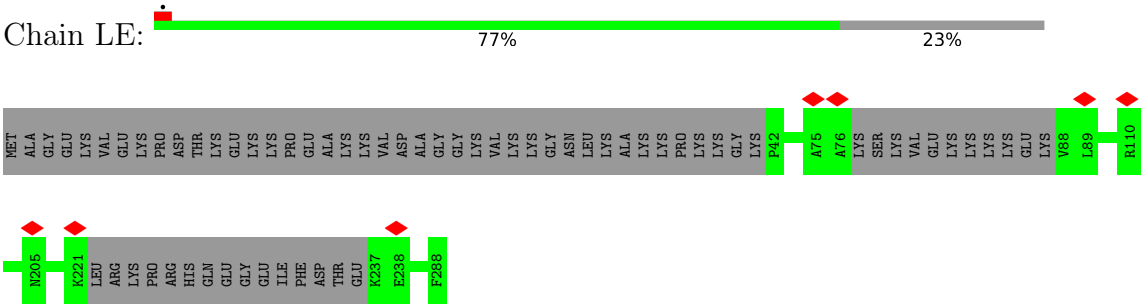
• Molecule 7: 60S ribosomal protein L5

Chain LD:



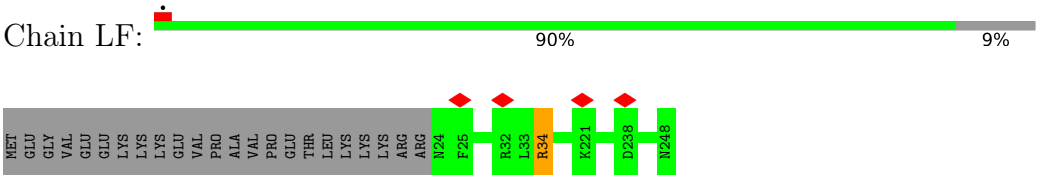
• Molecule 8: 60S ribosomal protein L6

Chain LE:



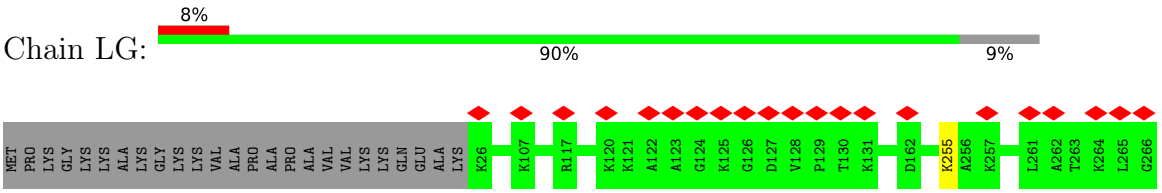
• Molecule 9: 60S ribosomal protein L7

Chain LF:



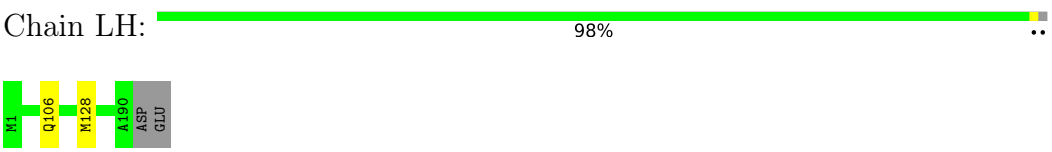
• Molecule 10: 60S ribosomal protein L7a

Chain LG:



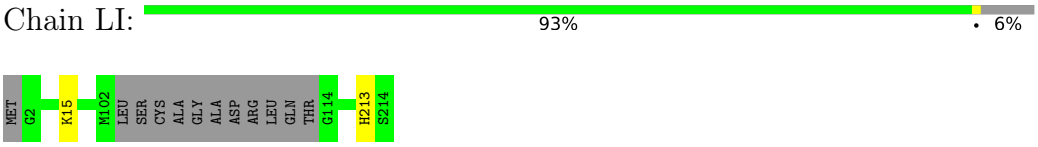
• Molecule 11: 60S ribosomal protein L9

Chain LH:



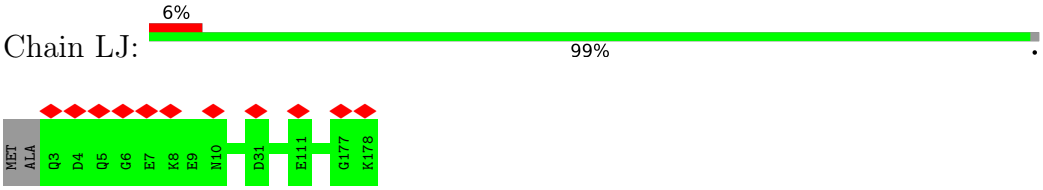
• Molecule 12: Large ribosomal subunit protein uL16

Chain LI:



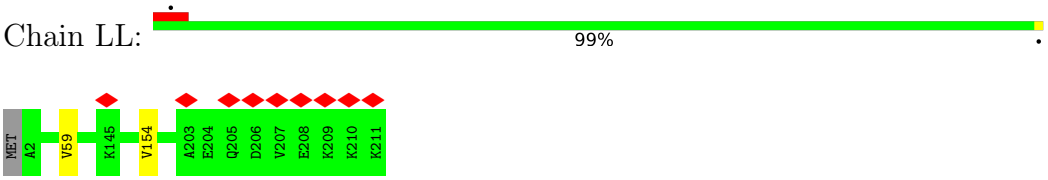
• Molecule 13: 60S ribosomal protein L11

Chain LJ:



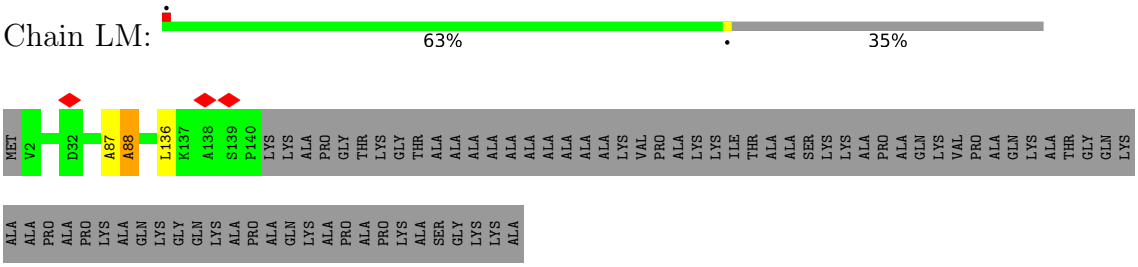
• Molecule 14: 60S ribosomal protein L13

Chain LL:



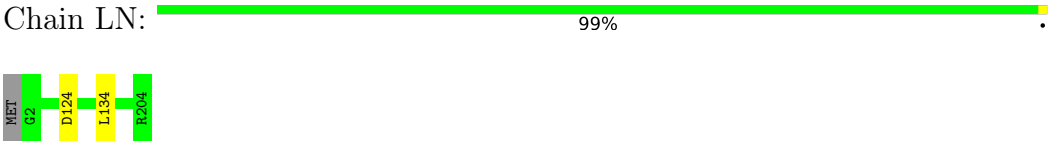
• Molecule 15: 60S ribosomal protein L14

Chain LM:



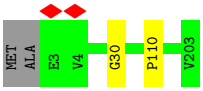
• Molecule 16: 60S ribosomal protein L15

Chain LN:



• Molecule 17: 60S ribosomal protein L13a

Chain LO:

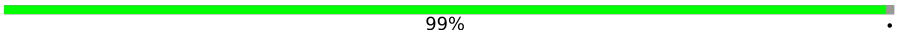


• Molecule 18: 60S ribosomal protein L17

Chain LP:

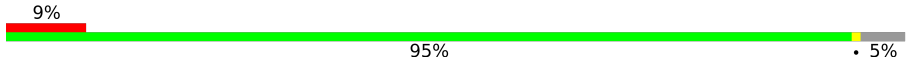
• Molecule 19: 60S ribosomal protein L18

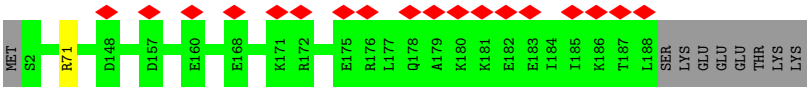
Chain LQ:



• Molecule 20: 60S ribosomal protein L19

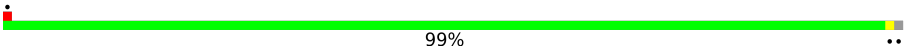
Chain LR:

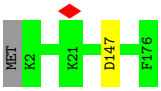




• Molecule 21: 60S ribosomal protein L18a

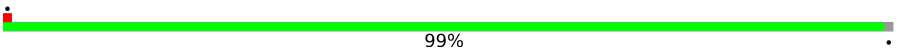
Chain LS:

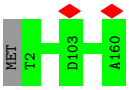




• Molecule 22: 60S ribosomal protein L21

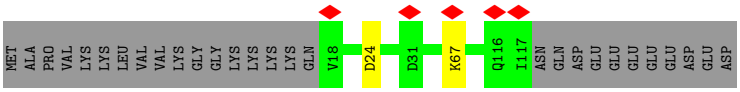
Chain LT:





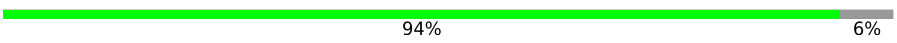
• Molecule 23: 60S ribosomal protein L22

Chain LU:



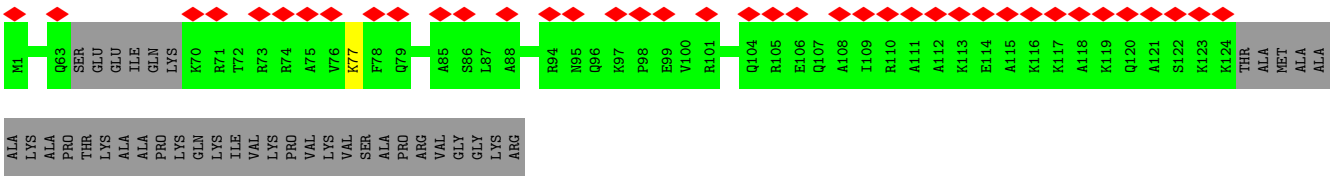
• Molecule 24: 60S ribosomal protein L23

Chain LV:



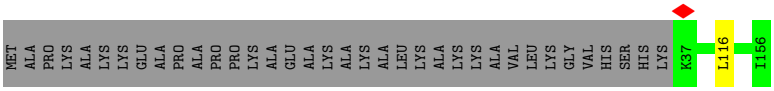
• Molecule 25: 60S ribosomal protein L24

Chain LW:



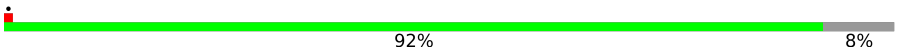
• Molecule 26: 60S ribosomal protein L23a

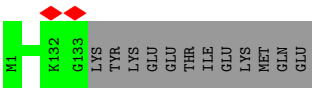
Chain LX:



• Molecule 27: 60S ribosomal protein L26

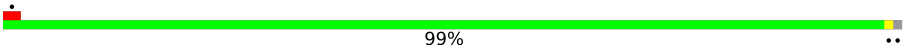
Chain LY:

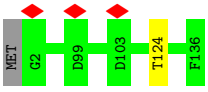




• Molecule 28: 60S ribosomal protein L27

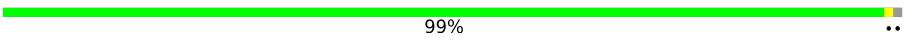
Chain LZ:

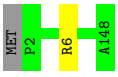




• Molecule 29: 60S ribosomal protein L27a

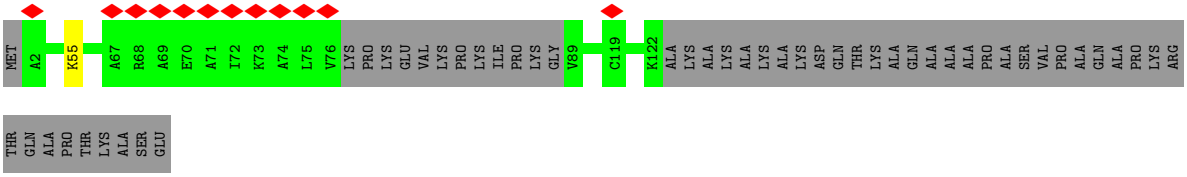
Chain La:



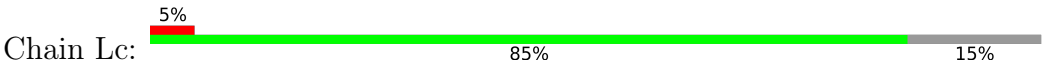


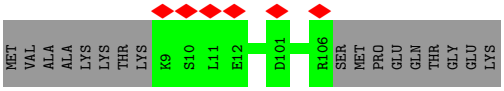
• Molecule 30: 60S ribosomal protein L29

Chain Lb:

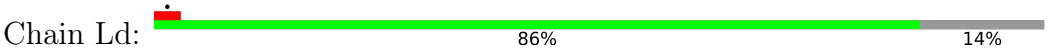


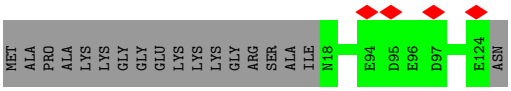
• Molecule 31: 60S ribosomal protein L30



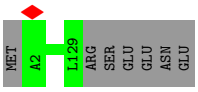


• Molecule 32: 60S ribosomal protein L31



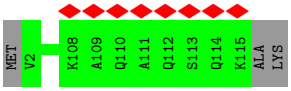


• Molecule 33: 60S ribosomal protein L32

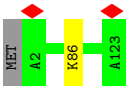


• Molecule 34: 60S ribosomal protein L35a

• Molecule 35: 60S ribosomal protein L34

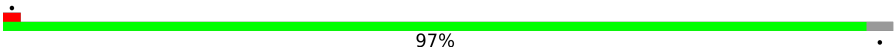


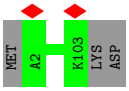
• Molecule 36: 60S ribosomal protein L35



• Molecule 37: 60S ribosomal protein L36

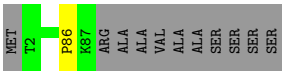
Chain Li:





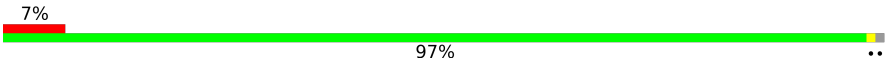
• Molecule 38: 60S ribosomal protein L37

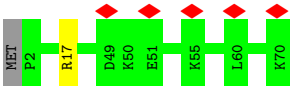
Chain Lj:



• Molecule 39: 60S ribosomal protein L38

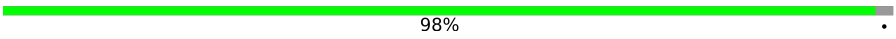
Chain Lk:





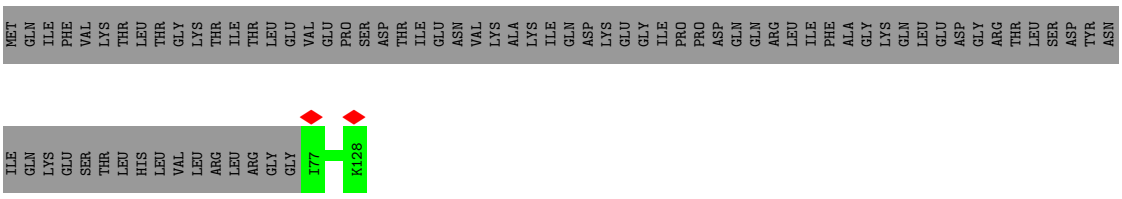
• Molecule 40: 60S ribosomal protein L39

Chain Ll:



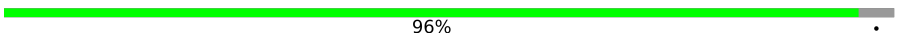
• Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Lm:



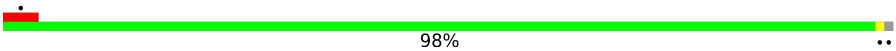
• Molecule 42: 60S ribosomal protein L41

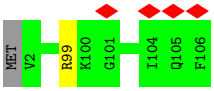
Chain Ln:



• Molecule 43: 60S ribosomal protein L36a

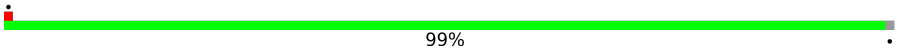
Chain Lo:





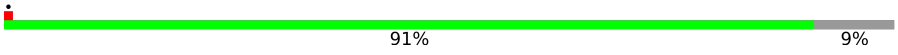
• Molecule 44: 60S ribosomal protein L37a

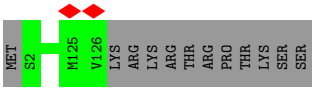
Chain Lp:



• Molecule 45: 60S ribosomal protein L28

Chain Lr:



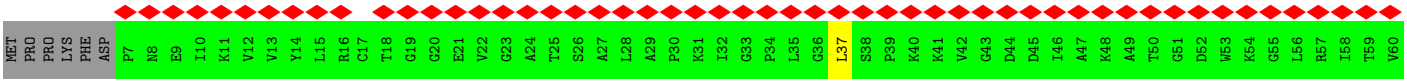


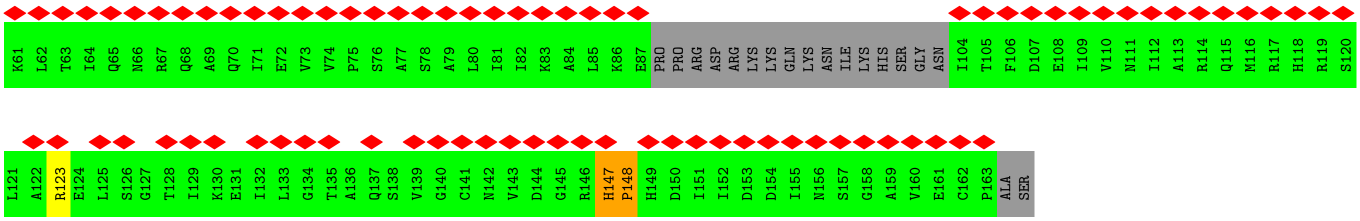
• Molecule 46: Large ribosomal subunit protein uL10

Chain Ls:

• Molecule 47: 60S ribosomal protein L12

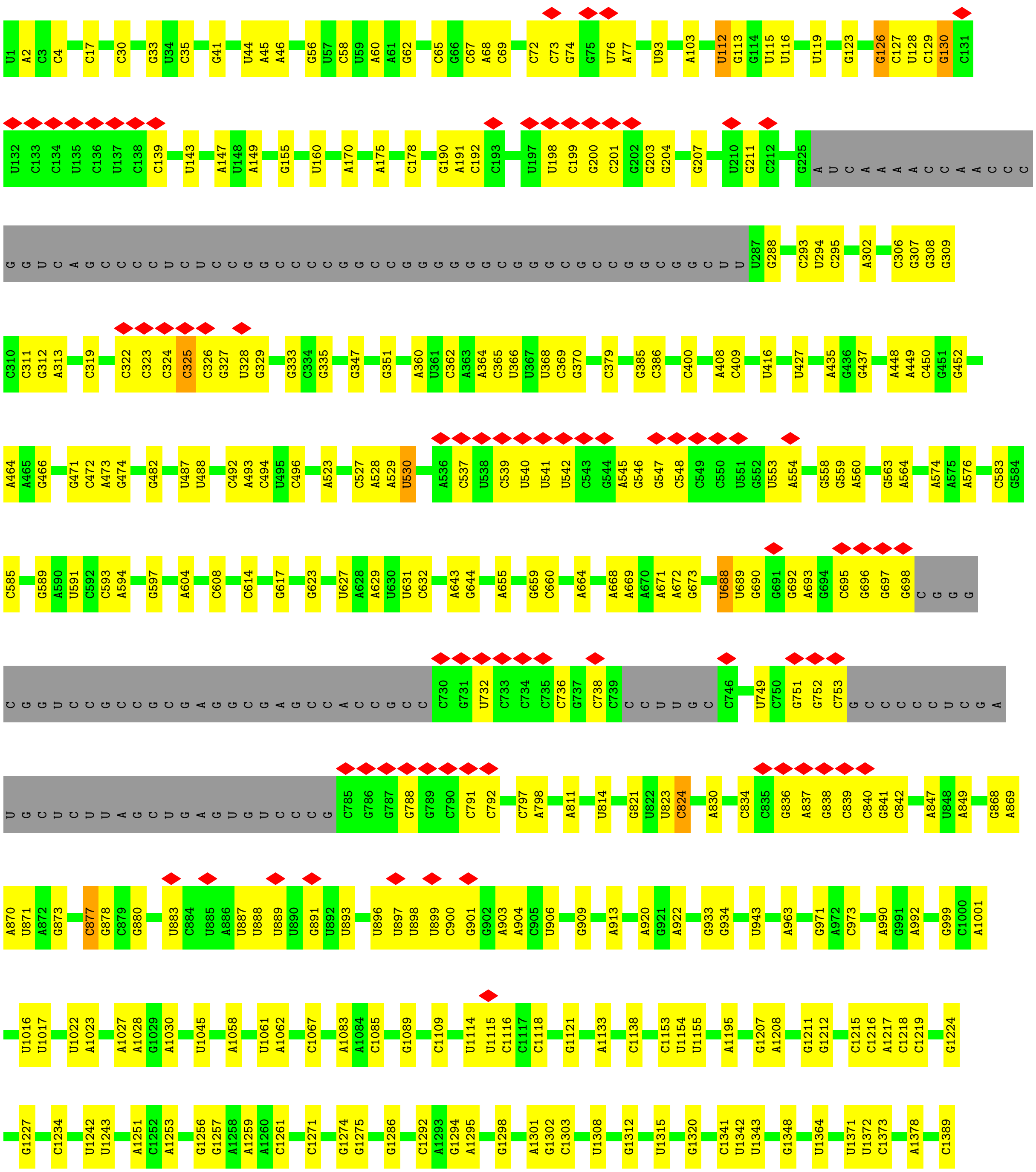
Chain Lt:

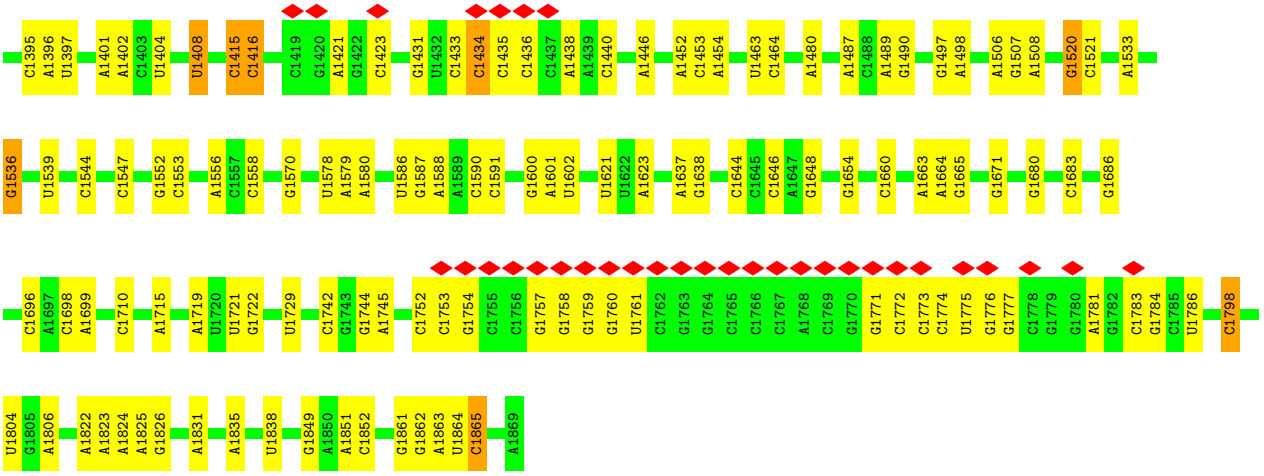




• Molecule 48: 18S rRNA

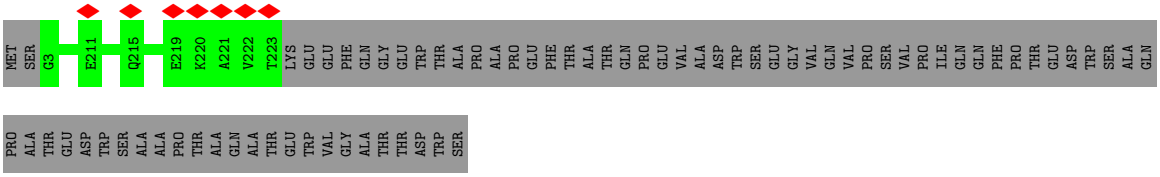
Chain S2:





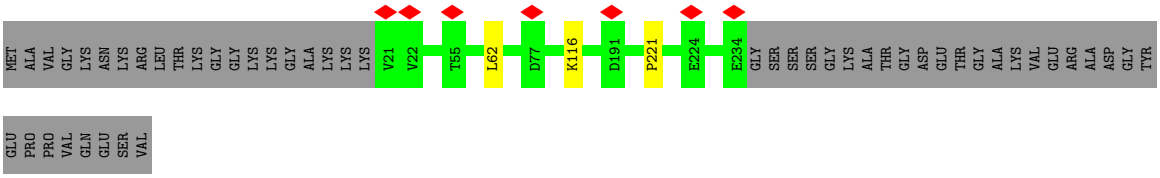
• Molecule 49: 40S ribosomal protein SA

Chain SA:



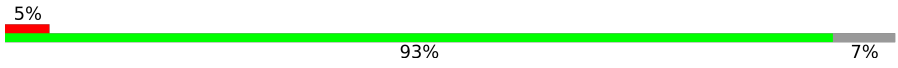
• Molecule 50: 40S ribosomal protein S3a

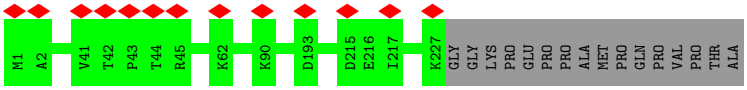
Chain SB:



• Molecule 51: 40S ribosomal protein S3

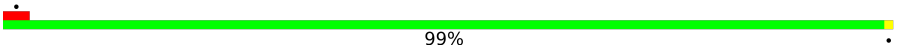
Chain SD:

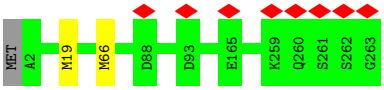




• Molecule 52: 40S ribosomal protein S4, X isoform

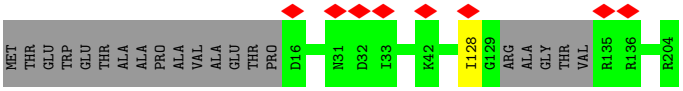
Chain SE:





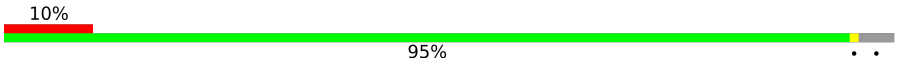
• Molecule 53: 40S ribosomal protein S5

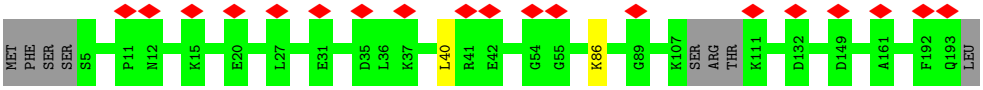
Chain SF:



• Molecule 54: 40S ribosomal protein S7

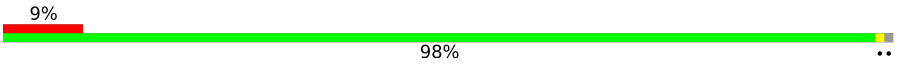
Chain SH:

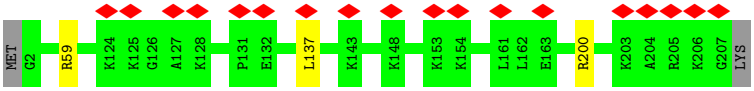




• Molecule 55: 40S ribosomal protein S8

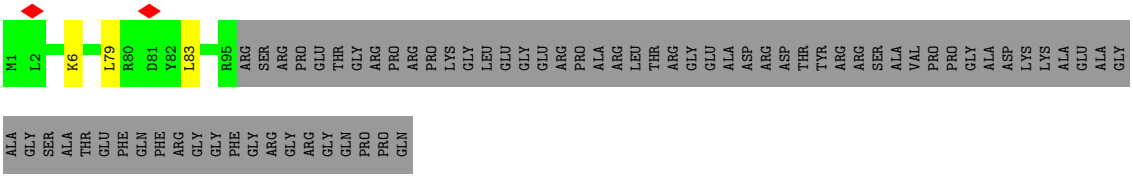
Chain SI:





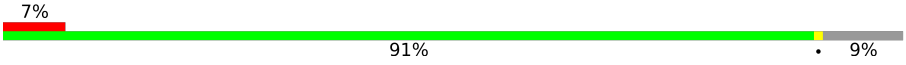
• Molecule 56: 40S ribosomal protein S10

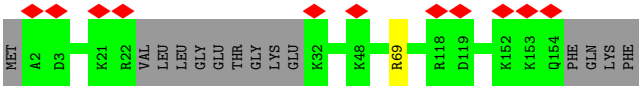
Chain SK:



• Molecule 57: 40S ribosomal protein S11

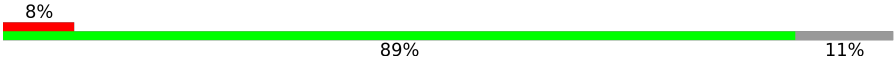
Chain SL:

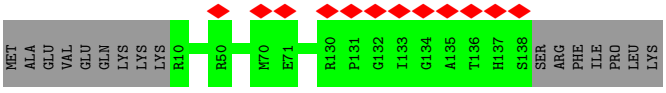




• Molecule 58: 40S ribosomal protein S15

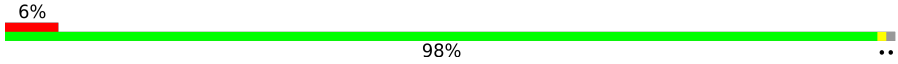
Chain SP:

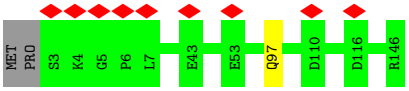




• Molecule 59: 40S ribosomal protein S16

Chain SQ:



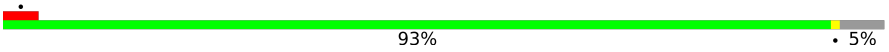


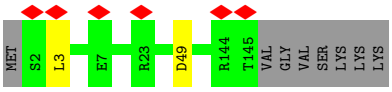
• Molecule 60: 40S ribosomal protein S17

Chain SR:

• Molecule 61: 40S ribosomal protein S18

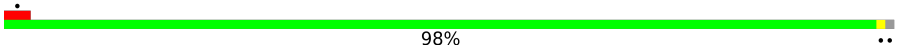
Chain SS:

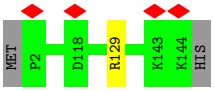




• Molecule 62: 40S ribosomal protein S19

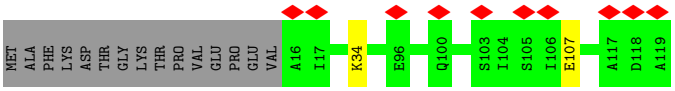
Chain ST:





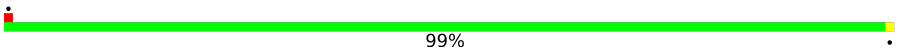
• Molecule 63: 40S ribosomal protein S20

Chain SU:



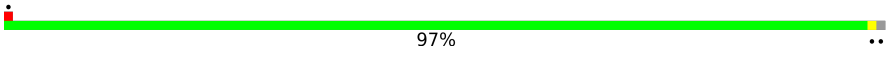
• Molecule 64: 40S ribosomal protein S21

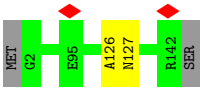
Chain SV:



• Molecule 65: 40S ribosomal protein S23

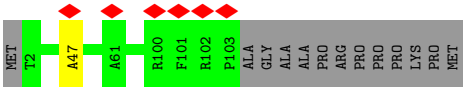
Chain SX:





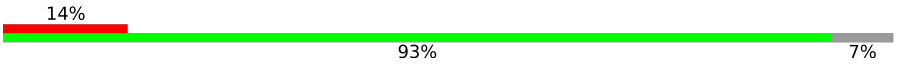
• Molecule 66: 40S ribosomal protein S26

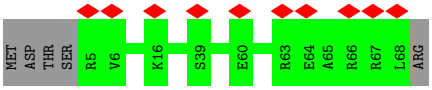
Chain Sa:



• Molecule 67: 40S ribosomal protein S28

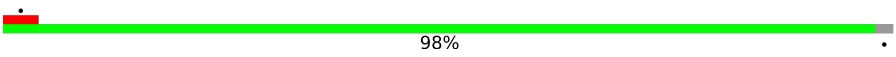
Chain Sc:

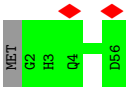




• Molecule 68: 40S ribosomal protein S29

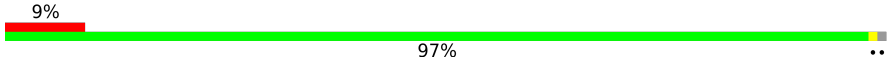
Chain Sd:

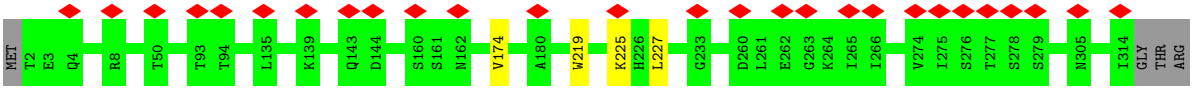




• Molecule 69: Receptor of activated protein C kinase 1

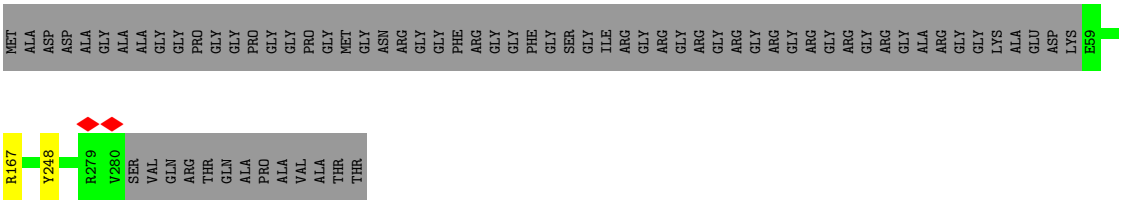
Chain Sg:





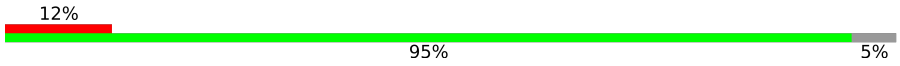
• Molecule 70: 40S ribosomal protein S2

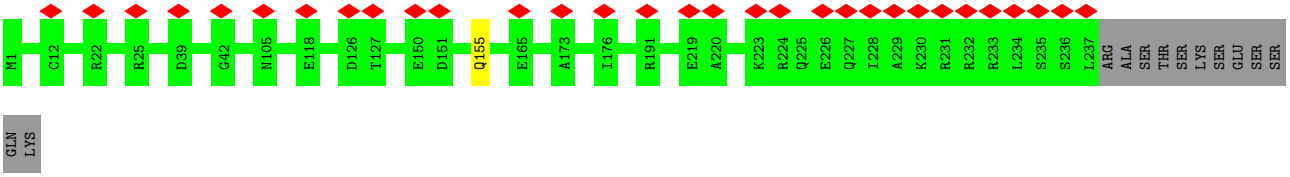
Chain SC:



• Molecule 71: 40S ribosomal protein S6

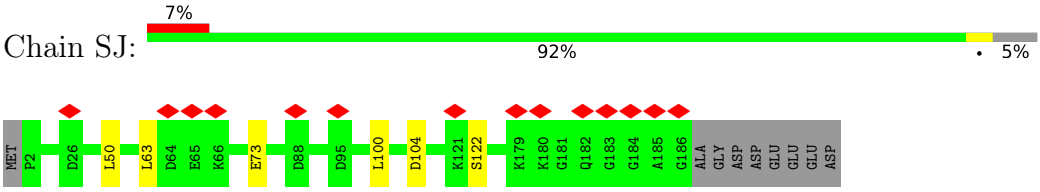
Chain SG:





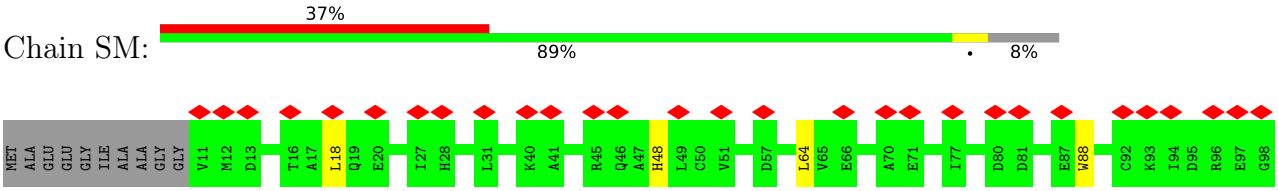
• Molecule 72: 40S ribosomal protein S9

Chain SJ:



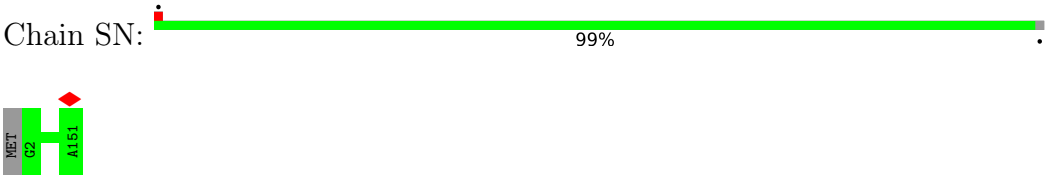
• Molecule 73: 40S ribosomal protein S12

Chain SM:



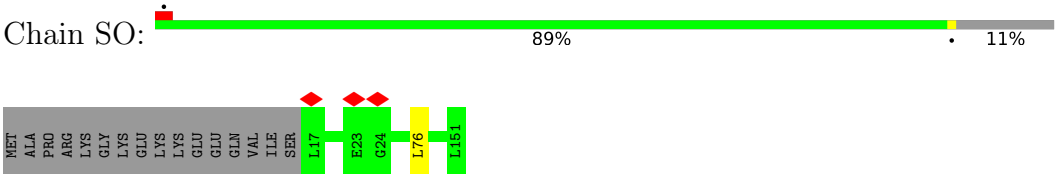
• Molecule 74: 40S ribosomal protein S13

Chain SN:



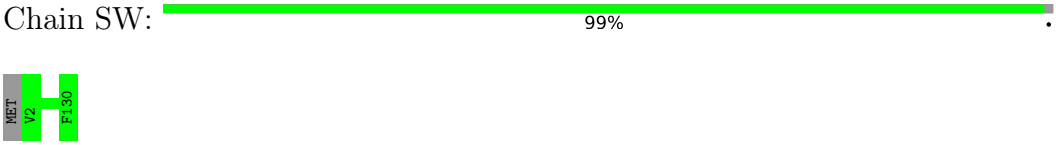
• Molecule 75: 40S ribosomal protein S14

Chain SO:



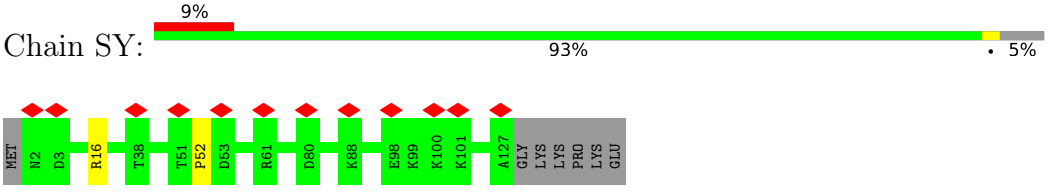
• Molecule 76: 40S ribosomal protein S15a

Chain SW:



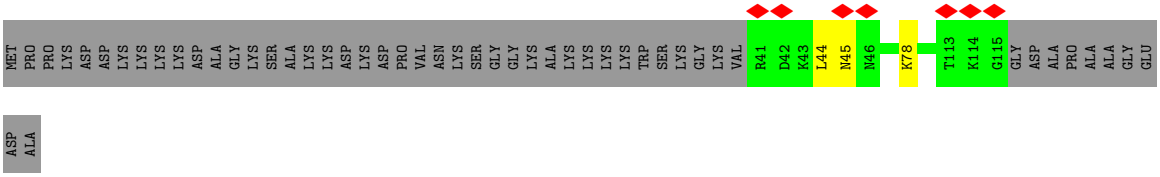
• Molecule 77: 40S ribosomal protein S24

Chain SY:



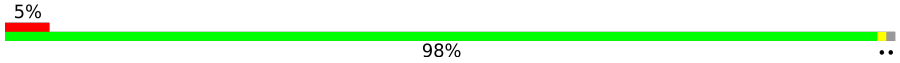
• Molecule 78: 40S ribosomal protein S25

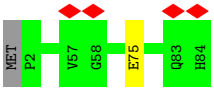
Chain SZ:



• Molecule 79: 40S ribosomal protein S27

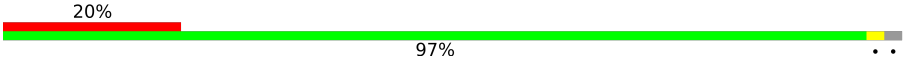
Chain Sb:

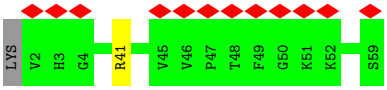




• Molecule 80: 40S ribosomal protein S30

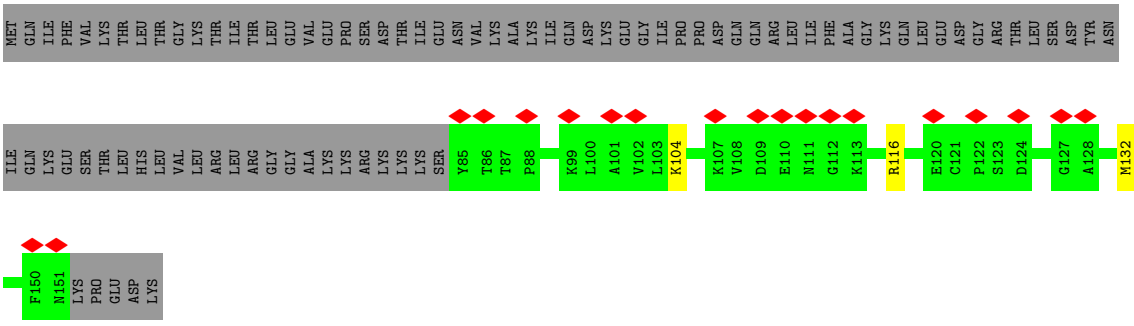
Chain Se:





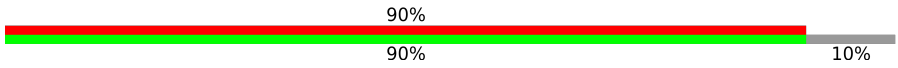
• Molecule 81: Ubiquitin-40S ribosomal protein S27a

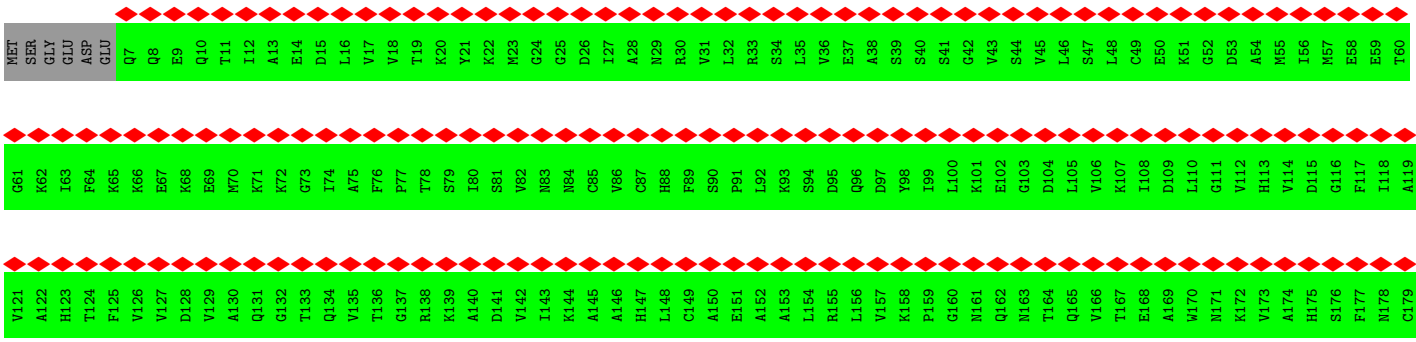
Chain Sf:

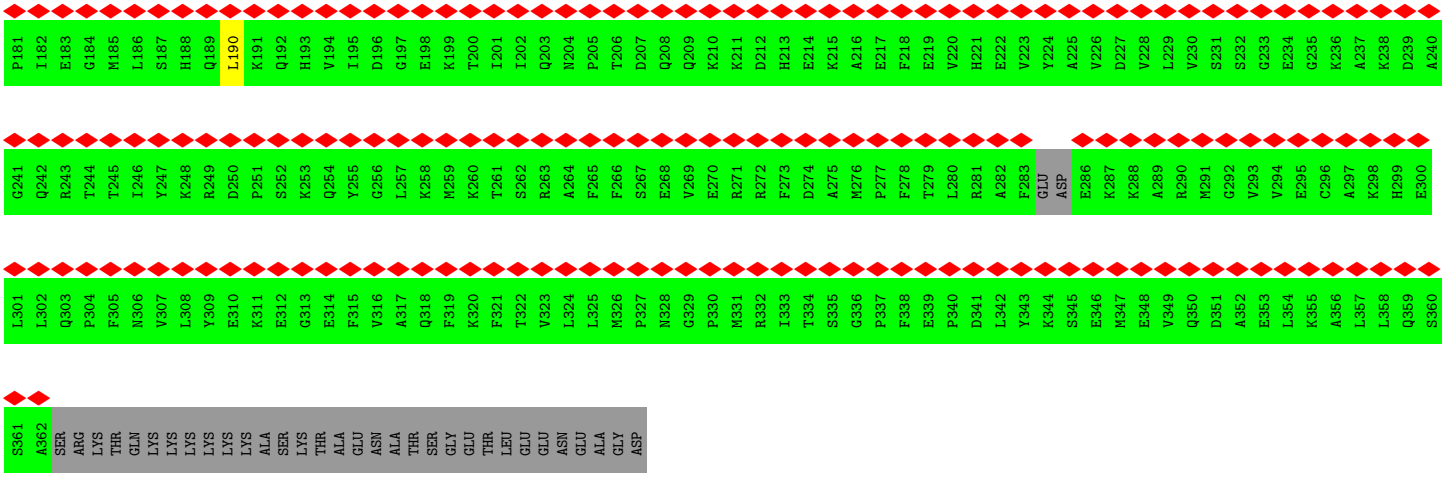


• Molecule 82: Proliferation-associated protein 2G4

Chain CA:

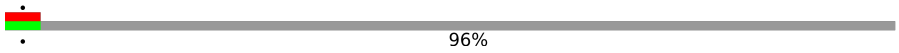


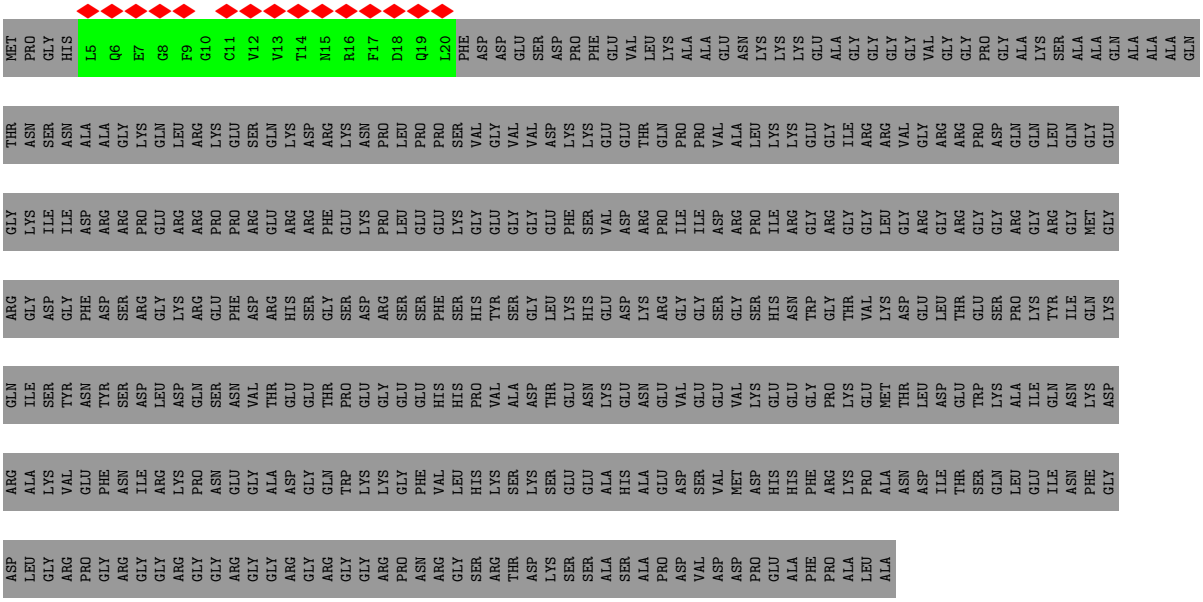




• Molecule 83: SERPINE1 mRNA-binding protein 1

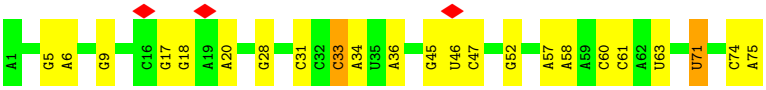
Chain CB:





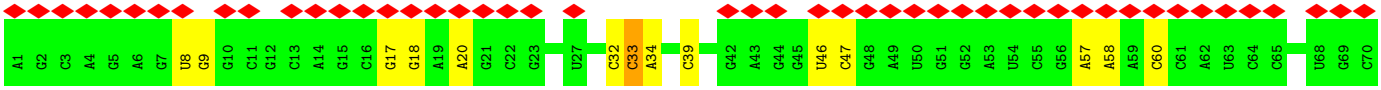
• Molecule 84: tRNA

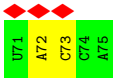
Chain CC:



• Molecule 84: tRNA

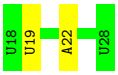
Chain CD:





• Molecule 85: mRNA

Chain CE:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32725	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	447.36, 447.36, 447.36	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, T1C, MLZ, ZN

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	L5	0.29	0/87961	0.97	225/137216 (0.2%)
2	L7	0.27	0/2861	0.96	10/4459 (0.2%)
3	L8	0.26	0/3701	0.89	3/5766 (0.1%)
4	LA	0.31	0/1936	0.65	0/2596
5	LB	0.30	0/3306	0.62	2/4424 (0.0%)
6	LC	0.28	0/2981	0.62	0/4002
7	LD	0.29	0/2428	0.56	0/3252
8	LE	0.28	0/1808	0.60	0/2425
9	LF	0.32	0/1905	0.61	1/2539 (0.0%)
10	LG	0.29	0/1960	0.58	0/2637
11	LH	0.31	0/1537	0.67	2/2066 (0.1%)
12	LI	0.29	0/1677	0.59	0/2237
13	LJ	0.30	0/1433	0.65	0/1915
14	LL	0.31	0/1732	0.65	1/2315 (0.0%)
15	LM	0.29	0/1161	0.67	1/1554 (0.1%)
16	LN	0.28	0/1746	0.63	1/2338 (0.0%)
17	LO	0.29	0/1682	0.57	0/2250
18	LP	0.29	0/1268	0.58	0/1701
19	LQ	0.26	0/1537	0.62	0/2052
20	LR	0.29	0/1582	0.61	0/2091
21	LS	0.29	0/1493	0.61	1/2003 (0.0%)
22	LT	0.29	0/1326	0.58	0/1770
23	LU	0.30	0/830	0.64	1/1114 (0.1%)
24	LV	0.27	0/993	0.58	0/1332
25	LW	0.28	0/979	0.62	0/1295
26	LX	0.29	0/1002	0.58	1/1345 (0.1%)
27	LY	0.29	0/1123	0.61	0/1493
28	LZ	0.29	0/1130	0.57	0/1507
29	La	0.31	0/1191	0.59	0/1591
30	Lb	0.27	0/889	0.64	0/1175
31	Lc	0.29	0/774	0.52	0/1038
32	Ld	0.28	0/903	0.62	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Le	0.27	0/1071	0.59	0/1429
34	Lf	0.28	0/895	0.64	0/1198
35	Lg	0.27	0/916	0.62	0/1220
36	Lh	0.29	0/1023	0.58	0/1351
37	Li	0.26	0/843	0.58	0/1115
38	Lj	0.32	0/720	0.68	1/952 (0.1%)
39	Lk	0.28	0/575	0.62	0/761
40	Ll	0.26	0/454	0.62	0/599
41	Lm	0.27	0/425	0.62	0/561
42	Ln	0.29	0/231	0.76	0/294
43	Lo	0.26	0/876	0.58	0/1156
44	Lp	0.27	0/718	0.55	0/953
45	Lr	0.27	0/1017	0.59	0/1364
46	Ls	0.28	0/1519	0.60	0/2052
47	Lt	0.28	0/1058	0.72	1/1430 (0.1%)
48	S2	0.29	0/41241	0.97	89/64258 (0.1%)
49	SA	0.29	0/1778	0.58	0/2416
50	SB	0.31	0/1765	0.67	3/2362 (0.1%)
51	SD	0.31	0/1793	0.63	0/2414
52	SE	0.31	0/2118	0.69	2/2849 (0.1%)
53	SF	0.26	0/1481	0.58	0/1988
54	SH	0.33	0/1519	0.67	1/2033 (0.0%)
55	SI	0.33	0/1715	0.72	1/2287 (0.0%)
56	SK	0.39	0/823	0.75	2/1111 (0.2%)
57	SL	0.27	0/1202	0.59	0/1606
58	SP	0.30	0/1082	0.64	0/1446
59	SQ	0.33	0/1160	0.70	1/1553 (0.1%)
60	SR	0.27	0/1105	0.58	0/1484
61	SS	0.33	0/1208	0.70	2/1618 (0.1%)
62	ST	0.34	0/1131	0.68	3/1515 (0.2%)
63	SU	0.35	0/831	0.78	1/1115 (0.1%)
64	SV	0.31	0/643	0.62	0/860
65	SX	0.30	0/1116	0.59	0/1490
66	Sa	0.28	0/836	0.63	0/1121
67	Sc	0.34	0/508	0.77	0/680
68	Sd	0.30	0/470	0.66	0/623
69	Sg	0.39	1/2493 (0.0%)	0.74	1/3394 (0.0%)
70	SC	0.37	1/1762 (0.1%)	0.60	0/2381
71	SG	0.30	0/1946	0.72	0/2590
72	SJ	0.40	1/1550 (0.1%)	0.80	5/2069 (0.2%)
73	SM	0.47	1/952 (0.1%)	0.87	2/1279 (0.2%)
74	SN	0.27	0/1232	0.56	0/1656
75	SO	0.32	0/1023	0.69	1/1372 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	SW	0.30	0/1051	0.61	0/1406
77	SY	0.31	0/1044	0.71	1/1388 (0.1%)
78	SZ	0.32	0/604	0.72	1/810 (0.1%)
79	Sb	0.30	0/665	0.57	0/891
80	Se	0.30	0/465	0.70	0/612
81	Sf	0.36	0/560	0.78	2/745 (0.3%)
82	CA	0.29	0/2810	0.62	1/3780 (0.0%)
83	CB	0.26	0/128	0.60	0/171
84	CC	0.29	0/1798	1.01	6/2802 (0.2%)
84	CD	0.26	0/1798	0.95	3/2802 (0.1%)
85	CE	0.25	0/258	0.92	0/399
All	All	0.29	4/238840 (0.0%)	0.86	379/350525 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	LA	0	1
5	LB	0	2
9	LF	0	1
11	LH	0	1
12	LI	0	1
14	LL	0	1
15	LM	0	2
17	LO	0	2
20	LR	0	1
28	LZ	0	1
34	Lf	0	2
36	Lh	0	1
47	Lt	0	2
50	SB	0	1
52	SE	0	1
55	SI	0	2
65	SX	0	1
69	Sg	0	1
73	SM	0	1
78	SZ	0	1
79	Sb	0	1
80	Se	0	1
All	All	0	28

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	SJ	73	GLU	CB-CG	-7.15	1.38	1.52
73	SM	88	TRP	CB-CG	6.74	1.62	1.50
70	SC	248	TYR	CD2-CE2	-6.11	1.30	1.39
69	Sg	219	TRP	CG-CD1	-5.11	1.29	1.36

The worst 5 of 379 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L5	1367	C	N1-C2-O2	13.03	126.72	118.90
1	L5	485	C	C2-N1-C1'	12.85	132.94	118.80
52	SE	19	MET	CB-CG-SD	-11.61	77.58	112.40
1	L5	1367	C	C2-N1-C1'	11.34	131.27	118.80
1	L5	1367	C	N3-C2-O2	-10.66	114.44	121.90

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	LA	110	GLY	Peptide
5	LB	258	HIS	Peptide
5	LB	303	ALA	Peptide
9	LF	34	ARG	Sidechain
11	LH	106	GLN	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/257 (96%)	224 (91%)	22 (9%)	0	100	100
5	LB	400/403 (99%)	374 (94%)	24 (6%)	2 (0%)	29	67
6	LC	366/427 (86%)	345 (94%)	21 (6%)	0	100	100
7	LD	291/297 (98%)	279 (96%)	12 (4%)	0	100	100
8	LE	215/288 (75%)	192 (89%)	23 (11%)	0	100	100
9	LF	223/248 (90%)	213 (96%)	10 (4%)	0	100	100
10	LG	239/266 (90%)	223 (93%)	16 (7%)	0	100	100
11	LH	188/192 (98%)	172 (92%)	16 (8%)	0	100	100
12	LI	198/214 (92%)	189 (96%)	8 (4%)	1 (0%)	29	67
13	LJ	174/178 (98%)	165 (95%)	9 (5%)	0	100	100
14	LL	208/211 (99%)	193 (93%)	15 (7%)	0	100	100
15	LM	137/215 (64%)	126 (92%)	10 (7%)	1 (1%)	22	61
16	LN	201/204 (98%)	187 (93%)	13 (6%)	1 (0%)	29	67
17	LO	199/203 (98%)	191 (96%)	8 (4%)	0	100	100
18	LP	151/184 (82%)	142 (94%)	9 (6%)	0	100	100
19	LQ	185/188 (98%)	176 (95%)	9 (5%)	0	100	100
20	LR	185/196 (94%)	181 (98%)	4 (2%)	0	100	100
21	LS	173/176 (98%)	161 (93%)	12 (7%)	0	100	100
22	LT	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
23	LU	98/128 (77%)	90 (92%)	7 (7%)	1 (1%)	15	54
24	LV	129/140 (92%)	122 (95%)	7 (5%)	0	100	100
25	LW	114/157 (73%)	107 (94%)	7 (6%)	0	100	100
26	LX	118/156 (76%)	115 (98%)	3 (2%)	0	100	100
27	LY	131/145 (90%)	127 (97%)	4 (3%)	0	100	100
28	LZ	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
29	La	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
30	Lb	105/159 (66%)	100 (95%)	5 (5%)	0	100	100
31	Lc	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
32	Ld	105/125 (84%)	98 (93%)	7 (7%)	0	100	100
33	Le	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
34	Lf	107/110 (97%)	96 (90%)	10 (9%)	1 (1%)	17	56
35	Lg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
37	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
38	Lj	84/97 (87%)	78 (93%)	6 (7%)	0	100	100
39	Lk	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
40	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
41	Lm	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
42	Ln	22/25 (88%)	21 (96%)	1 (4%)	0	100	100
43	Lo	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
44	Lp	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
45	Lr	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
46	Ls	194/317 (61%)	175 (90%)	19 (10%)	0	100	100
47	Lt	137/165 (83%)	107 (78%)	28 (20%)	2 (2%)	10	44
49	SA	219/295 (74%)	204 (93%)	15 (7%)	0	100	100
50	SB	212/264 (80%)	199 (94%)	13 (6%)	0	100	100
51	SD	225/243 (93%)	209 (93%)	16 (7%)	0	100	100
52	SE	260/263 (99%)	237 (91%)	23 (9%)	0	100	100
53	SF	180/204 (88%)	170 (94%)	9 (5%)	1 (1%)	25	64
54	SH	182/194 (94%)	170 (93%)	12 (7%)	0	100	100
55	SI	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
56	SK	93/165 (56%)	84 (90%)	9 (10%)	0	100	100
57	SL	140/158 (89%)	132 (94%)	8 (6%)	0	100	100
58	SP	127/145 (88%)	119 (94%)	8 (6%)	0	100	100
59	SQ	142/146 (97%)	132 (93%)	10 (7%)	0	100	100
60	SR	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
61	SS	142/152 (93%)	129 (91%)	13 (9%)	0	100	100
62	ST	141/145 (97%)	134 (95%)	7 (5%)	0	100	100
63	SU	102/119 (86%)	94 (92%)	7 (7%)	1 (1%)	15	54
64	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
65	SX	139/143 (97%)	131 (94%)	7 (5%)	1 (1%)	22	61
66	Sa	100/115 (87%)	91 (91%)	8 (8%)	1 (1%)	15	54
67	Sc	62/69 (90%)	58 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	Sd	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
69	Sg	311/317 (98%)	268 (86%)	43 (14%)	0	100	100
70	SC	220/293 (75%)	208 (94%)	12 (6%)	0	100	100
71	SG	235/249 (94%)	222 (94%)	13 (6%)	0	100	100
72	SJ	183/194 (94%)	173 (94%)	9 (5%)	1 (0%)	29	67
73	SM	120/132 (91%)	111 (92%)	9 (8%)	0	100	100
74	SN	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
75	SO	133/151 (88%)	120 (90%)	13 (10%)	0	100	100
76	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
77	SY	124/133 (93%)	115 (93%)	9 (7%)	0	100	100
78	SZ	73/125 (58%)	59 (81%)	13 (18%)	1 (1%)	11	46
79	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
80	Se	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
81	Sf	65/156 (42%)	57 (88%)	8 (12%)	0	100	100
82	CA	350/394 (89%)	333 (95%)	17 (5%)	0	100	100
83	CB	14/408 (3%)	13 (93%)	1 (7%)	0	100	100
All	All	11968/13972 (86%)	11194 (94%)	759 (6%)	15 (0%)	54	83

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	LB	360	LEU
12	LI	213	HIS
47	Lt	148	PRO
78	SZ	45	ASN
16	LN	124	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	LA	190/199 (96%)	190 (100%)	0	100	100
5	LB	348/349 (100%)	347 (100%)	1 (0%)	92	96
6	LC	306/348 (88%)	306 (100%)	0	100	100
7	LD	246/250 (98%)	246 (100%)	0	100	100
8	LE	195/252 (77%)	195 (100%)	0	100	100
9	LF	194/215 (90%)	194 (100%)	0	100	100
10	LG	203/223 (91%)	202 (100%)	1 (0%)	88	95
11	LH	169/171 (99%)	169 (100%)	0	100	100
12	LI	172/181 (95%)	172 (100%)	0	100	100
13	LJ	148/149 (99%)	148 (100%)	0	100	100
14	LL	176/177 (99%)	176 (100%)	0	100	100
15	LM	118/161 (73%)	118 (100%)	0	100	100
16	LN	171/172 (99%)	171 (100%)	0	100	100
17	LO	173/174 (99%)	173 (100%)	0	100	100
18	LP	134/163 (82%)	132 (98%)	2 (2%)	65	85
19	LQ	164/165 (99%)	164 (100%)	0	100	100
20	LR	166/175 (95%)	166 (100%)	0	100	100
21	LS	156/157 (99%)	156 (100%)	0	100	100
22	LT	139/140 (99%)	139 (100%)	0	100	100
23	LU	90/115 (78%)	90 (100%)	0	100	100
24	LV	101/107 (94%)	101 (100%)	0	100	100
25	LW	97/126 (77%)	96 (99%)	1 (1%)	76	90
26	LX	108/133 (81%)	108 (100%)	0	100	100
27	LY	123/135 (91%)	123 (100%)	0	100	100
28	LZ	117/118 (99%)	117 (100%)	0	100	100
29	La	120/121 (99%)	119 (99%)	1 (1%)	81	93
30	Lb	88/126 (70%)	87 (99%)	1 (1%)	73	88
31	Lc	83/97 (86%)	83 (100%)	0	100	100
32	Ld	98/110 (89%)	98 (100%)	0	100	100
33	Le	114/121 (94%)	114 (100%)	0	100	100
34	Lf	88/89 (99%)	88 (100%)	0	100	100
35	Lg	98/100 (98%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Lh	109/110 (99%)	109 (100%)	0	100	100
37	Li	86/89 (97%)	86 (100%)	0	100	100
38	Lj	73/80 (91%)	73 (100%)	0	100	100
39	Lk	64/65 (98%)	63 (98%)	1 (2%)	62	84
40	Ll	47/48 (98%)	47 (100%)	0	100	100
41	Lm	47/115 (41%)	47 (100%)	0	100	100
42	Ln	23/24 (96%)	23 (100%)	0	100	100
43	Lo	93/94 (99%)	92 (99%)	1 (1%)	73	88
44	Lp	74/75 (99%)	74 (100%)	0	100	100
45	Lr	109/121 (90%)	109 (100%)	0	100	100
46	Ls	162/258 (63%)	162 (100%)	0	100	100
47	Lt	112/137 (82%)	111 (99%)	1 (1%)	78	91
49	SA	183/243 (75%)	183 (100%)	0	100	100
50	SB	195/231 (84%)	195 (100%)	0	100	100
51	SD	190/202 (94%)	190 (100%)	0	100	100
52	SE	224/225 (100%)	224 (100%)	0	100	100
53	SF	156/170 (92%)	156 (100%)	0	100	100
54	SH	166/174 (95%)	165 (99%)	1 (1%)	86	94
55	SI	178/180 (99%)	178 (100%)	0	100	100
56	SK	86/136 (63%)	85 (99%)	1 (1%)	71	88
57	SL	130/142 (92%)	129 (99%)	1 (1%)	81	93
58	SP	115/130 (88%)	115 (100%)	0	100	100
59	SQ	119/121 (98%)	119 (100%)	0	100	100
60	SR	122/122 (100%)	122 (100%)	0	100	100
61	SS	125/132 (95%)	125 (100%)	0	100	100
62	ST	113/115 (98%)	113 (100%)	0	100	100
63	SU	94/107 (88%)	94 (100%)	0	100	100
64	SV	67/67 (100%)	66 (98%)	1 (2%)	65	85
65	SX	113/115 (98%)	113 (100%)	0	100	100
66	Sa	89/98 (91%)	89 (100%)	0	100	100
67	Sc	57/62 (92%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	Sd	48/49 (98%)	48 (100%)	0	100	100
69	Sg	272/275 (99%)	271 (100%)	1 (0%)	91	95
70	SC	188/225 (84%)	187 (100%)	1 (0%)	88	95
71	SG	207/218 (95%)	206 (100%)	1 (0%)	88	95
72	SJ	161/168 (96%)	161 (100%)	0	100	100
73	SM	102/108 (94%)	101 (99%)	1 (1%)	76	90
74	SN	130/131 (99%)	130 (100%)	0	100	100
75	SO	105/119 (88%)	105 (100%)	0	100	100
76	SW	112/113 (99%)	112 (100%)	0	100	100
77	SY	109/115 (95%)	108 (99%)	1 (1%)	78	91
78	SZ	66/103 (64%)	66 (100%)	0	100	100
79	Sb	75/76 (99%)	75 (100%)	0	100	100
80	Se	47/48 (98%)	47 (100%)	0	100	100
81	Sf	60/140 (43%)	57 (95%)	3 (5%)	24	60
82	CA	303/336 (90%)	303 (100%)	0	100	100
83	CB	14/328 (4%)	14 (100%)	0	100	100
All	All	10413/11859 (88%)	10391 (100%)	22 (0%)	93	98

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
69	Sg	225	LYS
73	SM	129	LYS
71	SG	155	GLN
77	SY	16	ARG
30	Lb	55	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
69	Sg	64	HIS
71	SG	56	ASN
82	CA	193	HIS
13	LJ	65	ASN
18	LP	80	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3656/5070 (72%)	809 (22%)	17 (0%)
2	L7	119/121 (98%)	10 (8%)	0
3	L8	155/157 (98%)	23 (14%)	0
48	S2	1717/1869 (91%)	400 (23%)	6 (0%)
84	CC	74/75 (98%)	21 (28%)	1 (1%)
84	CD	74/75 (98%)	16 (21%)	0
85	CE	10/11 (90%)	2 (20%)	0
All	All	5805/7378 (78%)	1281 (22%)	24 (0%)

5 of 1281 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	17	A
1	L5	30	C
1	L5	39	A
1	L5	42	A
1	L5	48	G

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	4378	A
48	S2	76	U
1	L5	4913	G
48	S2	112	U
1	L5	1977	C

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	MLZ	Lm	98	41	8,9,10	0.78	0	4,9,11	0.68	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
41	MLZ	Lm	98	41	-	3/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	Lm	98	MLZ	C-CA-CB-CG
41	Lm	98	MLZ	N-CA-CB-CG
41	Lm	98	MLZ	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 261 ligands modelled in this entry, 256 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
87	T1C	L5	5314	-	44,45,45	1.20	4 (9%)	53,72,72	1.34	3 (5%)
87	T1C	L5	5313	-	44,45,45	1.22	4 (9%)	53,72,72	1.34	7 (13%)
87	T1C	L5	5312	-	44,45,45	1.20	4 (9%)	53,72,72	1.12	3 (5%)
87	T1C	L5	5310	86	44,45,45	1.19	4 (9%)	53,72,72	0.98	2 (3%)
87	T1C	L5	5311	-	44,45,45	1.20	4 (9%)	53,72,72	1.18	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	T1C	L5	5314	-	-	8/22/80/80	0/4/4/4
87	T1C	L5	5313	-	-	9/22/80/80	0/4/4/4
87	T1C	L5	5312	-	-	9/22/80/80	0/4/4/4
87	T1C	L5	5310	86	-	12/22/80/80	0/4/4/4
87	T1C	L5	5311	-	-	16/22/80/80	0/4/4/4

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	L5	5313	T1C	C21-N21	5.52	1.48	1.33
87	L5	5312	T1C	C21-N21	5.51	1.48	1.33
87	L5	5314	T1C	C21-N21	5.48	1.48	1.33
87	L5	5311	T1C	C21-N21	5.44	1.47	1.33
87	L5	5310	T1C	C21-N21	5.42	1.47	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	L5	5314	T1C	C11-C1B-C12	5.02	122.77	118.80
87	L5	5313	T1C	C11-C1B-C12	4.99	122.75	118.80
87	L5	5310	T1C	C11-C1B-C12	4.19	122.11	118.80
87	L5	5312	T1C	C1C-C1-C2	4.11	122.28	115.75
87	L5	5312	T1C	C11-C1B-C12	4.05	122.01	118.80

There are no chirality outliers.

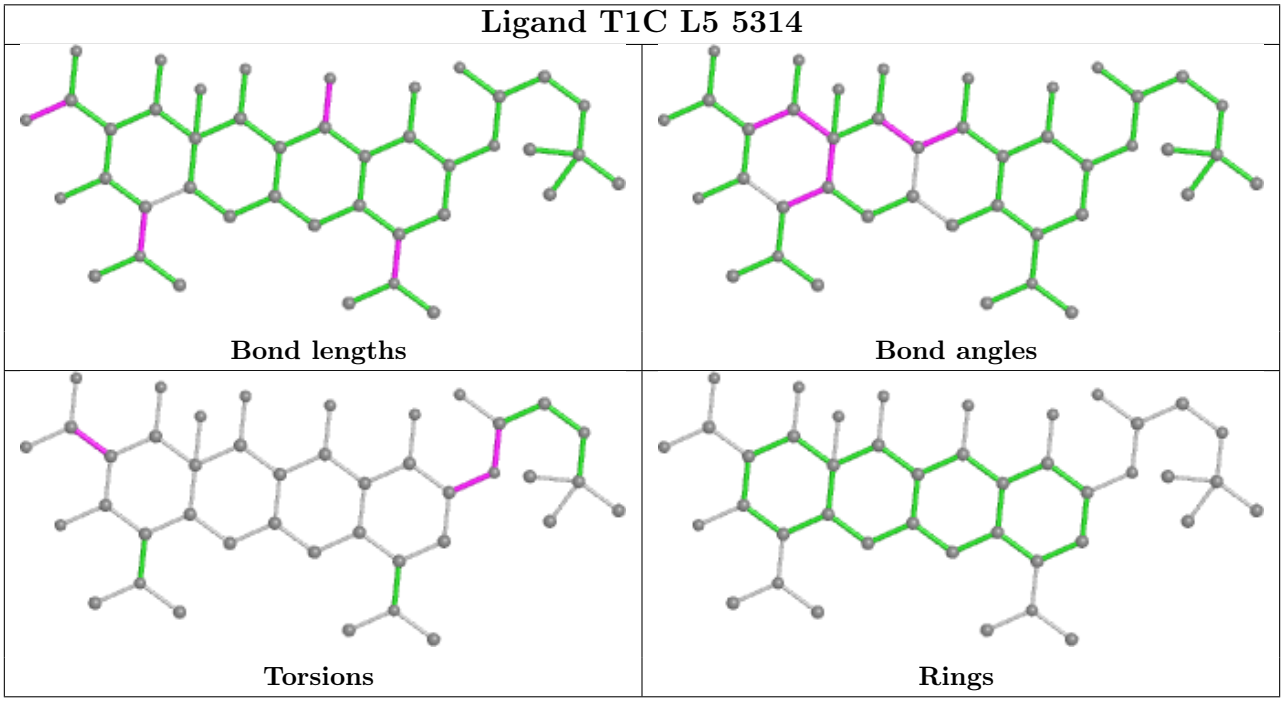
5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	L5	5310	T1C	C92-C91-N9-C9
87	L5	5310	T1C	C1-C2-C21-O21
87	L5	5310	T1C	C1-C2-C21-N21
87	L5	5311	T1C	C91-C92-N92-C93
87	L5	5311	T1C	C92-C91-N9-C9

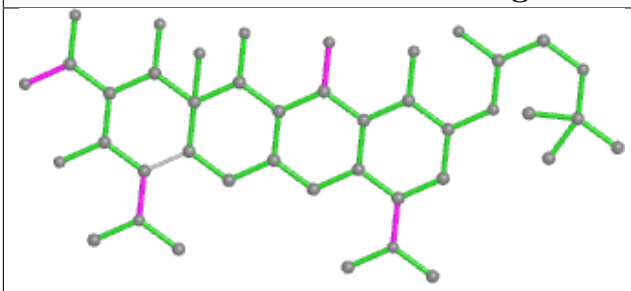
There are no ring outliers.

No monomer is involved in short contacts.

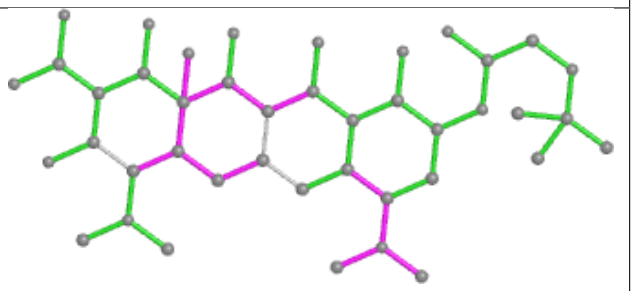
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



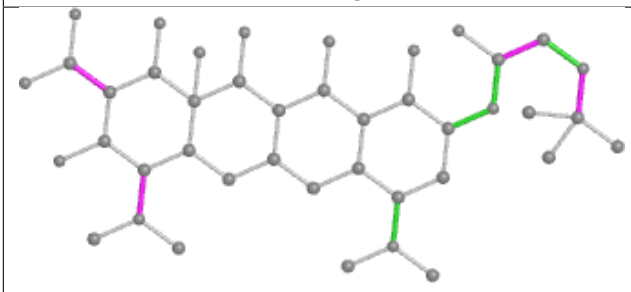
Ligand T1C L5 5313



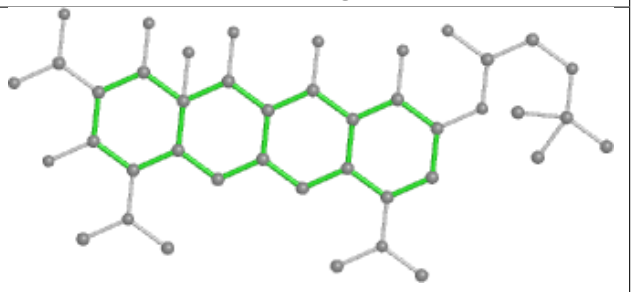
Bond lengths



Bond angles

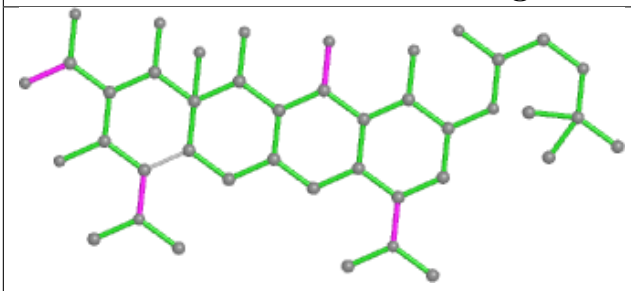


Torsions

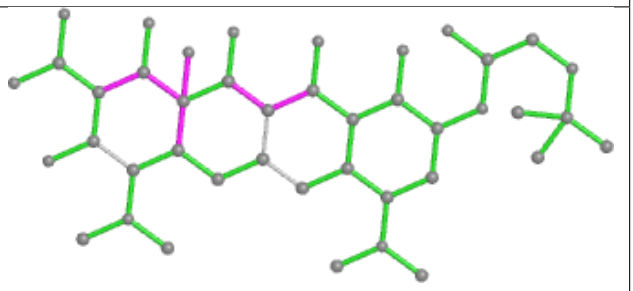


Rings

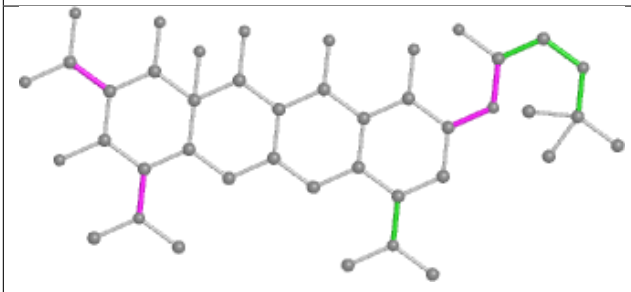
Ligand T1C L5 5312



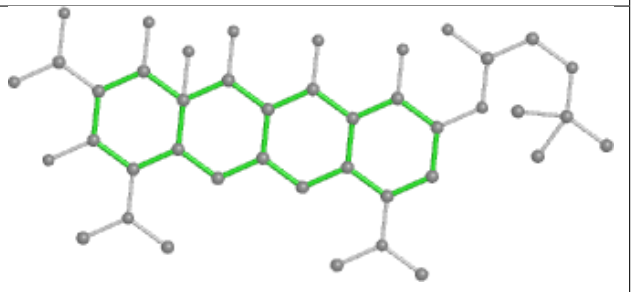
Bond lengths



Bond angles

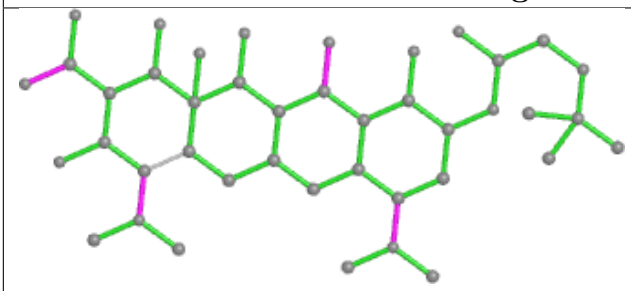


Torsions

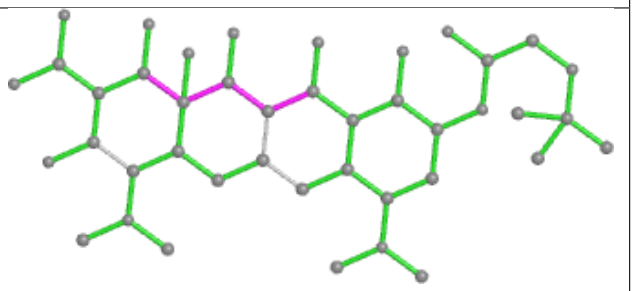


Rings

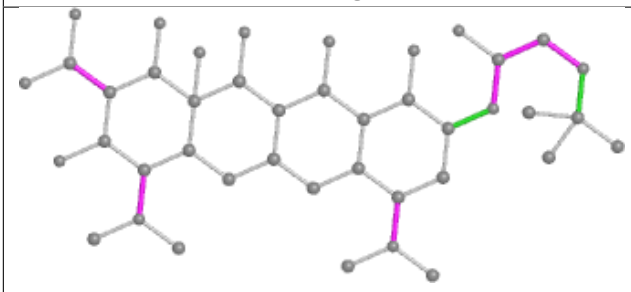
Ligand T1C L5 5310



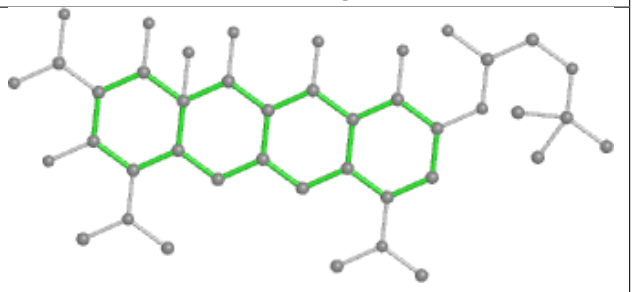
Bond lengths



Bond angles

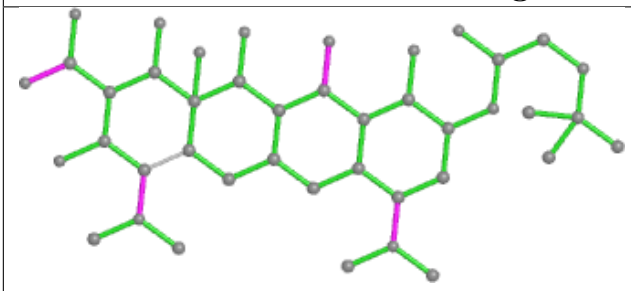


Torsions

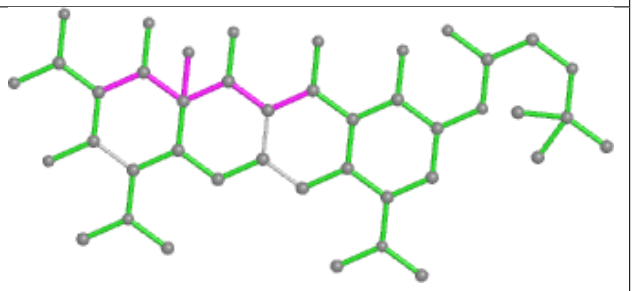


Rings

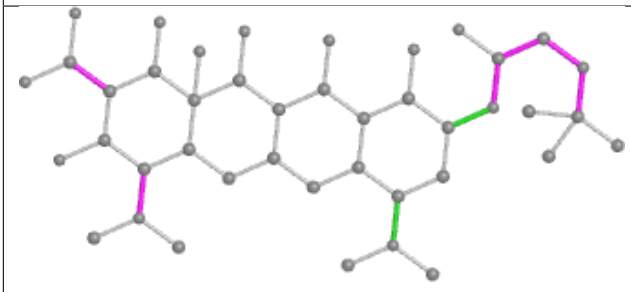
Ligand T1C L5 5311



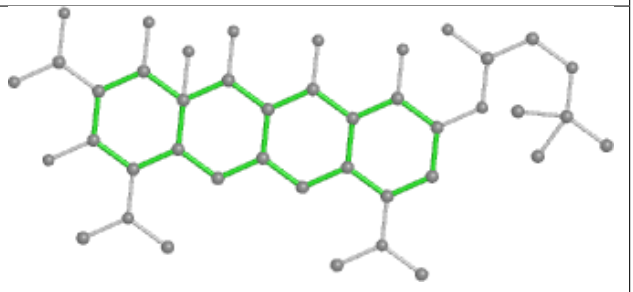
Bond lengths



Bond angles



Torsions



Rings

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.

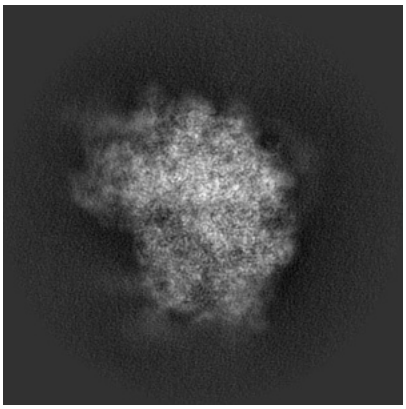
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38631. These allow visual inspection of the internal detail of the map and identification of artifacts.

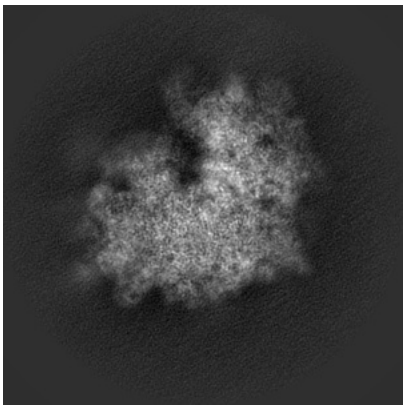
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

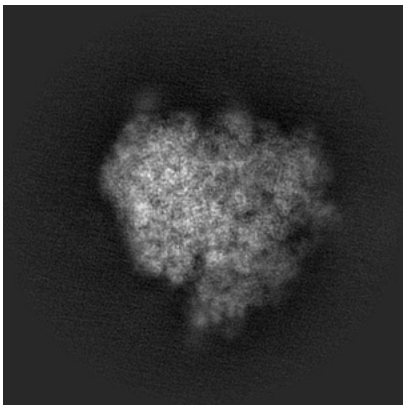
6.1.1 Primary map



X

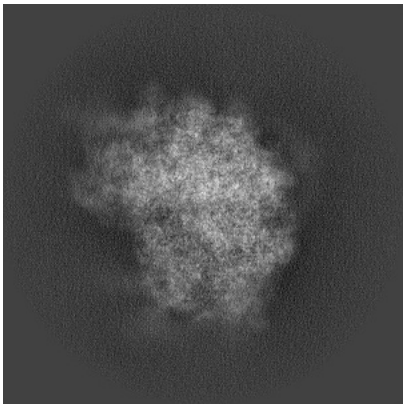


Y

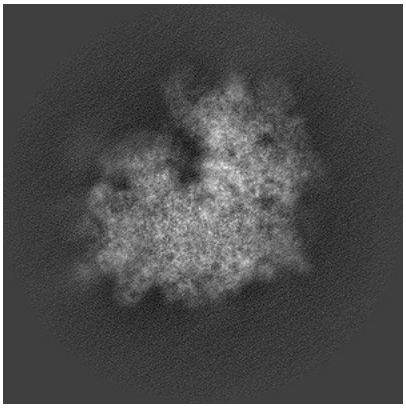


Z

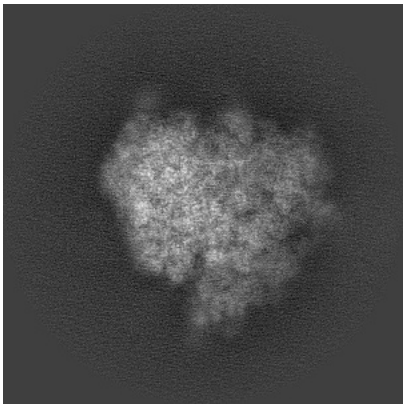
6.1.2 Raw map



X



Y

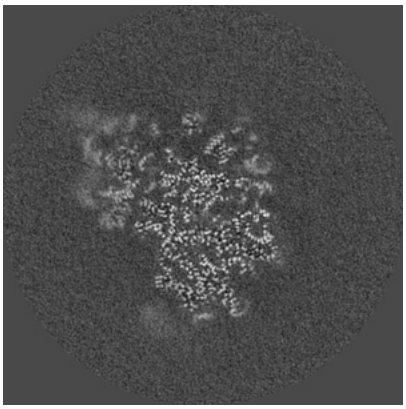


Z

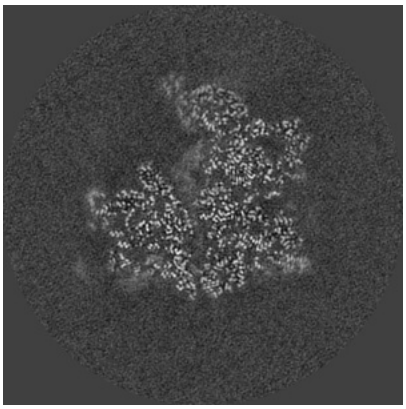
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

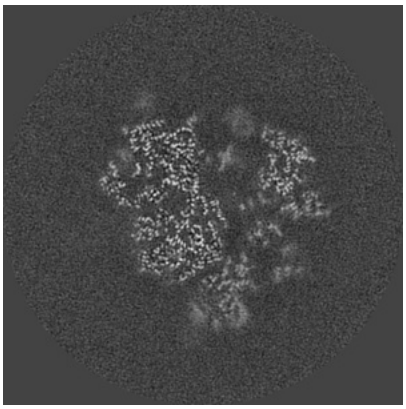
6.2.1 Primary map



X Index: 240

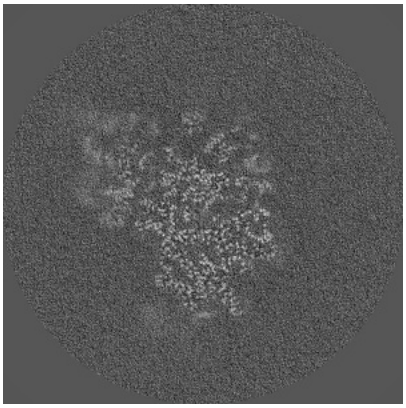


Y Index: 240

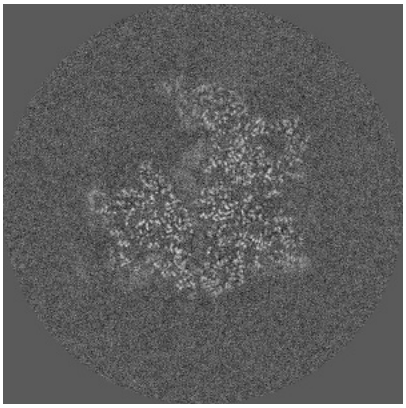


Z Index: 240

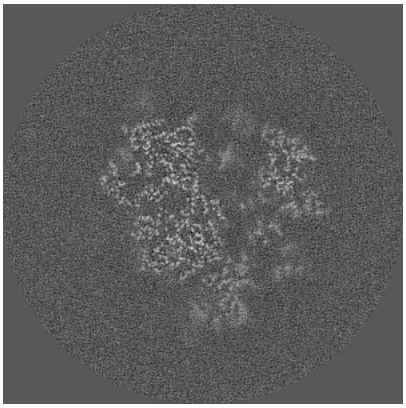
6.2.2 Raw map



X Index: 240



Y Index: 240

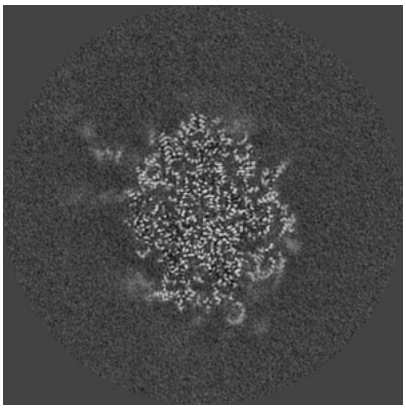


Z Index: 240

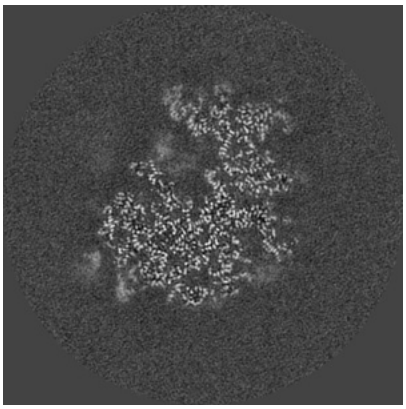
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

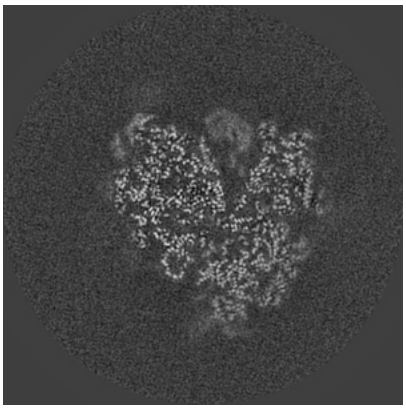
6.3.1 Primary map



X Index: 220

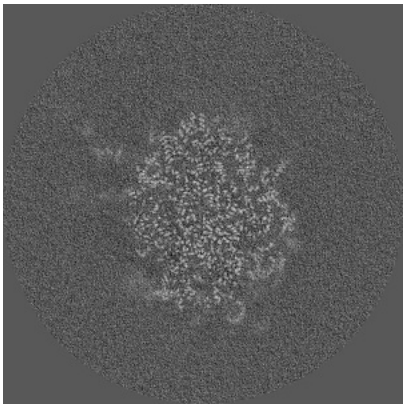


Y Index: 256

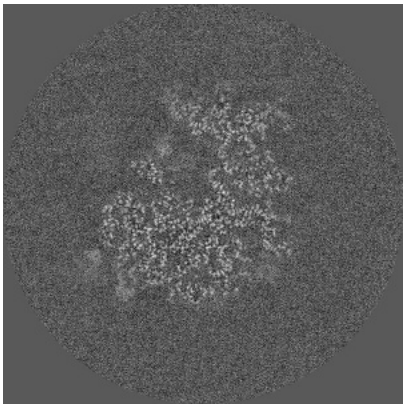


Z Index: 263

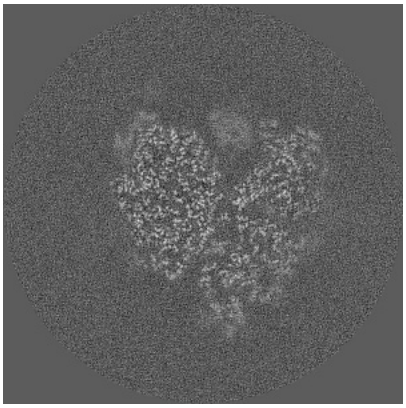
6.3.2 Raw map



X Index: 220



Y Index: 257

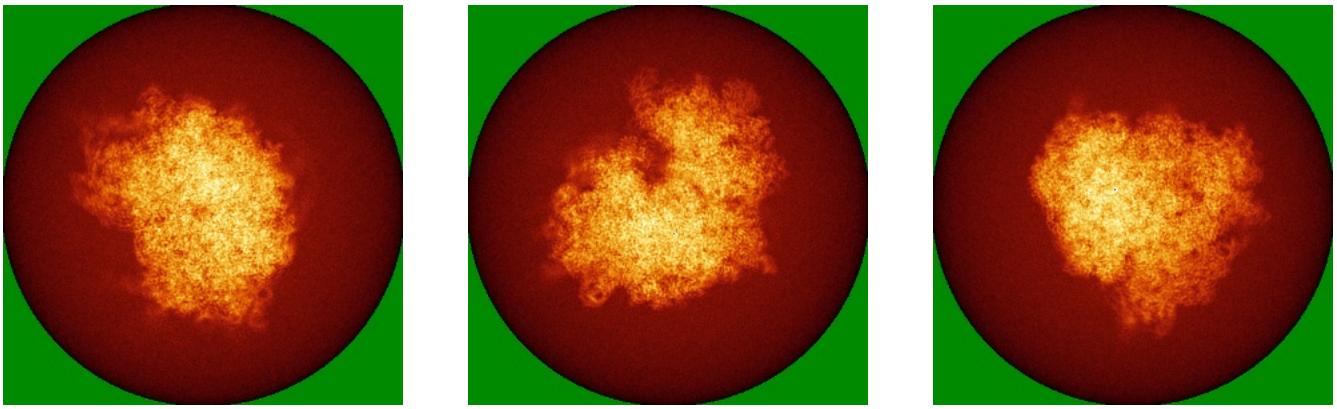


Z Index: 268

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

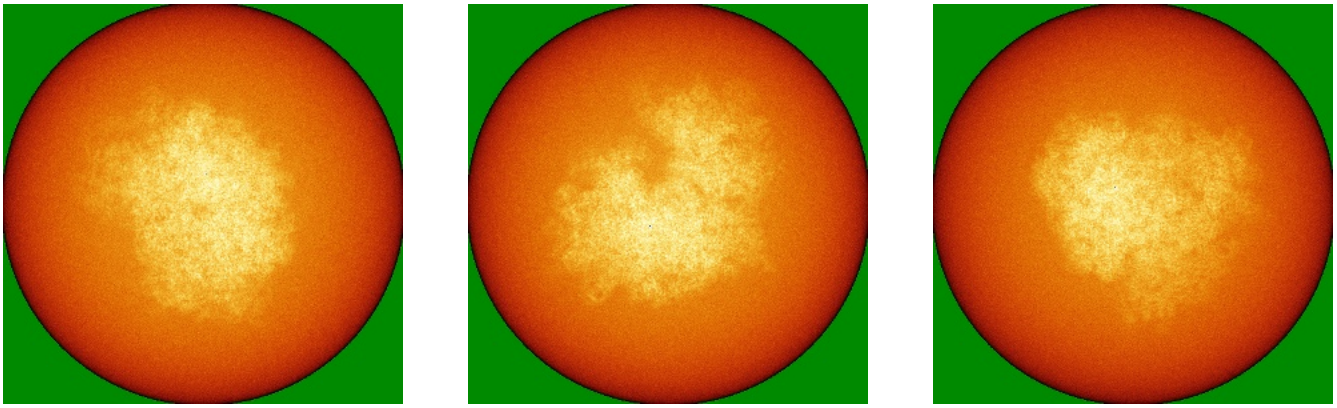
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

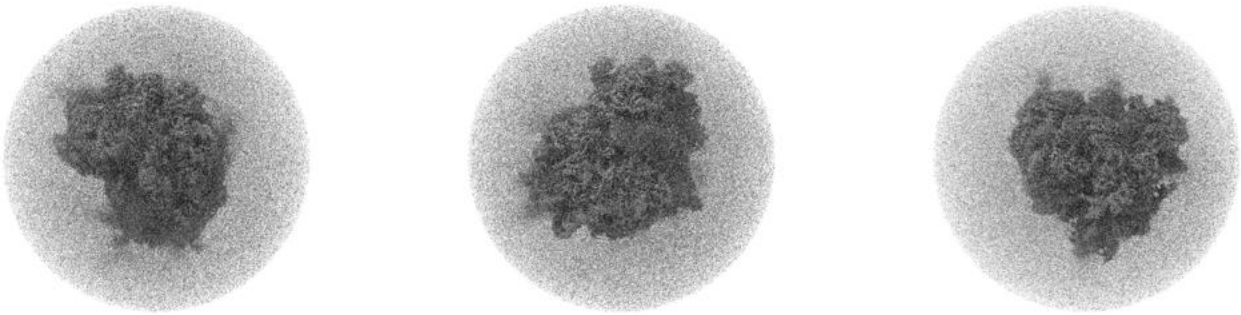
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

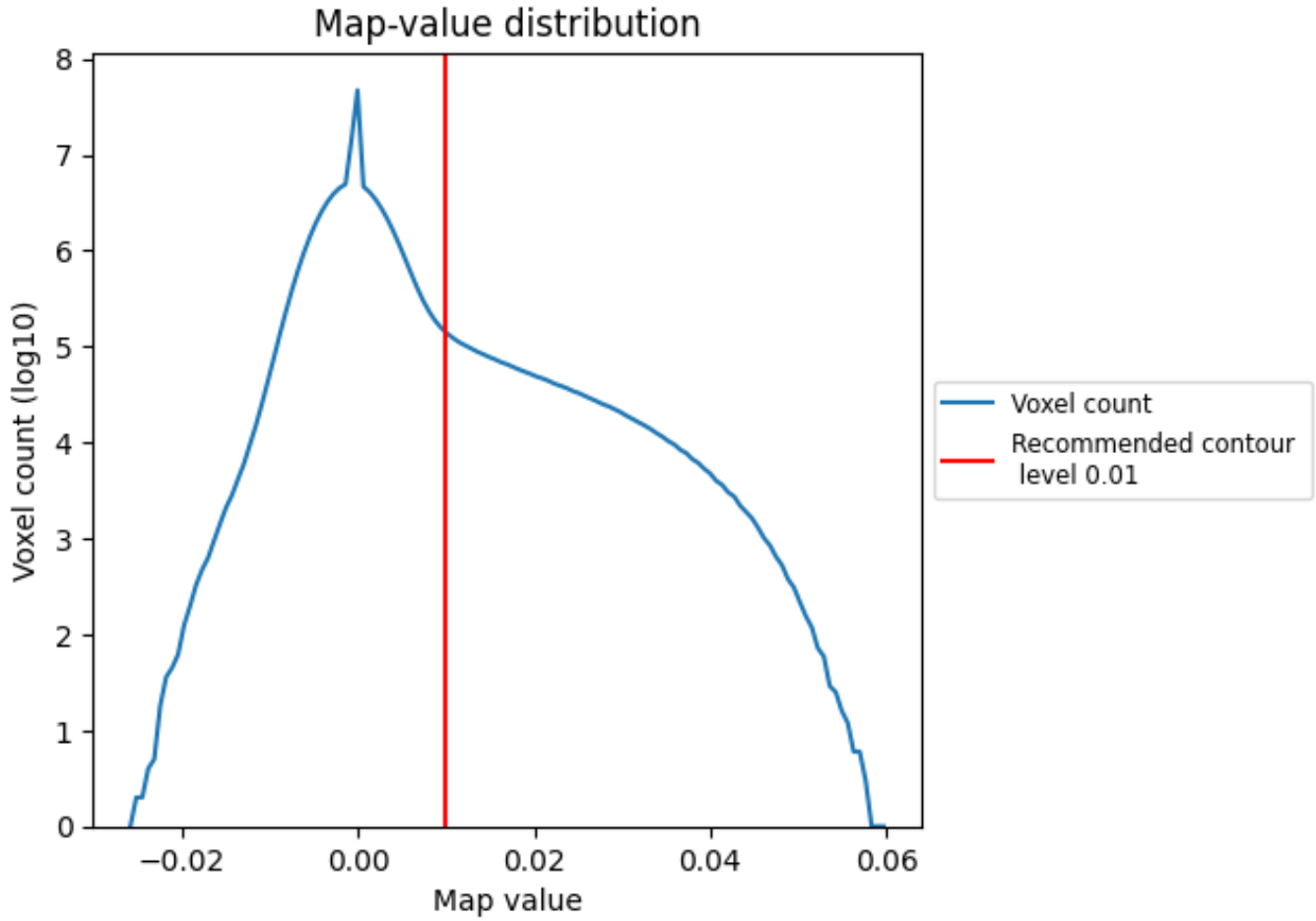
6.6 Mask visualisation (i)

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

7 Map analysis

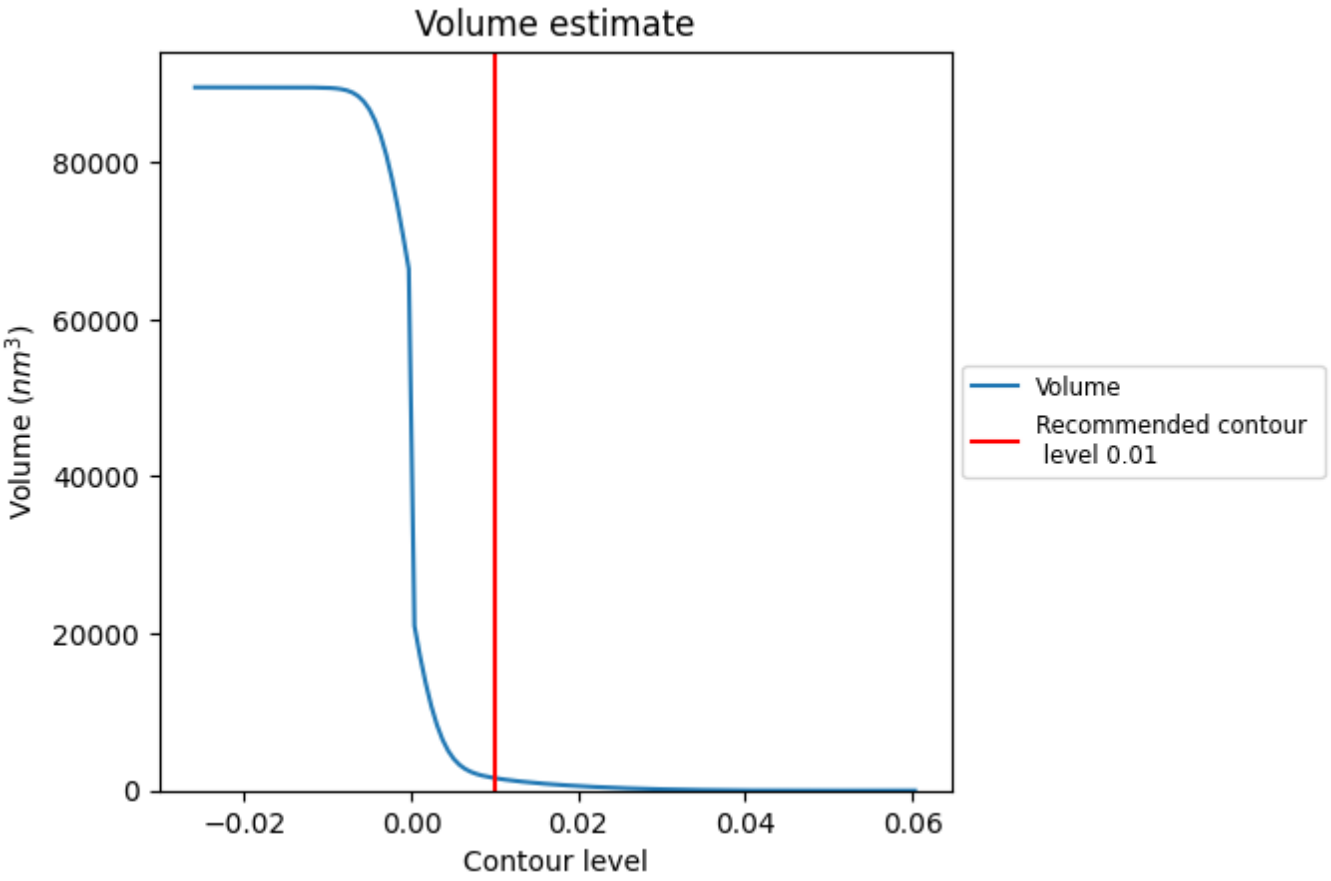
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

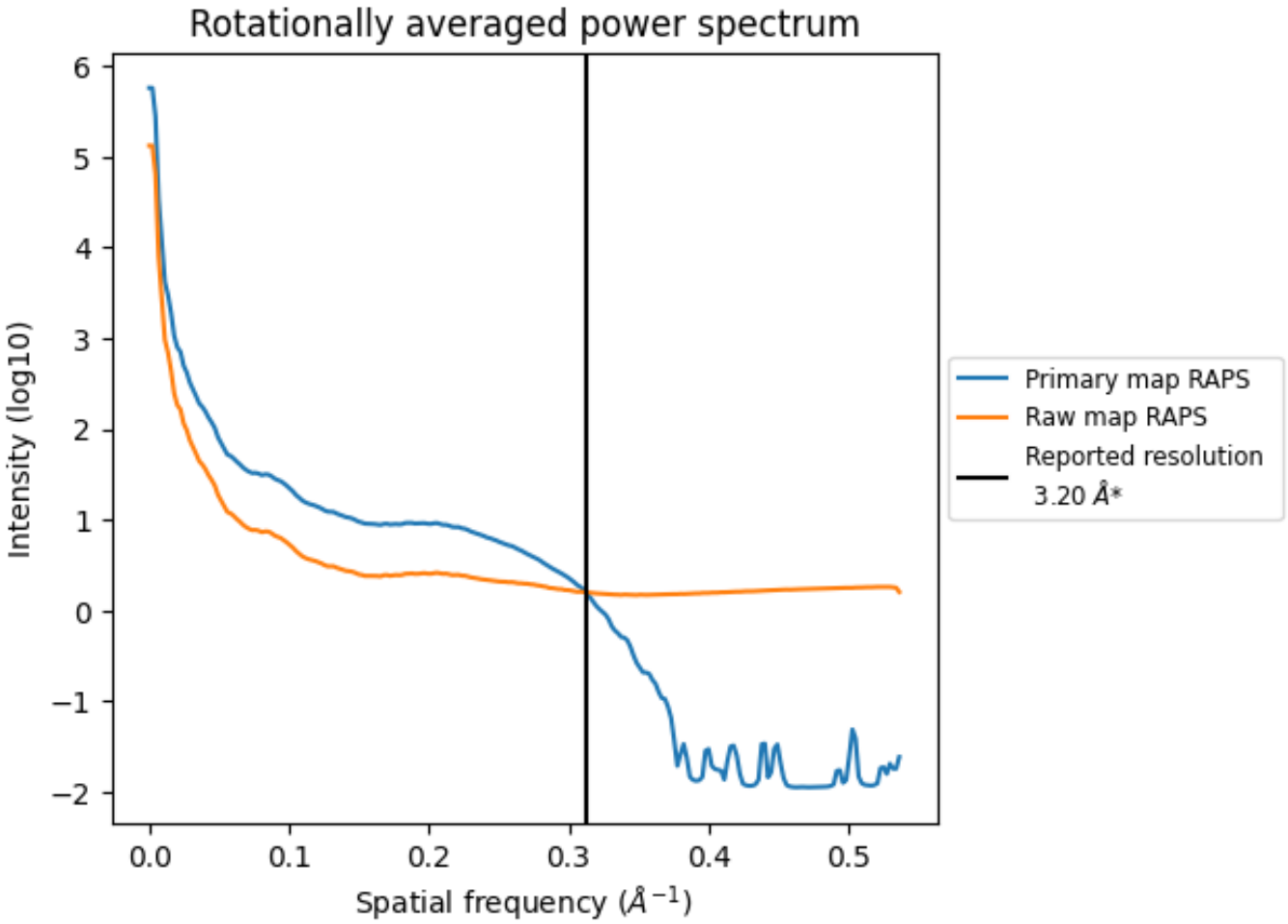
7.2 Volume estimate (i)



The volume at the recommended contour level is 1595 nm^3; this corresponds to an approximate mass of 1441 kDa.

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

7.3 Rotationally averaged power spectrum (i)

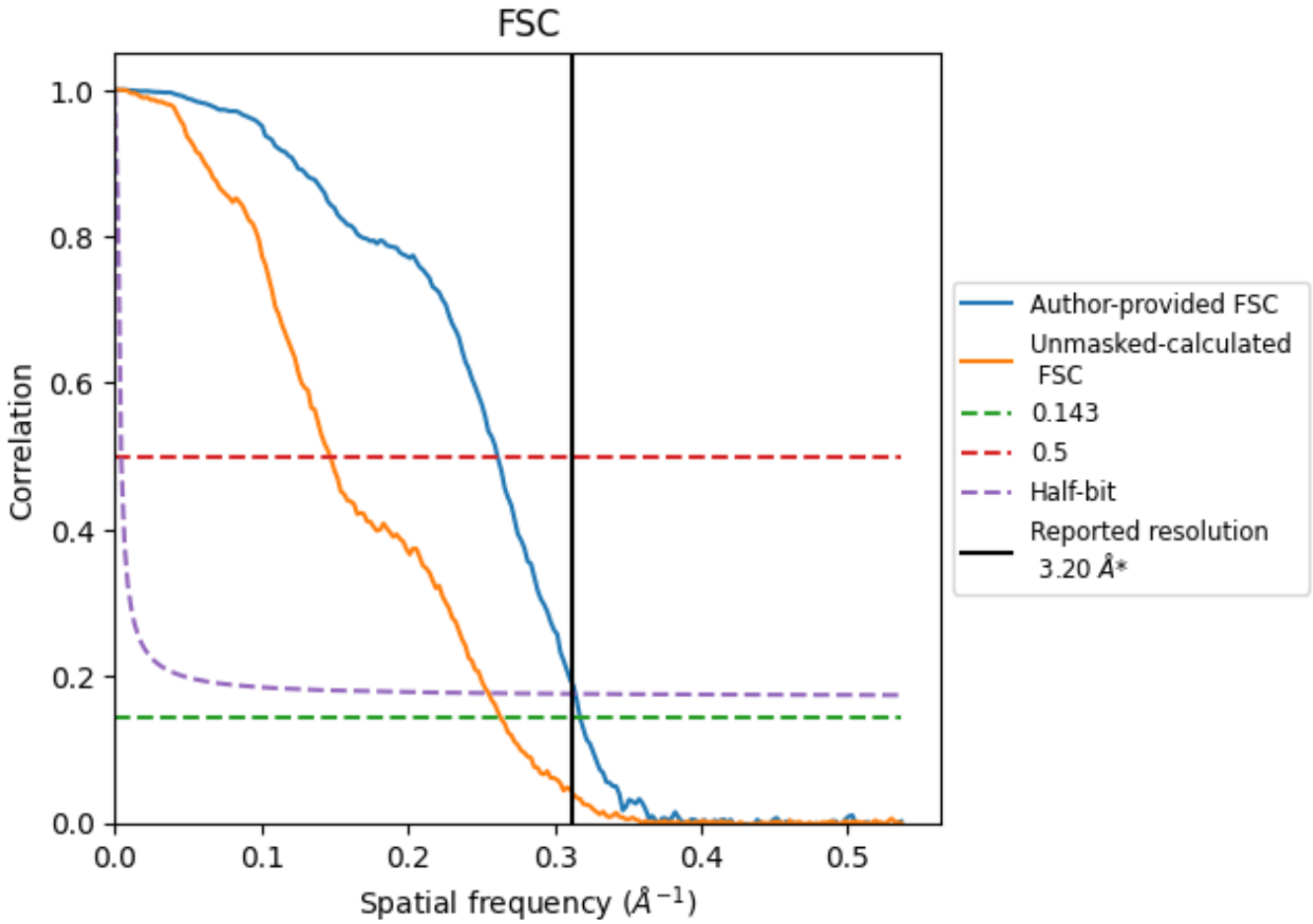


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

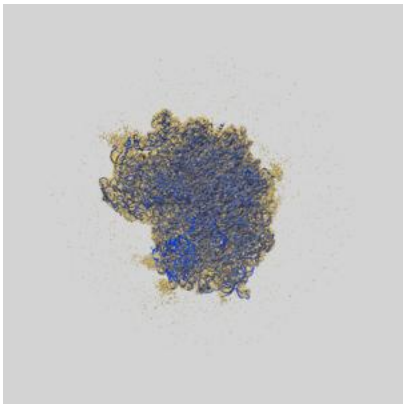
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.83	3.18
Unmasked-calculated*	3.80	6.80	3.92

*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 3.80 differs from the reported value 3.2 by more than 10 %

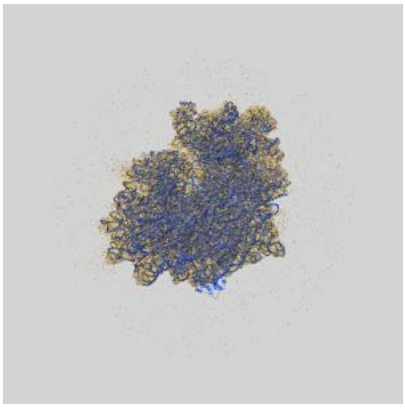
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38631 and PDB model 8XSZ. Per-residue inclusion information can be found in section 3 on page 22.

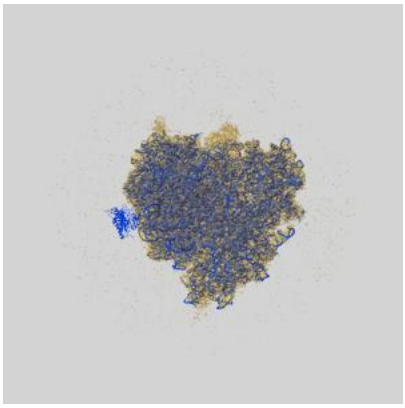
9.1 Map-model overlay



X



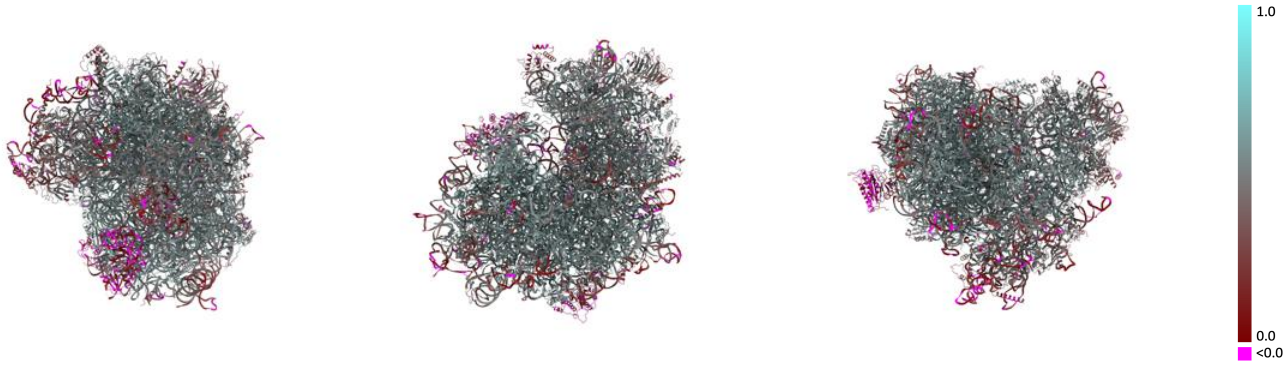
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

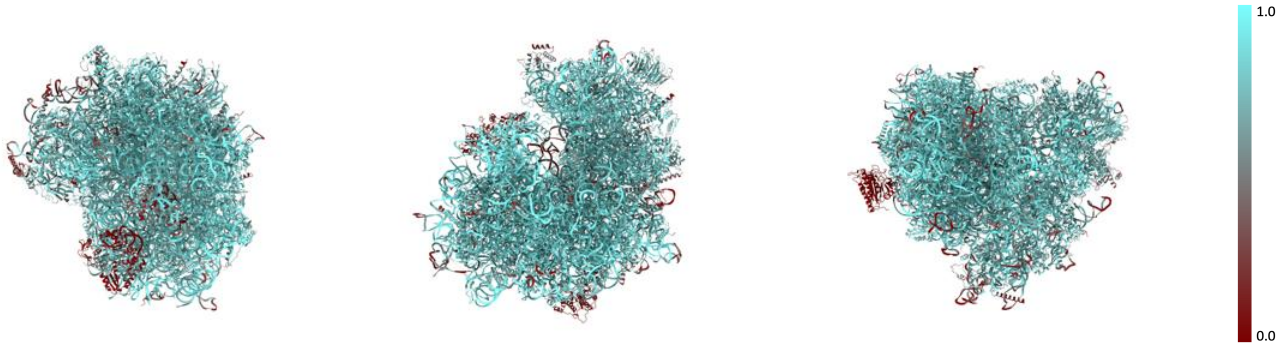
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

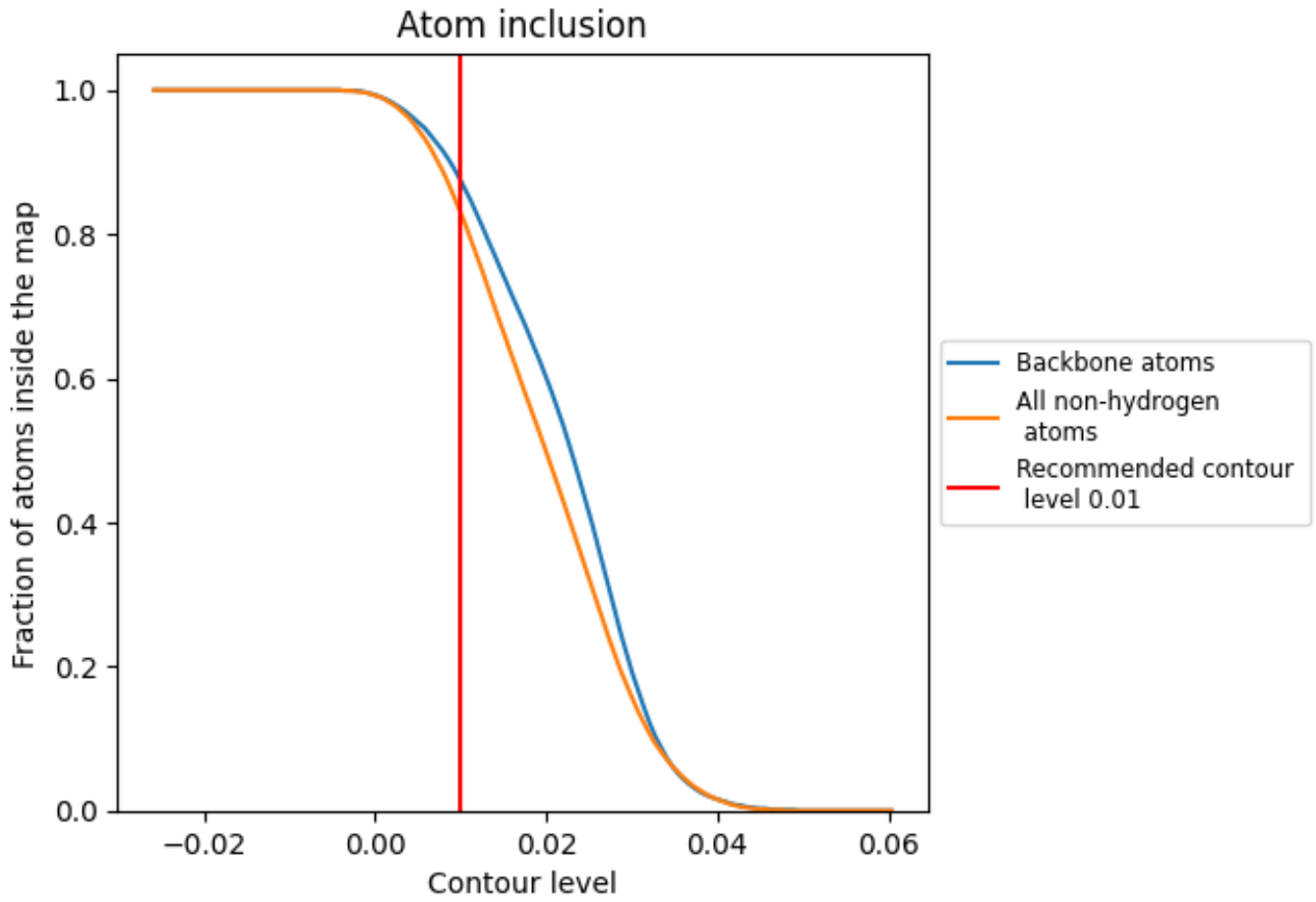
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.8290	0.4770
CA	0.0040	0.0910
CB	0.0560	0.2290
CC	0.8070	0.3670
CD	0.3200	0.2050
CE	0.8920	0.5240
L5	0.8960	0.4880
L7	0.9800	0.5560
L8	0.9180	0.5060
LA	0.8630	0.5640
LB	0.8530	0.5470
LC	0.8410	0.5370
LD	0.8590	0.5160
LE	0.8320	0.5140
LF	0.8540	0.5460
LG	0.7660	0.4840
LH	0.8390	0.5300
LI	0.8690	0.5560
LJ	0.7950	0.4970
LL	0.8210	0.5100
LM	0.8600	0.5330
LN	0.8760	0.5670
LO	0.8550	0.5470
LP	0.8700	0.5530
LQ	0.8680	0.5650
LR	0.7840	0.4920
LS	0.8960	0.5690
LT	0.8340	0.5350
LU	0.7880	0.4740
LV	0.8490	0.5610
LW	0.6100	0.3770
LX	0.8240	0.5340
LY	0.8580	0.5360
LZ	0.8430	0.5260
La	0.8890	0.5650

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Chain	Atom inclusion	Q-score
Lb	0.7560	0.4730
Lc	0.7990	0.5040
Ld	0.8370	0.5270
Le	0.8830	0.5650
Lf	0.8840	0.5660
Lg	0.8160	0.5340
Lh	0.8300	0.5270
Li	0.8310	0.5140
Lj	0.8640	0.5430
Lk	0.7400	0.4740
Ll	0.8560	0.5460
Lm	0.8680	0.5460
Ln	0.8230	0.5370
Lo	0.8420	0.5480
Lp	0.8300	0.5510
Lr	0.8660	0.5500
Ls	0.0910	0.0430
Lt	0.0690	0.0370
S2	0.8820	0.4640
SA	0.8170	0.5130
SB	0.7930	0.5090
SC	0.8210	0.5250
SD	0.7210	0.4600
SE	0.7450	0.4600
SF	0.7400	0.4710
SG	0.6670	0.3930
SH	0.7120	0.4210
SI	0.7350	0.4430
SJ	0.7280	0.4240
SK	0.7840	0.4490
SL	0.7680	0.5040
SM	0.4380	0.2140
SN	0.8290	0.5240
SO	0.8050	0.5090
SP	0.7650	0.4820
SQ	0.7560	0.4860
SR	0.7600	0.4880
SS	0.7950	0.4840
ST	0.7930	0.4940
SU	0.6990	0.4350
SV	0.8150	0.5180
SW	0.8500	0.5480

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Chain	Atom inclusion	Q-score
SX	0.7970	0.5050
SY	0.6830	0.3780
SZ	0.6950	0.4300
Sa	0.8030	0.5200
Sb	0.7860	0.4850
Sc	0.6440	0.4280
Sd	0.8480	0.5120
Se	0.5990	0.3940
Sf	0.5650	0.2700
Sg	0.6900	0.4020