



## wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 07:34 AM UTC

PDB ID : 9EVS / pdb\_00009evs  
EMDB ID : EMD-50011  
Title : Structure of the flowering plant mitoribosome with P-site tRNA  
Authors : Waltz, F.; Skaltsogiannis, V.; Giege, P.  
Deposited on : 2024-04-02  
Resolution : 3.05 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

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

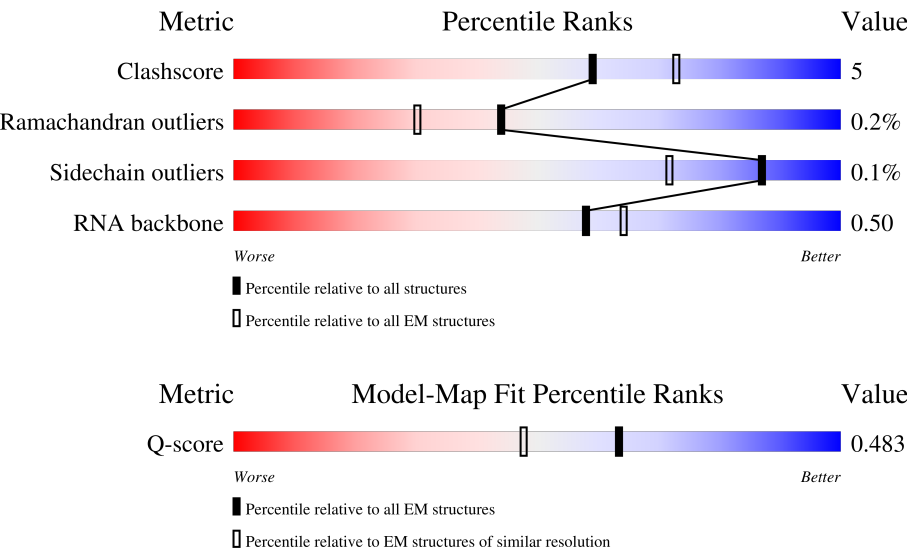


# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13971 ( 2.55 - 3.55 )



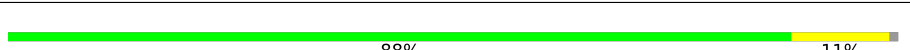
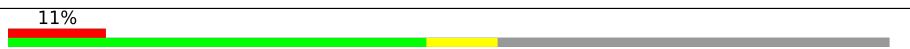
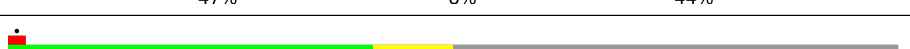
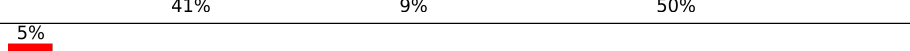
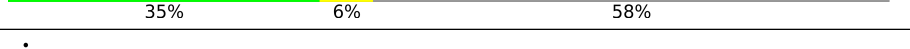





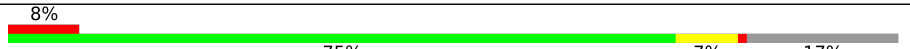


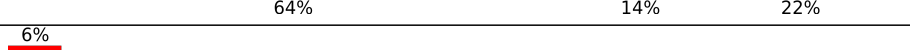


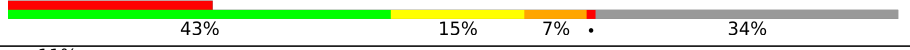





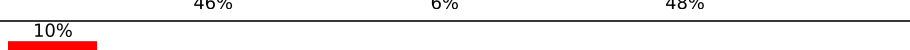
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	554	
2	C	362	
3	D	501	

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	138	
5	F	157	
6	G	129	
7	H	383	
8	I	228	
9	J	304	
10	K	125	
11	L	154	
12	M	155	
13	N	414	
14	O	136	
15	P	110	
16	Q	237	
17	R	212	
18	S	100	
19	T	94	
20	U	192	
21	V	193	
22	W	483	
23	X	496	
24	Y	102	
25	Z	153	
26	1	2922	
27	3	118	
28	1B	220	

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
29	1C	327	
30	1D	319	
31	1E	297	
32	1F	185	
33	1G	102	
34	1H	219	
35	1I	170	
36	1J	156	
37	1K	204	
38	1L	176	
39	1M	281	
40	1N	179	
41	1O	160	
42	1P	114	
43	1Q	233	
44	1R	126	
45	1S	270	
46	1T	264	
47	1U	180	
48	1V	159	
49	1W	249	
50	1X	271	
51	1Y	156	
52	1Z	212	
53	1a	144	

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
54	1b	109	
55	1c	135	
56	1d	139	
57	1e	63	
58	1f	146	
59	1g	162	
60	1h	103	
61	1i	247	
62	1j	90	
63	1k	119	
64	1l	233	
65	1m	128	
66	1o	125	
67	1p	130	
68	1q	79	
69	1r	167	
70	1s	181	
71	1t	491	
72	1u	757	
73	1v	521	
74	1x	4	
75	5	76	
76	2	1591	
77	6	6	
78	a	424	

Continued on next page...



*Continued from previous page...*

Mol	Chain	Length	Quality of chain
79	b	80	
80	c	128	
81	d	110	
82	e	383	
83	f	410	
84	h	384	
85	i	725	
86	j	408	
87	k	155	
88	A	212	



## 2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 211395 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 protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	467	Total	C	N	O	S	0	0
			3877	2520	701	643	13		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	TRP	ARG	conflict	UNP A0A068BCX1
B	172	LEU	SER	conflict	UNP A0A068BCX1
B	202	LYS	ARG	conflict	UNP A0A068BCX1
B	296	LEU	SER	conflict	UNP A0A068BCX1
B	512	CYS	ARG	conflict	UNP A0A068BCX1
B	524	VAL	ALA	conflict	UNP A0A068BCX1
B	533	LEU	SER	conflict	UNP A0A068BCX1

- Molecule 2 is a protein called uS4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	333	Total	C	N	O	S	0	0
			2811	1798	540	462	11		

- Molecule 3 is a protein called uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	417	Total	C	N	O	S	0	0
			3425	2146	603	664	12		

- Molecule 4 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	101	Total	C	N	O	S	0	0
			823	535	145	138	5		

- Molecule 5 is a protein called uS7m, Small ribosomal subunit protein uS7m.



Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	157	Total	C	N	O	S	0	0
			1254	793	244	213	4		

- Molecule 6 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	128	Total	C	N	O	S	0	0
			1037	652	193	189	3		

- Molecule 7 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	213	Total	C	N	O	S	0	0
			1682	1054	312	311	5		

- Molecule 8 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	113	Total	C	N	O	S	0	0
			941	602	174	159	6		

- Molecule 9 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	127	Total	C	N	O	S	0	0
			988	608	195	181	4		

- Molecule 10 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	124	Total	C	N	O	S	0	0
			992	613	208	167	4		

- Molecule 11 is a protein called uS13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	119	Total	C	N	O	S	0	0
			940	572	200	163	5		

- Molecule 12 is a protein called uS14m.



Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	101	Total	C	N	O	S	0	0
			843	524	174	140	5		

- Molecule 13 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	116	Total	C	N	O	S	0	0
			941	593	170	171	7		

- Molecule 14 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	110	Total	C	N	O	S	0	0
			869	550	169	144	6		

- Molecule 15 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	91	Total	C	N	O	S	0	0
			717	455	135	124	3		

- Molecule 16 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	90	Total	C	N	O	S	0	0
			724	460	127	134	3		

- Molecule 17 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	166	Total	C	N	O	S	0	0
			1299	819	236	237	7		

- Molecule 18 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	75	Total	C	N	O	S	0	0
			611	386	120	103	2		

- Molecule 19 is a protein called bTHXm.



Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	50	Total	C	N	O	S	0	0
			408	260	79	68	1		

- Molecule 20 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	127	Total	C	N	O	S	0	0
			1014	647	184	178	5		

- Molecule 21 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	164	Total	C	N	O	S	0	0
			1399	874	266	255	4		

- Molecule 22 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	380	Total	C	N	O	S	0	0
			3062	1955	535	559	13		

- Molecule 23 is a protein called mS31/mS46.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	204	Total	C	N	O	S	0	0
			1613	1011	262	329	11		

- Molecule 24 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	98	Total	C	N	O	S	0	0
			793	495	159	137	2		

- Molecule 25 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	80	Total	C	N	O	S	0	0
			649	422	121	104	2		

- Molecule 26 is a RNA chain called 26S rRNA.



Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	2922	Total	C	N	O	P	5	0
			62518	27942	11365	20289	2922		

- Molecule 27 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	118	Total	C	N	O	P	0	0
			2513	1124	453	819	117		

- Molecule 28 is a protein called uL2m C-ter.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1B	177	Total	C	N	O	S	0	0
			1325	819	259	233	14		

- Molecule 29 is a protein called Large ribosomal subunit protein uL2mz, N-terminal part.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1C	215	Total	C	N	O	S	0	0
			1696	1078	316	296	6		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1C	87	LYS	GLU	conflict	UNP P93311
1C	89	LEU	PHE	conflict	UNP P93311
1C	147	TYR	SER	conflict	UNP P93311
1C	155	SER	GLY	conflict	UNP P93311
1C	190	ASP	GLY	conflict	UNP P93311
1C	195	PRO	ALA	conflict	UNP P93311
1C	199	VAL	ALA	conflict	UNP P93311
1C	200	SER	LYS	conflict	UNP P93311
1C	201	THR	PRO	conflict	UNP P93311
1C	221	TYR	CYS	conflict	UNP P93311
1C	226	TRP	GLY	conflict	UNP P93311
1C	238	ASN	LYS	conflict	UNP P93311

- Molecule 30 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1D	264	Total	C	N	O	S	0	0
			2045	1309	367	358	11		



- Molecule 31 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1E	221	Total	C	N	O	S	0	0
			1753	1104	334	308	7		

- Molecule 32 is a protein called uL5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1F	158	Total	C	N	O	S	0	0
			1286	829	212	236	9		

- Molecule 33 is a protein called uL6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1G	98	Total	C	N	O	S	0	0
			779	508	136	130	5		

- Molecule 34 is a protein called bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1H	66	Total	C	N	O	S	0	0
			539	345	98	94	2		

- Molecule 35 is a protein called uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1I	130	Total	C	N	O	S	0	0
			1036	669	178	184	5		

- Molecule 36 is a protein called uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1J	147	Total	C	N	O	S	0	0
			1129	722	193	205	9		

- Molecule 37 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1K	189	Total	C	N	O	S	0	0
			1526	955	299	265	7		

- Molecule 38 is a protein called uL14m.



Mol	Chain	Residues	Atoms					AltConf	Trace
38	1L	127	Total	C	N	O	S	0	0
			966	609	184	168	5		

- Molecule 39 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1M	210	Total	C	N	O	S	0	0
			1649	1052	321	273	3		

- Molecule 40 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1N	148	Total	C	N	O	S	0	0
			1160	731	230	192	7		

- Molecule 41 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1O	151	Total	C	N	O	S	0	0
			1231	767	244	214	6		

- Molecule 42 is a protein called uL18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1P	113	Total	C	N	O	S	0	0
			878	564	160	149	5		

- Molecule 43 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1Q	122	Total	C	N	O	S	0	0
			1008	641	198	166	3		

- Molecule 44 is a protein called bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1R	110	Total	C	N	O	S	0	0
			915	572	184	154	5		

- Molecule 45 is a protein called bL21m.



Mol	Chain	Residues	Atoms					AltConf	Trace
45	1S	145	Total	C	N	O	S	0	0
			1170	750	207	211	2		

- Molecule 46 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1T	155	Total	C	N	O	S	0	0
			1241	782	249	205	5		

- Molecule 47 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1U	130	Total	C	N	O	S	0	0
			1048	675	190	181	2		

- Molecule 48 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1V	158	Total	C	N	O	S	0	0
			1223	770	229	220	4		

- Molecule 49 is a protein called bL25-2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1W	205	Total	C	N	O	S	0	0
			1588	1006	284	294	4		

- Molecule 50 is a protein called bL25m.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1X	216	Total	C	N	O	S	0	0
			1670	1069	298	302	1		

- Molecule 51 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1Y	98	Total	C	N	O	S	0	0
			768	484	152	131	1		

- Molecule 52 is a protein called bL28m.



Mol	Chain	Residues	Atoms					AltConf	Trace
52	1Z	177	Total	C	N	O	S	0	0
			1441	911	266	255	9		

- Molecule 53 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1a	110	Total	C	N	O	S	0	0
			928	588	172	158	10		

- Molecule 54 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1b	100	Total	C	N	O	S	0	0
			803	504	160	134	5		

- Molecule 55 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1c	59	Total	C	N	O	S	0	0
			489	313	98	73	5		

- Molecule 56 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	1d	49	Total	C	N	O	S	0	0
			379	240	80	55	4		

- Molecule 57 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	1e	54	Total	C	N	O	S	0	0
			459	300	85	72	2		

- Molecule 58 is a protein called bL34m.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	1f	44	Total	C	N	O	0	0
			364	224	88	52		

- Molecule 59 is a protein called bL35m.



Mol	Chain	Residues	Atoms					AltConf	Trace
59	1g	91	Total	C	N	O	S	0	0
			770	496	152	119	3		

- Molecule 60 is a protein called bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	1h	38	Total	C	N	O	S	0	0
			309	190	65	49	5		

- Molecule 61 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	1i	183	Total	C	N	O	S	0	0
			1424	885	255	274	10		

- Molecule 62 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	1j	71	Total	C	N	O	S	0	0
			570	369	102	97	2		

- Molecule 63 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	1k	118	Total	C	N	O	S	0	0
			952	599	184	165	4		

- Molecule 64 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	1l	211	Total	C	N	O	S	0	0
			1741	1131	286	316	8		

- Molecule 65 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	1m	122	Total	C	N	O	S	0	0
			970	610	170	184	6		

- Molecule 66 is a protein called mL54.



Mol	Chain	Residues	Atoms				AltConf	Trace
66	1o	76	Total	C	N	O	0	0
			626	397	114	115		

- Molecule 67 is a protein called mL59/mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	1p	117	Total	C	N	O	S	0	0
			992	626	189	169	8		

- Molecule 68 is a protein called mL60.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	1q	50	Total	C	N	O	S	0	0
			390	243	79	67	1		

- Molecule 69 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	1r	92	Total	C	N	O	S	0	0
			735	469	139	122	5		

- Molecule 70 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	1s	118	Total	C	N	O	S	0	0
			985	617	203	163	2		

- Molecule 71 is a protein called mL101 (rPPR4).

Mol	Chain	Residues	Atoms					AltConf	Trace
71	1t	484	Total	C	N	O	S	0	0
			3856	2433	665	733	25		

- Molecule 72 is a protein called mL102 (rPPR5).

Mol	Chain	Residues	Atoms					AltConf	Trace
72	1u	666	Total	C	N	O	S	0	0
			5264	3316	915	991	42		

- Molecule 73 is a protein called mL104 (rPPR9).



Mol	Chain	Residues	Atoms					AltConf	Trace
73	1v	433	Total	C	N	O	S	0	0
			3440	2173	599	640	28		

- Molecule 74 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
74	1x	4	Total	C	N	O	0	0
			19	11	4	4		

- Molecule 75 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	5	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 76 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	2	1591	Total	C	N	O	P	0	0
			34081	15222	6213	11055	1591		

- Molecule 77 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	6	6	Total	C	N	O	P	0	0
			130	59	27	38	6		

- Molecule 78 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	a	315	Total	C	N	O	S	0	0
			2487	1547	448	482	10		

- Molecule 79 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	b	77	Total	C	N	O	S	0	0
			610	378	116	108	8		

- Molecule 80 is a protein called mS38.



Mol	Chain	Residues	Atoms					AltConf	Trace
80	c	26	Total	C	N	O	S	0	0
			232	145	54	32	1		

- Molecule 81 is a protein called mS41.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	d	78	Total	C	N	O	S	0	0
			616	403	110	102	1		

- Molecule 82 is a protein called mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	e	246	Total	C	N	O	S	0	0
			2074	1310	374	380	10		

- Molecule 83 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	f	377	Total	C	N	O	S	0	0
			2922	1843	486	573	20		

- Molecule 84 is a protein called mS83 (rPPR10).

Mol	Chain	Residues	Atoms					AltConf	Trace
84	h	310	Total	C	N	O	S	0	0
			2460	1551	436	458	15		

- Molecule 85 is a protein called mS77 (NFD5).

Mol	Chain	Residues	Atoms					AltConf	Trace
85	i	306	Total	C	N	O	S	0	0
			2487	1567	419	487	14		

- Molecule 86 is a protein called mS76 (rPPR1).

Mol	Chain	Residues	Atoms					AltConf	Trace
86	j	381	Total	C	N	O	S	0	0
			2984	1885	510	567	22		

- Molecule 87 is a protein called mS86.



Mol	Chain	Residues	Atoms					AltConf	Trace
87	k	47	Total	C	N	O	S	0	0
			314	194	61	55	4		

- Molecule 88 is a protein called uS2m.

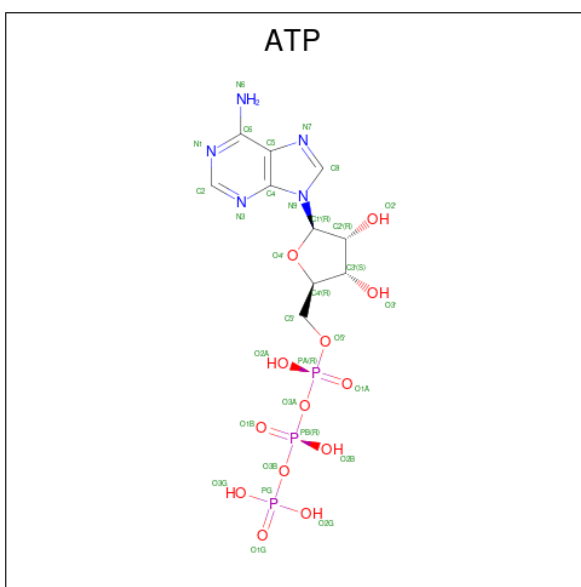
Mol	Chain	Residues	Atoms					AltConf	Trace
88	A	204	Total	C	N	O	S	0	0
			1611	1032	284	285	10		

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	T	1	Total	Mg	0
			1	1	
89	W	1	Total	Mg	0
			1	1	
89	1	249	Total	Mg	0
			249	249	
89	3	3	Total	Mg	0
			3	3	
89	1D	1	Total	Mg	0
			1	1	
89	1h	1	Total	Mg	0
			1	1	
89	1j	1	Total	Mg	0
			1	1	
89	1q	2	Total	Mg	0
			2	2	
89	2	98	Total	Mg	0
			98	98	

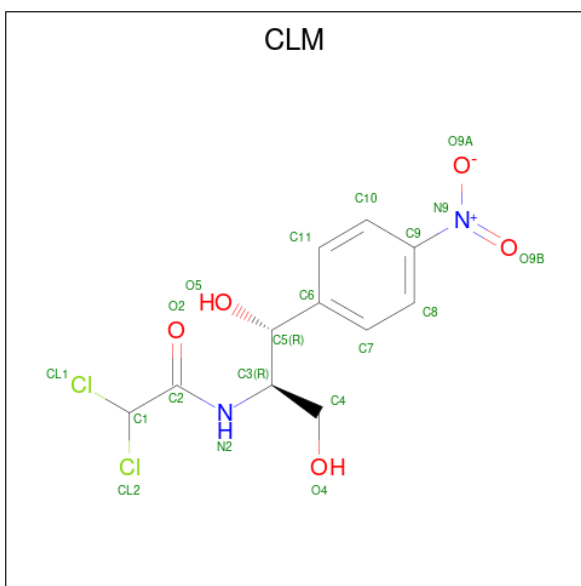
- Molecule 90 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).





Mol	Chain	Residues	Atoms					AltConf
90	W	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 91 is CHLORAMPHENICOL (CCD ID: CLM) (formula:  $C_{11}H_{12}Cl_2N_2O_5$ ).



Mol	Chain	Residues	Atoms					AltConf
91	1	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

- Molecule 92 is POTASSIUM ION (CCD ID: K) (formula: K).



Mol	Chain	Residues	Atoms		AltConf
92	1	56	Total 56	K 56	0
92	1B	3	Total 3	K 3	0
92	1E	1	Total 1	K 1	0
92	2	14	Total 14	K 14	0

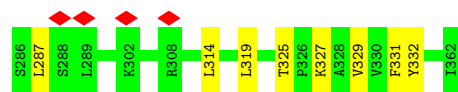
- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
93	1d	1	Total 1	Zn 1	0
93	1h	1	Total 1	Zn 1	0

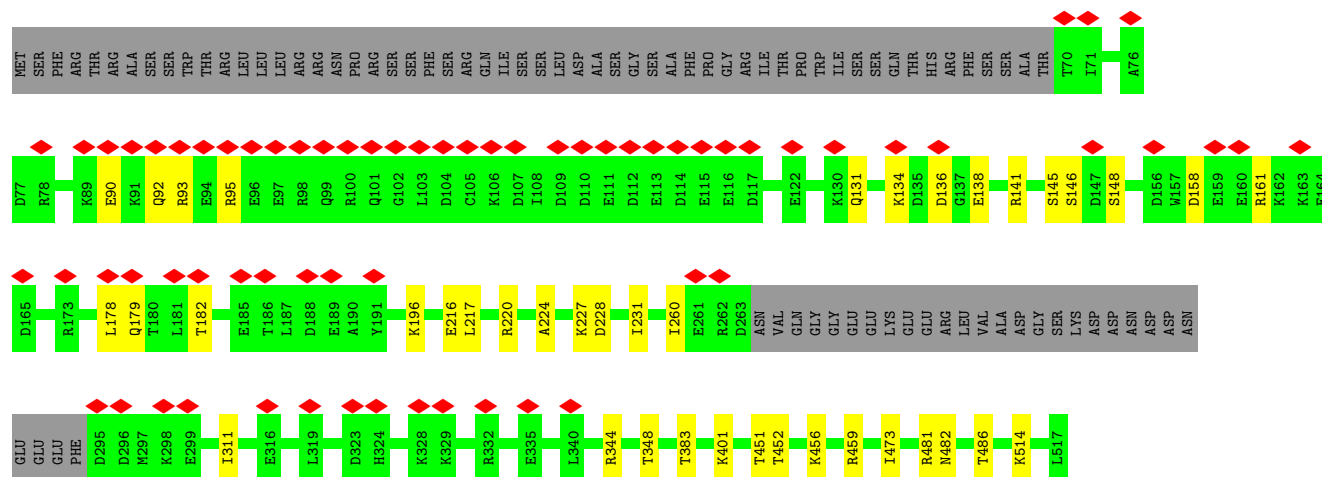
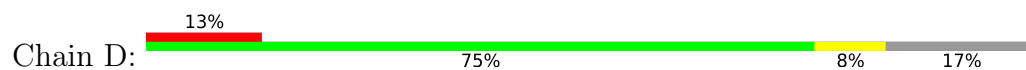




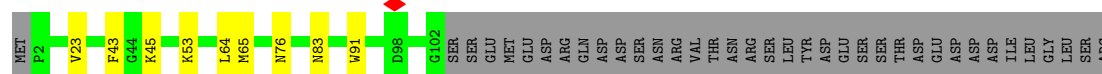




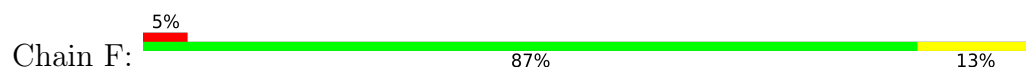
- Molecule 3: uS5m



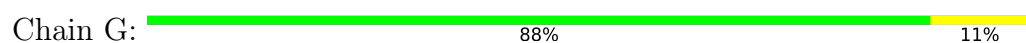
- Molecule 4: bS6m



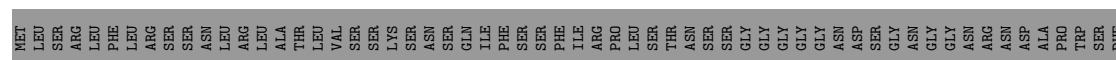
- Molecule 5: uS7m, Small ribosomal subunit protein uS7m



- Molecule 6: uS8m

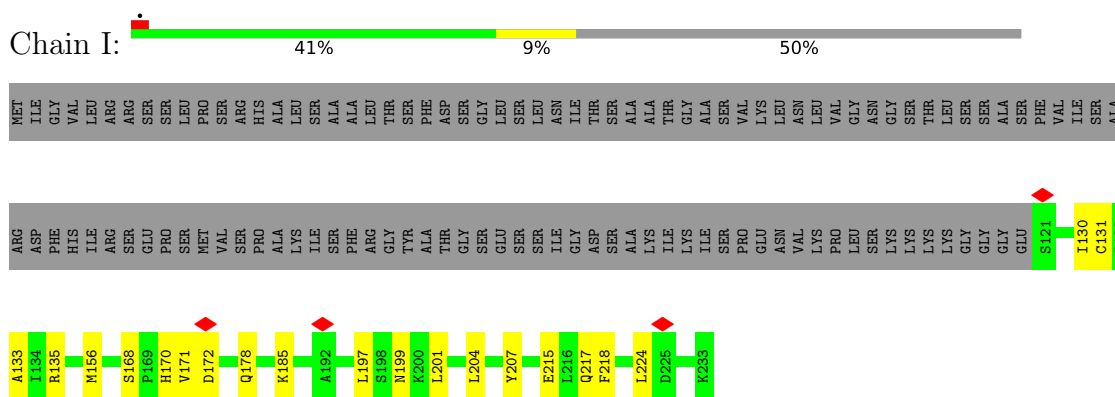


- Molecule 7: uS9m

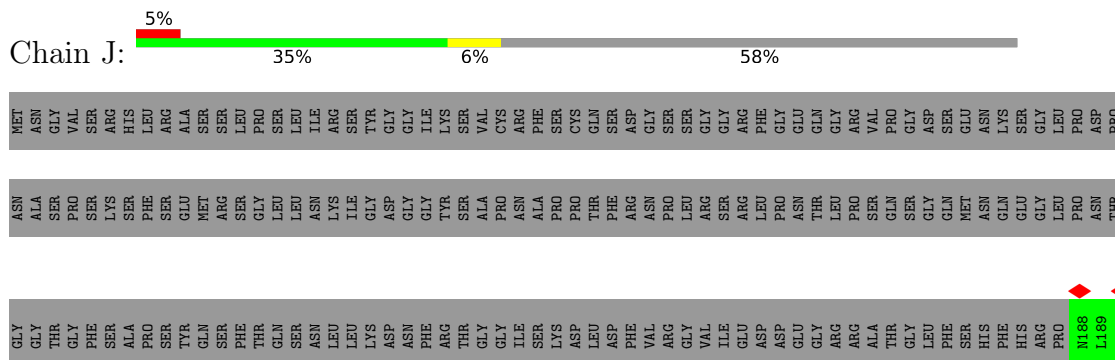




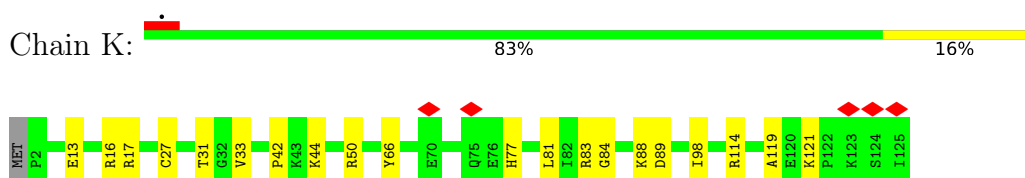
- Molecule 8: uS10m



- Molecule 9: uS11m



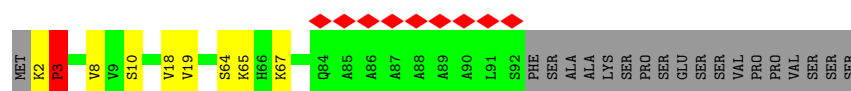
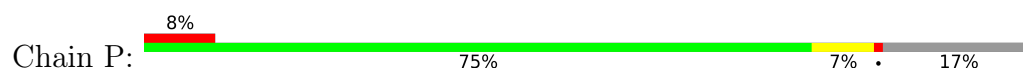
- Molecule 10: uS12m



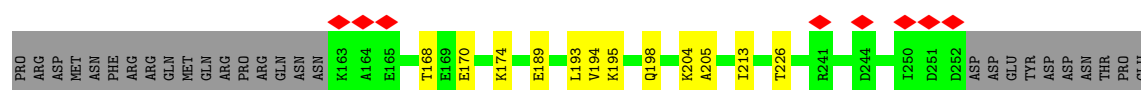
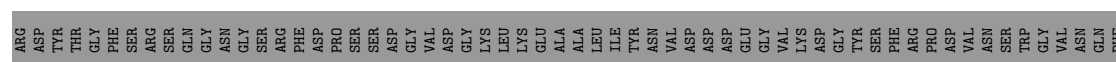
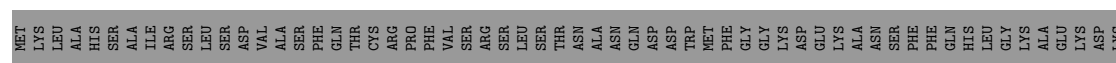




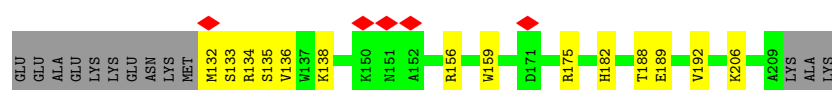
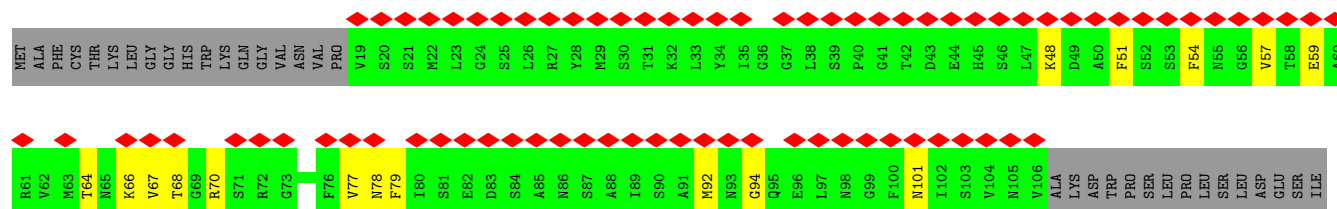
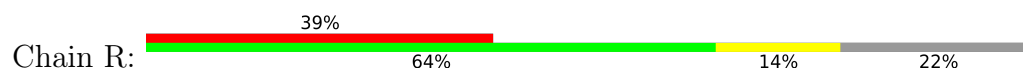




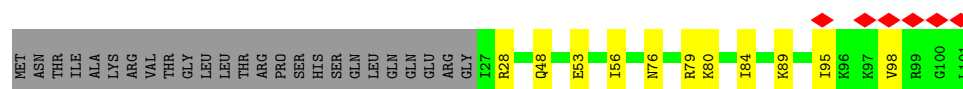
• Molecule 16: bS18m



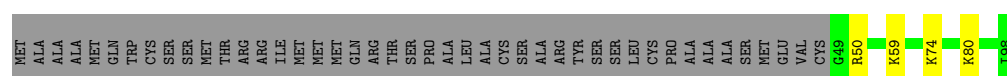
• Molecule 17: uS19m



• Molecule 18: bS21m



• Molecule 19: bTHXm



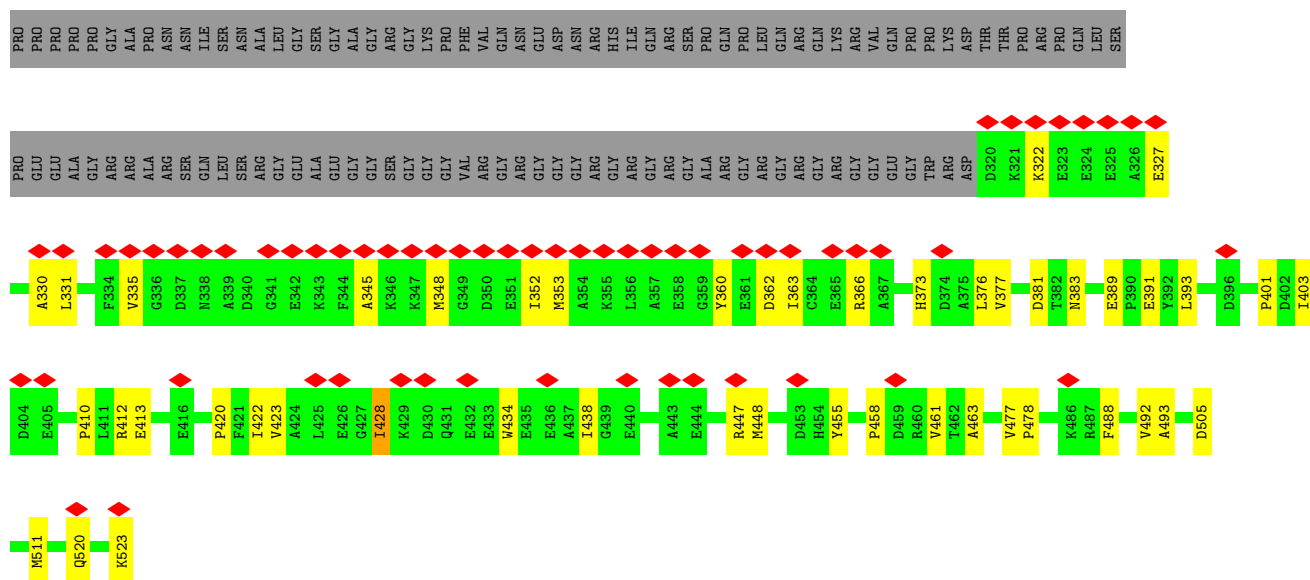
• Molecule 20: mS23



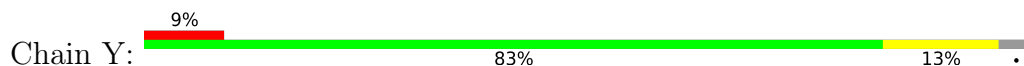




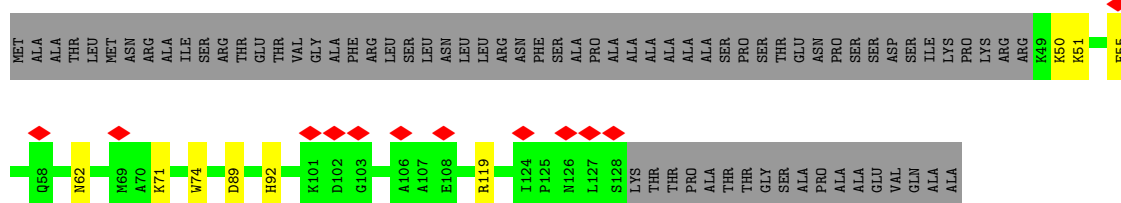




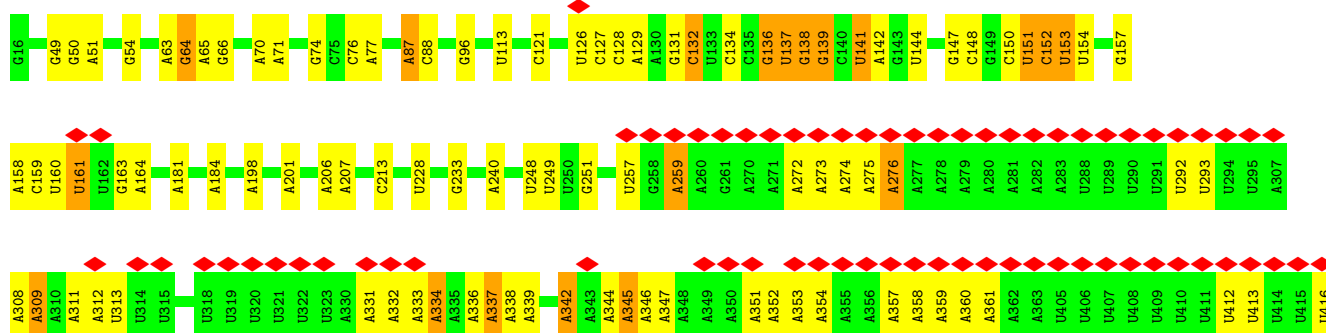
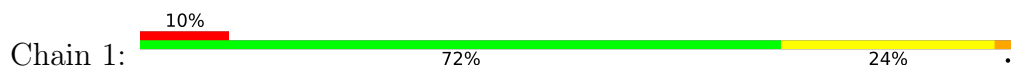
### • Molecule 24: mS33



### • Molecule 25: mS34



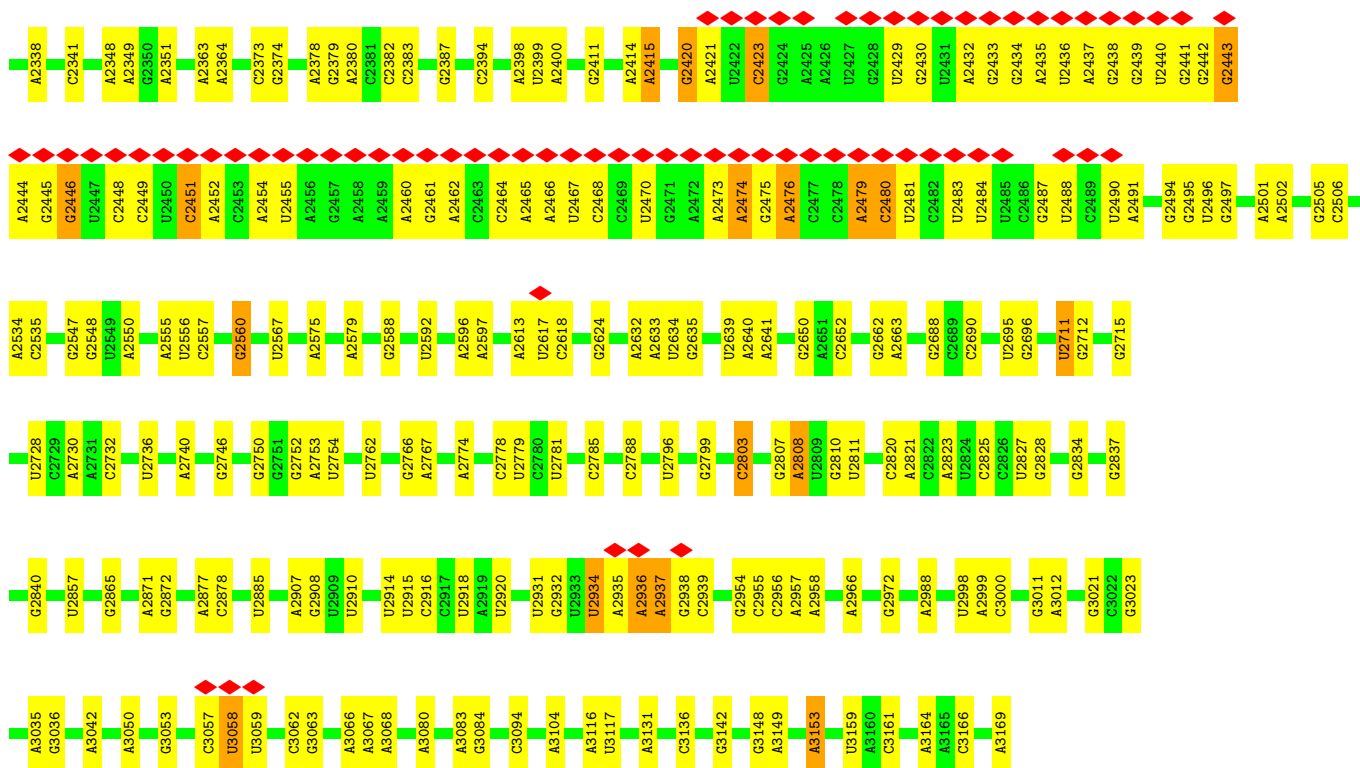
### • Molecule 26: 26S rRNA





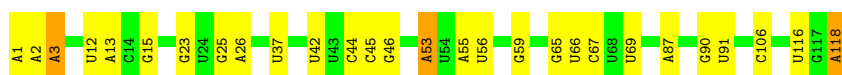






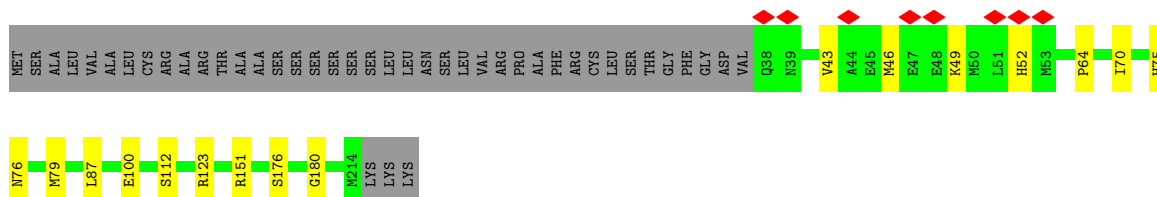
• Molecule 27: 5S rRNA

Chain 3: 76% 21% .



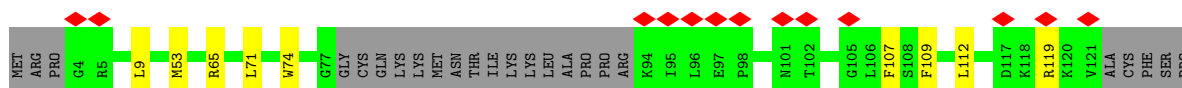
• Molecule 28: uL2m C-ter

Chain 1B: 73% 7% 20%

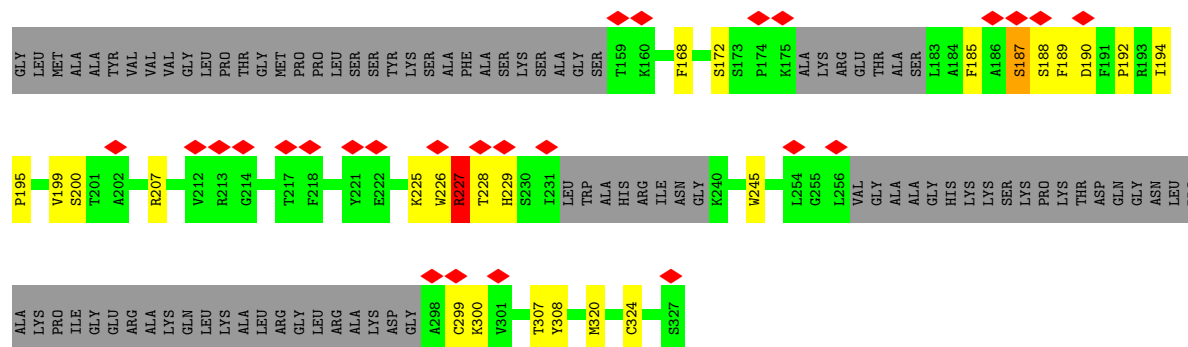


• Molecule 29: Large ribosomal subunit protein uL2mz, N-terminal part

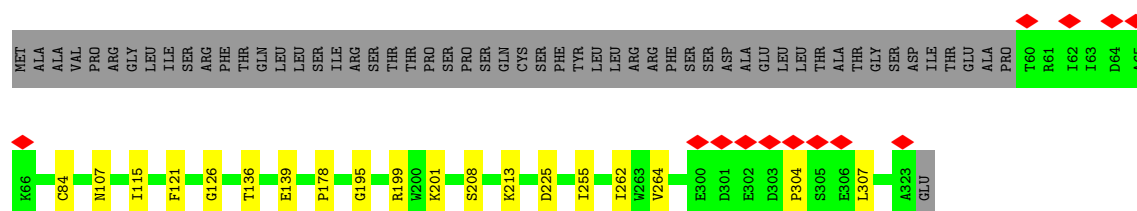
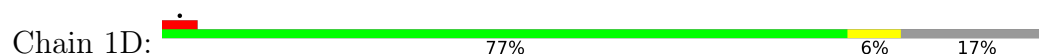
Chain 1C: 12% 55% 10% 34%



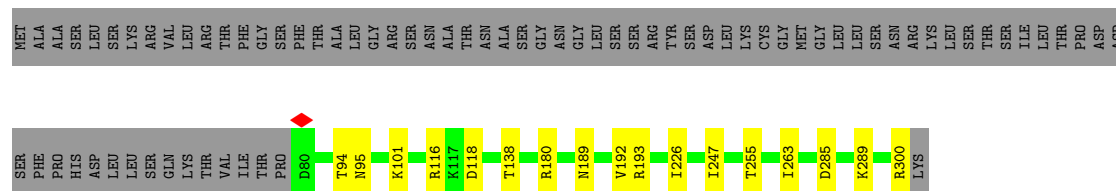




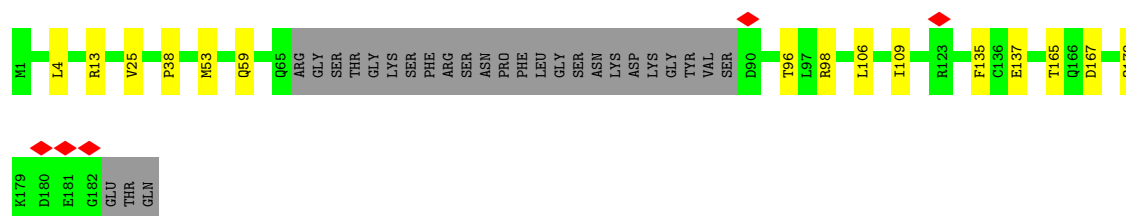
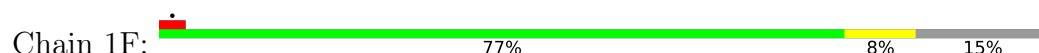
• Molecule 30: uL3m



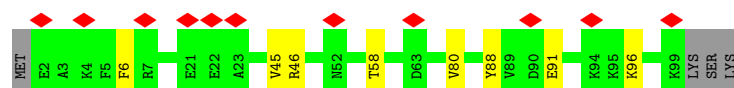
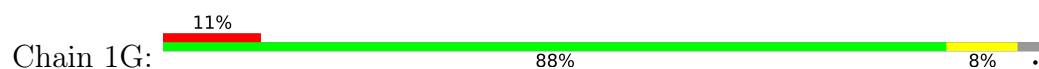
• Molecule 31: uL4m



• Molecule 32: uL5m

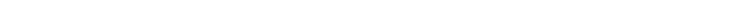


• Molecule 33: uL6m

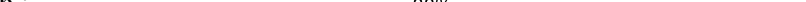




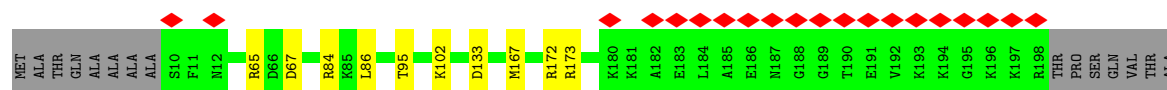
Chain 1H: 

Chain 1I: 

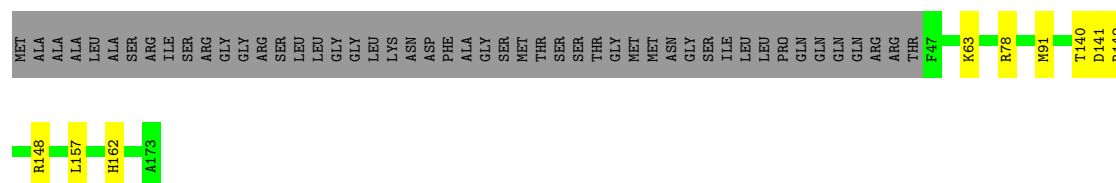
Chain 1J:  90% 71% 21% 6%

Chain 1K: 

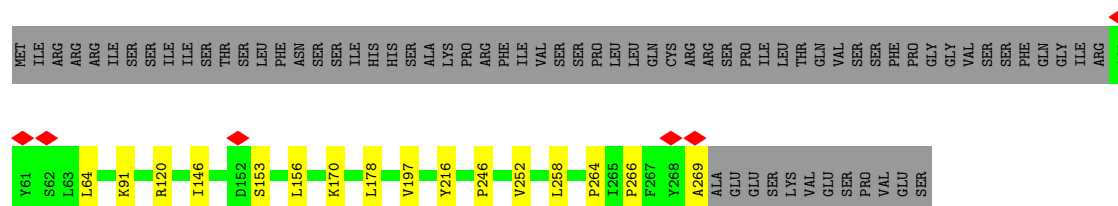




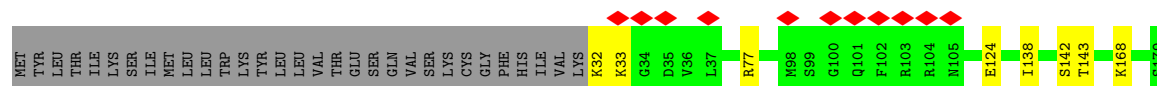
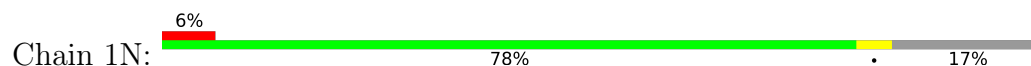
## • Molecule 38: uL14m



## • Molecule 39: uL15m



## • Molecule 40: uL16m



## • Molecule 41: bL17m



## • Molecule 42: uL18m

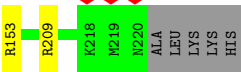
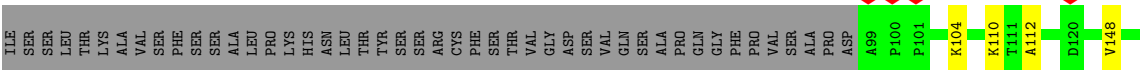


## • Molecule 43: bL19m

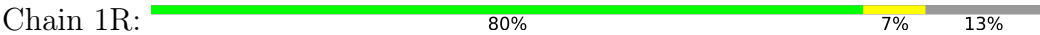




MET GLN SER SER ILE ARG SER SER THR ARG LEU LEU HIS ARG ASN ARG PHE SER ASN ALA ASN THR THR LEU SER PRO SER ARG PHE THR SER SER SER SER PRO THR LEU PRO ALA SER ASN PRO GLN SER ARG THR VAL ARG GLY PHE ASP SER ARG ARG THR GLY ALA PHE ASP SER ARG ARG THR ALA PHE ASP



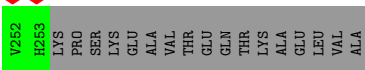
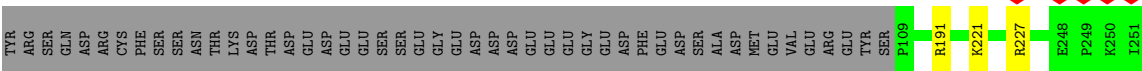
● Molecule 44: bL20m



● Molecule 45: bL21m



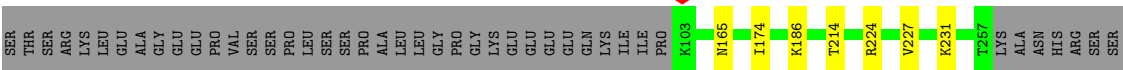
MET ALA SER SER ILE ARG SER SER THR ARG LEU LEU HIS ARG ASN ARG PHE SER ASN ALA ASN THR THR TYR THR SER SER GLN CYS PHE THR SER VAL GLN SER ALA PRO GLN GLY PHE ASP SER ARG ARG THR GLY ALA PHE ASP SER ARG ARG THR ALA PHE ASP



● Molecule 46: uL22m



MET ALA SER SER ILE ARG SER SER THR ARG LEU LEU HIS ARG ASN ARG PHE SER ASN ALA ASN THR THR TYR THR SER SER GLN CYS PHE THR SER VAL GLN SER ALA PRO GLN GLY PHE ASP SER ARG ARG THR GLY ALA PHE ASP SER ARG ARG THR ALA PHE ASP



GLU LEU VAL PRO SER ARG

● Molecule 47: uL23m

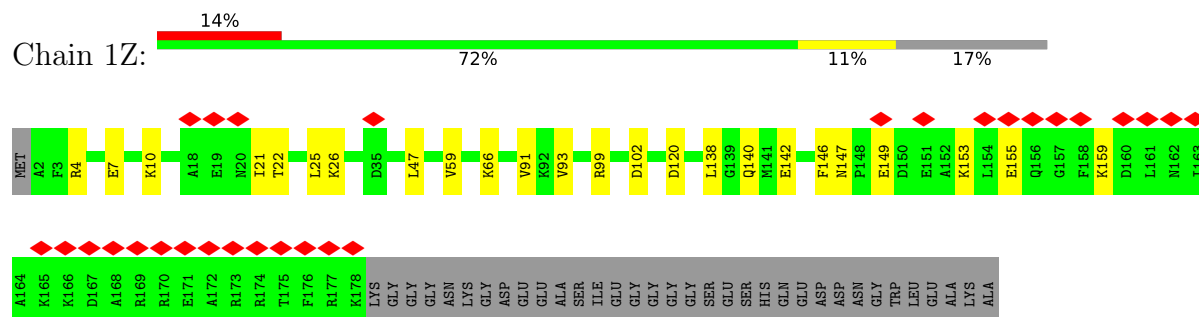




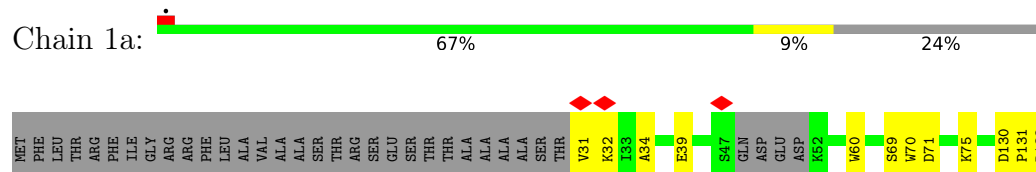




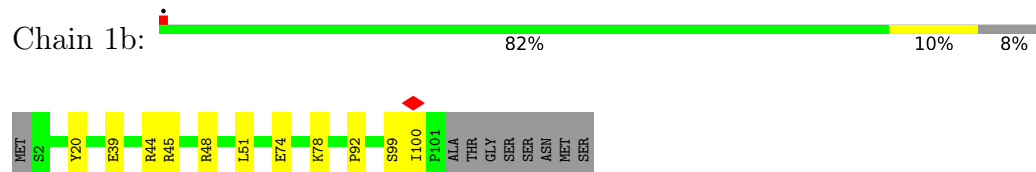
- Molecule 52: bL28m



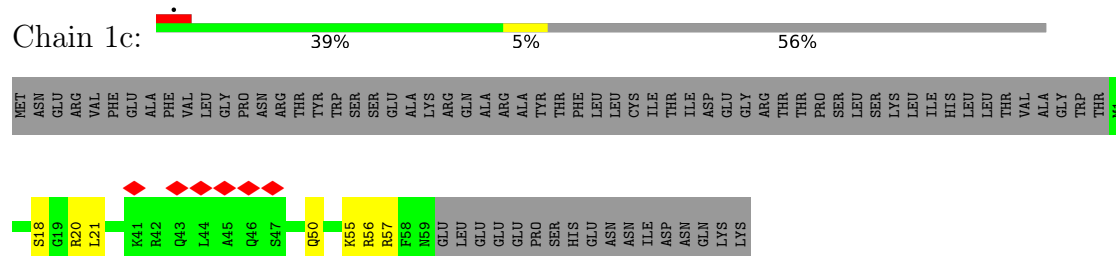
- Molecule 53: uL29m



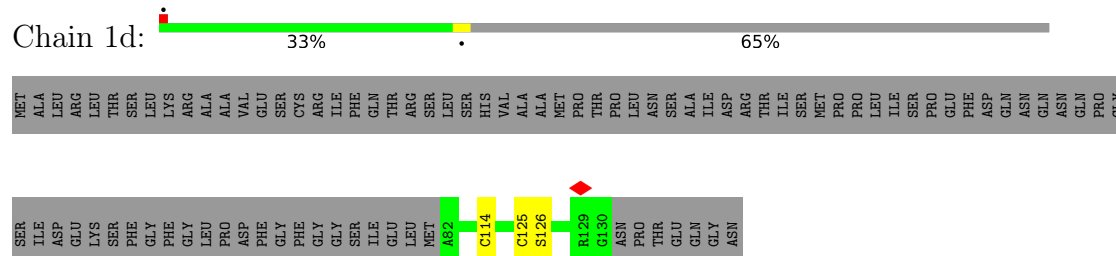
- Molecule 54: uL30m



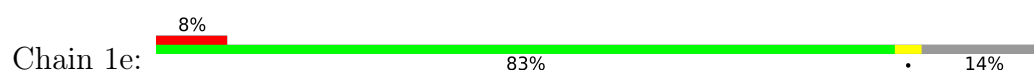
- Molecule 55: bL31m



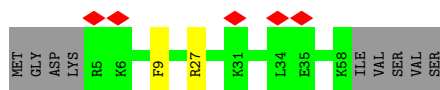
- Molecule 56: bL32m



- Molecule 57: bL33m

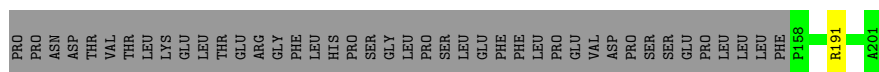






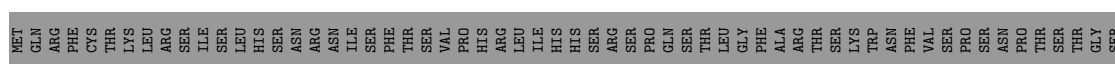
• Molecule 58: bL34m

Chain 1f: 29% 70%



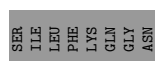
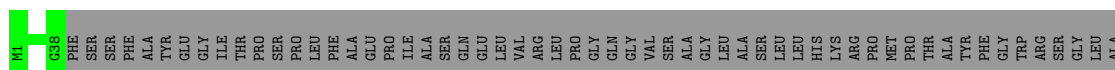
• Molecule 59: bL35m

Chain 1g: 51% 6% 44%



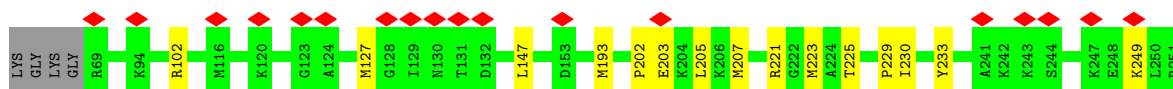
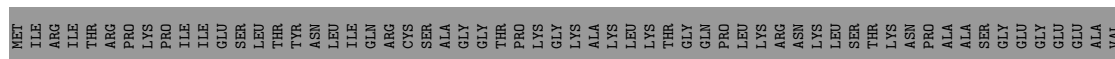
• Molecule 60: bL36m

Chain 1h: 37% 63%



• Molecule 61: mL40

Chain 1i: 7% 68% 6% 26%



• Molecule 62: mL41

Chain 1j: 71% 8% 21%






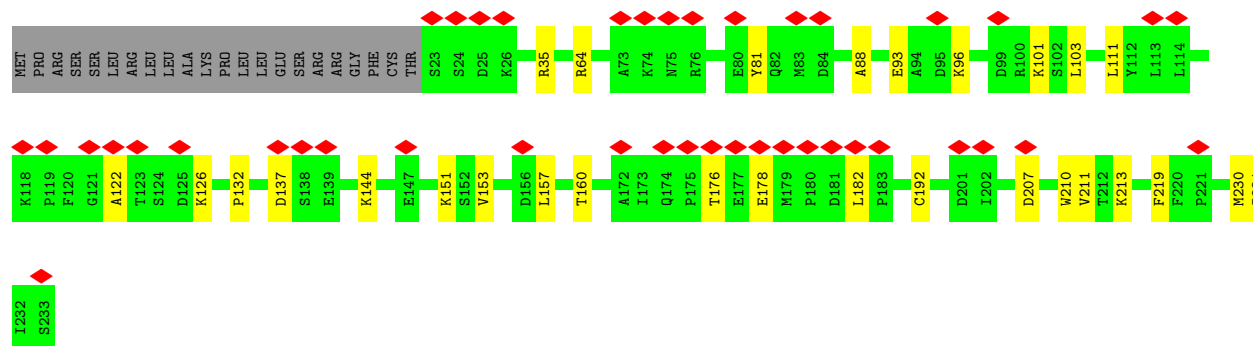
- Molecule 63: mL43

Chain 1k: 




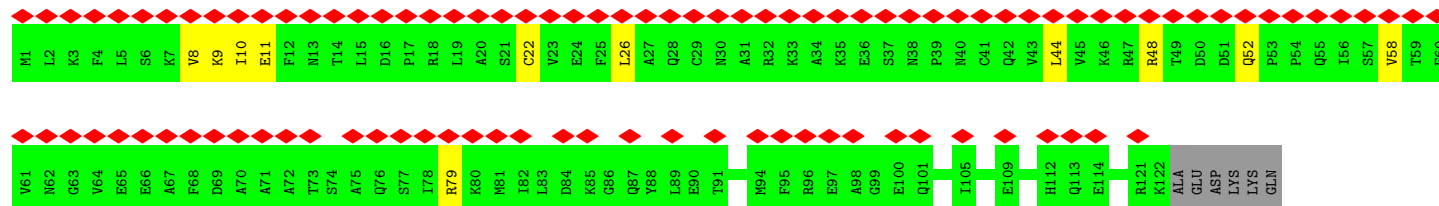
- Molecule 64: mL46

Chain 1l: 



- Molecule 65: mL53

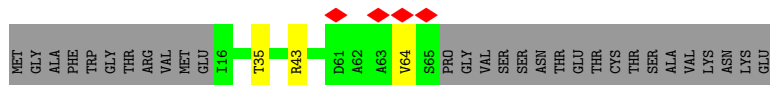
Chain 1m: 



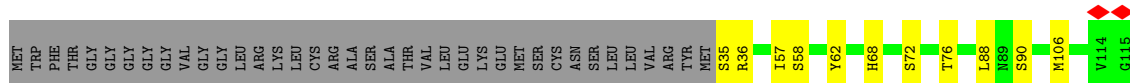




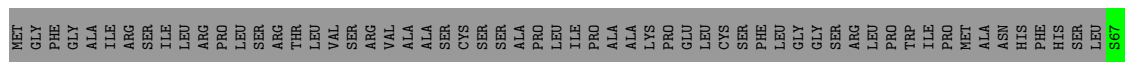
- Molecule 68: mL60



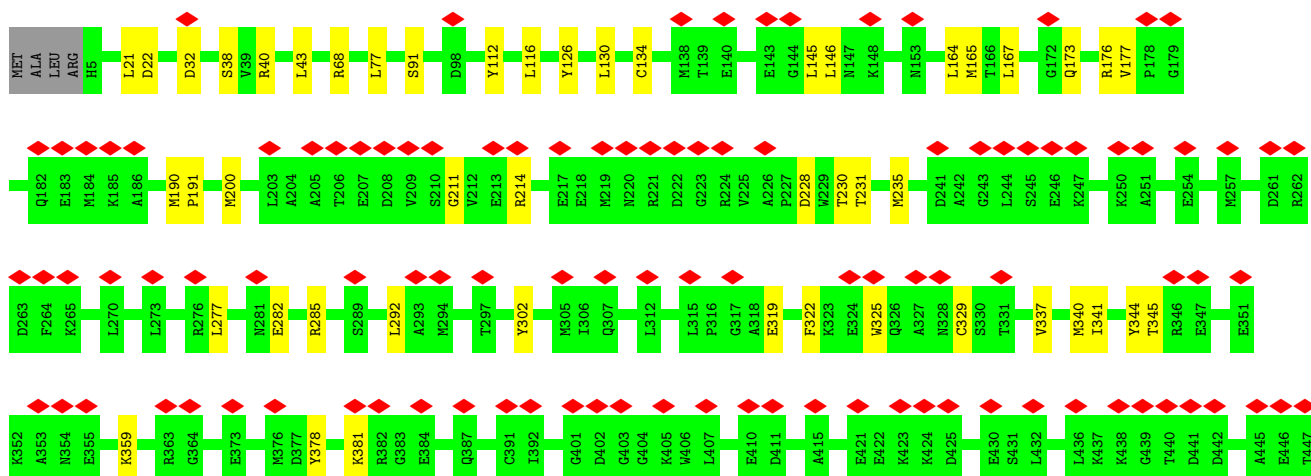
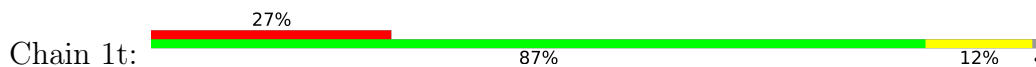
- Molecule 69: mL80



- Molecule 70: mL87



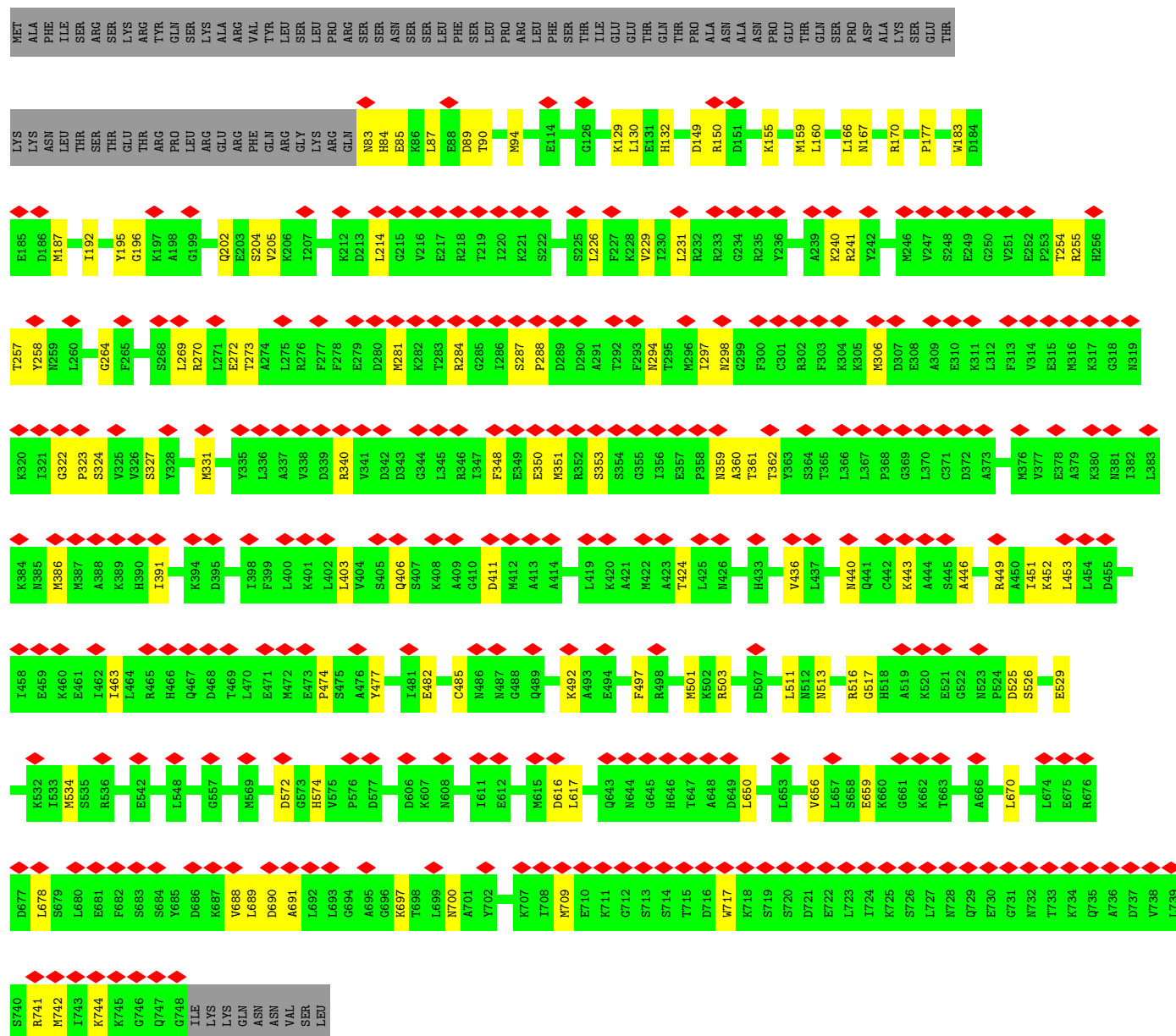
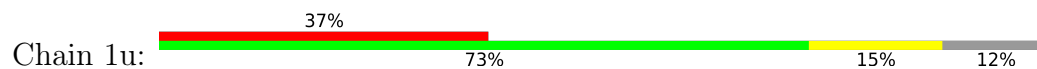
- Molecule 71: mL101 (rPPR4)



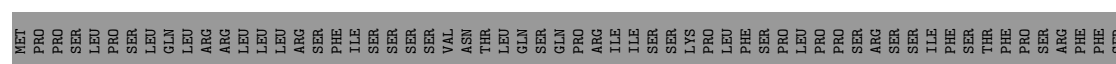
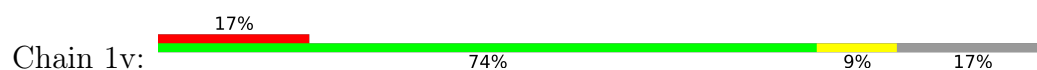




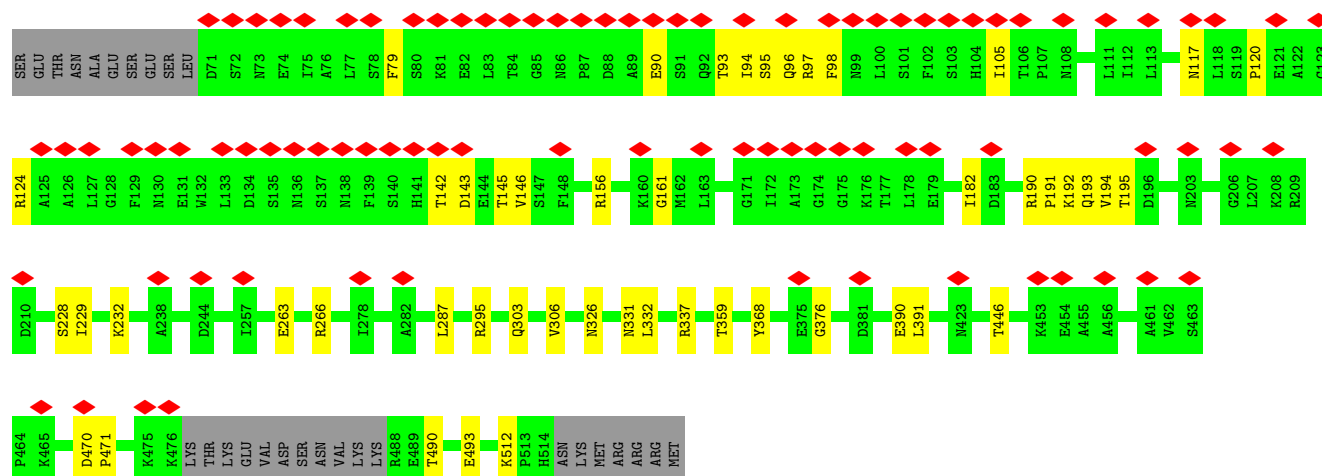
• Molecule 72: mL102 (rPPR5)



• Molecule 73: mL104 (rPPR9)







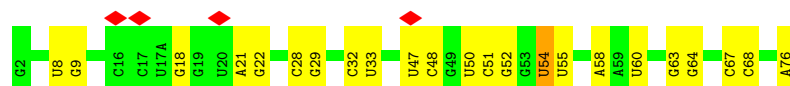
- Molecule 74: Nascent peptide

Chain 1x: 100%

There are no outlier residues recorded for this chain.

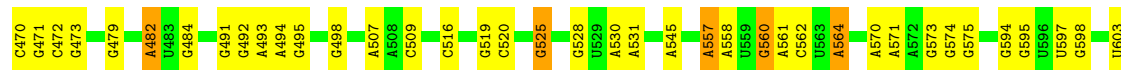
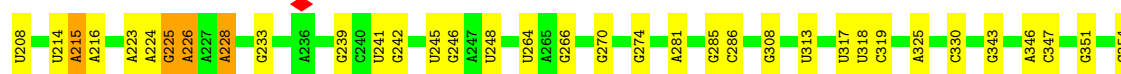
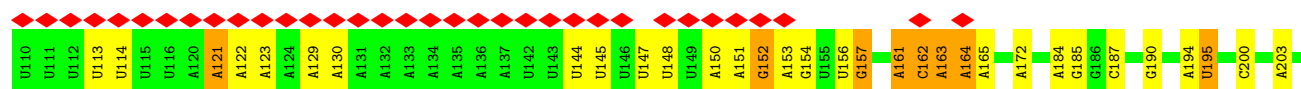
- Molecule 75: tRNA

Chain 5: 5% 70% 29%

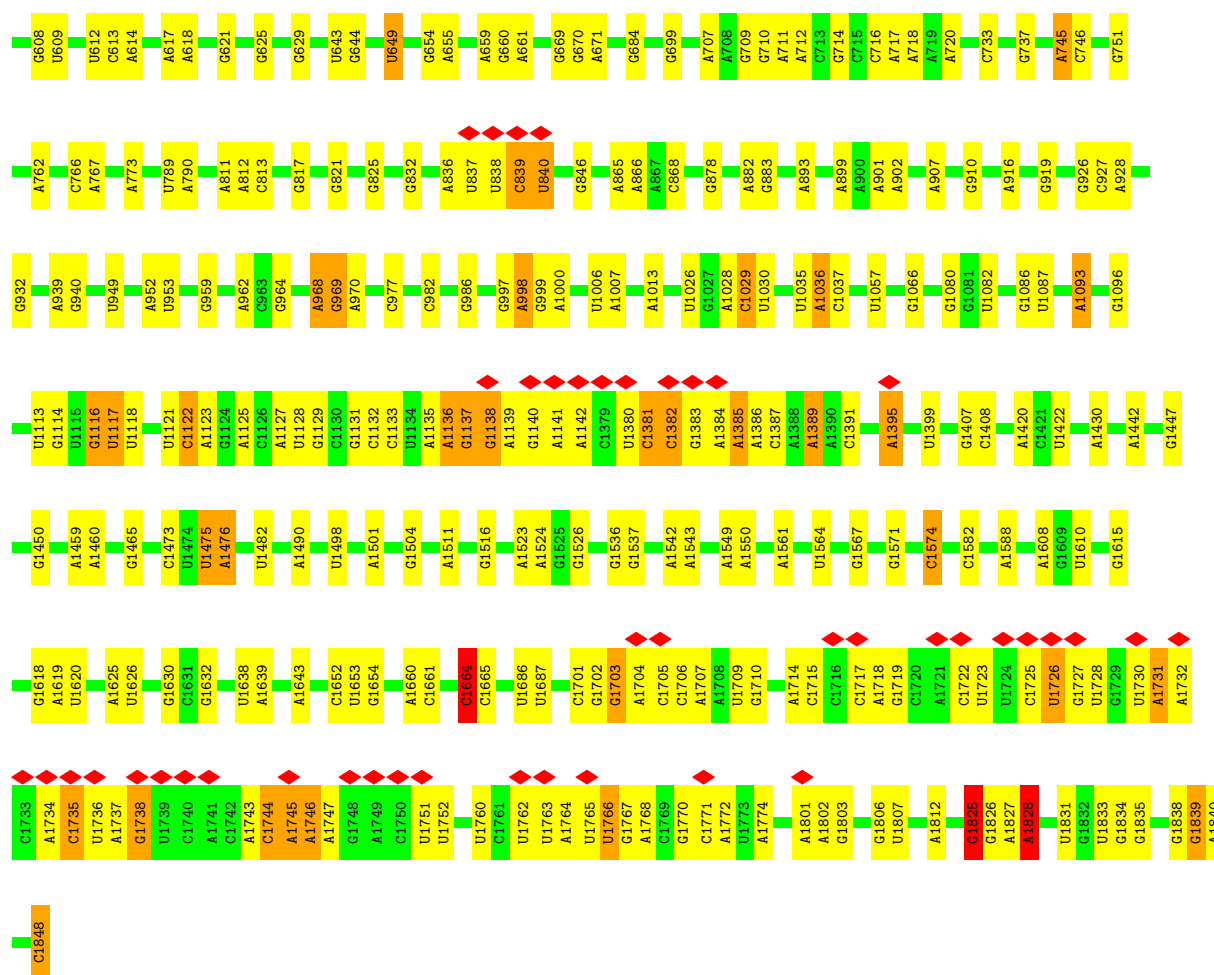


- Molecule 76: 18S rRNA

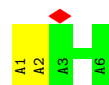
Chain 2: 7% 72% 25%







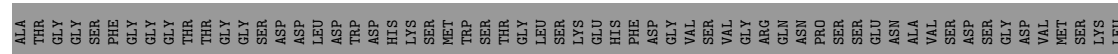
- Molecule 77: mRNA



- Molecule 78: mS35



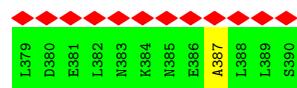




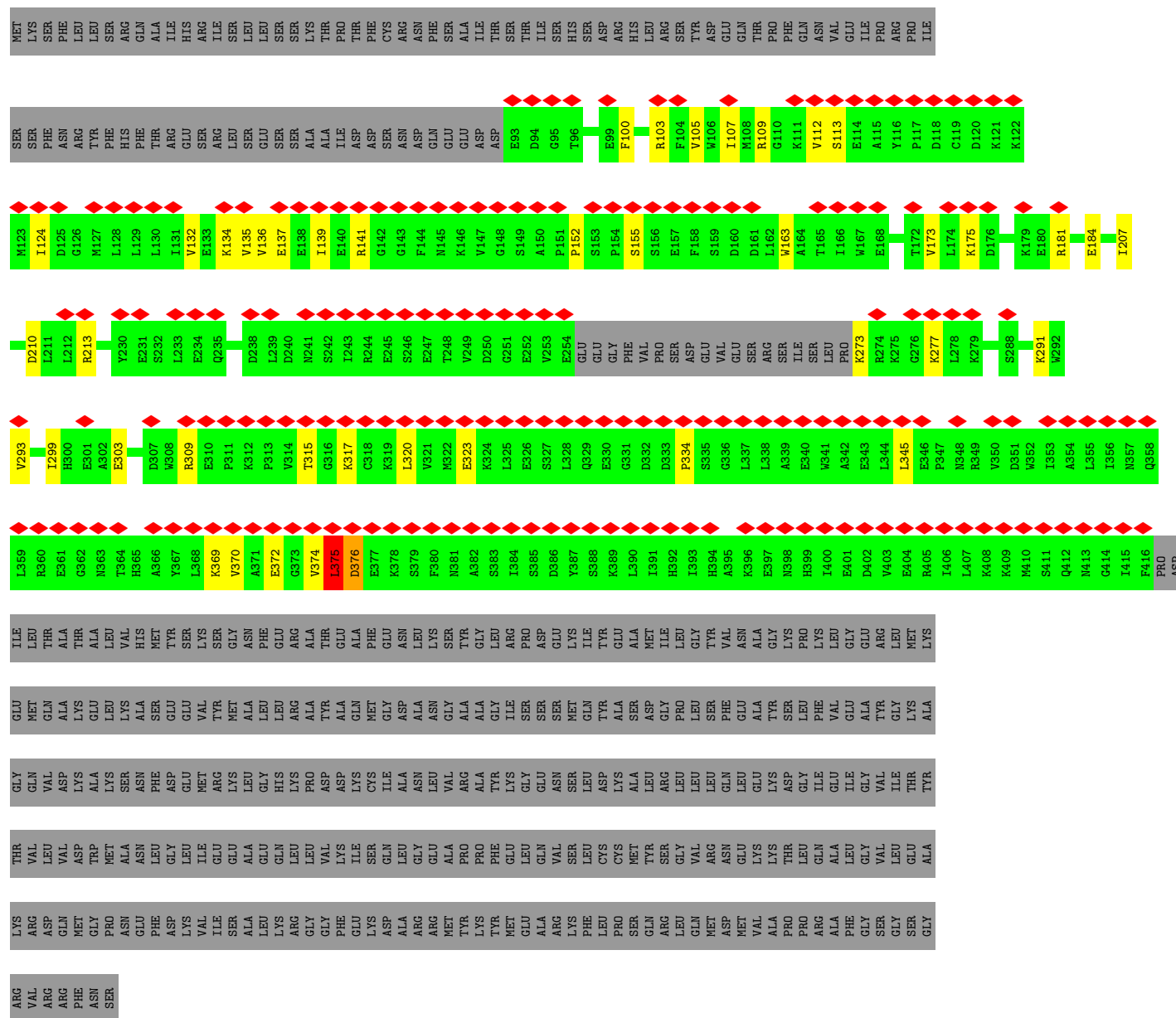
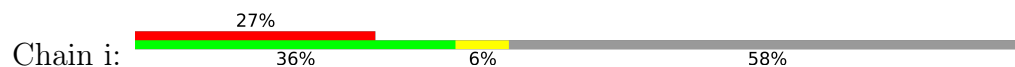




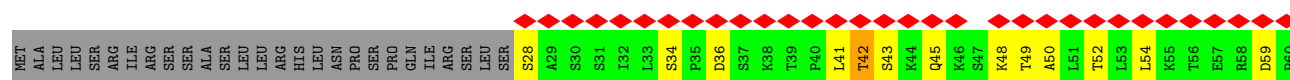




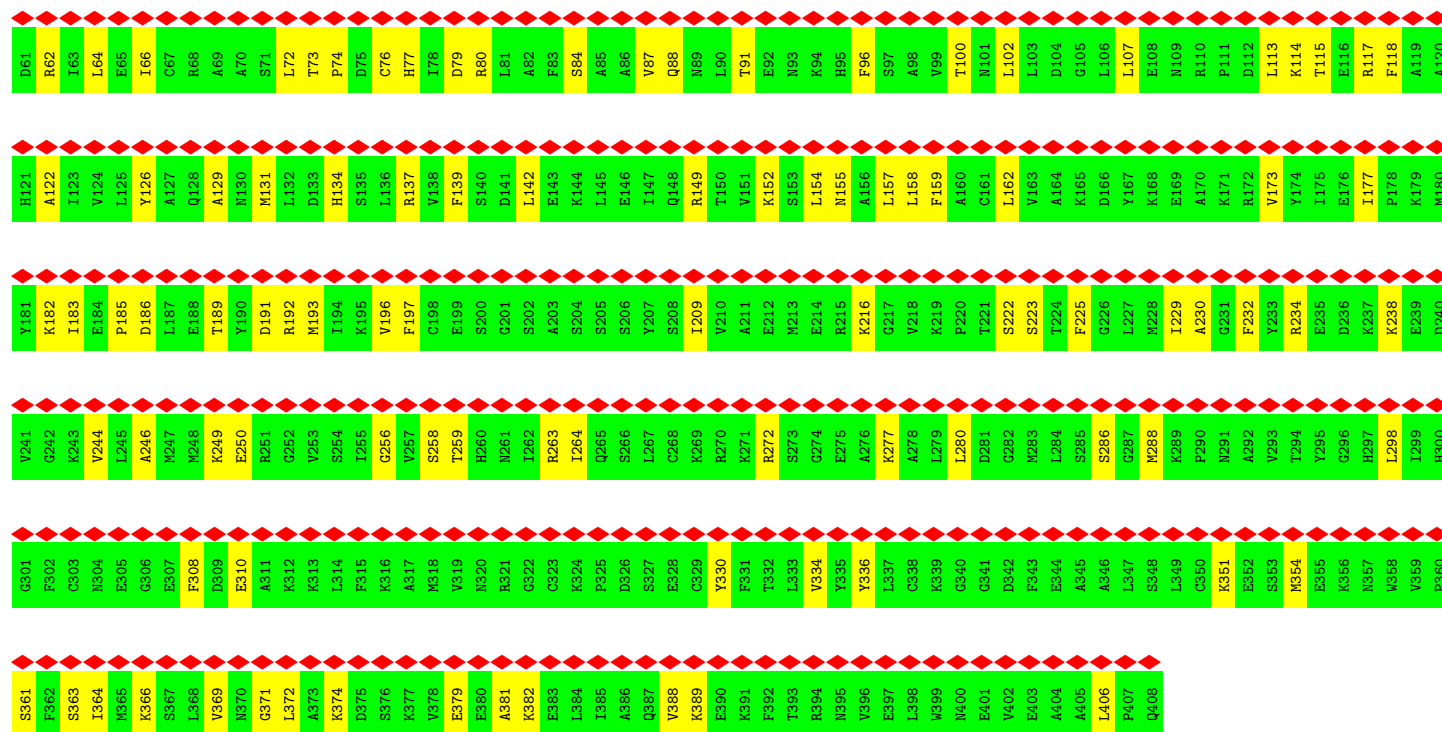
• Molecule 85: mS77 (NFD5)



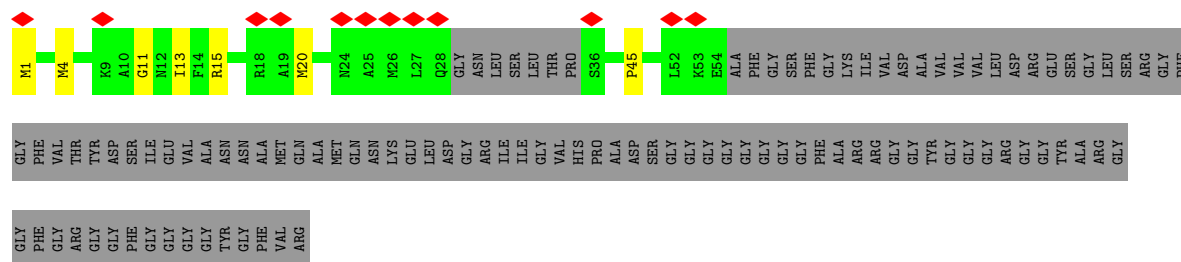
• Molecule 86: mS76 (rPPR1)



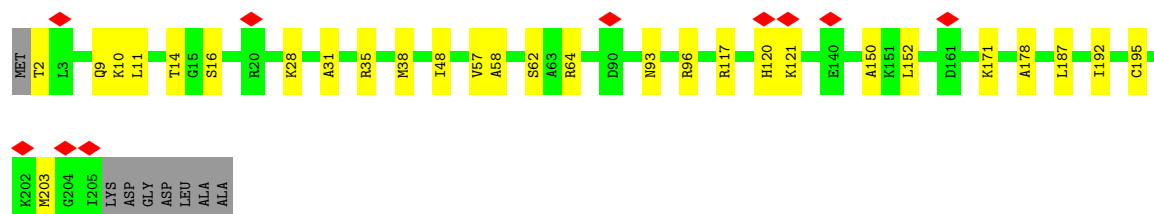
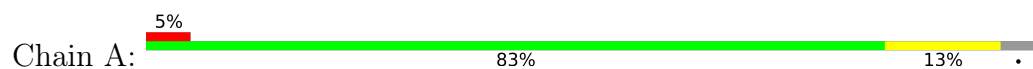




• Molecule 87: mS86



• Molecule 88: uS2m





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34964	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.541	Depositor
Minimum map value	-0.257	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.0796	Depositor
Map size (Å)	596.712, 596.712, 596.712	wwPDB
Map dimensions	564, 564, 564	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, ZN, ATP, 2MG, 4OC, OMG, CLM, OMU, UR3, K, MA6, 5MU, G7M, PSU, OMC, H2U, MG, 2MA, 4SU

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	B	0.26	0/3969	0.54	2/5320 (0.0%)
2	C	0.27	0/2865	0.45	0/3836
3	D	0.27	0/3474	0.46	0/4647
4	E	0.27	0/838	0.41	0/1121
5	F	0.27	0/1225	0.53	0/1641
6	G	0.27	0/1054	0.44	0/1418
7	H	0.37	1/1707 (0.1%)	0.59	1/2287 (0.0%)
8	I	0.27	0/964	0.46	0/1293
9	J	0.38	0/1000	0.50	0/1340
10	K	0.24	0/1009	0.39	0/1345
11	L	0.32	0/950	0.52	0/1263
12	M	0.44	0/856	0.52	0/1134
13	N	0.26	0/958	0.41	0/1280
14	O	0.30	0/890	0.50	0/1196
15	P	0.28	0/730	0.48	1/984 (0.1%)
16	Q	0.23	0/733	0.41	0/978
17	R	0.24	0/1323	0.48	0/1772
18	S	0.27	0/614	0.41	0/809
19	T	0.28	0/416	0.40	0/547
20	U	0.51	1/1036 (0.1%)	0.90	8/1395 (0.6%)
21	V	0.19	0/1423	0.39	0/1895
22	W	0.22	0/3139	0.41	0/4250
23	X	0.27	0/1644	0.53	0/2216
24	Y	0.37	0/807	0.46	0/1077
25	Z	0.18	0/669	0.39	0/900
26	1	0.35	0/69733	0.40	1/108691 (0.0%)
27	3	0.31	0/2810	0.39	0/4378
28	1B	0.31	0/1347	0.43	0/1797
29	1C	0.38	0/1727	0.57	4/2311 (0.2%)
30	1D	0.32	0/2099	0.43	0/2836
31	1E	0.31	0/1786	0.41	0/2412



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	1F	0.26	0/1313	0.48	0/1772
33	1G	0.22	0/796	0.43	0/1067
34	1H	0.27	0/547	0.47	0/731
35	1I	0.24	0/1054	0.56	0/1417
36	1J	0.27	0/1155	0.61	1/1563 (0.1%)
37	1K	0.29	0/1553	0.36	0/2080
38	1L	0.30	0/976	0.47	0/1304
39	1M	0.32	0/1682	0.46	2/2248 (0.1%)
40	1N	0.28	0/1184	0.42	0/1580
41	1O	0.30	0/1255	0.43	0/1687
42	1P	0.28	0/895	0.47	0/1206
43	1Q	0.30	0/1022	0.39	0/1368
44	1R	0.37	0/930	0.41	0/1234
45	1S	0.31	0/1192	0.39	0/1602
46	1T	0.32	0/1259	0.41	0/1687
47	1U	0.28	0/1065	0.39	0/1421
48	1V	0.28	0/1247	0.37	0/1681
49	1W	0.24	0/1613	0.49	0/2180
50	1X	0.24	0/1703	0.41	0/2307
51	1Y	0.32	0/785	0.38	0/1051
52	1Z	0.31	0/1466	0.47	2/1954 (0.1%)
53	1a	0.32	0/946	0.43	0/1262
54	1b	0.30	0/818	0.47	0/1099
55	1c	0.29	0/501	0.44	0/666
56	1d	0.44	0/387	0.63	1/514 (0.2%)
57	1e	0.33	0/468	0.39	0/618
58	1f	0.40	0/370	0.43	0/486
59	1g	0.37	0/789	0.45	0/1048
60	1h	0.29	0/312	0.38	0/409
61	1i	0.24	0/1440	0.38	0/1927
62	1j	0.35	0/586	0.41	0/789
63	1k	0.32	0/970	0.45	0/1309
64	1l	0.26	0/1792	0.45	0/2423
65	1m	0.23	0/987	0.48	0/1331
66	1o	0.17	0/637	0.43	0/860
67	1p	0.26	0/1014	0.39	0/1349
68	1q	0.31	0/394	0.40	0/527
69	1r	0.26	0/750	0.45	0/1005
70	1s	0.27	0/1001	0.41	0/1327
71	1t	0.26	0/3919	0.48	0/5272
72	1u	0.24	0/5345	0.51	0/7180
73	1v	0.25	0/3497	0.46	0/4681
74	1x	0.19	0/18	0.26	0/23



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	5	0.24	0/1725	0.33	0/2689
76	2	0.29	0/37992	0.37	0/59224
77	6	0.19	0/146	0.22	0/225
78	a	0.25	0/2524	0.54	2/3387 (0.1%)
79	b	0.29	0/618	0.68	0/822
80	c	0.27	0/233	0.40	0/296
81	d	0.26	0/628	0.47	0/840
82	e	0.25	0/2118	0.48	0/2828
83	f	0.25	0/2981	0.50	0/4033
84	h	0.29	0/2507	0.54	0/3384
85	i	0.24	0/2532	0.49	1/3400 (0.0%)
86	j	0.24	0/3032	0.56	1/4073 (0.0%)
87	k	0.25	0/317	0.58	1/424 (0.2%)
88	A	0.25	0/1647	0.47	0/2227
All	All	0.31	2/224428 (0.0%)	0.43	28/325466 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	H	0	1
11	L	0	1
30	1D	0	1
71	1t	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	404	LEU	CG-CD2	-5.93	1.32	1.52
20	U	81	PRO	N-CD	5.13	1.54	1.47

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U	80	ASP	C-N-CD	-14.93	63.78	125.00
20	U	71	PRO	N-CA-C	-9.97	99.67	113.53
20	U	81	PRO	CA-N-CD	-9.66	98.47	112.00
36	1J	38	PRO	CA-N-CD	-9.01	99.39	112.00
20	U	61	ARG	N-CA-C	-8.98	101.90	113.12



There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	1D	225	ASP	Peptide
71	1t	462	HIS	Peptide
7	H	225	ILE	Peptide
11	L	136	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3877	0	4008	100	0
2	C	2811	0	2986	26	0
3	D	3425	0	3453	28	0
4	E	823	0	879	6	0
5	F	1254	0	1268	14	0
6	G	1037	0	1058	9	0
7	H	1682	0	1726	27	0
8	I	941	0	970	15	0
9	J	988	0	1022	13	0
10	K	992	0	1051	15	0
11	L	940	0	989	9	0
12	M	843	0	884	11	0
13	N	941	0	978	4	0
14	O	869	0	898	12	0
15	P	717	0	755	10	0
16	Q	724	0	744	10	0
17	R	1299	0	1307	21	0
18	S	611	0	687	7	0
19	T	408	0	444	4	0
20	U	1014	0	1061	62	0
21	V	1399	0	1427	10	0
22	W	3062	0	3030	23	0
23	X	1613	0	1559	57	0
24	Y	793	0	834	12	0
25	Z	649	0	662	5	0
26	1	62518	0	31499	260	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	3	2513	0	1275	4	0
28	1B	1325	0	1398	12	0
29	1C	1696	0	1745	51	0
30	1D	2045	0	2080	18	0
31	1E	1753	0	1815	19	0
32	1F	1286	0	1280	10	0
33	1G	779	0	810	5	0
34	1H	539	0	574	22	0
35	1I	1036	0	1084	40	0
36	1J	1129	0	1166	52	0
37	1K	1526	0	1586	8	0
38	1L	966	0	1048	6	0
39	1M	1649	0	1765	10	0
40	1N	1160	0	1206	6	0
41	1O	1231	0	1262	7	0
42	1P	878	0	939	3	0
43	1Q	1008	0	1101	5	0
44	1R	915	0	946	6	0
45	1S	1170	0	1226	3	0
46	1T	1241	0	1346	5	0
47	1U	1048	0	1123	14	0
48	1V	1223	0	1278	12	0
49	1W	1588	0	1663	23	0
50	1X	1670	0	1751	10	0
51	1Y	768	0	792	7	0
52	1Z	1441	0	1485	17	0
53	1a	928	0	959	9	0
54	1b	803	0	845	12	0
55	1c	489	0	511	10	0
56	1d	379	0	416	1	0
57	1e	459	0	491	1	0
58	1f	364	0	398	1	0
59	1g	770	0	841	6	0
60	1h	309	0	337	0	0
61	1i	1424	0	1482	16	0
62	1j	570	0	593	9	0
63	1k	952	0	987	5	0
64	1l	1741	0	1707	19	0
65	1m	970	0	979	8	0
66	1o	626	0	657	11	0
67	1p	992	0	1027	8	0
68	1q	390	0	421	2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	1r	735	0	781	16	0
70	1s	985	0	1072	8	0
71	1t	3856	0	3912	37	0
72	1u	5264	0	5353	74	0
73	1v	3440	0	3497	29	0
74	1x	19	0	14	0	0
75	5	1625	0	828	5	0
76	2	34081	0	17178	192	0
77	6	130	0	66	1	0
78	a	2487	0	2382	69	0
79	b	610	0	626	6	0
80	c	232	0	278	3	0
81	d	616	0	674	11	0
82	e	2074	0	2074	24	0
83	f	2922	0	2868	73	0
84	h	2460	0	2478	73	0
85	i	2487	0	2450	39	0
86	j	2984	0	3044	84	0
87	k	314	0	261	12	0
88	A	1611	0	1633	22	0
89	1	249	0	0	0	0
89	1D	1	0	0	0	0
89	1h	1	0	0	0	0
89	1j	1	0	0	0	0
89	1q	2	0	0	0	0
89	2	98	0	0	0	0
89	3	3	0	0	0	0
89	T	1	0	0	0	0
89	W	1	0	0	0	0
90	W	31	0	12	0	0
91	1	20	0	11	0	0
92	1	56	0	0	0	0
92	1B	3	0	0	0	0
92	1E	1	0	0	0	0
92	2	14	0	0	0	0
93	1d	1	0	0	0	0
93	1h	1	0	0	0	0
All	All	211395	0	164066	1717	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1717 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:5:54:5MU:C4	75:5:54:5MU:C5	1.82	1.65
36:1J:42:ASN:HB2	36:1J:73:HIS:CE1	1.37	1.60
29:1C:227:ARG:NH2	29:1C:229:HIS:HB2	1.21	1.44
36:1J:42:ASN:HB2	36:1J:73:HIS:NE2	1.33	1.41
29:1C:199:VAL:CG1	34:1H:97:ARG:HD2	1.53	1.39

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	457/554 (82%)	425 (93%)	31 (7%)	1 (0%)	43	70
2	C	329/362 (91%)	317 (96%)	12 (4%)	0	100	100
3	D	413/501 (82%)	397 (96%)	15 (4%)	1 (0%)	43	70
4	E	99/138 (72%)	96 (97%)	3 (3%)	0	100	100
5	F	146/157 (93%)	140 (96%)	6 (4%)	0	100	100
6	G	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
7	H	209/383 (55%)	197 (94%)	11 (5%)	1 (0%)	24	52
8	I	111/228 (49%)	107 (96%)	4 (4%)	0	100	100
9	J	125/304 (41%)	121 (97%)	4 (3%)	0	100	100
10	K	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
11	L	117/154 (76%)	110 (94%)	7 (6%)	0	100	100
12	M	99/155 (64%)	96 (97%)	3 (3%)	0	100	100
13	N	114/414 (28%)	113 (99%)	1 (1%)	0	100	100
14	O	108/136 (79%)	104 (96%)	4 (4%)	0	100	100
15	P	89/110 (81%)	84 (94%)	4 (4%)	1 (1%)	11	34
16	Q	88/237 (37%)	87 (99%)	1 (1%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R	162/212 (76%)	152 (94%)	10 (6%)	0	100	100
18	S	73/100 (73%)	72 (99%)	1 (1%)	0	100	100
19	T	48/94 (51%)	44 (92%)	4 (8%)	0	100	100
20	U	125/192 (65%)	109 (87%)	9 (7%)	7 (6%)	1	7
21	V	162/193 (84%)	160 (99%)	2 (1%)	0	100	100
22	W	376/483 (78%)	368 (98%)	8 (2%)	0	100	100
23	X	202/496 (41%)	191 (95%)	8 (4%)	3 (2%)	8	28
24	Y	96/102 (94%)	95 (99%)	1 (1%)	0	100	100
25	Z	78/153 (51%)	74 (95%)	4 (5%)	0	100	100
28	1B	175/220 (80%)	171 (98%)	4 (2%)	0	100	100
29	1C	203/327 (62%)	194 (96%)	7 (3%)	2 (1%)	12	37
30	1D	262/319 (82%)	257 (98%)	5 (2%)	0	100	100
31	1E	219/297 (74%)	217 (99%)	2 (1%)	0	100	100
32	1F	154/185 (83%)	148 (96%)	6 (4%)	0	100	100
33	1G	96/102 (94%)	95 (99%)	1 (1%)	0	100	100
34	1H	64/219 (29%)	63 (98%)	1 (2%)	0	100	100
35	1I	128/170 (75%)	119 (93%)	8 (6%)	1 (1%)	16	42
36	1J	145/156 (93%)	132 (91%)	11 (8%)	2 (1%)	9	29
37	1K	187/204 (92%)	184 (98%)	3 (2%)	0	100	100
38	1L	125/176 (71%)	119 (95%)	6 (5%)	0	100	100
39	1M	208/281 (74%)	195 (94%)	13 (6%)	0	100	100
40	1N	146/179 (82%)	143 (98%)	3 (2%)	0	100	100
41	1O	149/160 (93%)	141 (95%)	8 (5%)	0	100	100
42	1P	111/114 (97%)	102 (92%)	9 (8%)	0	100	100
43	1Q	120/233 (52%)	116 (97%)	4 (3%)	0	100	100
44	1R	108/126 (86%)	107 (99%)	1 (1%)	0	100	100
45	1S	143/270 (53%)	139 (97%)	4 (3%)	0	100	100
46	1T	153/264 (58%)	148 (97%)	5 (3%)	0	100	100
47	1U	126/180 (70%)	120 (95%)	6 (5%)	0	100	100
48	1V	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
49	1W	203/249 (82%)	192 (95%)	11 (5%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	1X	214/271 (79%)	209 (98%)	5 (2%)	0	100	100
51	1Y	96/156 (62%)	94 (98%)	2 (2%)	0	100	100
52	1Z	175/212 (82%)	174 (99%)	1 (1%)	0	100	100
53	1a	106/144 (74%)	104 (98%)	2 (2%)	0	100	100
54	1b	98/109 (90%)	94 (96%)	4 (4%)	0	100	100
55	1c	57/135 (42%)	54 (95%)	3 (5%)	0	100	100
56	1d	47/139 (34%)	47 (100%)	0	0	100	100
57	1e	52/63 (82%)	51 (98%)	1 (2%)	0	100	100
58	1f	42/146 (29%)	42 (100%)	0	0	100	100
59	1g	89/162 (55%)	89 (100%)	0	0	100	100
60	1h	36/103 (35%)	34 (94%)	2 (6%)	0	100	100
61	1i	181/247 (73%)	176 (97%)	5 (3%)	0	100	100
62	1j	69/90 (77%)	68 (99%)	1 (1%)	0	100	100
63	1k	116/119 (98%)	111 (96%)	5 (4%)	0	100	100
64	1l	209/233 (90%)	198 (95%)	11 (5%)	0	100	100
65	1m	120/128 (94%)	119 (99%)	1 (1%)	0	100	100
66	1o	74/125 (59%)	70 (95%)	4 (5%)	0	100	100
67	1p	115/130 (88%)	112 (97%)	3 (3%)	0	100	100
68	1q	48/79 (61%)	47 (98%)	0	1 (2%)	5	21
69	1r	90/167 (54%)	84 (93%)	6 (7%)	0	100	100
70	1s	116/181 (64%)	113 (97%)	3 (3%)	0	100	100
71	1t	482/491 (98%)	468 (97%)	14 (3%)	0	100	100
72	1u	664/757 (88%)	624 (94%)	40 (6%)	0	100	100
73	1v	429/521 (82%)	412 (96%)	17 (4%)	0	100	100
74	1x	2/4 (50%)	2 (100%)	0	0	100	100
78	a	311/424 (73%)	305 (98%)	6 (2%)	0	100	100
79	b	75/80 (94%)	68 (91%)	7 (9%)	0	100	100
80	c	24/128 (19%)	23 (96%)	1 (4%)	0	100	100
81	d	76/110 (69%)	74 (97%)	2 (3%)	0	100	100
82	e	244/383 (64%)	236 (97%)	8 (3%)	0	100	100
83	f	375/410 (92%)	361 (96%)	14 (4%)	0	100	100

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	h	308/384 (80%)	301 (98%)	7 (2%)	0	100	100
85	i	302/725 (42%)	290 (96%)	10 (3%)	2 (1%)	18	45
86	j	379/408 (93%)	365 (96%)	14 (4%)	0	100	100
87	k	43/155 (28%)	37 (86%)	6 (14%)	0	100	100
88	A	202/212 (95%)	196 (97%)	6 (3%)	0	100	100
All	All	13521/19033 (71%)	13005 (96%)	494 (4%)	22 (0%)	44	70

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	225	ILE
20	U	64	PRO
20	U	81	PRO
29	1C	227	ARG
35	1I	133	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	421/492 (86%)	421 (100%)	0	100	100
2	C	314/343 (92%)	314 (100%)	0	100	100
3	D	370/444 (83%)	370 (100%)	0	100	100
4	E	90/126 (71%)	90 (100%)	0	100	100
5	F	124/124 (100%)	124 (100%)	0	100	100
6	G	112/113 (99%)	112 (100%)	0	100	100
7	H	176/320 (55%)	175 (99%)	1 (1%)	78	81
8	I	104/197 (53%)	104 (100%)	0	100	100
9	J	108/256 (42%)	107 (99%)	1 (1%)	70	78
10	K	107/108 (99%)	107 (100%)	0	100	100
11	L	99/128 (77%)	99 (100%)	0	100	100

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M	90/137 (66%)	90 (100%)	0	100	100
13	N	107/362 (30%)	107 (100%)	0	100	100
14	O	93/117 (80%)	93 (100%)	0	100	100
15	P	78/95 (82%)	78 (100%)	0	100	100
16	Q	75/203 (37%)	75 (100%)	0	100	100
17	R	141/180 (78%)	141 (100%)	0	100	100
18	S	68/90 (76%)	68 (100%)	0	100	100
19	T	44/79 (56%)	44 (100%)	0	100	100
20	U	109/170 (64%)	104 (95%)	5 (5%)	24	52
21	V	147/173 (85%)	147 (100%)	0	100	100
22	W	328/410 (80%)	328 (100%)	0	100	100
23	X	174/395 (44%)	174 (100%)	0	100	100
24	Y	84/86 (98%)	84 (100%)	0	100	100
25	Z	65/119 (55%)	65 (100%)	0	100	100
28	1B	141/176 (80%)	141 (100%)	0	100	100
29	1C	184/268 (69%)	183 (100%)	1 (0%)	81	82
30	1D	216/264 (82%)	216 (100%)	0	100	100
31	1E	192/257 (75%)	192 (100%)	0	100	100
32	1F	145/168 (86%)	145 (100%)	0	100	100
33	1G	82/86 (95%)	82 (100%)	0	100	100
34	1H	58/195 (30%)	58 (100%)	0	100	100
35	1I	113/143 (79%)	113 (100%)	0	100	100
36	1J	125/131 (95%)	125 (100%)	0	100	100
37	1K	161/170 (95%)	161 (100%)	0	100	100
38	1L	103/140 (74%)	103 (100%)	0	100	100
39	1M	169/235 (72%)	169 (100%)	0	100	100
40	1N	116/146 (80%)	116 (100%)	0	100	100
41	1O	129/139 (93%)	129 (100%)	0	100	100
42	1P	94/95 (99%)	94 (100%)	0	100	100
43	1Q	110/208 (53%)	110 (100%)	0	100	100
44	1R	96/110 (87%)	96 (100%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1S	130/244 (53%)	130 (100%)	0	100	100
46	1T	133/229 (58%)	133 (100%)	0	100	100
47	1U	114/147 (78%)	114 (100%)	0	100	100
48	1V	132/133 (99%)	132 (100%)	0	100	100
49	1W	181/216 (84%)	181 (100%)	0	100	100
50	1X	186/235 (79%)	186 (100%)	0	100	100
51	1Y	80/127 (63%)	80 (100%)	0	100	100
52	1Z	150/173 (87%)	150 (100%)	0	100	100
53	1a	102/128 (80%)	102 (100%)	0	100	100
54	1b	88/95 (93%)	88 (100%)	0	100	100
55	1c	51/119 (43%)	51 (100%)	0	100	100
56	1d	42/119 (35%)	42 (100%)	0	100	100
57	1e	49/57 (86%)	49 (100%)	0	100	100
58	1f	35/129 (27%)	35 (100%)	0	100	100
59	1g	84/152 (55%)	84 (100%)	0	100	100
60	1h	36/87 (41%)	36 (100%)	0	100	100
61	1i	152/203 (75%)	152 (100%)	0	100	100
62	1j	64/79 (81%)	64 (100%)	0	100	100
63	1k	105/106 (99%)	105 (100%)	0	100	100
64	1l	189/209 (90%)	189 (100%)	0	100	100
65	1m	107/112 (96%)	107 (100%)	0	100	100
66	1o	71/105 (68%)	71 (100%)	0	100	100
67	1p	101/108 (94%)	101 (100%)	0	100	100
68	1q	41/65 (63%)	41 (100%)	0	100	100
69	1r	83/138 (60%)	82 (99%)	1 (1%)	63	75
70	1s	103/155 (66%)	103 (100%)	0	100	100
71	1t	417/423 (99%)	417 (100%)	0	100	100
72	1u	578/663 (87%)	578 (100%)	0	100	100
73	1v	374/461 (81%)	374 (100%)	0	100	100
78	a	252/374 (67%)	252 (100%)	0	100	100
79	b	68/71 (96%)	68 (100%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
80	c	25/116 (22%)	25 (100%)	0	100	100
81	d	65/93 (70%)	65 (100%)	0	100	100
82	e	226/339 (67%)	226 (100%)	0	100	100
83	f	321/351 (92%)	321 (100%)	0	100	100
84	h	271/337 (80%)	271 (100%)	0	100	100
85	i	272/629 (43%)	271 (100%)	1 (0%)	84	84
86	j	330/355 (93%)	330 (100%)	0	100	100
87	k	22/106 (21%)	22 (100%)	0	100	100
88	A	177/182 (97%)	177 (100%)	0	100	100
All	All	11869/16368 (72%)	11859 (100%)	10 (0%)	87	89

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	1C	227	ARG
69	1r	68	HIS
85	i	375	LEU
20	U	65	GLU
20	U	69	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
65	1m	13	ASN
73	1v	330	ASN
68	1q	49	GLN
72	1u	83	ASN
78	a	397	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	1	2910/2922 (99%)	539 (18%)	28 (0%)
27	3	117/118 (99%)	24 (20%)	1 (0%)
75	5	75/76 (98%)	12 (16%)	0
76	2	1583/1591 (99%)	267 (16%)	11 (0%)
77	6	5/6 (83%)	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4690/4713 (99%)	842 (17%)	40 (0%)

5 of 842 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	1	49	G
26	1	50	G
26	1	51	A
26	1	54	G
26	1	63	A

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	3	12	U
76	2	1701	C
76	2	103	A
76	2	493	A
76	2	1706	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
26	PSU	1	2885	92,26	18,21,22	1.07	3 (16%)	21,30,33	1.97	5 (23%)
26	OMG	1	2560	92,75,26	23,26,27	2.38	7 (30%)	32,38,41	2.29	8 (25%)
75	4SU	5	8	75	18,21,22	4.12	7 (38%)	25,30,33	2.44	4 (16%)
76	2MG	2	1825	76	23,26,27	2.83	6 (26%)	33,38,41	3.05	14 (42%)
26	5MU	1	2257	92,26	19,22,23	1.47	4 (21%)	27,32,35	2.41	6 (22%)
26	PSU	1	2762	26	18,21,22	1.00	2 (11%)	21,30,33	1.89	4 (19%)
26	PSU	1	1105	26	18,21,22	1.04	2 (11%)	21,30,33	1.92	3 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
76	MA6	2	1827	76	23,26,27	1.83	6 (26%)	33,38,41	3.39	13 (39%)
26	PSU	1	891	26,89	18,21,22	1.09	2 (11%)	21,30,33	1.98	4 (19%)
76	UR3	2	1807	76	19,22,23	2.62	7 (36%)	26,32,35	1.68	2 (7%)
75	5MU	5	54	75	19,22,23	7.76	9 (47%)	27,32,35	3.50	10 (37%)
26	OMC	1	2803	26,89	19,22,23	2.74	7 (36%)	25,31,34	1.00	1 (4%)
26	PSU	1	2910	26	18,21,22	1.02	2 (11%)	21,30,33	1.83	5 (23%)
76	G7M	2	525	76	23,26,27	2.32	7 (30%)	34,39,42	3.11	10 (29%)
26	OMU	1	2857	26,89	19,22,23	3.01	8 (42%)	25,31,34	1.83	4 (16%)
76	MA6	2	1828	76	23,26,27	1.81	5 (21%)	33,38,41	3.41	12 (36%)
75	5MC	5	32	75	19,22,23	3.55	8 (42%)	26,32,35	1.15	2 (7%)
26	H2U	1	2754	26	18,21,22	0.69	0	19,30,33	1.19	1 (5%)
76	4OC	2	1664	76	20,23,24	3.19	8 (40%)	25,32,35	0.90	1 (4%)
26	2MA	1	2808	26,89	22,25,26	3.90	7 (31%)	32,37,40	2.45	10 (31%)
75	PSU	5	55	75	18,21,22	1.14	1 (5%)	21,30,33	1.92	4 (19%)

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
26	PSU	1	2885	92,26	-	1/7/25/26	0/2/2/2
26	OMG	1	2560	92,75,26	-	1/9/27/28	0/3/3/3
75	4SU	5	8	75	-	0/7/25/26	0/2/2/2
76	2MG	2	1825	76	-	2/9/27/28	0/3/3/3
26	5MU	1	2257	92,26	-	1/7/25/26	0/2/2/2
26	PSU	1	2762	26	-	0/7/25/26	0/2/2/2
26	PSU	1	1105	26	-	0/7/25/26	0/2/2/2
76	MA6	2	1827	76	-	0/11/29/30	0/3/3/3
26	PSU	1	891	26,89	-	1/7/25/26	0/2/2/2
76	UR3	2	1807	76	-	0/7/25/26	0/2/2/2
75	5MU	5	54	75	-	0/7/25/26	0/2/2/2
26	OMC	1	2803	26,89	-	0/9/27/28	0/2/2/2
26	PSU	1	2910	26	-	0/7/25/26	0/2/2/2
76	G7M	2	525	76	-	3/7/25/26	0/3/3/3
26	OMU	1	2857	26,89	-	0/9/27/28	0/2/2/2
76	MA6	2	1828	76	-	0/11/29/30	0/3/3/3
75	5MC	5	32	75	-	0/7/25/26	0/2/2/2
26	H2U	1	2754	26	-	0/7/38/39	0/2/2/2

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	4OC	2	1664	76	-	2/9/29/30	0/2/2/2
26	2MA	1	2808	26,89	-	2/7/25/26	0/3/3/3
75	PSU	5	55	75	-	0/7/25/26	0/2/2/2

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	5	54	5MU	C4-C5	22.99	1.82	1.44
75	5	54	5MU	C6-N1	15.66	1.64	1.38
75	5	54	5MU	C6-C5	-12.21	1.14	1.34
26	1	2808	2MA	C4-N3	12.21	1.50	1.34
75	5	54	5MU	C4-N3	-12.02	1.16	1.38

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	2	1828	MA6	N1-C6-N6	-11.92	102.33	116.86
76	2	1827	MA6	N1-C6-N6	-11.92	102.34	116.86
75	5	54	5MU	C5-C4-N3	10.84	124.75	115.32
76	2	525	G7M	CN7-N7-C5	9.01	138.03	126.80
75	5	8	4SU	C4-N3-C2	-8.30	119.36	127.31

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	1	2560	OMG	C1'-C2'-O2'-CM2
76	2	1664	4OC	O4'-C4'-C5'-O5'
76	2	1825	2MG	O4'-C4'-C5'-O5'
76	2	525	G7M	C3'-C4'-C5'-O5'
26	1	2808	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1	2560	OMG	2	0
76	2	1825	2MG	1	0
26	1	1105	PSU	1	0
26	1	891	PSU	2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	5	54	5MU	1	0
76	2	1828	MA6	2	0
76	2	1664	4OC	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 435 ligands modelled in this entry, 433 are monoatomic - leaving 2 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	$\# Z  > 2$
90	ATP	W	501	89	32,33,33	1.33	4 (12%)	48,52,52	1.80	11 (22%)
91	CLM	1	3201	-	20,20,20	1.64	3 (15%)	23,27,27	1.16	2 (8%)

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
90	ATP	W	501	89	-	0/22/38/38	0/3/3/3
91	CLM	1	3201	-	-	2/20/22/22	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	1	3201	CLM	C2-N2	4.75	1.44	1.34
90	W	501	ATP	C5-C4	4.32	1.46	1.39
91	1	3201	CLM	O9B-N9	-3.11	1.17	1.22
91	1	3201	CLM	O2-C2	-3.00	1.17	1.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	W	501	ATP	C5-C6	2.56	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	W	501	ATP	C5-C4-N3	-5.95	118.53	126.72
90	W	501	ATP	N3-C4-N9	4.81	135.34	127.17
90	W	501	ATP	C2-N3-C4	3.76	121.02	111.83
90	W	501	ATP	C4-C5-N7	-3.39	106.70	110.58
90	W	501	ATP	N3-C2-N1	-3.21	123.72	128.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

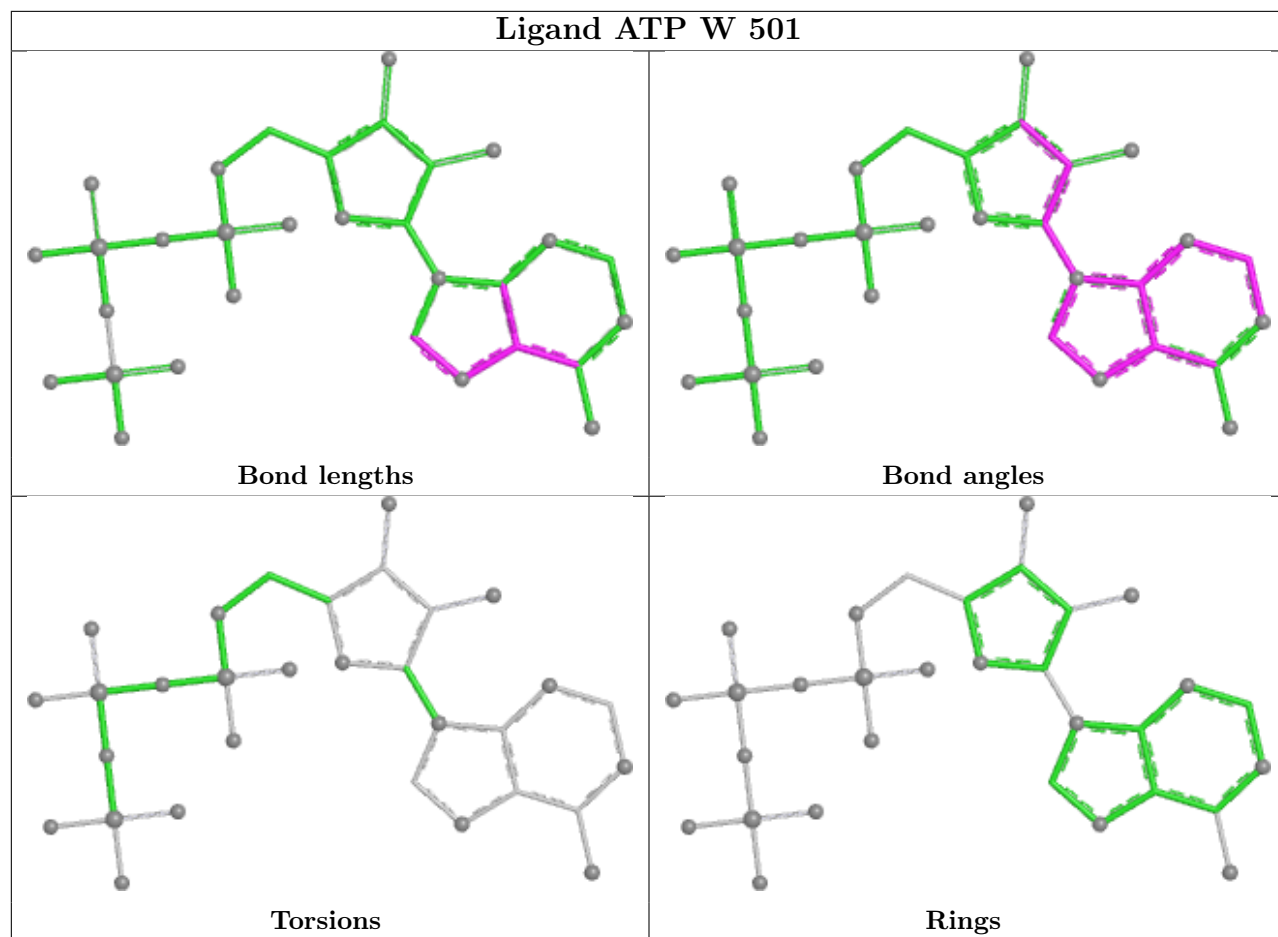
Mol	Chain	Res	Type	Atoms
91	1	3201	CLM	N2-C3-C4-O4
91	1	3201	CLM	C5-C3-C4-O4

There are no ring outliers.

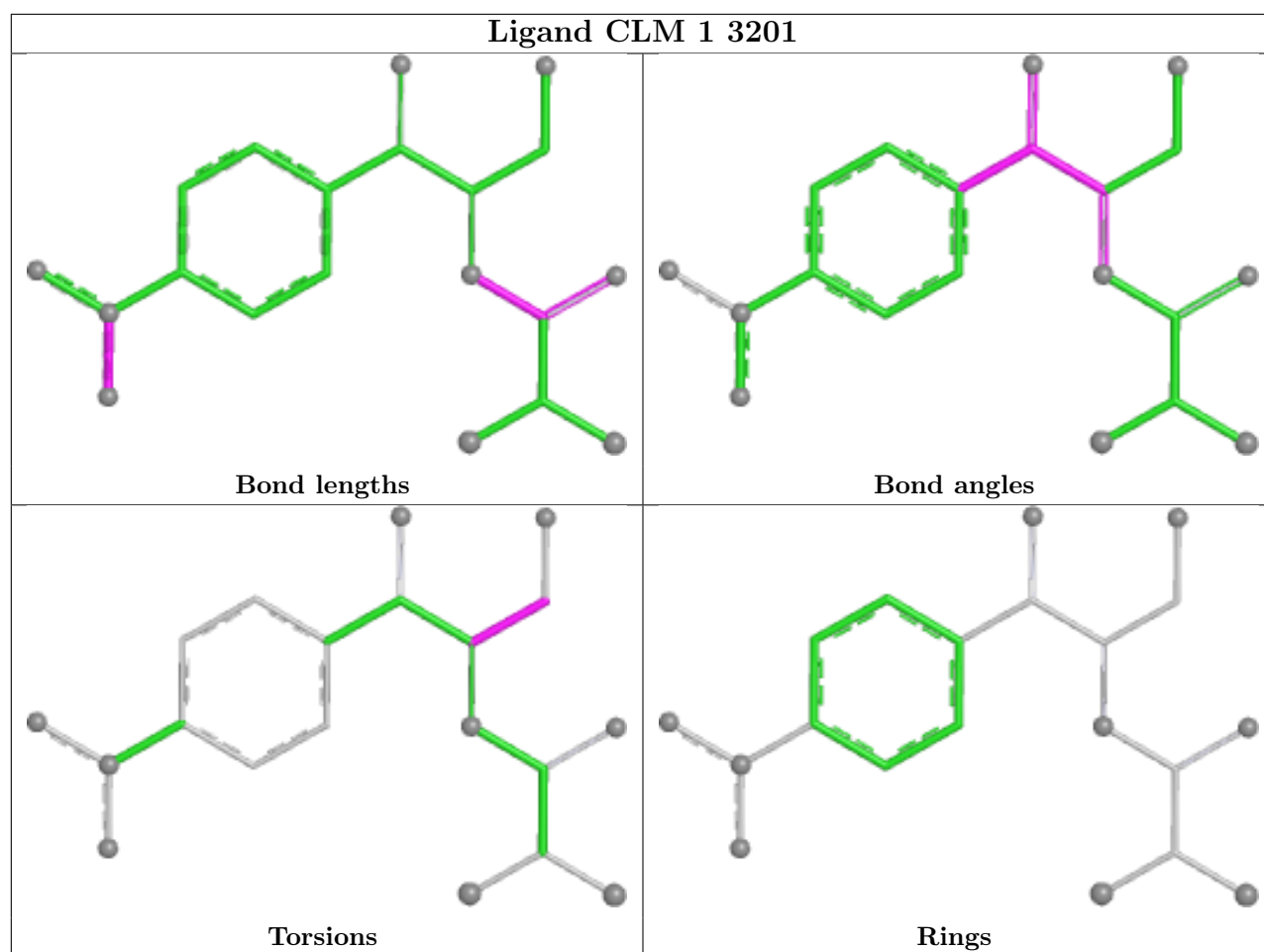
No monomer is involved in short contacts.

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
26	1	11
76	2	7

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	295:U	O3'	307:A	P	27.62
1	1	261:G	O3'	270:A	P	26.81
1	2	95:A	O3'	101:A	P	23.00

*Continued on next page...*



*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1704:U	O3'	1831:A	P	17.44
1	1	363:A	O3'	405:U	P	17.26



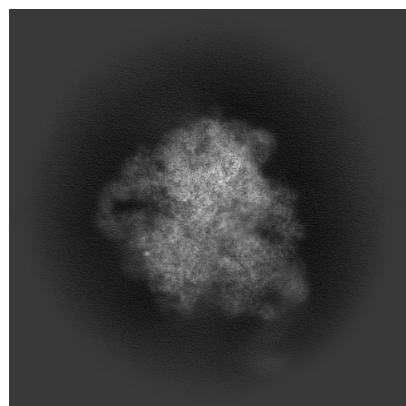
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50011. These allow visual inspection of the internal detail of the map and identification of artifacts.

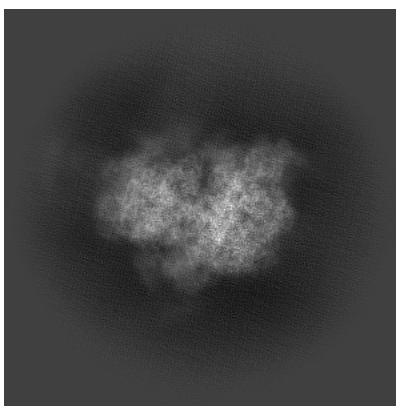
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

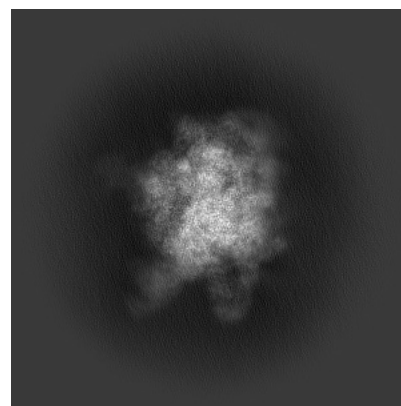
#### 6.1.1 Primary map



X

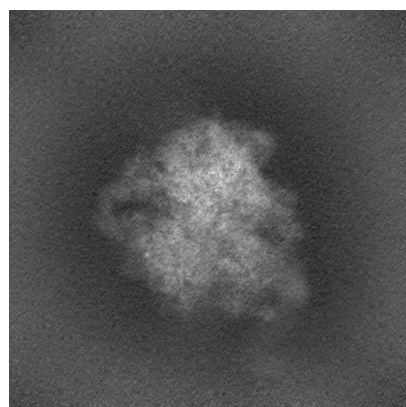


Y

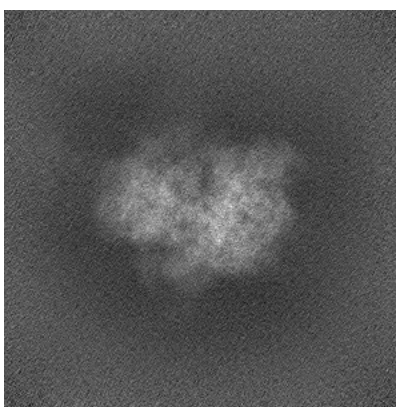


Z

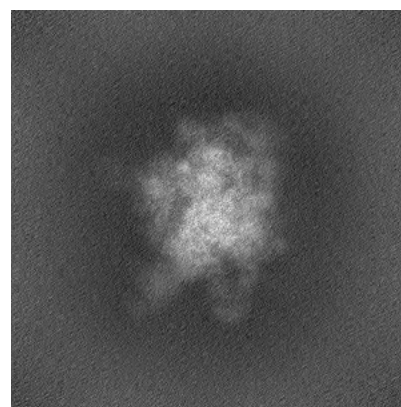
#### 6.1.2 Raw map



X



Y



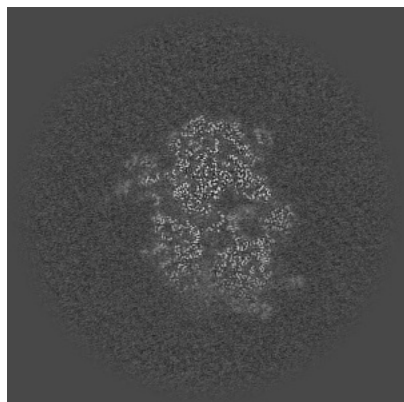
Z

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

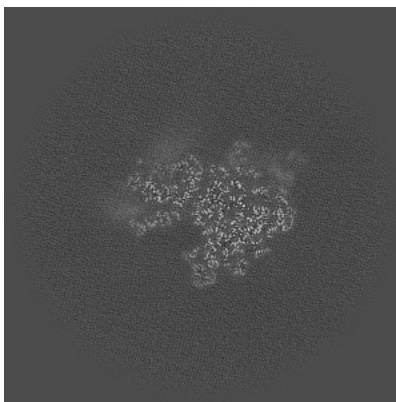


## 6.2 Central slices [i](#)

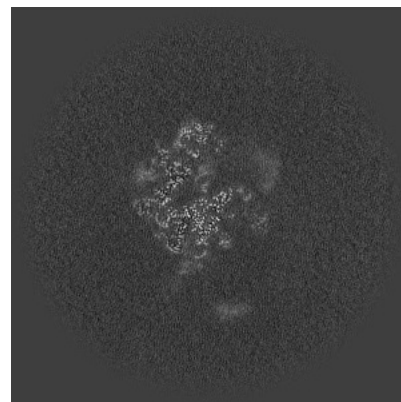
### 6.2.1 Primary map



X Index: 282

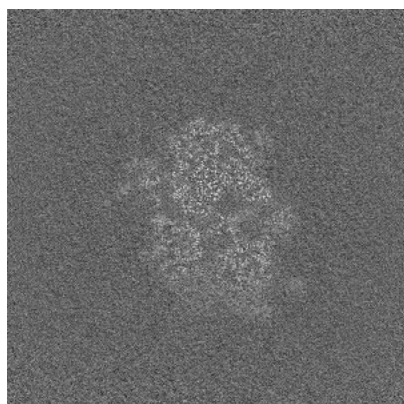


Y Index: 282

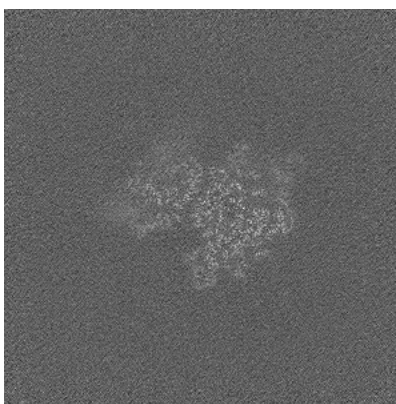


Z Index: 282

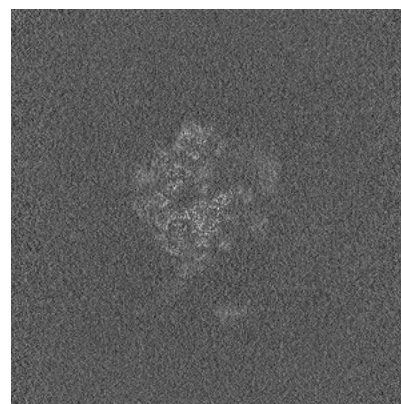
### 6.2.2 Raw map



X Index: 282



Y Index: 282



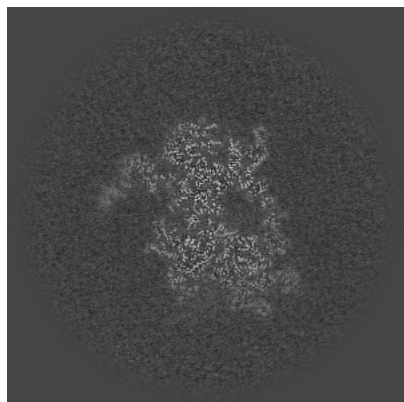
Z Index: 282

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

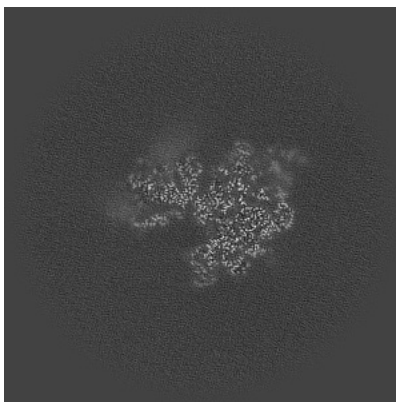


## 6.3 Largest variance slices [i](#)

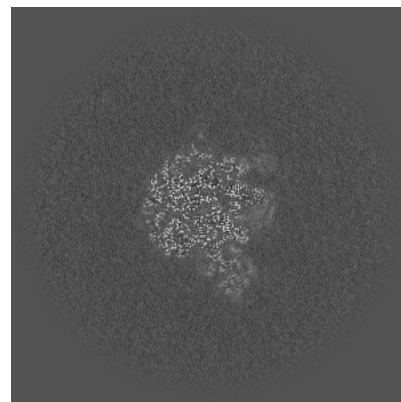
### 6.3.1 Primary map



X Index: 293

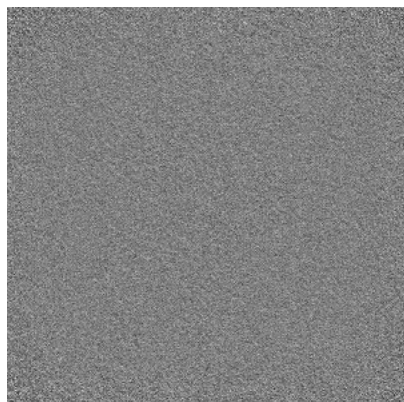


Y Index: 285

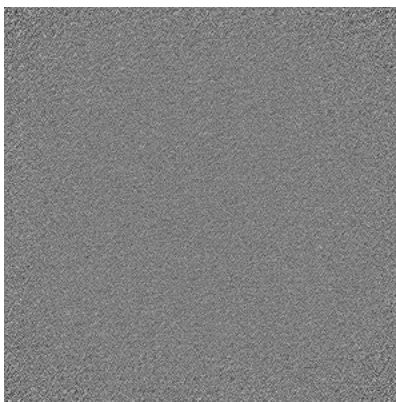


Z Index: 325

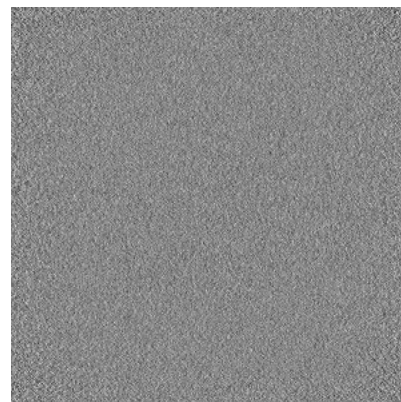
### 6.3.2 Raw map



X Index: 0



Y Index: 0



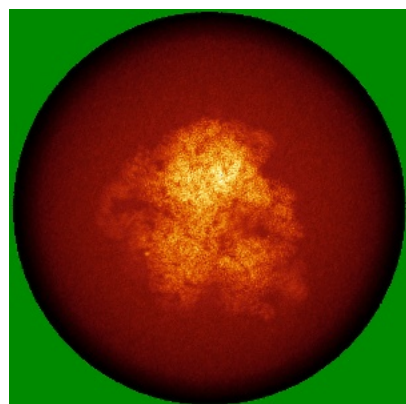
Z Index: 0

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

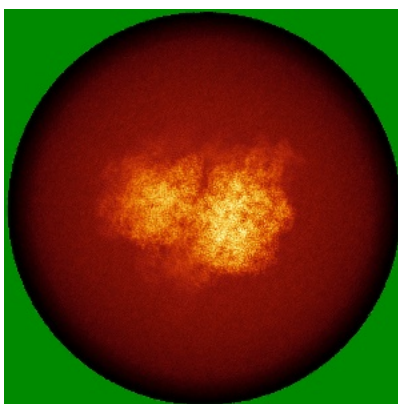


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

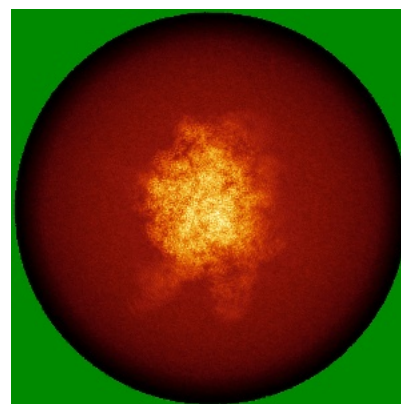
### 6.4.1 Primary map



X

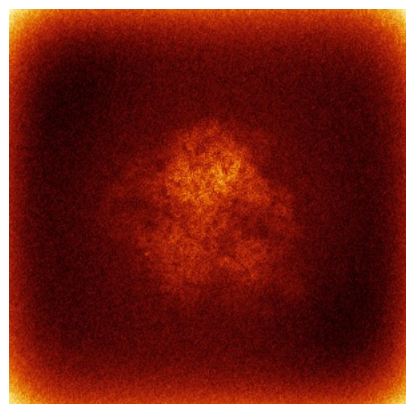


Y

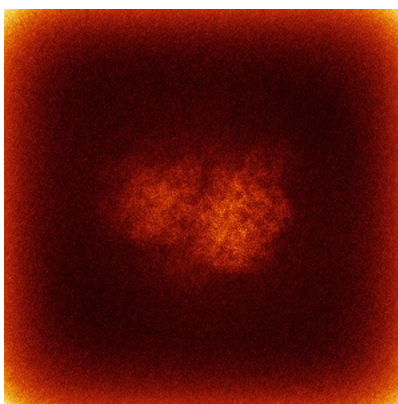


Z

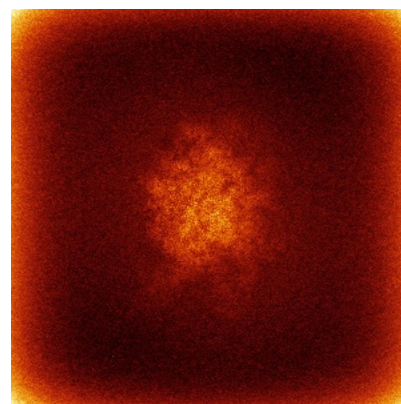
### 6.4.2 Raw map



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.



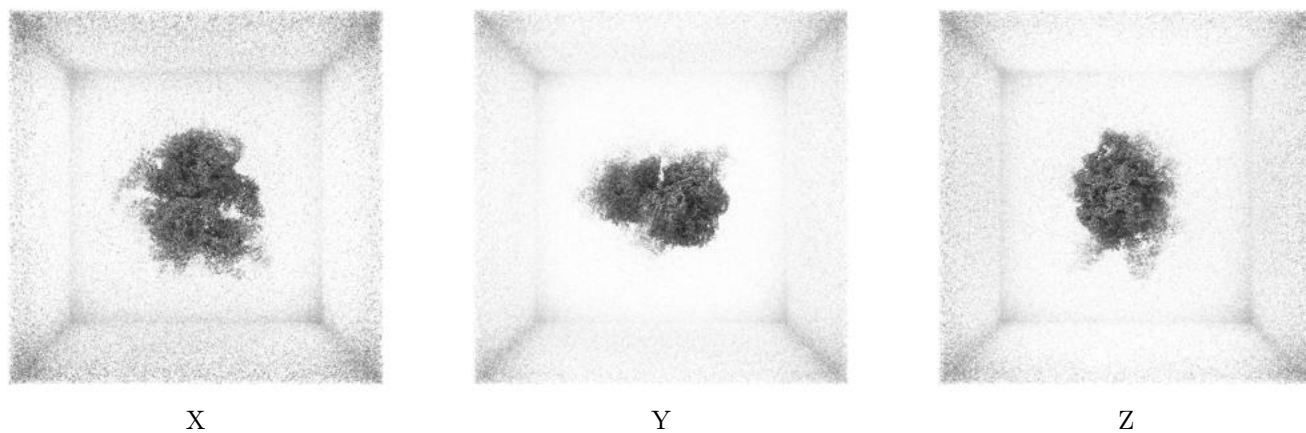
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0796. 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



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



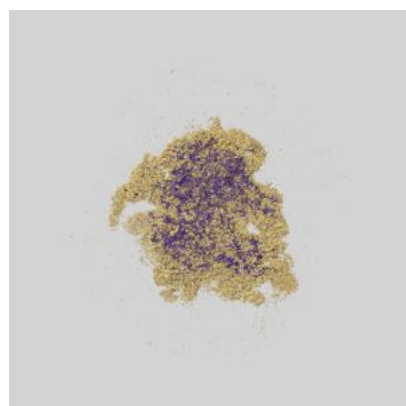
## 6.6 Mask visualisation [i](#)

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

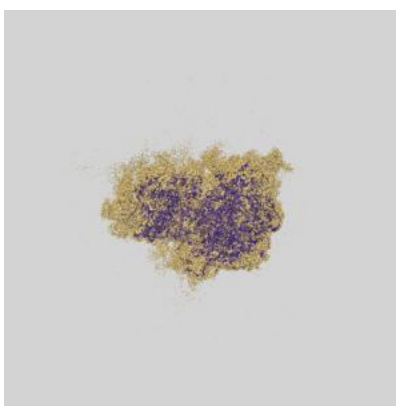
A mask typically either:

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

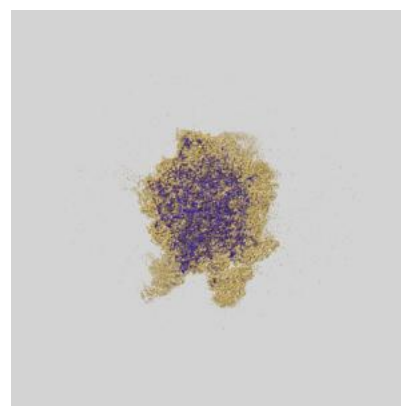
### 6.6.1 emd\_50011\_msk\_1.map [i](#)



X



Y



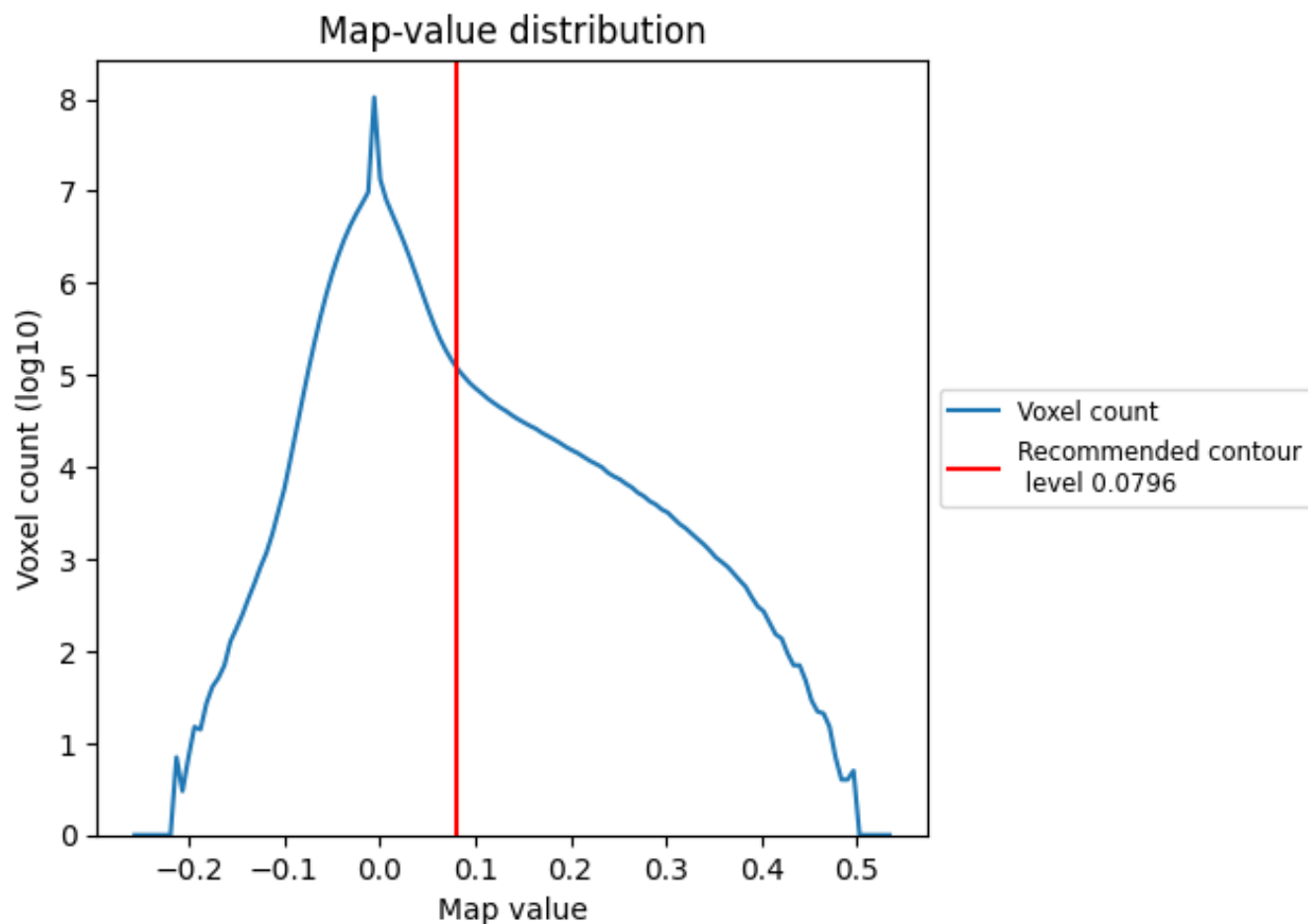
Z



## 7 Map analysis [i](#)

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

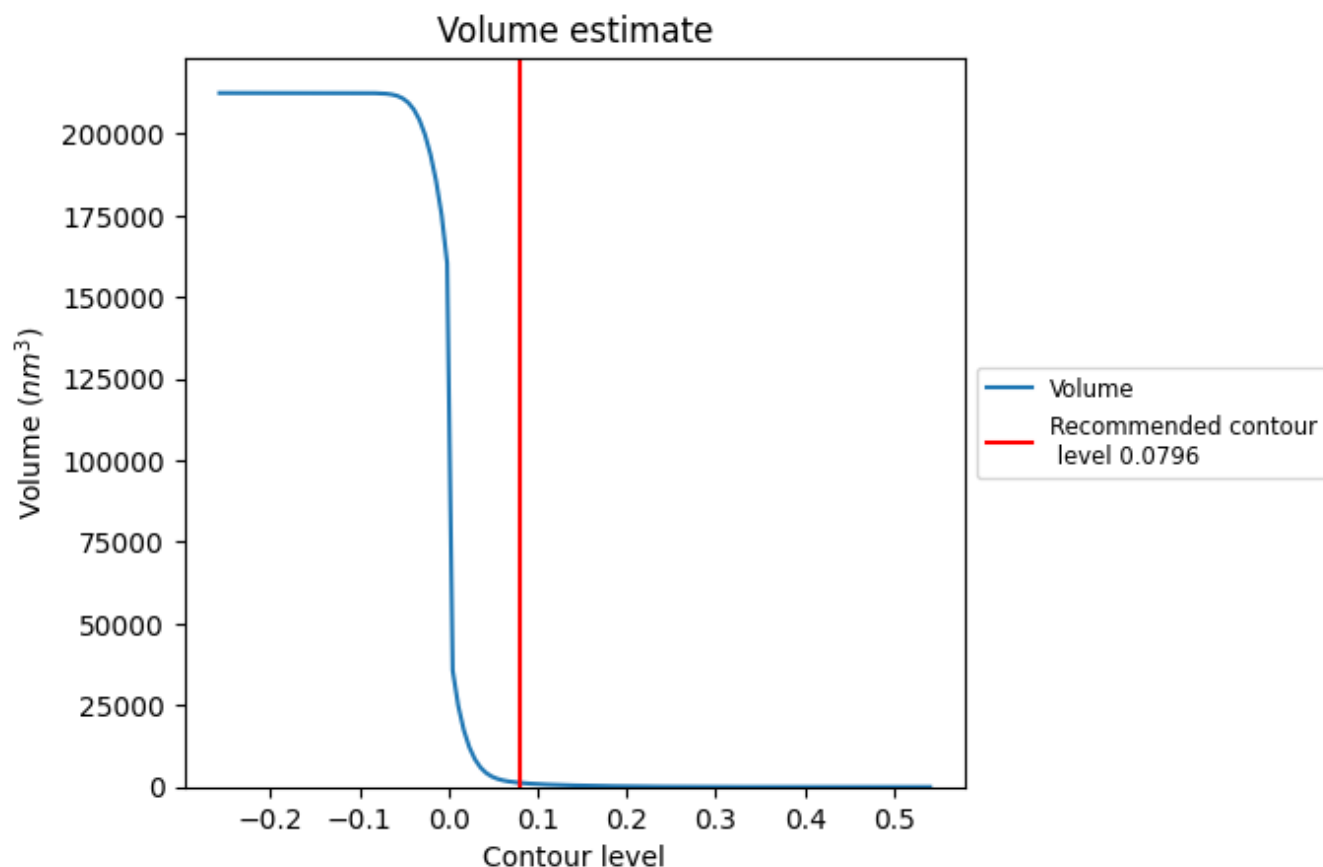
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [i](#)

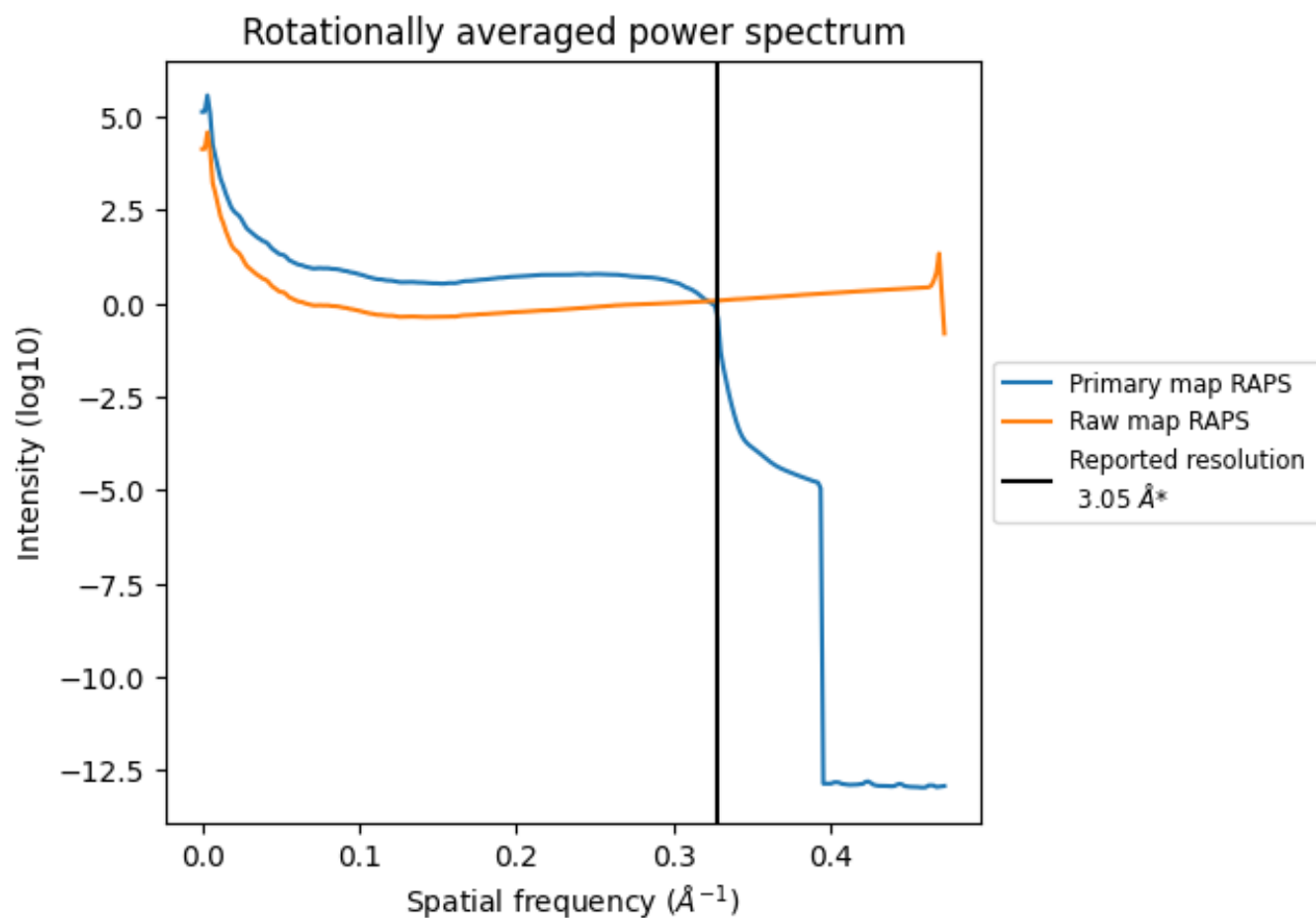


The volume at the recommended contour level is 1277 nm<sup>3</sup>; this corresponds to an approximate mass of 1154 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ



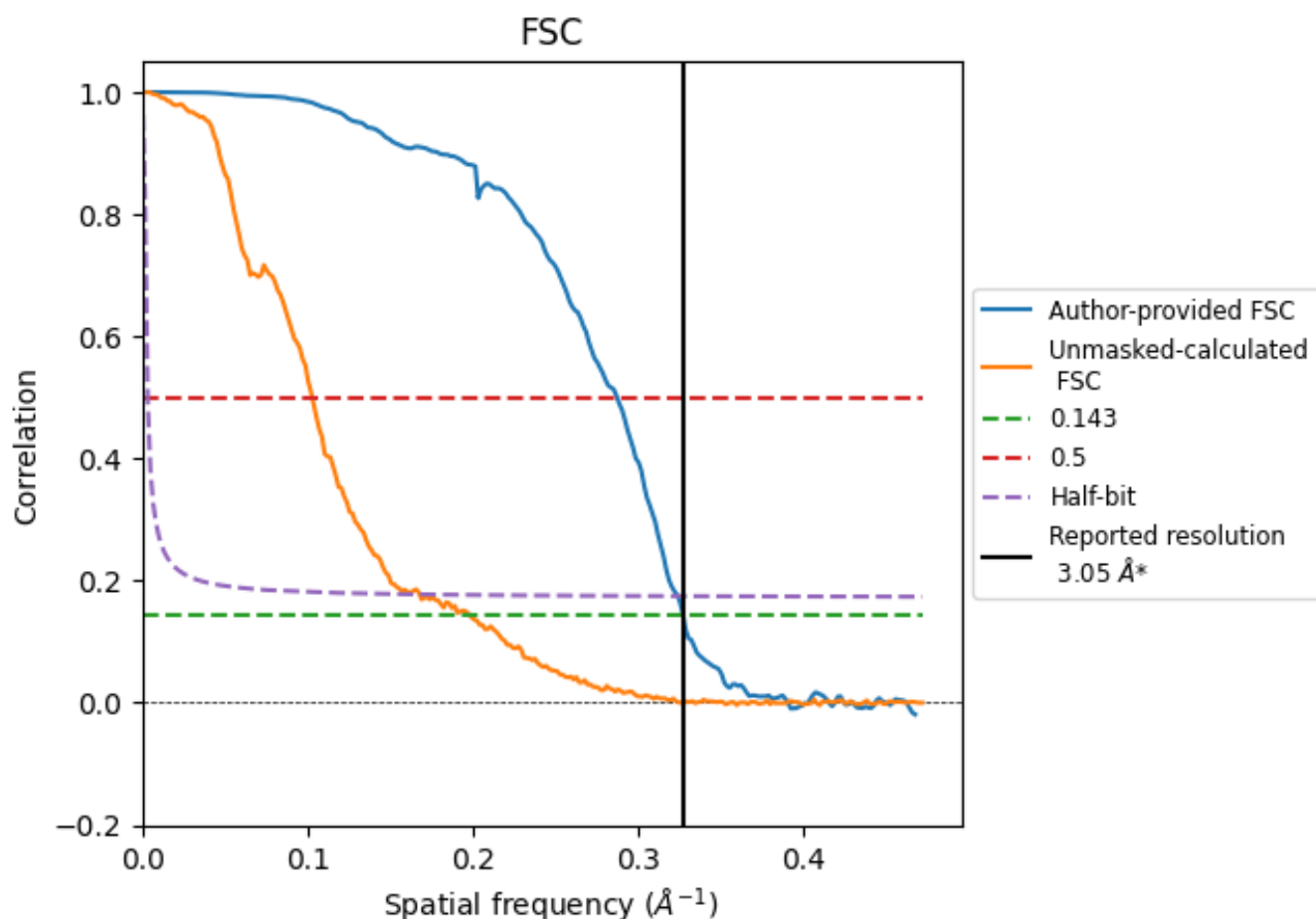
\*Reported resolution corresponds to spatial frequency of 0.328  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.328  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.05	3.48	3.08
Unmasked-calculated*	5.04	9.71	5.95

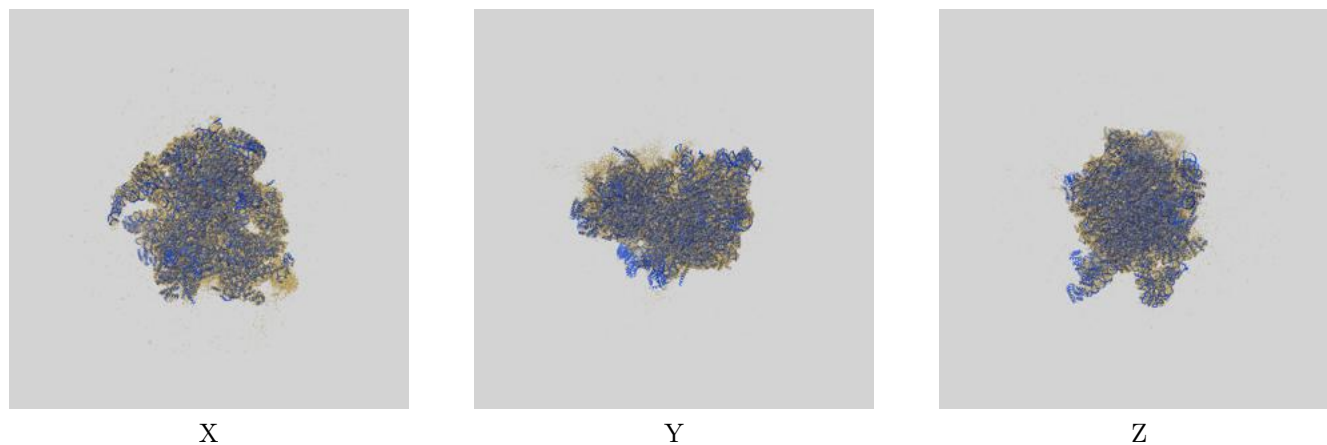
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.04 differs from the reported value 3.05 by more than 10 %



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50011 and PDB model 9EVS. Per-residue inclusion information can be found in section [3](#) on page [23](#).

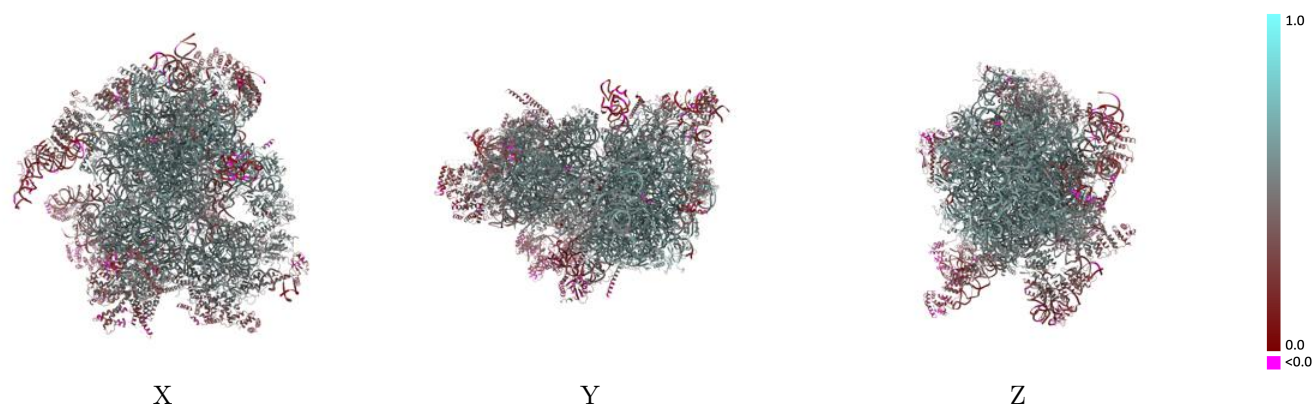
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0796 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

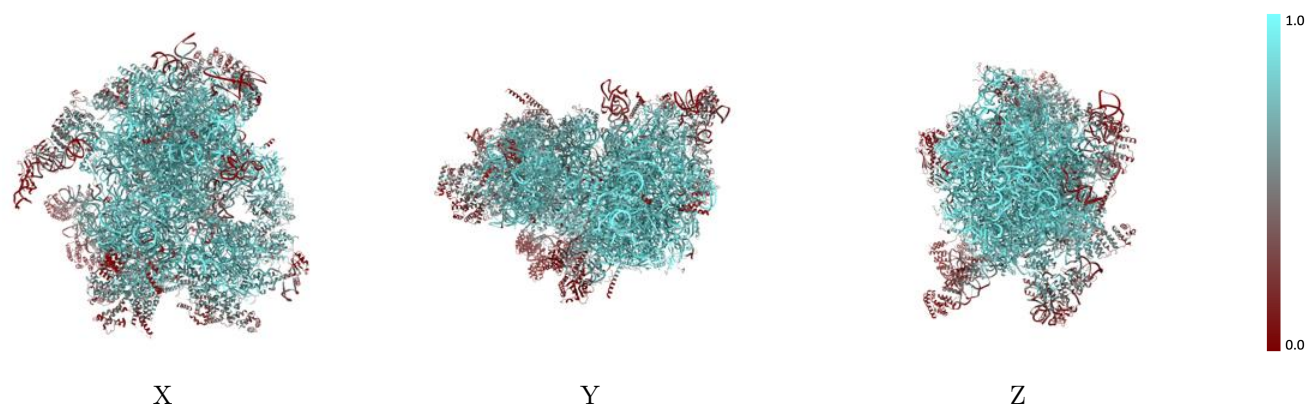


## 9.2 Q-score mapped to coordinate model [i](#)



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

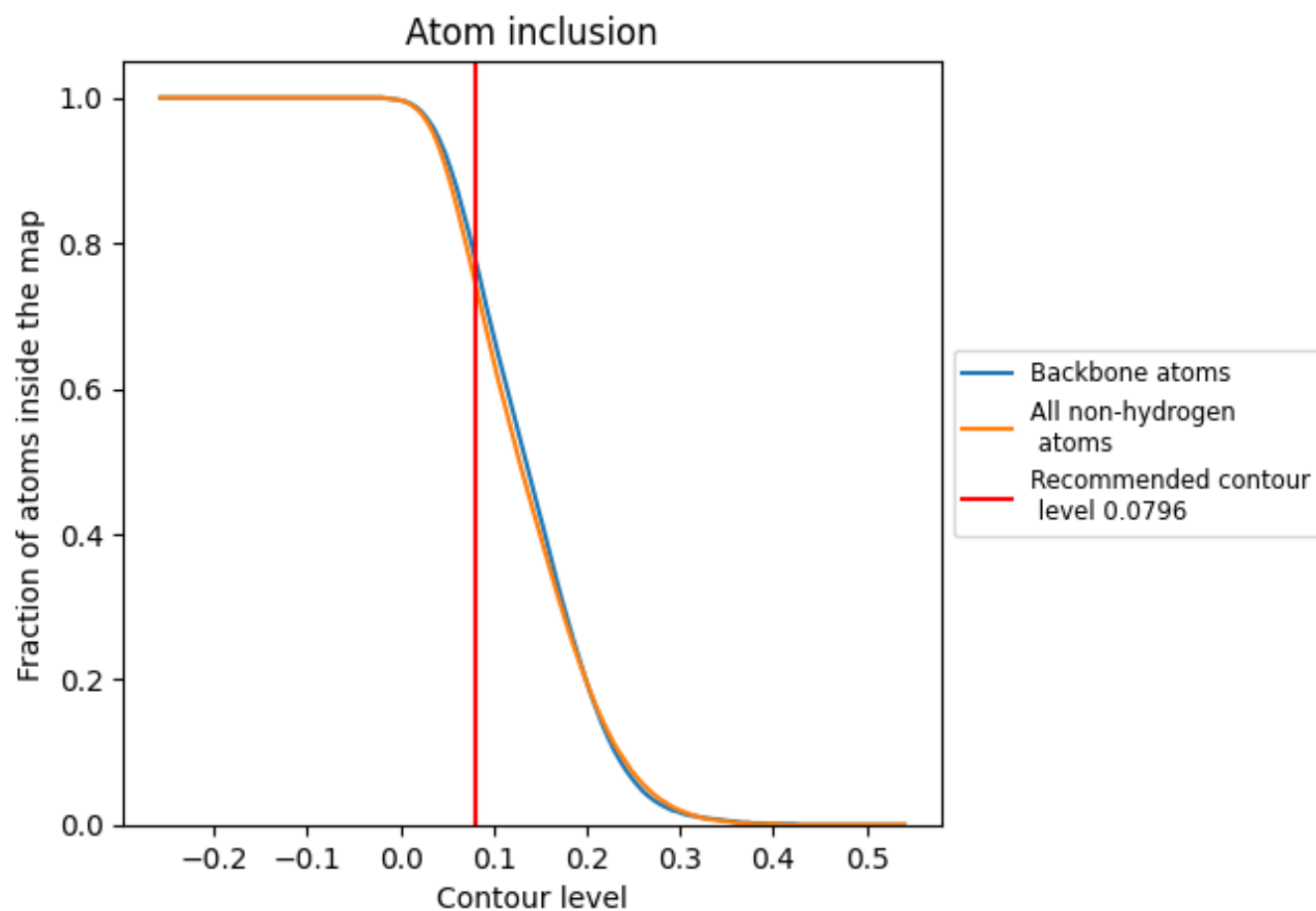
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0796).



## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 78% of all backbone atoms, 75% 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 (0.0796) and Q-score for the entire model and for each chain.





















































































Chain	Atom inclusion	Q-score
All	 0.7490	 0.4830
1	 0.8610	 0.5200
1B	 0.8510	 0.5650
1C	 0.7010	 0.5050
1D	 0.8610	 0.5710
1E	 0.8800	 0.5720
1F	 0.7420	 0.5240
1G	 0.6510	 0.4930
1H	 0.6770	 0.4830
1I	 0.0220	 0.1690
1J	 0.0920	 0.1880
1K	 0.8180	 0.5400
1L	 0.8220	 0.5680
1M	 0.8570	 0.5660
1N	 0.7890	 0.5350
1O	 0.8840	 0.5740
1P	 0.8430	 0.5530
1Q	 0.8110	 0.5530
1R	 0.9310	 0.5900
1S	 0.8270	 0.5670
1T	 0.8840	 0.5750
1U	 0.8200	 0.5590
1V	 0.8360	 0.5640
1W	 0.2130	 0.2470
1X	 0.7670	 0.5210
1Y	 0.8280	 0.5540
1Z	 0.7440	 0.5130
1a	 0.8600	 0.5550
1b	 0.8710	 0.5680
1c	 0.8050	 0.5300
1d	 0.9210	 0.5750
1e	 0.8200	 0.5520
1f	 0.9770	 0.6090
1g	 0.8910	 0.5810
1h	 0.8770	 0.5720



*Continued on next page...*



























*Continued from previous page...*

Chain	Atom inclusion	Q-score
1i	 0.6960	 0.5070
1j	 0.8940	 0.5730
1k	 0.8810	 0.5730
1l	 0.6310	 0.4620
1m	 0.2300	 0.2880
1o	 0.1180	 0.2320
1p	 0.7760	 0.5430
1q	 0.8400	 0.5550
1r	 0.8000	 0.5250
1s	 0.7830	 0.5280
1t	 0.5730	 0.4040
1u	 0.4600	 0.3640
1v	 0.6100	 0.4180
1x	 0.8950	 0.6300
2	 0.8760	 0.5060
3	 0.9400	 0.5490
5	 0.7550	 0.4260
6	 0.6610	 0.5240
A	 0.7660	 0.5170
B	 0.5750	 0.4150
C	 0.7130	 0.4830
D	 0.6730	 0.4740
E	 0.7820	 0.5330
F	 0.7040	 0.4850
G	 0.8330	 0.5470
H	 0.6380	 0.4690
I	 0.8060	 0.5270
J	 0.7400	 0.5030
K	 0.7660	 0.5340
L	 0.7530	 0.5200
M	 0.8250	 0.5460
N	 0.7780	 0.5340
O	 0.8180	 0.5280
P	 0.7660	 0.5260
Q	 0.7350	 0.5030
R	 0.4240	 0.3540
S	 0.6830	 0.5110
T	 0.8410	 0.5580
U	 0.5330	 0.3830
V	 0.6440	 0.4420
W	 0.7000	 0.4850
X	 0.5160	 0.3830

*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
Y	 0.6910	 0.4800
Z	 0.5970	 0.3770
a	 0.5220	 0.3680
b	 0.4680	 0.3790
c	 0.8340	 0.5570
d	 0.5750	 0.4190
e	 0.6980	 0.4680
f	 0.5830	 0.4150
h	 0.1910	 0.2040
i	 0.2840	 0.2850
j	 0.0290	 0.1450
k	 0.5630	 0.4150