wwPDB EM Validation Summary Report

Nov 19, 2022 – 03:24 pm GMT

PDB ID	:	5MRE
EMDB ID	:	EMD-3552
Title	:	Structure of the yeast mitochondrial ribosome - Class B
Authors	:	Desai, N.; Brown, A.; Amunts, A.; Ramakrishnan, V.
Deposited on	:	2016-12-22
Resolution	:	3.75 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

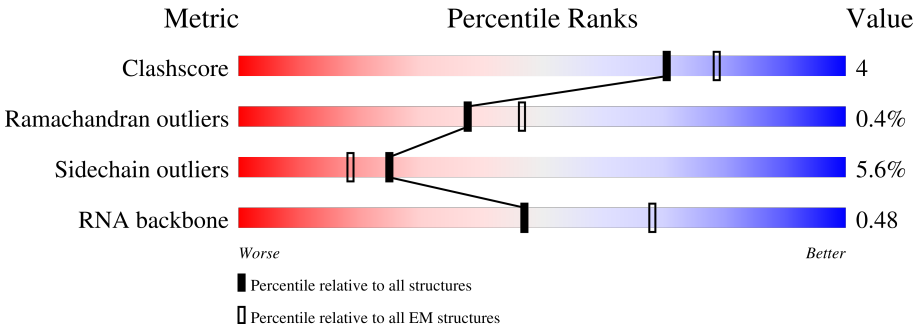
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.75 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)
Clashscore	158937	4297
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	A	3296	60% 19% • 18%
2	B	393	74% 7% • 18%
3	C	249	86% 13% •
4	D	252	88% 10% •
5	E	274	90% 9%
6	F	196	91% 9%
7	G	74	95% 5%

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Mol	Chain	Length	Quality of chain
8	H	160	90% 10%
9	I	138	84% 8% 8%
10	J	220	90% 10%
11	K	195	88% 12%
12	L	237	88% 8%
13	M	151	91% 9%
14	N	118	95%
15	O	225	93% 7%
16	P	207	94% 6%
17	Q	296	88% 7%
18	R	337	91% 7%
19	S	216	80% 6% 14%
20	T	225	85% 11%
21	U	82	89% 11%
22	V	177	50% 47%
23	W	112	95% 5%
24	X	64	84% 16%
25	Y	46	91% 9%
26	Z	62	94% 6%
27	0	38	89% 11%
28	1	348	94% 6%
29	2	113	88% 11%
30	3	130	94% 6%
31	4	138	91% 9%
32	5	324	90% 10%

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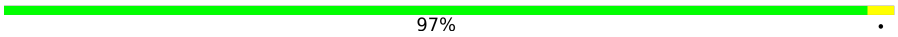
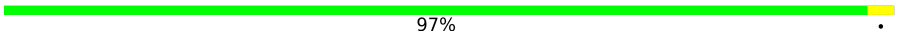
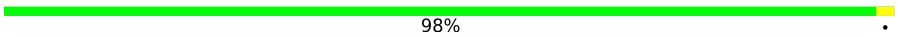
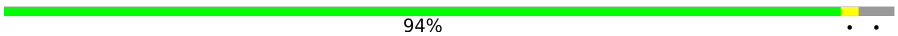
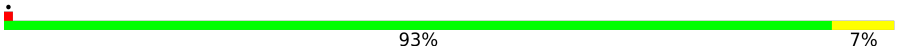
Mol	Chain	Length	Quality of chain
33	6	281	
34	7	106	
35	8	264	
36	9	215	
37	a	177	
38	b	155	
39	c	119	
40	d	215	
41	AA	344	
42	BB	266	
43	CC	398	
44	DD	486	
45	EE	293	
46	FF	125	
47	GG	161	
48	HH	154	
49	II	244	
50	JJ	186	
51	KK	148	
52	LL	124	
53	MM	120	
54	NN	115	
55	OO	253	
56	PP	119	
57	QQ	237	

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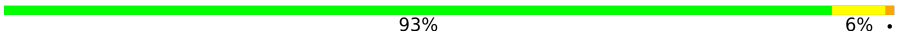
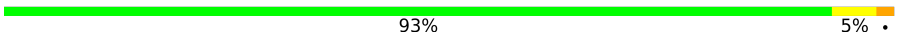
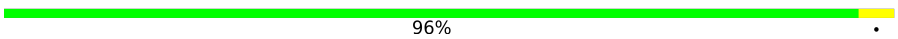
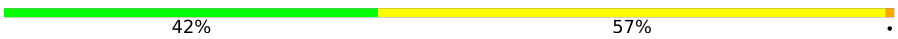
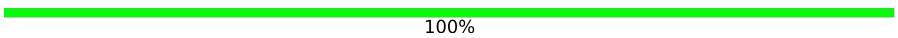
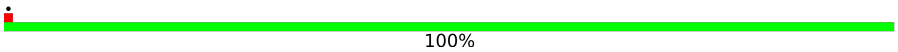
Mol	Chain	Length	Quality of chain
58	RR	99	
59	SS	80	
60	TT	92	
61	UU	233	
62	VV	233	
63	WW	401	
64	XX	96	
65	YY	273	
66	ZZ	91	
67	11	34	
68	22	99	
69	33	255	
70	44	321	
71	55	339	
72	66	319	
73	77	165	
74	88	457	
75	aa	1649	
76	bb	76	
77	cc	94	
78	dd	151	

2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 201462 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 21S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2709	57598	25914	10252	18729	2703	0	0

- Molecule 2 is a protein called uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	321	2527	1575	507	436	9	0	0

- Molecule 3 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	249	1932	1218	360	344	10	0	0

- Molecule 4 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	252	1991	1264	355	369	3	0	0

- Molecule 5 is a protein called uL5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	274	2187	1396	391	394	6	0	0

- Molecule 6 is a protein called uL6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	196	1524	967	273	280	4	0	0

- Molecule 7 is a protein called bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	74	Total	C	N	O	S	0	0
			617	393	110	113	1		

- Molecule 8 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	160	Total	C	N	O	S	0	0
			1275	807	240	224	4		

- Molecule 9 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	127	Total	C	N	O	S	0	0
			956	595	180	170	11		

- Molecule 10 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	220	Total	C	N	O	S	0	0
			1746	1119	326	298	3		

- Molecule 11 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	195	Total	C	N	O	S	0	0
			1573	1001	297	270	5		

- Molecule 12 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	229	Total	C	N	O	S	0	0
			1817	1140	333	336	8		

- Molecule 13 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	151	Total	C	N	O	S	0	0
			1206	766	220	217	3		

- Molecule 14 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	118	Total	C	N	O	S	0	0
			948	598	177	171	2		

- Molecule 15 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	225	Total	C	N	O	S	0	0
			1826	1169	332	320	5		

- Molecule 16 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	207	Total	C	N	O	S	0	0
			1729	1104	310	309	6		

- Molecule 17 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	284	Total	C	N	O	S	0	0
			2272	1451	396	417	8		

- Molecule 18 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	331	Total	C	N	O	S	0	0
			2738	1728	497	509	4		

- Molecule 19 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	185	Total	C	N	O	S	0	0
			1543	994	281	265	3		

- Molecule 20 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	216	Total	C	N	O	S	0	0
			1792	1139	324	325	4		

- Molecule 21 is a protein called uL30m.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	82	Total 639	C 410	N 116	O 113	0	0

- Molecule 22 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	93	Total 729	C 456	N 145	O 127	S 1	0	0

- Molecule 23 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	112	Total 937	C 587	N 181	O 163	S 6	0	0

- Molecule 24 is a protein called bL33m.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	64	Total 512	C 330	N 96	O 86	0	0

- Molecule 25 is a protein called bL34m.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	46	Total 385	C 245	N 82	O 58	0	0

- Molecule 26 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	62	Total 508	C 322	N 111	O 74	S 1	0	0

- Molecule 27 is a protein called bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	38	Total 324	C 205	N 66	O 50	S 3	0	0

- Molecule 28 is a protein called mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	348	Total	C	N	O	S	0	0
			2875	1847	499	523	6		

- Molecule 29 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	113	Total	C	N	O	S	0	0
			944	597	174	168	5		

- Molecule 30 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	130	Total	C	N	O	S	0	0
			1046	671	189	183	3		

- Molecule 31 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	138	Total	C	N	O	S	0	0
			1117	700	219	193	5		

- Molecule 32 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	324	Total	C	N	O	S	0	0
			2552	1630	431	480	11		

- Molecule 33 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	234	Total	C	N	O	S	0	0
			1932	1250	327	353	2		

- Molecule 34 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	106	Total	C	N	O	S	0	0
			858	553	151	152	2		

- Molecule 35 is a protein called mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	199	Total	C	N	O	S	0	0
			1629	1032	278	315	4		

- Molecule 36 is a protein called mL57.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	202	Total	C	N	O	S	0	0
			1587	1014	279	289	5		

- Molecule 37 is a protein called mL58.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	177	Total	C	N	O	S	0	0
			1440	907	267	260	6		

- Molecule 38 is a protein called mL59.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	155	Total	C	N	O	S	0	0
			1299	850	225	221	3		

- Molecule 39 is a protein called mL60.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	119	Total	C	N	O	S	0	0
			1004	645	191	164	4		

- Molecule 40 is a protein called mL67.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	206	Total	C	N	O	S	0	0
			1746	1117	318	304	7		

- Molecule 41 is a protein called bS1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AA	203	Total	C	N	O	S	0	0
			1610	1032	285	288	5		

- Molecule 42 is a protein called uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BB	266	Total	C	N	O	S	0	0
			2085	1313	366	404	2		

- Molecule 43 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	CC	339	Total	C	N	O	S	0	0
			2821	1772	502	517	30		

- Molecule 44 is a protein called uS4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	DD	287	Total	C	N	O	S	0	0
			2369	1542	420	403	4		

- Molecule 45 is a protein called uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	EE	288	Total	C	N	O	S	0	0
			2306	1473	408	417	8		

- Molecule 46 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	FF	125	Total	C	N	O	S	0	0
			1002	639	182	177	4		

- Molecule 47 is a protein called uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	GG	161	Total	C	N	O	S	0	0
			1282	811	238	228	5		

- Molecule 48 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	HH	154	Total	C	N	O	S	0	0
			1213	767	217	220	9		

- Molecule 49 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	II	226	Total	C	N	O	S	0	0
			1820	1167	332	316	5		

- Molecule 50 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	JJ	186	Total	C	N	O	S	0	0
			1508	964	259	281	4		

- Molecule 51 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	KK	142	Total	C	N	O	S	0	0
			1121	717	195	203	6		

- Molecule 52 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LL	124	Total	C	N	O	S	0	0
			948	585	194	165	4		

- Molecule 53 is a protein called uS13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	MM	120	Total	C	N	O	S	0	0
			942	596	179	161	6		

- Molecule 54 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	NN	115	Total	C	N	O	S	0	0
			953	612	182	154	5		

- Molecule 55 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	OO	238	Total	C	N	O	S	0	0
			1962	1227	371	356	8		

- Molecule 56 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	PP	116	Total	C	N	O	S	0	0
			919	586	172	159	2		

- Molecule 57 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	QQ	204	Total	C	N	O	S	0	0
			1683	1055	315	308	5		

- Molecule 58 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	RR	91	Total	C	N	O	S	0	0
			738	463	143	128	4		

- Molecule 59 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SS	80	Total	C	N	O	S	0	0
			636	408	115	111	2		

- Molecule 60 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	TT	92	Total	C	N	O	S	0	0
			760	475	150	130	5		

- Molecule 61 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	UU	233	Total	C	N	O	S	0	0
			1907	1211	331	358	7		

- Molecule 62 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	VV	233	Total	C	N	O	S	0	0
			1872	1189	338	342	3		

- Molecule 63 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	WW	401	Total	C	N	O	S	0	0
			3216	2072	540	596	8		

- Molecule 64 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	XX	96	Total	C	N	O	S	0	0
			774	496	140	135	3		

- Molecule 65 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	YY	269	Total	C	N	O	S	0	0
			2258	1429	404	421	4		

- Molecule 66 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	ZZ	87	Total	C	N	O	S	0	0
			687	435	128	118	6		

- Molecule 67 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	11	34	Total	C	N	O	S	0	0
			303	183	75	43	2		

- Molecule 68 is a protein called mS41.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	22	99	Total	C	N	O	S	0	0
			833	530	156	146	1		

- Molecule 69 is a protein called mS42.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	33	244	Total	C	N	O	S	0	0
			1953	1261	328	359	5		

- Molecule 70 is a protein called mS43.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	44	270	Total	C	N	O	S	0	0
			2169	1380	370	412	7		

- Molecule 71 is a protein called mS44.

Mol	Chain	Residues	Atoms				AltConf	Trace
71	55	59	Total	C	N	O	0	0
			508	338	84	86		

- Molecule 72 is a protein called mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	66	305	Total	C	N	O	S	0	0
			2488	1587	445	450	6		

- Molecule 73 is a protein called mS46.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	77	165	Total	C	N	O	S	0	0
			1330	854	214	259	3		

- Molecule 74 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	88	452	Total	C	N	O	S	0	0
			3573	2272	600	681	20		

- Molecule 75 is a RNA chain called 15S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	aa	1501	Total	C	N	O	P	0	0
			31883	14338	5633	10411	1501		

- Molecule 76 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	bb	76	Total	C	N	O	P	0	0
			1615	723	289	528	75		

- Molecule 77 is a protein called unknown protein sequence 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
77	cc	94	Total 470	C 282	N 94	O 94	0	0

- Molecule 78 is a protein called unknown protein sequence 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	dd	151	Total 755	C 453	N 151	O 151	0	0

- Molecule 79 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
79	A	183	Total 183	Mg 183	0
79	BB	1	Total 1	Mg 1	0
79	LL	1	Total 1	Mg 1	0
79	MM	1	Total 1	Mg 1	0
79	QQ	1	Total 1	Mg 1	0
79	WW	1	Total 1	Mg 1	0
79	aa	111	Total 111	Mg 111	0

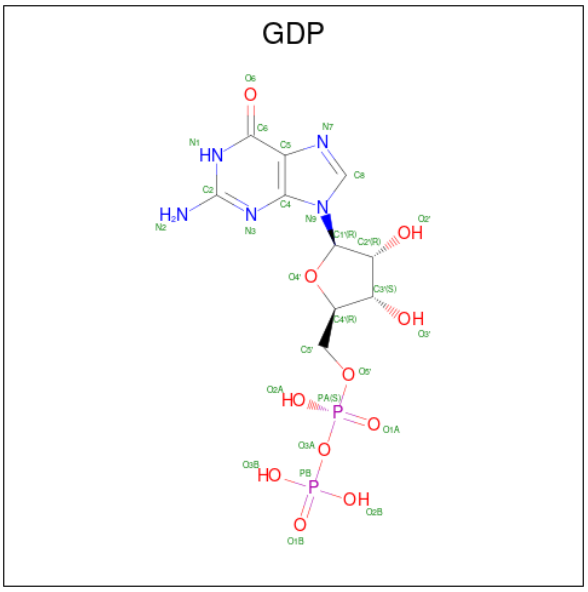
- Molecule 80 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
80	B	1	Total 1	Na 1	0

- Molecule 81 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	W	1	Total 1	Zn 1	0
81	0	1	Total 1	Zn 1	0

- Molecule 82 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



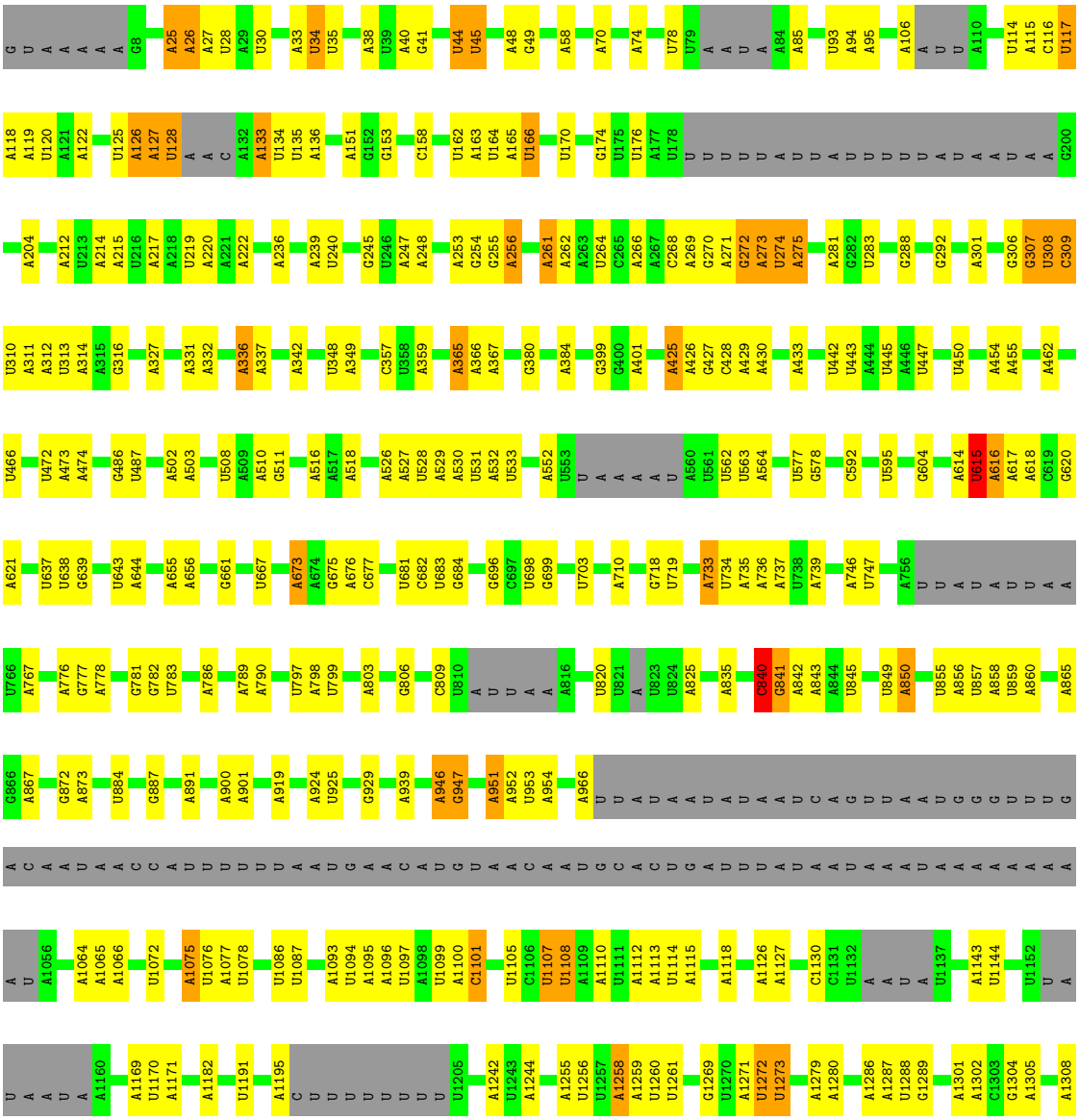
Mol	Chain	Residues	Atoms					AltConf
82	WW	1	Total	C	N	O	P	0
			28	10	5	11	2	

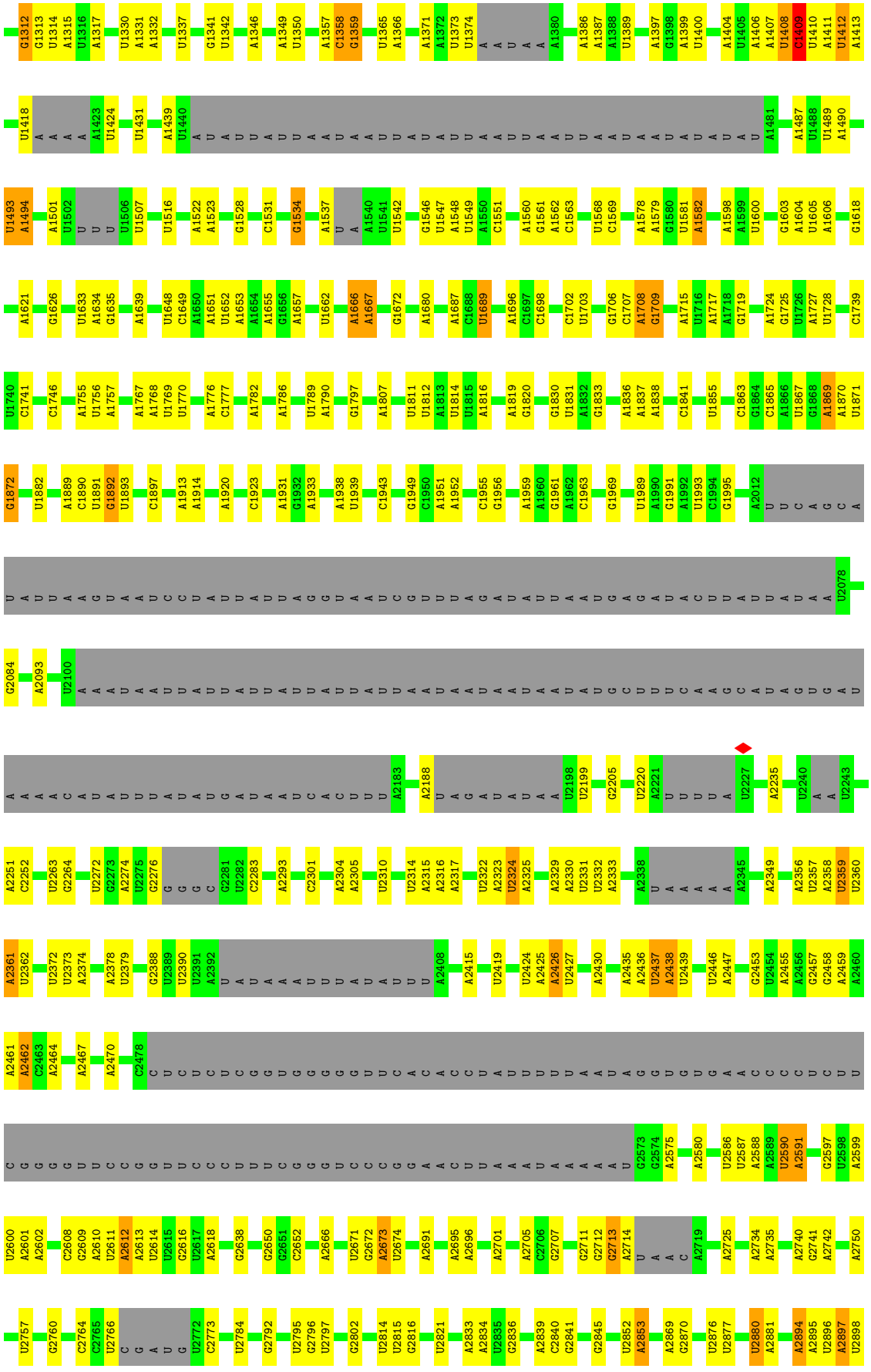
3 Residue-property plots (i)

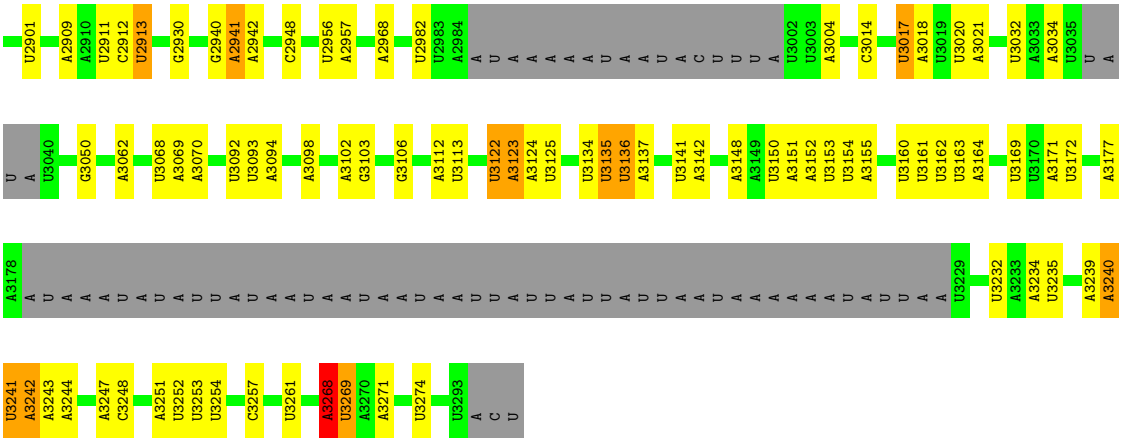
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 21S ribosomal RNA

Chain A:

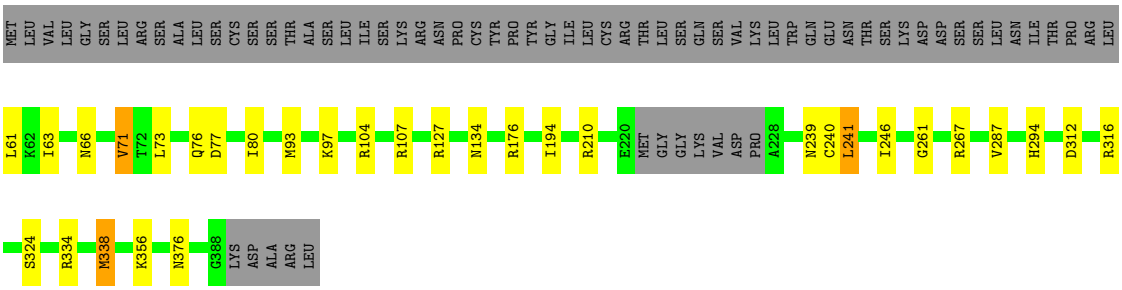






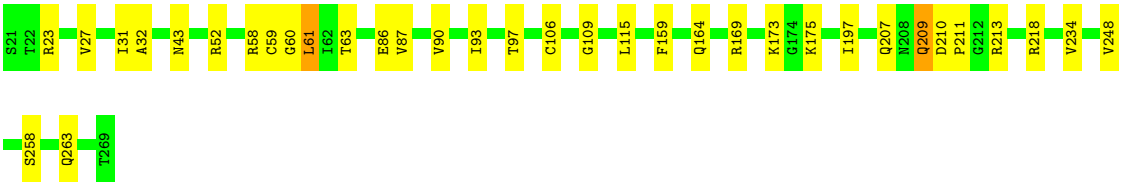
• Molecule 2: uL2m

Chain B:



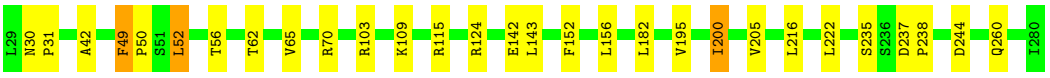
• Molecule 3: uL3m

Chain C:



• Molecule 4: uL4m

Chain D:



• Molecule 5: uL5m

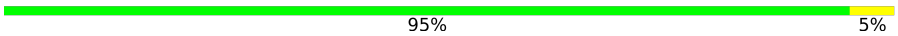
Chain E:

• Molecule 6: uL6m

Chain F:

• Molecule 7: bL9m

Chain G:



• Molecule 8: uL13m

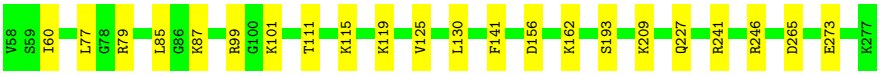
Chain H:

• Molecule 9: uL14m

Chain I:

• Molecule 10: uL15m

Chain J:



• Molecule 11: uL16m

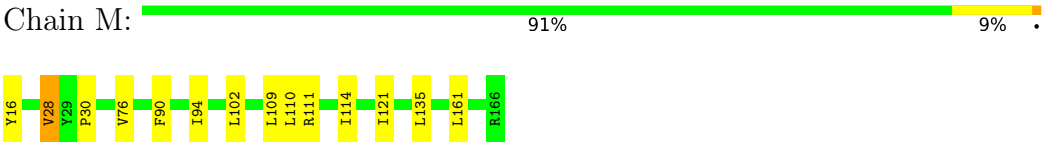
Chain K:

• Molecule 12: bL17m

Chain L:

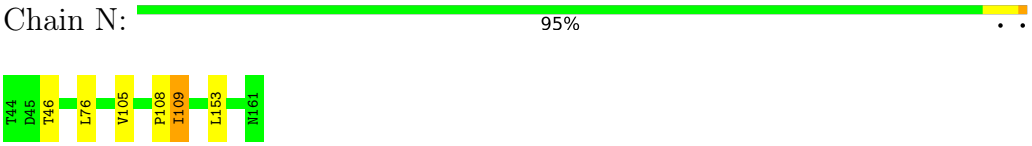
• Molecule 13: bL19m

Chain M:



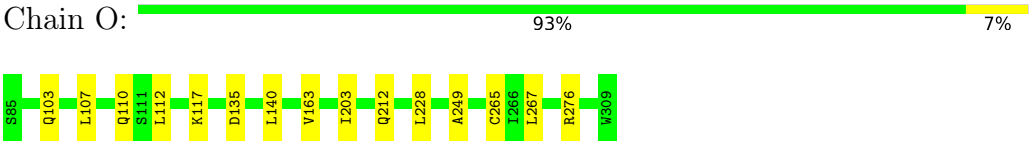
• Molecule 14: bL21m

Chain N:



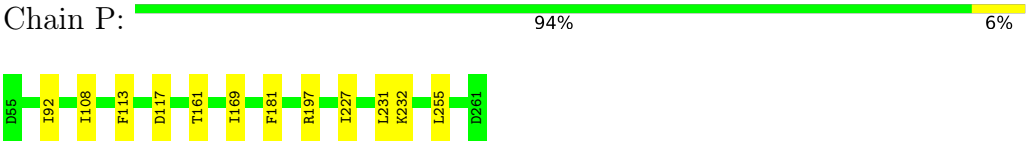
• Molecule 15: uL22m

Chain O:



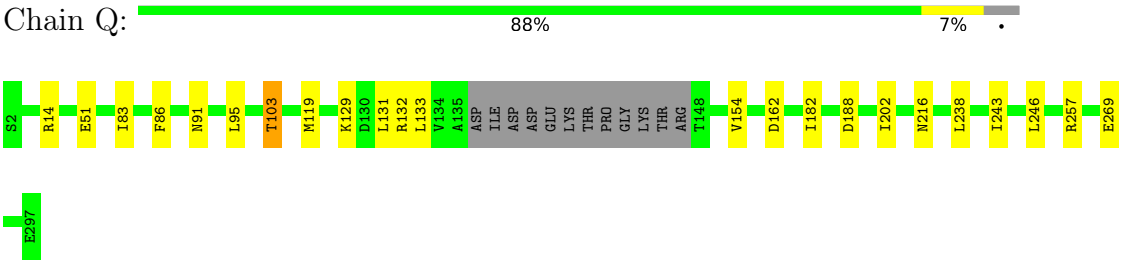
• Molecule 16: uL23m

Chain P:



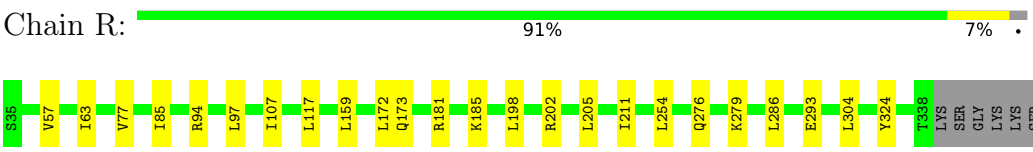
• Molecule 17: uL24m

Chain Q:



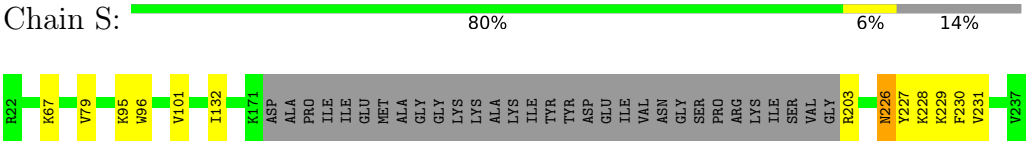
• Molecule 18: bL27m

Chain R:



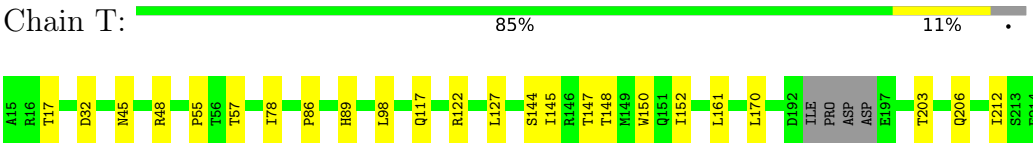
• Molecule 19: bL28m

Chain S:



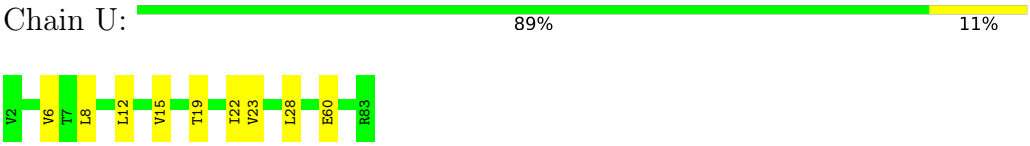
• Molecule 20: uL29m

Chain T:



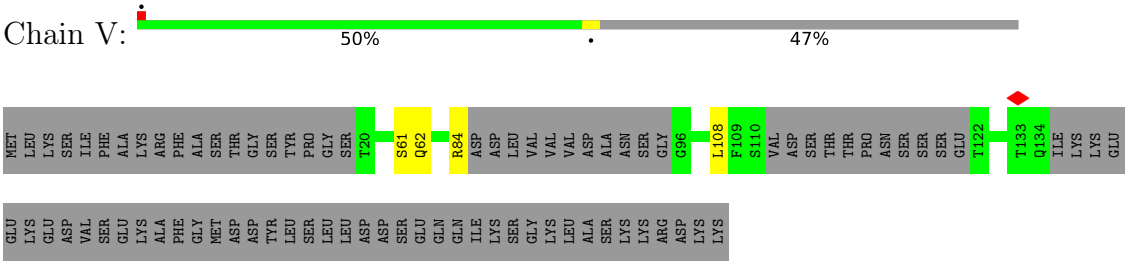
• Molecule 21: uL30m

Chain U:



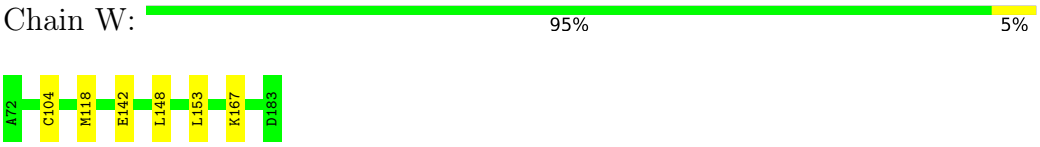
• Molecule 22: bL31m

Chain V:



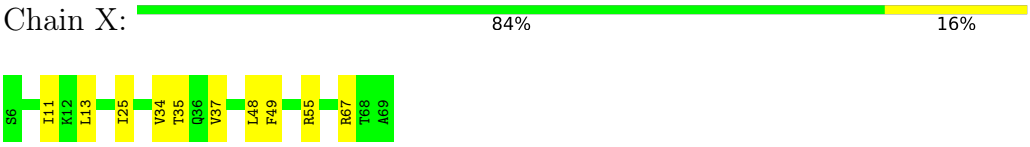
• Molecule 23: bL32m

Chain W:



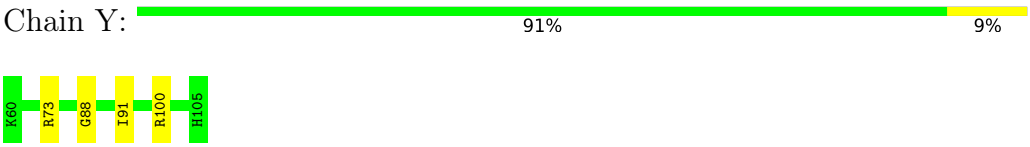
• Molecule 24: bL33m

Chain X:



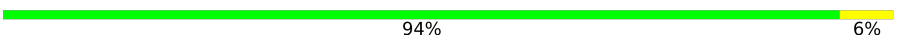
• Molecule 25: bL34m

Chain Y:



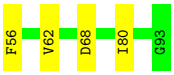
• Molecule 26: bL35m

Chain Z:



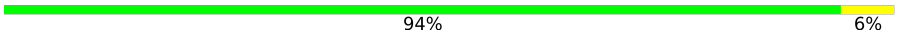
• Molecule 27: bL36m

Chain 0:



• Molecule 28: mL38

Chain 1:

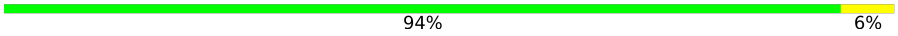


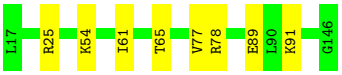
• Molecule 29: mL40

Chain 2:

• Molecule 30: mL41

Chain 3:



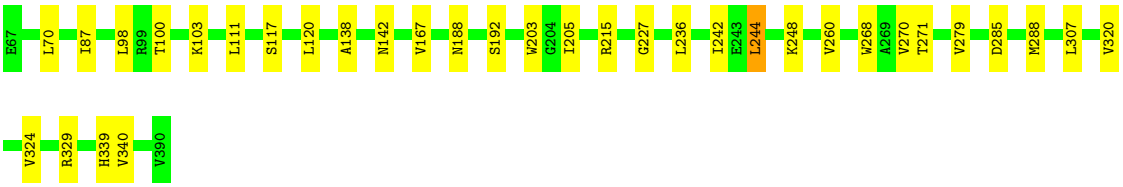


• Molecule 31: mL43

Chain 4:

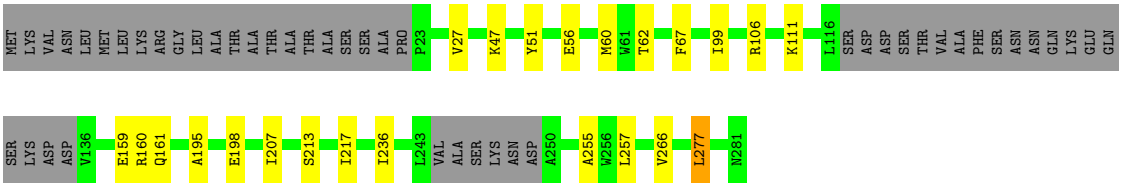
• Molecule 32: mL44

Chain 5:



• Molecule 33: mL46

Chain 6:

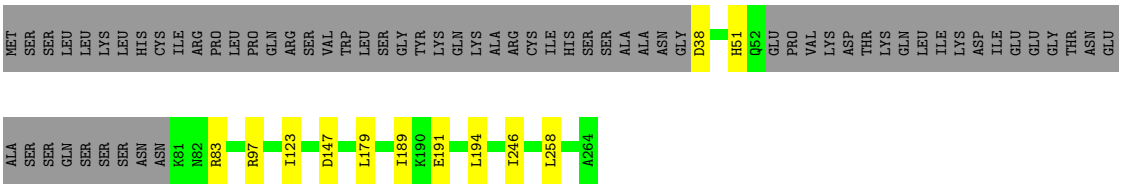


• Molecule 34: mL49

Chain 7:

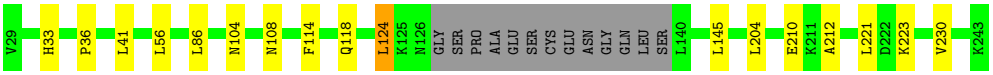
• Molecule 35: mL50

Chain 8:



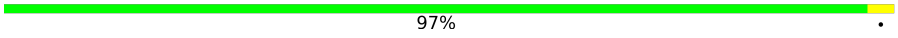
• Molecule 36: mL57

Chain 9:



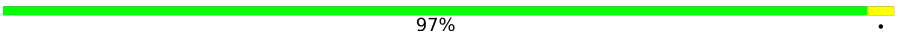
• Molecule 37: mL58

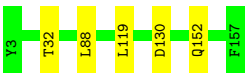
Chain a:



• Molecule 38: mL59

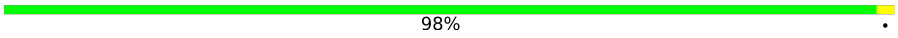
Chain b:

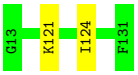




• Molecule 39: mL60

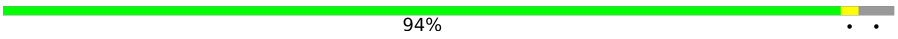
Chain c:

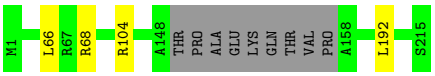




• Molecule 40: mL67

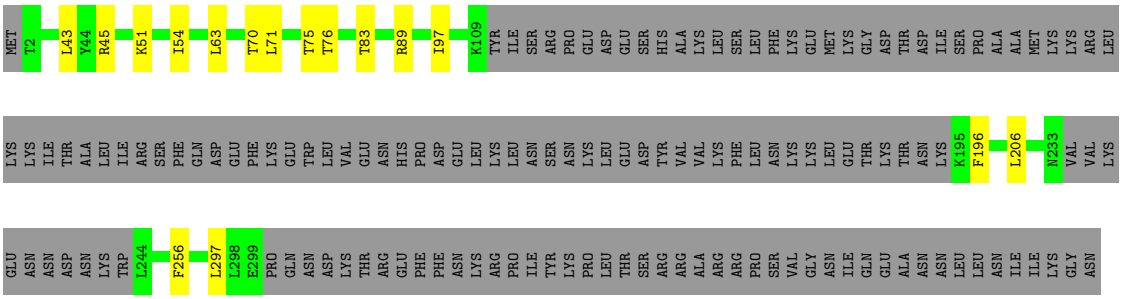
Chain d:





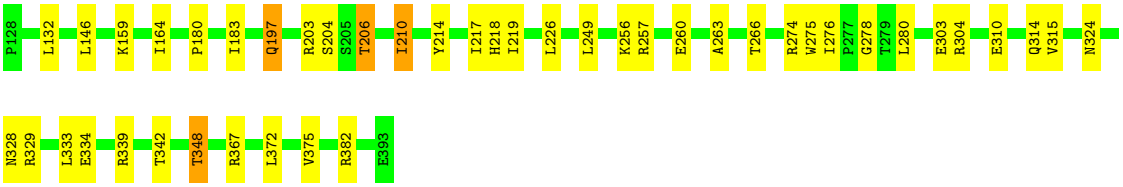
• Molecule 41: bS1m

Chain AA:



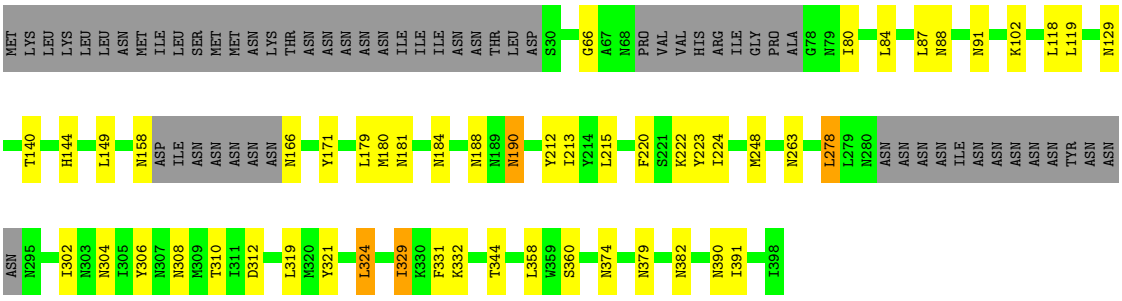
• Molecule 42: uS2m

Chain BB:



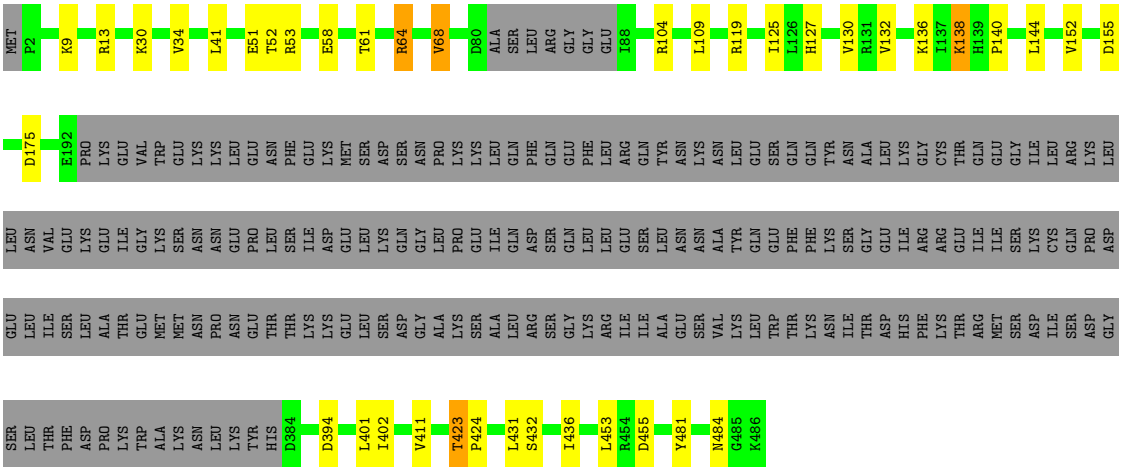
• Molecule 43: uS3m

Chain CC:



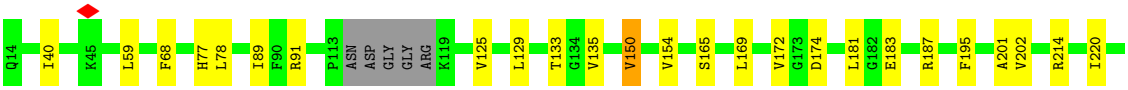
• Molecule 44: uS4m

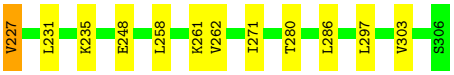
Chain DD:



• Molecule 45: uS5m

Chain EE:



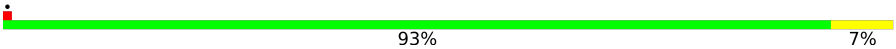


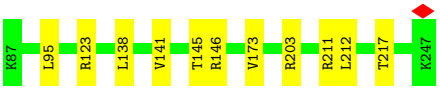
• Molecule 46: bS6m

Chain FF:

• Molecule 47: uS7m

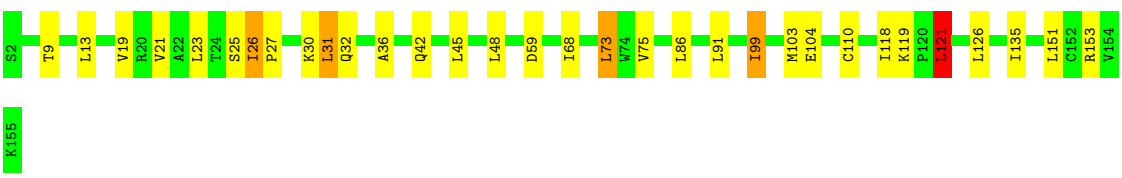
Chain GG:





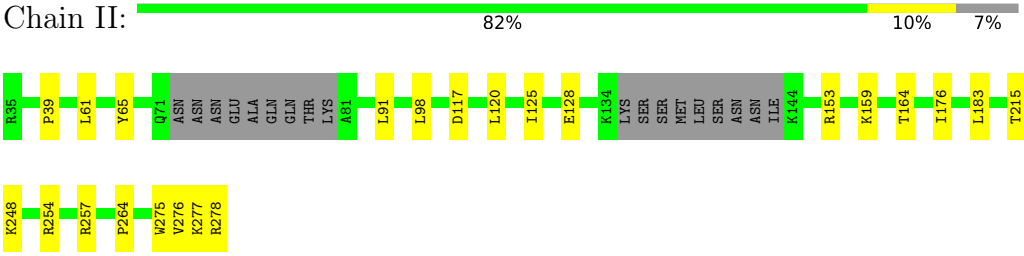
• Molecule 48: uS8m

Chain HH:



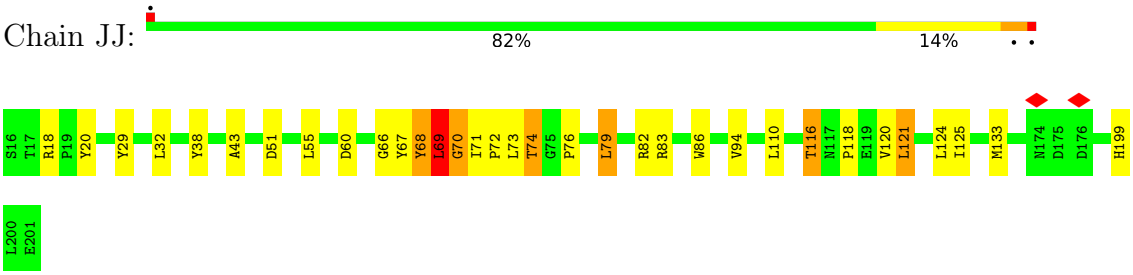
• Molecule 49: uS9m

Chain II:



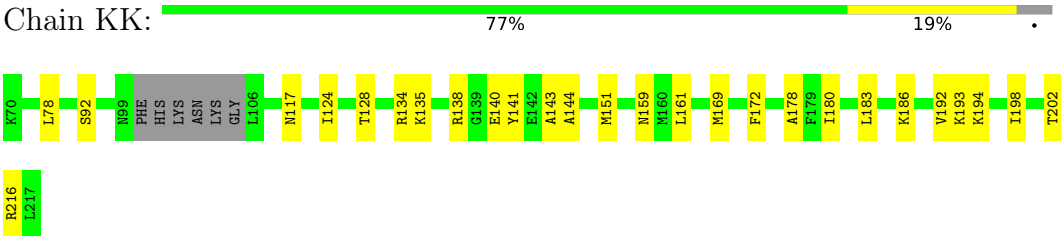
• Molecule 50: uS10m

Chain JJ:



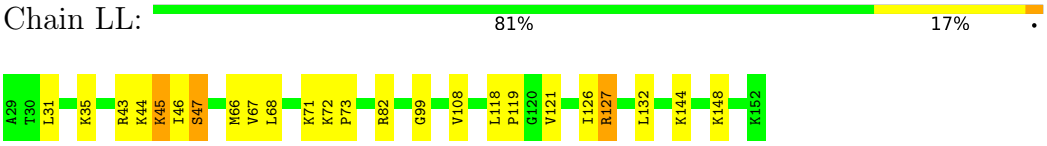
• Molecule 51: uS11m

Chain KK:



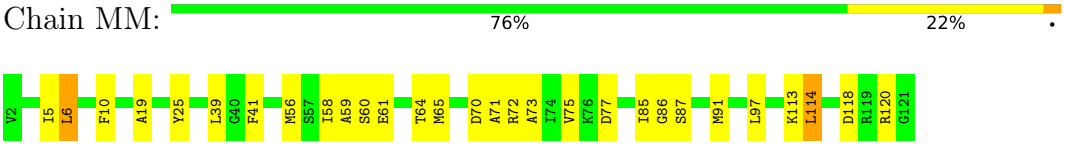
• Molecule 52: uS12m

Chain LL:



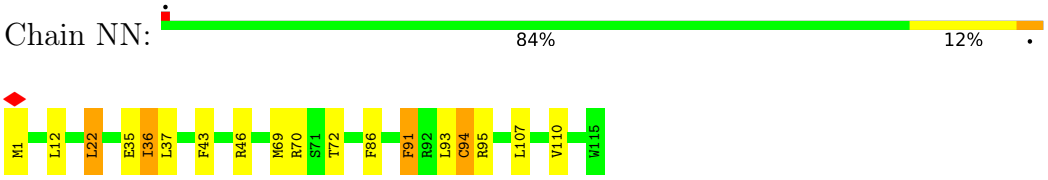
• Molecule 53: uS13m

Chain MM:



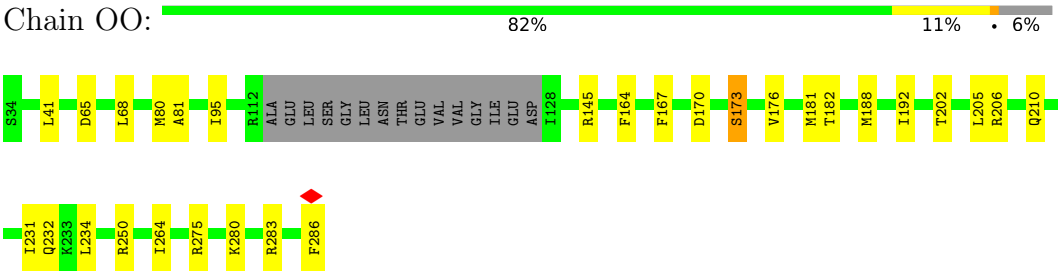
• Molecule 54: uS14m

Chain NN:



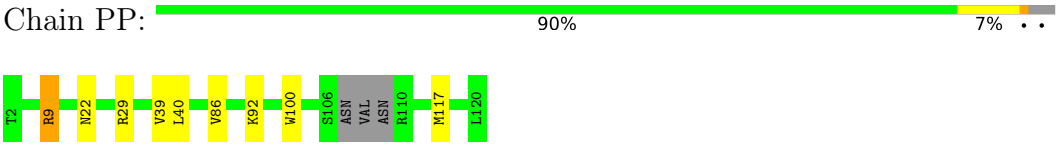
• Molecule 55: uS15m

Chain OO:



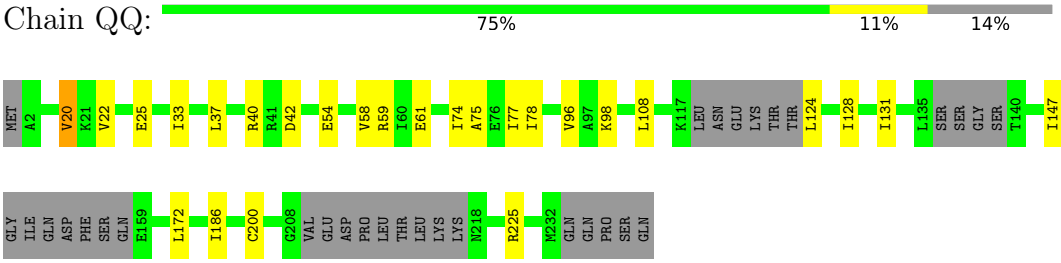
• Molecule 56: bS16m

Chain PP:



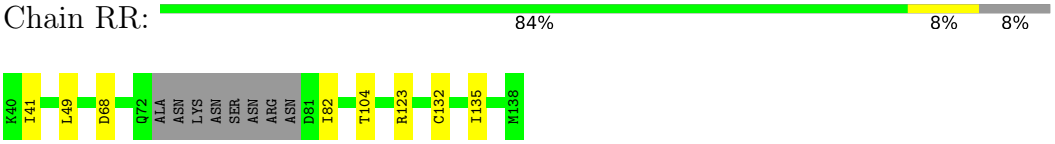
• Molecule 57: uS17m

Chain QQ:



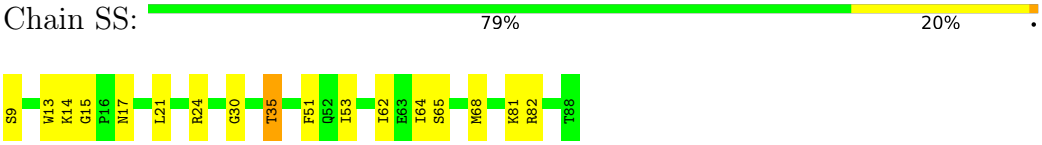
• Molecule 58: bS18m

Chain RR:



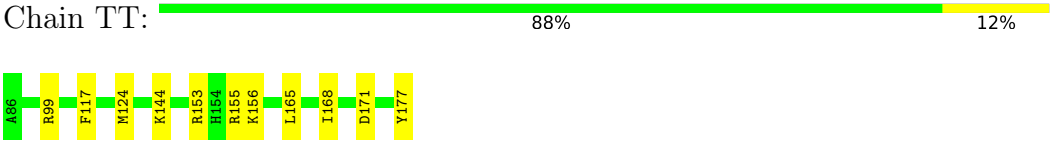
• Molecule 59: uS19m

Chain SS:



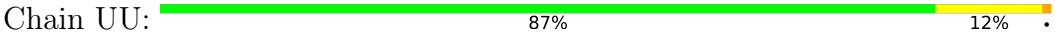
• Molecule 60: bS21m

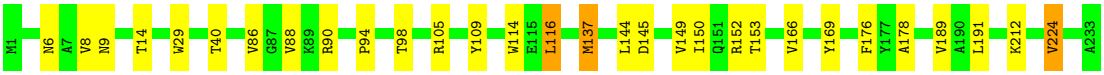
Chain TT:



• Molecule 61: mS23

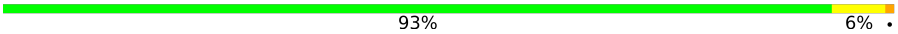
Chain UU:





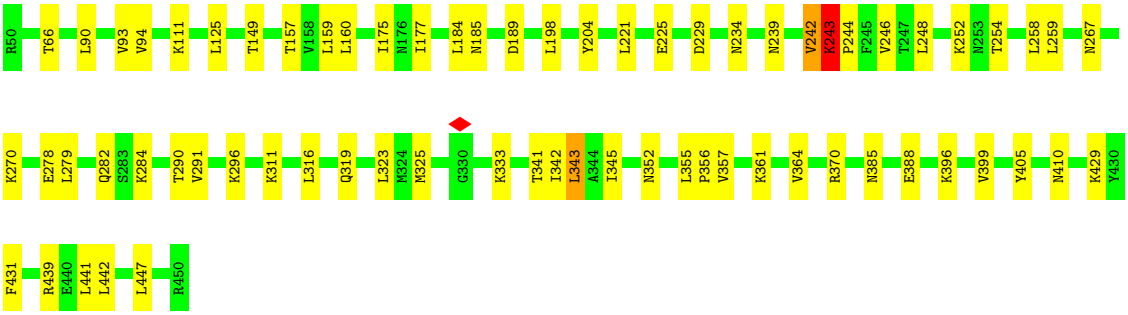
• Molecule 62: mS26

Chain VV:



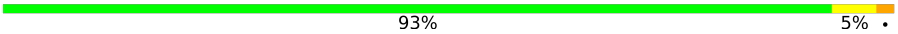
• Molecule 63: mS29

Chain WW:



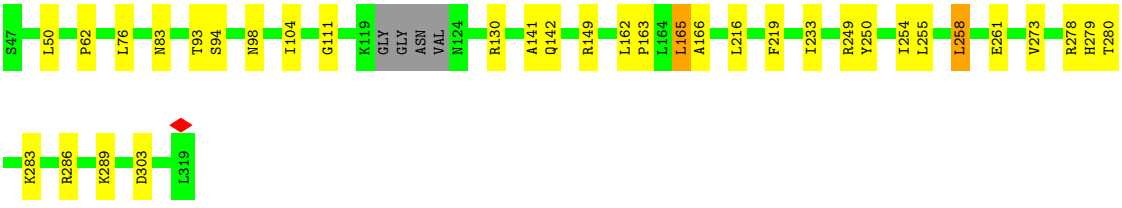
• Molecule 64: mS33

Chain XX:



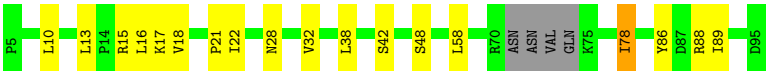
• Molecule 65: mS35

Chain YY:



• Molecule 66: mS37

Chain ZZ:

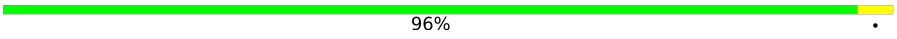


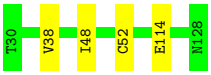
• Molecule 67: mS38

Chain 11:

• Molecule 68: mS41

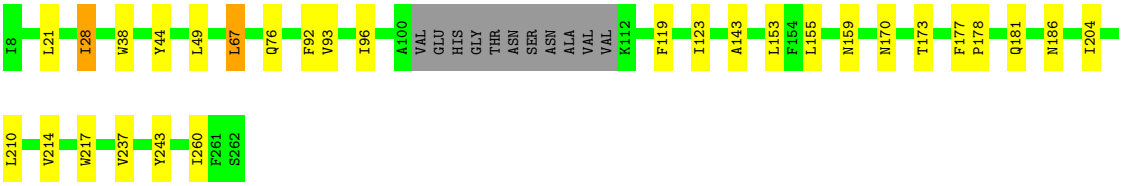
Chain 22:





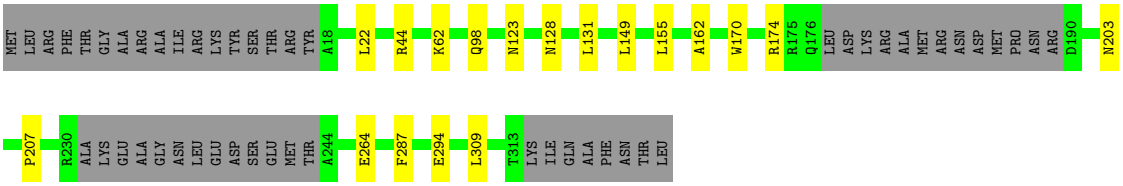
• Molecule 69: mS42

Chain 33:



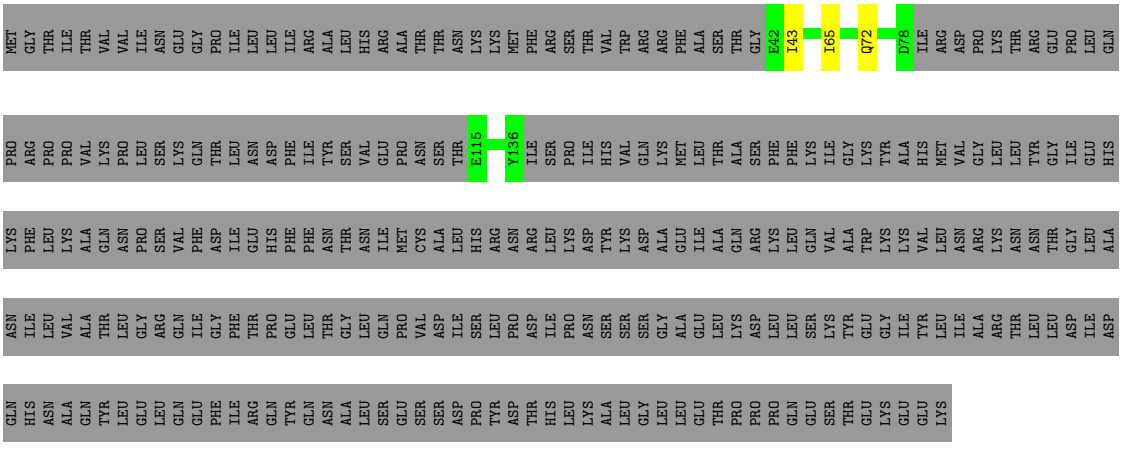
• Molecule 70: mS43

Chain 44:



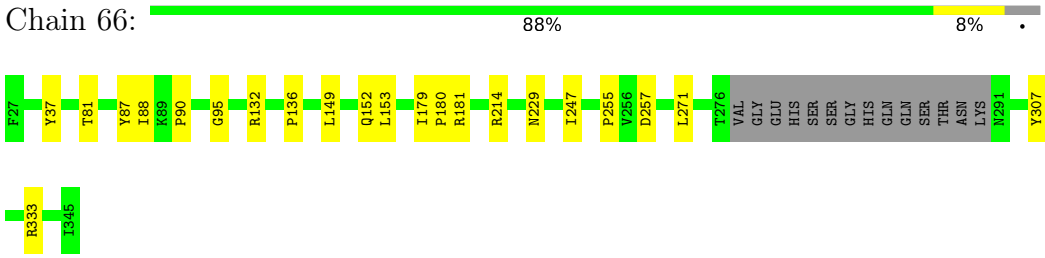
• Molecule 71: mS44

Chain 55:



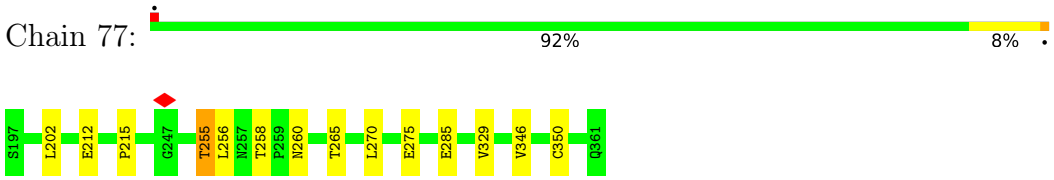
• Molecule 72: mS45

Chain 66:



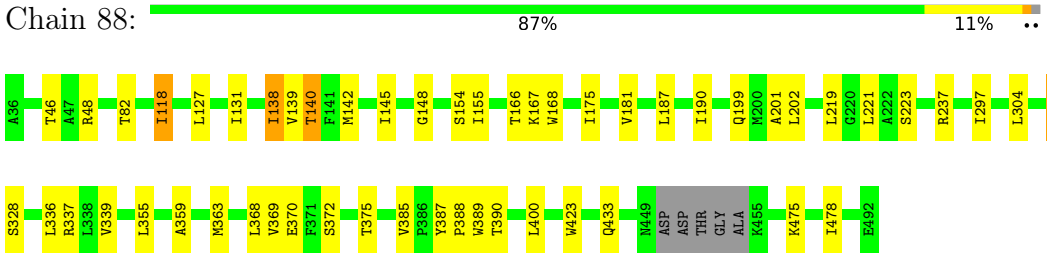
- Molecule 73: mS46

Chain 77:



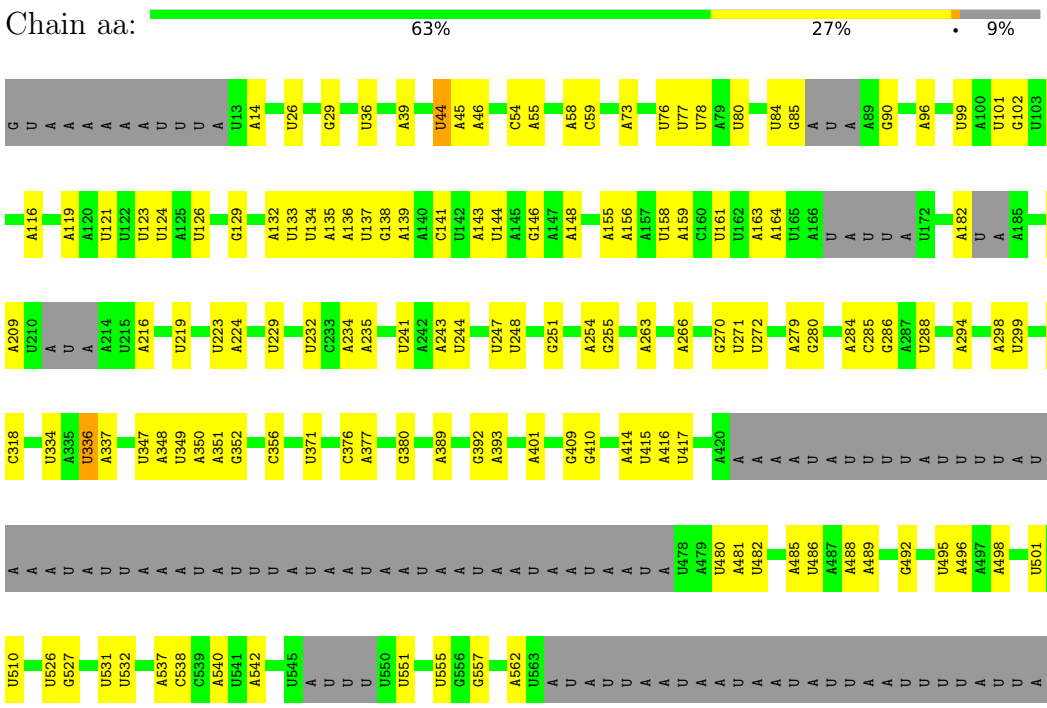
- Molecule 74: mS47

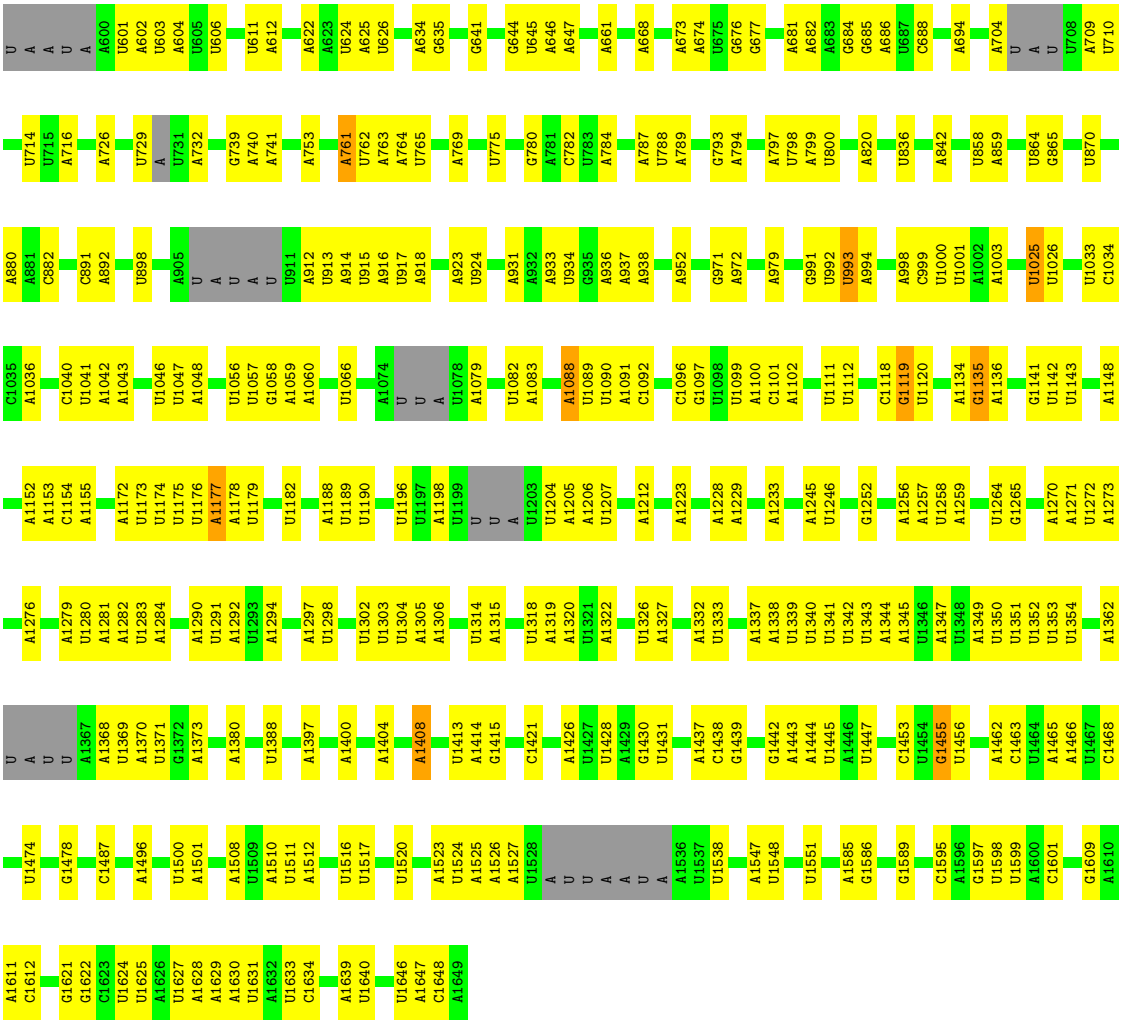
Chain 88:



- Molecule 75: 15S ribosomal RNA

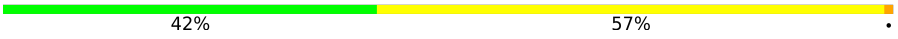
Chain aa:

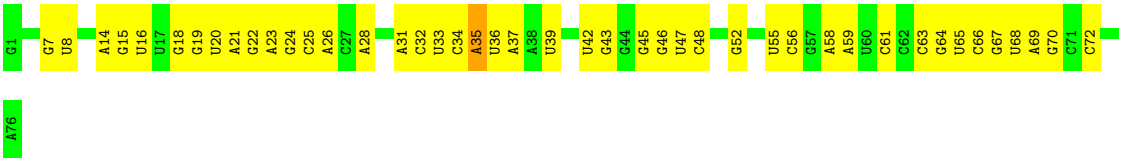




• Molecule 76: tRNA

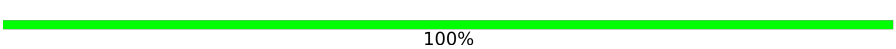
Chain bb:





• Molecule 77: unknown protein sequence 1

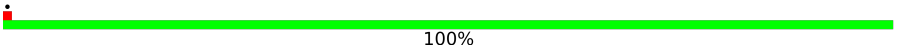
Chain cc:

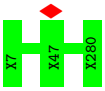


There are no outlier residues recorded for this chain.

• Molecule 78: unknown protein sequence 2

Chain dd:




X7
X47
X280

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55448	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	23.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.590	Depositor
Minimum map value	-0.375	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.00586	Depositor
Map size (Å)	442.2, 442.2, 442.2	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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	A	0.23	0/64517	0.70	14/100359 (0.0%)
2	B	0.34	0/2573	0.69	1/3456 (0.0%)
3	C	0.32	0/1975	0.61	0/2657
4	D	0.35	0/2031	0.66	0/2751
5	E	0.33	0/2244	0.57	0/3033
6	F	0.33	0/1551	0.57	0/2093
7	G	0.33	0/628	0.57	0/844
8	H	0.34	0/1302	0.62	0/1749
9	I	0.32	0/962	0.65	0/1285
10	J	0.33	0/1783	0.63	0/2384
11	K	0.34	0/1606	0.65	0/2148
12	L	0.33	0/1845	0.62	0/2489
13	M	0.34	0/1224	0.67	0/1651
14	N	0.32	0/961	0.65	0/1295
15	O	0.32	0/1859	0.62	0/2495
16	P	0.33	0/1773	0.60	0/2390
17	Q	0.34	0/2323	0.57	0/3135
18	R	0.33	0/2783	0.63	0/3723
19	S	0.34	0/1576	0.60	0/2104
20	T	0.34	0/1837	0.59	0/2486
21	U	0.34	0/648	0.61	0/870
22	V	0.35	0/741	0.61	0/995
23	W	0.31	0/955	0.59	0/1273
24	X	0.33	0/520	0.66	0/696
25	Y	0.35	0/392	0.72	0/515
26	Z	0.34	0/522	0.67	0/695
27	0	0.33	0/329	0.58	0/432
28	1	0.34	0/2949	0.58	0/3998
29	2	0.33	0/963	0.61	0/1295
30	3	0.34	0/1072	0.60	0/1442
31	4	0.34	0/1138	0.69	0/1526
32	5	0.32	0/2604	0.59	0/3526

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	6	0.35	0/1978	0.59	0/2664
34	7	0.35	0/873	0.61	0/1170
35	8	0.33	0/1659	0.56	0/2230
36	9	0.35	0/1616	0.56	0/2177
37	a	0.34	0/1471	0.64	0/1976
38	b	0.33	0/1333	0.57	0/1783
39	c	0.33	0/1028	0.61	0/1372
40	d	0.33	0/1791	0.61	0/2415
41	AA	0.33	0/1645	0.60	0/2218
42	BB	0.35	0/2128	0.67	0/2892
43	CC	0.34	0/2864	0.58	0/3853
44	DD	0.35	0/2434	0.63	0/3281
45	EE	0.33	0/2360	0.59	0/3180
46	FF	0.39	0/1014	0.64	0/1358
47	GG	0.34	0/1305	0.61	0/1763
48	HH	0.33	0/1232	0.70	1/1660 (0.1%)
49	II	0.34	0/1855	0.62	0/2492
50	JJ	0.34	0/1544	0.68	2/2091 (0.1%)
51	KK	0.36	0/1136	0.62	0/1515
52	LL	0.34	0/963	0.68	0/1292
53	MM	0.34	0/957	0.64	0/1277
54	NN	0.35	0/972	0.64	0/1300
55	OO	0.34	0/1985	0.65	0/2647
56	PP	0.34	0/934	0.64	0/1260
57	QQ	0.32	0/1694	0.64	0/2252
58	RR	0.37	0/749	0.66	0/998
59	SS	0.36	0/652	0.69	0/882
60	TT	0.37	0/771	0.63	0/1019
61	UU	0.33	0/1950	0.62	0/2636
62	VV	0.32	0/1900	0.60	0/2540
63	WW	0.34	0/3282	0.59	1/4438 (0.0%)
64	XX	0.35	0/786	0.63	0/1046
65	YY	0.35	0/2313	0.61	0/3119
66	ZZ	0.32	0/702	0.58	0/945
67	11	0.34	0/303	0.84	0/386
68	22	0.34	0/852	0.56	0/1142
69	33	0.35	0/2002	0.57	0/2721
70	44	0.34	0/2214	0.57	0/2990
71	55	0.35	0/521	0.57	0/701
72	66	0.34	0/2547	0.58	0/3438
73	77	0.35	0/1358	0.55	0/1839
74	88	0.35	0/3646	0.57	0/4935
75	aa	0.26	0/35686	0.75	33/55477 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	bb	0.45	0/1805	0.90	5/2811 (0.2%)
All	All	0.30	0/212996	0.67	57/307971 (0.0%)

There are no bond length outliers.

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
75	aa	1455	G	P-O3'-C3'	-11.24	106.21	119.70
75	aa	44	U	O4'-C1'-N1	10.73	116.78	108.20
75	aa	1119	G	C4'-C3'-O3'	-10.10	88.19	109.40
75	aa	1119	G	C2'-C3'-O3'	9.55	130.51	109.50
75	aa	44	U	C2'-C3'-O3'	-9.27	89.11	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	A	57598	0	28892	216	0
2	B	2527	0	2649	54	0
3	C	1932	0	1969	20	0
4	D	1991	0	2032	5	0
5	E	2187	0	2203	16	0
6	F	1524	0	1587	4	0
7	G	617	0	626	1	0
8	H	1275	0	1310	12	0
9	I	956	0	1037	4	0
10	J	1746	0	1840	5	0
11	K	1573	0	1629	5	0
12	L	1817	0	1878	9	0
13	M	1206	0	1283	7	0
14	N	948	0	1006	3	0
15	O	1826	0	1933	3	0
16	P	1729	0	1724	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	2272	0	2334	6	0
18	R	2738	0	2811	6	0
19	S	1543	0	1621	14	0
20	T	1792	0	1782	11	0
21	U	639	0	699	4	0
22	V	729	0	711	1	0
23	W	937	0	975	4	0
24	X	512	0	563	3	0
25	Y	385	0	423	3	0
26	Z	508	0	539	0	0
27	0	324	0	344	3	0
28	1	2875	0	2881	11	0
29	2	944	0	969	9	0
30	3	1046	0	1071	6	0
31	4	1117	0	1142	7	0
32	5	2552	0	2600	18	0
33	6	1932	0	1950	11	0
34	7	858	0	908	6	0
35	8	1629	0	1633	2	0
36	9	1587	0	1628	7	0
37	a	1440	0	1473	0	0
38	b	1299	0	1367	0	0
39	c	1004	0	1065	0	0
40	d	1746	0	1743	0	0
41	AA	1610	0	1639	6	0
42	BB	2085	0	2094	18	0
43	CC	2821	0	2829	17	0
44	DD	2369	0	2436	12	0
45	EE	2306	0	2324	17	0
46	FF	1002	0	1086	47	0
47	GG	1282	0	1338	2	0
48	HH	1213	0	1277	12	0
49	II	1820	0	1906	11	0
50	JJ	1508	0	1505	88	0
51	KK	1121	0	1171	11	0
52	LL	948	0	1002	14	0
53	MM	942	0	1001	17	0
54	NN	953	0	1007	9	0
55	OO	1962	0	2036	21	0
56	PP	919	0	982	4	0
57	QQ	1683	0	1769	16	0
58	RR	738	0	771	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	SS	636	0	654	19	0
60	TT	760	0	791	3	0
61	UU	1907	0	1898	18	0
62	VV	1872	0	1978	8	0
63	WW	3216	0	3315	45	0
64	XX	774	0	821	4	0
65	YY	2258	0	2229	49	0
66	ZZ	687	0	719	15	0
67	11	303	0	357	2	0
68	22	833	0	839	1	0
69	33	1953	0	1913	15	0
70	44	2169	0	2155	6	0
71	55	508	0	524	1	0
72	66	2488	0	2520	9	0
73	77	1330	0	1350	6	0
74	88	3573	0	3576	22	0
75	aa	31883	0	16005	0	0
76	bb	1615	0	821	0	0
77	cc	470	0	102	0	0
78	dd	755	0	167	0	0
79	A	183	0	0	0	0
79	BB	1	0	0	0	0
79	LL	1	0	0	0	0
79	MM	1	0	0	0	0
79	QQ	1	0	0	0	0
79	WW	1	0	0	0	0
79	aa	111	0	0	0	0
80	B	1	0	0	0	0
81	0	1	0	0	0	0
81	W	1	0	0	0	0
82	WW	28	0	12	1	0
All	All	201462	0	157749	837	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 4.

The worst 5 of 837 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)
50:JJ:71:ILE:CG1	50:JJ:116:THR:HG21	1.17	1.64
50:JJ:71:ILE:CD1	50:JJ:116:THR:HG21	1.32	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:JJ:71:ILE:HG12	50:JJ:116:THR:CG2	1.35	1.55
63:WW:243:LYS:NZ	63:WW:246:VAL:HG22	1.25	1.44
50:JJ:68:TYR:CE2	65:YY:163:PRO:HG3	1.55	1.42

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
2	B	317/393 (81%)	302 (95%)	15 (5%)	0	100 100
3	C	247/249 (99%)	234 (95%)	11 (4%)	2 (1%)	19 56
4	D	250/252 (99%)	237 (95%)	9 (4%)	4 (2%)	9 44
5	E	272/274 (99%)	256 (94%)	15 (6%)	1 (0%)	34 69
6	F	194/196 (99%)	183 (94%)	10 (5%)	1 (0%)	29 65
7	G	72/74 (97%)	70 (97%)	2 (3%)	0	100 100
8	H	158/160 (99%)	152 (96%)	6 (4%)	0	100 100
9	I	123/138 (89%)	114 (93%)	9 (7%)	0	100 100
10	J	218/220 (99%)	202 (93%)	15 (7%)	1 (0%)	29 65
11	K	193/195 (99%)	184 (95%)	9 (5%)	0	100 100
12	L	225/237 (95%)	217 (96%)	8 (4%)	0	100 100
13	M	149/151 (99%)	139 (93%)	10 (7%)	0	100 100
14	N	116/118 (98%)	105 (90%)	10 (9%)	1 (1%)	17 54
15	O	223/225 (99%)	211 (95%)	12 (5%)	0	100 100
16	P	205/207 (99%)	196 (96%)	9 (4%)	0	100 100
17	Q	280/296 (95%)	268 (96%)	12 (4%)	0	100 100
18	R	327/337 (97%)	314 (96%)	12 (4%)	1 (0%)	41 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	181/216 (84%)	171 (94%)	10 (6%)	0	100	100
20	T	210/225 (93%)	199 (95%)	11 (5%)	0	100	100
21	U	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
22	V	87/177 (49%)	83 (95%)	4 (5%)	0	100	100
23	W	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
24	X	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
25	Y	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
26	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
27	0	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
28	1	346/348 (99%)	330 (95%)	16 (5%)	0	100	100
29	2	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
30	3	128/130 (98%)	122 (95%)	6 (5%)	0	100	100
31	4	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
32	5	322/324 (99%)	306 (95%)	16 (5%)	0	100	100
33	6	228/281 (81%)	221 (97%)	7 (3%)	0	100	100
34	7	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
35	8	195/264 (74%)	192 (98%)	3 (2%)	0	100	100
36	9	198/215 (92%)	186 (94%)	12 (6%)	0	100	100
37	a	175/177 (99%)	163 (93%)	12 (7%)	0	100	100
38	b	153/155 (99%)	146 (95%)	7 (5%)	0	100	100
39	c	117/119 (98%)	112 (96%)	4 (3%)	1 (1%)	17	54
40	d	202/215 (94%)	189 (94%)	13 (6%)	0	100	100
41	AA	197/344 (57%)	190 (96%)	7 (4%)	0	100	100
42	BB	264/266 (99%)	247 (94%)	15 (6%)	2 (1%)	19	56
43	CC	331/398 (83%)	302 (91%)	27 (8%)	2 (1%)	25	61
44	DD	281/486 (58%)	265 (94%)	15 (5%)	1 (0%)	34	69
45	EE	284/293 (97%)	262 (92%)	20 (7%)	2 (1%)	22	59
46	FF	123/125 (98%)	113 (92%)	10 (8%)	0	100	100
47	GG	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	25	61
48	HH	152/154 (99%)	145 (95%)	7 (5%)	0	100	100
49	II	220/244 (90%)	206 (94%)	12 (6%)	2 (1%)	17	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
50	JJ	184/186 (99%)	164 (89%)	14 (8%)	6 (3%)	4 32
51	KK	138/148 (93%)	126 (91%)	11 (8%)	1 (1%)	22 59
52	LL	122/124 (98%)	110 (90%)	11 (9%)	1 (1%)	19 56
53	MM	118/120 (98%)	109 (92%)	8 (7%)	1 (1%)	19 56
54	NN	113/115 (98%)	109 (96%)	4 (4%)	0	100 100
55	OO	234/253 (92%)	227 (97%)	7 (3%)	0	100 100
56	PP	112/119 (94%)	105 (94%)	7 (6%)	0	100 100
57	QQ	194/237 (82%)	184 (95%)	9 (5%)	1 (0%)	29 65
58	RR	87/99 (88%)	81 (93%)	6 (7%)	0	100 100
59	SS	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	12 48
60	TT	90/92 (98%)	86 (96%)	4 (4%)	0	100 100
61	UU	231/233 (99%)	223 (96%)	8 (4%)	0	100 100
62	VV	231/233 (99%)	221 (96%)	10 (4%)	0	100 100
63	WW	399/401 (100%)	368 (92%)	29 (7%)	2 (0%)	29 65
64	XX	91/96 (95%)	88 (97%)	3 (3%)	0	100 100
65	YY	265/273 (97%)	244 (92%)	18 (7%)	3 (1%)	14 51
66	ZZ	83/91 (91%)	74 (89%)	9 (11%)	0	100 100
67	11	32/34 (94%)	31 (97%)	1 (3%)	0	100 100
68	22	97/99 (98%)	89 (92%)	7 (7%)	1 (1%)	15 52
69	33	240/255 (94%)	226 (94%)	13 (5%)	1 (0%)	34 69
70	44	264/321 (82%)	251 (95%)	10 (4%)	3 (1%)	14 51
71	55	55/339 (16%)	53 (96%)	2 (4%)	0	100 100
72	66	301/319 (94%)	291 (97%)	10 (3%)	0	100 100
73	77	163/165 (99%)	146 (90%)	16 (10%)	1 (1%)	25 61
74	88	448/457 (98%)	414 (92%)	31 (7%)	3 (1%)	22 59
All	All	13235/14689 (90%)	12478 (94%)	710 (5%)	47 (0%)	38 69

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	DD	423	THR
4	D	52	LEU
4	D	195	VAL

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Mol	Chain	Res	Type
14	N	109	ILE
42	BB	303	GLU

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
2	B	272/337 (81%)	256 (94%)	16 (6%)	19 51
3	C	210/210 (100%)	197 (94%)	13 (6%)	18 50
4	D	218/218 (100%)	197 (90%)	21 (10%)	8 34
5	E	242/242 (100%)	230 (95%)	12 (5%)	24 55
6	F	172/172 (100%)	164 (95%)	8 (5%)	26 56
7	G	68/68 (100%)	66 (97%)	2 (3%)	42 67
8	H	138/138 (100%)	131 (95%)	7 (5%)	24 55
9	I	108/117 (92%)	104 (96%)	4 (4%)	34 62
10	J	181/181 (100%)	165 (91%)	16 (9%)	10 38
11	K	167/167 (100%)	151 (90%)	16 (10%)	8 34
12	L	203/211 (96%)	194 (96%)	9 (4%)	28 58
13	M	136/136 (100%)	130 (96%)	6 (4%)	28 58
14	N	107/107 (100%)	105 (98%)	2 (2%)	57 76
15	O	200/200 (100%)	189 (94%)	11 (6%)	21 54
16	P	185/185 (100%)	181 (98%)	4 (2%)	52 73
17	Q	256/267 (96%)	242 (94%)	14 (6%)	21 54
18	R	303/308 (98%)	292 (96%)	11 (4%)	35 63
19	S	167/191 (87%)	161 (96%)	6 (4%)	35 63
20	T	204/213 (96%)	197 (97%)	7 (3%)	37 64
21	U	73/73 (100%)	71 (97%)	2 (3%)	44 69
22	V	74/161 (46%)	71 (96%)	3 (4%)	30 59
23	W	104/104 (100%)	101 (97%)	3 (3%)	42 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	X	56/56 (100%)	52 (93%)	4 (7%)	14 46
25	Y	40/40 (100%)	39 (98%)	1 (2%)	47 70
26	Z	50/50 (100%)	46 (92%)	4 (8%)	12 42
27	0	36/36 (100%)	35 (97%)	1 (3%)	43 68
28	1	323/323 (100%)	312 (97%)	11 (3%)	37 64
29	2	106/106 (100%)	100 (94%)	6 (6%)	20 53
30	3	112/112 (100%)	110 (98%)	2 (2%)	59 78
31	4	121/121 (100%)	118 (98%)	3 (2%)	47 70
32	5	284/284 (100%)	278 (98%)	6 (2%)	53 74
33	6	213/252 (84%)	205 (96%)	8 (4%)	33 61
34	7	95/95 (100%)	91 (96%)	4 (4%)	30 59
35	8	182/240 (76%)	173 (95%)	9 (5%)	25 55
36	9	176/186 (95%)	168 (96%)	8 (4%)	27 57
37	a	158/158 (100%)	152 (96%)	6 (4%)	33 61
38	b	144/144 (100%)	139 (96%)	5 (4%)	36 63
39	c	110/110 (100%)	109 (99%)	1 (1%)	78 88
40	d	191/199 (96%)	187 (98%)	4 (2%)	53 74
41	AA	177/309 (57%)	168 (95%)	9 (5%)	24 55
42	BB	233/233 (100%)	206 (88%)	27 (12%)	5 27
43	CC	328/385 (85%)	297 (90%)	31 (10%)	8 35
44	DD	256/437 (59%)	229 (90%)	27 (10%)	7 30
45	EE	249/252 (99%)	237 (95%)	12 (5%)	25 56
46	FF	114/114 (100%)	105 (92%)	9 (8%)	12 43
47	GG	138/138 (100%)	132 (96%)	6 (4%)	29 58
48	HH	141/141 (100%)	125 (89%)	16 (11%)	6 28
49	II	196/215 (91%)	186 (95%)	10 (5%)	24 55
50	JJ	167/167 (100%)	151 (90%)	16 (10%)	8 34
51	KK	122/127 (96%)	108 (88%)	14 (12%)	5 28
52	LL	103/103 (100%)	92 (89%)	11 (11%)	6 30
53	MM	100/100 (100%)	92 (92%)	8 (8%)	12 42
54	NN	103/103 (100%)	92 (89%)	11 (11%)	6 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	OO	208/220 (94%)	199 (96%)	9 (4%)	29	58
56	PP	101/104 (97%)	96 (95%)	5 (5%)	24	55
57	QQ	187/218 (86%)	178 (95%)	9 (5%)	25	56
58	RR	80/87 (92%)	74 (92%)	6 (8%)	13	44
59	SS	69/69 (100%)	63 (91%)	6 (9%)	10	39
60	TT	81/81 (100%)	73 (90%)	8 (10%)	8	33
61	UU	208/208 (100%)	198 (95%)	10 (5%)	25	56
62	VV	208/210 (99%)	199 (96%)	9 (4%)	29	58
63	WW	368/368 (100%)	328 (89%)	40 (11%)	6	29
64	XX	84/84 (100%)	79 (94%)	5 (6%)	19	51
65	YY	248/250 (99%)	231 (93%)	17 (7%)	15	47
66	ZZ	78/82 (95%)	71 (91%)	7 (9%)	9	37
67	11	32/32 (100%)	31 (97%)	1 (3%)	40	65
68	22	90/90 (100%)	89 (99%)	1 (1%)	73	85
69	33	216/231 (94%)	204 (94%)	12 (6%)	21	53
70	44	238/281 (85%)	229 (96%)	9 (4%)	33	61
71	55	53/303 (18%)	51 (96%)	2 (4%)	33	61
72	66	277/289 (96%)	269 (97%)	8 (3%)	42	67
73	77	158/158 (100%)	152 (96%)	6 (4%)	33	61
74	88	401/404 (99%)	377 (94%)	24 (6%)	19	51
All	All	11997/13111 (92%)	11320 (94%)	677 (6%)	25	53

5 of 677 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	LL	148	LYS
63	WW	325	MET
54	NN	37	LEU
52	LL	144	LYS
60	TT	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
19	S	226	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2677/3296 (81%)	608 (22%)	107 (3%)
75	aa	1473/1649 (89%)	444 (30%)	0
76	bb	75/76 (98%)	42 (56%)	0
All	All	4225/5021 (84%)	1094 (25%)	107 (2%)

5 of 1094 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	26	A
1	A	27	A
1	A	28	U
1	A	30	U
1	A	35	U

5 of 107 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1706	G
1	A	2329	A
1	A	3154	U
1	A	1708	A
1	A	2304	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 303 ligands modelled in this entry, 302 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
82	GDP	WW	501	79	24,30,30	0.98	1 (4%)	30,47,47	1.33	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	GDP	WW	501	79	-	5/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WW	501	GDP	C6-N1	-2.22	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	WW	501	GDP	PA-O3A-PB	-3.71	120.09	132.83
82	WW	501	GDP	C3'-C2'-C1'	2.58	104.87	100.98
82	WW	501	GDP	C5-C6-N1	2.47	118.32	113.95
82	WW	501	GDP	C8-N7-C5	2.44	107.64	102.99

There are no chirality outliers.

All (5) torsion outliers are listed below:

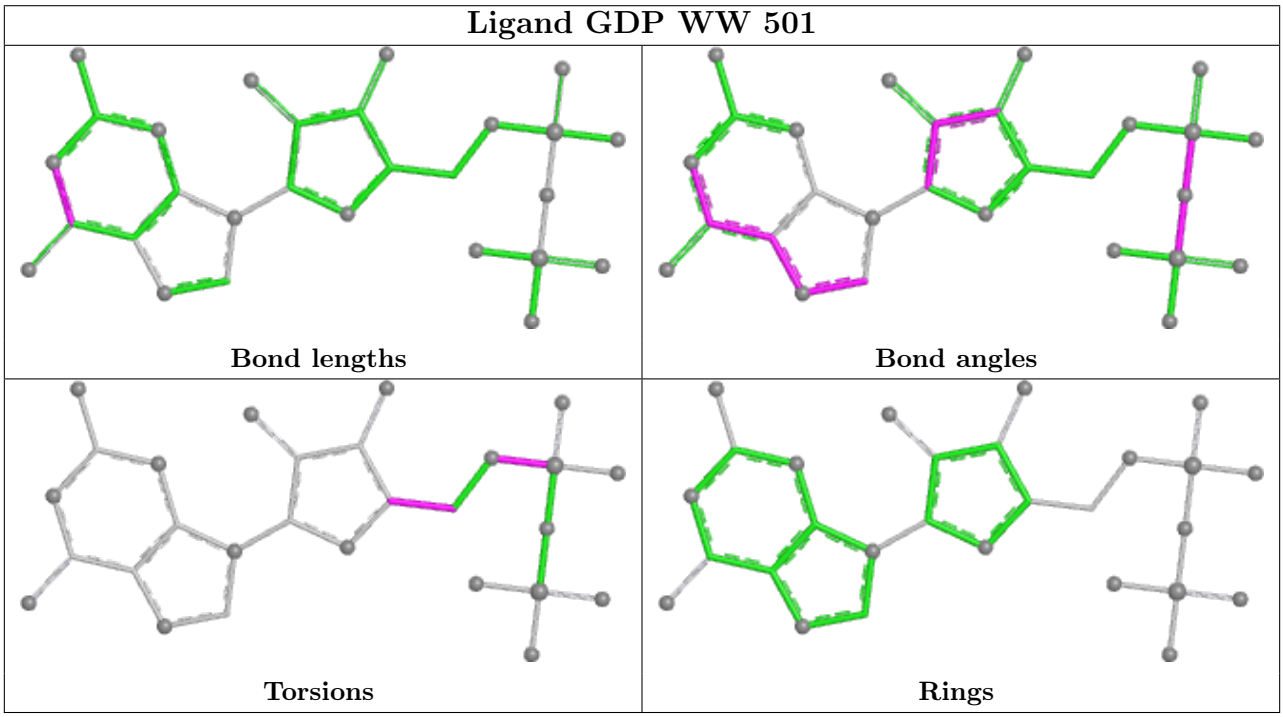
Mol	Chain	Res	Type	Atoms
82	WW	501	GDP	C5'-O5'-PA-O2A
82	WW	501	GDP	C3'-C4'-C5'-O5'
82	WW	501	GDP	O4'-C4'-C5'-O5'
82	WW	501	GDP	C5'-O5'-PA-O3A
82	WW	501	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	WW	501	GDP	1	0

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



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
75	aa	13
78	dd	7
77	cc	3
64	XX	2

The worst 5 of 25 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	dd	115:UNK	C	151:UNK	N	40.49
1	dd	220:UNK	C	265:UNK	N	35.53
1	dd	170:UNK	C	202:UNK	N	27.02
1	cc	59:UNK	C	76:UNK	N	22.66
1	cc	93:UNK	C	105:UNK	N	20.48

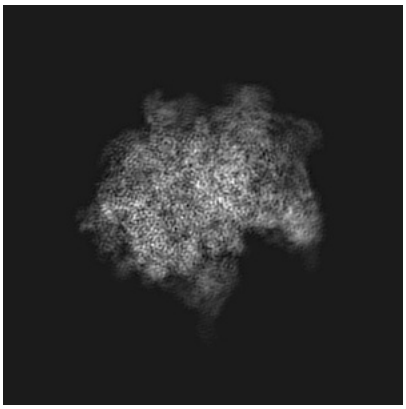
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3552. These allow visual inspection of the internal detail of the map and identification of artifacts.

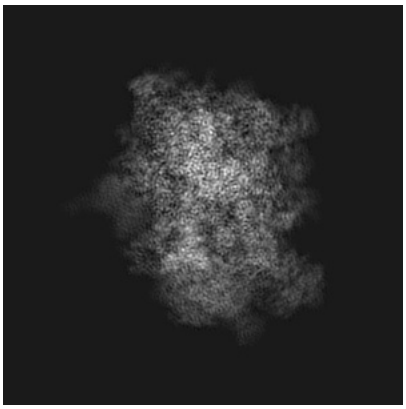
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

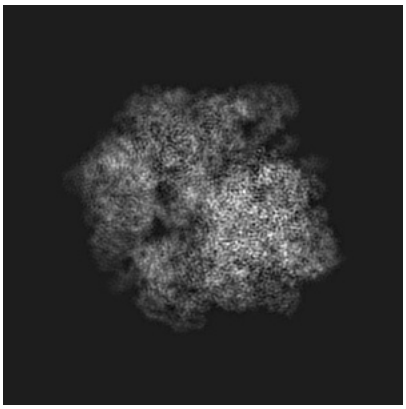
6.1.1 Primary map



X

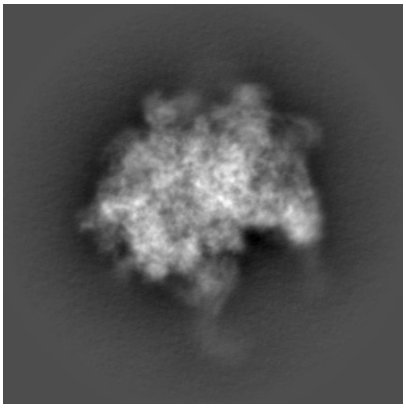


Y

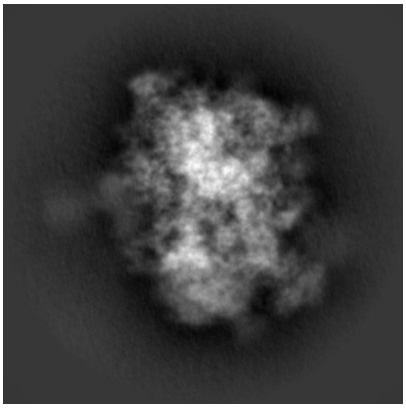


Z

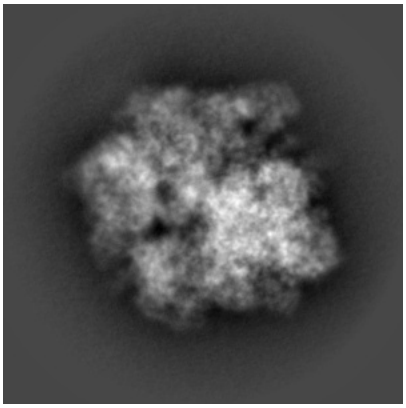
6.1.2 Raw map



X



Y



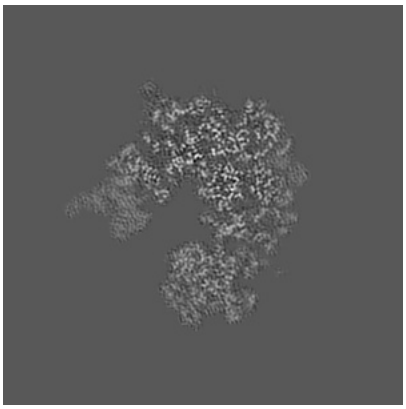
Z

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

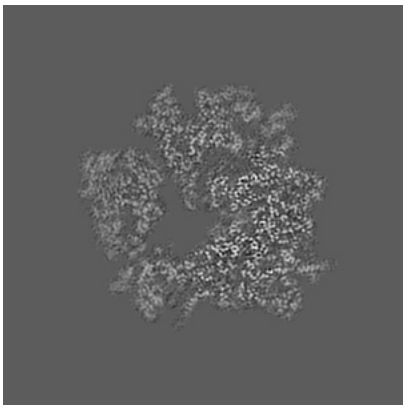
6.2 Central slices (i)

6.2.1 Primary map

X Index: 165

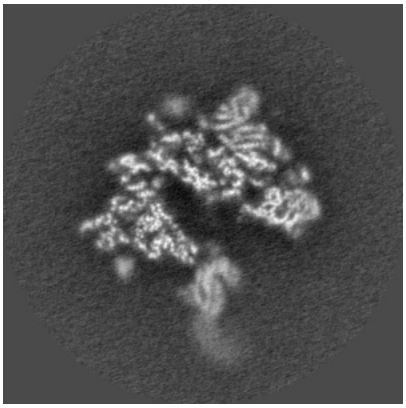


Y Index: 165

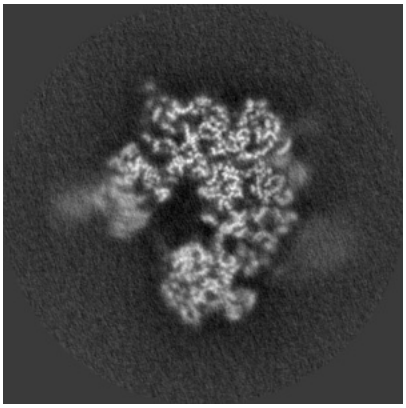


Z Index: 165

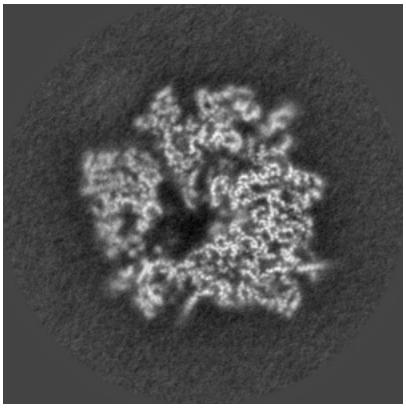
6.2.2 Raw map



X Index: 165



Y Index: 165

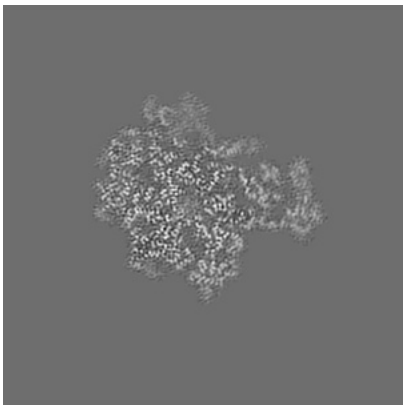


Z Index: 165

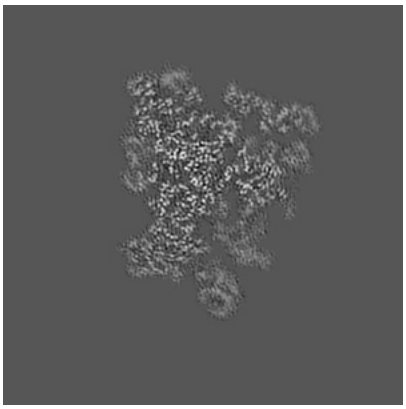
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

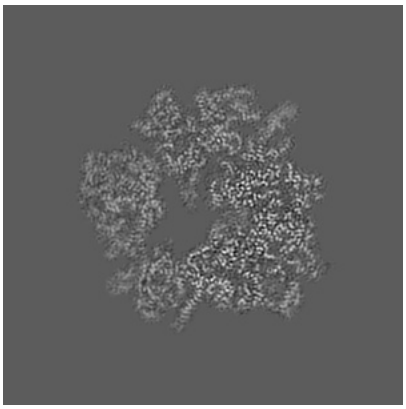
6.3.1 Primary map



X Index: 196

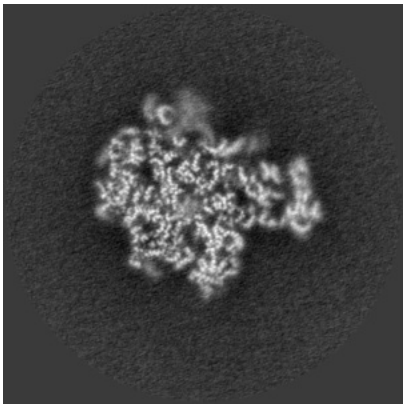


Y Index: 125

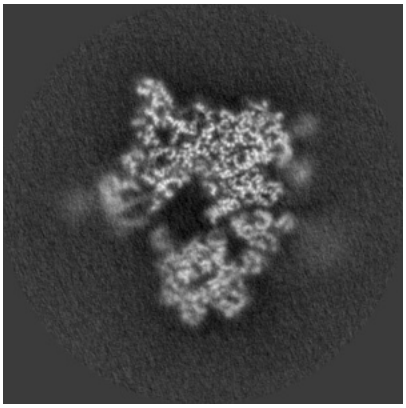


Z Index: 163

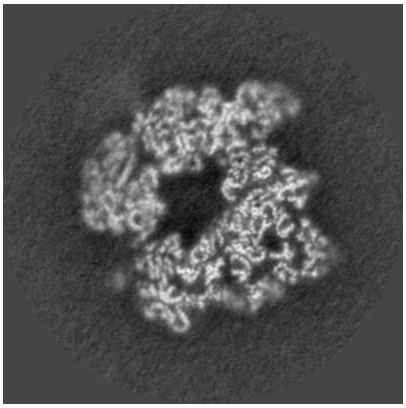
6.3.2 Raw map



X Index: 196



Y Index: 159

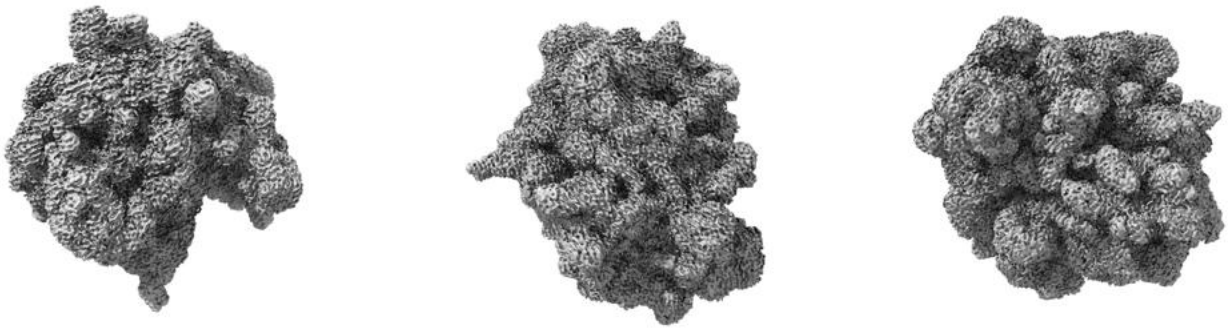


Z Index: 154

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

6.4 Orthogonal surface views (i)

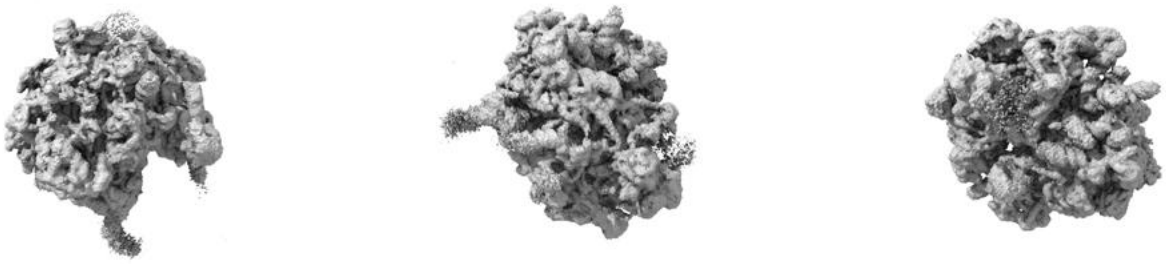
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00586. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

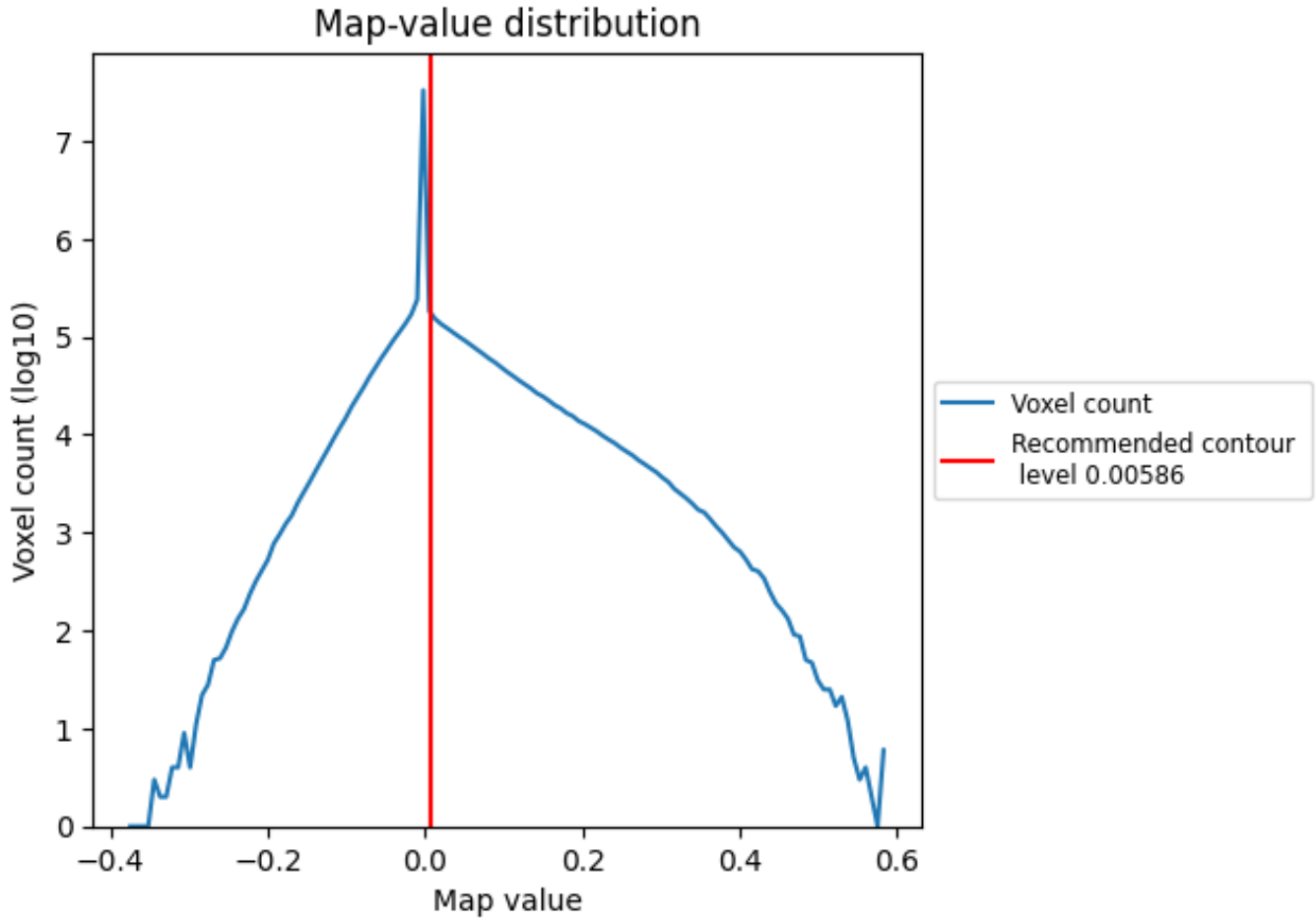
6.5 Mask visualisation (i)

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

7 Map analysis

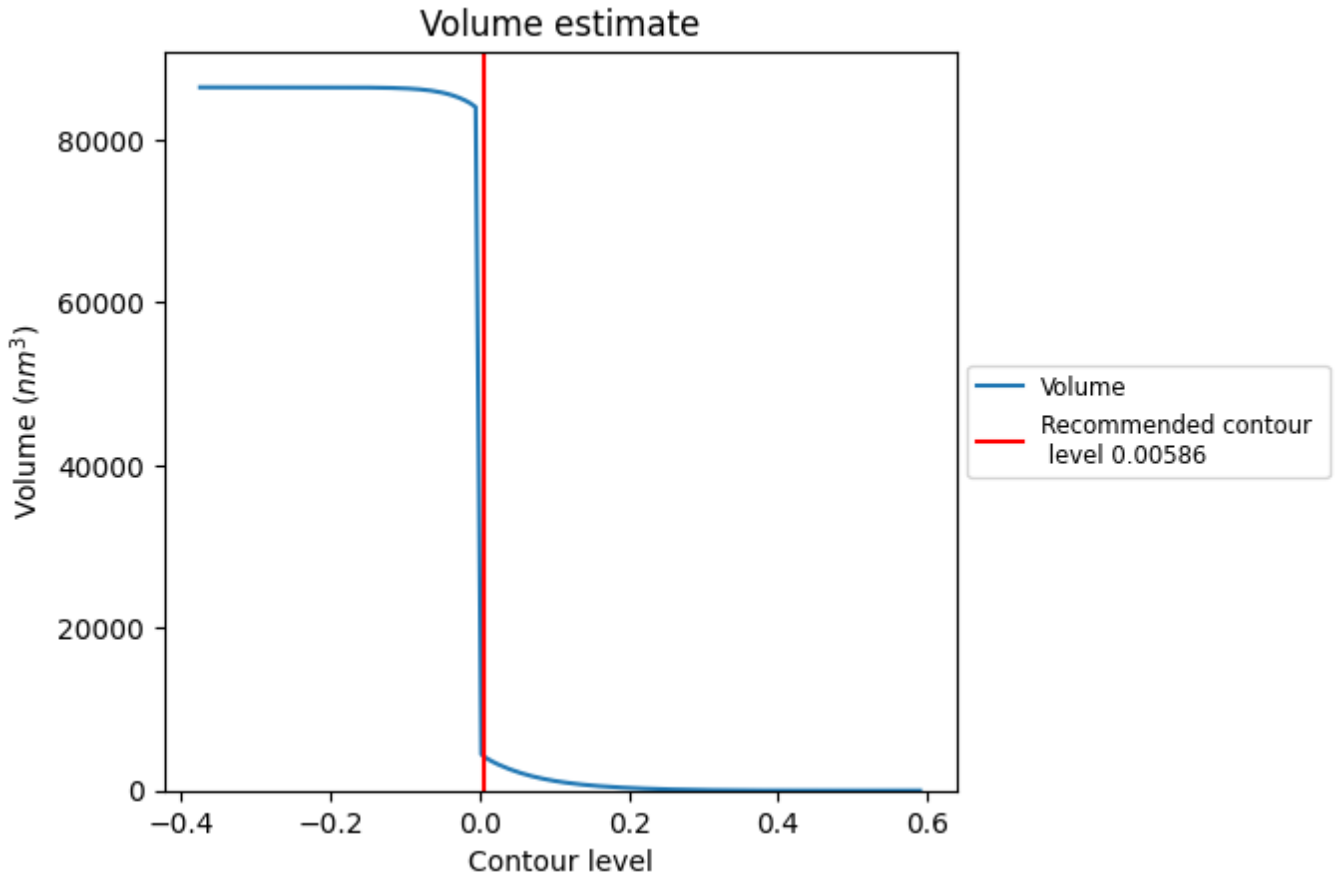
This section contains the results of statistical analysis of the map.

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.

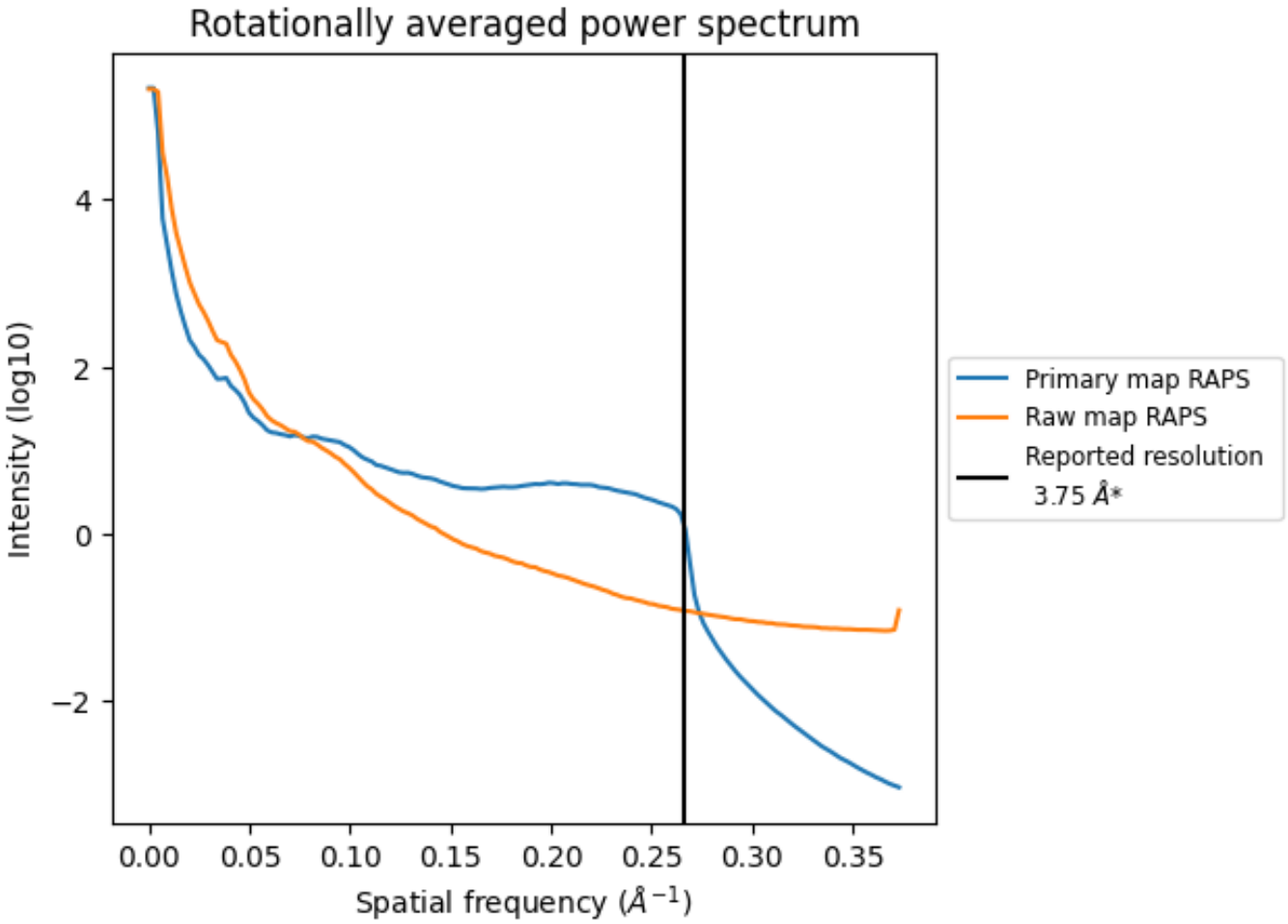
7.2 Volume estimate (i)



The volume at the recommended contour level is 4197 nm^3; this corresponds to an approximate mass of 3791 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)

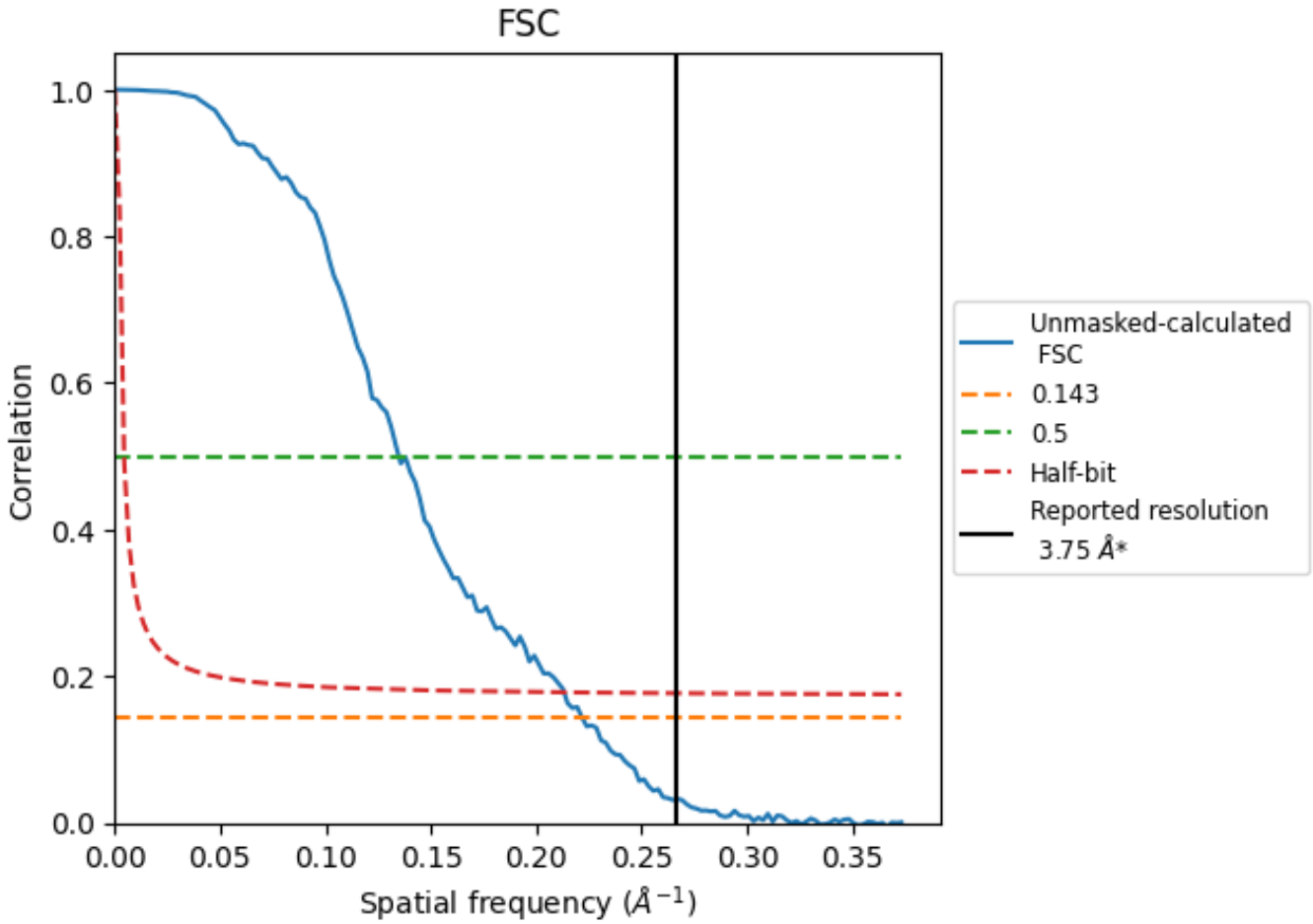


*Reported resolution corresponds to spatial frequency of 0.267 Å^{-1}

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 0.267 Å^{-1}

8.2 Resolution estimates (i)

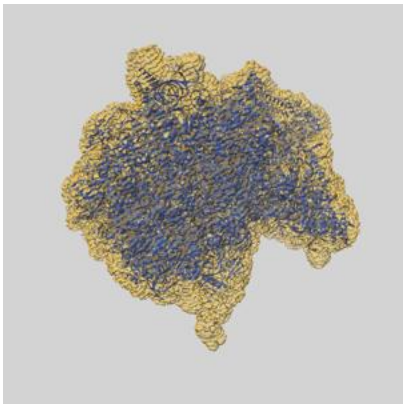
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.51	7.42	4.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 3.75 by more than 10 %

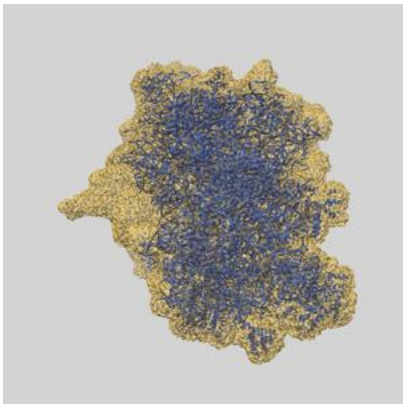
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3552 and PDB model 5MRE. Per-residue inclusion information can be found in section 3 on page 19.

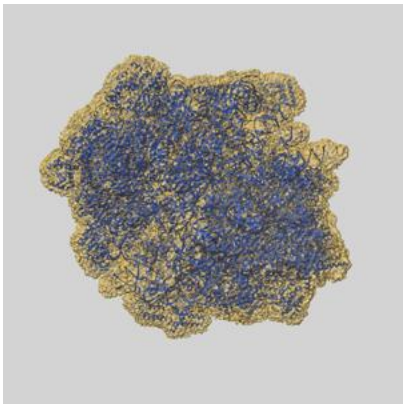
9.1 Map-model overlay



X



Y



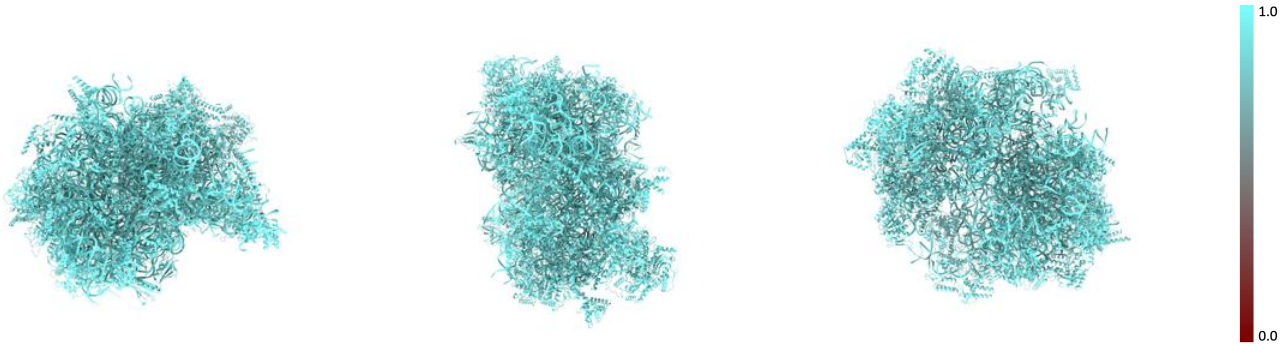
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00586 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

This section was not generated.

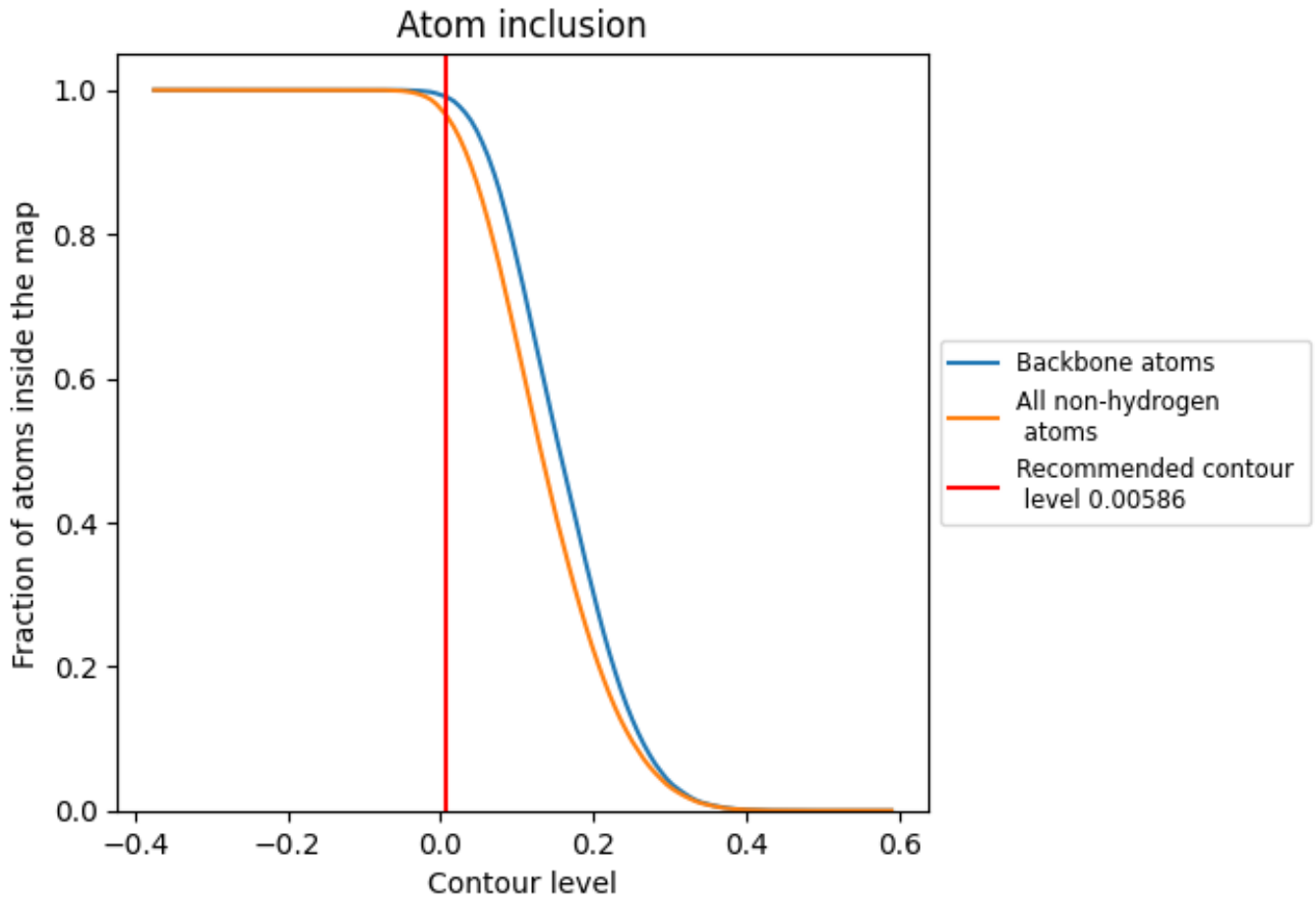
9.3 Atom inclusion mapped to coordinate model



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 (0.00586).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.00586) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.9671
0	0.9808
1	0.9665
11	0.9228
2	0.9674
22	0.9645
3	0.9646
33	0.9600
4	0.9593
44	0.9530
5	0.9589
55	0.9415
6	0.9483
66	0.9576
7	0.9597
77	0.9170
8	0.9532
88	0.9395
9	0.9669
A	0.9856
AA	0.9499
B	0.9525
BB	0.9593
C	0.9625
CC	0.9328
D	0.9584
DD	0.9538
E	0.9619
EE	0.9362
F	0.9647
FF	0.9070
G	0.9521
GG	0.9234
H	0.9624
HH	0.9497

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Chain	Atom inclusion
I	0.9477
II	0.9543
J	0.9654
JJ	0.9227
K	0.9621
KK	0.9347
L	0.9606
LL	0.9576
M	0.9564
MM	0.9457
N	0.9620
NN	0.9374
O	0.9641
OO	0.9270
P	0.9608
PP	0.9551
Q	0.9587
QQ	0.9373
R	0.9598
RR	0.9480
S	0.9567
SS	0.9452
T	0.9601
TT	0.9266
U	0.9553
UU	0.9517
V	0.9545
VV	0.9430
W	0.9573
WW	0.9439
X	0.9376
XX	0.9484
Y	0.9377
YY	0.9367
Z	0.9508
ZZ	0.9194
a	0.9743
aa	0.9880
b	0.9616
bb	0.9077
c	0.9641
cc	0.9468

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
d	0.9628
dd	0.9854