wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 03:23 pm GMT

PDB ID	:	5MRF
EMDB ID	:	EMD-3553
Title	:	Structure of the yeast mitochondrial ribosome - Class C
Authors	:	Desai, N.; Brown, A.; Amunts, A.; Ramakrishnan, V.
Deposited on	:	2016-12-22
Resolution	:	4.97 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:

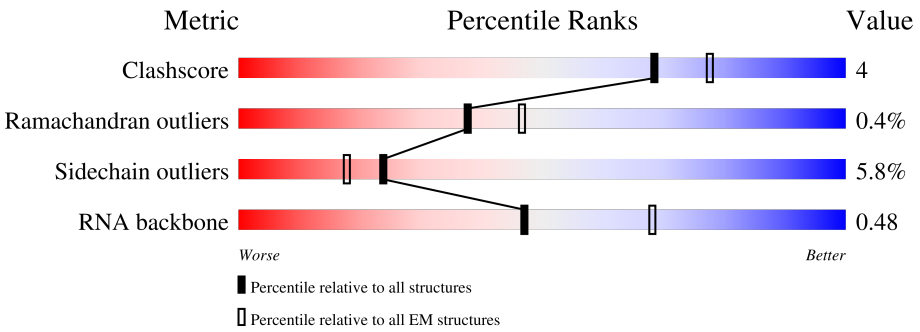
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.97 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% 20% • 18%
2	B	393	71% 10% • 18%
3	C	249	89% 10% •
4	D	252	88% 11% •
5	E	274	93% 7%
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% 8%
14	N	118	97%
15	O	225	92% 8%
16	P	207	94% 6%
17	Q	296	88% 7%
18	R	337	91% 7%
19	S	216	81% 14%
20	T	225	84% 12%
21	U	82	85% 15%
22	V	177	51% 47%
23	W	112	94% 6%
24	X	64	84% 16%
25	Y	46	91% 9%
26	Z	62	94% 6%
27	0	38	89% 11%
28	1	348	93% 7%
29	2	113	88% 12%
30	3	130	93% 7%
31	4	138	91% 9%
32	5	324	89% 11%

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Mol	Chain	Length	Quality of chain
33	6	281	75% 8% 17%
34	7	106	87% 13%
35	8	264	70% 5% 25%
36	9	215	86% 7% 6%
37	a	177	96%
38	b	155	97%
39	c	119	98%
40	d	215	94%
41	AA	344	55% 41%
42	BB	266	81% 17%
43	CC	398	71% 13% 15%
44	DD	486	50% 8% 41%
45	EE	293	86% 12%
46	FF	125	81% 18%
47	GG	161	93% 7%
48	HH	154	79% 18%
49	II	244	83% 9% 7%
50	JJ	186	84% 13%
51	KK	148	76% 18%
52	LL	124	82% 17%
53	MM	120	91% 8%
54	NN	115	81% 13% 5%
55	OO	253	80% 12% 6%
56	PP	119	89% 8%
57	QQ	237	74% 11% 14%

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Mol	Chain	Length	Quality of chain
58	RR	99	85% 7% 8%
59	SS	80	86% 12%
60	TT	92	88% 11%
61	UU	233	85% 14%
62	VV	233	93% 6%
63	WW	401	84% 15%
64	XX	96	93% 5%
65	YY	273	86% 12%
66	ZZ	91	67% 22% 5%
67	11	34	6% 91% 9%
68	22	99	96%
69	33	255	84% 11%
70	44	321	79% 6% 16%
71	55	339	17% 83%
72	66	319	88% 8%
73	77	165	92% 8%
74	88	457	87% 11%
75	aa	1649	63% 27% 9%
76	bb	76	49% 51%
77	cc	94	100%
78	dd	151	100%

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
			Total	C	N	O	S		
7	G	74	617	393	110	113	1	0	0

- Molecule 8 is a protein called uL13m.

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

- Molecule 9 is a protein called uL14m.

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

- Molecule 10 is a protein called uL15m.

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

- Molecule 11 is a protein called uL16m.

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

- Molecule 12 is a protein called bL17m.

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

- Molecule 13 is a protein called bL19m.

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

- Molecule 14 is a protein called bL21m.

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

- Molecule 15 is a protein called uL22m.

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

- Molecule 16 is a protein called uL23m.

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

- Molecule 17 is a protein called uL24m.

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

- Molecule 18 is a protein called bL27m.

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

- Molecule 19 is a protein called bL28m.

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

- Molecule 20 is a protein called uL29m.

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

- Molecule 21 is a protein called uL30m.

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

- Molecule 22 is a protein called bL31m.

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

- Molecule 23 is a protein called bL32m.

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

- Molecule 24 is a protein called bL33m.

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

- Molecule 25 is a protein called bL34m.

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

- Molecule 26 is a protein called bL35m.

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

- Molecule 27 is a protein called bL36m.

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

- Molecule 28 is a protein called mL38.

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

- Molecule 29 is a protein called mL40.

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

- Molecule 30 is a protein called mL41.

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

- Molecule 31 is a protein called mL43.

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

- Molecule 32 is a protein called mL44.

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

- Molecule 33 is a protein called mL46.

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

- Molecule 34 is a protein called mL49.

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

- Molecule 35 is a protein called mL50.

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

- Molecule 36 is a protein called mL57.

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

- Molecule 37 is a protein called mL58.

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

- Molecule 38 is a protein called mL59.

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

- Molecule 39 is a protein called mL60.

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

- Molecule 40 is a protein called mL67.

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

- Molecule 41 is a protein called bS1m.

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

- Molecule 42 is a protein called uS2m.

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

- Molecule 43 is a protein called uS3m.

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

- Molecule 44 is a protein called uS4m.

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

- Molecule 45 is a protein called uS5m.

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

- Molecule 46 is a protein called bS6m.

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

- Molecule 47 is a protein called uS7m.

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

- Molecule 48 is a protein called uS8m.

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

- Molecule 49 is a protein called uS9m.

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

- Molecule 50 is a protein called uS10m.

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

- Molecule 51 is a protein called uS11m.

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

- Molecule 52 is a protein called uS12m.

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

- Molecule 53 is a protein called uS13m.

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

- Molecule 54 is a protein called uS14m.

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

- Molecule 55 is a protein called uS15m.

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

- Molecule 56 is a protein called bS16m.

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

- Molecule 57 is a protein called uS17m.

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

- Molecule 58 is a protein called bS18m.

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

- Molecule 59 is a protein called uS19m.

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

- Molecule 60 is a protein called bS21m.

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

- Molecule 61 is a protein called mS23.

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

- Molecule 62 is a protein called mS26.

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

- Molecule 63 is a protein called mS29.

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

- Molecule 64 is a protein called mS33.

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

- Molecule 65 is a protein called mS35.

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

- Molecule 66 is a protein called mS37.

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

- Molecule 67 is a protein called mS38.

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

- Molecule 68 is a protein called mS41.

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

- Molecule 69 is a protein called mS42.

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

- Molecule 70 is a protein called mS43.

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

- Molecule 71 is a protein called mS44.

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

- Molecule 72 is a protein called mS45.

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

- Molecule 73 is a protein called mS46.

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

- Molecule 74 is a protein called mS47.

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

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

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

- Molecule 76 is a RNA chain called tRNA.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
79	A	182	182	182	0
79	R	1	1	1	0
79	BB	1	1	1	0
79	LL	1	1	1	0
79	MM	1	1	1	0
79	OO	1	1	1	0
79	PP	1	1	1	0
79	WW	1	1	1	0
79	aa	110	110	110	0

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

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

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

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

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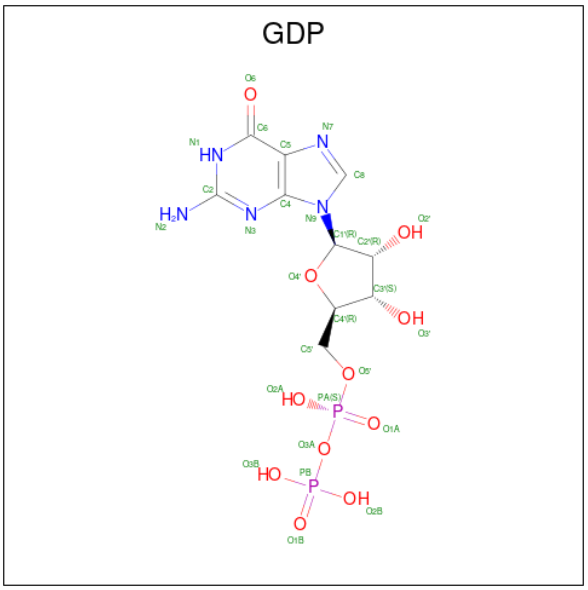
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
81	0	1	1	1	0

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



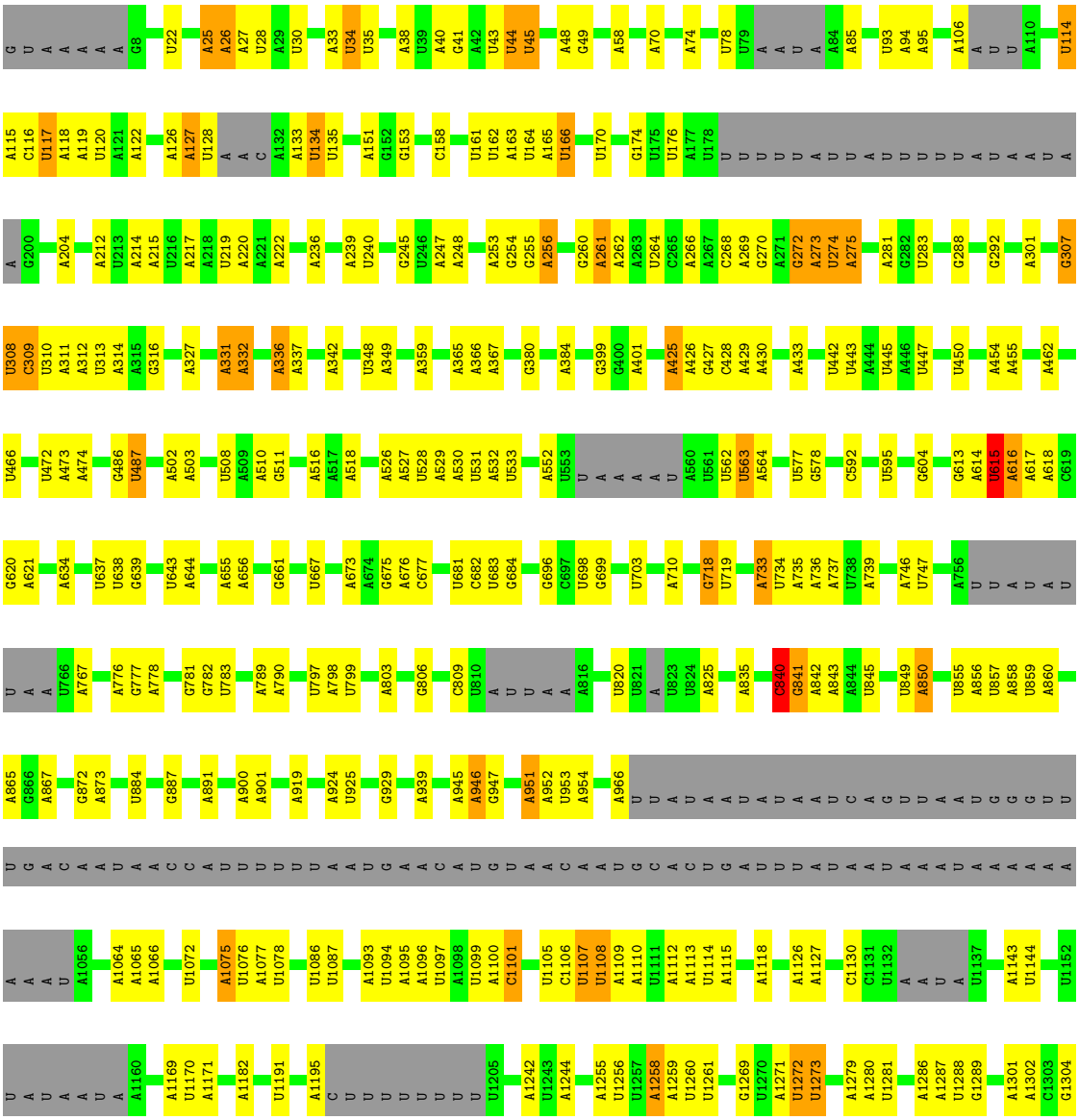
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
82	WW	1	28	10	5	11	2	0

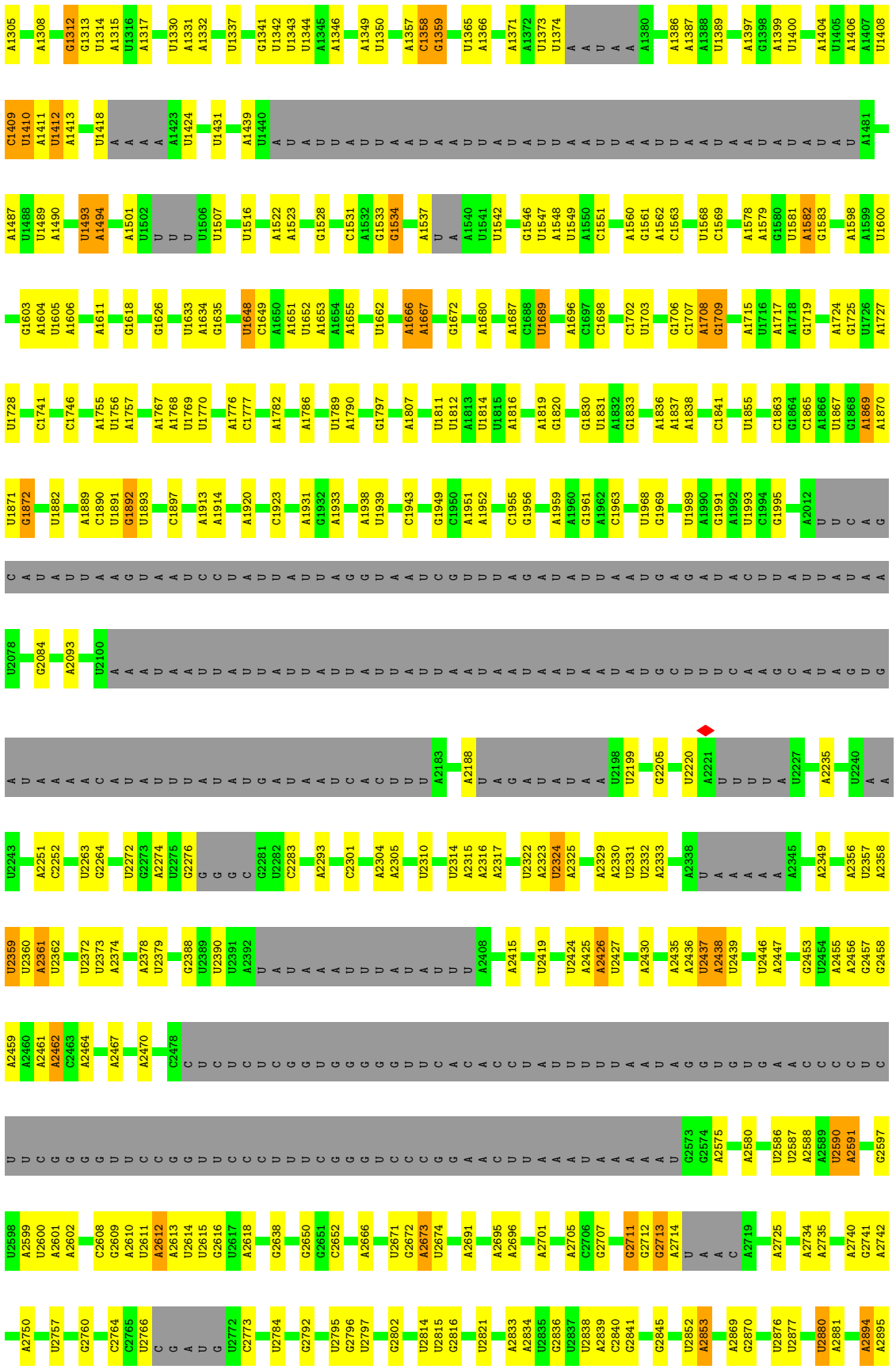
3 Residue-property plots (i)

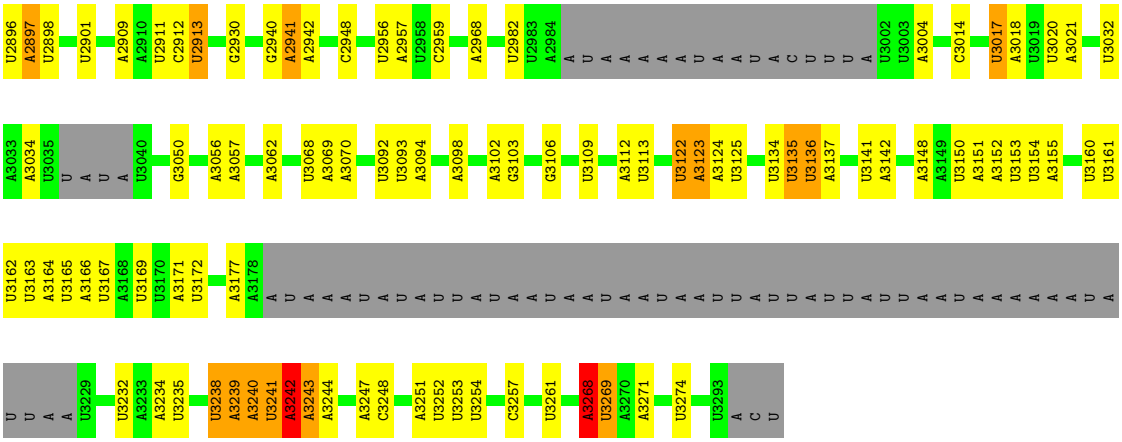
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 21S ribosomal RNA

Chain A: 60% 20% • 18%

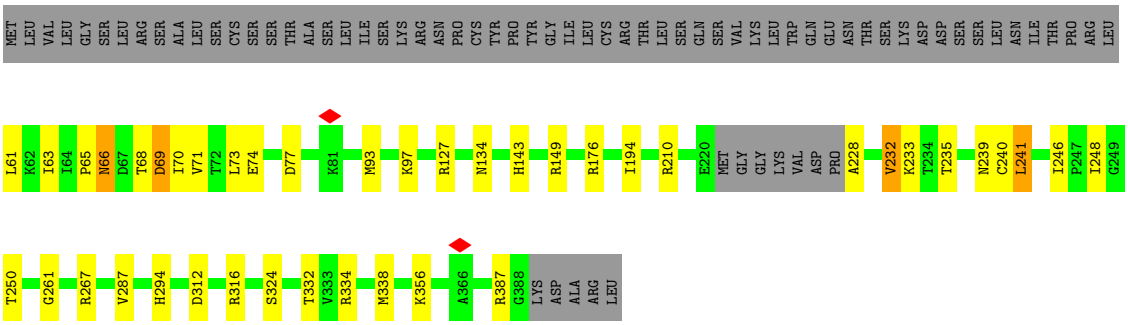



A1305 A1308 G1312 G1313 U1314 A1315 U1316 A1317 U1330 A1331 A1332 U1337 G1341 U1342 U1343 U1344 A1345 A1346 A1349 U1350 A1357 C1358 G1359 U1365 A1366 A1371 A1372 U1373 U1374 A1380 A1386 A1387 A1388 U1389 A1397 G1398 A1399 U1400 A1404 U1405 A1406 A1407 U1408
C1409 U1410 A1411 U1412 A1413 U1418 A1423 U1424 U1431 A1439 U1440 A1481
A1487 U1488 U1489 A1490 U1493 A1494 A1501 U1502 U1506 U1507 U1516 A1522 A1523 G1528 C1531 A1532 G1533 G1534 A1537 A1540 U1541 U1542 G1546 U1547 A1548 U1549 A1550 C1551 A1560 G1561 A1562 C1563 U1568 C1569 A1578 A1579 G1580 U1581 A1582 G1583 A1598 A1599 U1600
G1603 A1604 U1605 A1606 A1611 G1618 G1626 U1633 A1634 G1635 U1648 C1649 A1650 A1651 U1652 A1653 A1654 A1655 U1662 A1666 A1667 G1672 A1680 A1687 C1688 U1689 A1696 C1697 C1698 C1702 U1703 G1706 C1707 A1708 G1709 A1715 U1716 A1717 A1718 G1719 A1724 G1725 U1726 A1727
U1728 C1741 C1746 A1755 U1756 A1757 A1767 A1768 U1769 U1770 A1776 C1777 A1782 A1786 U1789 A1790 G1797 A1807 U1811 U1812 A1813 U1814 U1815 A1816 A1819 G1820 G1830 U1831 A1832 G1833 A1836 A1837 A1838 C1841 U1855 C1863 G1864 C1865 A1866 U1867 G1868 A1869 A1870
U1871 G1872 U1882 A1889 C1890 U1891 G1892 U1893 C1897 A1913 A1914 A1920 C1923 A1931 G1932 A1933 A1938 U1939 C1943 G1949 C1950 A1951 A1952 C1955 G1956 A1959 A1960 G1961 A1962 C1963 U1968 G1969 U1989 A1990 G1991 A1992 U1993 C1994 G1995 A2012
C A U A U U A A A G U A A U C C U A U U A A U U A U U A A G G U A A U C G U U U A A G A U A U U A A U U A A U U U A A U U U A A U U U A A U U G G A G A U A C U U U A A G
U2078 G2084 A2093 U2100
A U A A A A C A U A U U U A U A U U G A U U A A U C A C U U U A2183 A2188 U A G G A U A A U A A U2198 U2199 G2205 U2220 A2221 U U U U U A A U2227 A2235 U2240 A A A
U2243 A2251 C2252 U2263 G2264 U2272 G2273 A2274 U2275 G2276 G G G C G2281 U2282 C2283 A2293 C2301 A2304 A2305 U2310 U2314 A2315 A2316 A2317 U2322 A2323 U2324 A2325 A2329 A2330 U2331 U2332 A2333 A2338 U A A A A A2345 A2349 A2356 U2357 A2358
U2359 U2360 A2361 U2362 U2372 U2373 A2374 A2378 U2379 G2388 U2389 U2390 U2391 A2392 U A U A A A U U U U A U A2408 A2415 U2419 U2424 A2425 A2426 U2427 A2430 A2435 A2436 U2437 A2438 U2439 U2446 A2447 G2453 U2454 A2455 A2456 G2457 G2458
A2459 A2460 A2461 A2462 C2463 A2464 A2467 A2470 C2478 C U U C U C U C U C C U U C C G G G G G G U U U U C A C A A C C C U A U U A A U U C A G U U U C
U U C G G G G G U U U C C C C G G G G U U U C A A A C C U A A A U U A A U U A A U A A U U A A U U A A U



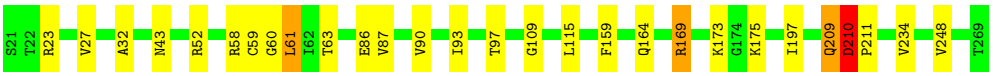
- Molecule 2: uL2m

Chain B:



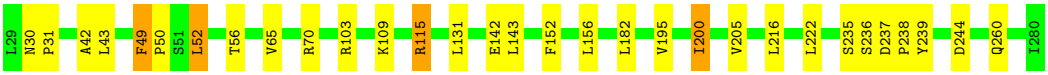
- Molecule 3: uL3m

Chain C:



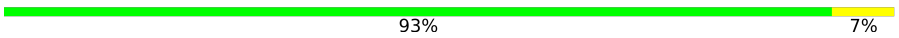
- Molecule 4: uL4m

Chain D:



- Molecule 5: uL5m

Chain E:



- Molecule 6: uL6m

Chain F: 91% 9%

S17 L24 V30 T48 L73 D78 E79 K80 V86 R97 V103 R104 I111 T115 E116 L122 R130 G196 V201 K212

• Molecule 7: bL9m

Chain G: 95% 5%

S10 A11 L12 V37 I65 L80 D83

• Molecule 8: uL13m

Chain H: 90% 10%

S2 R14 V19 T27 I37 R42 V46 T60 T68 G69 R83 K99 G102 L123 V128 N139 I158 Q161

• Molecule 9: uL14m

Chain I: 84% 8% 8%

M1 I2 F3 L4 K23 P33 V36 L50 THR GLN ASN ILE THR GLY THR ALA ASN THR ASN R62 I72 I99 T109 D119 D124 I138

• Molecule 10: uL15m

Chain J: 90% 10%

V58 L77 G78 R79 L85 G86 K87 R99 G100 K101 T111 K115 K119 V125 L130 F141 D156 K162 S193 K209 Q227 R241 R246 D265 E273 K277

• Molecule 11: uL16m

Chain K: 88% 12%

K38 H39 E40 K53 T68 A87 D94 I97 M98 L104 L109 L113 C114 T115 K130 M139 E150 E158 E163 A168 L184 S191 F192 Y215 L219 K227 R232

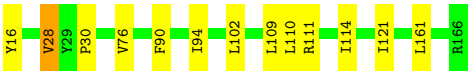
• Molecule 12: bL17m

Chain L: 88% 8%

T2 R7 K8 E42 T52 N62 E68 L69 L79 R107 R114 E125 V138 M145 L148 N169 K177 A178 E179 L194 L214 S221 LEU PRO LYS LYS THR LYS LYS PRO S230 R237 P238

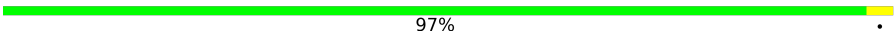
• Molecule 13: bL19m

Chain M: 91% 8%



- Molecule 14: bL21m

Chain N:

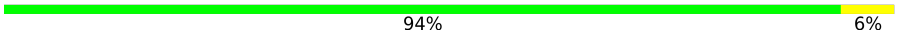


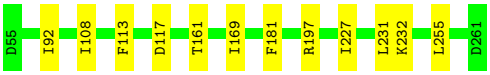
- Molecule 15: uL22m

Chain O:

- Molecule 16: uL23m

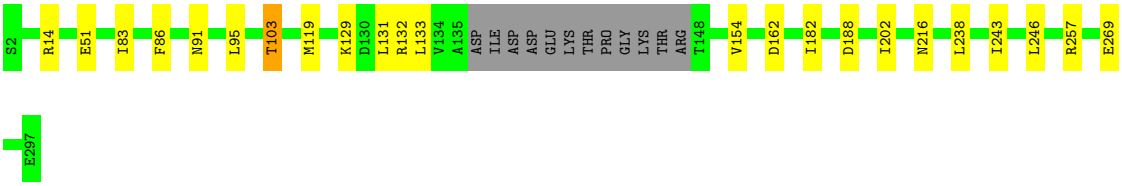
Chain P:





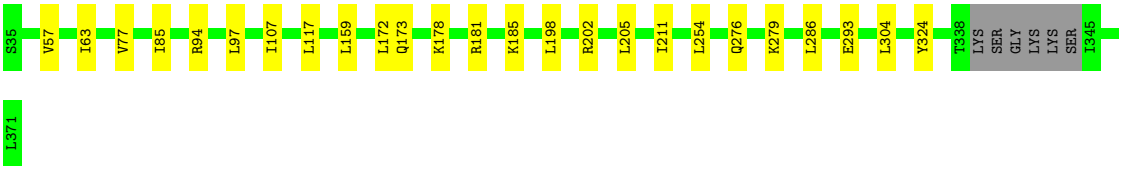
- Molecule 17: uL24m

Chain Q:



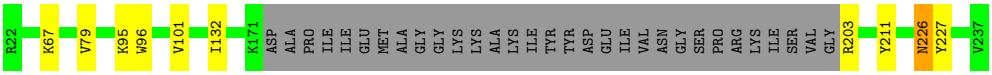
- Molecule 18: bL27m

Chain R:



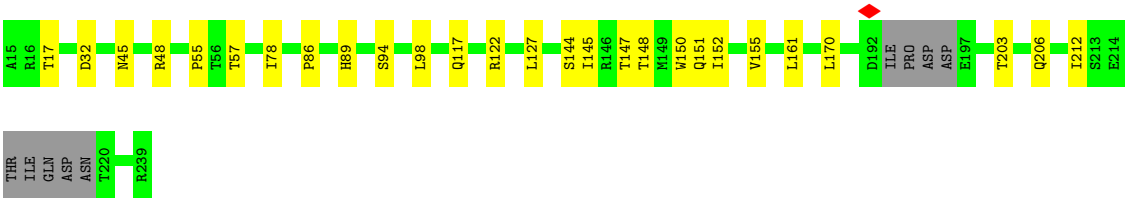
- Molecule 19: bL28m

Chain S:



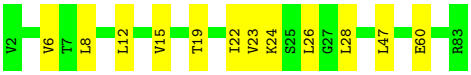
- Molecule 20: uL29m

Chain T: 84% 12% •



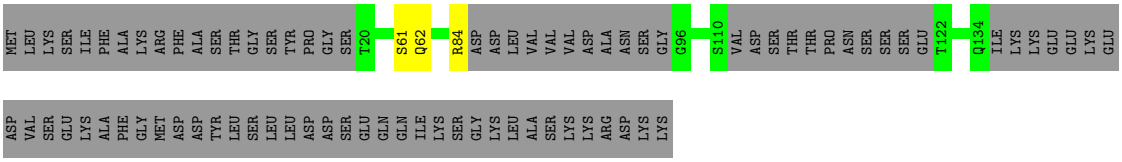
- Molecule 21: uL30m

Chain U: 85% 15%



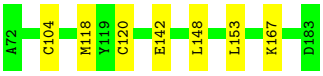
- Molecule 22: bL31m

Chain V: 51% • 47%



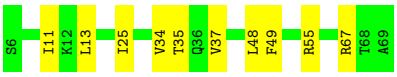
- Molecule 23: bL32m

Chain W: 94% 6%



- Molecule 24: bL33m

Chain X: 84% 16%



- Molecule 25: bL34m

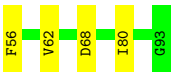
Chain Y: 91% 9%

- Molecule 26: bL35m

Chain Z: 94% 6%

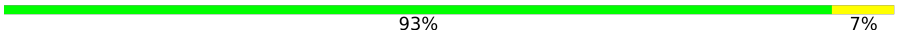
- Molecule 27: bL36m

Chain 0:



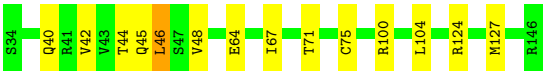
- Molecule 28: mL38

Chain 1:



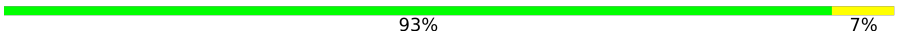
- Molecule 29: mL40

Chain 2:



- Molecule 30: mL41

Chain 3:

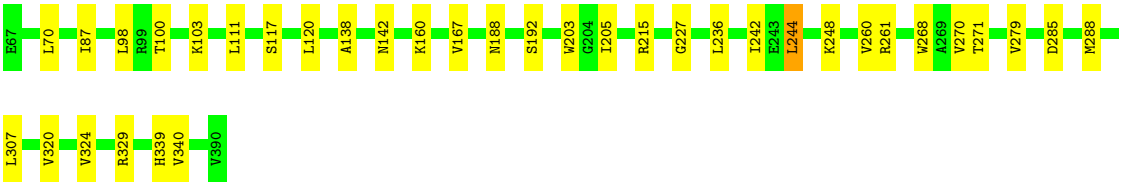


- Molecule 31: mL43

Chain 4:

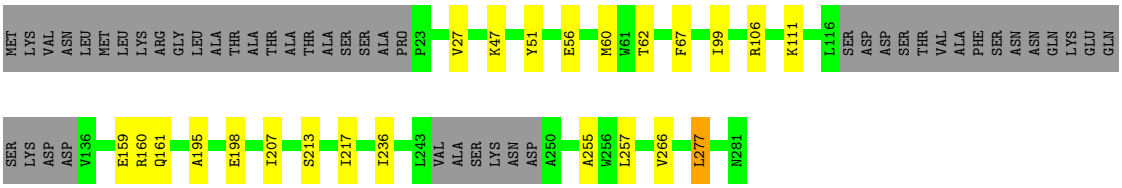
- Molecule 32: mL44

Chain 5:



- Molecule 33: mL46

Chain 6: 75% 8% 17%

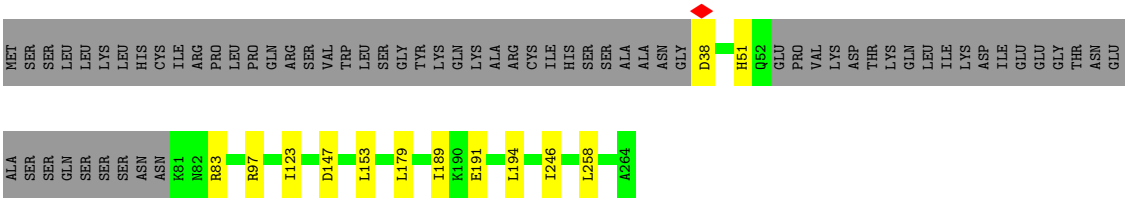


• Molecule 34: mL49

Chain 7: 87% 13%

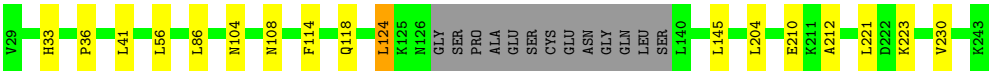
• Molecule 35: mL50

Chain 8: 70% 5% 25%



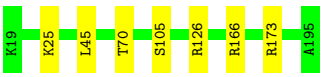
• Molecule 36: mL57

Chain 9: 86% 7% 6%



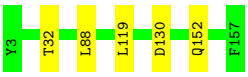
• Molecule 37: mL58

Chain a: 96%



• Molecule 38: mL59

Chain b: 97%

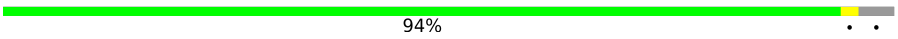


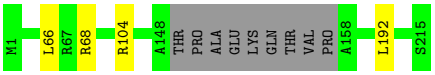
• Molecule 39: mL60

Chain c: 98%

- Molecule 40: mL67

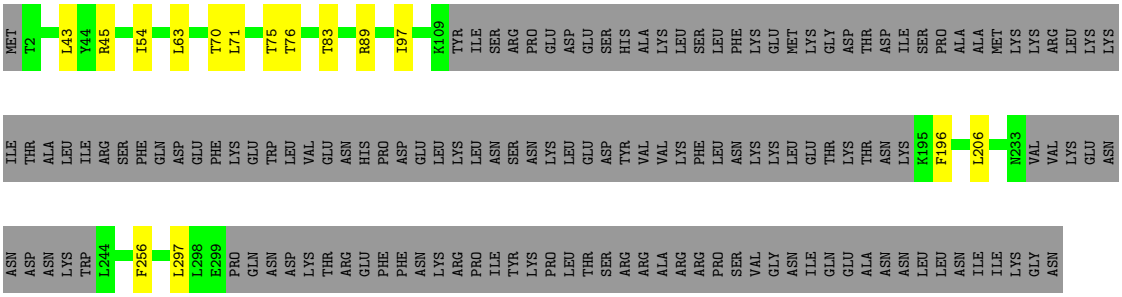
Chain d:





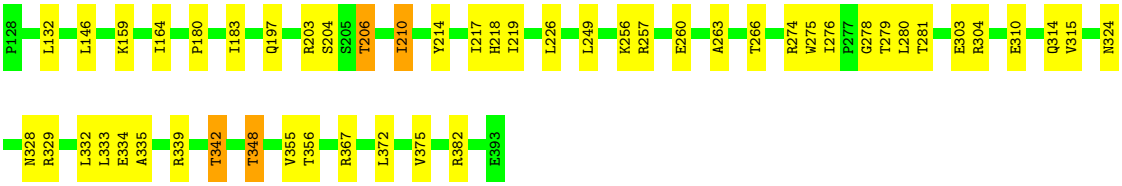
- Molecule 41: bS1m

Chain AA:



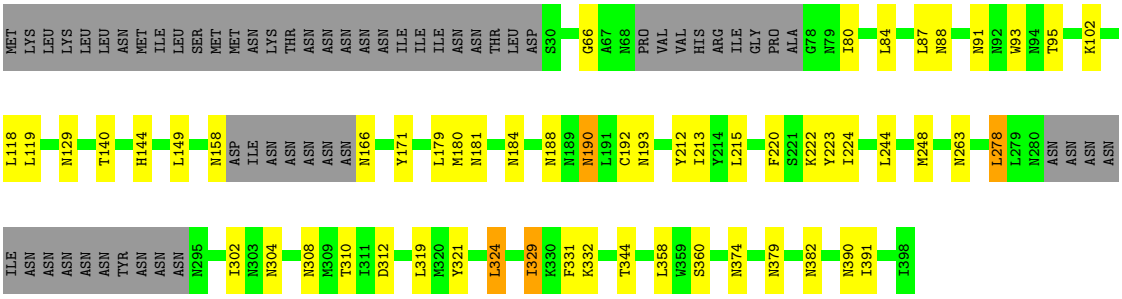
- Molecule 42: uS2m

Chain BB:



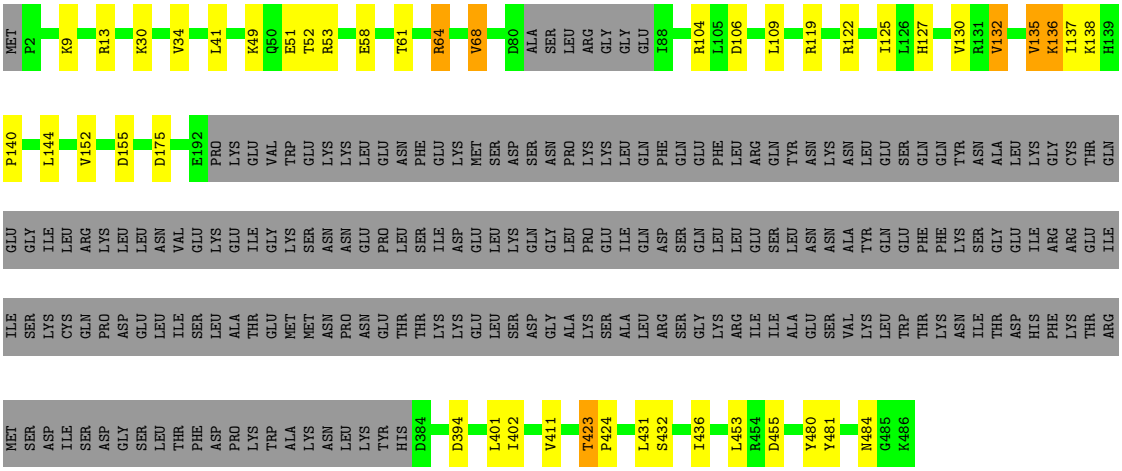
- Molecule 43: uS3m

Chain CC:



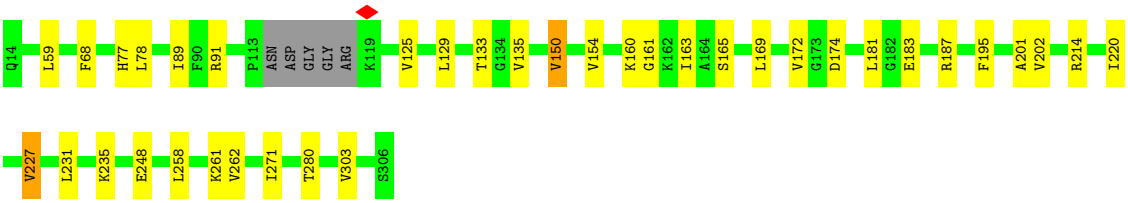
- Molecule 44: uS4m

Chain DD:



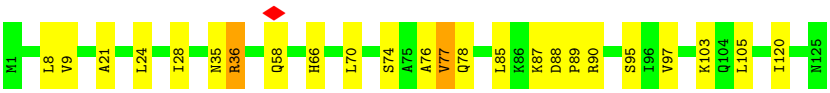
- Molecule 45: uS5m

Chain EE:



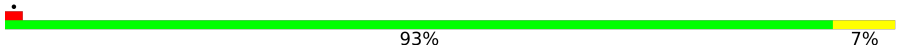
- Molecule 46: bS6m

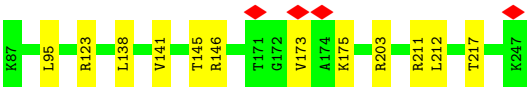
Chain FF:



- Molecule 47: uS7m

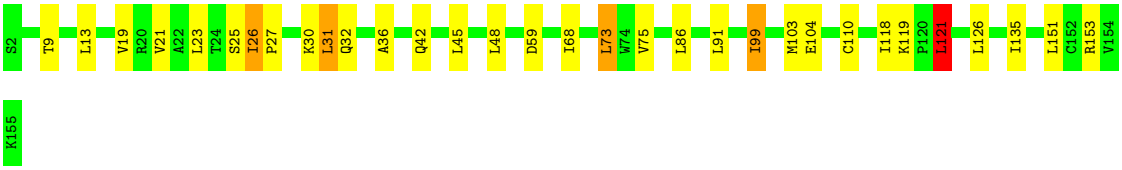
Chain GG:





- Molecule 48: uS8m

Chain HH:



- Molecule 49: uS9m

Chain II: 83% 9% 7%

R35 P39 L61 Y65 Q71 ASN ASN ASN GLU ALA GLN GLN THR LYS A81 L91 L98 D117 L120 I125 E128 K134 LYS SER SER MET LEU SER ASN ASN ILE K144 R153 K159 T164 I176 L183 L200 I211 T215

E225 M228 K248 R254 R257 P264 R278

- Molecule 50: uS10m

Chain JJ: 84% 13%

S16 T17 R18 P19 Y20 Y29 L34 Y38 D51 L55 D60 G66 Y67 Y68 L69 G70 I71 P72 L73 T74 G75 P76 L79 R82 R83 W86 V94 L110 T116 N117 P118 E119 V120 L121 L124 I125 M133 L152 H199 L200 E201

- Molecule 51: uS11m

Chain KK: 76% 18%

K70 L78 S92 N99 PHE HIS LYS ASN LYS GLY L106 N117 I124 T128 R134 K135 A136 A137 R138 G139 E140 Y141 E142 A143 A144 M151 N159 H160 L161 M169 F172 I180 L183 V192 K193 K194 I198 T202 R210 R216 L217

- Molecule 52: uS12m

Chain LL: 82% 17%

A29 T30 L31 K35 R42 R43 K44 K45 M66 V67 L68 R82 V91 E98 V108 L118 V121 I126 R127 L132 V135 R138 K144 K148 K152

- Molecule 53: uS13m

Chain MM: 91% 8%

V2 I5 L6 G9 F10 A19 Y25 G86 M91 L97 K113 L114 D118 R119 R120 G121

- Molecule 54: uS14m

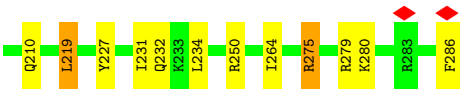
Chain NN: 81% 13% 5%

M1 L12 L22 E35 I36 L37 F43 M69 R70 S71 T72 C78 S81 F86 F91 R92 L93 C94 R95 N106 L107 P108 G109 V110 W115

- Molecule 55: uS15m

Chain OO: 80% 12% 6%

S34 D65 L68 T77 R78 Y79 M80 A81 K84 E85 P86 I95 R112 ALA GLU LEU SER GLY LEU ASN THR GLU VAL VAL GLY ILE GLU ASP I128 R145 F164 E165 R166 F167 D170 S173 V176 M181 T182 M188 I192 T202 L205 R206

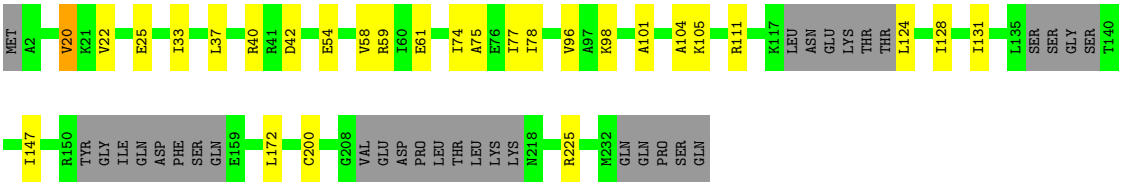


- Molecule 56: bS16m

Chain PP:

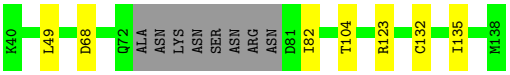
- Molecule 57: uS17m

Chain QQ:



- Molecule 58: bS18m

Chain RR:

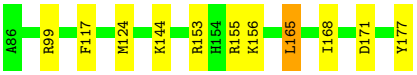


- Molecule 59: uS19m

Chain SS:

- Molecule 60: bS21m

Chain TT:

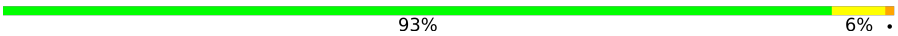


- Molecule 61: mS23

Chain UU:

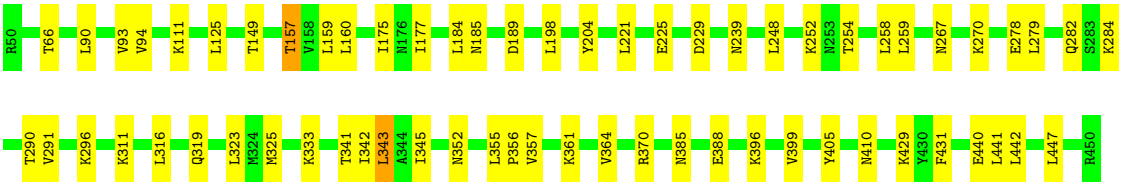
- Molecule 62: mS26

Chain VV:



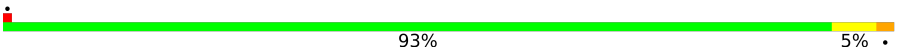
- Molecule 63: mS29

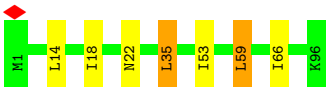
Chain WW:



- Molecule 64: mS33

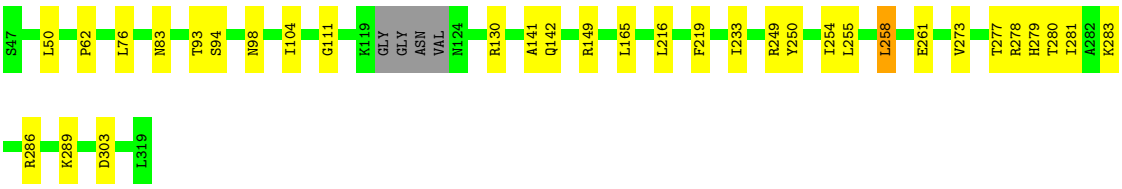
Chain XX:





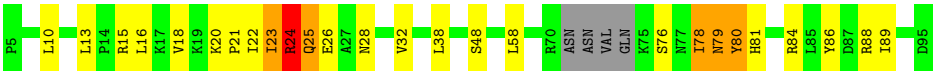
- Molecule 65: mS35

Chain YY:



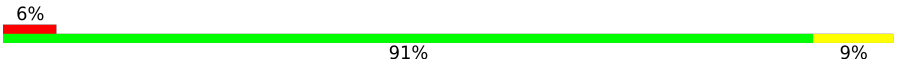
- Molecule 66: mS37

Chain ZZ:



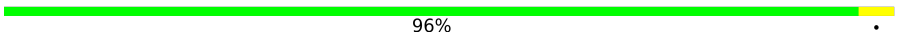
- Molecule 67: mS38

Chain 11:



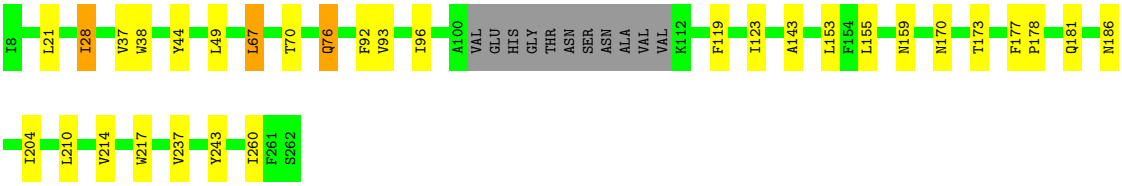
• Molecule 68: mS41

Chain 22:



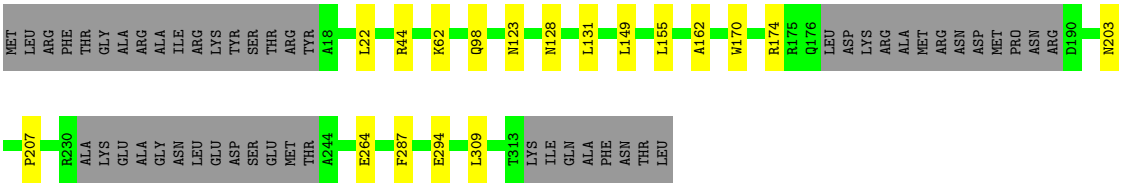
• Molecule 69: mS42

Chain 33:



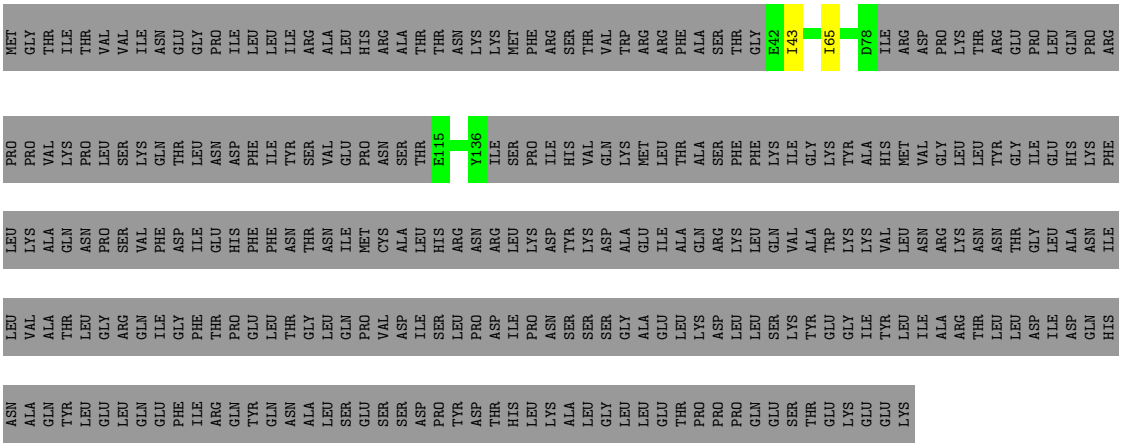
• Molecule 70: mS43

Chain 44:

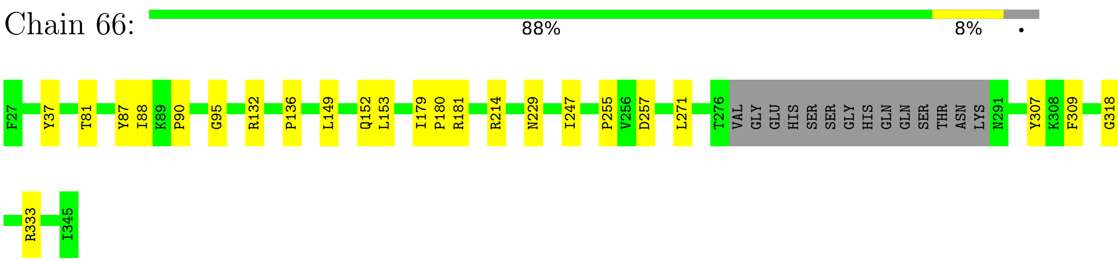


• Molecule 71: mS44

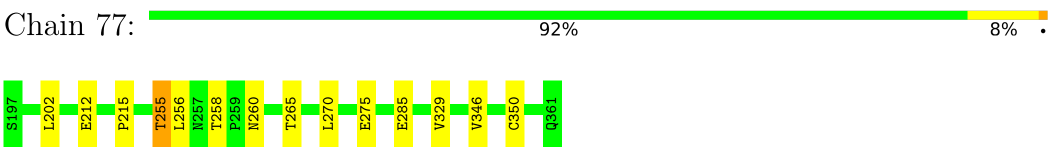
Chain 55:



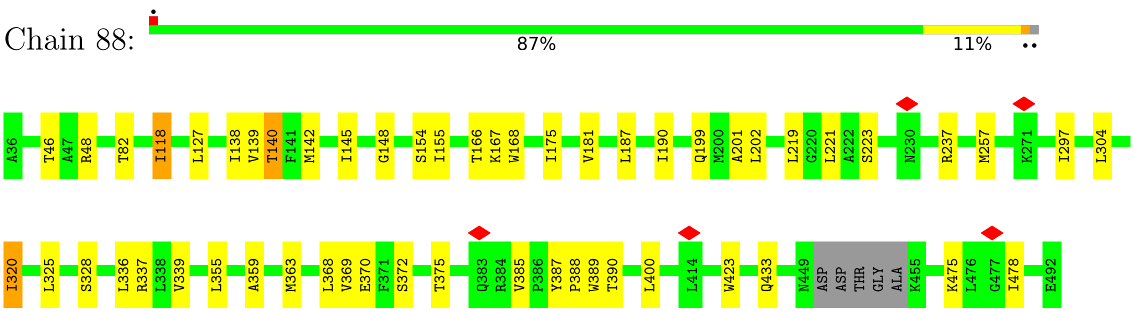
• Molecule 72: mS45



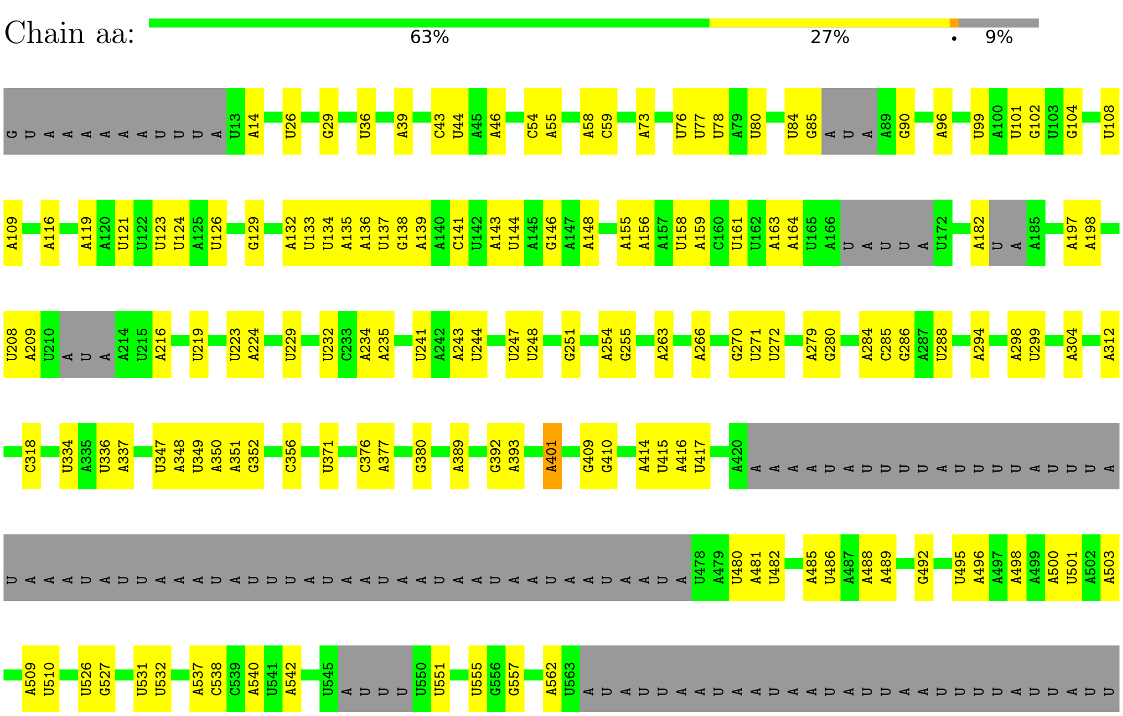
• Molecule 73: mS46

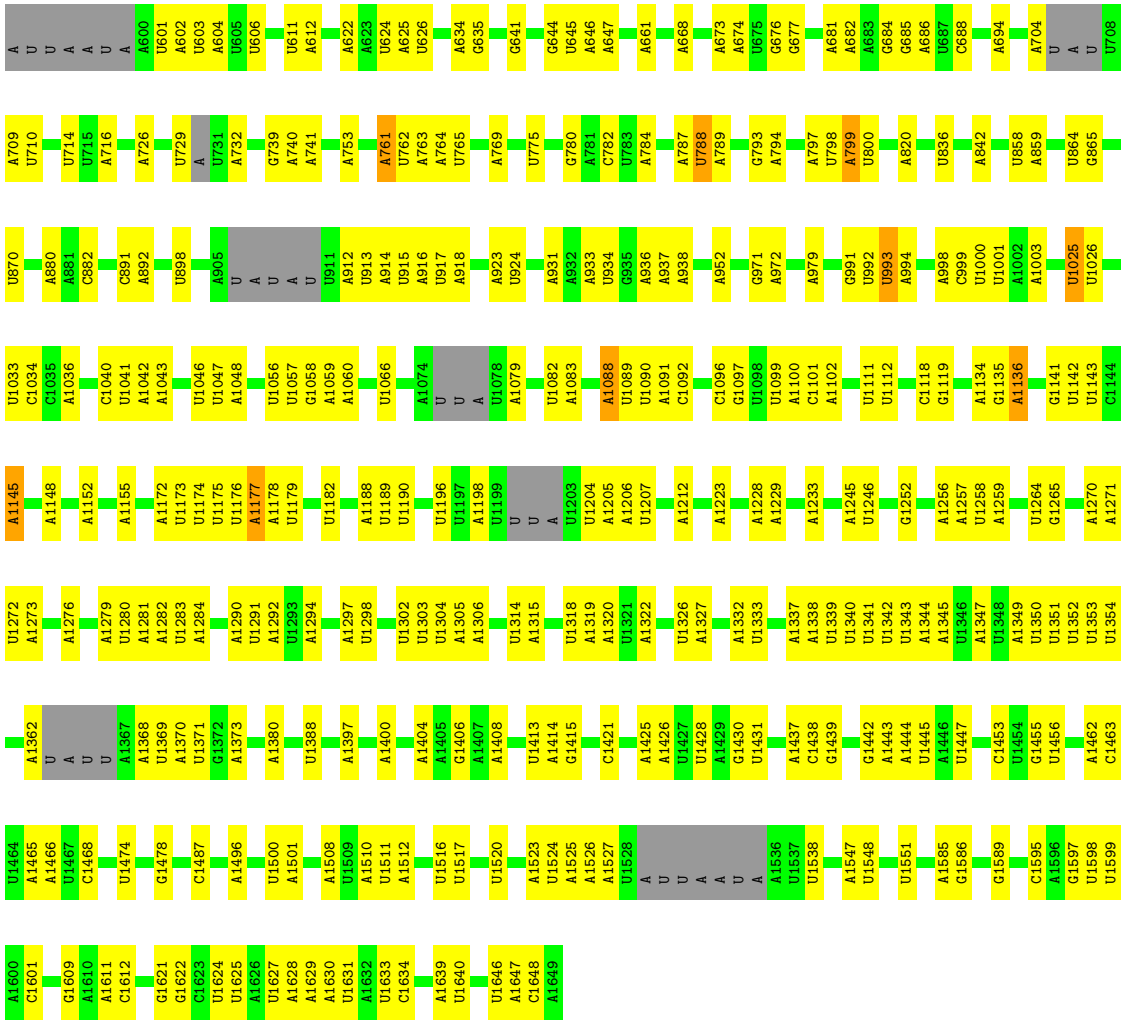


• Molecule 74: mS47



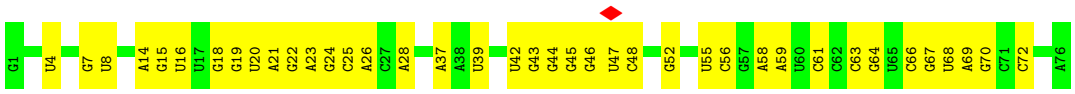
• Molecule 75: 15S ribosomal RNA





• Molecule 76: tRNA

Chain bb: 49% 51%



• Molecule 77: unknown protein sequence 1

Chain cc: 100%

There are no outlier residues recorded for this chain.

• Molecule 78: unknown protein sequence 2

Chain dd: 100%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24632	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	0.357	Depositor
Minimum map value	-0.234	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.0123	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 (i)

5.1 Standard geometry (i)

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

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	0.71	20/100359 (0.0%)
2	B	0.37	0/2573	0.73	1/3456 (0.0%)
3	C	0.32	0/1975	0.62	0/2657
4	D	0.35	0/2031	0.67	0/2751
5	E	0.32	0/2244	0.56	0/3033
6	F	0.33	0/1551	0.57	0/2093
7	G	0.33	0/628	0.58	0/844
8	H	0.34	0/1302	0.63	0/1749
9	I	0.31	0/962	0.66	0/1285
10	J	0.33	0/1783	0.64	0/2384
11	K	0.34	0/1606	0.66	0/2148
12	L	0.32	0/1845	0.63	0/2489
13	M	0.33	0/1224	0.66	0/1651
14	N	0.31	0/961	0.65	0/1295
15	O	0.32	0/1859	0.63	0/2495
16	P	0.33	0/1773	0.61	0/2390
17	Q	0.33	0/2323	0.57	0/3135
18	R	0.33	0/2783	0.64	0/3723
19	S	0.33	0/1576	0.61	0/2104
20	T	0.34	0/1837	0.60	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	0.73	0/515
26	Z	0.34	0/522	0.68	0/695
27	0	0.33	0/329	0.58	0/432
28	1	0.34	0/2949	0.59	0/3998
29	2	0.33	0/963	0.62	0/1295
30	3	0.34	0/1072	0.61	0/1442
31	4	0.34	0/1138	0.70	0/1526
32	5	0.32	0/2604	0.60	0/3526

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	6	0.34	0/1978	0.59	0/2664
34	7	0.35	0/873	0.62	0/1170
35	8	0.33	0/1659	0.56	0/2230
36	9	0.34	0/1616	0.57	0/2177
37	a	0.34	0/1471	0.65	0/1976
38	b	0.33	0/1333	0.58	0/1783
39	c	0.33	0/1028	0.62	0/1372
40	d	0.33	0/1791	0.62	0/2415
41	AA	0.33	0/1645	0.61	0/2218
42	BB	0.35	0/2128	0.69	0/2892
43	CC	0.34	0/2864	0.58	0/3853
44	DD	0.35	0/2434	0.64	0/3281
45	EE	0.33	0/2360	0.60	0/3180
46	FF	0.43	0/1014	0.70	1/1358 (0.1%)
47	GG	0.35	0/1305	0.62	0/1763
48	HH	0.33	0/1232	0.71	1/1660 (0.1%)
49	II	0.34	0/1855	0.62	0/2492
50	JJ	0.33	0/1544	0.63	0/2091
51	KK	0.36	0/1136	0.64	0/1515
52	LL	0.34	0/963	0.69	0/1292
53	MM	0.33	0/957	0.65	0/1277
54	NN	0.35	0/972	0.98	1/1300 (0.1%)
55	OO	0.36	0/1985	0.70	2/2647 (0.1%)
56	PP	0.33	0/934	0.64	0/1260
57	QQ	0.34	0/1694	0.65	0/2252
58	RR	0.37	0/749	0.67	0/998
59	SS	0.35	0/652	0.64	0/882
60	TT	0.37	0/771	0.64	0/1019
61	UU	0.33	0/1950	0.63	0/2636
62	VV	0.32	0/1900	0.60	0/2540
63	WW	0.34	0/3282	0.58	0/4438
64	XX	0.35	0/786	0.64	0/1046
65	YY	0.35	0/2313	0.62	0/3119
66	ZZ	0.32	0/702	0.61	0/945
67	11	0.33	0/303	0.80	0/386
68	22	0.34	0/852	0.56	0/1142
69	33	0.35	0/2002	0.58	0/2721
70	44	0.34	0/2214	0.58	0/2990
71	55	0.35	0/521	0.57	0/701
72	66	0.34	0/2547	0.59	0/3438
73	77	0.35	0/1358	0.56	0/1839
74	88	0.35	0/3646	0.58	0/4935
75	aa	0.25	0/35686	0.74	26/55477 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	bb	0.42	0/1805	0.80	4/2811 (0.1%)
All	All	0.30	0/212996	0.68	56/307971 (0.0%)

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	NN	107	LEU	C-N-CD	-26.29	62.77	120.60
1	A	3242	A	N9-C1'-C2'	-8.66	102.48	112.00
1	A	2897	A	C2'-C3'-O3'	8.34	127.85	109.50
1	A	840	C	C2'-C3'-O3'	8.32	127.81	109.50
1	A	3242	A	C2'-C3'-O3'	-8.01	91.88	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	28893	259	0
2	B	2527	0	2649	142	0
3	C	1932	0	1969	20	0
4	D	1991	0	2032	9	0
5	E	2187	0	2203	8	0
6	F	1524	0	1587	4	0
7	G	617	0	626	1	0
8	H	1275	0	1310	18	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	10	0
13	M	1206	0	1283	6	0
14	N	948	0	1006	1	0
15	O	1826	0	1933	13	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	13	0
20	T	1792	0	1782	12	0
21	U	639	0	699	5	0
22	V	729	0	711	0	0
23	W	937	0	975	5	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	12	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	19	0
33	6	1932	0	1950	12	0
34	7	858	0	908	6	0
35	8	1629	0	1633	3	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	5	0
42	BB	2085	0	2094	40	0
43	CC	2821	0	2829	39	0
44	DD	2369	0	2433	21	0
45	EE	2306	0	2324	23	0
46	FF	1002	0	1086	74	0
47	GG	1282	0	1342	5	0
48	HH	1213	0	1277	12	0
49	II	1820	0	1906	8	0
50	JJ	1508	0	1505	15	0
51	KK	1121	0	1172	32	0
52	LL	948	0	1003	12	0
53	MM	942	0	1001	3	0
54	NN	953	0	1007	37	0
55	OO	1962	0	2036	67	0
56	PP	919	0	982	4	0
57	QQ	1683	0	1769	42	0
58	RR	738	0	771	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	SS	636	0	654	2	0
60	TT	760	0	791	4	0
61	UU	1907	0	1898	21	0
62	VV	1872	0	1978	7	0
63	WW	3216	0	3315	15	0
64	XX	774	0	821	4	0
65	YY	2258	0	2229	10	0
66	ZZ	687	0	719	48	0
67	11	303	0	357	1	0
68	22	833	0	839	1	0
69	33	1953	0	1913	16	0
70	44	2169	0	2155	6	0
71	55	508	0	524	0	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	16010	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	182	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	OO	1	0	0	0	0
79	PP	1	0	0	0	0
79	R	1	0	0	0	0
79	WW	1	0	0	0	0
79	aa	110	0	0	0	0
80	B	1	0	0	0	0
81	0	1	0	0	0	0
81	W	1	0	0	1	0
82	WW	28	0	12	1	0
All	All	201462	0	157758	977	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 977 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)
2:B:63:ILE:HD11	57:QQ:104:ALA:CB	1.20	1.61
2:B:232:VAL:CG2	46:FF:87:LYS:HD2	1.30	1.59
2:B:73:LEU:HD23	46:FF:77:VAL:CG2	1.29	1.57
2:B:232:VAL:HG21	46:FF:87:LYS:CD	1.34	1.55
19:S:211:TYR:CE2	19:S:227:TYR:CE1	2.00	1.47

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%)	14 (4%)	1 (0%)	41 76
3	C	247/249 (99%)	234 (95%)	10 (4%)	3 (1%)	13 50
4	D	250/252 (99%)	237 (95%)	9 (4%)	4 (2%)	9 44
5	E	272/274 (99%)	254 (93%)	16 (6%)	2 (1%)	22 62
6	F	194/196 (99%)	182 (94%)	11 (6%)	1 (0%)	29 68
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%)	203 (93%)	14 (6%)	1 (0%)	29 68
11	K	193/195 (99%)	184 (95%)	9 (5%)	0	100 100
12	L	225/237 (95%)	218 (97%)	7 (3%)	0	100 100
13	M	149/151 (99%)	139 (93%)	10 (7%)	0	100 100
14	N	116/118 (98%)	108 (93%)	8 (7%)	0	100 100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	327/337 (97%)	314 (96%)	12 (4%)	1 (0%)	41	76
19	S	181/216 (84%)	172 (95%)	9 (5%)	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	56
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	60
43	CC	331/398 (83%)	303 (92%)	26 (8%)	2 (1%)	25	65
44	DD	281/486 (58%)	264 (94%)	16 (6%)	1 (0%)	34	72
45	EE	284/293 (97%)	262 (92%)	20 (7%)	2 (1%)	22	62
46	FF	123/125 (98%)	112 (91%)	11 (9%)	0	100	100
47	GG	159/161 (99%)	147 (92%)	11 (7%)	1 (1%)	25	65
48	HH	152/154 (99%)	144 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	II	220/244 (90%)	207 (94%)	11 (5%)	2 (1%)	17	56
50	JJ	184/186 (99%)	163 (89%)	15 (8%)	6 (3%)	4	29
51	KK	138/148 (93%)	124 (90%)	12 (9%)	2 (1%)	11	46
52	LL	122/124 (98%)	110 (90%)	10 (8%)	2 (2%)	9	44
53	MM	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
54	NN	113/115 (98%)	106 (94%)	4 (4%)	3 (3%)	5	33
55	OO	234/253 (92%)	222 (95%)	12 (5%)	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	68
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%)	220 (95%)	11 (5%)	0	100	100
63	WW	399/401 (100%)	368 (92%)	28 (7%)	3 (1%)	19	60
64	XX	91/96 (95%)	88 (97%)	3 (3%)	0	100	100
65	YY	265/273 (97%)	244 (92%)	18 (7%)	3 (1%)	14	52
66	ZZ	83/91 (91%)	70 (84%)	12 (14%)	1 (1%)	13	50
67	11	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
68	22	97/99 (98%)	89 (92%)	7 (7%)	1 (1%)	15	54
69	33	240/255 (94%)	225 (94%)	14 (6%)	1 (0%)	34	72
70	44	264/321 (82%)	251 (95%)	10 (4%)	3 (1%)	14	52
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	65
74	88	448/457 (98%)	414 (92%)	31 (7%)	3 (1%)	22	62
All	All	13235/14689 (90%)	12462 (94%)	718 (5%)	55 (0%)	38	72

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	DD	423	THR
51	KK	141	TYR

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Mol	Chain	Res	Type
52	LL	45	LYS
52	LL	98	GLU
54	NN	108	PRO

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%)	254 (93%)	18 (7%)	16	43
3	C	210/210 (100%)	200 (95%)	10 (5%)	25	51
4	D	218/218 (100%)	199 (91%)	19 (9%)	10	33
5	E	242/242 (100%)	231 (96%)	11 (4%)	27	53
6	F	172/172 (100%)	164 (95%)	8 (5%)	26	52
7	G	68/68 (100%)	66 (97%)	2 (3%)	42	64
8	H	138/138 (100%)	131 (95%)	7 (5%)	24	50
9	I	108/117 (92%)	104 (96%)	4 (4%)	34	58
10	J	181/181 (100%)	166 (92%)	15 (8%)	11	36
11	K	167/167 (100%)	151 (90%)	16 (10%)	8	29
12	L	203/211 (96%)	194 (96%)	9 (4%)	28	53
13	M	136/136 (100%)	130 (96%)	6 (4%)	28	53
14	N	107/107 (100%)	105 (98%)	2 (2%)	57	75
15	O	200/200 (100%)	188 (94%)	12 (6%)	19	46
16	P	185/185 (100%)	181 (98%)	4 (2%)	52	71
17	Q	256/267 (96%)	242 (94%)	14 (6%)	21	48
18	R	303/308 (98%)	291 (96%)	12 (4%)	31	56
19	S	167/191 (87%)	161 (96%)	6 (4%)	35	59
20	T	204/213 (96%)	196 (96%)	8 (4%)	32	56
21	U	73/73 (100%)	70 (96%)	3 (4%)	30	55
22	V	74/161 (46%)	71 (96%)	3 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	104/104 (100%)	101 (97%)	3 (3%)	42	64
24	X	56/56 (100%)	52 (93%)	4 (7%)	14	41
25	Y	40/40 (100%)	39 (98%)	1 (2%)	47	68
26	Z	50/50 (100%)	46 (92%)	4 (8%)	12	37
27	0	36/36 (100%)	35 (97%)	1 (3%)	43	64
28	1	323/323 (100%)	311 (96%)	12 (4%)	34	58
29	2	106/106 (100%)	99 (93%)	7 (7%)	16	43
30	3	112/112 (100%)	109 (97%)	3 (3%)	44	65
31	4	121/121 (100%)	118 (98%)	3 (2%)	47	68
32	5	284/284 (100%)	278 (98%)	6 (2%)	53	72
33	6	213/252 (84%)	205 (96%)	8 (4%)	33	57
34	7	95/95 (100%)	91 (96%)	4 (4%)	30	54
35	8	182/240 (76%)	173 (95%)	9 (5%)	25	51
36	9	176/186 (95%)	168 (96%)	8 (4%)	27	53
37	a	158/158 (100%)	151 (96%)	7 (4%)	28	53
38	b	144/144 (100%)	139 (96%)	5 (4%)	36	59
39	c	110/110 (100%)	109 (99%)	1 (1%)	78	88
40	d	191/199 (96%)	187 (98%)	4 (2%)	53	72
41	AA	177/309 (57%)	168 (95%)	9 (5%)	24	50
42	BB	233/233 (100%)	206 (88%)	27 (12%)	5	23
43	CC	328/385 (85%)	296 (90%)	32 (10%)	8	28
44	DD	256/437 (59%)	227 (89%)	29 (11%)	6	23
45	EE	249/252 (99%)	237 (95%)	12 (5%)	25	51
46	FF	114/114 (100%)	105 (92%)	9 (8%)	12	38
47	GG	138/138 (100%)	132 (96%)	6 (4%)	29	54
48	HH	141/141 (100%)	125 (89%)	16 (11%)	6	23
49	II	196/215 (91%)	185 (94%)	11 (6%)	21	47
50	JJ	167/167 (100%)	152 (91%)	15 (9%)	9	32
51	KK	122/127 (96%)	107 (88%)	15 (12%)	4	21
52	LL	103/103 (100%)	91 (88%)	12 (12%)	5	22
53	MM	100/100 (100%)	94 (94%)	6 (6%)	19	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	NN	103/103 (100%)	91 (88%)	12 (12%)	5	22
55	OO	208/220 (94%)	198 (95%)	10 (5%)	25	51
56	PP	101/104 (97%)	95 (94%)	6 (6%)	19	46
57	QQ	187/218 (86%)	178 (95%)	9 (5%)	25	51
58	RR	80/87 (92%)	74 (92%)	6 (8%)	13	39
59	SS	69/69 (100%)	62 (90%)	7 (10%)	7	27
60	TT	81/81 (100%)	73 (90%)	8 (10%)	8	28
61	UU	208/208 (100%)	196 (94%)	12 (6%)	20	46
62	VV	208/210 (99%)	199 (96%)	9 (4%)	29	54
63	WW	368/368 (100%)	328 (89%)	40 (11%)	6	25
64	XX	84/84 (100%)	79 (94%)	5 (6%)	19	46
65	YY	248/250 (99%)	231 (93%)	17 (7%)	15	42
66	ZZ	78/82 (95%)	67 (86%)	11 (14%)	3	18
67	11	32/32 (100%)	31 (97%)	1 (3%)	40	62
68	22	90/90 (100%)	89 (99%)	1 (1%)	73	85
69	33	216/231 (94%)	203 (94%)	13 (6%)	19	46
70	44	238/281 (85%)	229 (96%)	9 (4%)	33	57
71	55	53/303 (18%)	51 (96%)	2 (4%)	33	57
72	66	277/289 (96%)	269 (97%)	8 (3%)	42	64
73	77	158/158 (100%)	152 (96%)	6 (4%)	33	57
74	88	401/404 (99%)	376 (94%)	25 (6%)	18	45
All	All	11997/13111 (92%)	11302 (94%)	695 (6%)	24	46

5 of 695 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	LL	82	ARG
63	WW	258	LEU
53	MM	114	LEU
52	LL	67	VAL
58	RR	132	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2677/3296 (81%)	613 (22%)	109 (4%)
75	aa	1473/1649 (89%)	445 (30%)	0
76	bb	75/76 (98%)	36 (48%)	0
All	All	4225/5021 (84%)	1094 (25%)	109 (2%)

5 of 1094 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	22	U
1	A	26	A
1	A	27	A
1	A	28	U
1	A	30	U

5 of 109 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1727	A
1	A	2357	U
1	A	3171	A
1	A	1892	G
1	A	2322	U

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	0.97	1 (4%)	30,47,47	1.34	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	-2.24	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	-3.72	120.07	132.83
82	WW	501	GDP	C3'-C2'-C1'	2.56	104.83	100.98
82	WW	501	GDP	C5-C6-N1	2.51	118.39	113.95
82	WW	501	GDP	C8-N7-C5	2.45	107.66	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

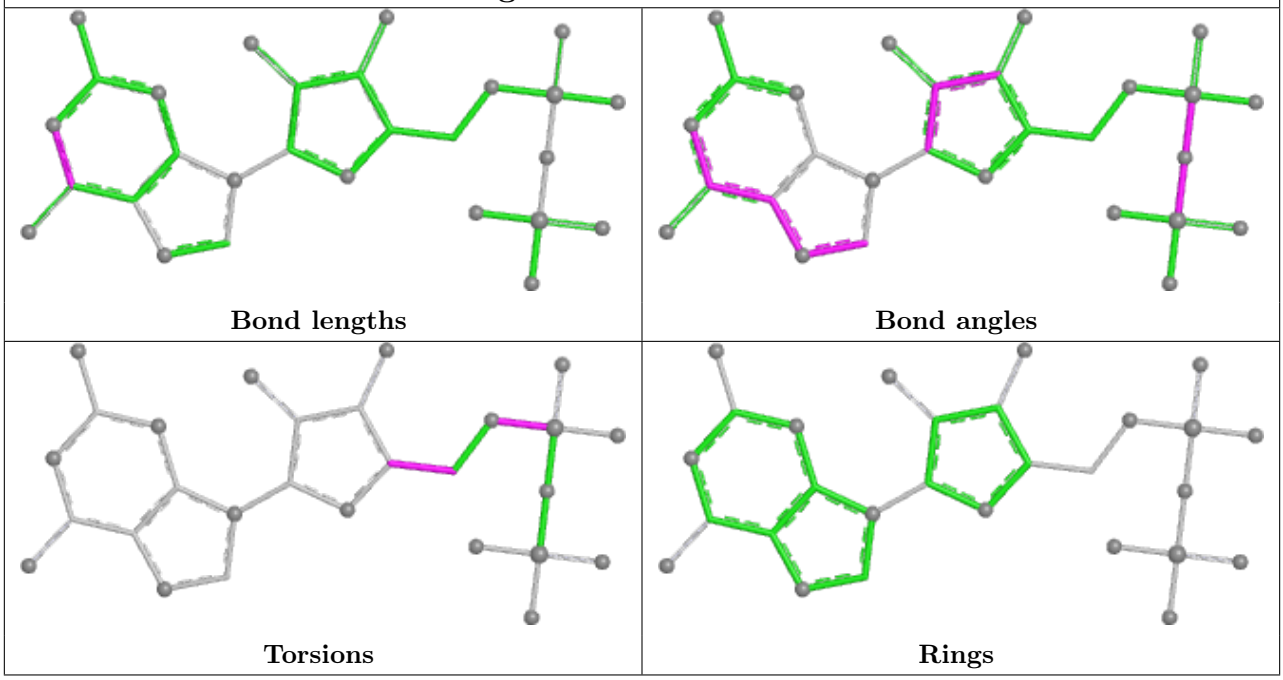
There are no ring outliers.

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.

Ligand GDP WW 501



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	35.54
1	dd	170:UNK	C	202:UNK	N	27.03
1	cc	59:UNK	C	76:UNK	N	22.66
1	cc	93:UNK	C	105:UNK	N	20.49

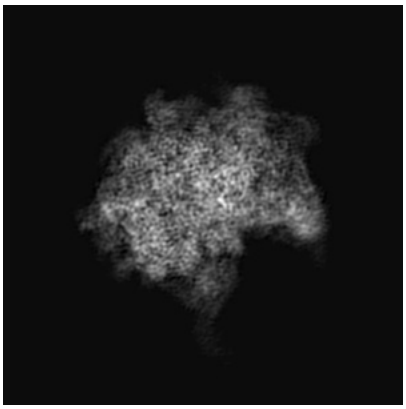
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3553. These allow visual inspection of the internal detail of the map and identification of artifacts.

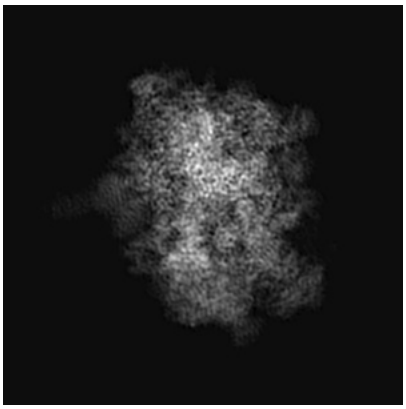
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

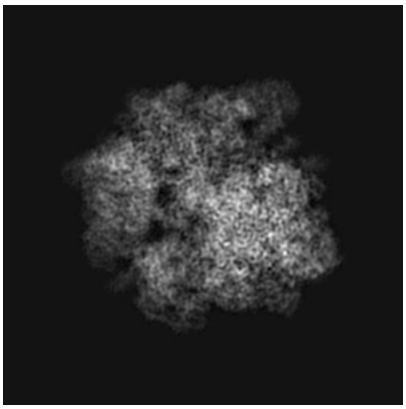
6.1.1 Primary map



X

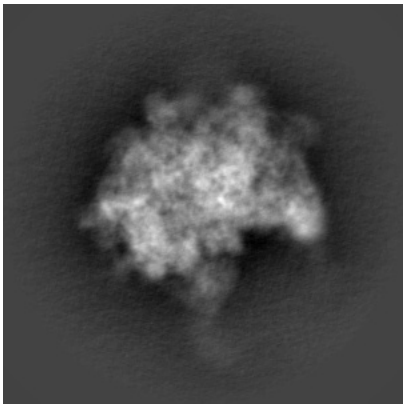


Y

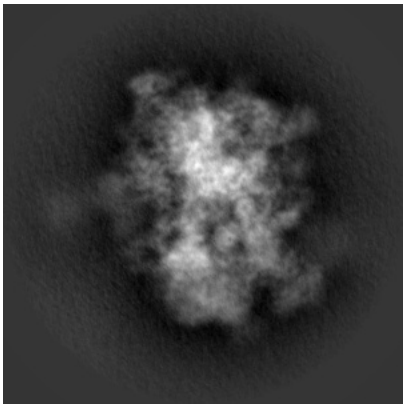


Z

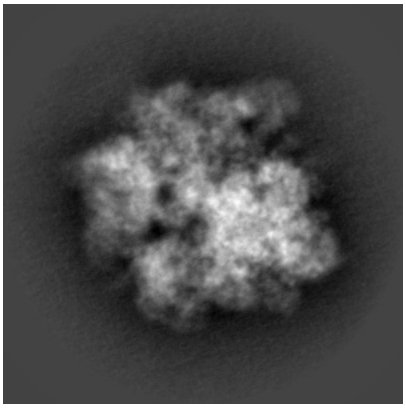
6.1.2 Raw map



X



Y

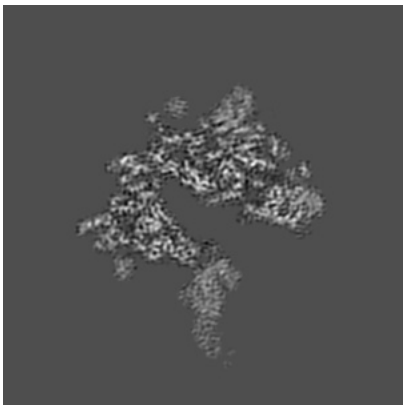


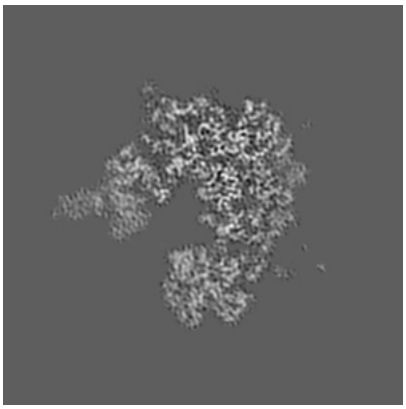
Z

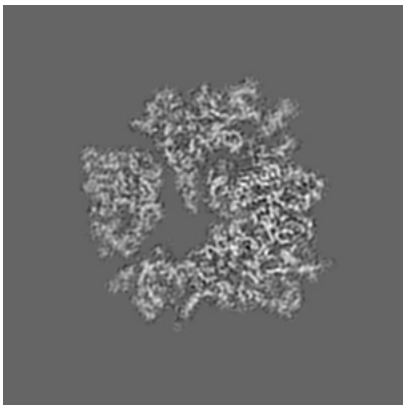
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

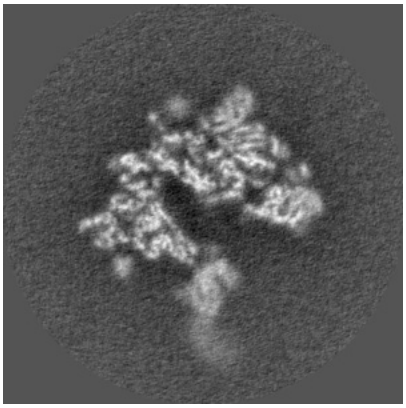
6.2.1 Primary map

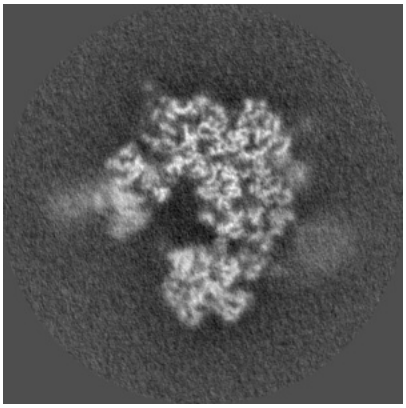

X Index: 165

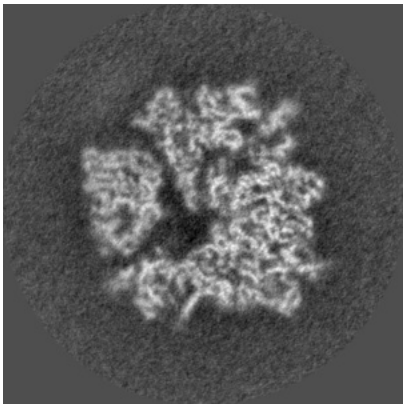

Y Index: 165


Z Index: 165

6.2.2 Raw map


X Index: 165

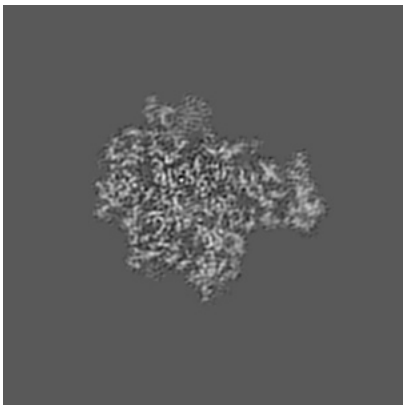

Y Index: 165


Z Index: 165

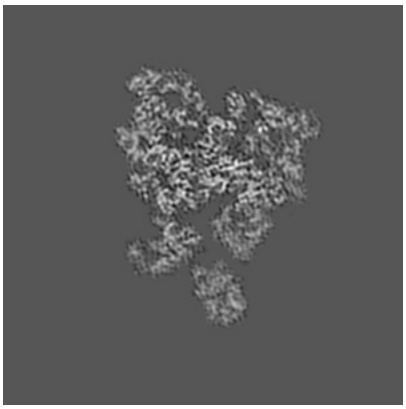
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

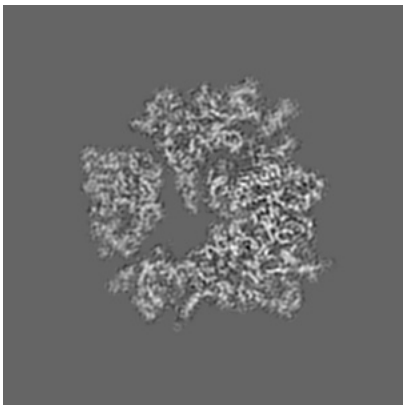
6.3.1 Primary map



X Index: 195

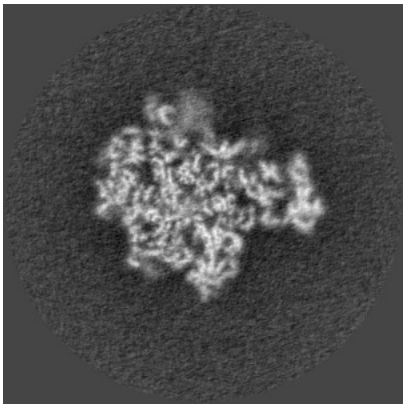


Y Index: 132

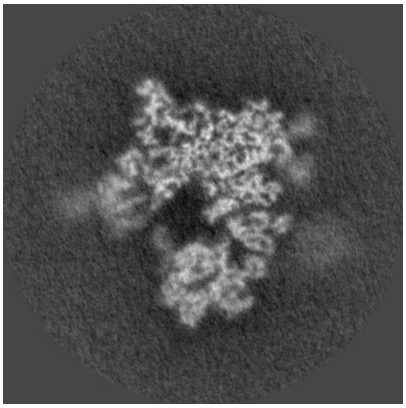


Z Index: 165

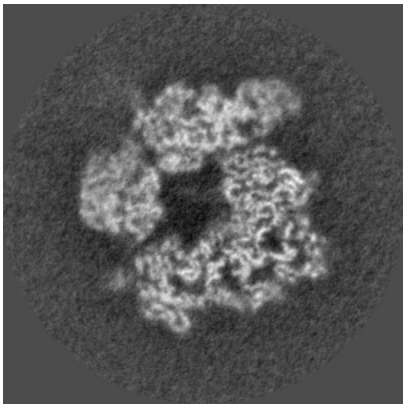
6.3.2 Raw map



X Index: 196



Y Index: 159

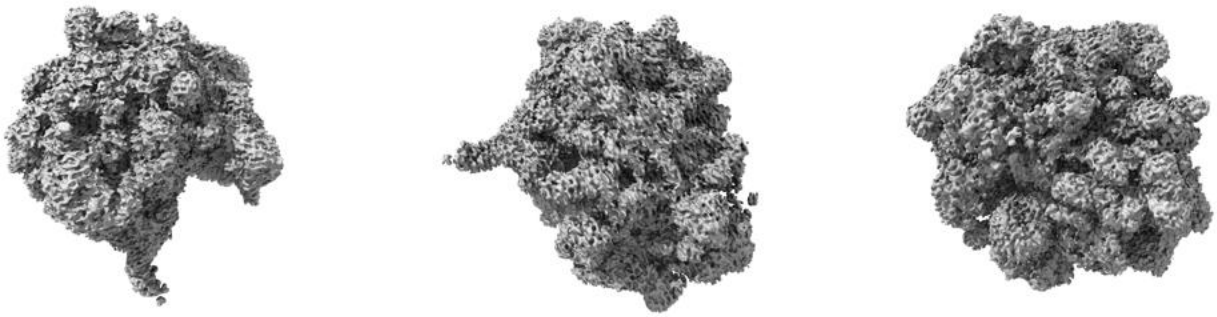


Z Index: 156

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

6.4 Orthogonal surface views (i)

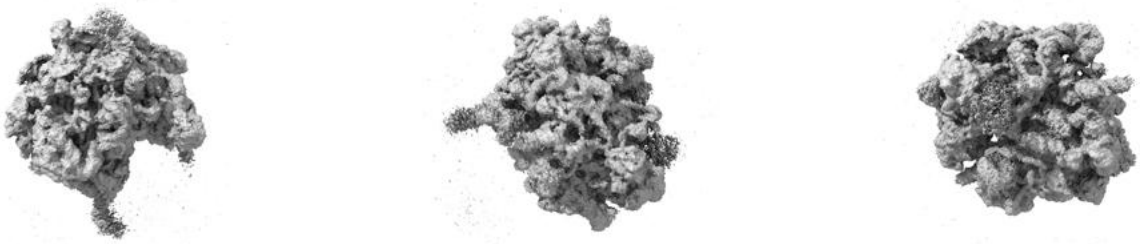
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0123. 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.

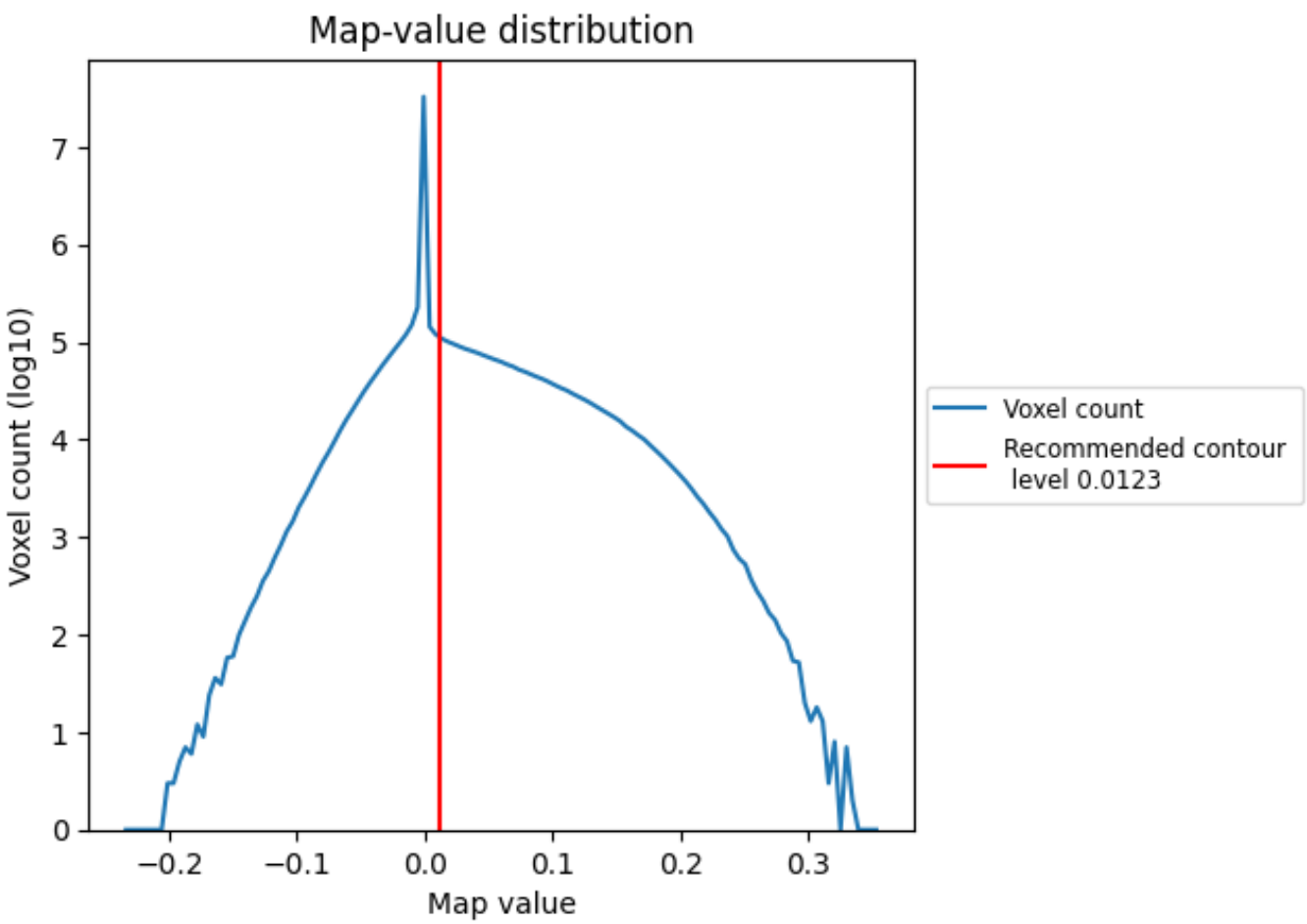
6.5 Mask visualisation (i)

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

7 Map analysis (i)

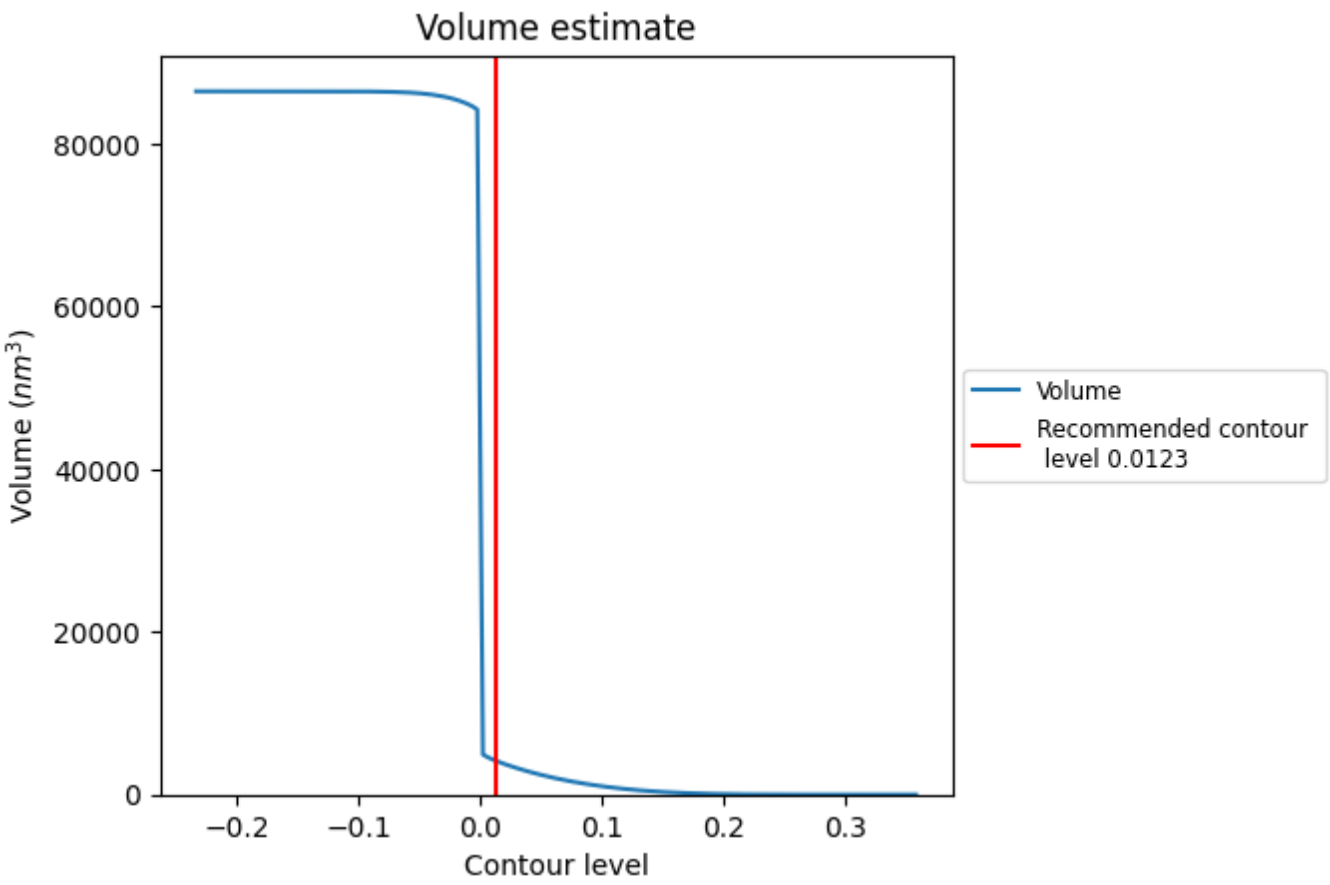
This section contains the results of statistical analysis of the map.

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.

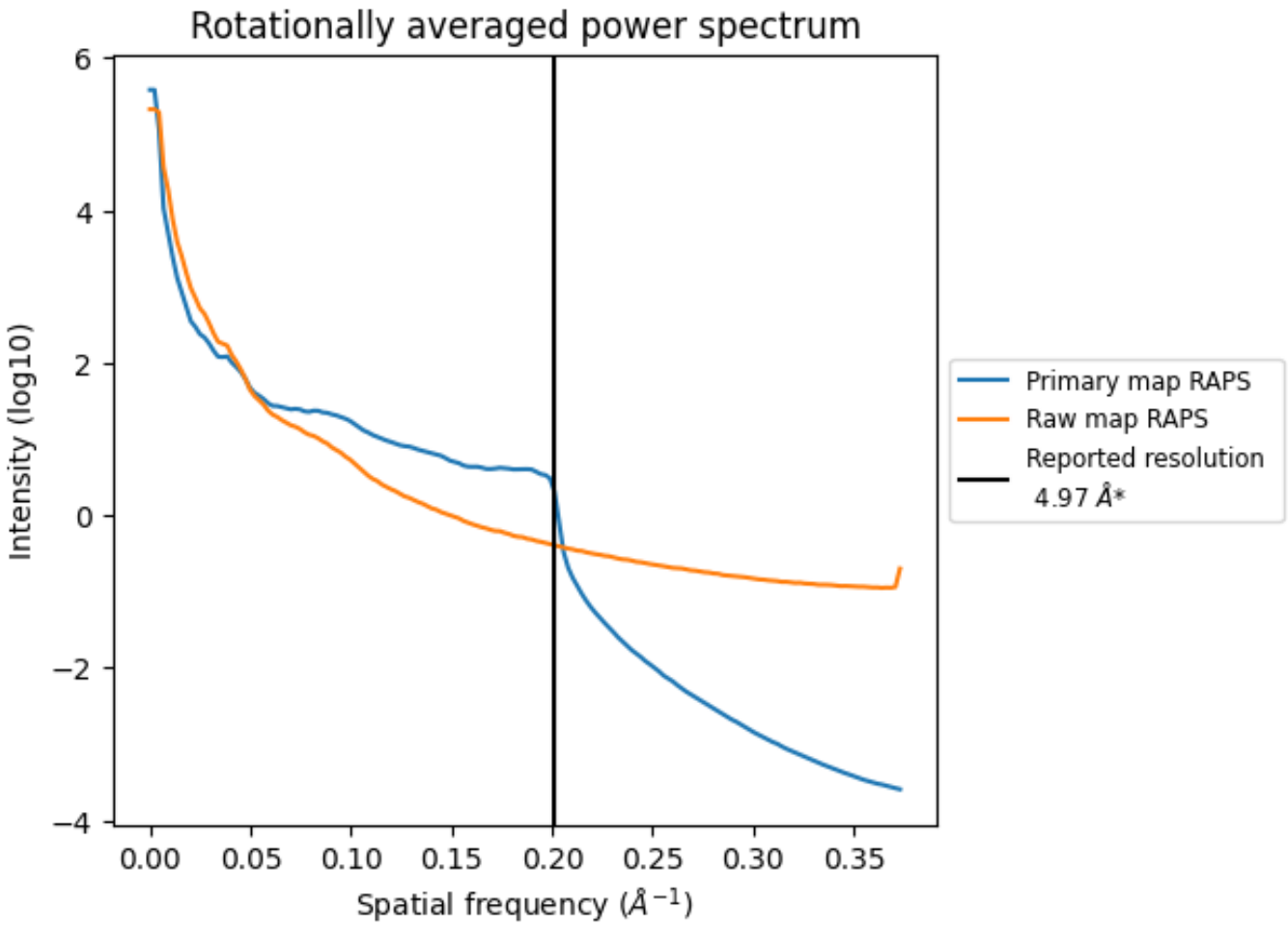
7.2 Volume estimate (i)



The volume at the recommended contour level is 4164 nm^3; this corresponds to an approximate mass of 3762 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)

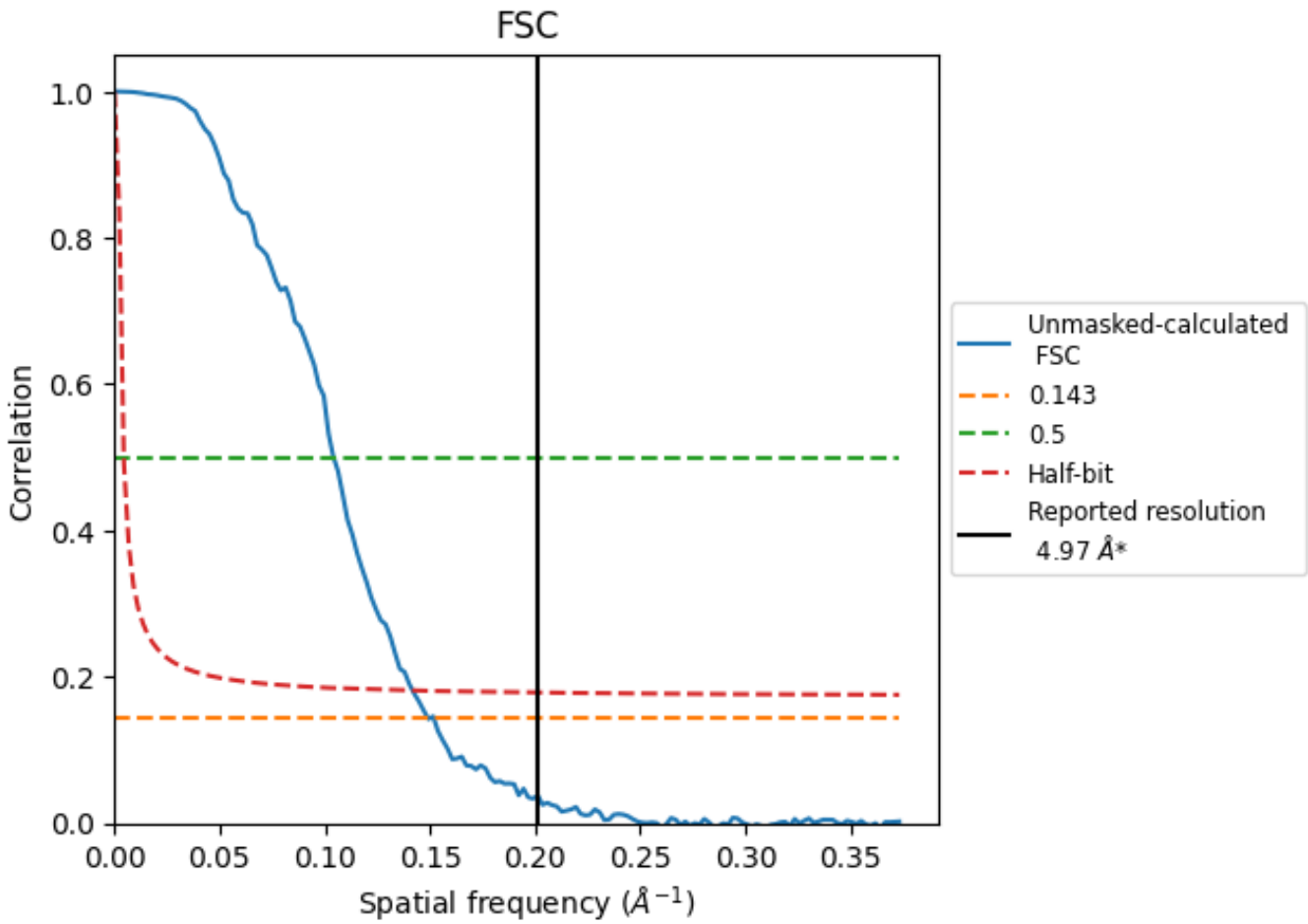


*Reported resolution corresponds to spatial frequency of 0.201 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.201 Å^{-1}

8.2 Resolution estimates (i)

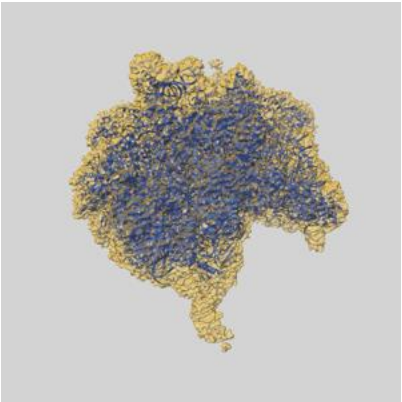
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.97	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.71	9.60	7.06

*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 6.71 differs from the reported value 4.97 by more than 10 %

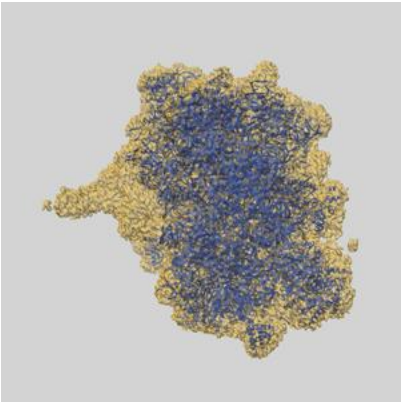
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3553 and PDB model 5MRF. Per-residue inclusion information can be found in section 3 on page 19.

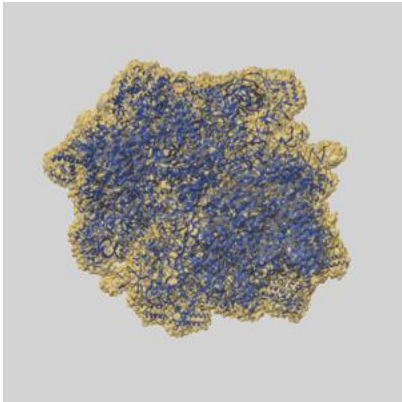
9.1 Map-model overlay (i)



X



Y



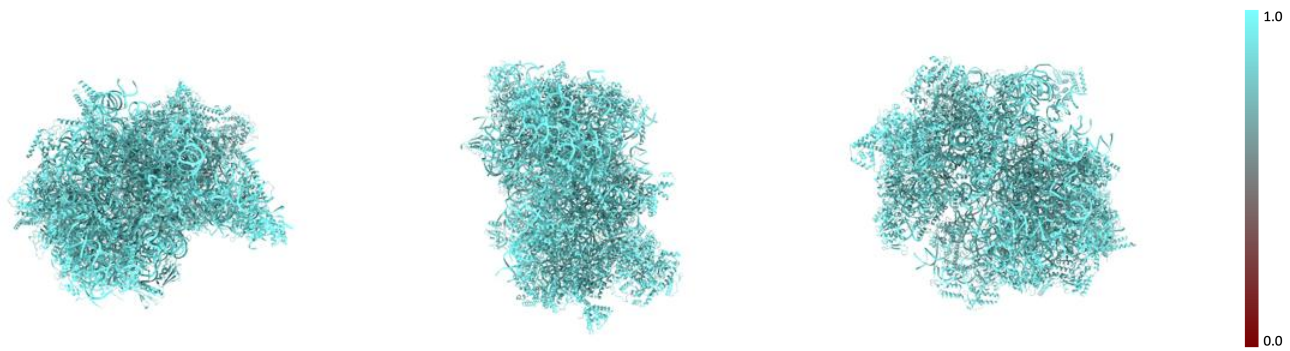
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0123 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)

This section was not generated.

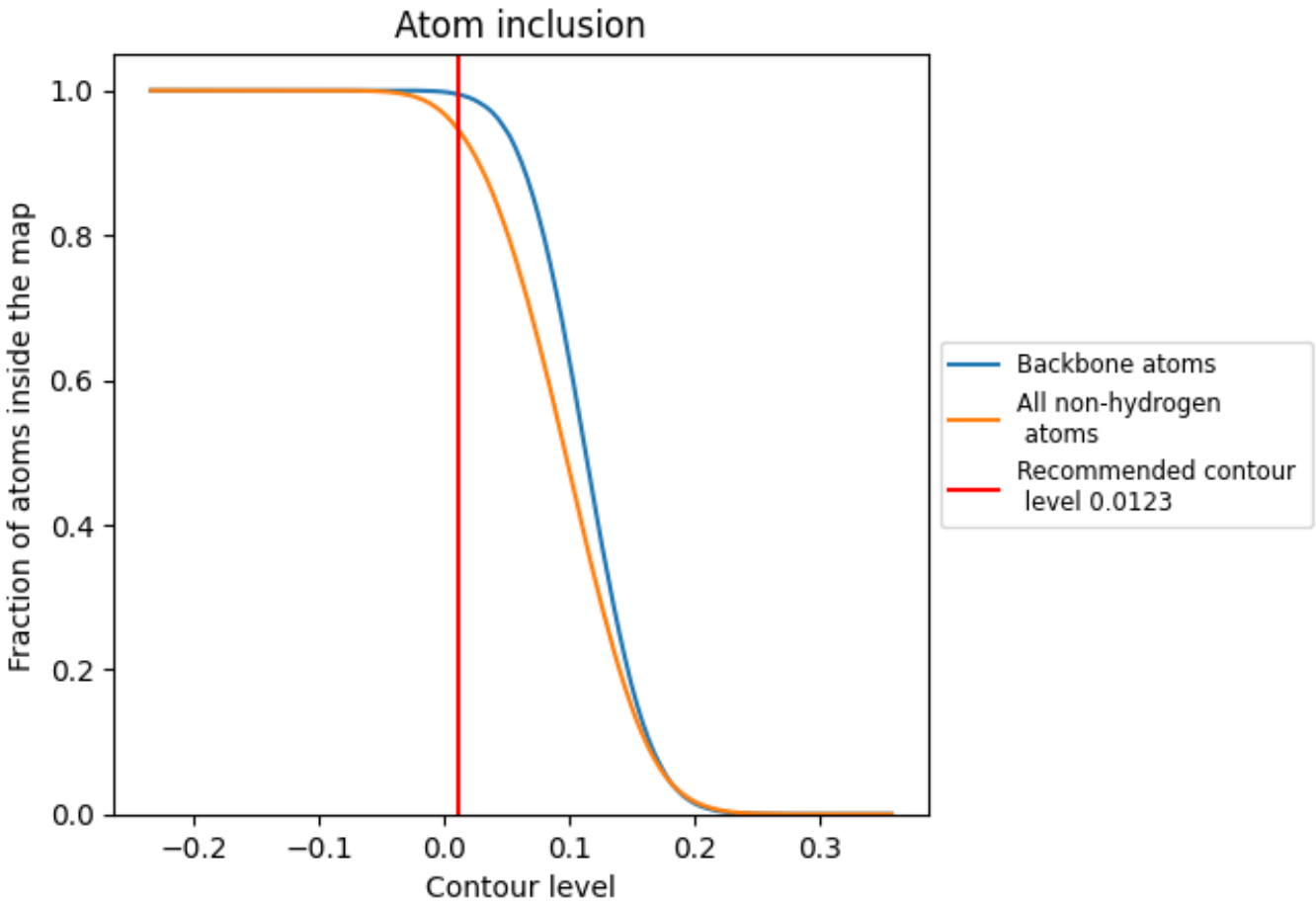
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0123).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0123) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.9440
0	0.9103
1	0.9352
11	0.7965
2	0.9064
22	0.9289
3	0.9283
33	0.9221
4	0.8882
44	0.9413
5	0.9146
55	0.8952
6	0.9245
66	0.9131
7	0.9181
77	0.9049
8	0.9151
88	0.8621
9	0.9395
A	0.9876
AA	0.8992
B	0.8919
BB	0.9035
C	0.9171
CC	0.9105
D	0.8889
DD	0.9236
E	0.8954
EE	0.9008
F	0.9175
FF	0.8611
G	0.9025
GG	0.8756
H	0.8919
HH	0.8716

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Chain	Atom inclusion
I	0.8794
II	0.9086
J	0.9126
JJ	0.8935
K	0.9093
KK	0.9065
L	0.8903
LL	0.9032
M	0.9137
MM	0.8958
N	0.8937
NN	0.9136
O	0.8978
OO	0.8688
P	0.9192
PP	0.9102
Q	0.9081
QQ	0.8996
R	0.9267
RR	0.9171
S	0.9015
SS	0.9114
T	0.9007
TT	0.8832
U	0.8947
UU	0.9034
V	0.9203
VV	0.9121
W	0.8992
WW	0.9214
X	0.8893
XX	0.9352
Y	0.8645
YY	0.9294
Z	0.8852
ZZ	0.9030
a	0.9392
aa	0.9880
b	0.9247
bb	0.9381
c	0.9119
cc	0.9702

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Chain	Atom inclusion
d	0.9156
dd	0.9709