Full wwPDB EM Validation Report (i)

Dec 19, 2022 – 01:13 pm GMT

PDB ID	:	6YXX
EMDB ID	:	EMD-10999
Title	:	State A of the Trypanosoma brucei mitoribosomal large subunit assembly intermediate
Authors	:	Jaskolowski, M.; Ramrath, D.J.F.; Bieri, P.; Niemann, M.; Mattei, S.; Calderaro, S.; Leibundgut, M.A.; Horn, E.K.; Boehringer, D.; Schneider, A.; Ban, N.
Deposited on	:	2020-05-04
Resolution	:	3.90 Å(reported)

This is a Full wwPDB EM Validation 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:

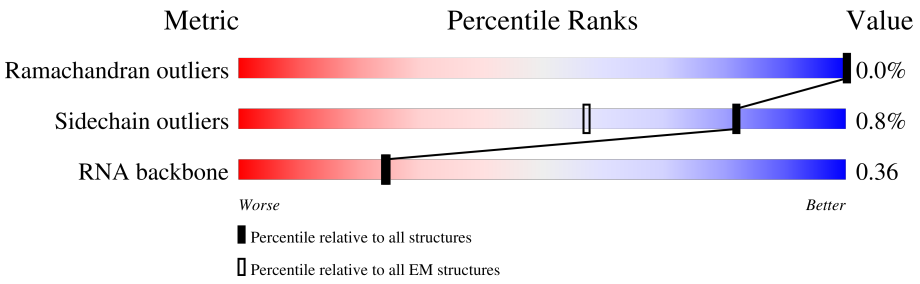
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A1	241	6% 89% • 10%
2	E1	482	14% 97% • •
3	A2	471	• 98% •
4	E2	568	8% 65% 35%
5	A3	218	69% 31%
6	E3	557	6% 72% 28%
7	E4	439	5% 96% • •
8	A5	80	68% • 31%

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Mol	Chain	Length	Quality of chain
9	E5	376	8% 87% 13%
10	E6	531	6% 81% 18%
11	A8	181	73% 27%
12	AA	1176	13% 50% 27% 23%
13	BA	831	92% 7%
14	EA	576	10% 92% 8%
15	UA	10	10% 100%
15	Uf	10	50% 100%
16	BB	541	75% 25%
17	EB	754	82% 17%
18	EC	406	91% 8%
19	BD	547	14% 76% 23%
20	ED	616	97%
21	AE	473	73% 27%
22	BE	449	79% 20%
23	EE	586	7% 73% 26%
24	AF	459	91% 9%
25	BF	426	81% 19%
26	EF	373	53% 79% 20%
27	EG	156	99%
28	BH	349	9% 67% 32%
29	EH	634	69% 30%
30	AI	263	10% 91% 9%
31	BI	342	88% 11%
32	UI	21	95% 100%

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Mol	Chain	Length	Quality of chain
32	Ur	21	100% / 100%
33	BJ	333	70% / 30%
34	AK	342	11% / 71% / 27%
35	BK	386	7% / 59% / 41%
36	UK	25	44% / 100%
37	BL	312	82% / 17%
38	EL	691	76% / 23%
39	EM	451	12% / 68% / 32%
40	UM	8	12% / 100%
41	AN	202	96%
42	BN	302	51% / 49%
43	EN	731	6% / 86% / 13%
44	BO	262	73% / 27%
45	EO	319	8% / 85% / 15%
45	EP	319	8% / 76% / 24%
46	AP	374	5% / 84% / 14%
47	BQ	231	6% / 94% / 6%
48	AR	301	88% / 11%
49	BR	205	94%
50	ER	148	56% / 43%
51	BS	198	7% / 79% / 19%
52	ES	524	29% / 71%
53	AT	144	98%
54	BT	191	91% / 9%
55	ET	102	99%

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Mol	Chain	Length	Quality of chain
56	AU	213	82% 18%
57	BU	185	8% 81% 19%
58	AV	188	95%
59	BV	190	26% 46% 53%
60	AW	278	99%
61	BW	188	98%
62	AX	246	67% 33%
63	AY	378	90% 10%
64	BZ	190	6% 99%
65	Ba	153	11% 99%
66	Bb	162	81% 18%
67	Bc	146	20% 91% 6%
68	Ae	197	64% 36%
69	Af	189	73% 26%
70	Bf	113	19% 75% 23%
71	Ag	260	72% 28%
72	E7	97	19% 100%
73	E8	786	8% 19% 80%
74	E9	343	14% 58% 42%
75	Al	218	83% 17%
76	Ul	238	39% 100%
77	Um	27	30% 100%
78	Un	28	11% 100%
79	Ao	1520	12% 88%
80	Ap	309	5% 84% 15%

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Mol	Chain	Length	Quality of chain
81	Up	87	99% / 100%
82	Us	79	97% / 100%
83	At	154	89% / 10%
84	Av	242	79% / 21%

2 Entry composition (i)

There are 92 unique types of molecules in this entry. The entry contains 183043 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A1	217	1788	1138	324	317	9	0	0

- Molecule 2 is a protein called mt-LAF21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E1	473	3836	2376	745	703	12	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E1	379	SER	ALA	conflict	UNP Q57WG6

- Molecule 3 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A2	463	3739	2381	651	694	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	238	GLY	ALA	conflict	UNP Q38EM7

- Molecule 4 is a protein called DUF4379 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E2	369	2933	1839	550	517	27	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E2	167	THR	LYS	conflict	UNP C9ZTN9

- Molecule 5 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A3	150	1226	781	236	203	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	198	UNK	ALA	conflict	UNP C9ZY77

- Molecule 6 is a protein called mt-LAF23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E3	403	3266	2062	590	591	23	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E3	1	MET	-	initiating methionine	UNP D0A795

- Molecule 7 is a protein called mt-LAF24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	E4	434	3418	2159	623	622	14	0	0

- Molecule 8 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A5	55	483	311	90	76	6	0	0

- Molecule 9 is a protein called mt-LAF25.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	E5	327	1635	981	327	327	0	0

- Molecule 10 is a protein called KRIPP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	E6	434	3405	2143	608	635	19	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E6	360	SER	ALA	conflict	UNP Q4GZA2

- Molecule 11 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A8	133	1136	712	233	184	7	0	0

- Molecule 12 is a RNA chain called 12S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	AA	904	18187	8161	2902	6220	904	0	0

- Molecule 13 is a protein called mL67.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	BA	769	6059	3847	1074	1104	34	0	0

- Molecule 14 is a protein called mt-EngA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	EA	532	4263	2672	785	785	21	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EA	12	UNK	ARG	conflict	UNP Q57TZ4

- Molecule 15 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	UA	10	50	30	10	10	0	0
15	Uf	10	50	30	10	10	0	0

- Molecule 16 is a protein called mL68.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	BB	407	3322	2114	589	599	20	0	0

- Molecule 17 is a protein called DEAD-box helicase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	EB	627	5039	3181	957	875	26	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EB	301	ALA	THR	conflict	UNP D0A9G9

- Molecule 18 is a protein called Pseudouridylate synthase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	EC	373	3005	1923	540	524	18	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EC	25	UNK	HIS	conflict	UNP Q38FJ3

- Molecule 19 is a protein called mL70.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	BD	419	3349	2134	586	609	20	0	0

- Molecule 20 is a protein called mt-LAF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	ED	598	4764	3026	850	865	23	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ED	252	ARG	LYS	conflict	UNP Q385G9

- Molecule 21 is a protein called Ribosomal protein L3 mitochondrial, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	AE	344	2802	1804	474	509	15	0	0

- Molecule 22 is a protein called mL71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	BE	357	2822	1801	477	535	9	0	0

- Molecule 23 is a protein called SpoU_methylase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	EE	431	3423	2132	646	632	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	337	ASP	GLY	conflict	UNP C9ZZ65

- Molecule 24 is a protein called Ribosomal protein L4/L1 family, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	AF	419	3414	2181	584	626	23	0	0

- Molecule 25 is a protein called Tetratricopeptide repeat.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	BF	346	2847	1803	519	512	13	0	0

- Molecule 26 is a protein called SpoU_methylase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	EF	297	2268	1439	401	420	8	0	0

- Molecule 27 is a protein called mt-LAF7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	EG	154	1295	812	256	218	9	0	0

- Molecule 28 is a protein called mL74.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BH	236	1948	1250	346	349	3	0	0

- Molecule 29 is a protein called mt-LAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	EH	443	3508	2214	635	640	19	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EH	166	UNK	GLY	conflict	UNP A0A1G4IEQ9
EH	495	ARG	LYS	conflict	UNP A0A1G4IEQ9

- Molecule 30 is a protein called RIBOSOMAL_L9 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	AI	240	1967	1260	345	353	9	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	249	UNK	LYS	conflict	UNP Q57UC5
AI	250	UNK	GLY	conflict	UNP Q57UC5
AI	251	UNK	PRO	conflict	UNP Q57UC5
AI	252	UNK	VAL	conflict	UNP Q57UC5

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Chain	Residue	Modelled	Actual	Comment	Reference
AI	253	UNK	LYS	conflict	UNP Q57UC5
AI	254	UNK	GLN	conflict	UNP Q57UC5
AI	255	UNK	ARG	conflict	UNP Q57UC5
AI	256	UNK	LYS	conflict	UNP Q57UC5
AI	257	UNK	ALA	conflict	UNP Q57UC5
AI	258	UNK	ARG	conflict	UNP Q57UC5

- Molecule 31 is a protein called mL75.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	BI	303	2475	1580	447	433	15	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BI	227	ASN	ASP	conflict	UNP D0A108

- Molecule 32 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	UI	21	105	63	21	21	0	0
32	Ur	21	105	63	21	21	0	0

- Molecule 33 is a protein called mL76.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	BJ	234	1944	1215	365	356	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BJ	329	GLU	ALA	conflict	UNP Q383M2

- Molecule 34 is a protein called Ribosomal protein L11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	AK	248	2088	1335	385	356	12	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	327	UNK	ALA	conflict	UNP Q586R9

- Molecule 35 is a protein called Chaperone protein DNAj, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	BK	228	1855	1153	353	341	8	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	33	UNK	HIS	conflict	UNP C9ZQR6
BK	60	UNK	PRO	conflict	UNP C9ZQR6
BK	348	VAL	LEU	conflict	UNP C9ZQR6

- Molecule 36 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	UK	25	125	75	25	25	0	0

- Molecule 37 is a protein called mL78.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	BL	258	2014	1236	395	373	10	0	0

- Molecule 38 is a protein called mt-LAF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	EL	532	4259	2732	744	754	29	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EL	104	UNK	ILE	conflict	UNP C9ZVC0
EL	108	GLU	GLY	conflict	UNP C9ZVC0
EL	126	VAL	LEU	conflict	UNP C9ZVC0
EL	188	SER	PHE	conflict	UNP C9ZVC0

- Molecule 39 is a protein called GTP-binding protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	EM	308	2432	1542	438	437	15	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EM	407	UNK	PRO	conflict	UNP Q38E75

- Molecule 40 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	UM	8	40	24	8	8	0	0

- Molecule 41 is a protein called 50S ribosomal protein L13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	AN	193	1639	1059	301	269	10	0	0

- Molecule 42 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	BN	154	1320	839	239	237	5	0	0

- Molecule 43 is a protein called mt-LAF14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	EN	638	5025	3152	909	936	28	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EN	18	GLU	GLY	conflict	UNP C9ZPS0
EN	310	LYS	ASN	conflict	UNP C9ZPS0
EN	676	CYS	TYR	conflict	UNP C9ZPS0

- Molecule 44 is a protein called mL81.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	BO	192	1498	936	268	281	13	0	0

- Molecule 45 is a protein called mt-LAF15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	EO	272	2126	1340	393	383	10	0	0
45	EP	243	1911	1208	347	347	9	0	0

- Molecule 46 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	AP	320	2615	1667	478	457	13	0	0

- Molecule 47 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	BQ	218	1651	1049	288	306	8	0	0

- Molecule 48 is a protein called 50S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	AR	267	2214	1399	403	399	13	0	0

- Molecule 49 is a protein called mL84.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	BR	196	1659	1064	299	287	9	0	0

- Molecule 50 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	ER	84	669	427	106	135	1	0	0

- Molecule 51 is a protein called mL85.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	BS	161	1120	694	206	214	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BS	45	ILE	VAL	conflict	UNP Q38FG8
BS	173	UNK	LEU	conflict	UNP Q38FG8

- Molecule 52 is a protein called Lipase (Class 3).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	ES	152	1259	779	246	230	4	0	0

- Molecule 53 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	AT	143	1180	743	224	206	7	0	0

- Molecule 54 is a protein called mL86.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	BT	173	1435	884	278	267	6	0	0

- Molecule 55 is a protein called mt-LAF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	ET	101	839	529	166	140	4	0	0

- Molecule 56 is a protein called bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	AU	175	1423	895	280	243	5	0	0

- Molecule 57 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	BU	150	1275	806	248	215	6	0	0

- Molecule 58 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	AV	181	1424	909	257	252	6	0	0

- Molecule 59 is a protein called mL88.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	BV	90	763	492	133	136	2	0	0

- Molecule 60 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	AW	278	2251	1427	417	393	14	0	0

- Molecule 61 is a protein called mL89.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	BW	188	1565	992	299	265	9	0	0

- Molecule 62 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	AX	164	1387	896	244	242	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	126	TYR	HIS	conflict	UNP Q387G3

- Molecule 63 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	AY	340	2790	1741	497	537	15	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	345	GLU	VAL	conflict	UNP C9ZK52

- Molecule 64 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	BZ	188	1396	883	241	266	6	0	0

- Molecule 65 is a protein called mL93.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	Ba	153	1287	820	237	223	7	0	0

- Molecule 66 is a protein called mL94.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	Bb	133	1048	661	196	188	3	0	0

- Molecule 67 is a protein called mL95.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	Bc	137	1194	776	216	201	1	0	0

- Molecule 68 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	Ae	127	1031	667	190	169	5	0	0

- Molecule 69 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	Af	139	1107	692	210	200	5	0	0

- Molecule 70 is a protein called mL98.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
70	Bf	87	725	462	131	132	0	0

- Molecule 71 is a protein called L51_S25_CI-B8 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	Ag	186	1564	979	295	283	7	0	0

- Molecule 72 is a protein called mt-LAF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	E7	97	815	501	175	135	4	0	0

- Molecule 73 is a protein called KRIPP9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
73	E8	154	1181	735	228	218	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E8	208	LYS	GLU	conflict	UNP Q57YZ6
E8	250	GLN	ARG	conflict	UNP Q57YZ6
E8	345	ILE	MET	conflict	UNP Q57YZ6
E8	630	UNK	LEU	conflict	UNP Q57YZ6

- Molecule 74 is a protein called mt-LAF29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	E9	200	1642	1022	326	285	9	0	0

- Molecule 75 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	Al	181	1440	936	250	247	7	0	0

- Molecule 76 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
76	Ul	238	1190	714	238	238	0	0

- Molecule 77 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
77	Um	27	135	81	27	27	0	0

- Molecule 78 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
78	Un	28	140	84	28	28	0	0

- Molecule 79 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	Ao	184	1443	903	263	270	7	0	0

- Molecule 80 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	Ap	263	2161	1402	374	373	12	0	0

- Molecule 81 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
81	Up	87	435	261	87	87	0	0

- Molecule 82 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
82	Us	79	395	237	79	79	0	0

- Molecule 83 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	At	138	1149	722	223	200	4	0	0

- Molecule 84 is a protein called mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	Av	192	1633	1038	304	279	12	0	0

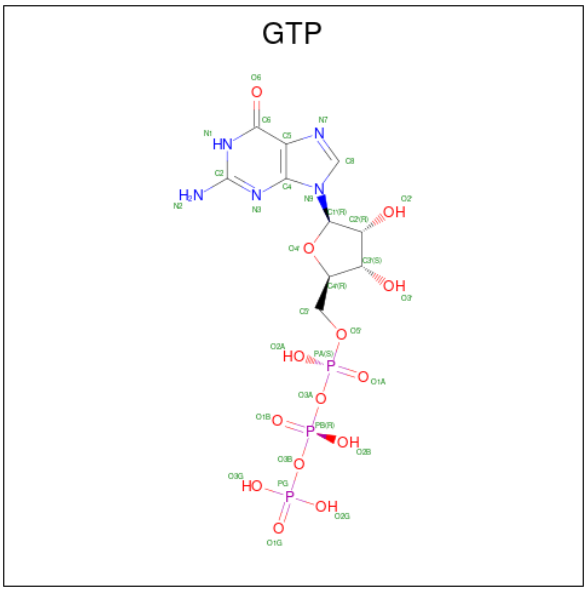
- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
85	E2	4	4	4	0
85	A5	1	1	1	0
85	EG	1	1	1	0
85	E9	1	1	1	0

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
86	A8	2	2	2	0
86	AA	12	12	12	0
86	EA	2	2	2	0
86	EB	1	1	1	0

- Molecule 87 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

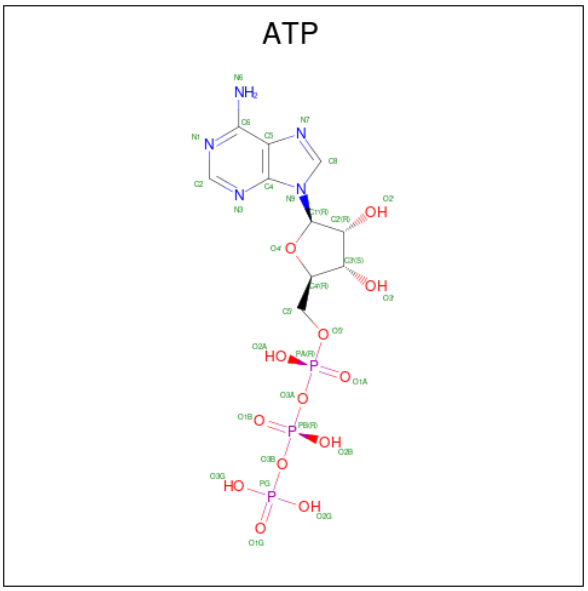


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
87	EA	1	64	20	10	28	6	0
			Total	C	N	O	P	
87	EA	1	64	20	10	28	6	0

- Molecule 88 is SODIUM ION (three-letter code: NA) (formula: Na).

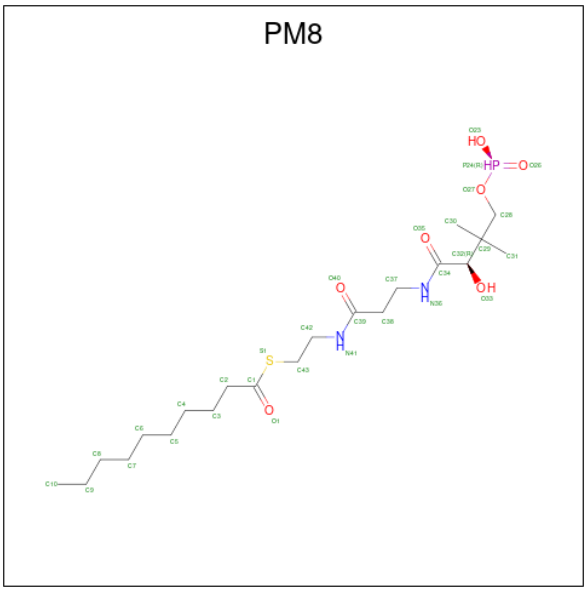
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
88	EA	2	2	2	0

- Molecule 89 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

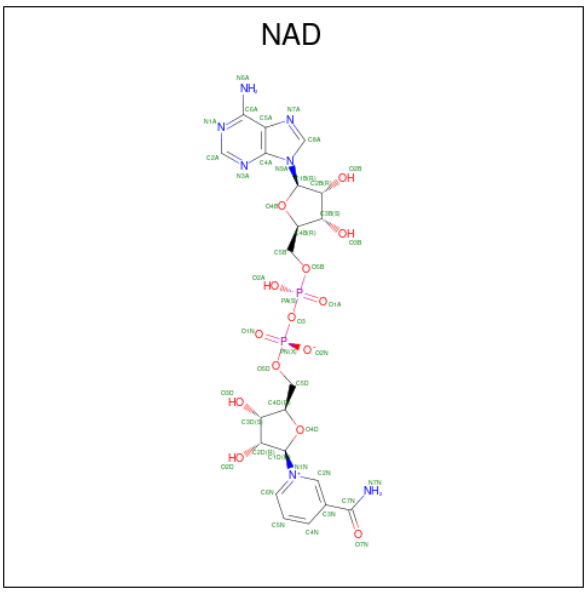
- Molecule 90 is S-(2-{[N-(2-HYDROXY-4-{[HYDROXY(OXIDO)PHOSPHINO]OXY}-3,3-DIMETHYLBUTANOYL)-BETA-ALANYL]AMINO}ETHYL) DECANETHIOATE (three-letter code: PM8) (formula: $C_{21}H_{41}N_2O_7PS$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
90	ER	1	32	21	2	7	1	1	0

- Molecule 91 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD)

(formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
91	Av	1	44	21	7	14	2	0

- Molecule 92 is water.

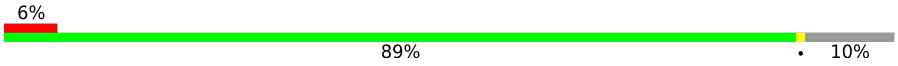
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
92	EA	4	4	4	0
			Total	O	
92	EB	4	4	4	0

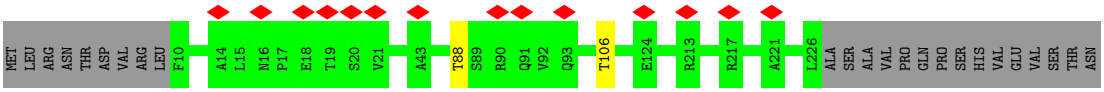
3 Residue-property plots (i)

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: bL28m

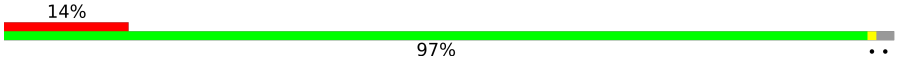
Chain A1:

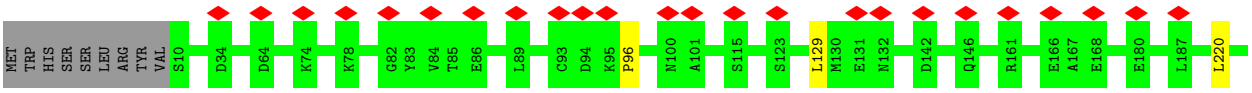


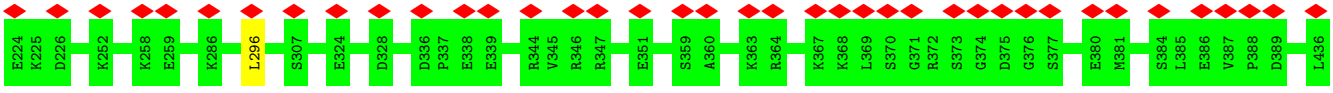


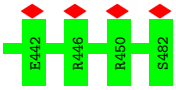
- Molecule 2: mt-LAF21

Chain E1:



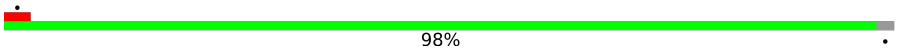


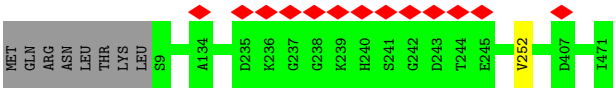




- Molecule 3: uL29m

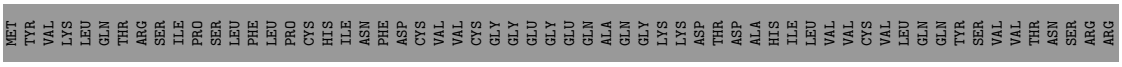
Chain A2:

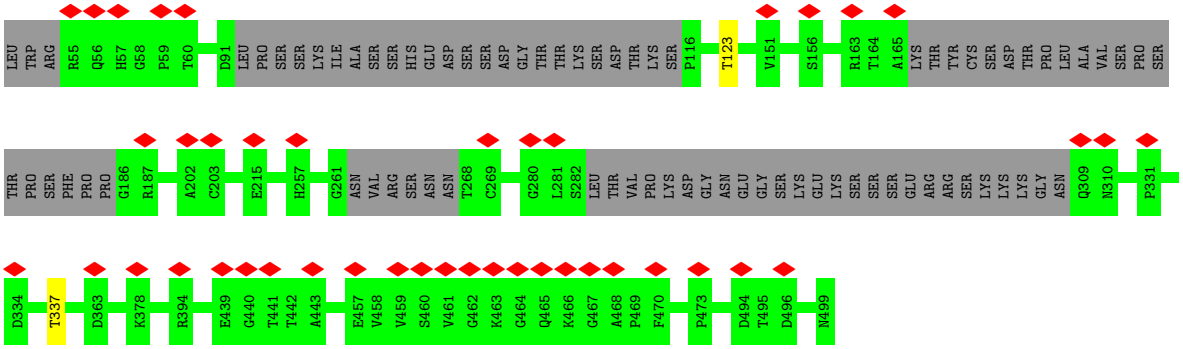




- Molecule 4: DUF4379 domain-containing protein

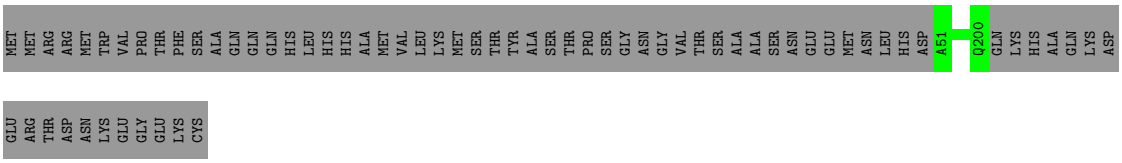
Chain E2:





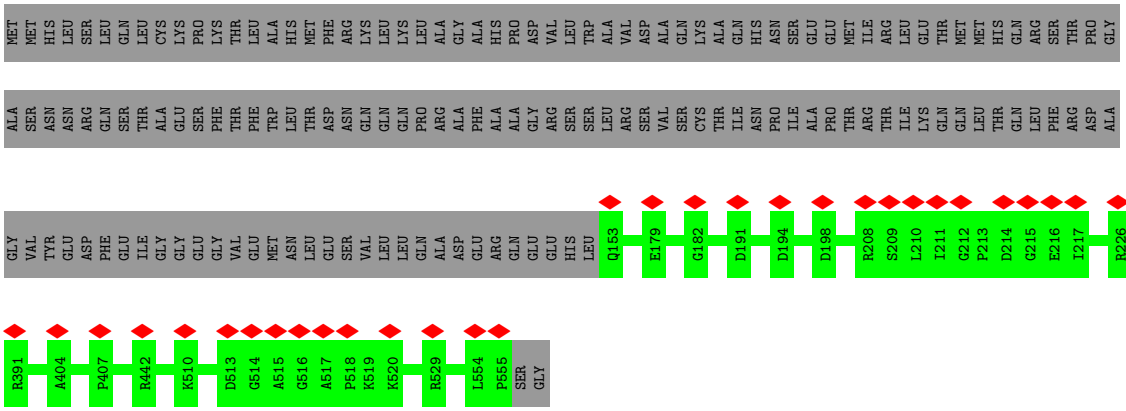
- Molecule 5: uL30m

Chain A3:



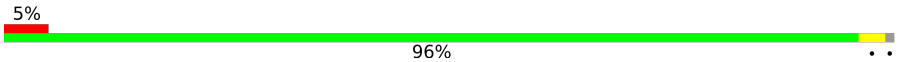
- Molecule 6: mt-LAF23

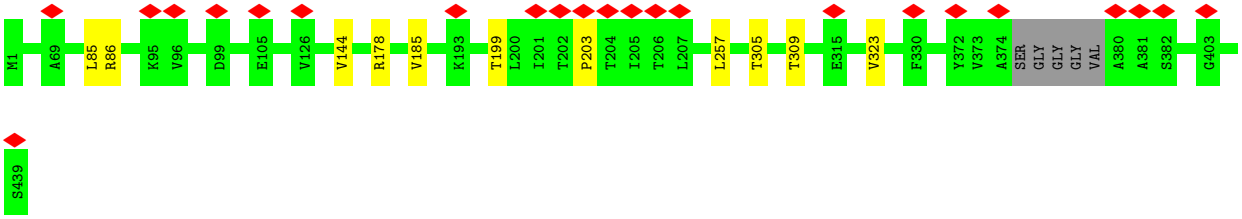
Chain E3:



- Molecule 7: mt-LAF24

Chain E4:



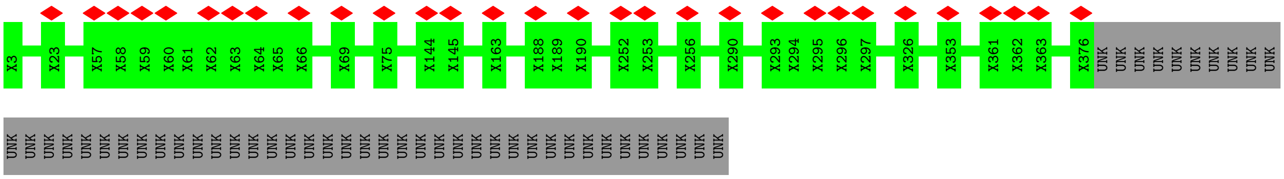


- Molecule 8: bL32m

Chain A5:

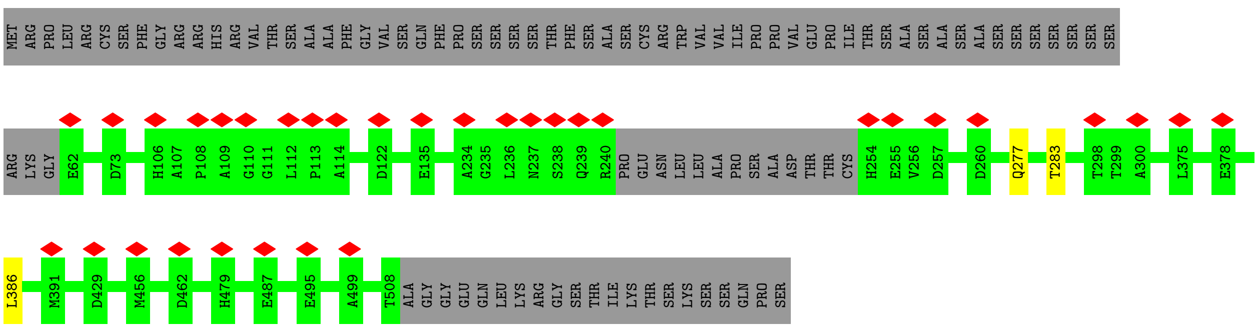
- Molecule 9: mt-LAF25

Chain E5:



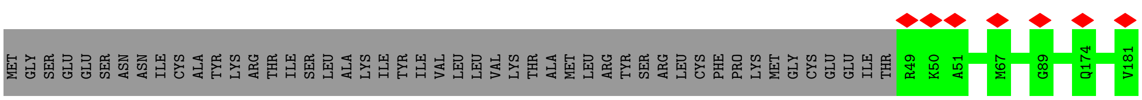
- Molecule 10: KRIPP3

Chain E6:



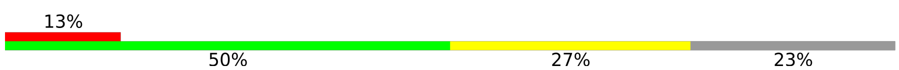
- Molecule 11: bL35m

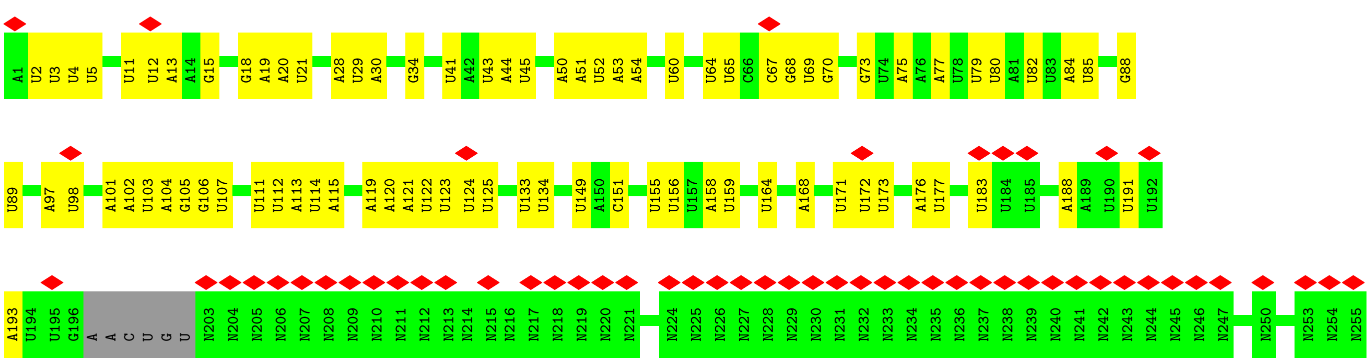
Chain A8:

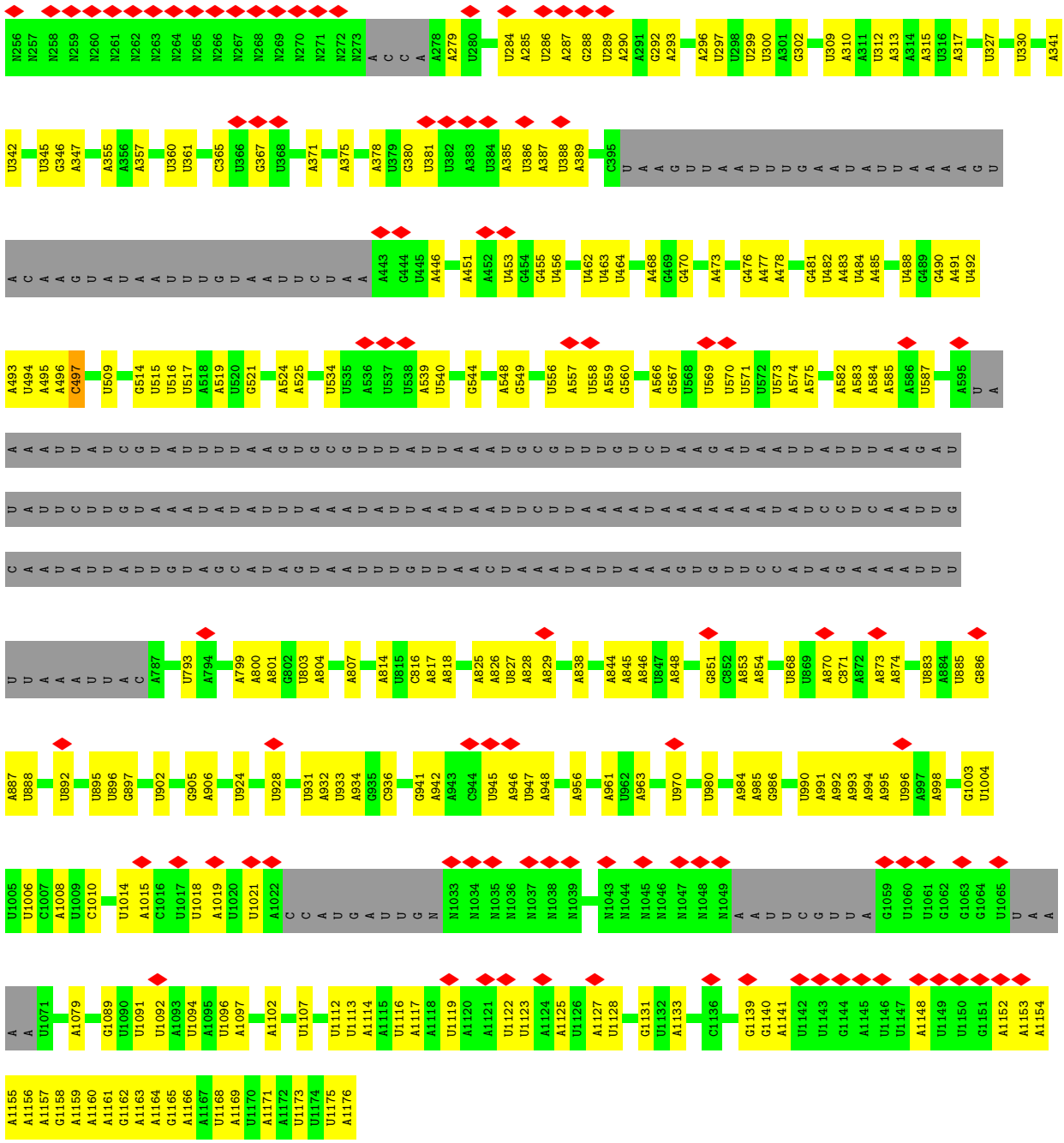


- Molecule 12: 12S ribosomal RNA

Chain AA:

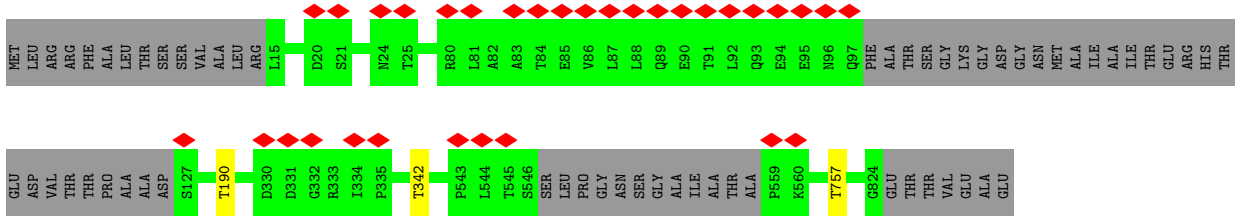






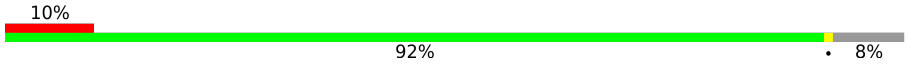
• Molecule 13: mL67

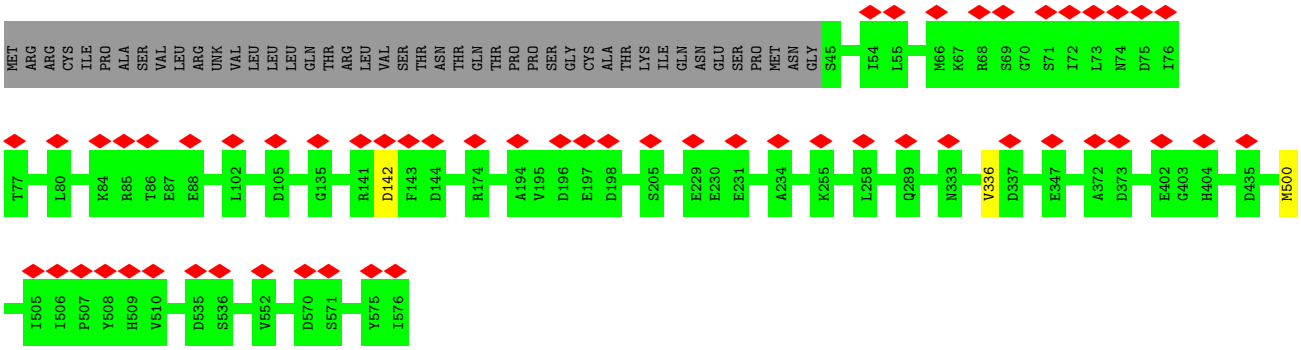
Chain BA: 92% 7%



• Molecule 14: mt-EngA

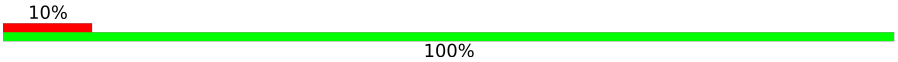
Chain EA:





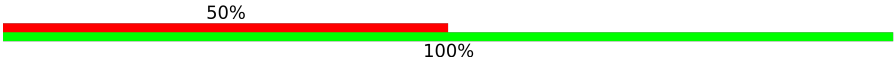
- Molecule 15: UNK

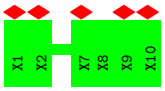
Chain UA:



- Molecule 15: UNK

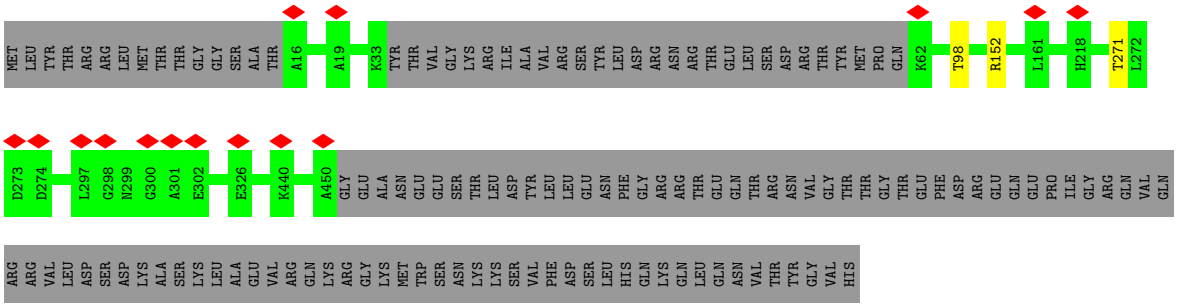
Chain Uf:





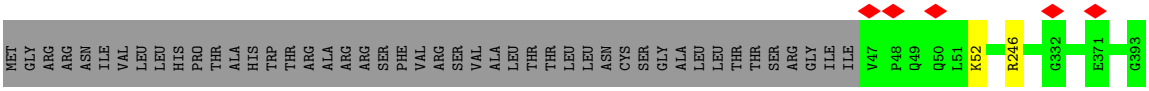
- Molecule 16: mL68

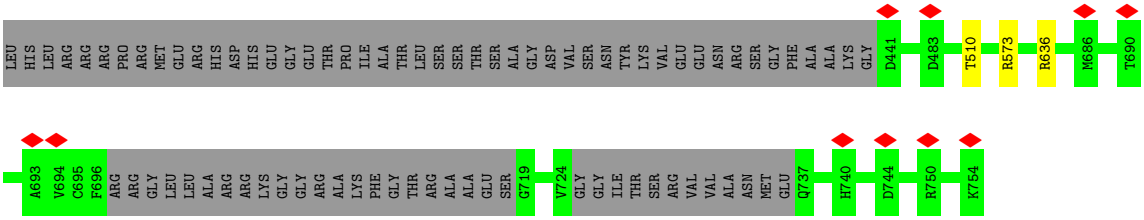
Chain BB:



- Molecule 17: DEAD-box helicase, putative

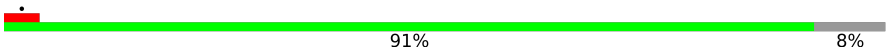
Chain EB:

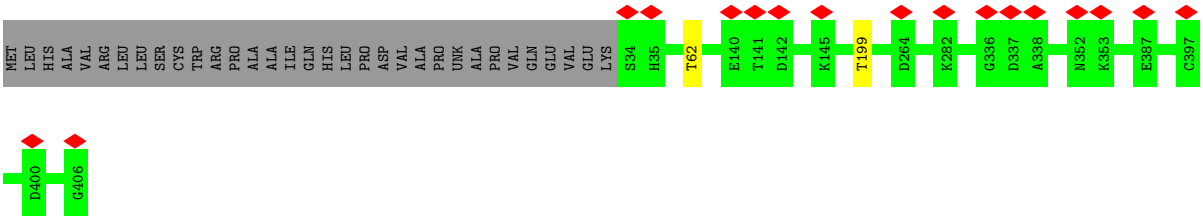




• Molecule 18: Pseudouridylate synthase, putative

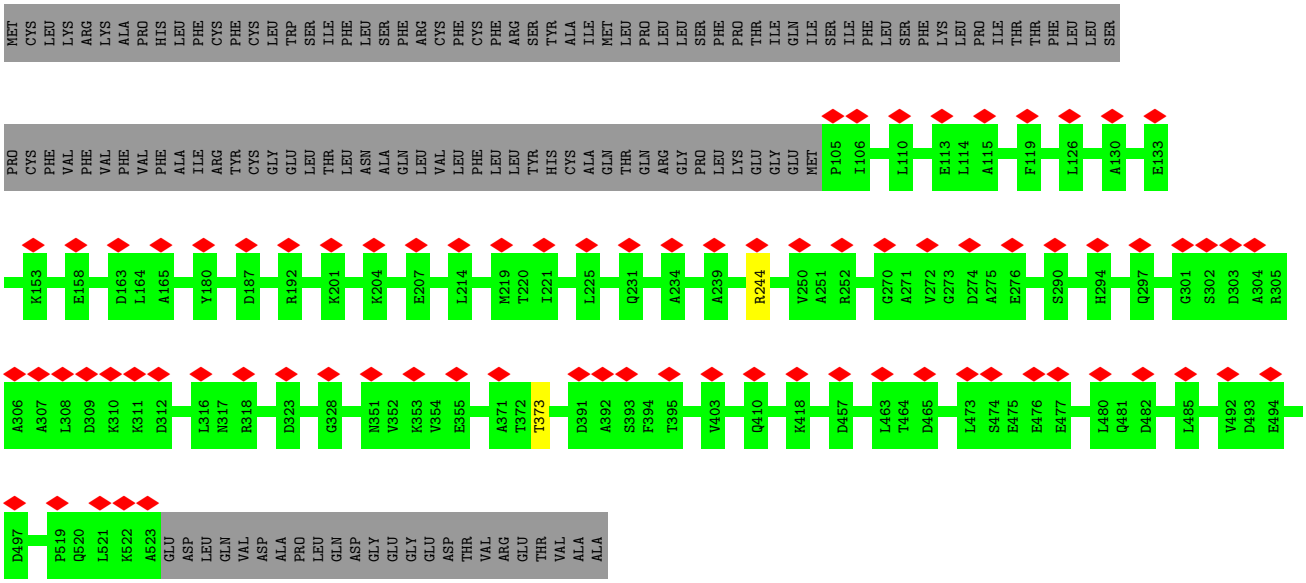
Chain EC:





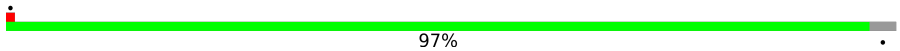
• Molecule 19: mL70

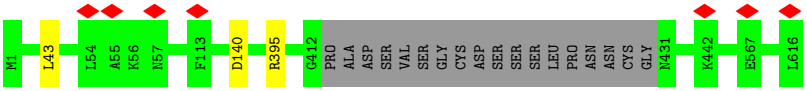
Chain BD:



• Molecule 20: mt-LAF4

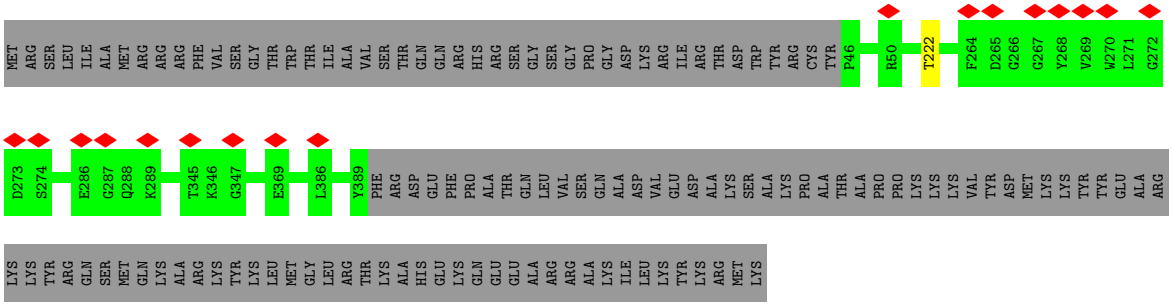
Chain ED:





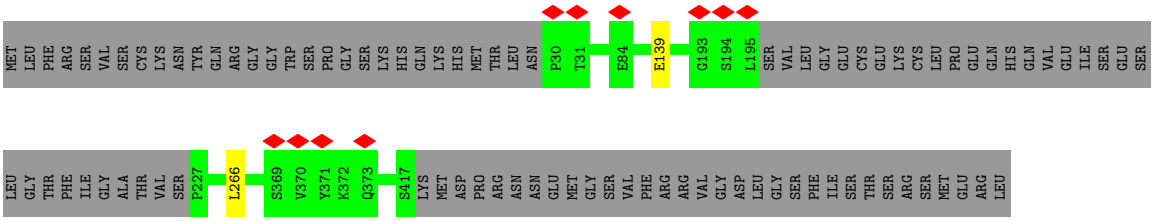
• Molecule 21: Ribosomal protein L3 mitochondrial, putative

Chain AE:



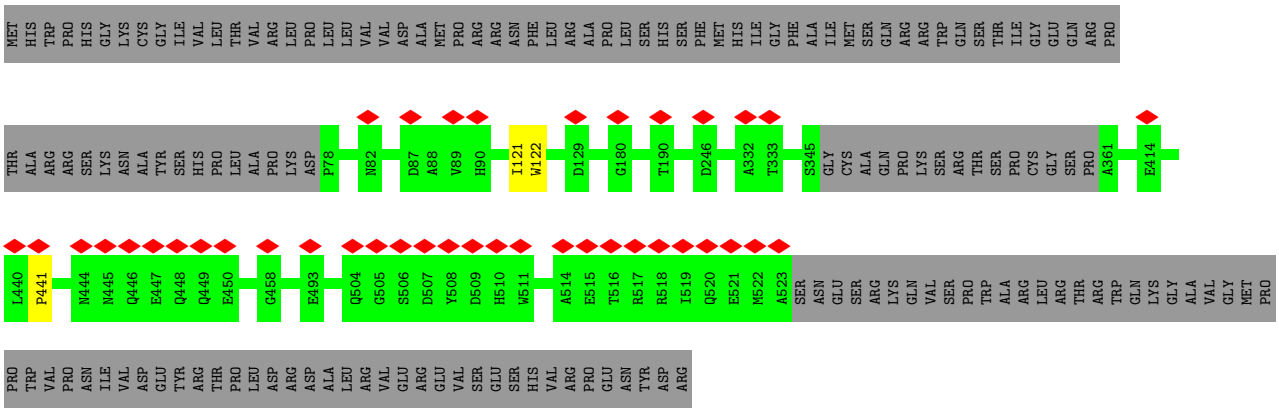
• Molecule 22: mL71

Chain BE:



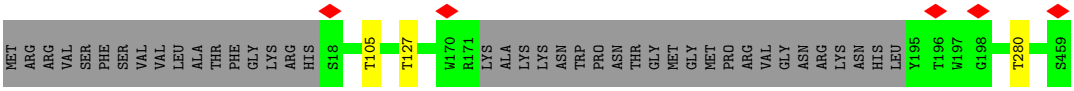
• Molecule 23: SpoU_methylase domain-containing protein

Chain EE:



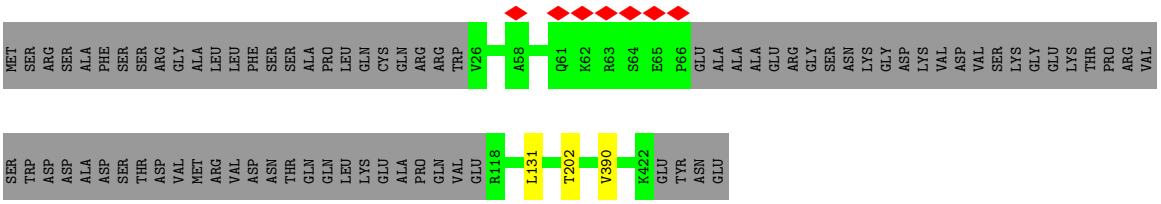
• Molecule 24: Ribosomal protein L4/L1 family, putative

Chain AF:



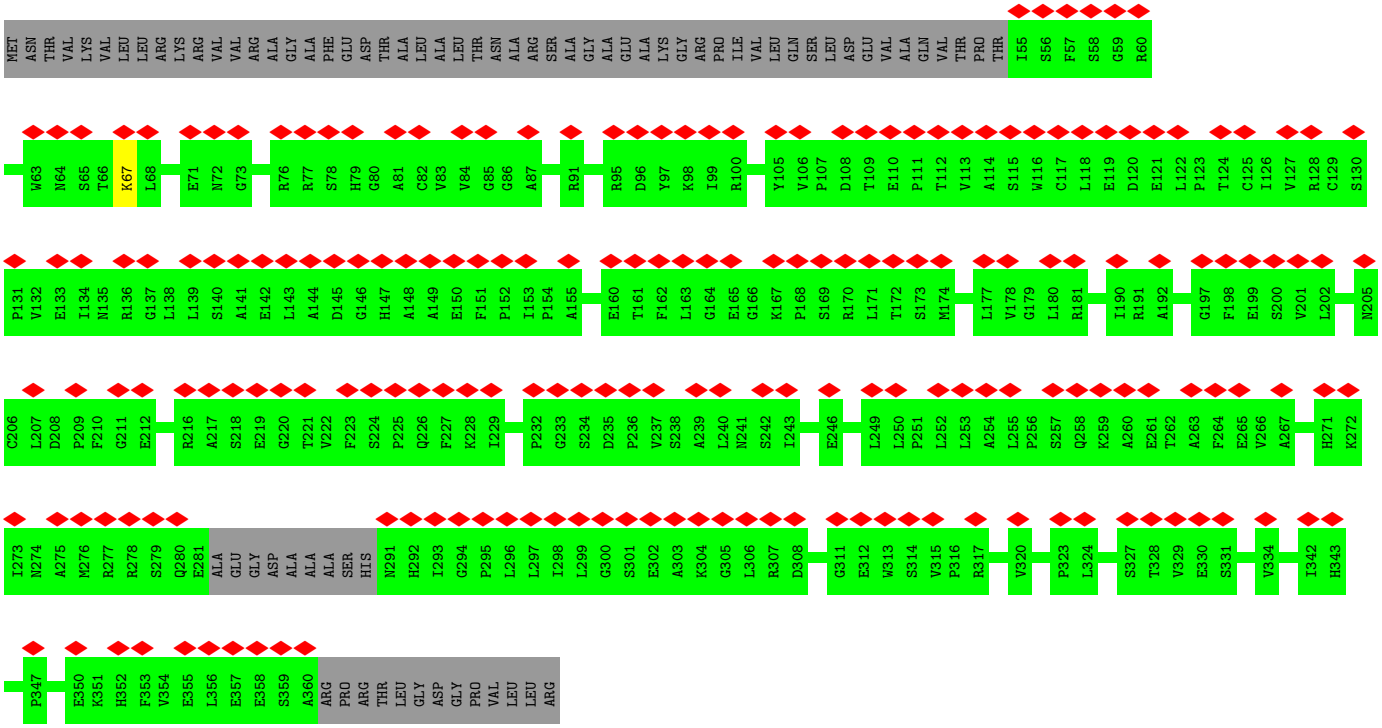
• Molecule 25: Tetratricopeptide repeat

Chain BF:



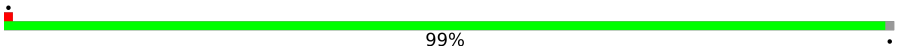
- Molecule 26: SpoU_methylase domain-containing protein

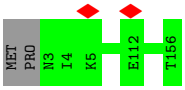
Chain EF:



- Molecule 27: mt-LAF7

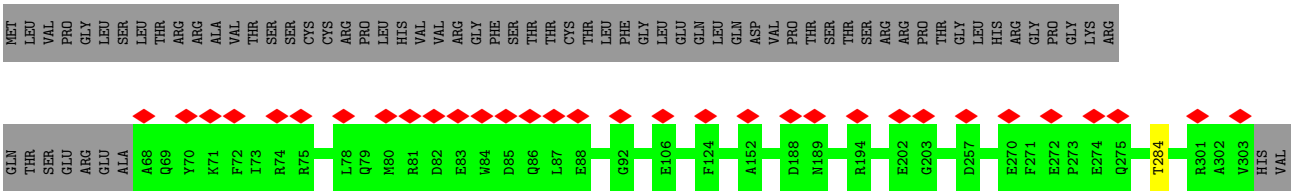
Chain EG:





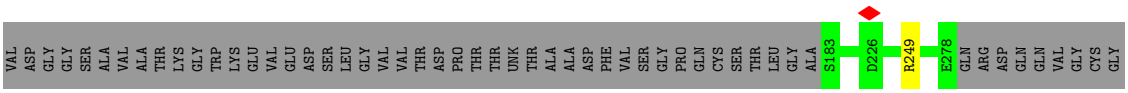
- Molecule 28: mL74

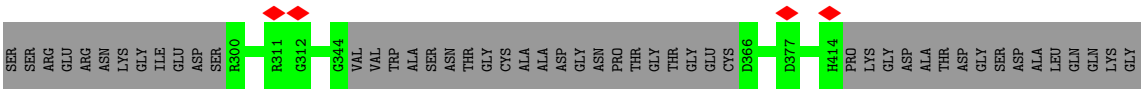
Chain BH:

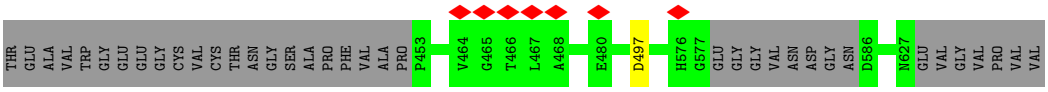


• Molecule 29: mt-LAF8

Chain EH:

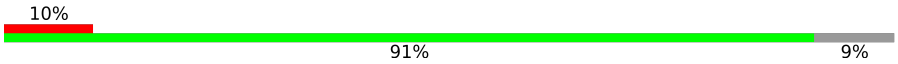


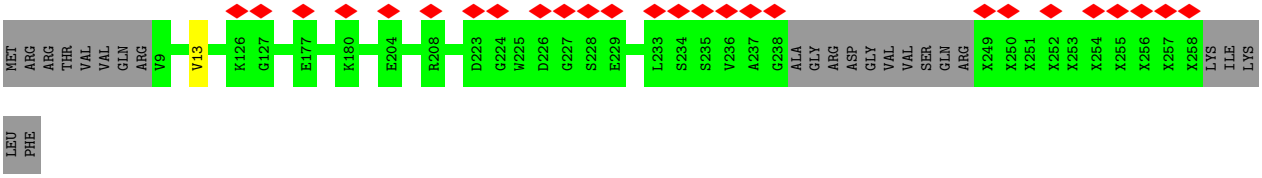




• Molecule 30: RIBOSOMAL_L9 domain-containing protein

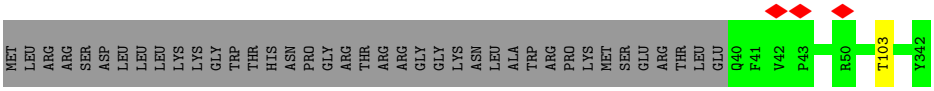
Chain AI:





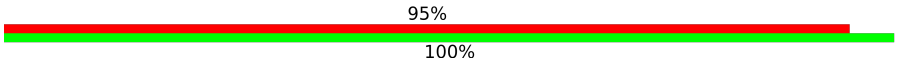
• Molecule 31: mL75

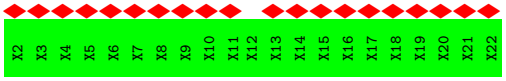
Chain BI:



• Molecule 32: UNK

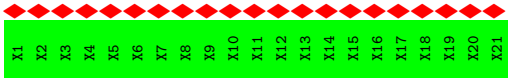
Chain UI:





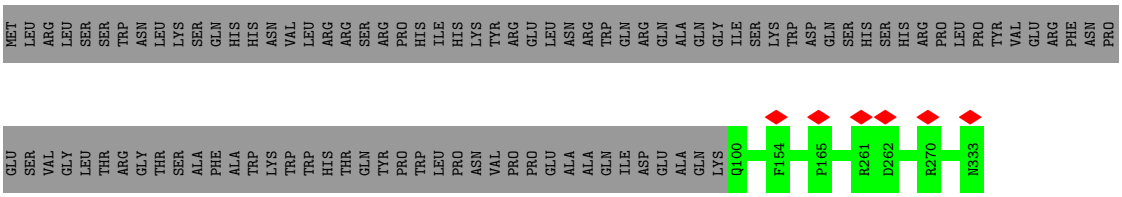
• Molecule 32: UNK

Chain Ur:



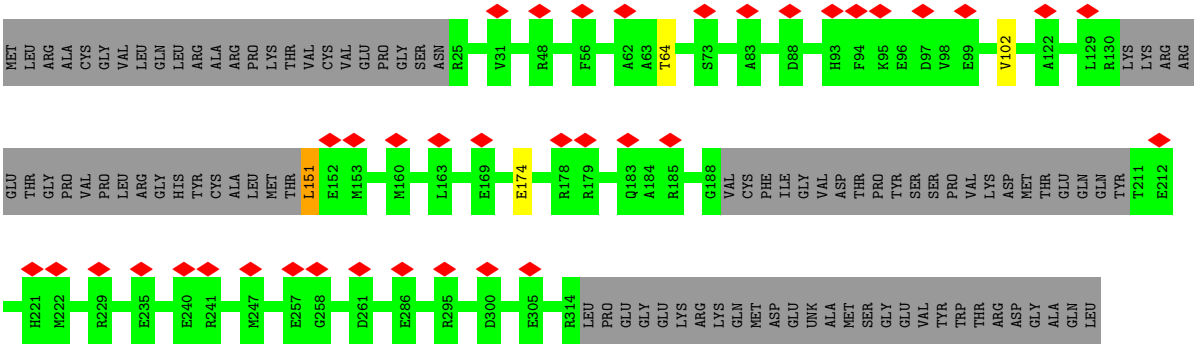
• Molecule 33: mL76

Chain BJ:



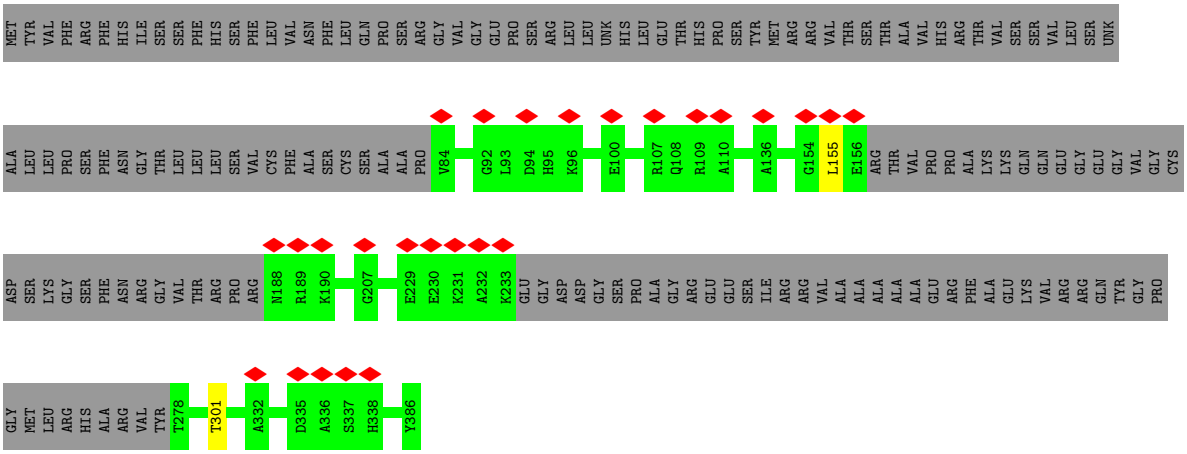
• Molecule 34: Ribosomal protein L11, putative

Chain AK:



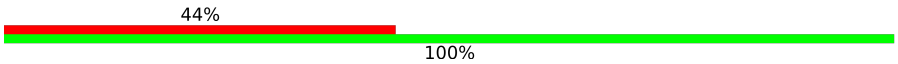
• Molecule 35: Chaperone protein DNAj, putative

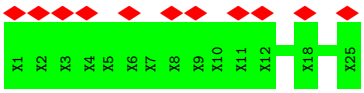
Chain BK:



• Molecule 36: UNK

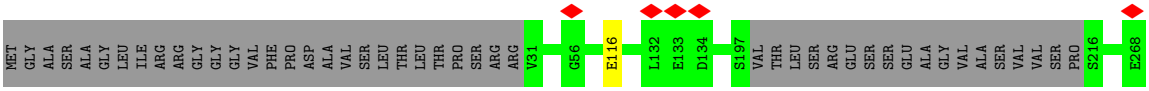
Chain UK:

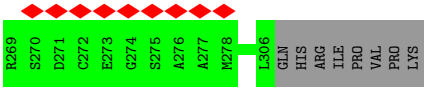




- Molecule 37: mL78

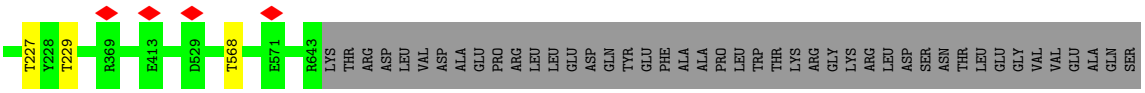
Chain BL:





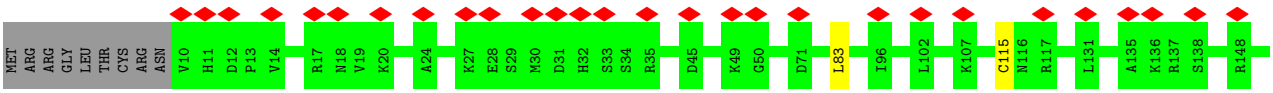
- Molecule 38: mt-LAF12

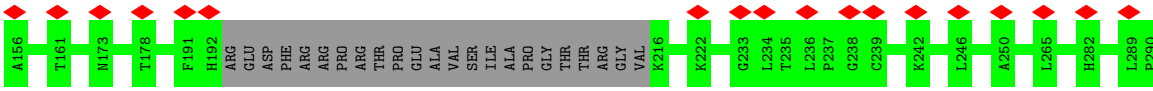
Chain EL:

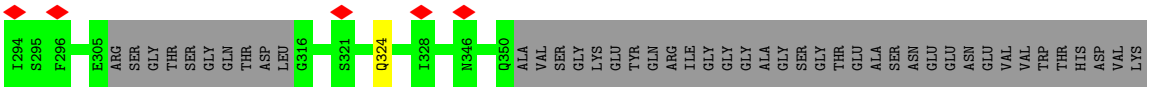


- Molecule 39: GTP-binding protein, putative

Chain EM:





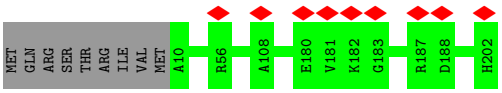


• Molecule 40: UNK

Chain UM: 12% 100%

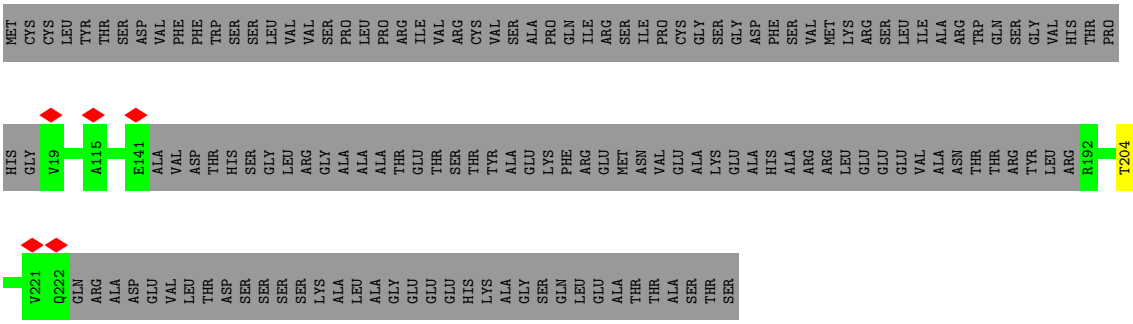
• Molecule 41: 50S ribosomal protein L13, putative

Chain AN: 96%



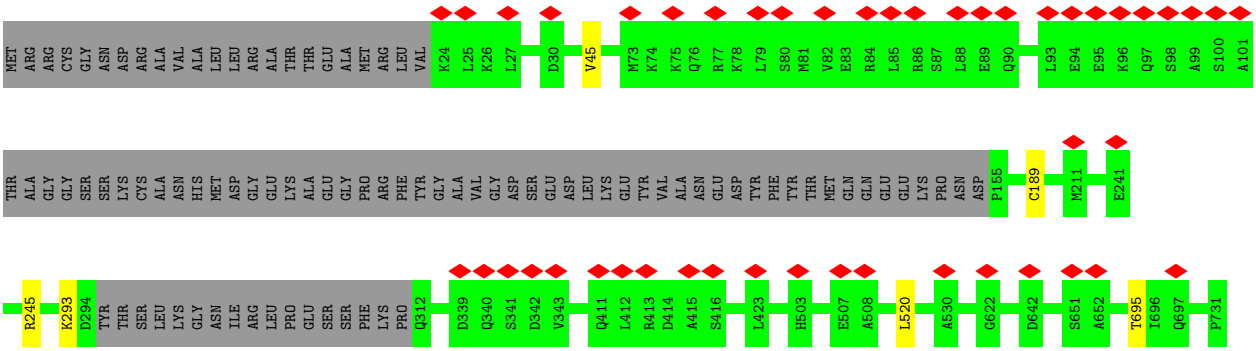
• Molecule 42: mL80

Chain BN: 51% 49%



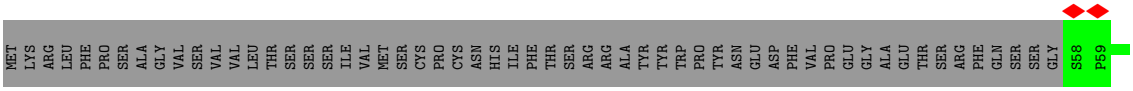
• Molecule 43: mt-LAF14

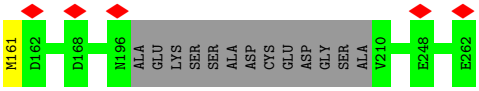
Chain EN: 6% 86% 13%



• Molecule 44: mL81

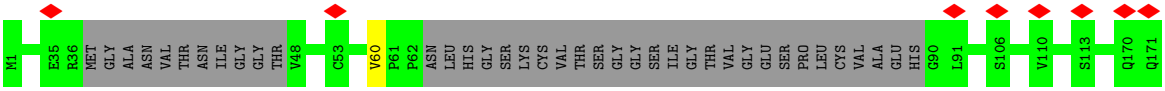
Chain BO: 73% 27%

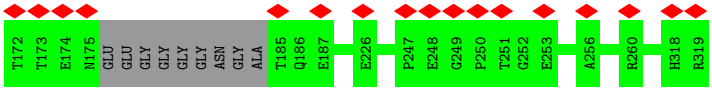




• Molecule 45: mt-LAF15a

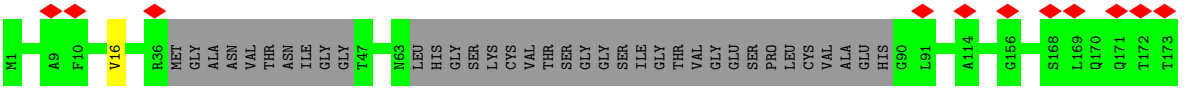
Chain EO:

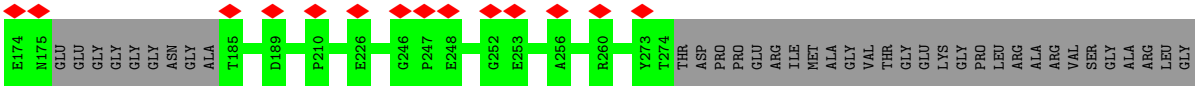


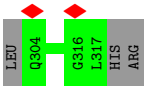


• Molecule 45: mt-LAF15a

Chain EP:

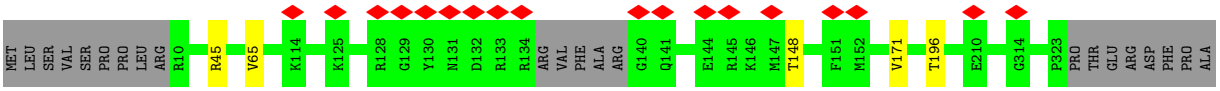


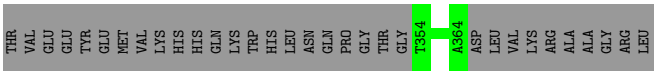




• Molecule 46: Ribosomal_L18e/L15P domain-containing protein

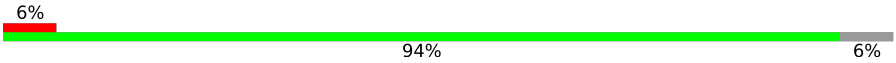
Chain AP:

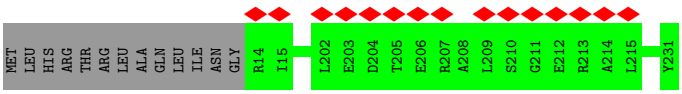




• Molecule 47: Peptidyl-prolyl cis-trans isomerase

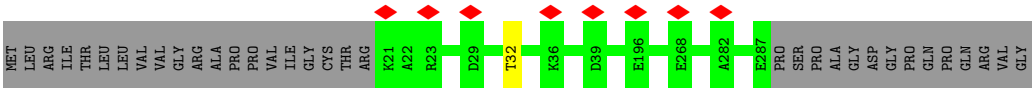
Chain BQ:





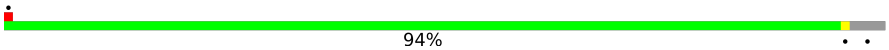
• Molecule 48: 50S ribosomal protein L17, putative

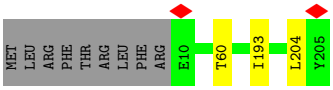
Chain AR:



• Molecule 49: mL84

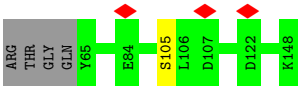
Chain BR:





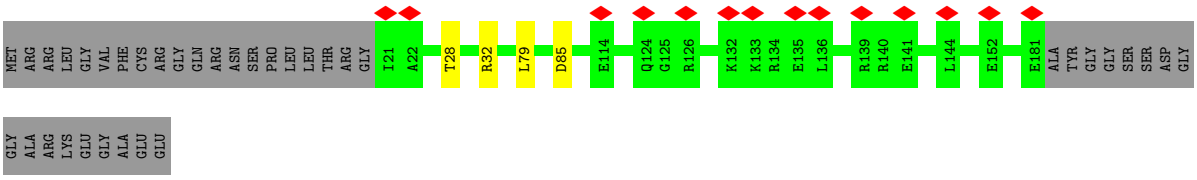
• Molecule 50: Acyl carrier protein

Chain ER:



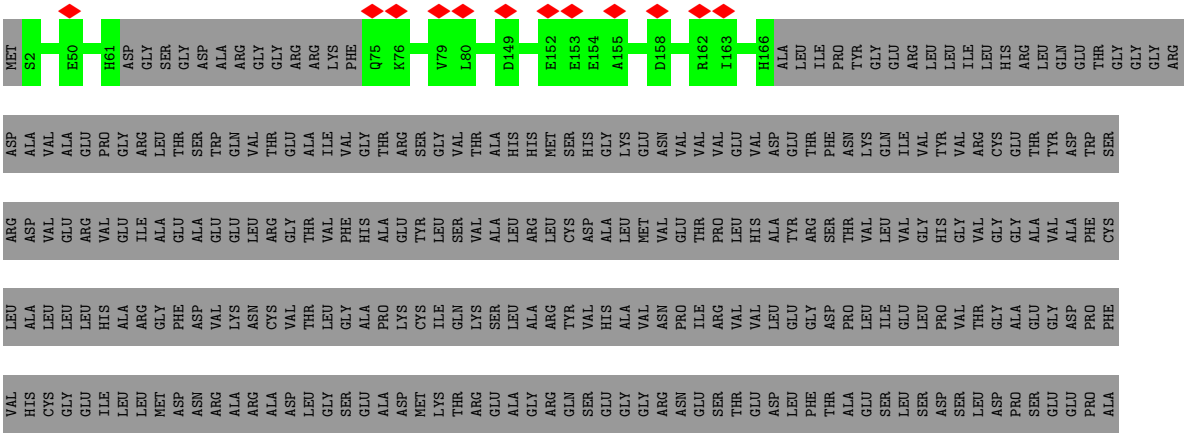
• Molecule 51: mL85

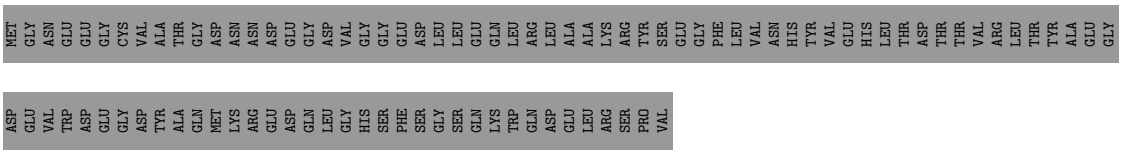
Chain BS:



• Molecule 52: Lipase (Class 3)

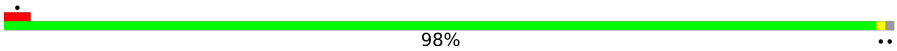
Chain ES:

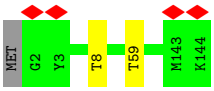




- Molecule 53: bL19m

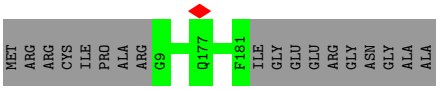
Chain AT:





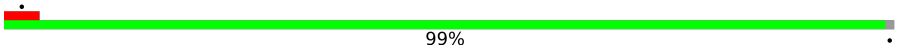
- Molecule 54: mL86

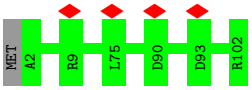
Chain BT:



- Molecule 55: mt-LAF19

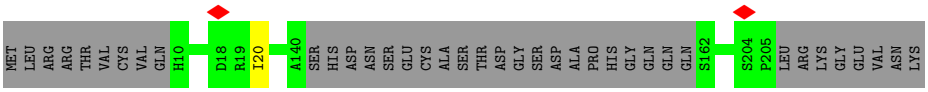
Chain ET:





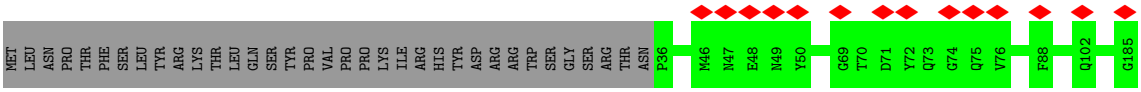
- Molecule 56: bL20m

Chain AU:



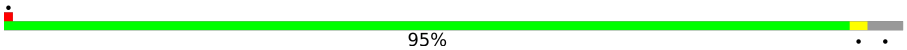
- Molecule 57: mL87

Chain BU:



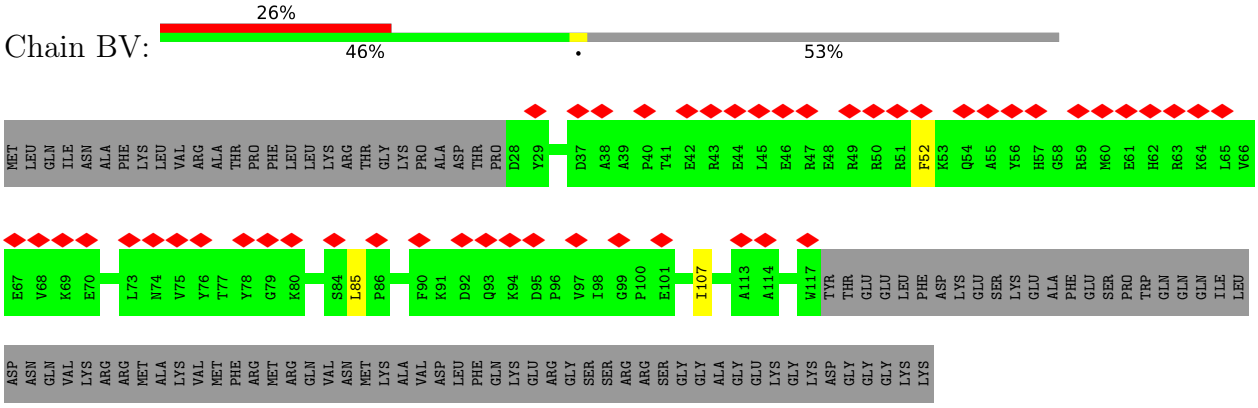
- Molecule 58: bL21m

Chain AV:



- Molecule 59: mL88

Chain BV:

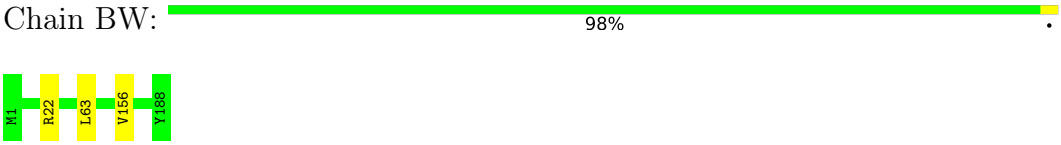


- Molecule 60: uL22m

Chain AW:

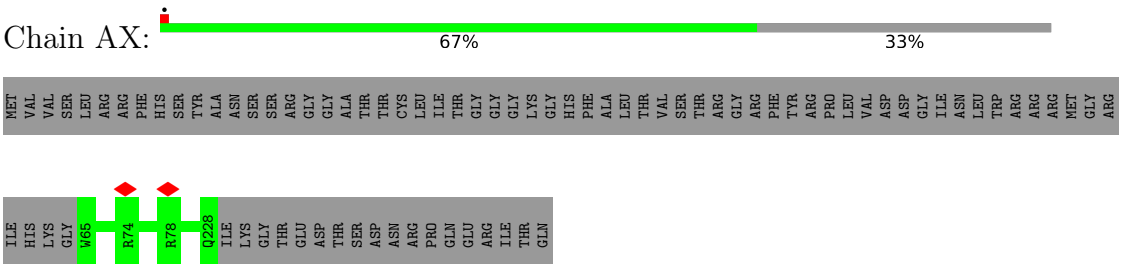
- Molecule 61: mL89

Chain BW:



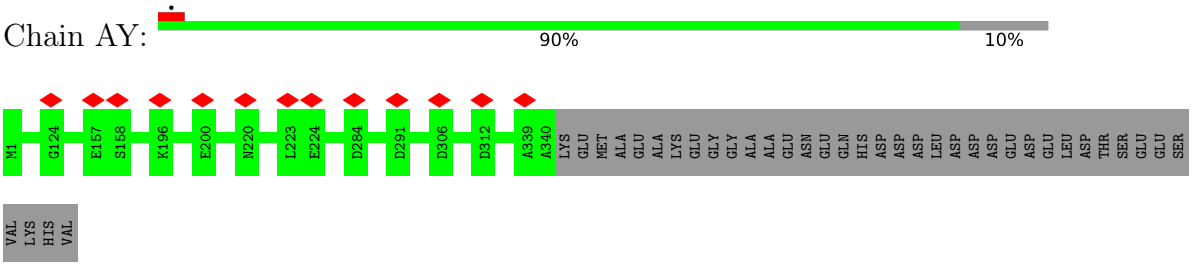
- Molecule 62: uL23m

Chain AX:



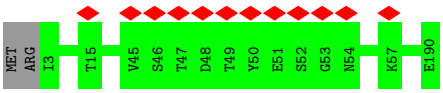
- Molecule 63: uL24m

Chain AY:



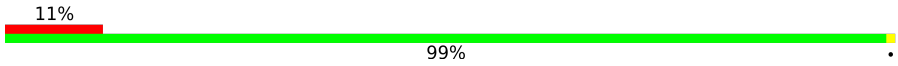
- Molecule 64: Peptidyl-prolyl cis-trans isomerase

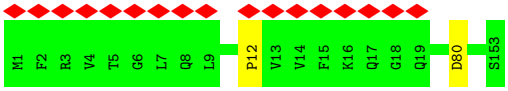
Chain BZ:



- Molecule 65: mL93

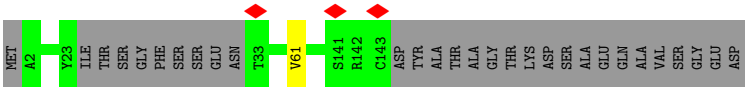
Chain Ba:





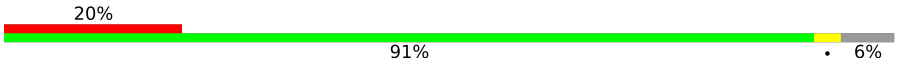
- Molecule 66: mL94

Chain Bb:



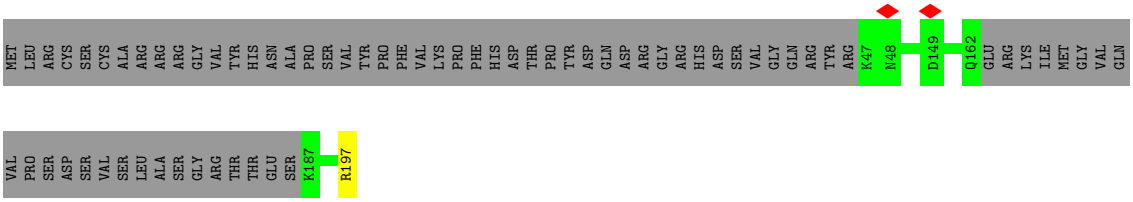
- Molecule 67: mL95

Chain Bc:



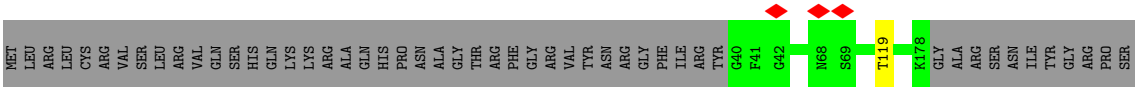
- Molecule 68: mL41

Chain Ae:



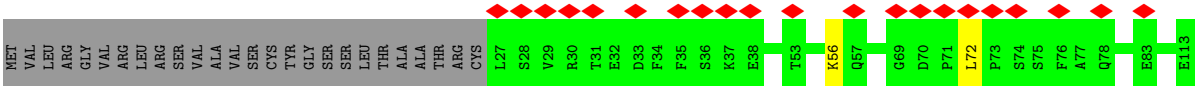
- Molecule 69: mL42

Chain Af:



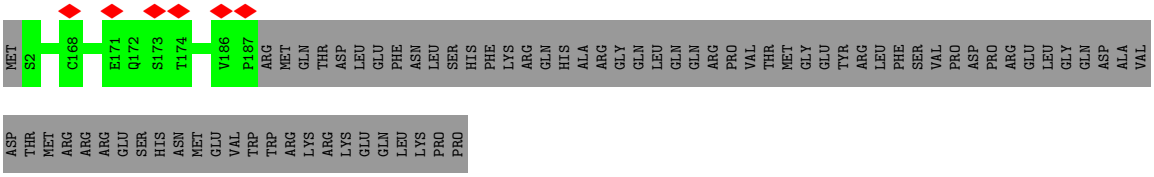
- Molecule 70: mL98

Chain Bf:



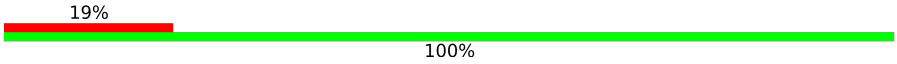
• Molecule 71: L51_S25_CI-B8 domain-containing protein

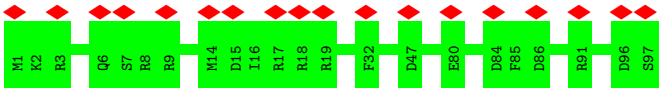
Chain Ag:



• Molecule 72: mt-LAF27

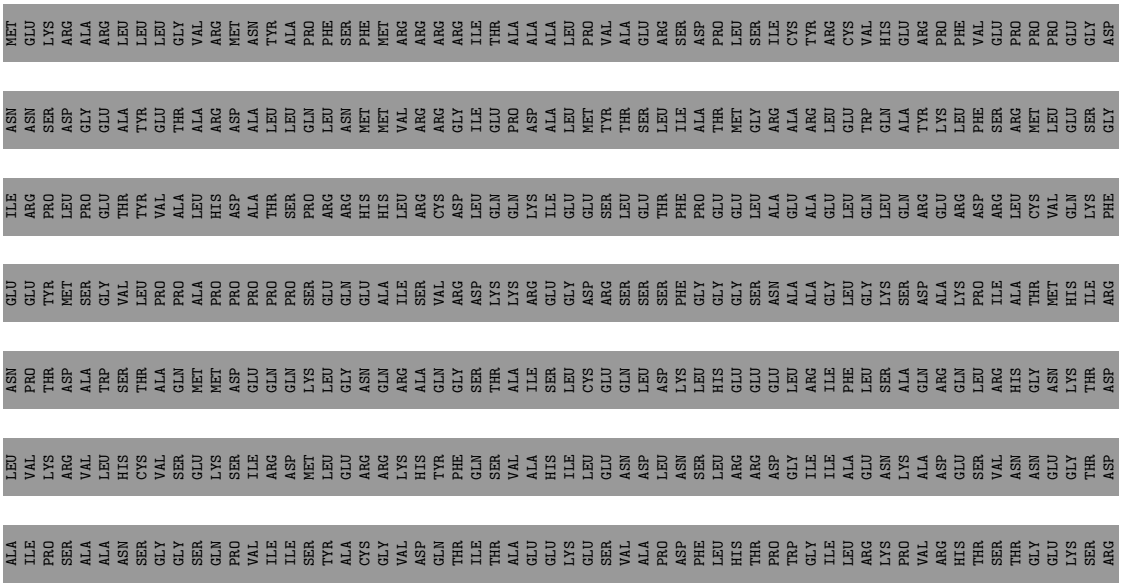
Chain E7:

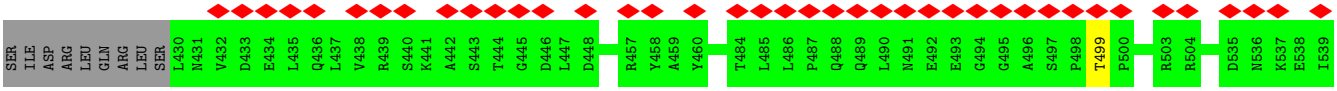


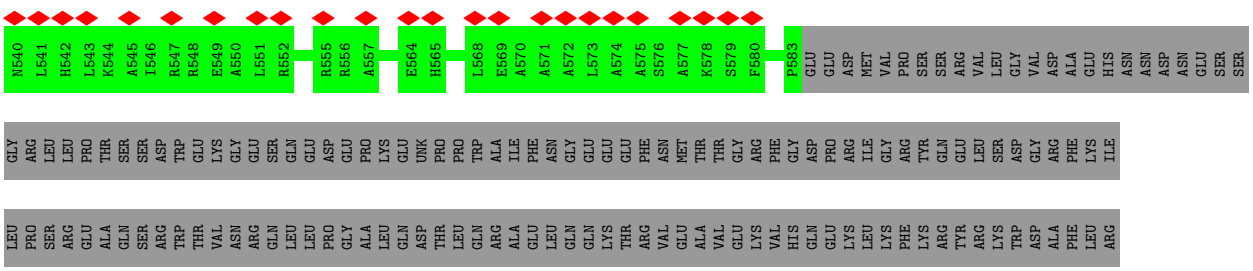


• Molecule 73: KRIPP9

Chain E8:







LYS ALA GLN ASP LYS GLN LYS GLY LYS PRO GLN THR ASP ASP LYS GLU GLY ASP GLY ASP GLY LYS LYS SER ALA GLY PRO LEU PRO ALA LYS LYS ARG LEU SER LEU LEU LEU ARG LYS GLY LYS ASP LYS ALA PRO ILE ASP ASP ALA VAL LYS ALA LYS TYR CYS LYS THR LEU

- Molecule 74: mt-LAF29

Chain E9:

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

SER GLY VAL VAL GLU GLU SER SER MET VAL SER ASN GLY ALA PHE ASP ALA VAL ARG PRO ALA ALA LEU GLY SER THR SER SER VAL ALA ASP GLU TYR LEU VAL PRO THR PRO ARG ALA THR LYS LEU LYS LYS ALA ALA MET ALA ALA SER ARG THR PRO THR PHE VAL LEU PRO ASN SER

ARG SER ALA THR ASP GLY GLU GLY GLY ALA ARG GLN ALA ASN ASP GLU ARG ASP GLY THR ASN SER SER P144 Q145 L146 F147 S148 I149 E150 E153 T154 Q155 Q156 R157 A158 N161 E165 H169 D176 E182 E183 R184 R185 A186 Q189 S190 H191 Q192 R193 A194 P195 T196

T197 K198 E199 V200 S201 D205 V206 A207 E231 R272 G273 E274 V275 A284 E285 A286 E287 K288 E289 R297 R298 R302 A316 N317 D318 L324 G343

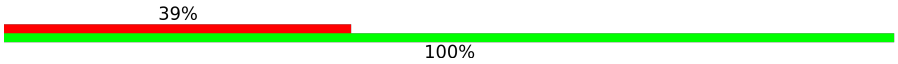
- Molecule 75: mL49

Chain Al:

MET LEU ASN ARG SER ARG LEU ARG ARG VAL TRP LEU GLY GLY THR ALA ALA ASN THR SER LEU GLY ARG ASP VAL MET PRO SER THR GLY LYS TYR ILE ASN ILE VAL SER P38 Q101 R102 C103 Q104 E105 E106 P107 E108 A109 V113 F218

- Molecule 76: UNK

Chain Ul:



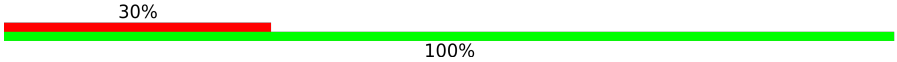
X1 X2 X3 X4 X5 X6 X7 X11 X21 X34 X35 X36 X37 X38 X39 X40 X41 X42 X43 X44 X45 X56 X57 X58 X59 X60 X66 X71 X77 X78 X79 X82 X85 X86 X89 X107 X111 X146 X147 X150 X151 X152 X153 X154 X155 X156 X157

X158 X179 X180 X186 X192 X193 X194 X197 X198 X199 X200 X201 X211 X214 X217 X218 X219 X220 X221 X232 X233 X234 X235 X236 X237 X249 X280 X281 X282 X283 X284 X285 X286 X287 X290 X295 X311 X312 X313 X314 X317 X318 X319 X326 X327 X332 X335

X336 X337 X348 X349 X350 X355 X356 X357 X358 X359 X360 X361 X362 X363

- Molecule 77: UNK

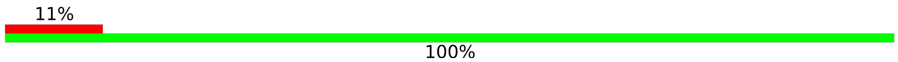
Chain Um:

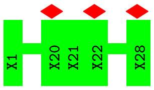


X1 X2 X10 X11 X12 X13 X14 X15 X104 X105

- Molecule 78: UNK

Chain Un:





- Molecule 79: mL52

Chain Ao:

MET HIS ILE TRP ARG THR ALA ALA SER ASN TRP VAL LYS ARG HIS ALA ARG SER ASN ALA ALA GLN TRP ARG ARG PRO GLU PRO ALA SER SER SER ALA ALA ALA LYS THR ILE ALA ARG LEU LEU ALA VAL GLY GLY HIS GLY CYS TRP SER GLU ALA THR ALA LEU TYR ALA GLU ALA

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

ILE ILE VAL PRO HIS SER ASP VAL GLY GLN GLU LYS GLU ALA ALA SER VAL ALA CYS ILE ALA VAL PHE ARG ALA LEU LEU THR SER GLY ARG THR HIS ALA ALA GLN ARG PHE ALA GLN GLN LEU LEU ARG SER ARG ASN SER ARG GLU HIS GLY LEU TRP ALA LEU ARG THR ILE

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

ARG ASP GLU VAL HIS ARG VAL ALA ALA ARG TRP CYS VAL ASP VAL ALA LEU HIS MET HIS THR CYS PRO TRP ARG PHE CYS LEU THR ASN GLU LYS GLU PRO ARG ARG GLU THR ALA PHE ASN SER GLU VAL THR SER TYR CYS CYS ALA LYS GLU LEU PRO MET PRO ALA PHE ALA VAL

THR MET LEU PRO PHE GLU VAL LEU ARG SER ASN ALA VAL GLY VAL LEU ARG CYS CYS THR ALA ALA GLY ASN GLY SER HIS GLY ASN GLU VAL VAL THR PHE ASP GLY THR ALA SER ASN VAL SER GLY GLY ARG SER GLY ASP SER THR SER CYS SER THR THR ALA PRO SER LEU GLY

LEU PRO ALA LEU LYS ARG LEU GLN ASP VAL VAL SER ALA ALA ILE GLU VAL PRO LEU SER THR HIS GLU PRO VAL GLU CYS LEU TYR LEU LEU LEU GLN ILE SER ARG ASP SER THR ALA PRO ASP PRO ARG ARG VAL MET PRO SER THR MET ASN ILE LEU TRP TRP ARG HIS LEU

GLN SER CYS VAL LEU GLU SER VAL LYS SER ALA VAL ARG TRP LYS SER VAL CYS ASP PHE VAL GLY LEU SER ARG LEU VAL THR GLU ARG VAL PRO HIS CYS PHE PRO LEU LEU VAL ALA HIS ALA ALA GLU SER PRO ASP ALA LEU ARG THR LEU PHE ASN GLU VAL SER ARG GLN GLU

GLY ALA ALA ALA UNK PRO VAL ASP ASP ILE PRO ARG SER CYS VAL MET GLY LEU LEU GLN MET CYS GLY ASP GLU ARG SER ALA ALA VAL ILE ASP TRP VAL VAL GLU HIS CYS UNK ASP HIS GLU SER ILE ALA GLN PHE VAL LEU ASP SER LEU GLY GLN HIS GLN GLU LEU ALA SER

VAL VAL VAL ARG ARG LEU PHE GLN ARG SER GLU GLN SER UNK ASP VAL ILE ASN ALA LEU SER ARG LEU LEU GLU LYS GLY THR CYS ARG THR LEU LEU ALA ASP VAL CYS SER LEU VAL PRO GLN ALA GLN GLN TRP THR VAL ALA LEU ARG PHE VAL SER GLY MET SER ALA PRO GLU

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

LEU GLY ALA GLU ARG LEU THR GLN ARG PRO GLU LEU LEU GLY LYS TYR ILE ARG TYR PHE SER LYS ARG VAL ALA VAL ASN SER ARG LEU TYR MET GLU LEU GLU ALA LEU LEU ALA CYS SER LYS VAL GLY GLY GLY SER ALA ARG ASN CYS GLY ARG SER SER ASN TRP ASN PRO ILE

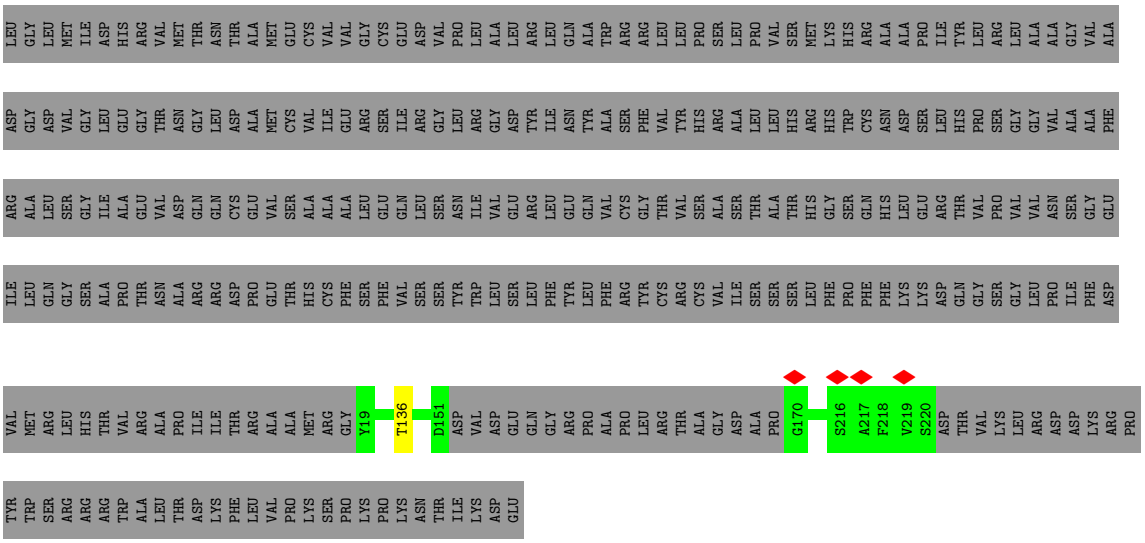
ALA SER THR VAL THR GLY GLY PRO PRO LEU GLU THR SER LEU VAL GLY VAL ARG THR GLU VAL LEU PRO LYS GLY ARG GLN TRP MET GLU ALA CYS ALA HIS ALA SER GLU VAL GLY VAL THR ARG GLY VAL LEU GLU ILE LEU ALA LYS ARG GLY ARG TRP GLU GLU ALA THR ILE LEU

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

PRO LEU GLU VAL VAL GLN LEU TRP LEU HIS ARG ARG SER VAL GLY GLU SER THR SER HIS VAL LEU PHE GLY LEU GLY PRO GLY SER SER LEU ARG THR GLU GLN ARG ASP ALA ASN ASP LYS HIS ASN VAL PHE GLY ASP ALA SER ARG TRP LEU GLY SER ALA GLN ALA GLU LEU

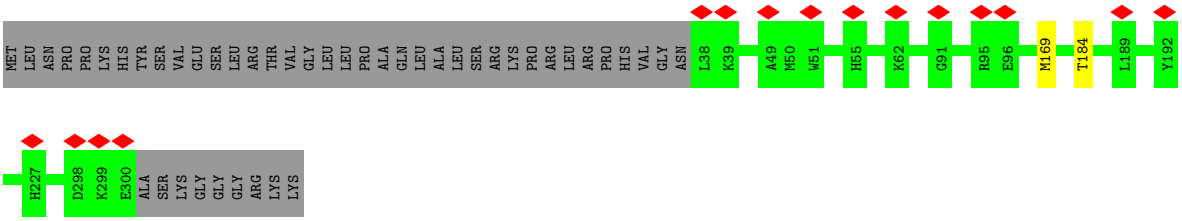
PHE PHE VAL LEU LEU GLU SER SER SER ARG SER SER ASP HIS GLN TRP ARG TYR ALA LEU GLN LEU LEU LYS GLU HIS VAL LEU LEU SER GLY GLY VAL PRO SER ALA ARG VAL PHE ARG SER THR TYR SER ILE LEU HIS ARG ALA GLU ARG TRP ARG GLU SER LEU GLN LEU LEU

GLY LEU GLN ARG SER VAL CYS GLY SER PRO THR VAL LYS CYS VAL HIS LEU VAL LEU SER THR LEU PRO SER THR ALA TRP GLN TYR ALA LEU GLY ALA LEU GLN CYS ILE PRO PRO GLY ASP SER GLY SER ILE HIS ARG VAL LEU PRO LEU LEU LEU PRO VAL SER TRP GLU SER ALA



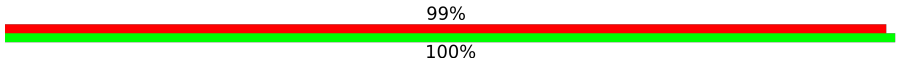
- Molecule 80: mL53

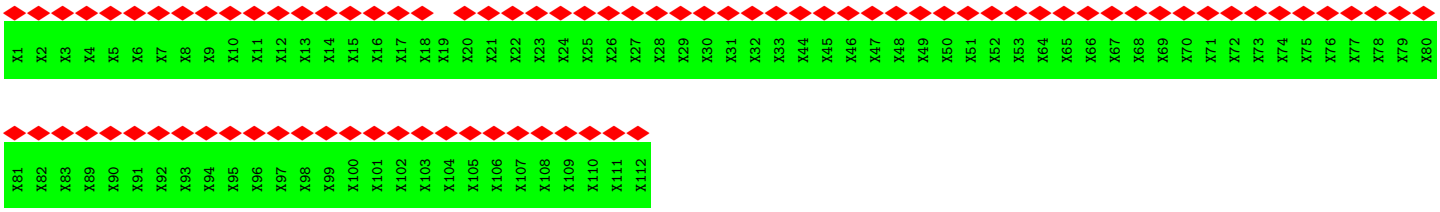
Chain Ap:



- Molecule 81: UNK

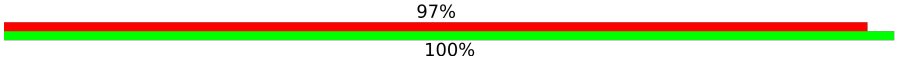
Chain Up:

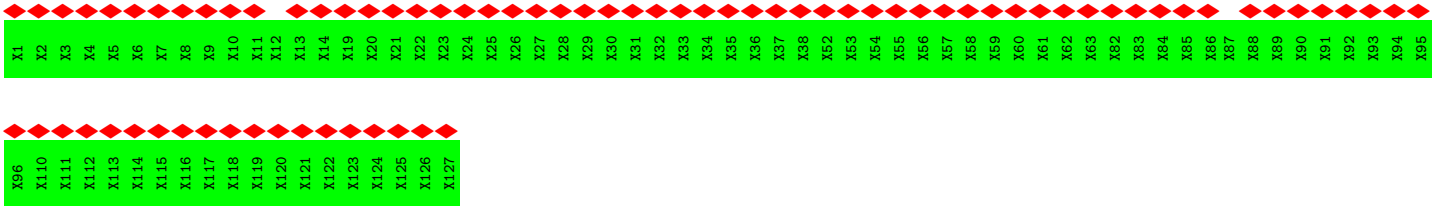




- Molecule 82: UNK

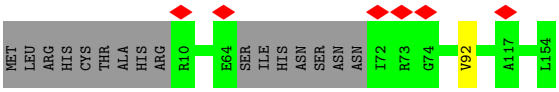
Chain Us:





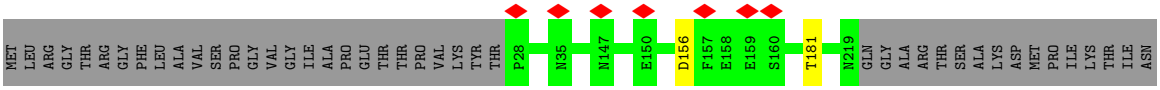
- Molecule 83: mL63

Chain At:



• Molecule 84: mL64

Chain Av:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16215	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 ($e^-/Å^2$)	75	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	434.001, 434.001, 434.001	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.44667, 1.44667, 1.44667	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, GTP, PM8, ZN, MG, ATP, NAD

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	A1	0.24	0/1828	0.39	0/2466
2	E1	0.23	0/3906	0.39	1/5236 (0.0%)
3	A2	0.25	0/3844	0.39	0/5234
4	E2	0.23	0/3000	0.39	0/4067
5	A3	0.24	0/1246	0.39	0/1678
6	E3	0.24	0/3331	0.38	0/4491
7	E4	0.24	0/3491	0.43	1/4740 (0.0%)
8	A5	0.23	0/498	0.37	0/663
10	E6	0.23	0/3471	0.39	0/4710
11	A8	0.23	0/1163	0.38	0/1558
12	AA	0.18	0/19045	0.75	7/29609 (0.0%)
13	BA	0.24	0/6192	0.39	0/8401
14	EA	0.23	0/4337	0.39	0/5856
16	BB	0.24	0/3411	0.39	0/4622
17	EB	0.23	0/5154	0.39	0/6977
18	EC	0.25	0/3090	0.41	0/4190
19	BD	0.24	0/3418	0.40	0/4629
20	ED	0.24	0/4877	0.40	0/6607
21	AE	0.26	0/2897	0.41	0/3938
22	BE	0.24	0/2896	0.39	0/3929
23	EE	0.23	0/3489	0.40	1/4722 (0.0%)
24	AF	0.25	0/3517	0.39	0/4775
25	BF	0.25	0/2909	0.41	0/3920
26	EF	0.24	0/2316	0.42	0/3148
27	EG	0.25	0/1331	0.40	0/1784
28	BH	0.24	0/2005	0.40	0/2734
29	EH	0.24	0/3586	0.39	0/4864
30	AI	0.24	0/1980	0.38	0/2693
31	BI	0.24	0/2548	0.37	0/3449
33	BJ	0.23	0/1985	0.37	0/2681
34	AK	0.34	1/2141 (0.0%)	0.46	1/2886 (0.0%)
35	BK	0.24	0/1897	0.37	0/2556

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	BL	0.23	0/2055	0.38	0/2782
38	EL	0.24	0/4384	0.38	0/5967
39	EM	0.24	0/2480	0.39	0/3352
41	AN	0.24	0/1698	0.39	0/2308
42	BN	0.24	0/1353	0.40	0/1827
43	EN	0.23	0/5115	0.38	0/6936
44	BO	0.24	0/1518	0.38	0/2051
45	EO	0.24	0/2173	0.40	0/2956
45	EP	0.23	0/1953	0.39	0/2659
46	AP	0.23	0/2695	0.40	0/3657
47	BQ	0.25	0/1691	0.41	0/2293
48	AR	0.24	0/2279	0.39	0/3079
49	BR	0.25	0/1702	0.40	0/2296
50	ER	0.24	0/679	0.38	0/923
51	BS	0.24	0/1131	0.37	0/1547
52	ES	0.23	0/1276	0.37	0/1715
53	AT	0.24	0/1210	0.40	0/1632
54	BT	0.24	0/1465	0.39	0/1970
55	ET	0.25	0/858	0.38	0/1148
56	AU	0.24	0/1456	0.37	0/1971
57	BU	0.24	0/1315	0.39	0/1776
58	AV	0.25	0/1454	0.45	0/1973
59	BV	0.40	0/786	0.51	1/1063 (0.1%)
60	AW	0.24	0/2307	0.40	0/3119
61	BW	0.25	0/1612	0.37	0/2177
62	AX	0.25	0/1432	0.40	0/1947
63	AY	0.24	0/2846	0.39	0/3847
64	BZ	0.25	0/1422	0.42	0/1925
65	Ba	0.24	0/1329	0.41	1/1798 (0.1%)
66	Bb	0.24	0/1073	0.42	0/1454
67	Bc	0.24	0/1238	0.38	0/1685
68	Ae	0.24	0/1068	0.39	0/1447
69	Af	0.24	0/1134	0.40	0/1536
70	Bf	0.25	0/749	0.43	0/1012
71	Ag	0.24	0/1608	0.39	0/2180
72	E7	0.23	0/834	0.38	0/1118
73	E8	0.23	0/1202	0.40	0/1631
74	E9	0.23	0/1678	0.37	0/2257
75	Al	0.25	0/1484	0.39	0/2019
79	Ao	0.24	0/1486	0.39	0/2022
80	Ap	0.24	0/2231	0.39	0/3030
83	At	0.23	0/1179	0.39	0/1596
84	Av	0.24	0/1678	0.37	0/2261

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.24	1/183115 (0.0%)	0.45	13/251755 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	AK	174	GLU	CB-CG	-5.46	1.41	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	AK	151	LEU	CA-CB-CG	-7.51	98.02	115.30
12	AA	159	U	C2-N1-C1'	6.69	125.73	117.70
23	EE	441	PRO	N-CA-CB	6.20	110.73	103.30
2	E1	96	PRO	N-CA-CB	6.05	110.56	103.30
12	AA	159	U	N1-C2-O2	6.01	127.00	122.80
7	E4	203	PRO	N-CA-CB	5.71	110.15	103.30
12	AA	571	U	C2-N1-C1'	5.71	124.55	117.70
65	Ba	12	PRO	N-CA-CB	5.71	110.15	103.30
12	AA	191	U	C2-N1-C1'	5.34	124.11	117.70
12	AA	159	U	N3-C2-O2	-5.34	118.46	122.20
12	AA	497	C	N1-C2-O2	5.15	121.99	118.90
59	BV	85	LEU	CB-CG-CD1	-5.05	102.41	111.00
12	AA	571	U	N1-C2-O2	5.03	126.32	122.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	215/241 (89%)	207 (96%)	8 (4%)	0	100	100
2	E1	471/482 (98%)	459 (98%)	12 (2%)	0	100	100
3	A2	461/471 (98%)	449 (97%)	12 (3%)	0	100	100
4	E2	359/568 (63%)	341 (95%)	18 (5%)	0	100	100
5	A3	147/218 (67%)	142 (97%)	5 (3%)	0	100	100
6	E3	401/557 (72%)	393 (98%)	8 (2%)	0	100	100
7	E4	430/439 (98%)	417 (97%)	13 (3%)	0	100	100
8	A5	53/80 (66%)	53 (100%)	0	0	100	100
10	E6	430/531 (81%)	417 (97%)	13 (3%)	0	100	100
11	A8	131/181 (72%)	129 (98%)	2 (2%)	0	100	100
13	BA	763/831 (92%)	741 (97%)	22 (3%)	0	100	100
14	EA	530/576 (92%)	520 (98%)	10 (2%)	0	100	100
16	BB	403/541 (74%)	385 (96%)	18 (4%)	0	100	100
17	EB	619/754 (82%)	603 (97%)	16 (3%)	0	100	100
18	EC	371/406 (91%)	359 (97%)	12 (3%)	0	100	100
19	BD	417/547 (76%)	402 (96%)	15 (4%)	0	100	100
20	ED	594/616 (96%)	577 (97%)	17 (3%)	0	100	100
21	AE	342/473 (72%)	328 (96%)	14 (4%)	0	100	100
22	BE	353/449 (79%)	345 (98%)	8 (2%)	0	100	100
23	EE	427/586 (73%)	413 (97%)	13 (3%)	1 (0%)	47	79
24	AF	415/459 (90%)	405 (98%)	10 (2%)	0	100	100
25	BF	342/426 (80%)	328 (96%)	14 (4%)	0	100	100
26	EF	293/373 (79%)	283 (97%)	10 (3%)	0	100	100
27	EG	152/156 (97%)	150 (99%)	2 (1%)	0	100	100
28	BH	234/349 (67%)	228 (97%)	6 (3%)	0	100	100
29	EH	429/634 (68%)	425 (99%)	4 (1%)	0	100	100
30	AI	228/263 (87%)	224 (98%)	4 (2%)	0	100	100
31	BI	301/342 (88%)	295 (98%)	6 (2%)	0	100	100
33	BJ	232/333 (70%)	227 (98%)	5 (2%)	0	100	100
34	AK	242/342 (71%)	237 (98%)	5 (2%)	0	100	100
35	BK	222/386 (58%)	220 (99%)	2 (1%)	0	100	100
37	BL	254/312 (81%)	245 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	EL	526/691 (76%)	513 (98%)	13 (2%)	0	100	100
39	EM	302/451 (67%)	296 (98%)	6 (2%)	0	100	100
41	AN	191/202 (95%)	185 (97%)	6 (3%)	0	100	100
42	BN	150/302 (50%)	145 (97%)	5 (3%)	0	100	100
43	EN	632/731 (86%)	612 (97%)	20 (3%)	0	100	100
44	BO	188/262 (72%)	185 (98%)	3 (2%)	0	100	100
45	EO	264/319 (83%)	256 (97%)	8 (3%)	0	100	100
45	EP	233/319 (73%)	226 (97%)	7 (3%)	0	100	100
46	AP	314/374 (84%)	308 (98%)	6 (2%)	0	100	100
47	BQ	216/231 (94%)	206 (95%)	10 (5%)	0	100	100
48	AR	265/301 (88%)	252 (95%)	13 (5%)	0	100	100
49	BR	194/205 (95%)	190 (98%)	4 (2%)	0	100	100
50	ER	82/148 (55%)	79 (96%)	3 (4%)	0	100	100
51	BS	158/198 (80%)	152 (96%)	6 (4%)	0	100	100
52	ES	148/524 (28%)	146 (99%)	2 (1%)	0	100	100
53	AT	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
54	BT	171/191 (90%)	165 (96%)	6 (4%)	0	100	100
55	ET	99/102 (97%)	96 (97%)	3 (3%)	0	100	100
56	AU	171/213 (80%)	167 (98%)	4 (2%)	0	100	100
57	BU	148/185 (80%)	141 (95%)	7 (5%)	0	100	100
58	AV	179/188 (95%)	172 (96%)	7 (4%)	0	100	100
59	BV	88/190 (46%)	86 (98%)	2 (2%)	0	100	100
60	AW	276/278 (99%)	270 (98%)	6 (2%)	0	100	100
61	BW	186/188 (99%)	178 (96%)	8 (4%)	0	100	100
62	AX	162/246 (66%)	161 (99%)	1 (1%)	0	100	100
63	AY	338/378 (89%)	336 (99%)	2 (1%)	0	100	100
64	BZ	186/190 (98%)	178 (96%)	8 (4%)	0	100	100
65	Ba	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
66	Bb	129/162 (80%)	123 (95%)	6 (5%)	0	100	100
67	Bc	135/146 (92%)	131 (97%)	4 (3%)	0	100	100
68	Ae	123/197 (62%)	118 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	Af	137/189 (72%)	137 (100%)	0	0	100	100
70	Bf	85/113 (75%)	80 (94%)	5 (6%)	0	100	100
71	Ag	184/260 (71%)	175 (95%)	9 (5%)	0	100	100
72	E7	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
73	E8	152/786 (19%)	146 (96%)	6 (4%)	0	100	100
74	E9	198/343 (58%)	193 (98%)	5 (2%)	0	100	100
75	Al	179/218 (82%)	177 (99%)	2 (1%)	0	100	100
79	Ao	180/1520 (12%)	175 (97%)	5 (3%)	0	100	100
80	Ap	261/309 (84%)	258 (99%)	3 (1%)	0	100	100
83	At	134/154 (87%)	128 (96%)	6 (4%)	0	100	100
84	Av	190/242 (78%)	185 (97%)	5 (3%)	0	100	100
All	All	19602/26562 (74%)	19044 (97%)	557 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	EE	121	ILE

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	
1	A1	195/217 (90%)	193 (99%)	2 (1%)	76	86
2	E1	393/419 (94%)	390 (99%)	3 (1%)	81	89
3	A2	405/413 (98%)	404 (100%)	1 (0%)	93	96
4	E2	328/505 (65%)	326 (99%)	2 (1%)	86	91
5	A3	134/193 (69%)	134 (100%)	0	100	100
6	E3	361/493 (73%)	361 (100%)	0	100	100
7	E4	367/378 (97%)	357 (97%)	10 (3%)	44	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	A5	52/73 (71%)	51 (98%)	1 (2%)	57	75
10	E6	372/454 (82%)	369 (99%)	3 (1%)	81	89
11	A8	118/161 (73%)	118 (100%)	0	100	100
13	BA	662/727 (91%)	659 (100%)	3 (0%)	88	93
14	EA	463/502 (92%)	460 (99%)	3 (1%)	86	91
16	BB	351/470 (75%)	348 (99%)	3 (1%)	78	87
17	EB	548/649 (84%)	543 (99%)	5 (1%)	78	87
18	EC	327/354 (92%)	325 (99%)	2 (1%)	86	91
19	BD	356/472 (75%)	354 (99%)	2 (1%)	86	91
20	ED	529/544 (97%)	526 (99%)	3 (1%)	86	91
21	AE	295/406 (73%)	294 (100%)	1 (0%)	92	95
22	BE	304/386 (79%)	302 (99%)	2 (1%)	84	90
23	EE	364/514 (71%)	363 (100%)	1 (0%)	92	95
24	AF	375/409 (92%)	372 (99%)	3 (1%)	81	89
25	BF	300/368 (82%)	297 (99%)	3 (1%)	76	86
26	EF	250/307 (81%)	249 (100%)	1 (0%)	91	94
27	EG	134/136 (98%)	134 (100%)	0	100	100
28	BH	206/297 (69%)	205 (100%)	1 (0%)	88	93
29	EH	389/527 (74%)	386 (99%)	3 (1%)	81	89
30	AI	205/225 (91%)	204 (100%)	1 (0%)	88	93
31	BI	254/288 (88%)	253 (100%)	1 (0%)	91	94
33	BJ	208/298 (70%)	208 (100%)	0	100	100
34	AK	221/301 (73%)	218 (99%)	3 (1%)	67	81
35	BK	200/329 (61%)	198 (99%)	2 (1%)	76	86
37	BL	202/262 (77%)	201 (100%)	1 (0%)	88	93
38	EL	461/598 (77%)	457 (99%)	4 (1%)	78	87
39	EM	266/386 (69%)	263 (99%)	3 (1%)	73	84
41	AN	173/182 (95%)	173 (100%)	0	100	100
42	BN	142/265 (54%)	141 (99%)	1 (1%)	84	90
43	EN	564/640 (88%)	558 (99%)	6 (1%)	73	84
44	BO	162/225 (72%)	161 (99%)	1 (1%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	EO	232/263 (88%)	231 (100%)	1 (0%)	91	94
45	EP	211/263 (80%)	210 (100%)	1 (0%)	88	93
46	AP	277/330 (84%)	272 (98%)	5 (2%)	59	77
47	BQ	172/195 (88%)	172 (100%)	0	100	100
48	AR	225/256 (88%)	224 (100%)	1 (0%)	91	94
49	BR	172/181 (95%)	169 (98%)	3 (2%)	60	78
50	ER	78/127 (61%)	77 (99%)	1 (1%)	69	82
51	BS	91/164 (56%)	87 (96%)	4 (4%)	28	56
52	ES	134/437 (31%)	134 (100%)	0	100	100
53	AT	123/124 (99%)	121 (98%)	2 (2%)	62	79
54	BT	151/163 (93%)	151 (100%)	0	100	100
55	ET	87/88 (99%)	87 (100%)	0	100	100
56	AU	151/184 (82%)	150 (99%)	1 (1%)	84	90
57	BU	134/168 (80%)	134 (100%)	0	100	100
58	AV	153/158 (97%)	150 (98%)	3 (2%)	55	74
59	BV	79/163 (48%)	77 (98%)	2 (2%)	47	69
60	AW	246/246 (100%)	244 (99%)	2 (1%)	81	89
61	BW	164/164 (100%)	161 (98%)	3 (2%)	59	77
62	AX	153/221 (69%)	153 (100%)	0	100	100
63	AY	305/337 (90%)	305 (100%)	0	100	100
64	BZ	148/160 (92%)	148 (100%)	0	100	100
65	Ba	130/144 (90%)	129 (99%)	1 (1%)	81	89
66	Bb	113/135 (84%)	112 (99%)	1 (1%)	78	87
67	Bc	127/134 (95%)	123 (97%)	4 (3%)	40	64
68	Ae	110/172 (64%)	109 (99%)	1 (1%)	78	87
69	Af	120/162 (74%)	119 (99%)	1 (1%)	81	89
70	Bf	77/98 (79%)	75 (97%)	2 (3%)	46	68
71	Ag	170/239 (71%)	170 (100%)	0	100	100
72	E7	87/87 (100%)	87 (100%)	0	100	100
73	E8	112/678 (16%)	111 (99%)	1 (1%)	78	87
74	E9	177/292 (61%)	175 (99%)	2 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	Al	155/186 (83%)	155 (100%)	0	100	100
79	Ao	151/1258 (12%)	150 (99%)	1 (1%)	84	90
80	Ap	229/267 (86%)	227 (99%)	2 (1%)	78	87
83	At	125/140 (89%)	124 (99%)	1 (1%)	81	89
84	Av	170/210 (81%)	168 (99%)	2 (1%)	71	83
All	All	17175/22967 (75%)	17046 (99%)	129 (1%)	82	89

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	88	THR
1	A1	106	THR
2	E1	129	LEU
2	E1	220	LEU
2	E1	296	LEU
3	A2	252	VAL
4	E2	123	THR
4	E2	337	THR
7	E4	85	LEU
7	E4	86	ARG
7	E4	144	VAL
7	E4	178	ARG
7	E4	185	VAL
7	E4	199	THR
7	E4	257	LEU
7	E4	305	THR
7	E4	309	THR
7	E4	323	VAL
8	A5	49	LEU
10	E6	277	GLN
10	E6	283	THR
10	E6	386	LEU
13	BA	190	THR
13	BA	342	THR
13	BA	757	THR
14	EA	142	ASP
14	EA	336	VAL
14	EA	500	MET
16	BB	98	THR
16	BB	152	ARG

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Mol	Chain	Res	Type
16	BB	271	THR
17	EB	52	LYS
17	EB	246	ARG
17	EB	510	THR
17	EB	573	ARG
17	EB	636	ARG
18	EC	62	THR
18	EC	199	THR
19	BD	244	ARG
19	BD	373	THR
20	ED	43	LEU
20	ED	140	ASP
20	ED	395	ARG
21	AE	222	THR
22	BE	139	GLU
22	BE	266	LEU
23	EE	122	TRP
24	AF	105	THR
24	AF	127	THR
24	AF	280	THR
25	BF	131	LEU
25	BF	202	THR
25	BF	390	VAL
26	EF	67	LYS
28	BH	284	THR
29	EH	52	THR
29	EH	249	ARG
29	EH	497	ASP
30	AI	13	VAL
31	BI	103	THR
34	AK	64	THR
34	AK	102	VAL
34	AK	151	LEU
35	BK	155	LEU
35	BK	301	THR
37	BL	116	GLU
38	EL	62	THR
38	EL	227	THR
38	EL	229	THR
38	EL	568	THR
39	EM	83	LEU
39	EM	115	CYS

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Mol	Chain	Res	Type
39	EM	324	GLN
42	BN	204	THR
43	EN	45	VAL
43	EN	189	CYS
43	EN	245	ARG
43	EN	293	LYS
43	EN	520	LEU
43	EN	695	THR
44	BO	161	MET
45	EO	60	VAL
46	AP	45	ARG
46	AP	65	VAL
46	AP	148	THR
46	AP	171	VAL
46	AP	196	THR
45	EP	16	VAL
48	AR	32	THR
49	BR	60	THR
49	BR	193	ILE
49	BR	204	LEU
50	ER	105	SER
51	BS	28	THR
51	BS	32	ARG
51	BS	79	LEU
51	BS	85	ASP
53	AT	8	THR
53	AT	59	THR
56	AU	20	ILE
58	AV	115	VAL
58	AV	124	THR
58	AV	128	ARG
59	BV	52	PHE
59	BV	107	ILE
60	AW	45	ARG
60	AW	266	THR
61	BW	22	ARG
61	BW	63	LEU
61	BW	156	VAL
65	Ba	80	ASP
66	Bb	61	VAL
67	Bc	18	ARG
67	Bc	109	ARG

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Mol	Chain	Res	Type
67	Bc	123	LYS
67	Bc	140	VAL
68	Ae	197	ARG
69	Af	119	THR
70	Bf	56	LYS
70	Bf	72	LEU
73	E8	499	THR
74	E9	298	ARG
74	E9	302	ARG
79	Ao	136	THR
80	Ap	169	MET
80	Ap	184	THR
83	At	92	VAL
84	Av	156	ASP
84	Av	181	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (267) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	138	ASN
2	E1	49	ASN
2	E1	146	GLN
2	E1	162	HIS
2	E1	165	ASN
2	E1	205	ASN
2	E1	278	HIS
2	E1	322	HIS
2	E1	366	HIS
3	A2	167	HIS
3	A2	194	GLN
3	A2	389	HIS
4	E2	234	HIS
4	E2	254	GLN
4	E2	343	ASN
4	E2	383	ASN
4	E2	388	GLN
4	E2	411	HIS
4	E2	488	ASN
5	A3	144	GLN
6	E3	295	GLN
6	E3	330	HIS
6	E3	448	GLN

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Mol	Chain	Res	Type
7	E4	29	GLN
7	E4	110	ASN
7	E4	138	ASN
7	E4	191	HIS
7	E4	195	HIS
7	E4	214	ASN
7	E4	293	ASN
7	E4	297	ASN
7	E4	338	GLN
7	E4	362	GLN
7	E4	370	HIS
10	E6	97	GLN
10	E6	150	HIS
10	E6	171	HIS
10	E6	173	ASN
10	E6	337	HIS
10	E6	373	ASN
10	E6	397	ASN
11	A8	136	GLN
11	A8	174	GLN
13	BA	301	HIS
13	BA	307	HIS
13	BA	502	HIS
13	BA	529	GLN
13	BA	693	HIS
13	BA	810	HIS
14	EA	59	HIS
14	EA	65	GLN
14	EA	317	ASN
14	EA	368	HIS
14	EA	386	ASN
14	EA	392	HIS
14	EA	469	ASN
14	EA	518	GLN
14	EA	544	GLN
16	BB	82	HIS
16	BB	170	GLN
16	BB	242	GLN
16	BB	313	HIS
16	BB	420	ASN
17	EB	159	GLN
17	EB	227	GLN

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Mol	Chain	Res	Type
17	EB	271	HIS
17	EB	336	HIS
17	EB	502	HIS
17	EB	515	HIS
17	EB	577	GLN
17	EB	603	GLN
17	EB	644	GLN
17	EB	683	GLN
18	EC	166	HIS
18	EC	315	GLN
18	EC	352	ASN
19	BD	193	GLN
19	BD	218	ASN
19	BD	297	GLN
19	BD	513	ASN
20	ED	75	ASN
20	ED	178	GLN
20	ED	312	HIS
20	ED	402	ASN
20	ED	543	GLN
20	ED	606	HIS
21	AE	380	GLN
22	BE	76	GLN
22	BE	78	HIS
22	BE	183	HIS
22	BE	279	HIS
22	BE	330	GLN
22	BE	373	GLN
23	EE	109	GLN
23	EE	160	HIS
23	EE	174	HIS
23	EE	270	ASN
23	EE	429	HIS
23	EE	434	HIS
24	AF	65	ASN
24	AF	147	ASN
24	AF	223	ASN
25	BF	132	GLN
25	BF	143	GLN
25	BF	288	GLN
25	BF	311	GLN
26	EF	74	ASN

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Mol	Chain	Res	Type
26	EF	292	HIS
27	EG	38	GLN
27	EG	69	HIS
27	EG	126	GLN
28	BH	79	GLN
28	BH	122	HIS
28	BH	253	GLN
28	BH	286	HIS
29	EH	505	GLN
29	EH	548	GLN
30	AI	76	HIS
30	AI	120	ASN
31	BI	125	ASN
31	BI	144	HIS
31	BI	152	GLN
31	BI	263	HIS
33	BJ	266	GLN
33	BJ	273	HIS
34	AK	87	ASN
34	AK	279	HIS
34	AK	293	ASN
35	BK	114	HIS
35	BK	212	GLN
37	BL	74	GLN
37	BL	95	GLN
37	BL	103	ASN
37	BL	226	HIS
37	BL	255	HIS
37	BL	262	GLN
38	EL	118	HIS
38	EL	278	GLN
38	EL	441	GLN
38	EL	484	ASN
38	EL	498	ASN
38	EL	582	GLN
38	EL	593	GLN
39	EM	57	HIS
39	EM	128	ASN
39	EM	173	ASN
39	EM	192	HIS
39	EM	282	HIS
39	EM	324	GLN

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Mol	Chain	Res	Type
41	AN	19	HIS
41	AN	82	HIS
41	AN	190	GLN
42	BN	81	HIS
42	BN	118	ASN
42	BN	133	GLN
43	EN	34	ASN
43	EN	55	HIS
43	EN	71	GLN
43	EN	312	GLN
43	EN	340	GLN
43	EN	374	HIS
43	EN	514	HIS
43	EN	537	HIS
43	EN	674	HIS
44	BO	186	GLN
45	EO	13	HIS
45	EO	170	GLN
45	EO	201	GLN
45	EO	235	GLN
45	EO	259	HIS
45	EO	315	GLN
45	EO	318	HIS
46	AP	46	ASN
46	AP	89	GLN
45	EP	13	HIS
45	EP	28	GLN
45	EP	99	HIS
45	EP	131	GLN
45	EP	157	ASN
45	EP	201	GLN
45	EP	233	HIS
45	EP	235	GLN
47	BQ	134	HIS
47	BQ	147	ASN
48	AR	67	GLN
48	AR	68	GLN
48	AR	113	GLN
48	AR	174	HIS
48	AR	242	HIS
49	BR	138	GLN
49	BR	160	GLN

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Mol	Chain	Res	Type
49	BR	164	HIS
51	BS	69	ASN
52	ES	52	ASN
52	ES	128	GLN
53	AT	9	ASN
53	AT	18	ASN
53	AT	99	ASN
53	AT	123	GLN
54	BT	26	HIS
55	ET	15	ASN
55	ET	71	ASN
55	ET	92	GLN
56	AU	65	ASN
56	AU	73	HIS
56	AU	165	HIS
57	BU	49	ASN
57	BU	81	GLN
57	BU	156	GLN
58	AV	143	GLN
58	AV	160	HIS
60	AW	12	HIS
60	AW	50	GLN
60	AW	75	GLN
60	AW	172	HIS
60	AW	183	GLN
61	BW	61	ASN
61	BW	138	HIS
63	AY	64	HIS
63	AY	89	GLN
63	AY	91	GLN
63	AY	145	ASN
63	AY	162	GLN
63	AY	248	GLN
63	AY	265	GLN
63	AY	321	GLN
64	BZ	96	GLN
65	Ba	25	GLN
65	Ba	31	GLN
65	Ba	129	GLN
66	Bb	79	HIS
67	Bc	66	HIS
67	Bc	67	GLN

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Mol	Chain	Res	Type
68	Ae	96	GLN
68	Ae	162	GLN
69	Af	86	ASN
69	Af	168	GLN
70	Bf	108	HIS
71	Ag	73	ASN
71	Ag	84	ASN
71	Ag	105	GLN
71	Ag	184	HIS
72	E7	6	GLN
72	E7	44	GLN
72	E7	67	ASN
73	E8	536	ASN
73	E8	542	HIS
74	E9	156	GLN
74	E9	161	ASN
74	E9	192	GLN
74	E9	203	HIS
74	E9	261	HIS
75	Al	167	GLN
75	Al	194	HIS
75	Al	211	HIS
79	Ao	107	GLN
79	Ao	139	GLN
80	Ap	78	HIS
80	Ap	132	HIS
80	Ap	146	GLN
80	Ap	150	HIS
80	Ap	170	HIS
83	At	116	GLN
83	At	148	GLN
84	Av	44	ASN
84	Av	118	ASN
84	Av	128	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	AA	810/1176 (68%)	310 (38%)	3 (0%)

All (310) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	AA	2	U
12	AA	3	U
12	AA	4	U
12	AA	5	U
12	AA	11	U
12	AA	12	U
12	AA	13	A
12	AA	15	G
12	AA	18	G
12	AA	19	A
12	AA	20	A
12	AA	21	U
12	AA	28	A
12	AA	29	U
12	AA	30	A
12	AA	34	G
12	AA	41	U
12	AA	43	U
12	AA	44	A
12	AA	45	U
12	AA	50	A
12	AA	51	A
12	AA	52	U
12	AA	53	A
12	AA	54	A
12	AA	60	U
12	AA	64	U
12	AA	65	U
12	AA	67	C
12	AA	68	G
12	AA	69	U
12	AA	70	G
12	AA	73	G
12	AA	75	A
12	AA	77	A
12	AA	79	U
12	AA	80	U
12	AA	82	U
12	AA	84	A
12	AA	85	U
12	AA	88	G
12	AA	89	U
12	AA	97	A

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Mol	Chain	Res	Type
12	AA	98	U
12	AA	101	A
12	AA	102	A
12	AA	103	U
12	AA	104	A
12	AA	105	G
12	AA	106	G
12	AA	107	U
12	AA	111	U
12	AA	112	U
12	AA	113	A
12	AA	114	U
12	AA	115	A
12	AA	119	A
12	AA	120	A
12	AA	121	A
12	AA	122	U
12	AA	123	U
12	AA	124	U
12	AA	125	U
12	AA	133	U
12	AA	134	U
12	AA	149	U
12	AA	151	C
12	AA	155	U
12	AA	156	U
12	AA	158	A
12	AA	164	U
12	AA	168	A
12	AA	171	U
12	AA	172	U
12	AA	173	U
12	AA	176	A
12	AA	177	U
12	AA	183	U
12	AA	188	A
12	AA	193	A
12	AA	279	A
12	AA	284	U
12	AA	285	A
12	AA	286	U
12	AA	287	A

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Mol	Chain	Res	Type
12	AA	288	G
12	AA	289	U
12	AA	290	A
12	AA	292	G
12	AA	293	A
12	AA	296	A
12	AA	297	U
12	AA	299	U
12	AA	300	U
12	AA	302	G
12	AA	309	U
12	AA	310	A
12	AA	312	U
12	AA	313	A
12	AA	315	A
12	AA	317	A
12	AA	327	U
12	AA	330	U
12	AA	341	A
12	AA	342	U
12	AA	345	U
12	AA	346	G
12	AA	347	A
12	AA	355	A
12	AA	357	A
12	AA	360	U
12	AA	361	U
12	AA	365	C
12	AA	367	G
12	AA	371	A
12	AA	375	A
12	AA	378	A
12	AA	380	G
12	AA	381	U
12	AA	385	A
12	AA	386	U
12	AA	387	A
12	AA	388	U
12	AA	389	A
12	AA	446	A
12	AA	451	A
12	AA	453	U

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Mol	Chain	Res	Type
12	AA	455	G
12	AA	456	U
12	AA	462	U
12	AA	463	U
12	AA	464	U
12	AA	468	A
12	AA	470	G
12	AA	473	A
12	AA	476	G
12	AA	477	A
12	AA	478	A
12	AA	481	G
12	AA	482	U
12	AA	483	A
12	AA	485	A
12	AA	488	U
12	AA	490	G
12	AA	491	A
12	AA	492	U
12	AA	493	A
12	AA	494	U
12	AA	495	A
12	AA	496	A
12	AA	497	C
12	AA	509	U
12	AA	514	G
12	AA	515	U
12	AA	516	U
12	AA	517	U
12	AA	519	A
12	AA	521	G
12	AA	524	A
12	AA	525	A
12	AA	534	U
12	AA	539	A
12	AA	540	U
12	AA	544	G
12	AA	548	A
12	AA	549	G
12	AA	556	U
12	AA	557	A
12	AA	558	U

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Mol	Chain	Res	Type
12	AA	559	A
12	AA	560	G
12	AA	566	A
12	AA	567	G
12	AA	569	U
12	AA	570	U
12	AA	573	U
12	AA	574	A
12	AA	575	A
12	AA	582	A
12	AA	583	A
12	AA	584	A
12	AA	585	A
12	AA	587	U
12	AA	793	U
12	AA	799	A
12	AA	800	A
12	AA	801	A
12	AA	803	U
12	AA	804	A
12	AA	807	A
12	AA	814	A
12	AA	816	C
12	AA	817	A
12	AA	818	A
12	AA	825	A
12	AA	826	A
12	AA	827	U
12	AA	828	A
12	AA	829	A
12	AA	838	A
12	AA	844	A
12	AA	845	A
12	AA	846	A
12	AA	848	A
12	AA	851	G
12	AA	853	A
12	AA	854	A
12	AA	868	U
12	AA	870	A
12	AA	871	C
12	AA	873	A

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Mol	Chain	Res	Type
12	AA	874	A
12	AA	883	U
12	AA	885	U
12	AA	886	G
12	AA	887	A
12	AA	888	U
12	AA	892	U
12	AA	895	U
12	AA	896	U
12	AA	897	G
12	AA	902	U
12	AA	905	G
12	AA	906	A
12	AA	924	U
12	AA	928	U
12	AA	931	U
12	AA	932	A
12	AA	933	U
12	AA	934	A
12	AA	936	C
12	AA	941	G
12	AA	942	A
12	AA	945	U
12	AA	946	A
12	AA	947	U
12	AA	948	A
12	AA	956	A
12	AA	961	A
12	AA	963	A
12	AA	970	U
12	AA	980	U
12	AA	984	A
12	AA	985	A
12	AA	986	G
12	AA	990	U
12	AA	991	A
12	AA	992	A
12	AA	993	A
12	AA	994	A
12	AA	995	A
12	AA	996	U
12	AA	998	A

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Mol	Chain	Res	Type
12	AA	1003	G
12	AA	1004	U
12	AA	1006	U
12	AA	1008	A
12	AA	1010	C
12	AA	1014	U
12	AA	1015	A
12	AA	1018	U
12	AA	1019	A
12	AA	1021	U
12	AA	1079	A
12	AA	1089	G
12	AA	1091	U
12	AA	1092	U
12	AA	1094	U
12	AA	1096	U
12	AA	1097	A
12	AA	1102	A
12	AA	1107	U
12	AA	1112	U
12	AA	1113	U
12	AA	1114	A
12	AA	1116	U
12	AA	1117	A
12	AA	1119	U
12	AA	1122	U
12	AA	1123	U
12	AA	1125	A
12	AA	1127	A
12	AA	1128	U
12	AA	1131	G
12	AA	1133	A
12	AA	1139	G
12	AA	1140	G
12	AA	1141	A
12	AA	1148	A
12	AA	1152	A
12	AA	1153	A
12	AA	1154	A
12	AA	1155	A
12	AA	1156	A
12	AA	1157	A

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Mol	Chain	Res	Type
12	AA	1158	G
12	AA	1159	A
12	AA	1160	A
12	AA	1161	A
12	AA	1162	G
12	AA	1163	A
12	AA	1164	A
12	AA	1165	G
12	AA	1166	A
12	AA	1168	U
12	AA	1169	A
12	AA	1171	A
12	AA	1173	U
12	AA	1175	U
12	AA	1176	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	AA	102	A
12	AA	484	U
12	AA	895	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 31 ligands modelled in this entry, 26 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	GTP	EA	1001	86,88	26,34,34	1.18	2 (7%)	32,54,54	1.54	7 (21%)
89	ATP	EB	1001	86	26,33,33	0.94	1 (3%)	31,52,52	1.50	5 (16%)
90	PM8	ER	200	50	25,31,31	0.54	0	30,38,38	1.34	2 (6%)
87	GTP	EA	1004	86,88	26,34,34	1.14	2 (7%)	32,54,54	1.46	7 (21%)
91	NAD	Av	301	-	42,48,48	0.64	1 (2%)	50,73,73	0.91	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	GTP	EA	1001	86,88	-	0/18/38/38	0/3/3/3
89	ATP	EB	1001	86	-	1/18/38/38	0/3/3/3
90	PM8	ER	200	50	-	11/36/38/38	-
87	GTP	EA	1004	86,88	-	2/18/38/38	0/3/3/3
91	NAD	Av	301	-	-	3/26/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	EA	1001	GTP	C5-C6	-4.04	1.39	1.47
87	EA	1004	GTP	C5-C6	-3.96	1.39	1.47
89	EB	1001	ATP	C5-C4	2.44	1.47	1.40
87	EA	1004	GTP	C2-N3	2.16	1.38	1.33
91	Av	301	NAD	C2N-N1N	2.14	1.37	1.35
87	EA	1001	GTP	C2-N3	2.09	1.38	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	Av	301	NAD	O4D-C1D-C2D	-3.72	101.48	106.93
89	EB	1001	ATP	PA-O3A-PB	-3.71	120.09	132.83
87	EA	1004	GTP	PB-O3B-PG	-3.57	120.56	132.83
87	EA	1001	GTP	PB-O3B-PG	-3.52	120.74	132.83
87	EA	1001	GTP	PA-O3A-PB	-3.27	121.61	132.83
87	EA	1001	GTP	C5-C6-N1	3.26	119.72	113.95

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	EA	1004	GTP	C8-N7-C5	3.23	109.14	102.99
89	EB	1001	ATP	N3-C2-N1	-3.22	123.64	128.68
87	EA	1004	GTP	C5-C6-N1	3.20	119.60	113.95
90	ER	200	PM8	O1-C1-C2	-3.15	120.27	123.99
87	EA	1001	GTP	C8-N7-C5	3.09	108.89	102.99
89	EB	1001	ATP	C3'-C2'-C1'	2.89	105.33	100.98
89	EB	1001	ATP	PB-O3B-PG	-2.86	123.01	132.83
87	EA	1004	GTP	C2-N1-C6	-2.86	119.84	125.10
89	EB	1001	ATP	C4-C5-N7	-2.77	106.52	109.40
90	ER	200	PM8	C3-C2-C1	-2.73	106.28	112.33
87	EA	1001	GTP	C2-N1-C6	-2.71	120.11	125.10
87	EA	1001	GTP	O3'-C3'-C2'	-2.44	103.92	111.82
91	Av	301	NAD	C6N-N1N-C2N	-2.29	119.89	121.97
91	Av	301	NAD	C5A-C6A-N6A	2.26	123.79	120.35
87	EA	1004	GTP	O4'-C1'-C2'	-2.15	103.78	106.93
87	EA	1004	GTP	PA-O3A-PB	-2.14	125.49	132.83
87	EA	1004	GTP	O6-C6-C5	-2.07	120.33	124.37
87	EA	1001	GTP	O6-C6-C5	-2.06	120.34	124.37

There are no chirality outliers.

All (17) torsion outliers are listed below:

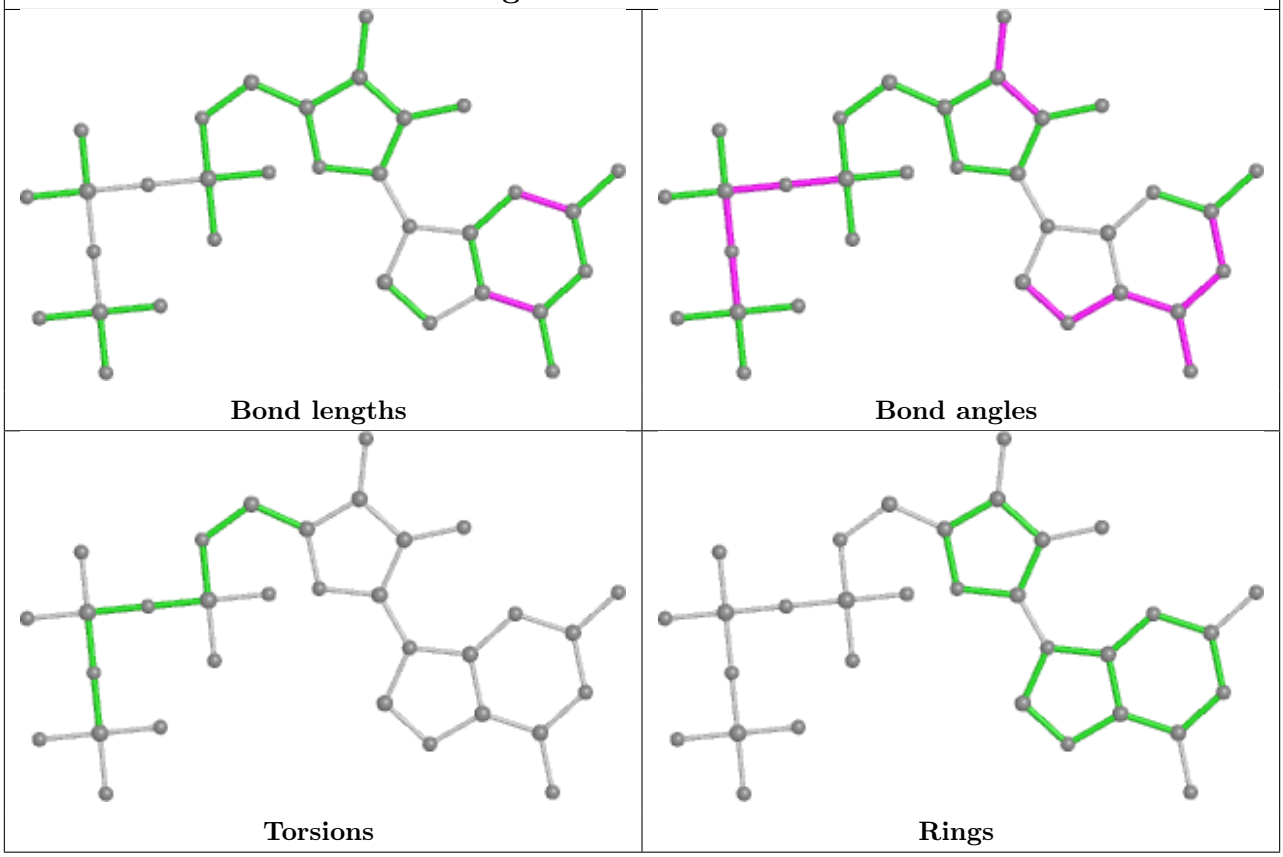
Mol	Chain	Res	Type	Atoms
90	ER	200	PM8	O27-C28-C29-C32
90	ER	200	PM8	O33-C32-C34-N36
90	ER	200	PM8	N41-C42-C43-S1
90	ER	200	PM8	O1-C1-S1-C43
90	ER	200	PM8	C2-C1-S1-C43
90	ER	200	PM8	C1-C2-C3-C4
90	ER	200	PM8	C38-C37-N36-C34
90	ER	200	PM8	O27-C28-C29-C30
90	ER	200	PM8	O27-C28-C29-C31
90	ER	200	PM8	O33-C32-C34-O35
91	Av	301	NAD	O4B-C4B-C5B-O5B
91	Av	301	NAD	O4D-C4D-C5D-O5D
87	EA	1004	GTP	C5'-O5'-PA-O3A
89	EB	1001	ATP	PA-O3A-PB-O1B
90	ER	200	PM8	C42-C43-S1-C1
91	Av	301	NAD	C3D-C4D-C5D-O5D
87	EA	1004	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

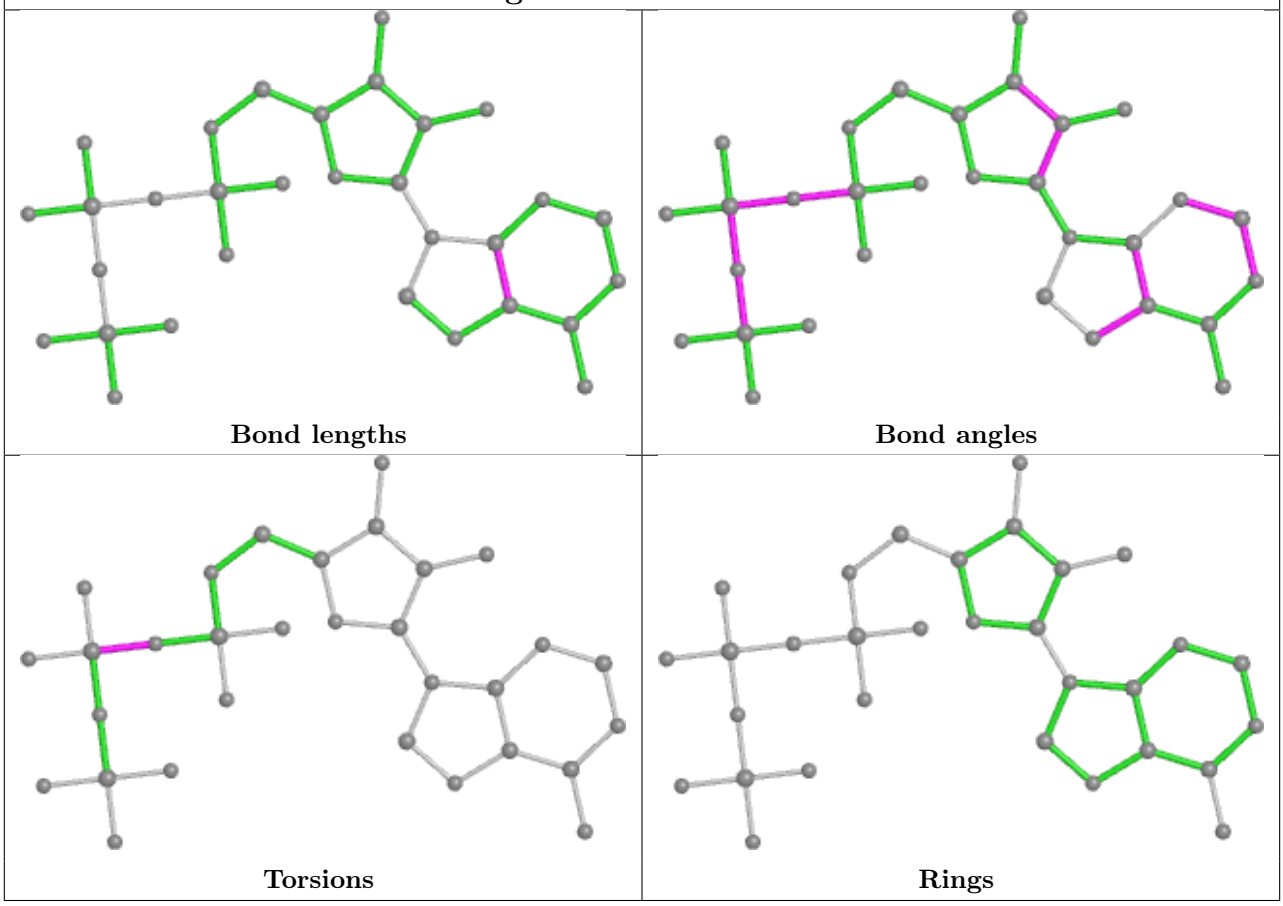
No monomer is involved in short contacts.

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

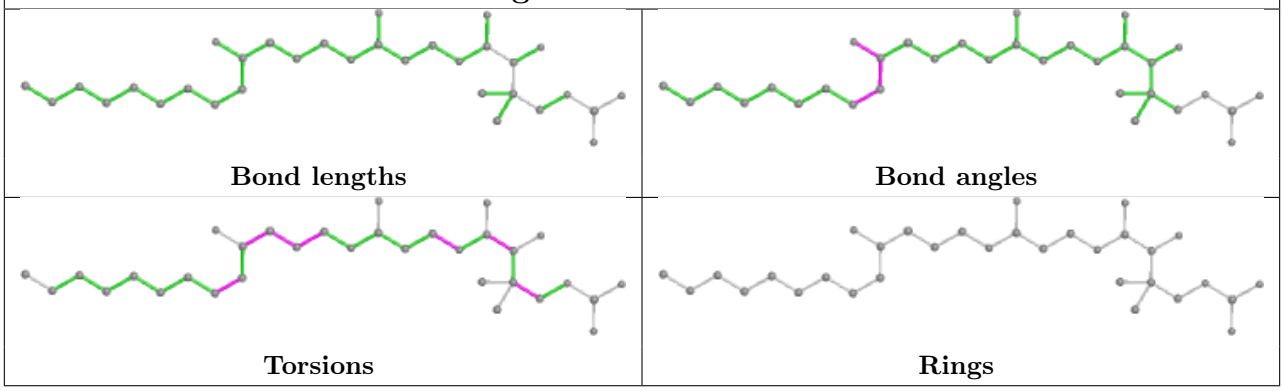
Ligand GTP EA 1001



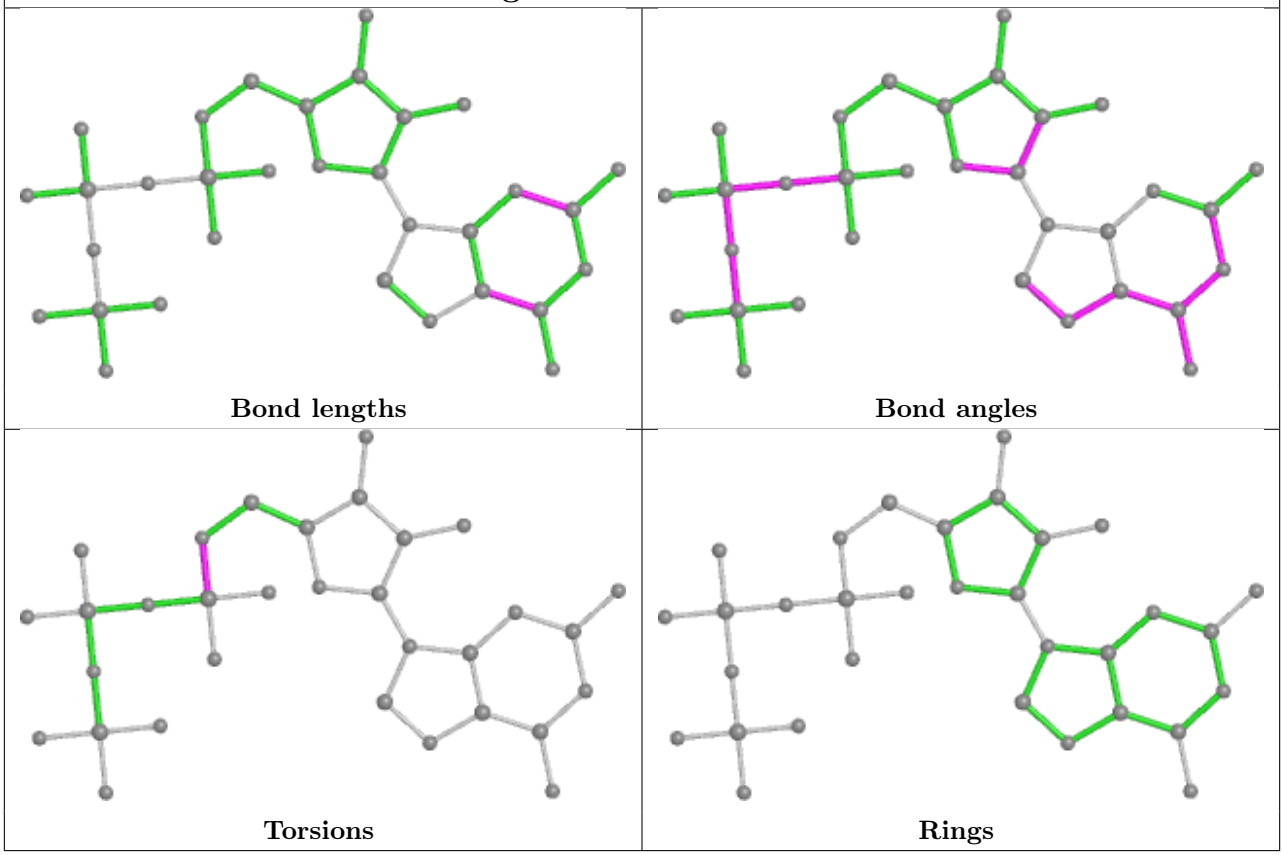
Ligand ATP EB 1001



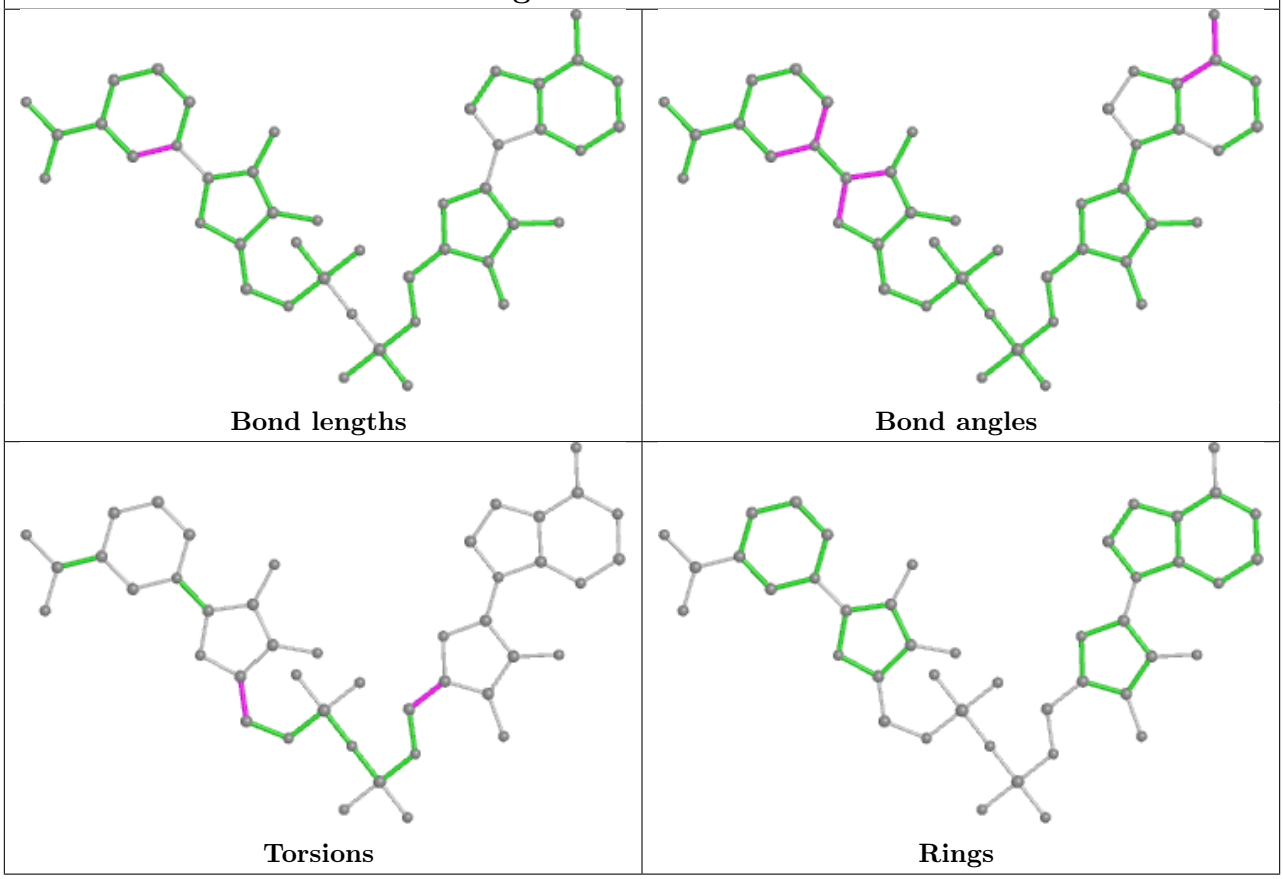
Ligand PM8 ER 200



Ligand GTP EA 1004



Ligand NAD Av 301



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
76	Ul	7
9	E5	5
82	Us	4
81	Up	3
77	Um	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ul	249:UNK	C	280:UNK	N	50.91
1	Ul	115:UNK	C	146:UNK	N	43.56
1	Ul	158:UNK	C	179:UNK	N	35.52
1	Us	63:UNK	C	82:UNK	N	32.92
1	Ul	295:UNK	C	311:UNK	N	29.90
1	Us	38:UNK	C	52:UNK	N	20.32
1	Us	96:UNK	C	110:UNK	N	17.98
1	Ul	337:UNK	C	348:UNK	N	15.67
1	E5	103:UNK	C	124:UNK	N	15.44
1	E5	133:UNK	C	144:UNK	N	15.38
1	Us	14:UNK	C	19:UNK	N	15.06
1	E5	88:UNK	C	94:UNK	N	13.57
1	E5	279:UNK	C	290:UNK	N	12.66
1	Up	83:UNK	C	89:UNK	N	11.90
1	Up	53:UNK	C	64:UNK	N	6.74
1	Ul	221:UNK	C	232:UNK	N	6.33
1	Um	21:UNK	C	100:UNK	N	5.55
1	Up	33:UNK	C	44:UNK	N	4.72
1	Ul	45:UNK	C	56:UNK	N	3.64
1	E5	311:UNK	C	314:UNK	N	3.12

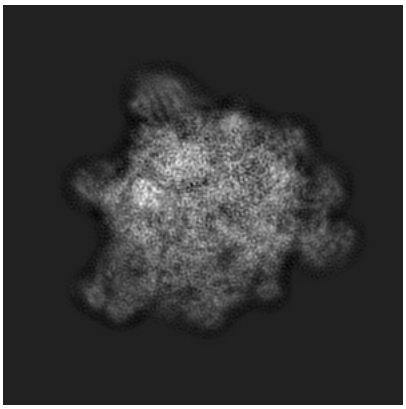
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10999. These allow visual inspection of the internal detail of the map and identification of artifacts.

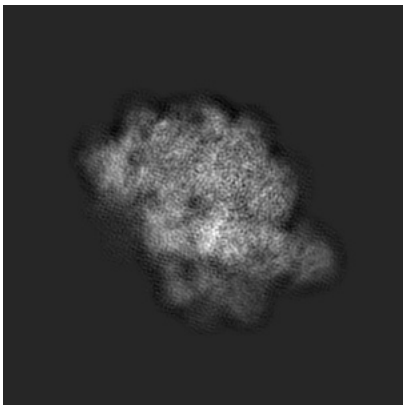
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

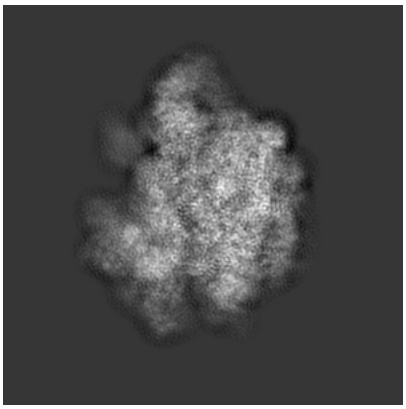
6.1.1 Primary map



X

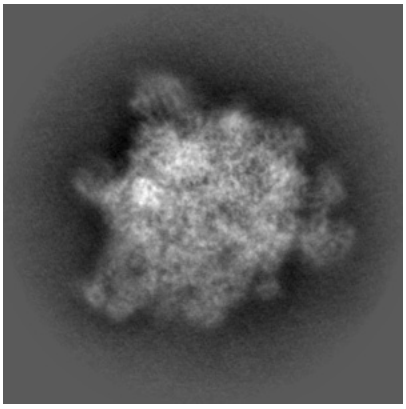


Y

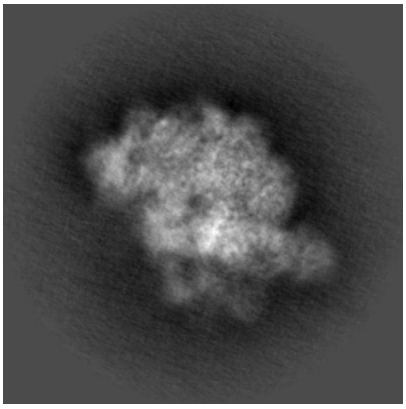


Z

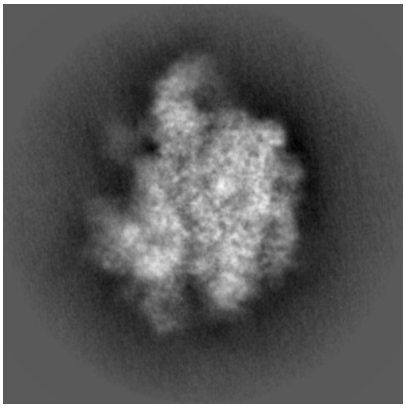
6.1.2 Raw map



X



Y

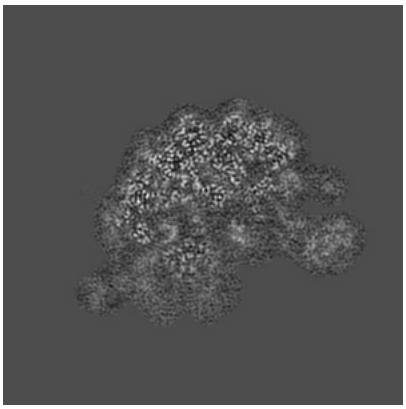


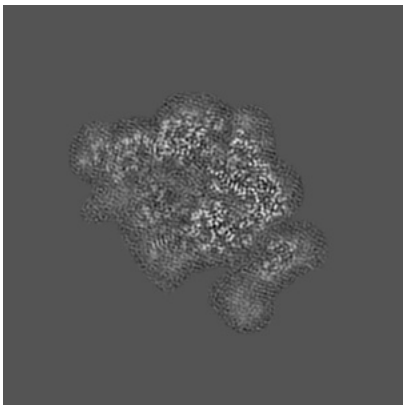
Z

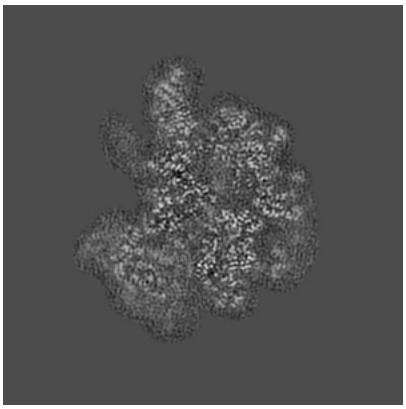
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

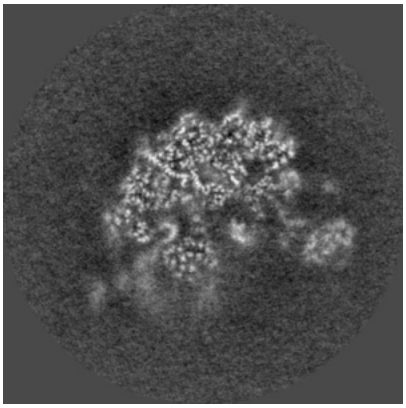
6.2.1 Primary map

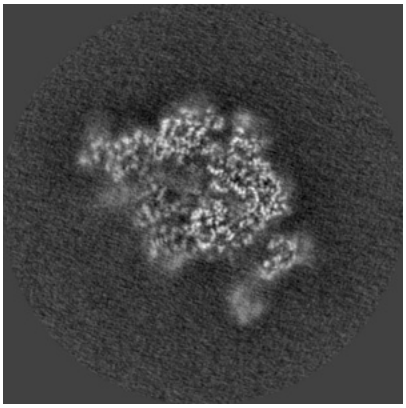

X Index: 150

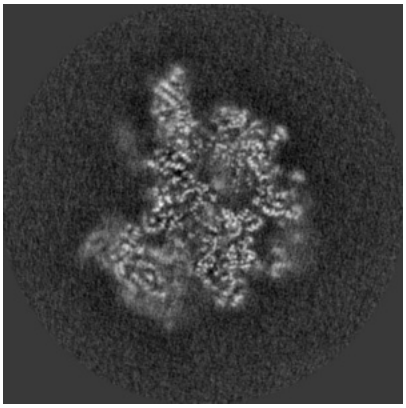

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

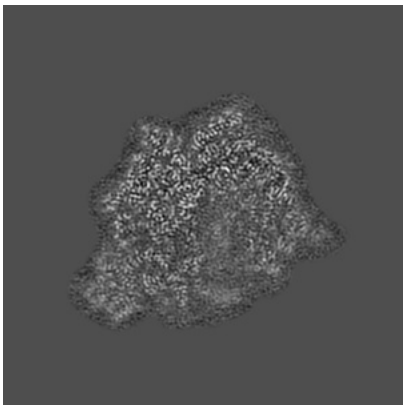

Y Index: 150


Z Index: 150

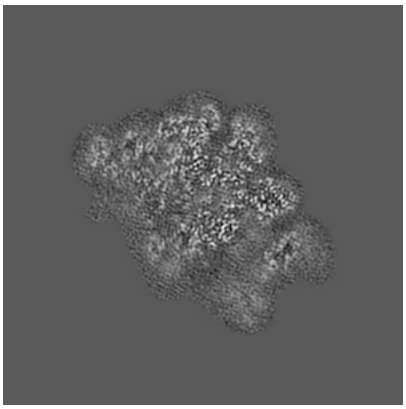
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

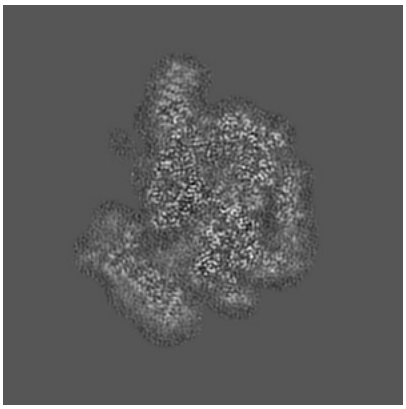
6.3.1 Primary map



X Index: 168

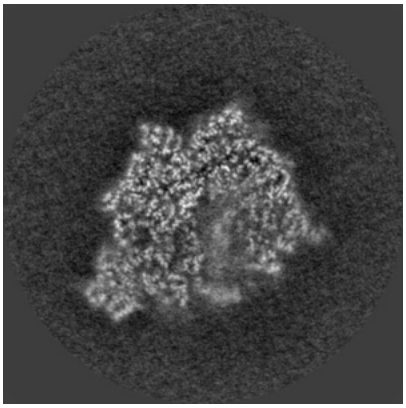


Y Index: 143

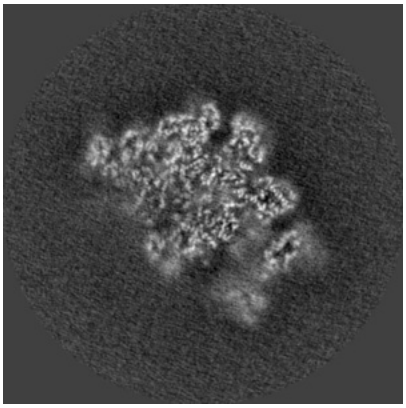


Z Index: 157

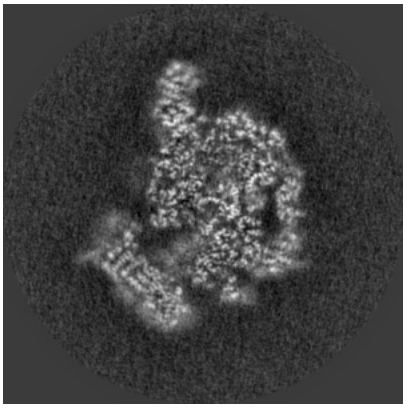
6.3.2 Raw map



X Index: 168



Y Index: 143



Z Index: 158

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 0.03. 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.

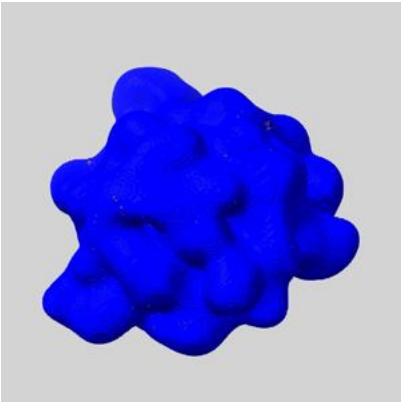
6.5 Mask visualisation (i)

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

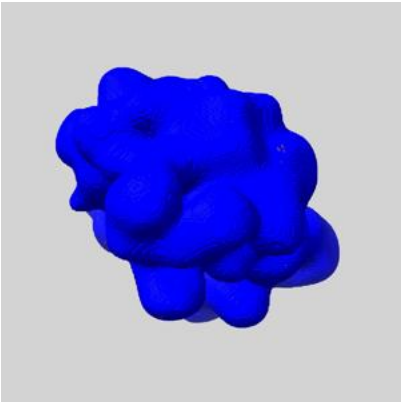
A mask typically either:

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

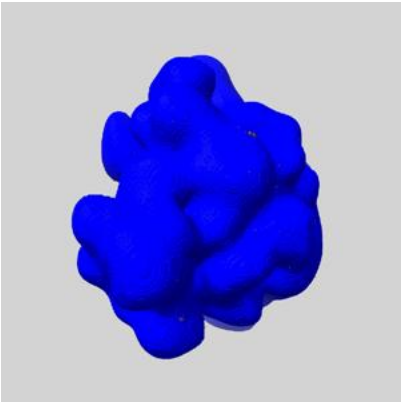
6.5.1 emd_10999_msk_1.map (i)



X



Y

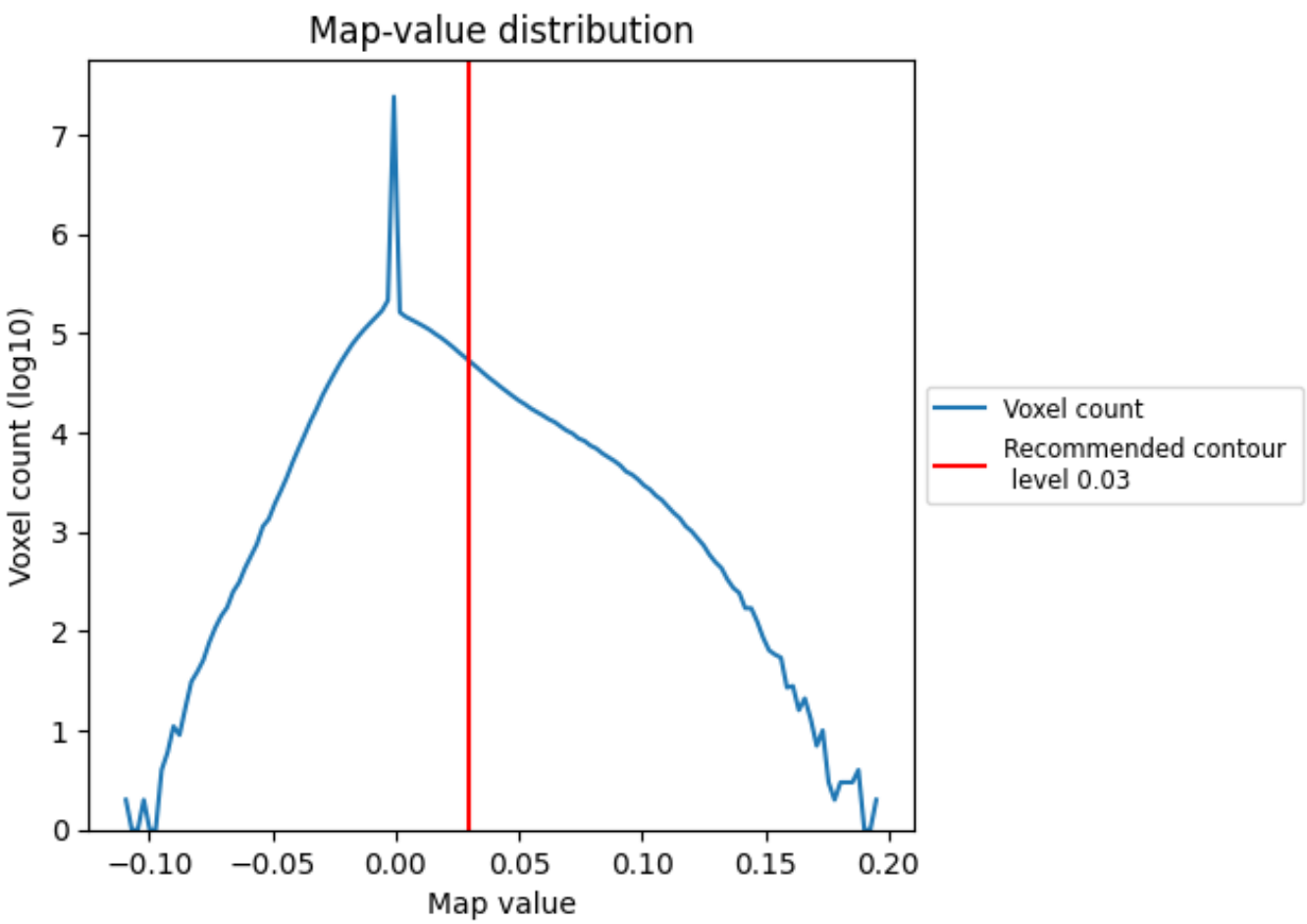


Z

7 Map analysis (i)

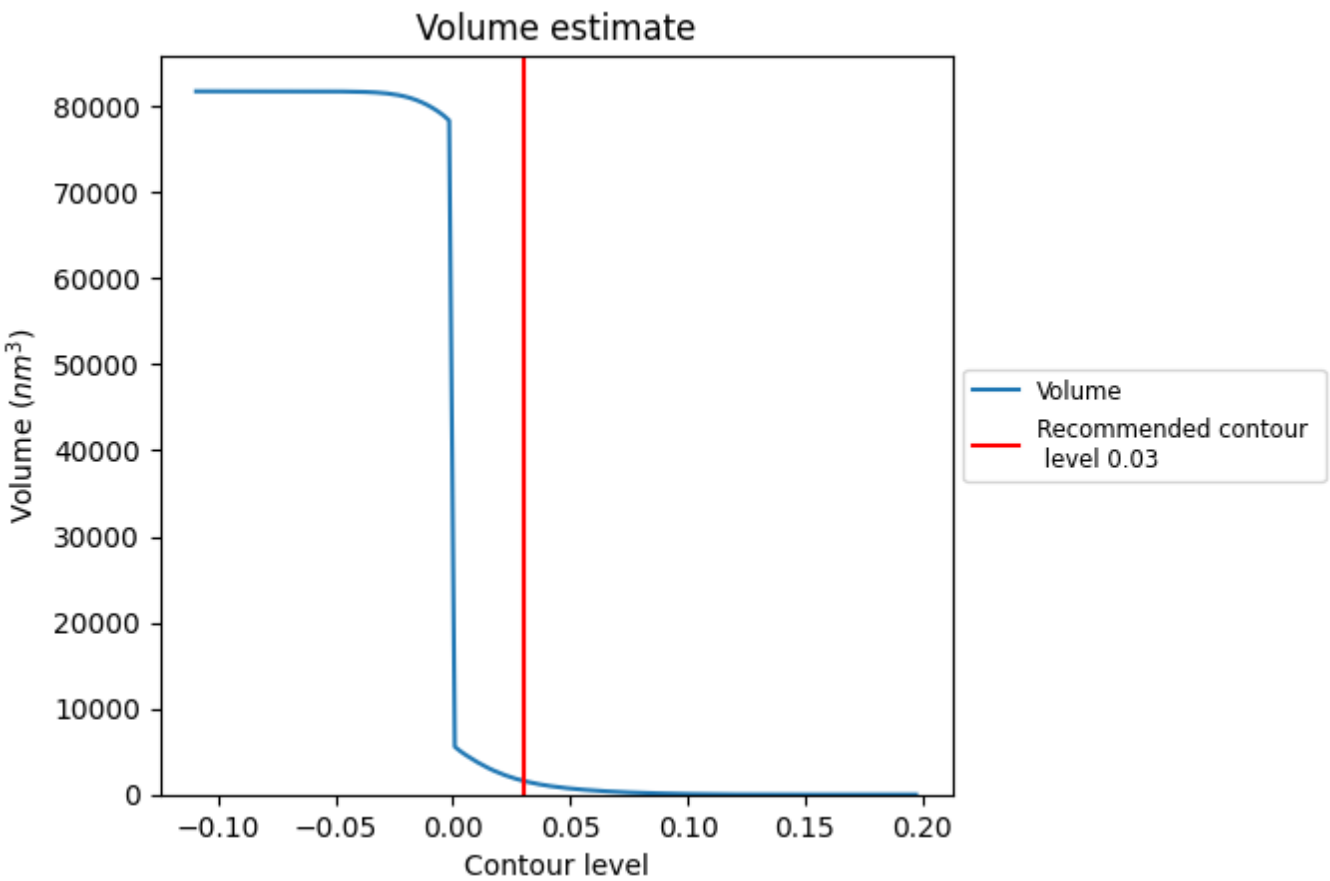
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

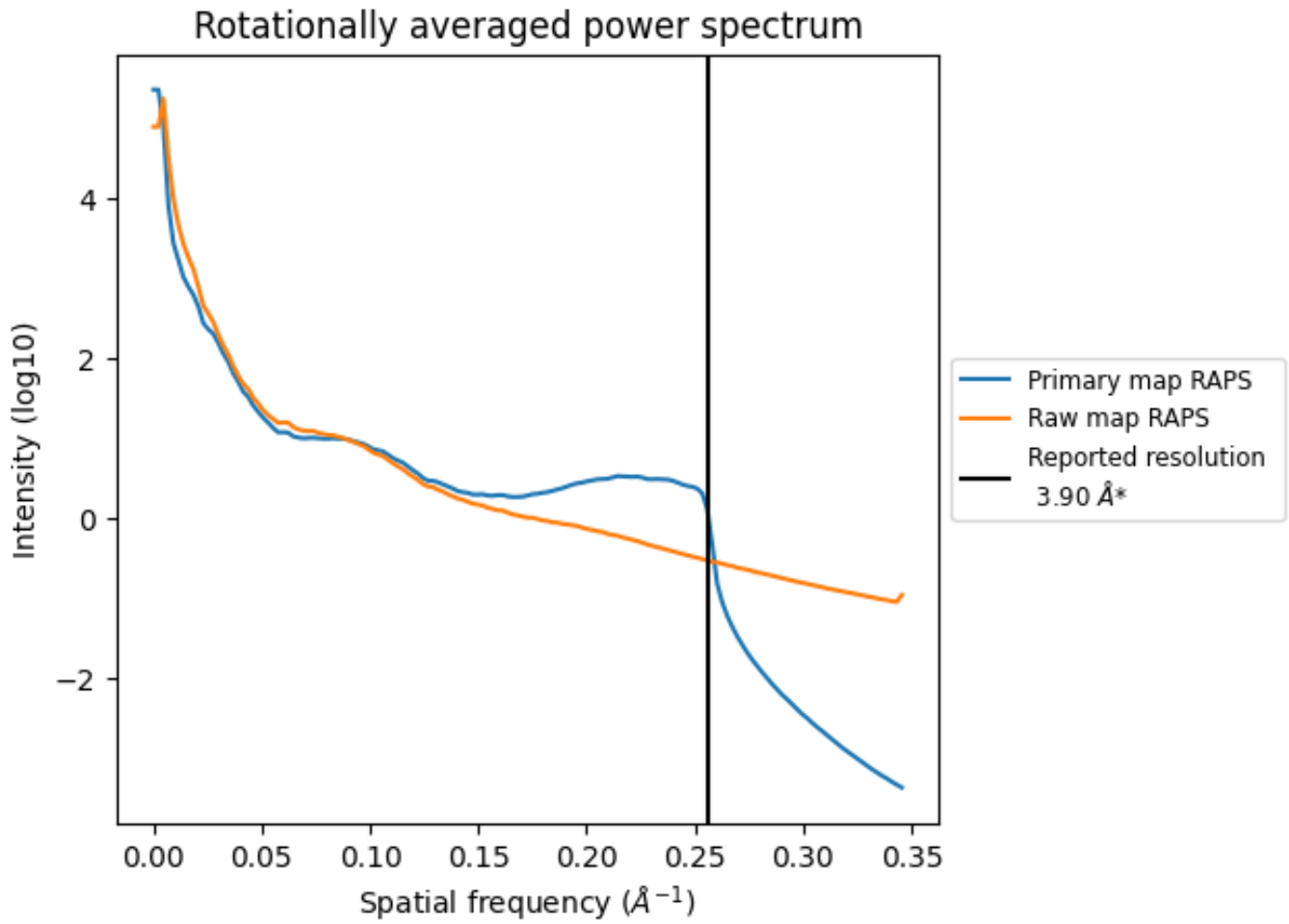
7.2 Volume estimate (i)



The volume at the recommended contour level is 1601 nm^3; this corresponds to an approximate mass of 1446 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)

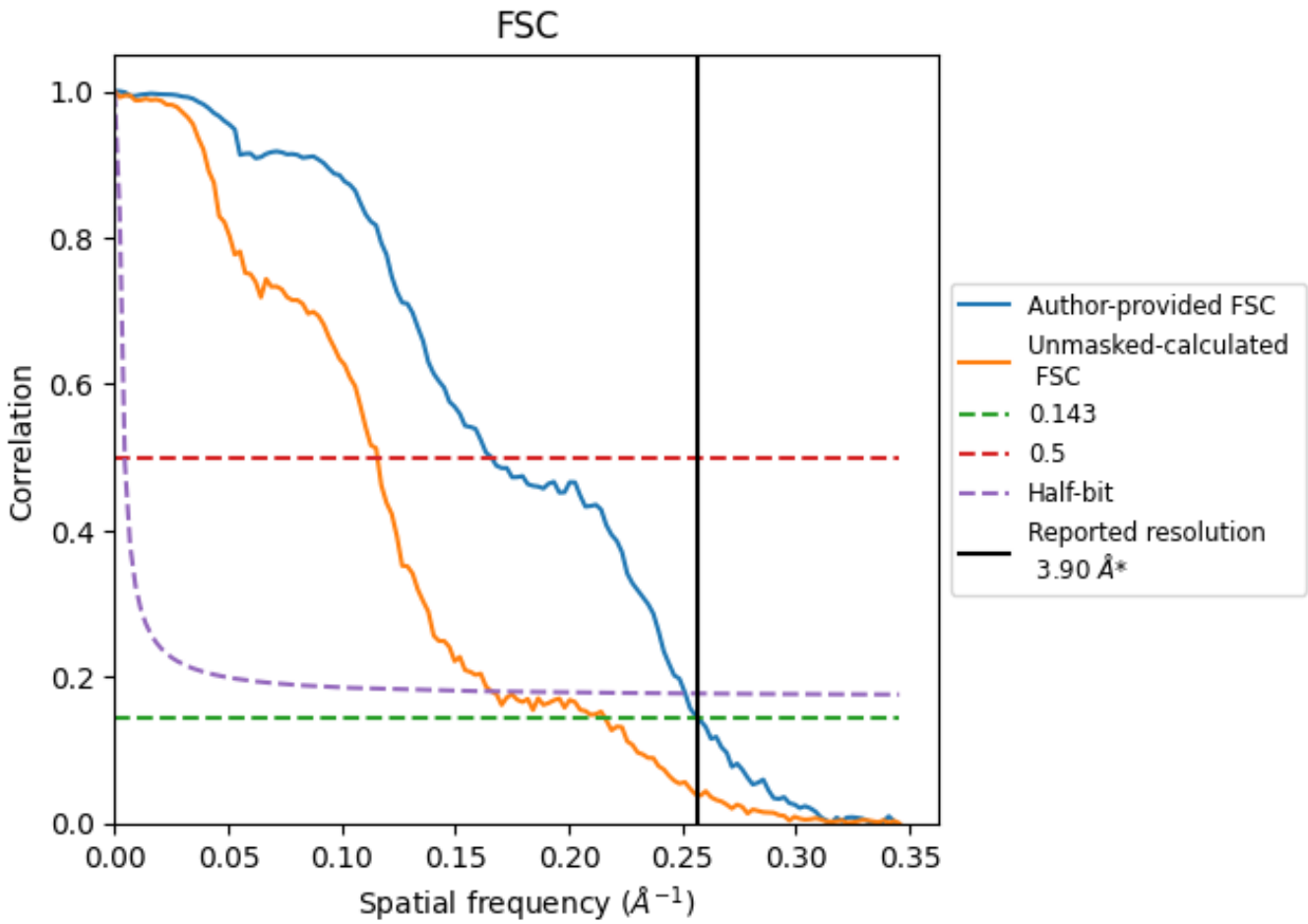


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

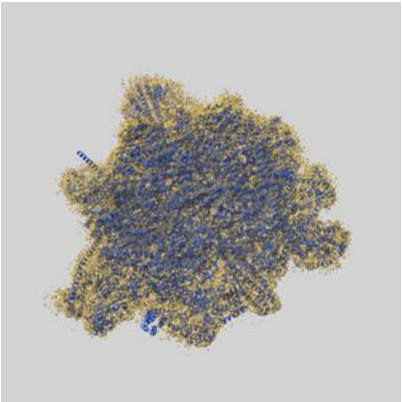
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.89	6.03	3.98
Unmasked-calculated*	4.63	8.64	6.02

*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 4.63 differs from the reported value 3.9 by more than 10 %

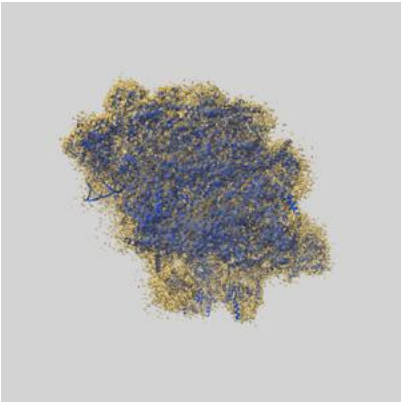
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10999 and PDB model 6YXX. Per-residue inclusion information can be found in section 3 on page 26.

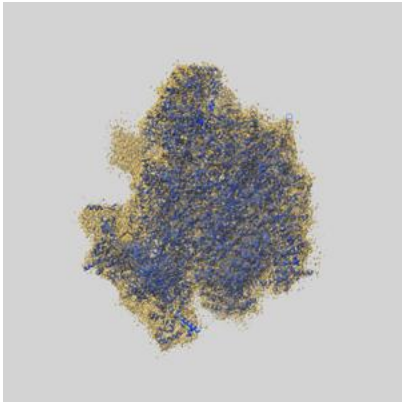
9.1 Map-model overlay (i)



X



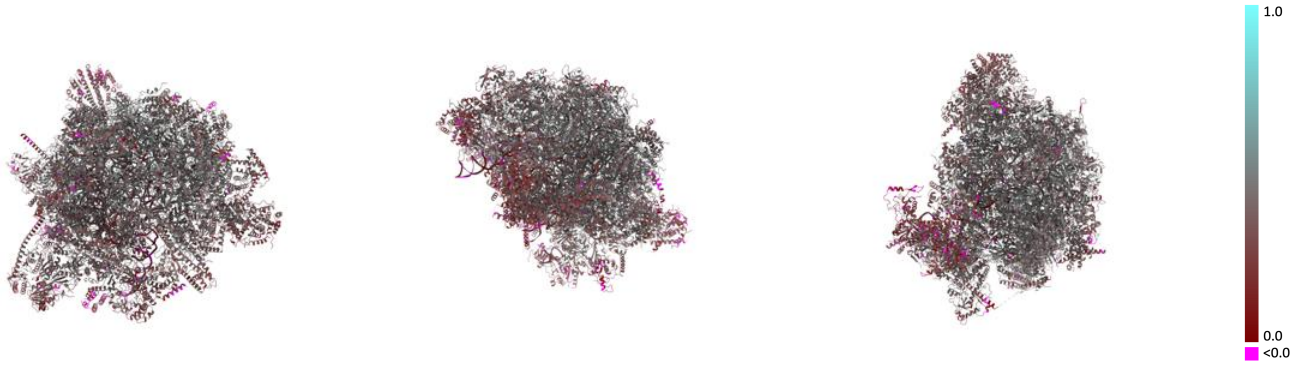
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

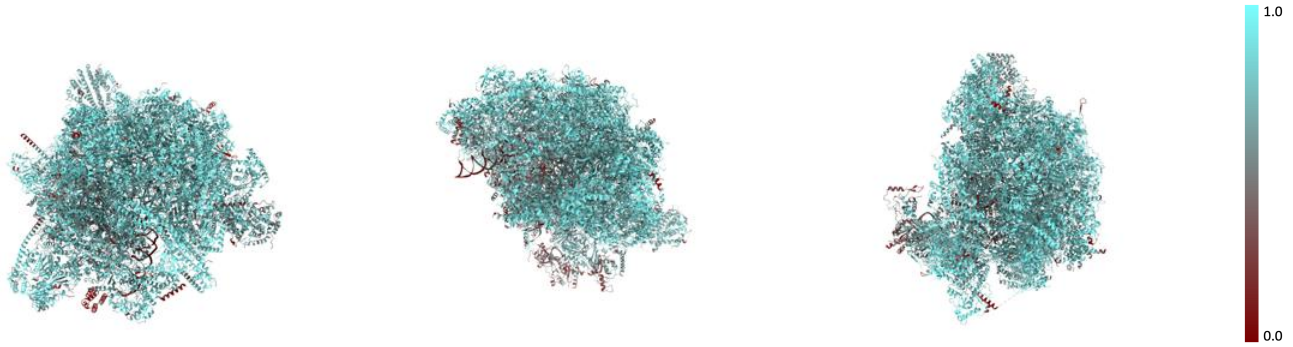
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

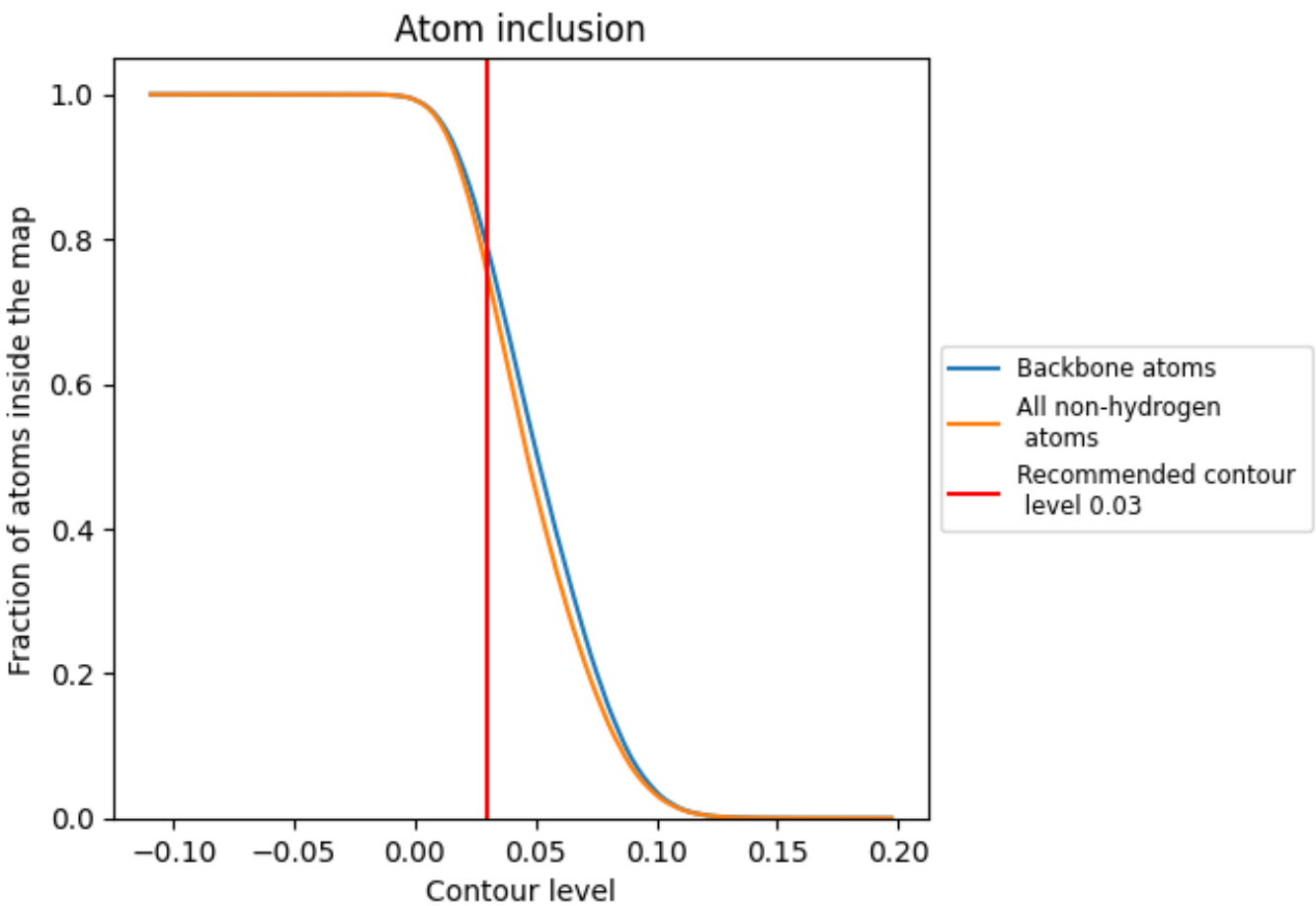
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 75% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7515	0.3890
A1	0.7496	0.3900
A2	0.8495	0.4290
A3	0.8045	0.4430
A5	0.8584	0.4800
A8	0.6972	0.4360
AA	0.7508	0.3430
AE	0.8064	0.4560
AF	0.8398	0.4530
AI	0.7459	0.3920
AK	0.6672	0.3000
AN	0.7855	0.4520
AP	0.7929	0.4350
AR	0.7968	0.4380
AT	0.7863	0.4370
AU	0.8332	0.4590
AV	0.8539	0.4670
AW	0.8071	0.4480
AX	0.8255	0.4500
AY	0.7970	0.4080
Ae	0.8240	0.4290
Af	0.8210	0.4340
Ag	0.8130	0.4310
Al	0.8045	0.4410
Ao	0.8181	0.4570
Ap	0.7959	0.4250
At	0.7940	0.4280
Av	0.7857	0.4260
BA	0.8301	0.4230
BB	0.7898	0.3550
BD	0.6262	0.3090
BE	0.8357	0.4090
BF	0.8476	0.4380
BH	0.6561	0.3800
BI	0.8393	0.4280

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Chain	Atom inclusion	Q-score
BJ	0.7849	0.3360
BK	0.7282	0.3670
BL	0.8176	0.4040
BN	0.7796	0.3940
BO	0.8109	0.4000
BQ	0.8228	0.4210
BR	0.8069	0.4390
BS	0.7905	0.3800
BT	0.8547	0.4260
BU	0.7227	0.3950
BV	0.4032	0.0930
BW	0.8769	0.4480
BZ	0.8301	0.3780
Ba	0.8071	0.4310
Bb	0.8283	0.3960
Bc	0.6577	0.3960
Bf	0.6501	0.3730
E1	0.6734	0.4160
E2	0.6848	0.3830
E3	0.6991	0.3940
E4	0.7622	0.3490
E5	0.8336	0.3500
E6	0.6933	0.3920
E7	0.7008	0.4230
E8	0.5009	0.3100
E9	0.5808	0.3770
EA	0.7046	0.3890
EB	0.7854	0.4530
EC	0.7651	0.4450
ED	0.8466	0.4290
EE	0.7242	0.3530
EF	0.3228	0.2350
EG	0.8029	0.4750
EH	0.8058	0.4040
EL	0.8361	0.4000
EM	0.6165	0.3150
EN	0.7689	0.3530
EO	0.7504	0.2990
EP	0.7047	0.2070
ER	0.7676	0.3110
ES	0.7642	0.2940
ET	0.7454	0.4380

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Chain	Atom inclusion	Q-score
UA	0.8400	0.4510
UI	0.1048	0.1140
UK	0.5360	0.2010
UM	0.7000	0.4390
Uf	0.5400	0.2210
Ul	0.5529	0.2870
Um	0.6667	0.2980
Un	0.7571	0.3850
Up	0.0621	0.1140
Ur	0.1143	0.1340
Us	0.0861	0.0630