wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 08:22 am GMT

PDB ID	:	6YXY
EMDB ID	:	EMD-11000
Title	:	State B 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	:	3.10 Å(reported)

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

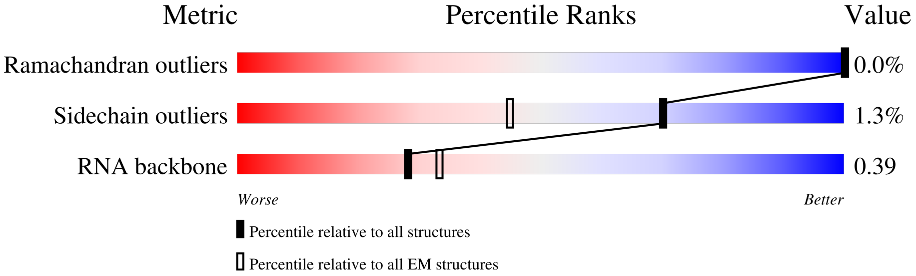
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance ⓘ

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

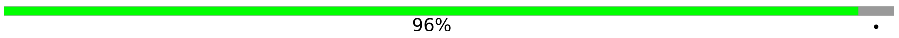
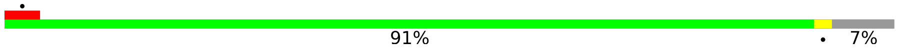
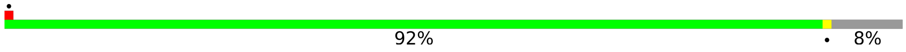
The reported resolution of this entry is 3.10 Å.

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	
2	A2	471	
3	A3	218	
4	A5	80	
5	A8	181	
6	AA	1176	
7	BA	831	
8	EA	576	

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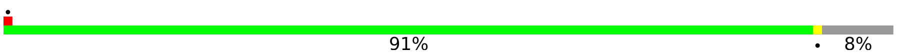
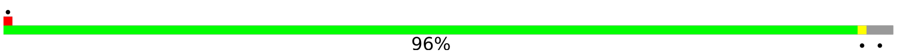
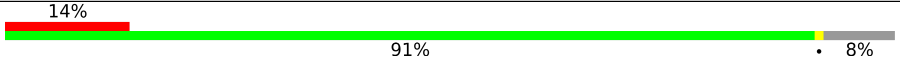
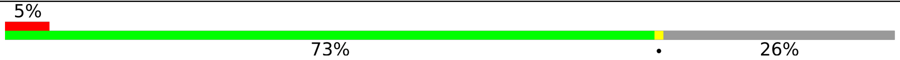
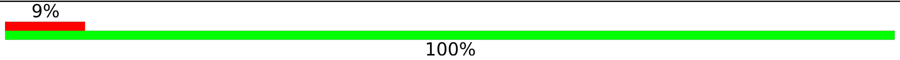
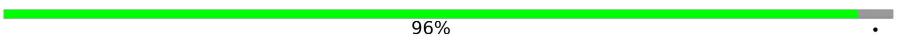
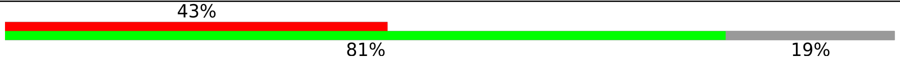
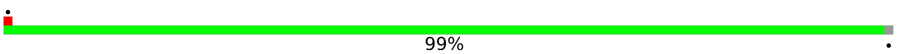
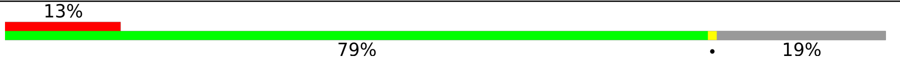
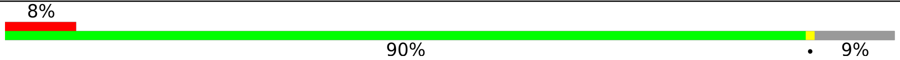
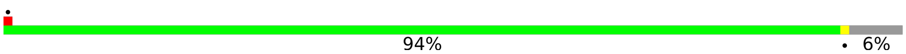
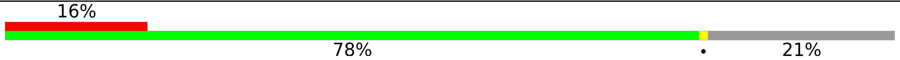
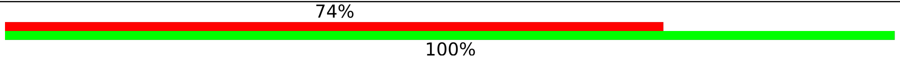
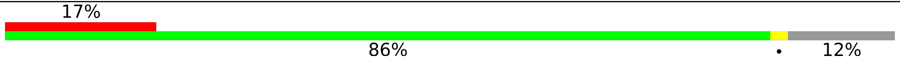
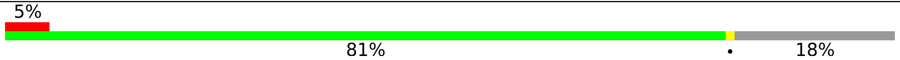
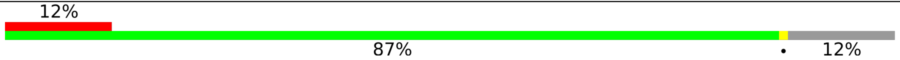
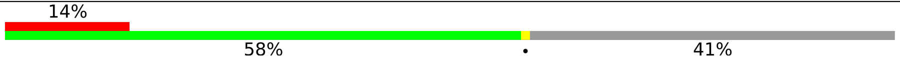
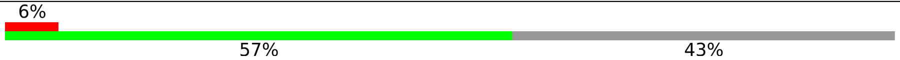
Mol	Chain	Length	Quality of chain
9	BB	541	 9% 74% 24%
10	EB	754	 88% 12%
11	EC	406	 91% 8%
12	BD	547	 75% 23%
13	ED	616	 96%
14	AE	473	 14% 91% 8%
15	BE	449	 88% 9%
16	EE	586	 5% 73% 26%
17	UE	33	 9% 100%
18	AF	459	 96%
19	BF	426	 81% 19%
20	EF	373	 43% 81% 19%
21	EG	156	 99%
22	BH	349	 13% 79% 19%
23	EH	634	 69% 31%
24	AI	263	 8% 90% 9%
25	BI	342	 94% 6%
26	EI	349	 16% 78% 21%
27	UI	23	 74% 100%
28	BJ	333	 17% 86% 12%
29	EJ	116	 5% 81% 18%
30	AK	342	 12% 87% 12%
31	BK	386	 14% 58% 41%
32	EK	148	 6% 57% 43%
32	ER	148	 57% 43%

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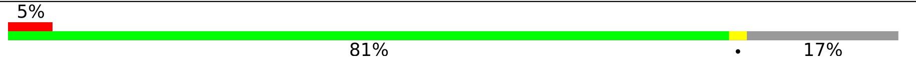
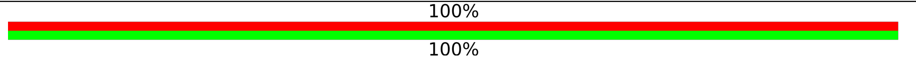
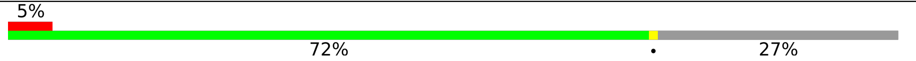
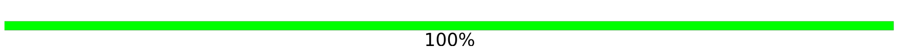
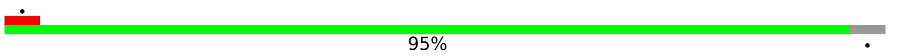
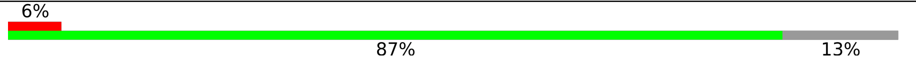
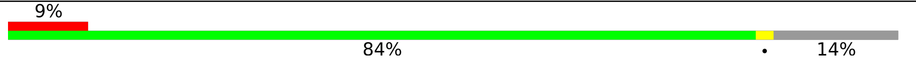
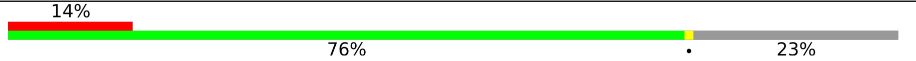
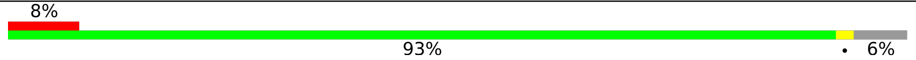
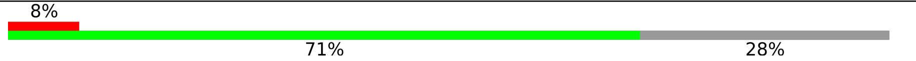
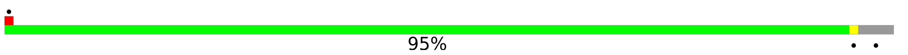
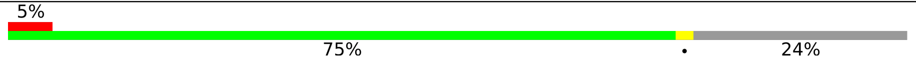
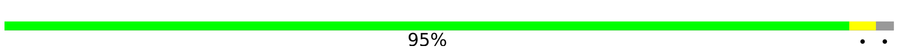
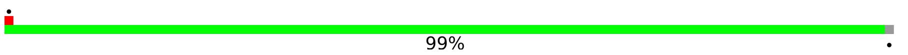
Mol	Chain	Length	Quality of chain
33	UK	25	
34	BL	312	
35	EL	691	
36	UL	72	
37	EM	451	
38	UM	8	
39	AN	202	
40	BN	302	
41	EN	731	
42	AO	217	
43	BO	262	
44	EO	319	
44	EP	319	
45	AP	374	
46	BQ	231	
47	EQ	655	
48	AR	301	
49	BR	205	
50	BS	198	
51	ES	524	
52	AT	144	
53	BT	191	
54	ET	102	
55	AU	213	
56	BU	185	

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Mol	Chain	Length	Quality of chain
57	EU	56	14% 82% • 16%
58	AV	188	95% • •
59	BV	190	22% 47% • 53%
60	AW	278	100%
61	BW	188	96% • •
62	AX	246	67% 33%
63	BX	190	45% 67% • 30%
64	UX	180	100% 100%
65	AY	378	• 89% • 10%
66	BZ	190	8% 97% •
67	Ba	153	• 92% • 7%
68	Bb	162	• 79% 21%
69	Bc	146	• 92% • 6%
70	Ae	197	• 64% • 36%
71	Af	189	72% • 26%
72	Bf	113	6% 76% • 23%
73	Ag	260	• 72% 28%
74	Bg	105	• 78% • 21%
75	Bh	92	• 98% ••
76	Bi	245	41% 76% • 22%
77	Al	218	• 83% 17%
78	Ao	1520	12% 88%
79	Ap	309	• 96% •
80	At	154	• 88% • 10%
81	Av	242	81% 19%

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 177224 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 uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A2	452	3661	2337	635	676	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 3 is a protein called uL30m.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	22	VAL	GLY	conflict	UNP Q38ED8
A3	26	SER	LEU	conflict	UNP Q38ED8
A3	35	ASN	SER	conflict	UNP Q38ED8
A3	198	UNK	ALA	conflict	UNP Q38ED8

- Molecule 4 is a protein called bL32m.

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

- Molecule 5 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A8	142	Total 1203	C 753	N 243	O 198	S 9	0	0

- Molecule 6 is a RNA chain called 12S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AA	903	Total 18833	C 8482	N 3157	O 6291	P 903	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1032	N	A	conflict	GB 343546
AA	1033	N	U	conflict	GB 343546
AA	1034	N	U	conflict	GB 343546
AA	1035	N	G	conflict	GB 343546
AA	1036	N	U	conflict	GB 343546
AA	1037	N	U	conflict	GB 343546
AA	1038	N	C	conflict	GB 343546
AA	1039	N	A	conflict	GB 343546
AA	1040	N	U	conflict	GB 343546
AA	1041	N	C	conflict	GB 343546
AA	1042	N	A	conflict	GB 343546
AA	1043	N	A	conflict	GB 343546
AA	1044	N	A	conflict	GB 343546
AA	1045	N	A	conflict	GB 343546
AA	1046	N	U	conflict	GB 343546
AA	1047	N	A	conflict	GB 343546
AA	1048	N	G	conflict	GB 343546
AA	1049	N	U	conflict	GB 343546

- Molecule 7 is a protein called mL67.

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

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	359	CYS	GLY	conflict	UNP Q386Z1

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Chain	Residue	Modelled	Actual	Comment	Reference
BA	385	PRO	SER	conflict	UNP Q386Z1
BA	387	SER	GLY	conflict	UNP Q386Z1
BA	456	ALA	VAL	conflict	UNP Q386Z1
BA	520	LEU	ARG	conflict	UNP Q386Z1

- Molecule 8 is a protein called mt-EngA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	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 9 is a protein called mL68.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	BB	412	3365	2142	595	607	21	0	0

- Molecule 10 is a protein called mt-LAF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	EB	663	5308	3344	1017	920	27	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 11 is a protein called mt-LAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	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 12 is a protein called mL70.

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

- Molecule 13 is a protein called mt-LAF4.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ED	252	ARG	LYS	conflict	UNP Q385G9
ED	326	UNK	GLY	conflict	UNP Q385G9

- Molecule 14 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AE	434	Total 3461	C 2215	N 598	O 630	S 18	0	0

- Molecule 15 is a protein called mL71.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BE	407	Total 3223	C 2044	N 558	O 608	S 13	0	0

- Molecule 16 is a protein called mt-LAF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	EE	433	Total 3444	C 2144	N 649	O 638	S 13	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	20	VAL	MET	conflict	UNP Q38DC9

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Chain	Residue	Modelled	Actual	Comment	Reference
EE	27	ARG	LYS	conflict	UNP Q38DC9
EE	337	ASP	GLY	conflict	UNP Q38DC9
EE	546	VAL	ALA	conflict	UNP Q38DC9

- Molecule 17 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	UE	33	165	99	33	33	0	0

- Molecule 18 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	AF	442	3597	2294	624	654	25	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	12	THR	ALA	conflict	UNP D0A7A6

- Molecule 19 is a protein called mL72.

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

- Molecule 20 is a protein called mt-LAF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	EF	302	2290	1451	406	425	8	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EF	47	UNK	GLU	conflict	UNP C9ZWD9
EF	48	UNK	VAL	conflict	UNP C9ZWD9
EF	49	UNK	ALA	conflict	UNP C9ZWD9
EF	50	UNK	GLN	conflict	UNP C9ZWD9
EF	51	UNK	VAL	conflict	UNP C9ZWD9

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Chain	Residue	Modelled	Actual	Comment	Reference
EF	52	UNK	THR	conflict	UNP C9ZWD9

- Molecule 21 is a protein called mt-LAF7.

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

- Molecule 22 is a protein called mL74.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	BH	282	2293	1457	423	409	4	0	0

- Molecule 23 is a protein called mt-LAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	EH	438	3471	2193	627	632	19	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EH	166	UNK	GLY	conflict	UNP Q57ZS6
EH	485	PRO	SER	conflict	UNP Q57ZS6
EH	495	ARG	LYS	conflict	UNP Q57ZS6

- Molecule 24 is a protein called bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	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
AI	253	UNK	LYS	conflict	UNP Q57UC5

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Chain	Residue	Modelled	Actual	Comment	Reference
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 25 is a protein called mL75.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	BI	323	2641	1681	483	461	16	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 26 is a protein called MALSU1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	EI	275	2101	1307	372	412	10	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EI	12	TYR	CYS	conflict	UNP Q584Y2
EI	70	PRO	LEU	conflict	UNP Q584Y2
EI	129	HIS	ARG	conflict	UNP Q584Y2
EI	144	SER	LEU	conflict	UNP Q584Y2

- Molecule 27 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	UI	23	115	69	23	23	0	0

- Molecule 28 is a protein called mL76.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BJ	293	Total 2433	C 1527	N 463	O 435	S 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 29 is a protein called L0R8F8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	EJ	95	Total 765	C 475	N 156	O 131	S 3	0	0

- Molecule 30 is a protein called uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AK	301	Total 2499	C 1593	N 456	O 433	S 17	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 31 is a protein called mL77.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BK	228	Total 1855	C 1153	N 353	O 341	S 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 32 is a protein called mt-ACP.

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

- Molecule 33 is a protein called UNK.

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

- Molecule 34 is a protein called mL78.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	259	Total 2023	C 1241	N 397	O 375	S 10	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BL	77	TYR	HIS	conflict	UNP Q389N4
BL	218	ALA	THR	conflict	UNP Q389N4
BL	292	SER	ASN	conflict	UNP Q389N4

- Molecule 35 is a protein called mt-LAF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	EL	559	Total 4484	C 2876	N 781	O 798	S 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 36 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	UL	72	Total 360	C 216	N 72	O 72	0	0

- Molecule 37 is a protein called Mtg1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	EM	330	Total 2606	C 1646	N 476	O 469	S 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 38 is a protein called UNK.

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

- Molecule 39 is a protein called uL13m.

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

- Molecule 40 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BN	214	Total 1714	C 1077	N 320	O 312	S 5	0	0

- Molecule 41 is a protein called mt-LAF14.

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

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

- Molecule 42 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	AO	165	1339	843	272	215	9	0	0

- Molecule 43 is a protein called mL81.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BO	215	1686	1058	294	321	13	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	30	THR	ILE	conflict	UNP Q385L5
BO	123	LEU	MET	conflict	UNP Q385L5
BO	134	PRO	SER	conflict	UNP Q385L5
BO	196	ASN	SER	conflict	UNP Q385L5
BO	238	ALA	GLU	conflict	UNP Q385L5

- Molecule 44 is a protein called mt-LAF15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	EO	275	2141	1348	396	387	10	0	0
			Total	C	N	O	S		
44	EP	245	1919	1212	349	349	9	0	0

- Molecule 45 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	AP	325	2691	1713	499	466	13	0	0

- Molecule 46 is a protein called mL83.

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

- Molecule 47 is a protein called mt-EngB.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	EQ	471	Total 3628	C 2286	N 657	O 666	S 19	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EQ	26	CYS	ARG	conflict	UNP Q380Y8
EQ	272	SER	ASN	conflict	UNP Q380Y8
EQ	325	ALA	THR	conflict	UNP Q380Y8
EQ	326	ALA	THR	conflict	UNP Q380Y8
EQ	379	UNK	PRO	conflict	UNP Q380Y8
EQ	400	SER	PRO	conflict	UNP Q380Y8
EQ	426	ARG	GLN	conflict	UNP Q380Y8
EQ	447	GLU	LYS	conflict	UNP Q380Y8
EQ	448	UNK	SER	conflict	UNP Q380Y8
EQ	468	SER	PRO	conflict	UNP Q380Y8
EQ	472	SER	PRO	conflict	UNP Q380Y8

- Molecule 48 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AR	257	Total 2146	C 1359	N 399	O 374	S 14	0	0

- Molecule 49 is a protein called mL84.

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

- Molecule 50 is a protein called mL85.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BS	151	Total 1218	C 753	N 232	O 226	S 7	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 51 is a protein called mt-LAF18.

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

- Molecule 52 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	AT	141	1163	732	221	204	6	0	0

- Molecule 53 is a protein called mL86.

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

- Molecule 54 is a protein called mt-LAF19.

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

- Molecule 55 is a protein called bL20m.

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

- Molecule 56 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	BU	83	705	442	143	116	4	0	0

- Molecule 57 is a protein called mt-LAF20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	EU	47	407	250	90	61	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	187	1557	987	298	264	8	0	0

- Molecule 62 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	AX	166	1400	904	247	244	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 mL90.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	BX	133	1088	695	201	183	9	0	0

- Molecule 64 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
64	UX	180	900	540	180	180	0	0

- Molecule 65 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	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 66 is a protein called mL92.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	BZ	190	1420	897	247	269	7	0	0

- Molecule 67 is a protein called mL93.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	Ba	142	1245	800	226	212	7	0	0

- Molecule 68 is a protein called mL94.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	Bb	128	1011	637	191	181	2	0	0

- Molecule 69 is a protein called mL95.

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

- Molecule 70 is a protein called mL41.

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

- Molecule 71 is a protein called mL42.

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

- Molecule 72 is a protein called mL98.

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

- Molecule 73 is a protein called mL43.

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

- Molecule 74 is a protein called mL99.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bg	83	Total 667	C 418	N 130	O 117	S 2	0	0

- Molecule 75 is a protein called mL100.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bh	91	Total 730	C 466	N 129	O 125	S 10	0	0

- Molecule 76 is a protein called mL101.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	Bi	192	1502	958	277	263	4	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bi	143	MET	ILE	conflict	UNP Q4GZ80
Bi	163	VAL	LEU	conflict	UNP Q4GZ80
Bi	213	ILE	PRO	conflict	UNP Q4GZ80

- Molecule 77 is a protein called mL49.

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

- Molecule 78 is a protein called mL52.

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

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ao	-1239	GLN	ARG	conflict	UNP Q385V2
Ao	-1157	ALA	GLU	conflict	UNP Q385V2
Ao	-1105	ALA	VAL	conflict	UNP Q385V2
Ao	-1062	GLY	SER	conflict	UNP Q385V2
Ao	-879	HIS	TYR	conflict	UNP Q385V2
Ao	-776	UNK	HIS	conflict	UNP Q385V2
Ao	-742	UNK	LYS	conflict	UNP Q385V2
Ao	-724	GLU	LYS	conflict	UNP Q385V2
Ao	-707	UNK	SER	conflict	UNP Q385V2
Ao	-521	GLU	GLY	conflict	UNP Q385V2
Ao	-515	ARG	GLN	conflict	UNP Q385V2
Ao	-481	LEU	VAL	conflict	UNP Q385V2
Ao	-214	ALA	VAL	conflict	UNP Q385V2
Ao	-175	LEU	VAL	conflict	UNP Q385V2
Ao	?	-	LEU	deletion	UNP Q385V2
Ao	?	-	LYS	deletion	UNP Q385V2

- Molecule 79 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	Ap	297	2428	1572	428	416	12	0	0

- Molecule 80 is a protein called mL63.

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

- Molecule 81 is a protein called mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	Av	196	1668	1062	309	285	12	0	0

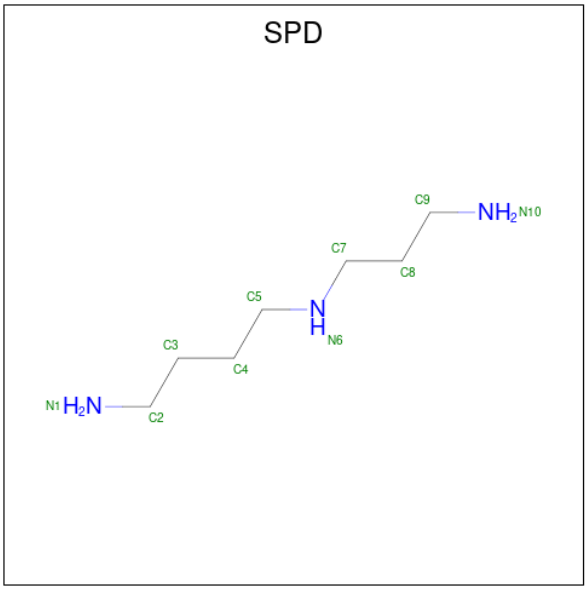
- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
82	A5	1	1	1	0
82	EG	1	1	1	0
82	BX	2	2	2	0
82	Bh	1	1	1	0

- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

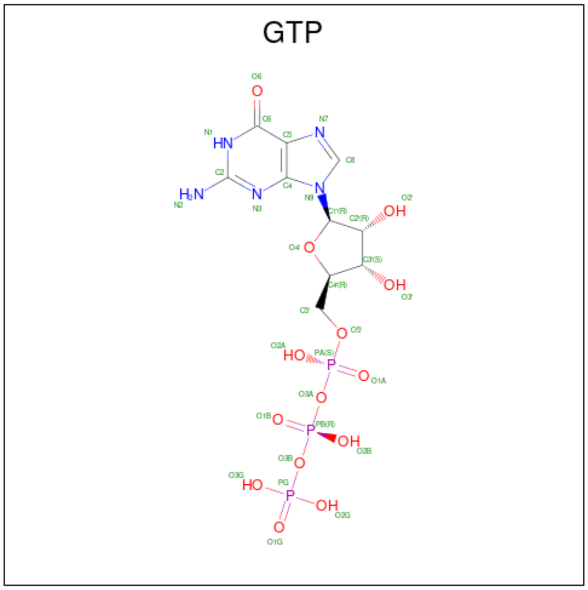
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
83	AA	29	29	29	0
83	EA	2	2	2	0
83	EB	1	1	1	0
83	EQ	1	1	1	0

- Molecule 84 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
84	AA	1	Total 10	C 7	N 3	0

- Molecule 85 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

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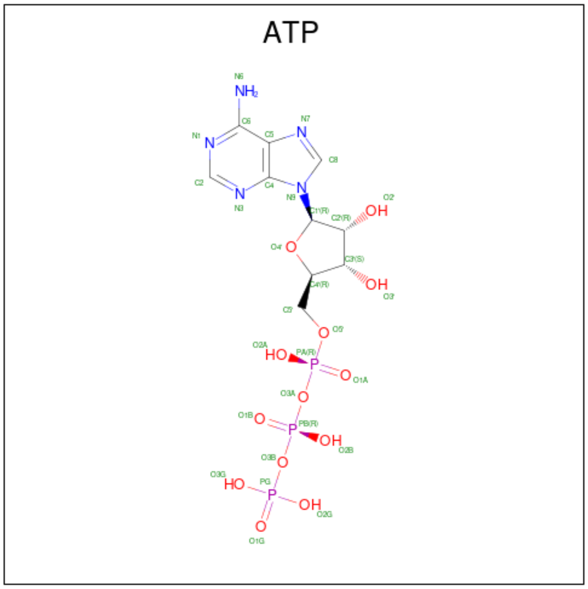
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
85	EQ	1	32	10	5	14	3	0

- Molecule 86 is SODIUM ION (three-letter code: NA) (formula: Na).

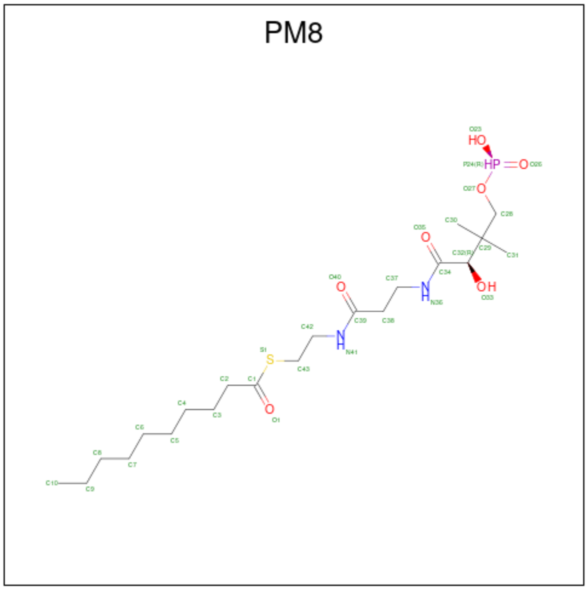
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
86	EA	2	2	2	0

- Molecule 87 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



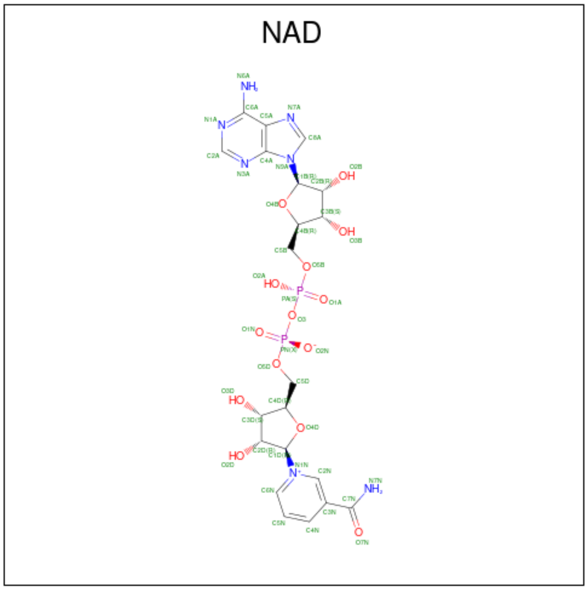
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
87	EB	1	31	10	5	13	3	0

- Molecule 88 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
88	EK	1	Total C N O P S 32 21 2 7 1 1	0
88	ER	1	Total C N O P S 32 21 2 7 1 1	0

- Molecule 89 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

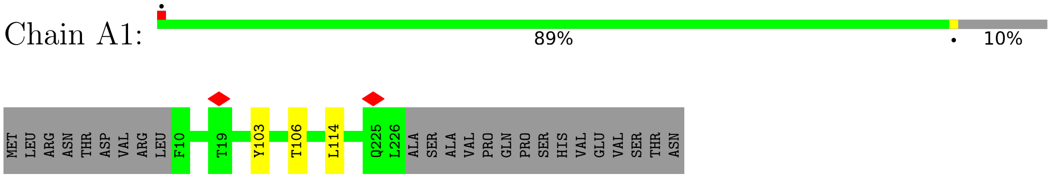
- Molecule 90 is water.

Mol	Chain	Residues	Atoms	AltConf
90	EA	2	Total O 4 4	0
90	EA	2	Total O 4 4	0
90	EB	4	Total O 4 4	0
90	EQ	2	Total O 2 2	0

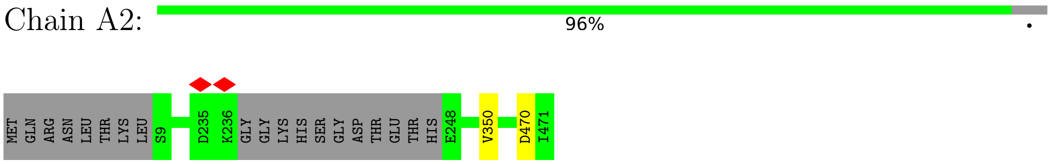
3 Residue-property plots ⓘ

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.

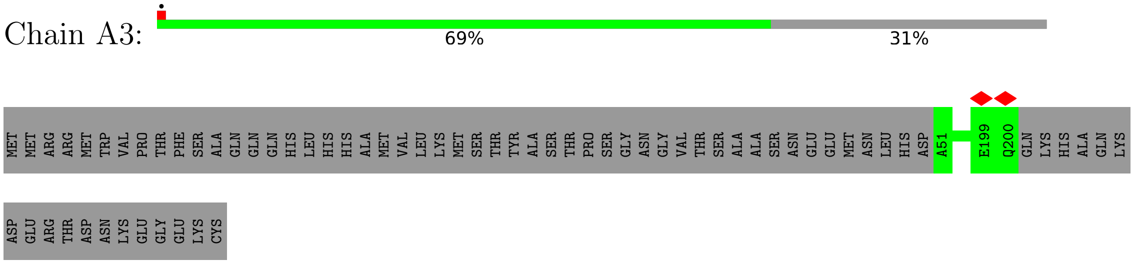
- Molecule 1: bL28m



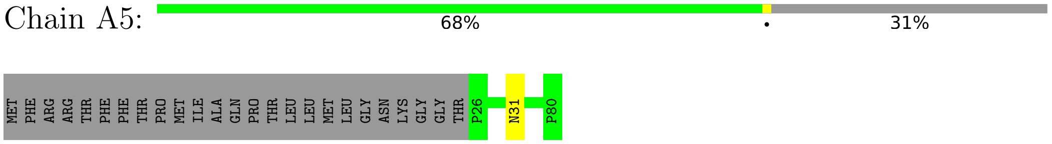
- Molecule 2: uL29m



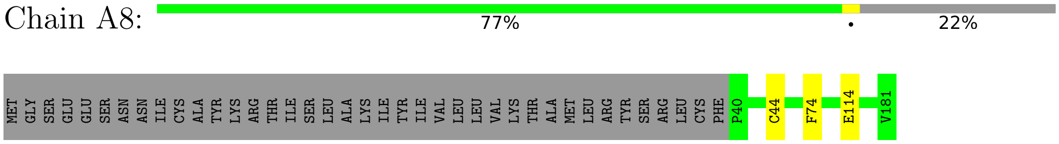
- Molecule 3: uL30m



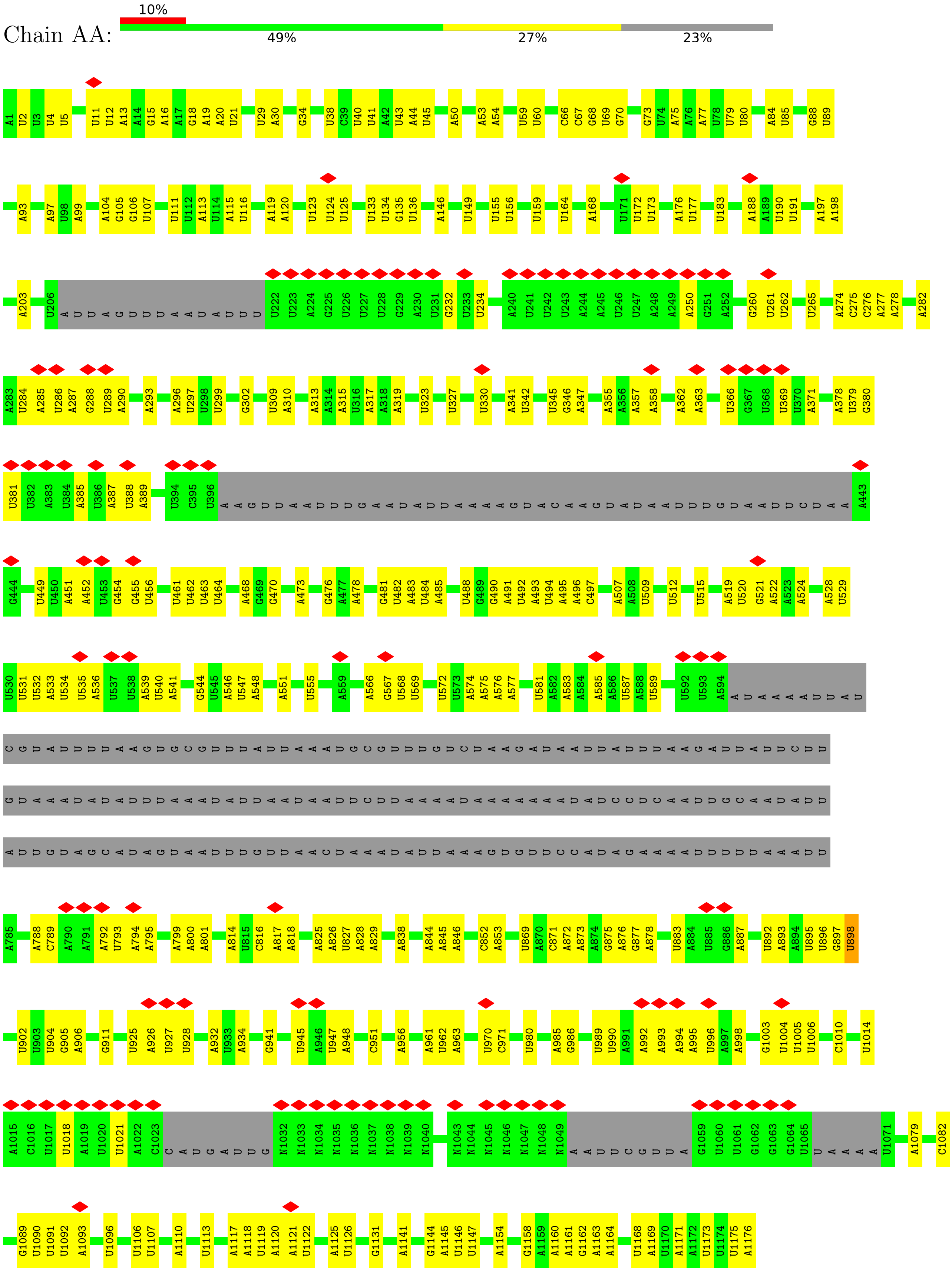
- Molecule 4: bL32m



- Molecule 5: bL35m

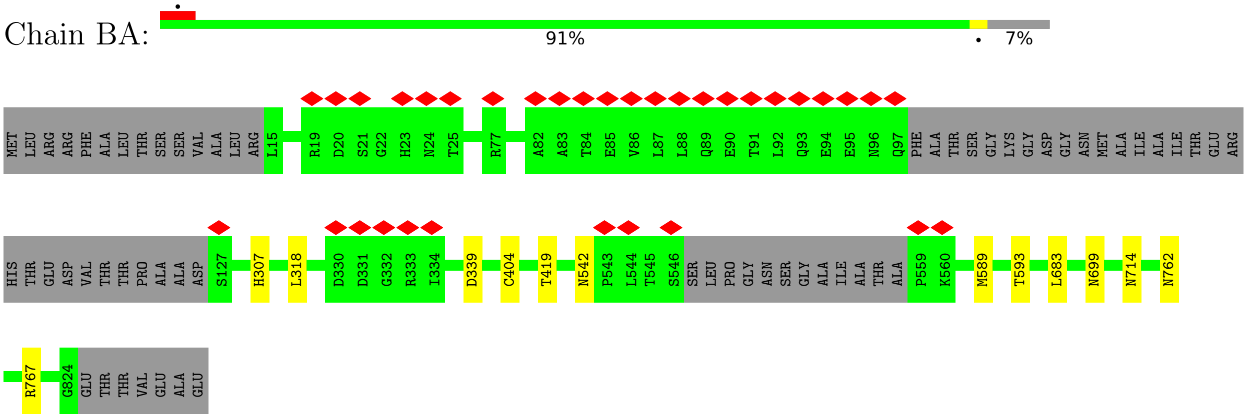


- Molecule 6: 12S ribosomal RNA



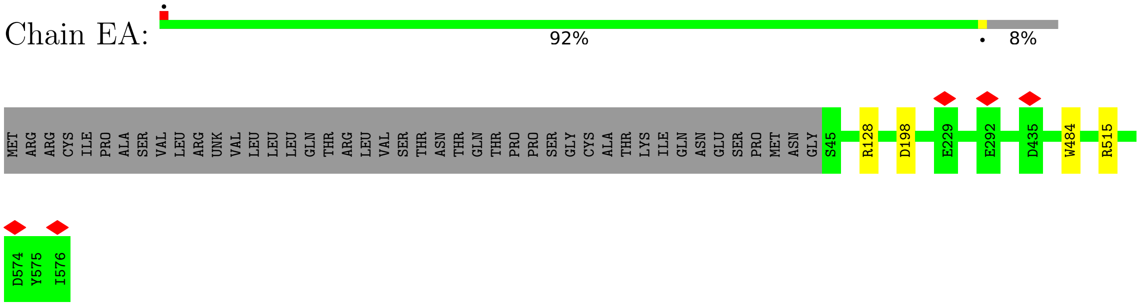
- Molecule 7: mL67

Chain BA:



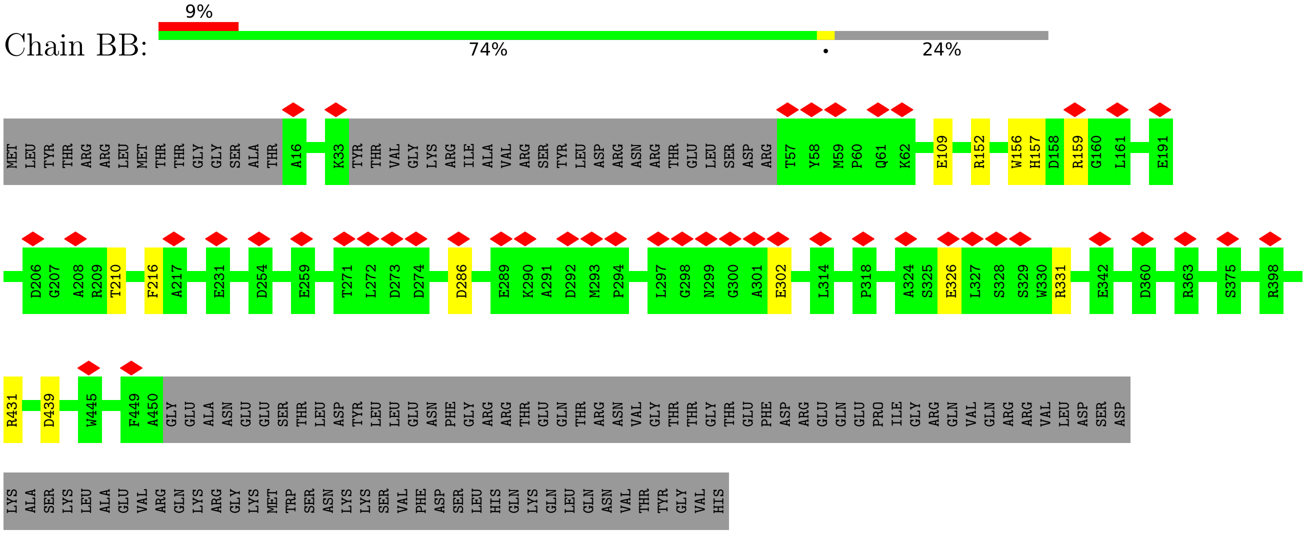
- Molecule 8: mt-EngA

Chain EA:



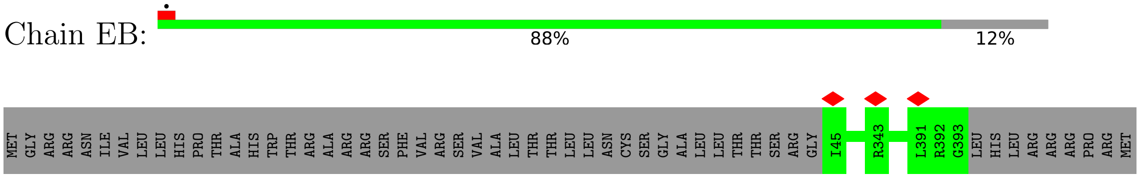
- Molecule 9: mL68

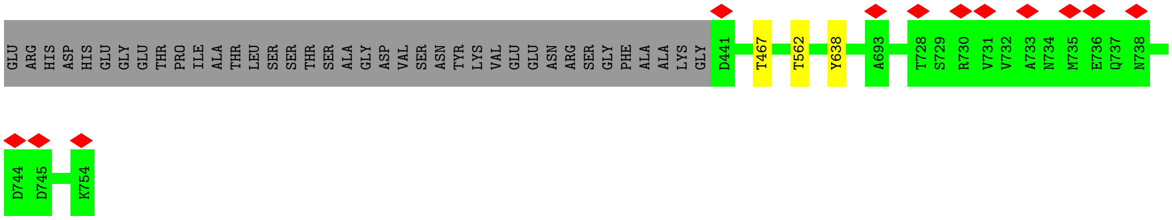
Chain BB:



- Molecule 10: mt-LAF2

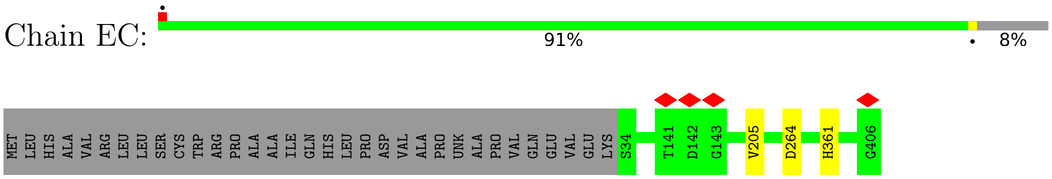
Chain EB:





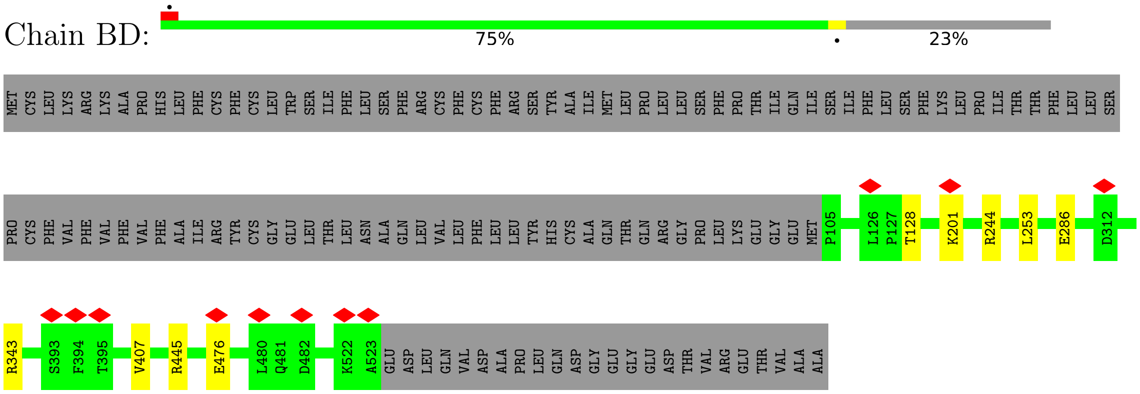
- Molecule 11: mt-LAF3

Chain EC:



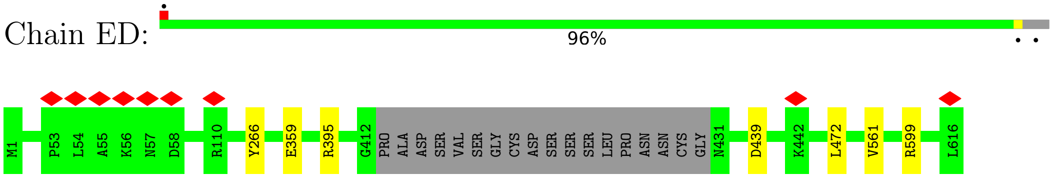
- Molecule 12: mL70

Chain BD:



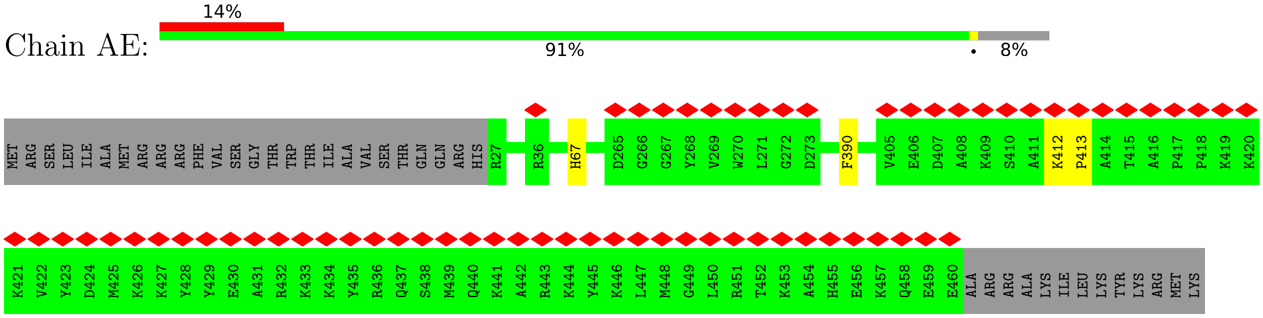
- Molecule 13: mt-LAF4

Chain ED:



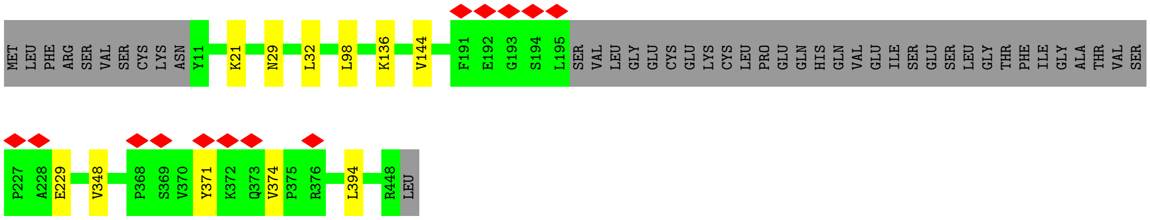
- Molecule 14: uL3m

Chain AE:



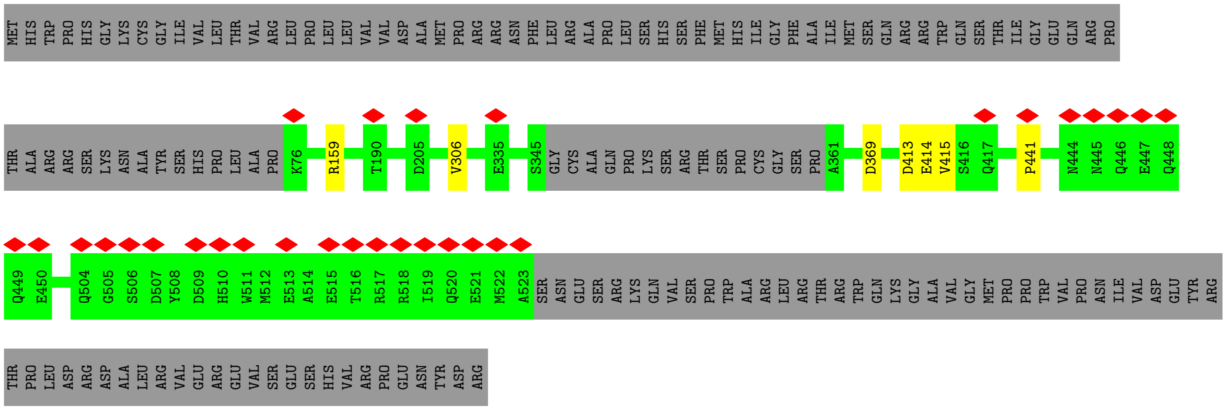
- Molecule 15: mL71

Chain BE:



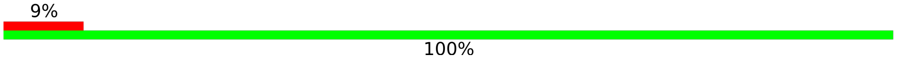
- Molecule 16: mt-LAF5

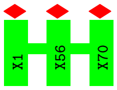
Chain EE:



- Molecule 17: UNK

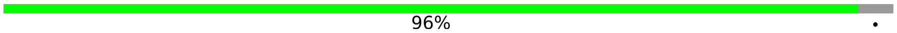
Chain UE:

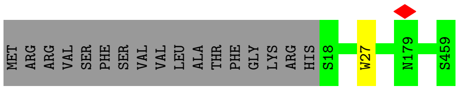




- Molecule 18: uL4m

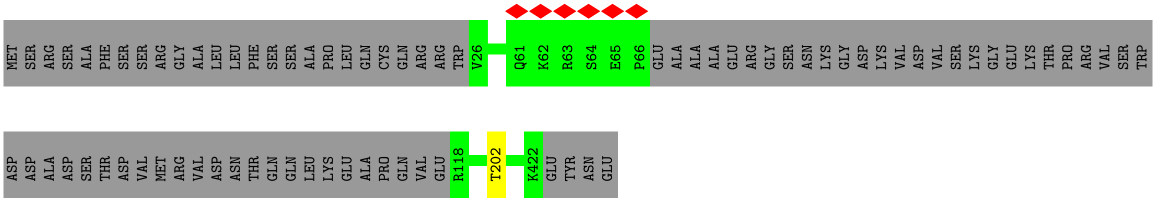
Chain AF:





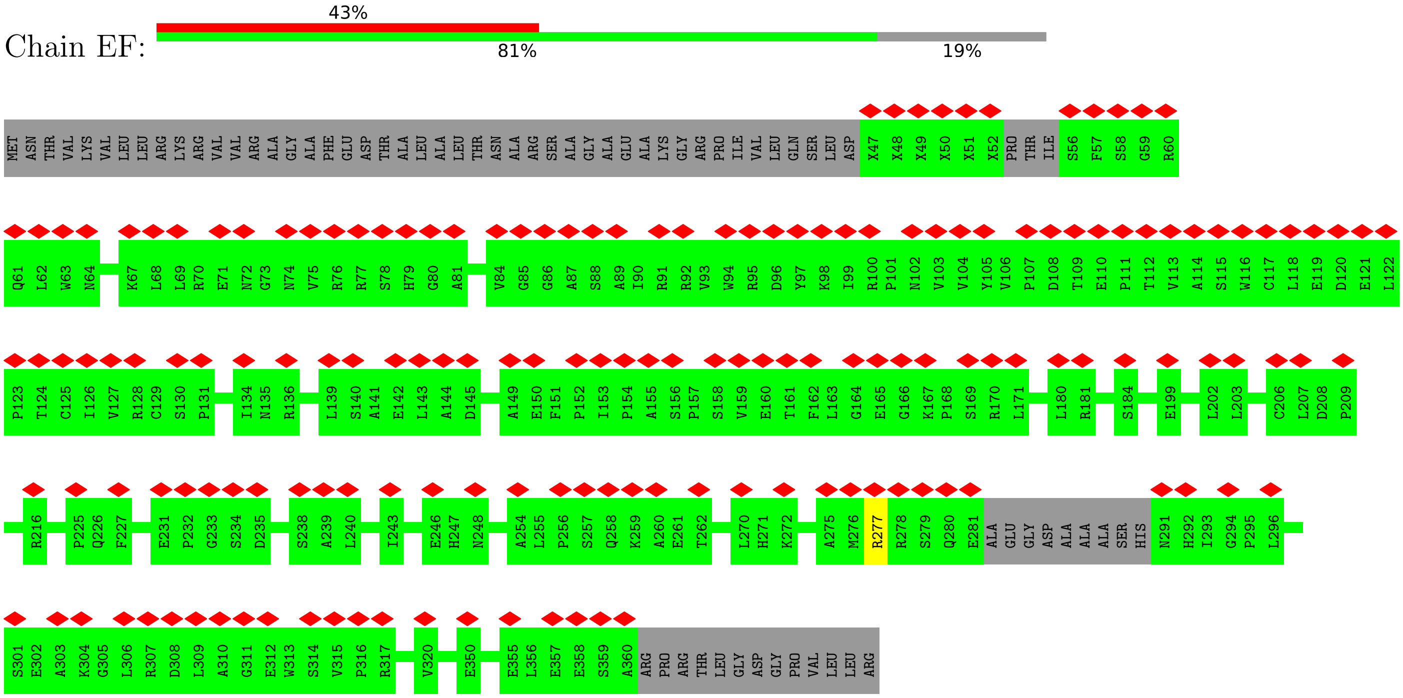
- Molecule 19: mL72

Chain BF:



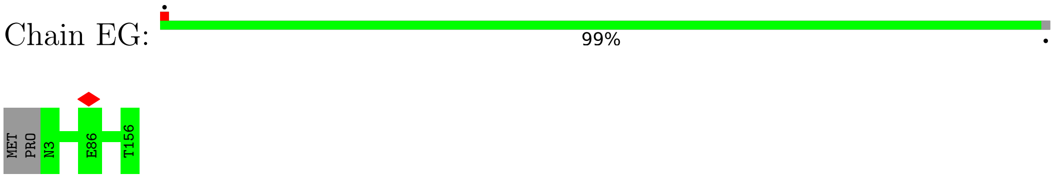
- Molecule 20: mt-LAF6

Chain EF:



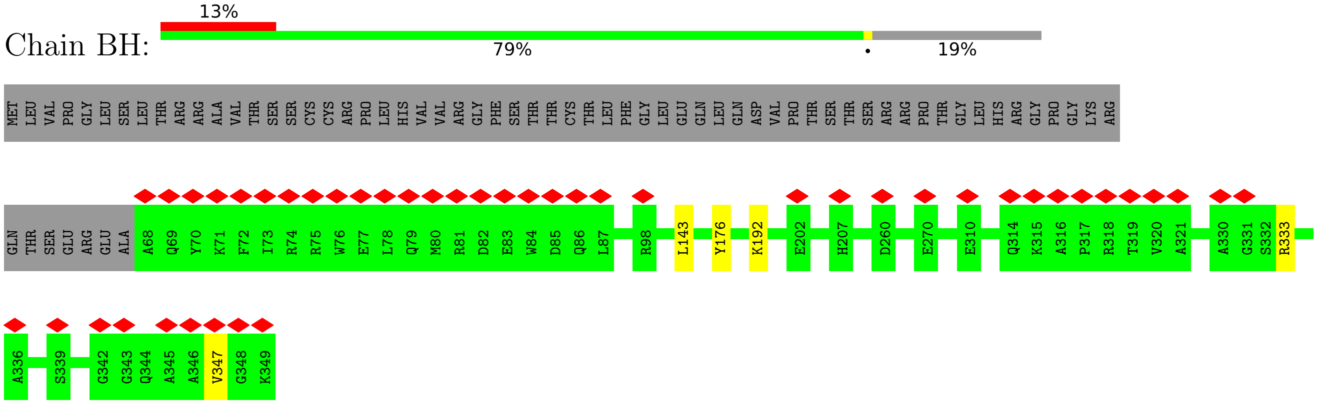
- Molecule 21: mt-LAF7

Chain EG:



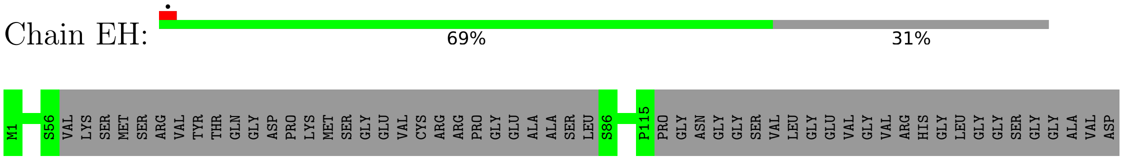
- Molecule 22: mL74

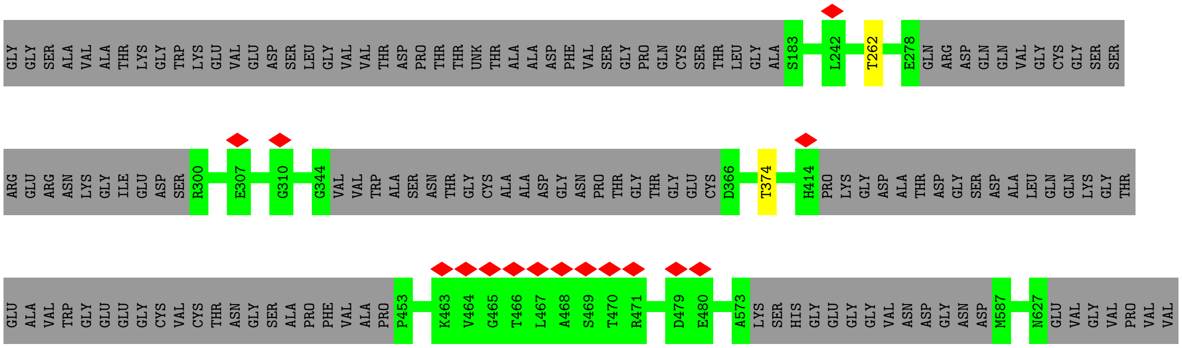
Chain BH:



- Molecule 23: mt-LAF8

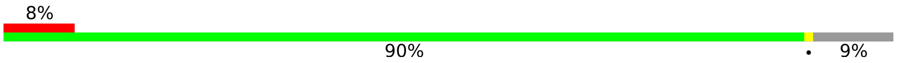
Chain EH:

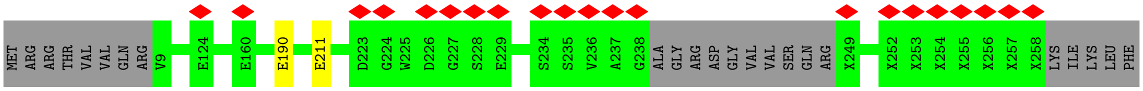




- Molecule 24: bL9m

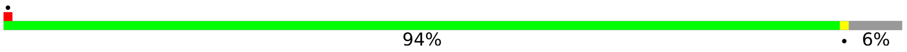
Chain AI:

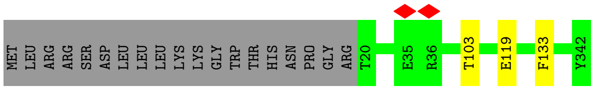




- Molecule 25: mL75

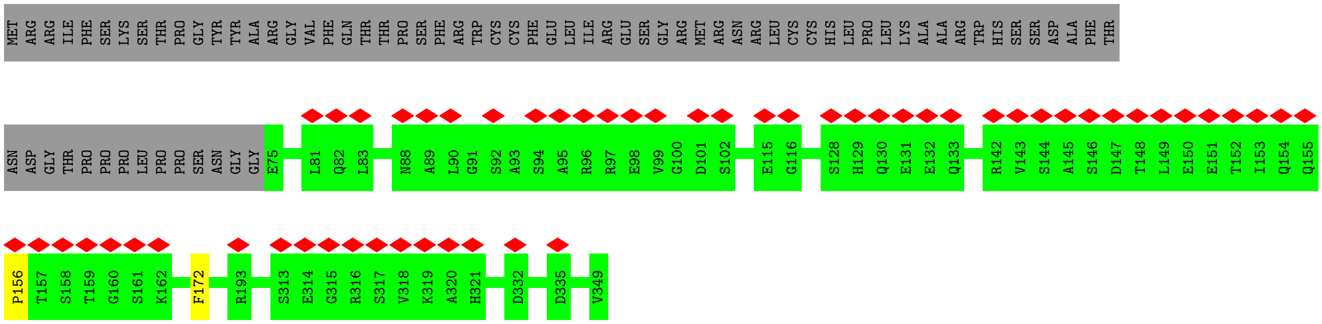
Chain BI:





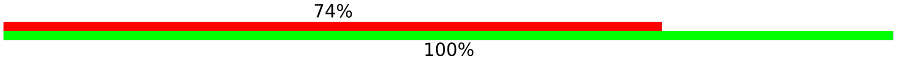
- Molecule 26: MALSU1

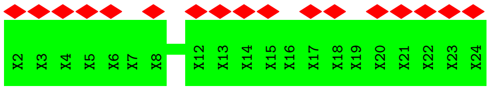
Chain EI:



- Molecule 27: UNK

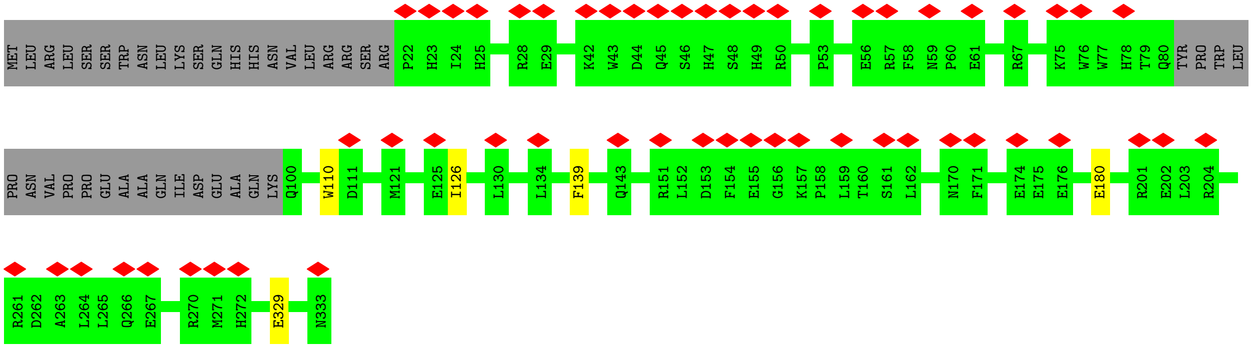
Chain UI:





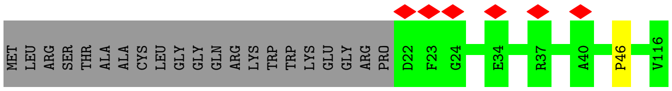
- Molecule 28: mL76

Chain BJ:



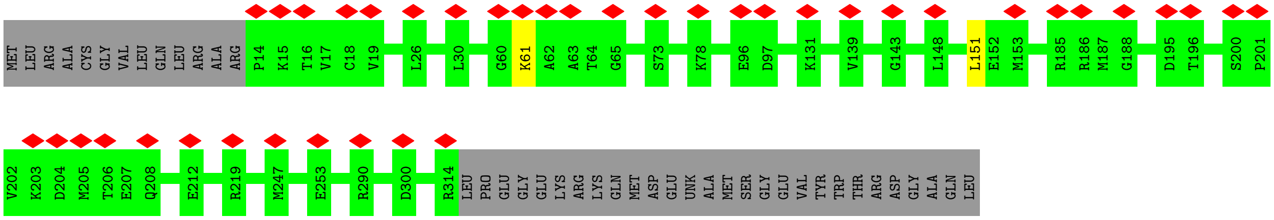
- Molecule 29: L0R8F8

Chain EJ:



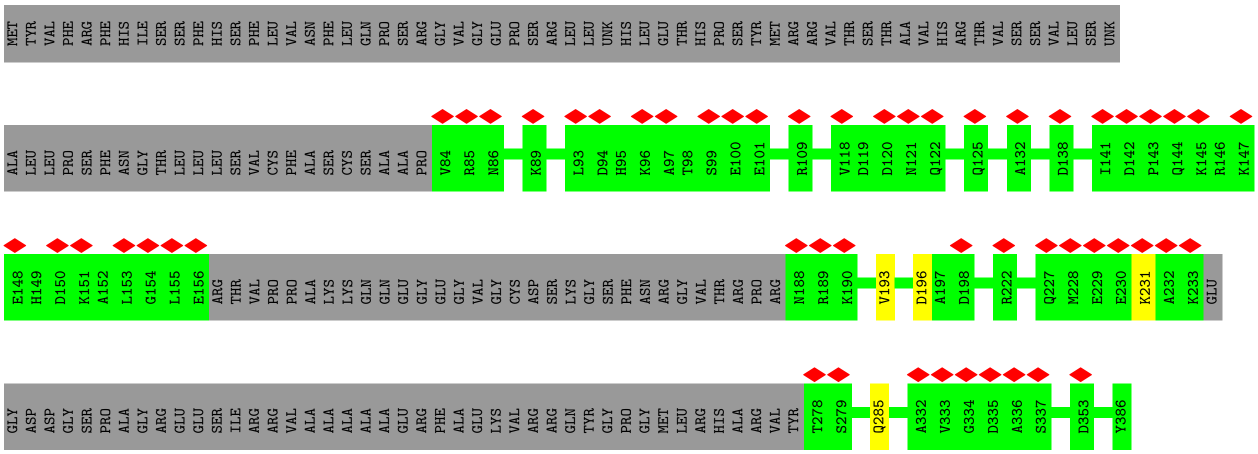
- Molecule 30: uL11m

Chain AK:



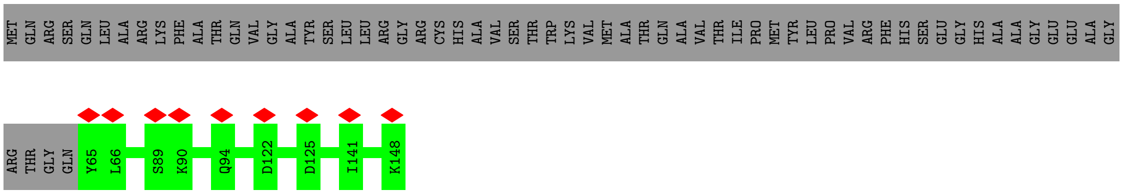
- Molecule 31: mL77

Chain BK:



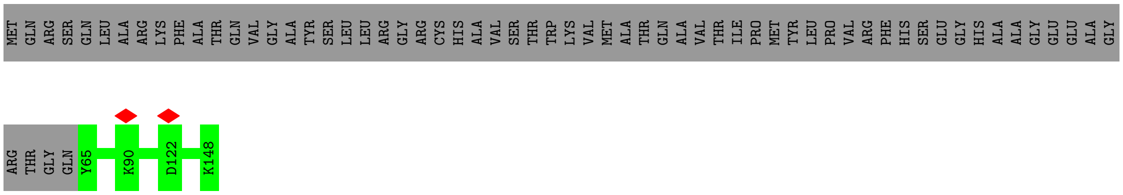
- Molecule 32: mt-ACP

Chain EK:



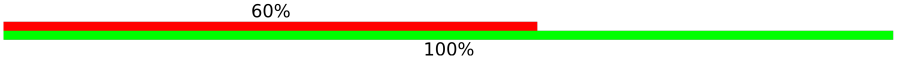
- Molecule 32: mt-ACP

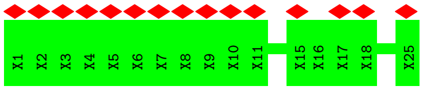
Chain ER:



- Molecule 33: UNK

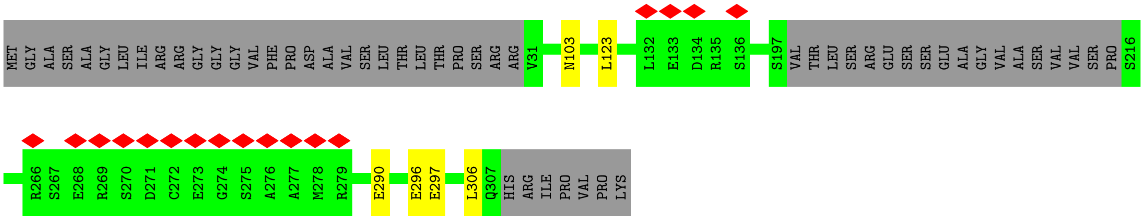
Chain UK:





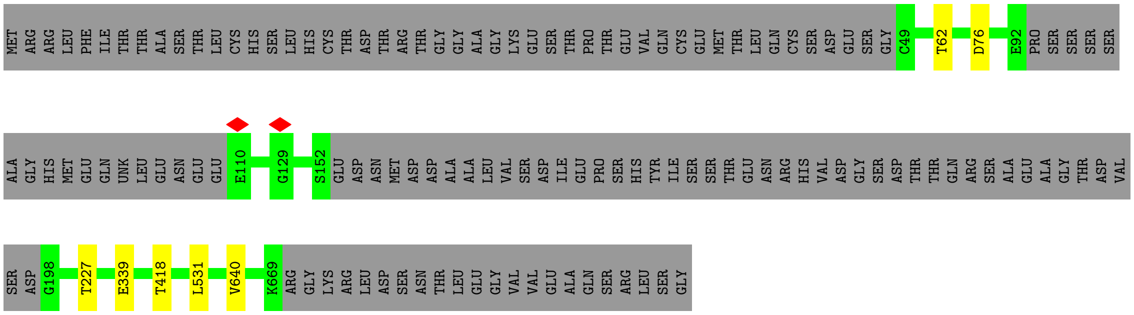
- Molecule 34: mL78

Chain BL:



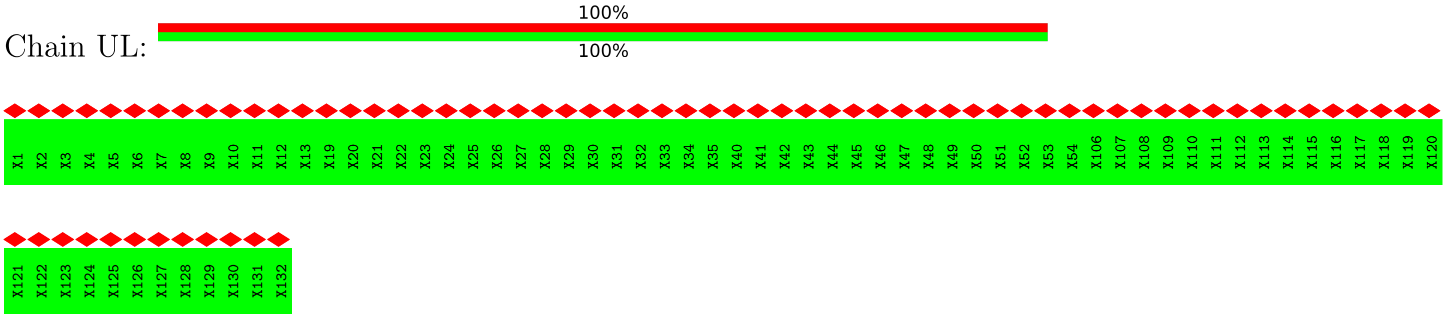
- Molecule 35: mt-LAF12

Chain EL:



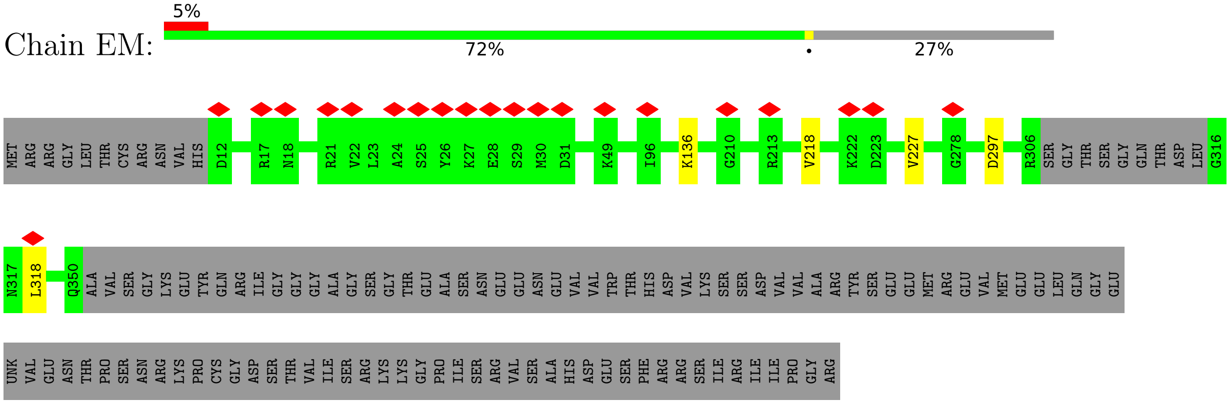
- Molecule 36: UNK

Chain UL:



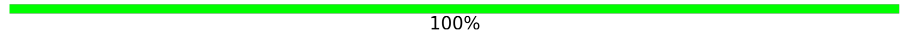
- Molecule 37: Mtg1

Chain EM:



- Molecule 38: UNK

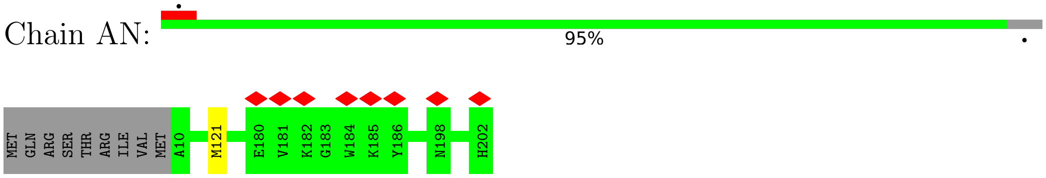
Chain UM:



There are no outlier residues recorded for this chain.

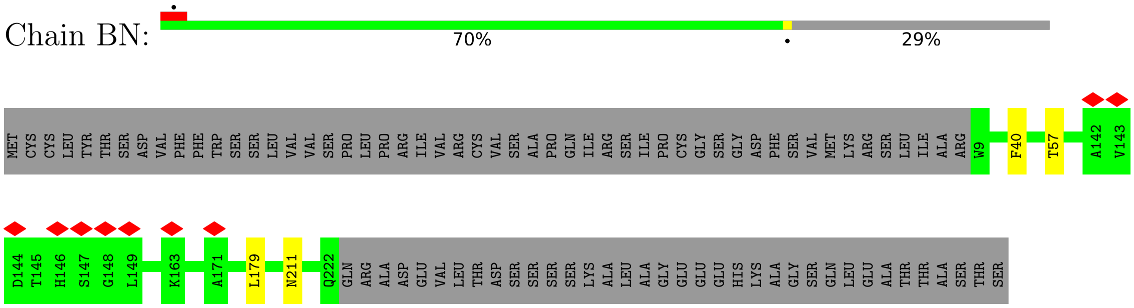
- Molecule 39: uL13m

Chain AN:



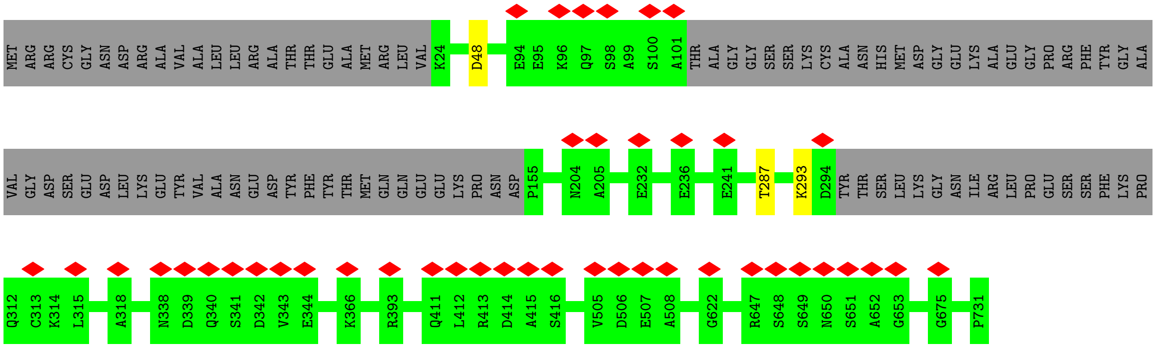
- Molecule 40: mL80

Chain BN:



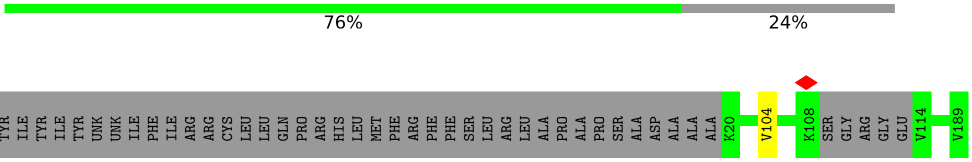
- Molecule 41: mt-LAF14

Chain EN:



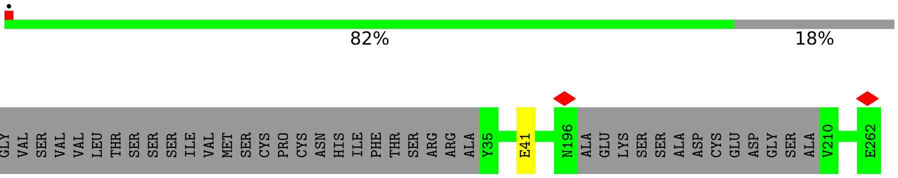
- Molecule 42: uL14m

Chain AO:



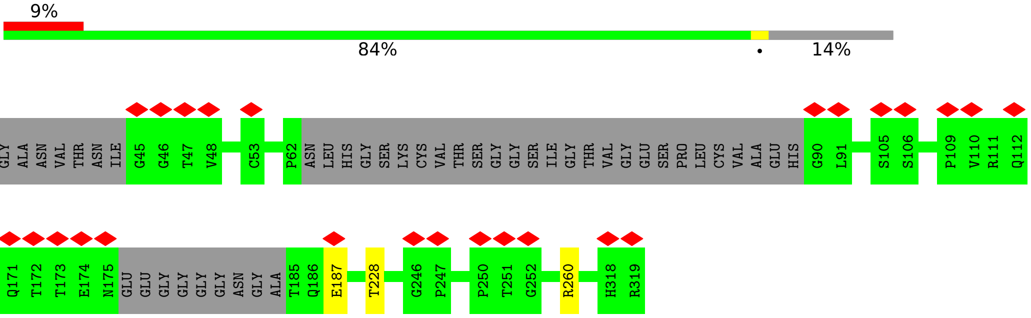
- Molecule 43: mL81

Chain BO:



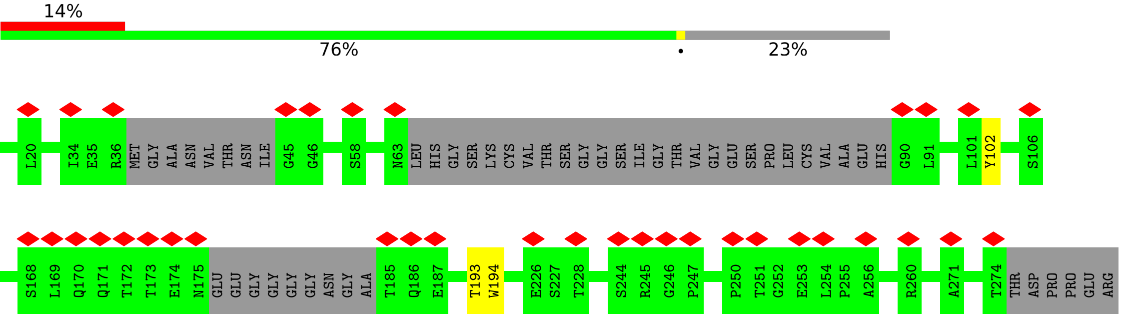
- Molecule 44: mt-LAF15a

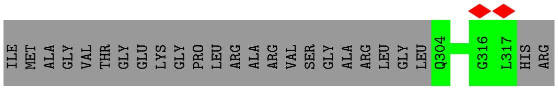
Chain EO:



- Molecule 44: mt-LAF15a

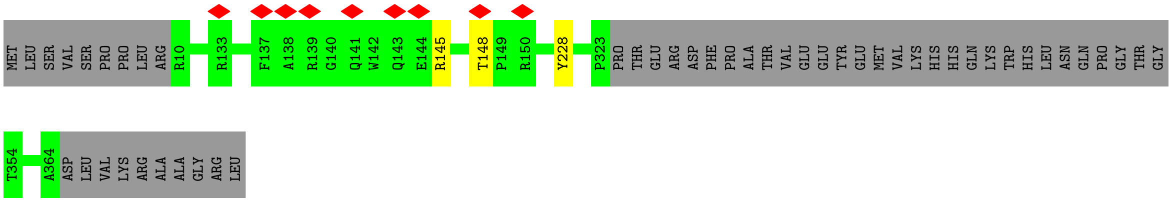
Chain EP:





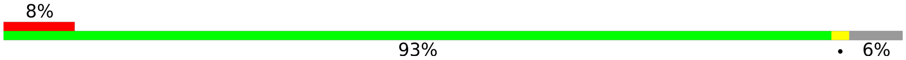
- Molecule 45: uL15m

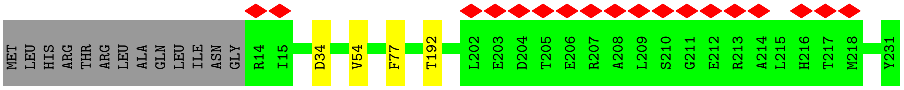
Chain AP:



- Molecule 46: mL83

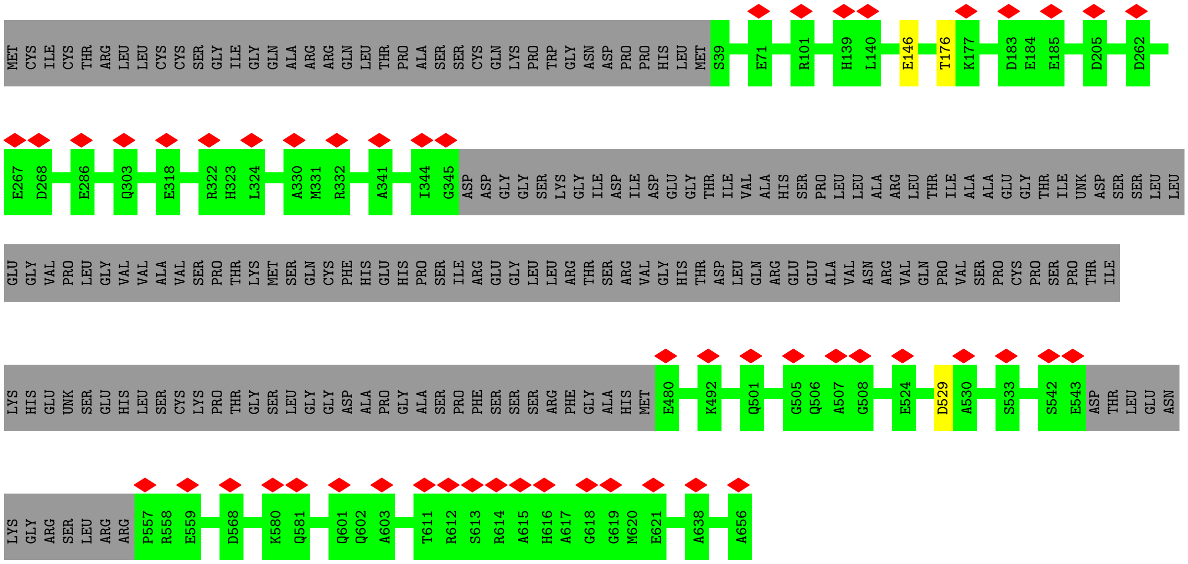
Chain BQ:





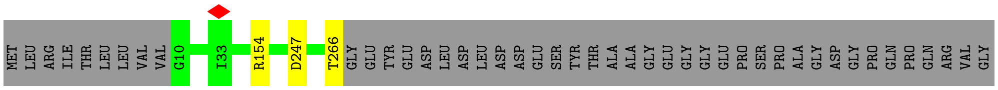
- Molecule 47: mt-EngB

Chain EQ:



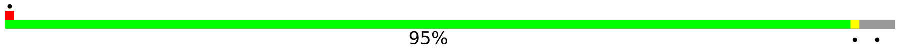
- Molecule 48: bL17m

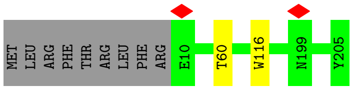
Chain AR:



- Molecule 49: mL84

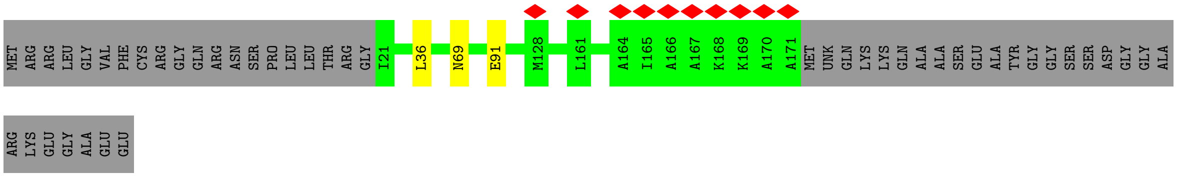
Chain BR:





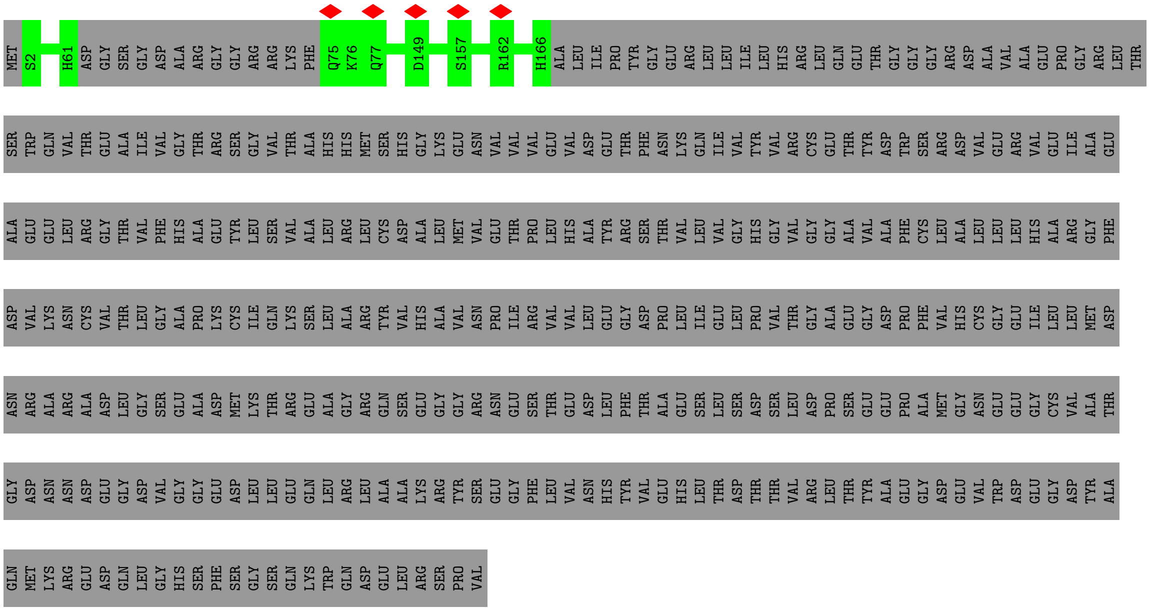
- Molecule 50: mL85

Chain BS:



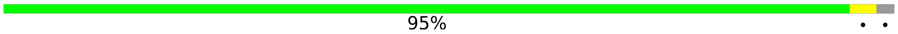
- Molecule 51: mt-LAF18

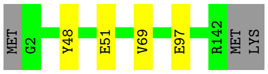
Chain ES:



- Molecule 52: bL19m

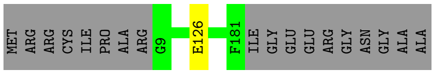
Chain AT:





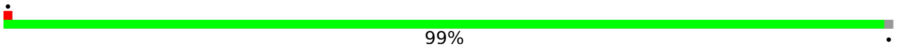
- Molecule 53: mL86

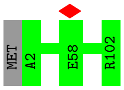
Chain BT:



- Molecule 54: mt-LAF19

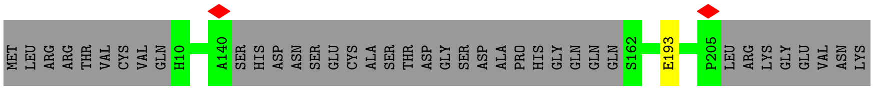
Chain ET:





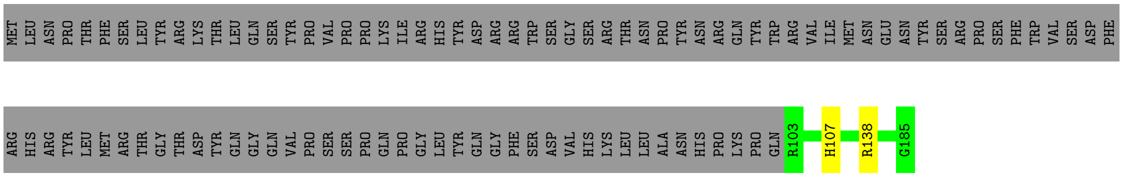
- Molecule 55: bL20m

Chain AU:



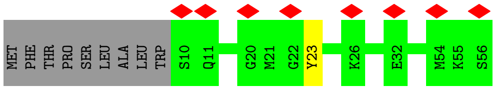
- Molecule 56: mL87

Chain BU:



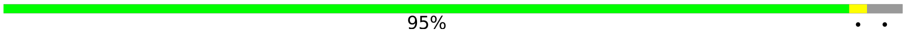
- Molecule 57: mt-LAF20

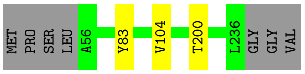
Chain EU:



- Molecule 58: bL21m

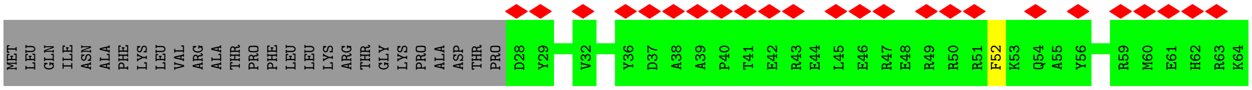
Chain AV:

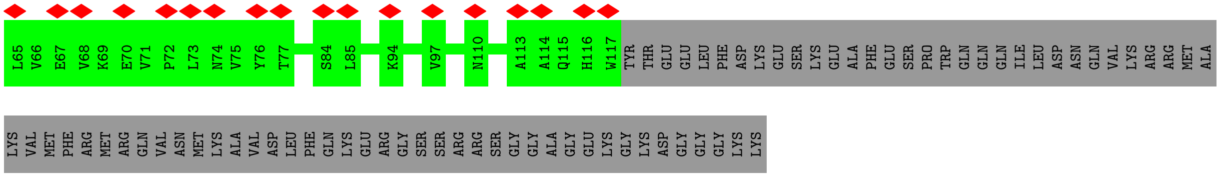




- Molecule 59: mL88

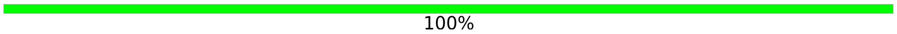
Chain BV:

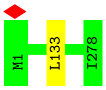




- Molecule 60: uL22m

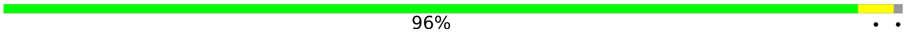
Chain AW:

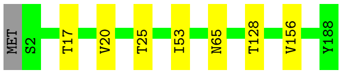




- Molecule 61: mL89

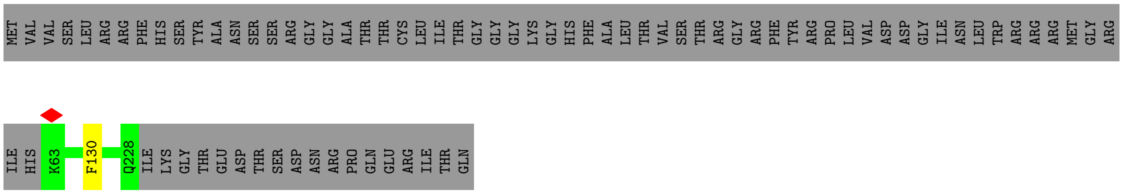
Chain BW:





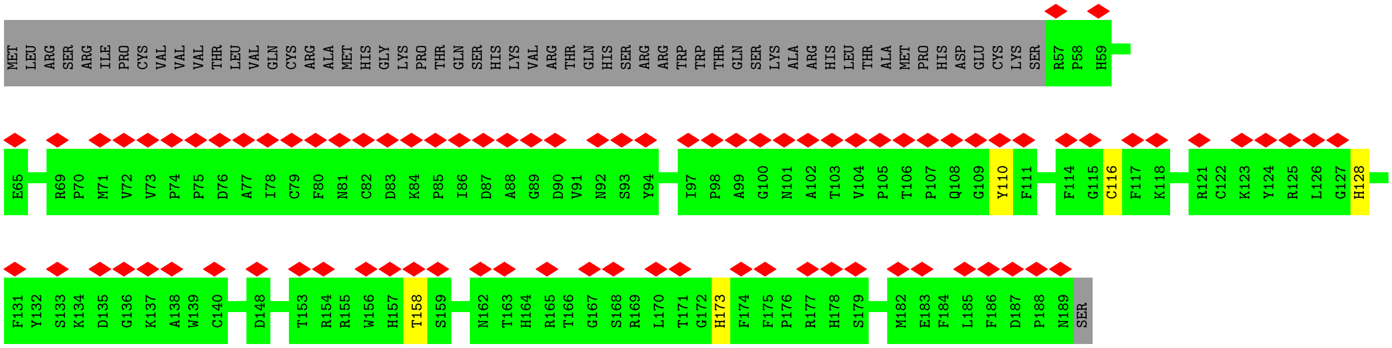
- Molecule 62: uL23m

Chain AX:



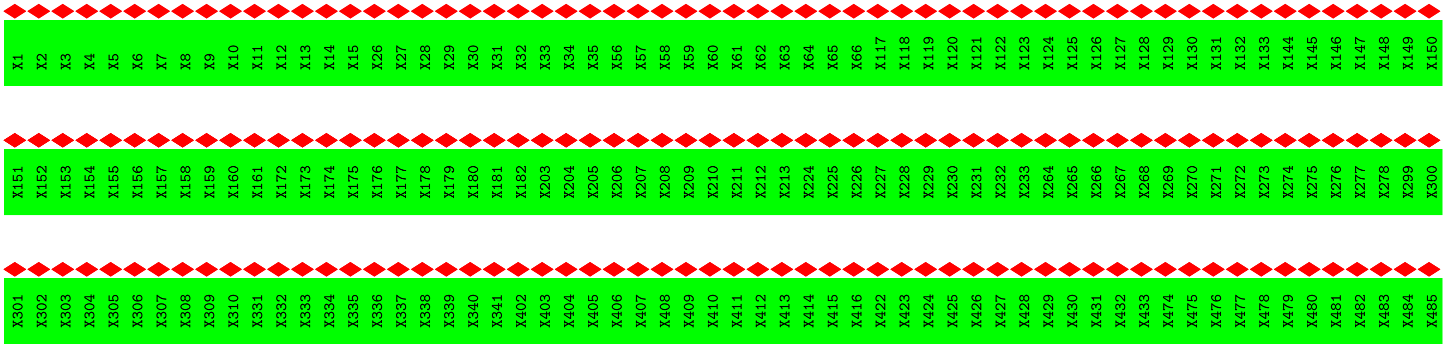
- Molecule 63: mL90

Chain BX:

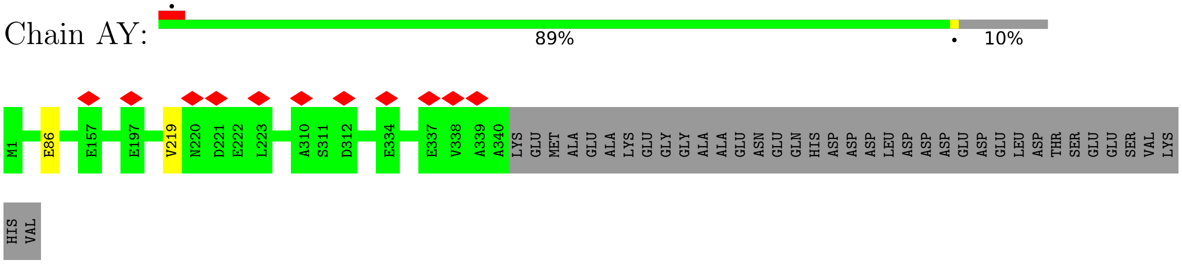


- Molecule 64: UNK

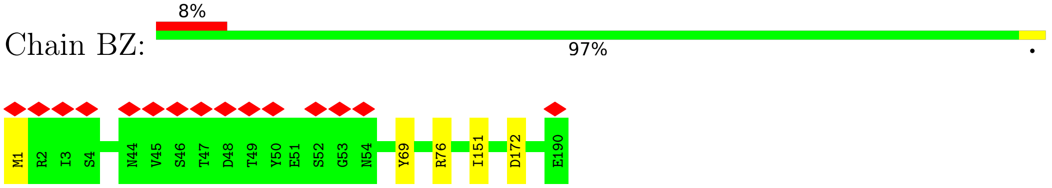
Chain UX:



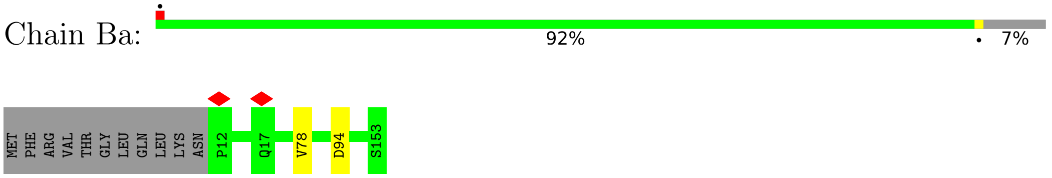
- Molecule 65: uL24m



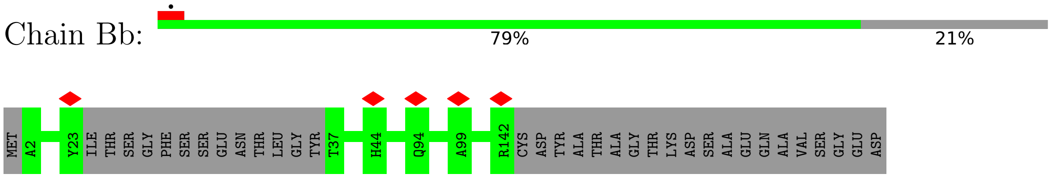
- Molecule 66: mL92



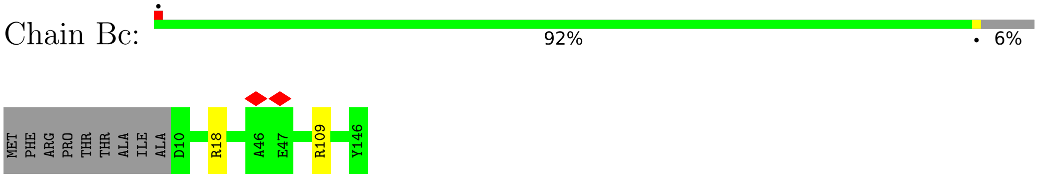
- Molecule 67: mL93



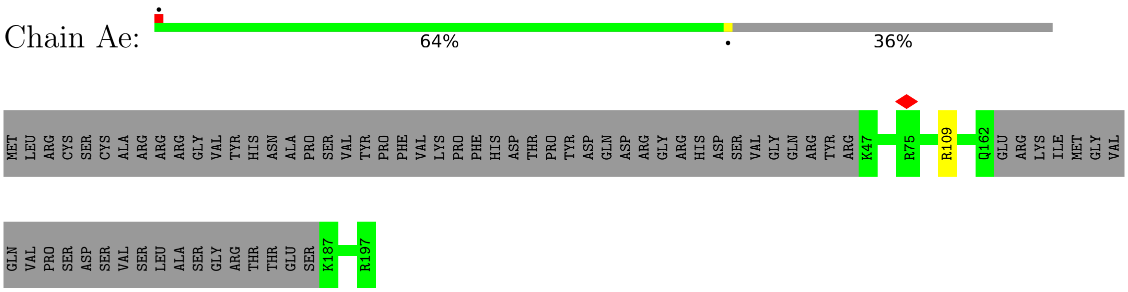
- Molecule 68: mL94



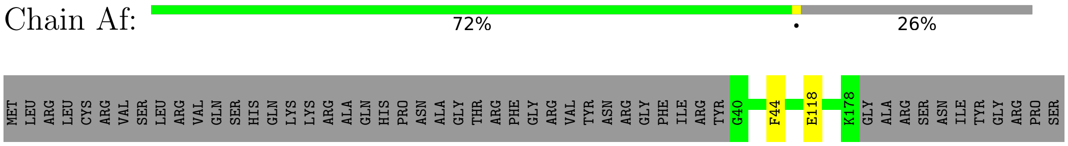
- Molecule 69: mL95



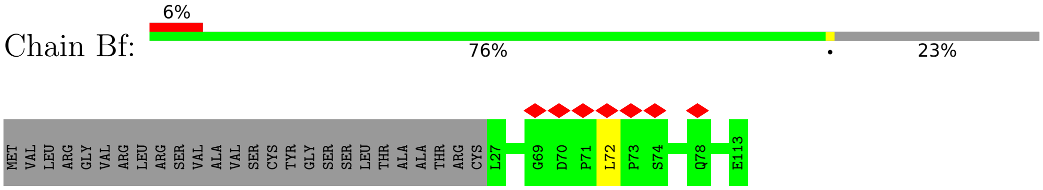
- Molecule 70: mL41



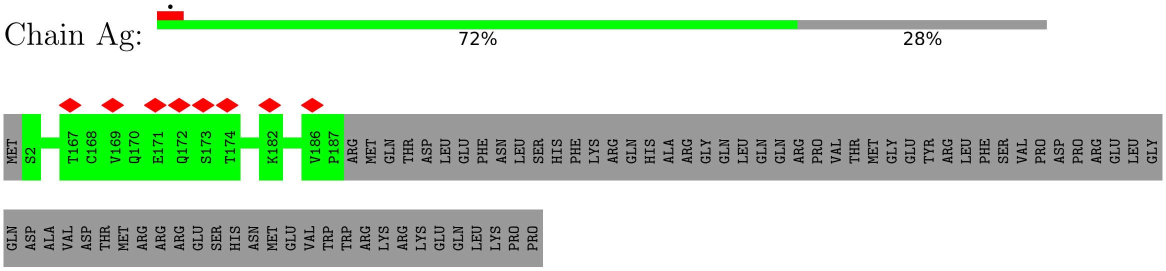
- Molecule 71: mL42



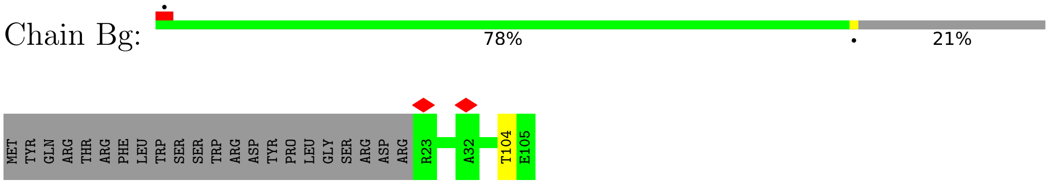
- Molecule 72: mL98



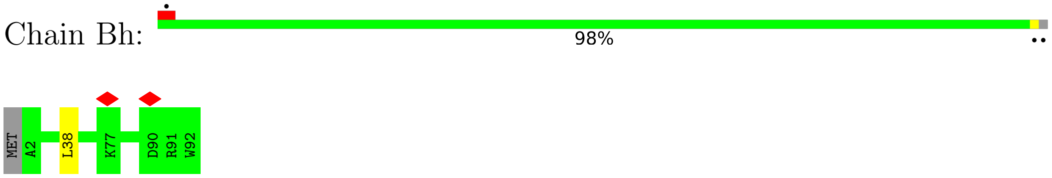
- Molecule 73: mL43



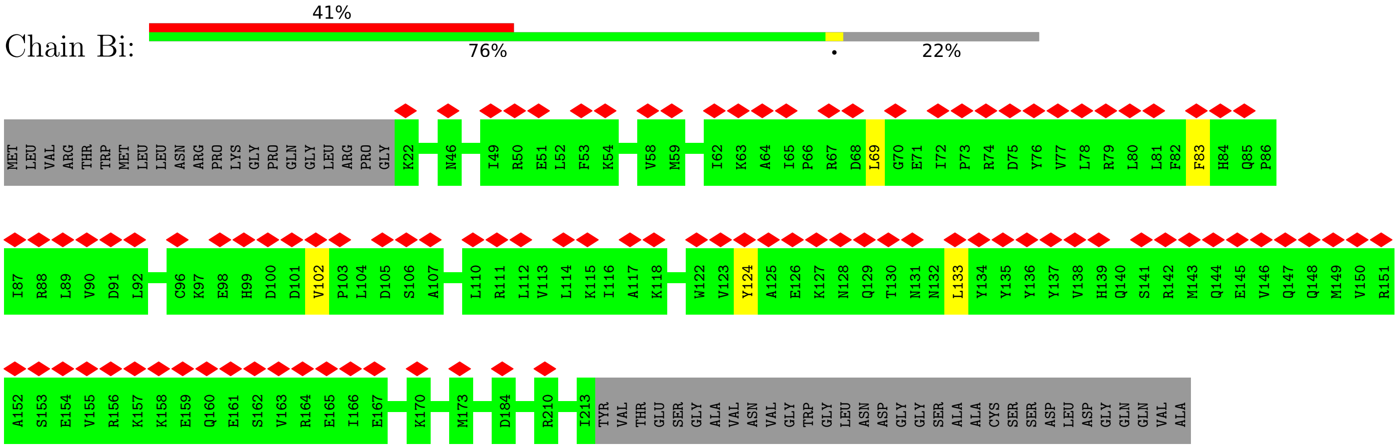
- Molecule 74: mL99



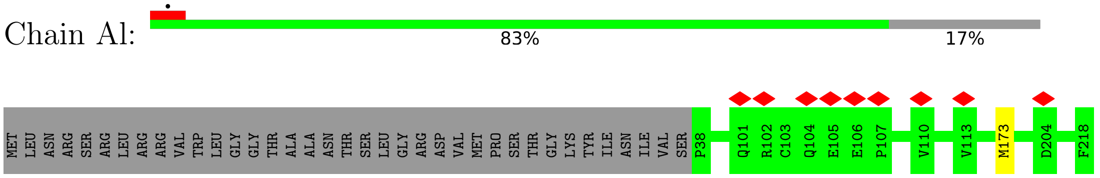
- Molecule 75: mL100



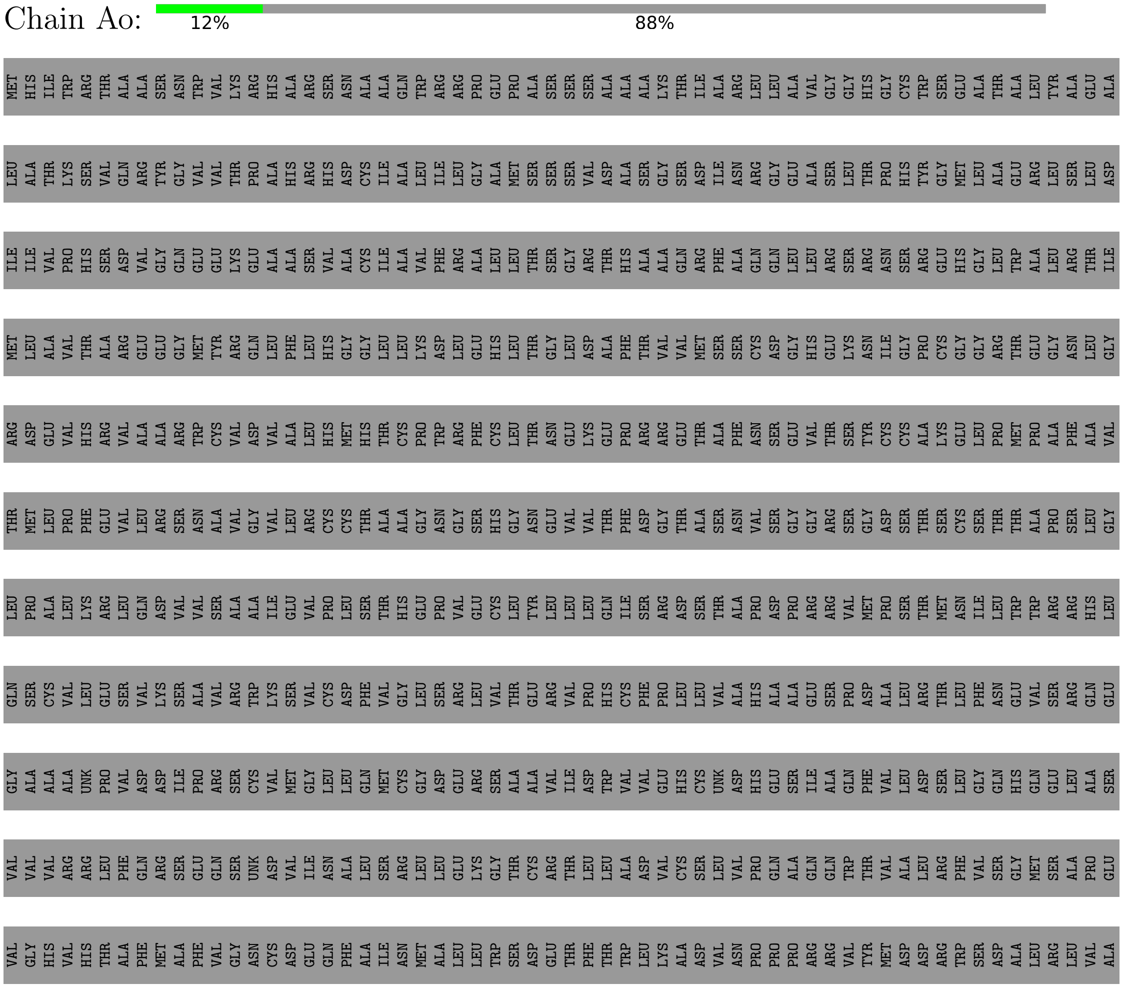
- Molecule 76: mL101

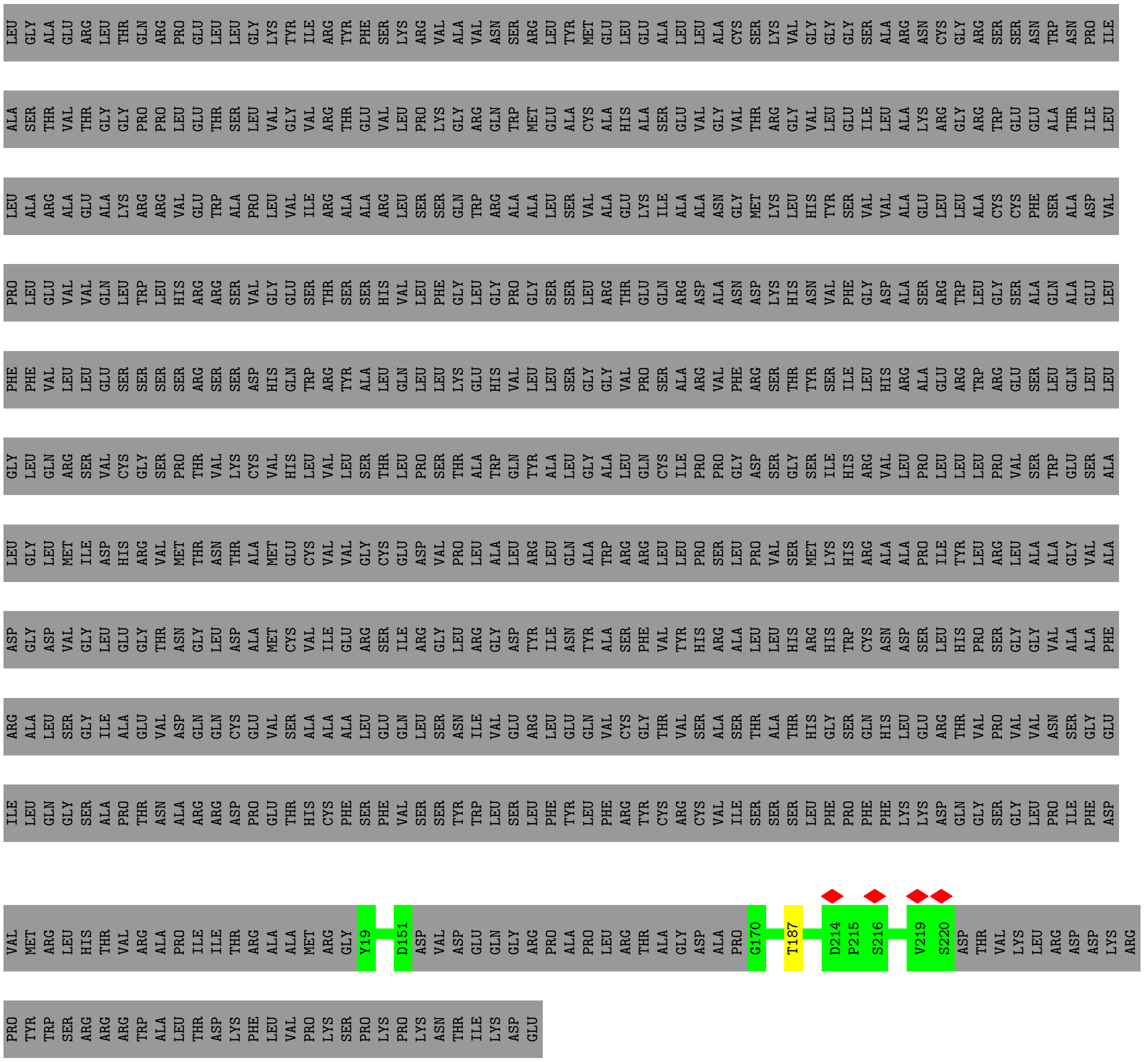


- Molecule 77: mL49

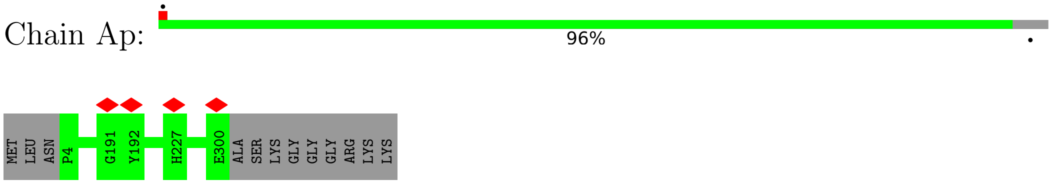


- Molecule 78: mL52

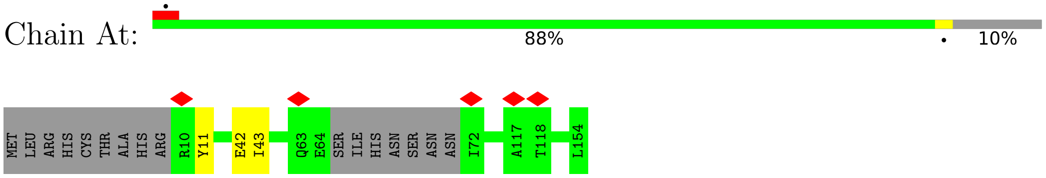




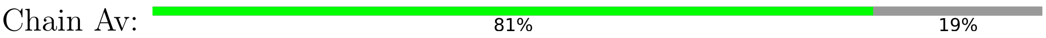
- Molecule 79: mL53

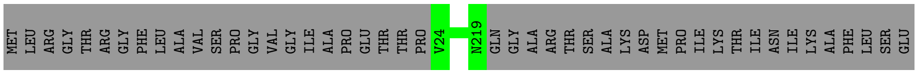


- Molecule 80: mL63



- Molecule 81: mL64




MET
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PRO
GLU
THR
THR
PRO
V24
N219
GLN
GLY
ALA
ARG
THR
SER
ALA
LYS
ASP
MET
PRO
ILE
LYS
THR
ILE
ASN
ILE
LYS
ALA
PHE
LEU
SER
GLU

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98508	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 ($e^-/\text{Å}^2$)	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	0.210	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	434.0, 434.0, 434.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	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: SPD, NAD, ZN, GTP, MG, ATP, PM8, NA

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	0.25	0/1828	0.39	0/2466
2	A2	0.25	0/3763	0.39	0/5124
3	A3	0.24	0/1246	0.40	0/1678
4	A5	0.24	0/498	0.40	0/663
5	A8	0.24	0/1231	0.40	0/1648
6	AA	0.21	0/20700	0.76	10/32183 (0.0%)
7	BA	0.24	0/6192	0.40	0/8401
8	EA	0.23	0/4337	0.39	0/5856
9	BB	0.24	0/3456	0.39	0/4684
10	EB	0.23	0/5426	0.40	0/7340
11	EC	0.25	0/3090	0.41	0/4190
12	BD	0.24	0/3418	0.39	0/4629
13	ED	0.24	0/4872	0.40	0/6599
14	AE	0.26	0/3570	0.42	1/4849 (0.0%)
15	BE	0.25	0/3306	0.40	0/4476
16	EE	0.23	0/3510	0.39	1/4751 (0.0%)
18	AF	0.25	0/3706	0.40	0/5029
19	BF	0.25	0/2909	0.41	0/3920
20	EF	0.24	0/2308	0.41	0/3137
21	EG	0.25	0/1331	0.41	0/1784
22	BH	0.24	0/2356	0.40	0/3203
23	EH	0.24	0/3548	0.39	0/4814
24	AI	0.25	0/1980	0.38	0/2693
25	BI	0.25	0/2717	0.39	0/3674
26	EI	0.23	0/2133	0.41	1/2894 (0.0%)
28	BJ	0.23	0/2494	0.38	0/3373
29	EJ	0.23	0/778	0.38	0/1047
30	AK	0.23	0/2565	0.39	0/3465
31	BK	0.24	0/1897	0.37	0/2556
32	EK	0.23	0/679	0.38	0/923
32	ER	0.24	0/679	0.39	0/923
34	BL	0.23	0/2064	0.39	0/2794

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	EL	0.24	0/4615	0.39	0/6282
37	EM	0.24	0/2658	0.39	0/3594
39	AN	0.24	0/1698	0.40	0/2308
40	BN	0.24	0/1755	0.38	0/2381
41	EN	0.23	0/5115	0.38	0/6936
42	AO	0.24	0/1371	0.42	0/1846
43	BO	0.25	0/1715	0.40	0/2322
44	EO	0.24	0/2188	0.40	0/2976
44	EP	0.24	0/1961	0.39	0/2669
45	AP	0.24	0/2774	0.41	0/3761
46	BQ	0.25	0/1691	0.42	0/2293
47	EQ	0.24	0/3701	0.39	0/4994
48	AR	0.24	0/2211	0.38	0/2988
49	BR	0.24	0/1702	0.40	0/2296
50	BS	0.23	0/1235	0.39	0/1665
51	ES	0.24	0/1276	0.37	0/1715
52	AT	0.24	0/1193	0.42	0/1611
53	BT	0.24	0/1465	0.40	0/1970
54	ET	0.25	0/858	0.37	0/1148
55	AU	0.24	0/1456	0.38	0/1971
56	BU	0.24	0/722	0.37	0/969
57	EU	0.24	0/412	0.38	0/538
58	AV	0.26	0/1454	0.45	0/1973
59	BV	0.23	0/786	0.39	0/1063
60	AW	0.24	0/2307	0.40	0/3119
61	BW	0.25	0/1604	0.40	0/2167
62	AX	0.25	0/1445	0.41	0/1963
63	BX	0.25	0/1131	0.42	0/1539
65	AY	0.24	0/2846	0.39	0/3847
66	BZ	0.25	0/1446	0.43	0/1956
67	Ba	0.24	0/1289	0.39	0/1742
68	Bb	0.24	0/1035	0.39	0/1402
69	Bc	0.25	0/1238	0.39	0/1685
70	Ae	0.24	0/1068	0.39	0/1447
71	Af	0.24	0/1134	0.40	0/1536
72	Bf	0.26	0/749	0.44	0/1012
73	Ag	0.24	0/1608	0.40	0/2180
74	Bg	0.24	0/682	0.40	0/919
75	Bh	0.24	0/752	0.40	0/1015
76	Bi	0.23	0/1530	0.38	0/2076
77	Al	0.25	0/1484	0.40	0/2019
78	Ao	0.25	0/1486	0.39	0/2022
79	Ap	0.24	0/2506	0.39	0/3404

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\lvert Z\rvert$ >5	RMSZ	#$\lvert Z\rvert$ >5
80	At	0.23	0/1179	0.39	0/1596
81	Av	0.24	0/1714	0.38	0/2311
All	All	0.24	0/180832	0.46	13/248992 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AA	951	C	C2-N1-C1'	8.17	127.79	118.80
6	AA	898	U	C2-N1-C1'	7.78	127.04	117.70
6	AA	951	C	N1-C2-O2	7.50	123.40	118.90
6	AA	898	U	N1-C2-O2	7.28	127.90	122.80
6	AA	898	U	N3-C2-O2	-6.55	117.61	122.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	205 (95%)	10 (5%)	0	100	100
2	A2	448/471 (95%)	438 (98%)	10 (2%)	0	100	100
3	A3	147/218 (67%)	143 (97%)	4 (3%)	0	100	100
4	A5	53/80 (66%)	53 (100%)	0	0	100	100
5	A8	140/181 (77%)	134 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	BA	763/831 (92%)	738 (97%)	25 (3%)	0	100	100
8	EA	530/576 (92%)	514 (97%)	16 (3%)	0	100	100
9	BB	408/541 (75%)	394 (97%)	14 (3%)	0	100	100
10	EB	659/754 (87%)	646 (98%)	13 (2%)	0	100	100
11	EC	371/406 (91%)	360 (97%)	11 (3%)	0	100	100
12	BD	417/547 (76%)	401 (96%)	16 (4%)	0	100	100
13	ED	593/616 (96%)	574 (97%)	19 (3%)	0	100	100
14	AE	432/473 (91%)	414 (96%)	17 (4%)	1 (0%)	47	79
15	BE	403/449 (90%)	381 (94%)	21 (5%)	1 (0%)	47	79
16	EE	429/586 (73%)	415 (97%)	14 (3%)	0	100	100
18	AF	440/459 (96%)	425 (97%)	15 (3%)	0	100	100
19	BF	342/426 (80%)	335 (98%)	7 (2%)	0	100	100
20	EF	292/373 (78%)	278 (95%)	14 (5%)	0	100	100
21	EG	152/156 (97%)	150 (99%)	2 (1%)	0	100	100
22	BH	280/349 (80%)	272 (97%)	8 (3%)	0	100	100
23	EH	424/634 (67%)	423 (100%)	1 (0%)	0	100	100
24	AI	228/263 (87%)	226 (99%)	2 (1%)	0	100	100
25	BI	321/342 (94%)	310 (97%)	11 (3%)	0	100	100
26	EI	273/349 (78%)	270 (99%)	3 (1%)	0	100	100
28	BJ	289/333 (87%)	278 (96%)	11 (4%)	0	100	100
29	EJ	93/116 (80%)	89 (96%)	3 (3%)	1 (1%)	14	46
30	AK	299/342 (87%)	289 (97%)	10 (3%)	0	100	100
31	BK	222/386 (58%)	218 (98%)	4 (2%)	0	100	100
32	EK	82/148 (55%)	82 (100%)	0	0	100	100
32	ER	82/148 (55%)	81 (99%)	1 (1%)	0	100	100
34	BL	255/312 (82%)	247 (97%)	8 (3%)	0	100	100
35	EL	553/691 (80%)	541 (98%)	12 (2%)	0	100	100
37	EM	326/451 (72%)	319 (98%)	7 (2%)	0	100	100
39	AN	191/202 (95%)	184 (96%)	7 (4%)	0	100	100
40	BN	212/302 (70%)	210 (99%)	2 (1%)	0	100	100
41	EN	632/731 (86%)	614 (97%)	18 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	AO	161/217 (74%)	156 (97%)	5 (3%)	0	100	100
43	BO	211/262 (80%)	209 (99%)	2 (1%)	0	100	100
44	EO	267/319 (84%)	257 (96%)	10 (4%)	0	100	100
44	EP	235/319 (74%)	227 (97%)	8 (3%)	0	100	100
45	AP	321/374 (86%)	309 (96%)	12 (4%)	0	100	100
46	BQ	216/231 (94%)	204 (94%)	12 (6%)	0	100	100
47	EQ	465/655 (71%)	460 (99%)	5 (1%)	0	100	100
48	AR	255/301 (85%)	250 (98%)	5 (2%)	0	100	100
49	BR	194/205 (95%)	185 (95%)	9 (5%)	0	100	100
50	BS	149/198 (75%)	146 (98%)	3 (2%)	0	100	100
51	ES	148/524 (28%)	145 (98%)	3 (2%)	0	100	100
52	AT	139/144 (96%)	134 (96%)	5 (4%)	0	100	100
53	BT	171/191 (90%)	165 (96%)	6 (4%)	0	100	100
54	ET	99/102 (97%)	95 (96%)	4 (4%)	0	100	100
55	AU	171/213 (80%)	165 (96%)	6 (4%)	0	100	100
56	BU	81/185 (44%)	81 (100%)	0	0	100	100
57	EU	45/56 (80%)	45 (100%)	0	0	100	100
58	AV	179/188 (95%)	174 (97%)	5 (3%)	0	100	100
59	BV	88/190 (46%)	86 (98%)	2 (2%)	0	100	100
60	AW	276/278 (99%)	273 (99%)	3 (1%)	0	100	100
61	BW	185/188 (98%)	183 (99%)	2 (1%)	0	100	100
62	AX	164/246 (67%)	162 (99%)	2 (1%)	0	100	100
63	BX	131/190 (69%)	122 (93%)	9 (7%)	0	100	100
65	AY	338/378 (89%)	334 (99%)	4 (1%)	0	100	100
66	BZ	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
67	Ba	140/153 (92%)	134 (96%)	6 (4%)	0	100	100
68	Bb	124/162 (76%)	120 (97%)	4 (3%)	0	100	100
69	Bc	135/146 (92%)	131 (97%)	4 (3%)	0	100	100
70	Ae	123/197 (62%)	119 (97%)	4 (3%)	0	100	100
71	Af	137/189 (72%)	136 (99%)	1 (1%)	0	100	100
72	Bf	85/113 (75%)	79 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	Ag	184/260 (71%)	178 (97%)	6 (3%)	0	100	100
74	Bg	81/105 (77%)	77 (95%)	4 (5%)	0	100	100
75	Bh	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
76	Bi	190/245 (78%)	183 (96%)	7 (4%)	0	100	100
77	Al	179/218 (82%)	175 (98%)	4 (2%)	0	100	100
78	Ao	180/1520 (12%)	179 (99%)	1 (1%)	0	100	100
79	Ap	295/309 (96%)	290 (98%)	5 (2%)	0	100	100
80	At	134/154 (87%)	129 (96%)	5 (4%)	0	100	100
81	Av	194/242 (80%)	190 (98%)	4 (2%)	0	100	100
All	All	19143/24932 (77%)	18599 (97%)	541 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	BE	348	VAL
29	EJ	46	PRO
14	AE	412	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	195/217 (90%)	192 (98%)	3 (2%)	65	85
2	A2	397/413 (96%)	395 (100%)	2 (0%)	88	94
3	A3	134/193 (69%)	134 (100%)	0	100	100
4	A5	52/73 (71%)	51 (98%)	1 (2%)	57	81
5	A8	126/161 (78%)	123 (98%)	3 (2%)	49	76
7	BA	662/727 (91%)	649 (98%)	13 (2%)	55	80
8	EA	463/502 (92%)	459 (99%)	4 (1%)	78	91
9	BB	356/470 (76%)	343 (96%)	13 (4%)	34	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	EB	573/649 (88%)	570 (100%)	3 (0%)	88	94
11	EC	327/354 (92%)	324 (99%)	3 (1%)	78	91
12	BD	356/472 (75%)	347 (98%)	9 (2%)	47	75
13	ED	529/544 (97%)	522 (99%)	7 (1%)	69	87
14	AE	349/406 (86%)	347 (99%)	2 (1%)	86	94
15	BE	348/386 (90%)	338 (97%)	10 (3%)	42	72
16	EE	367/514 (71%)	361 (98%)	6 (2%)	62	84
18	AF	394/409 (96%)	393 (100%)	1 (0%)	92	96
19	BF	300/368 (82%)	299 (100%)	1 (0%)	92	96
20	EF	249/302 (82%)	248 (100%)	1 (0%)	91	96
21	EG	134/136 (98%)	134 (100%)	0	100	100
22	BH	238/297 (80%)	233 (98%)	5 (2%)	53	79
23	EH	385/527 (73%)	383 (100%)	2 (0%)	88	94
24	AI	205/225 (91%)	203 (99%)	2 (1%)	76	90
25	BI	271/288 (94%)	268 (99%)	3 (1%)	73	89
26	EI	217/310 (70%)	216 (100%)	1 (0%)	88	94
28	BJ	255/298 (86%)	250 (98%)	5 (2%)	55	80
29	EJ	77/95 (81%)	77 (100%)	0	100	100
30	AK	269/301 (89%)	267 (99%)	2 (1%)	84	93
31	BK	200/329 (61%)	196 (98%)	4 (2%)	55	80
32	EK	78/127 (61%)	78 (100%)	0	100	100
32	ER	78/127 (61%)	78 (100%)	0	100	100
34	BL	203/262 (78%)	197 (97%)	6 (3%)	41	71
35	EL	485/598 (81%)	478 (99%)	7 (1%)	67	86
37	EM	284/386 (74%)	279 (98%)	5 (2%)	59	82
39	AN	173/182 (95%)	172 (99%)	1 (1%)	86	94
40	BN	167/265 (63%)	163 (98%)	4 (2%)	49	76
41	EN	564/640 (88%)	561 (100%)	3 (0%)	88	94
42	AO	143/185 (77%)	142 (99%)	1 (1%)	84	93
43	BO	181/225 (80%)	180 (99%)	1 (1%)	86	94
44	EO	233/263 (89%)	227 (97%)	6 (3%)	46	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	EP	211/263 (80%)	208 (99%)	3 (1%)	67	86
45	AP	287/330 (87%)	284 (99%)	3 (1%)	76	90
46	BQ	172/195 (88%)	168 (98%)	4 (2%)	50	77
47	EQ	382/539 (71%)	379 (99%)	3 (1%)	81	92
48	AR	222/256 (87%)	219 (99%)	3 (1%)	67	86
49	BR	172/181 (95%)	170 (99%)	2 (1%)	71	88
50	BS	127/164 (77%)	124 (98%)	3 (2%)	49	76
51	ES	134/437 (31%)	134 (100%)	0	100	100
52	AT	121/124 (98%)	117 (97%)	4 (3%)	38	69
53	BT	151/163 (93%)	150 (99%)	1 (1%)	84	93
54	ET	87/88 (99%)	87 (100%)	0	100	100
55	AU	151/184 (82%)	150 (99%)	1 (1%)	84	93
56	BU	72/168 (43%)	70 (97%)	2 (3%)	43	73
57	EU	43/51 (84%)	42 (98%)	1 (2%)	50	77
58	AV	153/158 (97%)	150 (98%)	3 (2%)	55	80
59	BV	79/163 (48%)	78 (99%)	1 (1%)	69	87
60	AW	246/246 (100%)	245 (100%)	1 (0%)	91	96
61	BW	163/164 (99%)	156 (96%)	7 (4%)	29	62
62	AX	154/221 (70%)	153 (99%)	1 (1%)	86	94
63	BX	117/170 (69%)	112 (96%)	5 (4%)	29	62
65	AY	305/337 (90%)	303 (99%)	2 (1%)	84	93
66	BZ	152/160 (95%)	147 (97%)	5 (3%)	38	69
67	Ba	134/144 (93%)	132 (98%)	2 (2%)	65	85
68	Bb	109/135 (81%)	109 (100%)	0	100	100
69	Bc	127/134 (95%)	125 (98%)	2 (2%)	62	84
70	Ae	110/172 (64%)	109 (99%)	1 (1%)	78	91
71	Af	120/162 (74%)	118 (98%)	2 (2%)	60	83
72	Bf	77/98 (79%)	76 (99%)	1 (1%)	69	87
73	Ag	170/239 (71%)	170 (100%)	0	100	100
74	Bg	66/87 (76%)	65 (98%)	1 (2%)	65	85
75	Bh	79/80 (99%)	78 (99%)	1 (1%)	69	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
76	Bi	147/217 (68%)	142 (97%)	5 (3%)	37	69
77	Al	155/186 (83%)	154 (99%)	1 (1%)	86	94
78	Ao	151/1258 (12%)	150 (99%)	1 (1%)	84	93
79	Ap	259/267 (97%)	259 (100%)	0	100	100
80	At	125/140 (89%)	122 (98%)	3 (2%)	49	76
81	Av	174/210 (83%)	174 (100%)	0	100	100
All	All	16721/21517 (78%)	16506 (99%)	215 (1%)	70	87

5 of 215 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	EL	339	GLU
44	EP	102	TYR
70	Ae	109	ARG
37	EM	136	LYS
41	EN	287	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 282 such sidechains are listed below:

Mol	Chain	Res	Type
65	AY	235	GLN
66	BZ	96	GLN
73	Ag	105	GLN
19	BF	362	HIS
19	BF	148	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	AA	879/1176 (74%)	318 (36%)	11 (1%)

5 of 318 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	AA	2	U
6	AA	4	U
6	AA	5	U
6	AA	11	U

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Mol	Chain	Res	Type
6	AA	12	U

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	AA	793	U
6	AA	895	U
6	AA	1004	U
6	AA	994	A
6	AA	493	A

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 48 ligands modelled in this entry, 40 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
88	PM8	ER	200	32	25,31,31	0.79	1 (4%)	30,38,38	1.03	1 (3%)
89	NAD	Av	301	-	42,48,48	0.64	1 (2%)	50,73,73	0.91	3 (6%)
84	SPD	AA	1250	-	9,9,9	0.33	0	8,8,8	0.87	0
85	GTP	EA	1001	86,83	26,34,34	1.16	2 (7%)	32,54,54	1.55	8 (25%)
88	PM8	EK	200	32	25,31,31	0.71	1 (4%)	30,38,38	0.97	2 (6%)
85	GTP	EQ	1000	83	26,34,34	1.16	2 (7%)	32,54,54	1.63	7 (21%)
85	GTP	EA	2001	86,83	26,34,34	1.15	2 (7%)	32,54,54	1.59	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
87	ATP	EB	1001	83	26,33,33	0.93	1 (3%)	31,52,52	1.43	5 (16%)

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
88	PM8	ER	200	32	-	17/36/38/38	-
89	NAD	Av	301	-	-	3/26/62/62	0/5/5/5
84	SPD	AA	1250	-	-	2/7/7/7	-
85	GTP	EA	1001	86,83	-	7/18/38/38	0/3/3/3
88	PM8	EK	200	32	-	12/36/38/38	-
85	GTP	EQ	1000	83	-	2/18/38/38	0/3/3/3
85	GTP	EA	2001	86,83	-	5/18/38/38	0/3/3/3
87	ATP	EB	1001	83	-	0/18/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	EQ	1000	GTP	C5-C6	-4.24	1.38	1.47
85	EA	1001	GTP	C5-C6	-4.02	1.39	1.47
85	EA	2001	GTP	C5-C6	-3.98	1.39	1.47
88	ER	200	PM8	C2-C1	2.51	1.53	1.50
87	EB	1001	ATP	C5-C4	2.42	1.47	1.40

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	EQ	1000	GTP	PB-O3B-PG	-3.89	119.47	132.83
85	EA	1001	GTP	PA-O3A-PB	-3.85	119.60	132.83
89	Av	301	NAD	O4D-C1D-C2D	-3.81	101.36	106.93
85	EQ	1000	GTP	PA-O3A-PB	-3.59	120.50	132.83
85	EA	1001	GTP	C5-C6-N1	3.43	120.01	113.95

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	EA	1001	GTP	PB-O3B-PG-O3G

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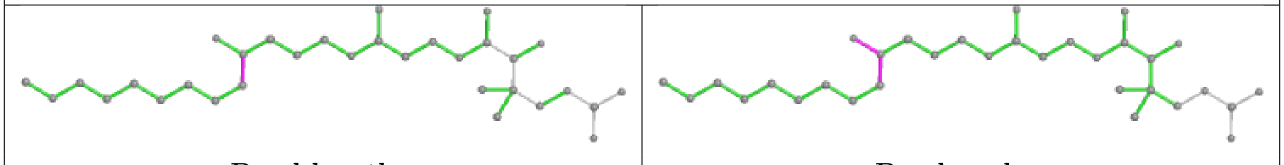
Mol	Chain	Res	Type	Atoms
85	EA	1001	GTP	C5'-O5'-PA-O3A
85	EA	1001	GTP	C5'-O5'-PA-O1A
85	EA	1001	GTP	C5'-O5'-PA-O2A
85	EA	1001	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

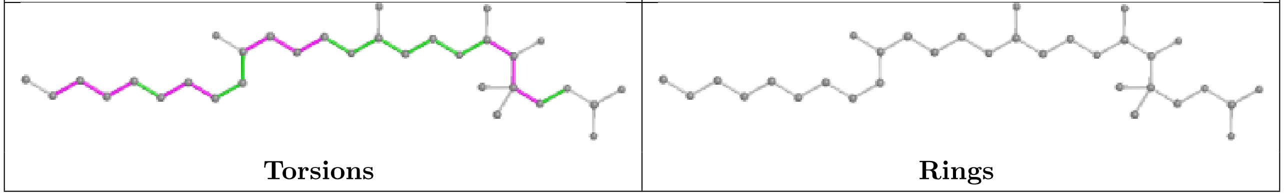
No monomer is involved in short contacts.

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 PM8 ER 200

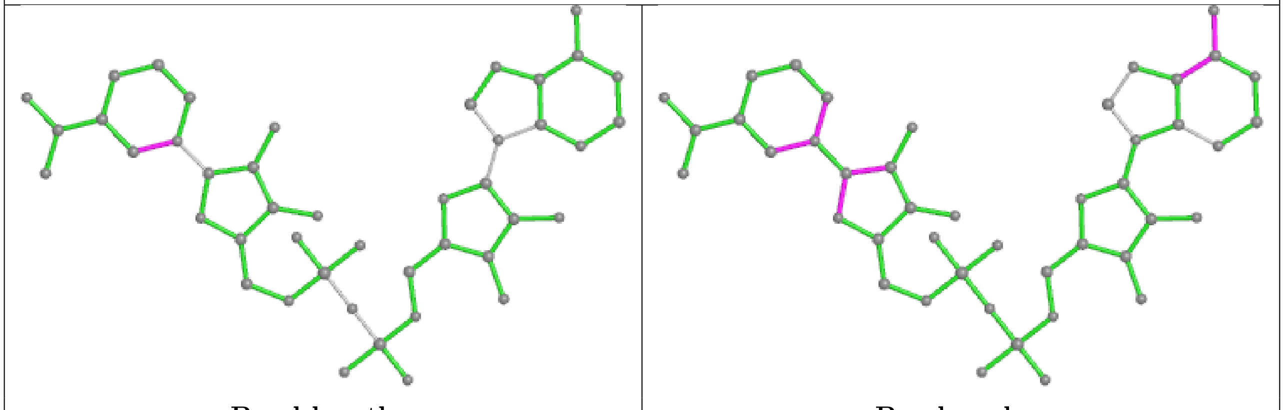


Bond lengths **Bond angles**

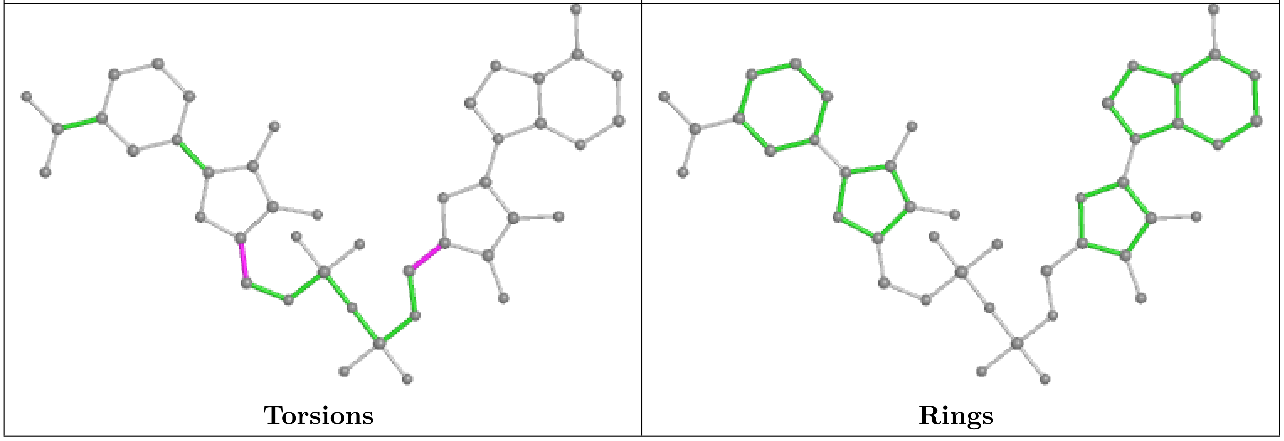


Torsions **Rings**

Ligand NAD Av 301

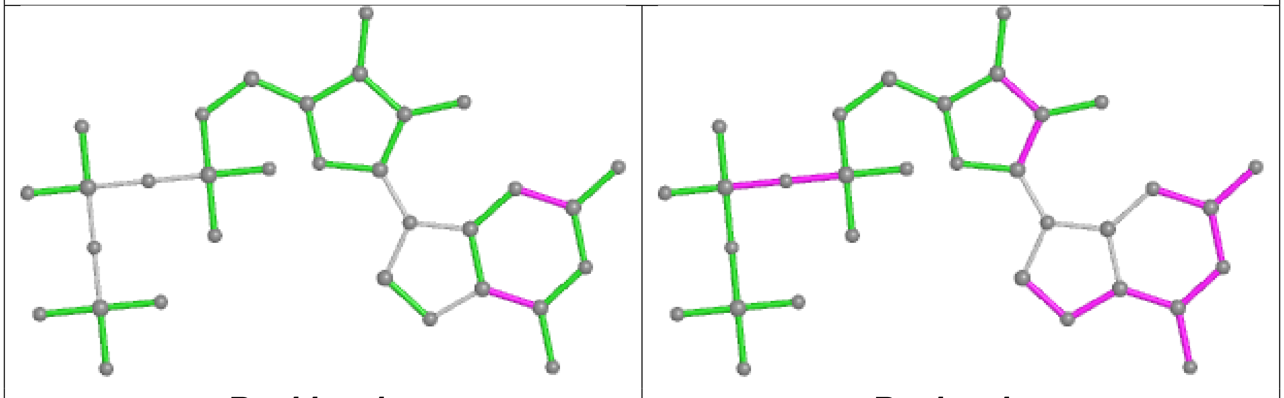


Bond lengths **Bond angles**

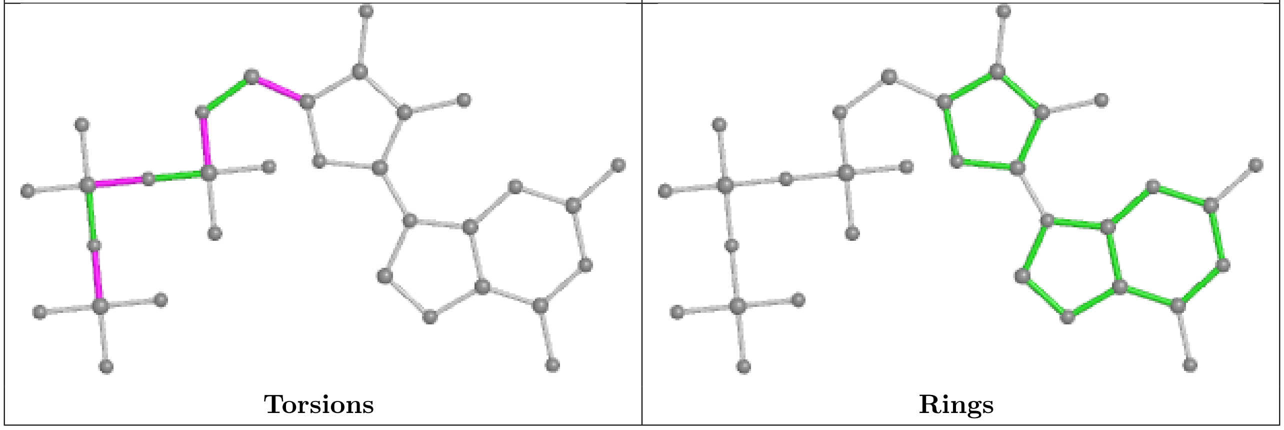


Torsions **Rings**

Ligand GTP EA 1001

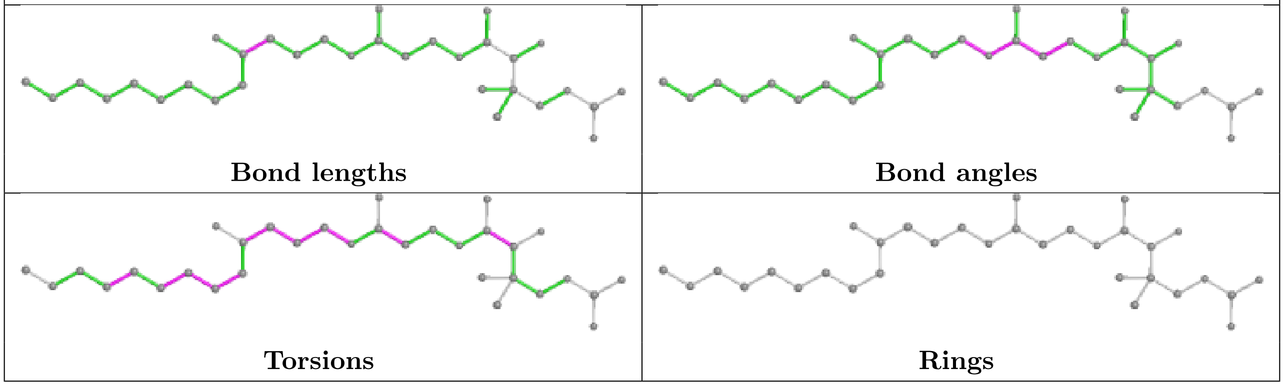


Bond lengths **Bond angles**

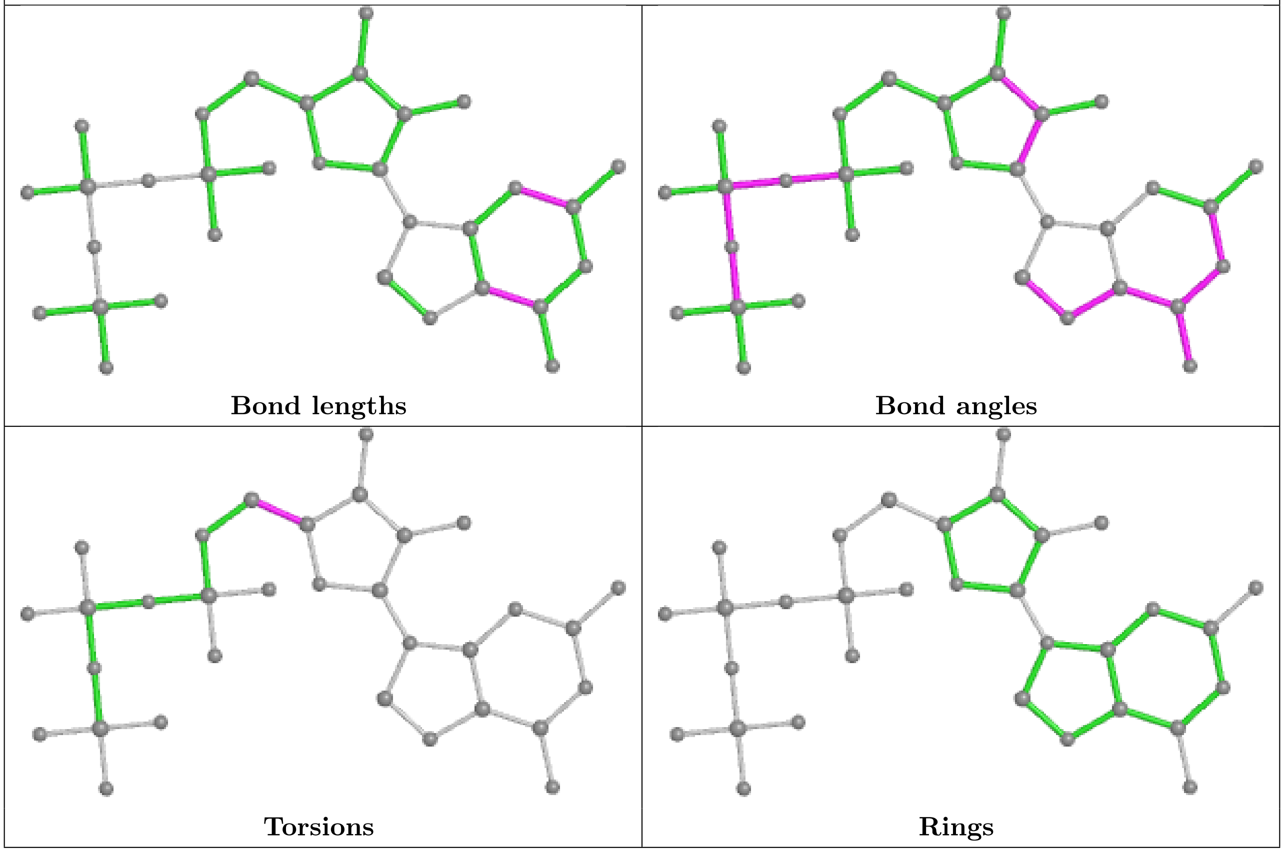


Torsions **Rings**

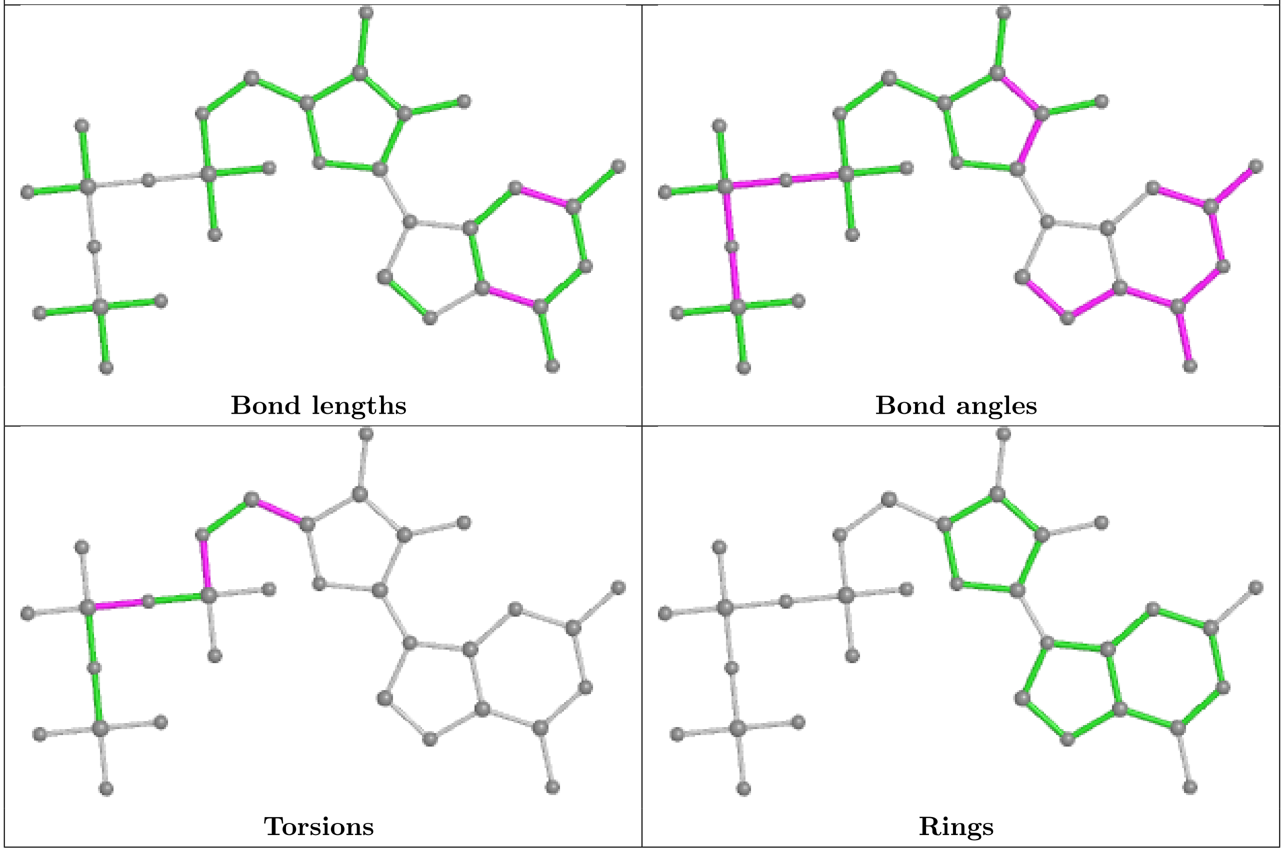
Ligand PM8 EK 200



Ligand GTP EQ 1000



Ligand GTP EA 2001



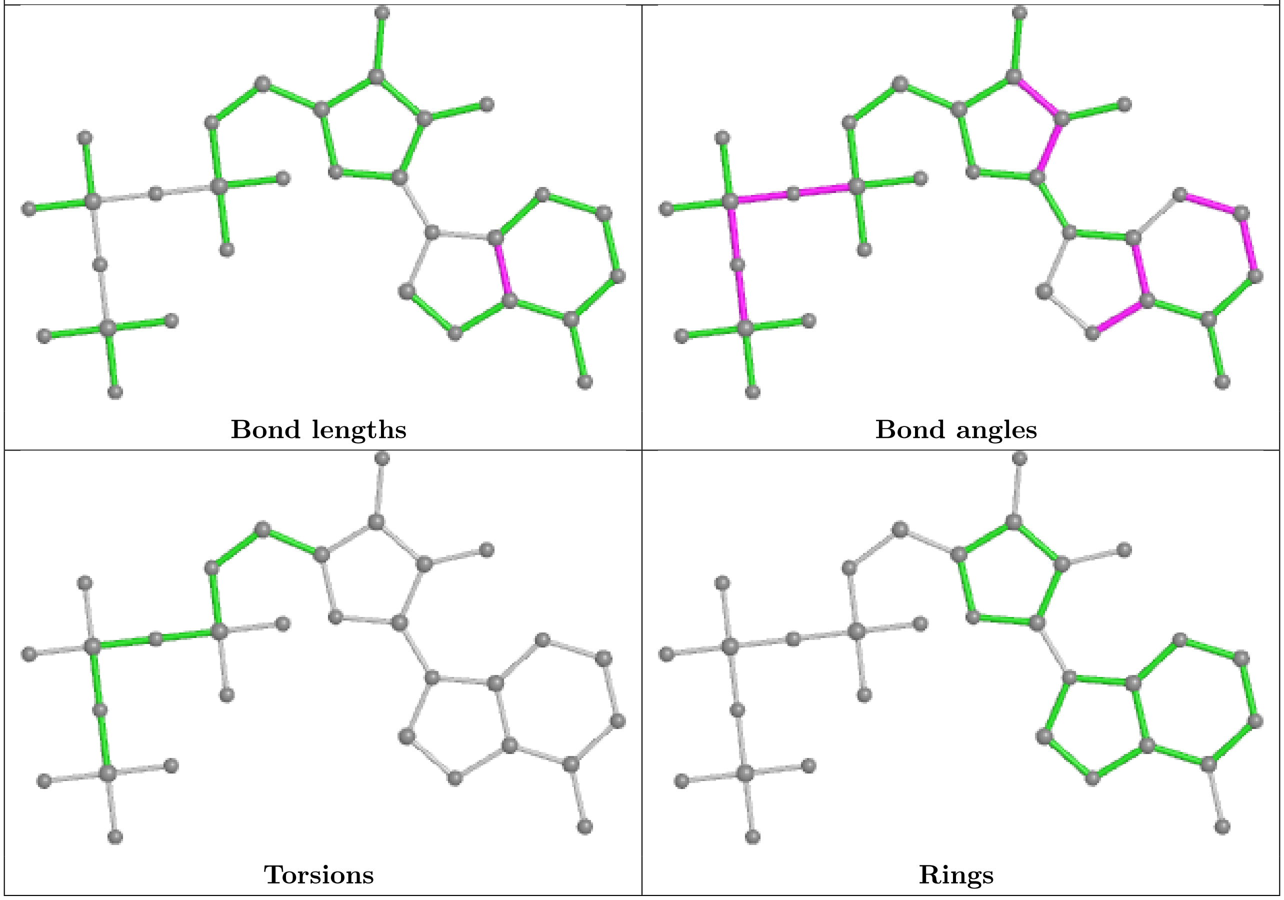
Bond lengths

Bond angles

Torsions

Rings

Ligand ATP EB 1001



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
64	UX	13
36	UL	3
17	UE	1

The worst 5 of 17 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UX	66:UNK	C	117:UNK	N	41.11
1	UX	341:UNK	C	402:UNK	N	39.28
1	UX	233:UNK	C	264:UNK	N	29.49

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UX	35:UNK	C	56:UNK	N	28.81
1	UX	15:UNK	C	26:UNK	N	26.47

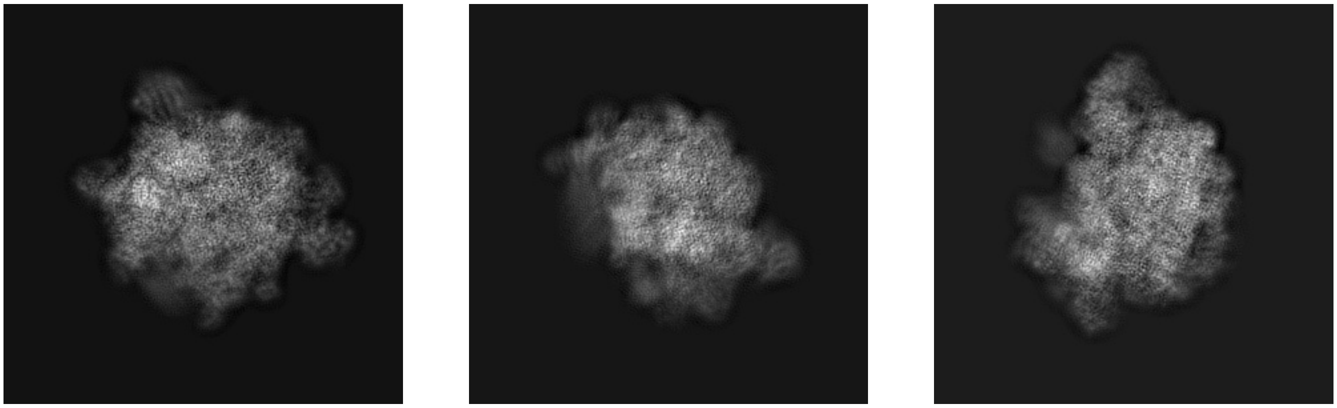
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-11000. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

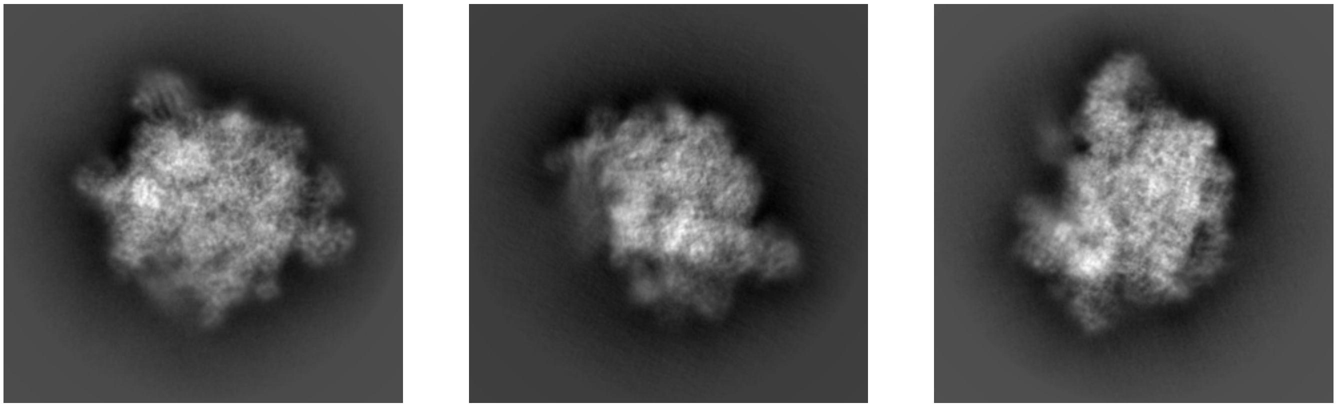
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

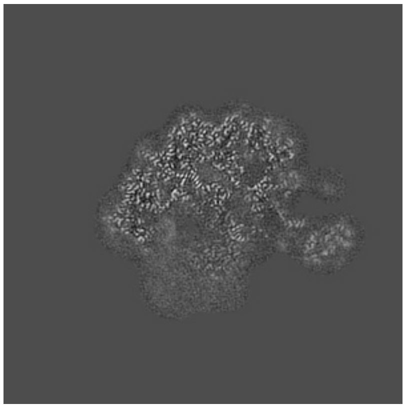


X Y Z

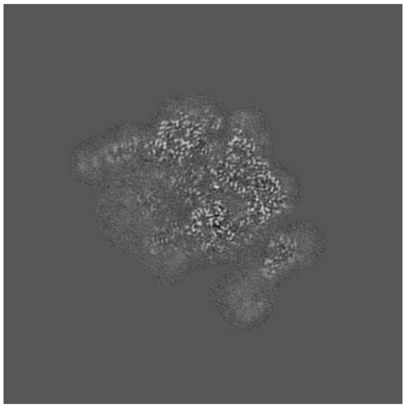
The images above show the map projected in three orthogonal directions.

6.2 Central slices

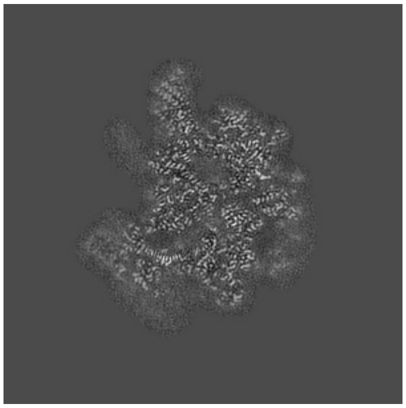
6.2.1 Primary map



X Index: 200

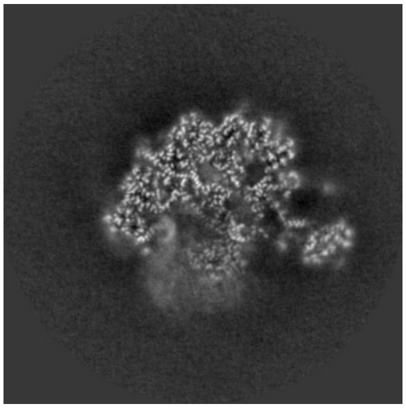


Y Index: 200

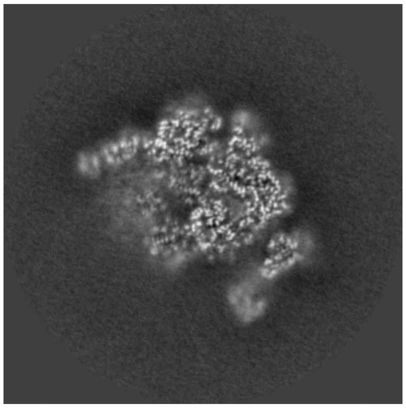


Z Index: 200

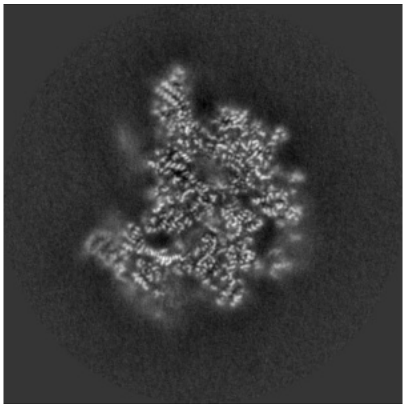
6.2.2 Raw map



X Index: 200



Y Index: 200

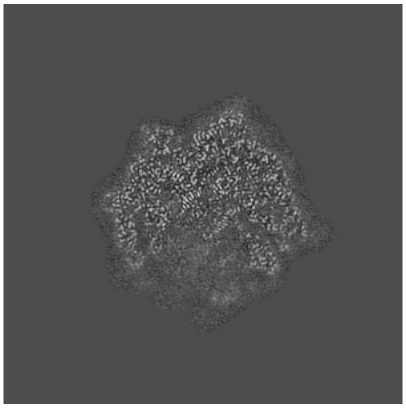


Z Index: 200

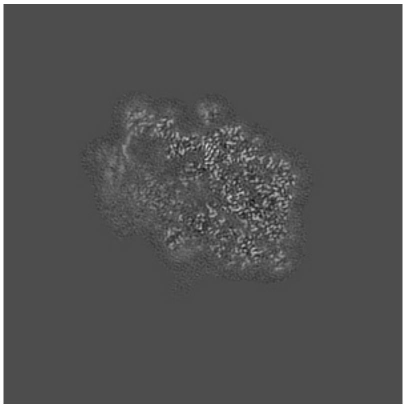
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

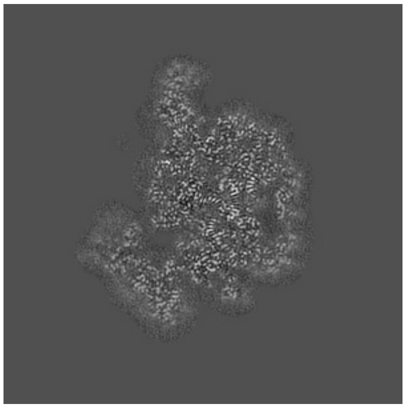
6.3.1 Primary map



X Index: 226

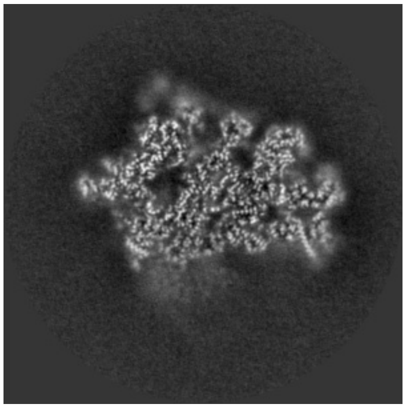


Y Index: 227

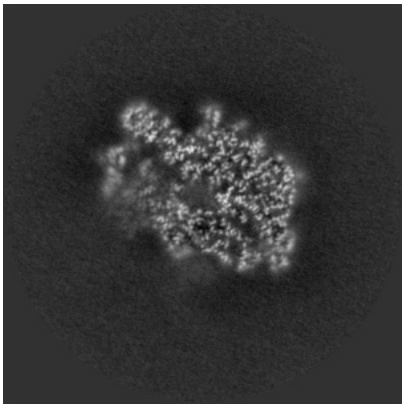


Z Index: 210

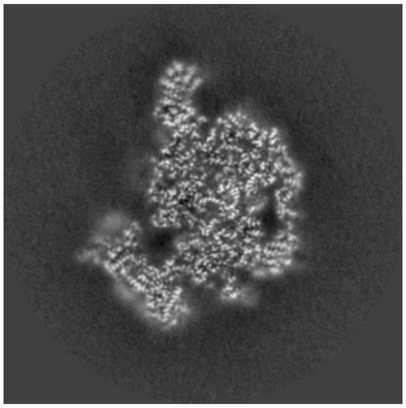
6.3.2 Raw map



X Index: 170



Y Index: 232



Z Index: 211

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

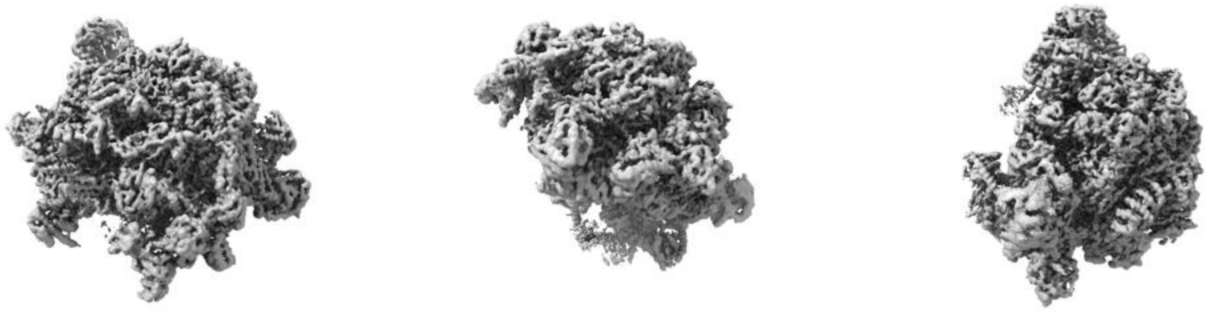
6.4 Orthogonal surface views

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

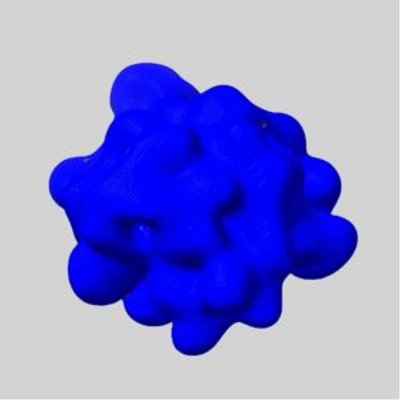
6.5 Mask visualisation ⓘ

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

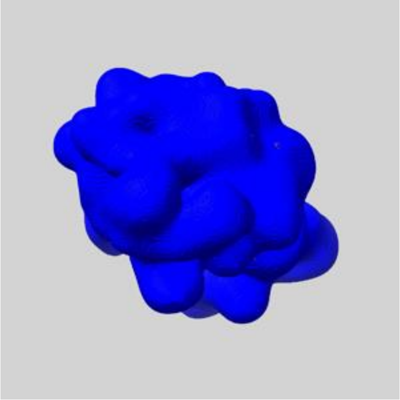
A mask typically either:

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

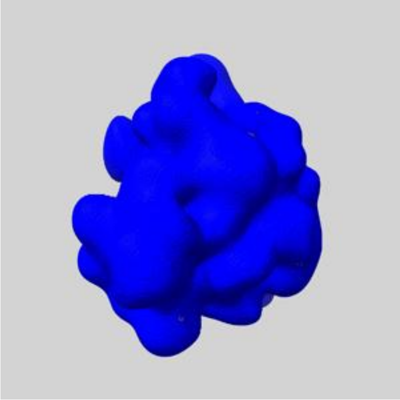
6.5.1 emd_11000_msk_1.map ⓘ



X



Y

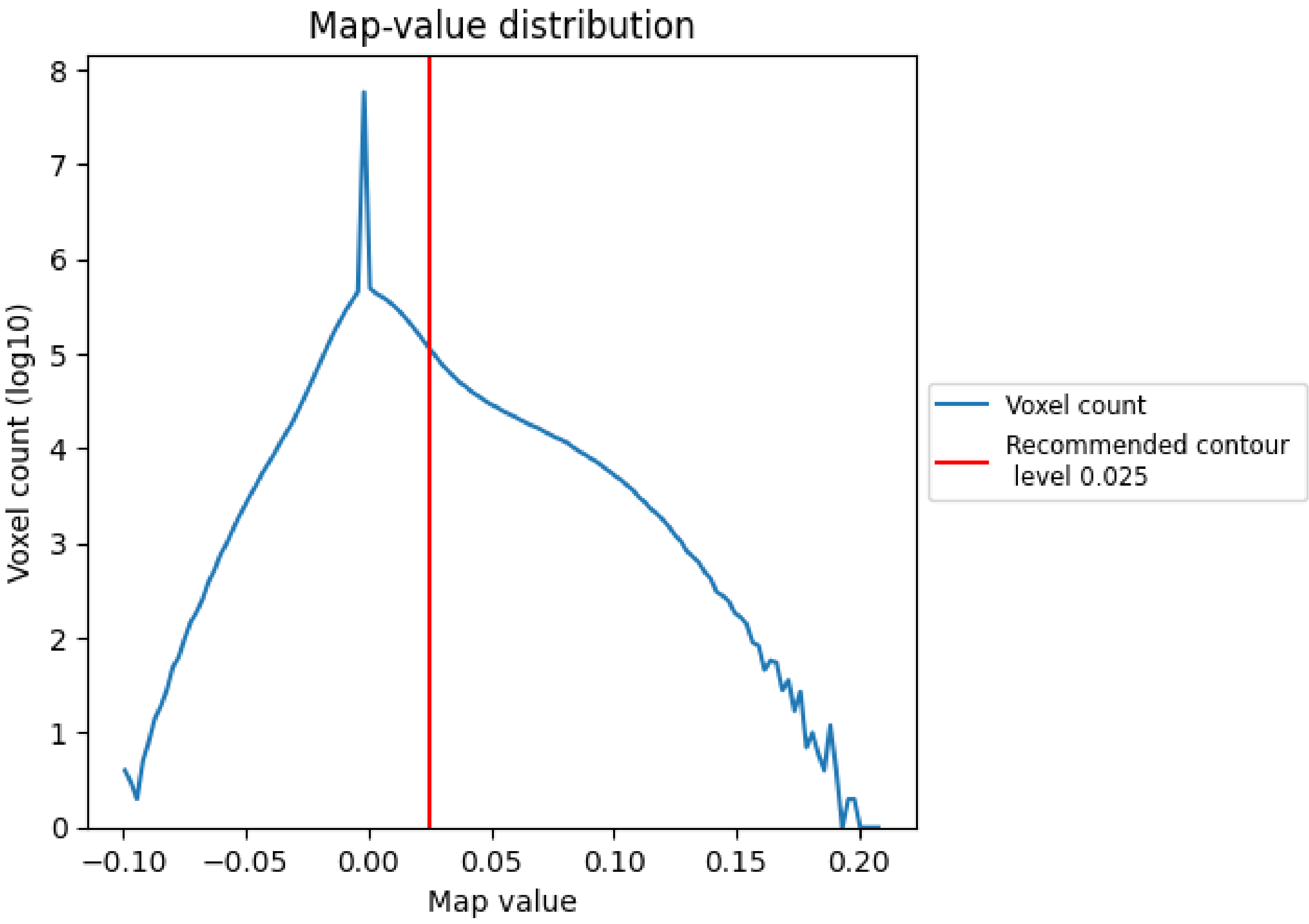


Z

7 Map analysis ⓘ

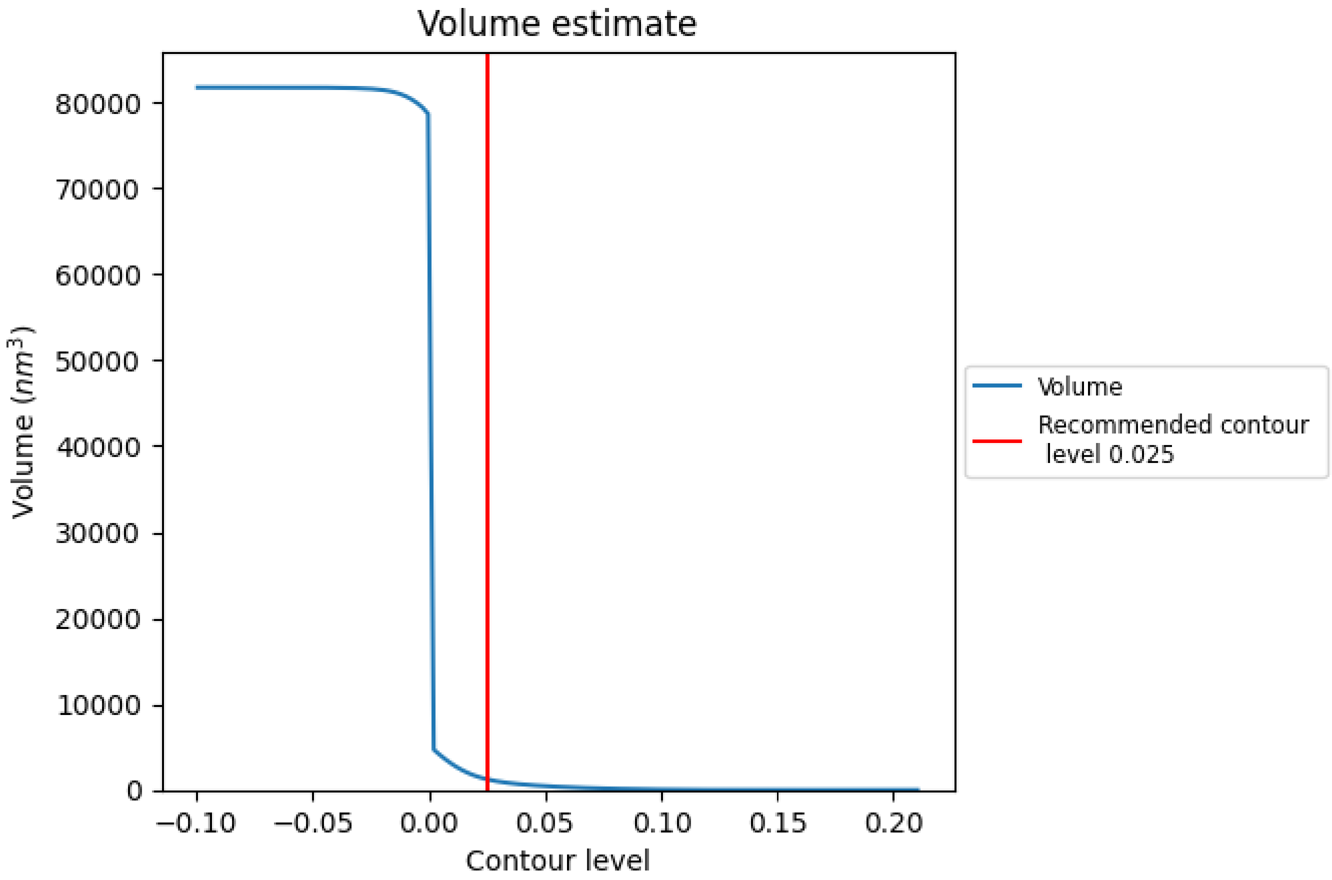
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

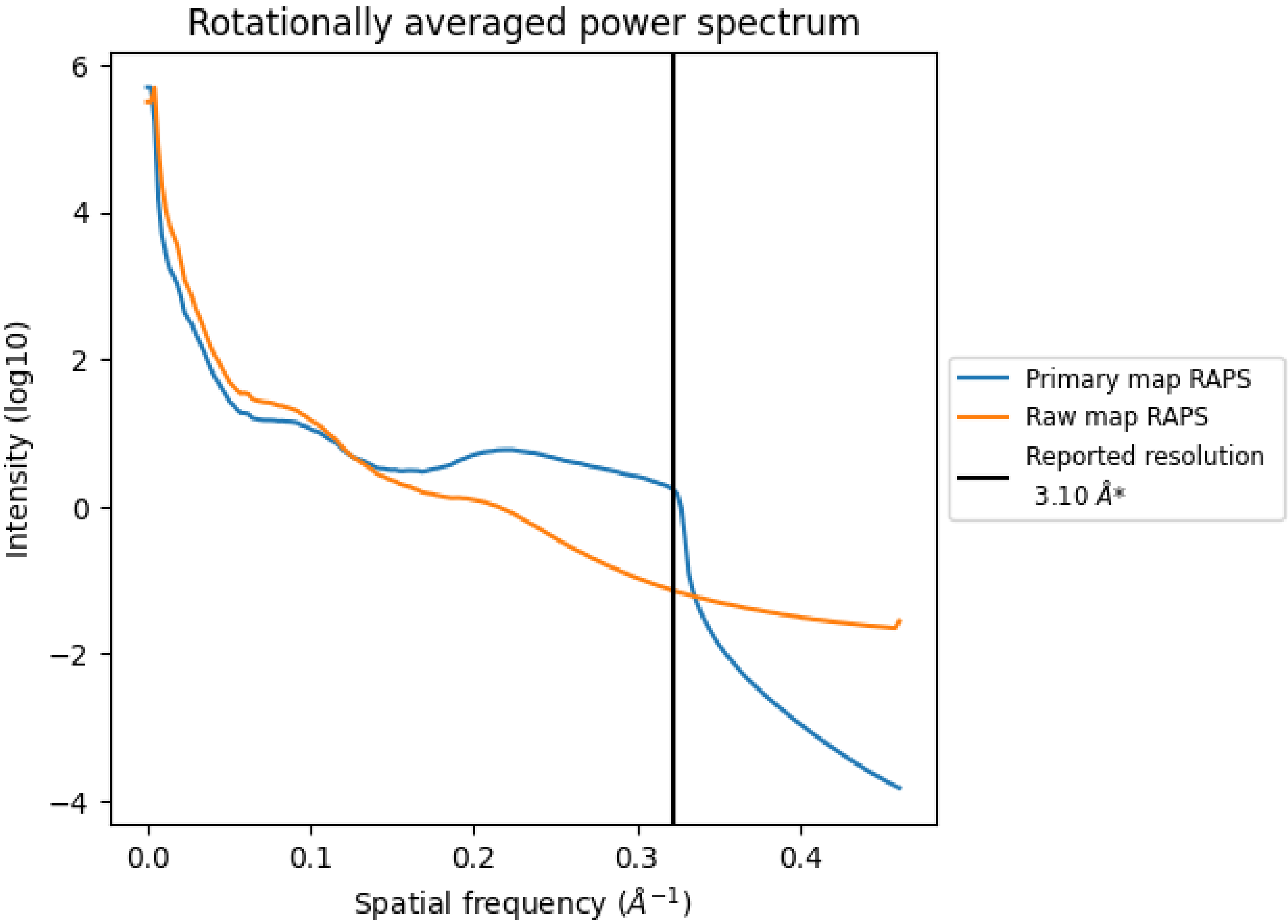
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1249 nm^3; this corresponds to an approximate mass of 1128 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

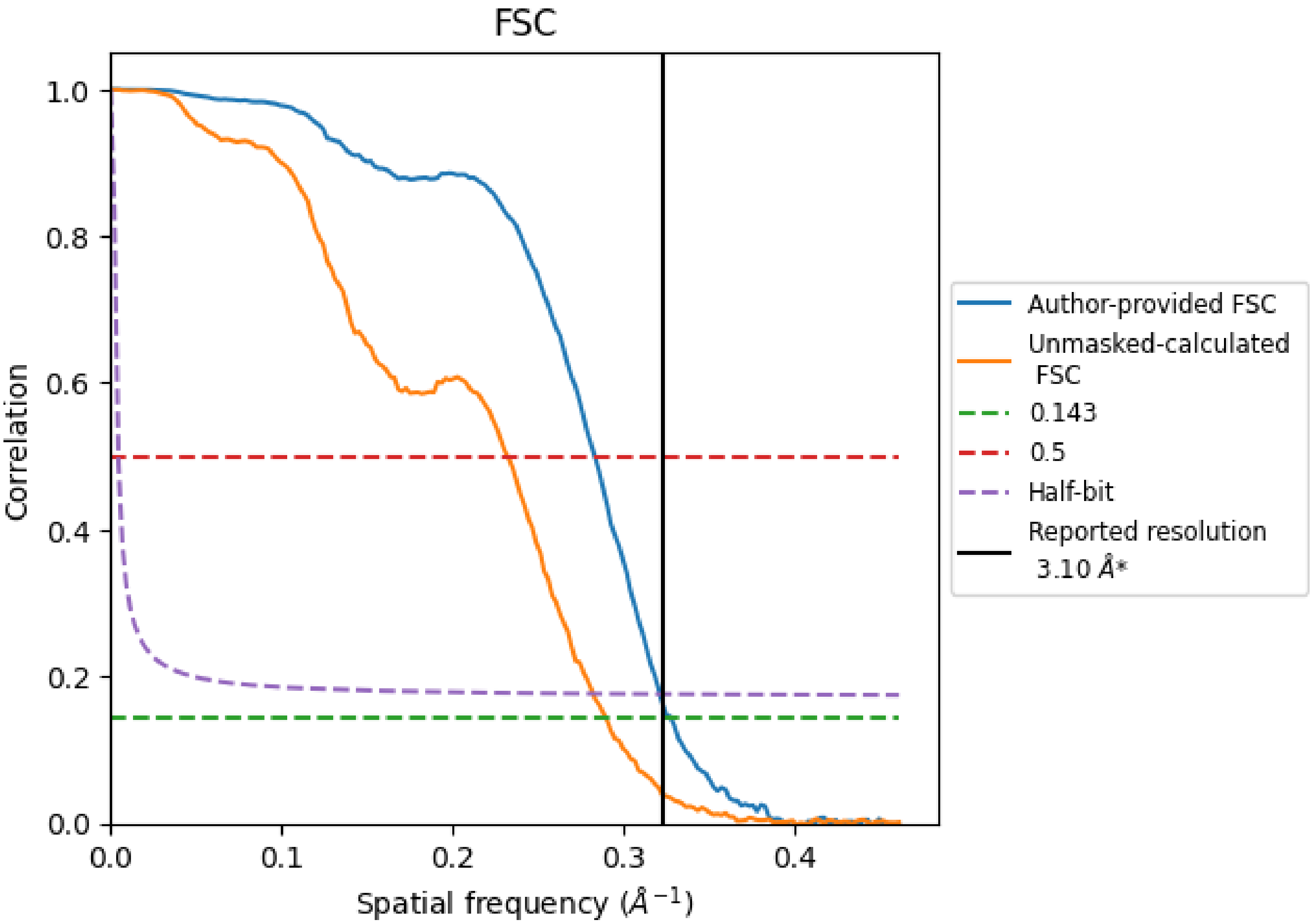


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8.2 Resolution estimates

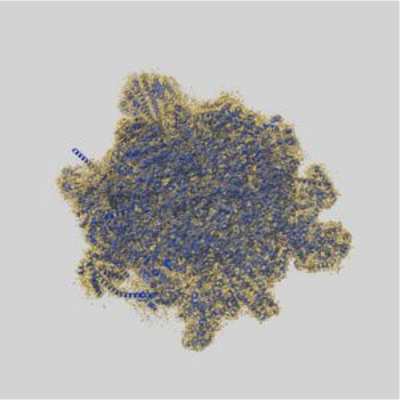
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.05	3.53	3.11
Unmasked-calculated*	3.45	4.31	3.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.45 differs from the reported value 3.1 by more than 10 %

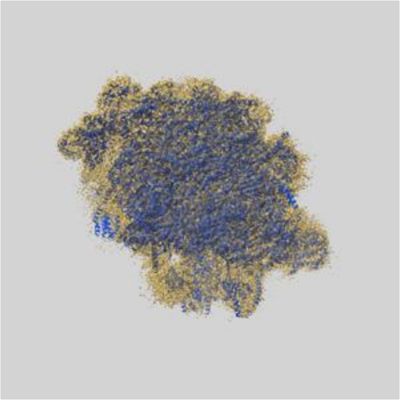
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11000 and PDB model 6YXY. Per-residue inclusion information can be found in section 3 on page 28.

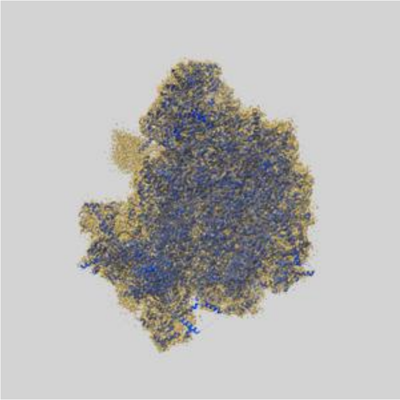
9.1 Map-model overlay (i)



X



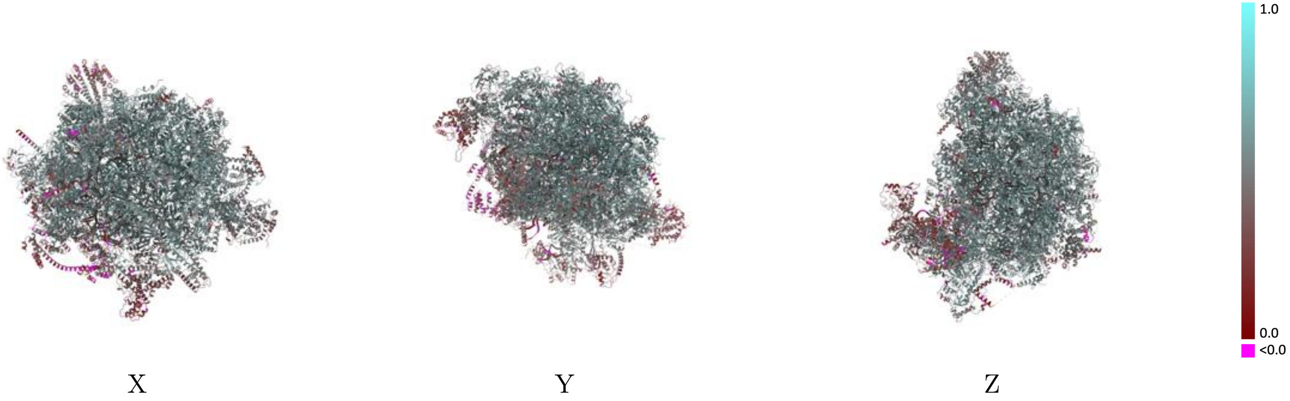
Y



Z

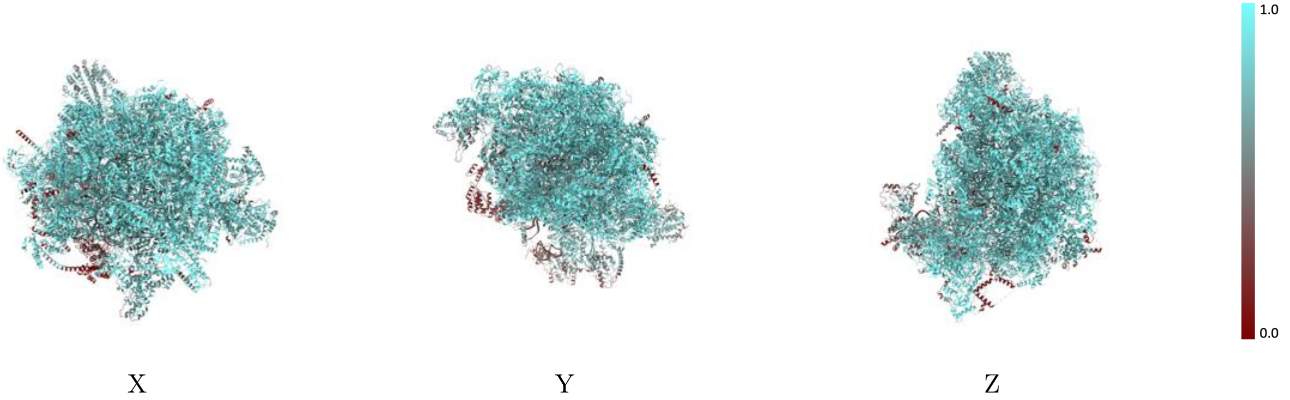
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



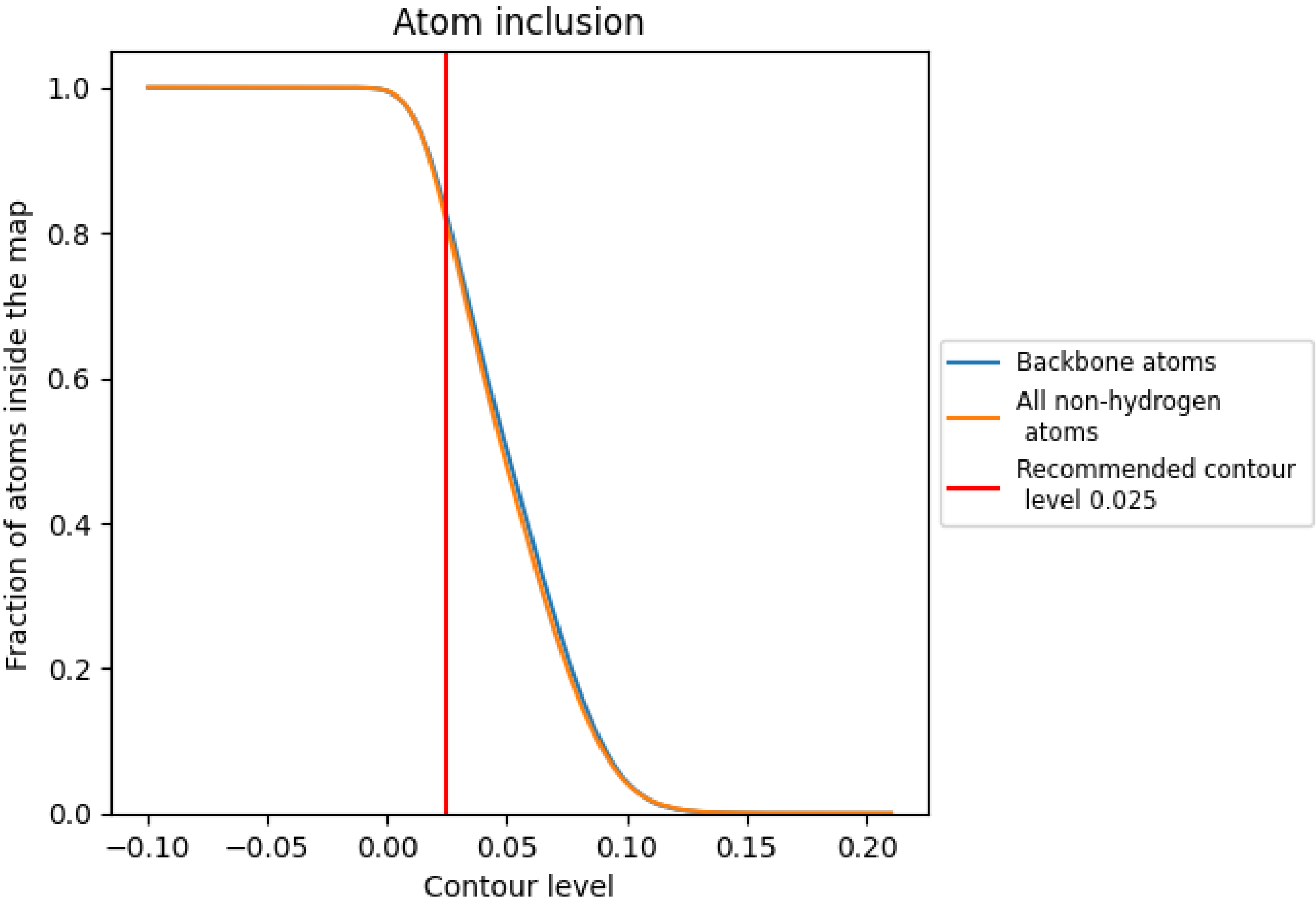
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8152	0.5080
A1	0.8647	0.5280
A2	0.9139	0.5520
A3	0.9048	0.5720
A5	0.8991	0.5690
A8	0.8803	0.5770
AA	0.8204	0.4900
AE	0.8098	0.5410
AF	0.9325	0.5840
AI	0.8556	0.5300
AK	0.6787	0.3790
AN	0.8826	0.5680
AO	0.8993	0.5800
AP	0.8985	0.5620
AR	0.8894	0.5660
AT	0.9232	0.5710
AU	0.9203	0.5710
AV	0.9316	0.5810
AW	0.9196	0.5780
AX	0.9143	0.5660
AY	0.8545	0.5220
Ae	0.8900	0.5510
Af	0.8887	0.5580
Ag	0.8767	0.5550
Al	0.8891	0.5650
Ao	0.8802	0.5720
Ap	0.9110	0.5670
At	0.8514	0.5380
Av	0.8960	0.5640
BA	0.8838	0.5420
BB	0.7289	0.3580
BD	0.7850	0.4450
BE	0.8521	0.5200
BF	0.9024	0.5570
BH	0.7517	0.5010

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Chain	Atom inclusion	Q-score
BI	0.9193	0.5640
BJ	0.6705	0.3940
BK	0.6676	0.4270
BL	0.8590	0.5030
BN	0.8445	0.4590
BO	0.8999	0.5500
BQ	0.8728	0.5360
BR	0.8600	0.5520
BS	0.8010	0.4910
BT	0.9190	0.5610
BU	0.8386	0.5070
BV	0.4709	0.2670
BW	0.9315	0.5660
BX	0.3201	0.4020
BZ	0.8242	0.4810
Ba	0.9185	0.5690
Bb	0.8332	0.4870
Bc	0.8700	0.5560
Bf	0.8045	0.5340
Bg	0.8375	0.5130
Bh	0.8390	0.5270
Bi	0.4556	0.3450
EA	0.8581	0.5460
EB	0.8818	0.5740
EC	0.8912	0.5780
ED	0.8935	0.5520
EE	0.8073	0.4970
EF	0.4007	0.3220
EG	0.9268	0.6010
EH	0.8520	0.5160
EI	0.7070	0.4690
EJ	0.8128	0.4580
EK	0.6786	0.3430
EL	0.9131	0.5460
EM	0.7492	0.5070
EN	0.7962	0.4840
EO	0.7498	0.3810
EP	0.6313	0.2550
EQ	0.6781	0.4960
ER	0.8049	0.4740
ES	0.7939	0.4480
ET	0.8455	0.5650

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Chain	Atom inclusion	Q-score
EU	0.6319	0.4880
UE	0.7636	0.4010
UI	0.2957	0.2930
UK	0.3600	0.1900
UL	0.0806	0.2040
UM	0.8750	0.5240
UX	0.0311	0.0710