



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 09:38 am GMT

PDB ID : 6HIX
EMDB ID : EMD-0231
Title : Cryo-EM structure of the Trypanosoma brucei mitochondrial ribosome - This entry contains the large mitoribosomal subunit
Authors : Ramrath, D.J.F.; Niemann, M.; Leibundgut, M.; Bieri, P.; Prange, C.; Horn, K.; Leitner, A.; Boehringer, D.; Schneider, A.; Ban, N.
Deposited on : 2018-08-31
Resolution : 3.39 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

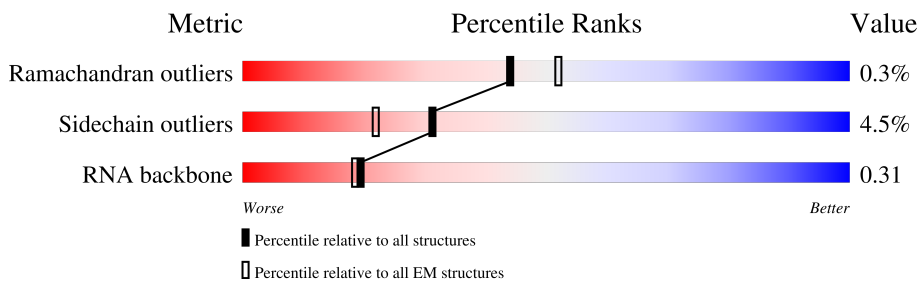
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.39 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.





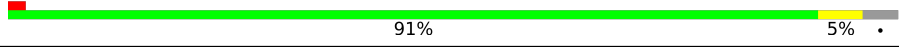
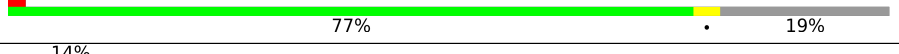



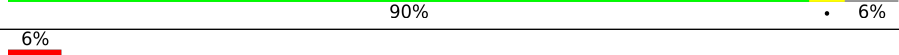
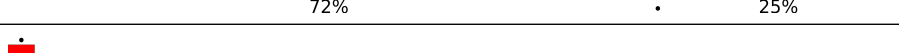

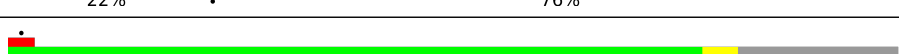

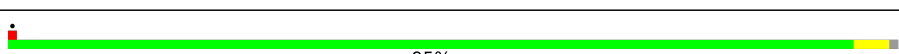
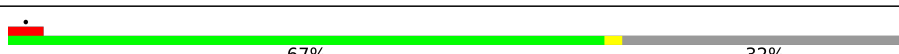
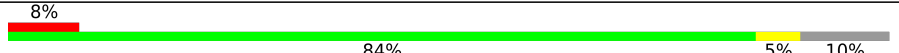




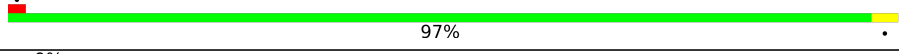
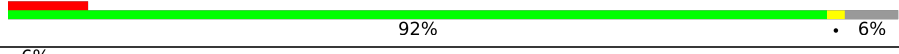
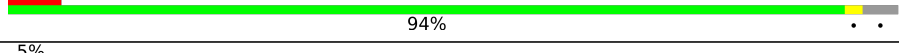



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A0	185	
2	A1	241	
3	A2	471	
4	A3	218	
5	A4	183	
6	A5	80	
7	A6	114	
8	A8	181	

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Mol	Chain	Length	Quality of chain
9	A9	184	
10	AE	473	
11	AF	459	
12	AI	263	
13	AJ	177	
14	AK	342	
15	AN	202	
16	AP	374	
17	AQ	167	
18	AR	301	
19	AT	144	
20	AU	213	
21	AV	188	
22	AW	278	
23	AX	246	
24	AY	378	
25	Ab	507	
26	Ad	289	
27	Ae	197	
28	Af	189	
29	Ag	260	
30	Aj	296	
31	Al	218	
32	Ao	259	
33	Ap	309	

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Mol	Chain	Length	Quality of chain
34	At	154	16% 88% 10%
35	Av	242	9% 82% 5% 12%
36	AB	56	54% 100%
37	AC	28	36% 100%
37	AD	28	100%
38	AG	27	100%
39	AA	1178	11% 25% 24% 50%
40	BA	831	78% 18%
41	BB	541	13% 65% 7% 28%
42	BC	523	88% 9%
43	BD	547	17% 72% 24%
44	BE	449	84% 13%
45	BF	426	79% 19%
46	BG	378	6% 79% 5% 16%
47	BH	349	55% 5% 40%
48	BI	343	89% 7%
49	BJ	333	8% 47% 50%
50	BK	386	28% 63% 33%
51	BL	312	72% 25%
52	BM	283	82% 5% 13%
53	BN	302	16% 67% 29%
54	BO	262	8% 52% 44%
55	BP	266	12% 71% 5% 24%
56	BQ	231	90% 6%
57	BR	205	90% 5% 5%

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Mol	Chain	Length	Quality of chain
58	BS	198	47% 51%
59	BT	191	84% 12%
60	BU	185	43% 56%
61	BV	190	8% 77% 18%
62	BW	188	97%
63	BX	190	33% 49% 7% 44%
64	BY	172	58% 41%
65	BZ	190	11% 99%
66	Ba	153	89% 9%
67	Bb	162	5% 57% 39%
68	Bc	146	7% 58% 38%
69	Bd	144	94%
70	Be	113	7% 86% 11%
71	Bf	113	6% 42% 56%
72	Bg	105	6% 73% 5% 22%
73	Bh	92	35% 90% 7%
74	UA	46	28% 100%
75	UB	40	25% 100%
76	UC	12	50% 100%
76	UH	12	17% 100%
77	UD	177	51% 99%
78	UE	22	5% 100%
79	UF	24	100%
79	UG	24	17% 100%
79	UN	24	88% 100%

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Mol	Chain	Length	Quality of chain
80	UI	17	 35% 100%
81	UK	10	 10% 100%
82	UL	15	 13% 100%
83	UM	6	 100%
84	UU	11	 27% 91% 9%
85	UV	8	 12% 100%
85	UX	8	 12% 100%
86	UW	7	 71% 100%

2 Entry composition i

There are 89 unique types of molecules in this entry. The entry contains 133849 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 bl27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A0	151	1269	801	236	227	5	0	0

- Molecule 2 is a protein called bl28m.

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

- Molecule 3 is a protein called ul29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A2	449	3638	2324	631	670	13	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is a protein called ul30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A3	150	1215	776	234	199	6	0	0

- Molecule 5 is a protein called bl31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A4	168	1387	880	262	240	5	0	0

- Molecule 6 is a protein called bl32m.

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

- Molecule 7 is a protein called bl33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A6	72	Total	C	N	O	S	0	0
			568	361	102	101	4		

- Molecule 8 is a protein called bl35m.

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

- Molecule 9 is a protein called bl36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A9	53	Total	C	N	O	S	0	0
			459	288	85	78	8		

- Molecule 10 is a protein called Ribosomal protein L3 mitochondrial, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AE	293	Total	C	N	O	S	0	0
			2390	1543	395	440	12		

- Molecule 11 is a protein called Ribosomal protein L4/L1 family, putative.

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

- Molecule 12 is a protein called bl9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AI	212	Total	C	N	O	S	0	0
			1790	1153	316	312	9		

- Molecule 13 is a protein called ul10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AJ	126	965	606	191	165	3	0	0

- Molecule 14 is a protein called Ribosomal protein L11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	AK	323	2676	1703	485	469	19	0	0

- Molecule 15 is a protein called 50S ribosomal protein L13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	AN	179	1508	973	275	251	9	0	0

- Molecule 16 is a protein called ul15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	AP	352	2904	1846	538	507	13	0	0

- Molecule 17 is a protein called 50S ribosomal protein L16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	AQ	125	1020	658	183	175	4	0	0

- Molecule 18 is a protein called 50S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	AR	227	1912	1211	356	332	13	0	0

- Molecule 19 is a protein called bl19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	AT	35	287	180	61	45	1	0	0

- Molecule 20 is a protein called bl20m.

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

- Molecule 21 is a protein called bl21m.

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

- Molecule 22 is a protein called ul22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	AW	276	2235	1416	415	391	13	0	0

- Molecule 23 is a protein called ul23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	AX	168	1416	913	253	245	5	0	0

- Molecule 24 is a protein called ul24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	AY	340	2712	1689	493	517	13	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 25 is a protein called ml38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Ab	453	3545	2252	621	657	15	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ab	290	SER	PHE	conflict	UNP Q381T7

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Chain	Residue	Modelled	Actual	Comment	Reference
Ab	299	GLU	LYS	conflict	UNP Q381T7
Ab	471	ASN	ILE	conflict	UNP Q381T7

- Molecule 26 is a protein called ml40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Ad	257	2122	1319	386	405	12	0	0

- Molecule 27 is a protein called ml41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Ae	116	927	594	170	158	5	0	0

- Molecule 28 is a protein called ml42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Af	126	1013	630	196	183	4	0	0

- Molecule 29 is a protein called ml43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Ag	259	2193	1368	422	392	11	0	0

- Molecule 30 is a protein called ml46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Aj	279	2246	1408	414	416	8	0	0

- Molecule 31 is a protein called ml49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Al	209	1618	1051	281	279	7	0	0

- Molecule 32 is a protein called ml52.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ao	183	Total	C	N	O	S	0	0
			1475	936	272	264	3		

- Molecule 33 is a protein called ml53.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ap	261	Total	C	N	O	S	0	0
			2143	1391	372	368	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ap	2	LEU	SER	conflict	UNP Q57YA9

- Molecule 34 is a protein called ml63.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	At	138	Total	C	N	O	S	0	0
			1100	690	210	196	4		

- Molecule 35 is a protein called ml64.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Av	213	Total	C	N	O	S	0	0
			1792	1138	333	308	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Av	164	ARG	GLN	conflict	UNP Q383B7

- Molecule 36 is a protein called bL12m.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	AB	56	Total	C	N	O	0	0
			280	168	56	56		

- Molecule 37 is a protein called bL12m.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	AC	28	Total	C	N	O	0	0
			140	84	28	28		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	AD	28	140	84	28	28	0	0

- Molecule 38 is a protein called bL12m.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	AG	27	135	81	27	27	0	0

- Molecule 39 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	AA	591	12491	5628	2125	4147	591	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	448	A	U	conflict	GB 343546
AA	622	A	U	conflict	GB 343546
AA	636	A	G	conflict	GB 343546
AA	702	G	A	conflict	GB 343546
AA	706	C	U	conflict	GB 343546
AA	743	C	G	conflict	GB 343546
AA	752	G	A	conflict	GB 343546
AA	757	U	A	conflict	GB 343546
AA	760	U	G	conflict	GB 343546
AA	762	U	G	conflict	GB 343546
AA	789	G	C	conflict	GB 343546
AA	793	G	U	conflict	GB 343546
AA	875	A	G	conflict	GB 343546
AA	876	G	A	conflict	GB 343546
AA	877	A	G	conflict	GB 343546

- Molecule 40 is a protein called ml67.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	BA	679	5384	3422	948	981	33	0	0

- Molecule 41 is a protein called ml68.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BB	389	2966	1879	535	539	13	0	0

- Molecule 42 is a protein called ml69.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	BC	478	3821	2451	670	680	20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	29	PRO	SER	conflict	UNP Q584V5
BC	42	GLY	SER	conflict	UNP Q584V5

- Molecule 43 is a protein called mL70.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	BD	417	2063	1229	417	417	0	0

- Molecule 44 is a protein called ml71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	BE	392	3105	1970	540	582	13	0	0

- Molecule 45 is a protein called ml72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BF	345	2838	1797	517	511	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	296	ILE	THR	conflict	UNP C9ZR63

- Molecule 46 is a protein called ml73.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BG	319	2503	1578	449	459	17	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	185	PHE	LEU	conflict	UNP Q57Y49

- Molecule 47 is a protein called ml74.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	BH	211	1729	1110	301	315	3	0	0

- Molecule 48 is a protein called ml75.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	BI	319	2609	1664	473	456	16	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BI	227	ASN	ASP	conflict	UNP Q38CK0
BI	319	ARG	GLN	conflict	UNP Q38CK0
BI	343	ALA	-	expression tag	UNP Q38CK0

- Molecule 49 is a protein called ml76.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	BJ	166	1339	832	262	239	6	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 50 is a protein called Chaperone protein DNAj, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	BK	258	1996	1237	383	368	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	348	VAL	LEU	conflict	UNP C9ZQR6

- Molecule 51 is a protein called ml78.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	BL	234	1887	1158	370	349	10	0	0

- Molecule 52 is a protein called ml79.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	BM	245	2015	1280	370	356	9	0	0

- Molecule 53 is a protein called ml80.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	145	THR	ALA	conflict	UNP Q585A3

- Molecule 54 is a protein called ml81.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	BO	147	1146	719	202	213	12	0	0

- Molecule 55 is a protein called ml82.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	BP	202	1550	973	292	276	9	0	0

- Molecule 56 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	BQ	216	1675	1061	291	315	8	0	0

- Molecule 57 is a protein called ml84.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	BR	195	1650	1059	298	284	9	0	0

- Molecule 58 is a protein called ml85.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	BS	97	784	493	141	144	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 59 is a protein called ml86.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	BT	168	1389	853	270	260	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	70	ARG	GLN	conflict	UNP C9ZPU8

- Molecule 60 is a protein called ml87.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	BU	82	694	436	139	115	4	0	0

- Molecule 61 is a protein called ml88.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	BV	155	1307	832	233	236	6	0	0

- Molecule 62 is a protein called ml89.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	BW	187	1557	987	298	264	8	0	0

- Molecule 63 is a protein called ml90.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	BX	107	867	552	160	147	8	0	0

- Molecule 64 is a protein called ml91.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	BY	102	877	549	171	154	3	0	0

- Molecule 65 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	BZ	190	1390	878	242	263	7	0	0

- Molecule 66 is a protein called ml93.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	Ba	139	1224	785	223	209	7	0	0

- Molecule 67 is a protein called ml94.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	Bb	99	770	482	144	143	1	0	0

- Molecule 68 is a protein called ml95.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	Bc	90	Total	C	N	O	0	0
			781	495	148	138		

- Molecule 69 is a protein called ml96.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bd	140	Total	C	N	O	S	0	0
			1113	689	209	204	11		

- Molecule 70 is a protein called ml97.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Be	101	Total	C	N	O	S	0	0
			822	517	152	144	9		

- Molecule 71 is a protein called ml98.

Mol	Chain	Residues	Atoms				AltConf	Trace
71	Bf	50	Total	C	N	O	0	0
			434	279	80	75		

- Molecule 72 is a protein called ml99.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bg	82	Total	C	N	O	S	0	0
			656	412	126	116	2		

- Molecule 73 is a protein called ml100.

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

- Molecule 74 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
74	UA	46	Total	C	N	O	0	0
			276	184	46	46		

- Molecule 75 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
75	UB	40	240	160	40	40	0	0

- Molecule 76 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
76	UC	12	72	48	12	12	0	0
76	UH	12	72	48	12	12	0	0

- Molecule 77 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
77	UD	177	1062	708	177	177	0	0

- Molecule 78 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
78	UE	22	132	88	22	22	0	0

- Molecule 79 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
79	UF	24	144	96	24	24	0	0
79	UG	24	144	96	24	24	0	0
79	UN	24	144	96	24	24	0	0

- Molecule 80 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
80	UI	17	102	68	17	17	0	0

- Molecule 81 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
81	UK	10	Total	C	N	O	0	0
			60	40	10	10		

- Molecule 82 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	UL	15	Total	C	N	O	0	0
			90	60	15	15		

- Molecule 83 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	UM	6	Total	C	N	O	0	0
			36	24	6	6		

- Molecule 84 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
84	UU	11	Total	C	N	O	0	0
			66	44	11	11		

- Molecule 85 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
85	UV	8	Total	C	N	O	0	0
			48	32	8	8		
85	UX	8	Total	C	N	O	0	0
			48	32	8	8		

- Molecule 86 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
86	UW	7	Total	C	N	O	0	0
			42	28	7	7		

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

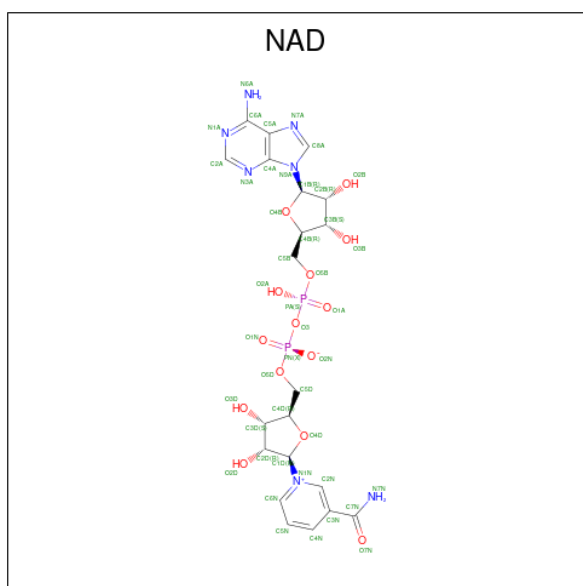
Mol	Chain	Residues	Atoms		AltConf
87	A5	1	Total	Zn	0
			1	1	
87	A9	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
87	BX	2	Total	Zn	0
			2	2	
87	Be	1	Total	Zn	0
			1	1	
87	Bh	1	Total	Zn	0
			1	1	

- Molecule 88 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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


- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

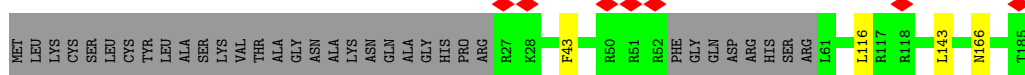
Mol	Chain	Residues	Atoms		AltConf
89	AA	7	Total	Mg	0
			7	7	

3 Residue-property plots [i](#)


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

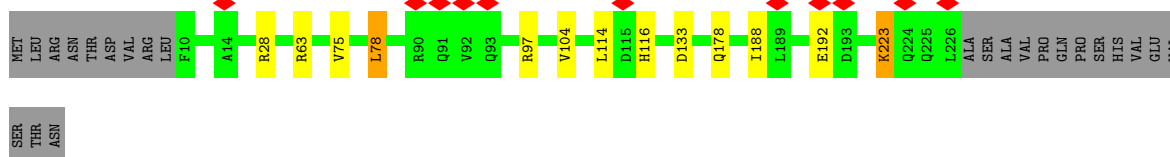
- Molecule 1: bl27m

Chain A0: 



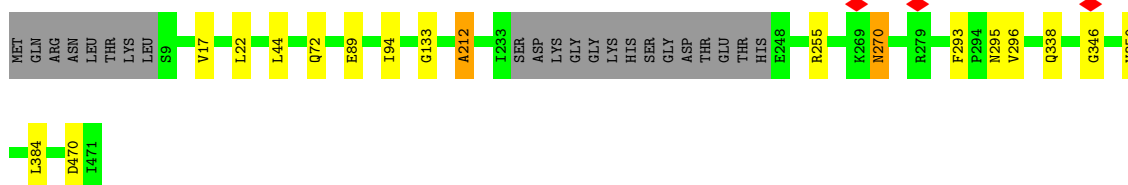
- Molecule 2: bl28m

Chain A1: 



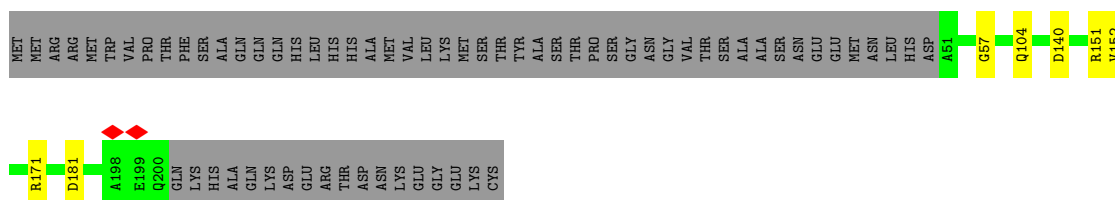
- Molecule 3: ul29m

Chain A2: 

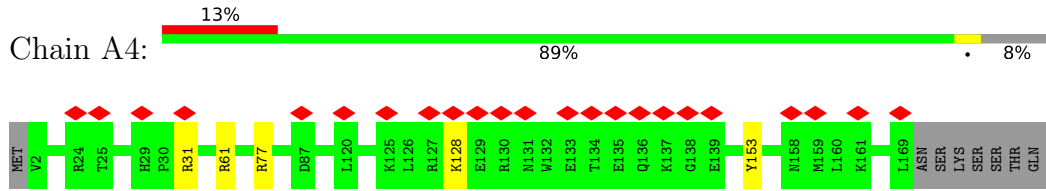


- Molecule 4: ul30m

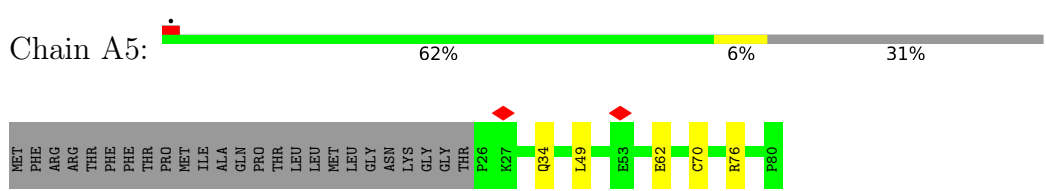
Chain A3: 



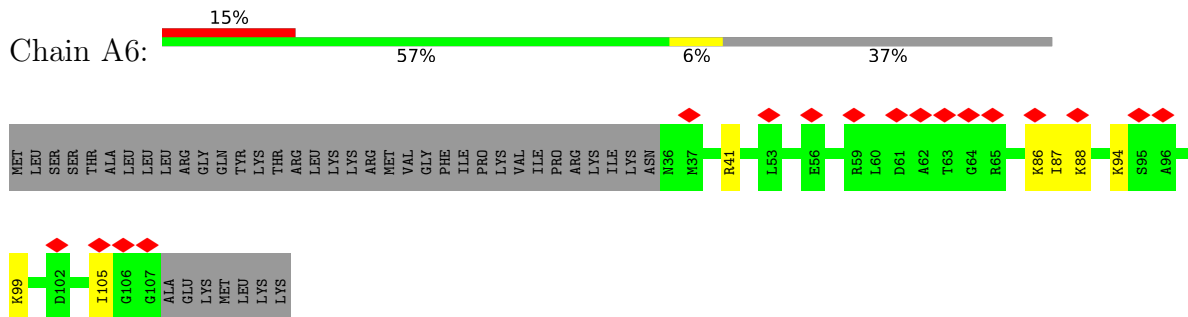
• Molecule 5: bl31m



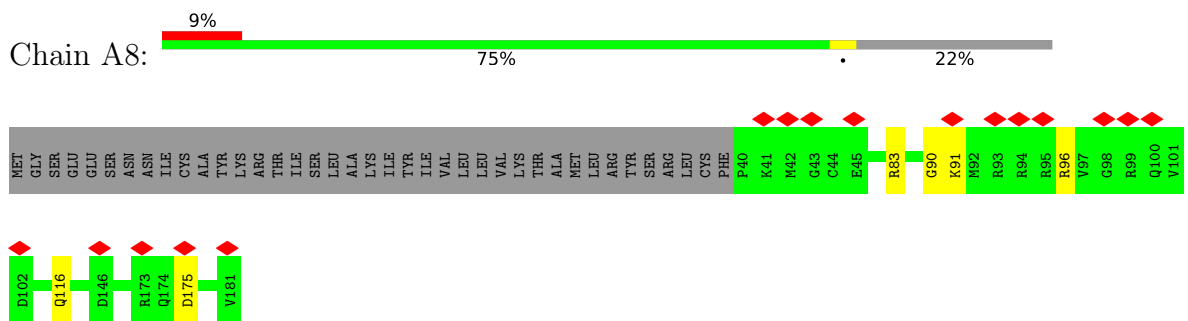
• Molecule 6: bl32m



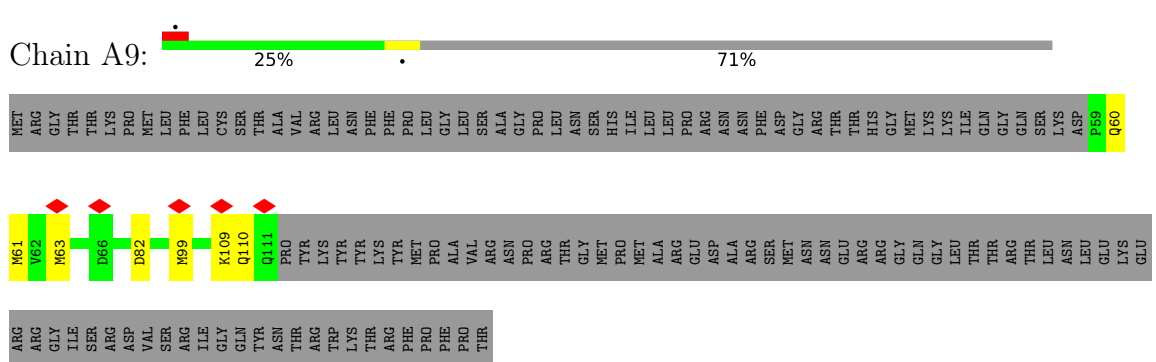
• Molecule 7: bl33m



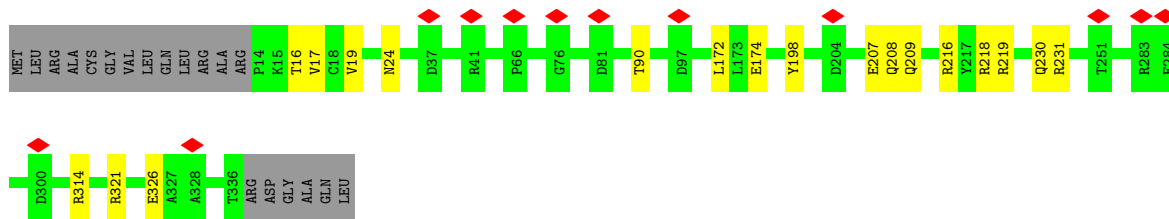
• Molecule 8: bl35m



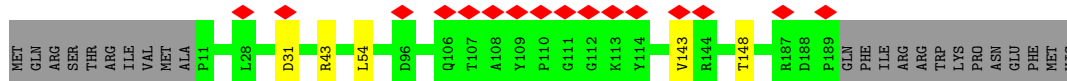
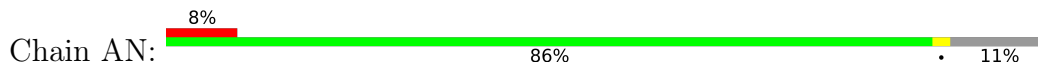
• Molecule 9: bl36m



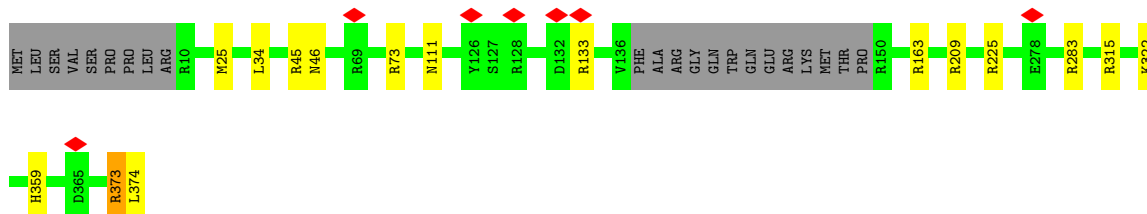
• Molecule 10: Ribosomal protein L3 mitochondrial, putative



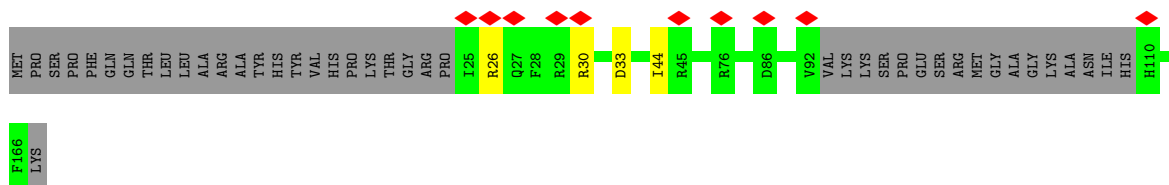
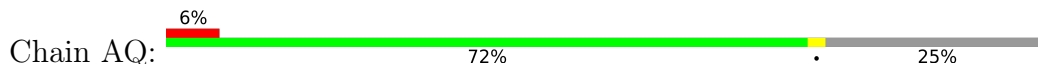
• Molecule 15: 50S ribosomal protein L13, putative



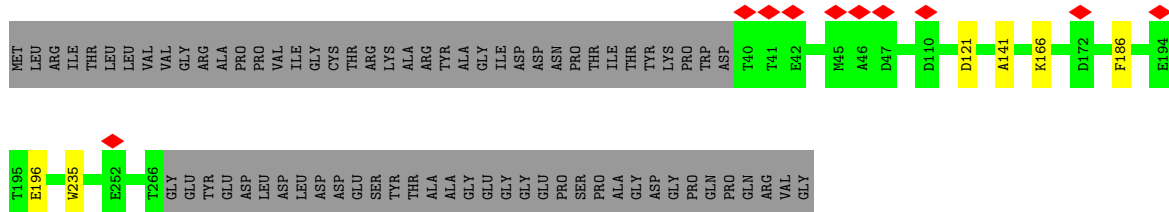
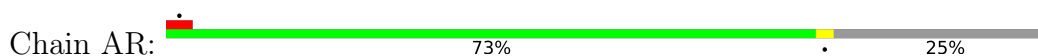
• Molecule 16: ul15m



• Molecule 17: 50S ribosomal protein L16, putative

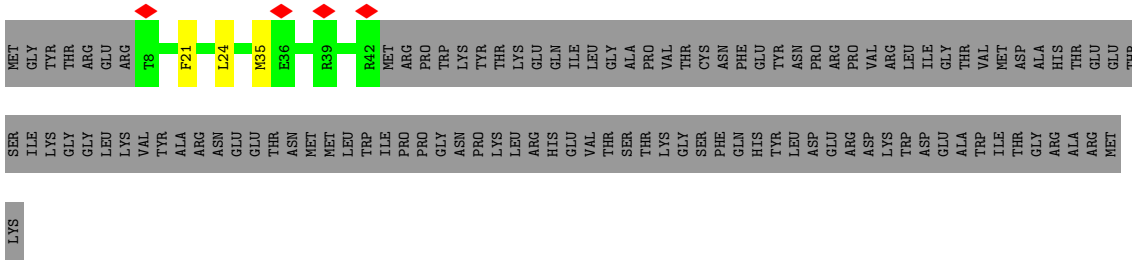


• Molecule 18: 50S ribosomal protein L17, putative

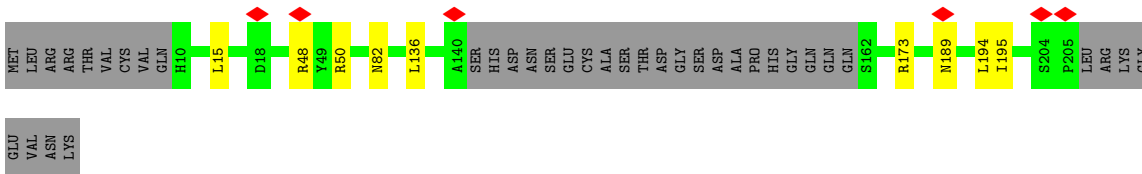
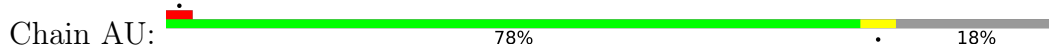


• Molecule 19: bl19m

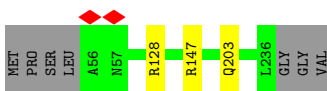




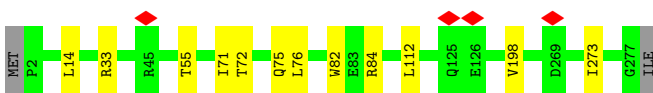
• Molecule 20: bl20m



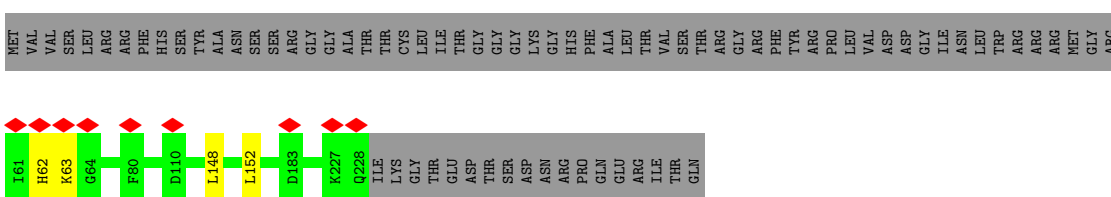
• Molecule 21: bl21m



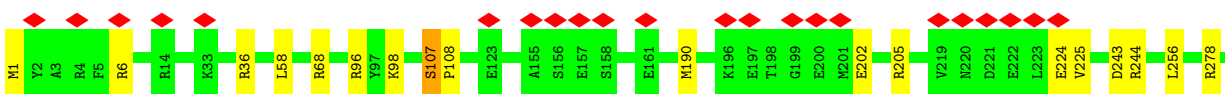
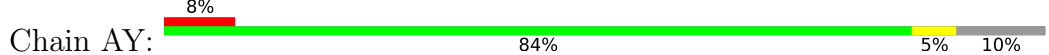
• Molecule 22: ul22m

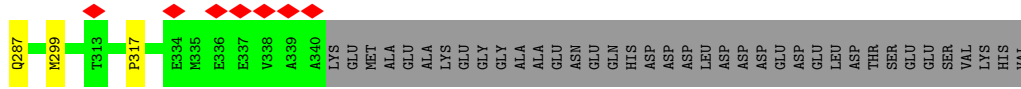


• Molecule 23: ul23m

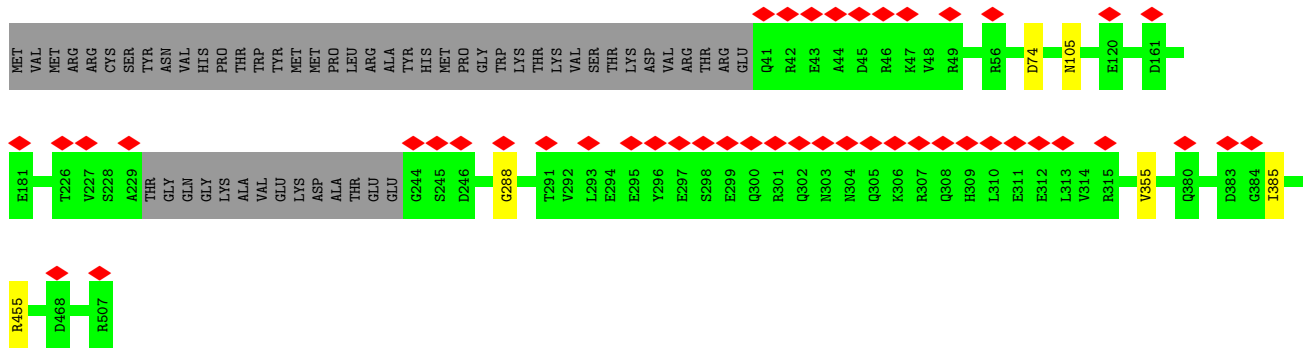
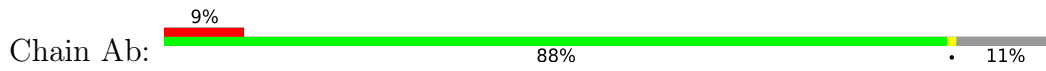


• Molecule 24: ul24m

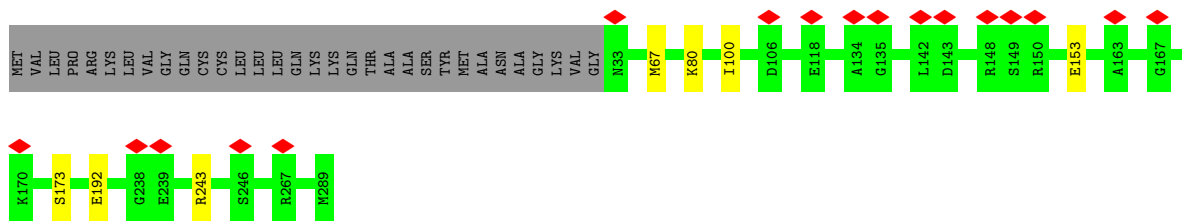
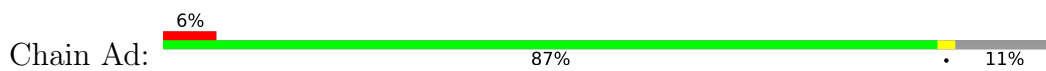




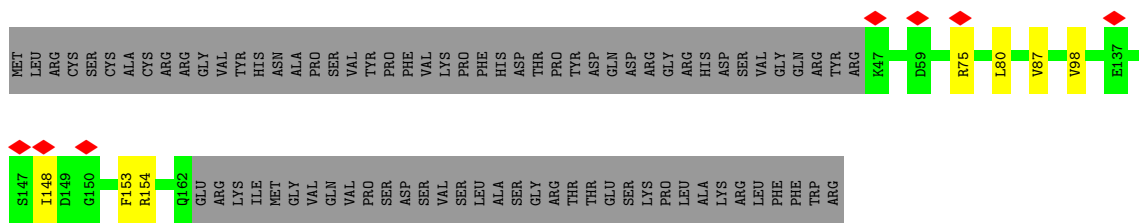
• Molecule 25: ml38



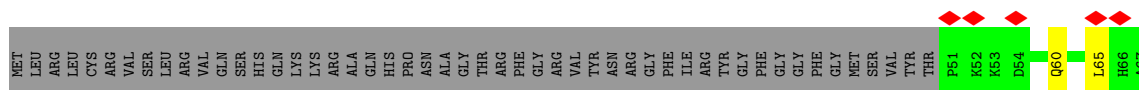
• Molecule 26: ml40

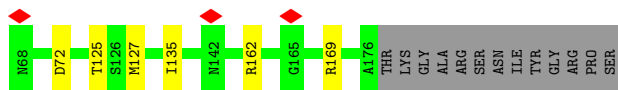


• Molecule 27: ml41

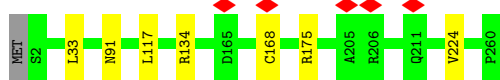


• Molecule 28: ml42

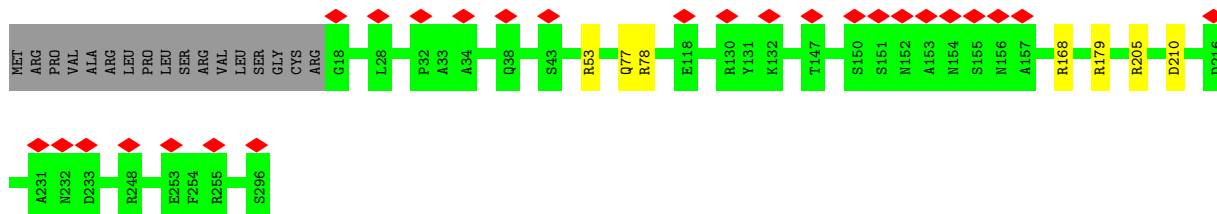




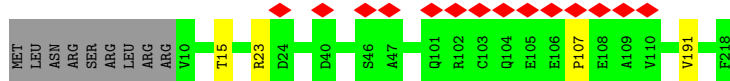
• Molecule 29: ml43



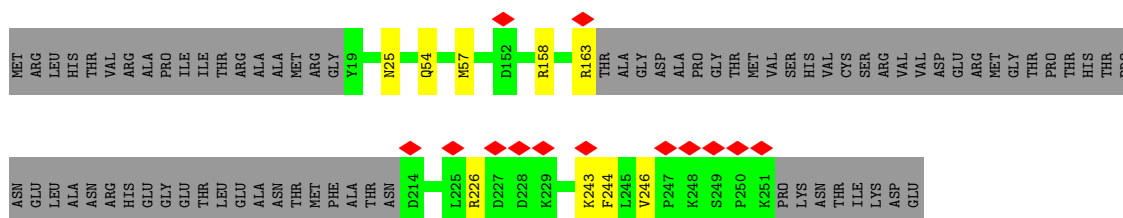
• Molecule 30: ml46



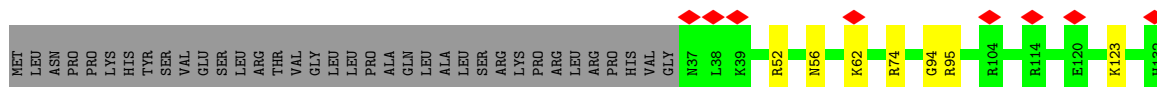
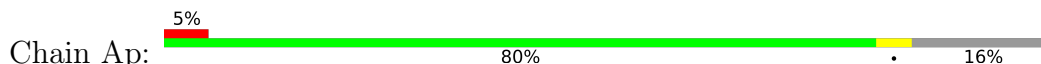
• Molecule 31: ml49

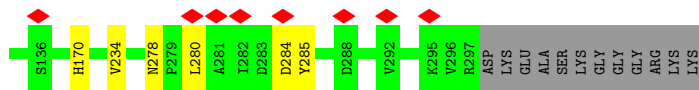


• Molecule 32: ml52

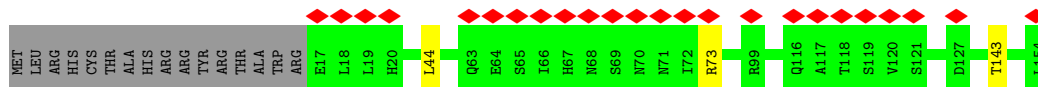
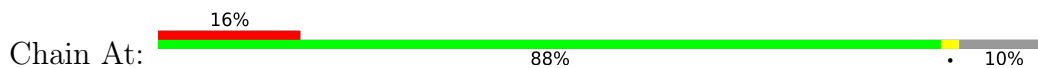


• Molecule 33: ml53

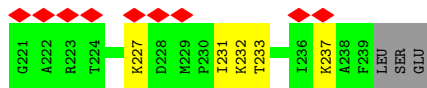
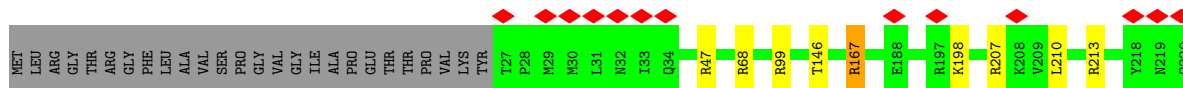
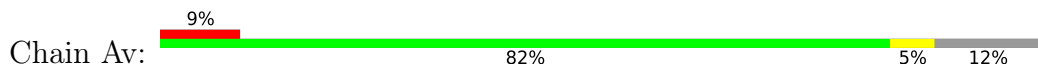




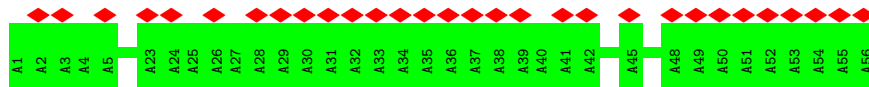
● Molecule 34: ml63



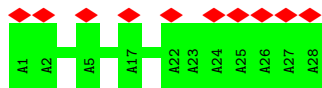
● Molecule 35: ml64



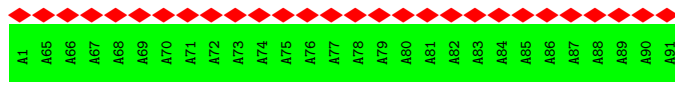
● Molecule 36: bL12m



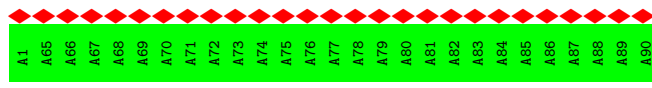
● Molecule 37: bL12m



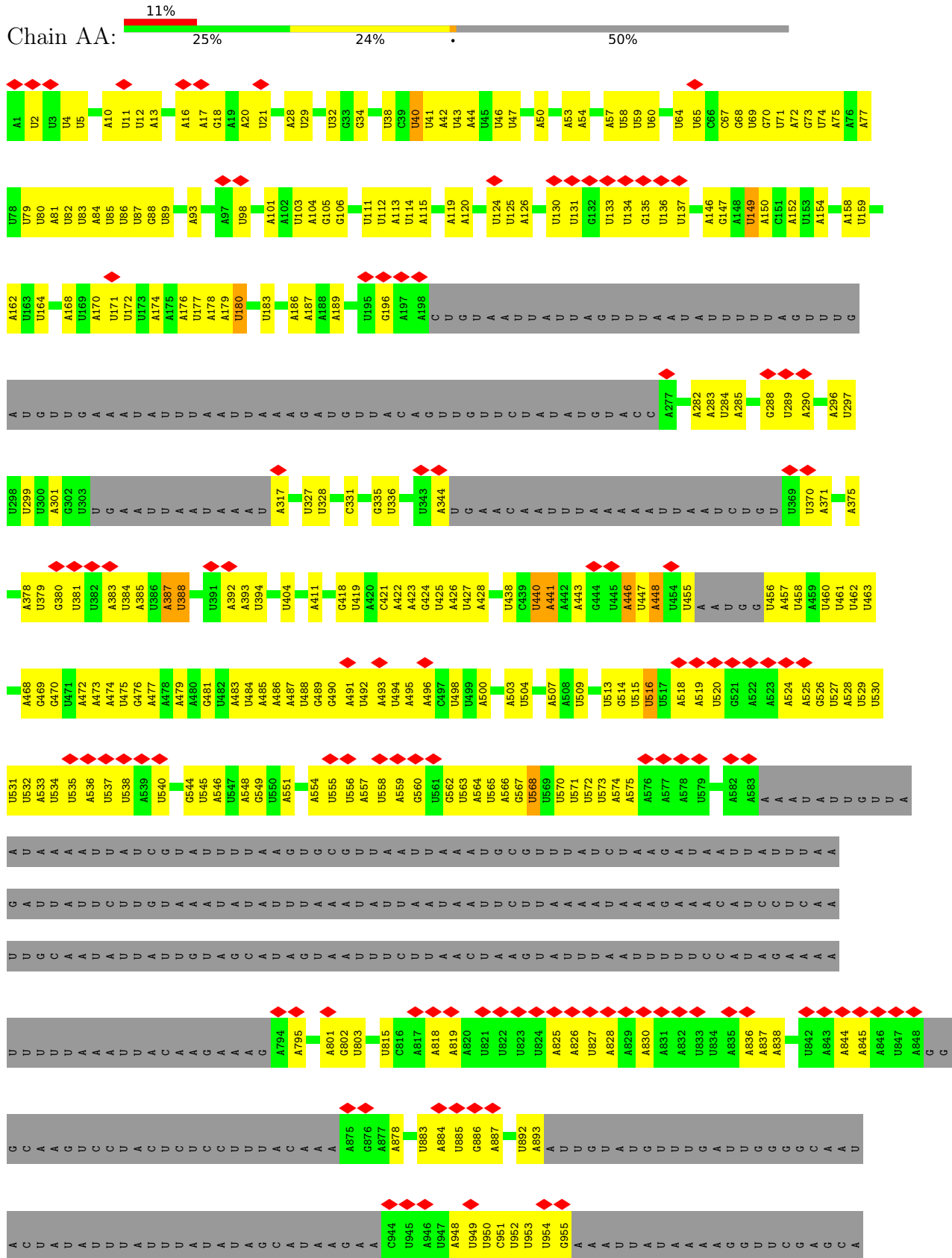
● Molecule 37: bL12m



● Molecule 38: bL12m

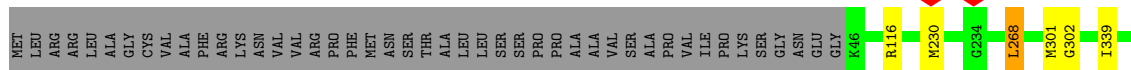
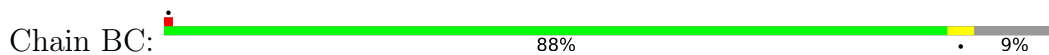


• Molecule 39: 12S rRNA

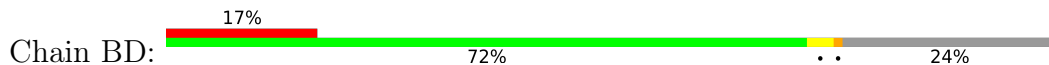


HIS
GLN
LYS
GLN
LEU
GLN
ASN
VAL
THR
GLY
VAL
HIS

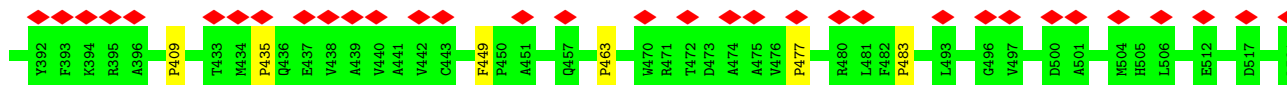
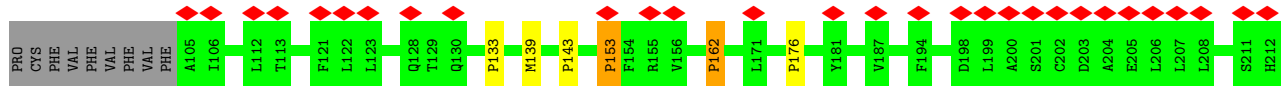
• Molecule 42: ml69



• Molecule 43: mL70



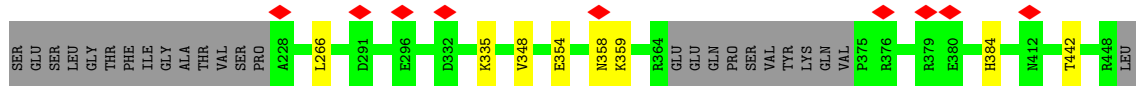
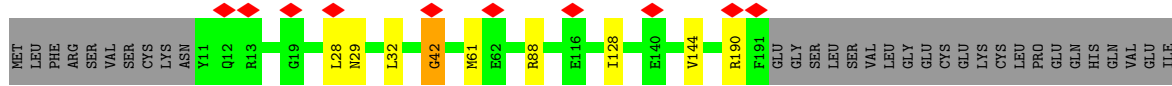
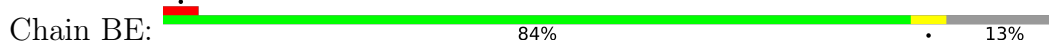
MET
CYS
LEU
LYS
LYS
ALA
PRO
HIS
LEU
PHE
CYS
PHE
CYS
TRP
LEU
SER
ILE
PHE
LEU
SER
PHE
ARG
CYS
PHE
CYS
PHE
ARG
CYS
PHE
CYS
PHE
SER
ILE
MET
LEU
PRO
LEU
LEU
SER
PHE
THR
ILE
ILE
SER
ILE
PHE
SER
PHE
LYS
PRO
ILE
THR
PHE
LEU
SER
PHE
THR
PHE
LEU
SER



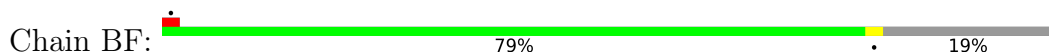
LYS
VAL
ARG
ARG
PHE
VAL
PHE
ASP
GLU
VAL
LYS
ASP
MET
TYR
GLU
THR
ASN
ILE
ASP
SER
VAL
LEU
LYS
ARG
VAL
ASP
ASP
ASN
PHE
LYS
GLN
VAL
VAL
PRO
GLN
LEU
LYS
ALA
GLU
ASP
GLN
VAL
GLY
ASP
ALA
PRO
SER
SER
LEU
SER
VAL
GLY
GLY
GLY
GLU
ASP
CYS
THR
VAL
LEU
PRO
GLU
THR
GLN
HIS
GLN
VAL
VAL
ILE

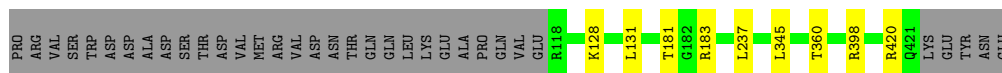
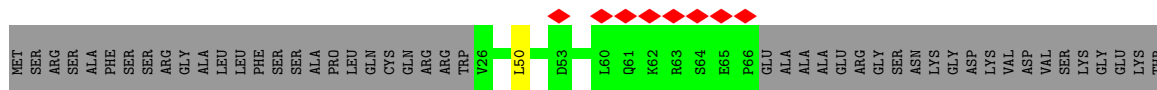
ALA

• Molecule 44: ml71

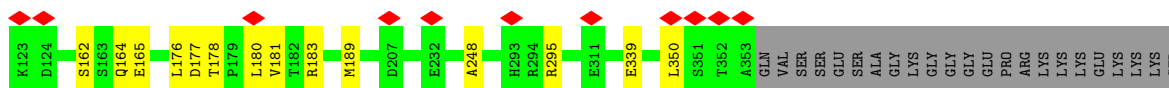
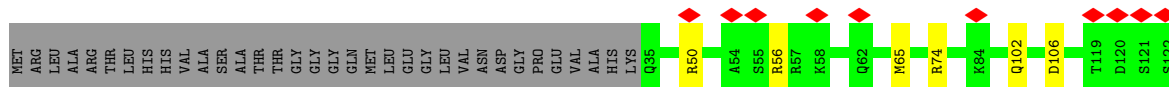
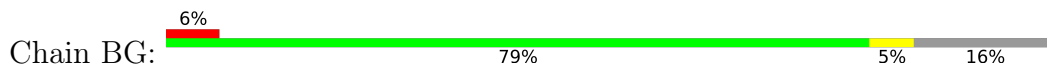


• Molecule 45: ml72



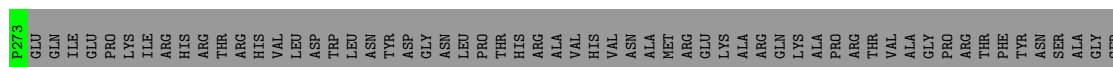
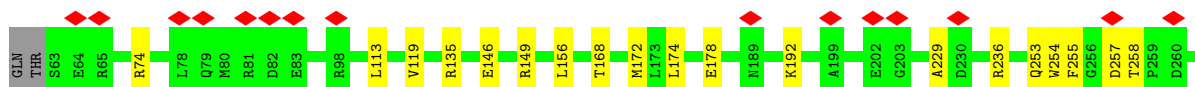
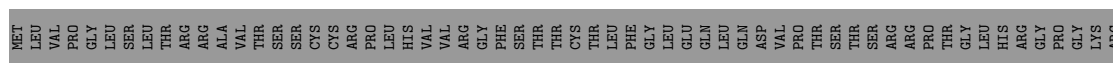


• Molecule 46: ml73



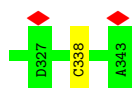
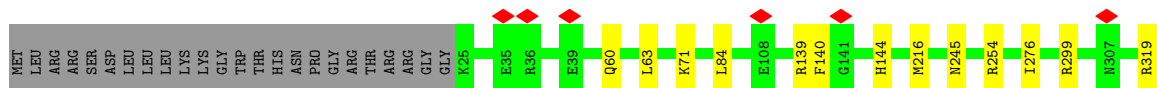
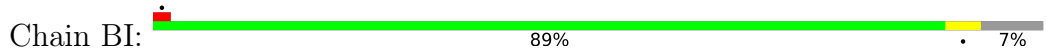
LYS
ALA

• Molecule 47: ml74



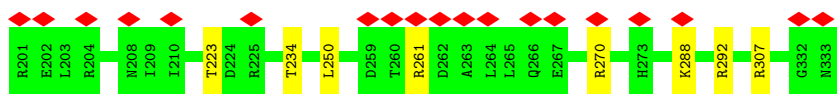
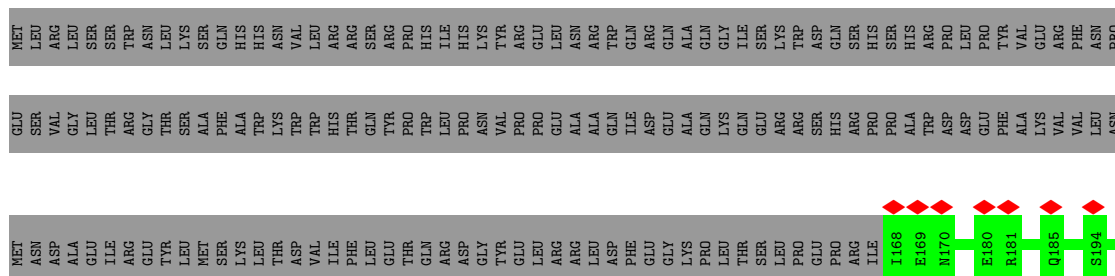
ARG
ALA
ASN
ALA
SER
SER
PHE
GLY
GLM
ALA
VAL
LYS

• Molecule 48: ml75

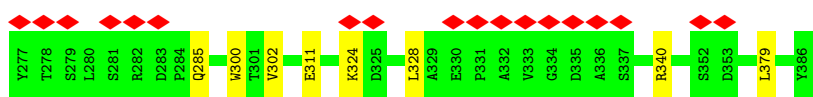
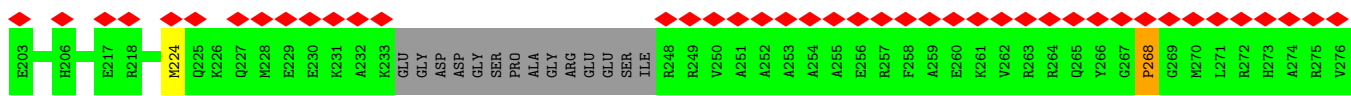
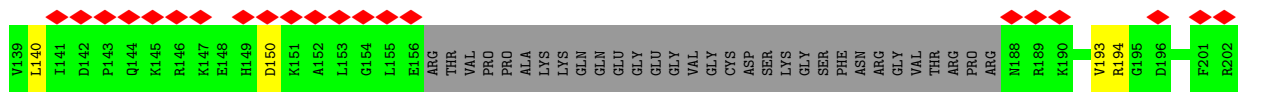
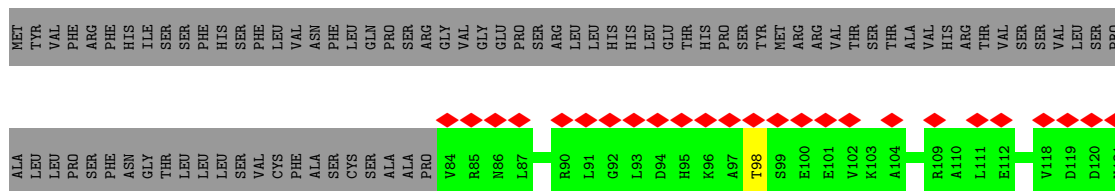


• Molecule 49: ml76

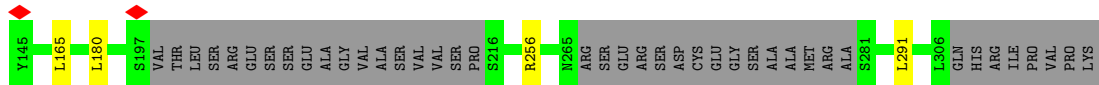
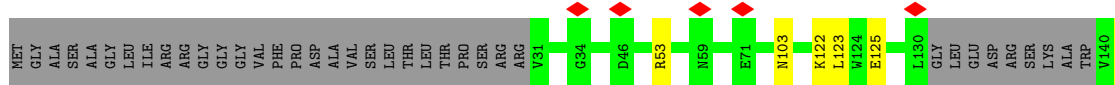
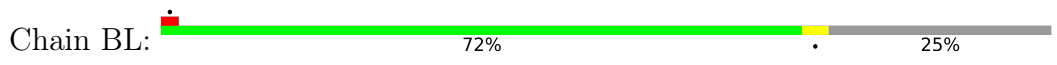




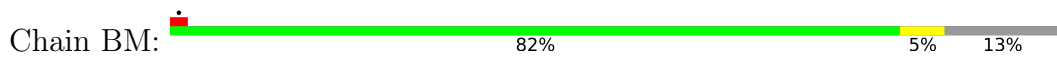
• Molecule 50: Chaperone protein DNAj, putative

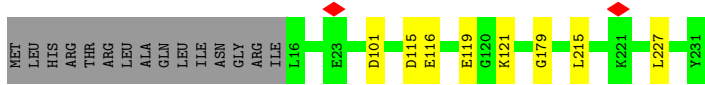
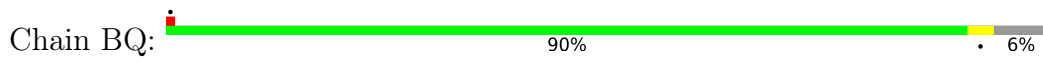


• Molecule 51: ml78

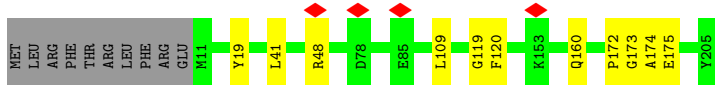
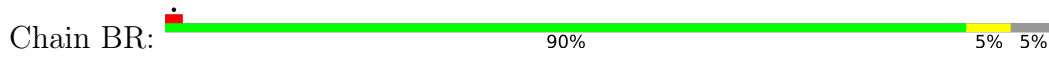


• Molecule 52: ml79

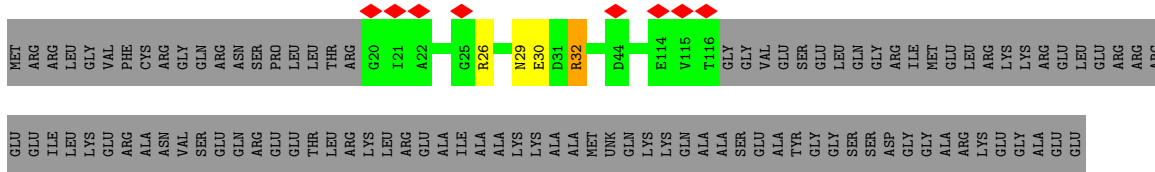




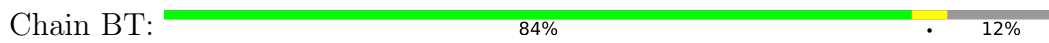
• Molecule 57: ml84



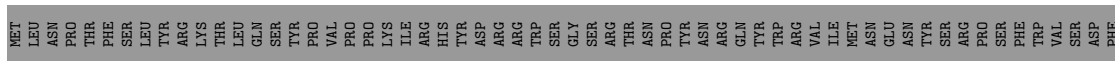
• Molecule 58: ml85



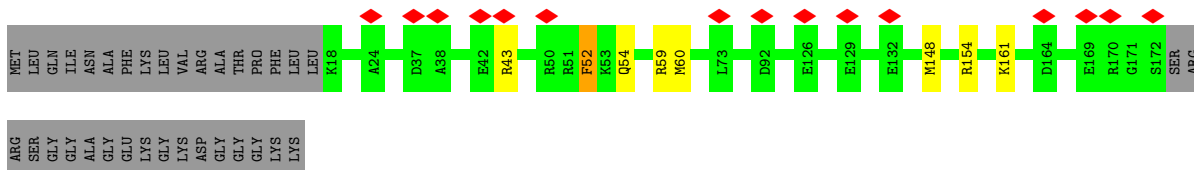
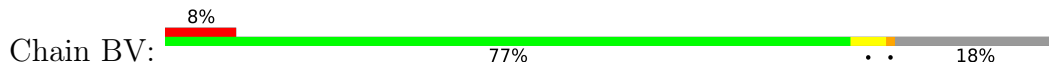
• Molecule 59: ml86



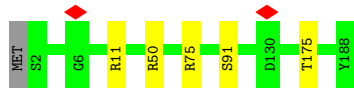
• Molecule 60: ml87



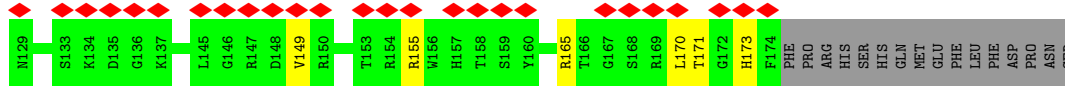
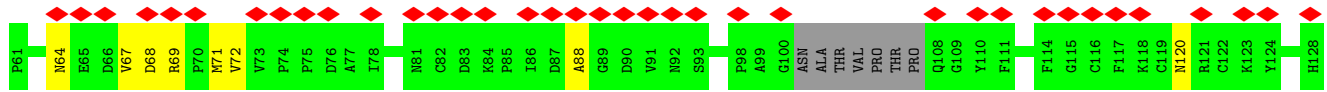
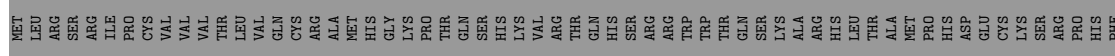
• Molecule 61: ml88



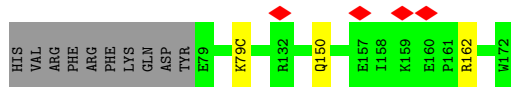
● Molecule 62: ml89



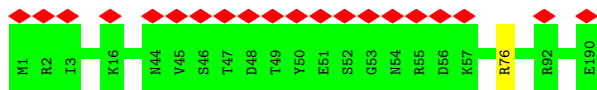
● Molecule 63: ml90



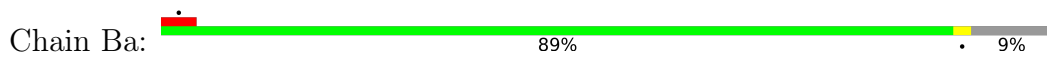
● Molecule 64: ml91



● Molecule 65: Peptidyl-prolyl cis-trans isomerase

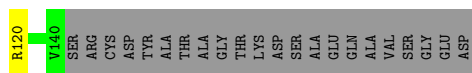
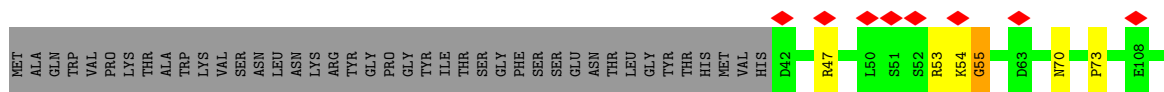


● Molecule 66: ml93

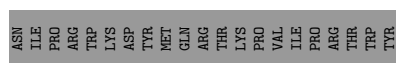
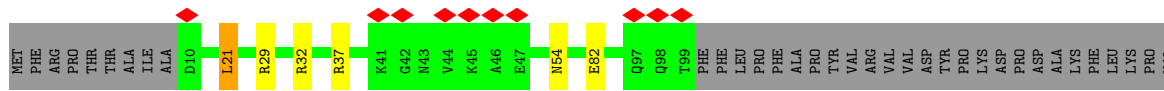


● Molecule 67: ml94

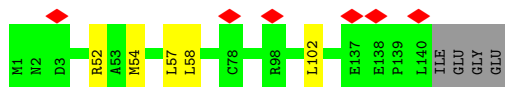




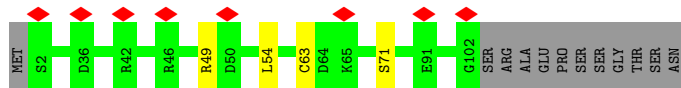
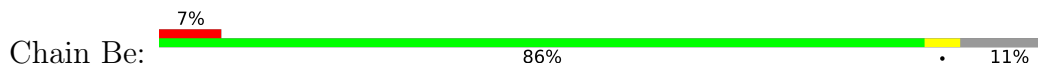
• Molecule 68: ml95



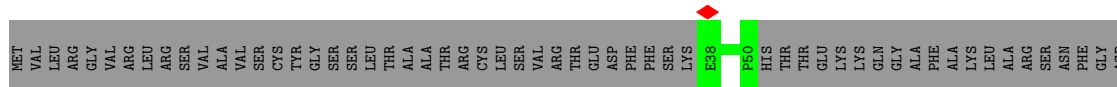
• Molecule 69: ml96



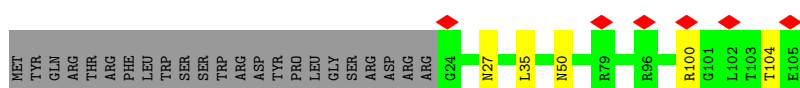
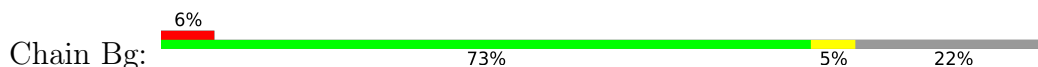
• Molecule 70: ml97



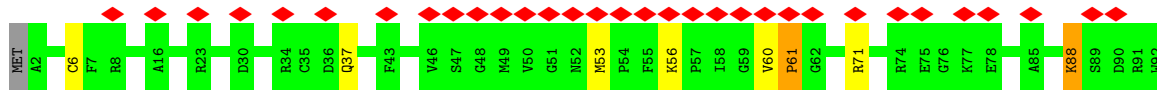
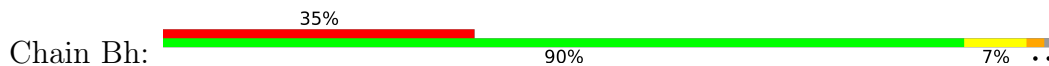
• Molecule 71: ml98



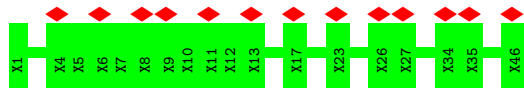
• Molecule 72: ml99



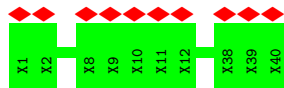
• Molecule 73: ml100



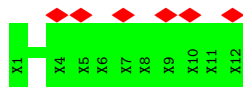
• Molecule 74: UNK



• Molecule 75: UNK



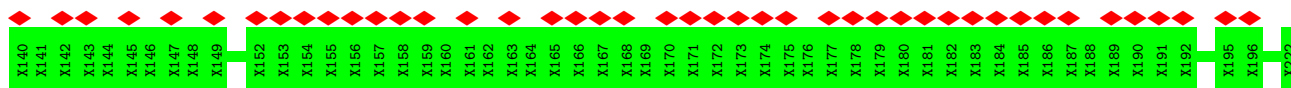
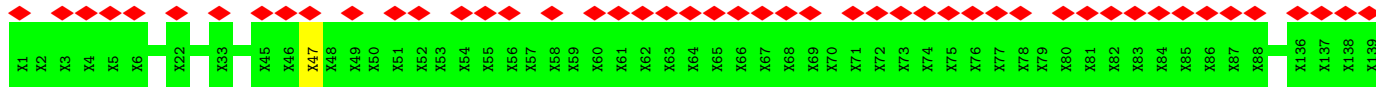
• Molecule 76: UNK



• Molecule 76: UNK



• Molecule 77: UNK



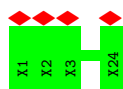
• Molecule 78: UNK



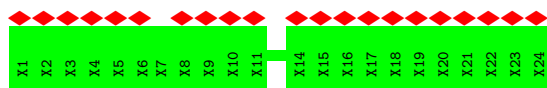
- Molecule 79: UNK



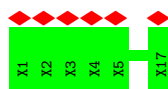
- Molecule 79: UNK



- Molecule 79: UNK



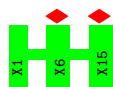
- Molecule 80: UNK



- Molecule 81: UNK



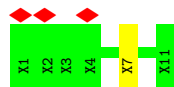
- Molecule 82: UNK



• Molecule 83: UNK



• Molecule 84: UNK



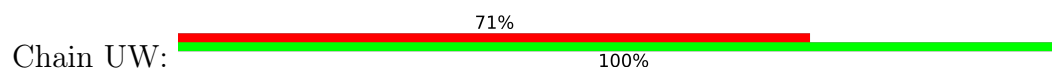
• Molecule 85: UNK



• Molecule 85: UNK



• Molecule 86: UNK



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31619	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 ($e^-/\text{\AA}^2$)	40	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	0.536	Depositor
Minimum map value	-0.224	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	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: NAD, MG, ZN

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	A0	0.32	0/1297	0.53	0/1750
2	A1	0.47	0/1828	0.66	2/2466 (0.1%)
3	A2	0.35	0/3740	0.57	1/5094 (0.0%)
4	A3	0.35	0/1241	0.53	0/1674
5	A4	0.33	0/1423	0.60	1/1924 (0.1%)
6	A5	0.34	0/498	0.56	0/663
7	A6	0.37	0/578	0.58	0/774
8	A8	0.40	0/1230	0.61	0/1645
9	A9	0.37	0/474	0.60	0/639
10	AE	0.42	0/2469	0.61	1/3364 (0.0%)
11	AF	0.37	0/3706	0.57	0/5029
12	AI	0.38	0/1850	0.65	2/2515 (0.1%)
13	AJ	0.32	0/986	0.55	1/1339 (0.1%)
14	AK	0.46	2/2745 (0.1%)	0.66	2/3705 (0.1%)
15	AN	0.39	0/1561	0.56	0/2123
16	AP	0.38	0/2993	0.61	1/4060 (0.0%)
17	AQ	0.36	0/1046	0.54	0/1415
18	AR	0.38	0/1969	0.59	0/2656
19	AT	0.34	0/292	0.54	0/390
20	AU	0.34	0/1456	0.55	1/1971 (0.1%)
21	AV	0.37	0/1453	0.59	0/1970
22	AW	0.36	0/2291	0.56	0/3097
23	AX	0.40	0/1462	0.60	1/1986 (0.1%)
24	AY	0.38	0/2763	0.60	1/3739 (0.0%)
25	Ab	0.34	0/3651	0.56	0/4988
26	Ad	0.32	0/2171	0.52	0/2930
27	Ae	0.37	0/960	0.60	0/1304
28	Af	0.34	0/1037	0.61	0/1406
29	Ag	0.33	0/2253	0.54	0/3046
30	Aj	0.35	0/2306	0.56	0/3136
31	Al	0.38	0/1665	0.60	1/2270 (0.0%)
32	Ao	0.35	0/1523	0.56	0/2070

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ap	0.41	0/2213	0.64	1/3007 (0.0%)
34	At	0.36	0/1128	0.59	0/1532
35	Av	0.38	0/1839	0.59	2/2478 (0.1%)
36	AB	0.26	0/279	0.43	0/389
37	AC	0.24	0/139	0.36	0/193
37	AD	0.30	0/139	0.35	0/193
38	AG	0.29	0/134	0.36	0/186
39	AA	0.42	1/13972 (0.0%)	0.95	51/21705 (0.2%)
40	BA	0.37	0/5501	0.61	1/7463 (0.0%)
41	BB	0.33	0/3038	0.58	7/4134 (0.2%)
42	BC	0.36	0/3919	0.59	1/5318 (0.0%)
43	BD	0.35	0/2062	0.66	18/2872 (0.6%)
44	BE	0.37	0/3184	0.59	2/4308 (0.0%)
45	BF	0.36	0/2900	0.57	0/3909
46	BG	0.35	0/2561	0.61	0/3469
47	BH	0.40	0/1778	0.61	0/2423
48	BI	0.34	0/2685	0.60	0/3633
49	BJ	0.32	0/1366	0.58	0/1846
50	BK	0.33	0/2038	0.51	1/2753 (0.0%)
51	BL	0.35	0/1924	0.60	1/2596 (0.0%)
52	BM	0.42	0/2082	0.63	0/2830
53	BN	0.33	0/1755	0.51	0/2381
54	BO	0.43	0/1160	0.62	1/1565 (0.1%)
55	BP	0.34	0/1593	0.58	1/2166 (0.0%)
56	BQ	0.41	0/1716	0.67	1/2324 (0.0%)
57	BR	0.38	0/1693	0.65	1/2284 (0.0%)
58	BS	0.44	0/801	0.72	1/1090 (0.1%)
59	BT	0.35	0/1417	0.60	1/1907 (0.1%)
60	BU	0.35	0/711	0.57	0/955
61	BV	0.62	3/1340 (0.2%)	0.68	2/1802 (0.1%)
62	BW	0.37	0/1604	0.56	0/2167
63	BX	0.35	0/897	0.73	3/1215 (0.2%)
64	BY	0.34	0/908	0.56	0/1231
65	BZ	0.35	0/1416	0.58	0/1919
66	Ba	0.42	1/1267 (0.1%)	0.58	0/1711
67	Bb	0.36	0/785	0.70	1/1063 (0.1%)
68	Bc	0.39	0/805	0.63	1/1091 (0.1%)
69	Bd	0.36	0/1133	0.59	0/1528
70	Be	0.36	0/844	0.62	0/1139
71	Bf	0.36	0/450	0.60	0/609
72	Bg	0.34	0/671	0.58	0/905
73	Bh	0.37	0/752	0.62	0/1015
All	All	0.38	7/135516 (0.0%)	0.65	113/186442 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A1	0	1
3	A2	0	2
4	A3	0	1
8	A8	0	2
11	AF	0	3
18	AR	0	2
21	AV	0	1
22	AW	0	1
23	AX	0	1
24	AY	0	2
25	Ab	0	1
33	Ap	0	1
35	Av	0	1
41	BB	0	1
42	BC	0	2
44	BE	0	1
46	BG	0	1
47	BH	0	1
50	BK	0	2
52	BM	0	2
53	BN	0	3
54	BO	0	3
55	BP	0	2
57	BR	0	3
67	Bb	0	4
71	Bf	0	1
73	Bh	0	3
77	UD	0	1
84	UU	0	1
All	All	0	50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BV	52	PHE	CE2-CZ	8.42	1.53	1.37
61	BV	52	PHE	CD1-CE1	8.27	1.55	1.39
14	AK	198	TYR	CB-CG	7.87	1.63	1.51
66	Ba	108	CYS	CB-SG	-5.99	1.72	1.81
14	AK	198	TYR	CD1-CE1	5.77	1.48	1.39

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	BX	69	ARG	NE-CZ-NH2	12.13	126.36	120.30
39	AA	40	U	C6-N1-C2	-11.67	114.00	121.00
39	AA	40	U	C5-C6-N1	11.29	128.35	122.70
39	AA	317	A	O5'-P-OP2	11.12	124.04	110.70
39	AA	40	U	N3-C4-C5	-9.58	108.85	114.60

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A1	78	LEU	Peptide
3	A2	133	GLY	Peptide
3	A2	346	GLY	Peptide
4	A3	57	GLY	Peptide
8	A8	90	GLY	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	147/185 (80%)	143 (97%)	4 (3%)	0	100	100
2	A1	215/241 (89%)	209 (97%)	5 (2%)	1 (0%)	29	61
3	A2	445/471 (94%)	432 (97%)	10 (2%)	3 (1%)	22	55
4	A3	148/218 (68%)	143 (97%)	5 (3%)	0	100	100
5	A4	166/183 (91%)	156 (94%)	10 (6%)	0	100	100
6	A5	53/80 (66%)	51 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	A6	70/114 (61%)	70 (100%)	0	0	100	100
8	A8	139/181 (77%)	128 (92%)	11 (8%)	0	100	100
9	A9	51/184 (28%)	49 (96%)	2 (4%)	0	100	100
10	AE	289/473 (61%)	277 (96%)	12 (4%)	0	100	100
11	AF	440/459 (96%)	415 (94%)	24 (6%)	1 (0%)	47	78
12	AI	210/263 (80%)	201 (96%)	7 (3%)	2 (1%)	15	46
13	AJ	124/177 (70%)	116 (94%)	8 (6%)	0	100	100
14	AK	319/342 (93%)	307 (96%)	11 (3%)	1 (0%)	41	72
15	AN	177/202 (88%)	169 (96%)	8 (4%)	0	100	100
16	AP	348/374 (93%)	327 (94%)	20 (6%)	1 (0%)	41	72
17	AQ	121/167 (72%)	117 (97%)	4 (3%)	0	100	100
18	AR	225/301 (75%)	211 (94%)	13 (6%)	1 (0%)	34	67
19	AT	33/144 (23%)	33 (100%)	0	0	100	100
20	AU	171/213 (80%)	168 (98%)	3 (2%)	0	100	100
21	AV	178/188 (95%)	174 (98%)	4 (2%)	0	100	100
22	AW	274/278 (99%)	267 (97%)	6 (2%)	1 (0%)	34	67
23	AX	166/246 (68%)	160 (96%)	6 (4%)	0	100	100
24	AY	338/378 (89%)	325 (96%)	9 (3%)	4 (1%)	13	41
25	Ab	449/507 (89%)	425 (95%)	24 (5%)	0	100	100
26	Ad	255/289 (88%)	249 (98%)	6 (2%)	0	100	100
27	Ae	114/197 (58%)	109 (96%)	5 (4%)	0	100	100
28	Af	124/189 (66%)	117 (94%)	7 (6%)	0	100	100
29	Ag	257/260 (99%)	250 (97%)	7 (3%)	0	100	100
30	Aj	277/296 (94%)	259 (94%)	18 (6%)	0	100	100
31	Al	207/218 (95%)	197 (95%)	10 (5%)	0	100	100
32	Ao	179/259 (69%)	169 (94%)	10 (6%)	0	100	100
33	Ap	259/309 (84%)	247 (95%)	11 (4%)	1 (0%)	34	67
34	At	136/154 (88%)	130 (96%)	5 (4%)	1 (1%)	22	55
35	Av	211/242 (87%)	205 (97%)	4 (2%)	2 (1%)	17	49
36	AB	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
37	AC	26/28 (93%)	26 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	AD	26/28 (93%)	25 (96%)	1 (4%)	0	100	100
38	AG	25/27 (93%)	25 (100%)	0	0	100	100
40	BA	675/831 (81%)	647 (96%)	27 (4%)	1 (0%)	51	82
41	BB	387/541 (72%)	361 (93%)	22 (6%)	4 (1%)	15	46
42	BC	476/523 (91%)	448 (94%)	24 (5%)	4 (1%)	19	51
43	BD	415/547 (76%)	386 (93%)	23 (6%)	6 (1%)	11	37
44	BE	386/449 (86%)	361 (94%)	23 (6%)	2 (0%)	29	61
45	BF	341/426 (80%)	328 (96%)	13 (4%)	0	100	100
46	BG	317/378 (84%)	290 (92%)	27 (8%)	0	100	100
47	BH	209/349 (60%)	202 (97%)	7 (3%)	0	100	100
48	BI	317/343 (92%)	300 (95%)	16 (5%)	1 (0%)	41	72
49	BJ	164/333 (49%)	157 (96%)	7 (4%)	0	100	100
50	BK	252/386 (65%)	241 (96%)	10 (4%)	1 (0%)	34	67
51	BL	226/312 (72%)	220 (97%)	6 (3%)	0	100	100
52	BM	243/283 (86%)	220 (90%)	22 (9%)	1 (0%)	34	67
53	BN	212/302 (70%)	204 (96%)	8 (4%)	0	100	100
54	BO	143/262 (55%)	136 (95%)	6 (4%)	1 (1%)	22	55
55	BP	200/266 (75%)	192 (96%)	6 (3%)	2 (1%)	15	46
56	BQ	214/231 (93%)	201 (94%)	13 (6%)	0	100	100
57	BR	193/205 (94%)	180 (93%)	11 (6%)	2 (1%)	15	46
58	BS	95/198 (48%)	93 (98%)	2 (2%)	0	100	100
59	BT	166/191 (87%)	160 (96%)	6 (4%)	0	100	100
60	BU	80/185 (43%)	79 (99%)	1 (1%)	0	100	100
61	BV	153/190 (80%)	147 (96%)	6 (4%)	0	100	100
62	BW	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
63	BX	103/190 (54%)	94 (91%)	8 (8%)	1 (1%)	15	46
64	BY	100/172 (58%)	90 (90%)	9 (9%)	1 (1%)	15	46
65	BZ	188/190 (99%)	176 (94%)	12 (6%)	0	100	100
66	Ba	137/153 (90%)	130 (95%)	7 (5%)	0	100	100
67	Bb	97/162 (60%)	88 (91%)	9 (9%)	0	100	100
68	Bc	88/146 (60%)	85 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	Bd	138/144 (96%)	132 (96%)	6 (4%)	0	100	100
70	Be	99/113 (88%)	97 (98%)	2 (2%)	0	100	100
71	Bf	46/113 (41%)	41 (89%)	4 (9%)	1 (2%)	6	29
72	Bg	80/105 (76%)	72 (90%)	8 (10%)	0	100	100
73	Bh	89/92 (97%)	84 (94%)	3 (3%)	2 (2%)	6	29
All	All	14660/18620 (79%)	13953 (95%)	658 (4%)	49 (0%)	44	72

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	AW	72	THR
35	Av	232	LYS
41	BB	294	PRO
43	BD	356	PRO
43	BD	389	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	140/167 (84%)	136 (97%)	4 (3%)	42	69
2	A1	195/217 (90%)	184 (94%)	11 (6%)	21	51
3	A2	394/413 (95%)	380 (96%)	14 (4%)	35	63
4	A3	131/193 (68%)	125 (95%)	6 (5%)	27	57
5	A4	153/164 (93%)	149 (97%)	4 (3%)	46	72
6	A5	52/73 (71%)	47 (90%)	5 (10%)	8	29
7	A6	61/99 (62%)	54 (88%)	7 (12%)	5	20
8	A8	126/161 (78%)	122 (97%)	4 (3%)	39	67
9	A9	51/166 (31%)	44 (86%)	7 (14%)	3	14
10	AE	258/406 (64%)	247 (96%)	11 (4%)	29	59
11	AF	394/409 (96%)	375 (95%)	19 (5%)	25	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AI	192/233 (82%)	184 (96%)	8 (4%)	30	59
13	AJ	90/151 (60%)	86 (96%)	4 (4%)	28	58
14	AK	287/301 (95%)	270 (94%)	17 (6%)	19	49
15	AN	160/182 (88%)	155 (97%)	5 (3%)	40	68
16	AP	310/330 (94%)	295 (95%)	15 (5%)	25	56
17	AQ	106/141 (75%)	102 (96%)	4 (4%)	33	61
18	AR	198/256 (77%)	195 (98%)	3 (2%)	65	82
19	AT	28/124 (23%)	25 (89%)	3 (11%)	6	24
20	AU	151/184 (82%)	143 (95%)	8 (5%)	22	52
21	AV	153/158 (97%)	151 (99%)	2 (1%)	69	84
22	AW	244/246 (99%)	234 (96%)	10 (4%)	30	59
23	AX	156/221 (71%)	154 (99%)	2 (1%)	69	84
24	AY	283/337 (84%)	268 (95%)	15 (5%)	22	52
25	Ab	373/451 (83%)	368 (99%)	5 (1%)	69	84
26	Ad	225/250 (90%)	218 (97%)	7 (3%)	40	68
27	Ae	100/172 (58%)	93 (93%)	7 (7%)	15	44
28	Af	111/162 (68%)	103 (93%)	8 (7%)	14	43
29	Ag	238/239 (100%)	231 (97%)	7 (3%)	42	69
30	Aj	237/260 (91%)	230 (97%)	7 (3%)	41	68
31	Al	170/186 (91%)	167 (98%)	3 (2%)	59	79
32	Ao	153/216 (71%)	144 (94%)	9 (6%)	19	49
33	Ap	227/267 (85%)	217 (96%)	10 (4%)	28	58
34	At	116/140 (83%)	114 (98%)	2 (2%)	60	80
35	Av	187/210 (89%)	176 (94%)	11 (6%)	19	49
40	BA	598/727 (82%)	572 (96%)	26 (4%)	29	59
41	BB	271/470 (58%)	240 (89%)	31 (11%)	5	21
42	BC	406/443 (92%)	396 (98%)	10 (2%)	47	72
44	BE	334/386 (86%)	321 (96%)	13 (4%)	32	61
45	BF	299/368 (81%)	289 (97%)	10 (3%)	38	66
46	BG	266/310 (86%)	247 (93%)	19 (7%)	14	44
47	BH	182/297 (61%)	164 (90%)	18 (10%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BI	268/288 (93%)	255 (95%)	13 (5%)	25	55
49	BJ	136/298 (46%)	128 (94%)	8 (6%)	19	49
50	BK	196/331 (59%)	184 (94%)	12 (6%)	18	48
51	BL	201/262 (77%)	192 (96%)	9 (4%)	27	58
52	BM	209/240 (87%)	197 (94%)	12 (6%)	20	50
53	BN	167/265 (63%)	158 (95%)	9 (5%)	22	52
54	BO	129/225 (57%)	122 (95%)	7 (5%)	22	52
55	BP	162/219 (74%)	155 (96%)	7 (4%)	29	59
56	BQ	182/195 (93%)	175 (96%)	7 (4%)	33	61
57	BR	171/181 (94%)	166 (97%)	5 (3%)	42	69
58	BS	85/164 (52%)	81 (95%)	4 (5%)	26	57
59	BT	147/163 (90%)	140 (95%)	7 (5%)	25	56
60	BU	71/168 (42%)	69 (97%)	2 (3%)	43	70
61	BV	138/163 (85%)	130 (94%)	8 (6%)	20	50
62	BW	163/164 (99%)	158 (97%)	5 (3%)	40	68
63	BX	92/170 (54%)	80 (87%)	12 (13%)	4	16
64	BY	89/151 (59%)	87 (98%)	2 (2%)	52	75
65	BZ	143/160 (89%)	142 (99%)	1 (1%)	84	92
66	Ba	131/144 (91%)	129 (98%)	2 (2%)	65	82
67	Bb	84/135 (62%)	81 (96%)	3 (4%)	35	63
68	Bc	82/134 (61%)	76 (93%)	6 (7%)	14	43
69	Bd	117/120 (98%)	112 (96%)	5 (4%)	29	59
70	Be	89/99 (90%)	85 (96%)	4 (4%)	27	58
71	Bf	45/98 (46%)	44 (98%)	1 (2%)	52	75
72	Bg	65/87 (75%)	60 (92%)	5 (8%)	13	40
73	Bh	79/80 (99%)	74 (94%)	5 (6%)	18	47
All	All	12247/15590 (79%)	11695 (96%)	552 (4%)	31	58

5 of 552 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	BP	121	ARG
57	BR	41	LEU

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Mol	Chain	Res	Type
55	BP	39	LEU
65	BZ	76	ARG
26	Ad	80	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 237 such sidechains are listed below:

Mol	Chain	Res	Type
33	Ap	197	GLN
64	BY	80	GLN
42	BC	62	GLN
64	BY	79(B)	HIS
73	Bh	37	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
39	AA	581/1178 (49%)	289 (49%)	19 (3%)

5 of 289 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
39	AA	2	U
39	AA	4	U
39	AA	5	U
39	AA	10	A
39	AA	11	U

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
39	AA	485	A
39	AA	951	C
39	AA	1164	A
39	AA	534	U
39	AA	387	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 13 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	NAD	Av	301	-	42,48,48	1.98	9 (21%)	50,73,73	1.82	10 (20%)

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	NAD	Av	301	-	-	3/26/62/62	0/5/5/5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	Av	301	NAD	C3N-C7N	-7.74	1.38	1.50
88	Av	301	NAD	C2A-N3A	4.51	1.39	1.32
88	Av	301	NAD	C2N-N1N	3.87	1.39	1.35
88	Av	301	NAD	C2A-N1A	3.03	1.39	1.33
88	Av	301	NAD	C5A-C4A	-2.84	1.33	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	Av	301	NAD	N3A-C2A-N1A	-6.69	118.23	128.68
88	Av	301	NAD	O4D-C1D-C2D	-4.68	100.08	106.93
88	Av	301	NAD	PN-O3-PA	-4.30	118.06	132.83
88	Av	301	NAD	C3D-C2D-C1D	-3.90	95.10	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	Av	301	NAD	C2B-C3B-C4B	-3.19	96.45	102.64

There are no chirality outliers.

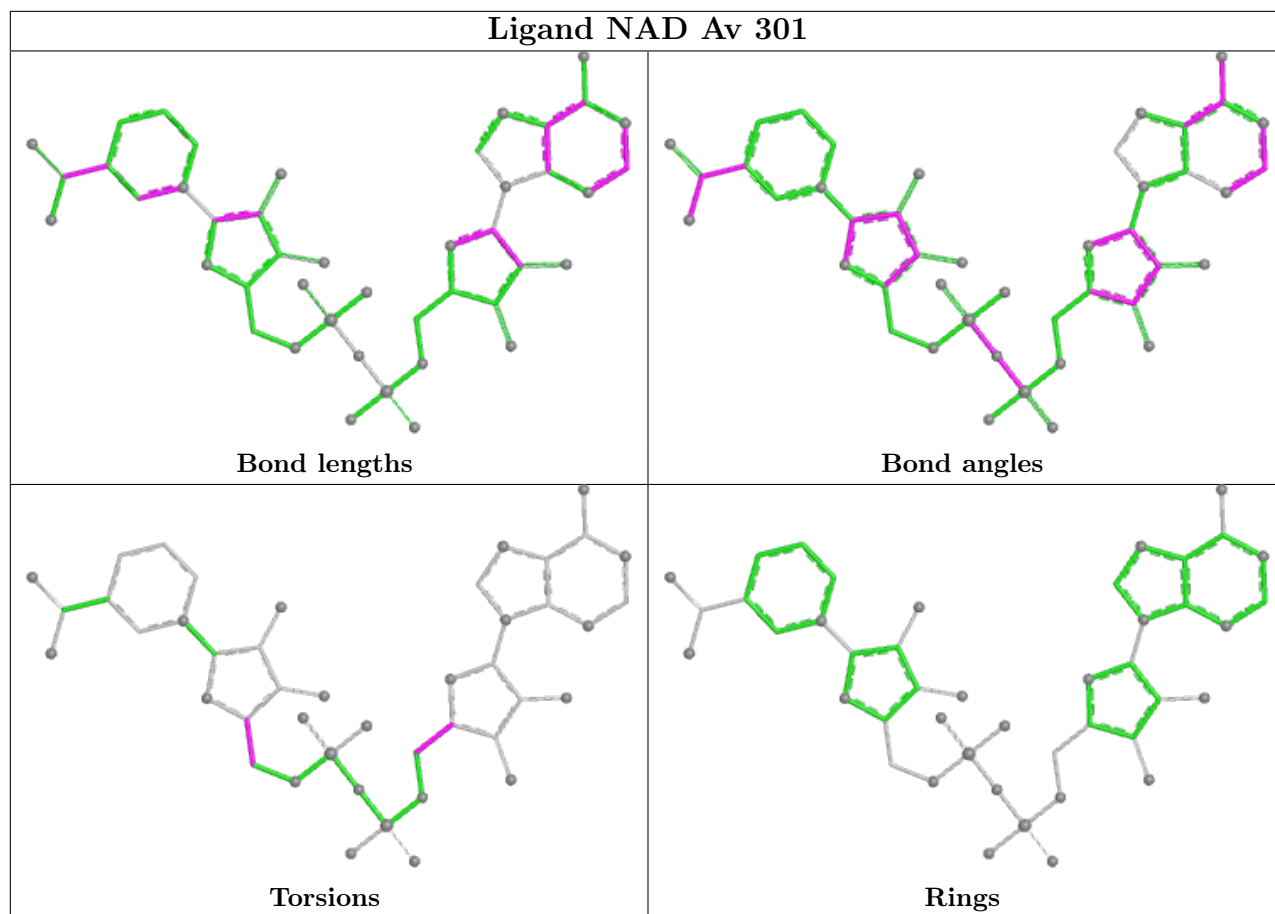
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	Av	301	NAD	O4D-C4D-C5D-O5D
88	Av	301	NAD	C3D-C4D-C5D-O5D
88	Av	301	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
77	UD	3
39	AA	1
14	AK	1
8	A8	1
21	AV	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UD	90:UNK	C	136:UNK	N	14.30
1	UD	158:UNK	C	159:UNK	N	11.31

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UD	68:UNK	C	69:UNK	N	9.93
1	AA	448:A	O3'	454:U	P	9.07
1	AK	250:LEU	C	251:THR	N	5.73

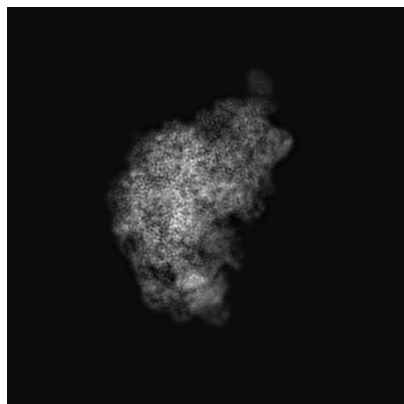
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0231. These allow visual inspection of the internal detail of the map and identification of artifacts.

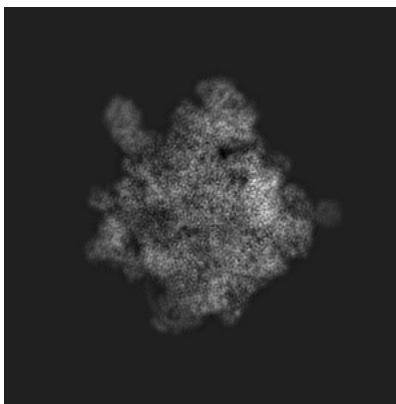
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

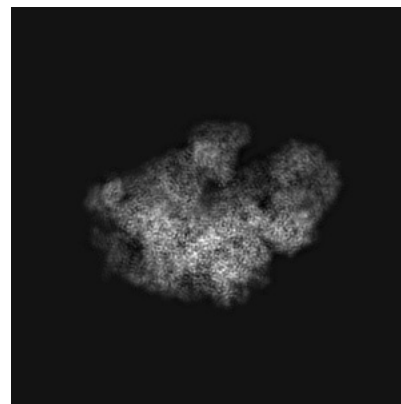
6.1.1 Primary map



X

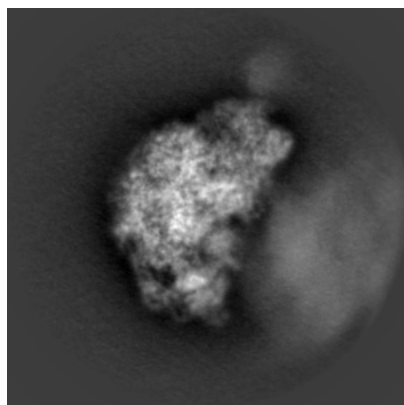


Y

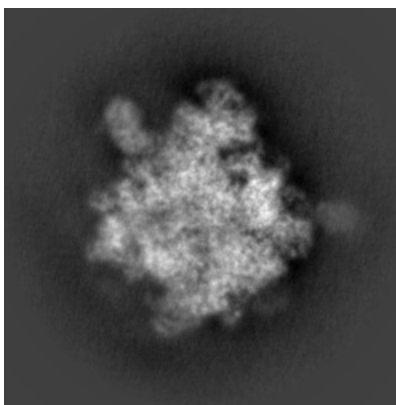


Z

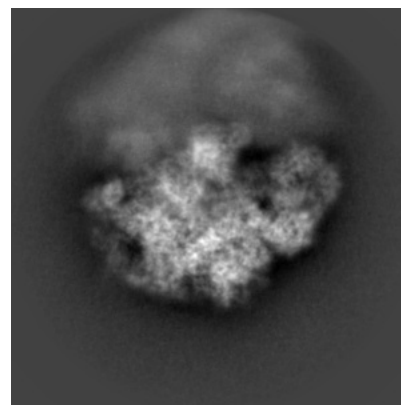
6.1.2 Raw map



X



Y

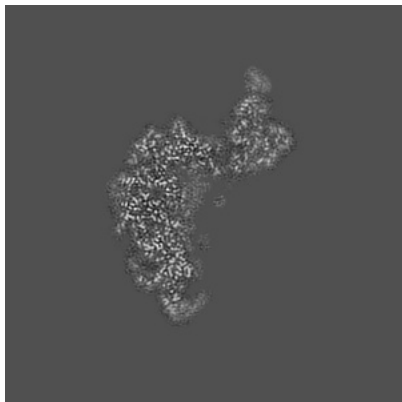


Z

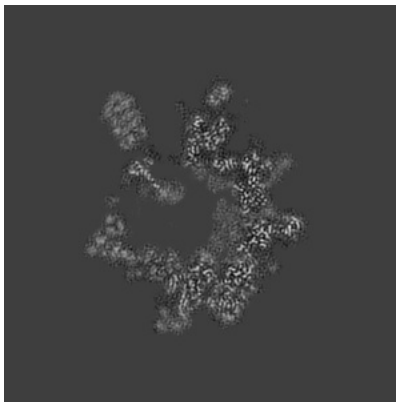
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

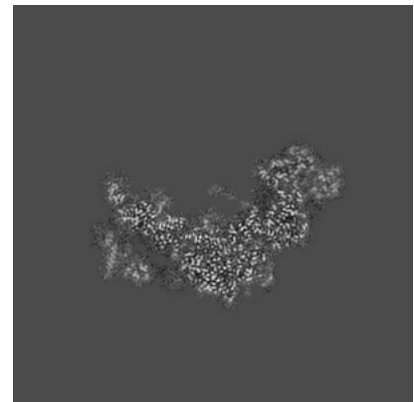
6.2.1 Primary map



X Index: 160

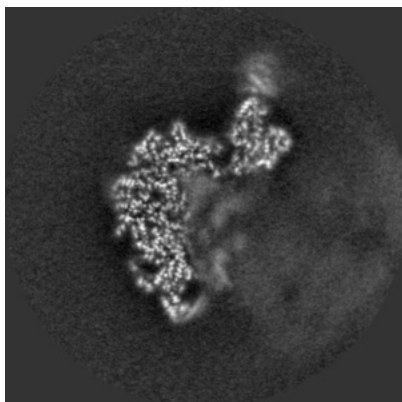


Y Index: 160

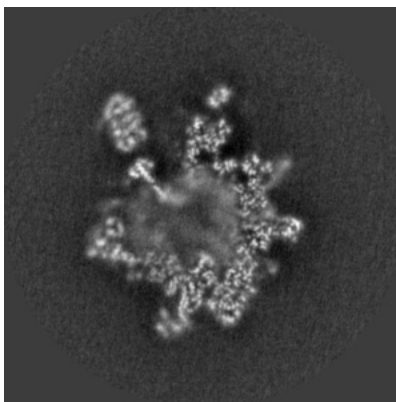


Z Index: 160

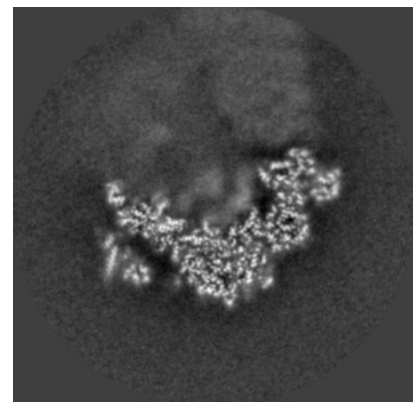
6.2.2 Raw map



X Index: 160



Y Index: 160

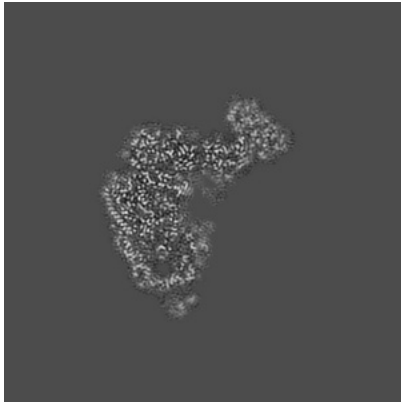


Z Index: 160

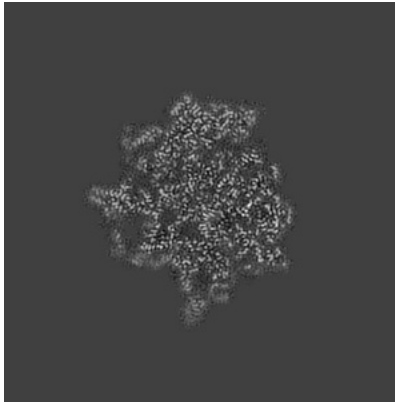
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

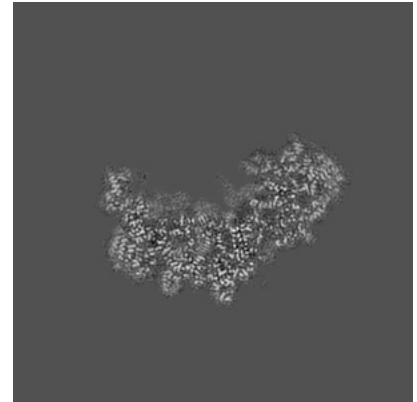
6.3.1 Primary map



X Index: 171

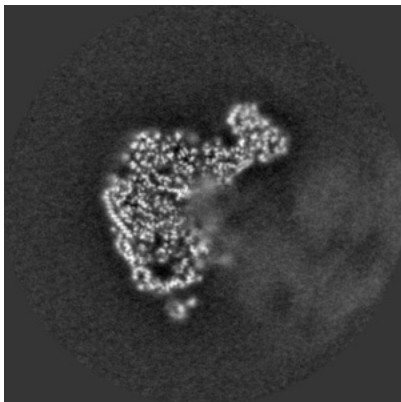


Y Index: 134

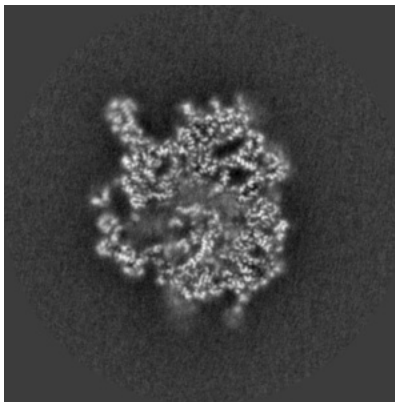


Z Index: 169

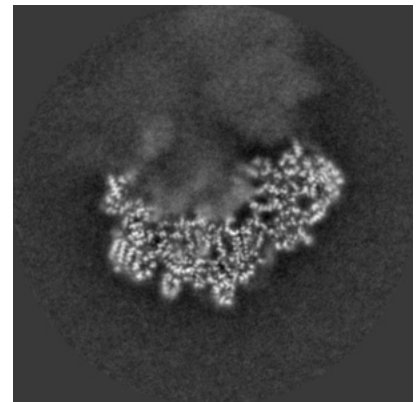
6.3.2 Raw map



X Index: 171



Y Index: 147

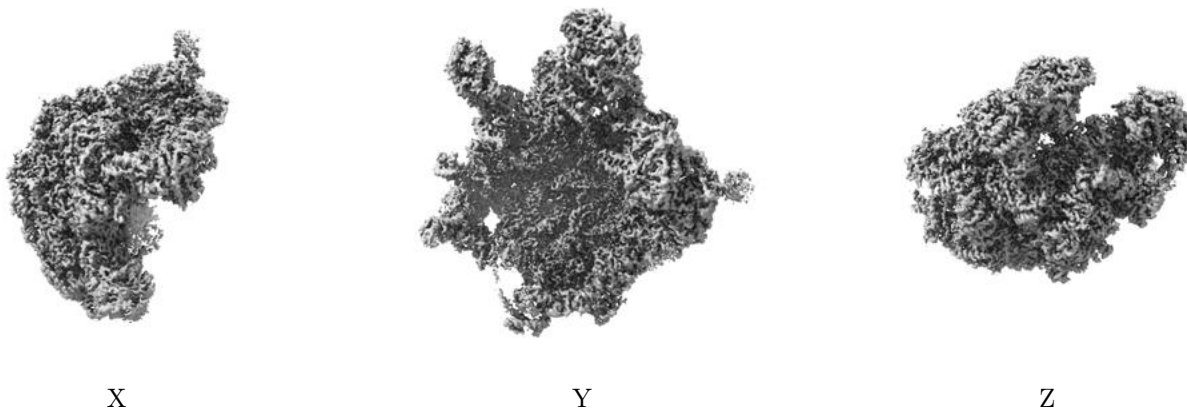


Z Index: 169

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

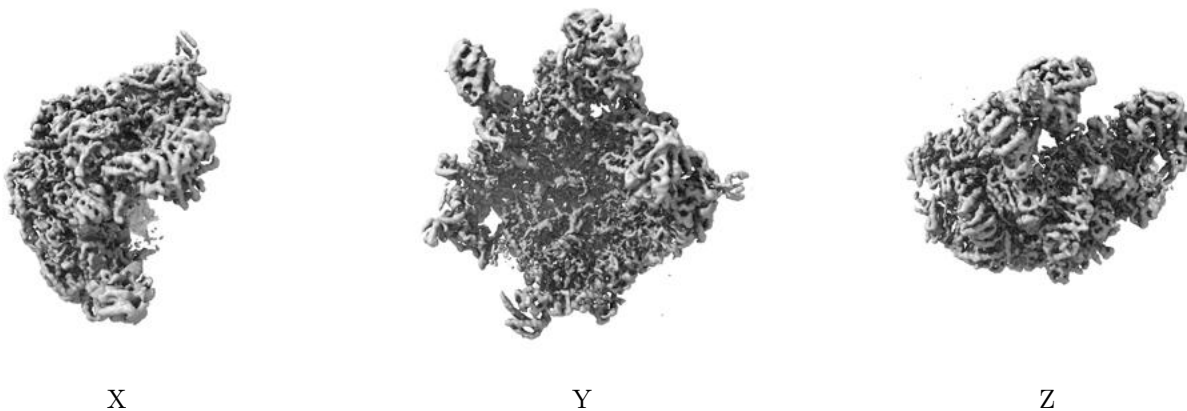
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



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

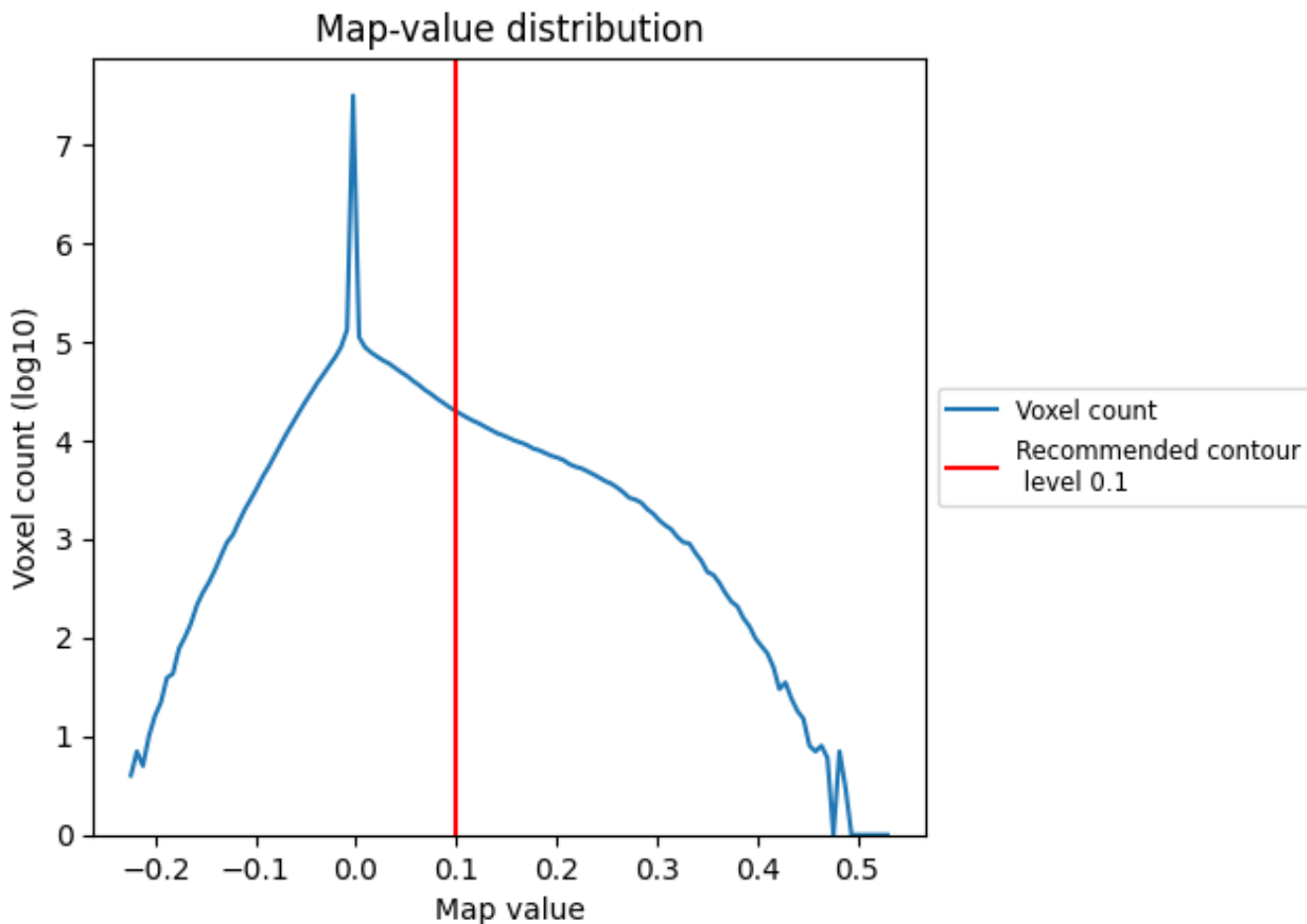
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

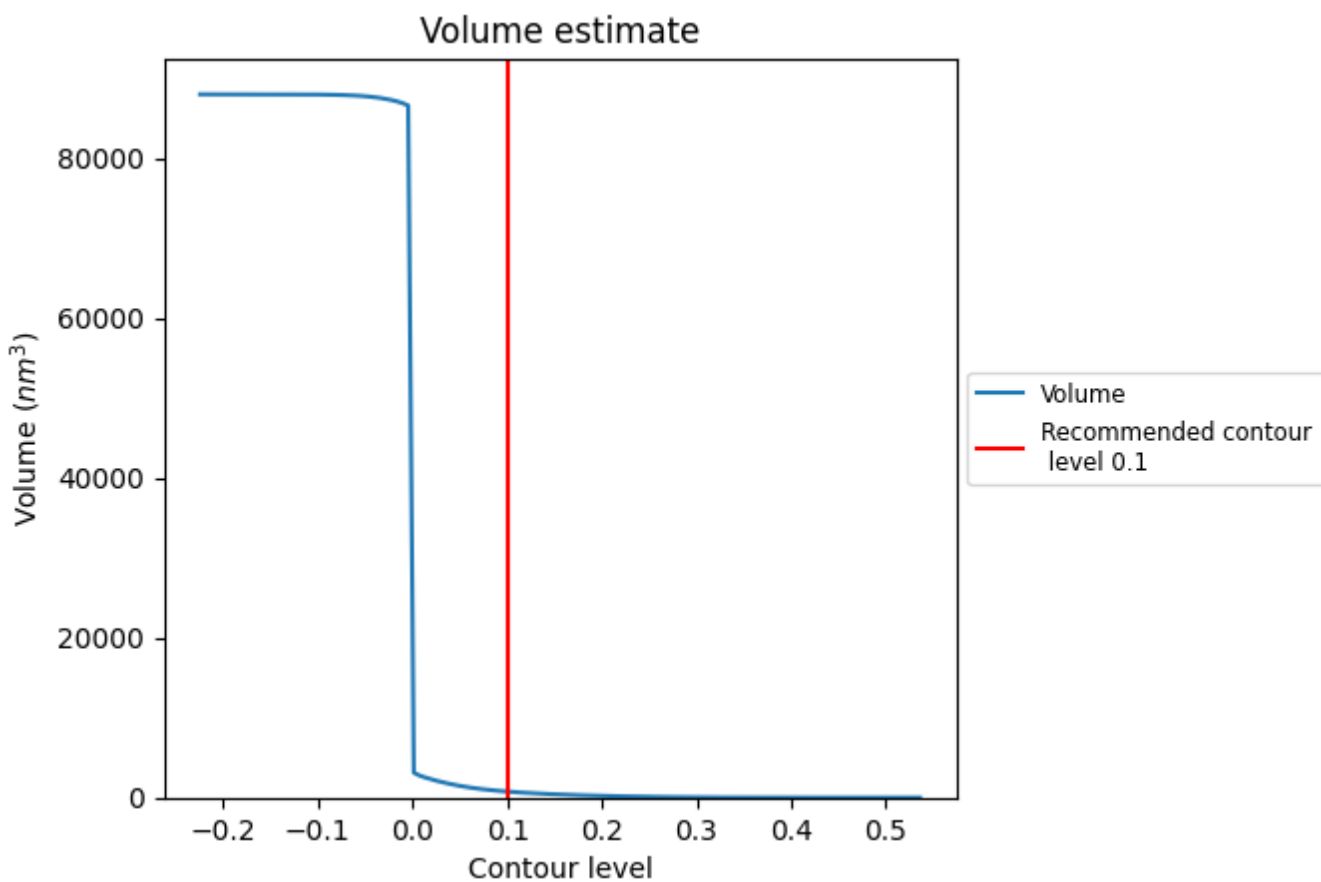
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

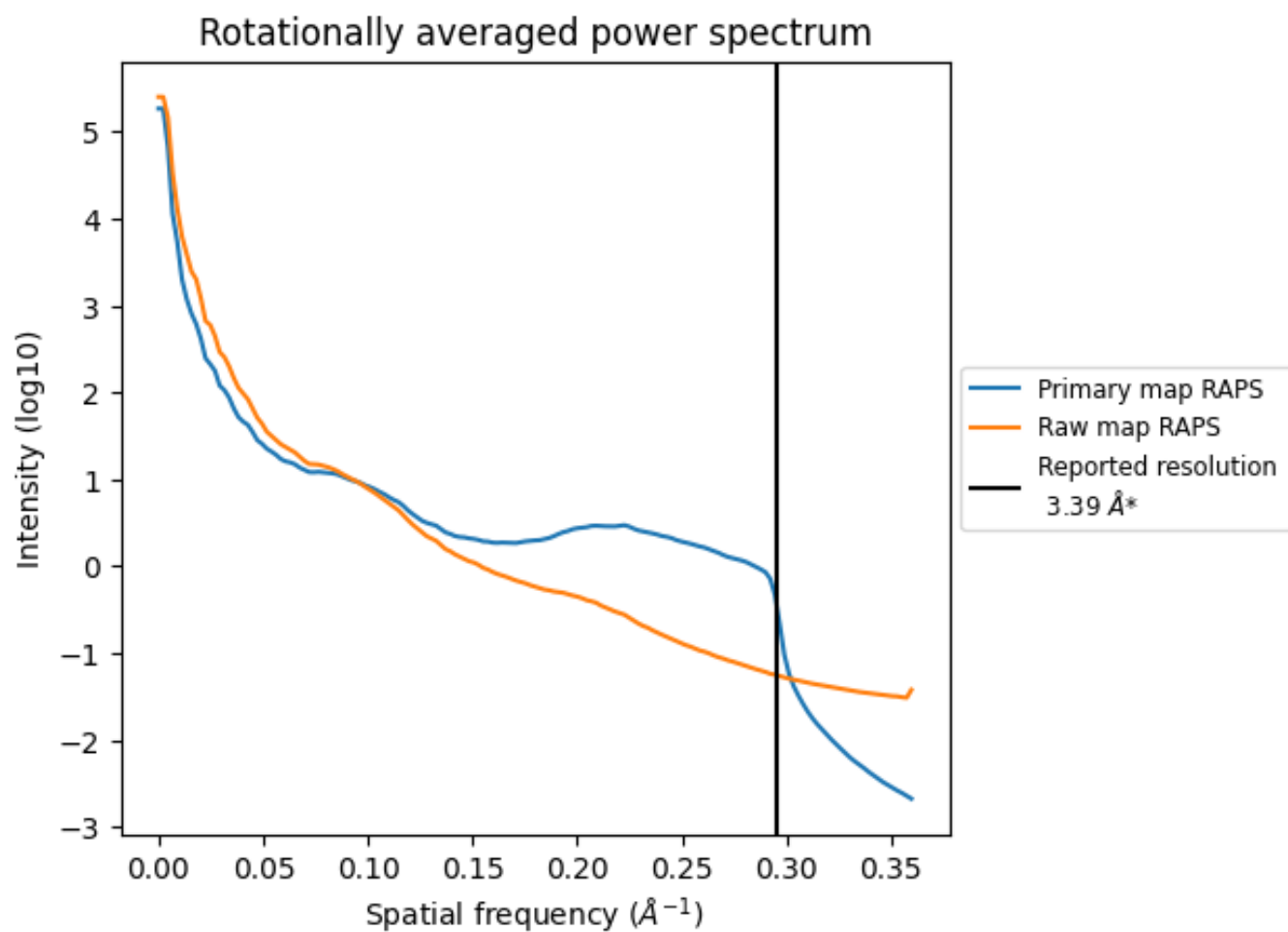
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 751 nm³; this corresponds to an approximate mass of 678 kDa.

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

7.3 Rotationally averaged power spectrum i

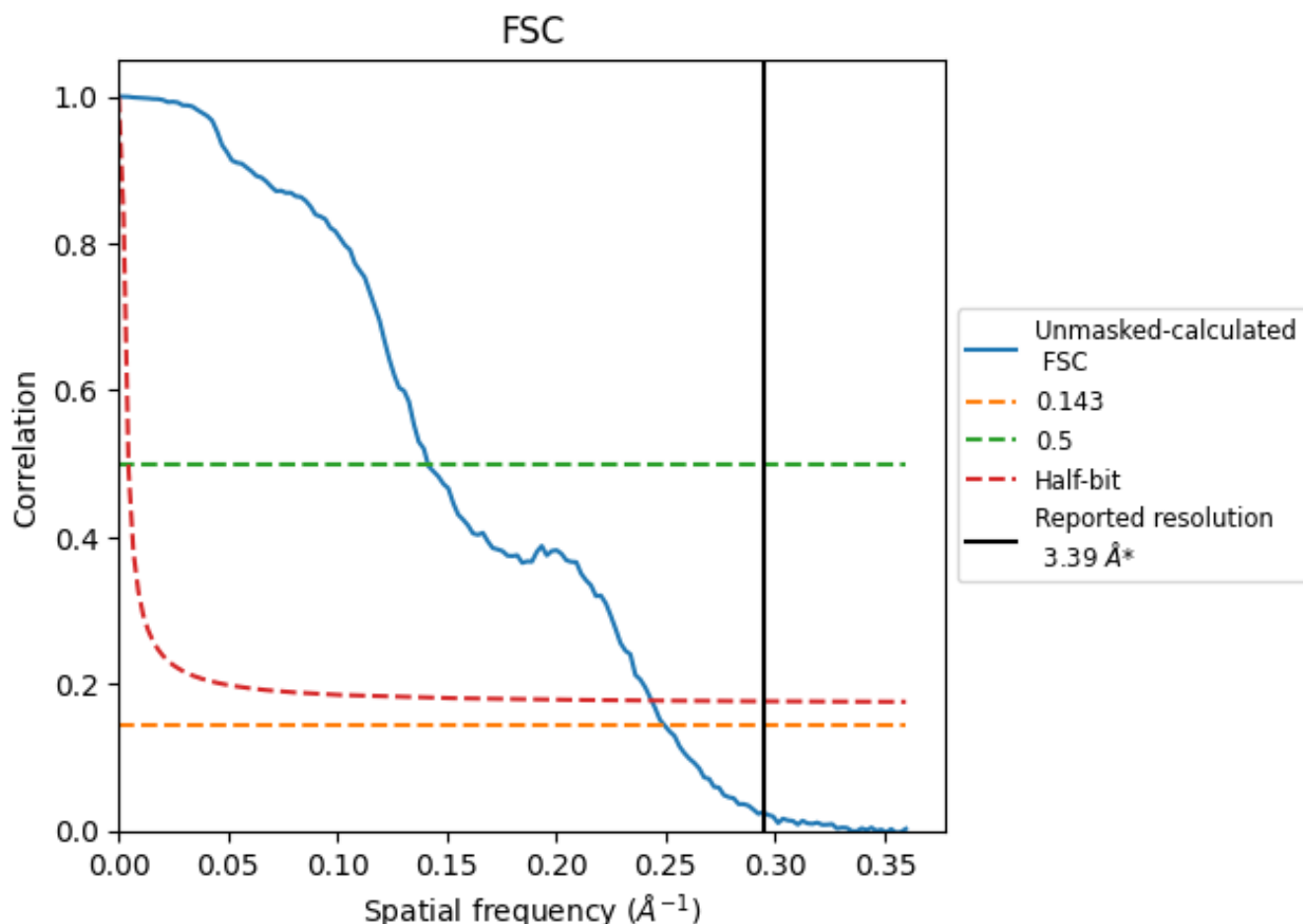


*Reported resolution corresponds to spatial frequency of 0.295 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.295 Å⁻¹

8.2 Resolution estimates [i](#)

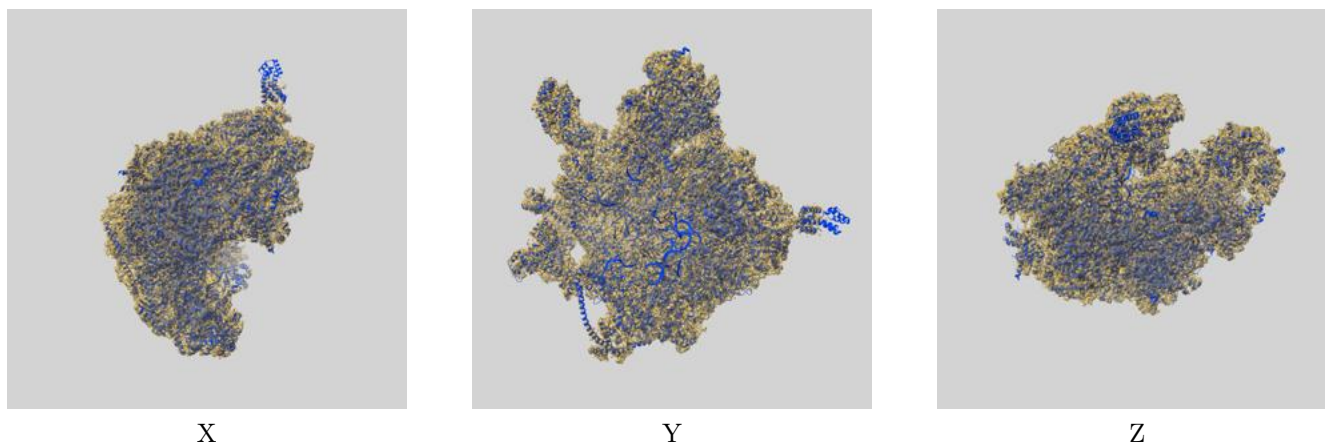
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.08	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.39 by more than 10 %

9 Map-model fit [i](#)

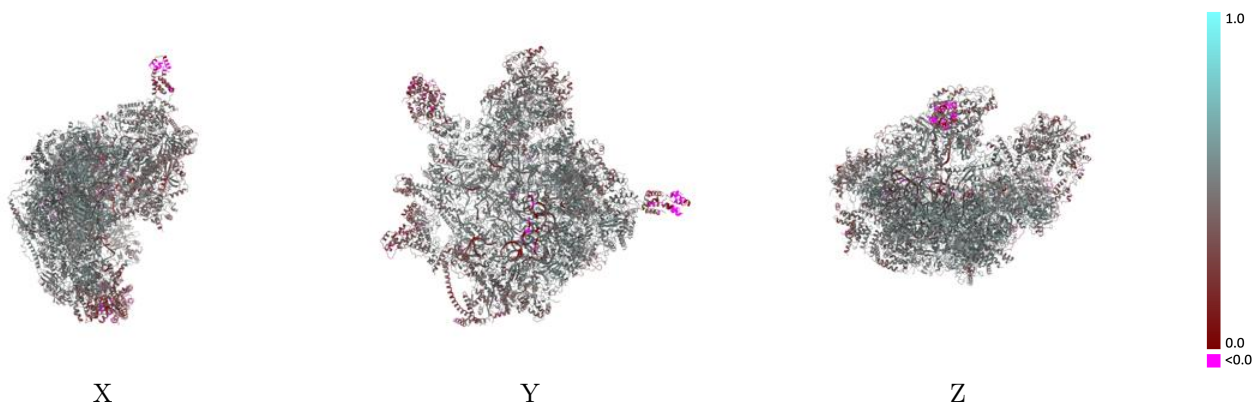
This section contains information regarding the fit between EMDB map EMD-0231 and PDB model 6HIX. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



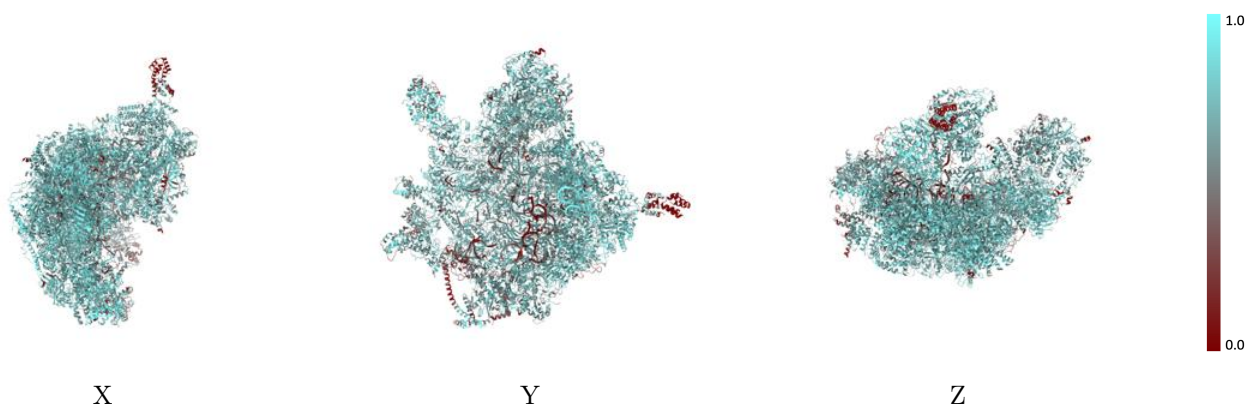
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



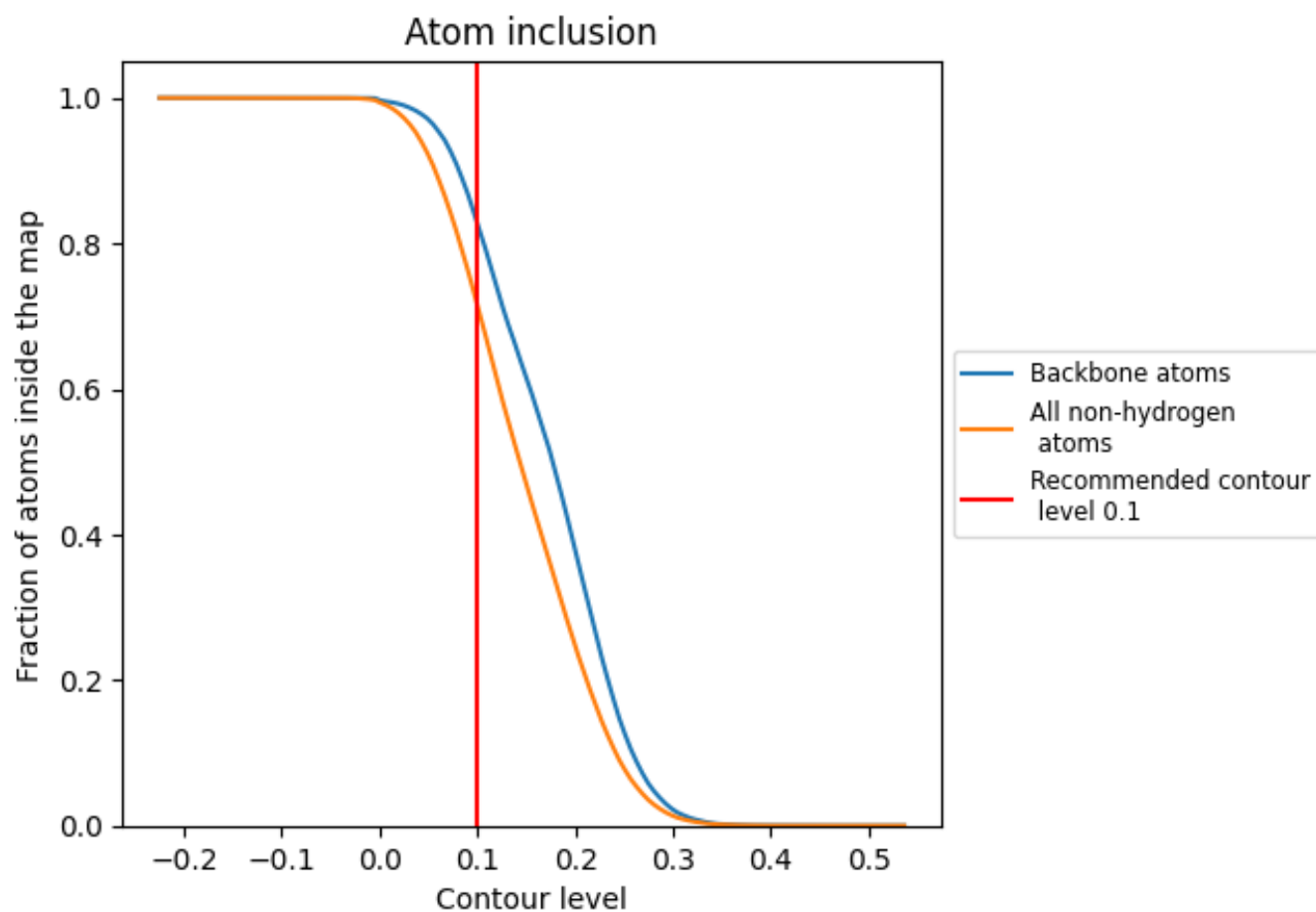
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 72% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7159	 0.4690
A0	 0.7174	 0.5000
A1	 0.7087	 0.4740
A2	 0.7984	 0.5020
A3	 0.7968	 0.5290
A4	 0.6252	 0.4470
A5	 0.7532	 0.5120
A6	 0.6129	 0.4720
A8	 0.6891	 0.4970
A9	 0.6539	 0.4950
AA	 0.6662	 0.4290
AB	 0.4571	 0.3200
AC	 0.5143	 0.2850
AD	 0.0000	 -0.0810
AE	 0.7383	 0.5000
AF	 0.7961	 0.5270
AG	 0.0148	 0.0120
AI	 0.7687	 0.5000
AJ	 0.6720	 0.4230
AK	 0.7180	 0.4390
AN	 0.7258	 0.5130
AP	 0.7804	 0.5170
AQ	 0.6805	 0.4990
AR	 0.7584	 0.4910
AT	 0.6777	 0.4690
AU	 0.7586	 0.5150
AV	 0.7696	 0.5100
AW	 0.7477	 0.5180
AX	 0.7411	 0.4970
AY	 0.7080	 0.4620
Ab	 0.7542	 0.4880
Ad	 0.6952	 0.4460
Ae	 0.7780	 0.4990
Af	 0.7371	 0.4950
Ag	 0.7727	 0.4930

































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Chain	Atom inclusion	Q-score
Aj	 0.6740	 0.3980
Al	 0.7511	 0.5160
Ao	 0.7590	 0.5150
Ap	 0.7418	 0.5020
At	 0.6938	 0.4710
Av	 0.7351	 0.4970
BA	 0.7644	 0.4990
BB	 0.6439	 0.3940
BC	 0.7875	 0.5060
BD	 0.6966	 0.2880
BE	 0.7347	 0.4730
BF	 0.7845	 0.5120
BG	 0.6847	 0.3960
BH	 0.7378	 0.4660
BI	 0.7883	 0.4930
BJ	 0.6494	 0.4060
BK	 0.4881	 0.3780
BL	 0.7405	 0.4820
BM	 0.7813	 0.5030
BN	 0.6154	 0.3960
BO	 0.6571	 0.4360
BP	 0.6846	 0.4790
BQ	 0.7923	 0.5100
BR	 0.7832	 0.5130
BS	 0.6837	 0.4540
BT	 0.8111	 0.5130
BU	 0.7348	 0.4630
BV	 0.6958	 0.4420
BW	 0.8317	 0.5190
BX	 0.3563	 0.4030
BY	 0.6848	 0.4450
BZ	 0.7243	 0.4600
Ba	 0.8010	 0.5200
Bb	 0.7373	 0.4550
Bc	 0.7086	 0.4810
Bd	 0.6992	 0.4680
Be	 0.7189	 0.5000
Bf	 0.6850	 0.4930
Bg	 0.7195	 0.4870
Bh	 0.4986	 0.4120
UA	 0.6014	 0.3140
UB	 0.6667	 0.4210

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Chain	Atom inclusion	Q-score
UC	 0.3889	 0.3870
UD	 0.4030	 0.3690
UE	 0.6742	 0.4730
UF	 0.7500	 0.4920
UG	 0.5972	 0.4630
UH	 0.7500	 0.5140
UI	 0.4118	 0.4170
UK	 0.7667	 0.4570
UL	 0.6333	 0.4470
UM	 0.1944	 0.3000
UN	 0.1806	 0.3030
UU	 0.4242	 0.3880
UV	 0.6667	 0.4970
UW	 0.2143	 0.2140
UX	 0.6667	 0.4540