



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 07:41 AM UTC

PDB ID : 6YWX / pdb_00006ywx
EMDB ID : EMD-10978
Title : The structure of the mitoribosome from *Neurospora crassa* with tRNA bound to the E-site
Authors : Amunts, A.; Itoh, Y.; Naschberger, A.
Deposited on : 2020-04-30
Resolution : 3.10 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

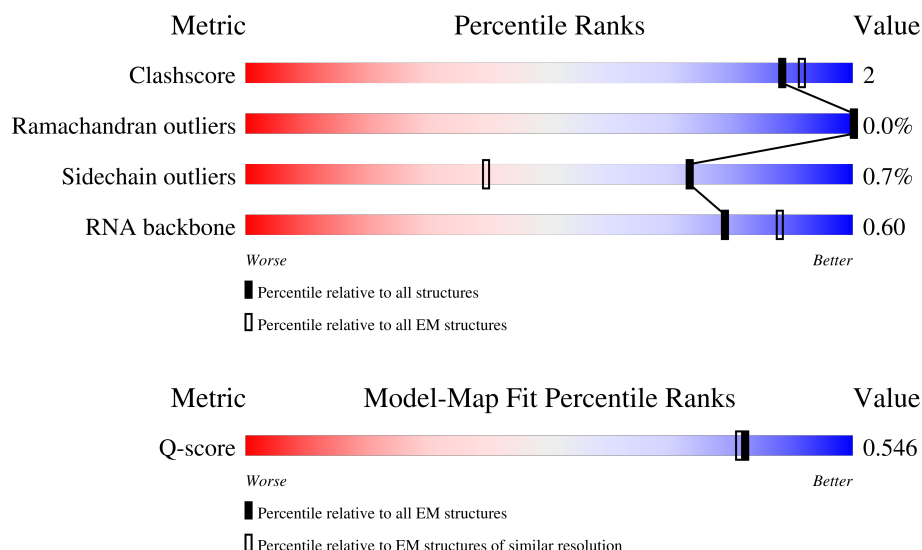
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



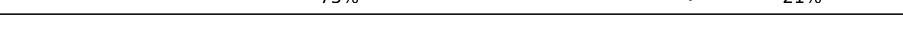
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	A	3464	
2	B	383	
3	C	384	

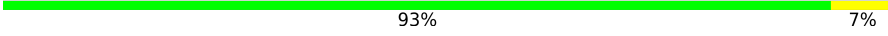
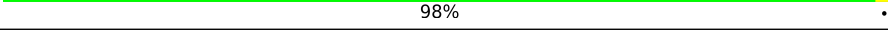
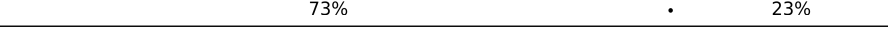
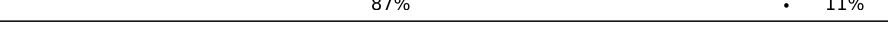
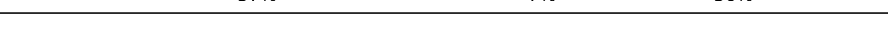
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Mol	Chain	Length	Quality of chain
4	D	325	
5	E	352	
6	F	255	
7	G	300	
8	f	347	
9	g	158	
10	H	183	
11	I	131	
12	J	312	
13	K	249	
14	L	193	
15	M	258	
16	N	217	
17	O	364	
18	P	228	
19	Q	396	
20	R	447	
21	S	274	
22	T	263	
23	U	161	
24	V	219	
25	W	129	
26	X	59	
27	Y	140	
28	0	124	

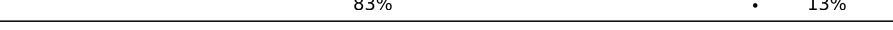
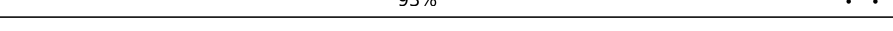
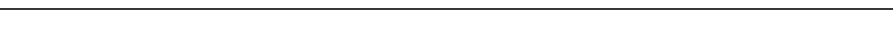
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Mol	Chain	Length	Quality of chain
29	1	449	
30	2	370	
31	3	103	
32	4	138	
33	5	439	
34	6	368	
35	7	165	
36	8	443	
37	h	98	
38	i	218	
39	9	267	
40	a	225	
41	b	162	
42	c	110	
43	d	292	
44	AA	470	
45	BB	428	
46	CC	508	
47	DD	453	
48	EE	477	
49	FF	117	
50	GG	309	
51	HH	161	
52	II	315	
53	JJ	268	

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Mol	Chain	Length	Quality of chain
54	KK	376	
55	LL	174	
56	MM	119	
57	NN	113	
58	OO	320	
59	PP	107	
60	QQ	165	
61	RR	256	
62	SS	91	
63	TT	236	
64	UU	253	
65	VV	316	
66	WW	396	
67	XX	469	
68	YY	108	
69	ZZ	382	
70	11	90	
71	22	344	
72	33	236	
73	44	310	
73	55	310	
74	66	348	
75	77	414	
76	88	508	
77	00	95	

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Mol	Chain	Length	Quality of chain
77	99	95	 38% 62%
78	aa	1864	 61% 15% • 23%
79	bb	61	 80% 16% •
80	e	303	 46% • 50%
81	j	201	 86% 11% •

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 390774 atoms, of which 173664 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2838	Total	C	H	N	O	P	0	0
			90895	27142	30363	10859	19693	2838		

- Molecule 2 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	317	Total	C	H	N	O	S	0	0
			4996	1537	2523	502	419	15		

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	307	Total	C	H	N	O	S	0	0
			4757	1468	2421	447	413	8		

- Molecule 4 is a protein called 60S ribosomal protein L4, variant.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	254	Total	C	H	N	O	S	0	0
			4068	1280	2040	372	371	5		

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	309	Total	C	H	N	O	S	0	0
			4910	1558	2461	436	443	12		

- Molecule 6 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	201	Total	C	H	N	O	S	0	0
			3253	1022	1645	290	288	8		

- Molecule 7 is a protein called RIBOSOMAL_L9 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	74	Total	C	H	N	O	S	0	0
			1245	390	627	121	104	3		

- Molecule 8 is a protein called uL10m.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	f	245	Total	C	H	N	O	S	0	0
			3801	1202	1925	325	346	3		

- Molecule 9 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	g	147	Total	C	H	N	O	S	0	0
			2257	700	1154	203	196	4		

- Molecule 10 is a protein called Ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	H	183	Total	C	H	N	O	S	0	0
			2885	899	1459	268	251	8		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	I	119	Total	C	H	N	O	S	0	0
			1898	564	985	182	159	8		

- Molecule 12 is a protein called 50S ribosomal subunit protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	J	243	Total	C	H	N	O	S	0	0
			3827	1198	1939	346	343	1		

- Molecule 13 is a protein called 60S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	K	168	Total	C	H	N	O	S	0	0
			2751	850	1401	263	231	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	L	192	Total	C	H	N	O	S	0	0
			3135	960	1590	294	285	6		

- Molecule 15 is a protein called Mitochondrial ribosomal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	M	194	Total	C	H	N	O	S	0	0
			3164	981	1628	292	253	10		

- Molecule 16 is a protein called Aconitate hydratase.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	N	133	Total	C	H	N	O	S	0	0
			2176	673	1120	195	182	6		

- Molecule 17 is a protein called Mitochondrial large ribosomal subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	O	272	Total	C	H	N	O	S	0	0
			4532	1392	2323	424	387	6		

- Molecule 18 is a protein called Mitochondrial ribosomal protein subunit L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	P	180	Total	C	H	N	O	S	0	0
			2975	953	1494	270	254	4		

- Molecule 19 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Q	353	Total	C	H	N	O	S	0	0
			5829	1786	2961	547	524	11		

- Molecule 20 is a protein called bL27m.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	R	249	Total	C	H	N	O	S	0	0
			4195	1283	2149	412	347	4		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	S	179	Total	C	H	N	O	S	0	0
			2979	937	1507	281	252	2		

- Molecule 22 is a protein called 54S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	T	180	Total	C	H	N	O	S	0	0
			2950	937	1453	279	278	3		

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	U	138	Total	C	H	N	O	S	0	0
			2263	698	1164	213	185	3		

- Molecule 24 is a protein called bL31m.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	V	56	Total	C	H	N	O	S	0	0
			921	291	462	85	82	1		

- Molecule 25 is a protein called Mitochondrial ribosomal protein subunit L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	W	59	Total	C	H	N	O	S	0	0
			949	282	489	98	72	8		

- Molecule 26 is a protein called bL33m.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	X	48	Total	C	H	N	O	S	0	0
			836	263	433	71	65	4		

- Molecule 27 is a protein called Related to ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Y	46	Total	C	H	N	O	S	0	0
			777	224	412	84	56	1		

- Molecule 28 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	0	46	Total	C	H	N	O	S	0	0
			797	240	409	86	58	4		

- Molecule 29 is a protein called Mitochondrial large ribosomal subunit YmL35.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	1	367	Total	C	H	N	O	S	0	0
			6014	1899	3029	547	531	8		

- Molecule 30 is a protein called mL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	2	123	Total	C	H	N	O	S	0	0
			2101	660	1055	211	171	4		

- Molecule 31 is a protein called mL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	3	95	Total	C	H	N	O	S	0	0
			1536	489	773	135	137	2		

- Molecule 32 is a protein called Mitochondrial ribosomal protein L43.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	4	137	Total	C	H	N	O	S	0	0
			2139	671	1087	192	183	6		

- Molecule 33 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	5	350	Total	C	H	N	O	S	0	0
			5429	1740	2710	477	493	9		

- Molecule 34 is a protein called 50S ribosomal subunit L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	6	273	Total	C	H	N	O	S	0	0
			4474	1418	2248	399	401	8		

- Molecule 35 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	7	84	Total	C	H	N	O	0	0
			1383	431	709	130	113		

- Molecule 36 is a protein called mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace	
36	8	331	Total	C	H	N	O	S	0	0
			5374	1683	2714	480	489	8		

- Molecule 37 is a protein called Mitochondrial ribosomal protein L44.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	h	98	Total	C	H	N	O	S	0	0
			1577	490	798	139	146	4		

- Molecule 38 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace	
38	i	124	Total	C	H	N	O	S	0	0
			1999	613	1022	181	178	5		

- Molecule 39 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	9	206	Total	C	H	N	O	S	0	0
			3341	1051	1698	295	290	7		

- Molecule 40 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	a	161	Total	C	H	N	O	S	0	0
			2671	837	1340	253	235	6		

- Molecule 41 is a protein called Mitochondrial 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	b	161	Total	C	H	N	O	S	0	0
			2693	840	1379	249	221	4		

- Molecule 42 is a protein called 54S ribosomal protein L31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	c	98	Total	C	H	N	O	S	0	0
			1700	528	873	162	134	3		

- Molecule 43 is a protein called mL67.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	d	235	Total	C	H	N	O	S	0	0
			3797	1180	1909	363	339	6		

- Molecule 44 is a protein called bS1m.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	AA	372	Total	C	H	N	O	S	0	0
			5790	1827	2907	507	543	6		

- Molecule 45 is a protein called Mito ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	BB	290	Total	C	H	N	O	S	0	0
			4570	1426	2301	423	414	6		

- Molecule 46 is a protein called Ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	CC	438	Total	C	H	N	O	S	0	0
			7538	2388	3897	636	612	5		

- Molecule 47 is a protein called Mito ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	DD	290	Total	C	H	N	O	S	0	0
			4716	1501	2373	430	401	11		

- Molecule 48 is a protein called 37S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	EE	367	Total	C	H	N	O	S	0	0
			5798	1799	2918	526	543	12		

- Molecule 49 is a protein called Mito ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	FF	117	Total	C	H	N	O	S	0	0
			1901	591	966	176	165	3		

- Molecule 50 is a protein called Ribosomal_S7 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	GG	217	Total	C	H	N	O	S	0	0
			3409	1063	1737	307	296	6		

- Molecule 51 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	HH	160	Total	C	H	N	O	S	0	0
			2521	783	1286	226	220	6		

- Molecule 52 is a protein called 37S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	II	247	Total	C	H	N	O	S	0	0
			3995	1253	2026	366	345	5		

- Molecule 53 is a protein called 37S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	JJ	188	Total	C	H	N	O	S	0	0
			3105	998	1554	273	272	8		

- Molecule 54 is a protein called Mitochondrial ribosomal protein subunit S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	KK	124	Total	C	H	N	O	S	0	0
			2020	625	1025	195	170	5		

- Molecule 55 is a protein called Mitochondrial 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	LL	128	Total	C	H	N	O	S	0	0
			1992	591	1033	198	165	5		

- Molecule 56 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	MM	118	Total	C	H	N	O	S	0	0
			1923	586	986	186	161	4		

- Molecule 57 is a protein called Mitochondrial 40S ribosomal protein MRP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	NN	112	Total	C	H	N	O	S	0	0
			1875	573	961	184	150	7		

- Molecule 58 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	OO	276	Total	C	H	N	O	S	0	0
			4428	1361	2230	431	401	5		

- Molecule 59 is a protein called Ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	PP	98	Total	C	H	N	O	S	0	0
			1612	510	826	141	135			

- Molecule 60 is a protein called Mitochondrial 37S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	QQ	158	Total	C	H	N	O	S	0	0
			2561	789	1314	234	219	5		

- Molecule 61 is a protein called Mito ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	RR	134	Total	C	H	N	O	S	0	0
			2169	679	1089	206	190	5		

- Molecule 62 is a protein called Mitochondrial ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	SS	81	Total	C	H	N	O	S	0	0
			1325	422	677	118	107	1		

- Molecule 63 is a protein called Mito ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	TT	88	Total	C	H	N	O	0	0
			1518	470	772	157	119		

- Molecule 64 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	UU	218	Total	C	H	N	O	S	0	0
			3600	1139	1801	334	319	7		

- Molecule 65 is a protein called mS26.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	VV	261	Total	C	H	N	O	S	0	0
			4192	1300	2112	390	387	3		

- Molecule 66 is a protein called mS27.

Mol	Chain	Residues	Atoms					AltConf	Trace	
66	WW	353	Total	C	H	N	O	S	0	0
			5744	1804	2901	514	515	10		

- Molecule 67 is a protein called Mitochondrial ribosomal protein DAP3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
67	XX	408	Total	C	H	N	O	S	0	0
			6446	2010	3271	562	587	16		

- Molecule 68 is a protein called mS33.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	YY	99	Total	C	H	N	O	S	0	0
			1609	491	823	152	142	1		

- Molecule 69 is a protein called 37S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	ZZ	312	Total	C	H	N	O	S	0	0
			5114	1631	2528	450	495	10		

- Molecule 70 is a protein called 37S ribosomal protein mrp10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	11	88	Total	C	H	N	O	S	0	0
			1358	417	686	128	121	6		

- Molecule 71 is a protein called DUF1713 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	22	33	Total	C	H	N	O	S	0	0
			660	187	359	70	43	1		

- Molecule 72 is a protein called IGR domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	33	193	Total	C	H	N	O	S	0	0
			3161	989	1607	295	268	2		

- Molecule 73 is a protein called Fe superoxide dismutase.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	44	260	Total	C	H	N	O	S	0	0
			4045	1318	1983	355	378	11		
73	55	232	Total	C	H	N	O	S	0	0
			3652	1195	1794	316	337	10		

- Molecule 74 is a protein called mS45.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	66	283	Total	C	H	N	O	S	0	0
			4628	1455	2330	425	414	4		

- Molecule 75 is a protein called mS46.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	77	179	Total	C	H	N	O	S	0	0
			2796	893	1396	227	277	3		

- Molecule 76 is a protein called 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	88	467	Total	C	H	N	O	S	0	0
			7327	2340	3650	634	691	12		

- Molecule 77 is a protein called IF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	00	48	Total	C	H	N	O	0	0
			823	252	417	77	77		
77	99	36	Total	C	H	N	O	0	0
			639	191	333	59	56		

- Molecule 78 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	aa	1435	Total	C	H	N	O	P	0	0
			45981	13712	15373	5486	9975	1435		

- Molecule 79 is a RNA chain called tRNA E-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	bb	61	Total	C	H	N	O	P	0	0
			1957	581	658	233	424	61		

- Molecule 80 is a protein called 60S ribosomal protein L1.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	e	150	Total	C	H	N	O	S	0	0
			2435	762	1234	212	220	7		

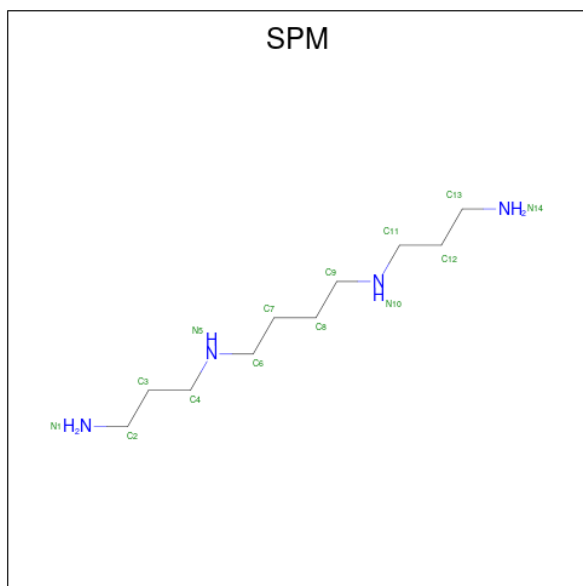
- Molecule 81 is a protein called L51_S25_CI-B8 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	j	195	Total	C	H	N	O	S	0	0
			3139	971	1586	290	284	8		

- Molecule 82 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
82	A	150	Total	Mg	0
			150	150	
82	BB	1	Total	Mg	0
			1	1	
82	XX	1	Total	Mg	0
			1	1	
82	00	1	Total	Mg	0
			1	1	
82	aa	96	Total	Mg	0
			96	96	

- Molecule 83 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).

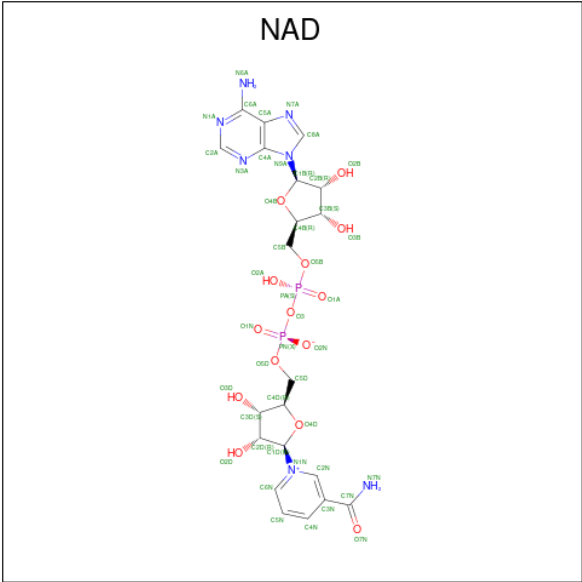


Mol	Chain	Residues	Atoms				AltConf
83	A	1	Total	C	H	N	0
			40	10	26	4	

- Molecule 84 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
84	A	28	Total	K	0
			28	28	
84	K	1	Total	K	0
			1	1	
84	2	1	Total	K	0
			1	1	
84	3	1	Total	K	0
			1	1	
84	77	1	Total	K	0
			1	1	
84	88	1	Total	K	0
			1	1	
84	aa	17	Total	K	0
			17	17	

- Molecule 85 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

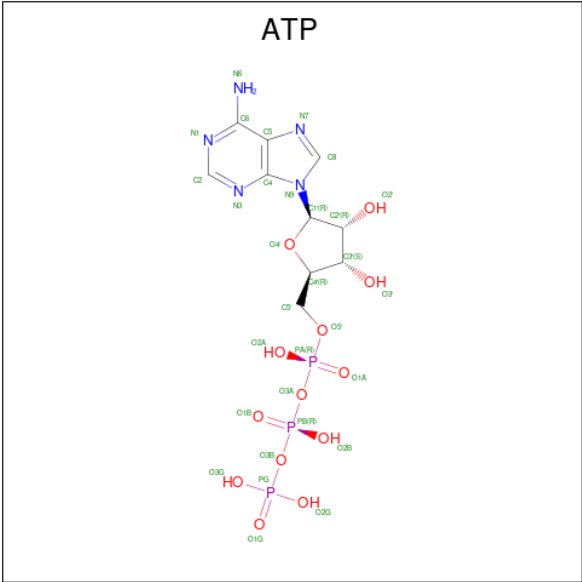


Mol	Chain	Residues	Atoms						AltConf
85	E	1	Total	C	H	N	O	P	0
			69	21	25	7	14	2	

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
86	W	1	Total	Zn	0
			1	1	
86	0	1	Total	Zn	0
			1	1	

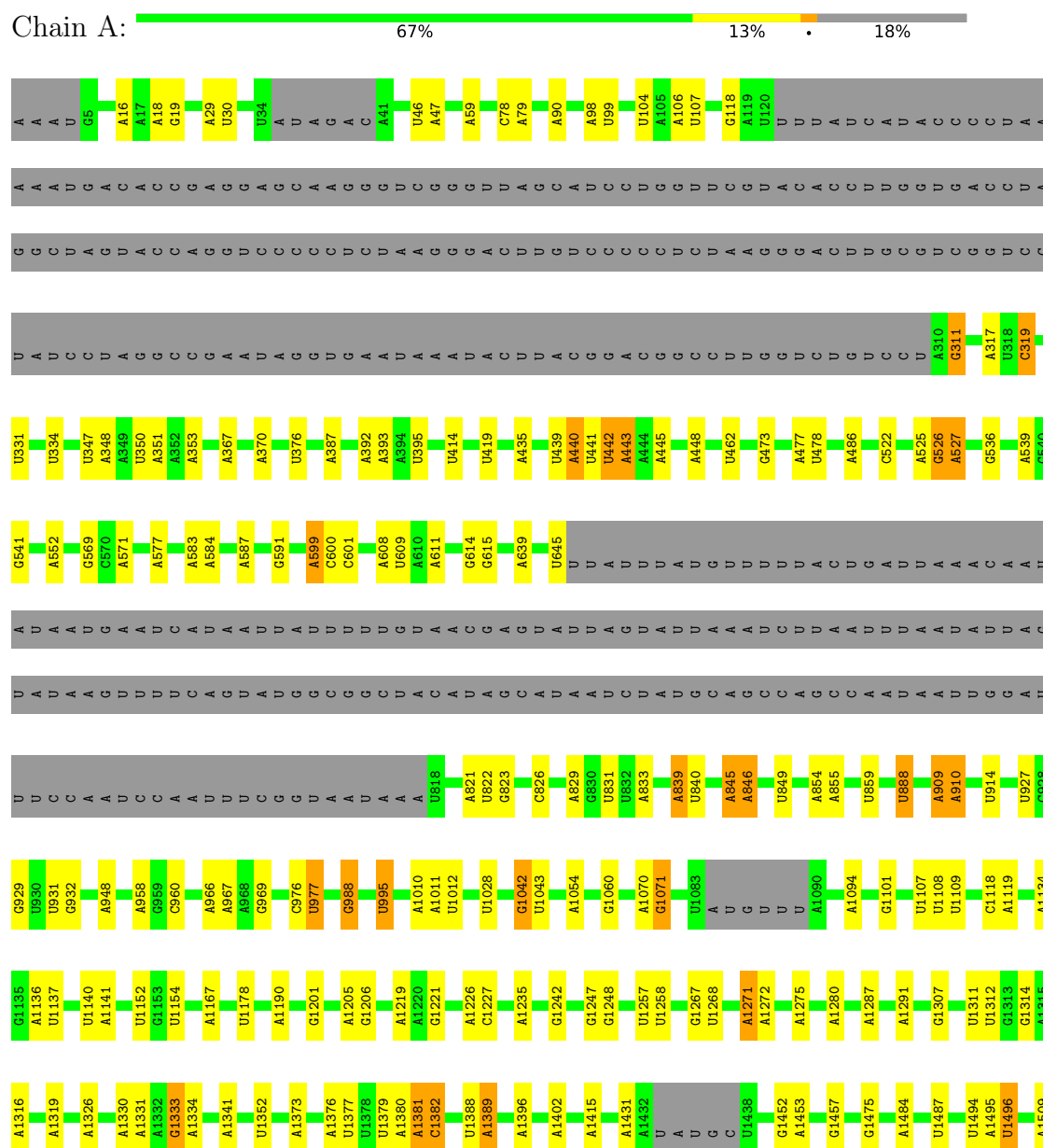
- Molecule 87 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

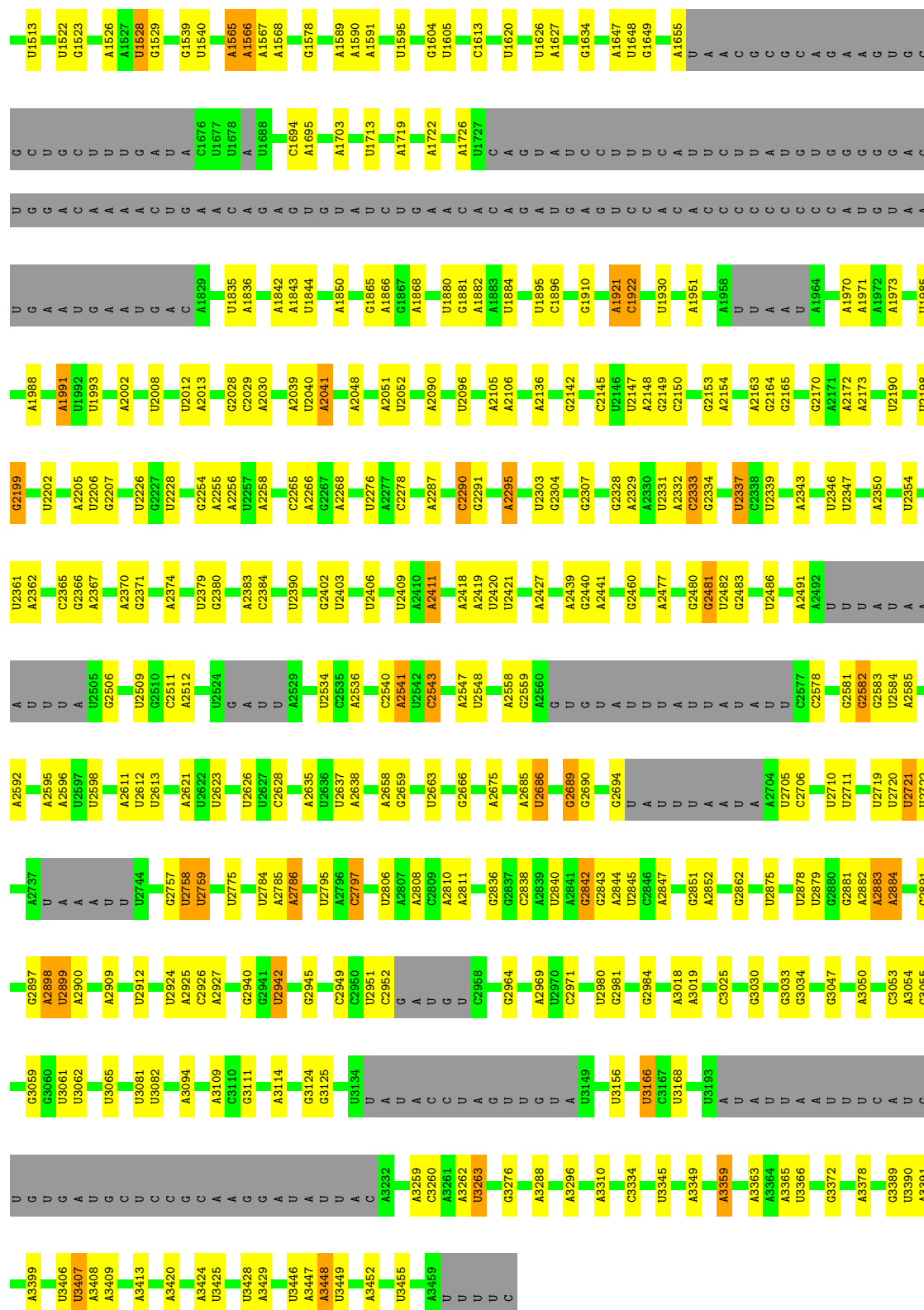


3 Residue-property plots

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.

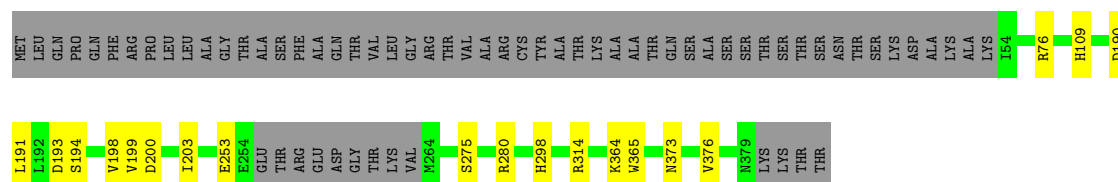
• Molecule 1: 23S rRNA





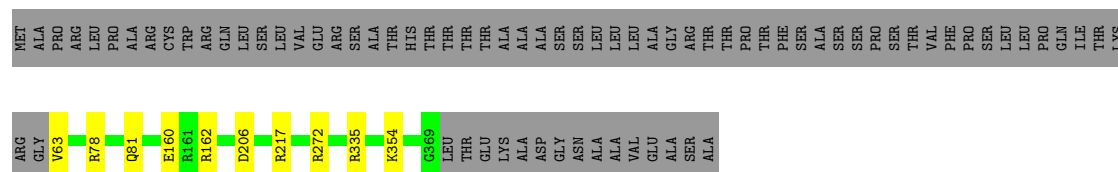
• Molecule 2: 60S ribosomal protein L2

Chain B: 78% 5% 17%



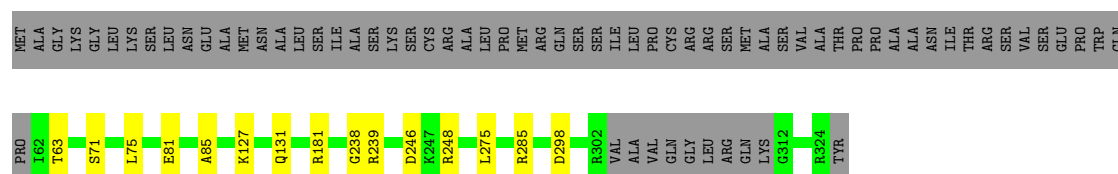
- Molecule 3: 60S ribosomal protein L3

Chain C: 77% 20%



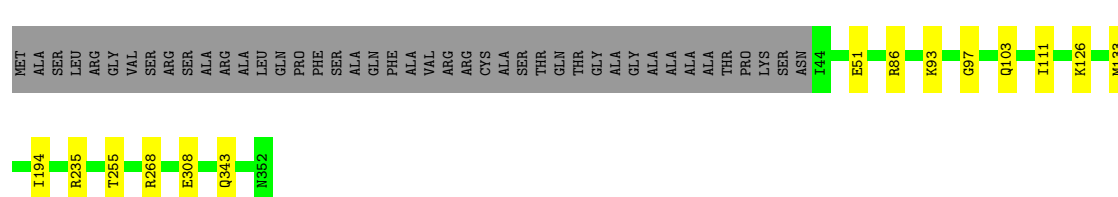
- Molecule 4: 60S ribosomal protein L4, variant

Chain D: 74% 5% 22%



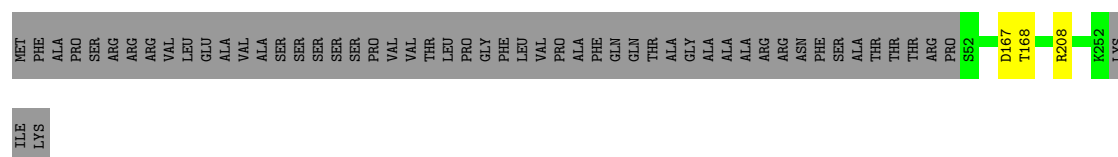
- Molecule 5: 50S ribosomal protein L5

Chain E: 84% 12%



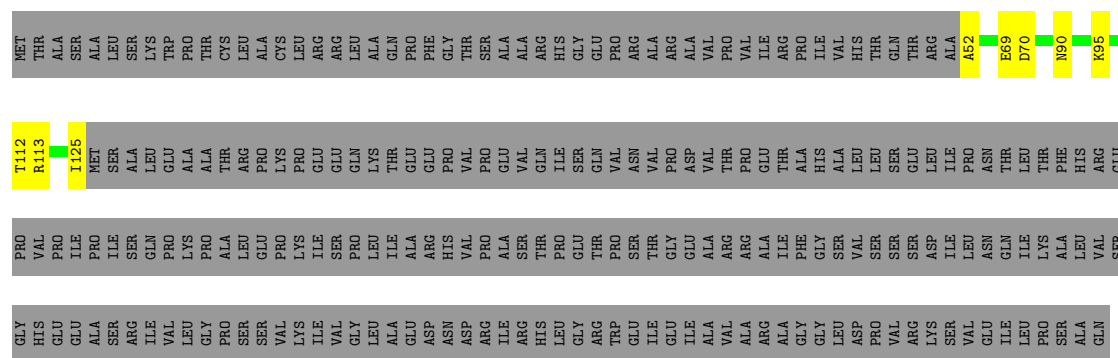
- Molecule 6: 60S ribosomal protein L6

Chain F: 78% 21%



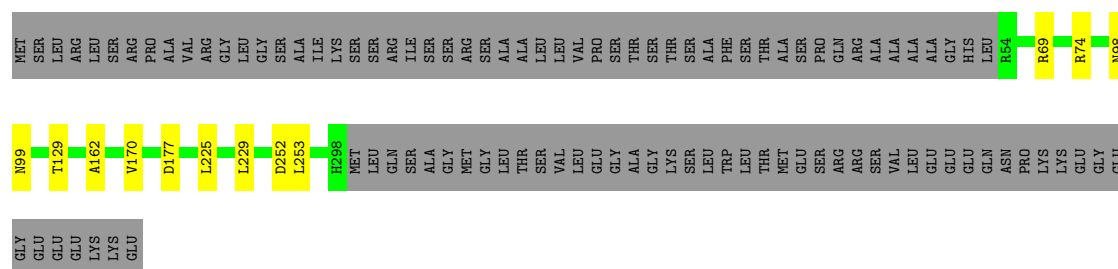
- Molecule 7: RIBOSOMAL_L9 domain-containing protein

Chain G: 22% 75%



• Molecule 8: uL10m

Chain f: 67% 29%



• Molecule 9: 60S ribosomal protein L19

Chain g: 89% 7%



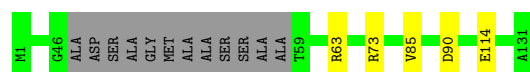
• Molecule 10: Ribosomal protein L13

Chain H: 97% 3%



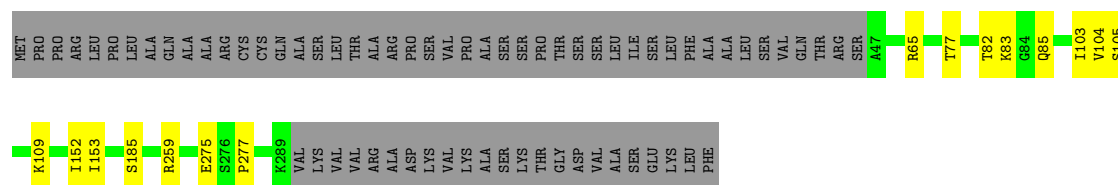
• Molecule 11: 50S ribosomal protein L14

Chain I: 87% 9%

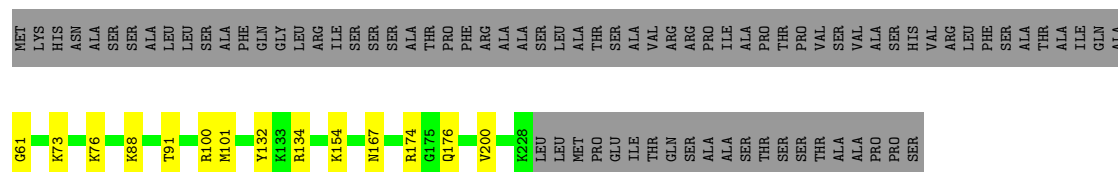


• Molecule 12: 50S ribosomal subunit protein L15

Chain J: 73% 5% 22%



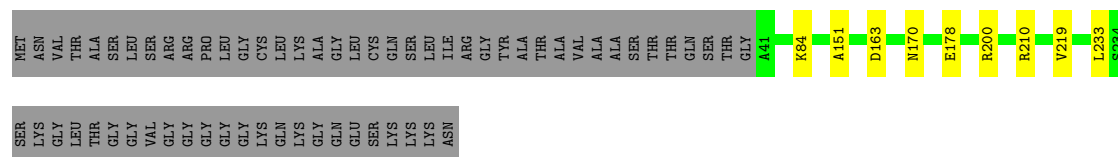
- Molecule 13: 60S ribosomal protein L16



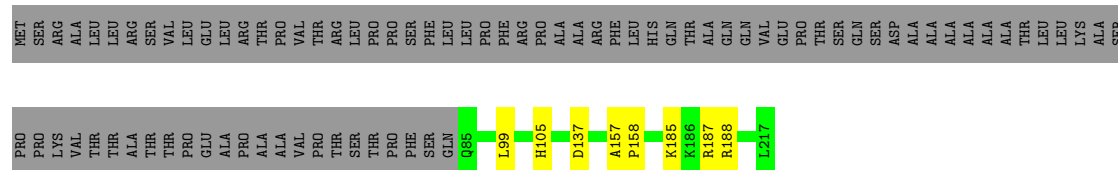
- Molecule 14: 50S ribosomal protein L17



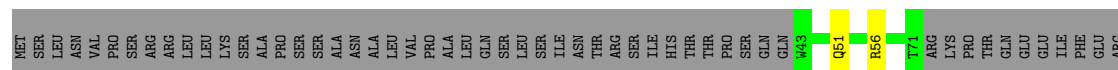
- Molecule 15: Mitochondrial ribosomal protein

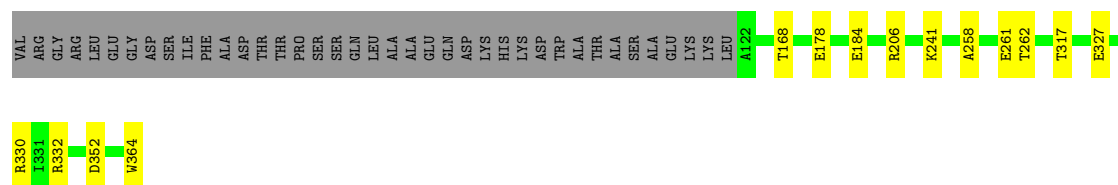


- Molecule 16: Aconitate hydratase



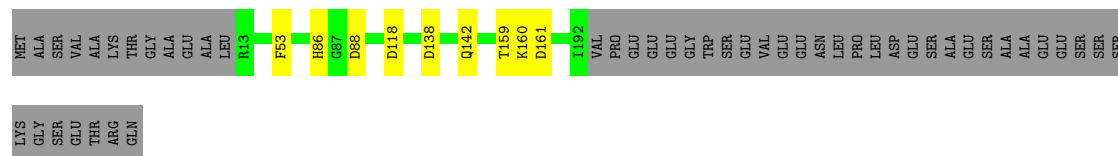
- Molecule 17: Mitochondrial large ribosomal subunit





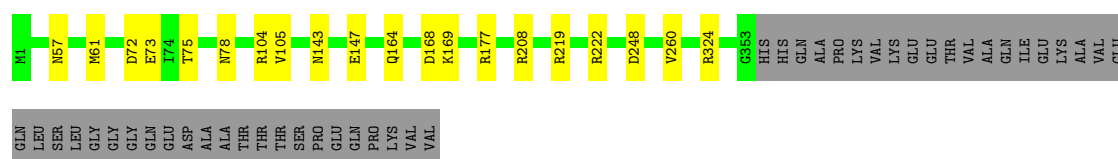
- Molecule 18: Mitochondrial ribosomal protein subunit L23

Chain P: 75% 21%



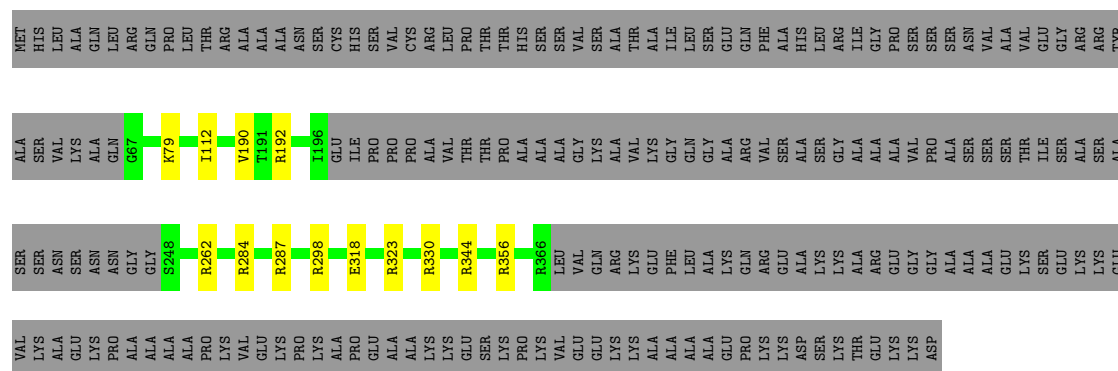
- Molecule 19: KOW domain-containing protein

Chain Q: 84% 5% 11%



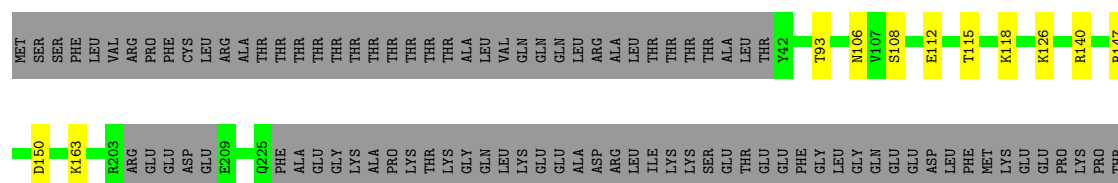
- Molecule 20: bL27m

Chain R: 53% 44%

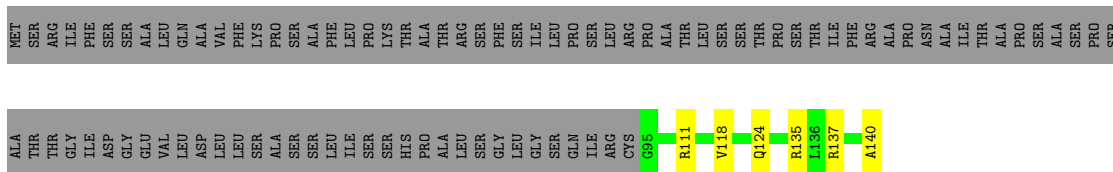


- Molecule 21: 50S ribosomal protein L24

Chain S: 61% 35%

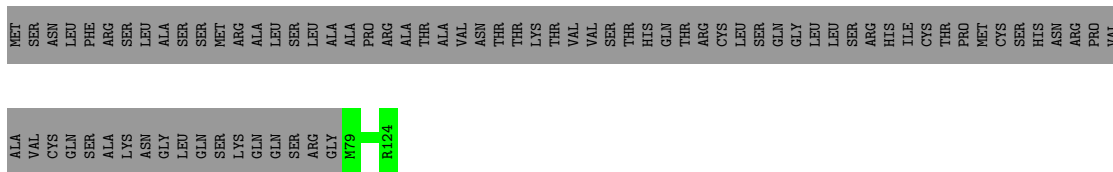


Chain Y:  29% . 67%

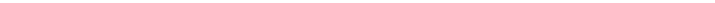


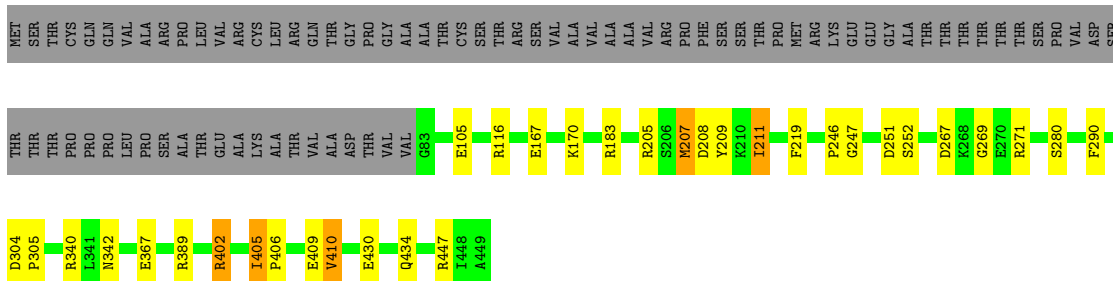
- Molecule 28: Ribosomal protein

Chain 0: 37% 63%

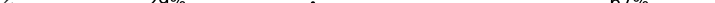


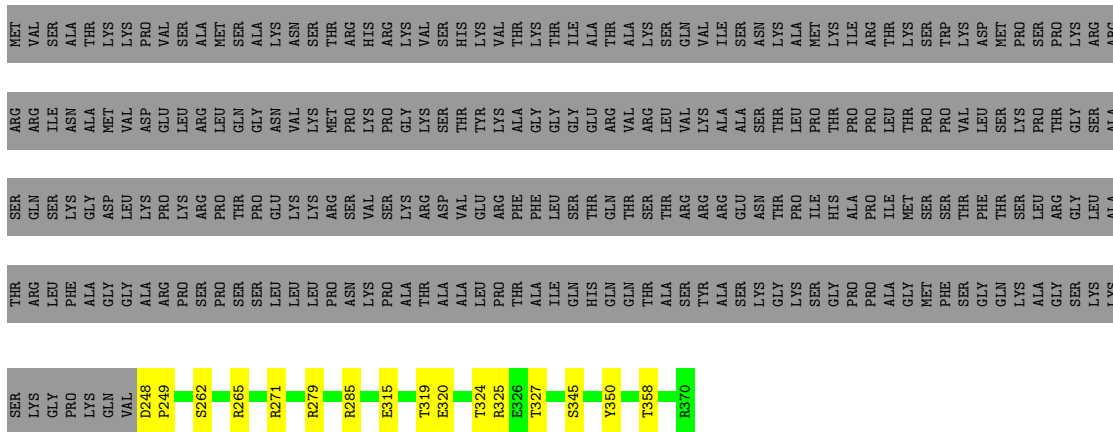
- Molecule 29: Mitochondrial large ribosomal subunit YmL35

Chain 1:  74% 6% 18%



- Molecule 30: mL40

Chain 2:  29% . 67%



- Molecule 31: mL41

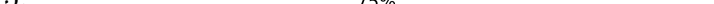
Chain 3: 89% .. 8%

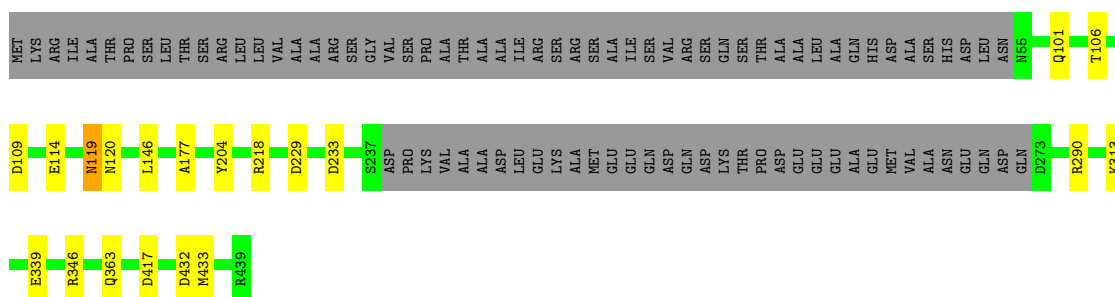
- Molecule 32: Mitochondrial ribosomal protein L43

Chain 4:  93% 7%



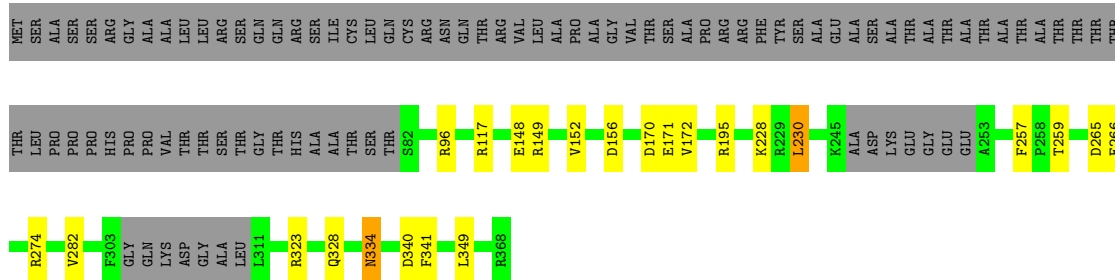
- Molecule 33: 60S ribosomal protein L3

Chain 5:  75% . 20%



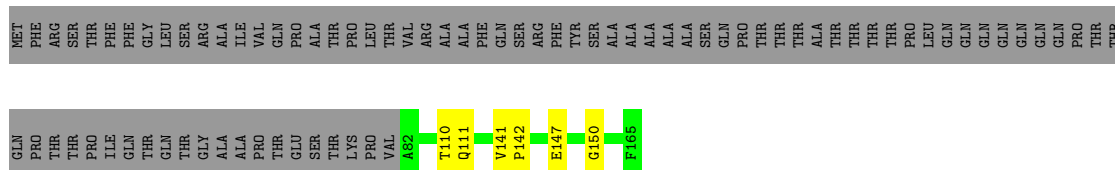
- Molecule 34: 50S ribosomal subunit L30

Chain 6: 68% 6% • 26%



- Molecule 35: mL49

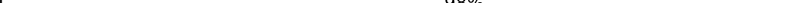
Chain 7:  47% . 49%



- Molecule 36: mL50

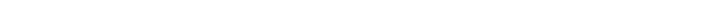
Chain 8: 71% . 25%

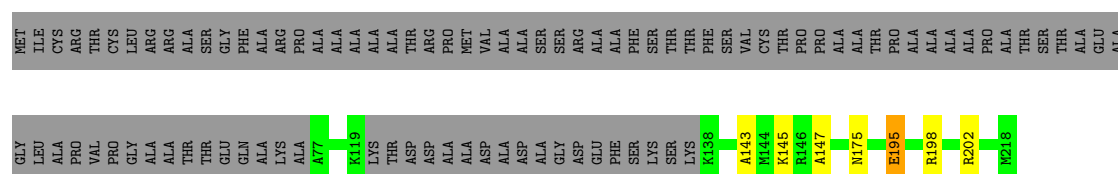
- Molecule 37: Mitochondrial ribosomal protein L44

Chain h:  98%

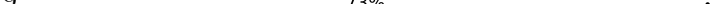


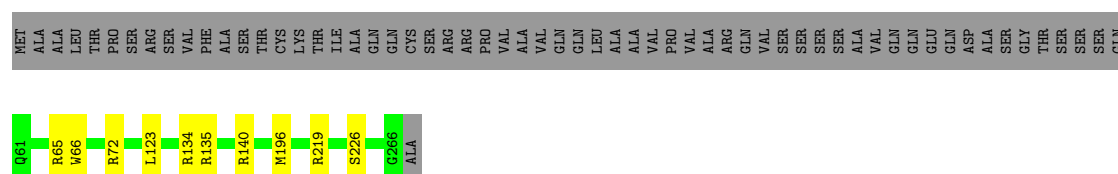
- Molecule 38: mL54

Chain i:  54% 1% 43%



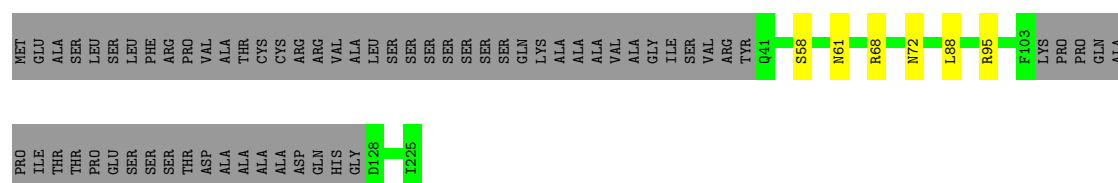
- Molecule 39: RNase III domain-containing protein

Chain 9:  73% . 23%



- Molecule 40: 60S ribosomal protein L20

Chain a:  69% 1% 30%

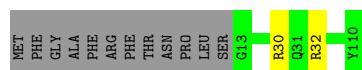


- Molecule 41: Mitochondrial 60S ribosomal protein L25

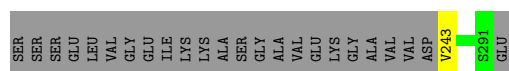
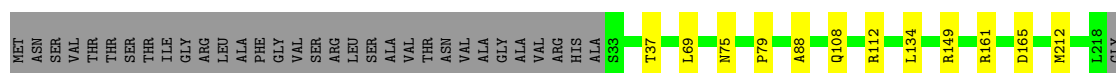
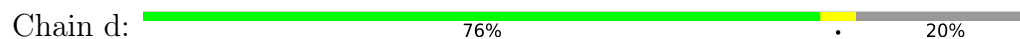
Chain b: 90% 10%



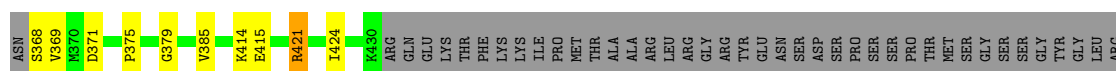
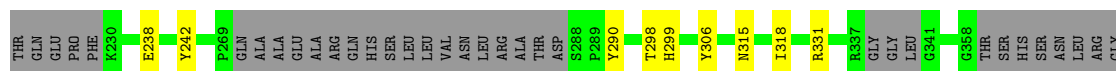
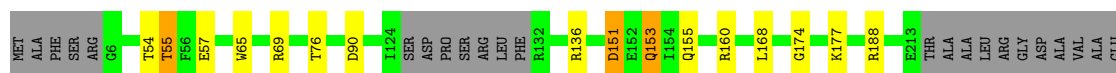
- Molecule 42: 54S ribosomal protein L31, mitochondrial



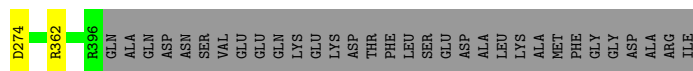
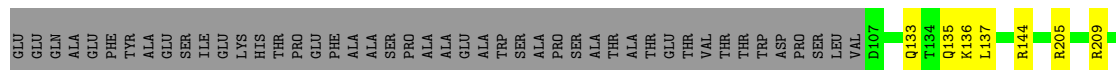
- Molecule 43: mL67



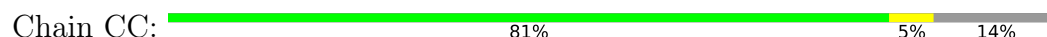
- Molecule 44: bS1m

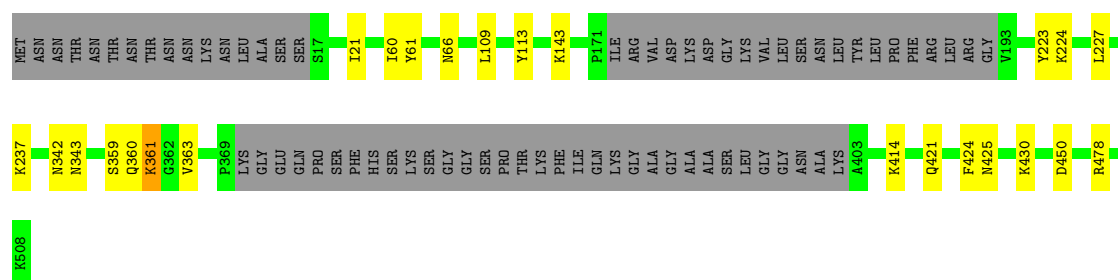


- Molecule 45: Mito ribosomal protein S2



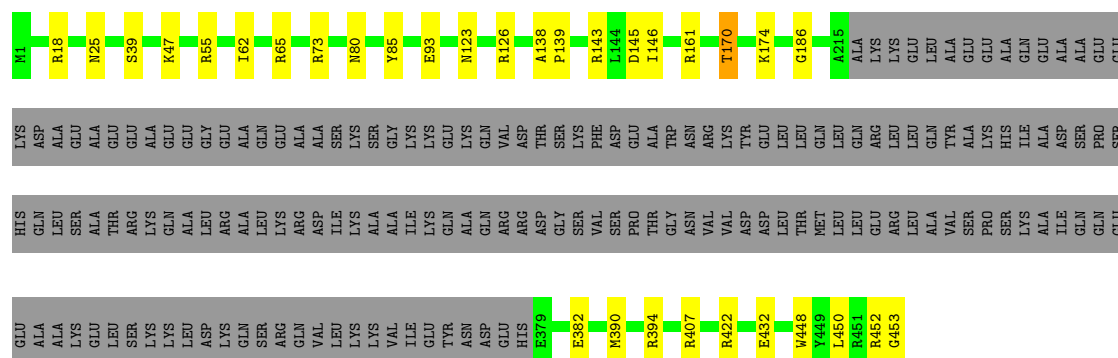
- Molecule 46: Ribosomal protein S5, mitochondrial





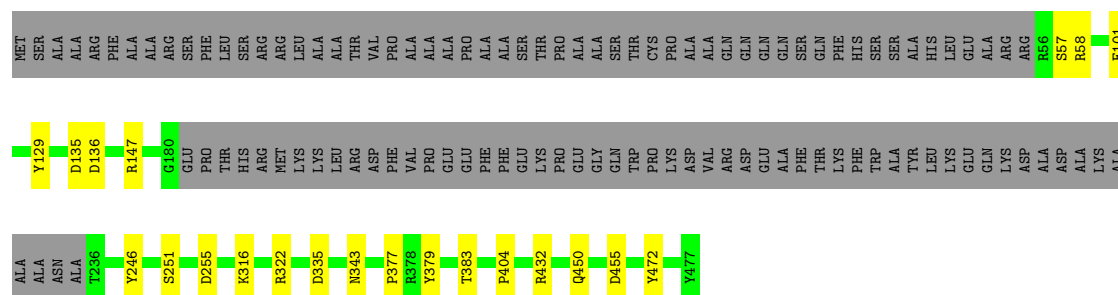
- Molecule 47: Mito ribosomal protein S4

Chain DD: 57% 7% 36%



- Molecule 48: 37S ribosomal protein S5

Chain EE: 72% 5% 23%



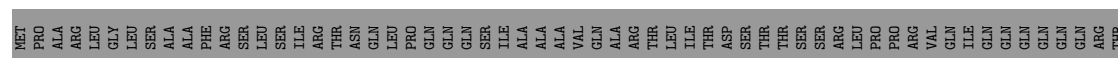
- Molecule 49: Mito ribosomal protein S6

Chain FF: 90% 10%



- Molecule 50: Ribosomal_S7 domain-containing protein

Chain GG: 66% 30% 4%



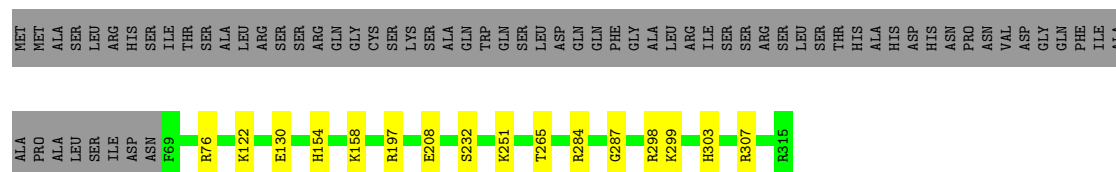
- Molecule 51: 40S ribosomal protein S8

Chain HH: 93% 7%



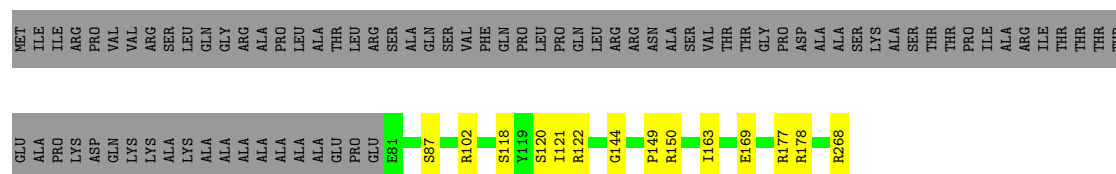
- Molecule 52: 37S ribosomal protein S9, mitochondrial

Chain II: 73% 5% 22%

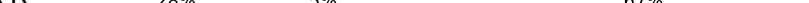


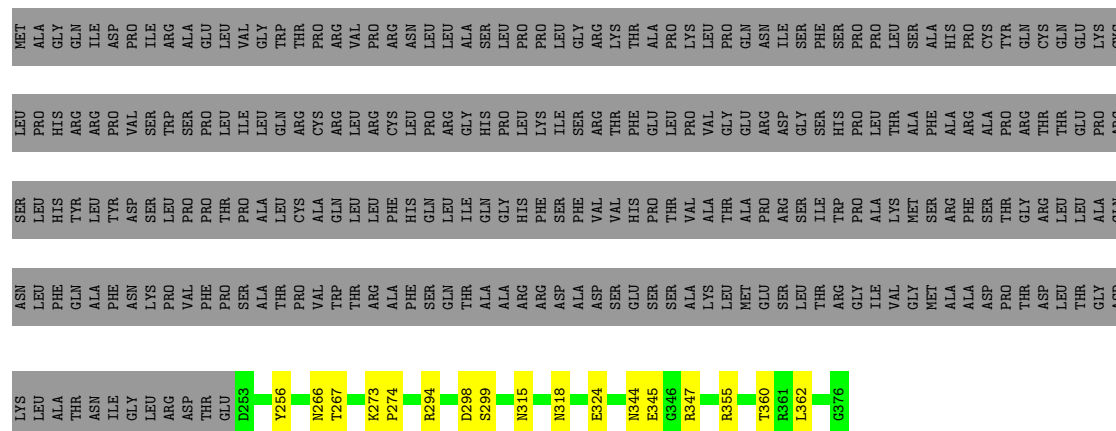
- Molecule 53: 37S ribosomal protein S10, mitochondrial

Chain JJ:  65% 5% 30%



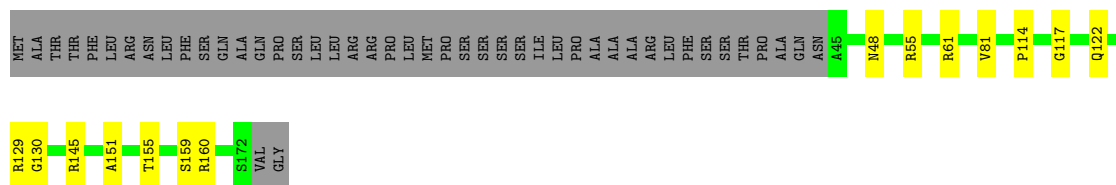
- Molecule 54: Mitochondrial ribosomal protein subunit S18

Chain KK:  28% 5% 67%



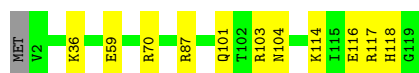
- Molecule 55: Mitochondrial 30S ribosomal protein S12

Chain LL:  66% 8% 26%



- Molecule 56: 40S ribosomal protein S13

Chain MM:  90% 9% .



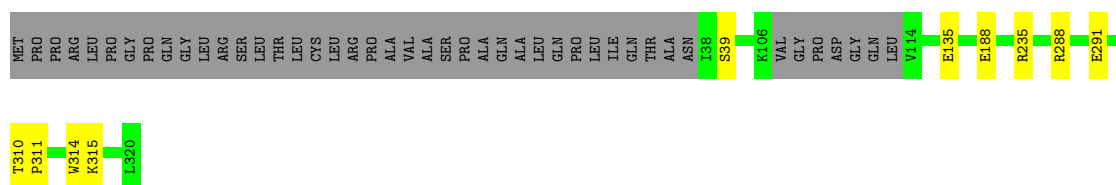
- Molecule 57: Mitochondrial 40S ribosomal protein MRP2

Chain NN:  88% 11% .



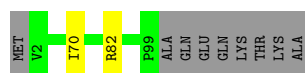
- Molecule 58: Ribosomal protein S15

Chain OO:  83% . 14%



- Molecule 59: Ribosomal protein S16, mitochondrial

Chain PP:  90% . 8%



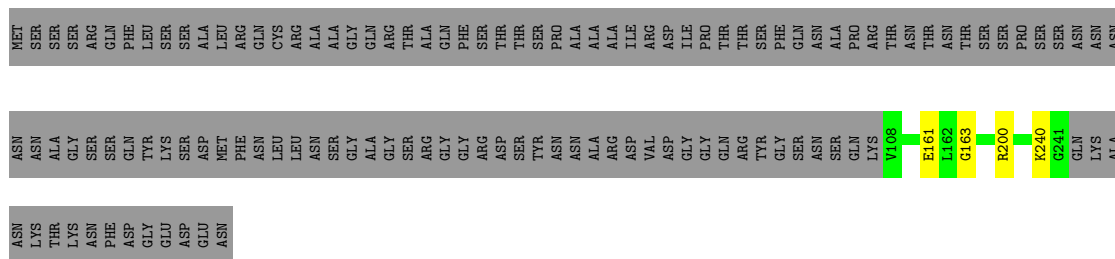
- Molecule 60: Mitochondrial 37S ribosomal protein S17

Chain QQ:  90% 6% .



- Molecule 61: Mito ribosomal protein S18

Chain RR:  51% 48%



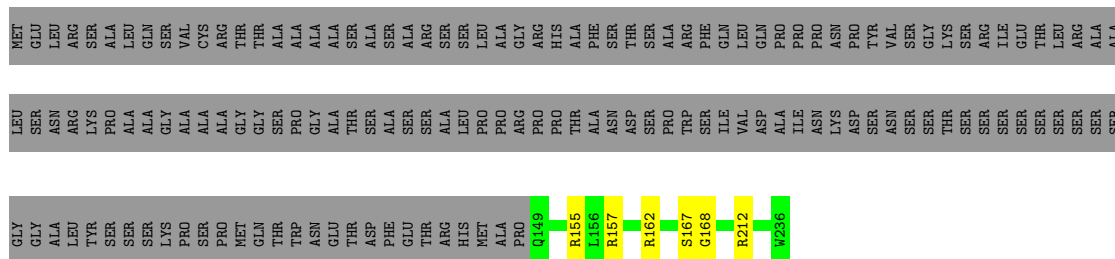
- Molecule 62: Mitochondrial ribosomal protein S19

Chain SS: 82% 7% 11%



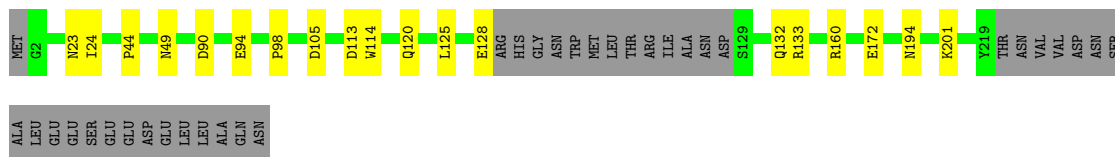
- Molecule 63: Mito ribosomal protein S21

Chain TT: 35% 0% 63%



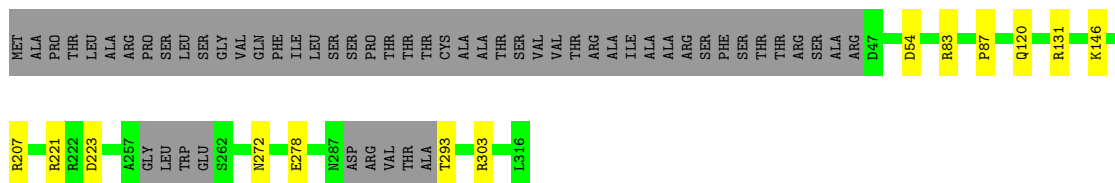
- Molecule 64: 37S ribosomal protein S25, mitochondrial

Chain UU: 79% 8% 14%



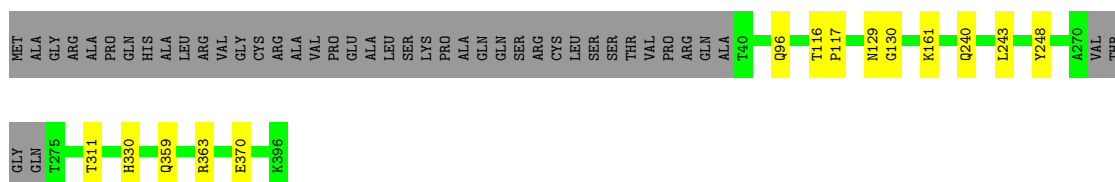
- Molecule 65: mS26

Chain VV: 78% 0% 17%



- Molecule 66: mS27

Chain WW: 86% 0% 11%



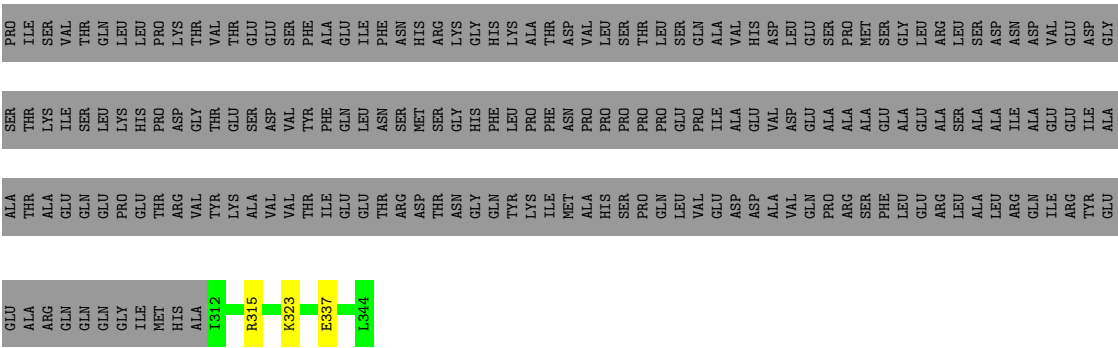
- Molecule 67: Mitochondrial ribosomal protein DAP3

- Molecule 68: mS33

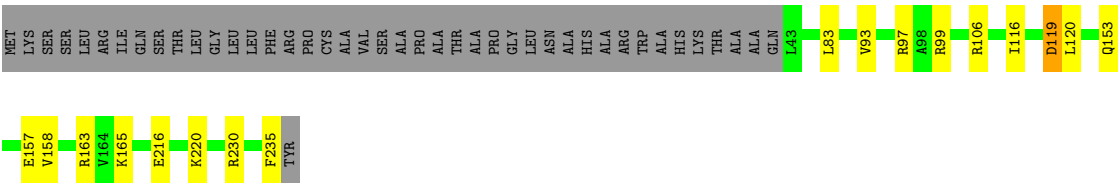
- Molecule 69: 37S ribosomal protein S24, mitochondrial

- Molecule 70: 37S ribosomal protein mrp10, mitochondrial

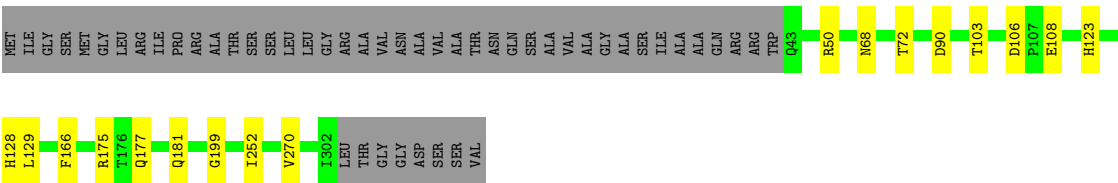
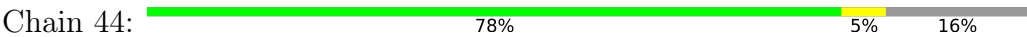
- Molecule 71: DUF1713 domain-containing protein



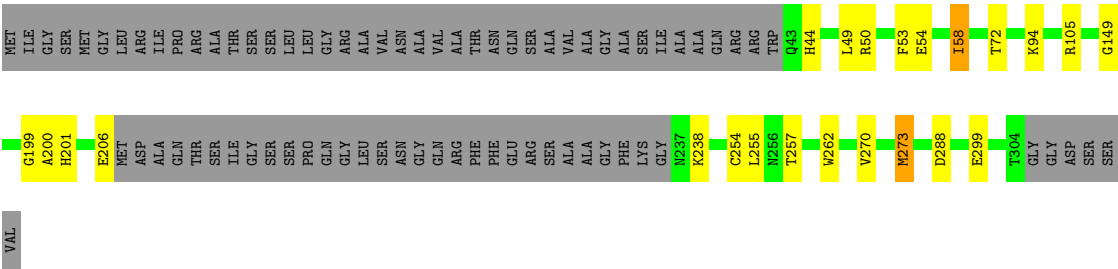
● Molecule 72: IGR domain-containing protein



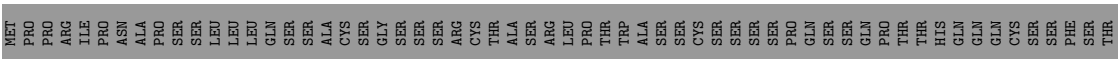
● Molecule 73: Fe superoxide dismutase



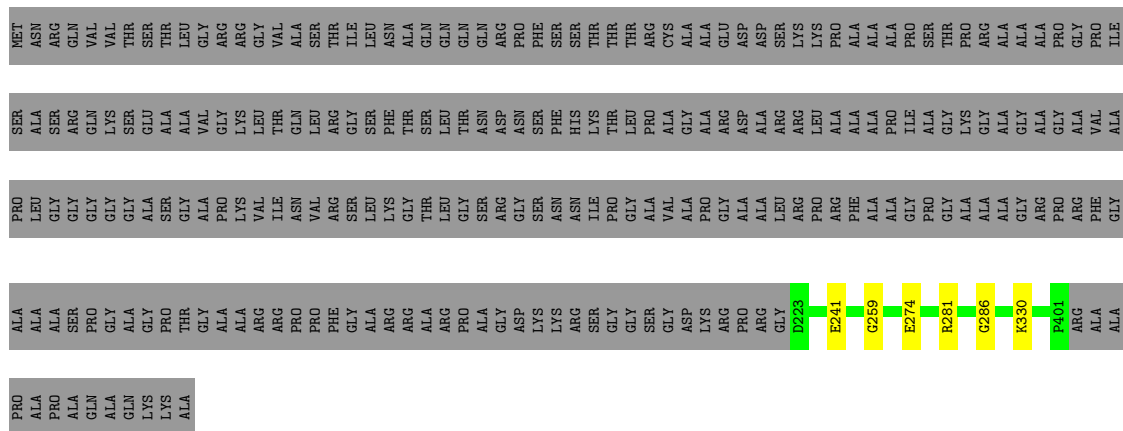
● Molecule 73: Fe superoxide dismutase



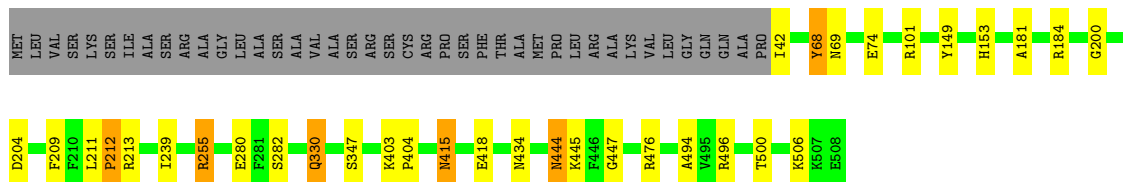
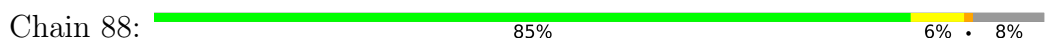
● Molecule 74: mS45



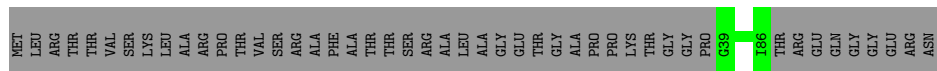
- Molecule 75: mS46



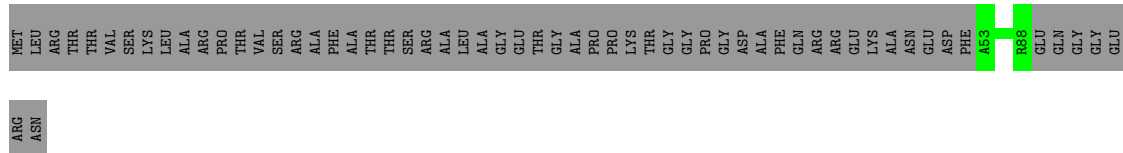
- Molecule 76: 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial



- Molecule 77: IF1



- Molecule 77: IF1



- Molecule 78: 16S rRNA



- Molecule 79: tRNA E-site

Chain bb:

80%

16%

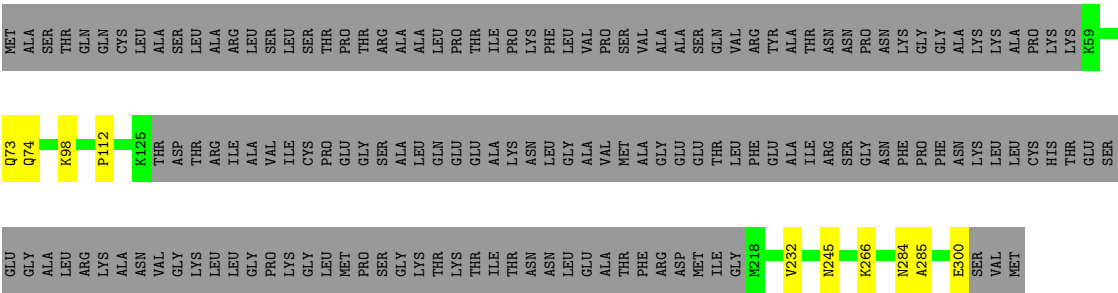


• Molecule 80: 60S ribosomal protein L1

Chain e:

46%

50%



• Molecule 81: L51_S25_CI-B8 domain-containing protein

Chain j:

86%

11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23802	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	37.985	Depositor
Minimum map value	-23.213	Depositor
Average map value	0.006	Depositor
Map value standard deviation	1.342	Depositor
Recommended contour level	0.0295	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ZN, K, NAD, SPM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.11	0/67790	0.19	0/105564
2	B	0.14	0/2531	0.31	0/3410
3	C	0.15	0/2380	0.30	0/3209
4	D	0.12	0/2072	0.26	0/2794
5	E	0.17	0/2518	0.31	0/3427
6	F	0.10	0/1644	0.24	0/2218
7	G	0.12	0/630	0.32	0/842
8	f	0.09	0/1923	0.24	0/2631
9	g	0.10	0/1126	0.27	0/1525
10	H	0.16	0/1460	0.30	0/1975
11	I	0.13	0/918	0.30	0/1225
12	J	0.13	0/1931	0.28	0/2597
13	K	0.13	0/1376	0.29	0/1842
14	L	0.14	0/1569	0.29	0/2106
15	M	0.12	0/1572	0.29	0/2117
16	N	0.14	0/1077	0.29	0/1452
17	O	0.13	0/2248	0.27	0/3015
18	P	0.13	0/1523	0.26	0/2058
19	Q	0.12	0/2916	0.27	0/3927
20	R	0.13	0/2083	0.30	0/2789
21	S	0.13	0/1510	0.30	0/2042
22	T	0.12	0/1538	0.28	0/2086
23	U	0.13	0/1117	0.31	0/1496
24	V	0.18	0/471	0.31	0/638
25	W	0.16	0/467	0.31	0/616
26	X	0.14	0/411	0.30	0/551
27	Y	0.18	0/368	0.36	0/485
28	0	0.15	0/395	0.29	0/523
29	1	0.15	0/3053	0.32	0/4108
30	2	0.19	0/1074	0.35	0/1449
31	3	0.13	0/783	0.27	0/1056
32	4	0.14	0/1077	0.27	0/1453

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	5	0.12	0/2790	0.27	0/3794
34	6	0.17	0/2274	0.32	0/3062
35	7	0.12	0/686	0.28	0/919
36	8	0.10	0/2714	0.27	0/3657
37	h	0.09	0/791	0.24	0/1065
38	i	0.10	0/990	0.28	0/1324
39	9	0.10	0/1678	0.27	0/2267
40	a	0.12	0/1364	0.27	0/1842
41	b	0.11	0/1348	0.26	0/1816
42	c	0.15	0/846	0.30	0/1134
43	d	0.12	0/1930	0.27	0/2597
44	AA	0.12	0/2948	0.28	0/3995
45	BB	0.14	0/2314	0.29	0/3142
46	CC	0.16	0/3712	0.27	0/4978
47	DD	0.15	0/2409	0.28	0/3255
48	EE	0.14	0/2928	0.28	0/3947
49	FF	0.13	0/952	0.29	0/1285
50	GG	0.13	0/1712	0.29	0/2324
51	HH	0.17	0/1259	0.30	0/1707
52	II	0.14	0/2013	0.28	0/2720
53	JJ	0.17	0/1590	0.30	0/2140
54	KK	0.12	0/1015	0.29	0/1357
55	LL	0.15	0/973	0.32	0/1305
56	MM	0.13	0/950	0.32	0/1274
57	NN	0.18	0/929	0.30	0/1243
58	OO	0.14	0/2242	0.30	0/3016
59	PP	0.18	0/806	0.27	0/1096
60	QQ	0.13	0/1268	0.26	0/1701
61	RR	0.13	0/1105	0.28	0/1491
62	SS	0.14	0/667	0.27	0/902
63	TT	0.14	0/761	0.29	0/1015
64	UU	0.13	0/1845	0.27	0/2491
65	VV	0.11	0/2120	0.26	0/2851
66	WW	0.11	0/2897	0.26	0/3911
67	XX	0.15	0/3234	0.28	0/4374
68	YY	0.14	0/797	0.31	0/1070
69	ZZ	0.13	0/2645	0.25	0/3566
70	11	0.12	0/686	0.25	0/929
71	22	0.16	0/301	0.31	0/388
72	33	0.14	0/1589	0.30	0/2140
73	44	0.09	0/2121	0.25	0/2879
73	55	0.09	0/1912	0.26	0/2600
74	66	0.13	0/2348	0.28	0/3163

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	77	0.15	0/1431	0.24	0/1934
76	88	0.12	0/3760	0.28	0/5085
77	00	0.09	0/409	0.24	0/540
77	99	0.08	0/307	0.19	0/405
78	aa	0.11	0/34270	0.18	0/53383
79	bb	0.05	0/1449	0.14	0/2248
80	e	0.09	0/1223	0.25	0/1645
81	j	0.10	0/1583	0.30	0/2130
All	All	0.12	0/230442	0.24	0/332328

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60532	30363	30379	161	0
2	B	2473	2523	2523	13	0
3	C	2336	2421	2420	8	0
4	D	2028	2040	2040	8	0
5	E	2449	2461	2461	8	0
6	F	1608	1645	1645	2	0
7	G	618	627	627	6	0
8	f	1876	1925	1925	8	0
9	g	1103	1154	1154	4	0
10	H	1426	1459	1459	4	0
11	I	913	985	985	4	0
12	J	1888	1939	1939	11	0
13	K	1350	1401	1401	10	0
14	L	1545	1590	1590	7	0
15	M	1536	1628	1628	6	0
16	N	1056	1120	1120	8	0
17	O	2209	2323	2323	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	P	1481	1494	1494	4	0
19	Q	2868	2961	2961	16	0
20	R	2046	2149	2149	12	0
21	S	1472	1507	1507	8	0
22	T	1497	1453	1453	7	0
23	U	1099	1164	1164	6	0
24	V	459	462	462	2	0
25	W	460	489	488	4	0
26	X	403	433	433	3	0
27	Y	365	412	412	4	0
28	0	388	409	409	0	0
29	1	2985	3029	3029	24	0
30	2	1046	1055	1055	11	0
31	3	763	773	773	2	0
32	4	1052	1087	1087	4	0
33	5	2719	2710	2710	15	0
34	6	2226	2248	2248	14	0
35	7	674	709	709	3	0
36	8	2660	2714	2714	9	0
37	h	779	798	798	1	0
38	i	977	1022	1022	6	0
39	9	1643	1698	1698	6	0
40	a	1331	1340	1340	3	0
41	b	1314	1379	1379	10	0
42	c	827	873	873	2	0
43	d	1888	1909	1909	6	0
44	AA	2883	2907	2907	28	0
45	BB	2269	2301	2301	7	0
46	CC	3641	3897	3897	14	0
47	DD	2343	2373	2373	21	0
48	EE	2880	2918	2918	19	0
49	FF	935	966	966	7	0
50	GG	1672	1737	1737	9	0
51	HH	1235	1286	1286	9	0
52	II	1969	2026	2026	12	0
53	JJ	1551	1554	1554	10	0
54	KK	995	1025	1025	12	0
55	LL	959	1033	1032	10	0
56	MM	937	986	986	8	0
57	NN	914	961	961	10	0
58	OO	2198	2230	2230	8	0
59	PP	786	826	826	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	QQ	1247	1314	1314	6	0
61	RR	1080	1089	1089	5	0
62	SS	648	677	677	5	0
63	TT	746	772	772	5	0
64	UU	1799	1801	1801	15	0
65	VV	2080	2112	2112	12	0
66	WW	2843	2901	2900	8	0
67	XX	3175	3271	3271	11	0
68	YY	786	823	823	4	0
69	ZZ	2586	2528	2528	6	0
70	11	672	686	686	3	0
71	22	301	359	359	3	0
72	33	1554	1607	1607	10	0
73	44	2062	1983	1982	13	0
73	55	1858	1794	1793	14	0
74	66	2298	2330	2330	18	0
75	77	1400	1396	1396	4	0
76	88	3677	3650	3650	24	0
77	00	406	417	417	0	0
77	99	306	333	333	0	0
78	aa	30608	15373	15376	101	0
79	bb	1299	658	661	2	0
80	e	1201	1234	1234	6	0
81	j	1553	1586	1586	13	0
82	00	1	0	0	0	0
82	A	150	0	0	0	0
82	BB	1	0	0	0	0
82	XX	1	0	0	0	0
82	aa	96	0	0	0	0
83	A	14	26	26	0	0
84	2	1	0	0	0	0
84	3	1	0	0	0	0
84	77	1	0	0	0	0
84	88	1	0	0	0	0
84	A	28	0	0	0	0
84	K	1	0	0	0	0
84	aa	17	0	0	0	0
85	E	44	25	26	3	0
86	0	1	0	0	0	0
86	W	1	0	0	0	0
87	XX	31	12	12	2	0
All	All	217110	173664	173681	715	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 715 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:EE:343:ASN:ND2	64:UU:24:ILE:O	2.06	0.89
30:2:350:TYR:OH	34:6:323:ARG:NH2	2.06	0.89
74:66:336:ARG:NH1	78:aa:549:C:O2	2.06	0.87
1:A:2757:G:OP2	30:2:285:ARG:NH1	2.09	0.85
1:A:966:A:OP1	2:B:314:ARG:NH1	2.14	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	313/383 (82%)	307 (98%)	6 (2%)	0	100	100
3	C	305/384 (79%)	301 (99%)	4 (1%)	0	100	100
4	D	250/325 (77%)	247 (99%)	3 (1%)	0	100	100
5	E	307/352 (87%)	304 (99%)	3 (1%)	0	100	100
6	F	199/255 (78%)	198 (100%)	1 (0%)	0	100	100
7	G	72/300 (24%)	68 (94%)	4 (6%)	0	100	100
8	f	243/347 (70%)	240 (99%)	3 (1%)	0	100	100
9	g	145/158 (92%)	142 (98%)	3 (2%)	0	100	100
10	H	181/183 (99%)	176 (97%)	5 (3%)	0	100	100
11	I	115/131 (88%)	114 (99%)	1 (1%)	0	100	100
12	J	241/312 (77%)	236 (98%)	4 (2%)	1 (0%)	30	61
13	K	166/249 (67%)	166 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	L	190/193 (98%)	186 (98%)	4 (2%)	0	100	100
15	M	192/258 (74%)	187 (97%)	5 (3%)	0	100	100
16	N	131/217 (60%)	124 (95%)	7 (5%)	0	100	100
17	O	268/364 (74%)	266 (99%)	2 (1%)	0	100	100
18	P	178/228 (78%)	178 (100%)	0	0	100	100
19	Q	351/396 (89%)	350 (100%)	1 (0%)	0	100	100
20	R	245/447 (55%)	241 (98%)	4 (2%)	0	100	100
21	S	175/274 (64%)	173 (99%)	2 (1%)	0	100	100
22	T	178/263 (68%)	177 (99%)	1 (1%)	0	100	100
23	U	134/161 (83%)	133 (99%)	1 (1%)	0	100	100
24	V	54/219 (25%)	54 (100%)	0	0	100	100
25	W	57/129 (44%)	54 (95%)	3 (5%)	0	100	100
26	X	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
27	Y	44/140 (31%)	44 (100%)	0	0	100	100
28	0	44/124 (36%)	44 (100%)	0	0	100	100
29	1	365/449 (81%)	358 (98%)	6 (2%)	1 (0%)	36	67
30	2	121/370 (33%)	120 (99%)	1 (1%)	0	100	100
31	3	93/103 (90%)	90 (97%)	3 (3%)	0	100	100
32	4	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
33	5	346/439 (79%)	344 (99%)	2 (1%)	0	100	100
34	6	267/368 (73%)	267 (100%)	0	0	100	100
35	7	82/165 (50%)	81 (99%)	1 (1%)	0	100	100
36	8	329/443 (74%)	328 (100%)	1 (0%)	0	100	100
37	h	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
38	i	120/218 (55%)	114 (95%)	6 (5%)	0	100	100
39	9	204/267 (76%)	199 (98%)	5 (2%)	0	100	100
40	a	157/225 (70%)	156 (99%)	1 (1%)	0	100	100
41	b	159/162 (98%)	158 (99%)	1 (1%)	0	100	100
42	c	96/110 (87%)	95 (99%)	1 (1%)	0	100	100
43	d	231/292 (79%)	229 (99%)	2 (1%)	0	100	100
44	AA	360/470 (77%)	351 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BB	288/428 (67%)	279 (97%)	9 (3%)	0	100	100
46	CC	432/508 (85%)	426 (99%)	6 (1%)	0	100	100
47	DD	286/453 (63%)	280 (98%)	6 (2%)	0	100	100
48	EE	363/477 (76%)	352 (97%)	11 (3%)	0	100	100
49	FF	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
50	GG	215/309 (70%)	213 (99%)	2 (1%)	0	100	100
51	HH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
52	II	245/315 (78%)	239 (98%)	6 (2%)	0	100	100
53	JJ	186/268 (69%)	180 (97%)	6 (3%)	0	100	100
54	KK	122/376 (32%)	118 (97%)	4 (3%)	0	100	100
55	LL	126/174 (72%)	118 (94%)	8 (6%)	0	100	100
56	MM	116/119 (98%)	111 (96%)	5 (4%)	0	100	100
57	NN	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
58	OO	272/320 (85%)	268 (98%)	4 (2%)	0	100	100
59	PP	96/107 (90%)	94 (98%)	2 (2%)	0	100	100
60	QQ	156/165 (94%)	154 (99%)	2 (1%)	0	100	100
61	RR	132/256 (52%)	128 (97%)	4 (3%)	0	100	100
62	SS	79/91 (87%)	77 (98%)	2 (2%)	0	100	100
63	TT	86/236 (36%)	86 (100%)	0	0	100	100
64	UU	216/253 (85%)	212 (98%)	4 (2%)	0	100	100
65	VV	255/316 (81%)	249 (98%)	6 (2%)	0	100	100
66	WW	349/396 (88%)	346 (99%)	3 (1%)	0	100	100
67	XX	404/469 (86%)	396 (98%)	8 (2%)	0	100	100
68	YY	97/108 (90%)	97 (100%)	0	0	100	100
69	ZZ	310/382 (81%)	303 (98%)	7 (2%)	0	100	100
70	11	86/90 (96%)	84 (98%)	2 (2%)	0	100	100
71	22	31/344 (9%)	31 (100%)	0	0	100	100
72	33	191/236 (81%)	182 (95%)	9 (5%)	0	100	100
73	44	258/310 (83%)	254 (98%)	4 (2%)	0	100	100
73	55	228/310 (74%)	223 (98%)	4 (2%)	1 (0%)	30	61
74	66	281/348 (81%)	279 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	77	177/414 (43%)	176 (99%)	1 (1%)	0	100	100
76	88	465/508 (92%)	447 (96%)	18 (4%)	0	100	100
77	00	46/95 (48%)	45 (98%)	1 (2%)	0	100	100
77	99	34/95 (36%)	34 (100%)	0	0	100	100
80	e	146/303 (48%)	141 (97%)	5 (3%)	0	100	100
81	j	193/201 (96%)	188 (97%)	5 (3%)	0	100	100
All	All	15335/21339 (72%)	15058 (98%)	274 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
73	55	200	ALA
12	J	83	LYS
29	1	410	VAL

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	
2	B	259/312 (83%)	257 (99%)	2 (1%)	73	81
3	C	242/303 (80%)	241 (100%)	1 (0%)	84	86
4	D	216/274 (79%)	216 (100%)	0	100	100
5	E	267/296 (90%)	263 (98%)	4 (2%)	57	75
6	F	173/216 (80%)	173 (100%)	0	100	100
7	G	64/254 (25%)	64 (100%)	0	100	100
8	f	206/287 (72%)	206 (100%)	0	100	100
9	g	120/124 (97%)	119 (99%)	1 (1%)	73	81
10	H	149/149 (100%)	148 (99%)	1 (1%)	76	82
11	I	100/105 (95%)	100 (100%)	0	100	100
12	J	198/255 (78%)	196 (99%)	2 (1%)	68	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	K	142/205 (69%)	142 (100%)	0	100	100
14	L	164/165 (99%)	164 (100%)	0	100	100
15	M	164/209 (78%)	163 (99%)	1 (1%)	78	83
16	N	119/188 (63%)	119 (100%)	0	100	100
17	O	235/315 (75%)	233 (99%)	2 (1%)	70	80
18	P	158/196 (81%)	155 (98%)	3 (2%)	50	73
19	Q	312/347 (90%)	312 (100%)	0	100	100
20	R	212/359 (59%)	210 (99%)	2 (1%)	70	80
21	S	159/242 (66%)	159 (100%)	0	100	100
22	T	161/224 (72%)	161 (100%)	0	100	100
23	U	118/138 (86%)	116 (98%)	2 (2%)	53	74
24	V	52/170 (31%)	52 (100%)	0	100	100
25	W	50/102 (49%)	50 (100%)	0	100	100
26	X	46/54 (85%)	46 (100%)	0	100	100
27	Y	38/116 (33%)	38 (100%)	0	100	100
28	0	41/108 (38%)	41 (100%)	0	100	100
29	1	316/384 (82%)	310 (98%)	6 (2%)	50	73
30	2	109/317 (34%)	107 (98%)	2 (2%)	51	73
31	3	83/91 (91%)	82 (99%)	1 (1%)	63	78
32	4	113/114 (99%)	110 (97%)	3 (3%)	39	67
33	5	279/351 (80%)	278 (100%)	1 (0%)	84	86
34	6	238/310 (77%)	234 (98%)	4 (2%)	53	74
35	7	69/136 (51%)	69 (100%)	0	100	100
36	8	285/378 (75%)	284 (100%)	1 (0%)	84	86
37	h	88/88 (100%)	87 (99%)	1 (1%)	65	78
38	i	101/162 (62%)	100 (99%)	1 (1%)	68	79
39	9	176/225 (78%)	174 (99%)	2 (1%)	65	78
40	a	146/196 (74%)	146 (100%)	0	100	100
41	b	141/141 (100%)	141 (100%)	0	100	100
42	c	86/96 (90%)	86 (100%)	0	100	100
43	d	201/243 (83%)	198 (98%)	3 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	AA	314/393 (80%)	307 (98%)	7 (2%)	45	71
45	BB	237/347 (68%)	236 (100%)	1 (0%)	84	86
46	CC	405/461 (88%)	399 (98%)	6 (2%)	57	75
47	DD	242/377 (64%)	239 (99%)	3 (1%)	63	78
48	EE	308/392 (79%)	308 (100%)	0	100	100
49	FF	99/99 (100%)	98 (99%)	1 (1%)	68	79
50	GG	181/260 (70%)	181 (100%)	0	100	100
51	HH	134/135 (99%)	133 (99%)	1 (1%)	76	82
52	II	206/263 (78%)	206 (100%)	0	100	100
53	JJ	166/227 (73%)	165 (99%)	1 (1%)	78	83
54	KK	108/324 (33%)	108 (100%)	0	100	100
55	LL	103/142 (72%)	102 (99%)	1 (1%)	68	79
56	MM	98/99 (99%)	98 (100%)	0	100	100
57	NN	96/97 (99%)	96 (100%)	0	100	100
58	OO	230/265 (87%)	230 (100%)	0	100	100
59	PP	85/92 (92%)	85 (100%)	0	100	100
60	QQ	132/138 (96%)	132 (100%)	0	100	100
61	RR	118/218 (54%)	118 (100%)	0	100	100
62	SS	70/80 (88%)	70 (100%)	0	100	100
63	TT	75/191 (39%)	75 (100%)	0	100	100
64	UU	187/218 (86%)	187 (100%)	0	100	100
65	VV	224/268 (84%)	224 (100%)	0	100	100
66	WW	300/333 (90%)	300 (100%)	0	100	100
67	XX	345/391 (88%)	340 (99%)	5 (1%)	59	76
68	YY	83/89 (93%)	83 (100%)	0	100	100
69	ZZ	278/328 (85%)	276 (99%)	2 (1%)	76	82
70	11	73/75 (97%)	73 (100%)	0	100	100
71	22	33/293 (11%)	33 (100%)	0	100	100
72	33	163/195 (84%)	161 (99%)	2 (1%)	63	78
73	44	215/250 (86%)	214 (100%)	1 (0%)	81	85
73	55	195/250 (78%)	192 (98%)	3 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	66	245/303 (81%)	243 (99%)	2 (1%)	73	81
75	77	153/304 (50%)	153 (100%)	0	100	100
76	88	388/419 (93%)	382 (98%)	6 (2%)	57	75
77	00	43/78 (55%)	43 (100%)	0	100	100
77	99	34/78 (44%)	34 (100%)	0	100	100
80	e	134/256 (52%)	134 (100%)	0	100	100
81	j	168/171 (98%)	167 (99%)	1 (1%)	78	83
All	All	13264/17844 (74%)	13175 (99%)	89 (1%)	73	82

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	CC	360	GLN
67	XX	463	SER
46	CC	363	VAL
53	JJ	121	ILE
72	33	119	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
54	KK	296	HIS
67	XX	114	ASN
56	MM	10	ASN
64	UU	32	ASN
69	ZZ	157	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2820/3464 (81%)	370 (13%)	11 (0%)
78	aa	1430/1864 (76%)	201 (14%)	0
79	bb	57/61 (93%)	11 (19%)	0
All	All	4307/5389 (79%)	582 (13%)	11 (0%)

5 of 582 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	18	A
1	A	19	G
1	A	29	A
1	A	46	U
1	A	47	A

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2720	U
1	A	2758	U
1	A	3054	A
1	A	2883	A
1	A	1205	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 304 ligands modelled in this entry, 301 are monoatomic - leaving 3 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	$\# Z > 2$
85	NAD	E	4301	84	46,48,48	0.90	1 (2%)	64,73,73	1.39	8 (12%)
83	SPM	A	3651	-	13,13,13	0.32	0	12,12,12	0.76	0
87	ATP	XX	501	82	32,33,33	2.46	6 (18%)	48,52,52	1.83	8 (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
85	NAD	E	4301	84	-	7/30/62/62	0/5/5/5
83	SPM	A	3651	-	-	2/11/11/11	-
87	ATP	XX	501	82	-	3/22/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	XX	501	ATP	C2'-C1'	-8.19	1.27	1.53
87	XX	501	ATP	PB-O3A	5.72	1.65	1.59
87	XX	501	ATP	PA-O3A	5.64	1.65	1.59
87	XX	501	ATP	PB-O3B	5.23	1.65	1.59
85	E	4301	NAD	C2N-N1N	-2.68	1.32	1.35

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	XX	501	ATP	C4-N9-C8	5.99	112.03	105.74
85	E	4301	NAD	C5A-C4A-N3A	-5.34	119.36	126.72
87	XX	501	ATP	N9-C8-N7	-5.01	106.82	113.94
87	XX	501	ATP	N3-C4-N9	4.52	134.85	127.17
87	XX	501	ATP	C5-C4-N3	-4.50	120.52	126.72

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	E	4301	NAD	C5D-O5D-PN-O3
87	XX	501	ATP	PB-O3B-PG-O2G
87	XX	501	ATP	PB-O3B-PG-O3G
83	A	3651	SPM	C12-C11-N10-C9
85	E	4301	NAD	C3D-C4D-C5D-O5D

There are no ring outliers.

2 monomers are involved in 5 short contacts:

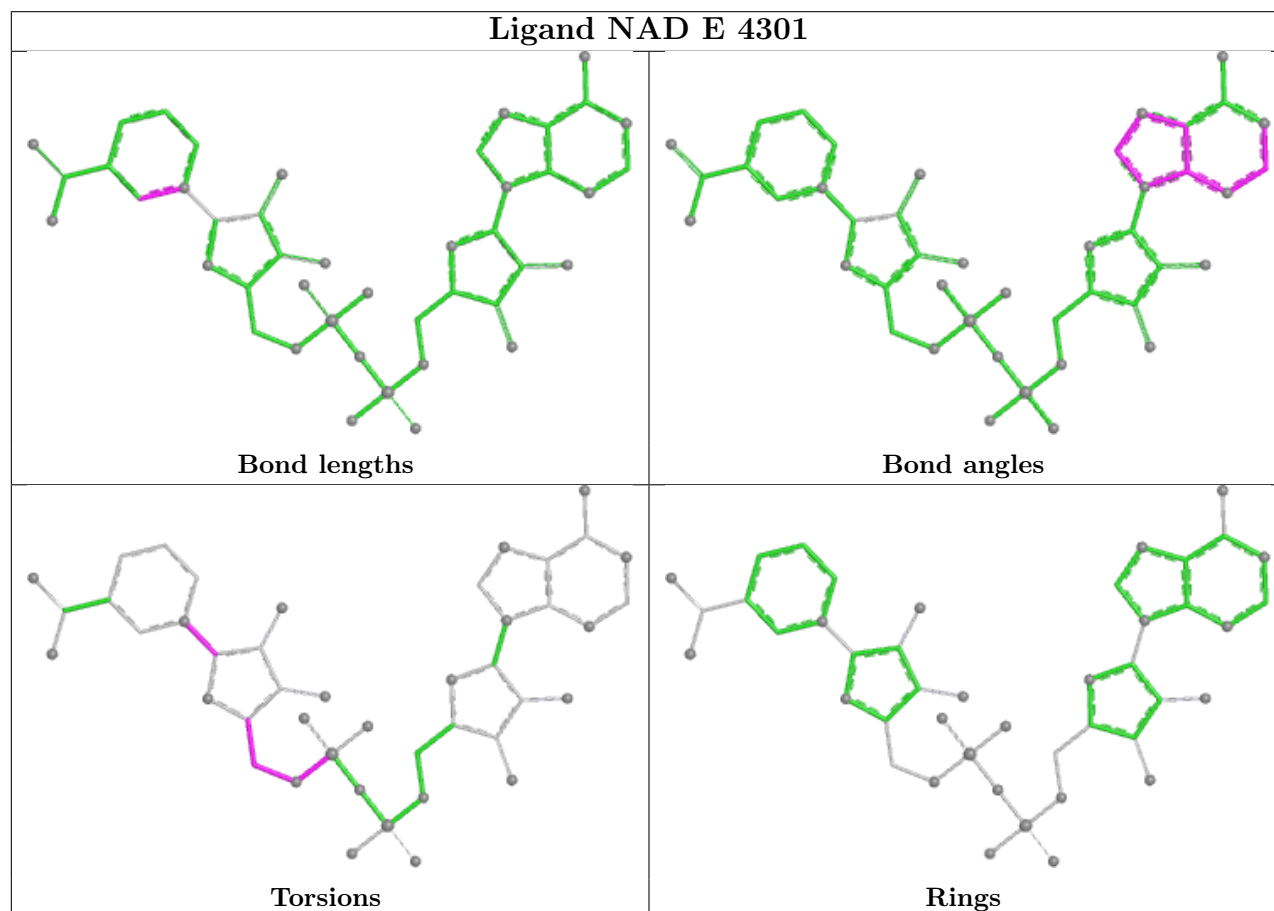
Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	E	4301	NAD	3	0

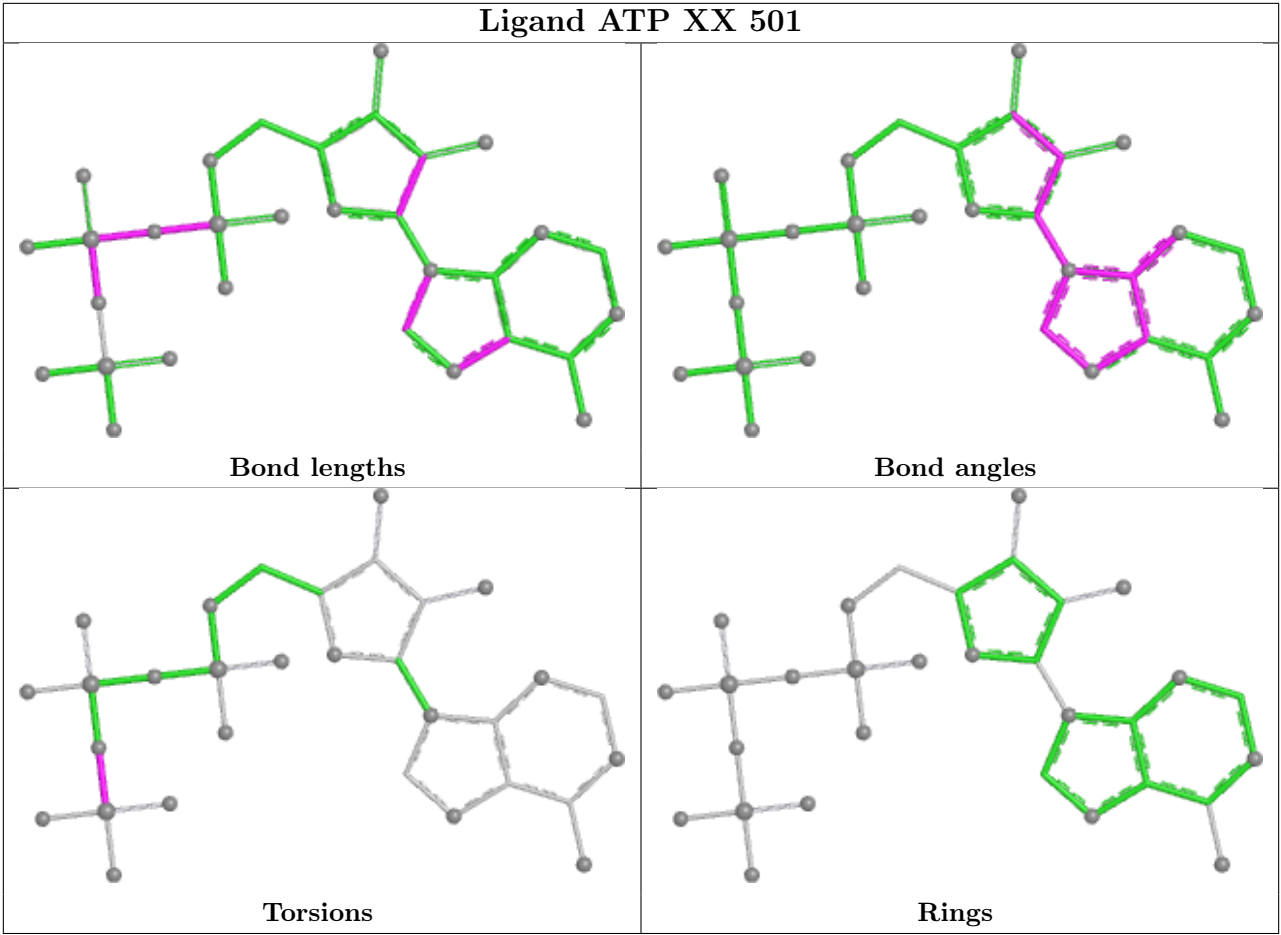
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	XX	501	ATP	2	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
79	bb	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	bb	28:A	O3'	41:G	P	18.21
1	bb	15:A	O3'	18:A	P	8.73
1	bb	46:G	O3'	48:U	P	3.74

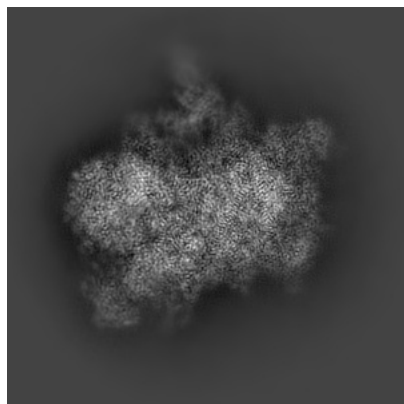
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10978. These allow visual inspection of the internal detail of the map and identification of artifacts.

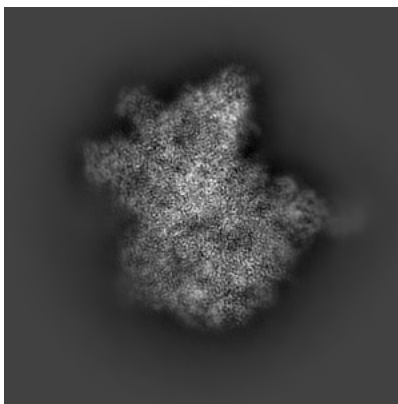
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

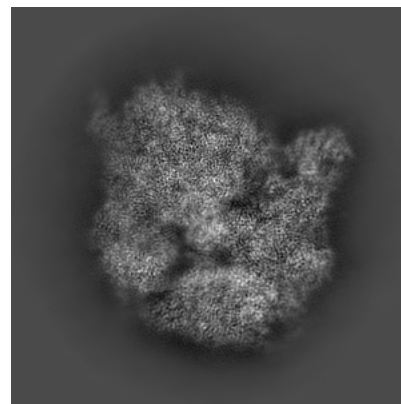
6.1.1 Primary map



X

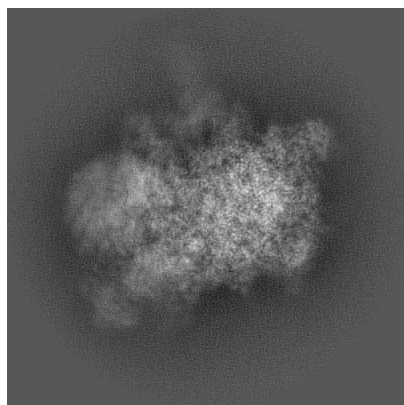


Y

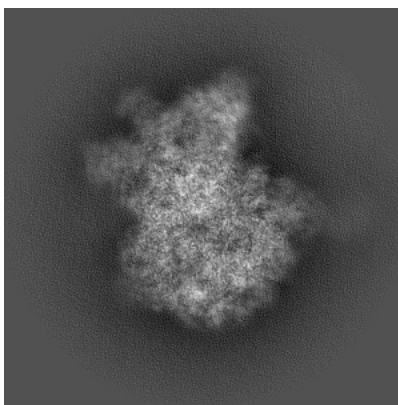


Z

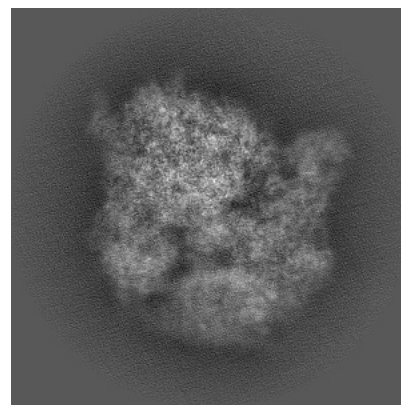
6.1.2 Raw map



X



Y

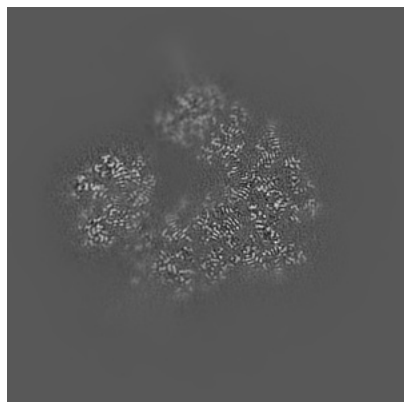


Z

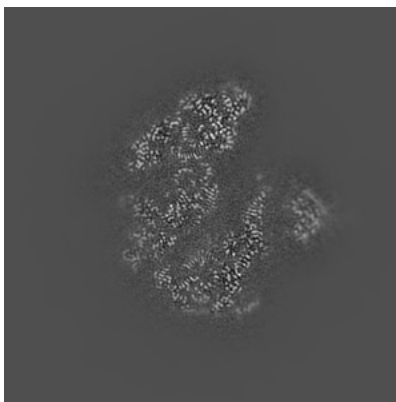
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

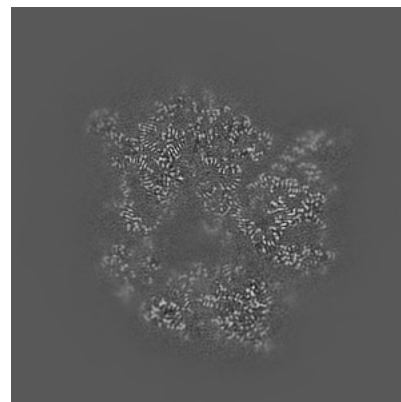
6.2.1 Primary map



X Index: 200

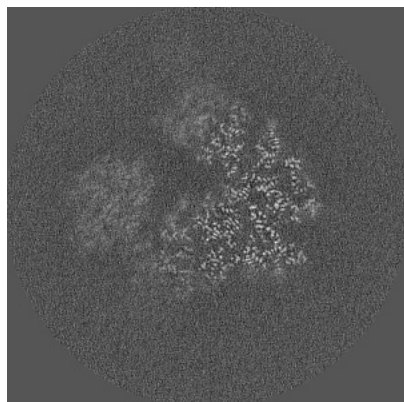


Y Index: 200

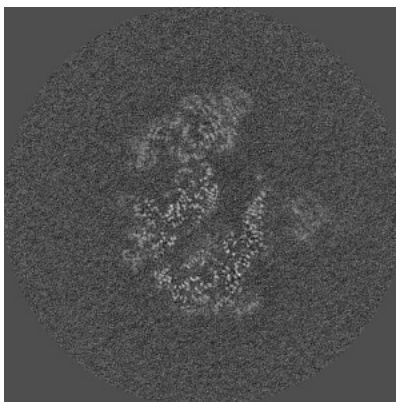


Z Index: 200

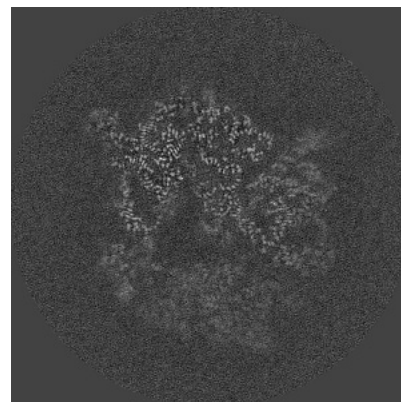
6.2.2 Raw map



X Index: 200



Y Index: 200

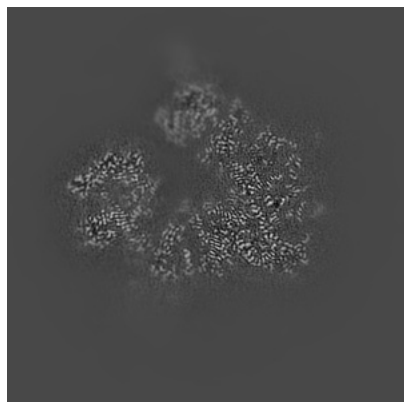


Z Index: 200

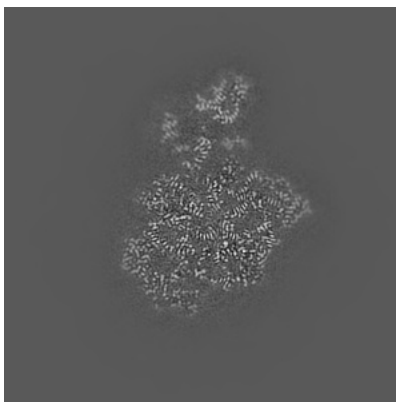
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

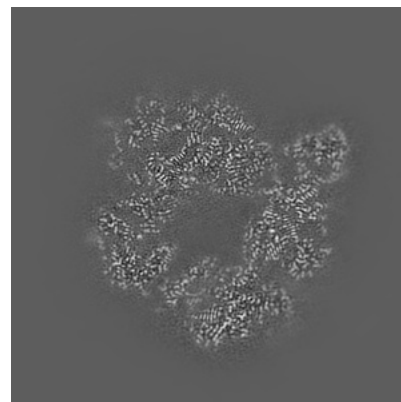
6.3.1 Primary map



X Index: 195

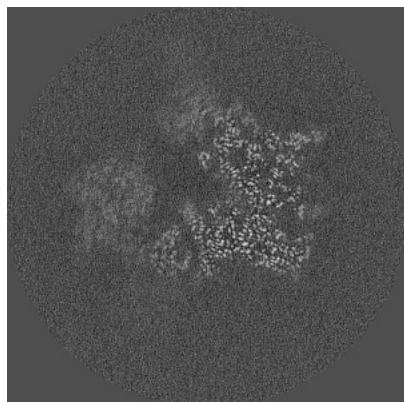


Y Index: 228

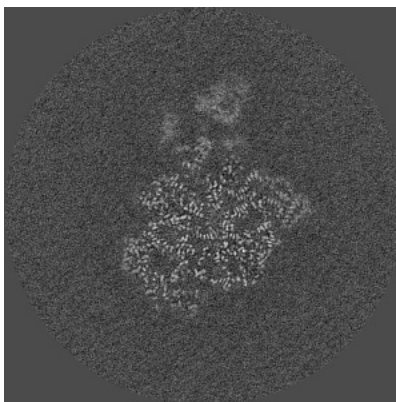


Z Index: 219

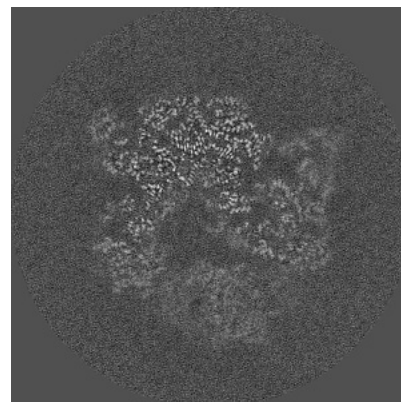
6.3.2 Raw map



X Index: 192



Y Index: 228

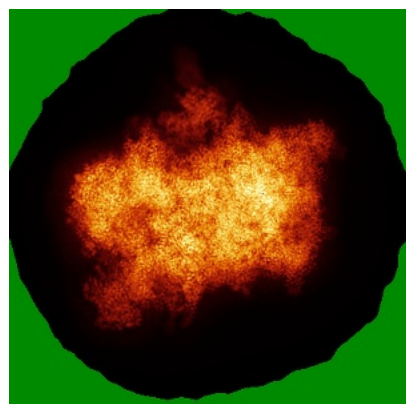


Z Index: 207

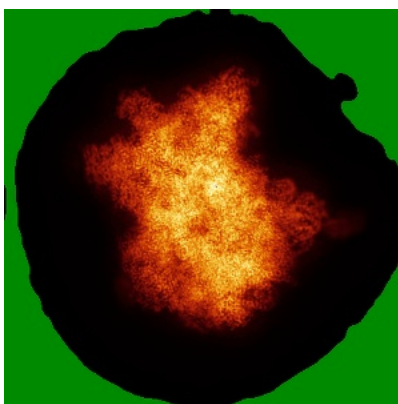
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

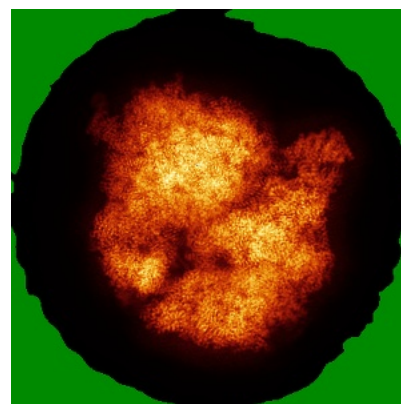
6.4.1 Primary map



X

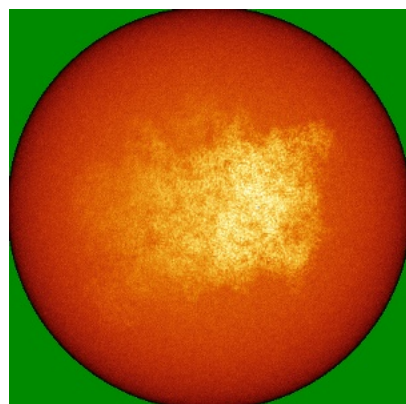


Y

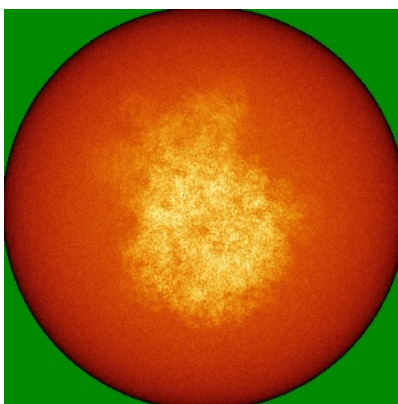


Z

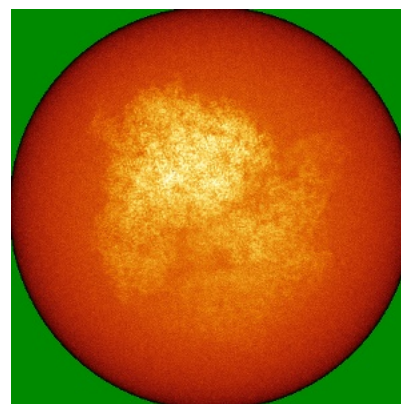
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

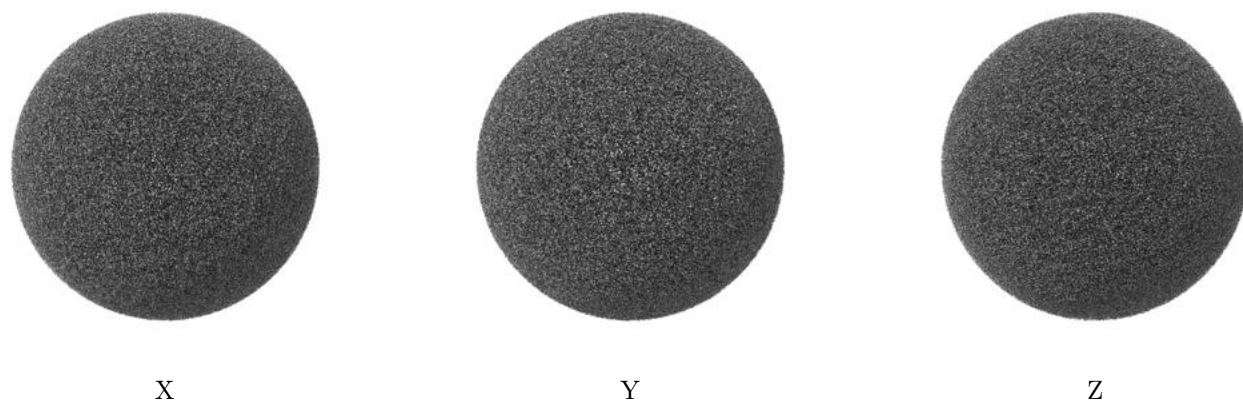
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0295. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

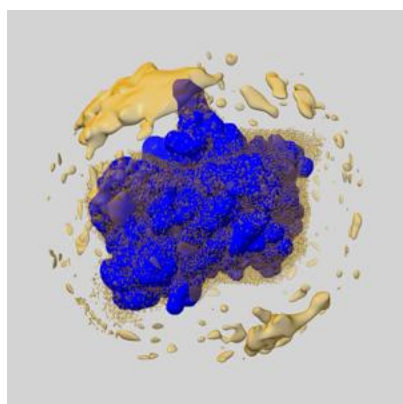
6.6 Mask visualisation [i](#)

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

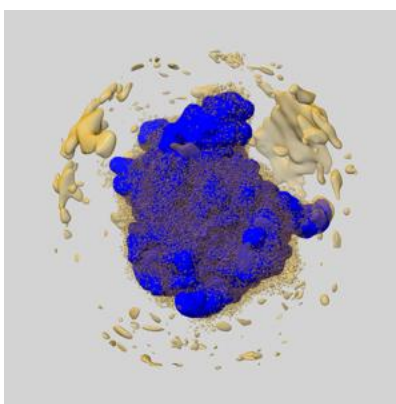
A mask typically either:

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

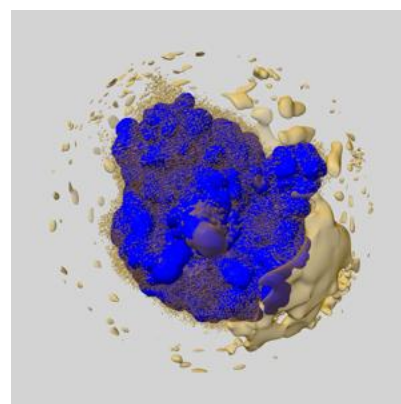
6.6.1 emd_10978_msk_1.map [i](#)



X



Y

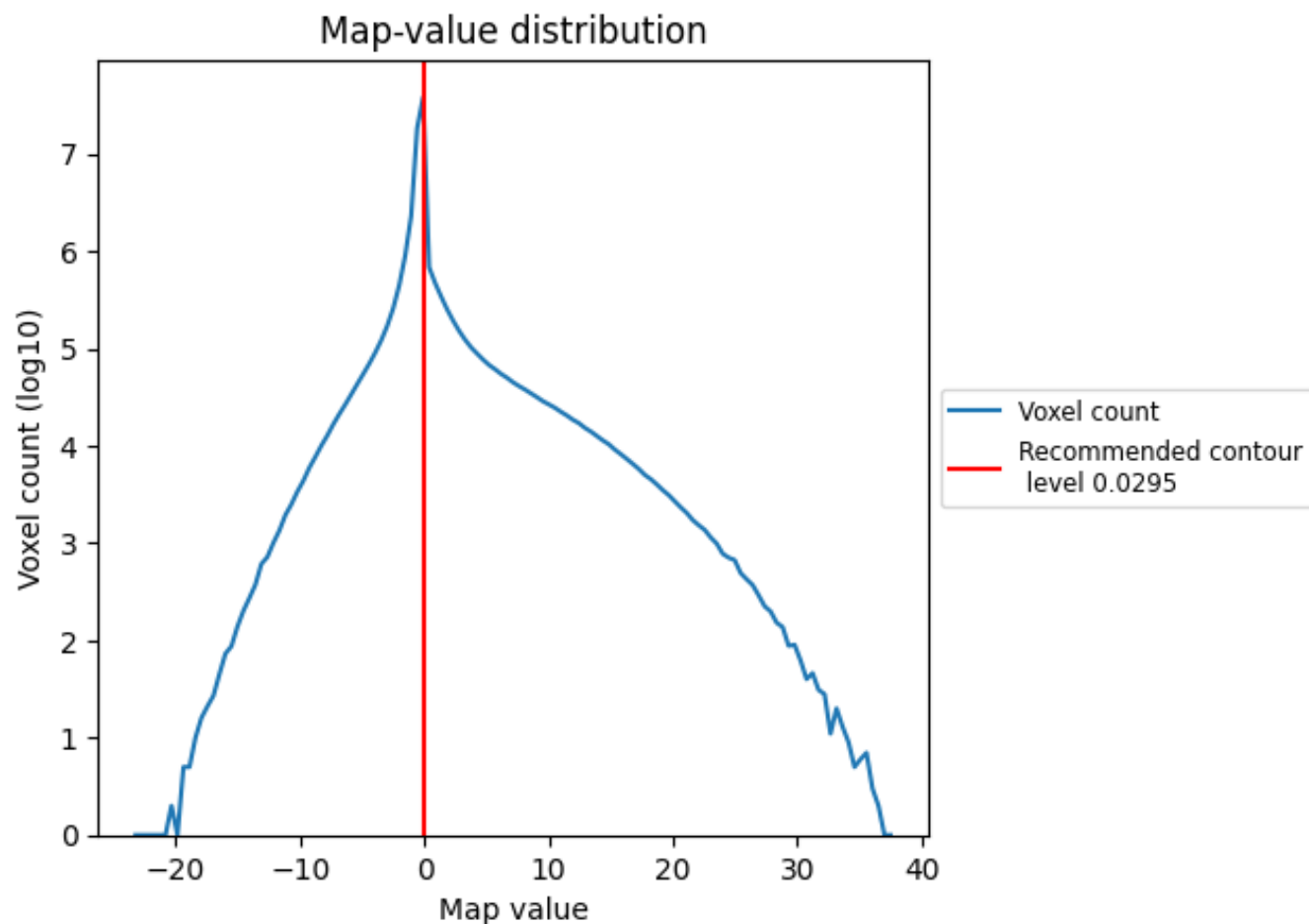


Z

7 Map analysis [i](#)

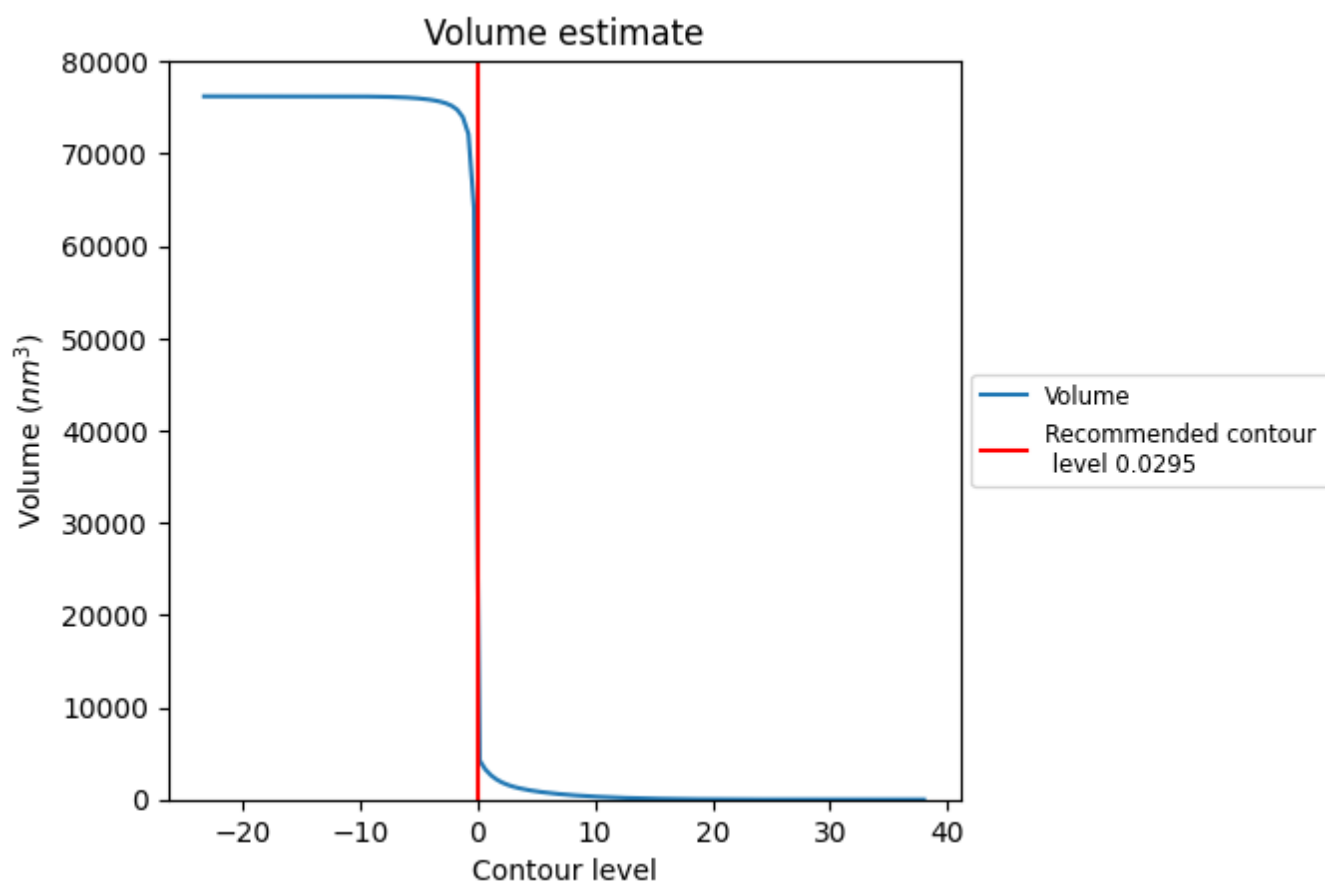
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

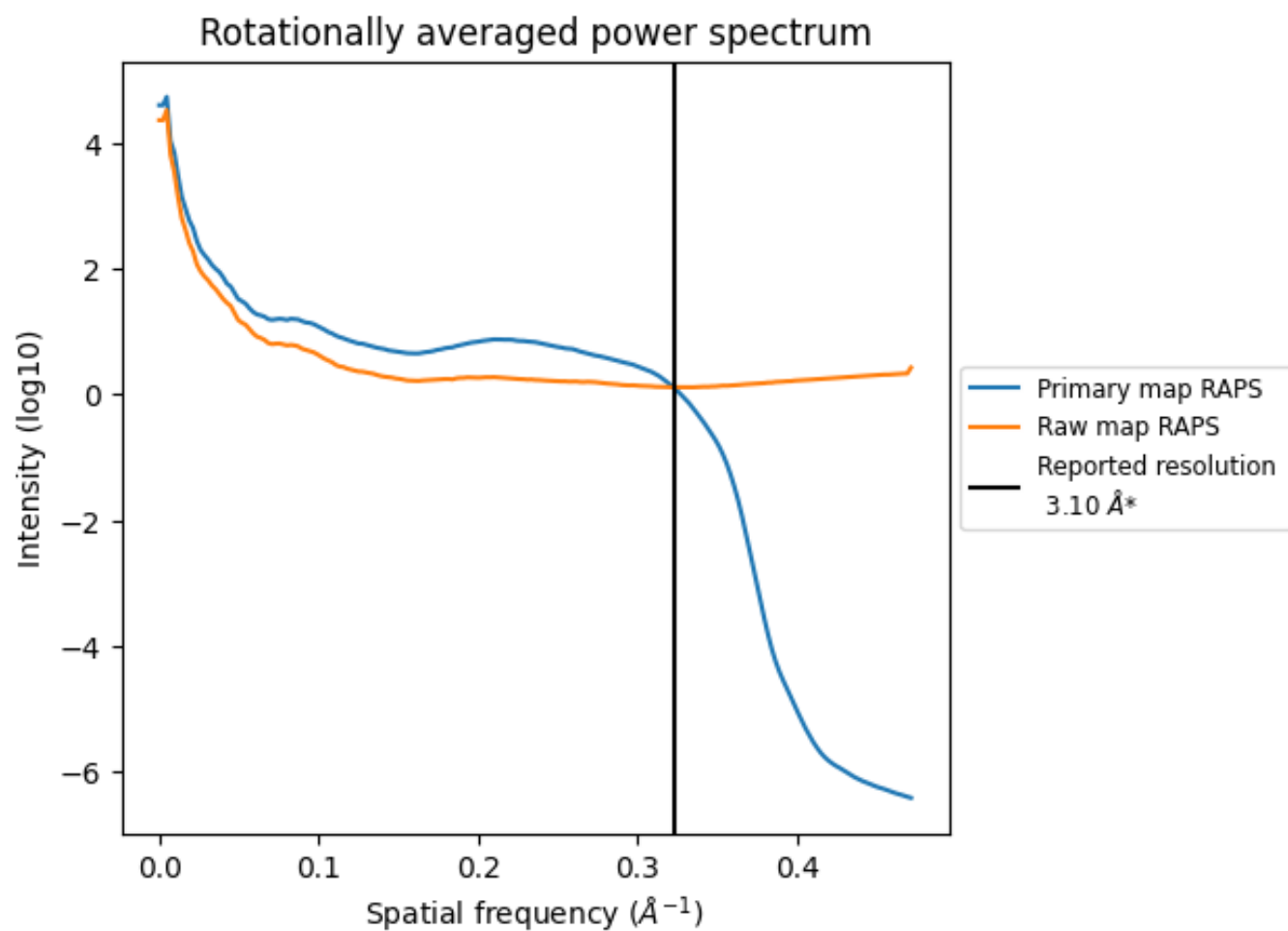
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 27404 nm³; this corresponds to an approximate mass of 24754 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 ⓘ

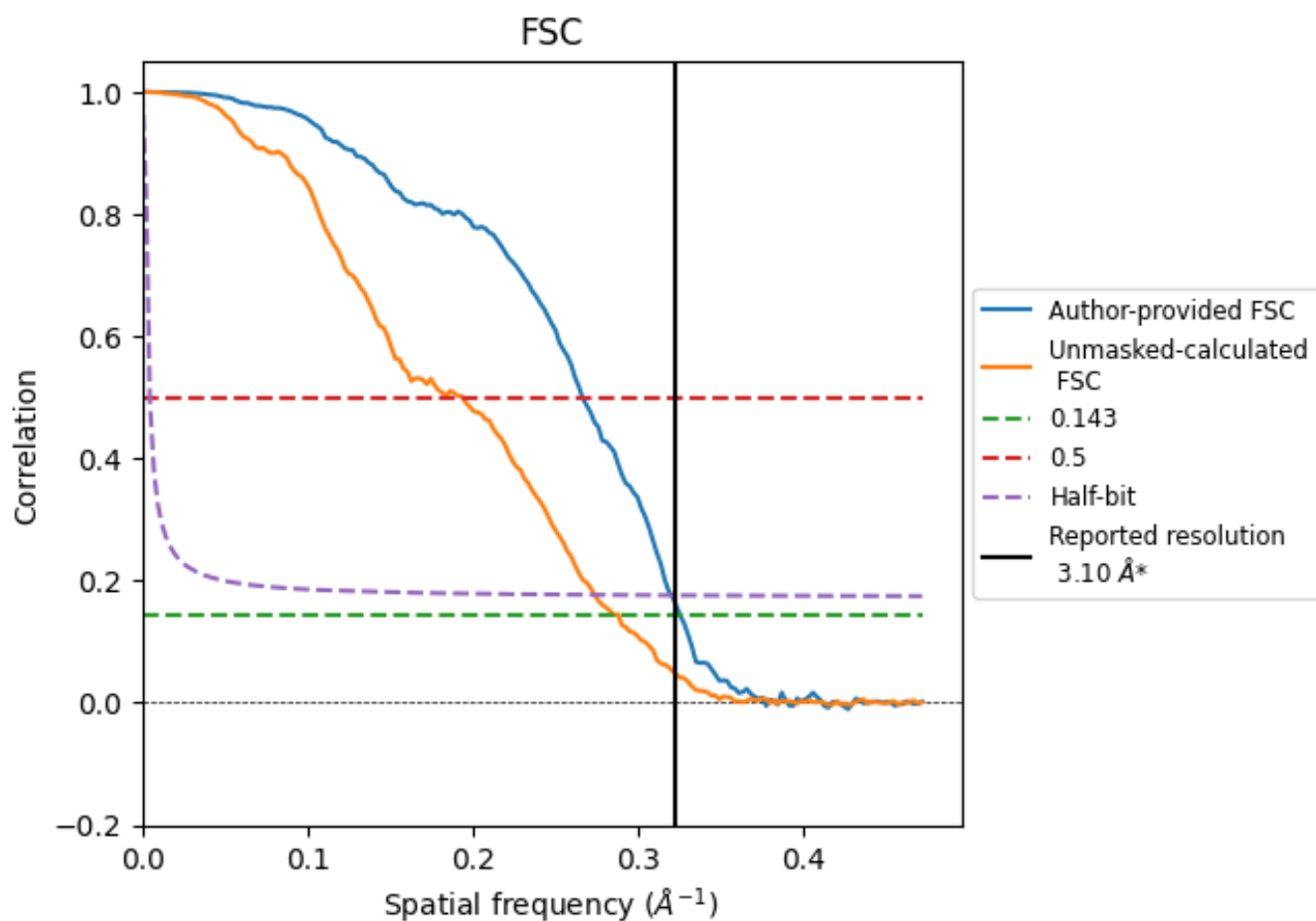


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

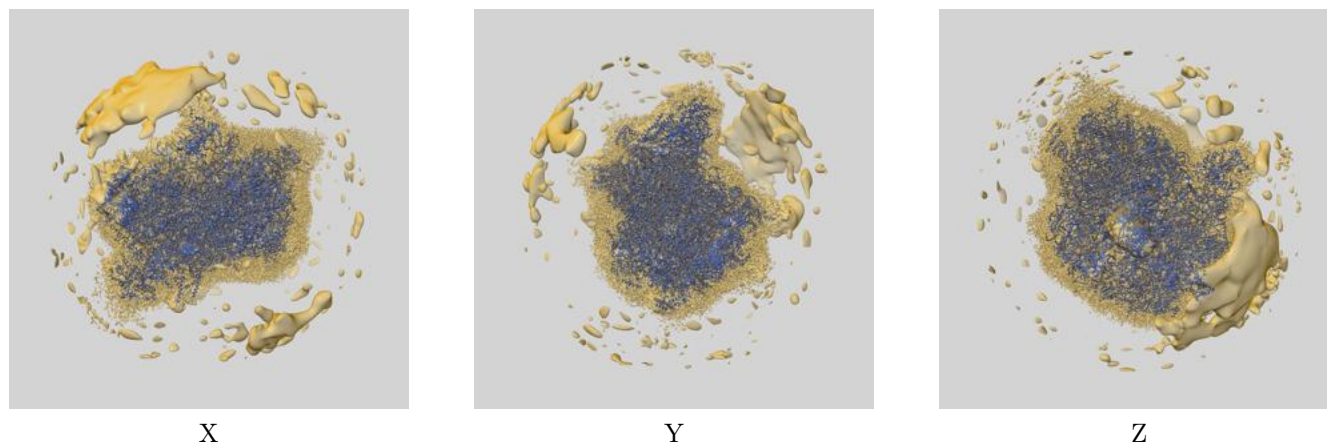
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.76	3.12
Unmasked-calculated*	3.47	5.16	3.65

*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 3.47 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

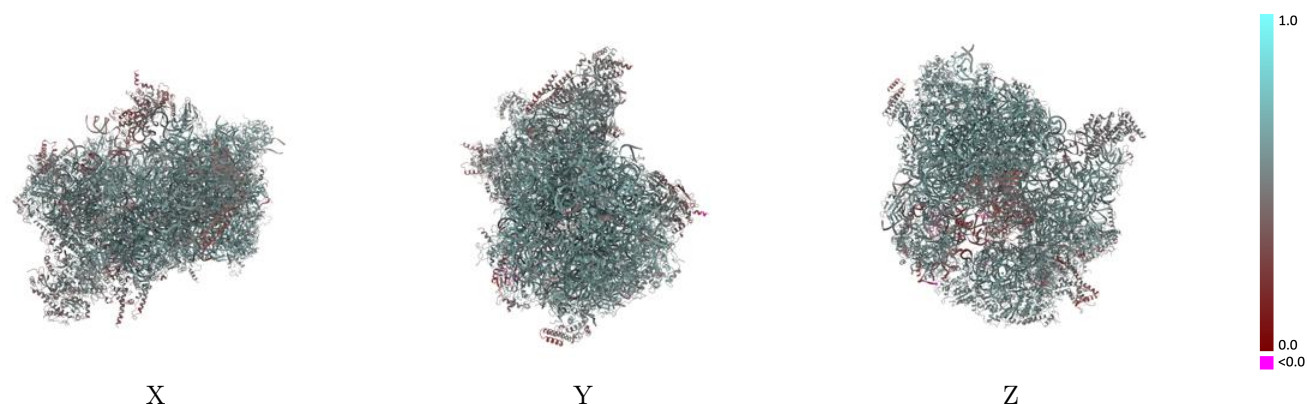
This section contains information regarding the fit between EMDB map EMD-10978 and PDB model 6YWX. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



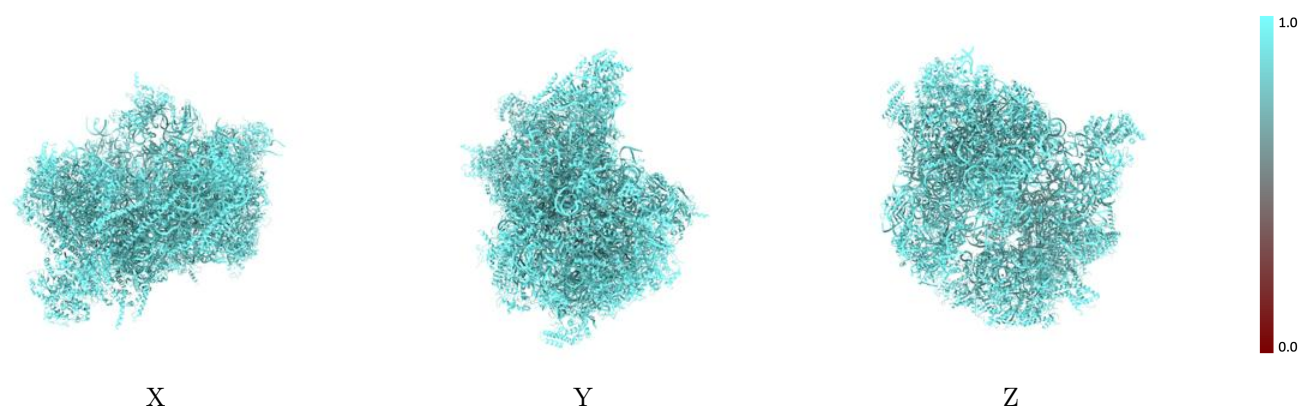
The images above show the 3D surface view of the map at the recommended contour level 0.0295 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



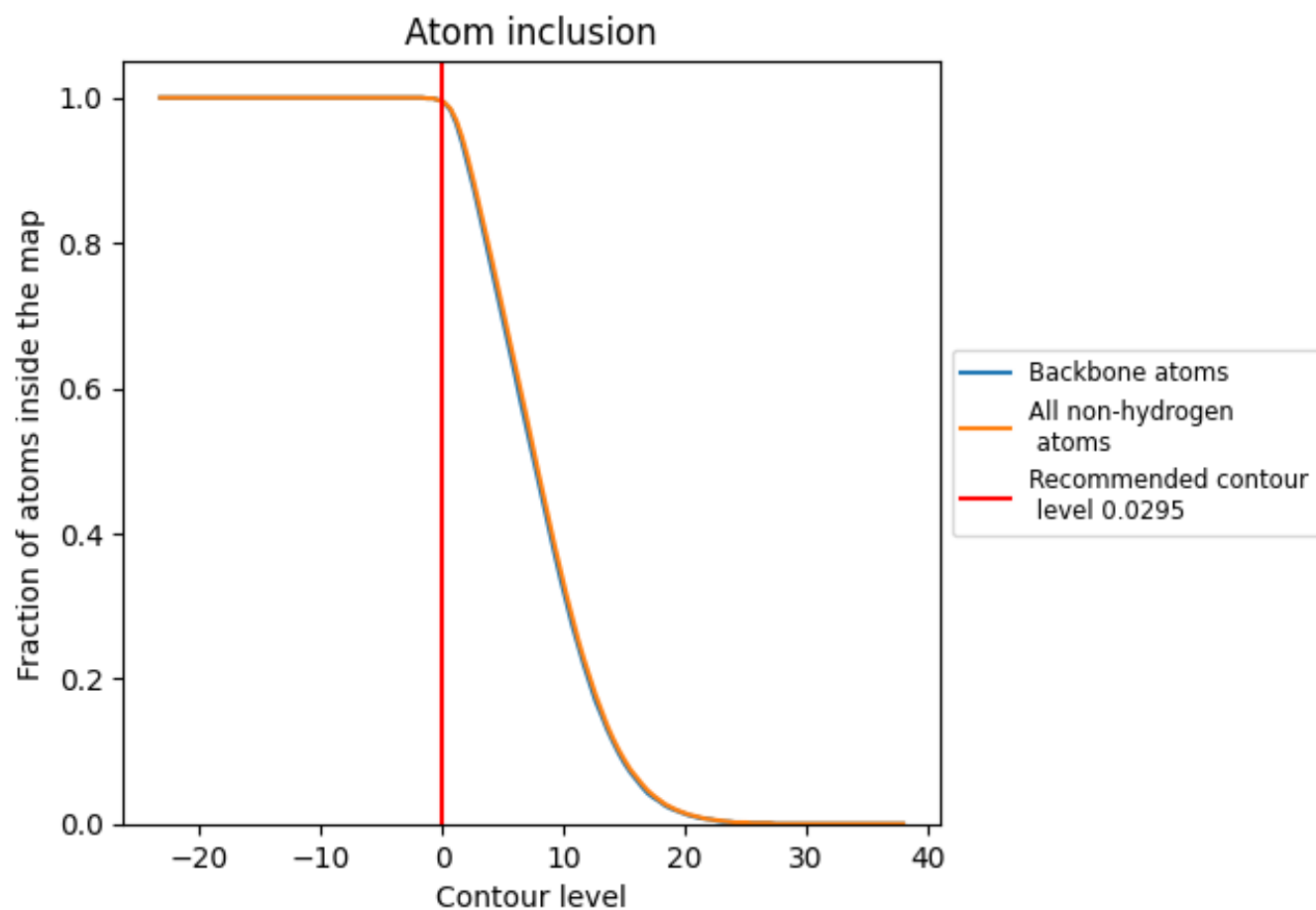
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0295).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0295) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9950	 0.5460
0	 0.9950	 0.6210
00	 0.9850	 0.3820
1	 0.9940	 0.5640
11	 0.9860	 0.4900
2	 0.9830	 0.5810
22	 0.9790	 0.5730
3	 0.9930	 0.5840
33	 0.9870	 0.5100
4	 0.9960	 0.6080
44	 0.9940	 0.4670
5	 0.9910	 0.5650
55	 0.9920	 0.4480
6	 0.9910	 0.5620
66	 0.9910	 0.5310
7	 0.9920	 0.5750
77	 0.9910	 0.5260
8	 0.9940	 0.4800
88	 0.9930	 0.5130
9	 0.9970	 0.5290
99	 0.9930	 0.3150
A	 0.9980	 0.5770
AA	 0.9900	 0.4750
B	 0.9980	 0.5960
BB	 0.9940	 0.5460
C	 0.9930	 0.6130
CC	 0.9890	 0.5160
D	 0.9950	 0.5750
DD	 0.9960	 0.5510
E	 0.9900	 0.5720
EE	 0.9950	 0.5480
F	 0.9920	 0.5320
FF	 0.9930	 0.5500
G	 0.9970	 0.5410
GG	 0.9890	 0.5240



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Chain	Atom inclusion	Q-score
H	 0.9930	 0.6130
HH	 0.9860	 0.5830
I	 0.9980	 0.5960
II	 0.9930	 0.5240
J	 0.9940	 0.5850
JJ	 0.9930	 0.5660
K	 0.9950	 0.5860
KK	 0.9970	 0.5560
L	 0.9940	 0.5960
LL	 0.9870	 0.5610
M	 0.9950	 0.5650
MM	 0.9930	 0.5430
N	 0.9980	 0.5980
NN	 0.9880	 0.5860
O	 0.9950	 0.5860
OO	 0.9910	 0.5340
P	 0.9890	 0.5870
PP	 0.9940	 0.5670
Q	 0.9950	 0.5600
QQ	 0.9940	 0.5230
R	 0.9960	 0.5190
RR	 0.9950	 0.5210
S	 0.9970	 0.5710
SS	 0.9870	 0.5320
T	 0.9960	 0.5750
TT	 0.9940	 0.5700
U	 0.9940	 0.5830
UU	 0.9900	 0.5300
V	 0.9980	 0.5850
VV	 0.9870	 0.5020
W	 0.9890	 0.6120
WW	 0.9870	 0.4710
X	 0.9950	 0.5860
XX	 0.9910	 0.5260
Y	 0.9890	 0.6290
YY	 0.9840	 0.5570
ZZ	 0.9920	 0.4950
a	 0.9930	 0.5600
aa	 0.9980	 0.5700
b	 0.9950	 0.5540
bb	 0.9680	 0.1900
c	 0.9940	 0.6140

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Chain	Atom inclusion	Q-score
d	 0.9950	 0.5830
e	 0.9800	 0.1300
f	 0.9920	 0.3740
g	 0.9950	 0.3400
h	 0.9800	 0.3400
i	 0.9860	 0.3080
j	 0.9930	 0.1450