



Full wwPDB EM Validation Report ⓘ

Jul 4, 2022 – 10:38 pm BST

PDB ID : 7QI4
EMDB ID : EMD-13980
Title : Human mitochondrial ribosome at 2.2 Å resolution
Authors : Singh, V.; Itoh, Y.; Amunts, A.
Deposited on : 2021-12-14
Resolution : 2.21 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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.dev8
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)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

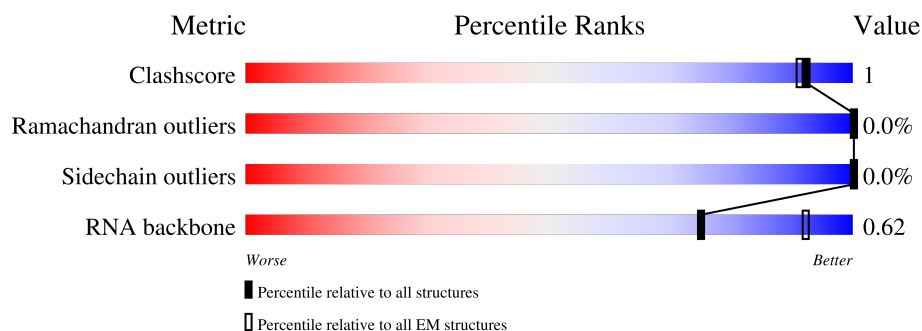
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.21 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AA	954	
2	AB	296	
3	AC	167	
4	AD	430	
5	AE	125	
6	AF	242	
7	AG	396	

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Mol	Chain	Length	Quality of chain
8	AH	201	
9	AI	194	
10	AJ	138	
11	AK	128	
12	AL	257	
13	AM	137	
14	AN	130	
15	AO	258	
16	AP	142	
17	AQ	87	
18	AR	360	
19	AS	190	
20	AT	173	
21	AU	205	
22	AV	414	
23	AW	187	
24	AX	398	
25	AY	395	
26	AZ	106	
27	A0	217	
28	A1	323	
29	A2	118	
30	A3	199	
31	A4	689	
32	Aw	22	

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Mol	Chain	Length	Quality of chain
33	Ax	70	
34	Ay	70	
35	Az	34	
36	A	1558	
37	B	73	
38	D	305	
39	E	348	
40	F	311	
41	H	267	
42	I	261	
43	J	192	
44	K	178	
45	L	145	
46	M	296	
47	N	251	
48	O	175	
49	P	180	
50	Q	292	
51	R	149	
52	S	205	
53	T	206	
54	U	153	
55	V	216	
56	W	148	
57	X	256	

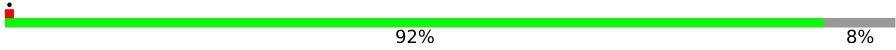





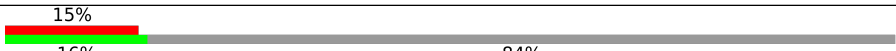




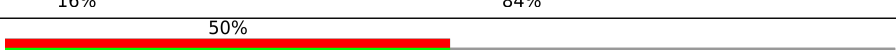
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Mol	Chain	Length	Quality of chain
58	Y	250	
59	Z	161	
60	0	188	
61	1	65	
62	2	92	
63	3	188	
64	4	103	
65	5	423	
66	6	380	
67	7	338	
68	8	206	
69	9	137	
70	a	142	
71	b	215	
72	c	332	
73	d	306	
74	e	279	
75	f	212	
76	g	166	
77	h	158	
78	i	128	
79	j	123	
80	k	112	
81	l	138	
82	m	128	

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Mol	Chain	Length	Quality of chain
83	o	102	
84	p	206	
85	q	222	
86	r	196	
87	s	439	
88	t	198	
88	u	198	
88	v	198	
88	w	198	
88	x	198	
88	y	198	
89	z	325	

2 Entry composition

There are 101 unique types of molecules in this entry. The entry contains 339115 atoms, of which 152402 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 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	AA	954	Total	C	H	N	O	P	0	0
			30565	9088	10305	3647	6571	954		

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AB	225	Total	C	H	N	O	S	0	0
			3654	1164	1826	331	323	10		

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	AC	132	Total	C	H	N	O	S	0	0
			2179	699	1096	195	185	4		

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	AD	343	Total	C	H	N	O	S	0	0
			5545	1713	2814	518	487	13		

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	AE	122	Total	C	H	N	O	S	0	0
			1976	614	1004	177	177	4		

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	AF	208	Total	C	H	N	O	S	0	0
			3503	1104	1778	312	298	11		

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	AG	327	Total	C	H	N	O	S	0	0
			5385	1710	2697	477	487	14		

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	AH	140	Total	C	H	N	O	S	0	0
			2343	745	1191	194	210	3		

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	AI	137	Total	C	H	N	O	S	0	0
			2086	642	1066	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	184	5F0	ASN	conflict	UNP P82912

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	AJ	108	Total	C	H	N	O	S	0	0
			1731	521	892	169	143	6		

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AK	101	Total	C	H	N	O	S	0	0
			1751	537	889	179	141	5		

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AL	174	Total	C	H	N	O	S	0	0
			2998	925	1545	270	251	7		

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AM	119	Total	C	H	N	O	S	0	0
			1914	594	972	185	157	6		

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AN	110	Total	C	H	N	O	S	0	0
			1801	562	933	156	147	3		

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	AO	193	Total	C	H	N	O	S	0	0
			3162	1014	1570	294	277	7		

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AP	97	Total	C	H	N	O	S	0	0
			1590	501	809	134	138	8		

- Molecule 17 is a protein called MRPS21 isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AQ	86	Total	C	H	N	O	S	0	0
			1504	460	760	150	126	8		

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AR	295	Total	C	H	N	O	S	0	0
			4845	1533	2436	413	455	8		

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AS	135	Total	C	H	N	O	S	0	0
			2228	716	1117	198	196	1		

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AT	168	Total	C	H	N	O	S	0	0
			2767	877	1396	239	244	11		

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	AU	176	Total	C	H	N	O	S	0	0
			2993	916	1505	301	267	4		

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AV	362	Total	C	H	N	O	S	0	0
			5941	1904	2972	495	558	12		

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	100	Total	C	H	N	O	S	0	0
			1595	498	806	141	146	4		

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	352	Total	C	H	N	O	S	0	0
			5708	1822	2859	499	517	11		

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AY	149	Total	C	H	N	O	S	0	0
			2449	801	1203	207	234	4		

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AZ	100	Total	C	H	N	O	S	0	0
			1701	534	862	153	148	4		

- Molecule 27 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	A0	215	Total	C	H	N	O	S	0	0
			3589	1130	1802	339	313	5		

- Molecule 28 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	A1	279	Total	C	H	N	O	S	0	0
			4565	1435	2300	387	432	11		

- Molecule 29 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	A2	117	Total	C	H	N	O	S	0	0
			1908	579	973	182	166	8		

- Molecule 30 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	A3	70	Total	C	H	N	O	S	0	0
			1327	401	702	134	89	1		

- Molecule 31 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	A4	588	Total	C	H	N	O	S	0	0
			9552	3053	4784	808	879	28		

- Molecule 32 is a RNA chain called A/A-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	Aw	22	Total	C	H	N	O	P	0	0
			701	209	237	82	151	22		

- Molecule 33 is a RNA chain called P/P-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	Ax	70	Total	C	H	N	O	P	0	0
			2234	665	752	261	486	70		

- Molecule 34 is a RNA chain called E/E-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	Ay	4	Total	C	H	N	O	P	0	0
			129	38	45	16	26	4		

- Molecule 35 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	Az	34	Total	C	H	N	O	P	0	0
			1080	324	360	123	239	34		

- Molecule 36 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	A	1558	Total	C	H	N	O	P	0	0
			49872	14843	16802	5963	10706	1558		

- Molecule 37 is a RNA chain called mitochondrial tRNA^{Val}.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	B	72	Total	C	H	N	O	P	0	0
			2303	685	779	269	498	72		

- Molecule 38 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	D	238	Total	C	H	N	O	S	0	0
			3787	1157	1928	376	317	9		

- Molecule 39 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	E	305	Total	C	H	N	O	S	0	0
			4830	1545	2424	418	432	11		

- Molecule 40 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	F	252	Total	C	H	N	O	S	0	0
			4106	1305	2075	370	350	6		

- Molecule 41 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	H	202	Total	C	H	N	O	S	0	0
			3401	1067	1740	304	286	4		

- Molecule 42 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	I	212	Total	C	H	N	O	S	0	0
			3489	1088	1794	304	292	11		

- Molecule 43 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	J	175	Total	C	H	N	O	S	0	0
			2739	847	1409	237	244	2		

- Molecule 44 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	K	177	Total	C	H	N	O	S	0	0
			2915	936	1460	259	253	7		

- Molecule 45 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	L	115	Total	C	H	N	O	S	0	0
			1835	559	945	171	155	5		

- Molecule 46 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	M	291	Total	C	H	N	O	S	0	0
			4725	1483	2398	430	408	6		

- Molecule 47 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	N	222	Total	C	H	N	O	S	0	0
			3610	1143	1824	326	307	10		

- Molecule 48 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	O	154	Total	C	H	N	O	S	0	0
			2557	792	1298	241	219	7		

- Molecule 49 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	P	144	Total	C	H	N	O	S	0	0
			2344	733	1171	224	211	5		

- Molecule 50 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	Q	238	Total	C	H	N	O	S	0	0
			4004	1268	2025	352	350	9		

- Molecule 51 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	R	140	Total	C	H	N	O	S	0	0
			2374	732	1220	231	187	4		

- Molecule 52 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	S	161	Total	C	H	N	O	S	0	0
			2662	835	1369	227	227	4		

- Molecule 53 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	T	166	Total	C	H	N	O	S	0	0
			2786	875	1417	254	233	7		

- Molecule 54 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	U	152	Total	C	H	N	O	S	0	0
			2486	788	1235	234	226	3		

- Molecule 55 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	V	205	Total	C	H	N	O	S	0	0
			3367	1068	1691	298	302	8		

- Molecule 56 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	W	116	Total	C	H	N	O	S	0	0
			1847	577	943	171	153	3		

- Molecule 57 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	X	244	Total	C	H	N	O	S	0	0
			4109	1322	2065	352	365	5		

- Molecule 58 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	Y	181	Total	C	H	N	O	S	0	0
			3159	995	1603	298	259	4		

- Molecule 59 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	Z	122	Total	C	H	N	O	S	0	0
			2048	636	1052	186	171	3		

- Molecule 60 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	0	110	Total	C	H	N	O	S	0	0
			1817	554	919	176	162	6		

- Molecule 61 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	1	56	Total	C	H	N	O	S	0	0
			977	296	513	89	77	2		

- Molecule 62 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	2	46	Total	C	H	N	O	S	0	0
			786	233	409	83	60	1		

- Molecule 63 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	3	95	Total	C	H	N	O	S	0	0
			1718	539	886	162	128	3		

- Molecule 64 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	4	38	Total	C	H	N	O	S	0	0
			705	217	363	72	49	4		

- Molecule 65 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	5	394	Total	C	H	N	O	S	0	0
			6432	2073	3222	560	566	11		

- Molecule 66 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	6	354	Total	C	H	N	O	S	0	0
			5802	1881	2854	525	533	9		

- Molecule 67 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	7	294	Total	C	H	N	O	S	0	0
			4796	1529	2406	405	438	18		

- Molecule 68 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	8	157	Total	C	H	N	O	S	0	0
			2698	844	1371	235	246	2		

- Molecule 69 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	9	124	Total	C	H	N	O	S	0	0
			1985	644	988	170	181	2		

- Molecule 70 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	a	100	Total	C	H	N	O	S	0	0
			1659	529	819	152	154	5		

- Molecule 71 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	b	150	Total	C	H	N	O	S	0	0
			2395	744	1199	231	218	3		

- Molecule 72 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	c	286	Total	C	H	N	O	S	0	0
			4624	1470	2325	397	423	9		

- Molecule 73 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	d	241	Total	C	H	N	O	S	0	0
			3972	1273	1987	340	359	13		

- Molecule 74 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	e	238	Total	C	H	N	O	S	0	0
			3853	1222	1922	339	364	6		

- Molecule 75 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	f	157	Total	C	H	N	O	S	0	0
			2529	799	1277	207	242	4		

- Molecule 76 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	g	134	Total	C	H	N	O	S	0	0
			2214	719	1101	193	199	2		

- Molecule 77 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	h	110	Total	C	H	N	O	S	0	0
			1780	568	885	156	168	3		

- Molecule 78 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	i	97	Total	C	H	N	O	S	0	0
			1690	532	862	165	127	4		

- Molecule 79 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	j	94	Total	C	H	N	O	S	0	0
			1492	463	747	144	136	2		

- Molecule 80 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	k	101	Total	C	H	N	O	S	0	0
			1562	479	788	148	142	5		

- Molecule 81 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	l	82	Total	C	H	N	O	S	0	0
			1364	437	676	120	128	3		

- Molecule 82 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	m	92	Total	C	H	N	O	S	0	0
			1554	488	763	159	142	2		

- Molecule 83 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	o	94	Total	C	H	N	O	S	0	0
			1608	501	810	165	129	3		

- Molecule 84 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	p	147	Total	C	H	N	O	S	0	0
			2433	748	1228	228	225	4		

- Molecule 85 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	q	161	Total	C	H	N	O	S	0	0
			2679	841	1329	260	244	5		

- Molecule 86 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	r	162	Total	C	H	N	O	S	0	0
			2677	839	1355	252	223	8		

- Molecule 87 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	s	386	Total	C	H	N	O	S	0	0
			6306	2023	3151	559	559	14		

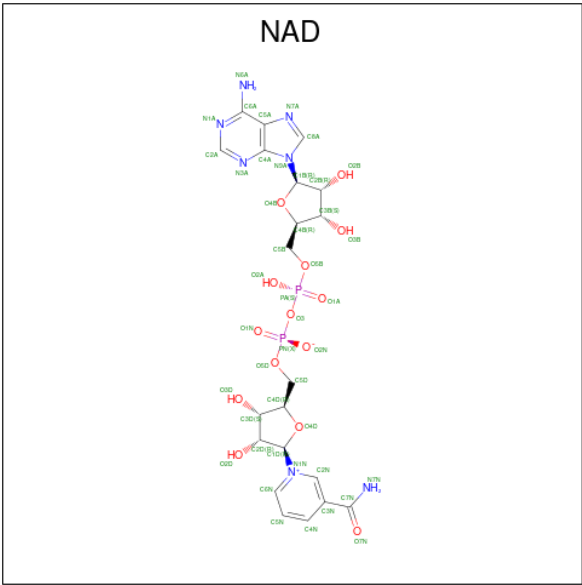
- Molecule 88 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
88	t	46	Total	C	H	N	O		0	0
			732	228	378	56	70			
88	u	32	Total	C	H	N	O		0	0
			541	168	284	40	49			
88	v	32	Total	C	H	N	O		0	0
			541	168	284	40	49			
88	w	31	Total	C	H	N	O		0	0
			520	159	275	39	47			
88	x	31	Total	C	H	N	O		0	0
			520	159	275	39	47			
88	y	31	Total	C	H	N	O		0	0
			520	159	275	39	47			

- Molecule 89 is a protein called 39S ribosomal protein L1, mitochondrial.

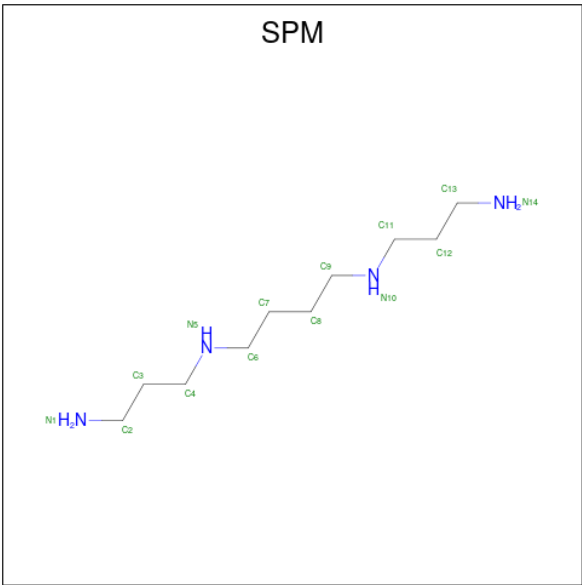
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
89	z	164	2685	856	1358	217	250	4	0	0

- Molecule 90 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



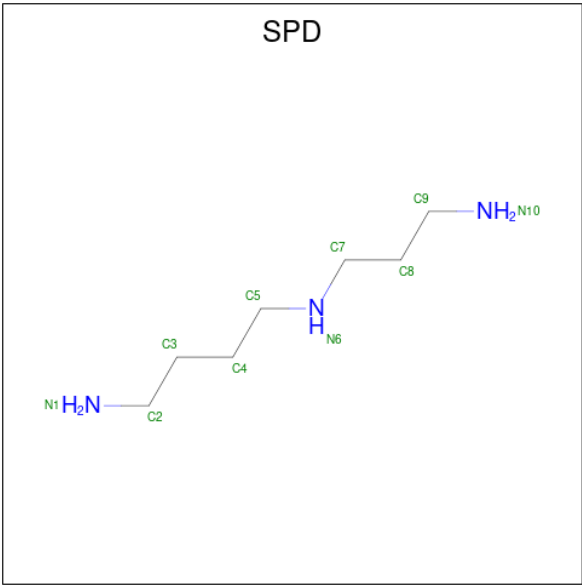
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
90	AA	1	70	21	26	7	14	2	0

- Molecule 91 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms				AltConf
91	AA	1	Total	C	H	N	0
			44	10	30	4	

- Molecule 92 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms				AltConf
92	AA	1	Total	C	H	N	0
			32	7	22	3	
92	A	1	Total	C	H	N	0
			96	21	66	9	
92	A	1	Total	C	H	N	0
			96	21	66	9	

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Mol	Chain	Residues	Atoms				AltConf
92	A	1	Total	C	H	N	0
			96	21	66	9	

- Molecule 93 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
93	AA	58	Total	Mg	0
			58	58	
93	AB	1	Total	Mg	0
			1	1	
93	AX	1	Total	Mg	0
			1	1	
93	A3	1	Total	Mg	0
			1	1	
93	Aw	1	Total	Mg	0
			1	1	
93	A	137	Total	Mg	0
			137	137	
93	D	2	Total	Mg	0
			2	2	
93	E	1	Total	Mg	0
			1	1	
93	g	1	Total	Mg	0
			1	1	

- Molecule 94 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
94	AA	20	Total	K	0
			20	20	
94	A4	1	Total	K	0
			1	1	
94	A	31	Total	K	0
			31	31	
94	D	1	Total	K	0
			1	1	
94	M	1	Total	K	0
			1	1	
94	W	1	Total	K	0
			1	1	
94	3	1	Total	K	0
			1	1	

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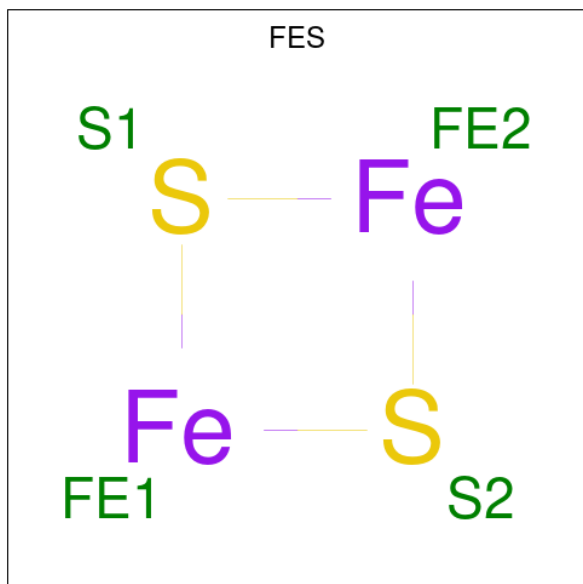
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Mol	Chain	Residues	Atoms	AltConf
94	6	1	Total K 1 1	0
94	i	1	Total K 1 1	0
94	o	1	Total K 1 1	0

- Molecule 95 is ZINC ION (three-letter code: ZN) (formula: Zn).

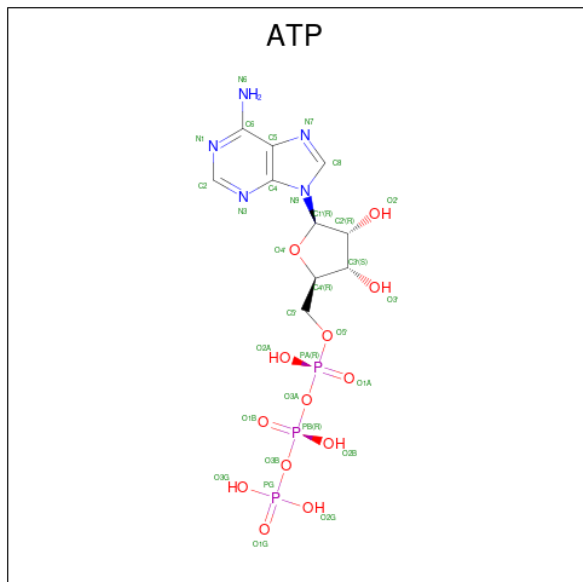
Mol	Chain	Residues	Atoms	AltConf
95	AO	1	Total Zn 1 1	0
95	0	1	Total Zn 1 1	0
95	4	1	Total Zn 1 1	0

- Molecule 96 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

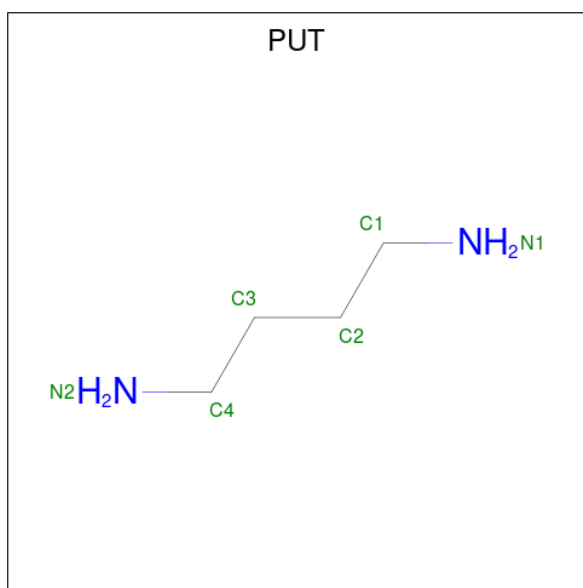


Mol	Chain	Residues	Atoms	AltConf
96	AP	1	Total Fe S 4 2 2	0
96	AT	1	Total Fe S 4 2 2	0
96	r	1	Total Fe S 4 2 2	0

- Molecule 97 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

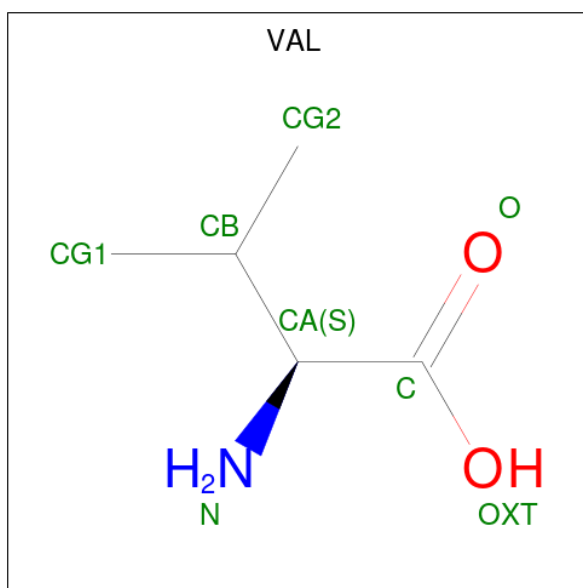


- Molecule 99 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms				AltConf
99	A	1	Total	C	H	N	0
			20	4	14	2	

- Molecule 100 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).



Mol	Chain	Residues	Atoms					AltConf
100	B	1	Total	C	H	N	O	0
			18	5	11	1	1	

- Molecule 101 is water.

Mol	Chain	Residues	Atoms		AltConf
101	AA	2149	Total 2149	O 2149	0
101	AB	77	Total 77	O 77	0
101	AC	55	Total 55	O 55	0
101	AD	79	Total 79	O 79	0
101	AE	29	Total 29	O 29	0
101	AF	37	Total 37	O 37	0
101	AG	71	Total 71	O 71	0
101	AH	50	Total 50	O 50	0
101	AI	45	Total 45	O 45	0
101	AJ	27	Total 27	O 27	0
101	AK	50	Total 50	O 50	0
101	AL	42	Total 42	O 42	0
101	AM	21	Total 21	O 21	0
101	AN	34	Total 34	O 34	0
101	AO	36	Total 36	O 36	0
101	AP	31	Total 31	O 31	0
101	AQ	67	Total 67	O 67	0
101	AR	12	Total 12	O 12	0
101	AS	25	Total 25	O 25	0
101	AT	43	Total 43	O 43	0
101	AU	8	Total 8	O 8	0
101	AW	16	Total 16	O 16	0

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Mol	Chain	Residues	Atoms		AltConf
101	AX	61	Total 61	O 61	0
101	AY	20	Total 20	O 20	0
101	AZ	27	Total 27	O 27	0
101	A0	1	Total 1	O 1	0
101	A1	36	Total 36	O 36	0
101	A2	35	Total 35	O 35	0
101	A3	52	Total 52	O 52	0
101	A4	11	Total 11	O 11	0
101	Aw	5	Total 5	O 5	0
101	Ax	5	Total 5	O 5	0
101	Ay	1	Total 1	O 1	0
101	Az	14	Total 14	O 14	0
101	A	3051	Total 3051	O 3051	0
101	B	64	Total 64	O 64	0
101	D	70	Total 70	O 70	0
101	E	72	Total 72	O 72	0
101	F	77	Total 77	O 77	0
101	H	9	Total 9	O 9	0
101	I	23	Total 23	O 23	0
101	J	1	Total 1	O 1	0
101	K	65	Total 65	O 65	0

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Mol	Chain	Residues	Atoms		AltConf
101	L	25	Total 25	O 25	0
101	M	67	Total 67	O 67	0
101	N	59	Total 59	O 59	0
101	O	38	Total 38	O 38	0
101	P	88	Total 88	O 88	0
101	Q	28	Total 28	O 28	0
101	R	58	Total 58	O 58	0
101	S	49	Total 49	O 49	0
101	T	48	Total 48	O 48	0
101	U	26	Total 26	O 26	0
101	V	5	Total 5	O 5	0
101	W	49	Total 49	O 49	0
101	X	12	Total 12	O 12	0
101	Y	27	Total 27	O 27	0
101	Z	33	Total 33	O 33	0
101	0	27	Total 27	O 27	0
101	1	3	Total 3	O 3	0
101	2	34	Total 34	O 34	0
101	3	40	Total 40	O 40	0
101	4	13	Total 13	O 13	0
101	5	16	Total 16	O 16	0

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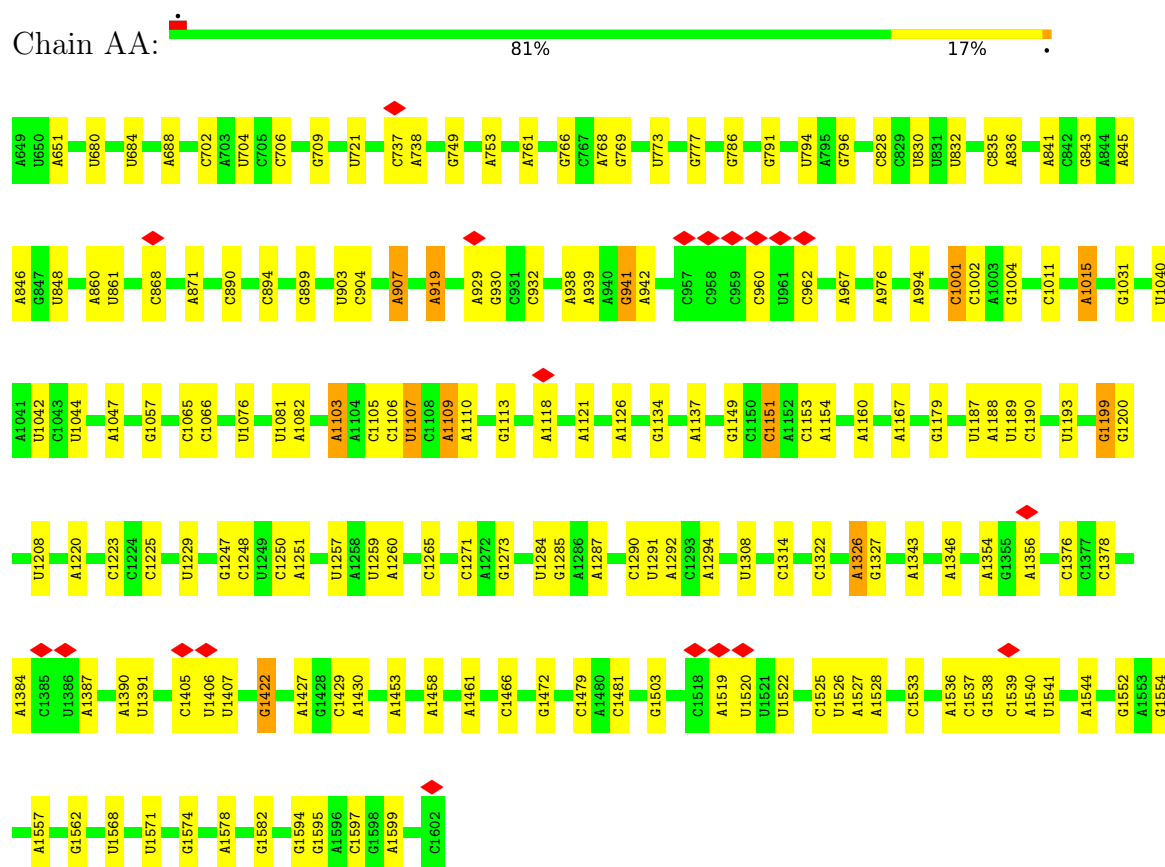
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Mol	Chain	Residues	Atoms		AltConf
101	6	98	Total 98	O 98	0
101	7	17	Total 17	O 17	0
101	8	17	Total 17	O 17	0
101	9	17	Total 17	O 17	0
101	a	13	Total 13	O 13	0
101	b	36	Total 36	O 36	0
101	c	19	Total 19	O 19	0
101	d	6	Total 6	O 6	0
101	e	13	Total 13	O 13	0
101	f	22	Total 22	O 22	0
101	g	13	Total 13	O 13	0
101	i	54	Total 54	O 54	0
101	j	23	Total 23	O 23	0
101	k	6	Total 6	O 6	0
101	l	5	Total 5	O 5	0
101	m	8	Total 8	O 8	0
101	o	34	Total 34	O 34	0
101	p	10	Total 10	O 10	0
101	r	46	Total 46	O 46	0
101	s	49	Total 49	O 49	0

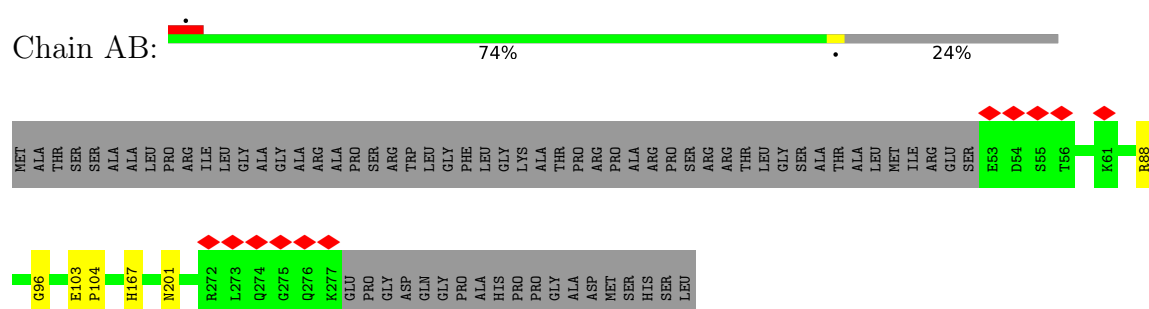
3 Residue-property plots

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


• Molecule 1: 12S mitochondrial rRNA

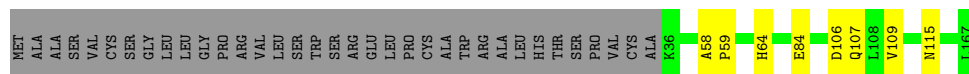


• Molecule 2: 28S ribosomal protein S2, mitochondrial




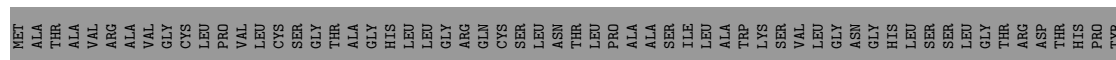
- Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain AC:  74% 5% 21%



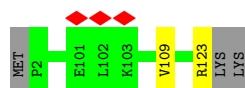
- Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain AD:  8% 77% 20%




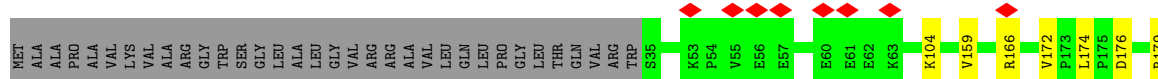
- Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain AE:  96% 4% 0%




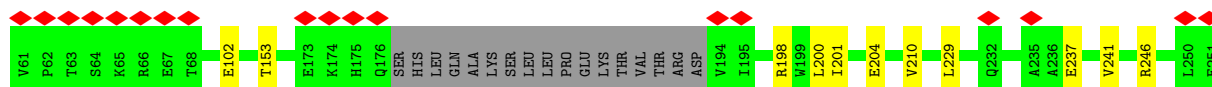
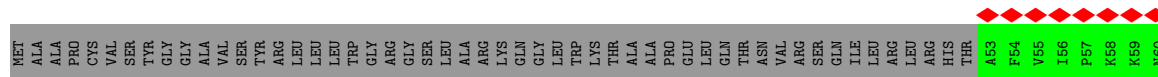
- Molecule 6: 28S ribosomal protein S7, mitochondrial

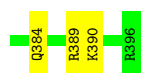
Chain AF:  81% 5% 14%



- Molecule 7: 28S ribosomal protein S9, mitochondrial

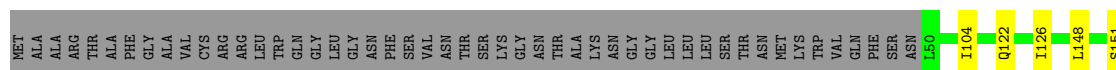
Chain AG:  7% 79% 17%





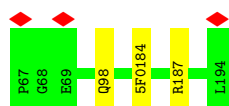
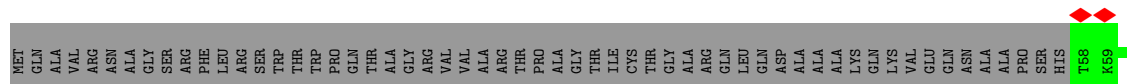
- Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain AH: 66% 30%



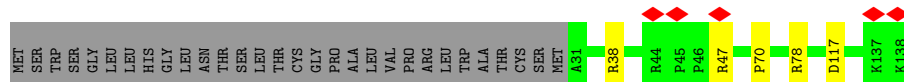
- Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain AI: 69% 29%



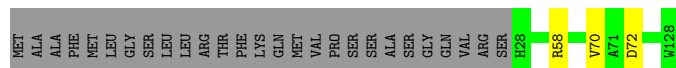
- Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain AJ: 75% 22%



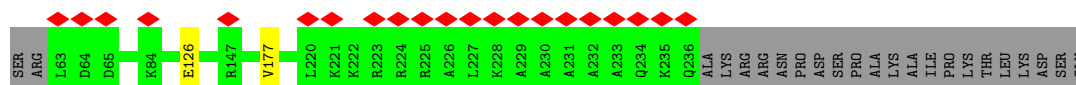
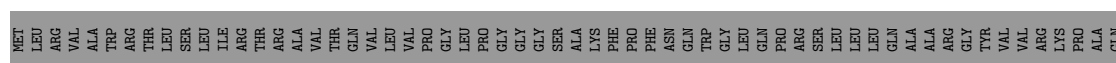
- Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain AK: 77% 21%

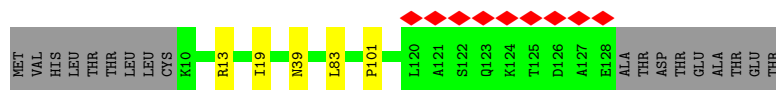
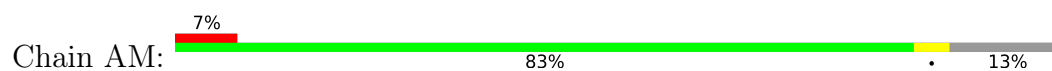


- Molecule 12: 28S ribosomal protein S15, mitochondrial

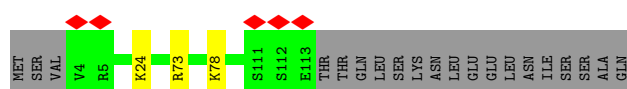
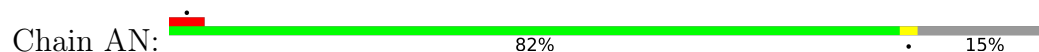
Chain AL: 8% 67% 32%



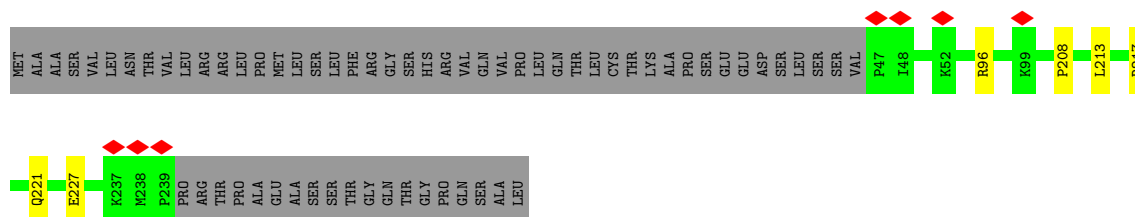
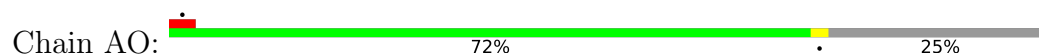
- Molecule 13: 28S ribosomal protein S16, mitochondrial



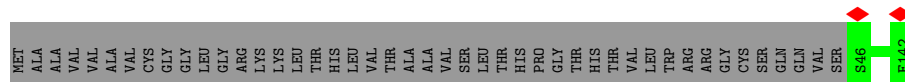
- Molecule 14: 28S ribosomal protein S17, mitochondrial



- Molecule 15: 28S ribosomal protein S18b, mitochondrial



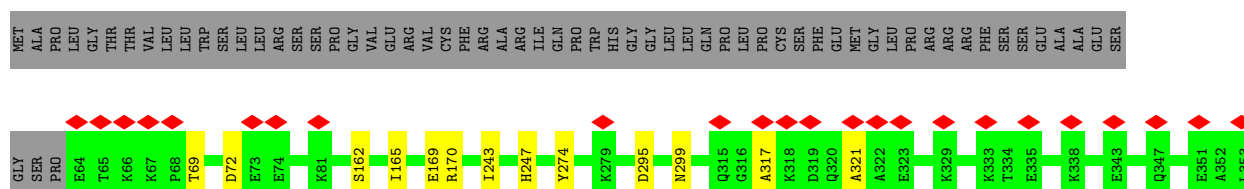
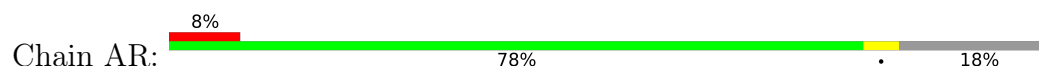
- Molecule 16: 28S ribosomal protein S18c, mitochondrial

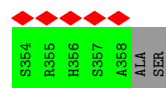


- Molecule 17: MRPS21 isoform 1

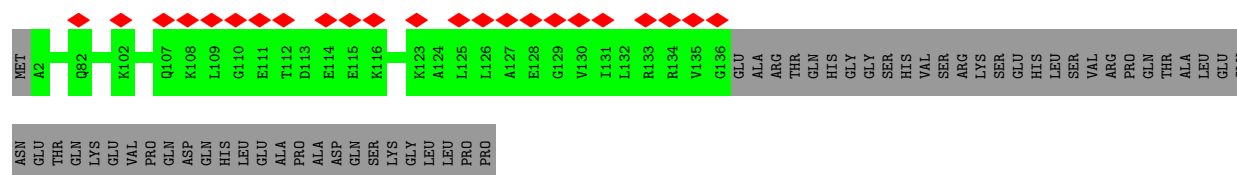
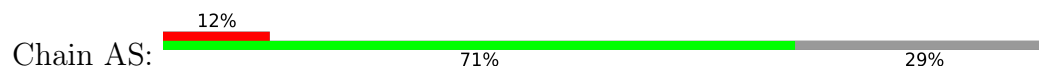


- Molecule 18: 28S ribosomal protein S22, mitochondrial

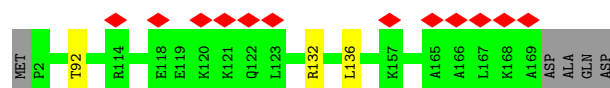




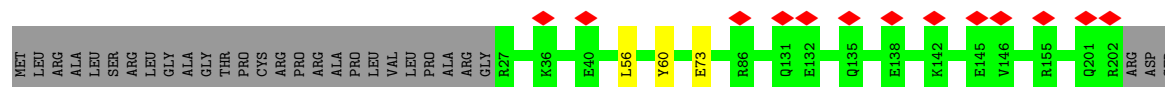
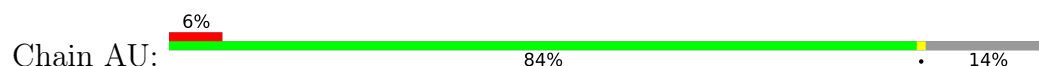
- Molecule 19: 28S ribosomal protein S23, mitochondrial



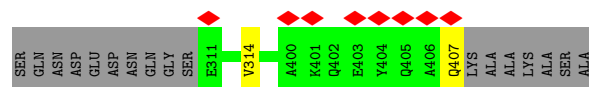
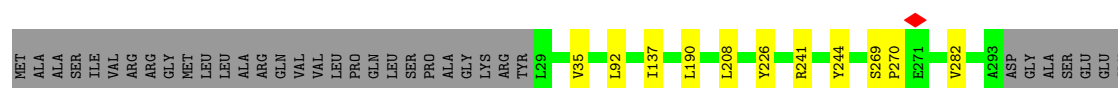
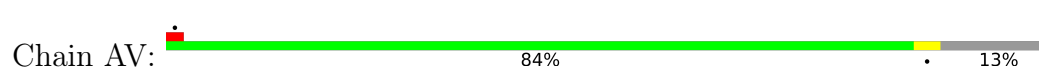
- Molecule 20: 28S ribosomal protein S25, mitochondrial



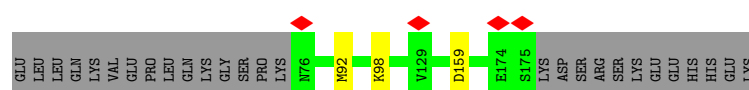
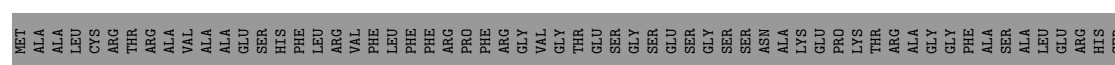
- Molecule 21: 28S ribosomal protein S26, mitochondrial




- Molecule 22: 28S ribosomal protein S27, mitochondrial

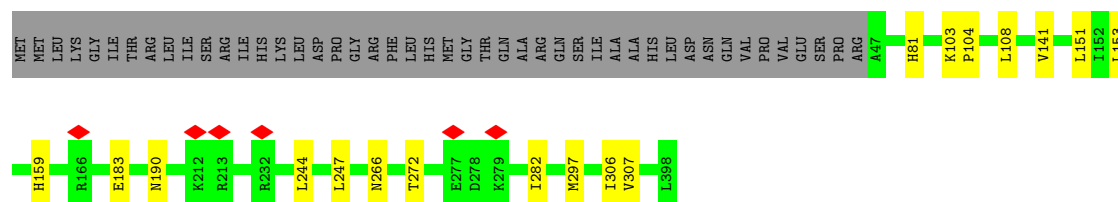


- Molecule 23: 28S ribosomal protein S28, mitochondrial



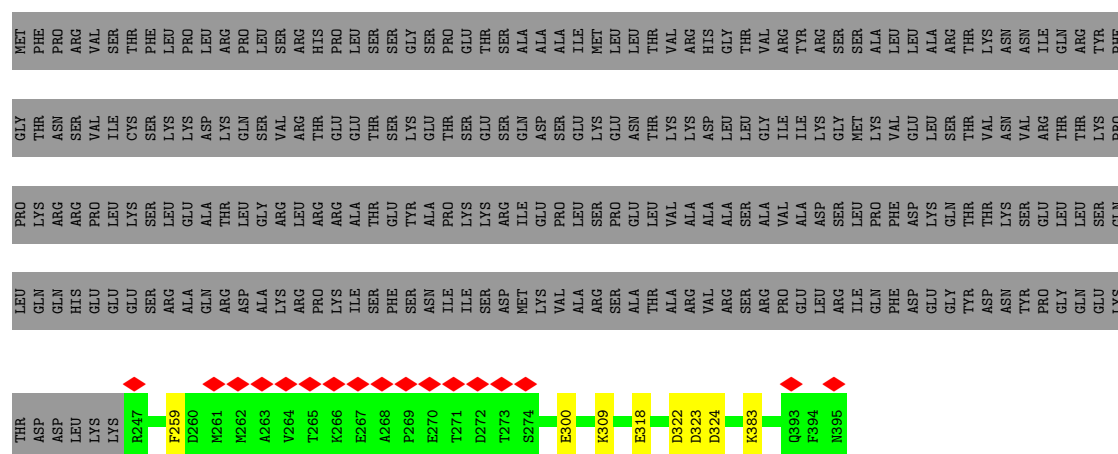
- Molecule 24: 28S ribosomal protein S29, mitochondrial

Chain AX:  84% 5% 12%



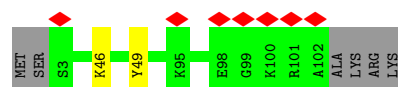
- Molecule 25: 28S ribosomal protein S31, mitochondrial

Chain AY:  36% 62%



- Molecule 26: 28S ribosomal protein S33, mitochondrial

Chain AZ:  7% 92% 6%




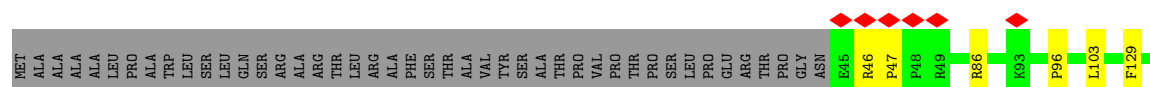
- Molecule 27: 28S ribosomal protein S34, mitochondrial

Chain A0:  93% 6%

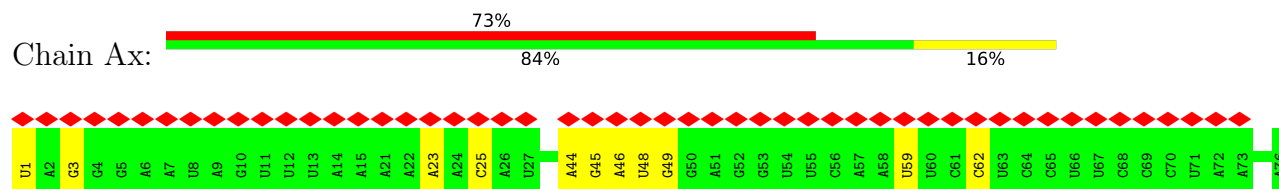


- Molecule 28: 28S ribosomal protein S35, mitochondrial

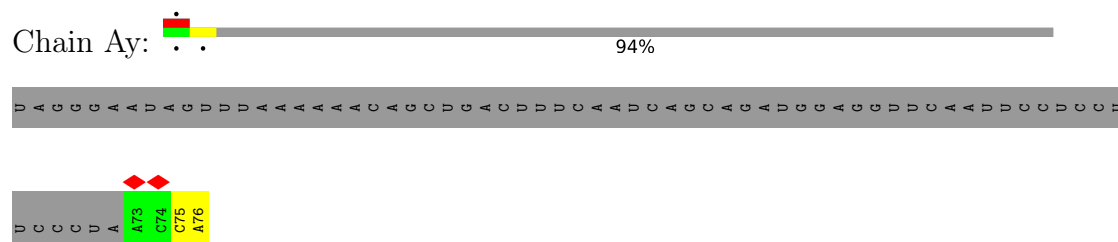
Chain A1:  6% 83% 14%



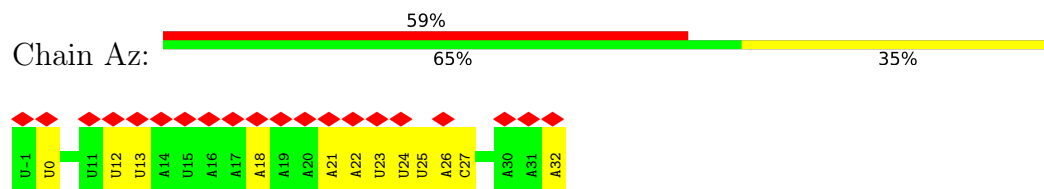
- Molecule 33: P/P-tRNA



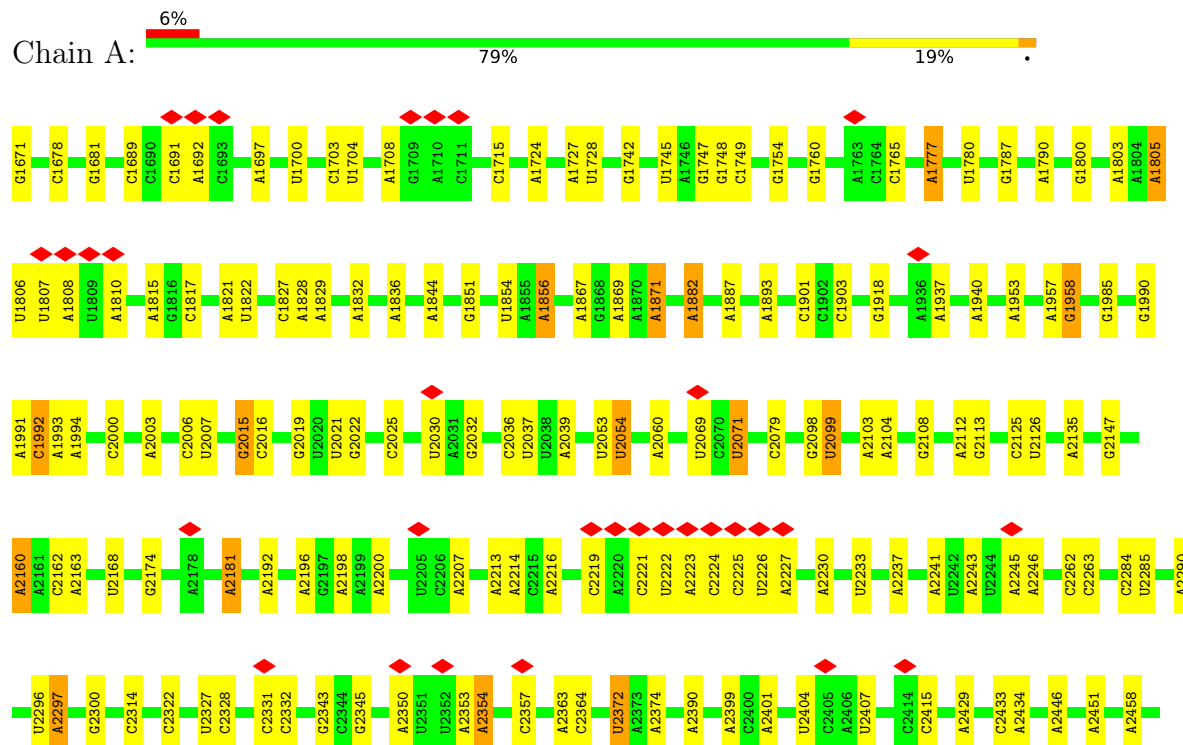
- Molecule 34: E/E-tRNA

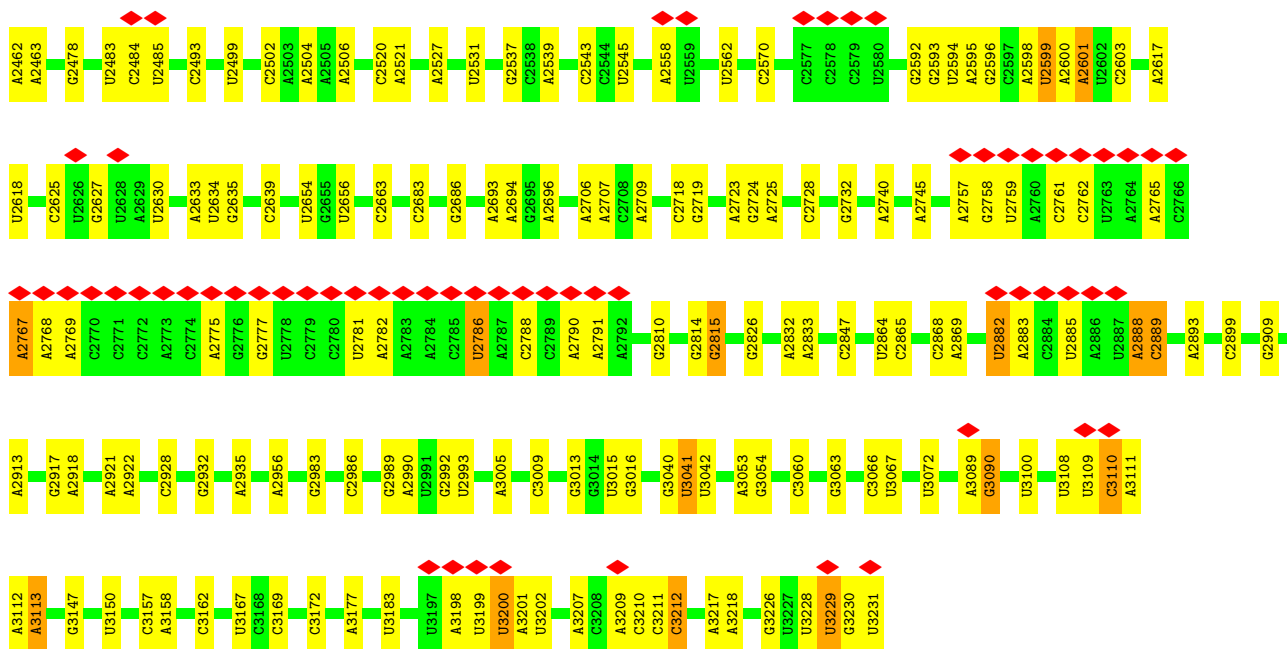


- Molecule 35: mRNA

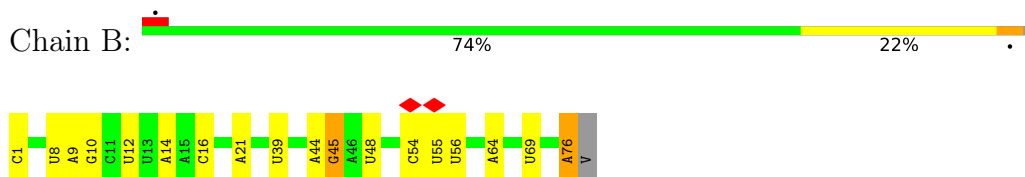


- Molecule 36: 16S mitochondrial rRNA

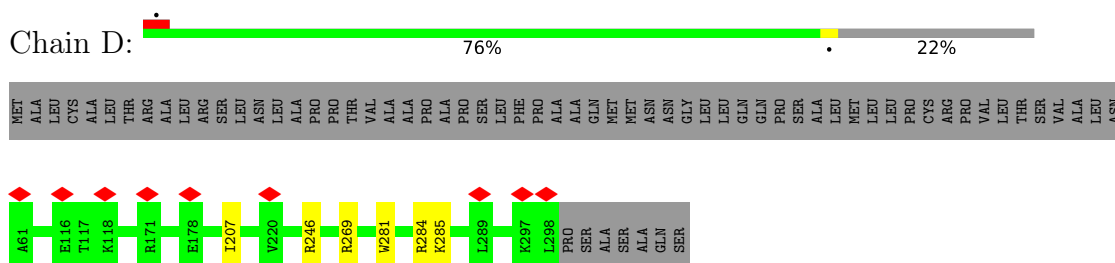




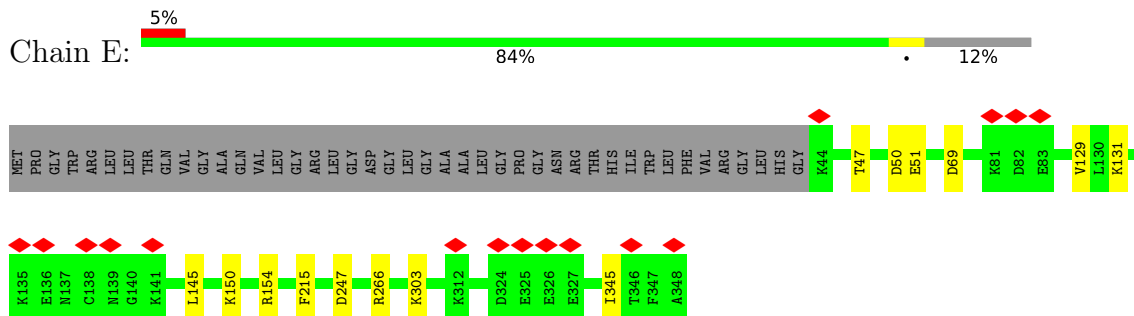
- Molecule 37: mitochondrial tRNA^{Val}




- Molecule 38: 39S ribosomal protein L2, mitochondrial

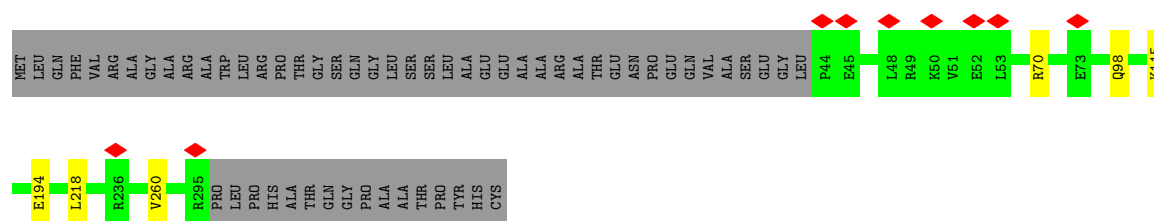


- Molecule 39: 39S ribosomal protein L3, mitochondrial



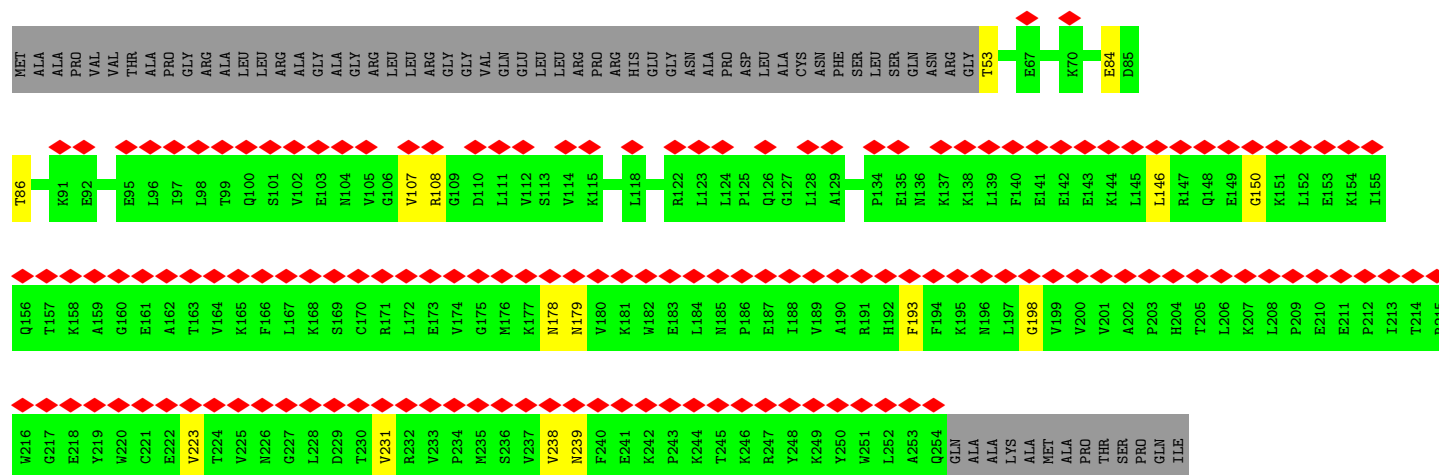
- Molecule 40: 39S ribosomal protein L4, mitochondrial

Chain F: 




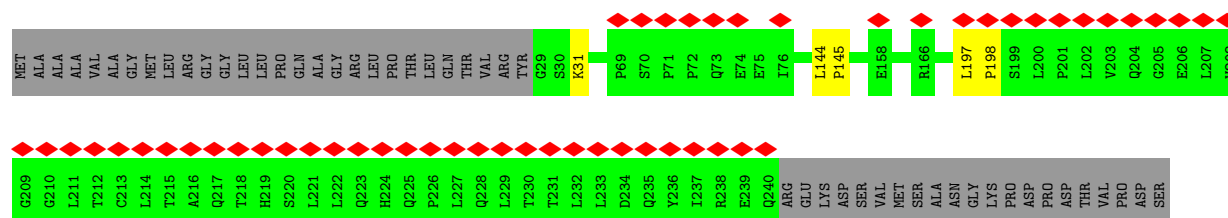
- Molecule 41: 39S ribosomal protein L9, mitochondrial

Chain H: 




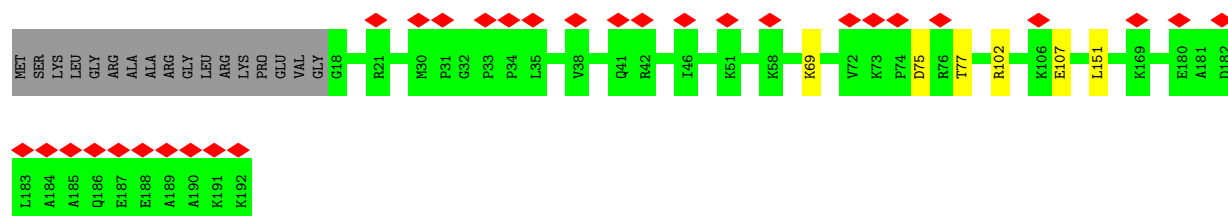
- Molecule 42: 39S ribosomal protein L10, mitochondrial

Chain I: 



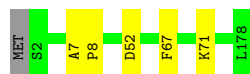
- Molecule 43: 39S ribosomal protein L11, mitochondrial

Chain J: 




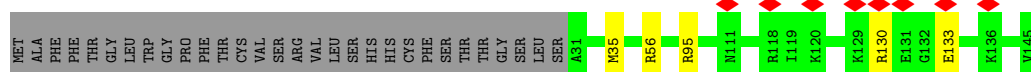
- Molecule 44: 39S ribosomal protein L13, mitochondrial

Chain K:  97%



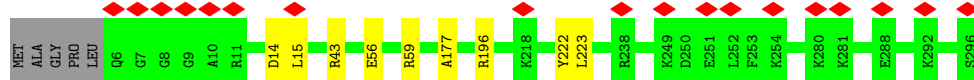
- Molecule 45: 39S ribosomal protein L14, mitochondrial

Chain L:  6% 76% 21%




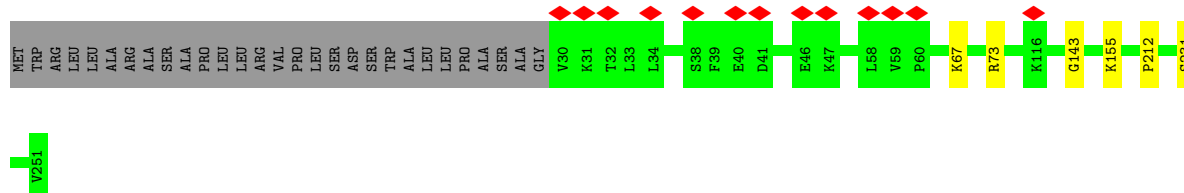
- Molecule 46: 39S ribosomal protein L15, mitochondrial

Chain M:  6% 95%




- Molecule 47: 39S ribosomal protein L16, mitochondrial

Chain N:  5% 86% 12%




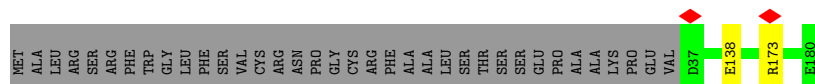
- Molecule 48: 39S ribosomal protein L17, mitochondrial

Chain O:  6% 82% 6% 12%

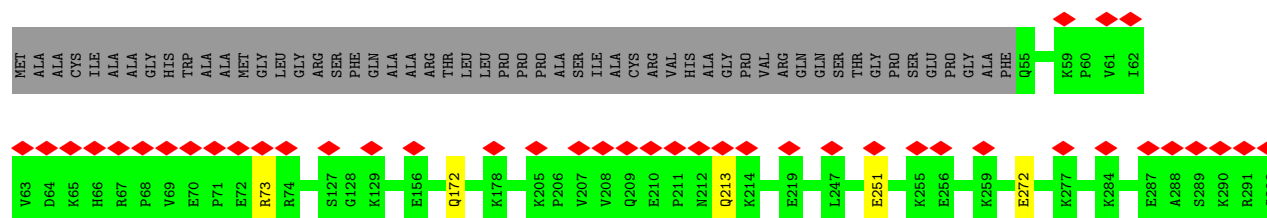
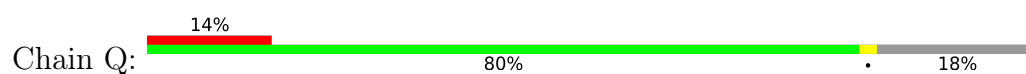


- Molecule 49: 39S ribosomal protein L18, mitochondrial

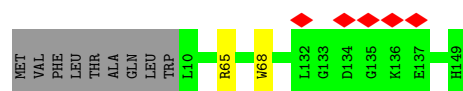
Chain P:  79% 20%



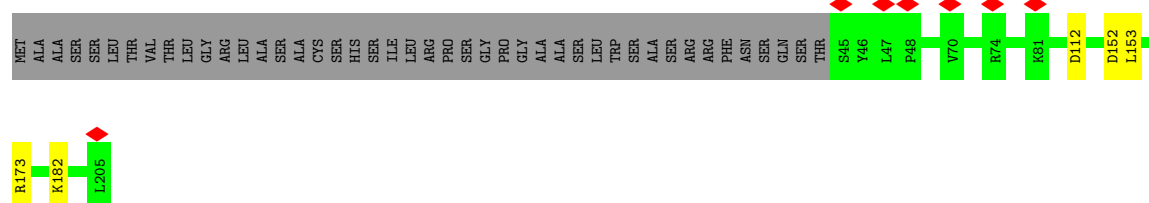
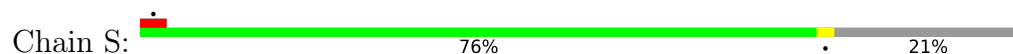
- Molecule 50: 39S ribosomal protein L19, mitochondrial



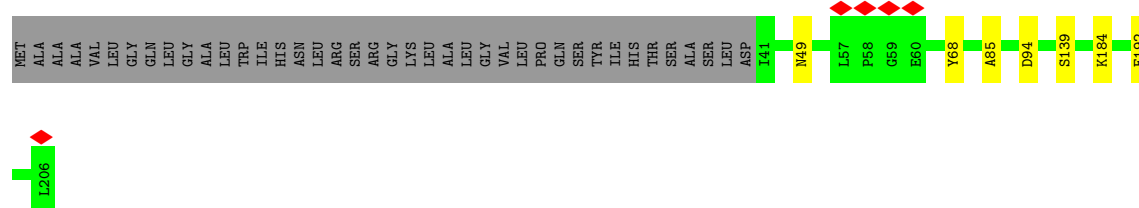
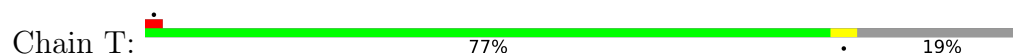
- Molecule 51: 39S ribosomal protein L20, mitochondrial



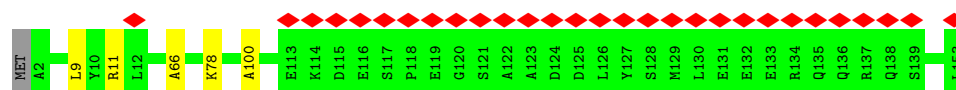
- Molecule 52: 39S ribosomal protein L21, mitochondrial



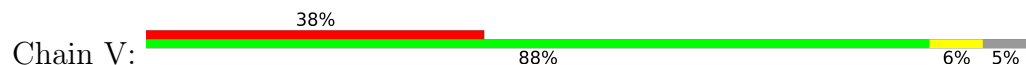
- Molecule 53: 39S ribosomal protein L22, mitochondrial

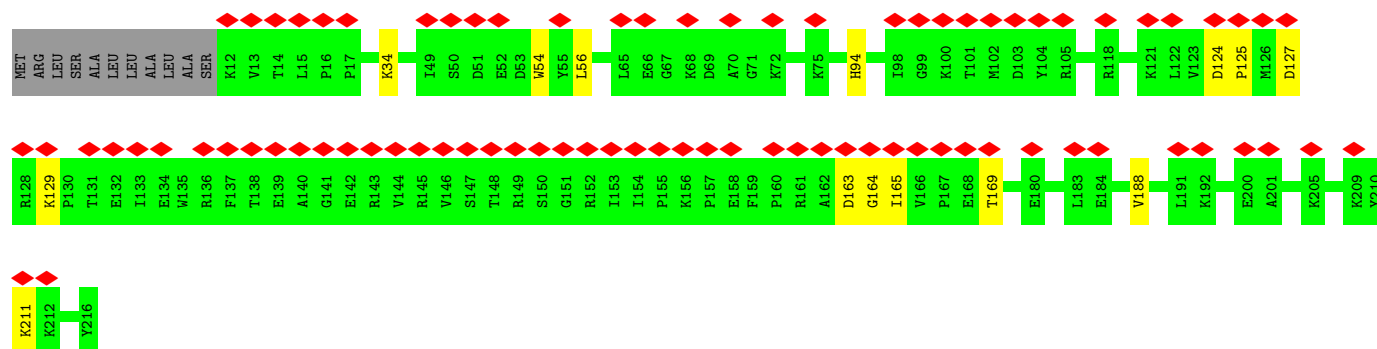


- Molecule 54: 39S ribosomal protein L23, mitochondrial



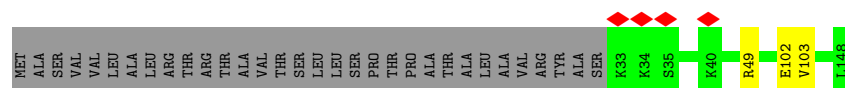
- Molecule 55: 39S ribosomal protein L24, mitochondrial





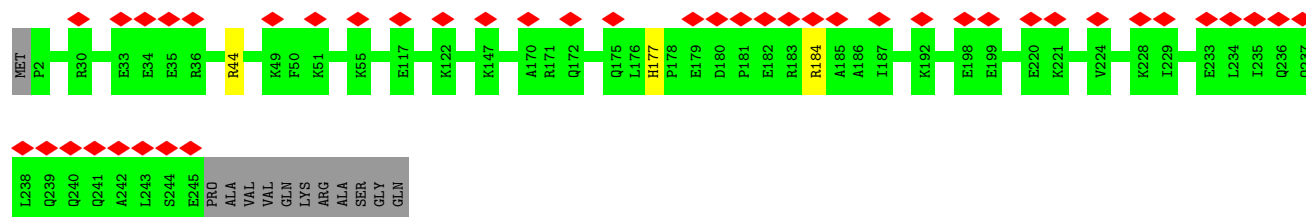
- Molecule 56: 39S ribosomal protein L27, mitochondrial

Chain W: 76% 22%



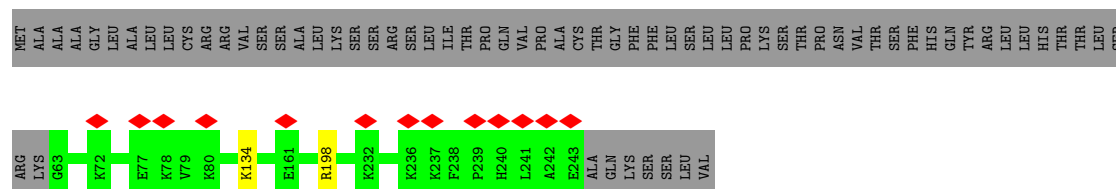
- Molecule 57: 39S ribosomal protein L28, mitochondrial

Chain X: 17% 94% 5%



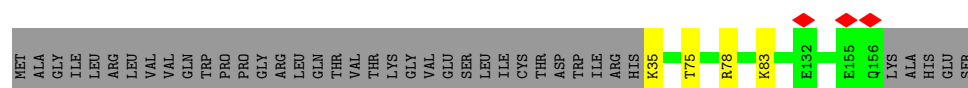
- Molecule 58: 39S ribosomal protein L47, mitochondrial

Chain Y: 5% 72% 28%



- Molecule 59: 39S ribosomal protein L30, mitochondrial

Chain Z: 5% 73% 24%



- Molecule 60: 39S ribosomal protein L32, mitochondrial

Chain 0: 5% 57% 41%

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

ASP THR SER GLY SER LYS GLU ASN SER SER LEU ASP SER SER PHE TRP MET A79 Q98 E112 E133 K143 Y160 T164 P165 S166 E167 Q168 D169 Q170 K180 Q187 N188

- Molecule 61: 39S ribosomal protein L33, mitochondrial

Chain 1: 20% 85% 14%

MET PHE LEU VAL ALA ALA PHE PHE ALA K10 S11 K12 S13 K14 L37 R38 E39 K40 K51 K59 K60 R63 S64 L65

- Molecule 62: 39S ribosomal protein L34, mitochondrial

Chain 2: 50% 50%

MET ALA VAL LEU LEU ALA GLY SER LEU LEU LEU GLY PRO THR ARG SER SER ALA LEU LEU LEU GLY ARG TRP LEU GLN PRO ARG ALA TRP LEU GLY PHE PRO ASP ALA TRP GLY LEU PRO THR PRO GLN ALA ARG K47 H92

- Molecule 63: 39S ribosomal protein L35, mitochondrial

Chain 3: 49% 49%

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

THR THR SER GLU ARG ASN THR CYS GLY HIS THR SER VAL ILE LEU ASN MET ALA PRO VAL LEU SER VAL SER THR LYS PRO VAL ARG SER L94 R104 K108 V188

- Molecule 64: 39S ribosomal protein L36, mitochondrial

Chain 4: 35% 63%

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

LEU PRO ALA LEU GLY F66 W88 M103

- Molecule 65: 39S ribosomal protein L37, mitochondrial

Chain 5: 11% 91% 7%

MET ALA LEU ALA SER GLY PRO ALA ARG ARG ALA LEU ALA GLY SER GLY GLN LEU GLY LEU GLY PHE PHE ALA PRO ARG ARG GLY A30 K40 S41 E42 P43 L46 E56 K63 E95 Y105 E130 E134 K135 D141 D142 P143 R144 N145 H146 I147 E148 N149



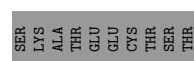
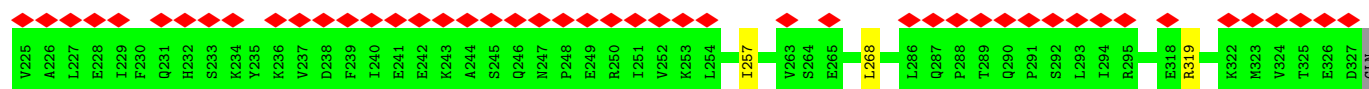
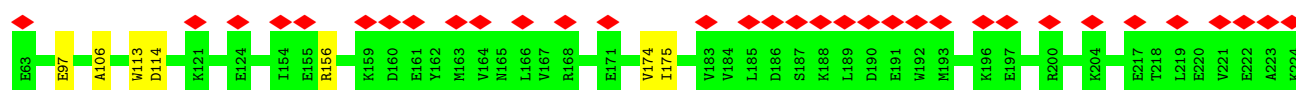
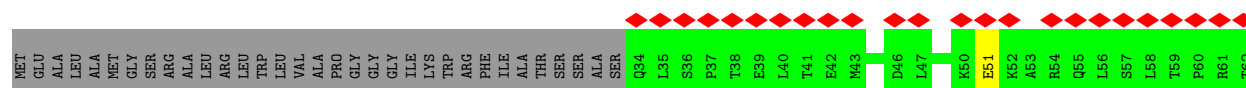
- Molecule 66: 39S ribosomal protein L38, mitochondrial

Chain 6: 89% 7%



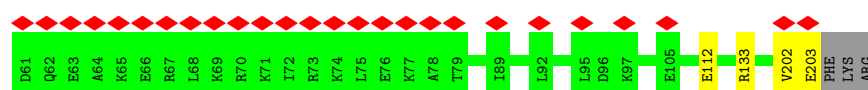
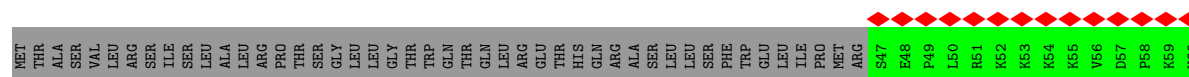
- Molecule 67: 39S ribosomal protein L39, mitochondrial

Chain 7: 31% 84% 13%



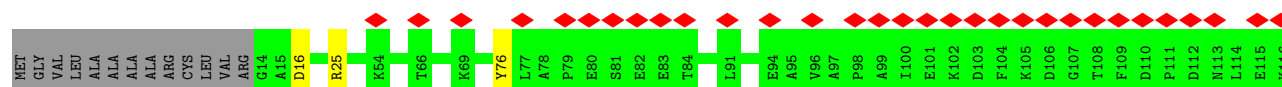
- Molecule 68: 39S ribosomal protein L40, mitochondrial

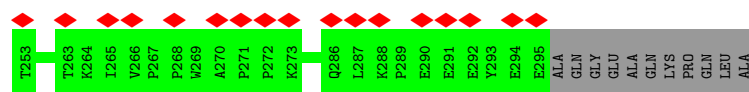
Chain 8: 19% 74% 24%



- Molecule 69: 39S ribosomal protein L41, mitochondrial

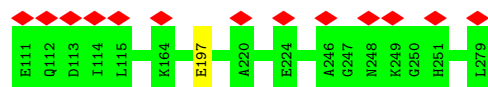
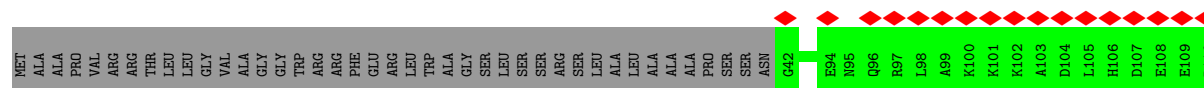
Chain 9: 25% 88% 9%





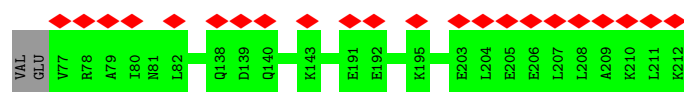
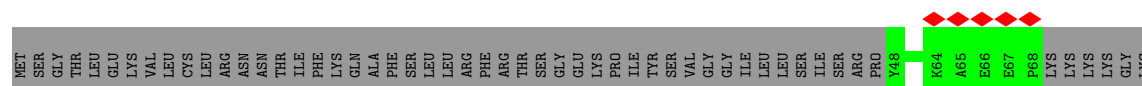
- Molecule 74: 39S ribosomal protein L46, mitochondrial

Chain e: 11% 85% 15%



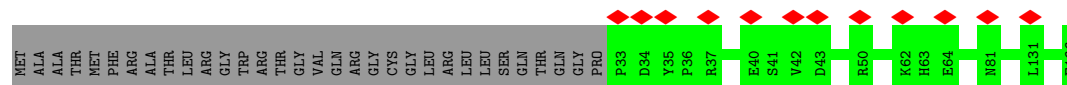
- Molecule 75: 39S ribosomal protein L48, mitochondrial

Chain f: 13% 74% 26%



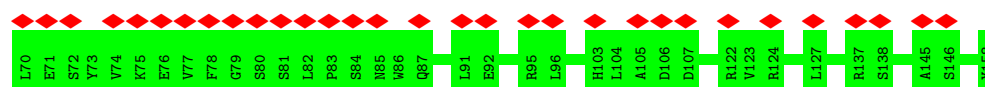
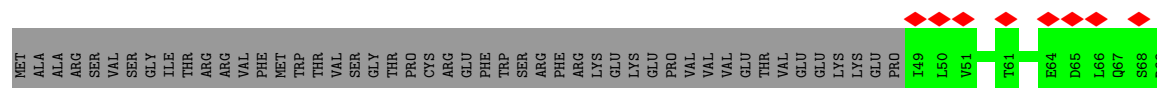
- Molecule 76: 39S ribosomal protein L49, mitochondrial

Chain g: 7% 81% 19%



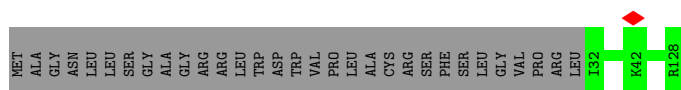
- Molecule 77: 39S ribosomal protein L50, mitochondrial

Chain h: 25% 70% 30%

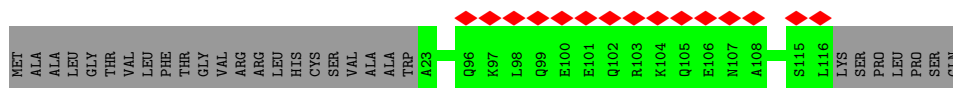
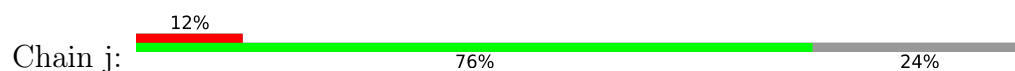


- Molecule 78: 39S ribosomal protein L51, mitochondrial

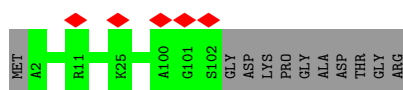
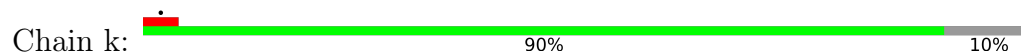
Chain i: 76% 24%



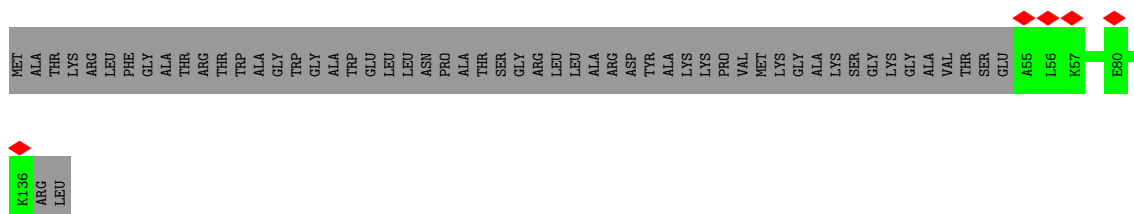
- Molecule 79: 39S ribosomal protein L52, mitochondrial



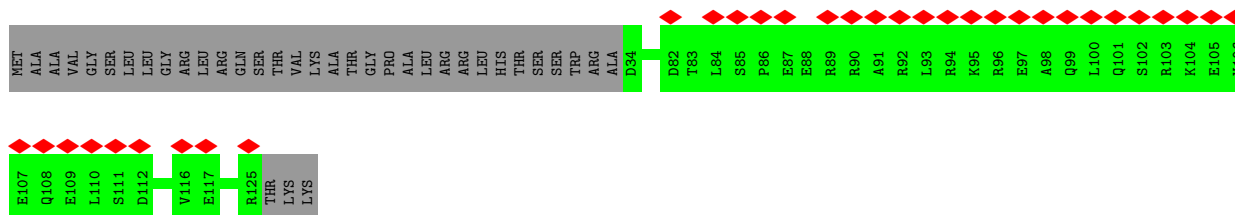
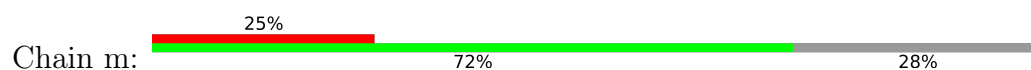
- Molecule 80: 39S ribosomal protein L53, mitochondrial



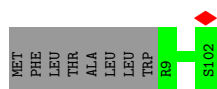
- Molecule 81: 39S ribosomal protein L54, mitochondrial



- Molecule 82: 39S ribosomal protein L55, mitochondrial



- Molecule 83: Ribosomal protein 63, mitochondrial



- Molecule 84: Peptidyl-tRNA hydrolase ICT1, mitochondrial

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

- Molecule 88: 39S ribosomal protein L12, mitochondrial



MET	LEU	PRO	ALA	ALA	ALA	ARG	PRO	LEU	TRP	GLY	PRO	CYS	LEU	GLY	LEU	ARG	ALA	ALA	ALA	PHE	ARG	LEU	ALA	ARG	ARG	ARG	GLN	VAL	PRO	CYS	CYS	VAL	ALA	VAL	ARG	HIS	MET	ARG	SER	SER	GLY	HIS	GLN	ARG	CYS	GLY	ALA	ALA	LEU	VAL	PRO	GLY	ALA	ALA	PRO	LYS	ASP	ASN	ALA	ALA	PRO	LYS	GLU	TRP		
P61	P62	K63	I64	Q65	Q66	L67	V68	Q69	D70	I71	A72	S73	L74	T76	L76	L77	E78	I79	S80	D81	L82	N83	E84	L85	L86	K87	K88	T89	L90	K91	ILE	GLN	ASP	VAL	GLY	LEU	VAL	VAL	PRO	MET	GLY	GLY	ALA	VAL	VAL	LEU	MET	SER	GLY	ALA	VAL	PRO	PRO	LYS	ASP	ASN	ALA	ALA	PRO	LYS	GLU	TRP				
ILE	PRO	ILE	ALA	LYS	GLU	ARG	THR	HIS	PHE	THR	VAL	ARG	LEU	THR	THR	VAL	ALA	LYS	PRO	VAL	ASP	LYS	VAL	ALA	LEU	ILE	LYS	GLU	TLE	LYS	ASN	TYR	ILE	GLN	GLY	ILE	ASN	LEU	VAL	GLN	ALA	LYS	VAL	LEU	VAL	GLY	LEU	VAL	VAL	LEU	PRO	PRO	GLN	GLU	TLE	LYS	ALA	ASN	VAL	VAL	ALA	LYS	GLU	ALA	GLU	
ALA	GLU	LYS	ILE	LYS	ALA	ALA	LEU	ALA	ALA	VAL	GLY	GLY	THR	VAL	VAL	LEU	GLU	ALA	LYS	PRO	VAL	ASP	LYS	VAL	ALA	LEU	ILE	LYS	GLU	TLE	LYS	ASN	TYR	ILE	GLN	GLY	ILE	ASN	LEU	VAL	GLN	ALA	LYS	VAL	LEU	VAL	GLY	LEU	VAL	VAL	LEU	PRO	PRO	GLN	GLU	TLE	LYS	ALA	ASN	VAL	VAL	ALA	LYS	GLU	ALA	GLU

- Molecule 88: 39S ribosomal protein L12, mitochondrial



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

- Molecule 89: 39S ribosomal protein L1, mitochondrial



MET	ALA	ALA	ALA	VAL	ARG	CYS	MET	GLY	ARG	ALA	ALA	ILE	HIS	HIS	GLN	ARG	HIS	SER	LEU	SER	SER	MET	VAL	TYR	GLN	THR	SER	LEU	CYS	SER	CYS	SER	VAL	ASN	ILE	ARG	VAL	PRO	ASN	ARG	HIS	PHE	ALA	ALA	ALA	THR	LYS	SER	LYS	LYS	GLY	ALA	LYS	GLU	LYS				
T61	P62	D63	E64	K65	K66	D67	E68	I69	E70	K71	I72	K73	A74	Y75	P76	Y77	M78	E79	G80	E81	P82	E83	D84	D85	V86	Y87	L88	X89	R90	L91	Y92	P93	R94	Q95	T96	Y97	E98	V99	E100	K101	A102	Y103	H104	L105	L106	K107	K108	F109	Q110	I111	L112	D113	F114	T115	S116	P117	K118	Q119	S120
V121	Y122	L123	D124	L125	T126	L127	D128	M129	A130	L131	G132	K133	K134	K135	N136	V137	E138	P139	F140	T141	S142	V143	L144	S145	L146	P147	Y148	P149	F150	A151	SER	GLU	ILE	ASN	LYS	VAL	VAL	VAL	PHE	THR	GLU	ASN	ALA	SER	SER	GLU	VAL	LYS	ILE	ALA	GLU	GLU	ASN	GLY	ALA	PHE	ALA	GLY	GLY

E301	G302	L303	L304	L305	K306	L307	D308	P309	L310	L311	P312	LYS	GLU	VAL	LYS	ASN	GLU	GLU	GLU	SER	GLU	GLU	LYS	LYS	GLU	ASP	ALA																															
H241	E242	L243	L244	V245	D246	E247	E248	R249	E250	M251	F252	L253	Q254	T255	K256	L257	A258	T259	L260	D261	M262	S263	S264	D265	Q266	L267	A268	A269	N270	L271	Q272	A273	V274	L275	N276	E277	V278	C279	R280	H281	R282	P283	L284	M285	L286	C287	P288	F289	V290	V291	R292	F294	L295	S296	S297	S298	T299	S300
THR	SER	LEU	ILE	GLN	LYS	ILE	TRP	ASP	ASP	GLU	ILE	VAL	ALA	VAL	PRO	GLU	ILE	MET	PRO	GLU	LEU	ASN	ARG	ARG	LYS	LYS	ASN	LYS	LYS	TRP	PRO	LYS	SER	ARG	ASN	SER	ILE	GLY	ARG	ASP	ILE	PRO	LYS	MET	LYS	LEU	GLU	LEU	PHE	LYS	ASN	G240						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	509691	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	71.473	Depositor
Minimum map value	-28.186	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.438	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, MG, GDP, 2MG, ATP, OMG, PUT, THC, SPD, AYA, B8T, SPM, OMU, 5MC, 5MU, FES, NAD, 1MA, MA6, K, SAC, ZN, 5F0

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	AA	0.20	0/22537	0.67	0/35085
2	AB	0.24	0/1871	0.49	0/2531
3	AC	0.25	0/1113	0.48	0/1505
4	AD	0.24	0/2783	0.51	0/3724
5	AE	0.24	0/989	0.51	0/1335
6	AF	0.24	0/1767	0.46	0/2373
7	AG	0.24	0/2746	0.48	0/3681
8	AH	0.24	0/1178	0.47	0/1598
9	AI	0.25	0/1030	0.49	0/1386
10	AJ	0.25	0/855	0.55	0/1148
11	AK	0.22	0/880	0.57	0/1182
12	AL	0.23	0/1477	0.47	0/1974
13	AM	0.24	0/963	0.54	0/1295
14	AN	0.24	0/886	0.50	0/1199
15	AO	0.24	0/1648	0.48	0/2243
16	AP	0.24	0/798	0.44	0/1070
17	AQ	0.23	0/748	0.56	0/994
18	AR	0.23	0/2456	0.44	0/3317
19	AS	0.24	0/1138	0.50	0/1533
20	AT	0.24	0/1402	0.46	0/1883
21	AU	0.23	0/1510	0.53	0/2025
22	AV	0.25	0/3030	0.41	0/4093
23	AW	0.25	0/801	0.50	0/1079
24	AX	0.24	0/2921	0.44	0/3954
25	AY	0.24	0/1280	0.39	0/1725
26	AZ	0.25	0/857	0.49	0/1141
27	A0	0.24	0/1834	0.54	0/2484
28	A1	0.24	0/2313	0.45	0/3129
29	A2	0.23	0/941	0.52	0/1257
30	A3	0.23	0/636	0.58	0/839
31	A4	0.24	0/4877	0.43	0/6598

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Aw	0.13	0/517	0.64	0/799
33	Ax	0.29	1/1655 (0.1%)	0.65	0/2569
34	Ay	0.13	0/93	0.68	0/142
35	Az	0.14	0/805	0.65	0/1250
36	A	0.19	1/36876 (0.0%)	0.68	0/57402
37	B	0.33	1/1627 (0.1%)	0.67	0/2527
38	D	0.23	0/1896	0.57	0/2549
39	E	0.24	0/2475	0.47	0/3355
40	F	0.23	0/2090	0.50	0/2842
41	H	0.23	0/1698	0.49	0/2292
42	I	0.24	0/1731	0.48	0/2345
43	J	0.25	0/1348	0.48	0/1813
44	K	0.24	0/1490	0.47	0/2021
45	L	0.23	0/905	0.53	0/1218
46	M	0.25	0/2381	0.53	0/3212
47	N	0.24	0/1833	0.51	0/2468
48	O	0.23	0/1283	0.54	0/1727
49	P	0.24	0/1199	0.54	0/1623
50	Q	0.24	0/2027	0.50	0/2734
51	R	0.23	0/1175	0.54	0/1572
52	S	0.23	0/1320	0.53	0/1789
53	T	0.25	0/1403	0.51	0/1886
54	U	0.24	0/1274	0.54	0/1723
55	V	0.24	0/1721	0.51	0/2333
56	W	0.25	0/926	0.49	0/1244
57	X	0.24	0/2099	0.47	0/2837
58	Y	0.23	0/1593	0.50	0/2136
59	Z	0.23	0/1021	0.47	0/1378
60	0	0.23	0/913	0.53	0/1224
61	1	0.24	0/469	0.55	0/621
62	2	0.22	0/383	0.58	0/507
63	3	0.23	0/853	0.53	0/1136
64	4	0.23	0/350	0.56	0/461
65	5	0.24	0/3305	0.48	0/4502
66	6	0.25	0/3043	0.52	0/4140
67	7	0.24	0/2447	0.47	0/3310
68	8	0.24	0/1354	0.48	0/1819
69	9	0.26	0/1025	0.48	0/1379
70	a	0.24	0/866	0.51	0/1174
71	b	0.23	0/1211	0.54	0/1639
72	c	0.24	0/2347	0.47	0/3171
73	d	0.24	0/2039	0.47	0/2759
74	e	0.24	0/1970	0.47	0/2658

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	f	0.24	0/1273	0.44	0/1716
76	g	0.25	0/1151	0.49	0/1569
77	h	0.23	0/918	0.45	0/1249
78	i	0.23	0/850	0.53	0/1135
79	j	0.24	0/760	0.50	0/1023
80	k	0.24	0/777	0.53	0/1048
81	l	0.24	0/707	0.48	0/960
82	m	0.23	0/805	0.57	0/1081
83	o	0.23	0/819	0.57	0/1097
84	p	0.23	0/1223	0.50	0/1641
85	q	0.23	0/1384	0.50	0/1869
86	r	0.24	0/1362	0.53	0/1846
87	s	0.24	0/3239	0.51	0/4400
88	t	0.23	0/358	0.35	0/486
88	u	0.22	0/259	0.33	0/350
88	v	0.22	0/259	0.34	0/350
88	w	0.21	0/246	0.35	0/331
88	x	0.22	0/246	0.34	0/331
88	y	0.22	0/246	0.34	0/331
89	z	0.25	0/1354	0.47	0/1831
All	All	0.23	3/187537 (0.0%)	0.57	0/266310

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	1671	G	OP3-P	-10.71	1.48	1.61
37	B	1	C	OP3-P	-10.58	1.48	1.61
33	Ax	1	U	OP3-P	-10.51	1.48	1.61

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	AA	20260	10305	10285	58	0
2	AB	1828	1826	1815	5	0
3	AC	1083	1096	1088	7	0
4	AD	2731	2814	2804	9	0
5	AE	972	1004	1000	2	0
6	AF	1725	1778	1769	8	0
7	AG	2688	2697	2687	10	0
8	AH	1152	1191	1183	7	0
9	AI	1020	1066	1052	2	0
10	AJ	839	892	887	5	0
11	AK	862	889	885	2	0
12	AL	1453	1545	1540	2	0
13	AM	942	972	965	4	0
14	AN	868	933	928	3	0
15	AO	1592	1570	1557	4	0
16	AP	781	809	806	0	0
17	AQ	744	760	758	1	0
18	AR	2409	2436	2428	9	0
19	AS	1111	1117	1115	0	0
20	AT	1371	1396	1393	2	0
21	AU	1488	1505	1499	4	0
22	AV	2969	2972	2961	11	0
23	AW	789	806	802	2	0
24	AX	2849	2859	2843	12	0
25	AY	1246	1203	1197	6	0
26	AZ	839	862	858	1	0
27	A0	1787	1802	1796	9	0
28	A1	2265	2300	2294	9	0
29	A2	935	973	971	4	0
30	A3	625	702	699	6	0
31	A4	4768	4784	4765	11	0
32	Aw	464	237	238	0	0
33	Ax	1482	752	753	0	0
34	Ay	84	45	45	0	0
35	Az	720	360	359	0	0
36	A	33070	16802	16794	95	0
37	B	1524	779	779	3	0
38	D	1859	1928	1920	5	0
39	E	2406	2424	2415	11	0
40	F	2031	2075	2065	4	0
41	H	1661	1740	1734	9	0
42	I	1695	1794	1785	3	0
43	J	1330	1409	1407	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	K	1455	1460	1452	3	0
45	L	890	945	941	3	0
46	M	2327	2398	2395	7	0
47	N	1786	1824	1817	5	0
48	O	1259	1298	1294	7	0
49	P	1173	1171	1165	2	0
50	Q	1979	2025	2022	4	0
51	R	1154	1220	1214	1	0
52	S	1293	1369	1365	4	0
53	T	1369	1417	1410	4	0
54	U	1251	1235	1232	4	0
55	V	1676	1691	1687	10	0
56	W	904	943	935	3	0
57	X	2044	2065	2060	2	0
58	Y	1556	1603	1597	1	0
59	Z	996	1052	1044	3	0
60	0	898	919	916	2	0
61	1	464	513	511	1	0
62	2	377	409	406	0	0
63	3	832	886	883	2	0
64	4	342	363	361	2	0
65	5	3210	3222	3206	6	0
66	6	2948	2854	2841	10	0
67	7	2390	2406	2397	8	0
68	8	1327	1371	1368	3	0
69	9	997	988	987	3	0
70	a	840	819	810	0	0
71	b	1196	1199	1195	0	0
72	c	2299	2325	2320	0	0
73	d	1985	1987	1976	0	0
74	e	1931	1922	1916	0	0
75	f	1252	1277	1269	0	0
76	g	1113	1101	1097	0	0
77	h	895	885	881	0	0
78	i	828	862	857	0	0
79	j	745	747	746	0	0
80	k	774	788	784	0	0
81	l	688	676	674	0	0
82	m	791	763	796	0	0
83	o	798	810	804	0	0
84	p	1205	1228	1223	0	0
85	q	1350	1329	1327	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	r	1322	1355	1348	0	0
87	s	3155	3151	3139	0	0
88	t	354	378	377	0	0
88	u	257	284	283	0	0
88	v	257	284	283	0	0
88	w	245	275	275	0	0
88	x	245	275	275	0	0
88	y	245	275	275	0	0
89	z	1327	1358	1353	0	0
90	AA	44	26	26	0	0
91	AA	14	30	26	0	0
92	A	30	66	57	0	0
92	AA	10	22	19	0	0
93	A	137	0	0	0	0
93	A3	1	0	0	0	0
93	AA	58	0	0	0	0
93	AB	1	0	0	0	0
93	AX	1	0	0	0	0
93	Aw	1	0	0	0	0
93	D	2	0	0	0	0
93	E	1	0	0	0	0
93	g	1	0	0	0	0
94	3	1	0	0	0	0
94	6	1	0	0	0	0
94	A	31	0	0	0	0
94	A4	1	0	0	0	0
94	AA	20	0	0	0	0
94	D	1	0	0	0	0
94	M	1	0	0	0	0
94	W	1	0	0	0	0
94	i	1	0	0	0	0
94	o	1	0	0	0	0
95	0	1	0	0	0	0
95	4	1	0	0	0	0
95	AO	1	0	0	0	0
96	AP	4	0	0	0	0
96	AT	4	0	0	0	0
96	r	4	0	0	0	0
97	AX	31	12	12	1	0
98	AX	28	12	12	0	0
99	A	6	14	12	0	0
100	B	7	11	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
101	0	27	0	0	0	0
101	1	3	0	0	0	0
101	2	34	0	0	0	0
101	3	40	0	0	0	0
101	4	13	0	0	0	0
101	5	16	0	0	0	0
101	6	98	0	0	1	0
101	7	17	0	0	0	0
101	8	17	0	0	1	0
101	9	17	0	0	0	0
101	A	3051	0	0	21	0
101	A0	1	0	0	0	0
101	A1	36	0	0	0	0
101	A2	35	0	0	0	0
101	A3	52	0	0	1	0
101	A4	11	0	0	0	0
101	AA	2149	0	0	22	0
101	AB	77	0	0	1	0
101	AC	55	0	0	0	0
101	AD	79	0	0	1	0
101	AE	29	0	0	0	0
101	AF	37	0	0	0	0
101	AG	71	0	0	1	0
101	AH	50	0	0	0	0
101	AI	45	0	0	0	0
101	AJ	27	0	0	1	0
101	AK	50	0	0	0	0
101	AL	42	0	0	0	0
101	AM	21	0	0	0	0
101	AN	34	0	0	0	0
101	AO	36	0	0	0	0
101	AP	31	0	0	0	0
101	AQ	67	0	0	0	0
101	AR	12	0	0	0	0
101	AS	25	0	0	0	0
101	AT	43	0	0	0	0
101	AU	8	0	0	0	0
101	AW	16	0	0	0	0
101	AX	61	0	0	1	0
101	AY	20	0	0	1	0
101	AZ	27	0	0	0	0
101	Aw	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
101	Ax	5	0	0	0	0
101	Ay	1	0	0	0	0
101	Az	14	0	0	0	0
101	B	64	0	0	0	0
101	D	70	0	0	0	0
101	E	72	0	0	1	0
101	F	77	0	0	2	0
101	H	9	0	0	0	0
101	I	23	0	0	1	0
101	J	1	0	0	0	0
101	K	65	0	0	1	0
101	L	25	0	0	1	0
101	M	67	0	0	1	0
101	N	59	0	0	2	0
101	O	38	0	0	0	0
101	P	88	0	0	1	0
101	Q	28	0	0	0	0
101	R	58	0	0	0	0
101	S	49	0	0	1	0
101	T	48	0	0	0	0
101	U	26	0	0	0	0
101	V	5	0	0	0	0
101	W	49	0	0	0	0
101	X	12	0	0	0	0
101	Y	27	0	0	0	0
101	Z	33	0	0	0	0
101	a	13	0	0	0	0
101	b	36	0	0	0	0
101	c	19	0	0	0	0
101	d	6	0	0	0	0
101	e	13	0	0	0	0
101	f	22	0	0	0	0
101	g	13	0	0	0	0
101	i	54	0	0	0	0
101	j	23	0	0	0	0
101	k	6	0	0	0	0
101	l	5	0	0	0	0
101	m	8	0	0	0	0
101	o	34	0	0	0	0
101	p	10	0	0	0	0
101	r	46	0	0	0	0
101	s	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	186713	152402	151885	369	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 1.

All (369) 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)
36:A:2103:A:HO2'	59:Z:35:LYS:N	1.73	0.84
7:AG:389:ARG:NH1	7:AG:390:LYS:O	2.12	0.83
1:AA:1472:G:O6	101:AA:1801:HOH:O	2.00	0.79
36:A:3063:G:O2'	36:A:3066:C:OP2	1.99	0.79
36:A:3042:U:OP2	101:A:3501:HOH:O	2.00	0.79
36:A:3198:A:O2'	36:A:3200:U:O2'	2.01	0.78
54:U:9:LEU:O	54:U:11:ARG:NH1	2.18	0.77
36:A:3147:G:OP1	101:A:3502:HOH:O	2.05	0.75
36:A:2098:G:O2'	36:A:2099:U:OP2	2.04	0.75
66:6:121:ARG:NH1	68:8:112:GLU:OE2	2.20	0.75
36:A:3226:G:O2'	36:A:3229:U:O4	2.04	0.74
36:A:3041:U:OP1	101:A:3504:HOH:O	2.06	0.74
22:AV:226:TYR:HE1	22:AV:282:VAL:HG21	1.52	0.73
40:F:115:LYS:NZ	101:F:401:HOH:O	2.20	0.73
24:AX:108:LEU:HD23	24:AX:141:VAL:HG21	1.72	0.72
1:AA:941:G:OP1	101:AA:1802:HOH:O	2.08	0.72
1:AA:1287:A:OP2	4:AD:260:LYS:NZ	2.22	0.71
54:U:11:ARG:NH2	55:V:211:LYS:O	2.22	0.71
36:A:3113:A:OP1	36:A:3167:U:O2'	2.03	0.71
1:AA:1047:A:OP2	101:AA:1803:HOH:O	2.09	0.70
68:8:133:ARG:NH1	101:8:301:HOH:O	2.19	0.70
36:A:1777:A:N6	36:A:1780:U:OP2	2.26	0.69
36:A:3015:U:OP1	101:A:3507:HOH:O	2.10	0.69
24:AX:272:THR:OG1	24:AX:282:ILE:O	2.09	0.69
1:AA:1314:C:OP2	101:AA:1804:HOH:O	2.10	0.68
31:A4:556:LYS:NZ	31:A4:560:GLU:OE2	2.27	0.68
25:AY:318:GLU:OE1	101:AY:401:HOH:O	2.11	0.68
47:N:143:GLY:O	101:N:301:HOH:O	2.12	0.68
66:6:217:LEU:HD11	66:6:271:LEU:HD12	1.75	0.68
18:AR:243:ILE:HG23	18:AR:247:HIS:CE1	2.29	0.68
36:A:2290:A:N7	101:A:3534:HOH:O	2.27	0.67
36:A:2181:A:OP1	101:A:3508:HOH:O	2.13	0.67
47:N:73:ARG:O	47:N:155:LYS:NZ	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:N:212:PRO:O	101:N:302:HOH:O	2.13	0.67
1:AA:1040:U:OP2	101:AA:1806:HOH:O	2.13	0.67
1:AA:1154:A:OP2	30:A3:155:ARG:NH2	2.29	0.66
52:S:112:ASP:OD2	101:S:301:HOH:O	2.14	0.66
45:L:95:ARG:NH2	101:L:201:HOH:O	2.29	0.66
1:AA:1151:C:N3	101:AA:1841:HOH:O	2.29	0.66
38:D:281:TRP:O	38:D:285:LYS:NZ	2.29	0.66
1:AA:976:A:N7	101:AA:1832:HOH:O	2.28	0.66
1:AA:1578:A:OP2	101:AA:1805:HOH:O	2.13	0.66
41:H:178:ASN:OD1	41:H:179:ASN:N	2.28	0.66
36:A:2372:U:OP2	101:A:3510:HOH:O	2.14	0.65
1:AA:894:C:OP1	101:AA:1807:HOH:O	2.14	0.65
66:6:322:ARG:NH1	101:6:502:HOH:O	2.28	0.65
97:AX:501:ATP:O1G	101:AX:601:HOH:O	2.15	0.65
36:A:2160:A:OP2	64:4:88:TRP:NE1	2.29	0.65
1:AA:828:C:OP2	101:AA:1808:HOH:O	2.14	0.65
36:A:1990:G:OP1	38:D:269:ARG:NH2	2.28	0.65
36:A:2826:G:OP1	56:W:49:ARG:NH1	2.30	0.64
36:A:3013:G:HO2'	64:4:66:PHE:N	1.96	0.64
37:B:76:A:O3'	100:B:101:VAL:HG12	1.97	0.64
36:A:2562:U:O2'	38:D:284:ARG:O	2.09	0.64
1:AA:930:G:O6	10:AJ:47:ARG:NH2	2.29	0.64
65:5:165:GLN:NE2	65:5:179:VAL:HG21	2.13	0.64
4:AD:244:LEU:HD22	4:AD:343:LEU:HD23	1.80	0.64
36:A:2314:C:OP2	101:A:3513:HOH:O	2.15	0.64
36:A:2543:C:OP1	101:A:3509:HOH:O	2.13	0.64
22:AV:208:LEU:HD13	22:AV:226:TYR:HD2	1.62	0.64
36:A:2216:A:O2'	101:A:3506:HOH:O	2.09	0.64
36:A:2539:A:OP1	101:A:3512:HOH:O	2.15	0.64
36:A:1856:A:OP2	36:A:2986:C:O2'	2.16	0.64
36:A:1745:U:O4	63:3:108:LYS:NZ	2.30	0.63
36:A:1882:A:N7	101:A:3549:HOH:O	2.30	0.63
36:A:2531:U:O4	38:D:246:ARG:NH2	2.32	0.63
25:AY:322:ASP:O	25:AY:324:ASP:N	2.31	0.63
7:AG:210:VAL:HG12	7:AG:210:VAL:O	1.99	0.62
39:E:129:VAL:CG1	39:E:145:LEU:HD11	2.29	0.62
8:AH:104:ILE:HG23	8:AH:148:LEU:HD21	1.83	0.61
36:A:1871:A:N3	63:3:104:ARG:NH2	2.48	0.61
36:A:1957:A:OP1	101:A:3514:HOH:O	2.16	0.61
36:A:2767:A:O2'	36:A:2769:A:N7	2.33	0.61
3:AC:109:VAL:HG23	28:A1:103:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:O:62:TYR:OH	50:Q:272:GLU:OE2	2.19	0.60
49:P:138:GLU:OE2	101:P:201:HOH:O	2.16	0.60
59:Z:78:ARG:O	59:Z:83:LYS:NZ	2.34	0.60
1:AA:684:U:OP1	101:AA:1809:HOH:O	2.15	0.60
36:A:1958:G:OP1	101:A:3515:HOH:O	2.16	0.60
36:A:1747:G:OP2	36:A:1749:C:N4	2.34	0.59
67:7:175:ILE:O	67:7:319:ARG:NH2	2.35	0.59
36:A:2108:G:O6	47:N:67:LYS:NZ	2.36	0.59
42:I:31:LYS:NZ	101:I:301:HOH:O	2.36	0.59
58:Y:134:LYS:NZ	69:9:76:TYR:OH	2.34	0.59
6:AF:240:ARG:NH2	6:AF:242:TRP:OXT	2.36	0.58
1:AA:769:G:OP2	14:AN:73:ARG:NH2	2.35	0.58
1:AA:1188:A:OP2	1:AA:1429:C:O2'	2.15	0.58
1:AA:1308:U:O2'	3:AC:64:HIS:ND1	2.37	0.58
69:9:16:ASP:OD1	69:9:25:ARG:NH2	2.35	0.58
1:AA:1346:A:OP2	101:AA:1811:HOH:O	2.16	0.58
36:A:2196:A:O2'	36:A:2213:A:N1	2.35	0.58
101:AA:1823:HOH:O	5:AE:123:ARG:NH2	2.36	0.58
36:A:2104:A:OP1	47:N:231:SER:OG	2.21	0.58
39:E:129:VAL:HG11	39:E:145:LEU:HD11	1.86	0.58
36:A:2021:U:OP1	101:A:3516:HOH:O	2.17	0.58
36:A:1805:A:OP2	55:V:94:HIS:NE2	2.37	0.57
45:L:130:ARG:NH1	45:L:133:GLU:OE2	2.36	0.57
11:AK:58:ARG:NE	11:AK:72:ASP:OD1	2.35	0.57
1:AA:1458:A:OP1	6:AF:104:LYS:NZ	2.30	0.57
36:A:2740:A:N3	36:A:2921:A:O2'	2.32	0.57
1:AA:1294:A:OP1	2:AB:201:ASN:ND2	2.37	0.57
1:AA:1554:G:OP2	101:AA:1815:HOH:O	2.17	0.57
4:AD:245:VAL:HG22	4:AD:271:ALA:HB1	1.86	0.57
6:AF:174:LEU:O	6:AF:179:ARG:NH1	2.37	0.57
1:AA:1208:U:OP1	101:AA:1812:HOH:O	2.16	0.57
1:AA:1015:A:OP2	101:AA:1814:HOH:O	2.17	0.57
36:A:3089:A:H3'	36:A:3090:G:C5'	2.34	0.57
36:A:3110:C:O2'	39:E:266:ARG:NH1	2.37	0.57
28:A1:152:ASP:OD2	28:A1:174:ARG:NH1	2.31	0.57
18:AR:69:THR:N	18:AR:72:ASP:OD2	2.38	0.56
36:A:2545:U:O2'	101:A:3511:HOH:O	2.15	0.56
1:AA:1109:A:OP2	101:AA:1816:HOH:O	2.18	0.56
39:E:50:ASP:O	48:O:138:ARG:NH2	2.39	0.56
4:AD:340:ILE:HG22	4:AD:340:ILE:O	2.06	0.55
36:A:2364:C:OP2	54:U:78:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:F:70:ARG:NH2	40:F:194:GLU:OE1	2.39	0.55
1:AA:1257:U:O2'	1:AA:1260:A:OP2	2.14	0.55
2:AB:88:ARG:NH1	101:AB:403:HOH:O	2.40	0.55
1:AA:843:G:N2	1:AA:846:A:OP2	2.34	0.55
1:AA:1044:U:OP1	1:AA:1110:A:O2'	2.21	0.55
6:AF:176:ASP:OD2	6:AF:180:ARG:NH1	2.40	0.54
36:A:1760:G:OP1	46:M:196:ARG:NE	2.40	0.54
24:AX:151:LEU:CD2	24:AX:247:LEU:HD22	2.38	0.54
1:AA:845:A:H4'	21:AU:60:TYR:CE2	2.43	0.54
18:AR:169:GLU:OE1	27:A0:180:LYS:NZ	2.29	0.53
22:AV:92:LEU:HD21	22:AV:137:ILE:HD11	1.90	0.53
36:A:2016:C:OP2	46:M:59:ARG:NH1	2.41	0.53
36:A:2071:U:O2'	66:6:28:ARG:NH2	2.42	0.53
36:A:1953:A:O2'	36:A:2463:A:OP1	2.26	0.53
36:A:2354:A:O2'	101:A:3503:HOH:O	2.05	0.53
10:AJ:117:ASP:OD1	101:AJ:201:HOH:O	2.19	0.53
36:A:2761:C:O2	36:A:2786:U:N3	2.42	0.53
24:AX:108:LEU:HD21	24:AX:307:VAL:HG11	1.91	0.52
7:AG:200:LEU:HD11	7:AG:204:GLU:HB3	1.91	0.52
15:AO:221:GLN:NE2	22:AV:314:VAL:O	2.37	0.52
1:AA:702:C:OP1	1:AA:848:U:O2'	2.26	0.52
65:5:173:ARG:HA	65:5:176:TYR:CE1	2.45	0.52
22:AV:208:LEU:HD13	22:AV:226:TYR:CD2	2.43	0.51
7:AG:229:LEU:HD21	7:AG:241:VAL:HG11	1.92	0.51
30:A3:144:ARG:NH2	101:A3:301:HOH:O	2.43	0.51
15:AO:208:PRO:HG2	15:AO:213:LEU:HD21	1.92	0.51
18:AR:243:ILE:HG23	18:AR:247:HIS:HE1	1.72	0.51
1:AA:1134:G:OP2	10:AJ:38:ARG:NH2	2.43	0.51
36:A:1742:G:O2'	36:A:1754:G:O6	2.23	0.51
1:AA:1479:C:OP1	101:AA:1819:HOH:O	2.19	0.51
24:AX:297:MET:HE3	24:AX:306:ILE:HG21	1.92	0.50
1:AA:841:A:OP1	13:AM:39:ASN:ND2	2.42	0.50
36:A:1749:C:OP2	36:A:2899:C:O2'	2.28	0.50
36:A:2462:A:N3	101:A:3575:HOH:O	2.34	0.50
41:H:53:THR:N	41:H:86:THR:HG1	2.09	0.50
53:T:184:LYS:NZ	53:T:192:GLU:OE1	2.38	0.50
55:V:188:VAL:O	55:V:188:VAL:HG23	2.11	0.50
66:6:161:LEU:HD13	66:6:271:LEU:HD11	1.93	0.50
24:AX:183:GLU:N	24:AX:183:GLU:OE1	2.42	0.50
55:V:163:ASP:OD1	55:V:164:GLY:N	2.45	0.50
57:X:177:HIS:O	57:X:184:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:217:ARG:NH1	15:AO:227:GLU:OE2	2.44	0.50
31:A4:303:CYS:SG	31:A4:344:ARG:NH2	2.85	0.50
52:S:173:ARG:HB2	52:S:182:LYS:HG2	1.92	0.50
17:AQ:63:ILE:HD13	29:A2:6:LEU:HD21	1.94	0.50
24:AX:108:LEU:HD21	24:AX:307:VAL:CG1	2.42	0.49
36:A:2537:G:O2'	36:A:2634:U:OP2	2.26	0.49
1:AA:1528:A:OP1	27:A0:101:ARG:NH2	2.45	0.49
18:AR:162:SER:O	18:AR:170:ARG:NH1	2.43	0.49
48:O:144:LEU:HD12	67:7:174:VAL:HG11	1.95	0.49
41:H:146:LEU:O	41:H:150:GLY:N	2.42	0.49
55:V:169:THR:HG22	55:V:169:THR:O	2.11	0.49
28:A1:46:ARG:HB2	28:A1:47:PRO:HD3	1.93	0.49
29:A2:64:ASP:OD1	29:A2:65:ALA:N	2.46	0.49
1:AA:768:A:O2'	14:AN:24:LYS:NZ	2.46	0.49
4:AD:283:GLU:O	4:AD:356:GLN:NE2	2.46	0.49
28:A1:46:ARG:HB2	28:A1:47:PRO:CD	2.43	0.49
6:AF:159:VAL:HG23	6:AF:172:VAL:HG21	1.95	0.49
48:O:64:LYS:NZ	48:O:100:GLN:O	2.46	0.49
8:AH:155:VAL:HG21	28:A1:129:PHE:CB	2.43	0.48
22:AV:269:SER:HB2	22:AV:270:PRO:HD2	1.94	0.48
1:AA:899:G:O2'	1:AA:907:A:N1	2.33	0.48
1:AA:1004:G:O2'	9:AI:98:GLN:NE2	2.46	0.48
10:AJ:78:ARG:NH2	10:AJ:117:ASP:OD2	2.47	0.48
36:A:2483:U:H2'	36:A:2484:C:O4'	2.14	0.48
50:Q:73:ARG:NH1	50:Q:213:GLN:O	2.47	0.48
36:A:2909:G:OP1	61:1:63:ARG:NH1	2.41	0.48
3:AC:106:ASP:OD1	3:AC:107:GLN:N	2.42	0.48
7:AG:384:GLN:NE2	101:AG:404:HOH:O	2.47	0.48
36:A:2499:U:OP2	36:A:2504:A:N6	2.36	0.48
1:AA:1520:U:OP2	22:AV:407:GLN:NE2	2.46	0.48
1:AA:1427:A:N7	101:AA:1868:HOH:O	2.35	0.48
31:A4:239:ARG:O	31:A4:242:ASN:ND2	2.45	0.48
36:A:2888:A:H3'	36:A:2889:C:C5'	2.44	0.48
3:AC:115:ASN:ND2	25:AY:309:LYS:O	2.48	0.47
20:AT:132:ARG:NH1	20:AT:136:LEU:O	2.48	0.47
42:I:197:LEU:HD12	42:I:198:PRO:HD2	1.96	0.47
36:A:1851:G:H2'	36:A:2693:A:N7	2.30	0.47
56:W:102:GLU:OE2	66:6:74:TYR:N	2.45	0.47
67:7:156:ARG:HG3	67:7:156:ARG:HH11	1.78	0.47
36:A:3201:A:H2'	36:A:3202:U:O4'	2.15	0.47
67:7:257:ILE:O	67:7:257:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1597:C:OP2	29:A2:24:ASN:ND2	2.47	0.47
24:AX:153:LEU:HD21	24:AX:244:LEU:CD2	2.45	0.47
1:AA:1453:A:OP1	101:AA:1820:HOH:O	2.20	0.47
4:AD:88:SER:N	101:AD:505:HOH:O	2.47	0.47
36:A:2663:C:OP1	48:O:13:ARG:NH2	2.46	0.47
44:K:52:ASP:OD1	101:K:201:HOH:O	2.20	0.47
8:AH:155:VAL:HG21	28:A1:129:PHE:HB2	1.97	0.47
3:AC:109:VAL:CG2	28:A1:103:LEU:HD11	2.45	0.47
12:AL:126:GLU:HG2	12:AL:177:VAL:HG11	1.97	0.47
36:A:1958:G:O2'	101:A:3517:HOH:O	2.18	0.47
53:T:85:ALA:O	53:T:139:SER:OG	2.33	0.47
1:AA:749:G:O3'	14:AN:78:LYS:NZ	2.41	0.47
22:AV:226:TYR:CE1	22:AV:282:VAL:HG21	2.42	0.47
40:F:218:LEU:HD23	40:F:260:VAL:HB	1.97	0.46
55:V:127:ASP:O	55:V:129:LYS:N	2.49	0.46
24:AX:159:HIS:NE2	24:AX:266:ASN:OD1	2.48	0.46
28:A1:250:GLU:OE2	28:A1:301:ASN:ND2	2.49	0.46
43:J:75:ASP:OD1	43:J:77:THR:HG22	2.16	0.46
44:K:67:PHE:HB3	44:K:71:LYS:HB2	1.98	0.46
8:AH:151:SER:O	8:AH:155:VAL:HG23	2.16	0.46
41:H:107:VAL:HG12	41:H:108:ARG:N	2.30	0.46
67:7:106:ALA:O	67:7:113:TRP:N	2.47	0.46
36:A:2777:G:N3	41:H:179:ASN:ND2	2.63	0.46
37:B:12:U:HO2'	37:B:14:A:P	2.39	0.46
60:0:133:GLU:OE2	60:0:160:TYR:OH	2.26	0.46
22:AV:190:LEU:HD11	22:AV:208:LEU:HD11	1.97	0.46
36:A:2458:A:O2'	39:E:215:PHE:O	2.29	0.46
4:AD:312:TYR:N	4:AD:331:ASP:OD2	2.48	0.46
7:AG:102:GLU:OE1	7:AG:102:GLU:N	2.45	0.46
36:A:2506:A:H1'	36:A:2601:A:N6	2.31	0.46
46:M:43:ARG:NH2	101:M:404:HOH:O	2.49	0.46
54:U:66:ALA:HB2	54:U:100:ALA:HA	1.98	0.46
7:AG:198:ARG:NH1	7:AG:201:ILE:HG23	2.32	0.45
20:AT:92:THR:O	20:AT:92:THR:HG22	2.16	0.45
66:6:257:PRO:HB3	66:6:268:LEU:HD21	1.98	0.45
31:A4:305:ILE:HG22	31:A4:306:ASN:N	2.32	0.45
36:A:3211:C:HO2'	36:A:3212:C:H5	1.58	0.45
39:E:47:THR:OG1	39:E:51:GLU:OE1	2.22	0.45
39:E:131:LYS:O	39:E:145:LEU:HD12	2.15	0.45
1:AA:1057:G:H4'	1:AA:1578:A:H4'	1.98	0.45
21:AU:56:LEU:HD11	21:AU:60:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AW:92:MET:O	23:AW:98:LYS:NZ	2.49	0.45
11:AK:70:VAL:HG11	25:AY:383:LYS:HE3	1.99	0.45
18:AR:317:ALA:O	18:AR:321:ALA:N	2.49	0.45
27:A0:41:LEU:HD13	27:A0:55:TRP:CG	2.52	0.45
36:A:1867:A:N1	36:A:2019:G:O2'	2.35	0.44
50:Q:251:GLU:OE1	50:Q:251:GLU:HA	2.16	0.44
1:AA:1265:C:H4'	8:AH:122:GLN:HG3	2.00	0.44
59:Z:75:THR:HB	59:Z:83:LYS:HG2	1.99	0.44
66:6:224:HIS:HA	66:6:232:TYR:CE2	2.52	0.44
41:H:84:GLU:OE1	57:X:44:ARG:NH2	2.50	0.44
46:M:177:ALA:HA	46:M:222:TYR:CD1	2.52	0.44
38:D:207:ILE:HG22	38:D:207:ILE:O	2.18	0.44
22:AV:35:VAL:O	22:AV:35:VAL:HG12	2.18	0.44
29:A2:43:ALA:HB1	29:A2:46:ILE:HD11	1.99	0.44
36:A:1822:U:O2	36:A:2707:A:O2'	2.33	0.44
39:E:247:ASP:O	101:E:501:HOH:O	2.21	0.44
1:AA:1259:U:H6	1:AA:1326:A:HO2'	1.58	0.44
27:A0:63:ARG:NH2	27:A0:110:ASP:OD2	2.51	0.44
37:B:44:A:H2'	37:B:45:G:O4'	2.18	0.44
1:AA:706:C:O2	27:A0:210:LYS:NZ	2.45	0.43
5:AE:109:VAL:HG23	5:AE:109:VAL:O	2.19	0.43
6:AF:193:ASP:OD1	6:AF:194:LYS:N	2.51	0.43
36:A:2598:A:H3'	36:A:2625:C:H42	1.83	0.43
65:5:105:TYR:CE1	65:5:262:ILE:HD12	2.54	0.43
41:H:223:VAL:N	41:H:231:VAL:O	2.46	0.43
36:A:2135:A:N3	36:A:2135:A:H2'	2.34	0.43
6:AF:237:ALA:O	6:AF:240:ARG:HG2	2.19	0.43
21:AU:73:GLU:OE2	27:A0:166:TYR:OH	2.37	0.43
31:A4:58:VAL:O	31:A4:58:VAL:HG23	2.18	0.43
1:AA:1461:A:N6	101:AA:1908:HOH:O	2.42	0.43
7:AG:237:GLU:OE1	7:AG:237:GLU:N	2.51	0.43
55:V:165:ILE:HG21	69:9:76:TYR:CD2	2.53	0.43
67:7:51:GLU:OE1	67:7:51:GLU:HA	2.19	0.43
36:A:2868:C:H2'	36:A:2869:A:O4'	2.19	0.43
36:A:1697:A:N3	36:A:1703:C:O2'	2.48	0.43
4:AD:198:TRP:HA	4:AD:201:ILE:HD12	2.01	0.43
31:A4:470:GLN:NE2	31:A4:472:ASP:OD2	2.52	0.43
36:A:1991:A:H5''	36:A:1992:C:OP1	2.18	0.43
36:A:2296:U:H5''	36:A:2297:A:OP1	2.19	0.43
36:A:2429:A:N1	36:A:2433:C:O2'	2.45	0.43
36:A:2053:U:HO2'	36:A:2054:U:H6	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1322:C:N3	4:AD:234:LYS:NZ	2.63	0.42
1:AA:1384:A:N7	101:AA:1873:HOH:O	2.37	0.42
36:A:1800:G:N1	36:A:1803:A:OP2	2.51	0.42
36:A:3089:A:H3'	36:A:3090:G:H5'	2.01	0.42
7:AG:200:LEU:HD13	7:AG:246:ARG:CZ	2.50	0.42
65:5:289:HIS:CE1	65:5:290:THR:HG1	2.35	0.42
1:AA:1199:G:N1	1:AA:1422:G:OP2	2.49	0.42
52:S:152:ASP:OD1	52:S:153:LEU:N	2.53	0.42
24:AX:151:LEU:HD23	24:AX:247:LEU:HD22	2.00	0.42
31:A4:458:TYR:HB3	31:A4:486:TYR:CD1	2.54	0.42
36:A:2025:C:OP1	52:S:182:LYS:HD3	2.19	0.42
66:6:215:THR:OG1	66:6:275:GLN:OE1	2.31	0.42
27:A0:158:GLU:O	27:A0:158:GLU:HG2	2.20	0.42
40:F:98:GLN:NE2	101:F:405:HOH:O	2.53	0.42
41:H:193:PHE:O	41:H:198:GLY:N	2.52	0.42
68:8:202:VAL:O	68:8:203:GLU:HB3	2.19	0.42
18:AR:247:HIS:HD2	18:AR:274:TYR:CE1	2.38	0.42
36:A:2728:C:H4'	36:A:2815:OMG:HM22	2.02	0.42
41:H:238:VAL:HG12	41:H:239:ASN:N	2.35	0.42
51:R:65:ARG:HA	51:R:68:TRP:CE3	2.55	0.42
31:A4:302:VAL:O	31:A4:312:LYS:NZ	2.51	0.42
36:A:2882:U:O4'	49:P:173:ARG:NH2	2.53	0.42
55:V:124:ASP:OD1	55:V:125:PRO:HD2	2.20	0.42
3:AC:58:ALA:HB1	3:AC:59:PRO:CD	2.50	0.41
3:AC:84:GLU:OE1	3:AC:84:GLU:N	2.45	0.41
27:A0:13:GLU:OE2	27:A0:16:ARG:NH1	2.53	0.41
53:T:49:ASN:ND2	53:T:68:TYR:O	2.52	0.41
1:AA:1103:A:N7	1:AA:1574:G:O2'	2.46	0.41
36:A:1787:G:N2	36:A:1790:A:OP2	2.51	0.41
36:A:1800:G:O6	55:V:34:LYS:NZ	2.52	0.41
65:5:273:VAL:HG12	65:5:273:VAL:O	2.20	0.41
1:AA:1065:C:H2'	1:AA:1066:C:O4'	2.21	0.41
8:AH:184:ILE:CG2	8:AH:184:ILE:O	2.69	0.41
65:5:56:GLU:O	65:5:56:GLU:HG3	2.19	0.41
67:7:114:ASP:OD1	67:7:268:LEU:N	2.53	0.41
13:AM:101:PRO:HB2	21:AU:60:TYR:CE1	2.55	0.41
39:E:69:ASP:OD1	39:E:154:ARG:NH1	2.53	0.41
12:AL:126:GLU:OE1	12:AL:126:GLU:N	2.41	0.41
18:AR:162:SER:HB2	18:AR:165:ILE:HD12	2.02	0.41
25:AY:300:GLU:OE1	31:A4:87:TYR:OH	2.30	0.41
28:A1:86:ARG:NH1	28:A1:96:PRO:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A:2174:G:H4'	43:J:151:LEU:HD23	2.01	0.41
25:AY:259:PHE:HB2	31:A4:363:ILE:HD11	2.03	0.41
36:A:1815:A:N1	101:A:3602:HOH:O	2.37	0.41
36:A:2015:G:O4'	46:M:56:GLU:HG3	2.21	0.41
2:AB:96:GLY:HA3	23:AW:159:ASP:OD2	2.21	0.41
8:AH:184:ILE:O	8:AH:184:ILE:HG22	2.20	0.41
10:AJ:70:PRO:HB3	10:AJ:117:ASP:HB3	2.03	0.41
36:A:2162:C:OP2	101:A:3521:HOH:O	2.22	0.41
36:A:2343:G:H3'	36:A:2343:G:N3	2.36	0.41
36:A:2595:A:H2'	36:A:2596:G:O4'	2.21	0.41
36:A:2598:A:O2'	36:A:2599:U:H5'	2.21	0.41
36:A:2814:G:O2'	36:A:2983:G:OP1	2.39	0.41
39:E:345:ILE:O	50:Q:172:GLN:NE2	2.51	0.41
43:J:102:ARG:N	43:J:107:GLU:OE2	2.52	0.41
44:K:7:ALA:HB3	44:K:8:PRO:HD3	2.03	0.41
46:M:14:ASP:OD1	46:M:15:LEU:N	2.54	0.41
53:T:94:ASP:OD2	67:7:97:GLU:N	2.39	0.41
1:AA:1107:U:O4	30:A3:128:LYS:NZ	2.47	0.41
22:AV:241:ARG:HA	22:AV:244:TYR:CE2	2.55	0.41
24:AX:81:HIS:ND1	24:AX:190:ASN:HB3	2.35	0.41
30:A3:159:GLU:OE2	36:A:2639:C:H5''	2.21	0.41
36:A:2709:A:N3	60:0:98:GLN:OE1	2.53	0.41
39:E:129:VAL:HG13	39:E:145:LEU:HD11	2.03	0.41
1:AA:919:A:OP2	15:AO:96:ARG:NH2	2.48	0.40
1:AA:994:A:O2'	6:AF:166:ARG:NH1	2.54	0.40
1:AA:1066:C:O2'	9:AI:187:ARG:O	2.39	0.40
1:AA:1149:G:OP2	30:A3:165:LYS:NZ	2.50	0.40
2:AB:167:HIS:CD2	7:AG:153:THR:HA	2.56	0.40
30:A3:173:LEU:HD12	30:A3:191:THR:HG23	2.02	0.40
31:A4:508:VAL:O	31:A4:508:VAL:HG12	2.20	0.40
1:AA:709:G:OP1	13:AM:13:ARG:NH2	2.54	0.40
42:I:144:LEU:N	42:I:145:PRO:HD2	2.37	0.40
43:J:69:LYS:HE3	43:J:69:LYS:HB2	1.96	0.40
45:L:35:MET:O	45:L:56:ARG:NH1	2.54	0.40
48:O:86:ILE:HB	48:O:87:PRO:HD3	2.03	0.40
56:W:103:VAL:HG11	66:6:61:ALA:HB1	2.03	0.40
1:AA:1001:C:N4	36:A:2558:A:O4'	2.55	0.40
26:AZ:46:LYS:HA	26:AZ:49:TYR:CE1	2.55	0.40
48:O:36:LEU:O	48:O:40:GLU:N	2.50	0.40
55:V:54:TRP:NE1	55:V:56:LEU:O	2.53	0.40
2:AB:103:GLU:N	2:AB:104:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A:2006:C:H2'	36:A:2007:U:C6	2.57	0.40
36:A:3009:C:O2	36:A:3009:C:O5'	2.38	0.40
13:AM:19:ILE:HB	13:AM:83:LEU:HD23	2.04	0.40
18:AR:295:ASP:O	18:AR:299:ASN:ND2	2.55	0.40
24:AX:103:LYS:N	24:AX:104:PRO:CD	2.84	0.40
27:A0:42:THR:HG22	27:A0:49:ARG:HG2	2.04	0.40
36:A:2327:U:H2'	36:A:2328:C:O4'	2.20	0.40
46:M:222:TYR:CE2	46:M:223:LEU:HG	2.57	0.40

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	AB	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
3	AC	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
4	AD	341/430 (79%)	331 (97%)	10 (3%)	0	100	100
5	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
6	AF	206/242 (85%)	203 (98%)	3 (2%)	0	100	100
7	AG	323/396 (82%)	319 (99%)	4 (1%)	0	100	100
8	AH	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	22	21
9	AI	133/194 (69%)	131 (98%)	2 (2%)	0	100	100
10	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
11	AK	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
12	AL	172/257 (67%)	171 (99%)	1 (1%)	0	100	100
13	AM	117/137 (85%)	117 (100%)	0	0	100	100
14	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	AO	191/258 (74%)	188 (98%)	3 (2%)	0	100	100
16	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
17	AQ	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
18	AR	293/360 (81%)	284 (97%)	9 (3%)	0	100	100
19	AS	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
20	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	AU	174/205 (85%)	174 (100%)	0	0	100	100
22	AV	358/414 (86%)	350 (98%)	8 (2%)	0	100	100
23	AW	98/187 (52%)	96 (98%)	2 (2%)	0	100	100
24	AX	350/398 (88%)	345 (99%)	5 (1%)	0	100	100
25	AY	147/395 (37%)	146 (99%)	0	1 (1%)	22	21
26	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
27	A0	213/217 (98%)	209 (98%)	4 (2%)	0	100	100
28	A1	277/323 (86%)	273 (99%)	4 (1%)	0	100	100
29	A2	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
30	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
31	A4	584/689 (85%)	577 (99%)	7 (1%)	0	100	100
38	D	236/305 (77%)	232 (98%)	4 (2%)	0	100	100
39	E	303/348 (87%)	296 (98%)	6 (2%)	1 (0%)	41	45
40	F	250/311 (80%)	247 (99%)	3 (1%)	0	100	100
41	H	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
42	I	210/261 (80%)	202 (96%)	8 (4%)	0	100	100
43	J	173/192 (90%)	173 (100%)	0	0	100	100
44	K	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
45	L	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
46	M	289/296 (98%)	283 (98%)	6 (2%)	0	100	100
47	N	220/251 (88%)	217 (99%)	3 (1%)	0	100	100
48	O	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
49	P	142/180 (79%)	142 (100%)	0	0	100	100
50	Q	236/292 (81%)	235 (100%)	1 (0%)	0	100	100
51	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
53	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
54	U	150/153 (98%)	147 (98%)	3 (2%)	0	100	100
55	V	203/216 (94%)	198 (98%)	5 (2%)	0	100	100
56	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
57	X	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
58	Y	179/250 (72%)	177 (99%)	2 (1%)	0	100	100
59	Z	120/161 (74%)	120 (100%)	0	0	100	100
60	0	108/188 (57%)	108 (100%)	0	0	100	100
61	1	54/65 (83%)	53 (98%)	1 (2%)	0	100	100
62	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
63	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
64	4	36/103 (35%)	36 (100%)	0	0	100	100
65	5	392/423 (93%)	382 (97%)	10 (3%)	0	100	100
66	6	352/380 (93%)	344 (98%)	8 (2%)	0	100	100
67	7	292/338 (86%)	286 (98%)	6 (2%)	0	100	100
68	8	155/206 (75%)	152 (98%)	3 (2%)	0	100	100
69	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
70	a	96/142 (68%)	95 (99%)	1 (1%)	0	100	100
71	b	148/215 (69%)	146 (99%)	2 (1%)	0	100	100
72	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100
73	d	235/306 (77%)	231 (98%)	4 (2%)	0	100	100
74	e	236/279 (85%)	228 (97%)	7 (3%)	1 (0%)	34	37
75	f	153/212 (72%)	152 (99%)	1 (1%)	0	100	100
76	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
77	h	108/158 (68%)	107 (99%)	1 (1%)	0	100	100
78	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
79	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
80	k	99/112 (88%)	99 (100%)	0	0	100	100
81	l	80/138 (58%)	80 (100%)	0	0	100	100
82	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
83	o	92/102 (90%)	92 (100%)	0	0	100	100
84	p	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
85	q	159/222 (72%)	159 (100%)	0	0	100	100
86	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
87	s	382/439 (87%)	374 (98%)	8 (2%)	0	100	100
88	t	44/198 (22%)	44 (100%)	0	0	100	100
88	u	30/198 (15%)	30 (100%)	0	0	100	100
88	v	30/198 (15%)	30 (100%)	0	0	100	100
88	w	29/198 (15%)	29 (100%)	0	0	100	100
88	x	29/198 (15%)	29 (100%)	0	0	100	100
88	y	29/198 (15%)	29 (100%)	0	0	100	100
89	z	160/325 (49%)	151 (94%)	8 (5%)	1 (1%)	25	25
All	All	14607/19484 (75%)	14384 (98%)	218 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	AH	126	ILE
25	AY	323	ASP
89	z	128	ASP
74	e	197	GLU
39	E	150	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	198/249 (80%)	198 (100%)	0	100	100
3	AC	115/143 (80%)	115 (100%)	0	100	100
4	AD	286/357 (80%)	286 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	104/107 (97%)	104 (100%)	0	100	100
6	AF	185/209 (88%)	185 (100%)	0	100	100
7	AG	285/342 (83%)	285 (100%)	0	100	100
8	AH	130/180 (72%)	130 (100%)	0	100	100
9	AI	104/146 (71%)	104 (100%)	0	100	100
10	AJ	93/118 (79%)	93 (100%)	0	100	100
11	AK	91/113 (80%)	91 (100%)	0	100	100
12	AL	158/226 (70%)	158 (100%)	0	100	100
13	AM	97/113 (86%)	97 (100%)	0	100	100
14	AN	96/115 (84%)	96 (100%)	0	100	100
15	AO	174/230 (76%)	174 (100%)	0	100	100
16	AP	88/123 (72%)	88 (100%)	0	100	100
17	AQ	78/79 (99%)	78 (100%)	0	100	100
18	AR	264/318 (83%)	264 (100%)	0	100	100
19	AS	116/164 (71%)	116 (100%)	0	100	100
20	AT	153/157 (98%)	153 (100%)	0	100	100
21	AU	152/174 (87%)	152 (100%)	0	100	100
22	AV	325/364 (89%)	325 (100%)	0	100	100
23	AW	87/158 (55%)	87 (100%)	0	100	100
24	AX	311/351 (89%)	311 (100%)	0	100	100
25	AY	137/357 (38%)	137 (100%)	0	100	100
26	AZ	90/95 (95%)	90 (100%)	0	100	100
27	A0	188/189 (100%)	188 (100%)	0	100	100
28	A1	257/291 (88%)	257 (100%)	0	100	100
29	A2	100/101 (99%)	100 (100%)	0	100	100
30	A3	65/166 (39%)	65 (100%)	0	100	100
31	A4	526/609 (86%)	526 (100%)	0	100	100
38	D	192/245 (78%)	192 (100%)	0	100	100
39	E	260/290 (90%)	259 (100%)	1 (0%)	91	95
40	F	219/262 (84%)	219 (100%)	0	100	100
41	H	182/228 (80%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	I	194/232 (84%)	194 (100%)	0	100	100
43	J	138/150 (92%)	138 (100%)	0	100	100
44	K	154/155 (99%)	154 (100%)	0	100	100
45	L	98/124 (79%)	98 (100%)	0	100	100
46	M	246/249 (99%)	246 (100%)	0	100	100
47	N	189/211 (90%)	189 (100%)	0	100	100
48	O	134/150 (89%)	134 (100%)	0	100	100
49	P	126/155 (81%)	126 (100%)	0	100	100
50	Q	220/256 (86%)	220 (100%)	0	100	100
51	R	118/126 (94%)	118 (100%)	0	100	100
52	S	146/180 (81%)	146 (100%)	0	100	100
53	T	146/176 (83%)	146 (100%)	0	100	100
54	U	134/135 (99%)	134 (100%)	0	100	100
55	V	183/191 (96%)	183 (100%)	0	100	100
56	W	94/119 (79%)	94 (100%)	0	100	100
57	X	220/229 (96%)	220 (100%)	0	100	100
58	Y	163/223 (73%)	162 (99%)	1 (1%)	86	92
59	Z	113/147 (77%)	113 (100%)	0	100	100
60	0	99/164 (60%)	99 (100%)	0	100	100
61	1	53/60 (88%)	53 (100%)	0	100	100
62	2	40/72 (56%)	40 (100%)	0	100	100
63	3	88/166 (53%)	88 (100%)	0	100	100
64	4	37/89 (42%)	37 (100%)	0	100	100
65	5	353/368 (96%)	352 (100%)	1 (0%)	92	96
66	6	313/332 (94%)	313 (100%)	0	100	100
67	7	270/303 (89%)	270 (100%)	0	100	100
68	8	146/190 (77%)	146 (100%)	0	100	100
69	9	104/112 (93%)	104 (100%)	0	100	100
70	a	96/133 (72%)	95 (99%)	1 (1%)	76	85
71	b	131/185 (71%)	131 (100%)	0	100	100
72	c	251/288 (87%)	251 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	d	223/274 (81%)	223 (100%)	0	100	100
74	e	207/236 (88%)	207 (100%)	0	100	100
75	f	139/188 (74%)	139 (100%)	0	100	100
76	g	124/148 (84%)	124 (100%)	0	100	100
77	h	104/148 (70%)	104 (100%)	0	100	100
78	i	86/110 (78%)	86 (100%)	0	100	100
79	j	74/97 (76%)	74 (100%)	0	100	100
80	k	83/90 (92%)	83 (100%)	0	100	100
81	l	76/116 (66%)	76 (100%)	0	100	100
82	m	85/113 (75%)	85 (100%)	0	100	100
83	o	80/87 (92%)	80 (100%)	0	100	100
84	p	135/181 (75%)	135 (100%)	0	100	100
85	q	138/178 (78%)	138 (100%)	0	100	100
86	r	147/169 (87%)	147 (100%)	0	100	100
87	s	340/381 (89%)	340 (100%)	0	100	100
88	t	40/158 (25%)	40 (100%)	0	100	100
88	u	31/158 (20%)	31 (100%)	0	100	100
88	v	31/158 (20%)	31 (100%)	0	100	100
88	w	30/158 (19%)	30 (100%)	0	100	100
88	x	30/158 (19%)	30 (100%)	0	100	100
88	y	30/158 (19%)	30 (100%)	0	100	100
89	z	150/287 (52%)	150 (100%)	0	100	100
All	All	13086/16790 (78%)	13082 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	E	303	LYS
58	Y	198	ARG
65	5	395	ARG
70	a	122	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
3	AC	156	GLN
4	AD	356	GLN
6	AF	113	GLN
6	AF	238	HIS
7	AG	384	GLN
8	AH	125	HIS
9	AI	92	HIS
9	AI	96	GLN
9	AI	98	GLN
12	AL	162	GLN
13	AM	50	GLN
21	AU	188	ASN
22	AV	380	GLN
23	AW	106	HIS
24	AX	250	GLN
26	AZ	56	HIS
26	AZ	63	GLN
28	A1	185	HIS
31	A4	257	HIS
31	A4	306	ASN
38	D	221	ASN
38	D	252	HIS
39	E	125	GLN
39	E	281	ASN
40	F	98	GLN
41	H	192	HIS
42	I	150	HIS
48	O	100	GLN
52	S	118	ASN
58	Y	179	HIS
59	Z	64	HIS
61	1	52	GLN
65	5	109	HIS
65	5	331	ASN
65	5	367	ASN
66	6	320	GLN
67	7	255	HIS
67	7	298	GLN
70	a	126	HIS
71	b	58	ASN
71	b	90	HIS
74	e	212	HIS
78	i	124	HIS

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Mol	Chain	Res	Type
83	o	21	HIS
83	o	94	HIS
85	q	107	GLN
85	q	142	ASN
86	r	96	HIS
86	r	131	HIS
89	z	104	HIS
89	z	241	HIS
89	z	266	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	950/954 (99%)	122 (12%)	0
32	Aw	20/22 (90%)	2 (10%)	0
33	Ax	68/70 (97%)	10 (14%)	0
34	Ay	3/70 (4%)	2 (66%)	0
35	Az	33/34 (97%)	12 (36%)	0
36	A	1556/1558 (99%)	220 (14%)	3 (0%)
37	B	71/73 (97%)	11 (15%)	0
All	All	2701/2781 (97%)	379 (14%)	3 (0%)

All (379) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	651	A
1	AA	680	U
1	AA	688	A
1	AA	704	U
1	AA	721	U
1	AA	737	C
1	AA	738	A
1	AA	753	A
1	AA	761	A
1	AA	766	G
1	AA	773	U
1	AA	777	G
1	AA	786	G
1	AA	791	G
1	AA	794	U
1	AA	796	G

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Mol	Chain	Res	Type
1	AA	830	U
1	AA	832	U
1	AA	835	C
1	AA	836	A
1	AA	860	A
1	AA	861	U
1	AA	868	C
1	AA	871	A
1	AA	890	C
1	AA	903	U
1	AA	904	C
1	AA	907	A
1	AA	919	A
1	AA	929	A
1	AA	932	C
1	AA	938	A
1	AA	939	A
1	AA	941	G
1	AA	942	A
1	AA	960	C
1	AA	962	C
1	AA	967	A
1	AA	1001	C
1	AA	1002	C
1	AA	1011	C
1	AA	1015	A
1	AA	1031	G
1	AA	1042	U
1	AA	1081	U
1	AA	1082	A
1	AA	1103	A
1	AA	1105	C
1	AA	1106	C
1	AA	1107	U
1	AA	1109	A
1	AA	1113	G
1	AA	1118	A
1	AA	1121	A
1	AA	1126	A
1	AA	1137	A
1	AA	1151	C
1	AA	1153	C

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Mol	Chain	Res	Type
1	AA	1160	A
1	AA	1167	A
1	AA	1179	G
1	AA	1187	U
1	AA	1189	U
1	AA	1190	C
1	AA	1193	U
1	AA	1199	G
1	AA	1200	G
1	AA	1220	A
1	AA	1223	C
1	AA	1225	C
1	AA	1229	U
1	AA	1247	G
1	AA	1248	C
1	AA	1250	C
1	AA	1251	A
1	AA	1271	C
1	AA	1273	G
1	AA	1284	U
1	AA	1285	G
1	AA	1290	C
1	AA	1291	U
1	AA	1292	A
1	AA	1326	A
1	AA	1327	G
1	AA	1343	A
1	AA	1354	A
1	AA	1356	A
1	AA	1376	C
1	AA	1378	C
1	AA	1387	A
1	AA	1390	A
1	AA	1391	U
1	AA	1405	C
1	AA	1406	U
1	AA	1407	U
1	AA	1422	G
1	AA	1430	A
1	AA	1466	C
1	AA	1481	C
1	AA	1503	G

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Mol	Chain	Res	Type
1	AA	1519	A
1	AA	1522	U
1	AA	1525	C
1	AA	1526	U
1	AA	1527	A
1	AA	1533	C
1	AA	1536	A
1	AA	1537	C
1	AA	1538	G
1	AA	1539	C
1	AA	1540	A
1	AA	1541	U
1	AA	1544	A
1	AA	1552	G
1	AA	1557	A
1	AA	1562	G
1	AA	1568	U
1	AA	1571	U
1	AA	1582	G
1	AA	1594	G
1	AA	1595	G
1	AA	1599	A
32	Aw	30	G
32	Aw	76	A
33	Ax	3	G
33	Ax	23	A
33	Ax	25	C
33	Ax	44	A
33	Ax	45	G
33	Ax	46	A
33	Ax	48	U
33	Ax	49	G
33	Ax	59	U
33	Ax	62	C
34	Ay	75	C
34	Ay	76	A
35	Az	0	U
35	Az	12	U
35	Az	13	U
35	Az	18	A
35	Az	21	A
35	Az	22	A

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Mol	Chain	Res	Type
35	Az	23	U
35	Az	24	U
35	Az	25	U
35	Az	26	A
35	Az	27	C
35	Az	32	A
36	A	1678	C
36	A	1681	G
36	A	1689	C
36	A	1692	A
36	A	1700	U
36	A	1704	U
36	A	1708	A
36	A	1715	C
36	A	1724	A
36	A	1727	A
36	A	1728	U
36	A	1748	G
36	A	1765	C
36	A	1777	A
36	A	1805	A
36	A	1806	U
36	A	1807	U
36	A	1808	A
36	A	1810	A
36	A	1817	C
36	A	1821	A
36	A	1827	C
36	A	1828	A
36	A	1829	A
36	A	1832	A
36	A	1836	A
36	A	1844	A
36	A	1854	U
36	A	1856	A
36	A	1869	A
36	A	1871	A
36	A	1882	A
36	A	1887	A
36	A	1893	A
36	A	1901	C
36	A	1903	C

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Mol	Chain	Res	Type
36	A	1918	G
36	A	1937	A
36	A	1940	A
36	A	1958	G
36	A	1985	G
36	A	1992	C
36	A	1993	A
36	A	1994	A
36	A	2000	C
36	A	2003	A
36	A	2015	G
36	A	2022	G
36	A	2030	U
36	A	2032	G
36	A	2036	C
36	A	2037	U
36	A	2039	A
36	A	2054	U
36	A	2060	A
36	A	2069	U
36	A	2071	U
36	A	2079	C
36	A	2099	U
36	A	2113	G
36	A	2125	C
36	A	2126	U
36	A	2147	G
36	A	2160	A
36	A	2163	A
36	A	2168	U
36	A	2181	A
36	A	2192	A
36	A	2198	A
36	A	2200	A
36	A	2207	A
36	A	2214	A
36	A	2219	C
36	A	2221	C
36	A	2222	U
36	A	2223	A
36	A	2224	C
36	A	2225	C

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Mol	Chain	Res	Type
36	A	2226	U
36	A	2227	A
36	A	2230	A
36	A	2233	U
36	A	2237	A
36	A	2241	A
36	A	2243	A
36	A	2245	A
36	A	2246	A
36	A	2262	C
36	A	2263	C
36	A	2284	C
36	A	2285	U
36	A	2297	A
36	A	2300	G
36	A	2322	C
36	A	2331	C
36	A	2332	C
36	A	2345	G
36	A	2350	A
36	A	2353	A
36	A	2354	A
36	A	2357	C
36	A	2363	A
36	A	2372	U
36	A	2374	A
36	A	2390	A
36	A	2399	A
36	A	2401	A
36	A	2404	U
36	A	2407	U
36	A	2415	C
36	A	2434	A
36	A	2446	A
36	A	2451	A
36	A	2478	G
36	A	2485	U
36	A	2493	C
36	A	2502	C
36	A	2520	C
36	A	2521	A
36	A	2527	A

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Mol	Chain	Res	Type
36	A	2570	C
36	A	2592	G
36	A	2593	G
36	A	2594	U
36	A	2599	U
36	A	2600	A
36	A	2601	A
36	A	2603	C
36	A	2618	U
36	A	2627	G
36	A	2630	U
36	A	2633	A
36	A	2635	G
36	A	2654	U
36	A	2656	U
36	A	2683	C
36	A	2686	G
36	A	2694	A
36	A	2696	A
36	A	2706	A
36	A	2718	C
36	A	2719	G
36	A	2723	A
36	A	2724	G
36	A	2725	A
36	A	2732	G
36	A	2745	A
36	A	2757	A
36	A	2758	G
36	A	2759	U
36	A	2762	C
36	A	2765	A
36	A	2767	A
36	A	2768	A
36	A	2775	A
36	A	2781	U
36	A	2782	A
36	A	2786	U
36	A	2788	C
36	A	2790	A
36	A	2791	A
36	A	2810	G

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Mol	Chain	Res	Type
36	A	2832	A
36	A	2833	A
36	A	2847	C
36	A	2864	U
36	A	2865	C
36	A	2882	U
36	A	2883	A
36	A	2885	U
36	A	2888	A
36	A	2889	C
36	A	2893	A
36	A	2913	A
36	A	2917	G
36	A	2918	A
36	A	2922	A
36	A	2928	C
36	A	2932	G
36	A	2935	A
36	A	2956	A
36	A	2989	G
36	A	2990	A
36	A	2992	G
36	A	2993	U
36	A	3005	A
36	A	3016	G
36	A	3041	U
36	A	3053	A
36	A	3054	G
36	A	3060	C
36	A	3072	U
36	A	3090	G
36	A	3100	U
36	A	3108	U
36	A	3109	U
36	A	3110	C
36	A	3111	A
36	A	3112	A
36	A	3113	A
36	A	3150	U
36	A	3157	C
36	A	3158	A
36	A	3162	C

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Mol	Chain	Res	Type
36	A	3169	C
36	A	3172	C
36	A	3177	A
36	A	3183	U
36	A	3199	U
36	A	3200	U
36	A	3207	A
36	A	3209	A
36	A	3210	C
36	A	3212	C
36	A	3217	A
36	A	3218	A
36	A	3228	U
36	A	3229	U
36	A	3230	G
36	A	3231	U
37	B	8	U
37	B	16	C
37	B	21	A
37	B	45	G
37	B	48	U
37	B	54	C
37	B	55	U
37	B	56	U
37	B	64	A
37	B	69	U
37	B	76	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	A	1691	C
36	A	2112	A
36	A	2245	A

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

20 non-standard protein/DNA/RNA residues are modelled in this entry.

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
36	OMG	A	2815	94,33,36	18,26,27	0.93	2 (11%)	19,38,41	0.62	0
80	AYA	k	2	80	6,7,8	0.80	0	5,8,10	0.47	0
36	OMU	A	3039	94,36	19,22,23	0.27	0	26,31,34	0.44	0
44	SAC	K	2	44	7,8,9	0.22	0	8,9,11	0.60	0
37	2MG	B	10	37	18,26,27	1.16	2 (11%)	16,38,41	0.87	1 (6%)
54	AYA	U	2	54	6,7,8	0.79	0	5,8,10	0.61	0
9	5F0	AI	184	9	8,8,9	0.58	0	7,9,11	1.15	1 (14%)
1	5MC	AA	1488	1	18,22,23	0.32	0	26,32,35	0.42	0
37	PSU	B	39	37	18,21,22	0.76	0	22,30,33	2.56	4 (18%)
1	MA6	AA	1583	1	19,26,27	0.76	0	18,38,41	0.52	0
36	1MA	A	2617	36	16,25,26	1.15	3 (18%)	18,37,40	0.92	1 (5%)
1	B8T	AA	1486	1,93	19,22,23	0.30	0	26,31,34	0.34	0
1	MA6	AA	1584	1	19,26,27	0.76	0	18,38,41	0.58	0
71	THC	b	2	71	8,9,10	0.28	0	9,11,13	0.49	0
36	OMG	A	3040	32,36	18,26,27	0.90	1 (5%)	19,38,41	0.60	0
37	1MA	B	9	37	16,25,26	1.17	2 (12%)	18,37,40	0.88	1 (5%)
1	5MU	AA	1076	1	19,22,23	0.62	0	28,32,35	1.22	3 (10%)
29	AYA	A2	2	29	6,7,8	0.80	0	5,8,10	0.50	0
17	AYA	AQ	2	17	6,7,8	0.80	0	5,8,10	0.79	0
36	PSU	A	3067	36	18,21,22	0.78	0	22,30,33	2.57	5 (22%)

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
36	OMG	A	2815	94,33,36	-	0/5/27/28	0/3/3/3
80	AYA	k	2	80	-	0/4/6/8	-
36	OMU	A	3039	94,36	-	0/9/27/28	0/2/2/2
44	SAC	K	2	44	-	0/7/8/10	-
37	2MG	B	10	37	-	0/5/27/28	0/3/3/3
54	AYA	U	2	54	-	1/4/6/8	-
9	5F0	AI	184	9	-	0/9/9/10	-
1	5MC	AA	1488	1	-	0/7/25/26	0/2/2/2
37	PSU	B	39	37	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	AA	1583	1	-	0/7/29/30	0/3/3/3
36	1MA	A	2617	36	-	0/3/25/26	0/3/3/3
1	B8T	AA	1486	1,93	-	0/7/27/28	0/2/2/2
1	MA6	AA	1584	1	-	2/7/29/30	0/3/3/3
71	THC	b	2	71	-	0/8/10/12	-
36	OMG	A	3040	32,36	-	0/5/27/28	0/3/3/3
37	1MA	B	9	37	-	0/3/25/26	0/3/3/3
1	5MU	AA	1076	1	-	0/7/25/26	0/2/2/2
29	AYA	A2	2	29	-	0/4/6/8	-
17	AYA	AQ	2	17	-	1/4/6/8	-
36	PSU	A	3067	36	-	0/7/25/26	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	2617	1MA	C6-N6	3.11	1.35	1.27
37	B	9	1MA	C6-N6	3.10	1.35	1.27
37	B	10	2MG	C8-N7	-3.06	1.29	1.35
37	B	10	2MG	C5-C6	-2.36	1.42	1.47
36	A	2815	OMG	C5-C6	-2.26	1.42	1.47
36	A	3040	OMG	C5-C6	-2.21	1.42	1.47
37	B	9	1MA	C5-C4	-2.17	1.37	1.43
36	A	2617	1MA	C5-C4	-2.10	1.37	1.43
36	A	2815	OMG	C8-N7	-2.02	1.31	1.35
36	A	2617	1MA	C8-N7	-2.02	1.31	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	3067	PSU	N1-C2-N3	8.10	124.31	115.13
37	B	39	PSU	N1-C2-N3	8.09	124.30	115.13
36	A	3067	PSU	C4-N3-C2	-6.56	116.88	126.34
37	B	39	PSU	C4-N3-C2	-6.55	116.90	126.34
1	AA	1076	5MU	C4-N3-C2	-4.81	121.12	127.35
36	A	3067	PSU	O2-C2-N1	-3.68	118.74	122.79
37	B	39	PSU	O2-C2-N1	-3.68	118.74	122.79
9	AI	184	5F0	OD1-C1-CB	-2.67	117.64	125.43
1	AA	1076	5MU	C5-C4-N3	2.66	117.58	115.31
36	A	3067	PSU	O2-C2-N3	-2.58	116.95	121.82
37	B	39	PSU	O2-C2-N3	-2.57	116.96	121.82
1	AA	1076	5MU	N3-C2-N1	2.26	117.89	114.89
36	A	2617	1MA	N1-C6-N6	2.23	125.43	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	3067	PSU	O4'-C1'-C2'	2.18	108.22	105.14
37	B	10	2MG	O6-C6-C5	2.11	128.50	124.37
37	B	9	1MA	N1-C6-N6	2.09	125.09	119.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	AQ	2	AYA	C-CA-N-CT
1	AA	1584	MA6	C5-C6-N6-C9
1	AA	1584	MA6	C4'-C5'-O5'-P
54	U	2	AYA	C-CA-N-CT

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	2815	OMG	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 278 ligands modelled in this entry, 265 are monoatomic - leaving 13 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	$\# Z > 2$
97	ATP	AX	501	93	26,33,33	0.76	0	31,52,52	0.63	0
91	SPM	AA	1702	-	13,13,13	0.28	0	12,12,12	0.99	0
92	SPD	A	3301	-	9,9,9	0.42	0	8,8,8	1.08	0
96	FES	AP	201	5,16	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
96	FES	r	201	86,42	0,4,4	-	-	-		
90	NAD	AA	1701	93	42,48,48	0.56	0	50,73,73	0.58	1 (2%)
100	VAL	B	101	37	4,6,7	0.55	0	6,7,9	0.71	0
99	PUT	A	3304	-	5,5,5	0.25	0	4,4,4	0.52	0
96	FES	AT	201	20,13	0,4,4	-	-	-		
92	SPD	A	3302	-	9,9,9	0.32	0	8,8,8	1.23	0
92	SPD	AA	1703	-	9,9,9	0.28	0	8,8,8	1.31	2 (25%)
92	SPD	A	3303	-	9,9,9	0.38	0	8,8,8	1.14	0
98	GDP	AX	503	-	24,30,30	0.89	2 (8%)	30,47,47	0.61	0

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
97	ATP	AX	501	93	-	0/18/38/38	0/3/3/3
91	SPM	AA	1702	-	-	1/11/11/11	-
92	SPD	A	3301	-	-	2/7/7/7	-
100	VAL	B	101	37	-	0/5/6/8	-
96	FES	AP	201	5,16	-	-	0/1/1/1
90	NAD	AA	1701	93	-	0/26/62/62	0/5/5/5
96	FES	r	201	86,42	-	-	0/1/1/1
99	PUT	A	3304	-	-	0/3/3/3	-
96	FES	AT	201	20,13	-	-	0/1/1/1
92	SPD	A	3302	-	-	0/7/7/7	-
92	SPD	AA	1703	-	-	0/7/7/7	-
92	SPD	A	3303	-	-	2/7/7/7	-
98	GDP	AX	503	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
98	AX	503	GDP	C5-C6	-2.23	1.42	1.47
98	AX	503	GDP	C8-N7	-2.02	1.31	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	AA	1701	NAD	C5A-C6A-N6A	2.26	123.79	120.35
92	AA	1703	SPD	C4-C5-N6	-2.23	106.11	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	AA	1703	SPD	C8-C7-N6	-2.12	106.41	112.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	A	3301	SPD	N6-C7-C8-C9
92	A	3301	SPD	C3-C4-C5-N6
92	A	3303	SPD	C4-C5-N6-C7
91	AA	1702	SPM	C12-C11-N10-C9
92	A	3303	SPD	C8-C7-N6-C5

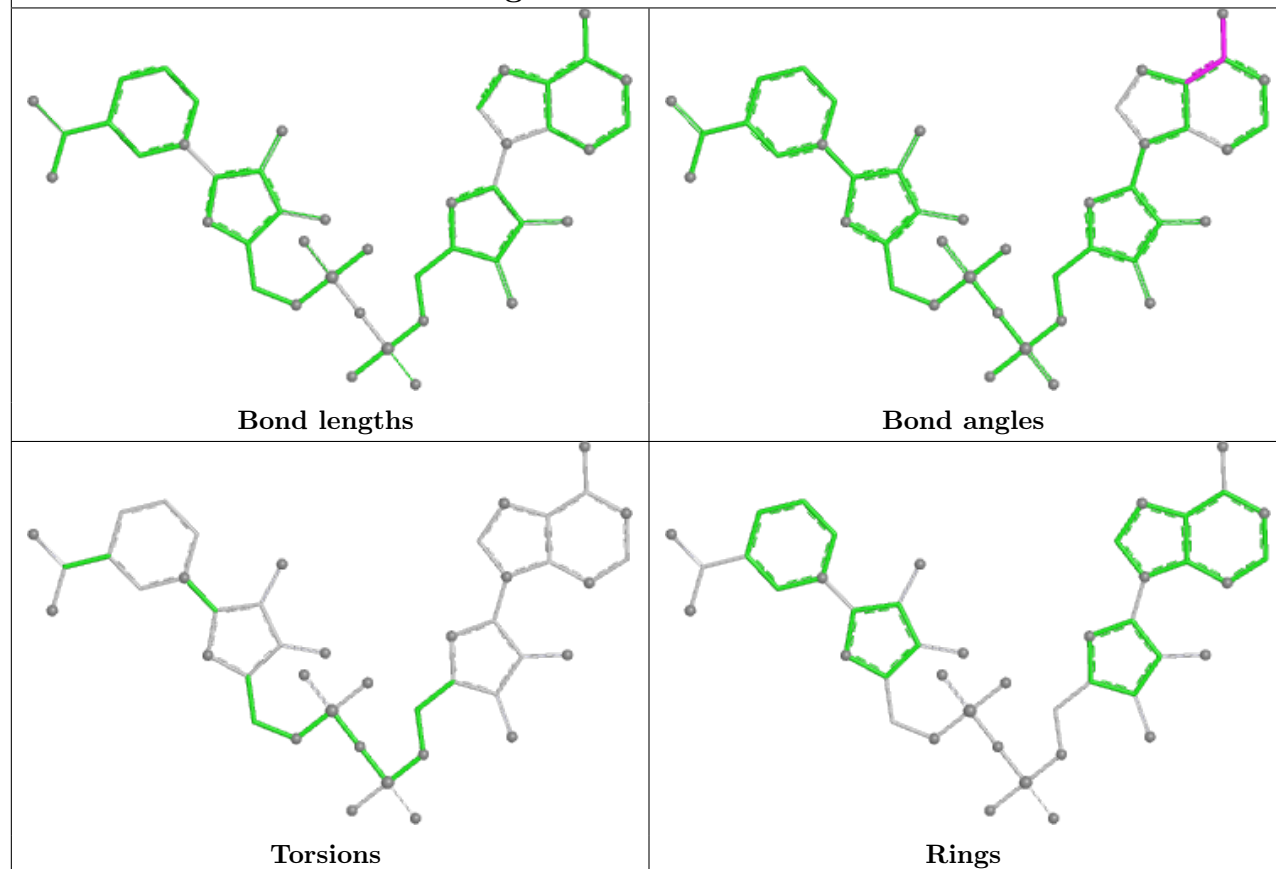
There are no ring outliers.

2 monomers are involved in 2 short contacts:

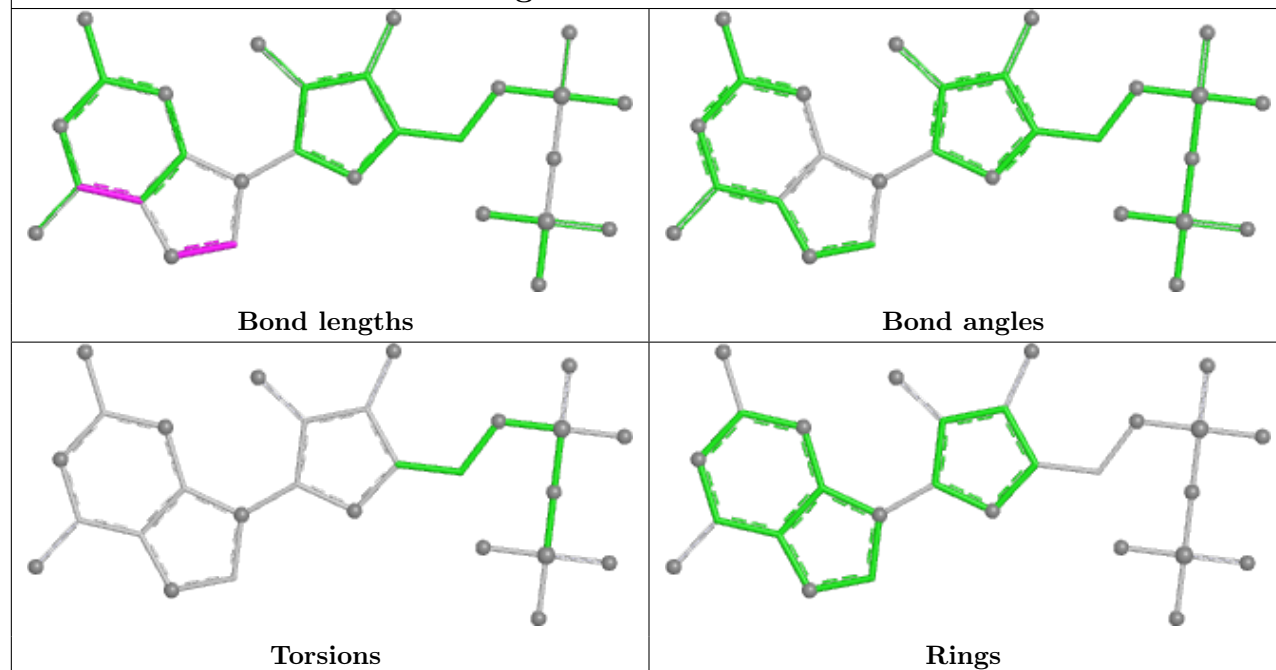
Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	AX	501	ATP	1	0
100	B	101	VAL	1	0

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

Ligand NAD AA 1701



Ligand GDP AX 503



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
32	Aw	1
36	A	1
33	Ax	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Aw	44:A	O3'	74:C	P	56.79
1	A	2357:C	O3'	2361:G	P	10.83
1	Ax	15:A	O3'	21:A	P	9.85

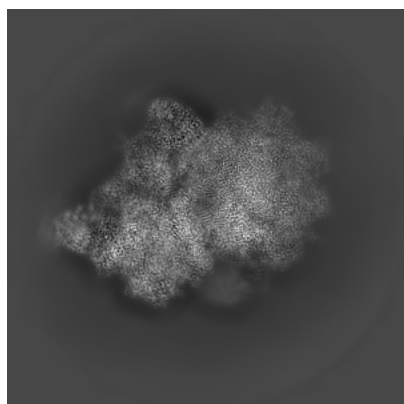
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13980. These allow visual inspection of the internal detail of the map and identification of artifacts.

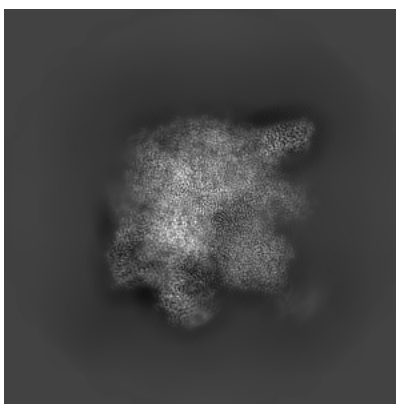
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

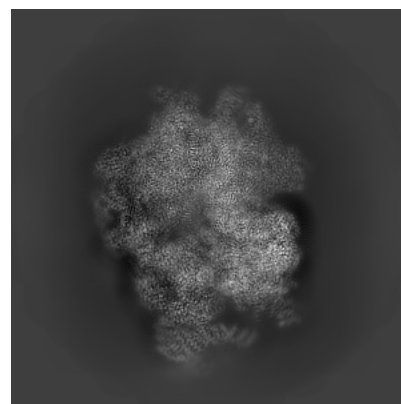
6.1.1 Primary map



X

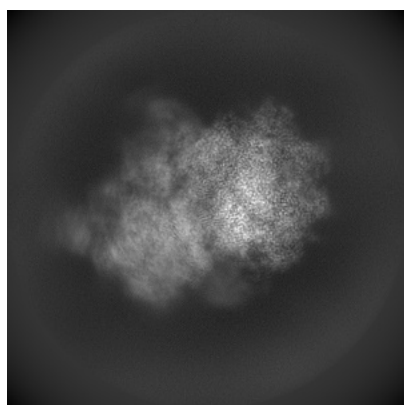


Y

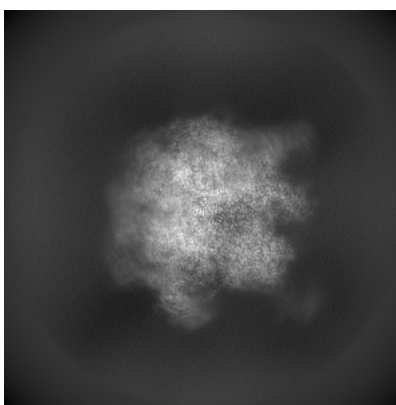


Z

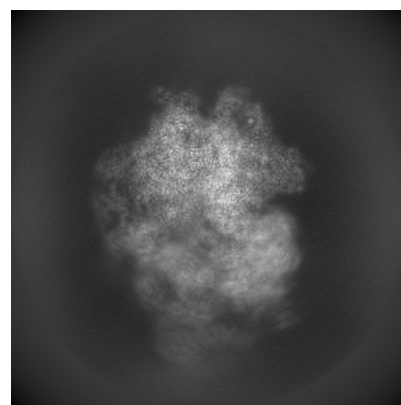
6.1.2 Raw map



X



Y

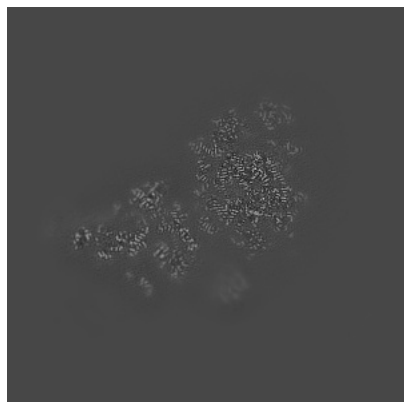


Z

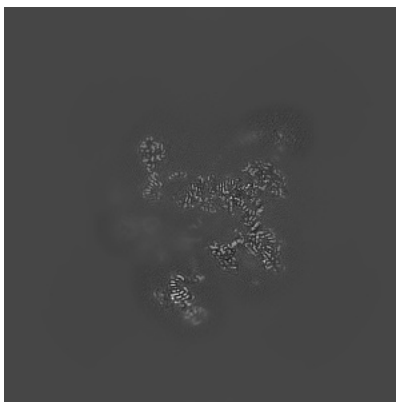
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

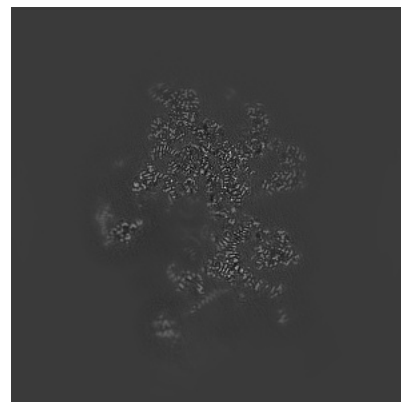
6.2.1 Primary map



X Index: 270

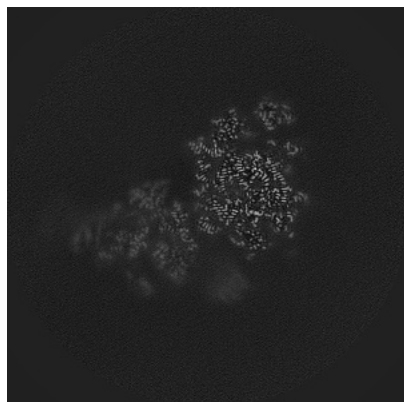


Y Index: 270

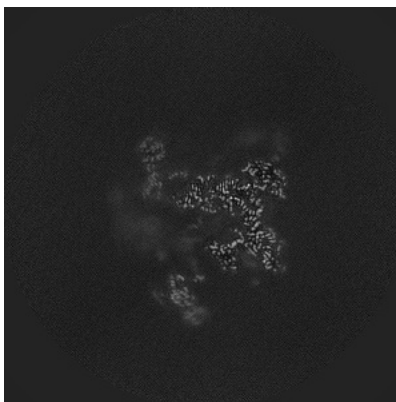


Z Index: 270

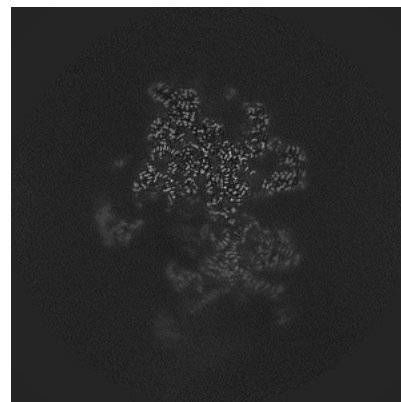
6.2.2 Raw map



X Index: 270



Y Index: 270

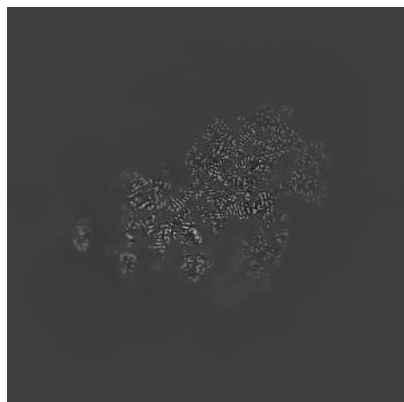


Z Index: 270

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

6.3 Largest variance slices [i](#)

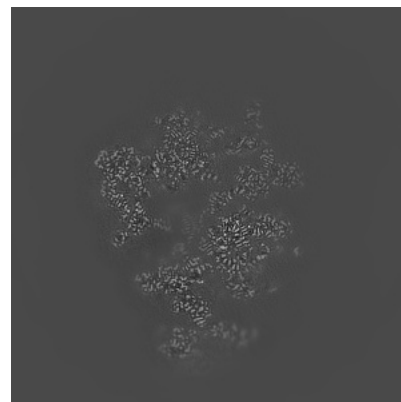
6.3.1 Primary map



X Index: 291

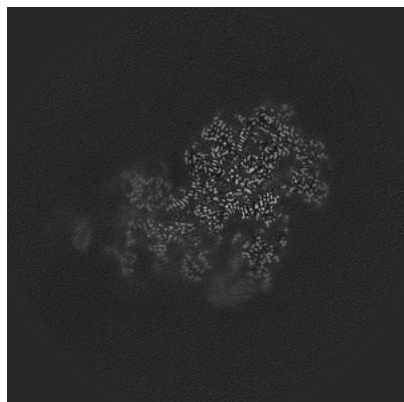


Y Index: 318

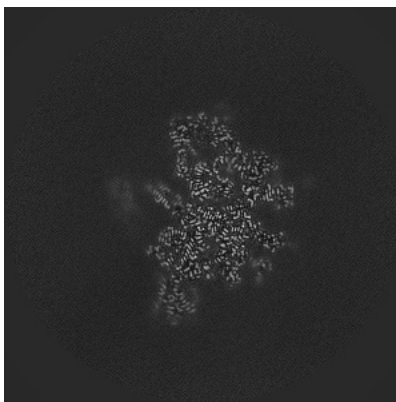


Z Index: 240

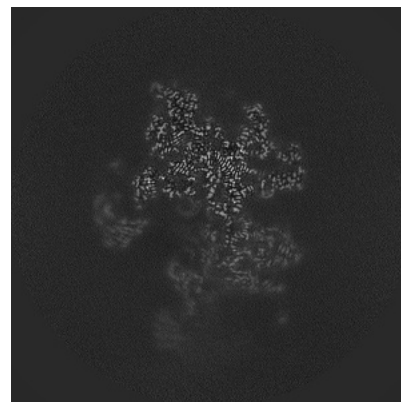
6.3.2 Raw map



X Index: 289



Y Index: 318



Z Index: 265

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

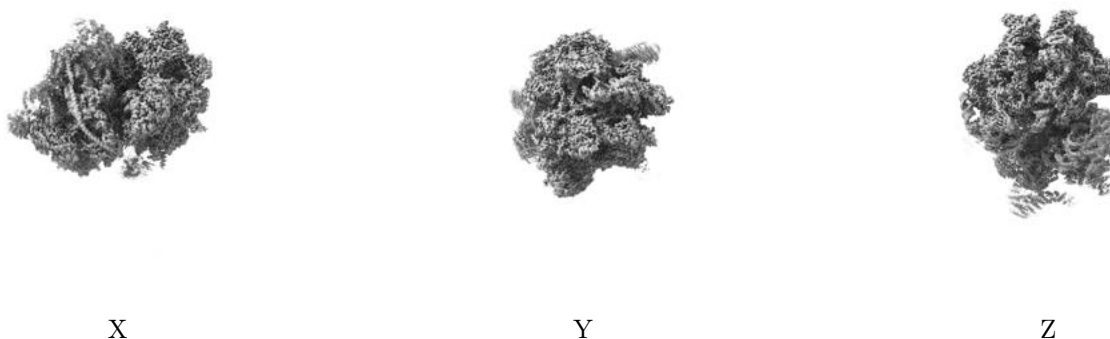
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. 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.

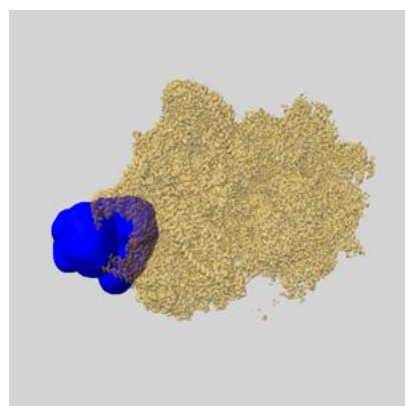
6.5 Mask visualisation [i](#)

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

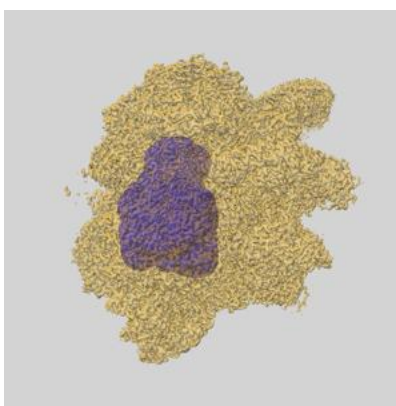
A mask typically either:

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

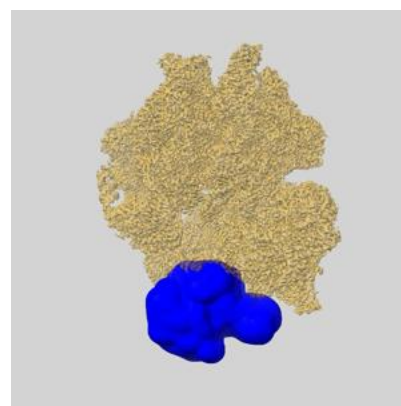
6.5.1 emd_13980_msk_9.map [i](#)



X

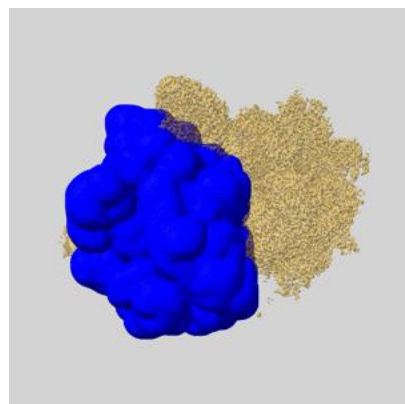


Y

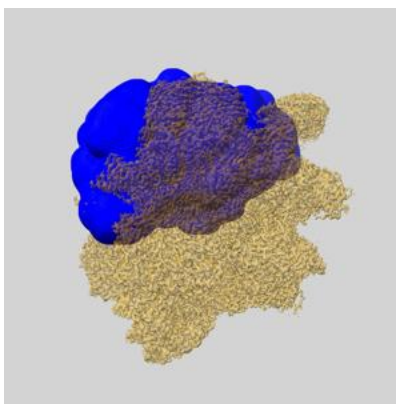


Z

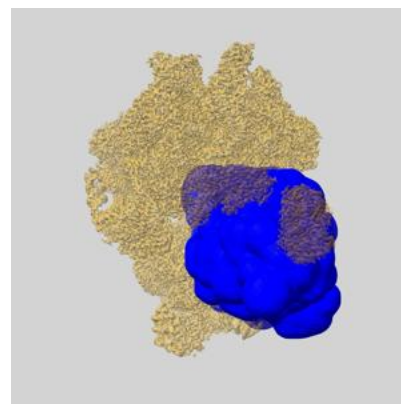
6.5.2 emd_13980_msk_8.map [i](#)



X

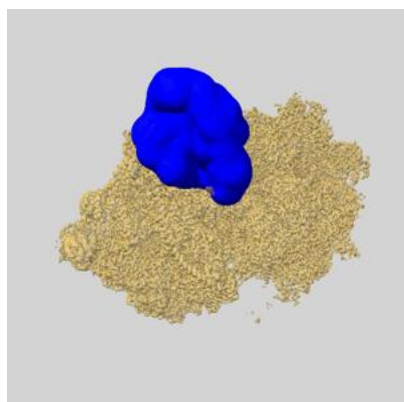


Y

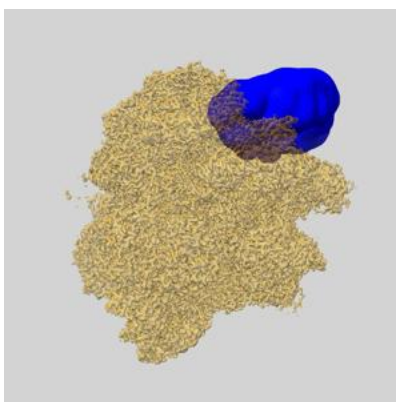


Z

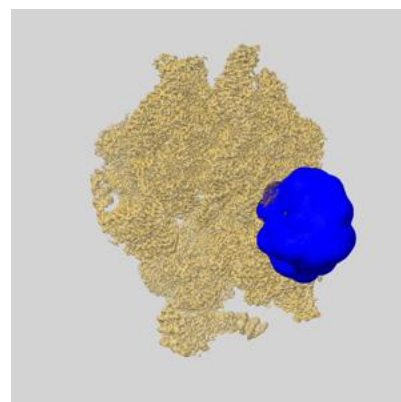
6.5.3 emd_13980_msk_7.map [i](#)



X

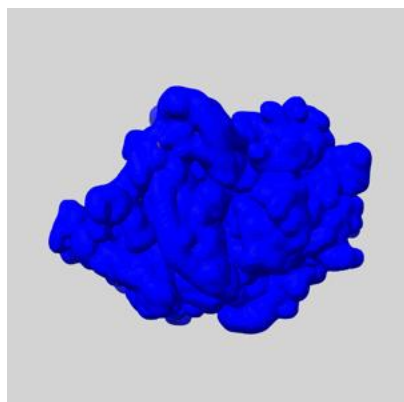


Y

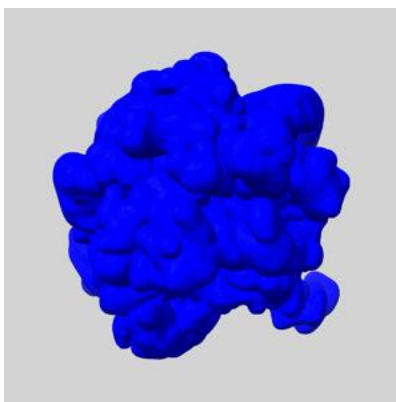


Z

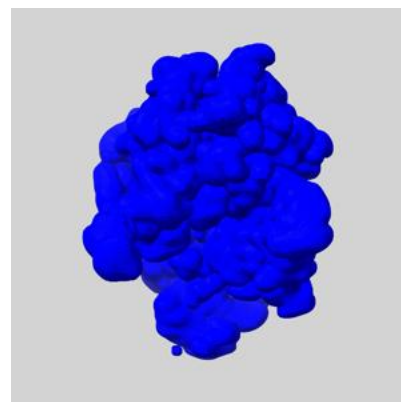
6.5.4 emd_13980_msk_6.map [i](#)



X

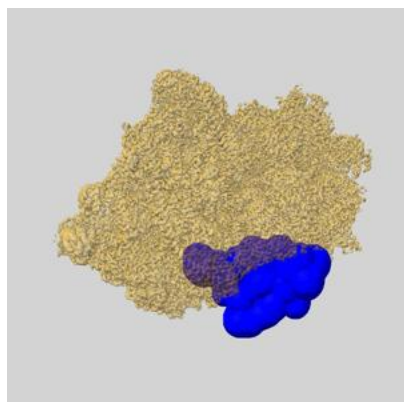


Y

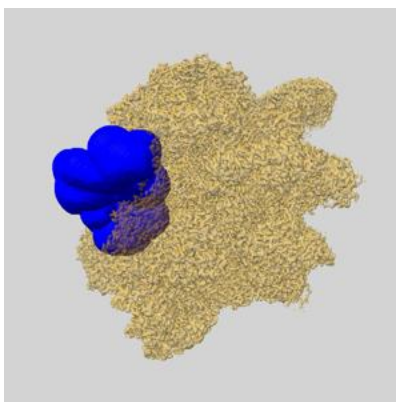


Z

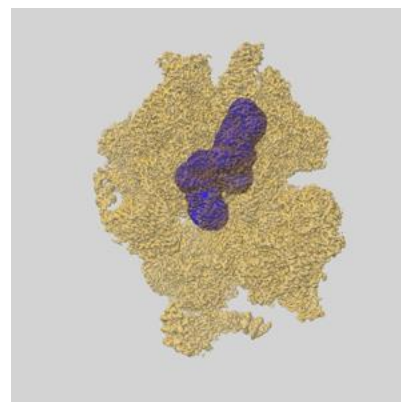
6.5.5 emd_13980_msk_5.map [i](#)



X

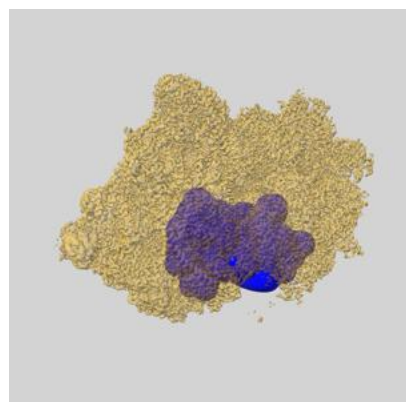


Y

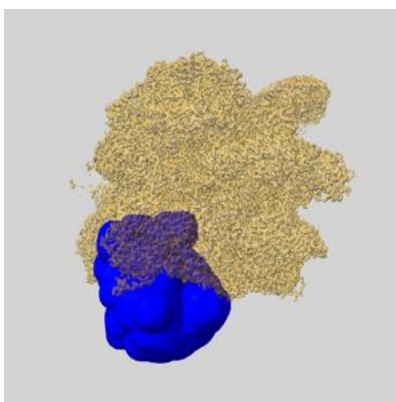


Z

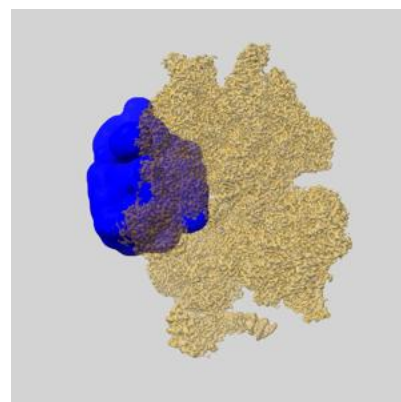
6.5.6 emd_13980_msk_4.map [i](#)



X

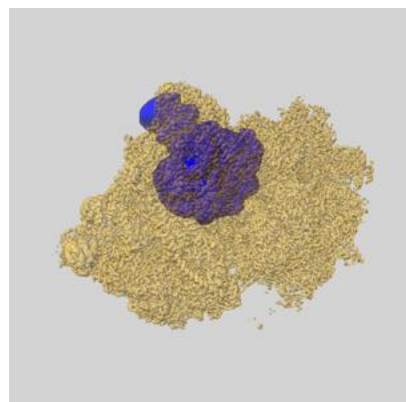


Y

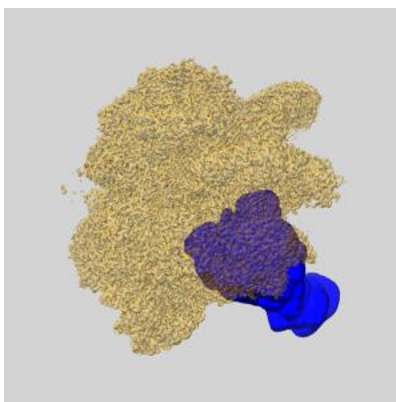


Z

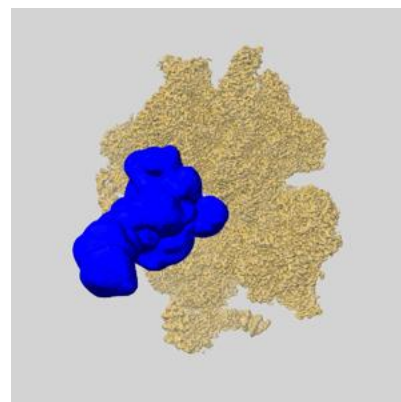
6.5.7 emd_13980_msk_3.map [i](#)



X

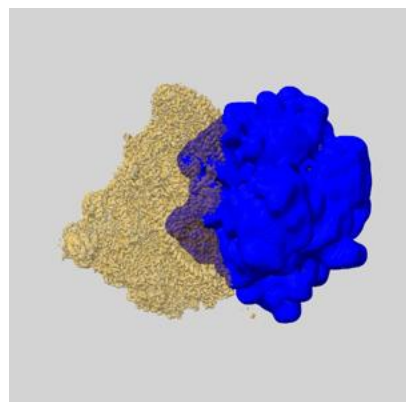


Y

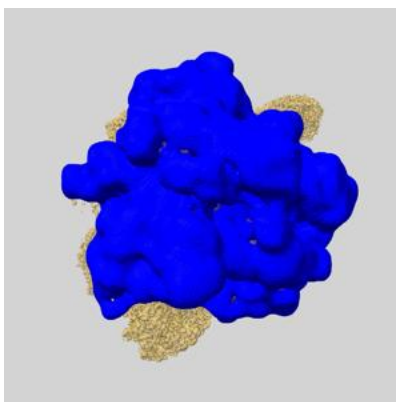


Z

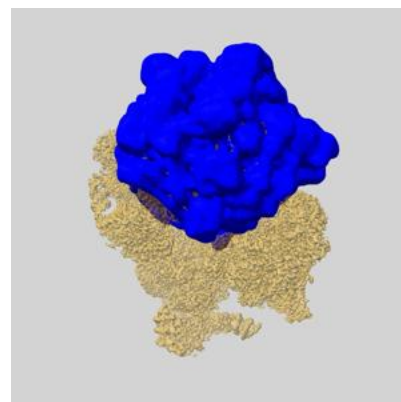
6.5.8 emd_13980_msk_2.map [i](#)



X

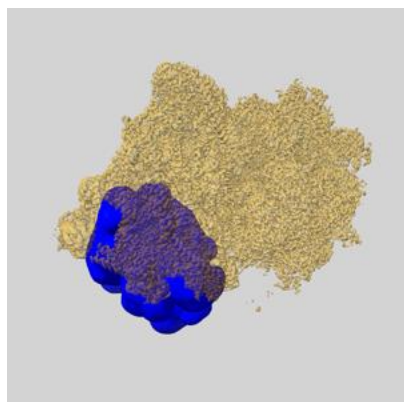


Y

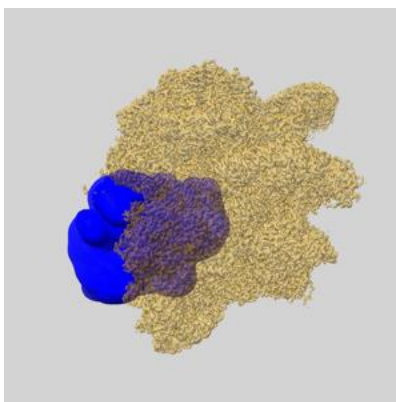


Z

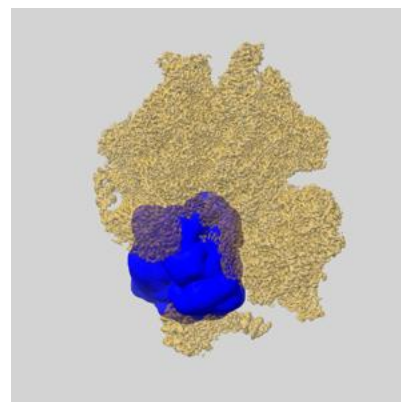
6.5.9 emd_13980_msk_1.map [i](#)



X



Y

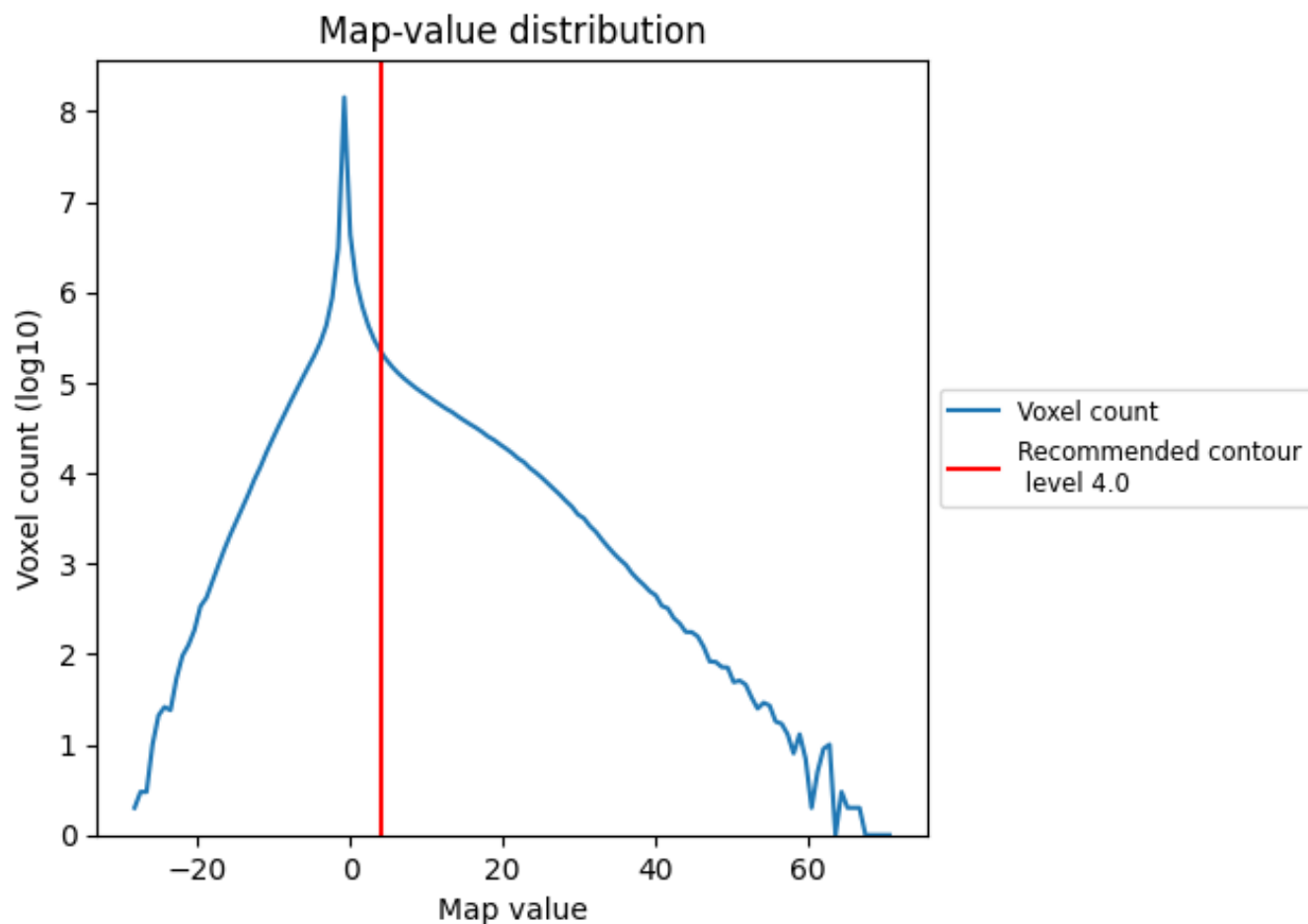


Z

7 Map analysis [i](#)

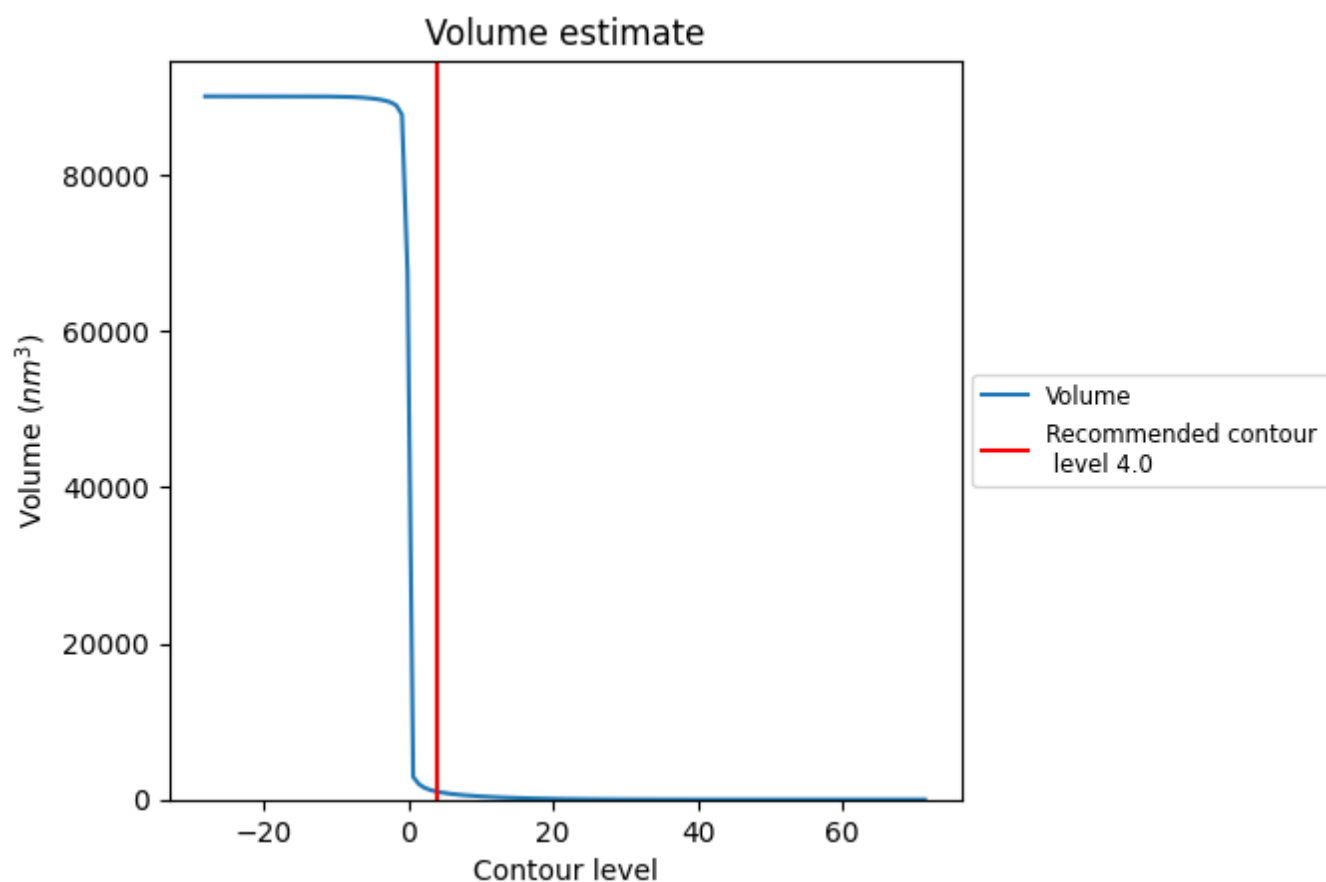
This section contains the results of statistical analysis of the map.

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.

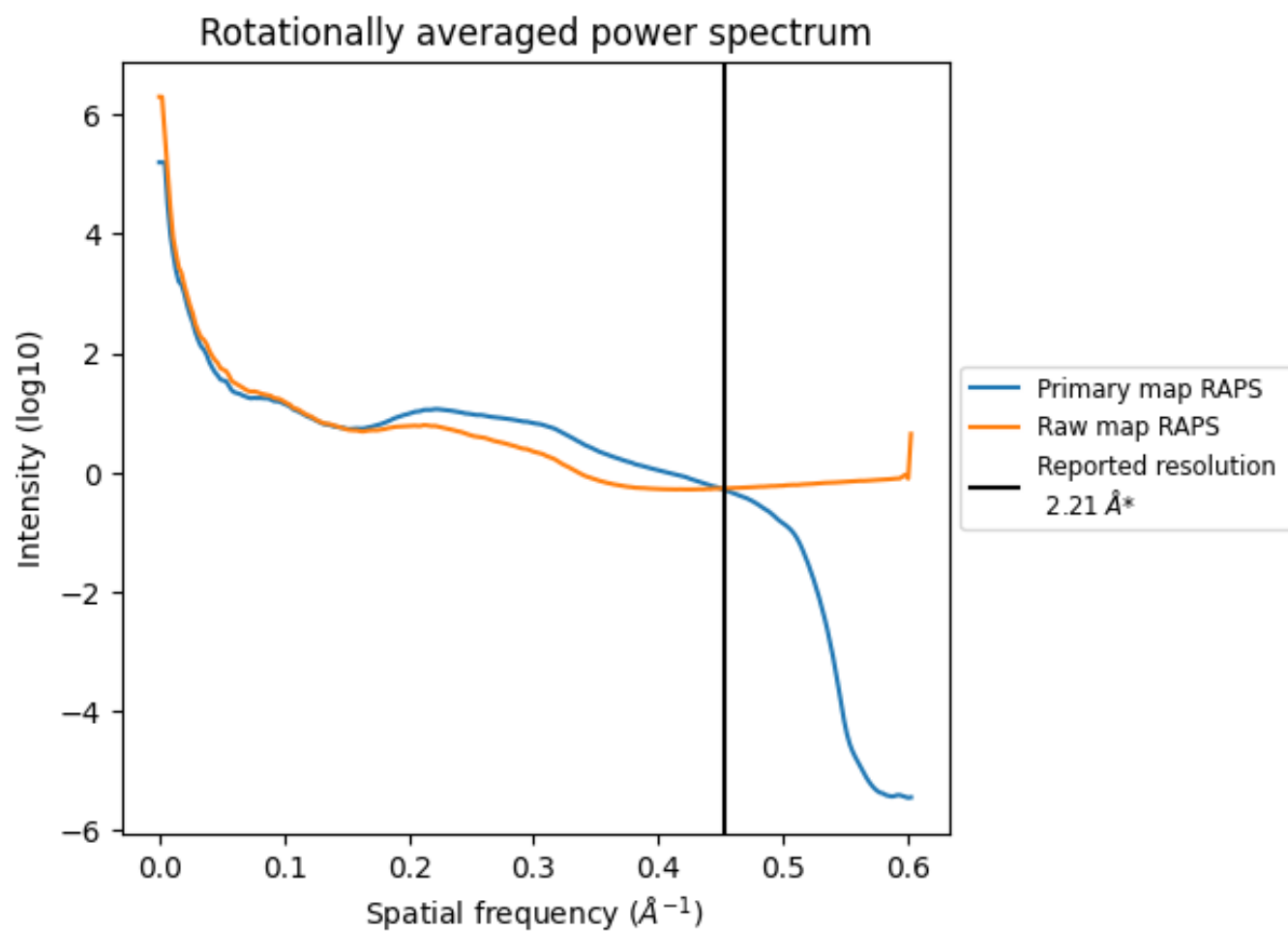
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 998 nm^3 ; this corresponds to an approximate mass of 902 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 ⓘ

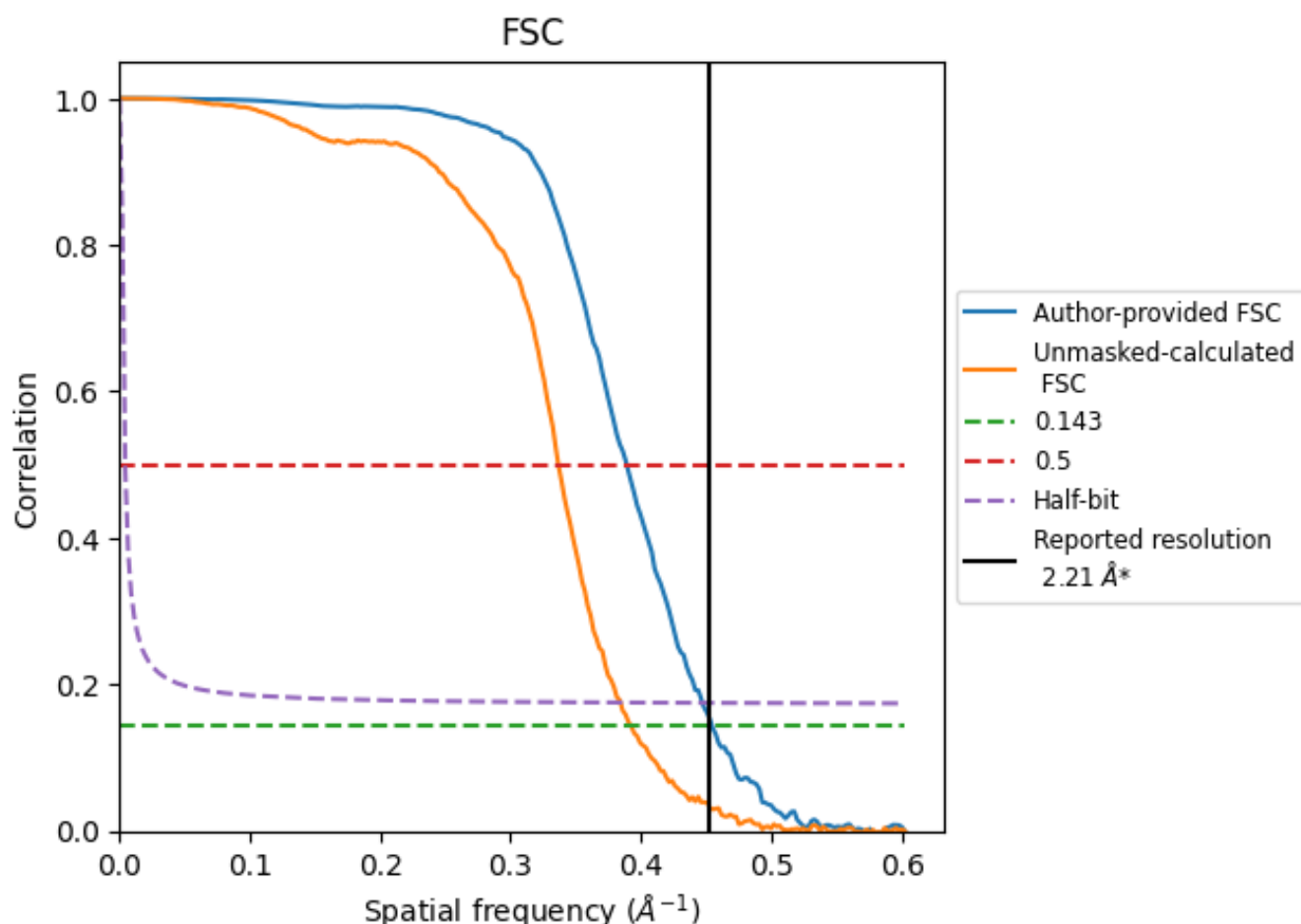


*Reported resolution corresponds to spatial frequency of 0.452 \AA^{-1}

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 0.452 Å⁻¹

8.2 Resolution estimates [i](#)

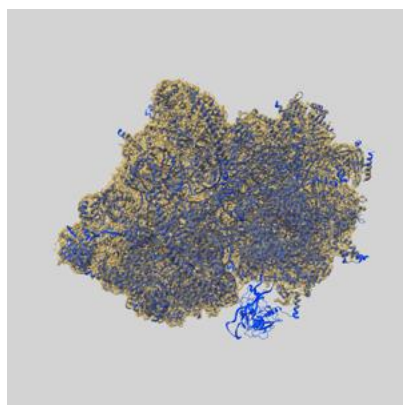
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.21	-	-
Author-provided FSC curve	2.20	2.57	2.24
Unmasked-calculated*	2.55	2.97	2.60

*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 2.55 differs from the reported value 2.21 by more than 10 %

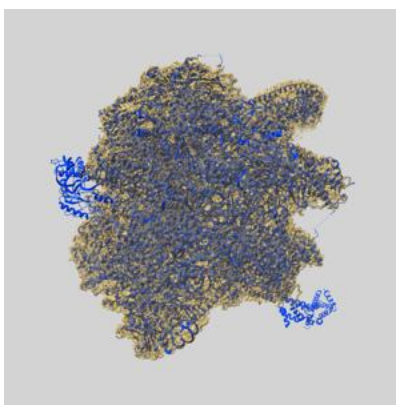
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13980 and PDB model 7QI4. Per-residue inclusion information can be found in section 3 on page 30.

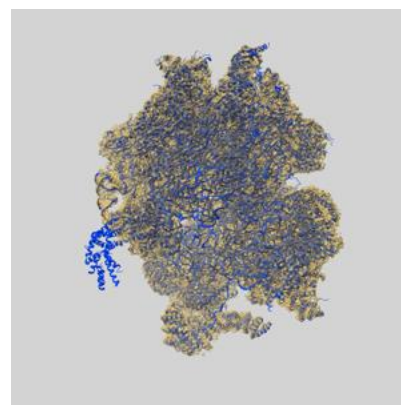
9.1 Map-model overlay [i](#)



X



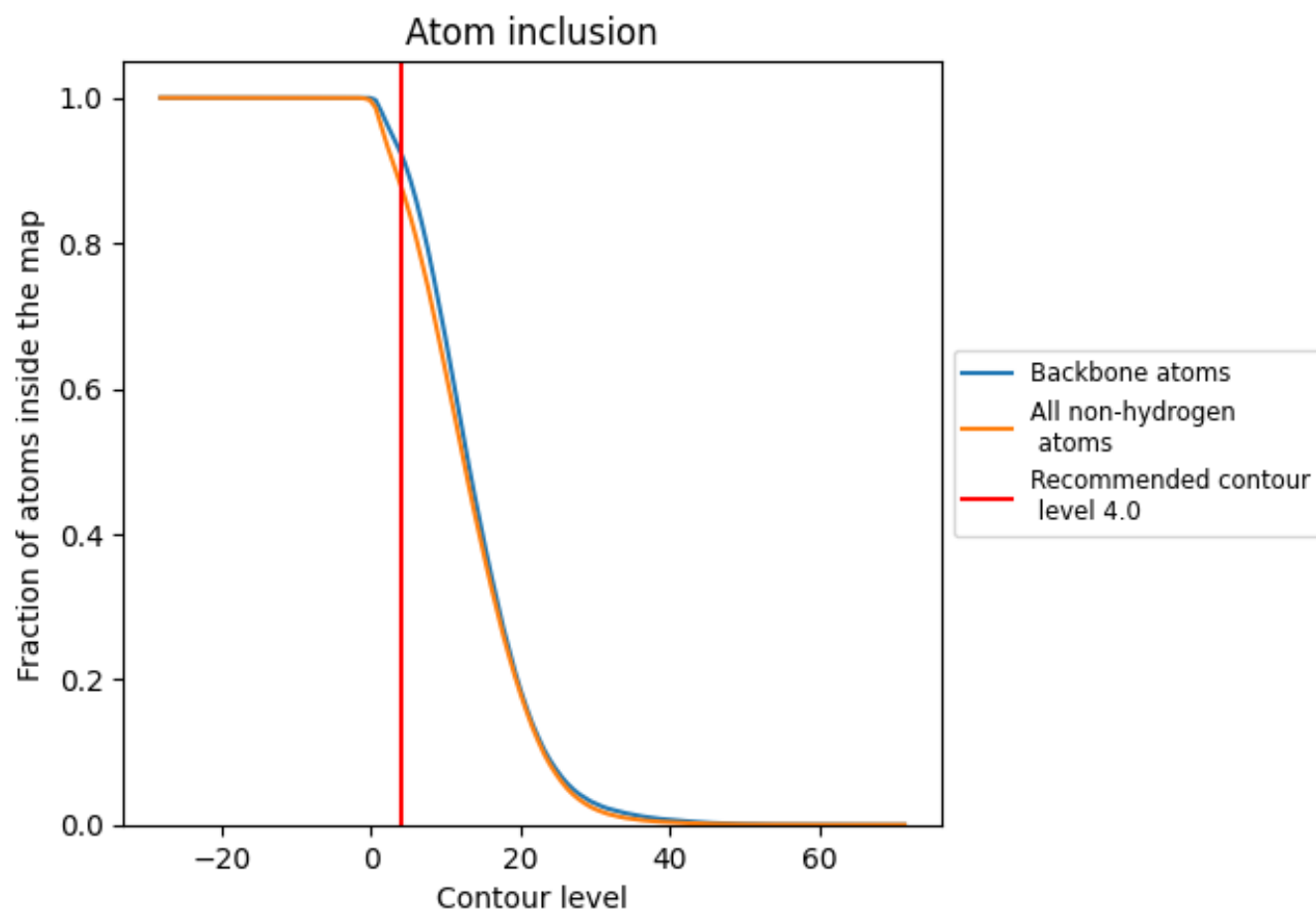
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 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 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.