Full wwPDB EM Validation Report ⓘ

Jan 11, 2024 – 06:33 pm GMT

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

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

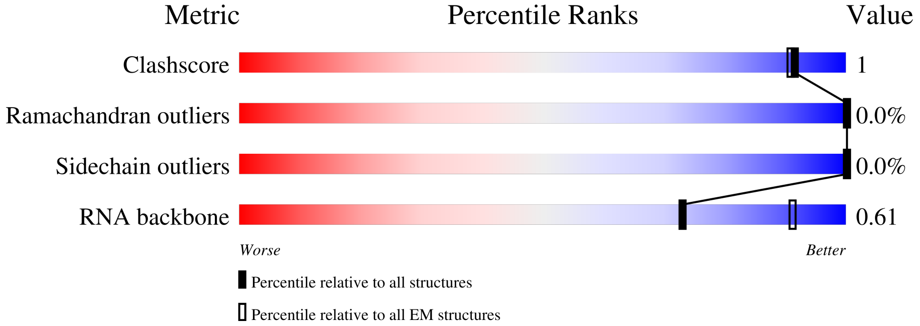
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

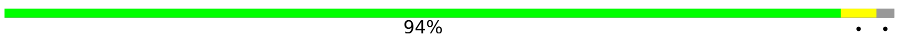
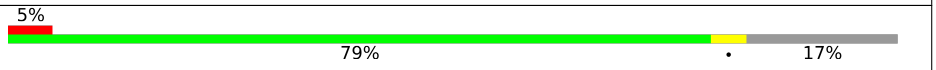
The reported resolution of this entry is 2.21 Å.

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.



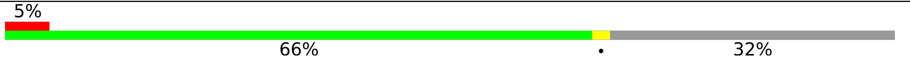
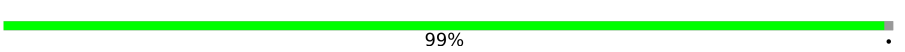
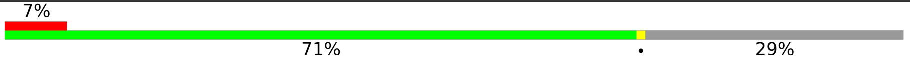
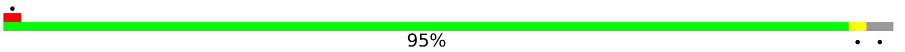
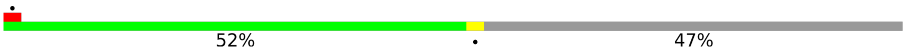
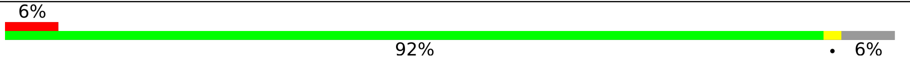
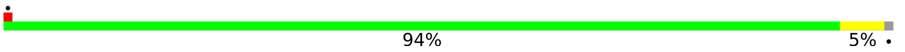
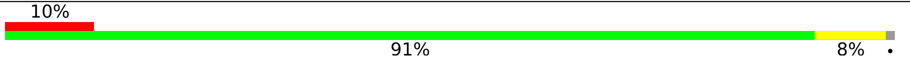
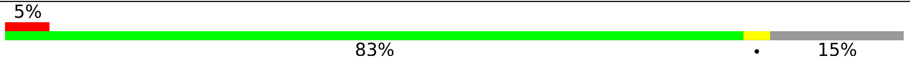
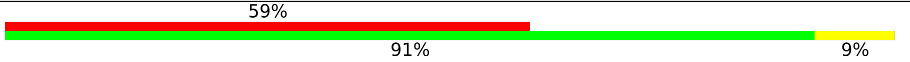
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	

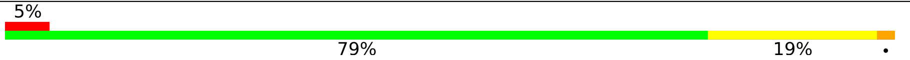
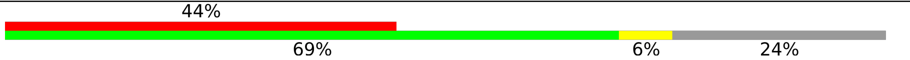
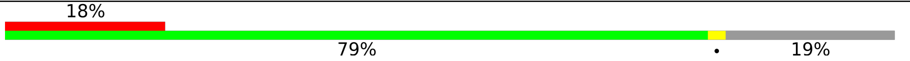
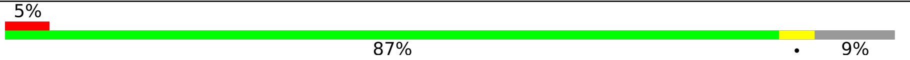
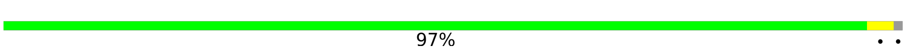
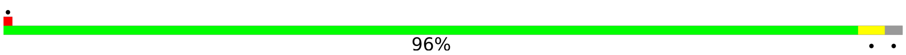
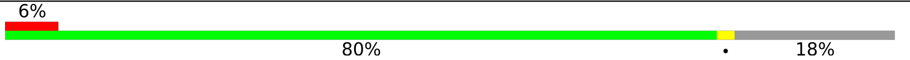
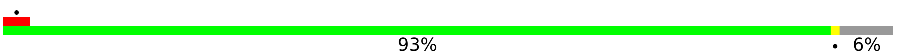
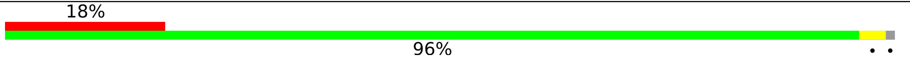
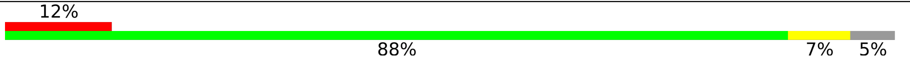
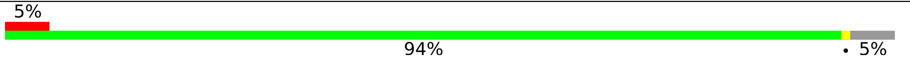
Continued on next page...

Continued from previous page...

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	

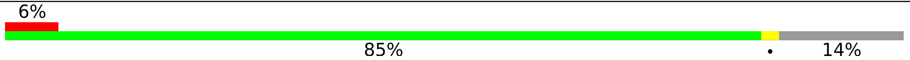
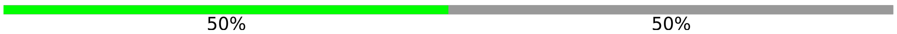
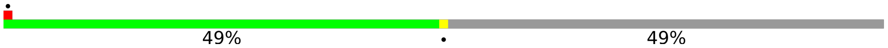
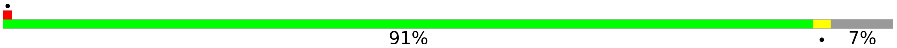
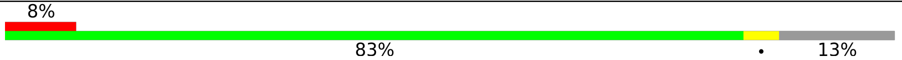
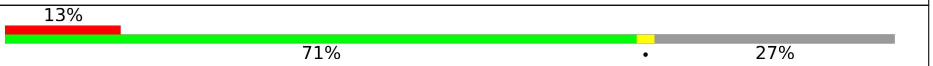
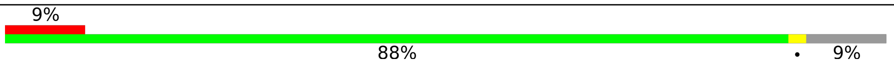
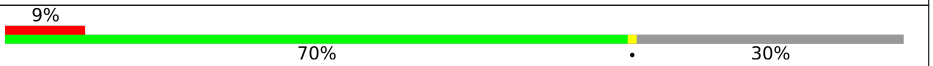
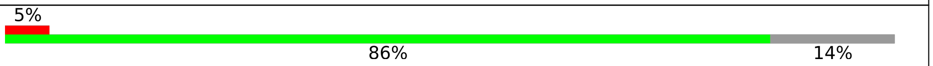
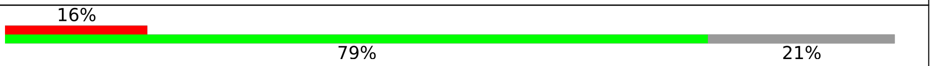
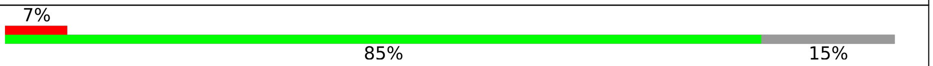
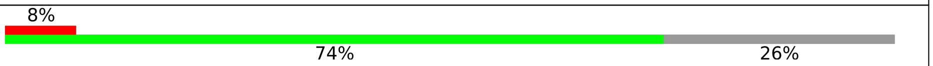
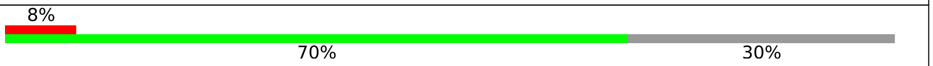
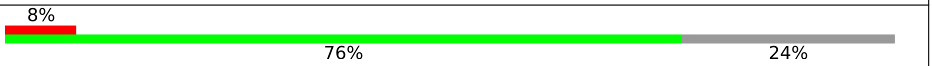
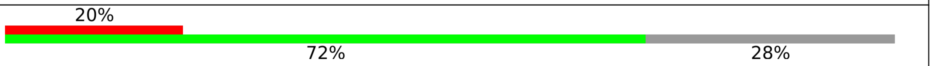
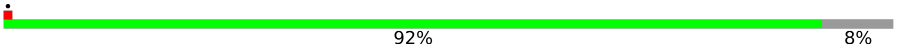
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	Ax	70	70% 84% 16%
34	Az	34	56% 65% 35%
35	A	1558	5% 79% 19%
36	B	72	75% 24%
37	D	305	76% 22%
38	E	348	84% 12%
39	F	311	79% 19%
40	H	267	44% 69% 6% 24%
41	I	261	18% 79% 19%
42	J	192	5% 87% 9%
43	K	178	97%
44	L	145	77% 21%
45	M	296	96%
46	N	251	84% 5% 12%
47	O	175	81% 7% 12%
48	P	180	79% 20%
49	Q	292	6% 80% 18%
50	R	149	93% 6%
51	S	205	76% 21%
52	T	206	77% 19%
53	U	153	18% 96%
54	V	216	12% 88% 7% 5%
55	W	148	76% 22%
56	X	256	5% 94% 5%
57	Y	250	72% 28%

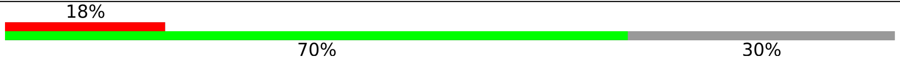
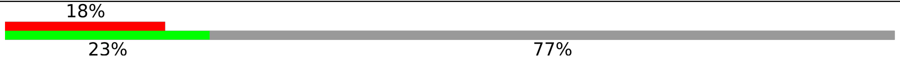
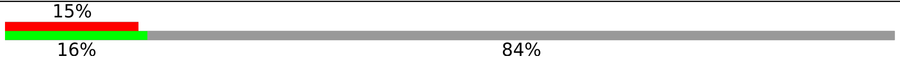
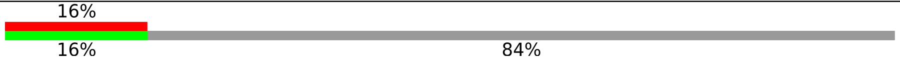
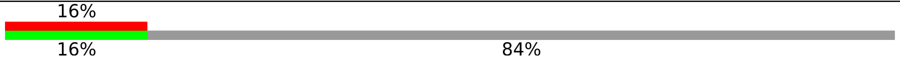
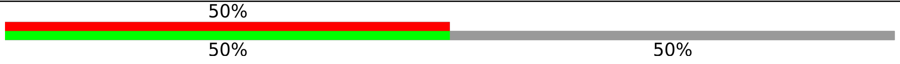
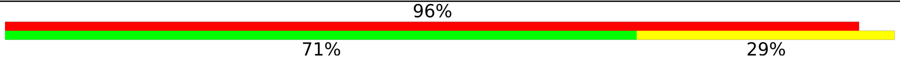
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
58	Z	161	 73% 24%
59	0	188	 57% 41%
60	1	65	 6% 85% 14%
61	2	92	 50% 50%
62	3	188	 49% 49%
63	4	103	 35% 63%
64	5	423	 91% 7%
65	6	380	 89% 7%
66	7	338	 8% 83% 13%
67	8	206	 13% 71% 27%
68	9	137	 9% 88% 9%
69	a	142	 9% 70% 30%
70	b	215	 70% 30%
71	c	332	 5% 86% 14%
72	d	306	 16% 79% 21%
73	e	279	 7% 85% 15%
74	f	212	 8% 74% 26%
75	g	166	 81% 19%
76	h	158	 8% 70% 30%
77	i	128	 76% 24%
78	j	123	 8% 76% 24%
79	k	112	 90% 10%
80	l	138	 59% 41%
81	m	128	 20% 72% 28%
82	o	102	 92% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
83	p	206	
84	q	222	
85	r	196	
86	s	439	
87	t	198	
87	u	198	
87	v	198	
87	w	198	
87	x	198	
87	y	198	
88	z	325	
89	Ay	52	

2 Entry composition

There are 101 unique types of molecules in this entry. The entry contains 340116 atoms, of which 152427 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
			Total	C	H	N	O	P		
1	AA	954	30564	9088	10304	3647	6571	954	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	AB	225	3644	1164	1816	331	323	10	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	AC	132	2172	699	1089	195	185	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	AD	343	5536	1713	2805	518	487	13	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	AE	122	1972	614	1000	177	177	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	AF	208	3496	1104	1771	312	298	11	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	AG	327	5377	1710	2689	477	487	14	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	AH	140	2339	745	1187	194	210	3	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	AI	137	2081	642	1061	192	182	4	0	0

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
			Total	C	H	N	O	S		
10	AJ	108	1727	521	888	169	143	6	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	AK	101	1748	537	886	179	141	5	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	AL	174	2994	925	1541	270	251	7	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	AM	119	1908	594	966	185	157	6	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	AN	110	1797	562	929	156	147	3	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	AO	193	3149	1014	1557	294	277	7	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	AP	97	1587	501	806	134	138	8	0	0

- Molecule 17 is a protein called MRPS21 isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	AQ	86	1502	460	758	150	126	8	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	AR	295	4839	1533	2430	413	455	8	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	AS	135	2227	716	1116	198	196	1	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	AT	168	2764	877	1393	239	244	11	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	AU	176	2989	916	1501	301	267	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	AV	362	5933	1904	2964	495	558	12	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	AW	100	1593	498	804	141	146	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	AX	352	5694	1822	2845	499	517	11	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	AY	149	2444	801	1198	207	234	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	AZ	100	1698	534	859	153	148	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
27	A0	215	Total 3584	C 1130	H 1797	N 339	O 313	S 5	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
28	A1	279	Total 4561	C 1435	H 2296	N 387	O 432	S 11	0	0

- 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 1906	C 579	H 971	N 182	O 166	S 8	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	A3	70	Total 1326	C 401	H 701	N 134	O 89	S 1	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
31	A4	588	Total 9538	C 3053	H 4770	N 808	O 879	S 28	0	0

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
33	Ax	70	Total 2233	C 665	H 751	N 260	O 487	P 70	0	0

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
34	Az	34	1079	324	360	123	238	34	0	0

- Molecule 35 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
35	A	1558	49871	14843	16801	5963	10706	1558	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	A	deletion	GB 1563835895
A	?	-	C	deletion	GB 1563835895
A	?	-	U	deletion	GB 1563835895

- Molecule 36 is a RNA chain called mitochondrial tRNAVal.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	74	C	G	conflict	GB NC_012920.1
B	76	A	U	conflict	GB NC_012920.1

- Molecule 37 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
37	D	238	3780	1157	1921	376	317	9	0	0

- Molecule 38 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	E	305	4822	1545	2416	418	432	11	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
39	F	252	Total	C	H	N	O	S	0	0
			4097	1305	2066	370	350	6		

- Molecule 40 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	H	202	Total	C	H	N	O	S	0	0
			3397	1067	1736	304	286	4		

- Molecule 41 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	I	212	Total	C	H	N	O	S	0	0
			3481	1088	1786	304	292	11		

- Molecule 42 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	J	175	Total	C	H	N	O	S	0	0
			2738	847	1408	237	244	2		

- Molecule 43 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	K	177	Total	C	H	N	O	S	0	0
			2907	936	1452	259	253	7		

- Molecule 44 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	L	115	Total	C	H	N	O	S	0	0
			1832	559	942	171	155	5		

- Molecule 45 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	M	291	Total	C	H	N	O	S	0	0
			4723	1483	2396	430	408	6		

- Molecule 46 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	N	222	3604	1143	1818	326	307	10	0	0

- Molecule 47 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	O	154	2554	792	1295	241	219	7	0	0

- Molecule 48 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	P	144	2339	733	1166	224	211	5	0	0

- Molecule 49 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
49	Q	239	4021	1277	2031	353	351	9	0	0

- Molecule 50 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	R	140	2369	732	1215	231	187	4	0	0

- Molecule 51 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
51	S	161	2659	835	1366	227	227	4	0	0

- Molecule 52 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
52	T	166	2781	875	1412	254	233	7	0	0

- Molecule 53 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
53	U	152	2483	788	1232	234	226	3	0	0

- Molecule 54 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
54	V	205	3365	1068	1689	298	302	8	0	0

- Molecule 55 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
55	W	116	1840	577	936	171	153	3	0	0

- Molecule 56 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
56	X	244	4105	1322	2061	352	365	5	0	0

- Molecule 57 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
57	Y	181	3154	995	1598	298	259	4	0	0

- Molecule 58 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
58	Z	122	2041	636	1045	186	171	3	0	0

- Molecule 59 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
59	0	110	1815	554	917	176	162	6	0	0

- Molecule 60 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
60	1	56	977	296	513	89	77	2	0	0

- Molecule 61 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
61	2	46	784	233	407	83	60	1	0	0

- Molecule 62 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
62	3	95	1716	539	884	162	128	3	0	0

- Molecule 63 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
63	4	38	704	217	362	72	49	4	0	0

- Molecule 64 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
64	5	394	6419	2073	3209	560	566	11	0	0

- Molecule 65 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
65	6	354	5792	1881	2844	525	533	9	0	0

- Molecule 66 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
66	7	294	4789	1529	2399	405	438	18	0	0

- Molecule 67 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
67	8	151	2588	812	1310	226	238	2	0	0

- Molecule 68 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
68	9	124	1985	644	988	170	181	2	0	0

- Molecule 69 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
69	a	100	1652	529	812	152	154	5	0	0

- Molecule 70 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
70	b	150	2392	744	1196	231	218	3	0	0

- Molecule 71 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
71	c	286	4621	1470	2322	397	423	9	0	0

- Molecule 72 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
72	d	241	3965	1273	1980	340	359	13	0	0

- Molecule 73 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
73	e	238	3848	1222	1917	339	364	6	0	0

- Molecule 74 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	f	157	Total 2523	C 799	H 1271	N 207	O 242	S 4	0	0

- Molecule 75 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	g	134	Total 2210	C 719	H 1097	N 193	O 199	S 2	0	0

- Molecule 76 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	h	110	Total 1778	C 568	H 883	N 156	O 168	S 3	0	0

- Molecule 77 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	i	97	Total 1687	C 532	H 859	N 165	O 127	S 4	0	0

- Molecule 78 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 79 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	k	101	Total 1559	C 479	H 785	N 148	O 142	S 5	0	0

- Molecule 80 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	l	82	Total 1363	C 437	H 675	N 120	O 128	S 3	0	0

- Molecule 81 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	m	92	Total 1551	C 488	H 760	N 159	O 142	S 2	0	0

- Molecule 82 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	o	94	Total 1604	C 501	H 806	N 165	O 129	S 3	0	0

- Molecule 83 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	p	147	Total 2430	C 748	H 1225	N 228	O 225	S 4	0	0

- Molecule 84 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	q	155	Total 2571	C 809	H 1273	N 251	O 233	S 5	0	0

- Molecule 85 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	r	162	Total 2671	C 839	H 1349	N 252	O 223	S 8	0	0

- Molecule 86 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	s	386	Total 6300	C 2023	H 3145	N 559	O 559	S 14	0	0

- Molecule 87 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	t	46	Total 732	C 228	H 378	N 56	O 70	0	0
87	u	32	Total 541	C 168	H 284	N 40	O 49	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
87	v	32	541	168	284	40	49	0	0
87	w	31	520	159	275	39	47	0	0
87	x	31	520	159	275	39	47	0	0
87	y	31	520	159	275	39	47	0	0

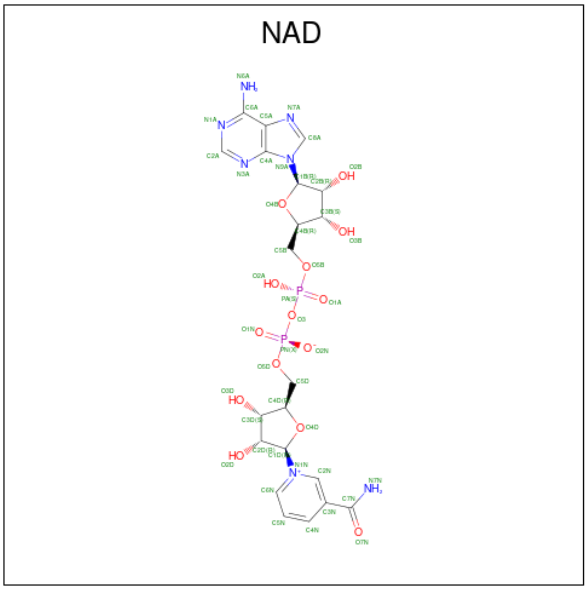
- Molecule 88 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
88	z	164	2682	856	1355	217	250	4	0	0

- Molecule 89 is a RNA chain called E/E-tRNA.

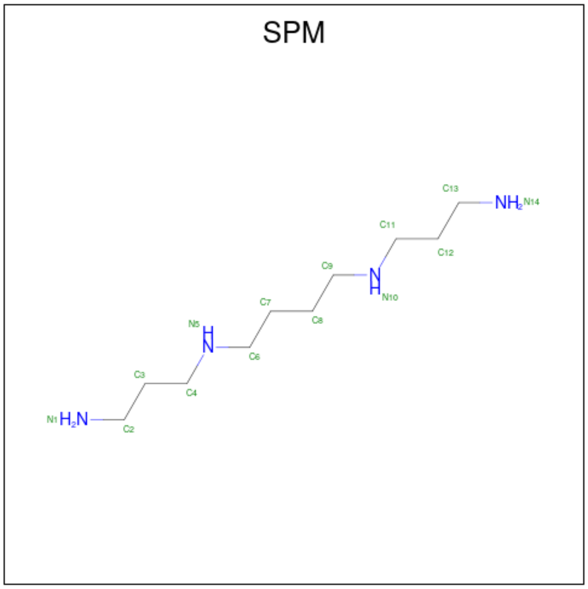
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
89	Ay	52	1667	496	560	199	360	52	0	0

- Molecule 90 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



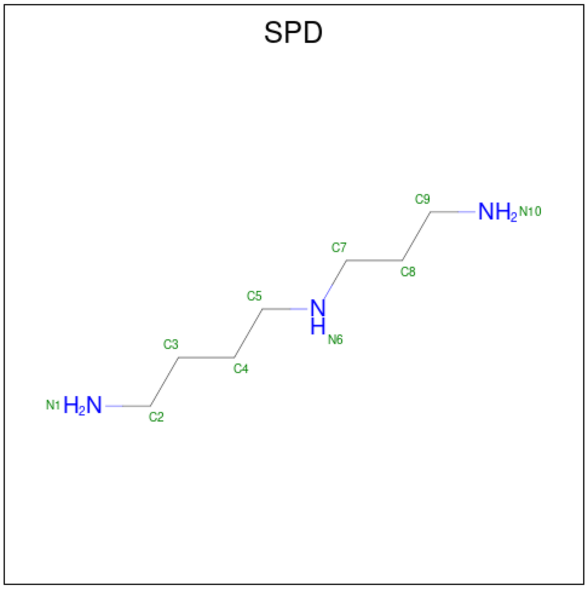
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
90	AA	1	70	21	26	7	14	2	0

- Molecule 91 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 92 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



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

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

Mol	Chain	Residues	Atoms	AltConf
93	AA	61	Total Mg 61 61	0
93	AB	1	Total Mg 1 1	0
93	AX	1	Total Mg 1 1	0
93	A3	1	Total Mg 1 1	0
93	Aw	1	Total Mg 1 1	0
93	A	137	Total Mg 137 137	0
93	D	2	Total Mg 2 2	0
93	E	1	Total Mg 1 1	0
93	g	1	Total Mg 1 1	0

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

Mol	Chain	Residues	Atoms	AltConf
94	AA	18	Total K 18 18	0
94	A	29	Total K 29 29	0
94	D	1	Total K 1 1	0
94	M	1	Total K 1 1	0
94	W	1	Total K 1 1	0

Continued on next page...

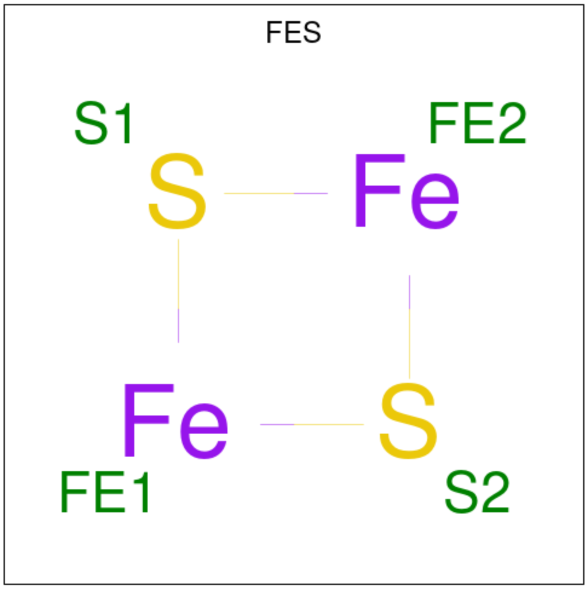
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
94	3	1	Total K 1 1	0
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: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



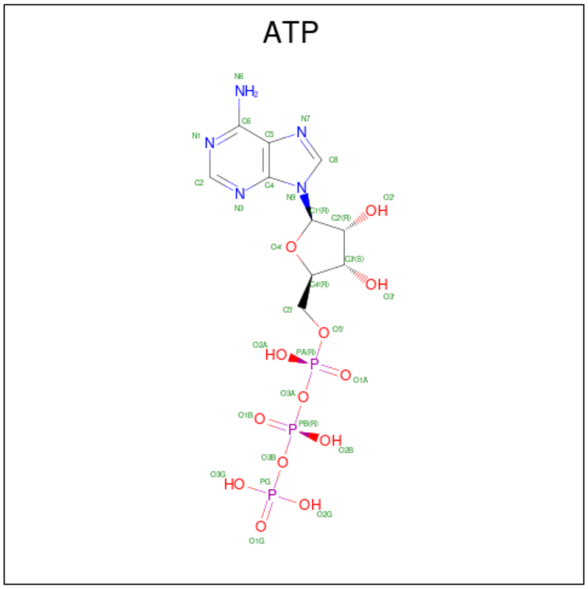
Mol	Chain	Residues	Atoms	AltConf
96	AP	1	Total Fe S 4 2 2	0
96	AT	1	Total Fe S 4 2 2	0

Continued on next page...

Continued from previous page...

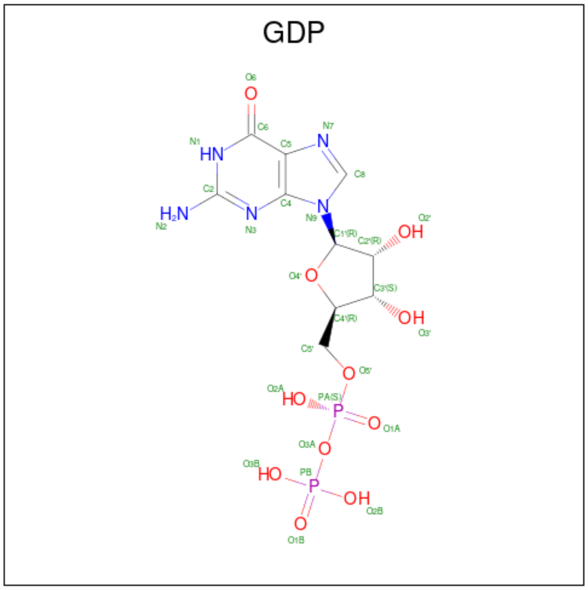
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
96	r	1	4	2	2	0

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



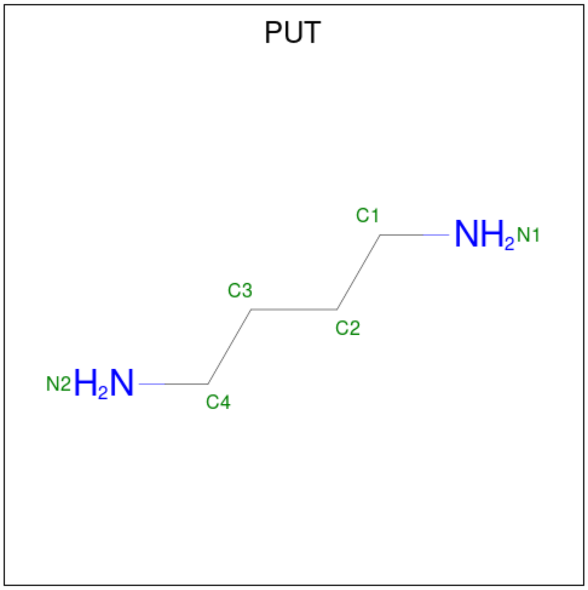
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
97	AX	1	43	10	12	5	13	3	0

- Molecule 98 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



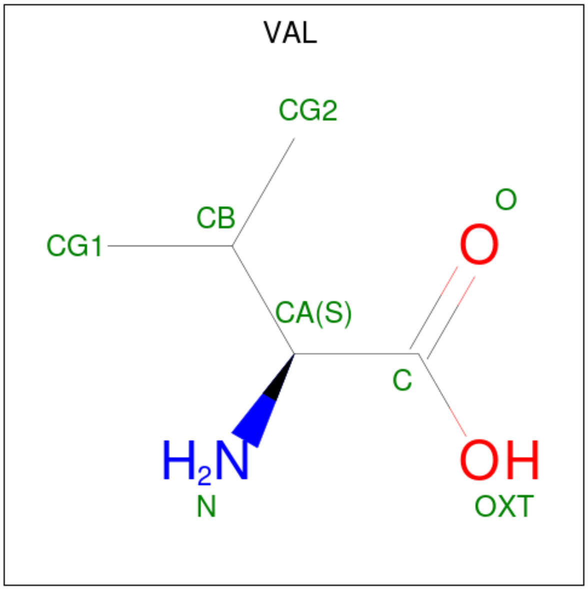
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
98	AX	1	40	10	12	5	11	2	0

- Molecule 99 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).



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

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



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

- Molecule 101 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
101	AA	2157	2157	2157	0
101	AB	80	80	80	0
101	AC	58	58	58	0
101	AD	79	79	79	0
101	AE	30	30	30	0
101	AF	36	36	36	0
101	AG	70	70	70	0
101	AH	50	50	50	0
101	AI	44	44	44	0
101	AJ	29	29	29	0
101	AK	51	51	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
101	AL	43	Total O 43 43	0
101	AM	21	Total O 21 21	0
101	AN	34	Total O 34 34	0
101	AO	37	Total O 37 37	0
101	AP	31	Total O 31 31	0
101	AQ	68	Total O 68 68	0
101	AR	12	Total O 12 12	0
101	AS	23	Total O 23 23	0
101	AT	43	Total O 43 43	0
101	AU	8	Total O 8 8	0
101	AW	15	Total O 15 15	0
101	AX	61	Total O 61 61	0
101	AY	20	Total O 20 20	0
101	AZ	27	Total O 27 27	0
101	A0	1	Total O 1 1	0
101	A1	36	Total O 36 36	0
101	A2	35	Total O 35 35	0
101	A3	52	Total O 52 52	0
101	A4	11	Total O 11 11	0
101	Aw	5	Total O 5 5	0
101	Ax	5	Total O 5 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
101	Az	15	Total O 15 15	0
101	A	3056	Total O 3056 3056	0
101	B	63	Total O 63 63	0
101	D	73	Total O 73 73	0
101	E	74	Total O 74 74	0
101	F	78	Total O 78 78	0
101	H	9	Total O 9 9	0
101	I	23	Total O 23 23	0
101	J	1	Total O 1 1	0
101	K	65	Total O 65 65	0
101	L	25	Total O 25 25	0
101	M	66	Total O 66 66	0
101	N	60	Total O 60 60	0
101	O	38	Total O 38 38	0
101	P	89	Total O 89 89	0
101	Q	27	Total O 27 27	0
101	R	57	Total O 57 57	0
101	S	49	Total O 49 49	0
101	T	48	Total O 48 48	0
101	U	26	Total O 26 26	0
101	V	5	Total O 5 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
101	W	48	Total O 48 48	0
101	X	12	Total O 12 12	0
101	Y	29	Total O 29 29	0
101	Z	34	Total O 34 34	0
101	0	27	Total O 27 27	0
101	1	3	Total O 3 3	0
101	2	34	Total O 34 34	0
101	3	40	Total O 40 40	0
101	4	13	Total O 13 13	0
101	5	22	Total O 22 22	0
101	6	100	Total O 100 100	0
101	7	17	Total O 17 17	0
101	8	19	Total O 19 19	0
101	9	17	Total O 17 17	0
101	a	13	Total O 13 13	0
101	b	39	Total O 39 39	0
101	c	20	Total O 20 20	0
101	d	5	Total O 5 5	0
101	e	13	Total O 13 13	0
101	f	22	Total O 22 22	0
101	g	13	Total O 13 13	0

Continued on next page...

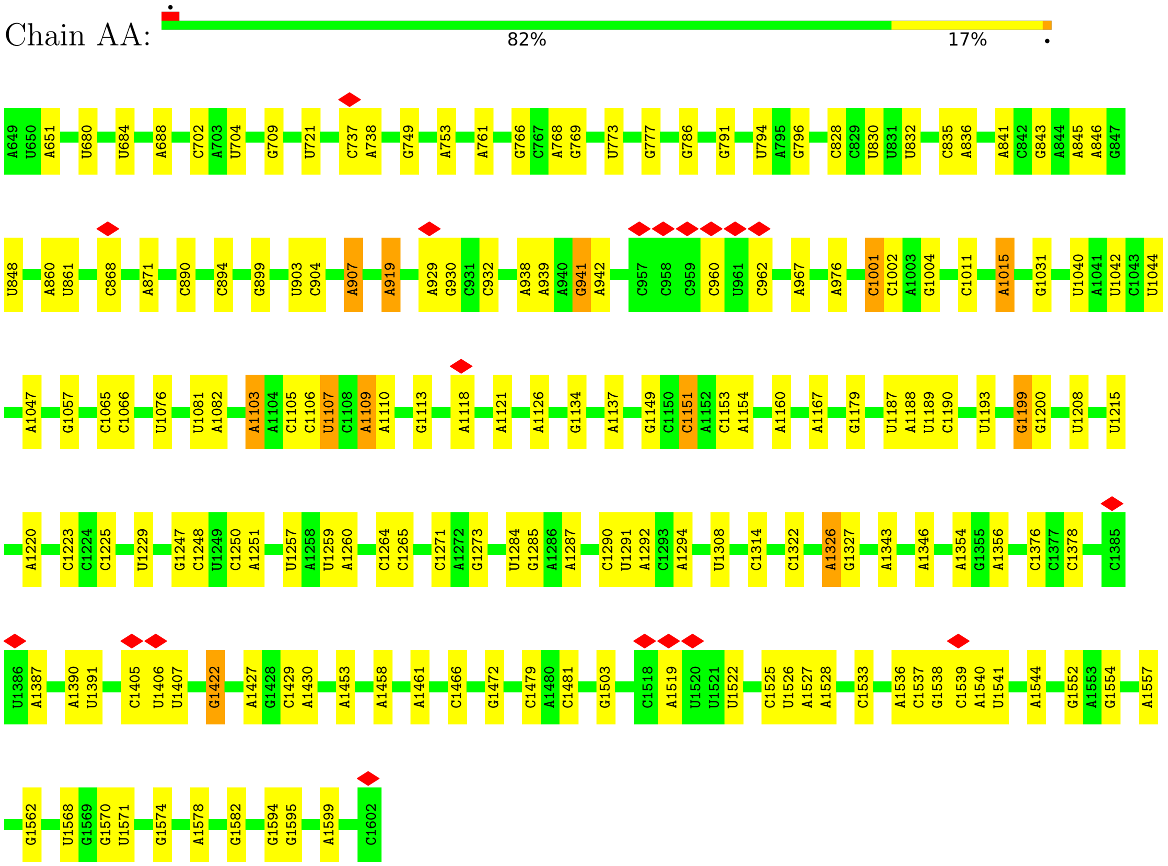
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
101	i	54	Total O 54 54	0
101	j	23	Total O 23 23	0
101	k	6	Total O 6 6	0
101	l	5	Total O 5 5	0
101	m	8	Total O 8 8	0
101	o	34	Total O 34 34	0
101	p	10	Total O 10 10	0
101	r	50	Total O 50 50	0
101	s	51	Total O 51 51	0
101	Ay	1	Total O 1 1	0

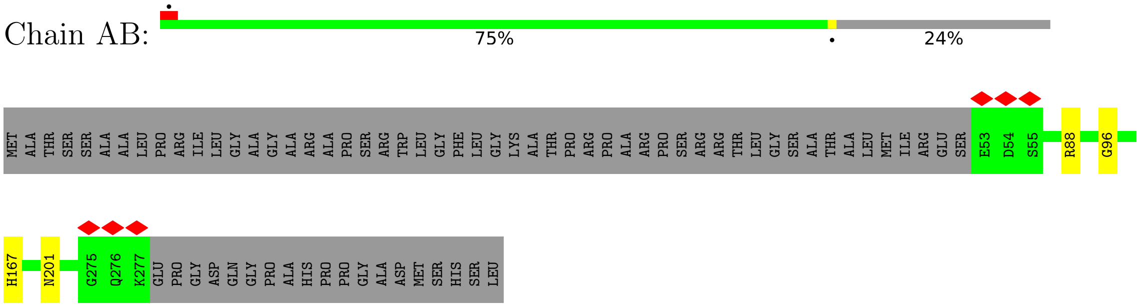
3 Residue-property plots ⓘ

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.

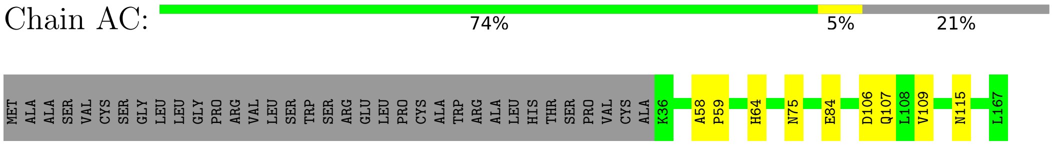
- Molecule 1: 12S mitochondrial rRNA



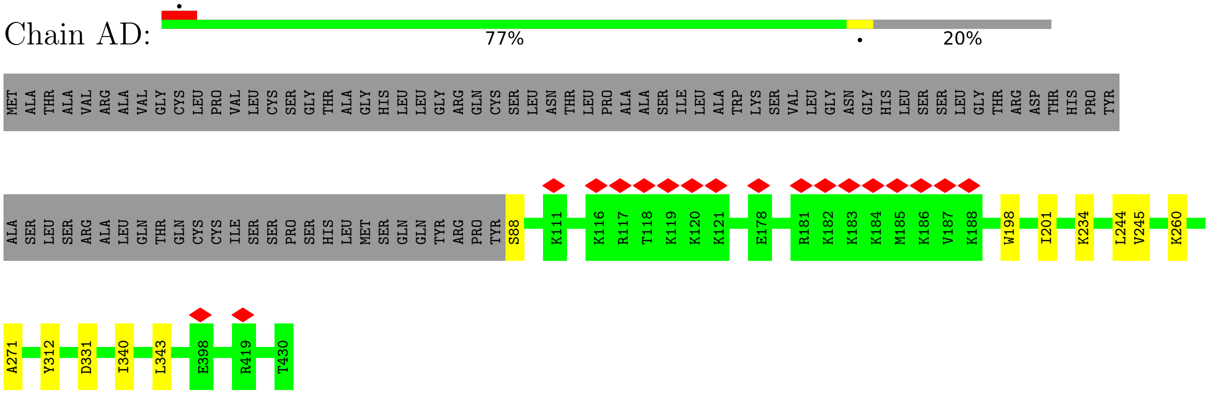
- Molecule 2: 28S ribosomal protein S2, mitochondrial



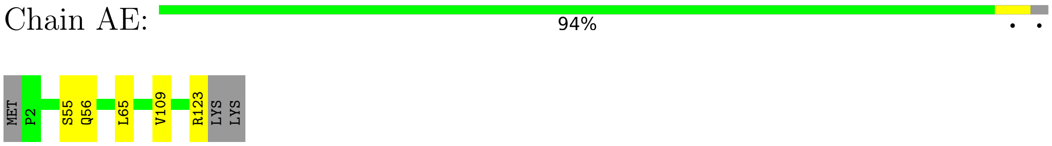
- Molecule 3: 28S ribosomal protein S24, mitochondrial



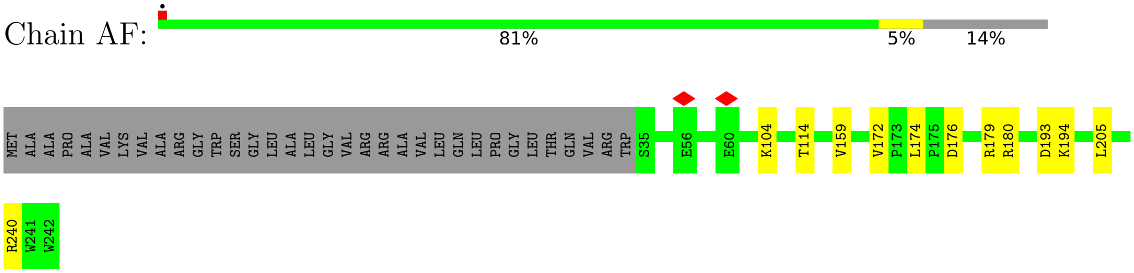
- Molecule 4: 28S ribosomal protein S5, mitochondrial



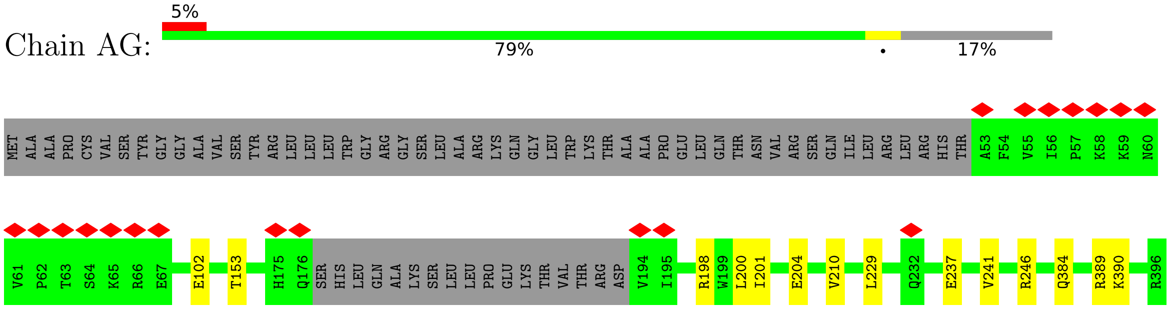
- Molecule 5: 28S ribosomal protein S6, mitochondrial



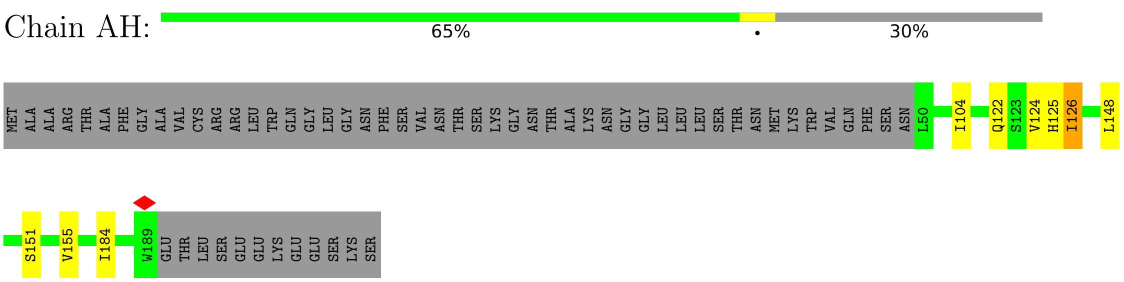
- Molecule 6: 28S ribosomal protein S7, mitochondrial



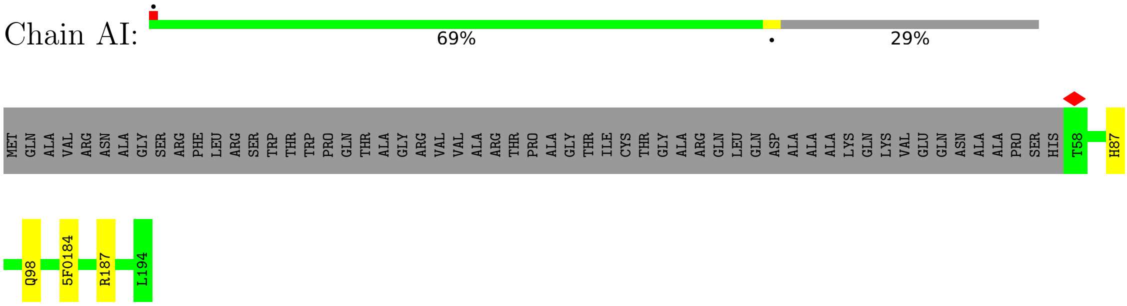
- Molecule 7: 28S ribosomal protein S9, mitochondrial



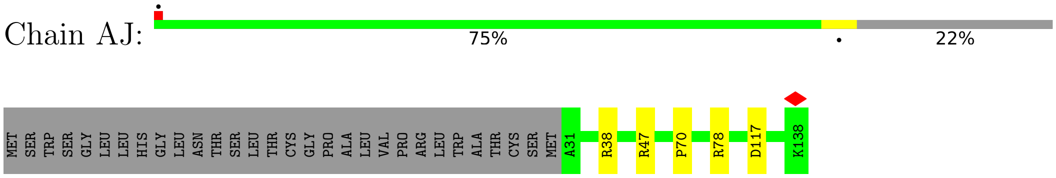
- Molecule 8: 28S ribosomal protein S10, mitochondrial



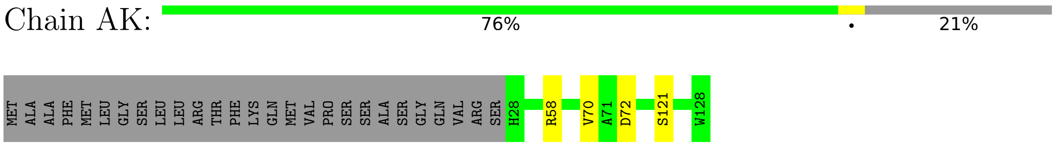
- Molecule 9: 28S ribosomal protein S11, mitochondrial



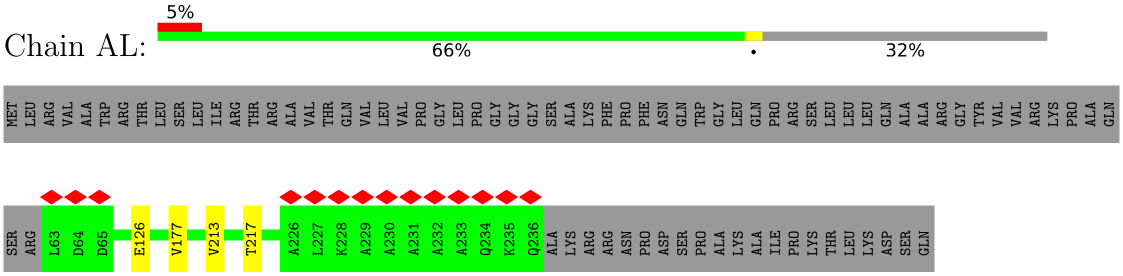
- Molecule 10: 28S ribosomal protein S12, mitochondrial



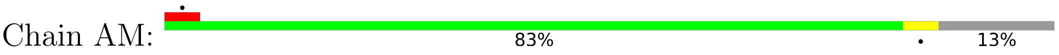
- Molecule 11: 28S ribosomal protein S14, mitochondrial

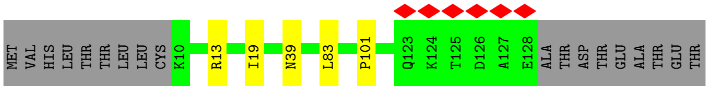


- Molecule 12: 28S ribosomal protein S15, mitochondrial



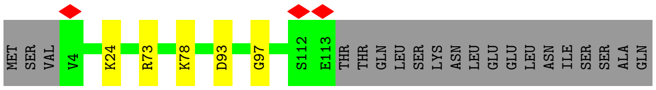
- Molecule 13: 28S ribosomal protein S16, mitochondrial





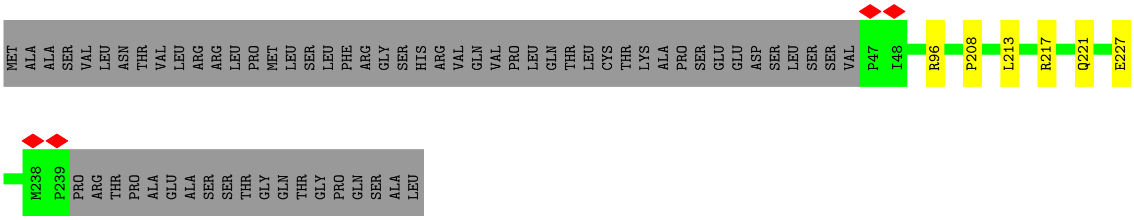
- Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain AN:



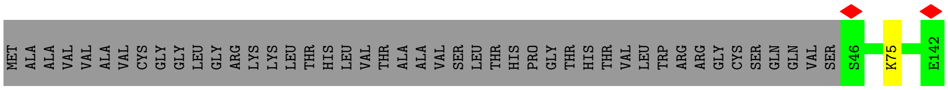
- Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain AO:



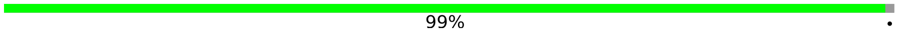
- Molecule 16: 28S ribosomal protein S18c, mitochondrial

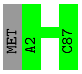
Chain AP:



- Molecule 17: MRPS21 isoform 1

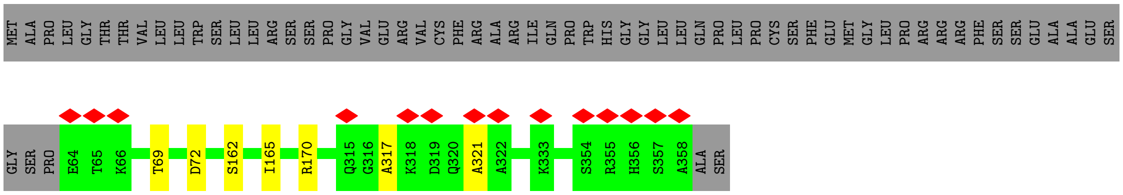
Chain AQ:





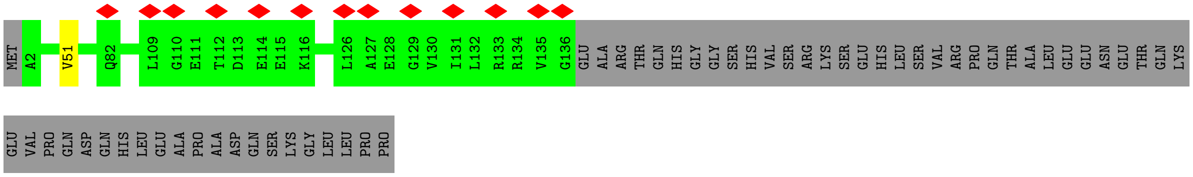
- Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain AR:



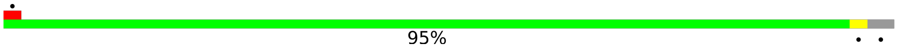
- Molecule 19: 28S ribosomal protein S23, mitochondrial

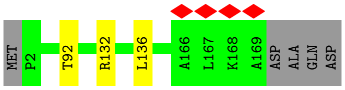
Chain AS:



- Molecule 20: 28S ribosomal protein S25, mitochondrial

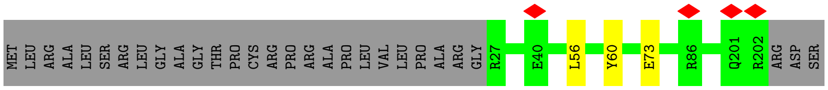
Chain AT:





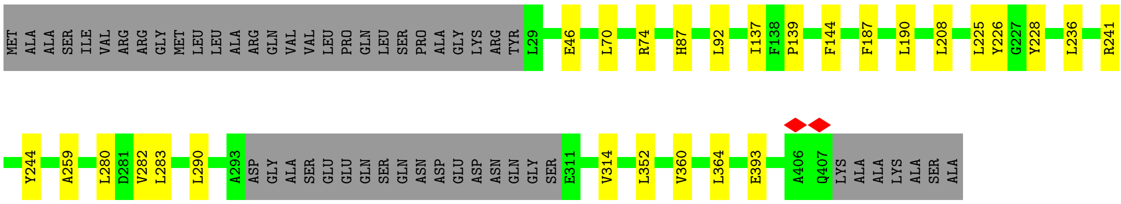
- Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain AU:



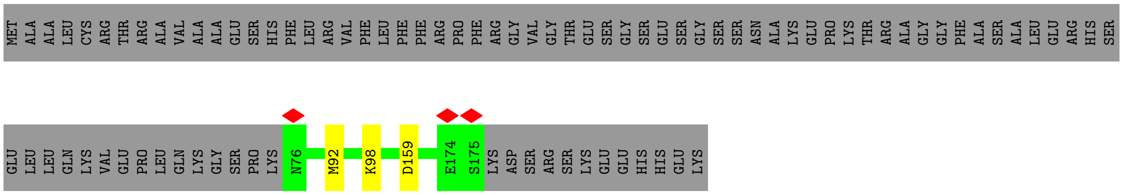
- Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain AV:



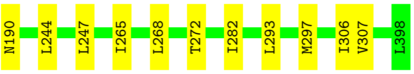
- Molecule 23: 28S ribosomal protein S28, mitochondrial

Chain AW:



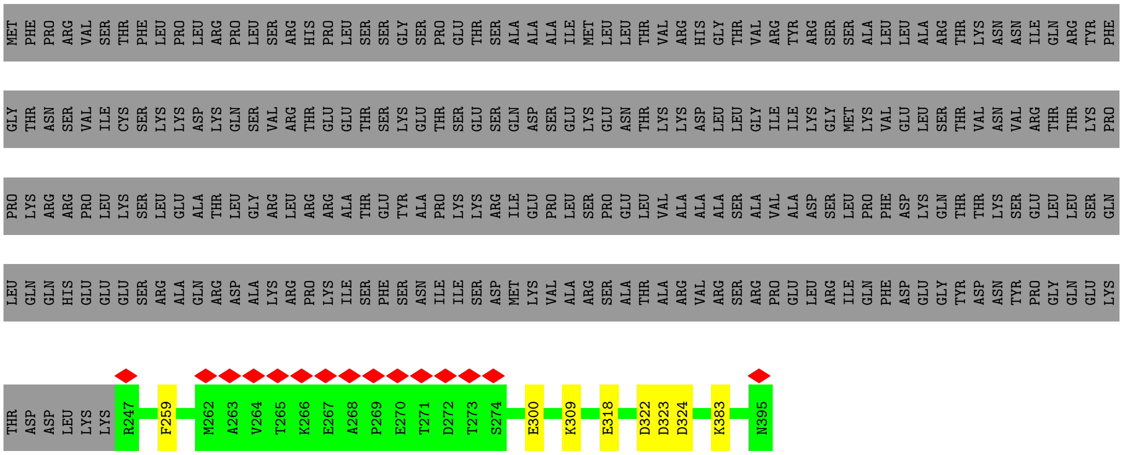
- Molecule 24: 28S ribosomal protein S29, mitochondrial

Chain AX:



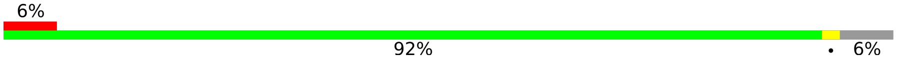
- Molecule 25: 28S ribosomal protein S31, mitochondrial

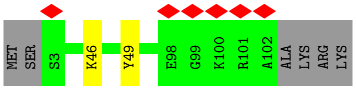
Chain AY:



- Molecule 26: 28S ribosomal protein S33, mitochondrial

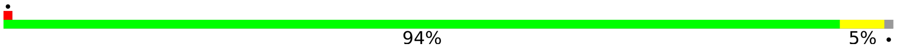
Chain AZ:

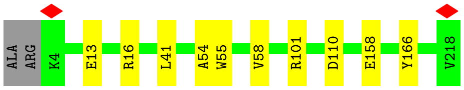




- Molecule 27: 28S ribosomal protein S34, mitochondrial

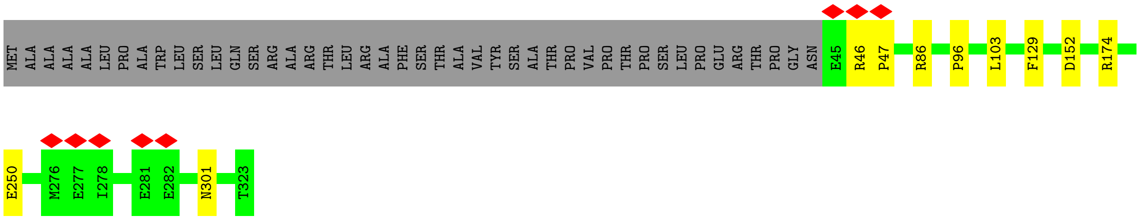
Chain A0:





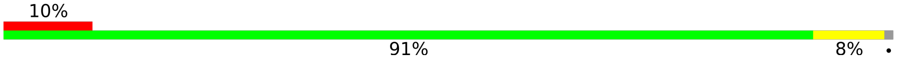
- Molecule 28: 28S ribosomal protein S35, mitochondrial

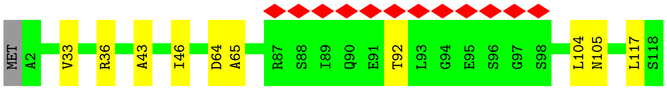
Chain A1:



- Molecule 29: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

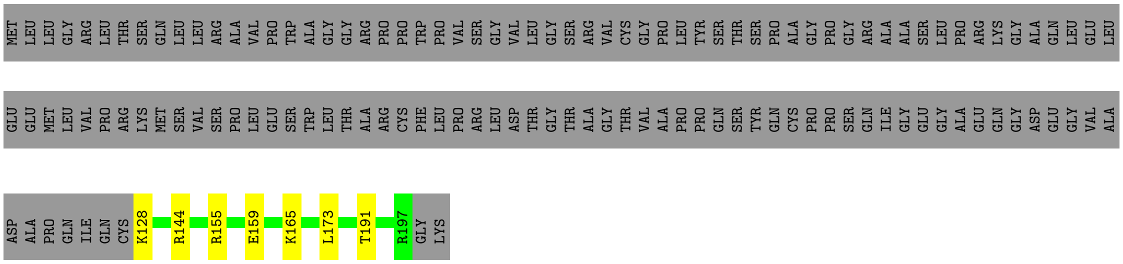
Chain A2:





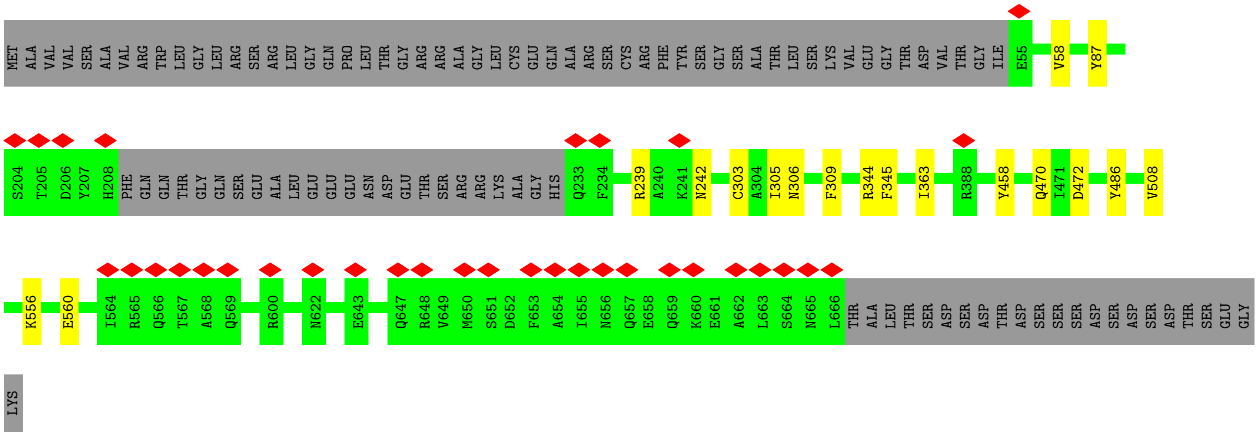
- Molecule 30: Aurora kinase A-interacting protein

Chain A3:



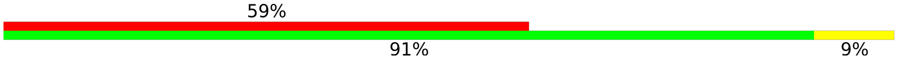
- Molecule 31: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

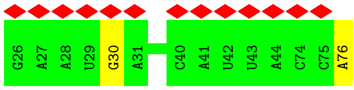
Chain A4:



- Molecule 32: A/A-tRNA

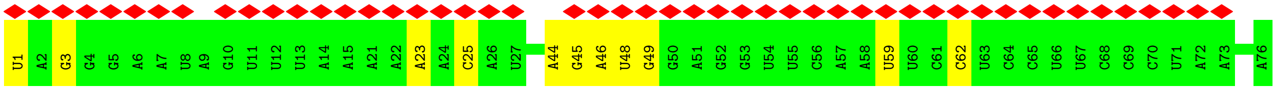
Chain Aw:



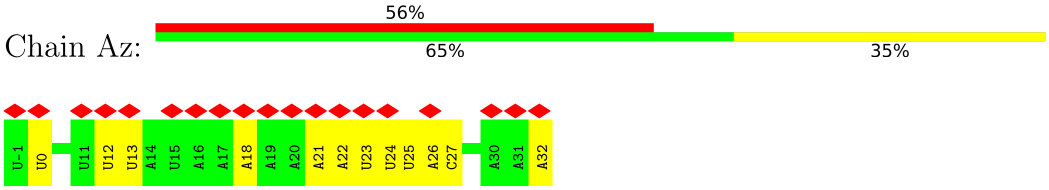


- Molecule 33: P/P-tRNA

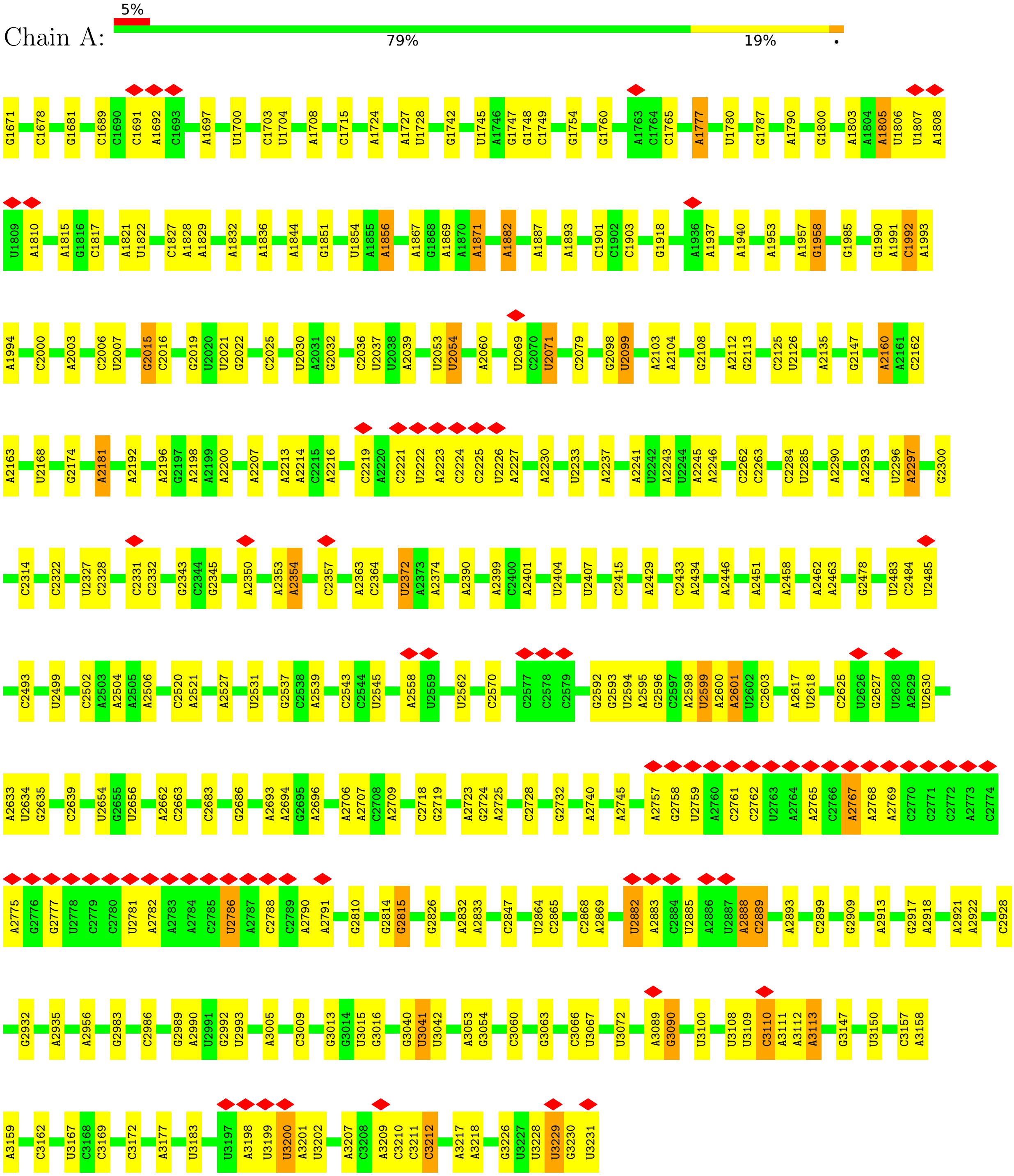
Chain Ax:



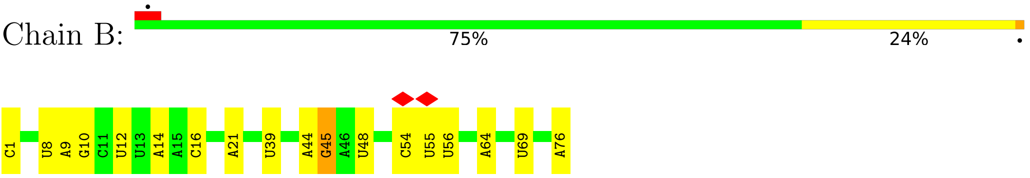
- Molecule 34: mRNA



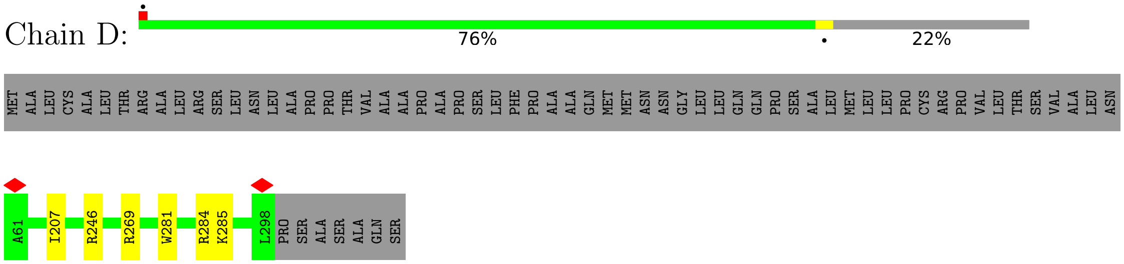
- Molecule 35: 16S mitochondrial rRNA



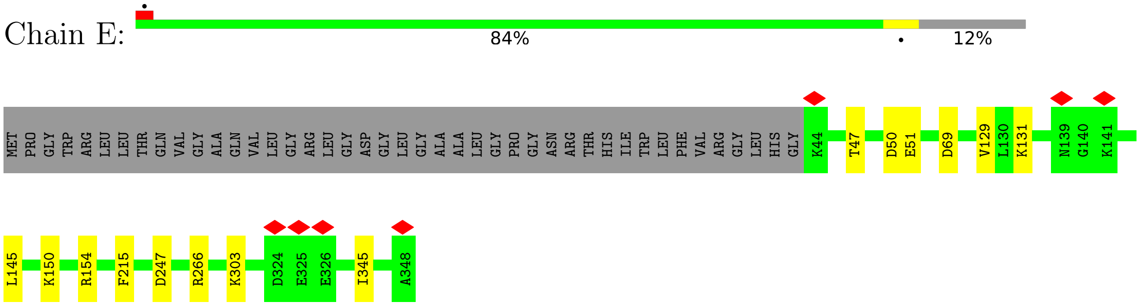
- Molecule 36: mitochondrial tRNAVal



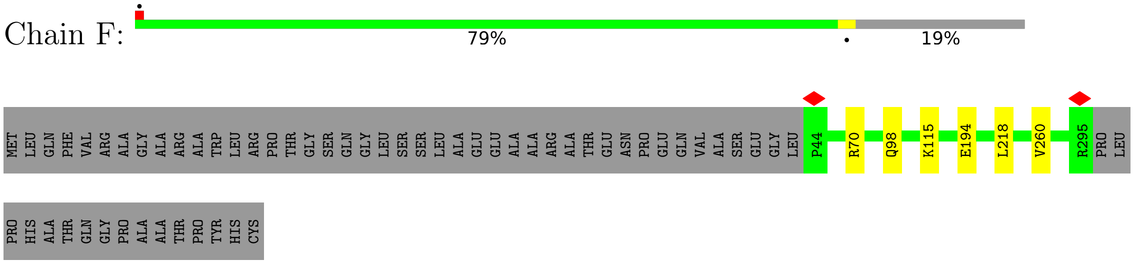
- Molecule 37: 39S ribosomal protein L2, mitochondrial



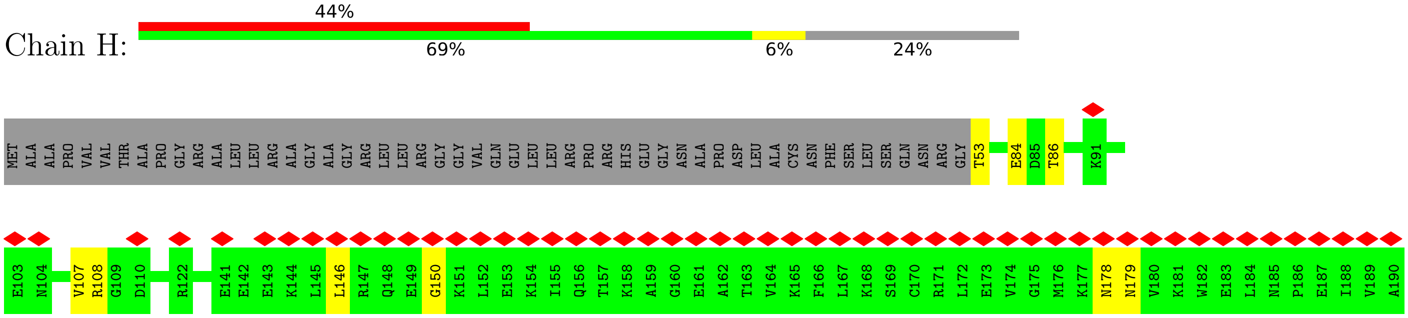
- Molecule 38: 39S ribosomal protein L3, mitochondrial

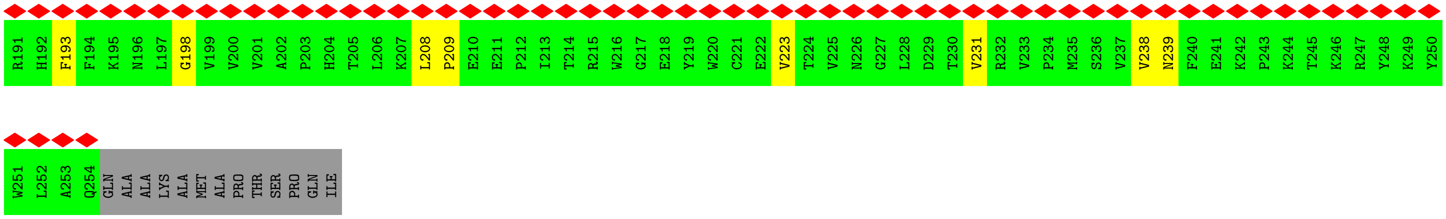


- Molecule 39: 39S ribosomal protein L4, mitochondrial

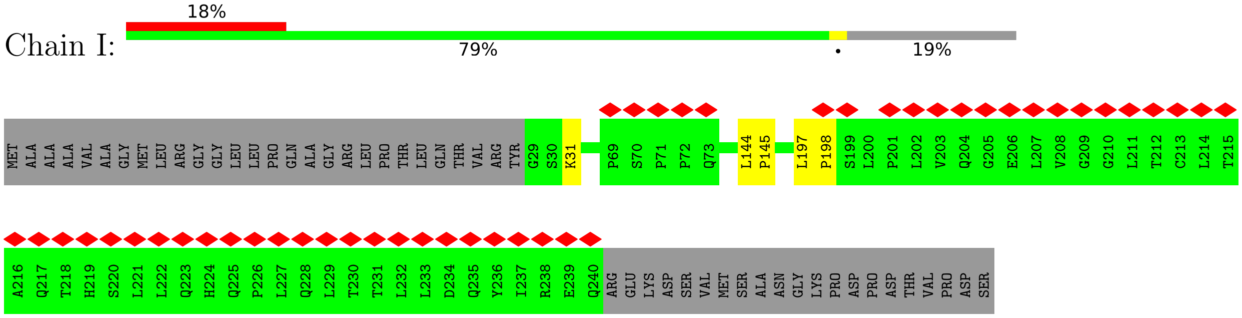


- Molecule 40: 39S ribosomal protein L9, mitochondrial

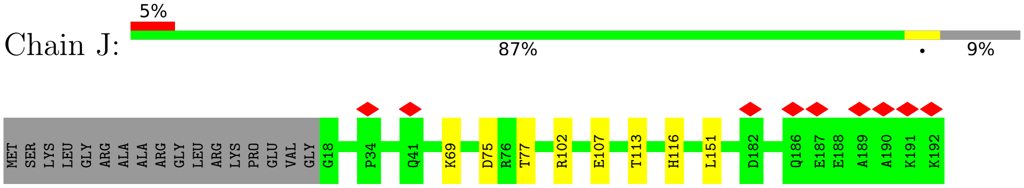




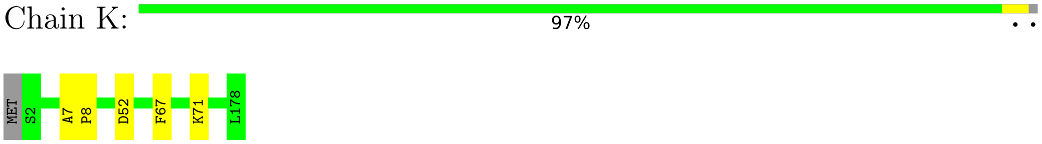
- Molecule 41: 39S ribosomal protein L10, mitochondrial



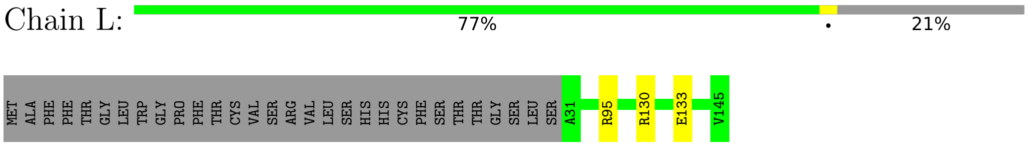
- Molecule 42: 39S ribosomal protein L11, mitochondrial



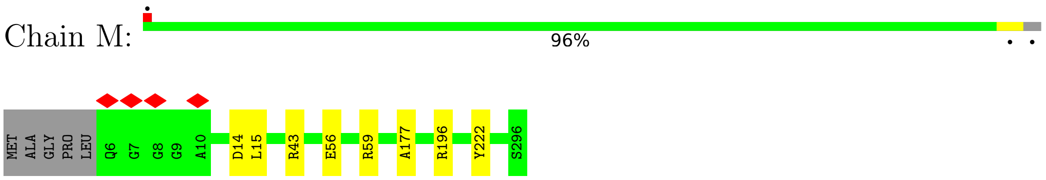
- Molecule 43: 39S ribosomal protein L13, mitochondrial



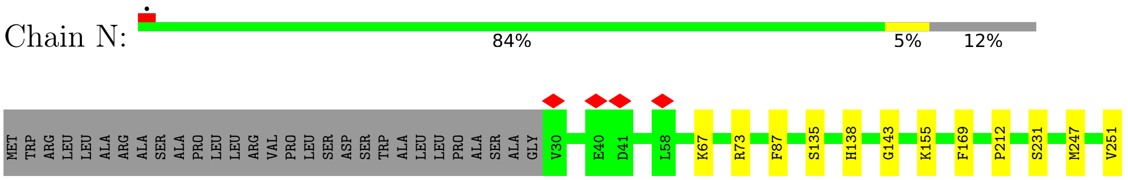
- Molecule 44: 39S ribosomal protein L14, mitochondrial



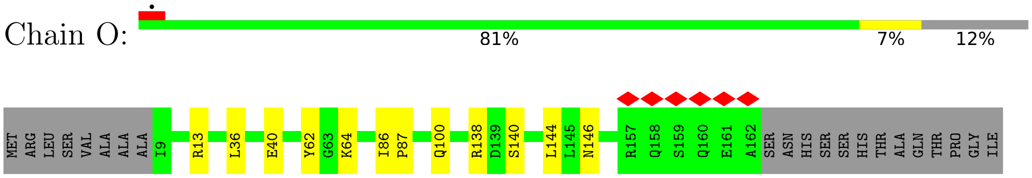
- Molecule 45: 39S ribosomal protein L15, mitochondrial



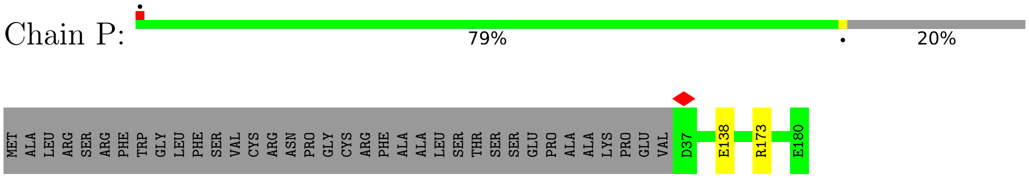
- Molecule 46: 39S ribosomal protein L16, mitochondrial



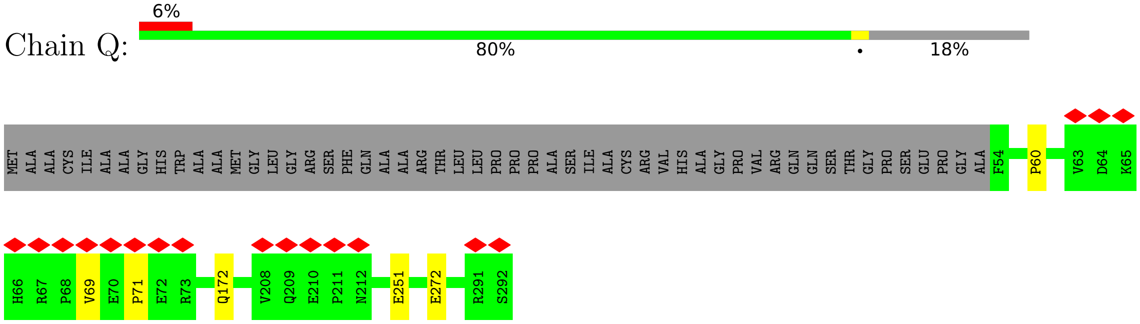
- Molecule 47: 39S ribosomal protein L17, mitochondrial



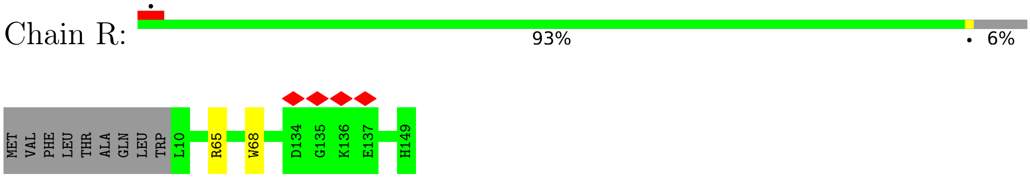
- Molecule 48: 39S ribosomal protein L18, mitochondrial



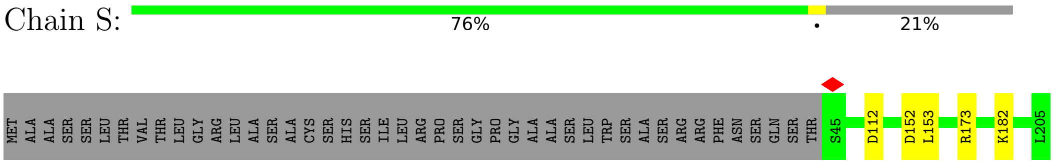
- Molecule 49: 39S ribosomal protein L19, mitochondrial



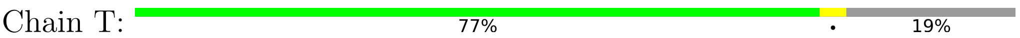
- Molecule 50: 39S ribosomal protein L20, mitochondrial

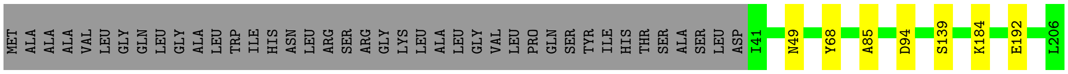


- Molecule 51: 39S ribosomal protein L21, mitochondrial



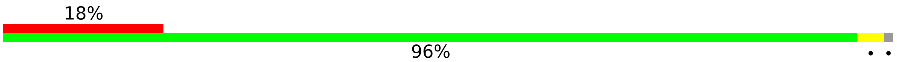
- Molecule 52: 39S ribosomal protein L22, mitochondrial

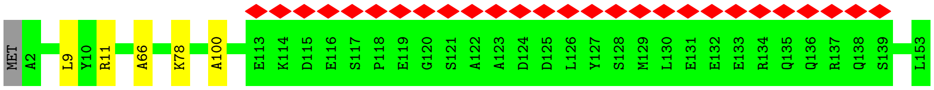




- Molecule 53: 39S ribosomal protein L23, mitochondrial

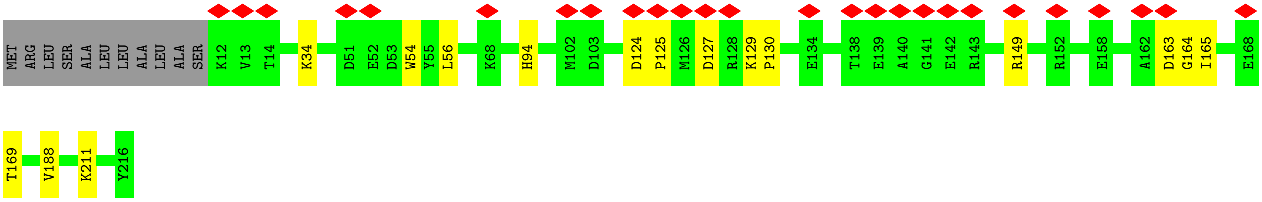
Chain U:





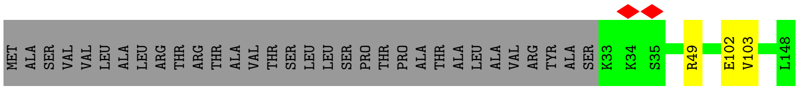
- Molecule 54: 39S ribosomal protein L24, mitochondrial

Chain V:



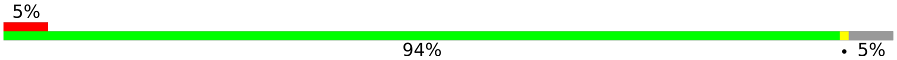
- Molecule 55: 39S ribosomal protein L27, mitochondrial

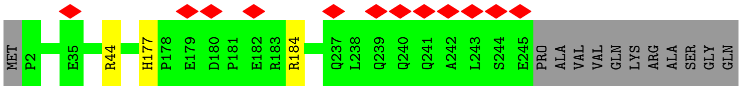
Chain W:



- Molecule 56: 39S ribosomal protein L28, mitochondrial

Chain X:



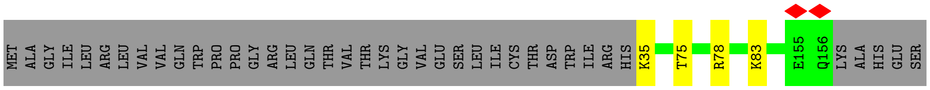


- Molecule 57: 39S ribosomal protein L47, mitochondrial

Chain Y:

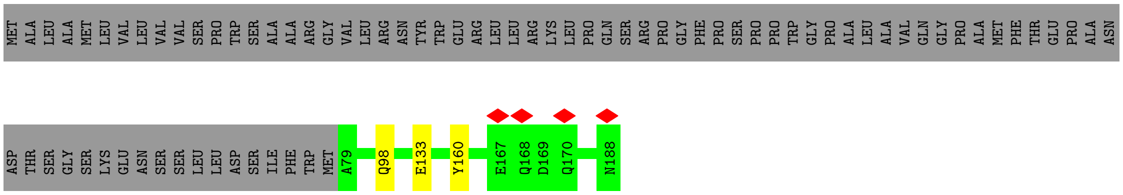
- Molecule 58: 39S ribosomal protein L30, mitochondrial

Chain Z:



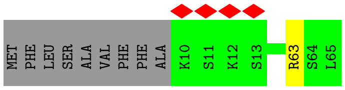
- Molecule 59: 39S ribosomal protein L32, mitochondrial

Chain 0:



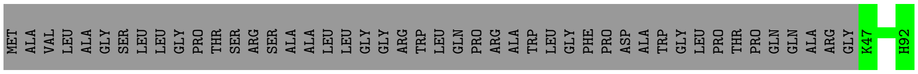
- Molecule 60: 39S ribosomal protein L33, mitochondrial

Chain 1:



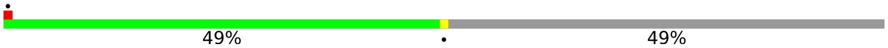
- Molecule 61: 39S ribosomal protein L34, mitochondrial

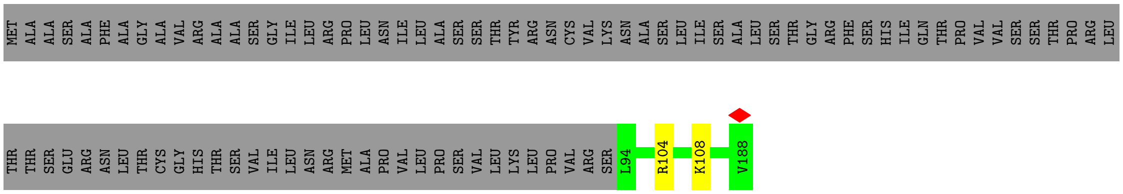
Chain 2:



- Molecule 62: 39S ribosomal protein L35, mitochondrial

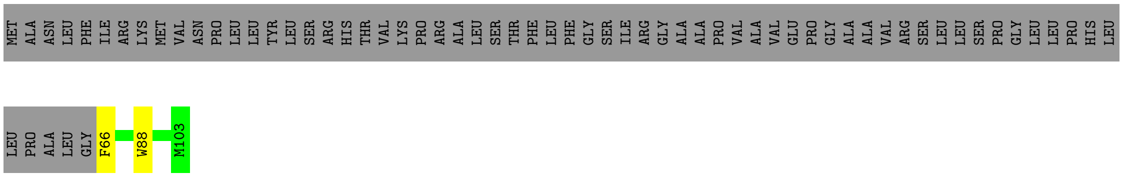
Chain 3:



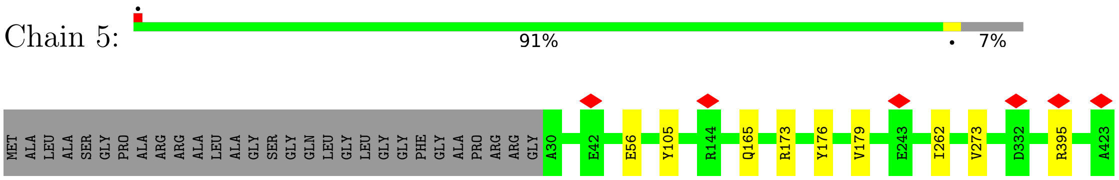


- Molecule 63: 39S ribosomal protein L36, mitochondrial

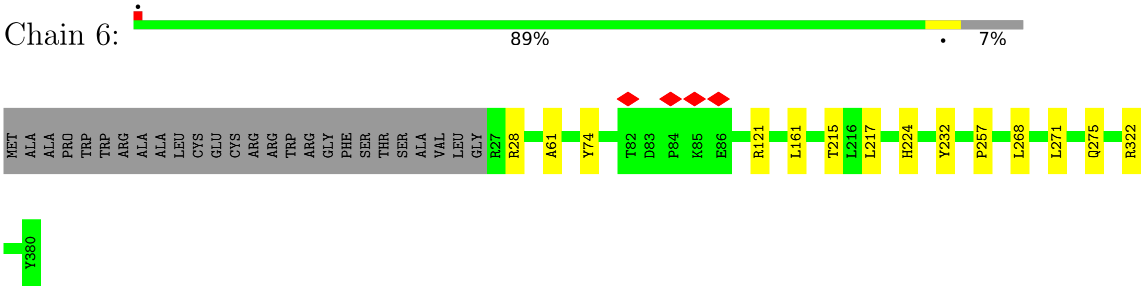
Chain 4:



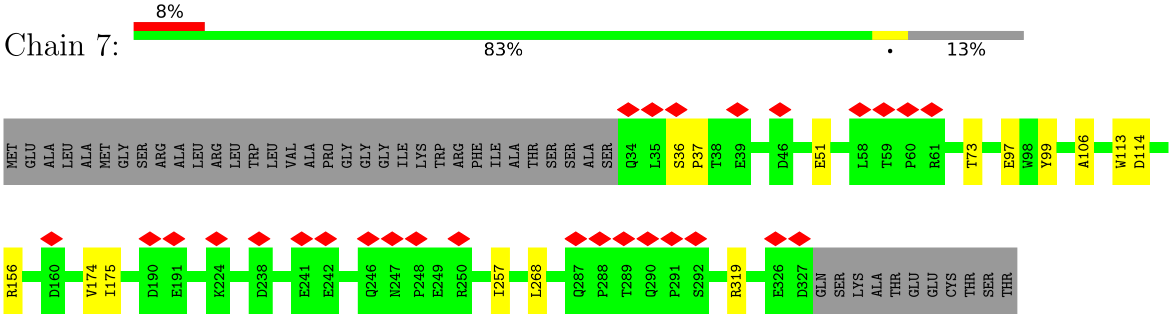
- Molecule 64: 39S ribosomal protein L37, mitochondrial



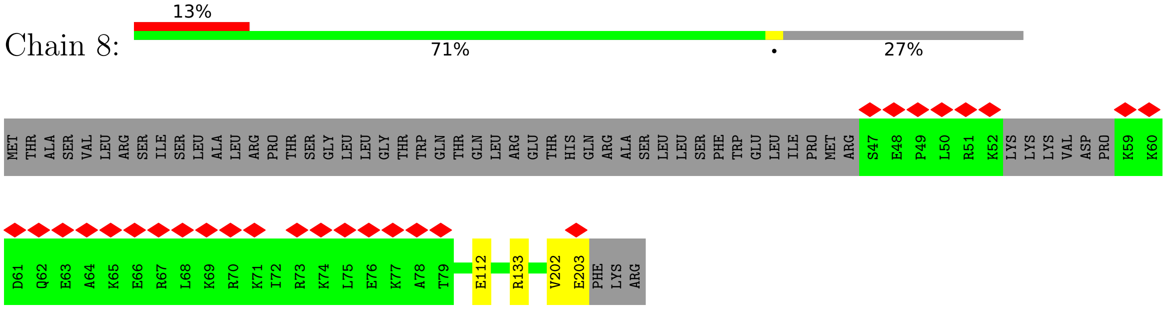
- Molecule 65: 39S ribosomal protein L38, mitochondrial



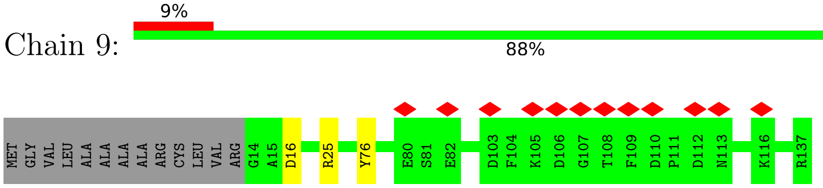
- Molecule 66: 39S ribosomal protein L39, mitochondrial



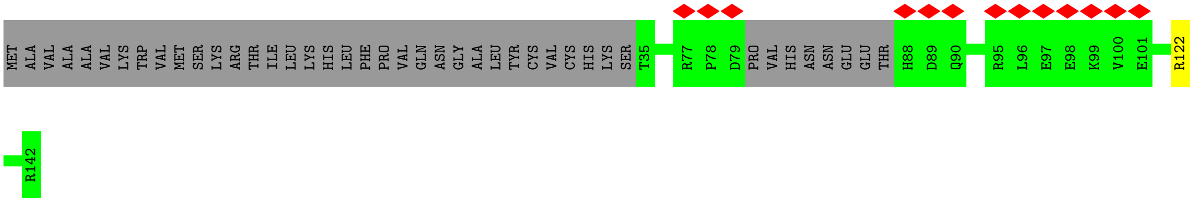
- Molecule 67: 39S ribosomal protein L40, mitochondrial



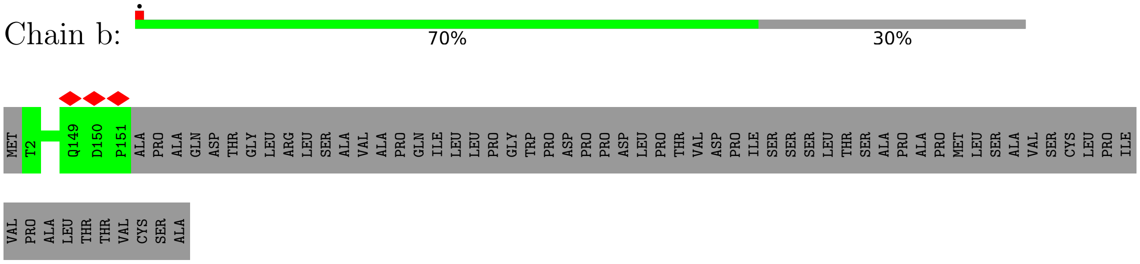
- Molecule 68: 39S ribosomal protein L41, mitochondrial



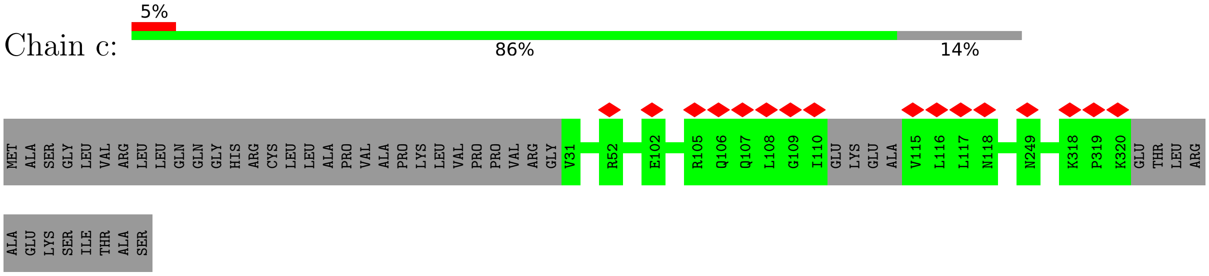
- Molecule 69: 39S ribosomal protein L42, mitochondrial



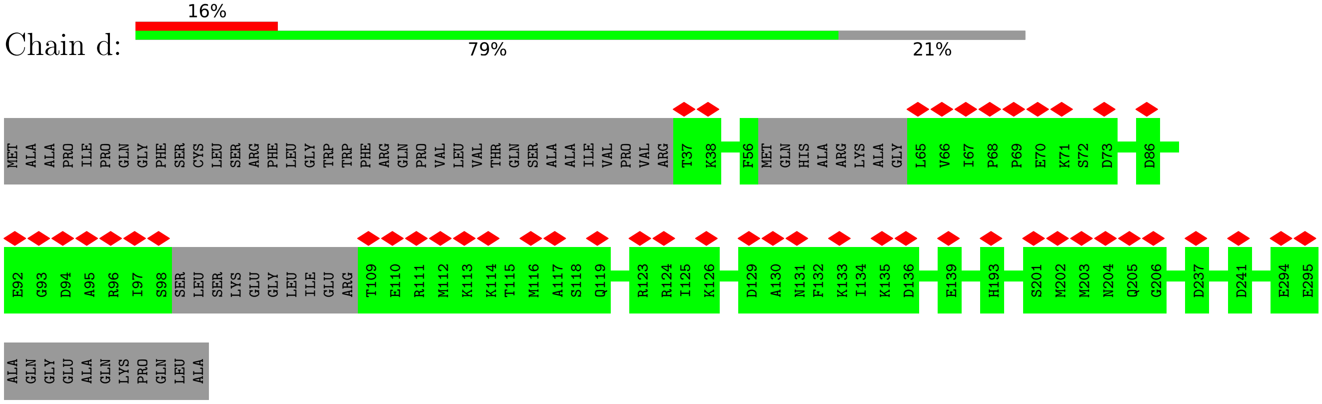
- Molecule 70: 39S ribosomal protein L43, mitochondrial



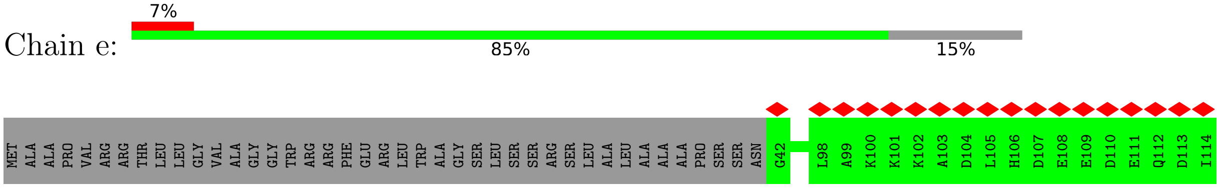
- Molecule 71: 39S ribosomal protein L44, mitochondrial

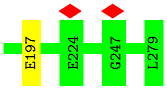


- Molecule 72: 39S ribosomal protein L45, mitochondrial

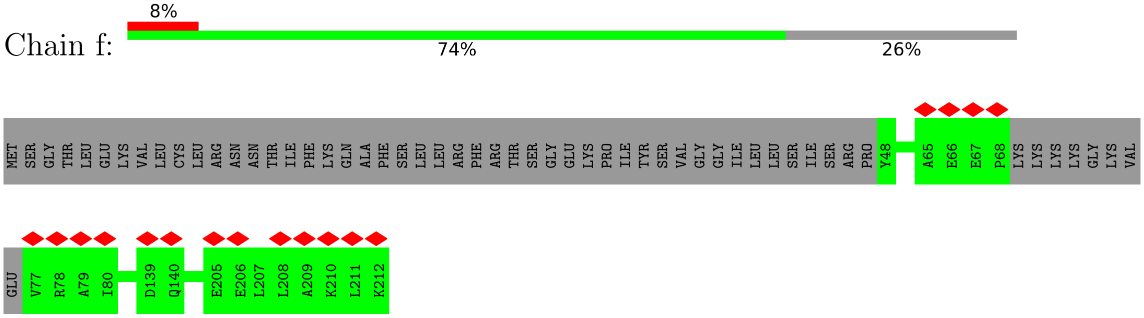


- Molecule 73: 39S ribosomal protein L46, mitochondrial

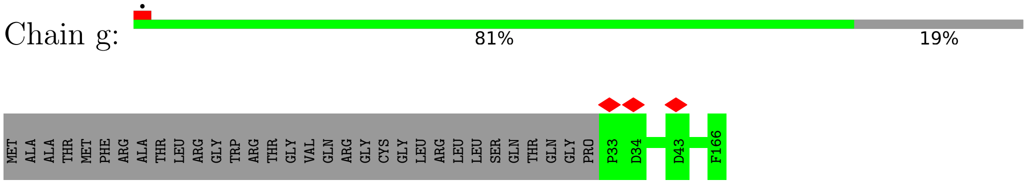




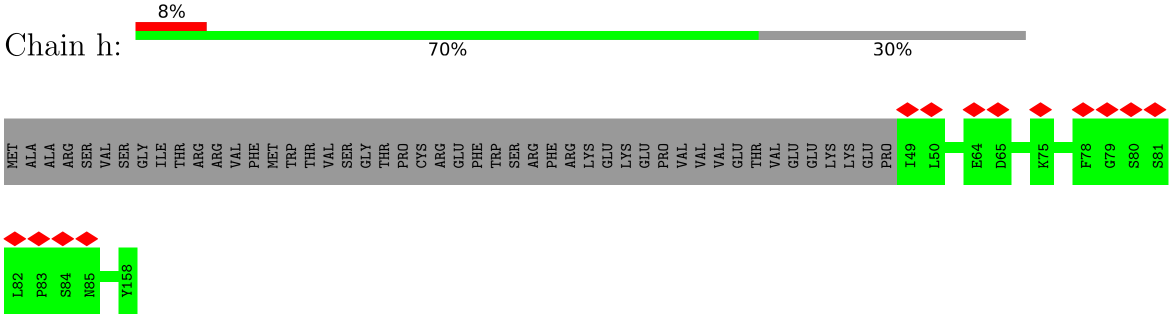
- Molecule 74: 39S ribosomal protein L48, mitochondrial



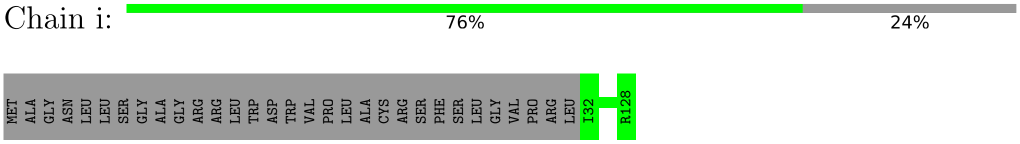
- Molecule 75: 39S ribosomal protein L49, mitochondrial



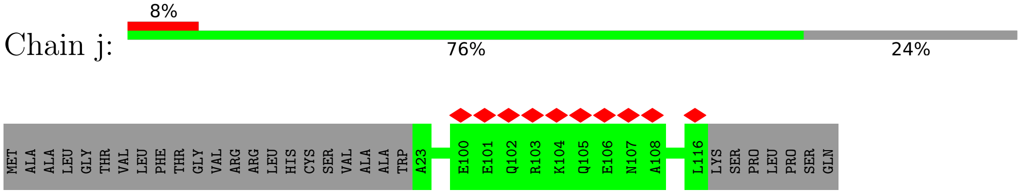
- Molecule 76: 39S ribosomal protein L50, mitochondrial



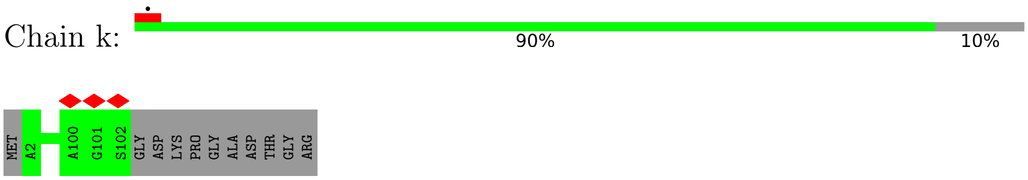
- Molecule 77: 39S ribosomal protein L51, mitochondrial



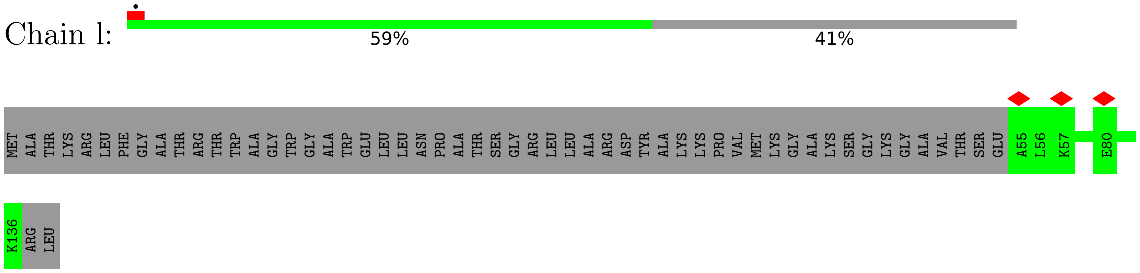
- Molecule 78: 39S ribosomal protein L52, mitochondrial



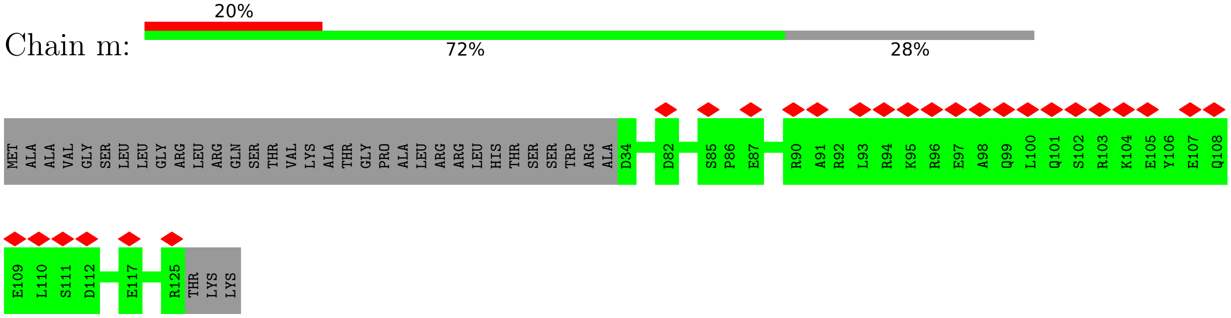
- Molecule 79: 39S ribosomal protein L53, mitochondrial



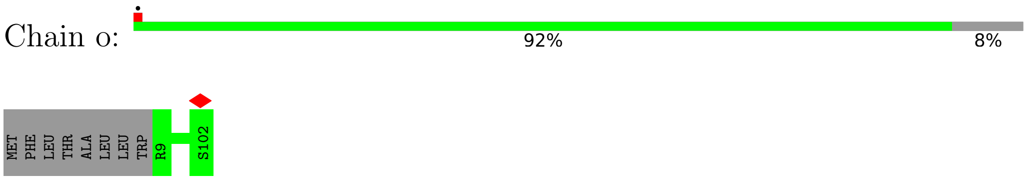
- Molecule 80: 39S ribosomal protein L54, mitochondrial



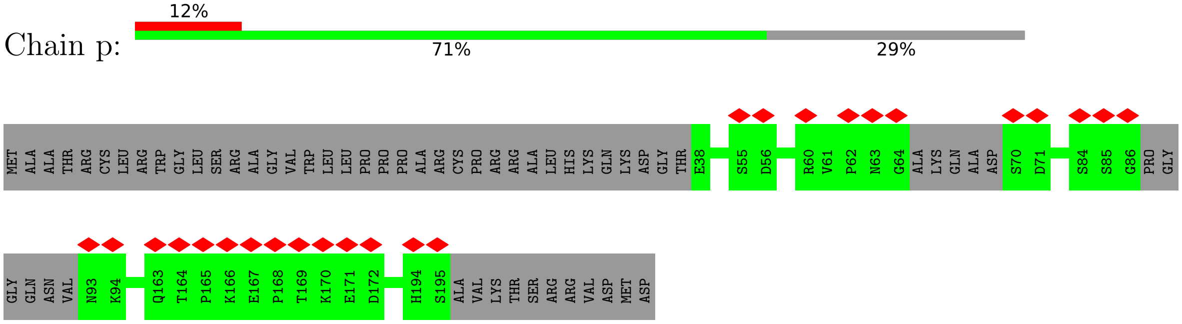
- Molecule 81: 39S ribosomal protein L55, mitochondrial



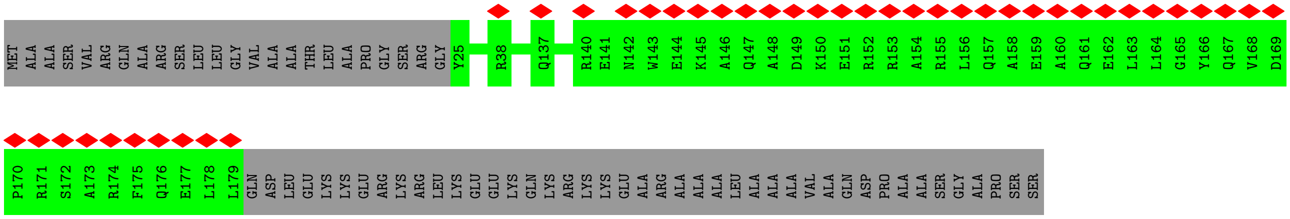
- Molecule 82: Ribosomal protein 63, mitochondrial



- Molecule 83: Peptidyl-tRNA hydrolase ICT1, mitochondrial

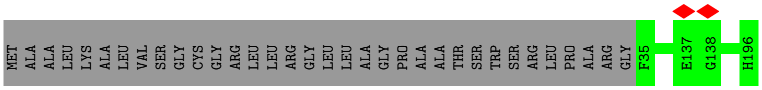


- Molecule 84: Growth arrest and DNA damage-inducible proteins-interacting protein 1



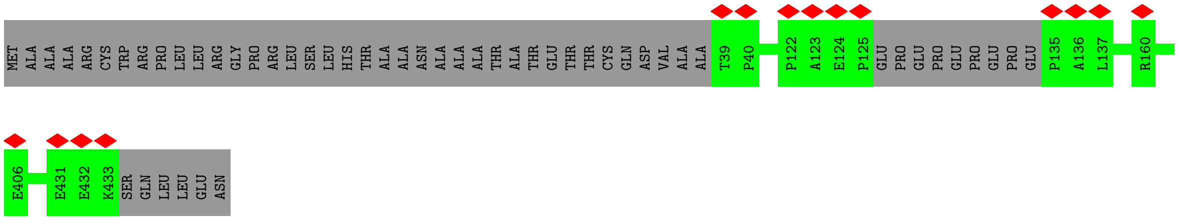
- Molecule 85: 39S ribosomal protein S18a, mitochondrial

Chain r:



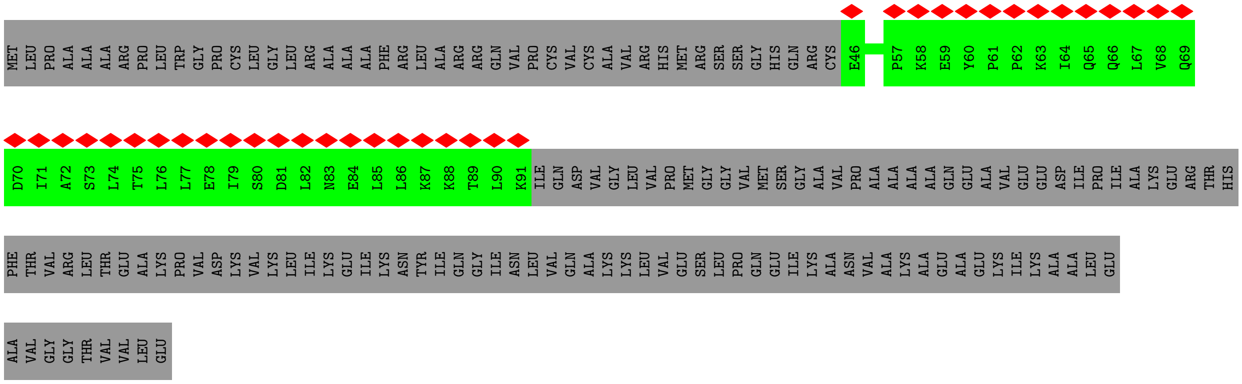
- Molecule 86: 39S ribosomal protein S30, mitochondrial

Chain s:



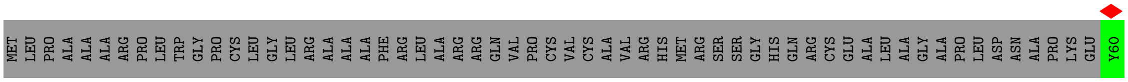
- Molecule 87: 39S ribosomal protein L12, mitochondrial

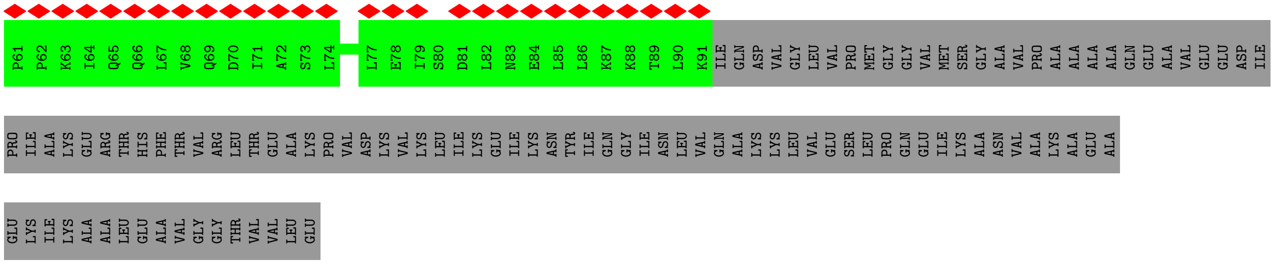
Chain t:



- Molecule 87: 39S ribosomal protein L12, mitochondrial

Chain u:



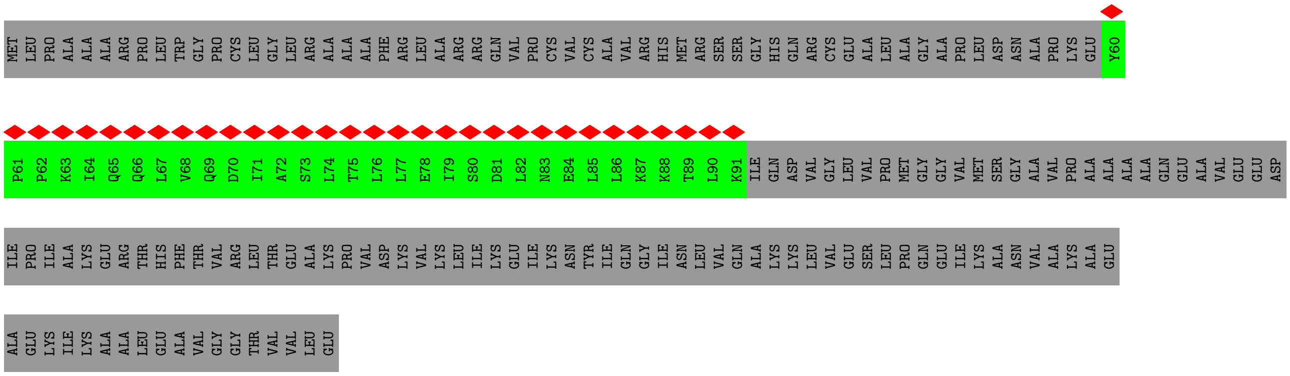

P61 P62 K63 I64 Q65 Q66 L67 V68 Q69 D70 I71 A72 S73 L74 L77 E78 I79 S80 D81 L82 N83 E84 L85 L86 K87 K88 T89 L90 K91 ILE GLN ASP VAL GLY LEU VAL PRO MET GLY GLY VAL MET SER GLY ALA VAL PRO ALA ALA ALA GLN GLU ALA VAL GLU GLU ASP ILE

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

GLU LYS ILE LYS ALA ALA LEU GLU ALA VAL GLY GLY THR VAL VAL LEU GLU

- Molecule 87: 39S ribosomal protein L12, mitochondrial

Chain v:


MET LEU PRO ALA ALA ALA ARG PRO LEU TRP GLY PRO CYS LEU GLY LEU ARG ALA ALA PHE ARG LEU ALA ARG ARG GLN VAL PRO CYS VAL CYS ALA VAL ARG HIS MET ARG SER SER GLY HIS GLN ARG CYS GLU ALA LEU ALA GLY ALA PRO LEU ASP ASN ALA PRO LYS GLU Y60

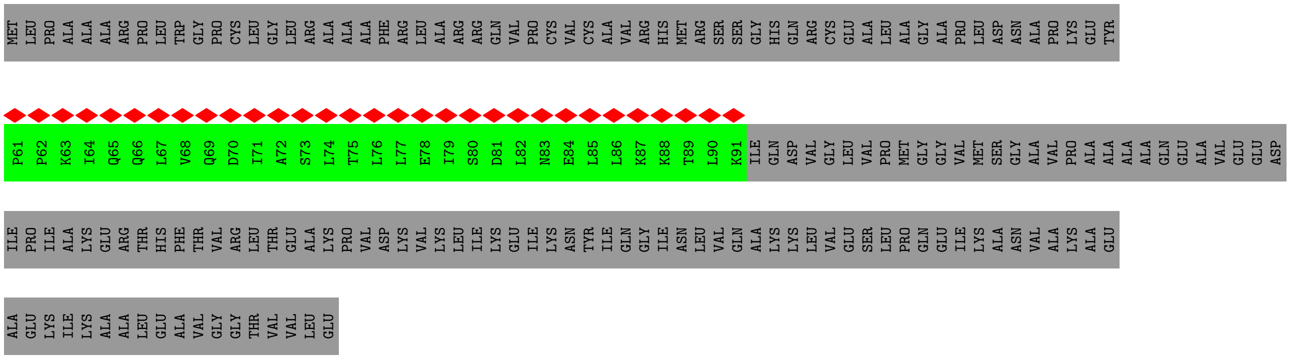
P61 P62 K63 I64 Q65 Q66 L67 V68 Q69 D70 I71 A72 S73 L74 T75 L76 L77 E78 I79 S80 D81 L82 N83 E84 L85 L86 K87 K88 T89 L90 K91 ILE GLN ASP VAL GLY LEU VAL PRO MET GLY GLY VAL MET SER GLY ALA VAL PRO ALA ALA ALA GLN GLU ALA VAL GLU GLU ASP

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

ALA GLU LYS ILE LYS ALA ALA LEU GLU ALA VAL GLY GLY THR VAL VAL LEU GLU

- Molecule 87: 39S ribosomal protein L12, mitochondrial

Chain w:


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

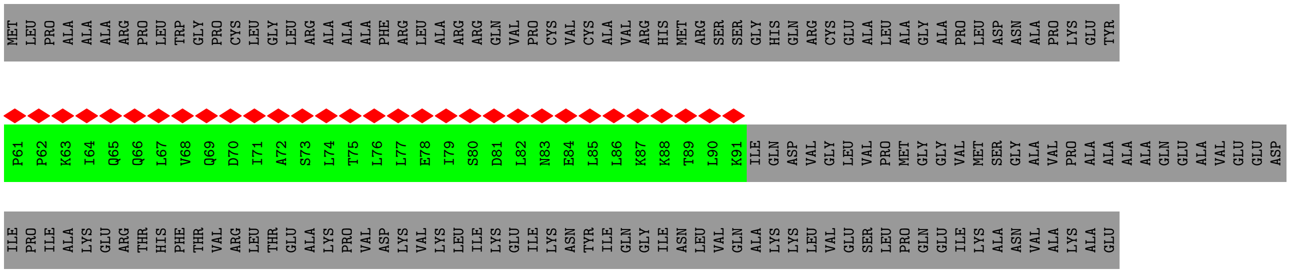
P61 P62 K63 I64 Q65 Q66 L67 V68 Q69 D70 I71 A72 S73 L74 T75 L76 L77 E78 I79 S80 D81 L82 N83 E84 L85 L86 K87 K88 T89 L90 K91 ILE GLN ASP VAL GLY LEU VAL PRO MET GLY GLY VAL MET SER GLY ALA VAL PRO ALA ALA ALA GLN GLU ALA VAL GLU GLU ASP

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

ALA GLU LYS ILE LYS ALA ALA LEU GLU ALA VAL GLY GLY THR VAL VAL LEU GLU

- Molecule 87: 39S ribosomal protein L12, mitochondrial

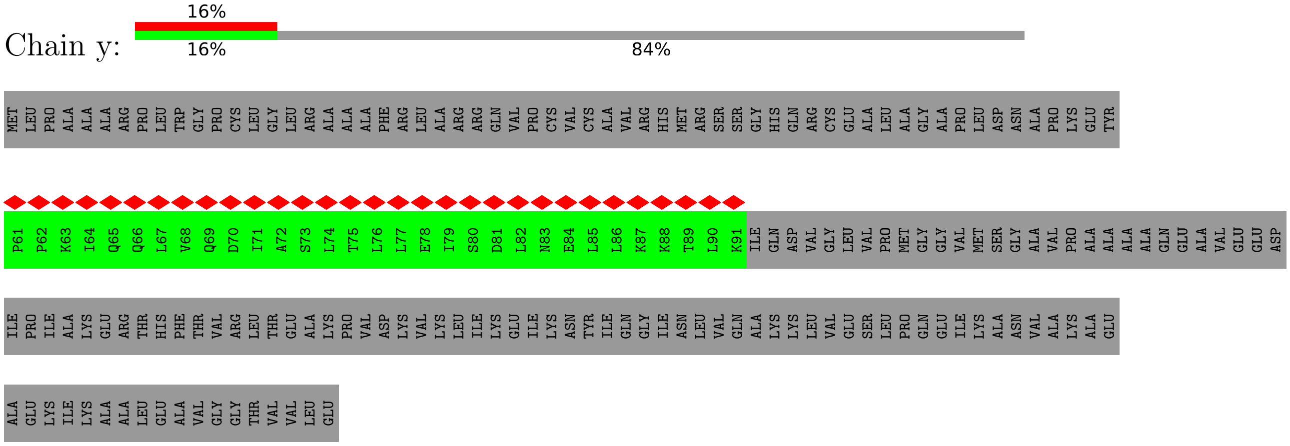
Chain x:


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

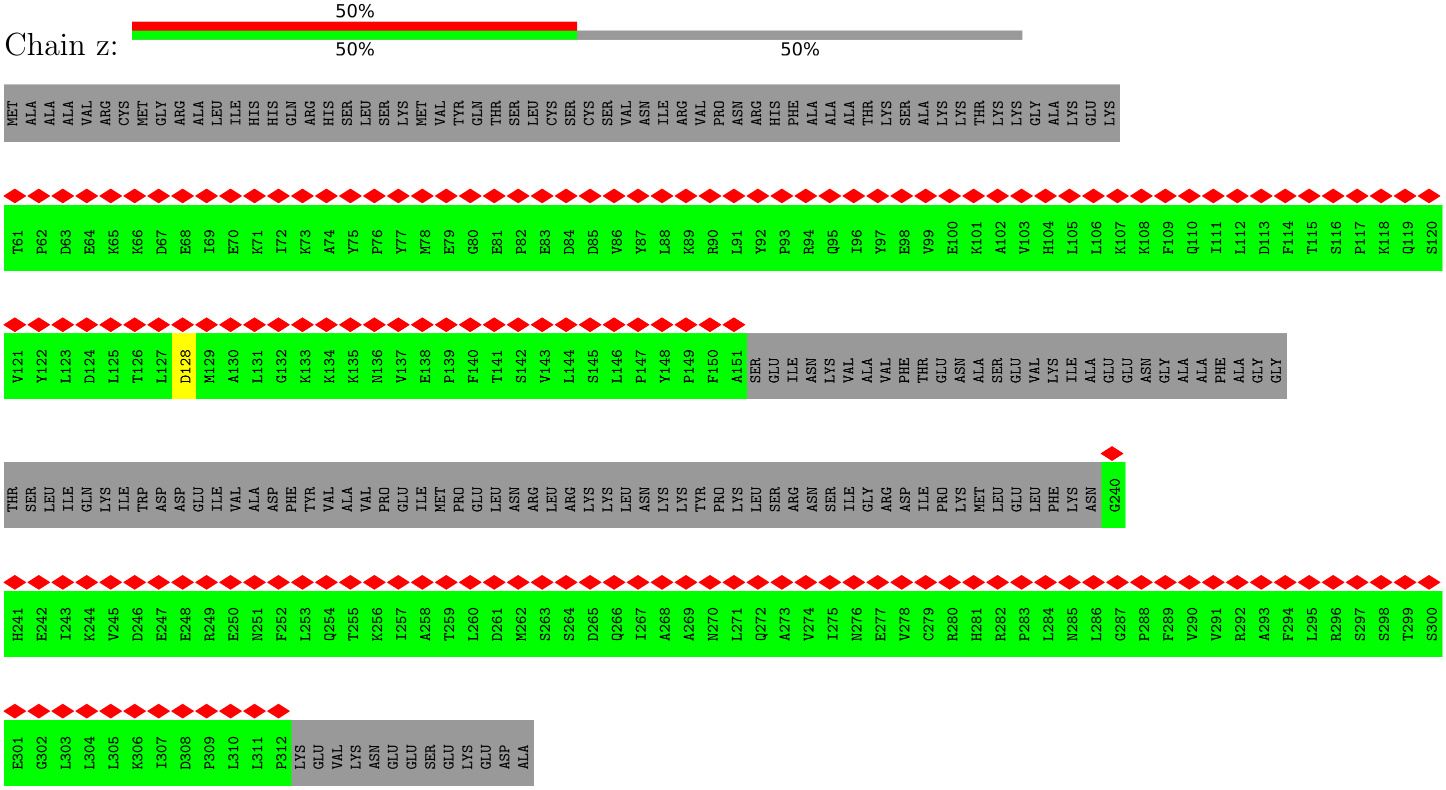
P61 P62 K63 I64 Q65 Q66 L67 V68 Q69 D70 I71 A72 S73 L74 T75 L76 L77 E78 I79 S80 D81 L82 N83 E84 L85 L86 K87 K88 T89 L90 K91 ILE GLN ASP VAL GLY LEU VAL PRO MET GLY GLY VAL MET SER GLY ALA VAL PRO ALA ALA ALA GLN GLU ALA VAL GLU GLU ASP

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

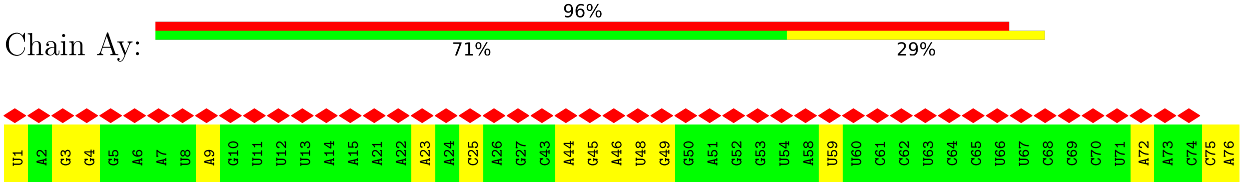
- Molecule 87: 39S ribosomal protein L12, mitochondrial



- Molecule 88: 39S ribosomal protein L1, mitochondrial



- Molecule 89: E/E-tRNA



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 $(e^-/\text{Å}^2)$	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: 5MC, AYA, 5MU, SAC, ZN, OMG, GDP, 1MA, OMU, MA6, SPM, SPD, FES, 2MG, K, ATP, THC, B8T, NAD, 5F0, MG, PUT, PSU

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	0.19	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	0.52	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	0.53	0/1295
14	AN	0.23	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	0.26	0/3030	0.43	0/4093
23	AW	0.25	0/801	0.51	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	0.50	0/1141
27	A0	0.24	0/1834	0.54	0/2484
28	A1	0.24	0/2313	0.45	0/3129
29	A2	0.24	0/941	0.54	0/1257
30	A3	0.23	0/636	0.57	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	Az	0.13	0/803	0.65	0/1244
35	A	0.19	1/36876 (0.0%)	0.68	0/57402
36	B	0.33	1/1627 (0.1%)	0.67	0/2527
37	D	0.23	0/1896	0.56	0/2549
38	E	0.24	0/2475	0.47	0/3355
39	F	0.23	0/2090	0.50	0/2842
40	H	0.23	0/1698	0.49	0/2292
41	I	0.24	0/1731	0.48	0/2345
42	J	0.25	0/1348	0.48	0/1813
43	K	0.24	0/1490	0.47	0/2021
44	L	0.23	0/905	0.54	0/1218
45	M	0.25	0/2381	0.53	0/3212
46	N	0.24	0/1833	0.51	0/2468
47	O	0.23	0/1283	0.53	0/1727
48	P	0.24	0/1199	0.53	0/1623
49	Q	0.24	0/2039	0.50	0/2750
50	R	0.23	0/1175	0.54	0/1572
51	S	0.23	0/1320	0.53	0/1789
52	T	0.25	0/1403	0.51	0/1886
53	U	0.24	0/1274	0.54	0/1723
54	V	0.24	0/1721	0.51	0/2333
55	W	0.25	0/926	0.49	0/1244
56	X	0.24	0/2099	0.47	0/2837
57	Y	0.23	0/1593	0.49	0/2136
58	Z	0.23	0/1021	0.47	0/1378
59	0	0.23	0/913	0.53	0/1224
60	1	0.25	0/469	0.55	0/621
61	2	0.23	0/383	0.58	0/507
62	3	0.23	0/853	0.53	0/1136
63	4	0.23	0/350	0.56	0/461
64	5	0.24	0/3305	0.48	0/4502
65	6	0.25	0/3043	0.52	0/4140
66	7	0.24	0/2447	0.47	0/3310
67	8	0.24	0/1303	0.48	0/1750
68	9	0.26	0/1025	0.48	0/1379
69	a	0.24	0/866	0.51	0/1174
70	b	0.23	0/1211	0.54	0/1639
71	c	0.24	0/2347	0.47	0/3171
72	d	0.24	0/2039	0.47	0/2759
73	e	0.24	0/1970	0.47	0/2658
74	f	0.24	0/1273	0.44	0/1716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	g	0.25	0/1151	0.49	0/1569
76	h	0.23	0/918	0.45	0/1249
77	i	0.23	0/850	0.53	0/1135
78	j	0.24	0/760	0.51	0/1023
79	k	0.23	0/777	0.53	0/1048
80	l	0.24	0/707	0.49	0/960
81	m	0.23	0/805	0.57	0/1081
82	o	0.23	0/819	0.57	0/1097
83	p	0.23	0/1223	0.50	0/1641
84	q	0.23	0/1332	0.50	0/1801
85	r	0.24	0/1362	0.53	0/1846
86	s	0.24	0/3239	0.51	0/4400
87	t	0.23	0/358	0.35	0/486
87	u	0.22	0/259	0.33	0/350
87	v	0.22	0/259	0.34	0/350
87	w	0.21	0/246	0.35	0/331
87	x	0.22	0/246	0.34	0/331
87	y	0.22	0/246	0.34	0/331
88	z	0.25	0/1354	0.47	0/1831
89	Ay	0.32	1/1235 (0.1%)	0.66	0/1912
All	All	0.23	4/188586 (0.0%)	0.57	0/267953

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	1671	G	OP3-P	-10.76	1.48	1.61
36	B	1	C	OP3-P	-10.61	1.48	1.61
33	Ax	1	U	OP3-P	-10.58	1.48	1.61
89	Ay	1	U	OP3-P	-10.56	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	10304	10285	56	0
2	AB	1828	1816	1815	4	0
3	AC	1083	1089	1088	8	0
4	AD	2731	2805	2804	8	0
5	AE	972	1000	1000	6	0
6	AF	1725	1771	1769	8	0
7	AG	2688	2689	2687	10	0
8	AH	1152	1187	1183	9	0
9	AI	1020	1061	1053	3	0
10	AJ	839	888	887	5	0
11	AK	862	886	885	3	0
12	AL	1453	1541	1540	3	0
13	AM	942	966	965	4	0
14	AN	868	929	928	4	0
15	AO	1592	1557	1557	4	0
16	AP	781	806	806	3	0
17	AQ	744	758	758	0	0
18	AR	2409	2430	2428	5	0
19	AS	1111	1116	1115	1	0
20	AT	1371	1393	1393	2	0
21	AU	1488	1501	1499	4	0
22	AV	2969	2964	2961	19	0
23	AW	789	804	802	2	0
24	AX	2849	2845	2843	12	0
25	AY	1246	1198	1197	6	0
26	AZ	839	859	858	1	0
27	A0	1787	1797	1796	7	0
28	A1	2265	2296	2294	9	0
29	A2	935	971	971	6	0
30	A3	625	701	699	6	0
31	A4	4768	4770	4766	11	0
32	Aw	464	237	238	0	0
33	Ax	1482	751	752	0	0
34	Az	719	360	360	0	0
35	A	33070	16801	16794	97	0
36	B	1524	779	779	2	0
37	D	1859	1921	1920	5	0
38	E	2406	2416	2415	10	0
39	F	2031	2066	2065	4	0
40	H	1661	1736	1734	10	0
41	I	1695	1786	1785	3	0
42	J	1330	1408	1407	5	0
43	K	1455	1452	1452	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	L	890	942	941	2	0
45	M	2327	2396	2395	6	0
46	N	1786	1818	1817	10	0
47	O	1259	1295	1294	8	0
48	P	1173	1166	1165	2	0
49	Q	1990	2031	2031	5	0
50	R	1154	1215	1214	1	0
51	S	1293	1366	1365	4	0
52	T	1369	1412	1410	4	0
53	U	1251	1232	1232	4	0
54	V	1676	1689	1687	11	0
55	W	904	936	935	3	0
56	X	2044	2061	2060	2	0
57	Y	1556	1598	1597	1	0
58	Z	996	1045	1044	3	0
59	0	898	917	916	2	0
60	1	464	513	511	1	0
61	2	377	407	406	0	0
62	3	832	884	883	2	0
63	4	342	362	361	2	0
64	5	3210	3209	3206	5	0
65	6	2948	2844	2841	10	0
66	7	2390	2399	2397	10	0
67	8	1278	1310	1308	3	0
68	9	997	988	987	3	0
69	a	840	812	810	0	0
70	b	1196	1196	1190	0	0
71	c	2299	2322	2320	0	0
72	d	1985	1980	1976	0	0
73	e	1931	1917	1916	0	0
74	f	1252	1271	1269	0	0
75	g	1113	1097	1097	0	0
76	h	895	883	881	0	0
77	i	828	859	857	0	0
78	j	745	747	746	0	0
79	k	774	785	784	0	0
80	l	688	675	674	0	0
81	m	791	760	796	0	0
82	o	798	806	804	0	0
83	p	1205	1225	1223	0	0
84	q	1298	1273	1272	0	0
85	r	1322	1349	1348	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	s	3155	3145	3139	0	0
87	t	354	378	377	0	0
87	u	257	284	283	0	0
87	v	257	284	283	0	0
87	w	245	275	275	0	0
87	x	245	275	275	0	0
87	y	245	275	275	0	0
88	z	1327	1355	1353	0	0
89	Ay	1107	560	563	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	61	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	29	0	0	0	0
94	AA	18	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	0	0
101	0	27	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	22	0	0	0	0
101	6	100	0	0	1	0
101	7	17	0	0	0	0
101	8	19	0	0	1	0
101	9	17	0	0	0	0
101	A	3056	0	0	22	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	2157	0	0	23	0
101	AB	80	0	0	1	0
101	AC	58	0	0	0	0
101	AD	79	0	0	1	0
101	AE	30	0	0	0	0
101	AF	36	0	0	0	0
101	AG	70	0	0	1	0
101	AH	50	0	0	0	0
101	AI	44	0	0	1	0
101	AJ	29	0	0	1	0
101	AK	51	0	0	0	0
101	AL	43	0	0	0	0
101	AM	21	0	0	0	0
101	AN	34	0	0	0	0
101	AO	37	0	0	0	0
101	AP	31	0	0	0	0
101	AQ	68	0	0	0	0
101	AR	12	0	0	0	0
101	AS	23	0	0	0	0
101	AT	43	0	0	0	0
101	AU	8	0	0	0	0
101	AW	15	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
101	Ax	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
101	Ay	1	0	0	0	0
101	Az	15	0	0	0	0
101	B	63	0	0	0	0
101	D	73	0	0	0	0
101	E	74	0	0	1	0
101	F	78	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	66	0	0	1	0
101	N	60	0	0	4	0
101	O	38	0	0	0	0
101	P	89	0	0	1	0
101	Q	27	0	0	0	0
101	R	57	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	48	0	0	0	0
101	X	12	0	0	0	0
101	Y	29	0	0	0	0
101	Z	34	0	0	0	0
101	a	13	0	0	0	0
101	b	39	0	0	0	0
101	c	20	0	0	0	0
101	d	5	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	50	0	0	0	0
101	s	51	0	0	0	0
All	All	187689	152427	152294	391	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 (391) 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)
35:A:2103:A:HO2’	58:Z:35:LYS:N	1.72	0.86
22:AV:226:TYR:HE1	22:AV:282:VAL:HG21	1.42	0.83
7:AG:389:ARG:NH1	7:AG:390:LYS:O	2.12	0.83
6:AF:159:VAL:HG23	6:AF:172:VAL:HG21	1.63	0.80
35:A:3063:G:O2’	35:A:3066:C:OP2	2.00	0.79
35:A:3042:U:OP2	101:A:3501:HOH:O	2.00	0.79
35:A:3198:A:O2’	35:A:3200:U:O2’	2.01	0.78
53:U:9:LEU:O	53:U:11:ARG:NH1	2.16	0.78
1:AA:1472:G:O6	101:AA:1801:HOH:O	2.01	0.78
65:6:121:ARG:NH1	67:8:112:GLU:OE2	2.19	0.76
35:A:3147:G:OP1	101:A:3502:HOH:O	2.04	0.75
35:A:2098:G:O2’	35:A:2099:U:OP2	2.04	0.75
22:AV:92:LEU:HD21	22:AV:137:ILE:HD11	1.69	0.74
35:A:3226:G:O2’	35:A:3229:U:O4	2.04	0.74
31:A4:303:CYS:SG	31:A4:344:ARG:NH2	2.60	0.74
35:A:3041:U:OP1	101:A:3504:HOH:O	2.05	0.74
35:A:3113:A:OP1	35:A:3167:U:O2’	2.04	0.73
24:AX:108:LEU:HD23	24:AX:141:VAL:HG21	1.71	0.73
39:F:115:LYS:NZ	101:F:401:HOH:O	2.21	0.72
1:AA:1287:A:OP2	4:AD:260:LYS:NZ	2.21	0.72
53:U:11:ARG:NH2	54:V:211:LYS:O	2.22	0.72
1:AA:941:G:OP1	101:AA:1802:HOH:O	2.07	0.72
22:AV:208:LEU:HD13	22:AV:226:TYR:HD2	1.56	0.71
22:AV:46:GLU:OE2	22:AV:74:ARG:NE	2.21	0.70
1:AA:1047:A:OP2	101:AA:1804:HOH:O	2.09	0.70
22:AV:226:TYR:CE1	22:AV:282:VAL:HG21	2.27	0.69
1:AA:1570:G:O6	101:AA:1803:HOH:O	2.09	0.69
65:6:217:LEU:HD11	65:6:271:LEU:HD12	1.74	0.69
35:A:1777:A:N6	35:A:1780:U:OP2	2.25	0.69
35:A:3015:U:OP1	101:A:3506:HOH:O	2.10	0.69
35:A:2290:A:N7	101:A:3533:HOH:O	2.26	0.69
25:AY:318:GLU:OE1	101:AY:401:HOH:O	2.11	0.68
24:AX:272:THR:OG1	24:AX:282:ILE:O	2.10	0.68
31:A4:556:LYS:NZ	31:A4:560:GLU:OE2	2.27	0.68
1:AA:976:A:N7	101:AA:1832:HOH:O	2.25	0.68
1:AA:1578:A:OP2	101:AA:1806:HOH:O	2.11	0.68
35:A:2181:A:OP1	101:A:3509:HOH:O	2.12	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1314:C:OP2	101:AA:1805:HOH:O	2.11	0.68
44:L:95:ARG:NH2	101:L:201:HOH:O	2.28	0.67
51:S:112:ASP:OD2	101:S:301:HOH:O	2.13	0.67
46:N:73:ARG:O	46:N:155:LYS:NZ	2.27	0.67
1:AA:1040:U:OP2	101:AA:1807:HOH:O	2.14	0.66
46:N:212:PRO:O	101:N:301:HOH:O	2.13	0.66
35:A:2543:C:OP1	101:A:3508:HOH:O	2.11	0.66
1:AA:1154:A:OP2	30:A3:155:ARG:NH2	2.29	0.66
1:AA:684:U:OP1	101:AA:1808:HOH:O	2.14	0.66
37:D:281:TRP:O	37:D:285:LYS:NZ	2.29	0.66
1:AA:1151:C:N3	101:AA:1843:HOH:O	2.29	0.66
40:H:178:ASN:OD1	40:H:179:ASN:N	2.28	0.66
46:N:143:GLY:O	101:N:302:HOH:O	2.14	0.66
64:5:165:GLN:NE2	64:5:179:VAL:HG21	2.11	0.66
35:A:2372:U:OP2	101:A:3511:HOH:O	2.14	0.66
97:AX:501:ATP:O1G	101:AX:601:HOH:O	2.15	0.65
35:A:1957:A:OP1	101:A:3510:HOH:O	2.13	0.65
35:A:2314:C:OP2	101:A:3512:HOH:O	2.14	0.65
1:AA:894:C:OP1	101:AA:1809:HOH:O	2.14	0.65
35:A:2160:A:OP2	63:4:88:TRP:NE1	2.29	0.65
65:6:322:ARG:NH1	101:6:502:HOH:O	2.29	0.65
1:AA:930:G:O6	10:AJ:47:ARG:NH2	2.29	0.65
67:8:133:ARG:NH1	101:8:301:HOH:O	2.24	0.65
35:A:1990:G:OP1	37:D:269:ARG:NH2	2.28	0.64
35:A:2826:G:OP1	55:W:49:ARG:NH1	2.31	0.64
35:A:2562:U:O2’	37:D:284:ARG:O	2.09	0.64
35:A:1882:A:N7	101:A:3546:HOH:O	2.29	0.64
1:AA:828:C:OP2	101:AA:1810:HOH:O	2.15	0.64
35:A:2216:A:O2’	101:A:3505:HOH:O	2.09	0.64
35:A:3013:G:HO2’	63:4:66:PHE:N	1.96	0.64
35:A:2539:A:OP1	101:A:3515:HOH:O	2.15	0.64
35:A:1856:A:OP2	35:A:2986:C:O2’	2.16	0.64
35:A:2531:U:O4	37:D:246:ARG:NH2	2.31	0.64
35:A:1745:U:O4	62:3:108:LYS:NZ	2.30	0.63
4:AD:244:LEU:HD22	4:AD:343:LEU:HD23	1.81	0.63
7:AG:210:VAL:HG12	7:AG:210:VAL:O	1.98	0.63
25:AY:322:ASP:O	25:AY:324:ASP:N	2.32	0.62
3:AC:109:VAL:HG23	28:A1:103:LEU:HD11	1.82	0.61
35:A:1871:A:N3	62:3:104:ARG:NH2	2.48	0.61
38:E:129:VAL:CG1	38:E:145:LEU:HD11	2.30	0.61
6:AF:174:LEU:O	6:AF:179:ARG:NH1	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:2767:A:O2'	35:A:2769:A:N7	2.33	0.61
47:O:62:TYR:OH	49:Q:272:GLU:OE2	2.18	0.61
57:Y:134:LYS:NZ	68:9:76:TYR:OH	2.32	0.61
58:Z:78:ARG:O	58:Z:83:LYS:NZ	2.34	0.60
8:AH:104:ILE:HG23	8:AH:148:LEU:HD21	1.84	0.60
1:AA:1554:G:OP2	101:AA:1814:HOH:O	2.17	0.60
35:A:1747:G:OP2	35:A:1749:C:N4	2.34	0.59
42:J:113:THR:OG1	42:J:116:HIS:ND1	2.26	0.59
66:7:175:ILE:O	66:7:319:ARG:NH2	2.35	0.59
29:A2:64:ASP:OD1	29:A2:65:ALA:N	2.36	0.59
41:I:31:LYS:NZ	101:I:301:HOH:O	2.35	0.59
68:9:16:ASP:OD1	68:9:25:ARG:NH2	2.35	0.59
35:A:1958:G:OP1	101:A:3516:HOH:O	2.17	0.58
35:A:2108:G:O6	46:N:67:LYS:NZ	2.36	0.58
1:AA:1188:A:OP2	1:AA:1429:C:O2'	2.15	0.58
1:AA:1294:A:OP1	2:AB:201:ASN:ND2	2.36	0.58
35:A:2196:A:O2'	35:A:2213:A:N1	2.35	0.58
38:E:129:VAL:HG11	38:E:145:LEU:HD11	1.86	0.58
1:AA:769:G:OP2	14:AN:73:ARG:NH2	2.35	0.58
44:L:130:ARG:NH1	44:L:133:GLU:OE2	2.36	0.58
22:AV:208:LEU:HD13	22:AV:226:TYR:CD2	2.36	0.58
1:AA:1208:U:OP1	101:AA:1813:HOH:O	2.16	0.57
101:AA:1827:HOH:O	5:AE:123:ARG:NH2	2.36	0.57
35:A:2021:U:OP1	101:A:3517:HOH:O	2.17	0.57
35:A:2740:A:N3	35:A:2921:A:O2'	2.32	0.57
38:E:50:ASP:O	47:O:138:ARG:NH2	2.37	0.57
39:F:70:ARG:NH2	39:F:194:GLU:OE1	2.37	0.57
11:AK:58:ARG:NE	11:AK:72:ASP:OD1	2.36	0.57
35:A:3089:A:H3'	35:A:3090:G:C5'	2.34	0.57
28:A1:152:ASP:OD2	28:A1:174:ARG:NH1	2.31	0.57
35:A:3110:C:O2'	38:E:266:ARG:NH1	2.38	0.57
1:AA:1015:A:OP2	101:AA:1816:HOH:O	2.18	0.56
18:AR:69:THR:N	18:AR:72:ASP:OD2	2.38	0.56
1:AA:1109:A:OP2	101:AA:1815:HOH:O	2.17	0.56
2:AB:88:ARG:NH1	101:AB:403:HOH:O	2.38	0.56
4:AD:245:VAL:HG22	4:AD:271:ALA:HB1	1.86	0.56
6:AF:172:VAL:HG12	6:AF:240:ARG:HD3	1.86	0.56
35:A:2545:U:O2'	101:A:3514:HOH:O	2.15	0.56
29:A2:43:ALA:HB1	29:A2:46:ILE:HD11	1.88	0.56
35:A:2364:C:OP2	53:U:78:LYS:NZ	2.38	0.56
22:AV:236:LEU:CD1	22:AV:290:LEU:HD13	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1308:U:O2'	3:AC:64:HIS:ND1	2.36	0.55
48:P:138:GLU:OE2	101:P:201:HOH:O	2.18	0.55
4:AD:340:ILE:HG22	4:AD:340:ILE:O	2.07	0.55
35:A:1760:G:OP1	45:M:196:ARG:NE	2.40	0.55
1:AA:1257:U:O2'	1:AA:1260:A:OP2	2.14	0.55
29:A2:33:VAL:HG21	29:A2:104:LEU:HD23	1.87	0.55
35:A:1805:A:OP2	54:V:94:HIS:NE2	2.36	0.55
1:AA:1346:A:OP2	101:AA:1818:HOH:O	2.18	0.54
1:AA:845:A:H4'	21:AU:60:TYR:CE2	2.43	0.54
22:AV:228:TYR:HB3	22:AV:259:ALA:HB2	1.89	0.54
1:AA:843:G:N2	1:AA:846:A:OP2	2.35	0.54
1:AA:1044:U:OP1	1:AA:1110:A:O2'	2.22	0.54
22:AV:236:LEU:HD12	22:AV:290:LEU:HD13	1.89	0.54
24:AX:151:LEU:CD2	24:AX:247:LEU:HD22	2.38	0.54
35:A:2016:C:OP2	45:M:59:ARG:NH1	2.41	0.54
1:AA:1264:C:H1'	8:AH:124:VAL:HG13	1.90	0.53
10:AJ:117:ASP:OD1	101:AJ:201:HOH:O	2.17	0.53
35:A:2761:C:O2	35:A:2786:U:N3	2.42	0.53
8:AH:184:ILE:O	8:AH:184:ILE:HG22	2.08	0.53
24:AX:108:LEU:HD21	24:AX:307:VAL:HG11	1.90	0.53
35:A:1953:A:O2'	35:A:2463:A:OP1	2.26	0.53
35:A:2462:A:N3	101:A:3569:HOH:O	2.34	0.53
1:AA:1458:A:OP1	6:AF:104:LYS:NZ	2.29	0.53
35:A:2071:U:O2'	65:6:28:ARG:NH2	2.42	0.52
35:A:2354:A:O2'	101:A:3503:HOH:O	2.05	0.52
29:A2:36:ARG:NH2	29:A2:92:THR:HG23	2.25	0.52
7:AG:229:LEU:HD21	7:AG:241:VAL:HG11	1.91	0.52
1:AA:702:C:OP1	1:AA:848:U:O2'	2.26	0.52
7:AG:200:LEU:HD11	7:AG:204:GLU:HB3	1.91	0.52
65:6:161:LEU:HD13	65:6:271:LEU:HD11	1.91	0.52
64:5:173:ARG:HA	64:5:176:TYR:CE1	2.45	0.52
9:AI:87:HIS:NE2	101:AI:201:HOH:O	2.25	0.51
30:A3:144:ARG:NH2	101:A3:301:HOH:O	2.43	0.51
35:A:1742:G:O2'	35:A:1754:G:O6	2.23	0.51
54:V:163:ASP:OD1	54:V:164:GLY:N	2.44	0.51
1:AA:1134:G:OP2	10:AJ:38:ARG:NH2	2.43	0.51
22:AV:187:PHE:CE1	22:AV:352:LEU:HD13	2.46	0.51
5:AE:65:LEU:HD11	16:AP:75:LYS:CD	2.41	0.51
46:N:247:MET:SD	101:N:331:HOH:O	2.60	0.50
52:T:184:LYS:NZ	52:T:192:GLU:OE1	2.38	0.50
35:A:1749:C:OP2	35:A:2899:C:O2'	2.28	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N:251:VAL:OXT	101:N:303:HOH:O	2.19	0.50
40:H:53:THR:N	40:H:86:THR:HG1	2.10	0.50
54:V:188:VAL:O	54:V:188:VAL:HG23	2.11	0.50
1:AA:841:A:OP1	13:AM:39:ASN:ND2	2.42	0.50
22:AV:225:LEU:HD11	22:AV:283:LEU:HD22	1.94	0.50
24:AX:108:LEU:HD21	24:AX:307:VAL:CG1	2.42	0.50
24:AX:183:GLU:N	24:AX:183:GLU:OE1	2.42	0.50
28:A1:250:GLU:OE2	28:A1:301:ASN:ND2	2.45	0.50
56:X:177:HIS:O	56:X:184:ARG:NH1	2.44	0.50
35:A:2162:C:OP2	101:A:3519:HOH:O	2.19	0.49
35:A:2537:G:O2'	35:A:2634:U:OP2	2.26	0.49
28:A1:46:ARG:HB2	28:A1:47:PRO:HD3	1.93	0.49
1:AA:768:A:O2'	14:AN:24:LYS:NZ	2.45	0.49
1:AA:1004:G:O2'	9:AI:98:GLN:NE2	2.45	0.49
51:S:173:ARG:HB2	51:S:182:LYS:HG2	1.92	0.49
40:H:146:LEU:O	40:H:150:GLY:N	2.42	0.49
1:AA:1215:U:O4	101:AA:1819:HOH:O	2.18	0.49
43:K:52:ASP:OD1	101:K:201:HOH:O	2.19	0.49
29:A2:33:VAL:HG22	29:A2:105:ASN:OD1	2.13	0.49
35:A:2483:U:H2'	35:A:2484:C:O4'	2.13	0.49
15:AO:208:PRO:HG2	15:AO:213:LEU:HD21	1.94	0.48
28:A1:46:ARG:HB2	28:A1:47:PRO:CD	2.43	0.48
1:AA:899:G:O2'	1:AA:907:A:N1	2.33	0.48
24:AX:268:LEU:HD21	24:AX:293:LEU:HD23	1.96	0.48
54:V:169:THR:HG22	54:V:169:THR:O	2.12	0.48
3:AC:106:ASP:OD1	3:AC:107:GLN:N	2.43	0.48
6:AF:159:VAL:CG2	6:AF:172:VAL:HG21	2.40	0.48
7:AG:384:GLN:NE2	101:AG:404:HOH:O	2.47	0.48
31:A4:239:ARG:O	31:A4:242:ASN:ND2	2.44	0.48
35:A:2909:G:OP1	60:1:63:ARG:NH1	2.42	0.48
10:AJ:78:ARG:NH2	10:AJ:117:ASP:OD2	2.47	0.48
55:W:102:GLU:OE2	65:6:74:TYR:N	2.45	0.48
8:AH:155:VAL:HG21	28:A1:129:PHE:CB	2.43	0.48
24:AX:297:MET:HE3	24:AX:306:ILE:HG21	1.95	0.48
35:A:2104:A:OP1	46:N:231:SER:OG	2.21	0.48
35:A:2888:A:H3'	35:A:2889:C:C5'	2.44	0.48
47:O:64:LYS:NZ	47:O:100:GLN:O	2.47	0.48
35:A:2499:U:OP2	35:A:2504:A:N6	2.36	0.48
1:AA:1427:A:N7	101:AA:1873:HOH:O	2.35	0.48
66:7:156:ARG:HG3	66:7:156:ARG:HH11	1.78	0.48
1:AA:749:G:O3'	14:AN:78:LYS:NZ	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:217:ARG:NH1	15:AO:227:GLU:OE2	2.46	0.47
22:AV:360:VAL:HG13	22:AV:364:LEU:HD22	1.96	0.47
1:AA:1479:C:OP1	101:AA:1820:HOH:O	2.20	0.47
22:AV:190:LEU:HD13	22:AV:226:TYR:CE2	2.49	0.47
35:A:1851:G:H2'	35:A:2693:A:N7	2.29	0.47
47:O:144:LEU:HD12	66:7:174:VAL:HG11	1.97	0.47
3:AC:115:ASN:ND2	25:AY:309:LYS:O	2.48	0.47
35:A:3201:A:H2'	35:A:3202:U:O4'	2.15	0.47
3:AC:109:VAL:CG2	28:A1:103:LEU:HD11	2.45	0.47
4:AD:88:SER:N	101:AD:504:HOH:O	2.47	0.47
12:AL:126:GLU:HG2	12:AL:177:VAL:HG11	1.97	0.47
41:I:197:LEU:HD12	41:I:198:PRO:HD2	1.97	0.47
20:AT:132:ARG:NH1	20:AT:136:LEU:O	2.48	0.47
1:AA:1453:A:OP1	101:AA:1822:HOH:O	2.21	0.47
8:AH:125:HIS:CE1	8:AH:126:ILE:HG23	2.49	0.47
15:AO:221:GLN:NE2	22:AV:314:VAL:O	2.39	0.47
42:J:75:ASP:OD1	42:J:77:THR:HG22	2.15	0.47
66:7:257:ILE:O	66:7:257:ILE:HG13	2.15	0.47
35:A:1958:G:O2'	101:A:3518:HOH:O	2.18	0.47
35:A:2663:C:OP1	47:O:13:ARG:NH2	2.47	0.47
6:AF:176:ASP:OD2	6:AF:180:ARG:NH1	2.48	0.47
66:7:106:ALA:O	66:7:113:TRP:N	2.47	0.47
52:T:85:ALA:O	52:T:139:SER:OG	2.33	0.46
8:AH:155:VAL:HG21	28:A1:129:PHE:HB2	1.97	0.46
24:AX:153:LEU:HD21	24:AX:244:LEU:CD2	2.46	0.46
53:U:66:ALA:HB2	53:U:100:ALA:HA	1.98	0.46
54:V:127:ASP:O	54:V:129:LYS:N	2.49	0.46
59:0:133:GLU:OE2	59:0:160:TYR:OH	2.26	0.46
38:E:47:THR:OG1	38:E:51:GLU:OE1	2.22	0.46
22:AV:225:LEU:HD21	22:AV:280:LEU:HD23	1.97	0.46
40:H:107:VAL:HG12	40:H:108:ARG:N	2.30	0.46
22:AV:87:HIS:ND1	49:Q:60:PRO:HB2	2.30	0.46
35:A:2458:A:O2'	38:E:215:PHE:O	2.29	0.46
8:AH:184:ILE:O	8:AH:184:ILE:CG2	2.63	0.46
39:F:218:LEU:HD23	39:F:260:VAL:HB	1.98	0.46
7:AG:102:GLU:OE1	7:AG:102:GLU:N	2.44	0.46
27:A0:54:ALA:O	27:A0:58:VAL:HG23	2.16	0.46
35:A:2777:G:N3	40:H:179:ASN:ND2	2.63	0.46
36:B:12:U:HO2'	36:B:14:A:P	2.39	0.46
8:AH:151:SER:O	8:AH:155:VAL:HG23	2.16	0.46
24:AX:81:HIS:ND1	24:AX:190:ASN:HB3	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A4:305:ILE:HG22	31:A4:306:ASN:N	2.31	0.46
35:A:2506:A:H1'	35:A:2601:A:N6	2.31	0.46
6:AF:193:ASP:OD1	6:AF:194:LYS:N	2.49	0.45
20:AT:92:THR:O	20:AT:92:THR:HG22	2.16	0.45
21:AU:56:LEU:HD11	21:AU:60:TYR:CZ	2.52	0.45
65:6:215:THR:OG1	65:6:275:GLN:OE1	2.31	0.45
27:A0:41:LEU:HD13	27:A0:55:TRP:CG	2.52	0.45
43:K:67:PHE:HB3	43:K:71:LYS:HB2	1.99	0.45
45:M:43:ARG:NH2	101:M:404:HOH:O	2.50	0.45
1:AA:1057:G:H4'	1:AA:1578:A:H4'	1.98	0.45
4:AD:312:TYR:N	4:AD:331:ASP:OD2	2.49	0.45
35:A:3211:C:HO2'	35:A:3212:C:H5	1.58	0.45
65:6:224:HIS:HA	65:6:232:TYR:CE2	2.51	0.45
7:AG:198:ARG:NH1	7:AG:201:ILE:HG23	2.32	0.45
11:AK:70:VAL:HG11	25:AY:383:LYS:HE3	1.99	0.45
23:AW:92:MET:O	23:AW:98:LYS:NZ	2.49	0.45
31:A4:309:PHE:HB2	31:A4:345:PHE:CD1	2.52	0.45
18:AR:317:ALA:O	18:AR:321:ALA:N	2.49	0.45
38:E:131:LYS:O	38:E:145:LEU:HD12	2.16	0.45
49:Q:251:GLU:OE1	49:Q:251:GLU:HA	2.16	0.45
58:Z:75:THR:HB	58:Z:83:LYS:HG2	1.99	0.45
45:M:177:ALA:HA	45:M:222:TYR:CD1	2.52	0.45
18:AR:162:SER:O	18:AR:170:ARG:NH1	2.48	0.44
40:H:84:GLU:OE1	56:X:44:ARG:NH2	2.50	0.44
19:AS:51:VAL:HG13	29:A2:117:LEU:HD11	1.99	0.44
35:A:1867:A:N1	35:A:2019:G:O2'	2.36	0.44
46:N:135:SER:HG	46:N:138:HIS:CE1	2.36	0.44
64:5:105:TYR:CE1	64:5:262:ILE:HD12	2.53	0.44
39:F:98:GLN:NE2	101:F:406:HOH:O	2.51	0.44
65:6:257:PRO:HB3	65:6:268:LEU:HD21	2.00	0.44
35:A:1822:U:O2	35:A:2707:A:O2'	2.33	0.44
1:AA:1259:U:H6	1:AA:1326:A:HO2'	1.58	0.44
36:B:44:A:H2'	36:B:45:G:O4'	2.18	0.44
37:D:207:ILE:HG22	37:D:207:ILE:O	2.19	0.43
7:AG:237:GLU:OE1	7:AG:237:GLU:N	2.50	0.43
35:A:2598:A:H3'	35:A:2625:C:H42	1.83	0.43
5:AE:65:LEU:HD11	16:AP:75:LYS:HD2	2.00	0.43
1:AA:1461:A:N6	101:AA:1898:HOH:O	2.41	0.43
5:AE:109:VAL:HG23	5:AE:109:VAL:O	2.19	0.43
40:H:223:VAL:N	40:H:231:VAL:O	2.46	0.43
7:AG:200:LEU:HD13	7:AG:246:ARG:CZ	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AU:73:GLU:OE2	27:A0:166:TYR:OH	2.37	0.43
35:A:2135:A:N3	35:A:2135:A:H2'	2.34	0.43
66:7:51:GLU:OE1	66:7:51:GLU:HA	2.19	0.43
31:A4:58:VAL:O	31:A4:58:VAL:HG23	2.18	0.43
35:A:1697:A:N3	35:A:1703:C:O2'	2.48	0.43
35:A:2293:A:N1	101:A:3603:HOH:O	2.37	0.43
35:A:2868:C:H2'	35:A:2869:A:O4'	2.19	0.43
5:AE:55:SER:O	5:AE:56:GLN:NE2	2.51	0.43
13:AM:101:PRO:HB2	21:AU:60:TYR:CE1	2.53	0.43
35:A:1991:A:H5"	35:A:1992:C:OP1	2.18	0.43
35:A:2053:U:HO2'	35:A:2054:U:H6	1.65	0.43
35:A:2429:A:N1	35:A:2433:C:O2'	2.45	0.43
35:A:2296:U:H5"	35:A:2297:A:OP1	2.19	0.42
49:Q:69:VAL:HG12	49:Q:71:PRO:HD3	2.00	0.42
31:A4:470:GLN:NE2	31:A4:472:ASP:OD2	2.52	0.42
35:A:3089:A:H3'	35:A:3090:G:H5'	2.01	0.42
46:N:135:SER:OG	46:N:138:HIS:CE1	2.72	0.42
35:A:2882:U:O4'	48:P:173:ARG:NH2	2.52	0.42
51:S:152:ASP:OD1	51:S:153:LEU:N	2.53	0.42
31:A4:458:TYR:HB3	31:A4:486:TYR:CD1	2.54	0.42
35:A:1800:G:N1	35:A:1803:A:OP2	2.51	0.42
24:AX:151:LEU:HD23	24:AX:247:LEU:HD22	2.00	0.42
54:V:165:ILE:HG21	68:9:76:TYR:CD2	2.54	0.42
50:R:65:ARG:HA	50:R:68:TRP:CE3	2.55	0.42
67:8:202:VAL:O	67:8:203:GLU:HB3	2.19	0.42
1:AA:1199:G:N1	1:AA:1422:G:OP2	2.49	0.42
1:AA:1322:C:N3	4:AD:234:LYS:NZ	2.64	0.42
12:AL:213:VAL:O	12:AL:217:THR:HG23	2.20	0.42
35:A:2728:C:H4'	35:A:2815:OMG:HM22	2.01	0.42
3:AC:84:GLU:OE1	3:AC:84:GLU:N	2.44	0.42
28:A1:86:ARG:NH1	28:A1:96:PRO:O	2.50	0.42
1:AA:1528:A:OP1	27:A0:101:ARG:NH2	2.51	0.42
4:AD:198:TRP:HA	4:AD:201:ILE:HD12	2.02	0.42
6:AF:114:THR:HG21	6:AF:205:LEU:HG	2.02	0.42
22:AV:241:ARG:HA	22:AV:244:TYR:CE2	2.55	0.42
27:A0:158:GLU:O	27:A0:158:GLU:HG2	2.20	0.42
1:AA:1265:C:H4'	8:AH:122:GLN:HG3	2.02	0.42
27:A0:110:ASP:OD1	27:A0:110:ASP:N	2.50	0.42
66:7:73:THR:HG1	66:7:99:TYR:HH	1.62	0.42
3:AC:58:ALA:HB1	3:AC:59:PRO:CD	2.50	0.41
27:A0:13:GLU:OE2	27:A0:16:ARG:NH1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:1787:G:N2	35:A:1790:A:OP2	2.51	0.41
35:A:2174:G:H4’	42:J:151:LEU:HD23	2.00	0.41
54:V:124:ASP:OD1	54:V:125:PRO:HD2	2.20	0.41
1:AA:1103:A:N7	1:AA:1574:G:O2’	2.46	0.41
40:H:238:VAL:HG12	40:H:239:ASN:N	2.35	0.41
47:O:140:SER:O	47:O:146:ASN:ND2	2.50	0.41
64:5:56:GLU:O	64:5:56:GLU:HG3	2.19	0.41
66:7:114:ASP:OD1	66:7:268:LEU:N	2.53	0.41
12:AL:126:GLU:OE1	12:AL:126:GLU:N	2.41	0.41
22:AV:139:PRO:HD2	22:AV:144:PHE:CZ	2.55	0.41
35:A:1800:G:O6	54:V:34:LYS:NZ	2.52	0.41
35:A:2025:C:OP1	51:S:182:LYS:HD3	2.20	0.41
64:5:273:VAL:HG12	64:5:273:VAL:O	2.20	0.41
1:AA:1065:C:H2’	1:AA:1066:C:O4’	2.21	0.41
30:A3:173:LEU:HD12	30:A3:191:THR:HG23	2.02	0.41
35:A:1815:A:N1	101:A:3599:HOH:O	2.37	0.41
3:AC:75:ASN:ND2	11:AK:121:SER:O	2.53	0.41
18:AR:162:SER:O	18:AR:170:ARG:NH2	2.53	0.41
38:E:247:ASP:O	101:E:501:HOH:O	2.22	0.41
42:J:102:ARG:N	42:J:107:GLU:OE2	2.51	0.41
43:K:7:ALA:HB3	43:K:8:PRO:HD3	2.02	0.41
24:AX:265:ILE:HD11	24:AX:297:MET:HE2	2.02	0.41
30:A3:159:GLU:OE2	35:A:2639:C:H5”	2.21	0.41
35:A:2015:G:O4’	45:M:56:GLU:HG3	2.21	0.41
35:A:2662:A:OP1	35:A:3159:A:O2’	2.33	0.41
38:E:69:ASP:OD1	38:E:154:ARG:NH1	2.54	0.41
52:T:49:ASN:ND2	52:T:68:TYR:O	2.53	0.41
1:AA:1149:G:OP2	30:A3:165:LYS:NZ	2.50	0.41
2:AB:96:GLY:HA3	23:AW:159:ASP:OD2	2.21	0.41
2:AB:167:HIS:CD2	7:AG:153:THR:HA	2.56	0.41
18:AR:162:SER:HB2	18:AR:165:ILE:HD12	2.02	0.41
25:AY:259:PHE:HB2	31:A4:363:ILE:HD11	2.03	0.41
35:A:2598:A:O2’	35:A:2599:U:H5’	2.21	0.41
52:T:94:ASP:OD2	66:7:97:GLU:N	2.38	0.41
1:AA:709:G:OP1	13:AM:13:ARG:NH2	2.53	0.41
1:AA:1001:C:N4	35:A:2558:A:O4’	2.54	0.41
14:AN:93:ASP:O	14:AN:97:GLY:N	2.48	0.41
25:AY:300:GLU:OE1	31:A4:87:TYR:OH	2.31	0.41
26:AZ:46:LYS:HA	26:AZ:49:TYR:CE1	2.55	0.41
35:A:2595:A:H2’	35:A:2596:G:O4’	2.21	0.41
46:N:87:PHE:HE1	46:N:169:PHE:HB2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1107:U:O4	30:A3:128:LYS:NZ	2.47	0.41
10:AJ:70:PRO:HB3	10:AJ:117:ASP:HB3	2.03	0.41
35:A:2343:G:H3'	35:A:2343:G:N3	2.36	0.41
45:M:14:ASP:OD1	45:M:15:LEU:N	2.54	0.41
55:W:103:VAL:HG11	65:6:61:ALA:HB1	2.03	0.41
1:AA:1066:C:O2'	9:AI:187:ARG:O	2.39	0.40
13:AM:19:ILE:HB	13:AM:83:LEU:HD23	2.03	0.40
31:A4:508:VAL:O	31:A4:508:VAL:HG12	2.20	0.40
35:A:2709:A:N3	59:0:98:GLN:OE1	2.53	0.40
40:H:193:PHE:O	40:H:198:GLY:N	2.54	0.40
54:V:130:PRO:O	54:V:149:ARG:NH1	2.54	0.40
66:7:36:SER:HB2	66:7:37:PRO:HD2	2.02	0.40
5:AE:65:LEU:HD11	16:AP:75:LYS:HD3	2.03	0.40
22:AV:70:LEU:HD23	22:AV:393:GLU:OE1	2.22	0.40
35:A:2814:G:O2'	35:A:2983:G:OP1	2.39	0.40
41:I:144:LEU:N	41:I:145:PRO:HD2	2.37	0.40
47:O:36:LEU:O	47:O:40:GLU:N	2.50	0.40
1:AA:919:A:OP2	15:AO:96:ARG:NH2	2.49	0.40
35:A:2327:U:H2'	35:A:2328:C:O4'	2.20	0.40
35:A:3009:C:O2	35:A:3009:C:O5'	2.38	0.40
38:E:345:ILE:O	49:Q:172:GLN:NE2	2.51	0.40
42:J:69:LYS:HE3	42:J:69:LYS:HB2	1.96	0.40
47:O:86:ILE:HB	47:O:87:PRO:HD3	2.03	0.40
35:A:2006:C:H2'	35:A:2007:U:C6	2.57	0.40
40:H:208:LEU:HB3	40:H:209:PRO:HD2	2.04	0.40
54:V:54:TRP:NE1	54:V:56:LEU:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	204 (99%)	2 (1%)	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	134/194 (69%)	132 (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
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%)	353 (99%)	5 (1%)	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%)	97 (99%)	1 (1%)	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
37	D	236/305 (77%)	232 (98%)	4 (2%)	0	100	100
38	E	303/348 (87%)	296 (98%)	6 (2%)	1 (0%)	41	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	F	250/311 (80%)	247 (99%)	3 (1%)	0	100	100
40	H	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
41	I	210/261 (80%)	203 (97%)	7 (3%)	0	100	100
42	J	173/192 (90%)	173 (100%)	0	0	100	100
43	K	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
44	L	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
45	M	289/296 (98%)	283 (98%)	6 (2%)	0	100	100
46	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
47	O	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
48	P	142/180 (79%)	142 (100%)	0	0	100	100
49	Q	237/292 (81%)	237 (100%)	0	0	100	100
50	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
51	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
52	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
53	U	150/153 (98%)	147 (98%)	3 (2%)	0	100	100
54	V	203/216 (94%)	199 (98%)	4 (2%)	0	100	100
55	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
56	X	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
57	Y	179/250 (72%)	177 (99%)	2 (1%)	0	100	100
58	Z	120/161 (74%)	120 (100%)	0	0	100	100
59	0	108/188 (57%)	108 (100%)	0	0	100	100
60	1	54/65 (83%)	53 (98%)	1 (2%)	0	100	100
61	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
62	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
63	4	36/103 (35%)	36 (100%)	0	0	100	100
64	5	392/423 (93%)	382 (97%)	10 (3%)	0	100	100
65	6	352/380 (93%)	344 (98%)	8 (2%)	0	100	100
66	7	292/338 (86%)	286 (98%)	6 (2%)	0	100	100
67	8	147/206 (71%)	144 (98%)	3 (2%)	0	100	100
68	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
69	a	96/142 (68%)	94 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	b	148/215 (69%)	146 (99%)	2 (1%)	0	100	100
71	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100
72	d	235/306 (77%)	231 (98%)	4 (2%)	0	100	100
73	e	236/279 (85%)	229 (97%)	6 (2%)	1 (0%)	34	37
74	f	153/212 (72%)	152 (99%)	1 (1%)	0	100	100
75	g	132/166 (80%)	129 (98%)	3 (2%)	0	100	100
76	h	108/158 (68%)	107 (99%)	1 (1%)	0	100	100
77	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
78	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
79	k	99/112 (88%)	99 (100%)	0	0	100	100
80	l	80/138 (58%)	80 (100%)	0	0	100	100
81	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
82	o	92/102 (90%)	92 (100%)	0	0	100	100
83	p	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
84	q	153/222 (69%)	153 (100%)	0	0	100	100
85	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
86	s	382/439 (87%)	374 (98%)	8 (2%)	0	100	100
87	t	44/198 (22%)	44 (100%)	0	0	100	100
87	u	30/198 (15%)	30 (100%)	0	0	100	100
87	v	30/198 (15%)	30 (100%)	0	0	100	100
87	w	29/198 (15%)	29 (100%)	0	0	100	100
87	x	29/198 (15%)	29 (100%)	0	0	100	100
87	y	29/198 (15%)	29 (100%)	0	0	100	100
88	z	160/325 (49%)	151 (94%)	8 (5%)	1 (1%)	25	25
All	All	14595/19484 (75%)	14379 (98%)	211 (1%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	AH	126	ILE
25	AY	323	ASP
88	z	128	ASP
38	E	150	LYS
73	e	197	GLU

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
37	D	192/245 (78%)	192 (100%)	0	100	100
38	E	260/290 (90%)	259 (100%)	1 (0%)	91	95
39	F	219/262 (84%)	219 (100%)	0	100	100
40	H	182/228 (80%)	182 (100%)	0	100	100
41	I	194/232 (84%)	194 (100%)	0	100	100
42	J	138/150 (92%)	138 (100%)	0	100	100
43	K	154/155 (99%)	154 (100%)	0	100	100
44	L	98/124 (79%)	98 (100%)	0	100	100
45	M	246/249 (99%)	246 (100%)	0	100	100
46	N	189/211 (90%)	189 (100%)	0	100	100
47	O	134/150 (89%)	134 (100%)	0	100	100
48	P	126/155 (81%)	126 (100%)	0	100	100
49	Q	221/256 (86%)	221 (100%)	0	100	100
50	R	118/126 (94%)	118 (100%)	0	100	100
51	S	146/180 (81%)	146 (100%)	0	100	100
52	T	146/176 (83%)	146 (100%)	0	100	100
53	U	134/135 (99%)	134 (100%)	0	100	100
54	V	183/191 (96%)	183 (100%)	0	100	100
55	W	94/119 (79%)	94 (100%)	0	100	100
56	X	220/229 (96%)	220 (100%)	0	100	100
57	Y	163/223 (73%)	162 (99%)	1 (1%)	86	92
58	Z	113/147 (77%)	113 (100%)	0	100	100
59	0	99/164 (60%)	99 (100%)	0	100	100
60	1	53/60 (88%)	53 (100%)	0	100	100
61	2	40/72 (56%)	40 (100%)	0	100	100
62	3	88/166 (53%)	88 (100%)	0	100	100
63	4	37/89 (42%)	37 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	5	353/368 (96%)	352 (100%)	1 (0%)	92	96
65	6	313/332 (94%)	313 (100%)	0	100	100
66	7	270/303 (89%)	270 (100%)	0	100	100
67	8	140/190 (74%)	140 (100%)	0	100	100
68	9	104/112 (93%)	104 (100%)	0	100	100
69	a	96/133 (72%)	95 (99%)	1 (1%)	76	85
70	b	131/185 (71%)	131 (100%)	0	100	100
71	c	251/288 (87%)	251 (100%)	0	100	100
72	d	223/274 (81%)	223 (100%)	0	100	100
73	e	207/236 (88%)	207 (100%)	0	100	100
74	f	139/188 (74%)	139 (100%)	0	100	100
75	g	124/148 (84%)	124 (100%)	0	100	100
76	h	104/148 (70%)	104 (100%)	0	100	100
77	i	86/110 (78%)	86 (100%)	0	100	100
78	j	74/97 (76%)	74 (100%)	0	100	100
79	k	83/90 (92%)	83 (100%)	0	100	100
80	l	76/116 (66%)	76 (100%)	0	100	100
81	m	85/113 (75%)	85 (100%)	0	100	100
82	o	80/87 (92%)	80 (100%)	0	100	100
83	p	135/181 (75%)	135 (100%)	0	100	100
84	q	132/178 (74%)	132 (100%)	0	100	100
85	r	147/169 (87%)	147 (100%)	0	100	100
86	s	340/381 (89%)	340 (100%)	0	100	100
87	t	40/158 (25%)	40 (100%)	0	100	100
87	u	31/158 (20%)	31 (100%)	0	100	100
87	v	31/158 (20%)	31 (100%)	0	100	100
87	w	30/158 (19%)	30 (100%)	0	100	100
87	x	30/158 (19%)	30 (100%)	0	100	100
87	y	30/158 (19%)	30 (100%)	0	100	100
88	z	150/287 (52%)	150 (100%)	0	100	100
All	All	13075/16790 (78%)	13071 (100%)	4 (0%)	100	100

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

Mol	Chain	Res	Type
38	E	303	LYS
57	Y	198	ARG
64	5	395	ARG
69	a	122	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
4	AD	356	GLN
6	AF	113	GLN
6	AF	238	HIS
7	AG	384	GLN
9	AI	96	GLN
9	AI	98	GLN
12	AL	162	GLN
13	AM	50	GLN
17	AQ	41	HIS
21	AU	188	ASN
22	AV	380	GLN
23	AW	106	HIS
24	AX	159	HIS
24	AX	250	GLN
26	AZ	63	GLN
28	A1	185	HIS
31	A4	257	HIS
31	A4	306	ASN
37	D	221	ASN
38	E	125	GLN
38	E	281	ASN
39	F	98	GLN
41	I	36	HIS
41	I	150	HIS
47	O	100	GLN
51	S	118	ASN
55	W	62	HIS
58	Z	150	HIS
59	0	118	GLN
59	0	120	HIS
60	1	52	GLN
64	5	109	HIS
64	5	331	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
64	5	367	ASN
65	6	320	GLN
66	7	298	GLN
69	a	126	HIS
70	b	58	ASN
73	e	212	HIS
73	e	252	HIS
77	i	124	HIS
82	o	21	HIS
82	o	94	HIS
84	q	107	GLN
84	q	142	ASN
85	r	96	HIS
88	z	104	HIS
88	z	241	HIS
88	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	Az	32/34 (94%)	12 (37%)	0
35	A	1556/1558 (99%)	220 (14%)	3 (0%)
36	B	71/72 (98%)	11 (15%)	0
89	Ay	48/52 (92%)	14 (29%)	0
All	All	2745/2762 (99%)	391 (14%)	3 (0%)

All (391) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	Az	0	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	Az	12	U
34	Az	13	U
34	Az	18	A
34	Az	21	A
34	Az	22	A
34	Az	23	U
34	Az	24	U
34	Az	25	U
34	Az	26	A
34	Az	27	C
34	Az	32	A
35	A	1678	C
35	A	1681	G
35	A	1689	C
35	A	1692	A
35	A	1700	U
35	A	1704	U
35	A	1708	A
35	A	1715	C
35	A	1724	A
35	A	1727	A
35	A	1728	U
35	A	1748	G
35	A	1765	C
35	A	1777	A
35	A	1805	A
35	A	1806	U
35	A	1807	U
35	A	1808	A
35	A	1810	A
35	A	1817	C
35	A	1821	A
35	A	1827	C
35	A	1828	A
35	A	1829	A
35	A	1832	A
35	A	1836	A
35	A	1844	A
35	A	1854	U
35	A	1856	A
35	A	1869	A
35	A	1871	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	A	1882	A
35	A	1887	A
35	A	1893	A
35	A	1901	C
35	A	1903	C
35	A	1918	G
35	A	1937	A
35	A	1940	A
35	A	1958	G
35	A	1985	G
35	A	1992	C
35	A	1993	A
35	A	1994	A
35	A	2000	C
35	A	2003	A
35	A	2015	G
35	A	2022	G
35	A	2030	U
35	A	2032	G
35	A	2036	C
35	A	2037	U
35	A	2039	A
35	A	2054	U
35	A	2060	A
35	A	2069	U
35	A	2071	U
35	A	2079	C
35	A	2099	U
35	A	2113	G
35	A	2125	C
35	A	2126	U
35	A	2147	G
35	A	2160	A
35	A	2163	A
35	A	2168	U
35	A	2181	A
35	A	2192	A
35	A	2198	A
35	A	2200	A
35	A	2207	A
35	A	2214	A
35	A	2219	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	A	2221	C
35	A	2222	U
35	A	2223	A
35	A	2224	C
35	A	2225	C
35	A	2226	U
35	A	2227	A
35	A	2230	A
35	A	2233	U
35	A	2237	A
35	A	2241	A
35	A	2243	A
35	A	2245	A
35	A	2246	A
35	A	2262	C
35	A	2263	C
35	A	2284	C
35	A	2285	U
35	A	2297	A
35	A	2300	G
35	A	2322	C
35	A	2331	C
35	A	2332	C
35	A	2345	G
35	A	2350	A
35	A	2353	A
35	A	2354	A
35	A	2357	C
35	A	2363	A
35	A	2372	U
35	A	2374	A
35	A	2390	A
35	A	2399	A
35	A	2401	A
35	A	2404	U
35	A	2407	U
35	A	2415	C
35	A	2434	A
35	A	2446	A
35	A	2451	A
35	A	2478	G
35	A	2485	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	A	2493	C
35	A	2502	C
35	A	2520	C
35	A	2521	A
35	A	2527	A
35	A	2570	C
35	A	2592	G
35	A	2593	G
35	A	2594	U
35	A	2599	U
35	A	2600	A
35	A	2601	A
35	A	2603	C
35	A	2618	U
35	A	2627	G
35	A	2630	U
35	A	2633	A
35	A	2635	G
35	A	2654	U
35	A	2656	U
35	A	2683	C
35	A	2686	G
35	A	2694	A
35	A	2696	A
35	A	2706	A
35	A	2718	C
35	A	2719	G
35	A	2723	A
35	A	2724	G
35	A	2725	A
35	A	2732	G
35	A	2745	A
35	A	2757	A
35	A	2758	G
35	A	2759	U
35	A	2762	C
35	A	2765	A
35	A	2767	A
35	A	2768	A
35	A	2775	A
35	A	2781	U
35	A	2782	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	A	2786	U
35	A	2788	C
35	A	2790	A
35	A	2791	A
35	A	2810	G
35	A	2832	A
35	A	2833	A
35	A	2847	C
35	A	2864	U
35	A	2865	C
35	A	2882	U
35	A	2883	A
35	A	2885	U
35	A	2888	A
35	A	2889	C
35	A	2893	A
35	A	2913	A
35	A	2917	G
35	A	2918	A
35	A	2922	A
35	A	2928	C
35	A	2932	G
35	A	2935	A
35	A	2956	A
35	A	2989	G
35	A	2990	A
35	A	2992	G
35	A	2993	U
35	A	3005	A
35	A	3016	G
35	A	3041	U
35	A	3053	A
35	A	3054	G
35	A	3060	C
35	A	3072	U
35	A	3090	G
35	A	3100	U
35	A	3108	U
35	A	3109	U
35	A	3110	C
35	A	3111	A
35	A	3112	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	A	3113	A
35	A	3150	U
35	A	3157	C
35	A	3158	A
35	A	3162	C
35	A	3169	C
35	A	3172	C
35	A	3177	A
35	A	3183	U
35	A	3199	U
35	A	3200	U
35	A	3207	A
35	A	3209	A
35	A	3210	C
35	A	3212	C
35	A	3217	A
35	A	3218	A
35	A	3228	U
35	A	3229	U
35	A	3230	G
35	A	3231	U
36	B	8	U
36	B	16	C
36	B	21	A
36	B	45	G
36	B	48	U
36	B	54	C
36	B	55	U
36	B	56	U
36	B	64	A
36	B	69	U
36	B	76	A
89	Ay	3	G
89	Ay	4	G
89	Ay	9	A
89	Ay	23	A
89	Ay	25	C
89	Ay	44	A
89	Ay	45	G
89	Ay	46	A
89	Ay	48	U
89	Ay	49	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
89	Ay	59	U
89	Ay	72	A
89	Ay	75	C
89	Ay	76	A

All (3) RNA pucker outliers are listed below:

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

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

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	$\#\|Z\| > 2$
9	5F0	AI	184	9	8,8,9	0.58	0	7,9,11	1.16	1 (14%)
36	2MG	B	10	36	18,26,27	1.16	2 (11%)	16,38,41	0.87	1 (6%)
36	1MA	B	9	36	16,25,26	1.16	3 (18%)	18,37,40	0.88	1 (5%)
1	MA6	AA	1583	1	19,26,27	0.76	0	18,38,41	0.56	0
1	B8T	AA	1486	1,93	19,22,23	0.29	0	26,31,34	0.34	0
35	PSU	A	3067	35	18,21,22	0.78	0	22,30,33	2.56	5 (22%)
1	5MC	AA	1488	1	18,22,23	0.32	0	26,32,35	0.42	0
35	OMU	A	3039	94,35	19,22,23	0.27	0	26,31,34	0.44	0
1	MA6	AA	1584	1	19,26,27	0.77	0	18,38,41	0.55	0
35	OMG	A	2815	94,35,33	18,26,27	0.94	2 (11%)	19,38,41	0.63	0
1	5MU	AA	1076	1	19,22,23	0.62	0	28,32,35	1.21	3 (10%)
53	AYA	U	2	53	6,7,8	0.80	0	5,8,10	0.58	0
29	AYA	A2	2	29	6,7,8	0.81	0	5,8,10	0.45	0
79	AYA	k	2	79	6,7,8	0.81	0	5,8,10	0.46	0
43	SAC	K	2	43	7,8,9	0.22	0	8,9,11	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
36	PSU	B	39	36	18,21,22	0.76	0	22,30,33	2.54	4 (18%)
35	OMG	A	3040	35,32	18,26,27	0.91	2 (11%)	19,38,41	0.60	0
35	1MA	A	2617	35	16,25,26	1.15	3 (18%)	18,37,40	0.92	1 (5%)
17	AYA	AQ	2	17	6,7,8	0.80	0	5,8,10	0.81	0
70	THC	b	2	70	8,9,10	0.28	0	9,11,13	0.48	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
9	5F0	AI	184	9	-	0/9/9/10	-
36	2MG	B	10	36	-	0/5/27/28	0/3/3/3
36	1MA	B	9	36	-	0/3/25/26	0/3/3/3
1	MA6	AA	1583	1	-	0/7/29/30	0/3/3/3
1	B8T	AA	1486	1,93	-	0/7/27/28	0/2/2/2
35	PSU	A	3067	35	-	0/7/25/26	0/2/2/2
1	5MC	AA	1488	1	-	0/7/25/26	0/2/2/2
35	OMU	A	3039	94,35	-	0/9/27/28	0/2/2/2
1	MA6	AA	1584	1	-	2/7/29/30	0/3/3/3
35	OMG	A	2815	94,35,33	-	0/5/27/28	0/3/3/3
1	5MU	AA	1076	1	-	0/7/25/26	0/2/2/2
53	AYA	U	2	53	-	1/4/6/8	-
29	AYA	A2	2	29	-	0/4/6/8	-
79	AYA	k	2	79	-	0/4/6/8	-
43	SAC	K	2	43	-	0/7/8/10	-
36	PSU	B	39	36	-	0/7/25/26	0/2/2/2
35	OMG	A	3040	35,32	-	0/5/27/28	0/3/3/3
35	1MA	A	2617	35	-	0/3/25/26	0/3/3/3
17	AYA	AQ	2	17	-	1/4/6/8	-
70	THC	b	2	70	-	0/8/10/12	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	10	2MG	C8-N7	-3.11	1.29	1.35
35	A	2617	1MA	C6-N6	3.11	1.35	1.27
36	B	9	1MA	C6-N6	3.08	1.35	1.27
36	B	10	2MG	C5-C6	-2.38	1.42	1.47
35	A	2815	OMG	C5-C6	-2.32	1.42	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	3040	OMG	C5-C6	-2.21	1.42	1.47
36	B	9	1MA	C5-C4	-2.13	1.37	1.43
35	A	2617	1MA	C5-C4	-2.10	1.37	1.43
35	A	2815	OMG	C8-N7	-2.04	1.31	1.35
36	B	9	1MA	C8-N7	-2.02	1.31	1.35
35	A	2617	1MA	C8-N7	-2.01	1.31	1.35
35	A	3040	OMG	C8-N7	-2.01	1.31	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	B	39	PSU	N1-C2-N3	8.06	124.26	115.13
35	A	3067	PSU	N1-C2-N3	8.06	124.26	115.13
35	A	3067	PSU	C4-N3-C2	-6.55	116.90	126.34
36	B	39	PSU	C4-N3-C2	-6.50	116.97	126.34
1	AA	1076	5MU	C4-N3-C2	-4.77	121.18	127.35
36	B	39	PSU	O2-C2-N1	-3.68	118.74	122.79
35	A	3067	PSU	O2-C2-N1	-3.64	118.78	122.79
9	AI	184	5F0	O-C-CB	-2.69	117.58	125.43
1	AA	1076	5MU	C5-C4-N3	2.63	117.56	115.31
35	A	3067	PSU	O2-C2-N3	-2.58	116.96	121.82
36	B	39	PSU	O2-C2-N3	-2.56	117.00	121.82
1	AA	1076	5MU	N3-C2-N1	2.23	117.84	114.89
35	A	2617	1MA	N1-C6-N6	2.21	125.39	119.77
35	A	3067	PSU	O4'-C1'-C2'	2.15	108.17	105.14
36	B	10	2MG	O6-C6-C5	2.12	128.52	124.37
36	B	9	1MA	N1-C6-N6	2.10	125.11	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
53	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
35	A	2815	OMG	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 276 ligands modelled in this entry, 263 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 $\lvert Z\rvert > 2$ 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	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
92	SPD	A	3301	-	9,9,9	0.42	0	8,8,8	1.07	0
98	GDP	AX	503	-	24,30,30	0.88	1 (4%)	30,47,47	0.61	0
91	SPM	AA	1702	-	13,13,13	0.28	0	12,12,12	0.98	0
90	NAD	AA	1701	93	42,48,48	0.57	0	50,73,73	0.59	1 (2%)
96	FES	r	201	85,41	0,4,4	-	-	-		
100	VAL	B	101	36	4,6,7	0.51	0	6,7,9	0.95	0
92	SPD	AA	1703	-	9,9,9	0.28	0	8,8,8	1.31	2 (25%)
96	FES	AP	201	5,16	0,4,4	-	-	-		
97	ATP	AX	501	93	26,33,33	0.75	0	31,52,52	0.64	0
99	PUT	A	3304	-	5,5,5	0.25	0	4,4,4	0.53	0
92	SPD	A	3303	-	9,9,9	0.38	0	8,8,8	1.14	0
92	SPD	A	3302	-	9,9,9	0.33	0	8,8,8	1.22	0
96	FES	AT	201	13,20	0,4,4	-	-	-		

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
92	SPD	A	3301	-	-	2/7/7/7	-
98	GDP	AX	503	-	-	0/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	SPM	AA	1702	-	-	1/11/11/11	-
90	NAD	AA	1701	93	-	0/26/62/62	0/5/5/5
96	FES	r	201	85,41	-	-	0/1/1/1
100	VAL	B	101	36	-	1/5/6/8	-
92	SPD	AA	1703	-	-	0/7/7/7	-
96	FES	AP	201	5,16	-	-	0/1/1/1
99	PUT	A	3304	-	-	0/3/3/3	-
92	SPD	A	3303	-	-	2/7/7/7	-
96	FES	AT	201	13,20	-	-	0/1/1/1
92	SPD	A	3302	-	-	0/7/7/7	-
97	ATP	AX	501	93	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
98	AX	503	GDP	C5-C6	-2.22	1.42	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
90	AA	1701	NAD	C5A-C6A-N6A	2.32	123.88	120.35
92	AA	1703	SPD	C4-C5-N6	-2.24	106.09	112.14
92	AA	1703	SPD	C8-C7-N6	-2.13	106.38	112.14

There are no chirality outliers.

All (6) 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
100	B	101	VAL	O-C-CA-CB

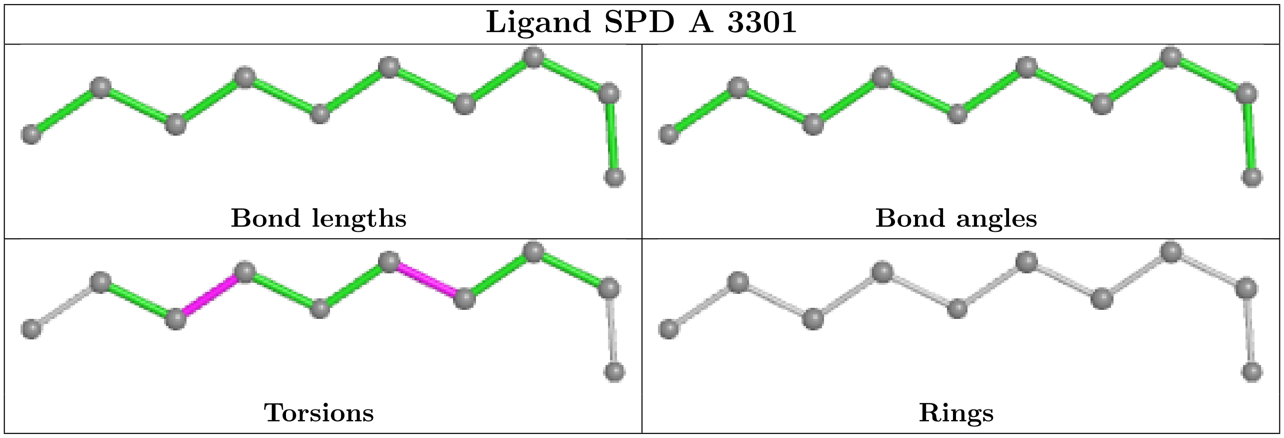
There are no ring outliers.

1 monomer is involved in 1 short contact:

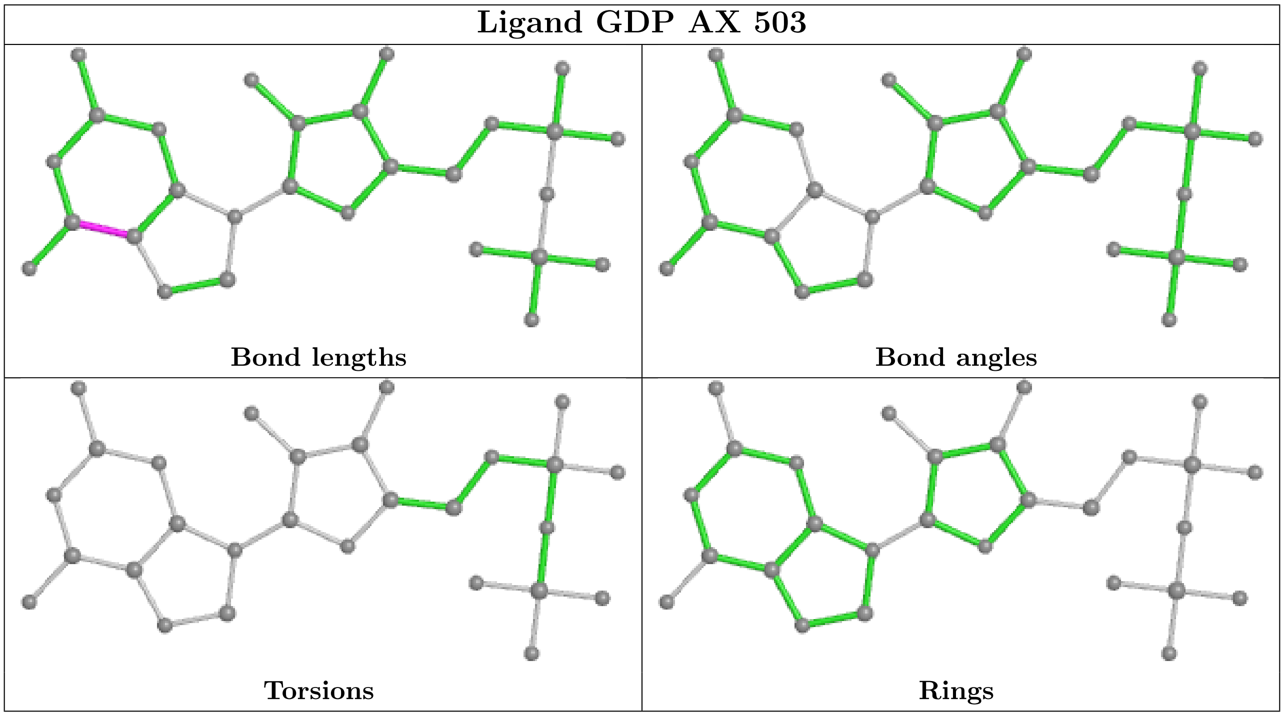
Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	AX	501	ATP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

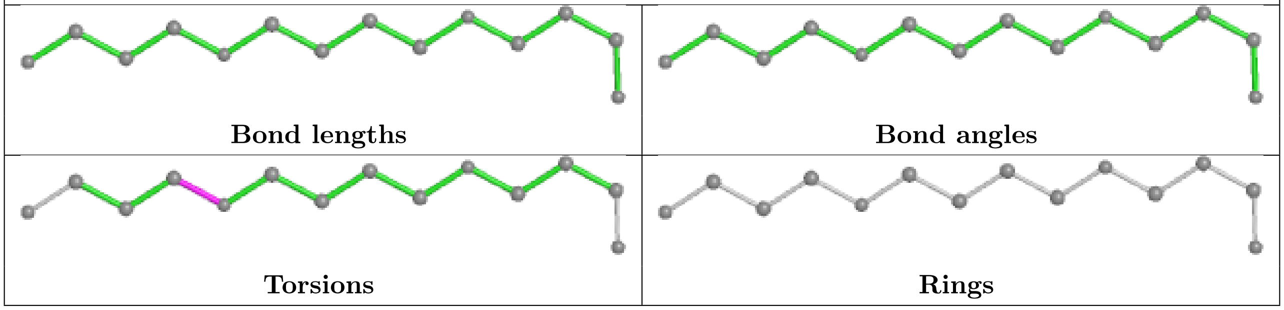
Ligand SPD A 3301



Ligand GDP AX 503



Ligand SPM AA 1702



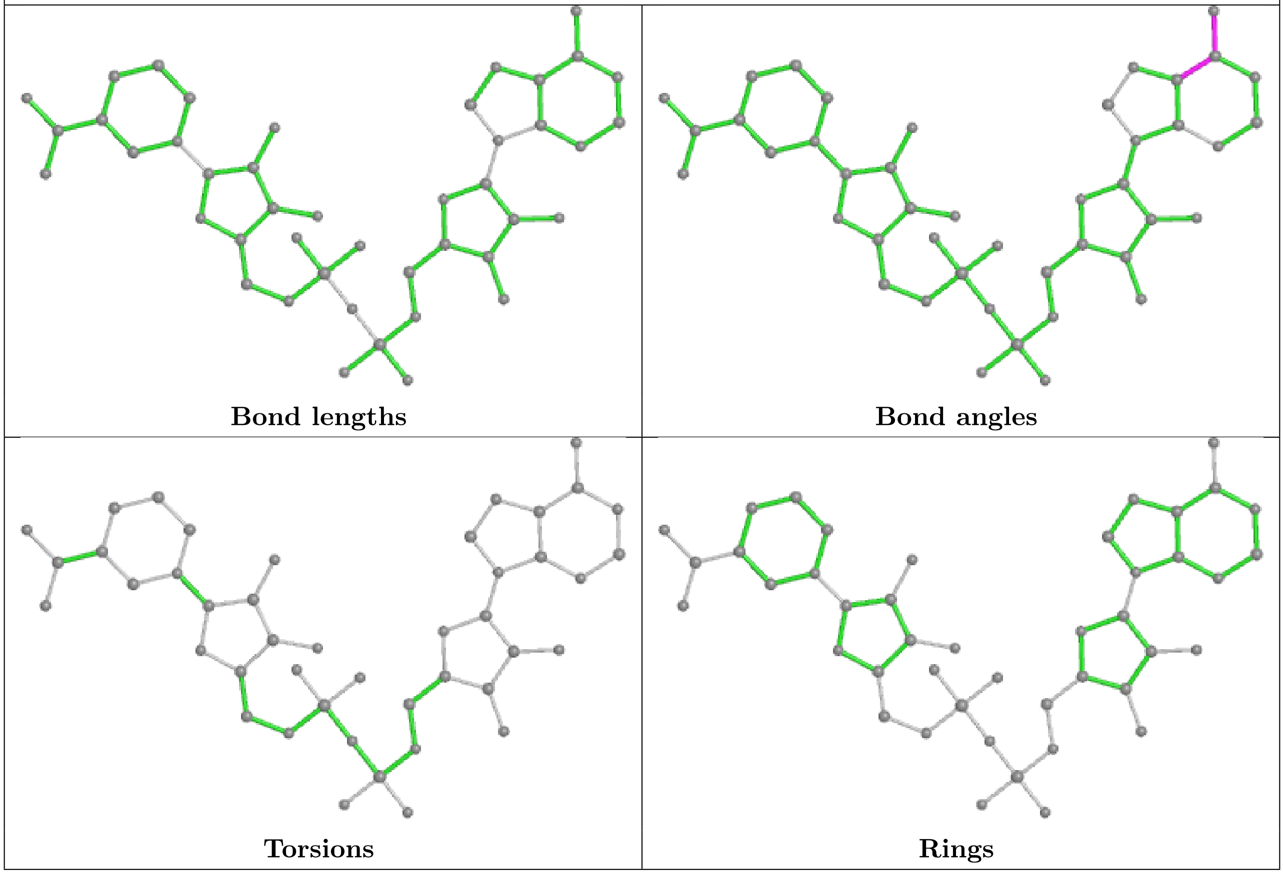
Bond lengths

Bond angles

Torsions

Rings

Ligand NAD AA 1701



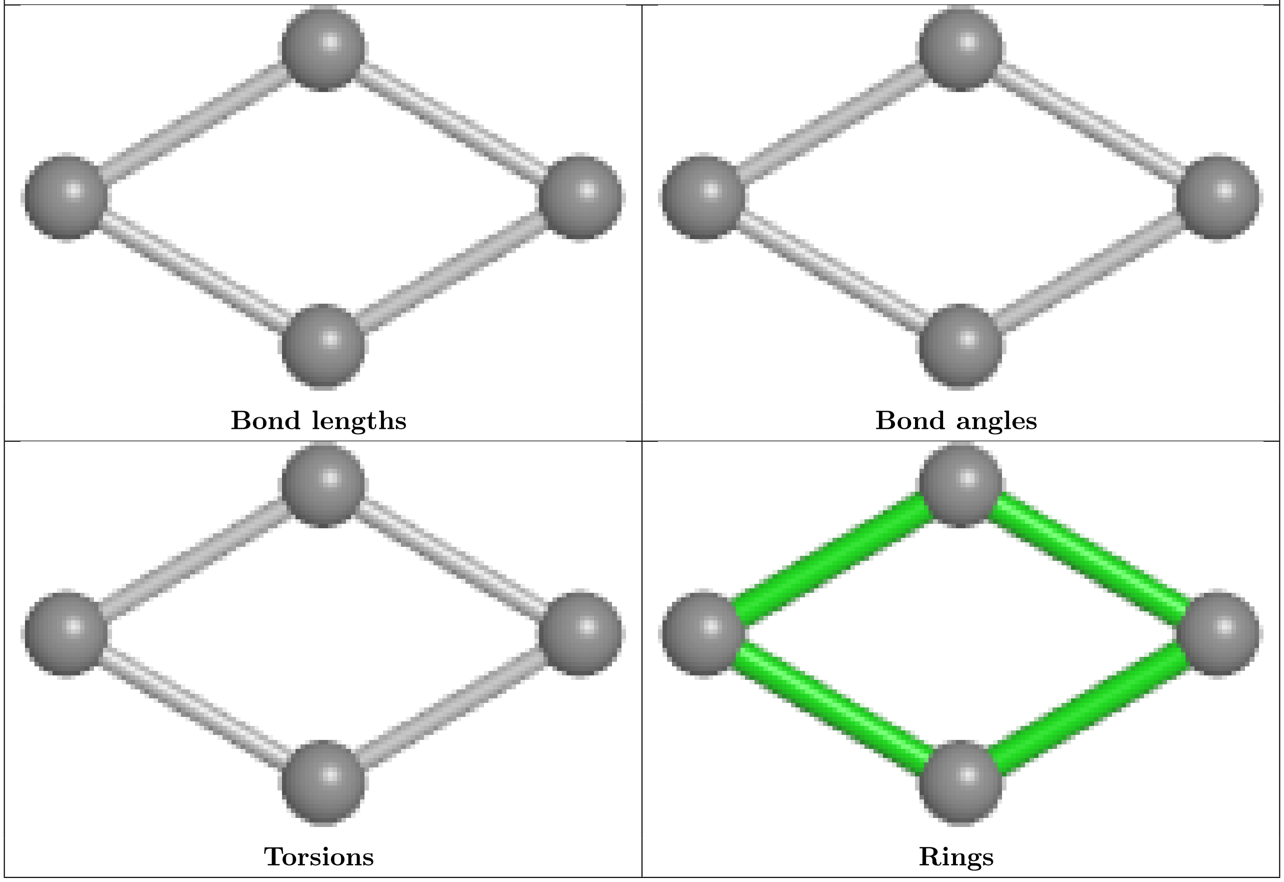
Bond lengths

Bond angles

Torsions

Rings

Ligand FES r 201



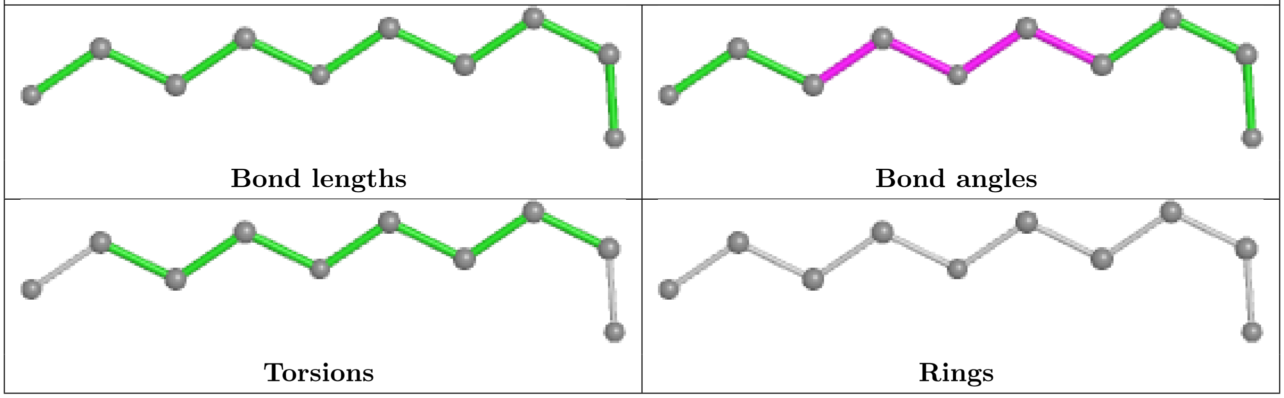
Bond lengths

Bond angles

Torsions

Rings

Ligand SPD AA 1703



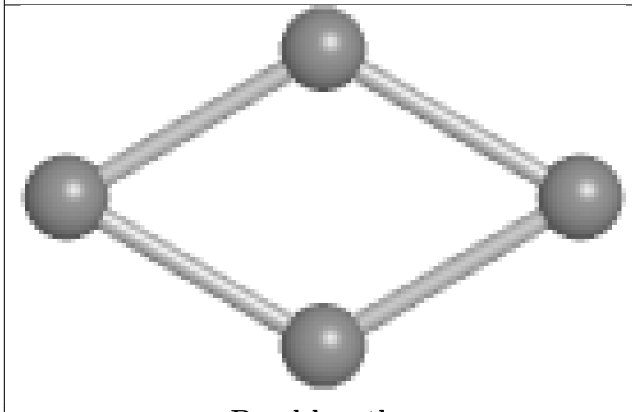
Bond lengths

Bond angles

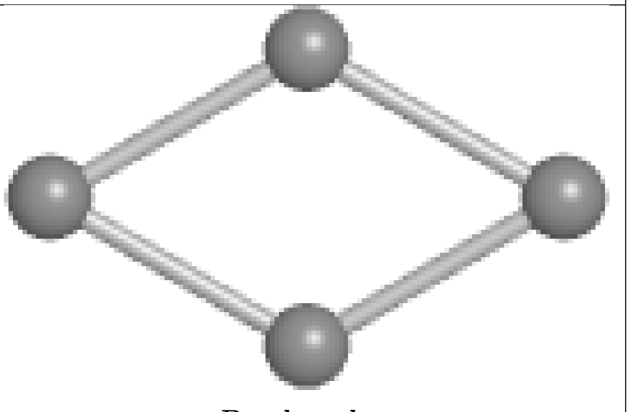
Torsions

Rings

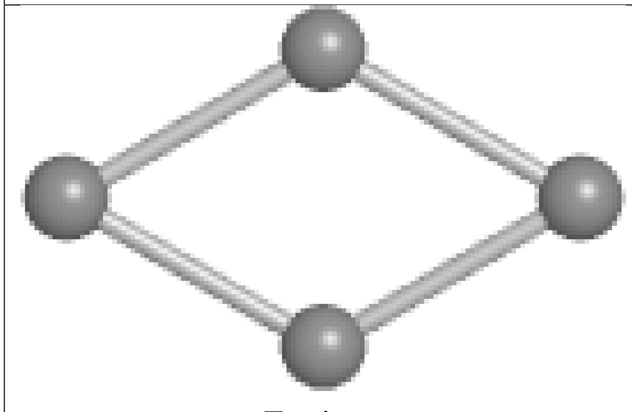
Ligand FES AP 201



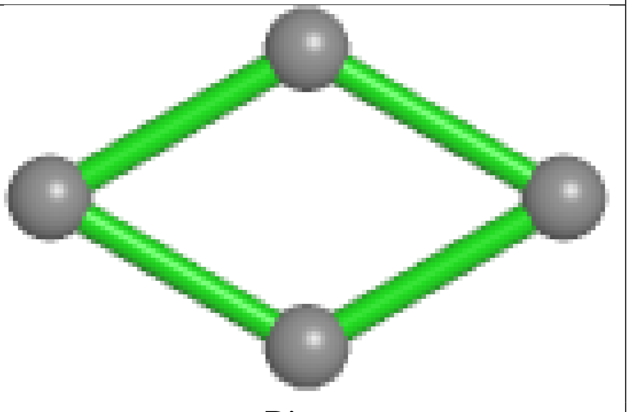
Bond lengths



Bond angles

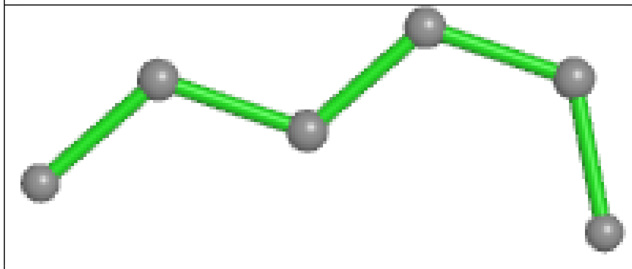


Torsions

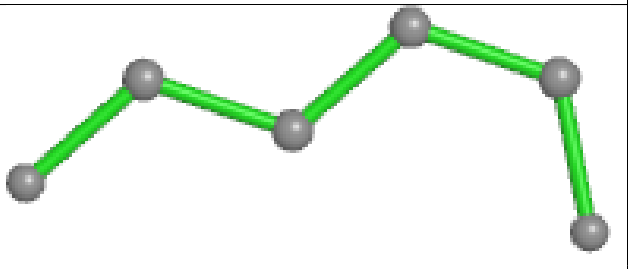


Rings

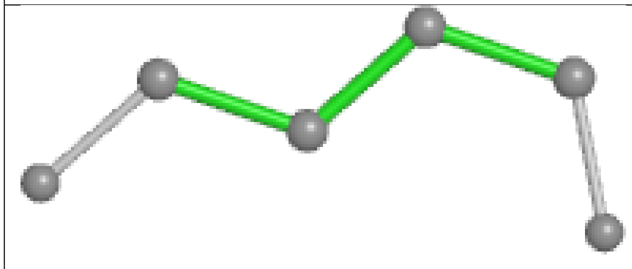
Ligand PUT A 3304



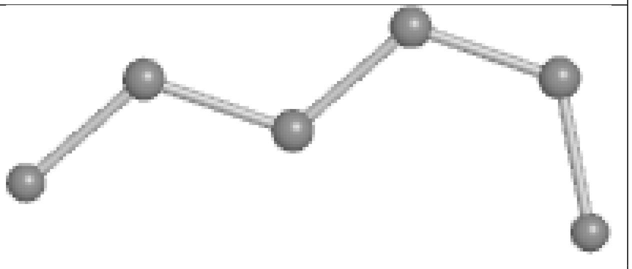
Bond lengths



Bond angles

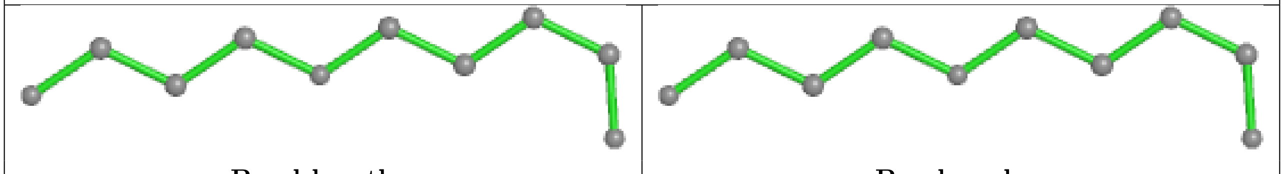


Torsions

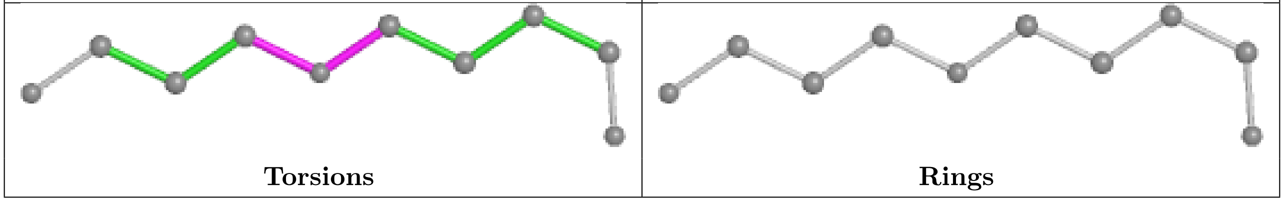


Rings

Ligand SPD A 3303

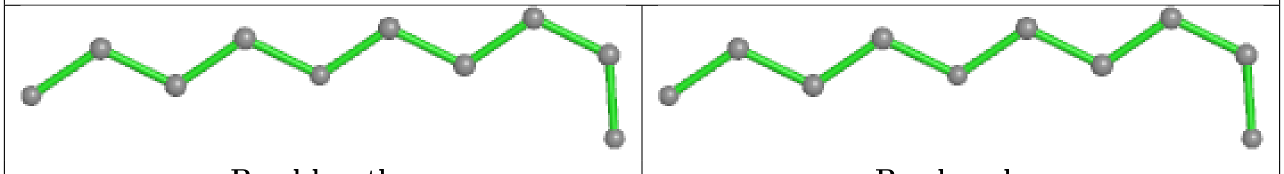


Bond lengths **Bond angles**

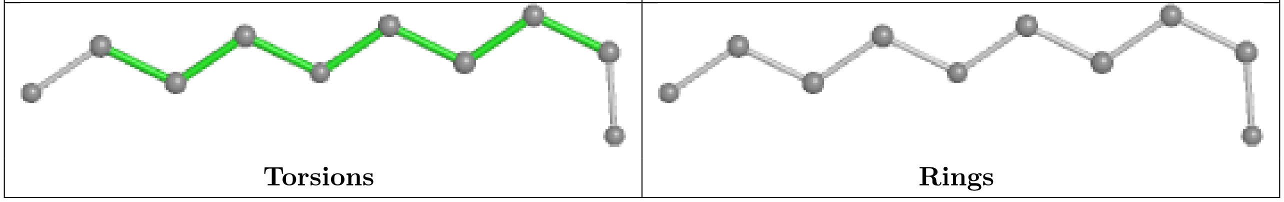


Torsions **Rings**

Ligand SPD A 3302

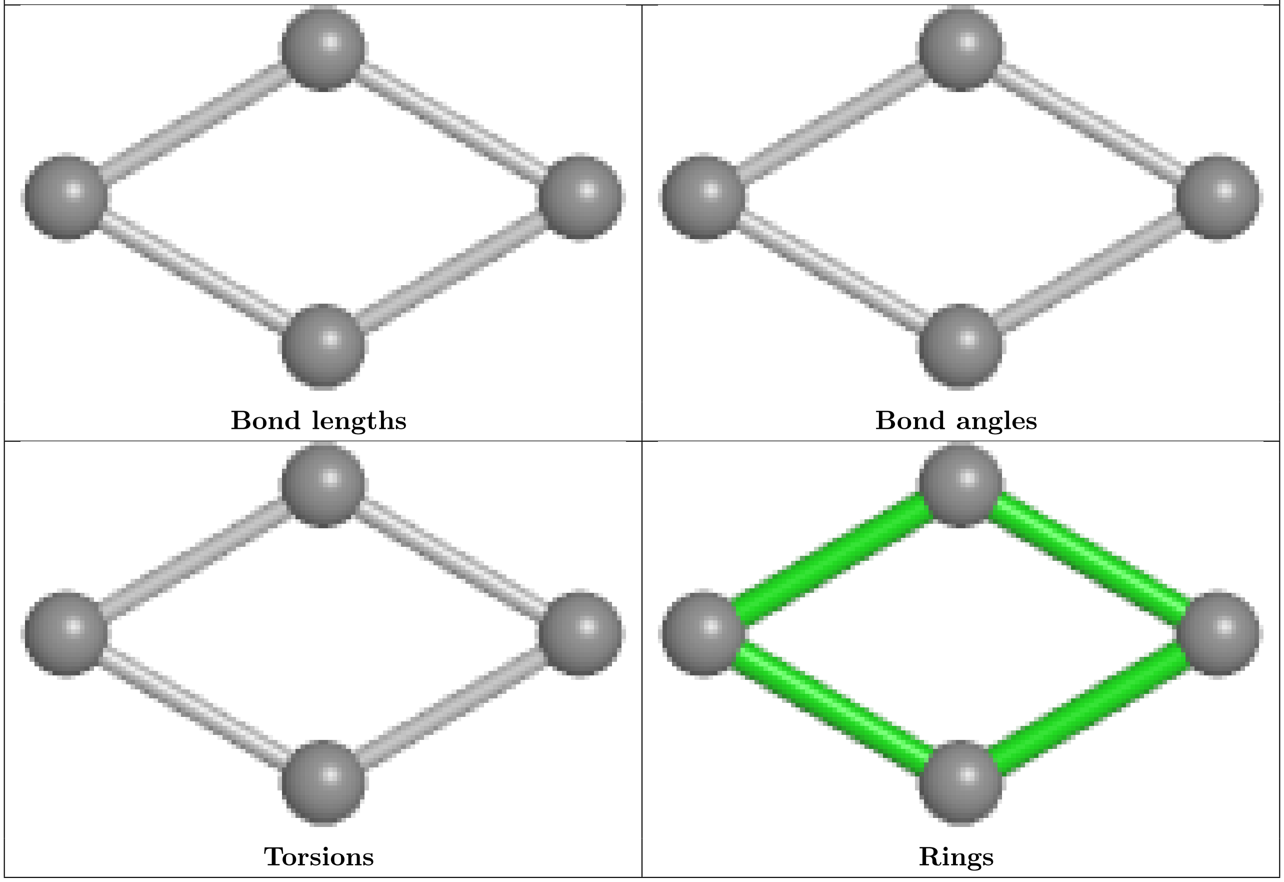


Bond lengths **Bond angles**



Torsions **Rings**

Ligand FES AT 201



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
89	Ay	3
32	Aw	1
35	A	1
33	Ax	1
34	Az	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

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ay	27:G	O3'	43:C	P	17.81
1	Ay	54:U	O3'	58:A	P	12.21
1	A	2357:C	O3'	2361:G	P	10.83
1	Ax	15:A	O3'	21:A	P	9.85
1	Ay	15:A	O3'	21:A	P	9.25
1	Az	3:A	O3'	4:A	P	3.05

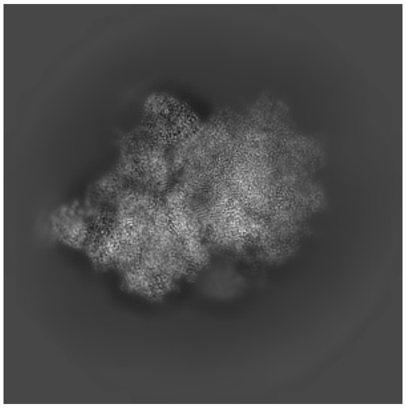
6 Map visualisation

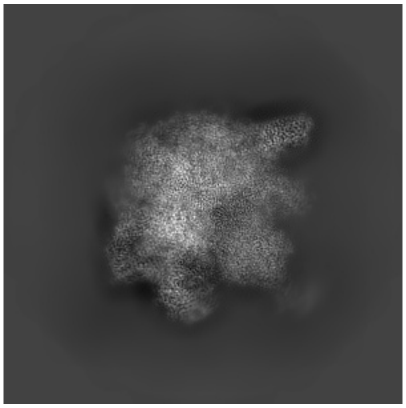
This section contains visualisations of the EMDB entry EMD-13980. These allow visual inspection of the internal detail of the map and identification of artifacts.

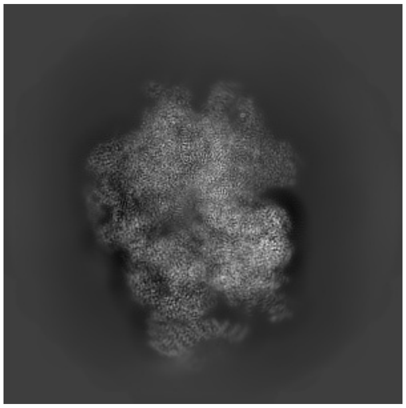
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

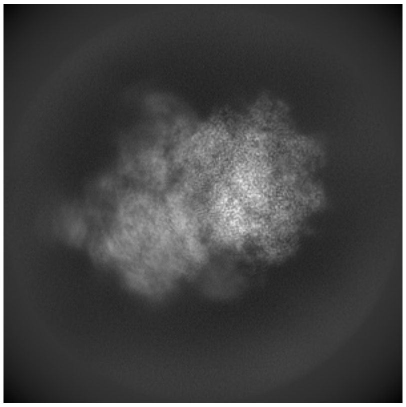
6.1.1 Primary map

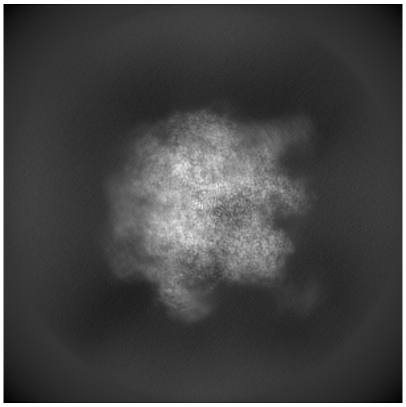

X

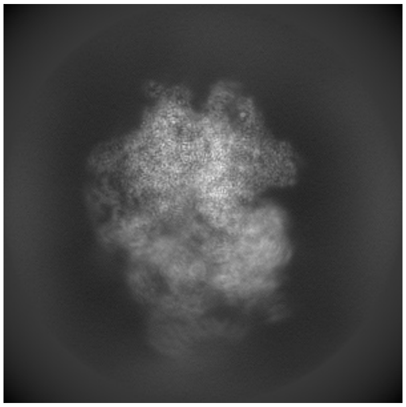

Y


Z

6.1.2 Raw map


X

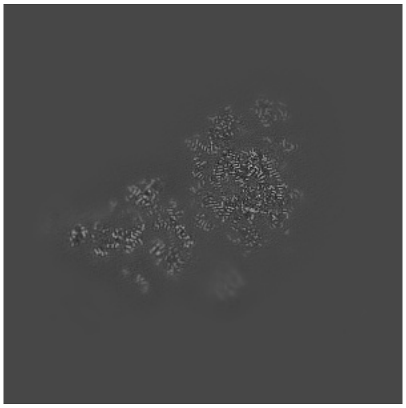

Y

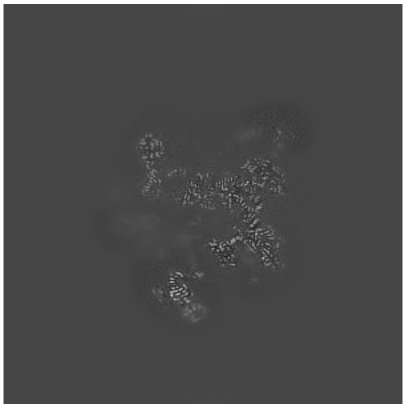

Z

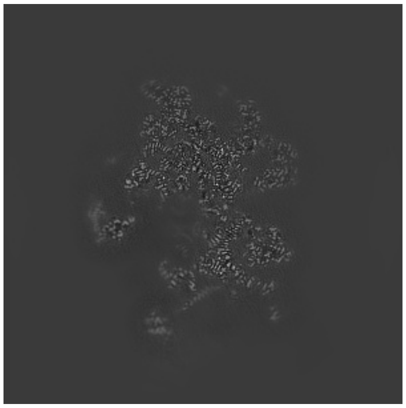
The images above show the map projected in three orthogonal directions.

6.2 Central slices

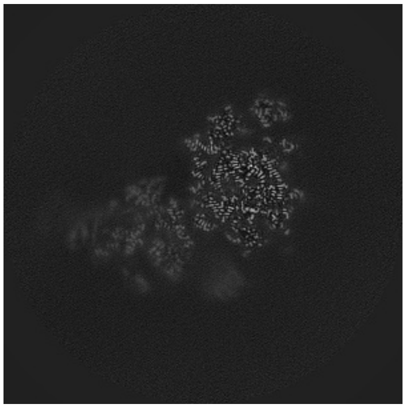
6.2.1 Primary map

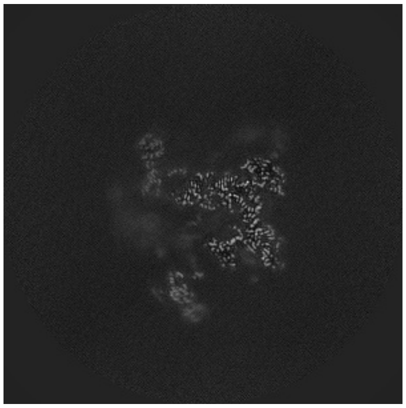

X Index: 270

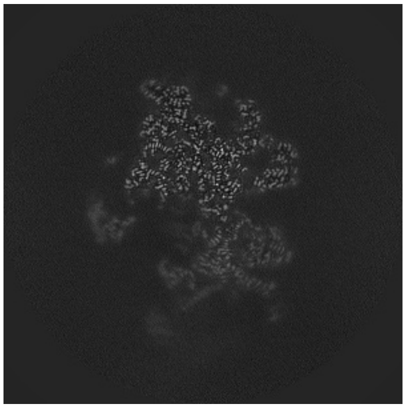

Y Index: 270


Z Index: 270

6.2.2 Raw map


X Index: 270


Y Index: 270


Z Index: 270

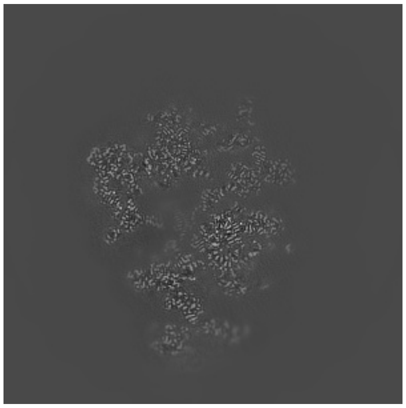
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

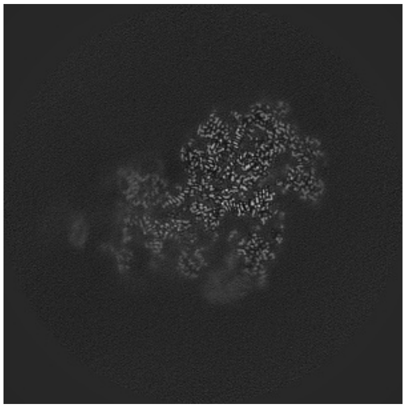
6.3.1 Primary map

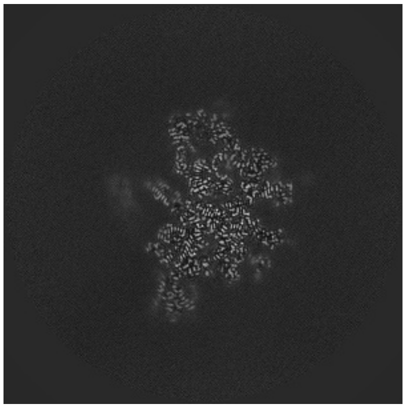

X Index: 291

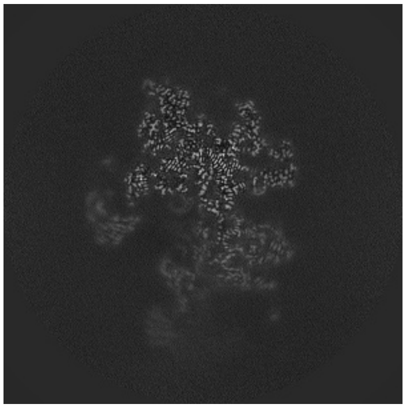

Y Index: 318


Z Index: 240

6.3.2 Raw map


X Index: 289

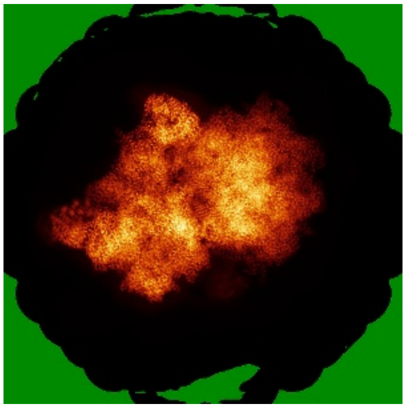

Y Index: 318


Z Index: 265

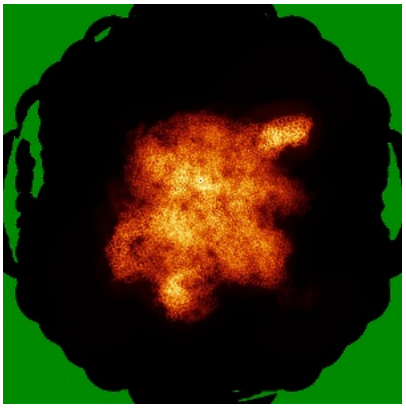
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

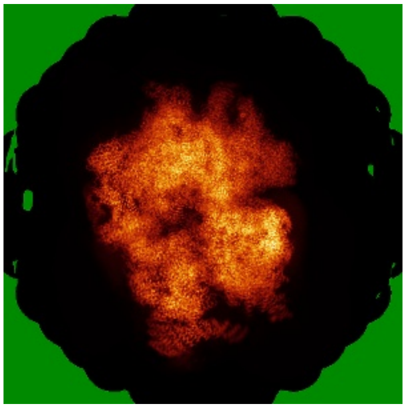
6.4.1 Primary map



X

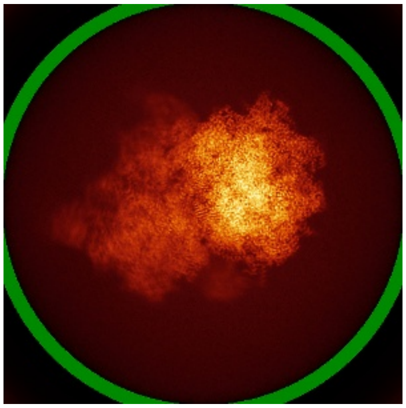


Y

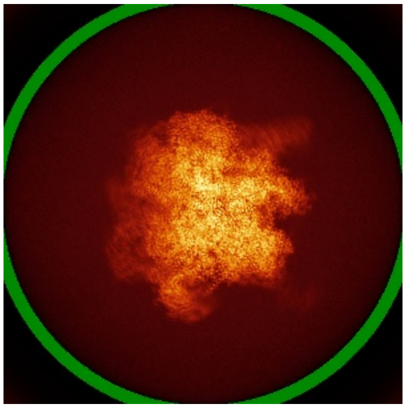


Z

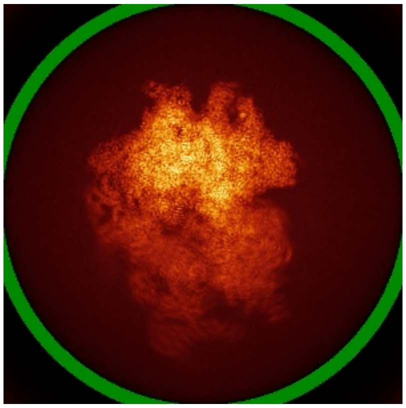
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

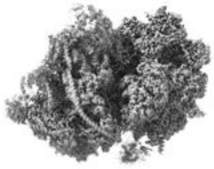
X

Y

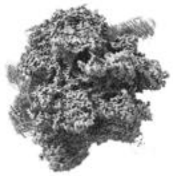
Z

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.

6.5.2 Raw map



X



Y

Z

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

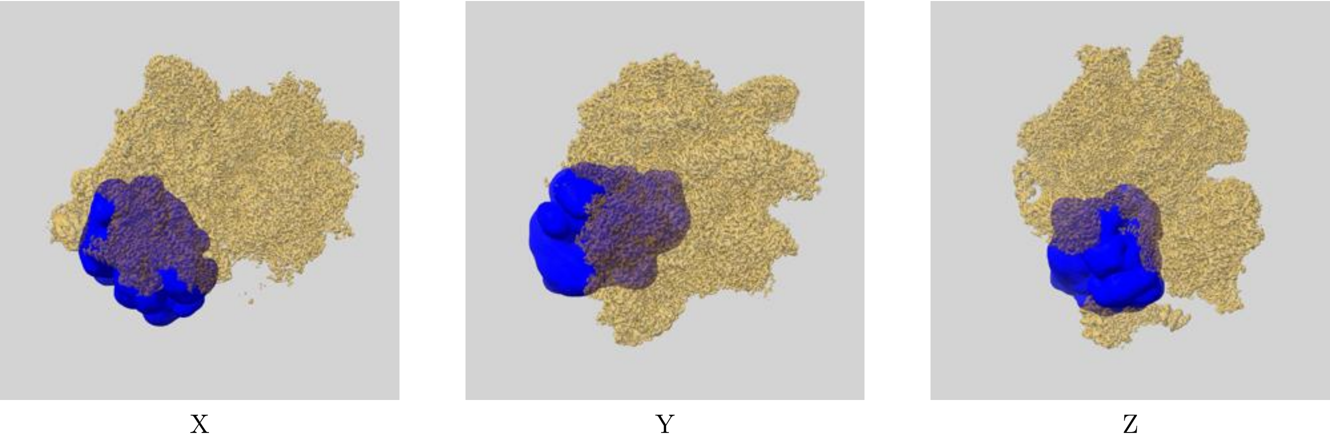
6.6 Mask visualisation ⓘ

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

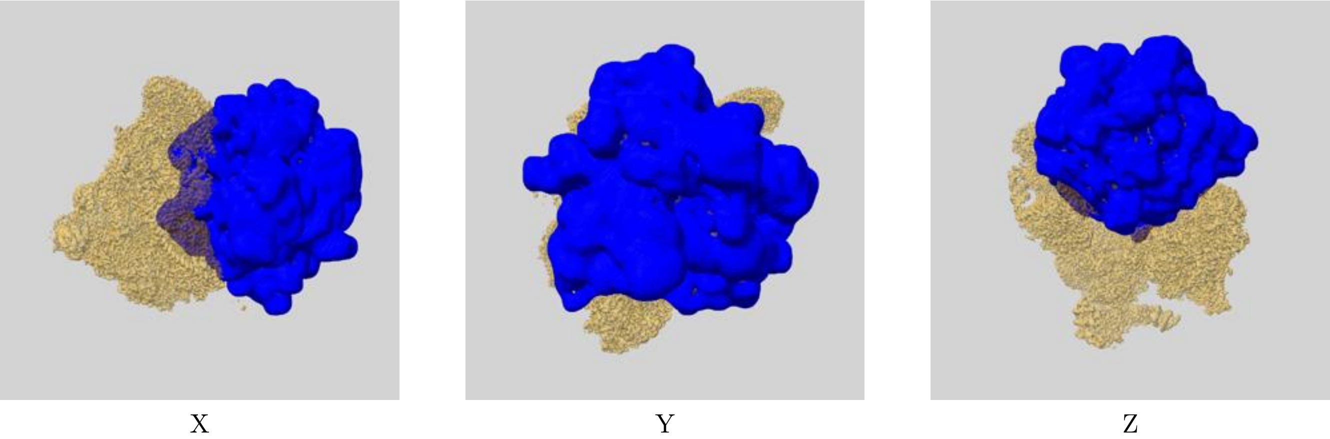
A mask typically either:

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

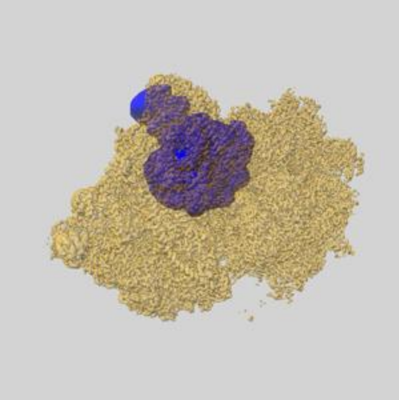
6.6.1 emd_13980_msk_1.map ⓘ



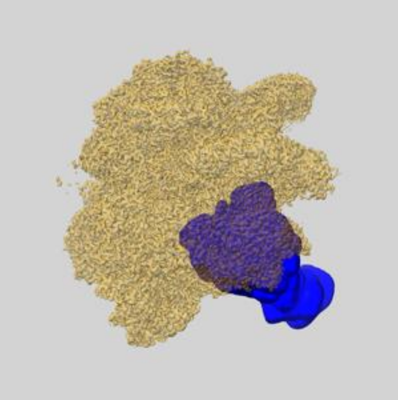
6.6.2 emd_13980_msk_2.map ⓘ



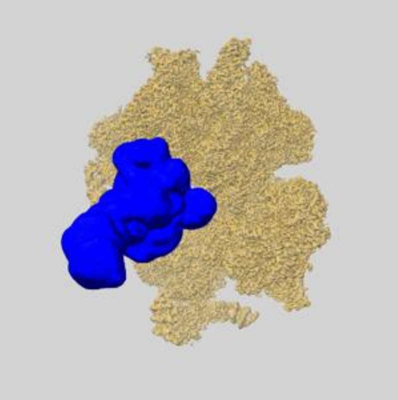
6.6.3 emd_13980_msk_3.map ⓘ



X

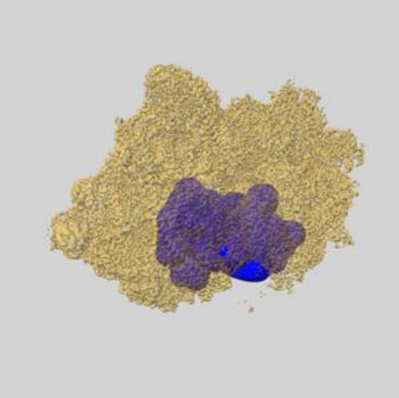


Y

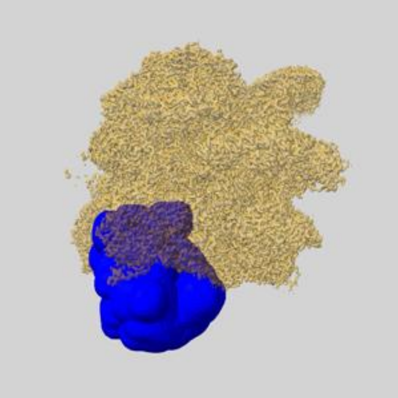


Z

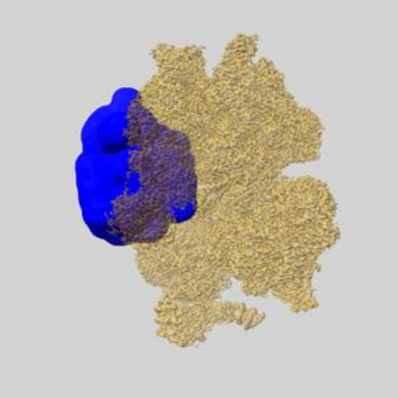
6.6.4 emd_13980_msk_4.map ⓘ



X

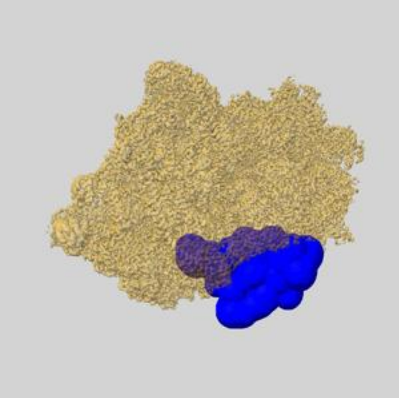


Y

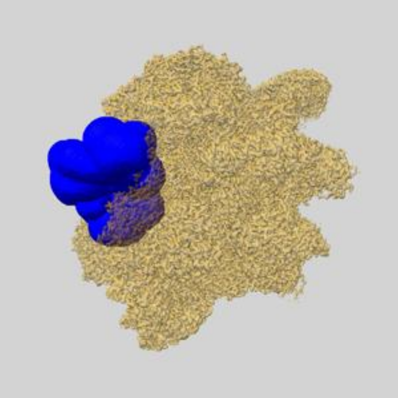


Z

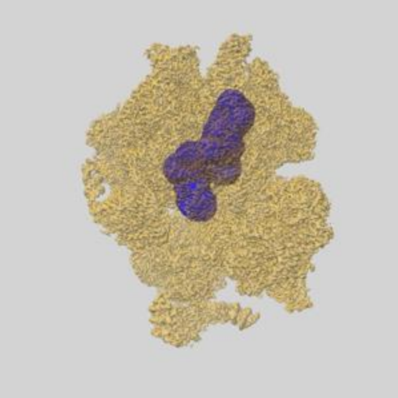
6.6.5 emd_13980_msk_5.map ⓘ



X

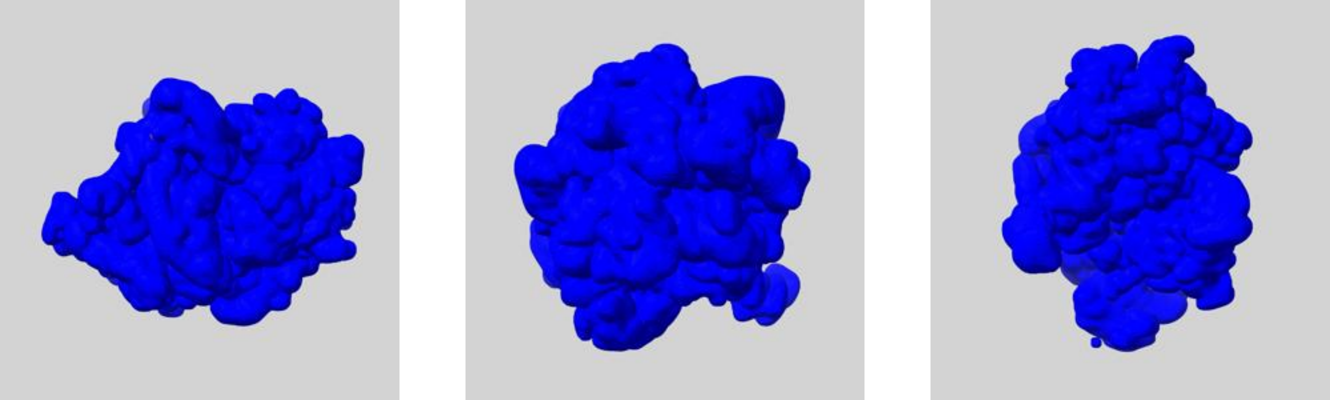


Y



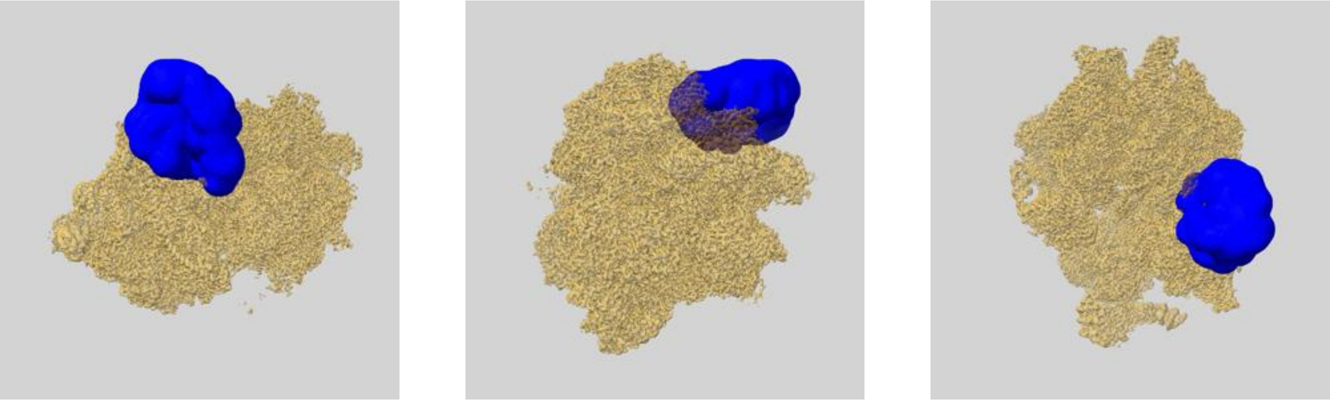
Z

6.6.6 emd_13980_msk_6.map



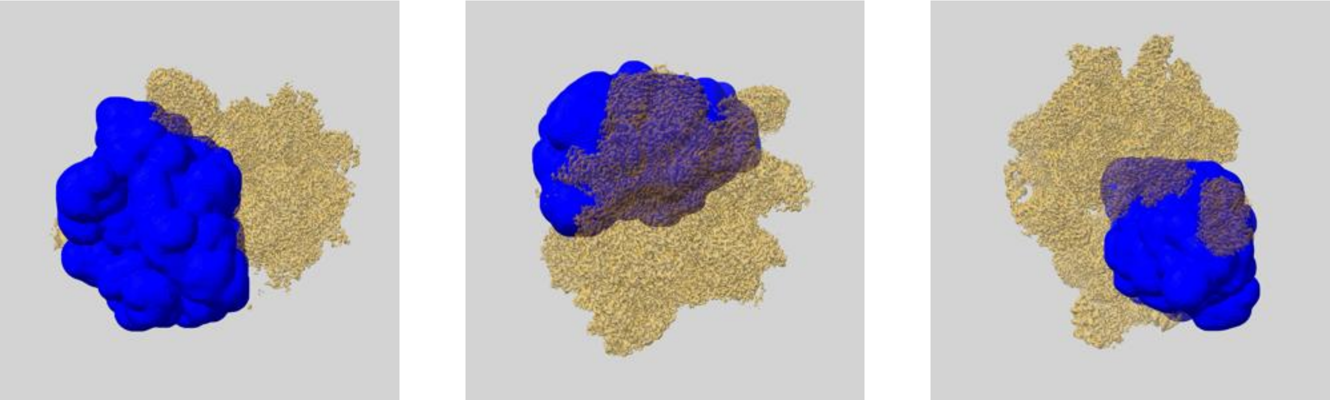
X Y Z

6.6.7 emd_13980_msk_7.map



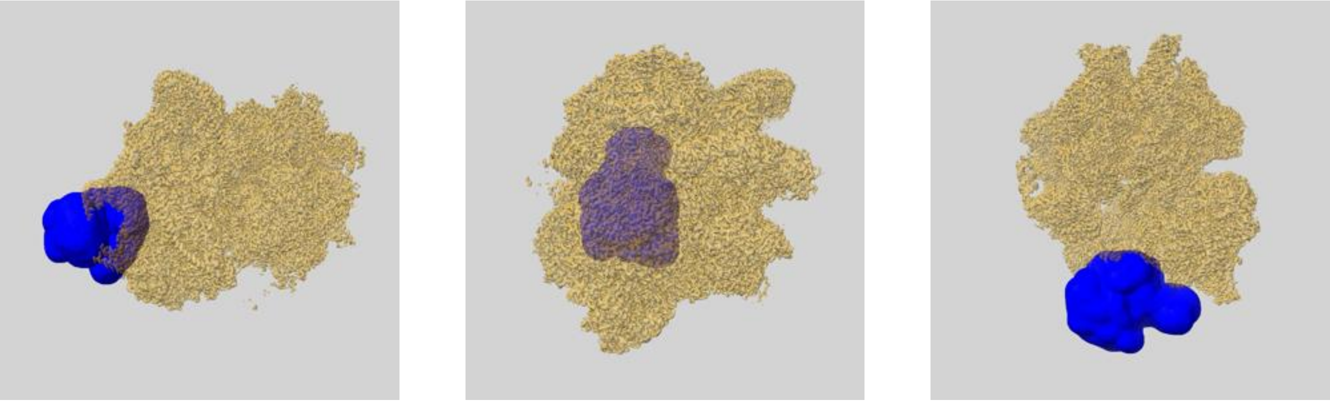
X Y Z

6.6.8 emd_13980_msk_8.map



X Y Z

6.6.9 emd_13980_msk_9.map ⓘ

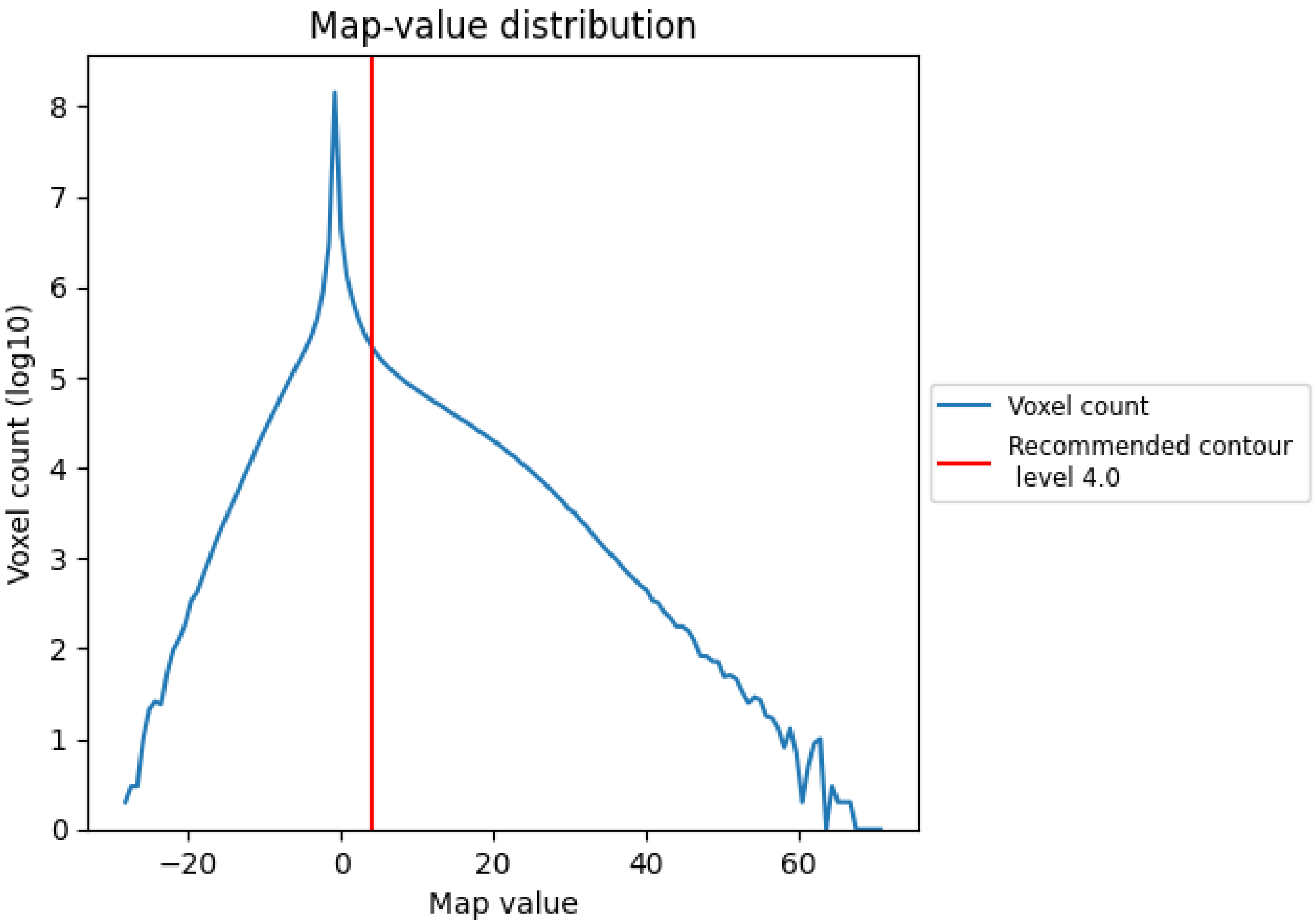


X Y Z

7 Map analysis ⓘ

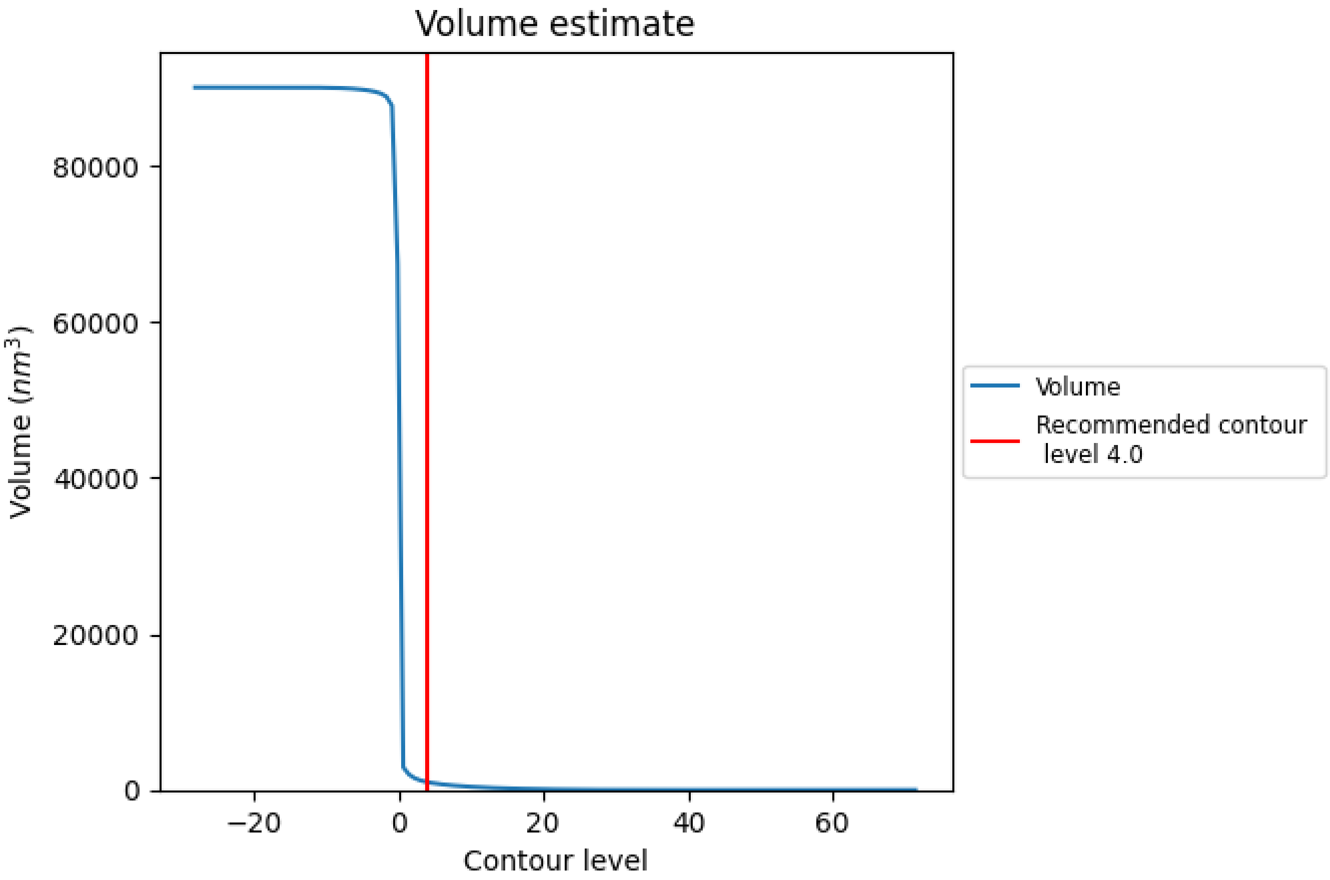
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

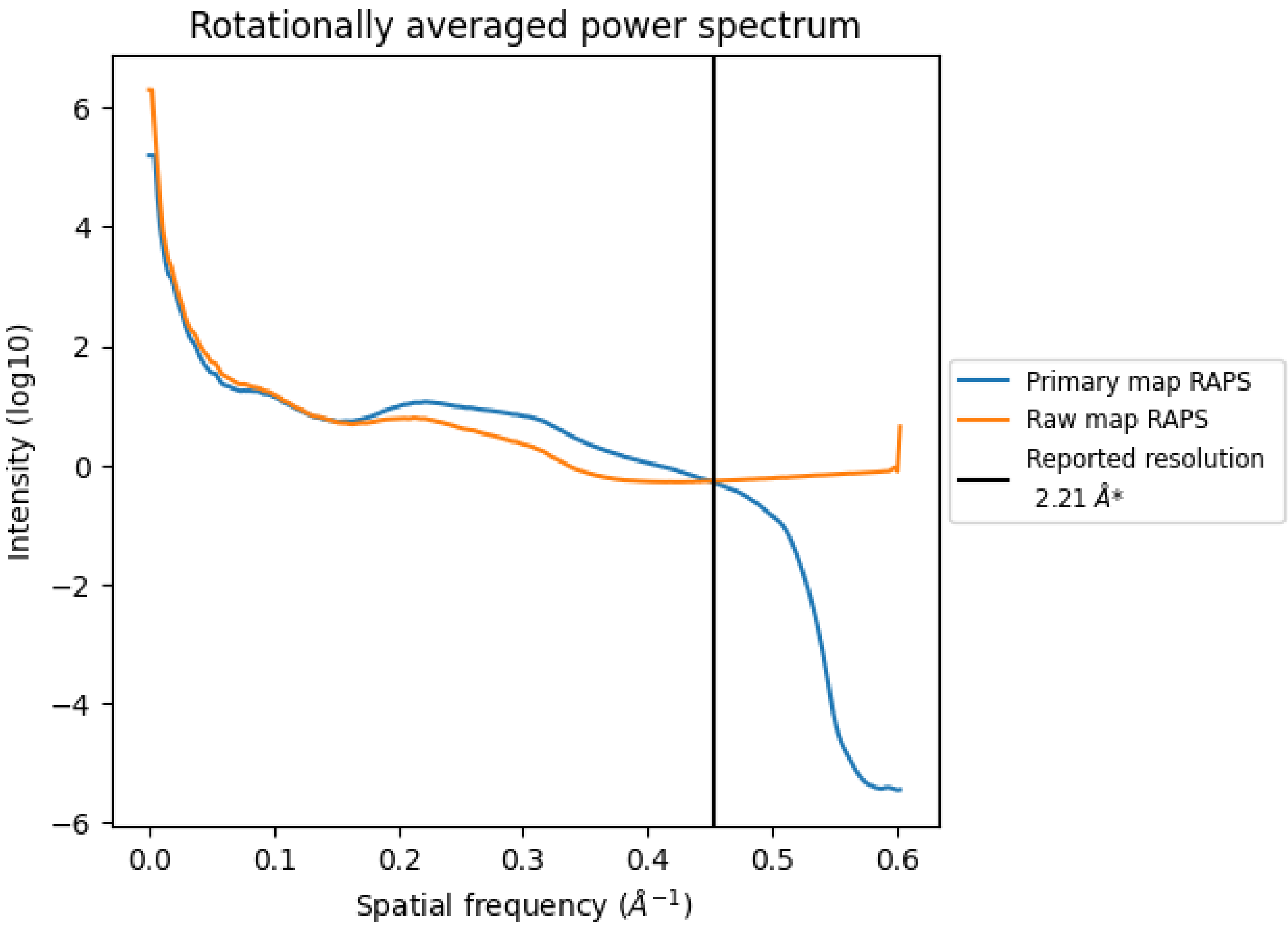
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 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 ⓘ

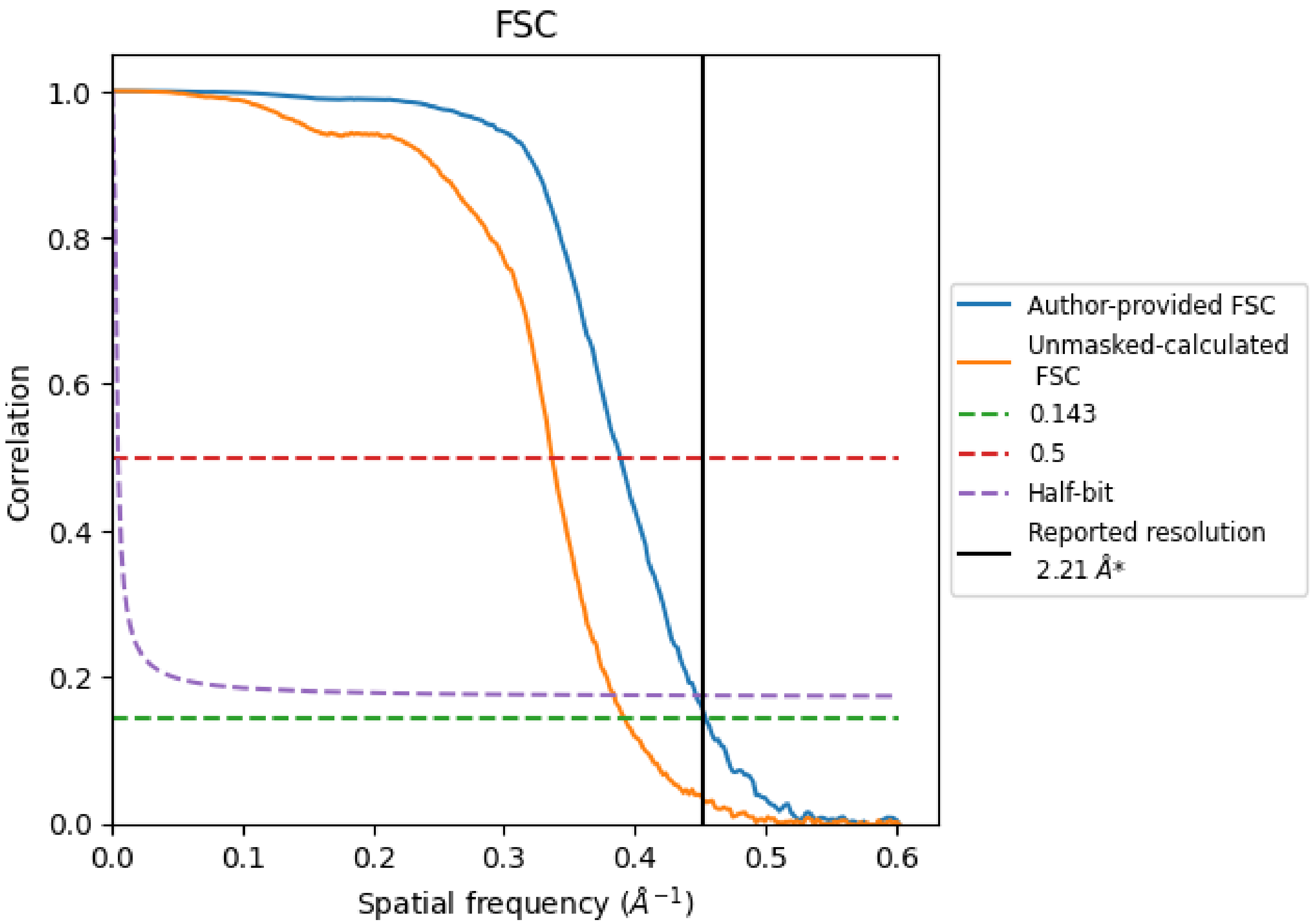


*Reported resolution corresponds to spatial frequency of 0.452 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.452 $Å^{-1}$

8.2 Resolution estimates ⓘ

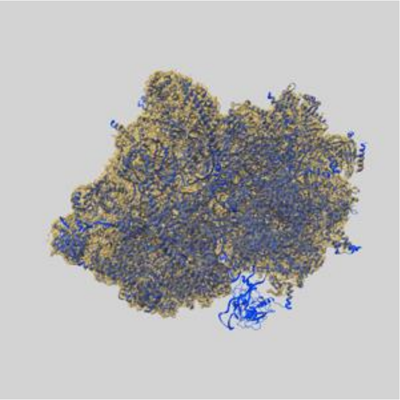
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.21	-	-
Author-provided FSC curve	2.20	2.57	2.24
Unmasked-calculated*	2.55	2.97	2.60

*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 %

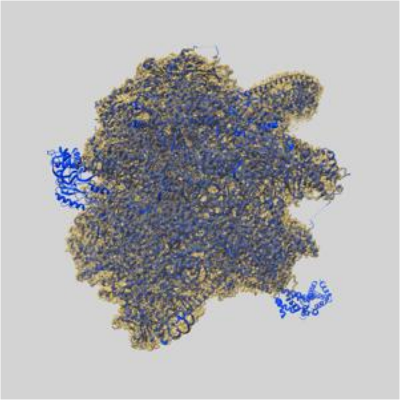
9 Map-model fit ⓘ

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 31.

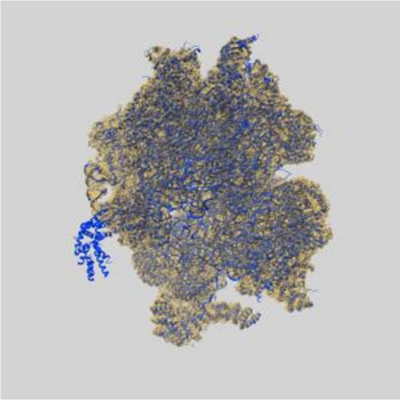
9.1 Map-model overlay ⓘ



X



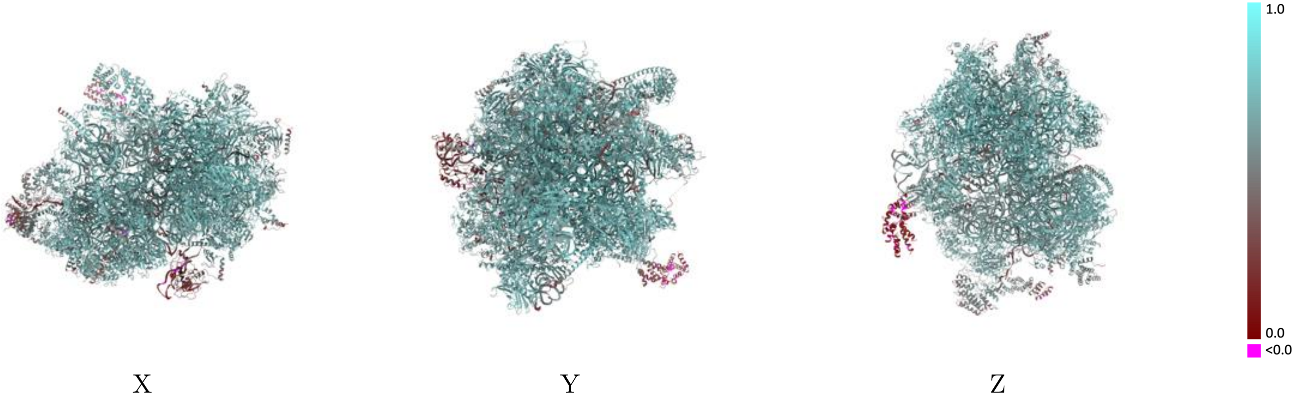
Y



Z

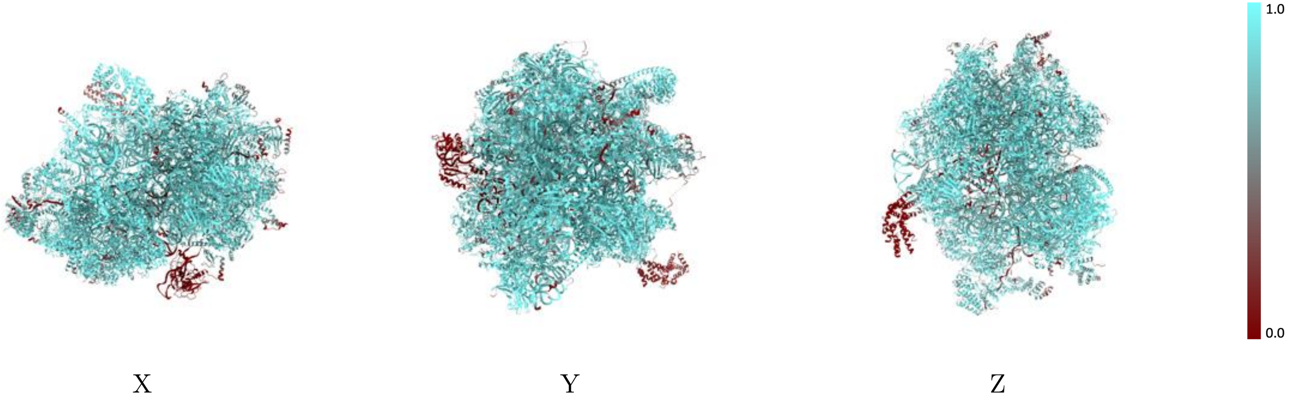
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



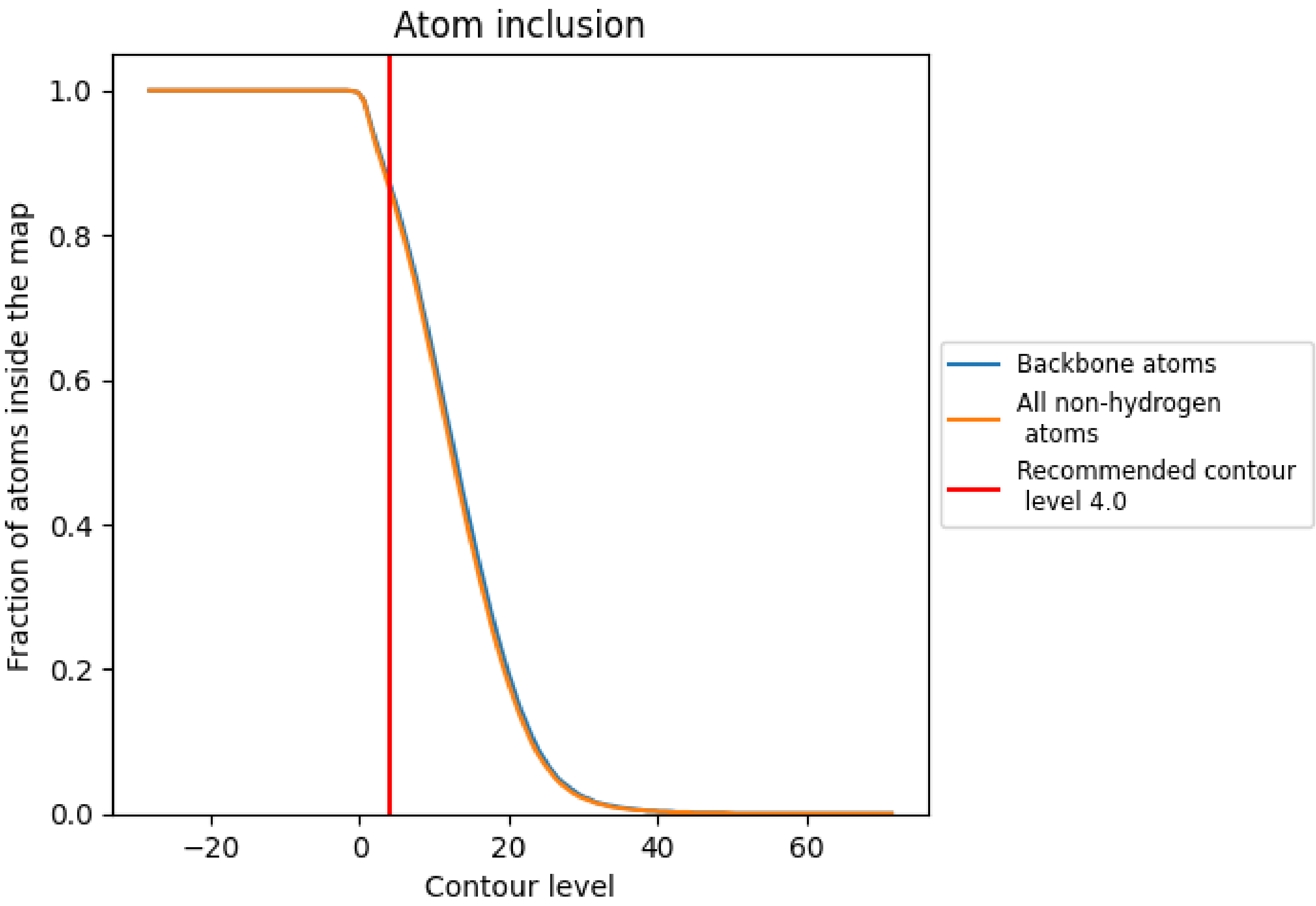
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.0).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8660	0.6580
0	0.8910	0.7120
1	0.8340	0.6530
2	0.9970	0.7990
3	0.9800	0.7760
4	0.9570	0.7280
5	0.8920	0.6790
6	0.9470	0.6840
7	0.7770	0.6380
8	0.7300	0.5620
9	0.8140	0.6560
A	0.9310	0.7150
A0	0.9350	0.6560
A1	0.9030	0.6410
A2	0.8240	0.6160
A3	0.9400	0.6960
A4	0.8330	0.5170
AA	0.9690	0.6790
AB	0.9370	0.6800
AC	0.9790	0.7080
AD	0.8780	0.6410
AE	0.9280	0.6750
AF	0.9240	0.6620
AG	0.8650	0.6250
AH	0.9420	0.6690
AI	0.9470	0.6810
AJ	0.9250	0.6580
AK	0.9770	0.7220
AL	0.8710	0.6390
AM	0.9230	0.6580
AN	0.9400	0.6820
AO	0.9200	0.6490
AP	0.9330	0.6880
AQ	0.9700	0.7130
AR	0.8420	0.5910

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AS	0.8420	0.5980
AT	0.9180	0.6630
AU	0.8410	0.6050
AV	0.9450	0.6500
AW	0.9120	0.6420
AX	0.9440	0.6610
AY	0.8320	0.5840
AZ	0.9020	0.6580
Aw	0.4040	0.5580
Ax	0.3350	0.4630
Ay	0.0320	0.3360
Az	0.3840	0.3970
B	0.9290	0.6060
D	0.9450	0.7310
E	0.9310	0.7300
F	0.9500	0.7440
H	0.3380	0.4460
I	0.7310	0.5550
J	0.8260	0.5930
K	0.9680	0.7450
L	0.9410	0.7310
M	0.9400	0.7310
N	0.9210	0.6940
O	0.9380	0.7350
P	0.9700	0.7200
Q	0.8570	0.6850
R	0.9550	0.7670
S	0.9370	0.7330
T	0.9450	0.7360
U	0.8140	0.6740
V	0.7520	0.6230
W	0.9560	0.7350
X	0.8590	0.6760
Y	0.9190	0.7130
Z	0.9310	0.7310
a	0.8030	0.6550
b	0.9450	0.7370
c	0.8580	0.6730
d	0.6790	0.5740
e	0.8310	0.5750
f	0.8300	0.6020
g	0.8990	0.7070

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
h	0.7470	0.6260
i	0.9710	0.7750
j	0.8340	0.6530
k	0.9150	0.6390
l	0.8770	0.6230
m	0.6820	0.5220
o	0.9670	0.7590
p	0.7550	0.5880
q	0.6110	0.5270
r	0.9320	0.6980
s	0.9060	0.7060
t	0.1870	0.3060
u	0.1050	0.2870
v	0.0000	0.1330
w	0.0000	0.0340
x	0.0000	0.0990
y	0.0000	0.0580
z	0.0080	0.2250