



Full wwPDB EM Validation Report ⓘ

Mar 16, 2026 – 08:31 PM UTC

PDB ID : 6YWY / pdb_00006ywy
EMDB ID : EMD-10985
Title : The structure of the mitoribosome from *Neurospora crassa* with bound tRNA at the P-site
Authors : Amunts, A.; Itoh, Y.; Naschberger, A.
Deposited on : 2020-04-30
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

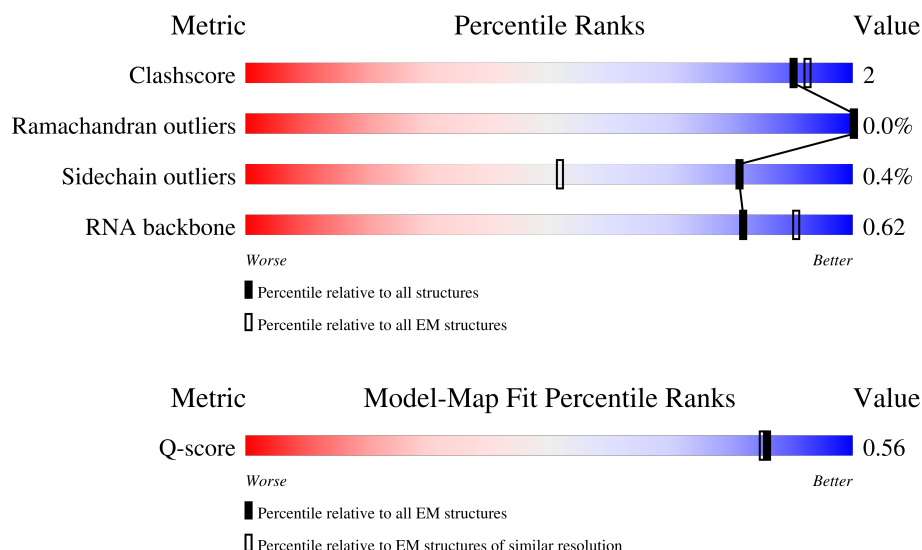
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.05 Å.

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



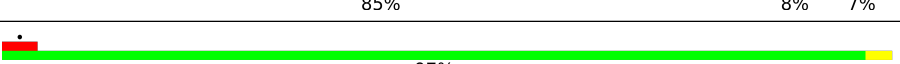
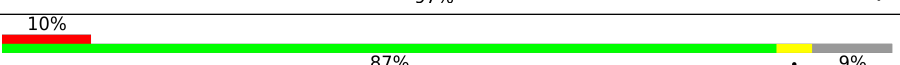
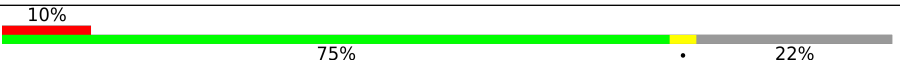
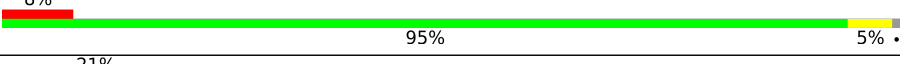
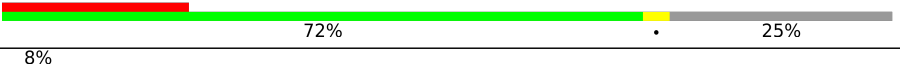
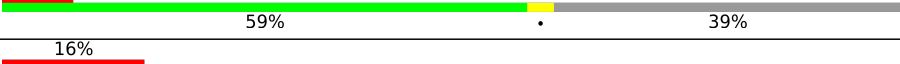
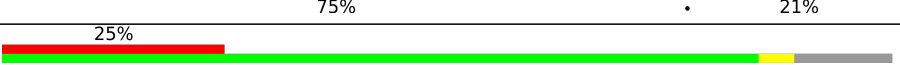
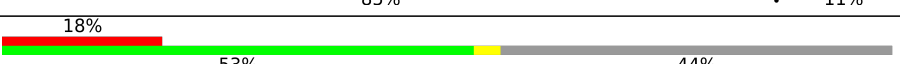
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13971 (2.55 - 3.55)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3464	
2	B	383	
3	C	384	

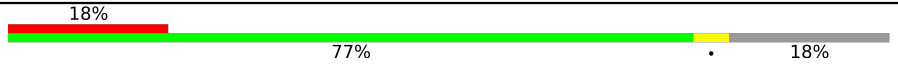
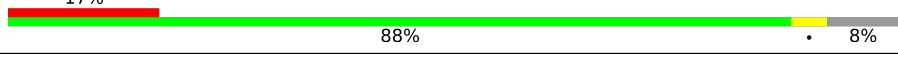
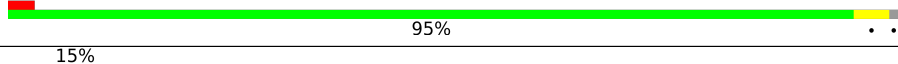
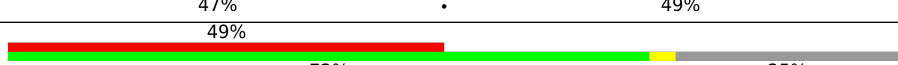
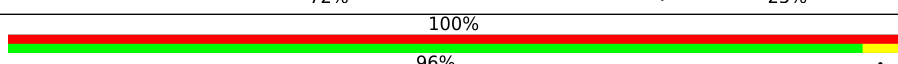
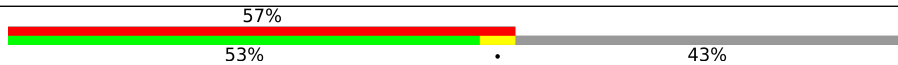
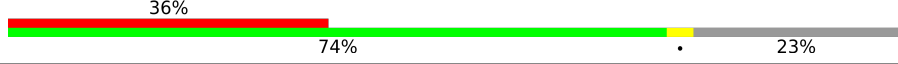
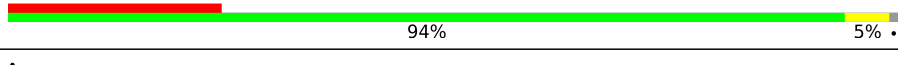
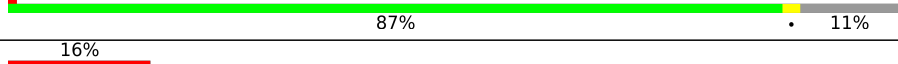
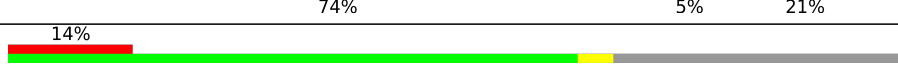
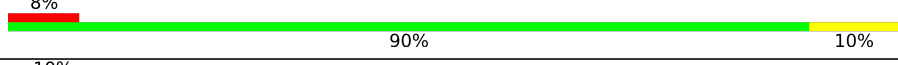
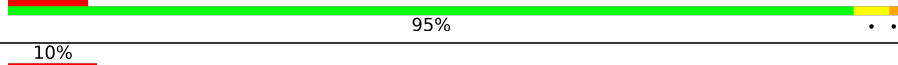
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
77	99	95	
78	aa	1864	
79	bb	73	
80	ee	11	
81	cc	7	
82	e	303	
83	j	201	

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 392401 atoms, of which 174325 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2843	Total	C	H	N	O	P	0	0
			91056	27190	30416	10878	19729	2843		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	315	Total	C	H	N	O	S	0	0
			4964	1527	2508	500	415	14		

- Molecule 3 is a protein called Related to ribosomal protein L3, mitochondrial.

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

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

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

- Molecule 5 is a protein called Related to ribosomal protein L5, mitochondrial.

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

- Molecule 6 is a protein called uL6m.

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

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

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

- Molecule 8 is a protein called Related to ribosomal protein YmL11, mitochondrial.

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

- Molecule 9 is a protein called uL11m.

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

- Molecule 10 is a protein called uL13m.

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

- Molecule 11 is a protein called Ribosomal protein L14.

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

- Molecule 12 is a protein called Ribosomal protein L15.

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

- Molecule 13 is a protein called Related to ribosomal protein L16, mitochondrial.

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

- Molecule 14 is a protein called uL17m.

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

- Molecule 15 is a protein called bL19m.

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

- Molecule 16 is a protein called Related to ribosomal protein YmL49, mitochondrial.

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

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

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

- Molecule 18 is a protein called uL23m.

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

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

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

- Molecule 20 is a protein called Related to 60s ribosomal protein L2 (Mitochondrial).

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

- Molecule 21 is a protein called bL28m.

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

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

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

- Molecule 23 is a protein called Related to ribosomal protein L30.

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

- Molecule 24 is a protein called Related to ribosomal protein YmL36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	V	94	Total	C	H	N	O	S	0	0
			1485	472	735	136	140	2		

- Molecule 25 is a protein called Related to ribosomal protein YmL32 (Mitochondrial).

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

- Molecule 26 is a protein called bL33m.

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

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

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

- Molecule 28 is a protein called Ribosomal protein.

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

- Molecule 29 is a protein called PEBP-like protein.

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

- Molecule 30 is a protein called mL40.

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

- Molecule 31 is a protein called mL41.

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

- Molecule 32 is a protein called L51_S25_CI-B8 domain-containing protein.

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

- Molecule 33 is a protein called Ribonuclease III.

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

- Molecule 34 is a protein called mL46.

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

- Molecule 35 is a protein called mL49.

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

- Molecule 36 is a protein called mL50.

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

- Molecule 37 is a protein called Probable ribosomal protein YmL44, mitochondrial.

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

- Molecule 38 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace	
38	i	124	Total	C	H	N	O	S	0	0
			1998	613	1022	181	177	5		

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

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

- Molecule 40 is a protein called Related to ribosomal protein YmL20, mitochondrial.

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

- Molecule 41 is a protein called Mitoc_mL59 domain-containing protein.

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

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

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

- Molecule 43 is a protein called mL67.

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

- Molecule 44 is a protein called bS1m.

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

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

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

- Molecule 46 is a protein called Ribosomal protein S5.

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

- Molecule 47 is a protein called S4 RNA-binding domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	DD	290	Total	C	H	N	O	S	0	0
			4715	1501	2373	430	400	11		

- Molecule 48 is a protein called Related to ribosomal protein S5 (Mitochondrial).

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

- Molecule 49 is a protein called Ribosomal protein S6.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
50	GG	223	Total	C	H	N	O	S	0	0
			3523	1098	1799	318	302	6		

- Molecule 51 is a protein called uS8m.

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

- Molecule 52 is a protein called uS9m.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	II	247	Total	C	H	N	O	S	0	0
			3994	1253	2026	366	344	5		

- Molecule 53 is a protein called 30S ribosomal protein S10, mitochondrial.

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

- Molecule 54 is a protein called Translational machinery component.

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

- Molecule 55 is a protein called Ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	LL	128	Total	C	H	N	O	S	0	0
			1991	591	1032	198	165	5		

- Molecule 56 is a protein called Probable ribosomal protein S13.

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

- Molecule 57 is a protein called Mitochondrial 37S ribosomal protein MRP2.

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

- Molecule 58 is a protein called Related to ribosomal protein S15 (Mitochondrial).

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

- Molecule 59 is a protein called bS16m.

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

- Molecule 60 is a protein called uS17m.

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

- Molecule 61 is a protein called Ribosomal protein S18.

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

- Molecule 62 is a protein called Ribosomal protein S19/S15.

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

- Molecule 63 is a protein called bS21m.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
64	UU	224	Total	C	H	N	O	S	0	0
			3687	1165	1843	342	330	7		

- Molecule 65 is a protein called mS26.

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

- Molecule 66 is a protein called mS27.

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

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

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

- Molecule 68 is a protein called mS33.

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

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

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

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

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

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

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

- Molecule 72 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	33	191	Total	C	H	N	O	S	0	0
			3134	978	1595	293	266	2		

- Molecule 73 is a protein called Manganese and iron superoxide dismutase.

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

- Molecule 74 is a protein called mS45.

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

- Molecule 75 is a protein called mS46.

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

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

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

- Molecule 77 is a protein called IF1.

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
79	bb	73	Total	C	H	N	O	P	0	0
			2346	697	789	284	503	73		

- Molecule 80 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	ee	11	Total	C	H	N	O	P	0	0
			344	103	115	34	81	11		

- Molecule 81 is a protein called Poly-Peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	cc	7	Total	C	H	N	O	0	0
			69	21	34	7	7		

- Molecule 82 is a protein called 60S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	e	148	Total	C	H	N	O	S	0	0
			2396	751	1212	209	218	6		

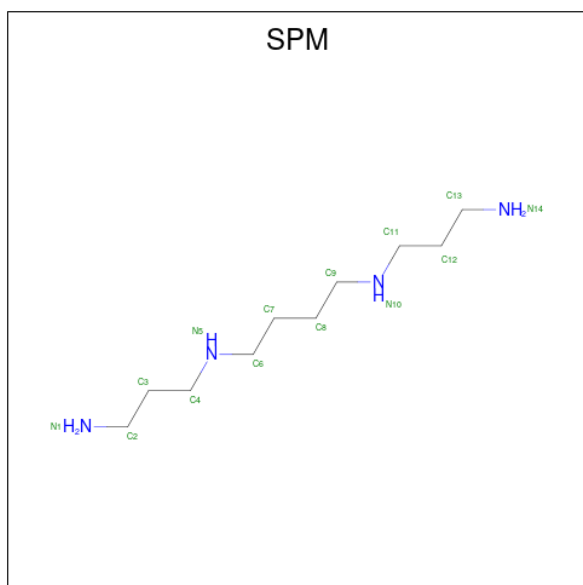
- Molecule 83 is a protein called L51_S25_CI-B8 domain-containing protein.

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

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	A	144	Total	Mg	0
			144	144	
84	K	1	Total	Mg	0
			1	1	
84	L	1	Total	Mg	0
			1	1	
84	BB	1	Total	Mg	0
			1	1	
84	KK	1	Total	Mg	0
			1	1	
84	QQ	1	Total	Mg	0
			1	1	
84	XX	1	Total	Mg	0
			1	1	
84	YY	1	Total	Mg	0
			1	1	
84	00	1	Total	Mg	0
			1	1	
84	aa	97	Total	Mg	0
			97	97	
84	ee	1	Total	Mg	0
			1	1	

- Molecule 85 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



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

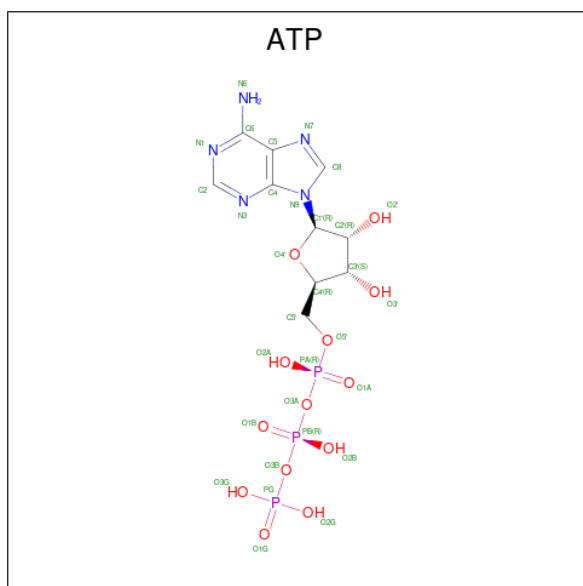
- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
87	W	1	Total Zn 1 1	0
87	0	1	Total Zn 1 1	0

- # NAD

Mol	Chain	Residues	Atoms						AltConf
88	2	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

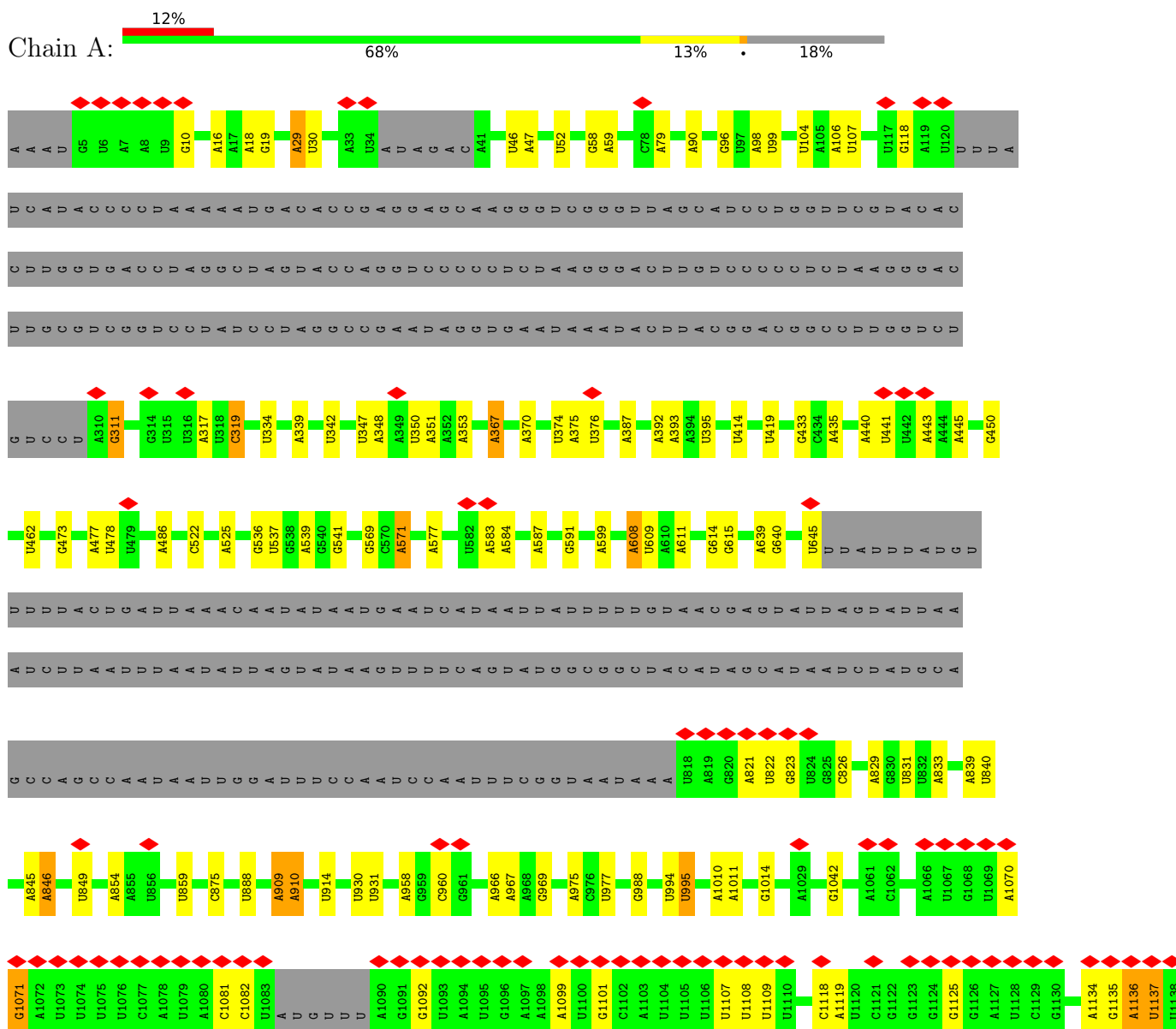
- Molecule 89 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



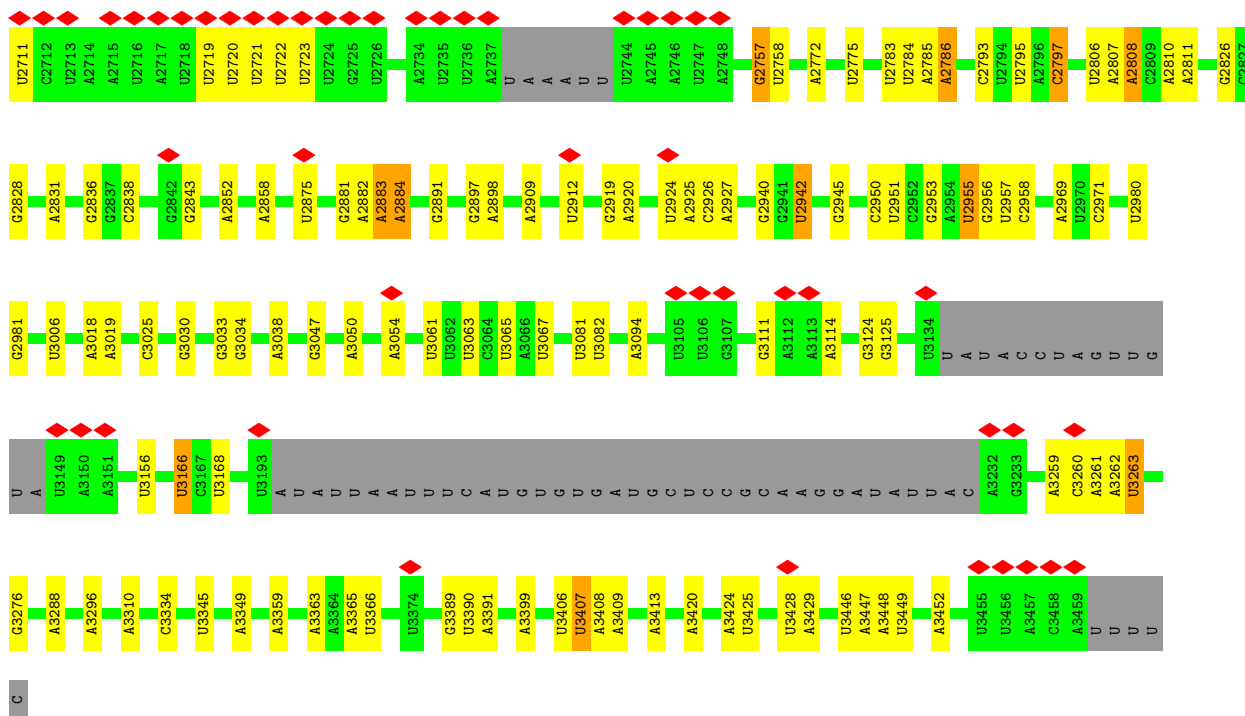
3 Residue-property plots [i](#)

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

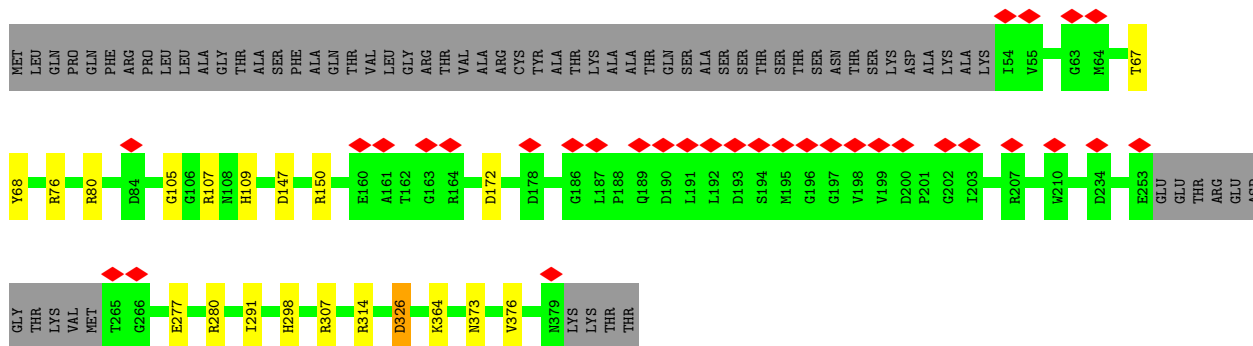
• Molecule 1: 23S rRNA



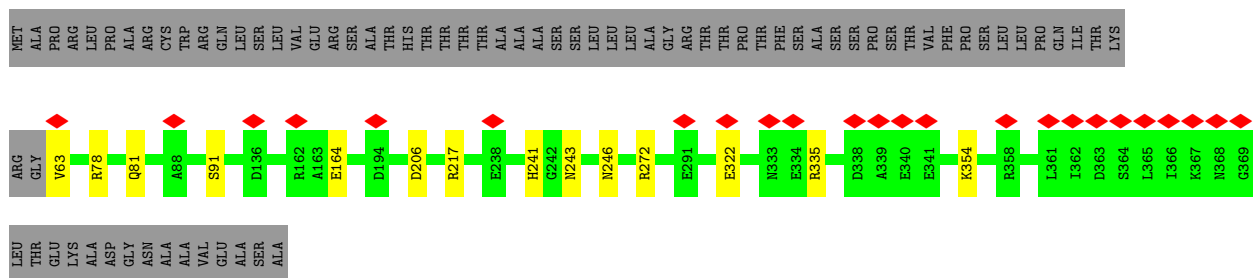
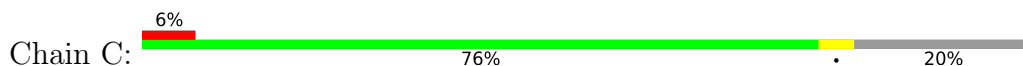




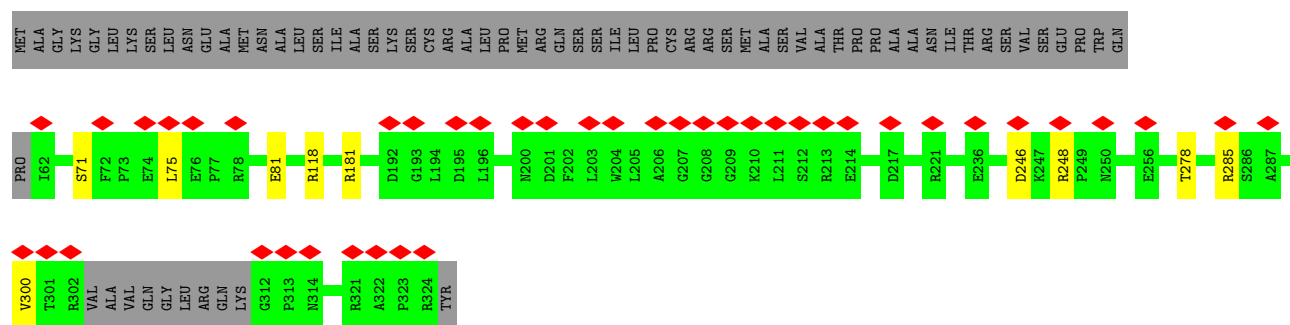
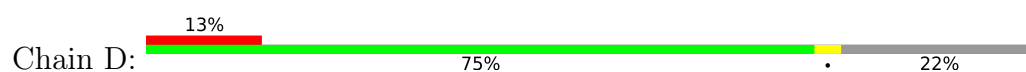
- Molecule 2: 60S ribosomal protein L2, mitochondrial



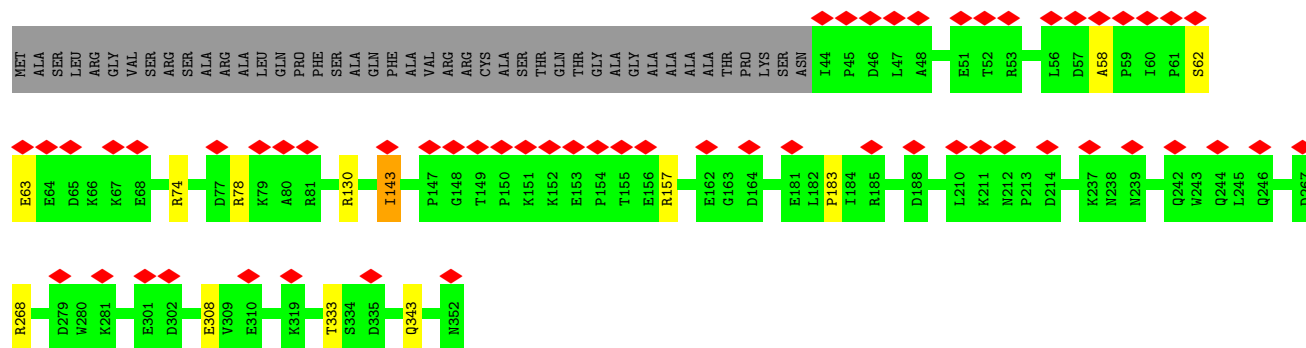
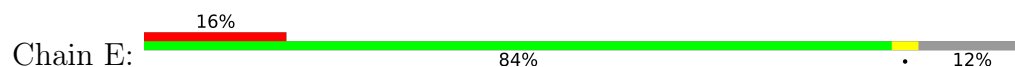
- Molecule 3: Related to ribosomal protein L3, mitochondrial



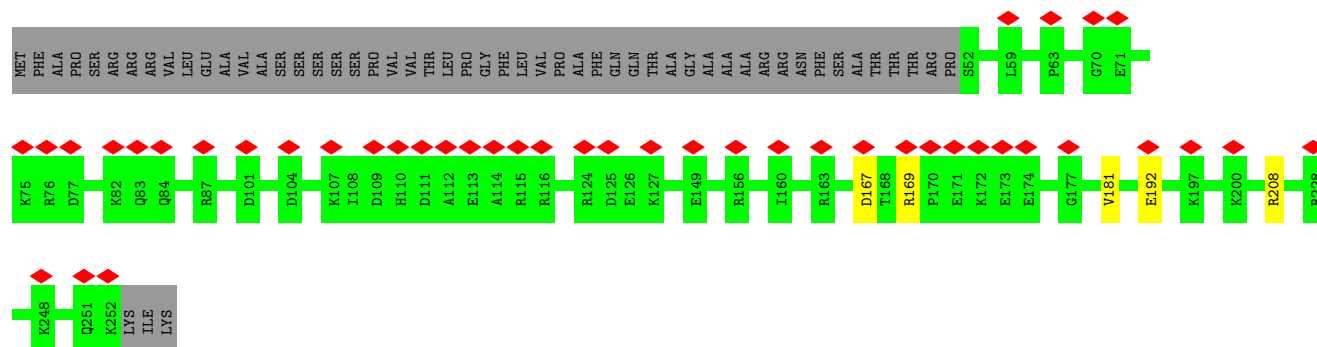
- Molecule 4: 60S ribosomal protein L4, variant



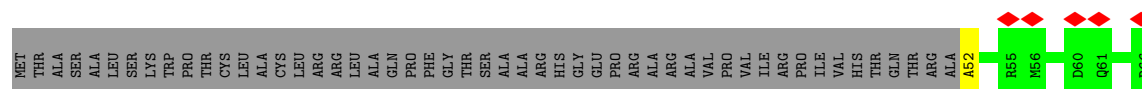
- Molecule 5: Related to ribosomal protein L5, mitochondrial

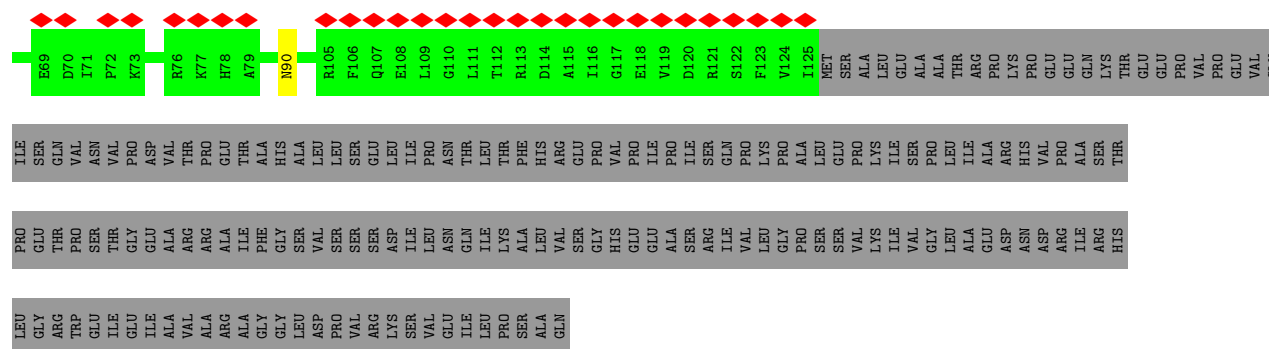


- Molecule 6: uL6m

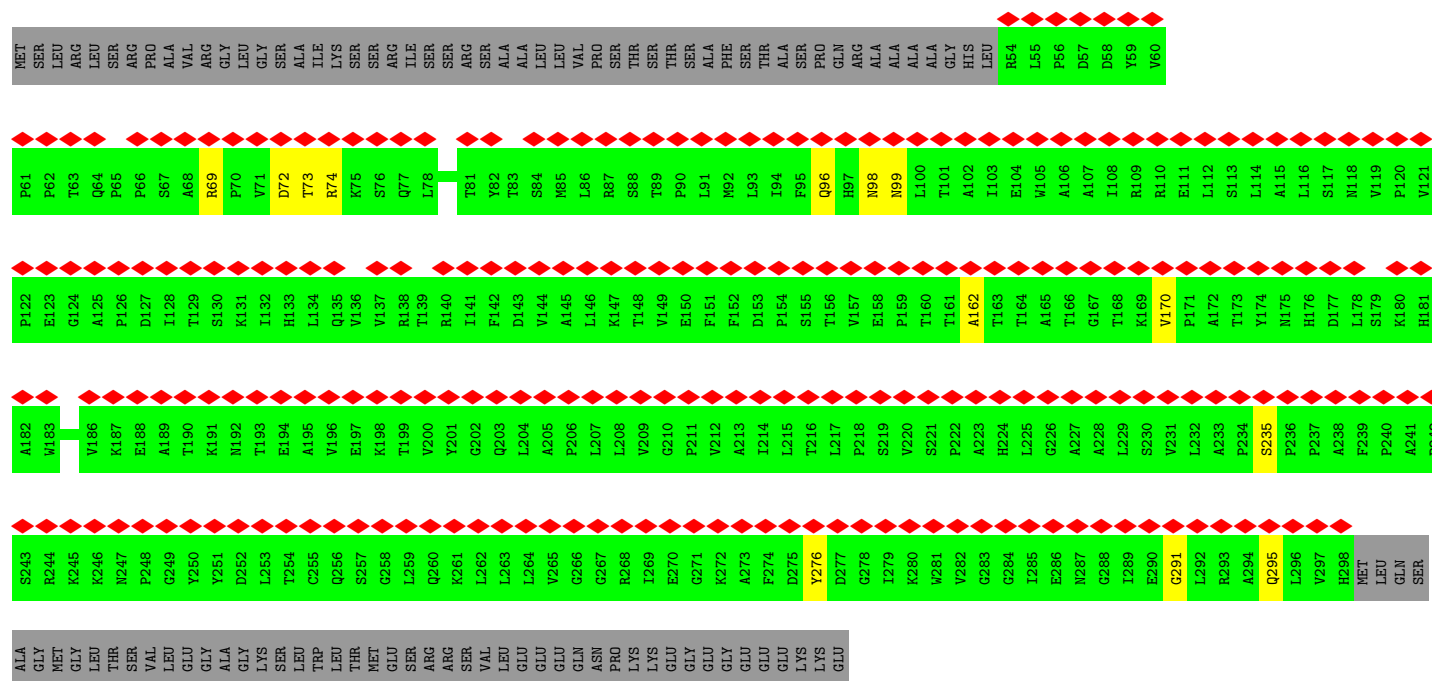


- Molecule 7: RIBOSOMAL_L9 domain-containing protein

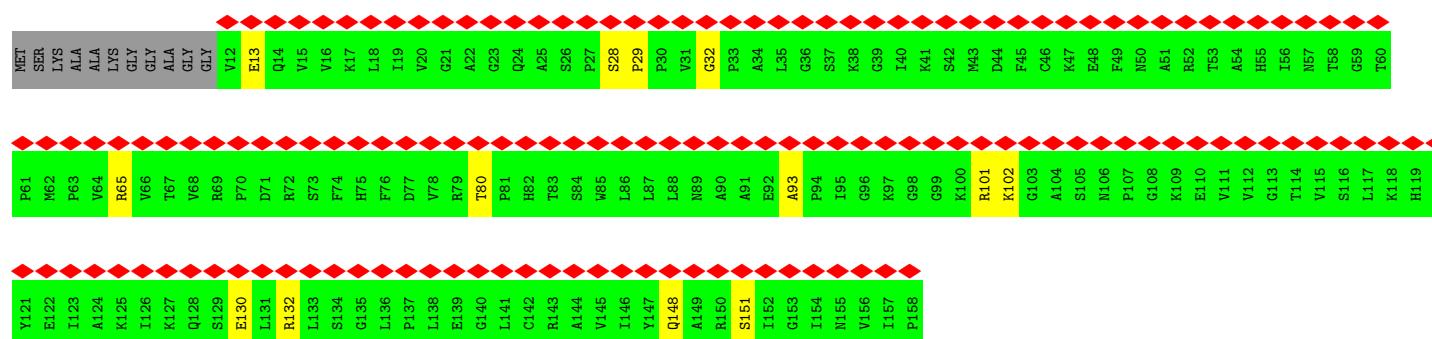
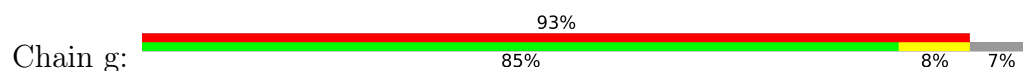




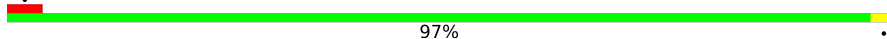
- Molecule 8: Related to ribosomal protein YmL11, mitochondrial



- Molecule 9: uL11m



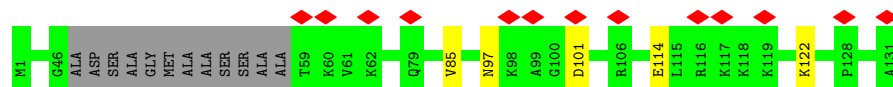
- Molecule 10: uL13m

Chain H:  97%



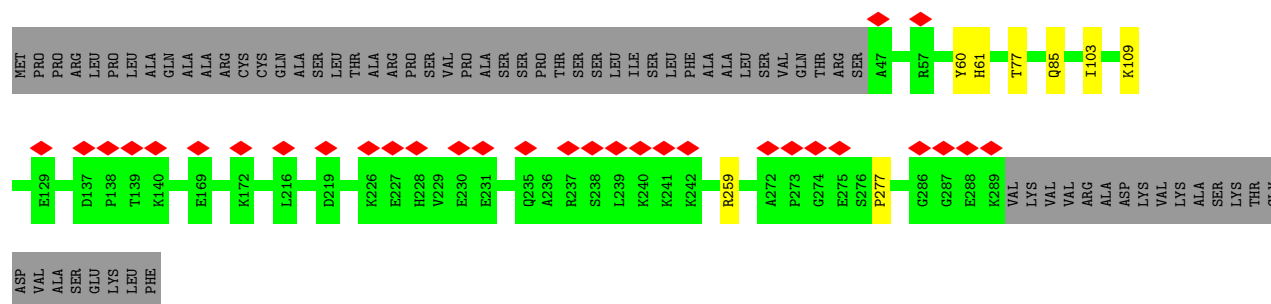
- Molecule 11: Ribosomal protein L14

Chain I:  10% 87% 9%



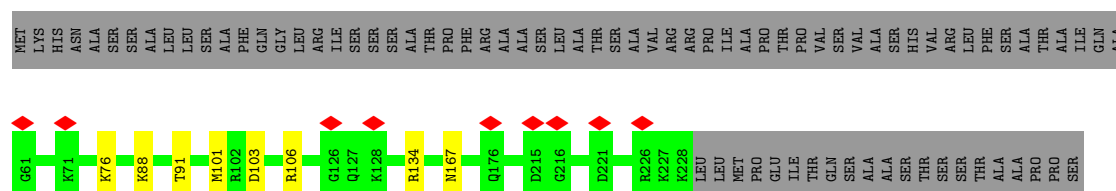
- Molecule 12: Ribosomal protein L15

Chain J:  10% 75% 22%

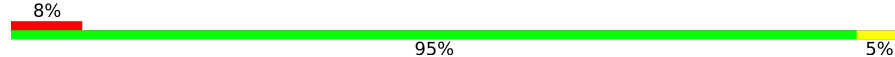


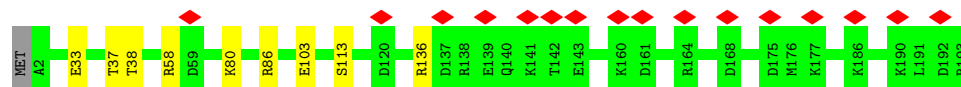
- Molecule 13: Related to ribosomal protein L16, mitochondrial

Chain K:  64% 33%



- Molecule 14: uL17m

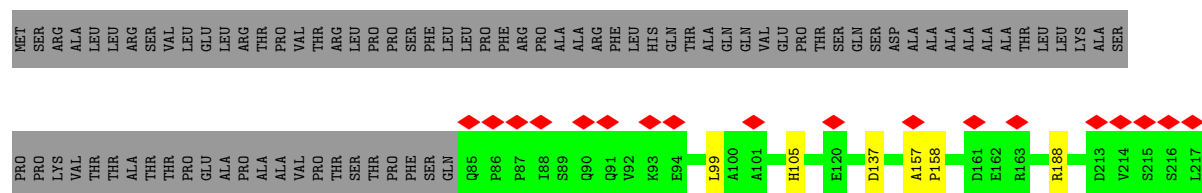
Chain L:  8% 95% 5%



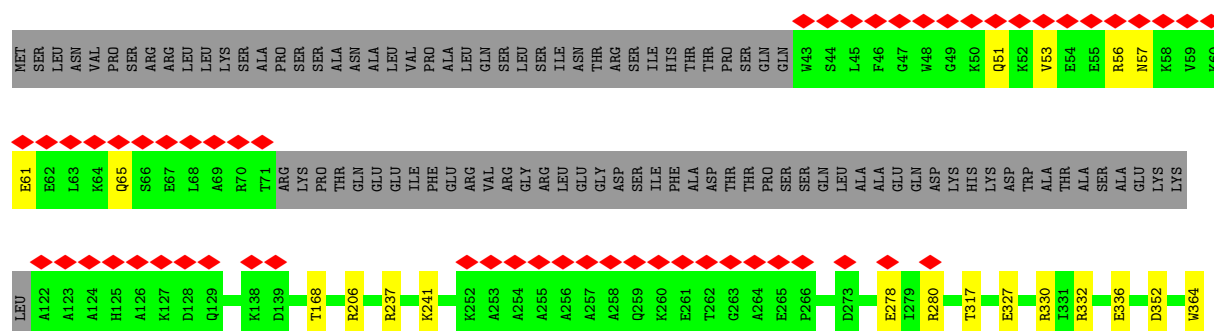
- Molecule 15: bL19m

Chain M:  21% 72% 25%

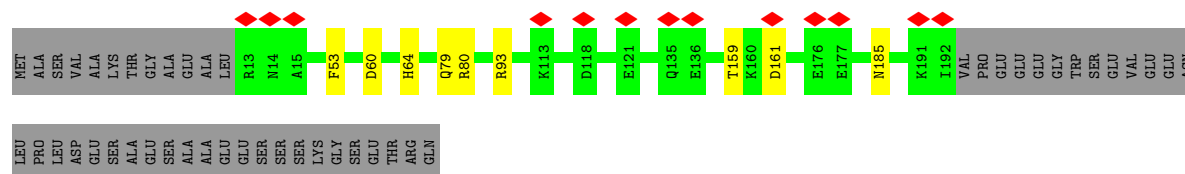
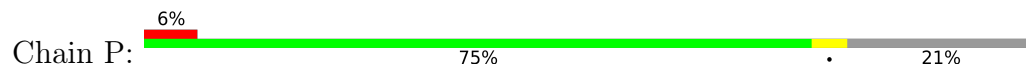
- Molecule 16: Related to ribosomal protein YmL49, mitochondrial



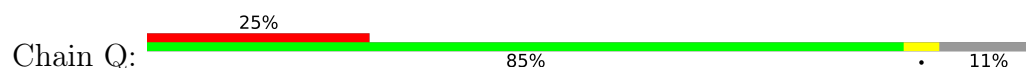
- Molecule 17: Mitochondrial large ribosomal subunit



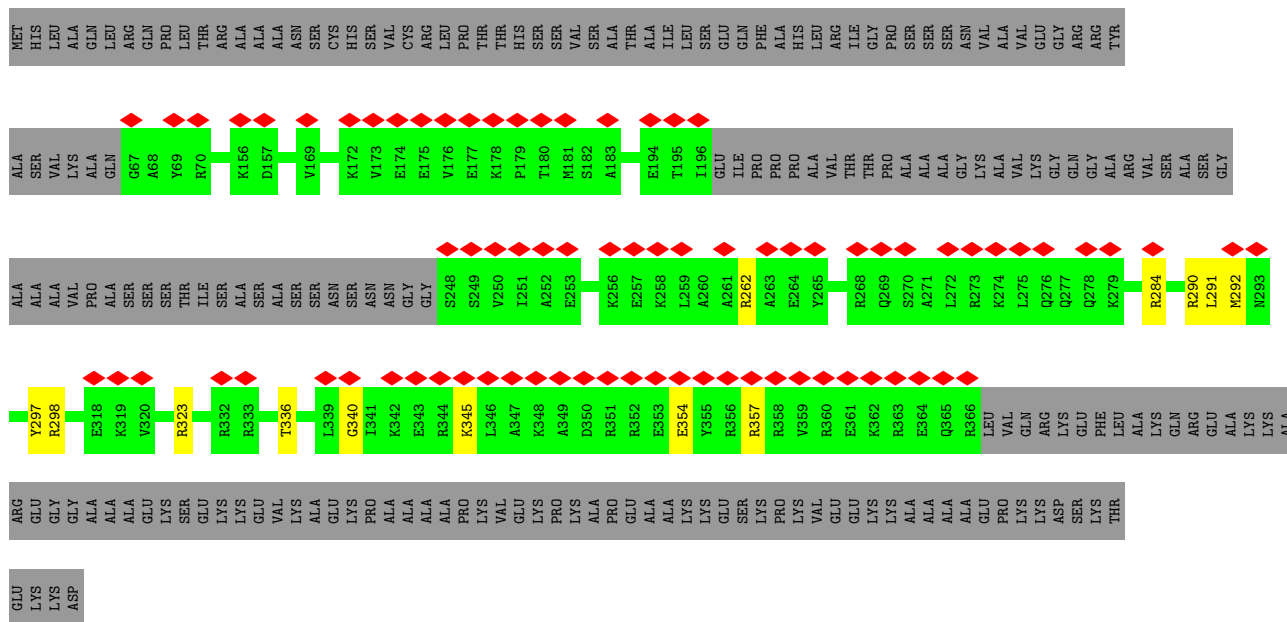
- Molecule 18: uL23m



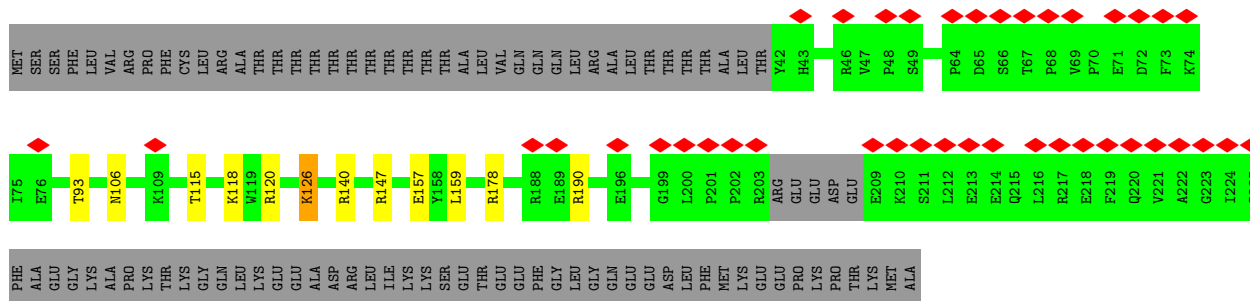
- Molecule 19: KOW domain-containing protein



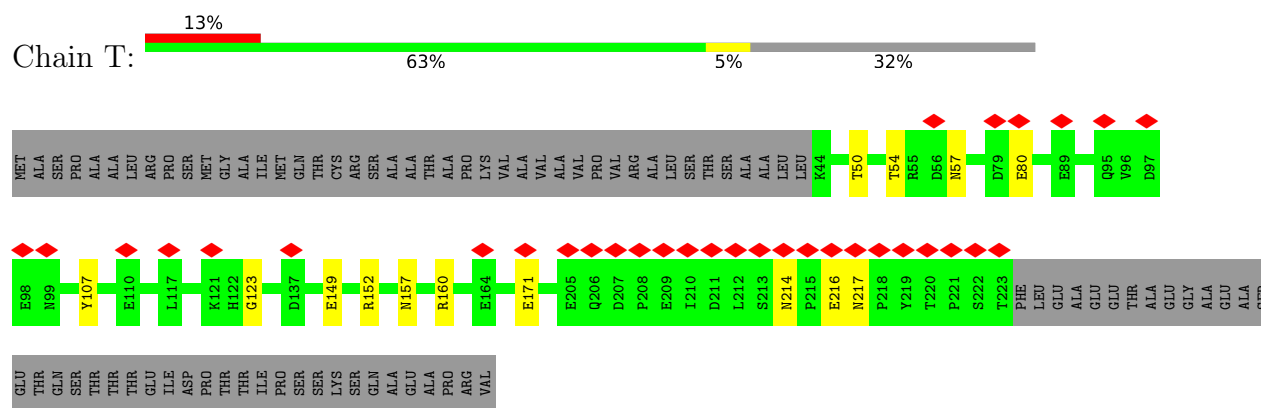
- Molecule 20: Related to 60s ribosomal protein L2 (Mitochondrial)



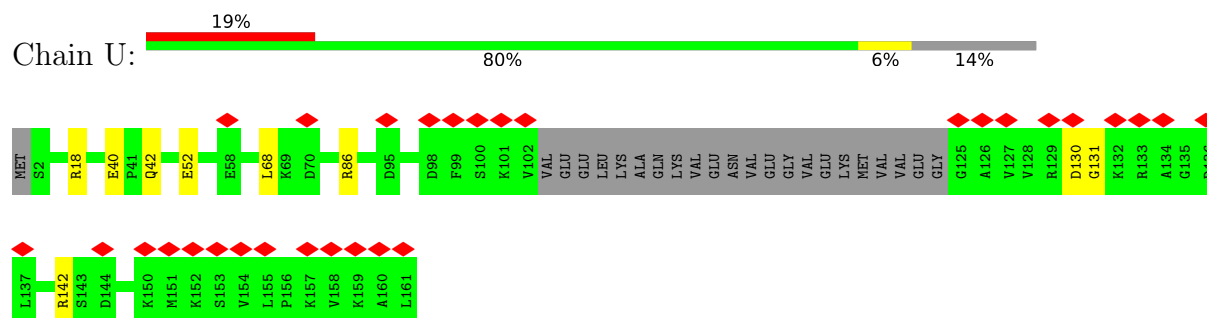
- Molecule 21: bL28m



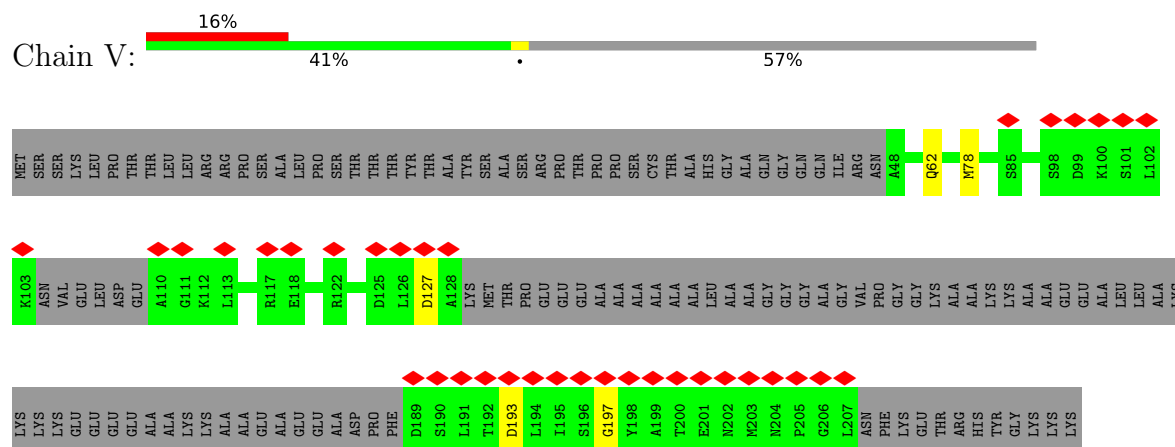
- Molecule 22: 54S ribosomal protein L4, mitochondrial



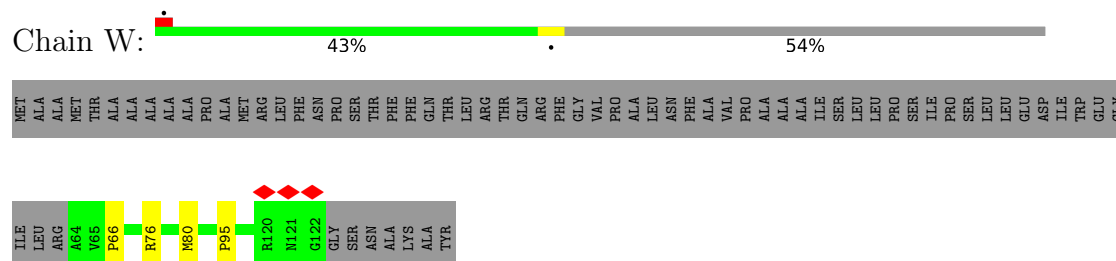
- Molecule 23: Related to ribosomal protein L30



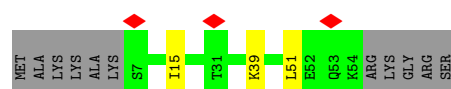
- Molecule 24: Related to ribosomal protein YmL36, mitochondrial



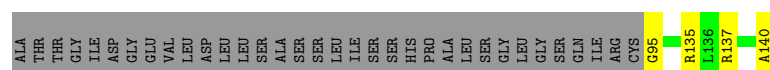
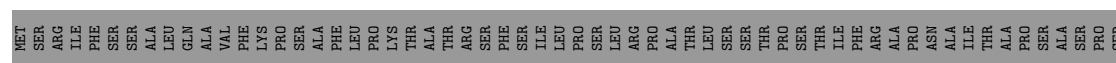
- Molecule 25: Related to ribosomal protein YmL32 (Mitochondrial)



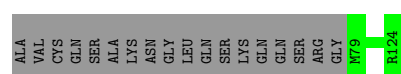
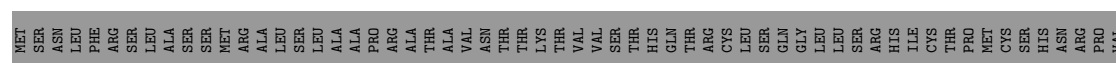
- Molecule 26: bL33m



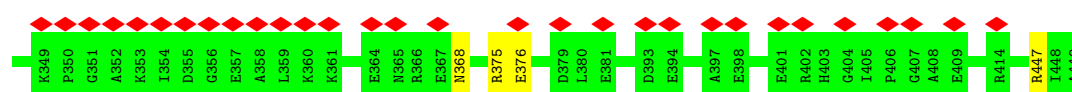
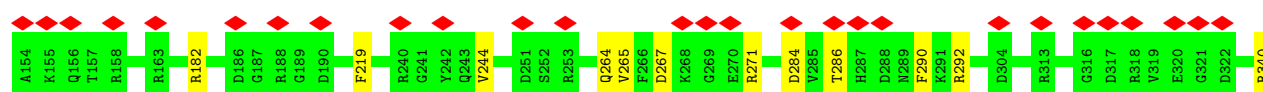
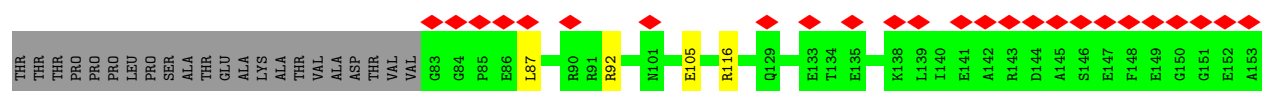
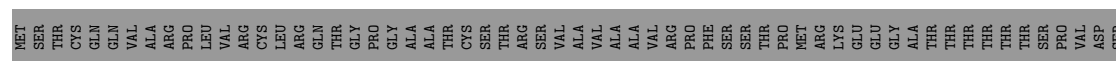
- Chain Y:  30% 3% 67%

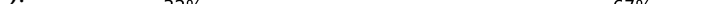


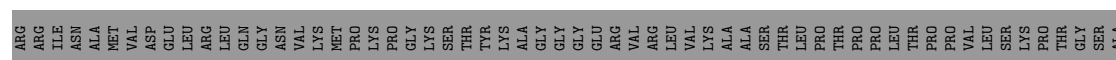
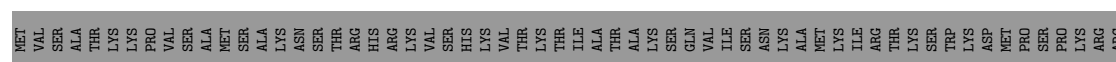
- Chain 0: 37% 63%



- Chain 1:  18% 77% 5%

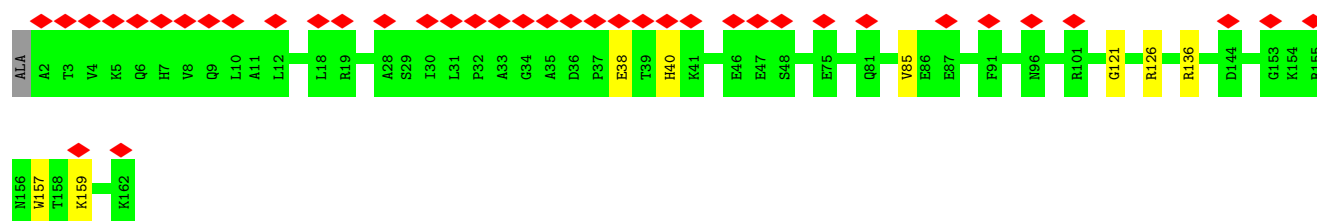
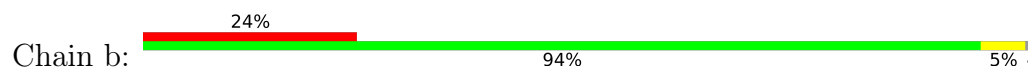


- Chain 2:  5% 32% 67%

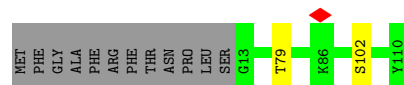
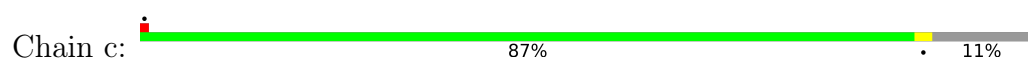




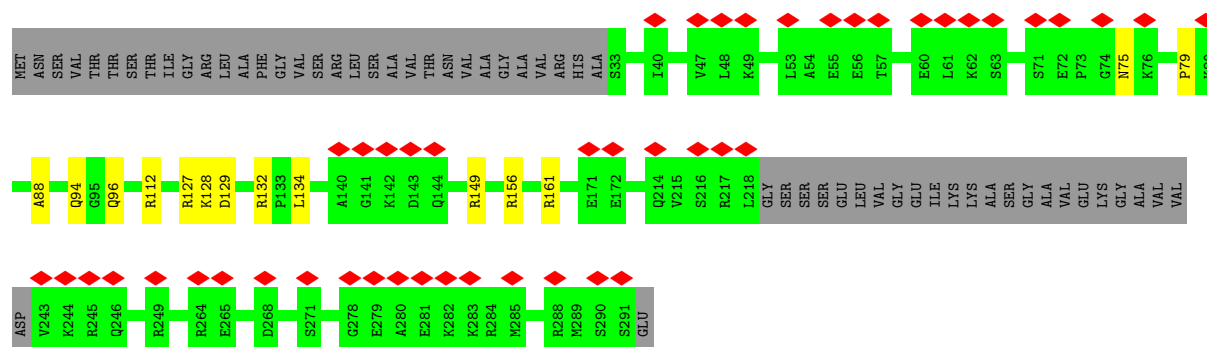
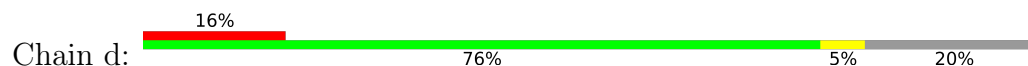
- Molecule 41: Mitoc mL59 domain-containing protein



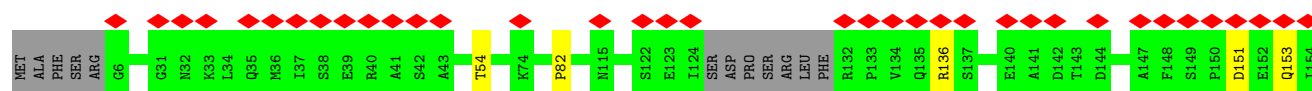
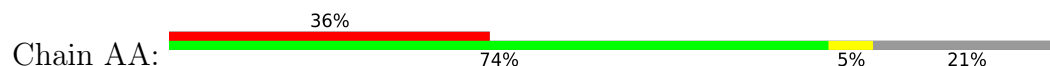
- Molecule 42: 54S ribosomal protein L31, mitochondrial



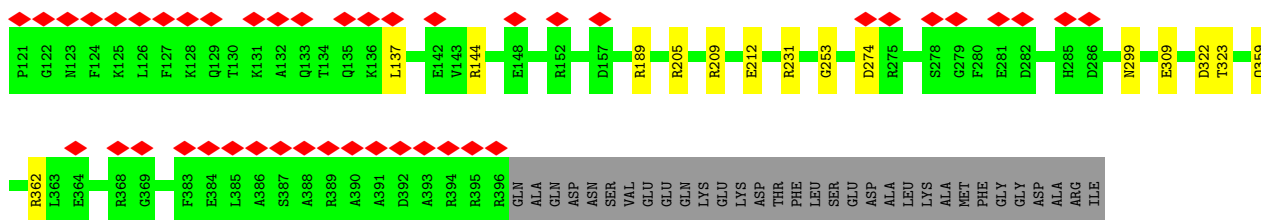
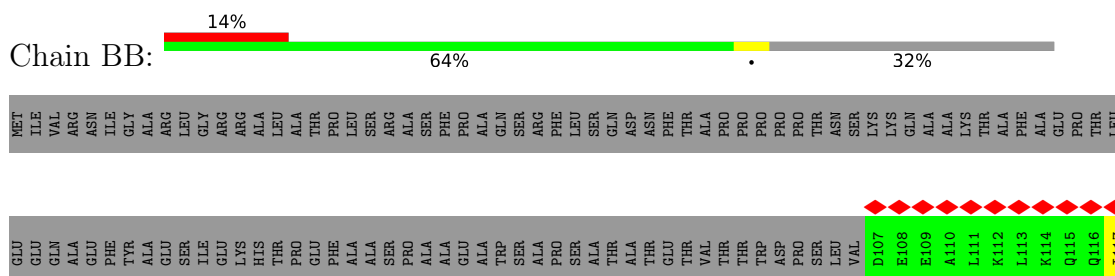
- Molecule 43: mL67



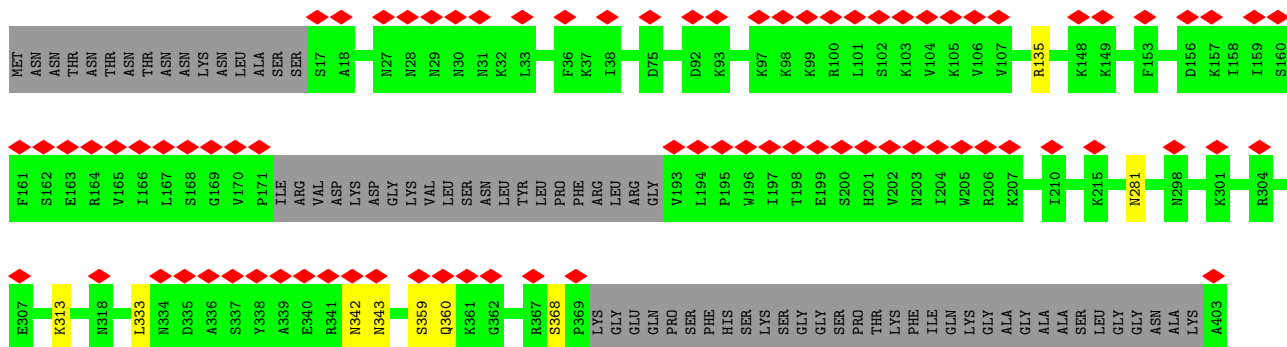
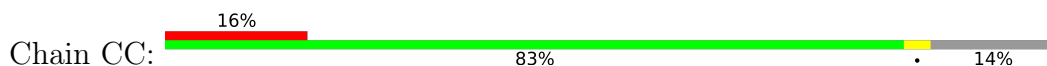
- Molecule 44: bS1m



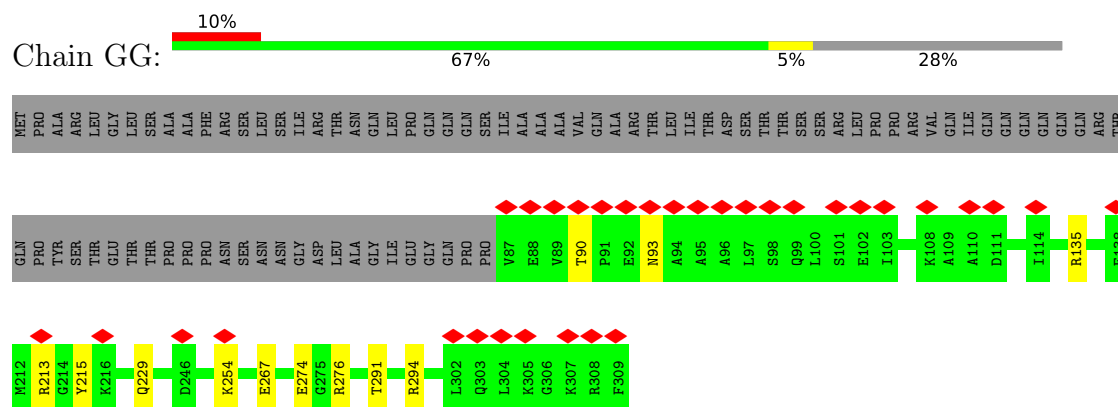
- Molecule 45: Mito ribosomal protein S2



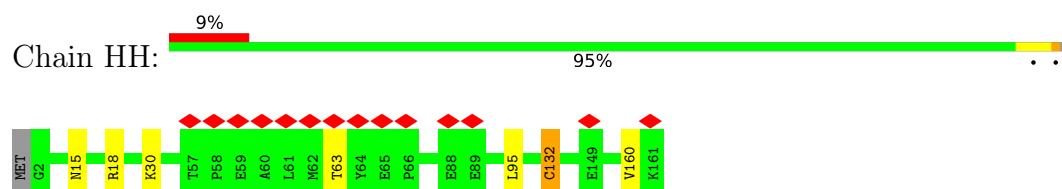
- Molecule 46: Ribosomal protein S5



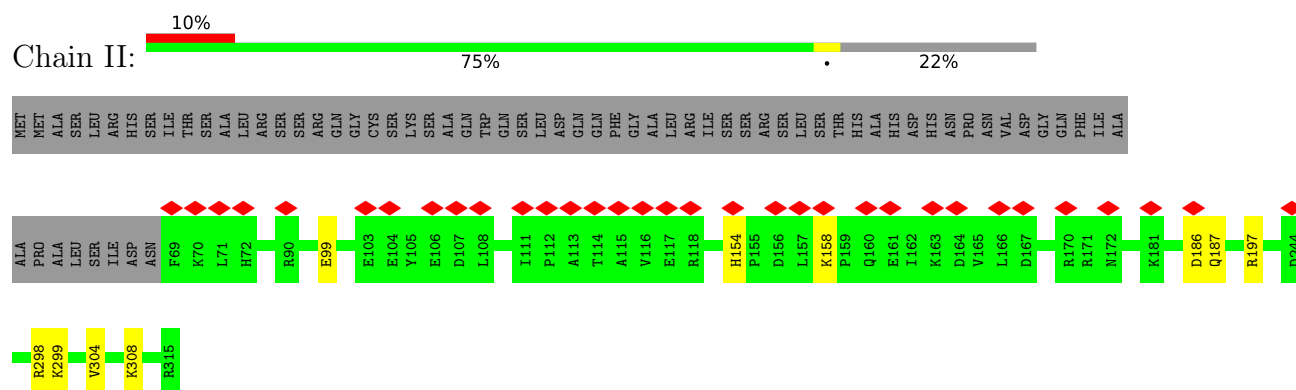
- Molecule 50: Ribosomal_S7 domain-containing protein



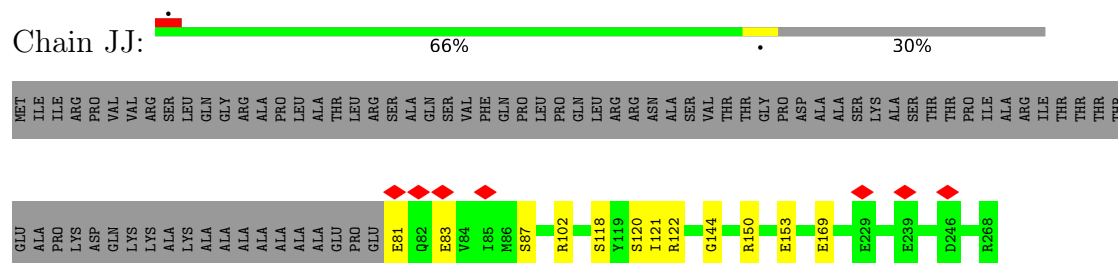
- Molecule 51: uS8m



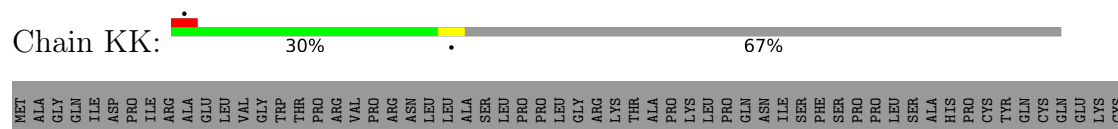
- Molecule 52: uS9m

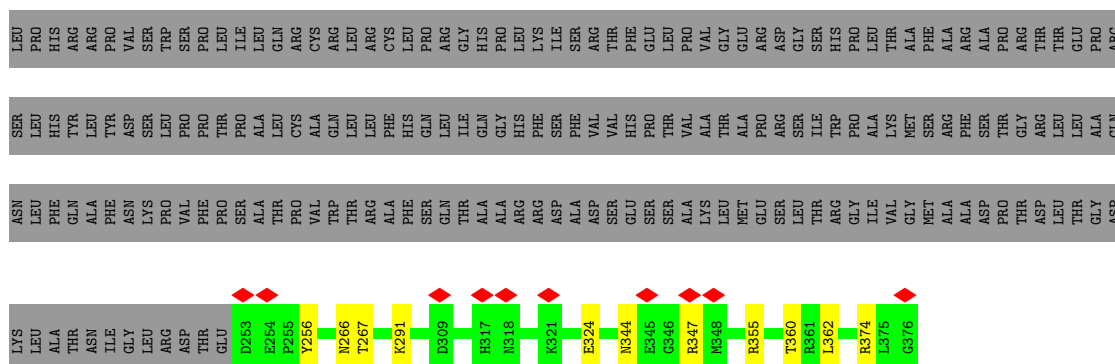


- Molecule 53: 30S ribosomal protein S10, mitochondrial

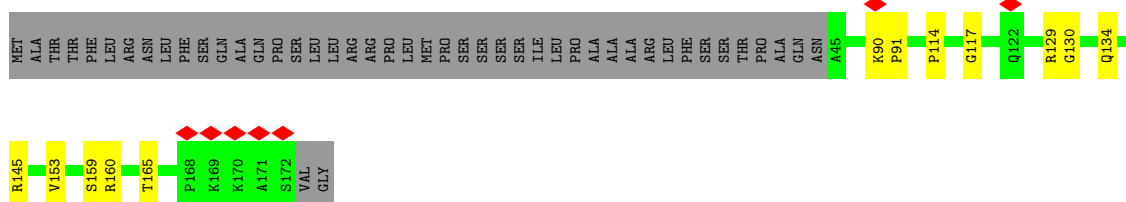


- Molecule 54: Translational machinery component

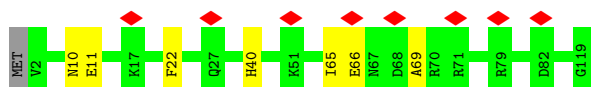




- Molecule 55: Ribosomal protein S12



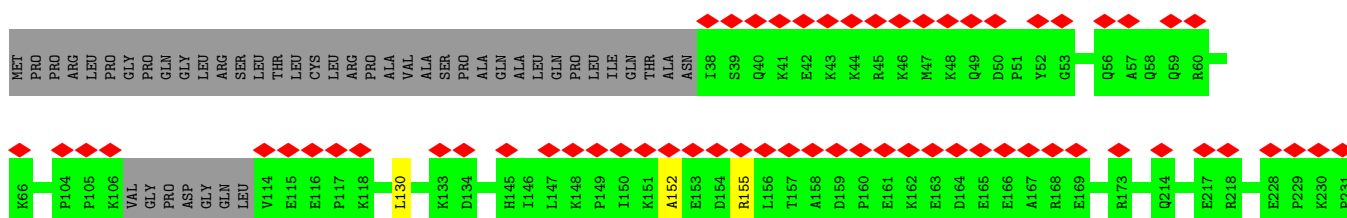
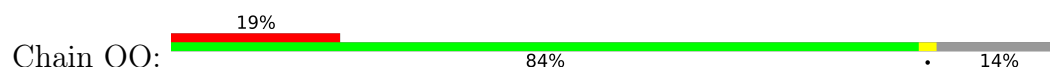
- Molecule 56: Probable ribosomal protein S13

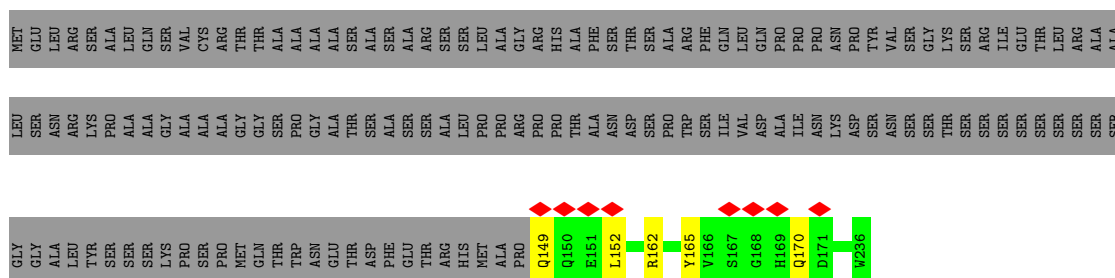


- Molecule 57: Mitochondrial 37S ribosomal protein MRP2

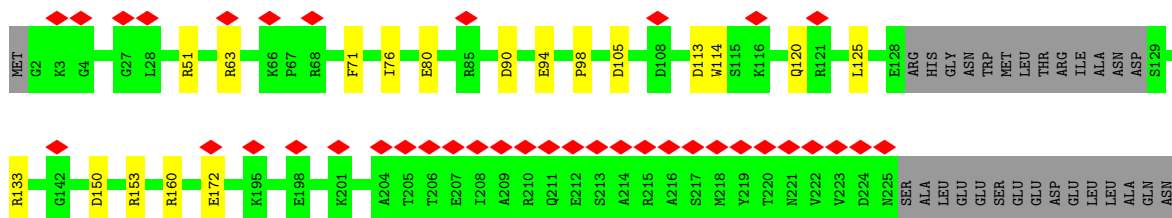
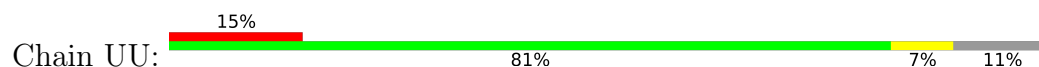


- Molecule 58: Related to ribosomal protein S15 (Mitochondrial)

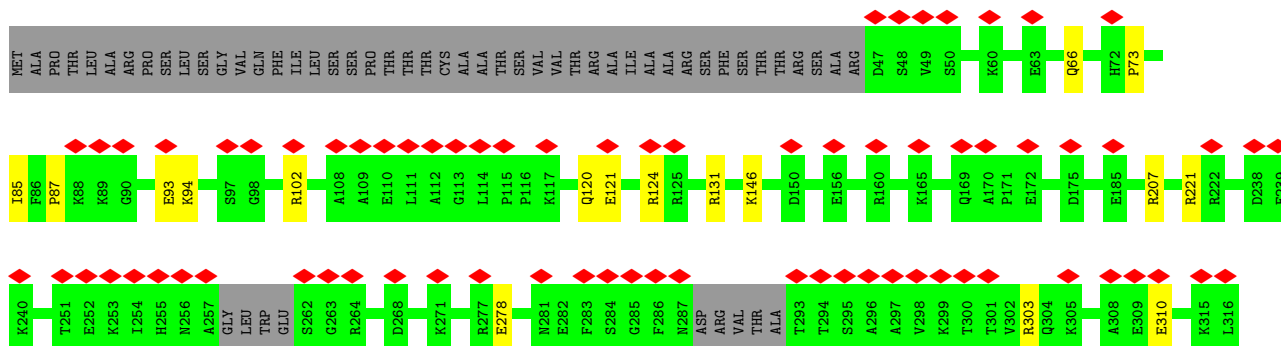
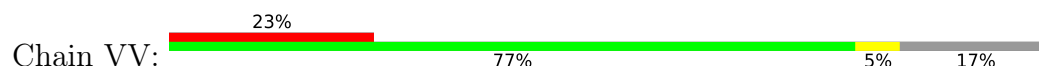




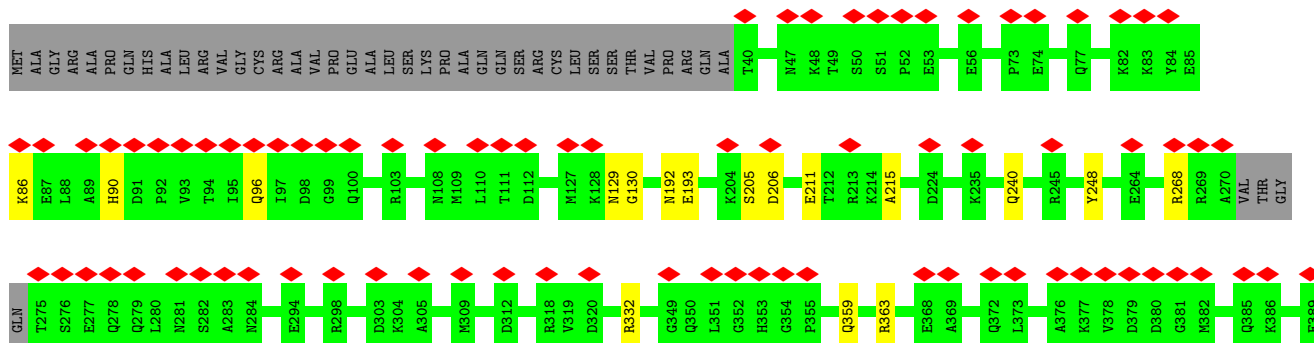
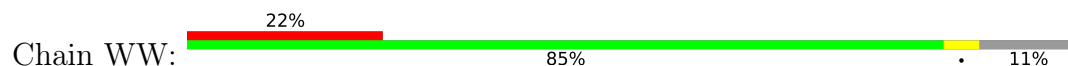
• Molecule 64: 37S ribosomal protein S25, mitochondrial

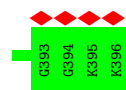


• Molecule 65: mS26



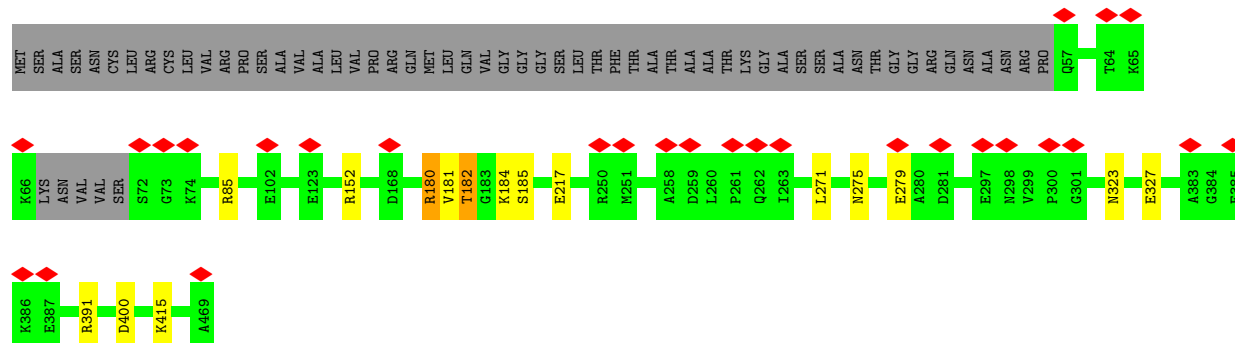
• Molecule 66: mS27





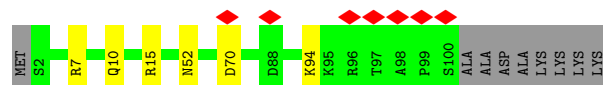
• Molecule 67: Mitochondrial ribosomal protein DAP3

Chain XX: 6% 84% 13%



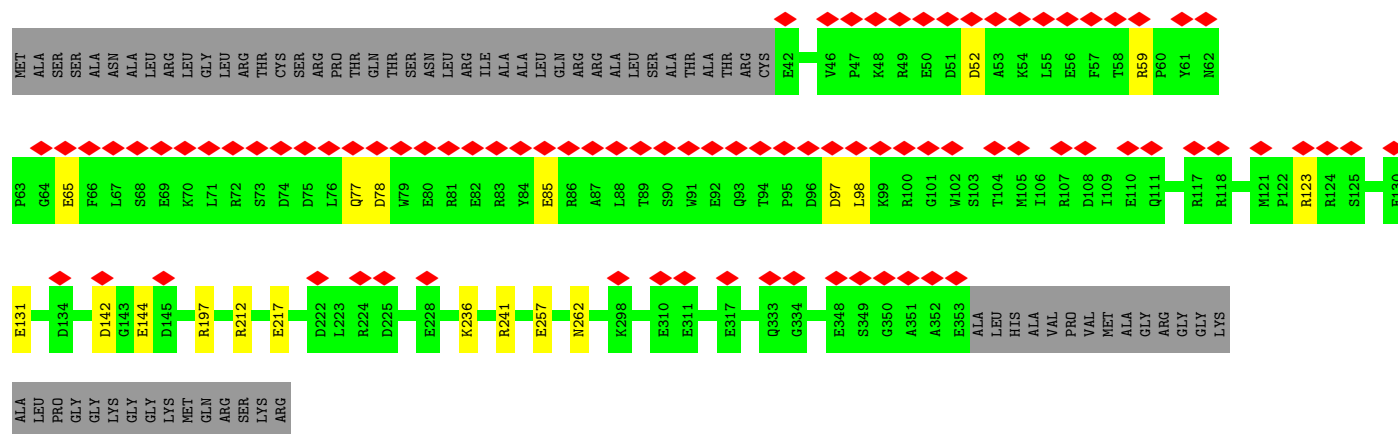
• Molecule 68: mS33

Chain YY: 6% 86% 6% 8%



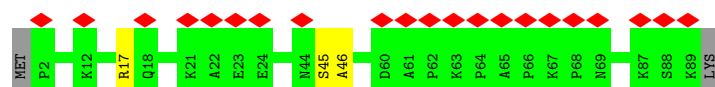
• Molecule 69: 37S ribosomal protein S24, mitochondrial

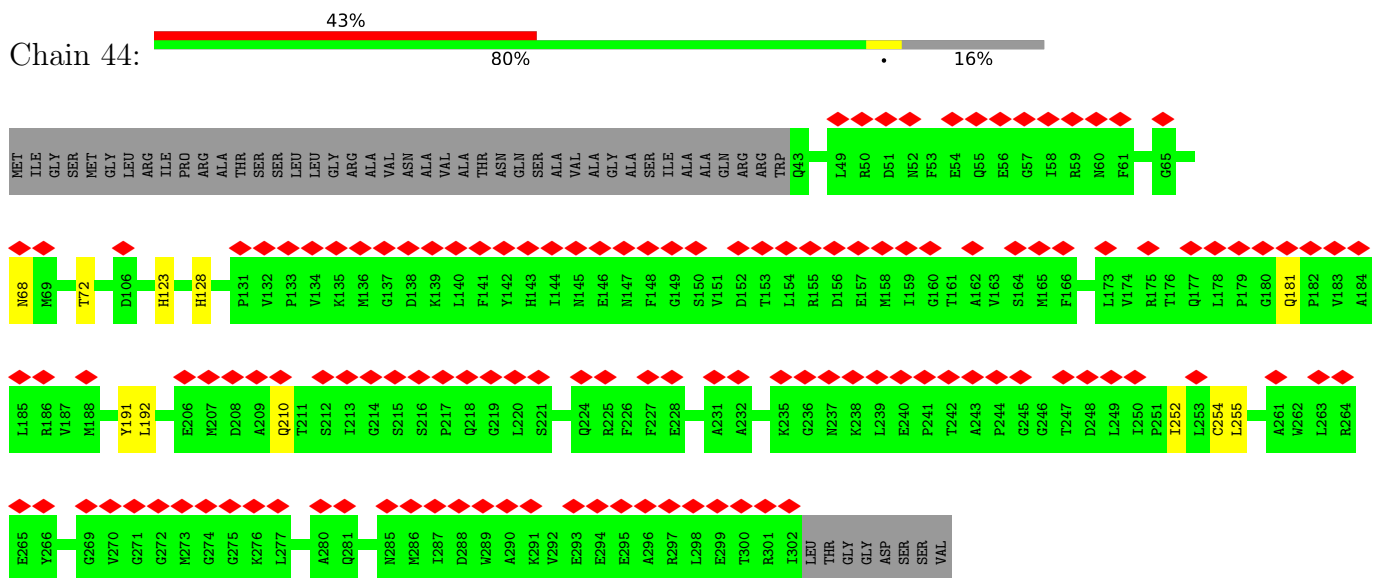
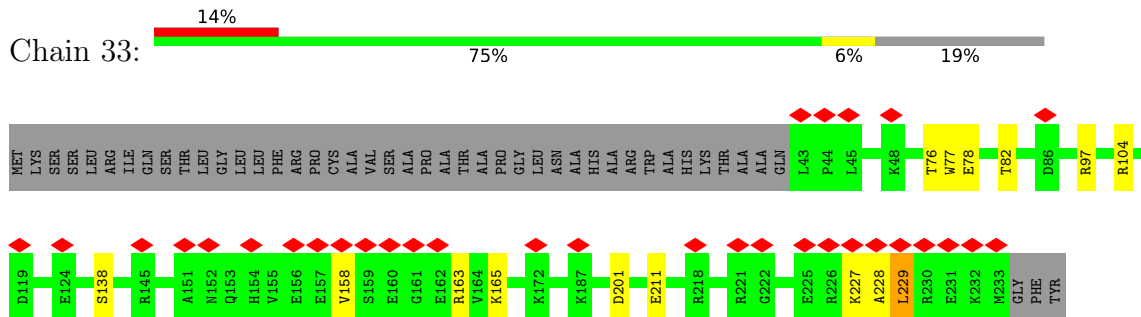
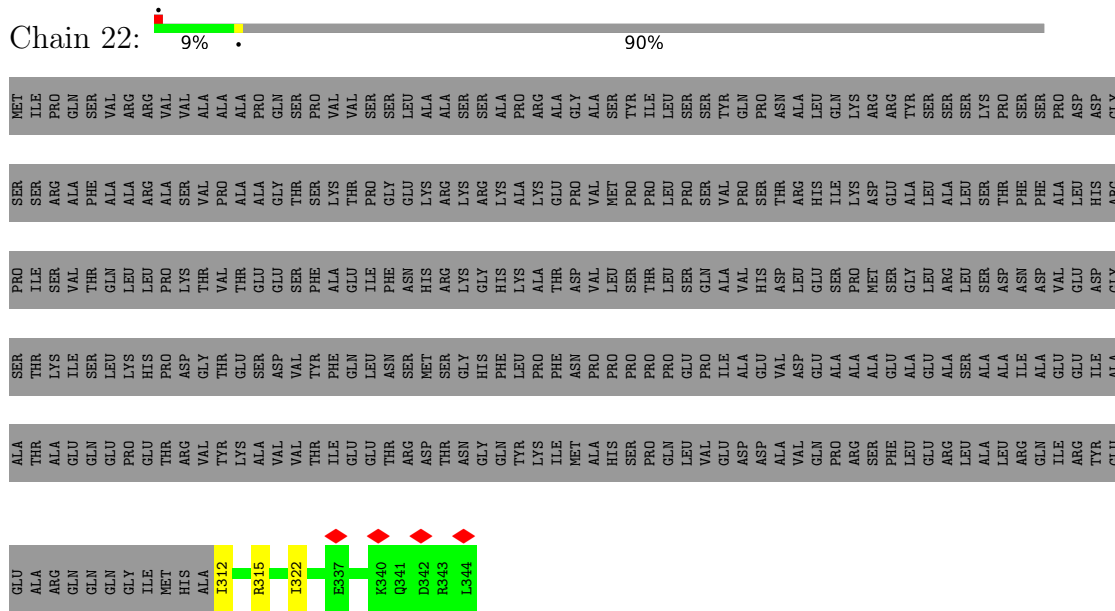
Chain ZZ: 23% 77% 5% 18%



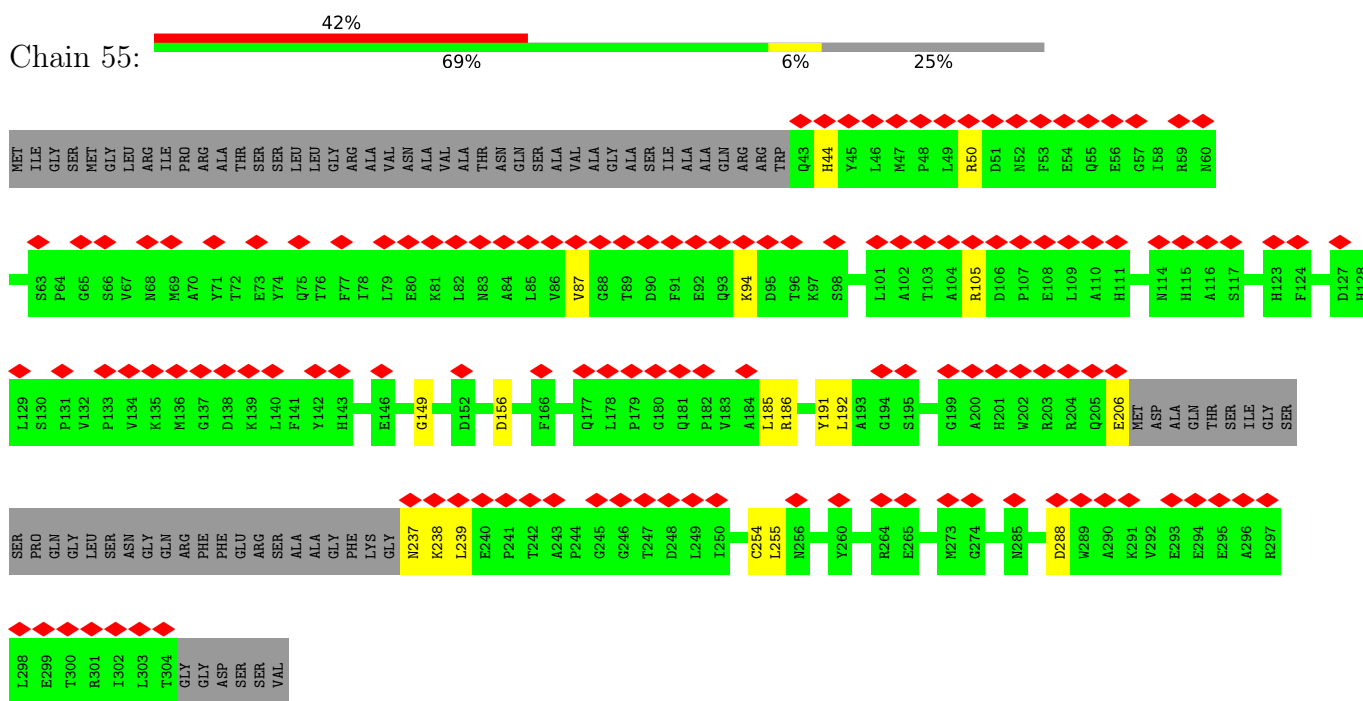
• Molecule 70: 37S ribosomal protein mrp10, mitochondrial

Chain 11: 23% 94% 2%

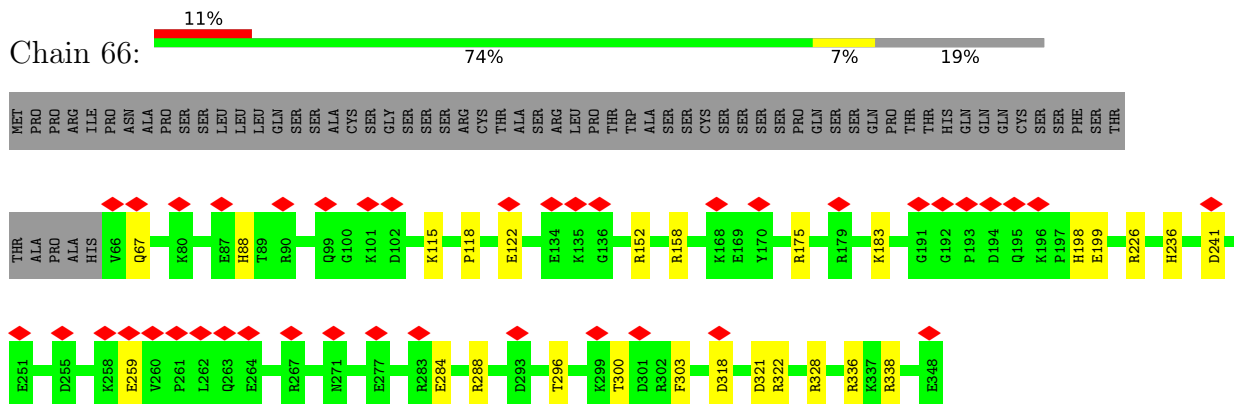




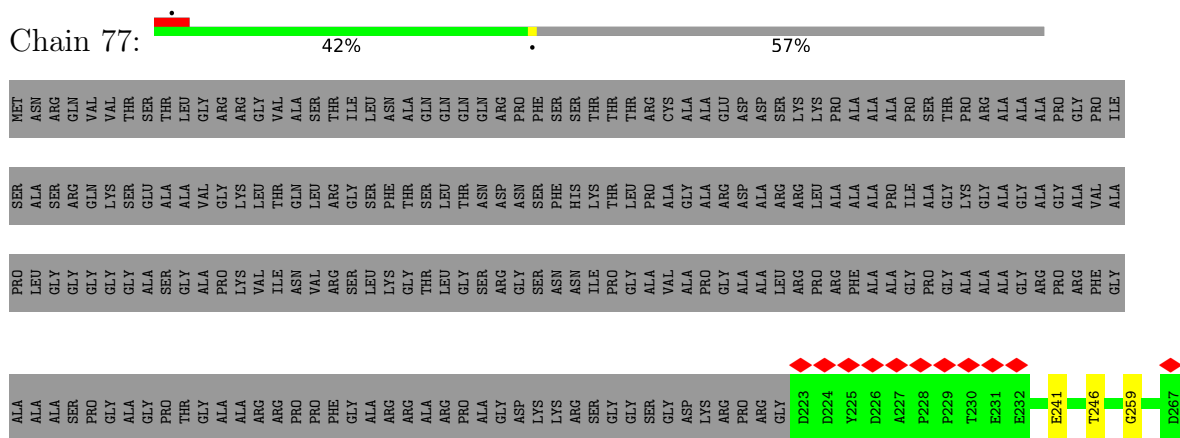
- 

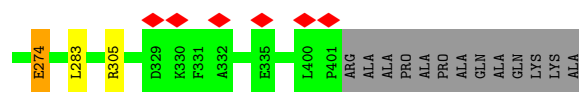


- Molecule 74: mS45



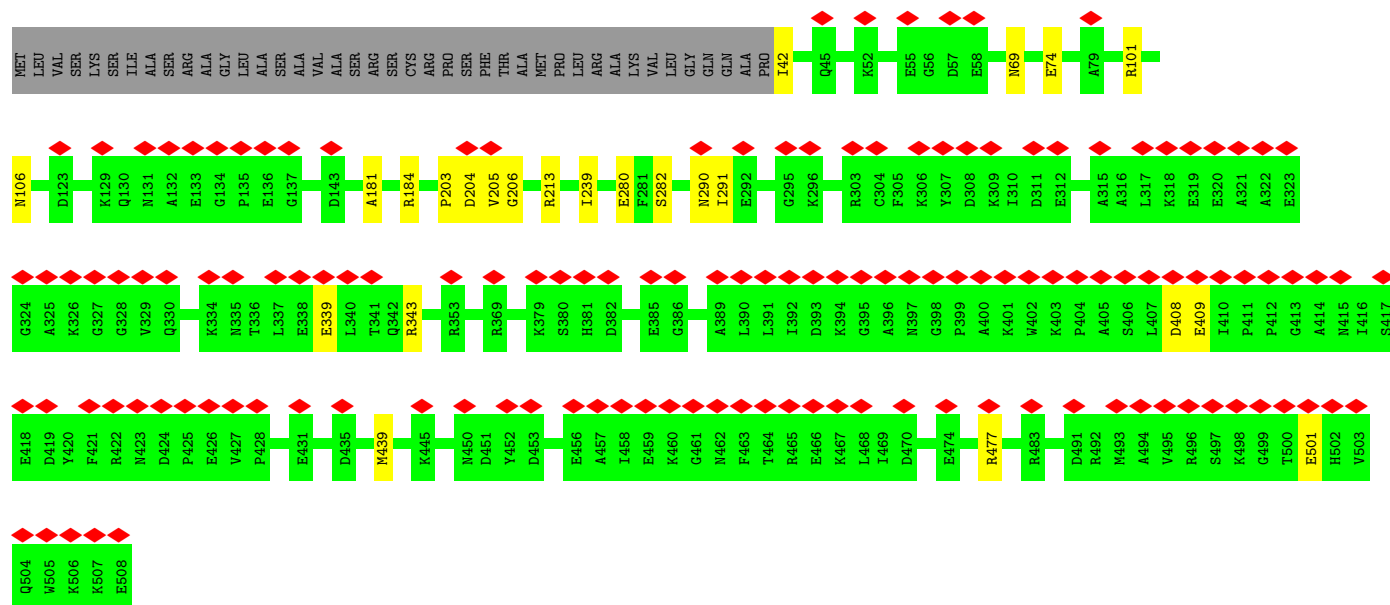
- Molecule 75: mS46





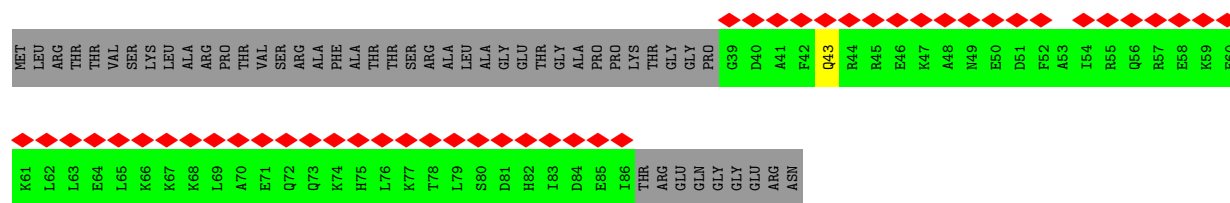
- Molecule 76: 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial

Chain 88: 27% 87% 5% 8%



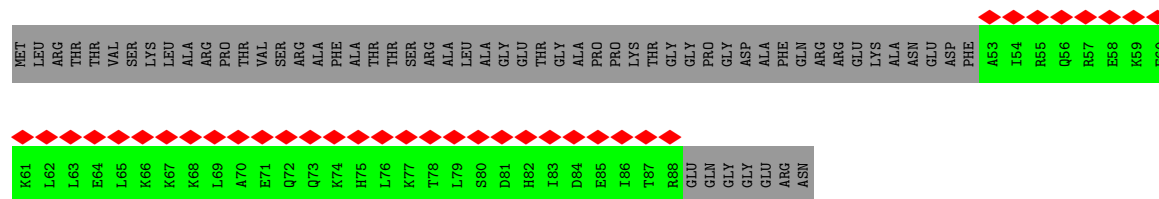
- Molecule 77: IF1

Chain 00: 49% 49% 49%



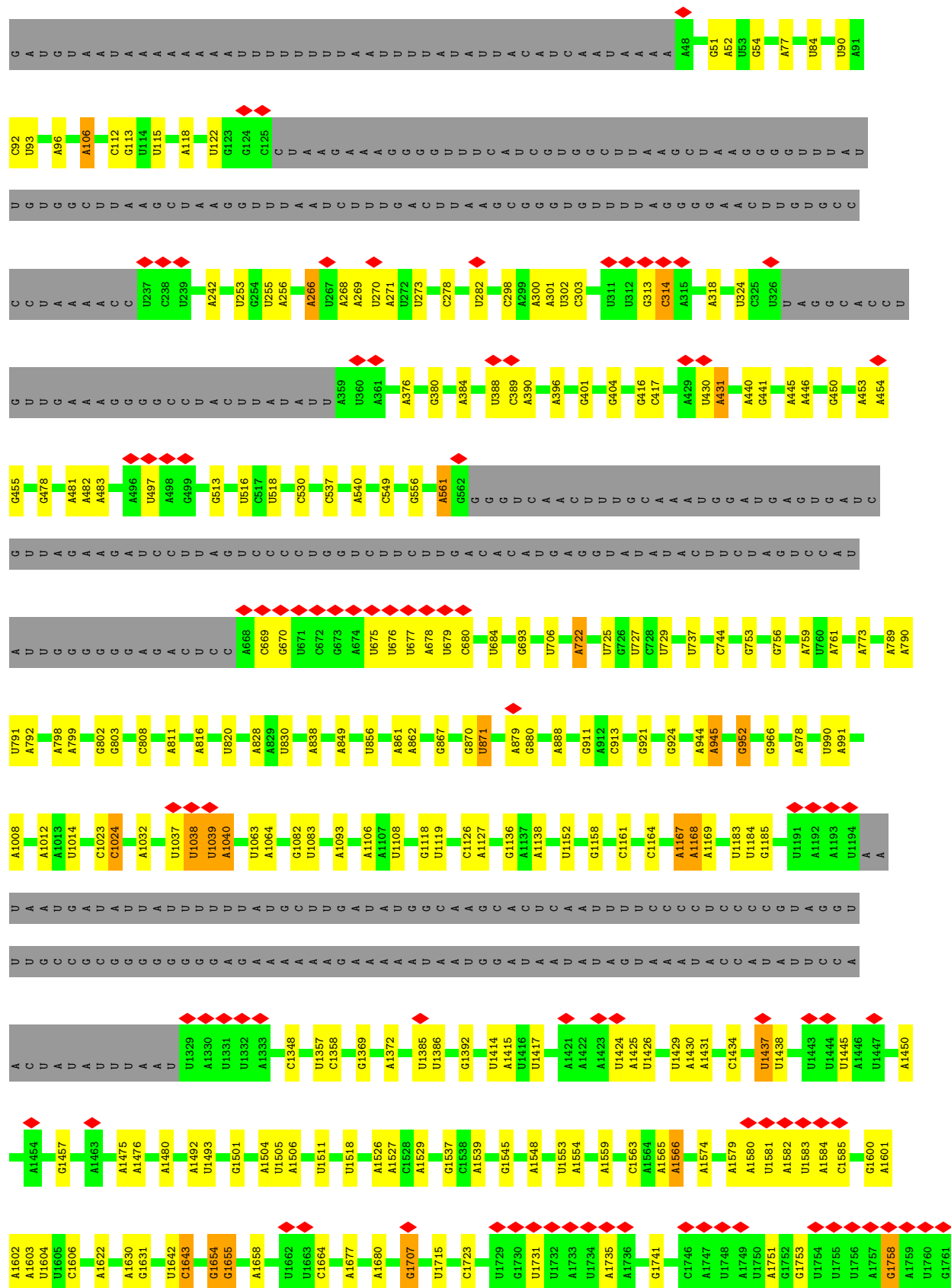
- Molecule 77: IF1

Chain 99: 38% 38% 62%

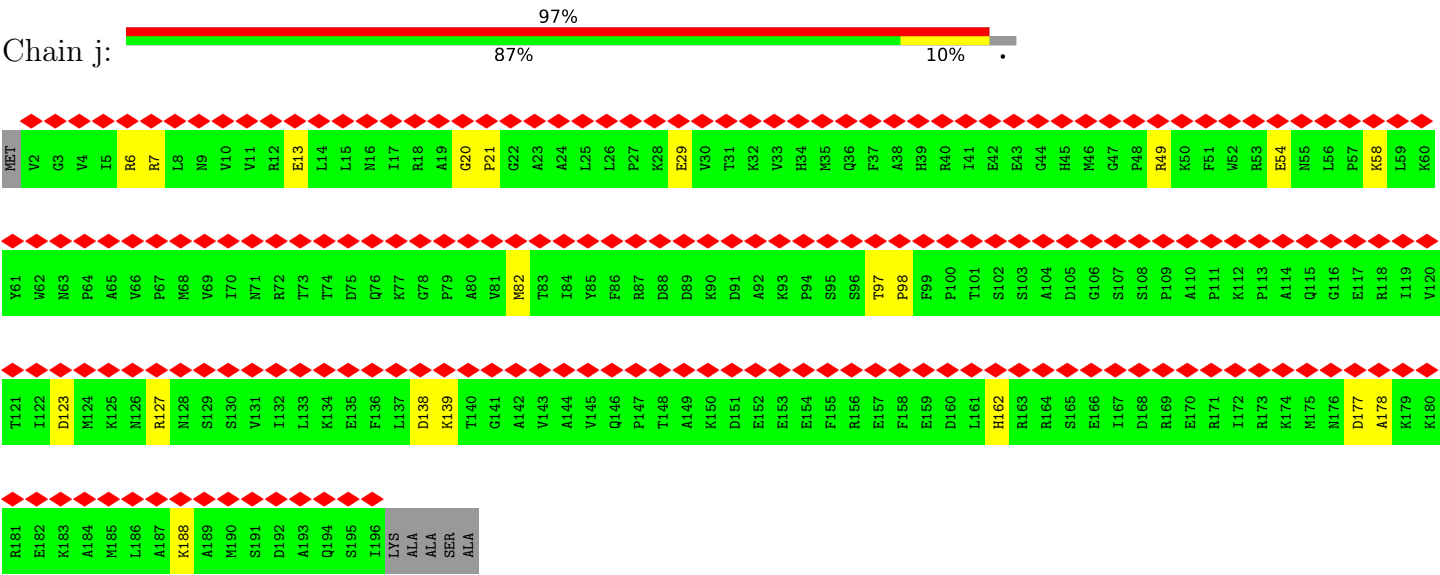


- Molecule 78: 16S rRNA

Chain aa: 6% 63% 13% 23%



● Molecule 83: L51_S25_CI-B8 domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	38.193	Depositor
Minimum map value	-22.800	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.186	Depositor
Recommended contour level	4.77	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.11	0/67912	0.18	0/105757
2	B	0.14	0/2514	0.29	0/3388
3	C	0.14	0/2380	0.28	0/3209
4	D	0.13	0/2072	0.26	0/2794
5	E	0.12	0/2518	0.26	0/3427
6	F	0.11	0/1644	0.24	0/2218
7	G	0.11	0/630	0.29	0/842
8	f	0.08	0/1923	0.22	0/2631
9	g	0.09	0/1126	0.25	0/1525
10	H	0.16	0/1460	0.28	0/1975
11	I	0.13	0/918	0.28	0/1225
12	J	0.13	0/1931	0.26	0/2597
13	K	0.15	0/1376	0.29	0/1842
14	L	0.13	0/1569	0.28	0/2106
15	M	0.12	0/1572	0.27	0/2117
16	N	0.14	0/1077	0.28	0/1452
17	O	0.13	0/2248	0.26	0/3015
18	P	0.13	0/1523	0.24	0/2058
19	Q	0.11	0/2916	0.26	0/3927
20	R	0.14	0/2083	0.29	0/2789
21	S	0.13	0/1510	0.28	0/2042
22	T	0.12	0/1538	0.26	0/2086
23	U	0.13	0/1117	0.28	0/1496
24	V	0.11	0/766	0.25	0/1034
25	W	0.16	0/467	0.31	0/616
26	X	0.15	0/411	0.29	0/551
27	Y	0.19	0/368	0.36	0/485
28	0	0.16	0/395	0.29	0/523
29	1	0.12	0/3053	0.26	0/4108
30	2	0.13	0/1074	0.30	0/1449
31	3	0.13	0/783	0.25	0/1056
32	4	0.13	0/1077	0.25	0/1453

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	5	0.12	0/2790	0.25	0/3794
34	6	0.11	0/2274	0.26	0/3062
35	7	0.12	0/686	0.29	0/919
36	8	0.09	0/2714	0.25	0/3657
37	h	0.08	0/791	0.23	0/1065
38	i	0.09	0/989	0.24	0/1324
39	9	0.09	0/1678	0.26	0/2267
40	a	0.12	0/1364	0.26	0/1842
41	b	0.12	0/1348	0.25	0/1816
42	c	0.17	0/846	0.30	0/1134
43	d	0.11	0/1930	0.25	0/2597
44	AA	0.11	0/2948	0.24	0/3995
45	BB	0.14	0/2314	0.28	0/3142
46	CC	0.15	0/3712	0.26	0/4978
47	DD	0.16	0/2408	0.28	0/3255
48	EE	0.14	0/2928	0.27	0/3947
49	FF	0.13	0/952	0.27	0/1285
50	GG	0.13	0/1765	0.28	0/2392
51	HH	0.16	0/1259	0.28	0/1707
52	II	0.13	0/2012	0.27	0/2720
53	JJ	0.17	0/1590	0.28	0/2140
54	KK	0.14	0/1015	0.29	0/1357
55	LL	0.15	0/973	0.31	0/1305
56	MM	0.13	0/950	0.30	0/1274
57	NN	0.18	0/929	0.29	0/1243
58	OO	0.13	0/2242	0.27	0/3016
59	PP	0.17	0/806	0.26	0/1096
60	QQ	0.12	0/1268	0.25	0/1701
61	RR	0.13	0/1105	0.27	0/1491
62	SS	0.13	0/667	0.25	0/902
63	TT	0.15	0/761	0.29	0/1015
64	UU	0.13	0/1890	0.27	0/2554
65	VV	0.11	0/2120	0.24	0/2851
66	WW	0.10	0/2897	0.25	0/3911
67	XX	0.14	0/3234	0.27	0/4374
68	YY	0.14	0/797	0.31	0/1070
69	ZZ	0.13	0/2645	0.25	0/3566
70	11	0.12	0/686	0.24	0/929
71	22	0.17	0/301	0.30	0/388
72	33	0.14	0/1573	0.30	0/2119
73	44	0.09	0/2121	0.23	0/2879
73	55	0.08	0/1912	0.22	0/2600
74	66	0.13	0/2348	0.27	0/3163

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	77	0.13	0/1431	0.21	0/1934
76	88	0.11	0/3760	0.25	0/5085
77	00	0.08	0/409	0.21	0/540
77	99	0.09	0/307	0.19	0/405
78	aa	0.11	0/34270	0.18	0/53383
79	bb	0.06	0/1741	0.15	0/2708
80	ee	0.08	0/254	0.19	0/392
81	cc	0.06	0/34	0.21	0/46
82	e	0.08	0/1206	0.24	0/1624
83	j	0.11	0/1583	0.29	0/2130
All	All	0.12	0/231484	0.23	0/333882

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60640	30416	30431	146	0
2	B	2456	2508	2508	11	0
3	C	2336	2421	2420	13	0
4	D	2028	2040	2040	6	0
5	E	2449	2461	2461	10	0
6	F	1608	1645	1645	3	0
7	G	618	627	627	2	0
8	f	1876	1925	1925	8	0
9	g	1103	1154	1154	9	0
10	H	1426	1459	1459	4	0
11	I	913	985	985	4	0
12	J	1888	1939	1939	6	0
13	K	1350	1401	1401	6	0
14	L	1545	1590	1590	5	0
15	M	1536	1628	1628	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	N	1056	1120	1120	5	0
17	O	2209	2323	2323	11	0
18	P	1481	1494	1494	5	0
19	Q	2868	2961	2961	14	0
20	R	2046	2149	2149	9	0
21	S	1472	1507	1507	8	0
22	T	1497	1453	1453	10	0
23	U	1099	1164	1164	6	0
24	V	750	735	735	5	0
25	W	460	489	488	4	0
26	X	403	433	433	2	0
27	Y	365	412	412	3	0
28	0	388	409	409	0	0
29	1	2985	3029	3029	13	0
30	2	1046	1055	1055	4	0
31	3	763	773	773	3	0
32	4	1052	1087	1087	4	0
33	5	2719	2710	2710	10	0
34	6	2226	2248	2248	7	0
35	7	674	709	709	4	0
36	8	2660	2714	2714	8	0
37	h	779	798	798	3	0
38	i	976	1022	1022	7	0
39	9	1643	1698	1698	6	0
40	a	1331	1340	1340	2	0
41	b	1314	1379	1379	5	0
42	c	827	873	873	1	0
43	d	1888	1909	1909	8	0
44	AA	2883	2907	2907	19	0
45	BB	2269	2301	2301	13	0
46	CC	3641	3897	3897	12	0
47	DD	2342	2373	2373	17	0
48	EE	2880	2918	2918	15	0
49	FF	935	966	966	6	0
50	GG	1724	1799	1799	7	0
51	HH	1235	1286	1286	4	0
52	II	1968	2026	2026	8	0
53	JJ	1551	1554	1554	8	0
54	KK	995	1025	1025	8	0
55	LL	959	1032	1032	8	0
56	MM	937	986	986	5	0
57	NN	914	961	961	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	OO	2198	2230	2230	6	0
59	PP	786	826	826	2	0
60	QQ	1247	1314	1314	5	0
61	RR	1080	1089	1089	5	0
62	SS	648	677	677	4	0
63	TT	746	772	772	3	0
64	UU	1844	1843	1842	12	0
65	VV	2080	2112	2112	14	0
66	WW	2843	2901	2900	9	0
67	XX	3175	3271	3271	11	0
68	YY	786	823	823	3	0
69	ZZ	2586	2528	2528	14	0
70	11	672	686	686	2	0
71	22	301	359	359	2	0
72	33	1539	1595	1595	9	0
73	44	2062	1983	1982	8	0
73	55	1858	1794	1793	11	0
74	66	2298	2330	2330	20	0
75	77	1400	1396	1396	3	0
76	88	3677	3650	3650	15	0
77	00	406	417	417	1	0
77	99	306	333	333	0	0
78	aa	30608	15373	15377	83	0
79	bb	1557	789	790	1	0
80	ee	229	115	115	0	0
81	cc	35	34	34	0	0
82	e	1184	1212	1212	6	0
83	j	1553	1586	1586	12	0
84	00	1	0	0	0	0
84	A	144	0	0	0	0
84	BB	1	0	0	0	0
84	K	1	0	0	0	0
84	KK	1	0	0	0	0
84	L	1	0	0	0	0
84	QQ	1	0	0	0	0
84	XX	1	0	0	0	0
84	YY	1	0	0	0	0
84	aa	97	0	0	0	0
84	ee	1	0	0	0	0
85	A	14	26	26	0	0
86	2	1	0	0	0	0
86	3	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	88	1	0	0	0	0
86	A	32	0	0	0	0
86	ZZ	1	0	0	0	0
86	aa	13	0	0	0	0
87	0	1	0	0	0	0
87	W	1	0	0	0	0
88	2	44	26	26	3	0
89	XX	31	12	12	2	0
All	All	218076	174325	174339	631	0

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

All (631) 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)
57:NN:75:ARG:NH1	57:NN:80:GLY:O	2.08	0.86
67:XX:152:ARG:NH1	67:XX:415:LYS:O	2.09	0.85
1:A:2337:U:O2'	1:A:2339:U:OP1	1.96	0.83
69:ZZ:212:ARG:NH1	69:ZZ:257:GLU:OE1	2.12	0.82
57:NN:22:ASP:OD2	57:NN:26:ARG:NH1	2.12	0.82
1:A:3094:A:OP1	10:H:94:ARG:NH1	2.14	0.81
14:L:136:ARG:NH1	25:W:95:PRO:O	2.13	0.81
47:DD:407:ARG:NH1	74:66:198:HIS:O	2.14	0.81
1:A:2757:G:OP2	30:2:285:ARG:NH1	2.15	0.80
5:E:268:ARG:NH2	5:E:308:GLU:OE1	2.14	0.80
1:A:445:A:OP2	19:Q:324:ARG:NH2	2.16	0.79
1:A:3452:A:OP2	33:5:218:ARG:NH1	2.17	0.78
71:22:315:ARG:NH2	78:aa:1108:U:OP1	2.17	0.78
33:5:146:LEU:O	39:9:140:ARG:NH2	2.18	0.77
72:33:165:LYS:NZ	78:aa:324:U:OP2	2.17	0.77
46:CC:478:ARG:NH1	57:NN:101:LEU:O	2.17	0.77
1:A:29:A:O3'	3:C:78:ARG:NH1	2.17	0.77
5:E:343:GLN:OE1	30:2:345:SER:OG	2.03	0.76
1:A:2797:C:OP1	26:X:39:LYS:NZ	2.18	0.76
14:L:58:ARG:O	14:L:86:ARG:NH1	2.19	0.76
67:XX:180:ARG:O	67:XX:182:THR:N	2.19	0.76
74:66:284:GLU:OE2	74:66:288:ARG:NH2	2.20	0.76
21:S:93:THR:OG1	21:S:140:ARG:NH1	2.19	0.75
74:66:336:ARG:NH1	78:aa:549:C:O2	2.18	0.75
43:d:75:ASN:ND2	43:d:79:PRO:O	2.20	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:219:PHE:O	29:1:340:ARG:NH1	2.19	0.75
54:KK:362:LEU:O	78:aa:871:U:O2'	2.05	0.75
58:OO:130:LEU:O	65:VV:221:ARG:NH1	2.18	0.75
41:b:121:GLY:O	41:b:126:ARG:NH2	2.20	0.74
64:UU:150:ASP:OD1	64:UU:153:ARG:NH2	2.20	0.74
64:UU:63:ARG:NH2	78:aa:945:A:OP1	2.21	0.74
15:M:232:VAL:O	66:WW:96:GLN:NE2	2.20	0.74
47:DD:126:ARG:NH2	48:EE:472:TYR:O	2.21	0.74
1:A:2481:G:O2'	1:A:2483:G:OP2	2.05	0.73
33:5:229:ASP:OD1	33:5:233:ASP:N	2.21	0.73
19:Q:164:GLN:NE2	19:Q:169:LYS:O	2.21	0.73
47:DD:80:ASN:O	47:DD:126:ARG:NH1	2.20	0.73
44:AA:168:LEU:O	65:VV:303:ARG:NH1	2.21	0.73
1:A:2366:G:OP2	83:j:49:ARG:NH2	2.22	0.72
50:GG:165:ASN:OD1	50:GG:168:ARG:NH2	2.22	0.72
1:A:2158:U:O2'	79:bb:12:U:O2'	2.06	0.72
53:JJ:150:ARG:NH2	78:aa:1431:A:OP2	2.23	0.72
1:A:2536:A:OP1	20:R:262:ARG:NH1	2.23	0.71
5:E:268:ARG:NH1	24:V:62:GLN:OE1	2.23	0.71
8:f:96:GLN:OE1	37:h:24:ARG:NH2	2.24	0.71
48:EE:147:ARG:NH2	75:77:241:GLU:O	2.24	0.70
1:A:2925:A:OP2	1:A:2926:C:N4	2.24	0.70
1:A:3334:C:OP1	3:C:217:ARG:NH1	2.25	0.70
29:1:375:ARG:NH1	29:1:376:GLU:OE2	2.25	0.70
1:A:1291:A:N6	1:A:1358:A:OP2	2.25	0.70
1:A:2008:U:OP2	1:A:2013:A:N6	2.22	0.70
46:CC:333:LEU:O	48:EE:82:LYS:NZ	2.24	0.69
1:A:2276:U:OP1	3:C:63:VAL:N	2.25	0.69
40:a:61:ASN:O	40:a:68:ARG:NH2	2.25	0.69
49:FF:76:GLU:OE1	49:FF:79:ARG:NH1	2.25	0.69
46:CC:343:ASN:ND2	53:JJ:87:SER:O	2.26	0.69
29:1:292:ARG:NH2	29:1:368:ASN:OD1	2.25	0.69
1:A:3363:A:O2'	1:A:3365:A:OP2	2.11	0.69
49:FF:112:ARG:NH1	65:VV:278:GLU:OE1	2.24	0.69
72:33:211:GLU:N	78:aa:106:A:OP2	2.24	0.69
1:A:2153:G:OP2	1:A:2153:G:N2	2.25	0.68
45:BB:209:ARG:NH2	76:88:280:GLU:OE2	2.25	0.68
72:33:97:ARG:NH2	78:aa:537:C:OP2	2.27	0.68
1:A:831:U:OP1	1:A:854:A:O2'	2.12	0.68
38:i:143:ALA:O	38:i:147:ALA:N	2.27	0.67
54:KK:324:GLU:OE1	54:KK:355:ARG:NH1	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:HH:15:ASN:OD1	51:HH:18:ARG:NH2	2.28	0.67
45:BB:359:GLN:OE1	45:BB:362:ARG:NH2	2.27	0.67
82:e:73:GLN:OE1	82:e:74:GLN:N	2.27	0.67
1:A:2951:U:O2'	1:A:2955:U:OP1	2.12	0.67
29:1:105:GLU:O	29:1:116:ARG:NH1	2.27	0.67
17:O:364:TRP:O	32:4:125:ARG:NH1	2.28	0.67
1:A:1330:A:OP2	38:i:198:ARG:NH2	2.28	0.67
1:A:2512:A:OP2	29:1:182:ARG:NH2	2.27	0.67
78:aa:1039:U:O2'	78:aa:1040:A:O4'	2.13	0.66
83:j:54:GLU:O	83:j:58:LYS:NZ	2.29	0.66
47:DD:186:GLY:O	74:66:158:ARG:NH1	2.27	0.66
48:EE:318:LEU:O	48:EE:413:ARG:NH2	2.29	0.66
48:EE:129:TYR:OH	53:JJ:122:ARG:NH1	2.29	0.66
29:1:267:ASP:OD1	29:1:271:ARG:NH2	2.29	0.65
55:LL:129:ARG:NH2	55:LL:130:GLY:O	2.29	0.65
76:88:42:ILE:O	76:88:101:ARG:NH2	2.29	0.65
82:e:300:GLU:N	82:e:300:GLU:OE1	2.29	0.65
51:HH:63:THR:OG1	76:88:74:GLU:OE2	2.14	0.65
1:A:3033:G:N2	1:A:3033:G:OP2	2.30	0.64
1:A:1271:A:OP1	1:A:1382:C:O2'	2.14	0.64
1:A:966:A:OP1	2:B:314:ARG:NH1	2.30	0.64
1:A:3166:U:O2'	15:M:163:ASP:OD2	2.15	0.64
78:aa:1136:G:N1	78:aa:1622:A:OP2	2.28	0.64
35:7:111:GLN:NE2	35:7:147:GLU:OE2	2.30	0.64
69:ZZ:212:ARG:O	69:ZZ:262:ASN:ND2	2.30	0.64
53:JJ:102:ARG:NH2	53:JJ:144:GLY:O	2.31	0.64
1:A:2492:A:O2'	1:A:2634:A:N6	2.31	0.63
44:AA:160:ARG:NH2	44:AA:262:ASP:OD1	2.31	0.63
67:XX:271:LEU:O	67:XX:275:ASN:ND2	2.31	0.63
78:aa:1429:U:O4	78:aa:1430:A:N6	2.32	0.63
1:A:2380:G:N1	1:A:2383:A:OP2	2.31	0.63
47:DD:407:ARG:NH2	74:66:118:PRO:O	2.32	0.63
2:B:280:ARG:NH2	2:B:364:LYS:O	2.32	0.63
1:A:2332:A:H4'	1:A:2332:A:OP1	1.98	0.63
78:aa:1037:U:O2'	78:aa:1039:U:O4	2.16	0.63
41:b:40:HIS:O	41:b:40:HIS:ND1	2.32	0.62
32:4:81:ARG:NH1	32:4:107:GLY:O	2.32	0.62
73:44:181:GLN:N	73:44:181:GLN:OE1	2.33	0.62
78:aa:513:G:N2	78:aa:516:U:OP2	2.31	0.62
83:j:29:GLU:OE1	83:j:29:GLU:N	2.32	0.62
73:44:68:ASN:ND2	73:44:72:THR:OG1	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:88:339:GLU:O	76:88:343:ARG:NH2	2.32	0.62
41:b:157:TRP:NE1	41:b:159:LYS:O	2.32	0.62
1:A:3366:U:O4	3:C:272:ARG:NH2	2.31	0.62
13:K:91:THR:O	13:K:134:ARG:NH1	2.32	0.62
78:aa:298:C:N4	78:aa:301:A:OP2	2.32	0.61
6:F:169:ARG:NE	6:F:192:GLU:OE2	2.33	0.61
1:A:2584:U:O4	1:A:2585:A:N6	2.33	0.61
11:I:114:GLU:N	11:I:114:GLU:OE2	2.33	0.61
55:LL:134:GLN:N	55:LL:134:GLN:OE1	2.33	0.61
67:XX:184:LYS:NZ	89:XX:501:ATP:O1G	2.33	0.61
34:6:149:ARG:NH2	34:6:152:VAL:O	2.32	0.61
66:WW:129:ASN:OD1	66:WW:130:GLY:N	2.34	0.61
1:A:846:A:OP2	20:R:298:ARG:NH2	2.33	0.61
29:1:264:GLN:NE2	29:1:265:VAL:O	2.33	0.61
63:TT:149:GLN:N	63:TT:152:LEU:O	2.33	0.61
78:aa:1642:U:OP2	78:aa:1643:C:N4	2.33	0.61
45:BB:231:ARG:NH2	52:II:99:GLU:OE2	2.34	0.61
17:O:241:LYS:NZ	19:Q:72:ASP:OD1	2.34	0.60
83:j:177:ASP:OD1	83:j:178:ALA:N	2.34	0.60
59:PP:70:ILE:O	65:VV:131:ARG:NH1	2.33	0.60
61:RR:217:SER:OG	78:aa:871:U:OP1	2.19	0.60
46:CC:368:SER:O	53:JJ:81:GLU:N	2.35	0.60
67:XX:323:ASN:OD1	67:XX:327:GLU:N	2.34	0.60
19:Q:147:GLU:OE1	19:Q:177:ARG:NH1	2.34	0.60
55:LL:160:ARG:NH2	78:aa:727:U:OP1	2.34	0.60
9:g:93:ALA:O	9:g:101:ARG:NH1	2.35	0.60
76:88:69:ASN:ND2	76:88:106:ASN:OD1	2.34	0.60
1:A:3111:G:N2	1:A:3114:A:OP2	2.34	0.59
64:UU:113:ASP:O	64:UU:120:GLN:NE2	2.34	0.59
65:VV:87:PRO:O	65:VV:146:LYS:NZ	2.34	0.59
1:A:1314:G:N2	1:A:1341:A:O2'	2.36	0.59
38:i:195:GLU:OE1	38:i:195:GLU:N	2.35	0.59
65:VV:121:GLU:OE1	65:VV:124:ARG:NH1	2.36	0.59
1:A:1634:G:OP1	21:S:120:ARG:NH2	2.35	0.59
52:II:298:ARG:NH1	52:II:299:LYS:O	2.36	0.59
1:A:537:U:O2'	31:3:13:ARG:NH1	2.36	0.59
34:6:197:SER:OG	34:6:199:ASP:OD1	2.18	0.59
34:6:266:GLU:OE1	34:6:274:ARG:NH2	2.35	0.59
45:BB:137:LEU:O	73:44:123:HIS:ND1	2.35	0.59
4:D:81:GLU:OE2	4:D:285:ARG:NE	2.36	0.59
45:BB:117:ILE:O	52:II:154:HIS:NE2	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SS:40:ARG:NH2	78:aa:1604:U:O2	2.36	0.58
78:aa:870:G:O2'	78:aa:871:U:OP1	2.21	0.58
60:QQ:84:ARG:NH1	78:aa:384:A:OP2	2.37	0.58
1:A:473:G:N7	21:S:147:ARG:NH2	2.52	0.58
1:A:2332:A:C8	1:A:2332:A:H5''	2.38	0.58
23:U:142:ARG:NH1	36:8:388:LEU:O	2.37	0.58
47:DD:73:ARG:NH1	47:DD:450:LEU:O	2.37	0.57
33:5:204:TYR:OH	39:9:196:MET:O	2.22	0.57
47:DD:65:ARG:O	74:66:338:ARG:NH1	2.37	0.57
1:A:3389:G:O2'	1:A:3409:A:N6	2.37	0.57
1:A:1976:G:O2'	78:aa:1723:C:N4	2.38	0.57
17:O:278:GLU:OE2	17:O:280:ARG:NH2	2.37	0.57
40:a:88:LEU:O	40:a:95:ARG:NH2	2.38	0.57
49:FF:4:GLU:OE2	61:RR:171:ARG:NE	2.37	0.57
1:A:833:A:OP1	12:J:109:LYS:NZ	2.38	0.57
36:8:195:GLU:OE1	36:8:339:ARG:NE	2.37	0.57
78:aa:693:G:N1	78:aa:722:A:OP2	2.36	0.57
1:A:2785:A:O2'	1:A:2786:A:OP2	2.22	0.57
78:aa:1758:G:N2	78:aa:1758:G:OP2	2.36	0.57
19:Q:248:ASP:OD1	22:T:123:GLY:N	2.37	0.56
1:A:2540:C:OP2	20:R:323:ARG:NH2	2.36	0.56
1:A:2251:U:O2'	25:W:66:PRO:O	2.23	0.56
50:GG:291:THR:O	50:GG:294:ARG:NH2	2.33	0.56
57:NN:57:GLN:NE2	62:SS:16:PRO:O	2.38	0.56
76:88:184:ARG:NE	76:88:239:ILE:O	2.33	0.56
83:j:138:ASP:OD1	83:j:139:LYS:N	2.38	0.56
8:f:98:ASN:OD1	8:f:99:ASN:ND2	2.36	0.56
22:T:214:ASN:ND2	22:T:217:ASN:O	2.39	0.56
1:A:1565:A:O2'	1:A:1566:A:OP2	2.21	0.56
78:aa:678:A:O2'	78:aa:679:U:O4'	2.16	0.56
1:A:1291:A:OP1	8:f:69:ARG:NE	2.39	0.56
1:A:2687:G:OP2	29:1:292:ARG:NH1	2.38	0.56
10:H:8:THR:N	17:O:352:ASP:OD1	2.37	0.56
65:VV:93:GLU:OE2	65:VV:102:ARG:NH1	2.38	0.56
17:O:332:ARG:NH1	17:O:336:GLU:OE1	2.39	0.56
58:OO:152:ALA:O	58:OO:155:ARG:NH2	2.39	0.56
1:A:2390:U:OP1	83:j:7:ARG:NH1	2.39	0.56
1:A:2635:A:O2'	1:A:2636:U:O3'	2.24	0.56
38:i:185:GLN:OE1	38:i:185:GLN:N	2.36	0.56
56:MM:10:ASN:OD1	56:MM:11:GLU:N	2.39	0.55
45:BB:144:ARG:NH2	64:UU:105:ASP:OD1	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:88:213:ARG:NH1	76:88:439:MET:O	2.38	0.55
1:A:822:U:N3	1:A:823:G:O6	2.39	0.55
69:ZZ:52:ASP:OD1	69:ZZ:52:ASP:N	2.38	0.55
14:L:103:GLU:O	14:L:113:SER:OG	2.23	0.55
17:O:206:ARG:NH1	25:W:80:MET:SD	2.79	0.55
44:AA:155:GLN:N	44:AA:155:GLN:OE1	2.39	0.55
49:FF:37:ASP:OD1	49:FF:38:ILE:N	2.40	0.55
76:88:204:ASP:O	76:88:206:GLY:N	2.40	0.55
53:JJ:169:GLU:OE1	57:NN:97:ARG:NH2	2.38	0.55
1:A:3446:U:O2'	1:A:3448:A:OP1	2.24	0.55
18:P:60:ASP:OD1	18:P:64:HIS:ND1	2.39	0.55
59:PP:57:LYS:NZ	78:aa:706:U:OP1	2.39	0.55
12:J:109:LYS:O	29:1:447:ARG:NH1	2.40	0.55
44:AA:306:TYR:OH	64:UU:94:GLU:OE2	2.24	0.55
64:UU:125:LEU:O	64:UU:160:ARG:NH2	2.39	0.55
76:88:290:ASN:OD1	76:88:291:ILE:N	2.40	0.55
27:Y:137:ARG:NE	27:Y:140:ALA:O	2.40	0.54
78:aa:478:G:N1	78:aa:481:A:OP2	2.40	0.54
78:aa:1008:A:O2'	78:aa:1093:A:N1	2.40	0.54
66:WW:359:GLN:OE1	66:WW:363:ARG:NH1	2.40	0.54
10:H:14:ARG:NH1	10:H:67:ASP:O	2.40	0.54
78:aa:1437:U:O2'	78:aa:1438:U:OP2	2.18	0.54
9:g:28:SER:O	9:g:32:GLY:N	2.35	0.54
36:8:163:ASP:OD2	36:8:167:GLN:NE2	2.41	0.54
44:AA:308:ARG:NH2	73:55:156:ASP:OD2	2.41	0.54
82:e:232:VAL:O	82:e:245:ASN:ND2	2.38	0.54
73:44:254:CYS:SG	73:44:255:LEU:N	2.81	0.54
1:A:1178:U:O2	1:A:1178:U:C2'	2.56	0.54
76:88:181:ALA:O	76:88:184:ARG:NH1	2.41	0.54
1:A:1014:G:O2'	12:J:85:GLN:OE1	2.26	0.54
44:AA:298:THR:OG1	44:AA:299:HIS:N	2.41	0.54
60:QQ:94:ALA:O	60:QQ:101:ARG:NH2	2.40	0.54
1:A:2362:A:N1	1:A:2374:A:O2'	2.40	0.53
30:2:299:GLU:OE2	88:2:4301:NAD:O2D	2.26	0.53
63:TT:165:TYR:O	63:TT:170:GLN:NE2	2.41	0.53
22:T:171:GLU:OE1	22:T:171:GLU:N	2.40	0.53
37:h:72:ASN:OD1	37:h:73:MET:N	2.40	0.53
49:FF:54:GLN:N	49:FF:54:GLN:OE1	2.41	0.53
74:66:321:ASP:O	74:66:328:ARG:NH1	2.39	0.53
8:f:162:ALA:N	8:f:170:VAL:O	2.41	0.53
55:LL:117:GLY:O	55:LL:145:ARG:NH2	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:ZZ:123:ARG:NH2	69:ZZ:142:ASP:OD1	2.41	0.53
19:Q:104:ARG:NH1	19:Q:143:ASN:O	2.42	0.53
69:ZZ:197:ARG:NH1	69:ZZ:217:GLU:OE2	2.41	0.53
1:A:2541:A:OP2	20:R:323:ARG:NH1	2.42	0.53
47:DD:39:SER:O	48:EE:316:LYS:NZ	2.41	0.53
70:11:17:ARG:NH1	78:aa:1846:U:OP2	2.42	0.53
1:A:645:U:O2'	1:A:821:A:N6	2.42	0.53
1:A:1461:G:OP1	12:J:77:THR:OG1	2.24	0.53
67:XX:279:GLU:N	67:XX:279:GLU:OE1	2.42	0.53
1:A:2090:A:N7	7:G:52:ALA:N	2.57	0.53
1:A:2919:G:O2'	1:A:2920:A:OP2	2.23	0.53
44:AA:315:ASN:N	64:UU:172:GLU:OE2	2.39	0.53
46:CC:313:LYS:NZ	78:aa:1434:C:OP1	2.42	0.53
78:aa:1369:G:N2	78:aa:1372:A:OP2	2.39	0.53
4:D:71:SER:O	4:D:75:LEU:N	2.38	0.53
11:I:101:ASP:OD2	11:I:122:LYS:NZ	2.40	0.52
52:II:187:GLN:NE2	78:aa:1424:U:O4	2.42	0.52
65:VV:85:ILE:O	65:VV:94:LYS:NZ	2.41	0.52
46:CC:281:ASN:ND2	69:ZZ:131:GLU:OE1	2.43	0.52
78:aa:1545:G:N2	78:aa:1548:A:OP2	2.37	0.52
62:SS:9:LYS:N	78:aa:1603:A:OP1	2.42	0.52
62:SS:9:LYS:NZ	78:aa:1602:A:OP1	2.35	0.52
1:A:311:G:O6	19:Q:219:ARG:NH1	2.40	0.52
18:P:185:ASN:ND2	19:Q:67:PRO:O	2.38	0.52
47:DD:429:GLY:O	74:66:115:LYS:NZ	2.43	0.52
1:A:2379:U:N3	1:A:2383:A:N7	2.58	0.52
17:O:327:GLU:OE2	17:O:330:ARG:NH1	2.42	0.52
51:HH:30:LYS:N	78:aa:816:A:OP1	2.43	0.52
5:E:130:ARG:NH1	88:2:4301:NAD:O1A	2.40	0.52
58:OO:235:ARG:O	65:VV:207:ARG:NH1	2.42	0.52
1:A:3263:U:O2'	22:T:54:THR:O	2.28	0.51
73:44:128:HIS:NE2	73:44:252:ILE:O	2.43	0.51
73:55:185:LEU:O	73:55:186:ARG:NH1	2.43	0.51
78:aa:966:G:H4'	78:aa:1824:A:H4'	1.93	0.51
65:VV:120:GLN:N	65:VV:120:GLN:OE1	2.42	0.51
83:j:123:ASP:O	83:j:127:ARG:NH1	2.43	0.51
1:A:2346:U:OP1	1:A:2354:U:N3	2.43	0.51
1:A:614:G:OP1	1:A:1528:U:O2'	2.21	0.51
2:B:326:ASP:OD1	2:B:326:ASP:N	2.43	0.51
17:O:51:GLN:O	17:O:56:ARG:NH1	2.39	0.51
44:AA:343:ASP:N	44:AA:343:ASP:OD1	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:NN:10:ASP:OD1	57:NN:10:ASP:N	2.44	0.51
1:A:1305:A:OP1	9:g:132:ARG:NH2	2.43	0.51
24:V:127:ASP:OD1	24:V:127:ASP:N	2.44	0.51
29:1:87:LEU:O	29:1:92:ARG:NH2	2.44	0.51
1:A:339:A:N6	31:3:24:LYS:O	2.43	0.50
1:A:2772:A:N6	1:A:2783:U:O4	2.44	0.50
1:A:3345:U:OP2	3:C:354:LYS:NZ	2.45	0.50
61:RR:142:PRO:O	61:RR:146:LYS:N	2.40	0.50
66:WW:206:ASP:O	66:WW:268:ARG:NH1	2.44	0.50
19:Q:208:ARG:N	19:Q:222:ARG:O	2.43	0.50
48:EE:236:THR:OG1	48:EE:237:GLY:N	2.44	0.50
69:ZZ:77:GLN:N	69:ZZ:77:GLN:OE1	2.45	0.50
1:A:2510:G:OP2	5:E:78:ARG:NH1	2.41	0.50
23:U:52:GLU:OE2	42:c:102:SER:OG	2.29	0.50
44:AA:188:ARG:NE	65:VV:310:GLU:O	2.45	0.50
1:A:875:C:OP1	4:D:118:ARG:NH2	2.41	0.50
60:QQ:80:SER:OG	78:aa:404:G:OP1	2.29	0.50
78:aa:791:U:OP2	78:aa:792:A:O2'	2.27	0.50
83:j:20:GLY:N	83:j:21:PRO:CD	2.75	0.50
1:A:608:A:OP2	16:N:188:ARG:NH1	2.42	0.50
1:A:2883:A:O2'	1:A:2884:A:P	2.69	0.50
33:5:432:ASP:OD1	33:5:433:MET:N	2.44	0.50
50:GG:254:LYS:NZ	50:GG:267:GLU:OE1	2.41	0.50
61:RR:200:ARG:NH2	78:aa:1032:A:OP1	2.43	0.50
78:aa:450:G:N2	78:aa:453:A:OP2	2.36	0.50
1:A:1071:G:O6	1:A:1099:A:N6	2.45	0.50
2:B:373:ASN:ND2	2:B:376:VAL:O	2.39	0.49
34:6:96:ARG:NH1	34:6:230:LEU:O	2.41	0.49
36:8:213:ALA:O	36:8:339:ARG:NH2	2.45	0.49
17:O:237:ARG:NH1	19:Q:73:GLU:OE1	2.43	0.49
41:b:38:GLU:OE1	41:b:38:GLU:N	2.41	0.49
8:f:291:GLY:O	8:f:295:GLN:NE2	2.45	0.49
5:E:143:ILE:HD12	5:E:143:ILE:O	2.13	0.49
74:66:88:HIS:NE2	74:66:183:LYS:O	2.43	0.49
48:EE:379:TYR:N	48:EE:383:THR:O	2.44	0.49
75:77:283:LEU:O	75:77:305:ARG:NH2	2.45	0.49
58:OO:288:ARG:NH1	78:aa:808:C:OP1	2.45	0.49
70:11:45:SER:OG	70:11:46:ALA:N	2.45	0.49
1:A:2343:A:OP2	83:j:6:ARG:NH1	2.46	0.49
78:aa:789:A:O2'	78:aa:792:A:O2'	2.30	0.49
83:j:97:THR:OG1	83:j:98:PRO:HD3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:CC:442:ARG:NH2	46:CC:448:ARG:O	2.36	0.49
53:JJ:118:SER:OG	53:JJ:120:SER:O	2.31	0.49
44:AA:136:ARG:NH2	73:55:149:GLY:O	2.46	0.48
48:EE:287:ASP:OD1	48:EE:288:ASP:N	2.46	0.48
73:44:68:ASN:O	73:44:72:THR:OG1	2.26	0.48
83:j:13:GLU:OE2	83:j:162:HIS:NE2	2.44	0.48
1:A:2924:U:O4	1:A:2925:A:N6	2.47	0.48
75:77:259:GLY:N	75:77:274:GLU:OE2	2.42	0.48
78:aa:1082:G:O2'	78:aa:1083:U:OP2	2.32	0.48
1:A:1906:C:O2	3:C:241:HIS:NE2	2.43	0.48
73:44:210:GLN:OE1	73:55:105:ARG:NH1	2.46	0.48
1:A:1201:G:O6	13:K:76:LYS:NZ	2.47	0.48
1:A:1352:U:OP1	8:f:74:ARG:NH1	2.46	0.48
44:AA:54:THR:HG23	64:UU:98:PRO:HB3	1.95	0.48
3:C:206:ASP:OD2	3:C:335:ARG:NH2	2.41	0.48
38:i:181:ASN:O	38:i:181:ASN:ND2	2.46	0.48
47:DD:197:LEU:O	47:DD:201:GLY:N	2.43	0.48
74:66:226:ARG:NH2	74:66:241:ASP:OD2	2.46	0.48
1:A:59:A:OP1	25:W:76:ARG:NE	2.42	0.48
1:A:1930:U:O2'	2:B:76:ARG:NH1	2.47	0.48
24:V:193:ASP:OD1	24:V:193:ASP:N	2.46	0.48
45:BB:205:ARG:NH2	76:88:282:SER:O	2.46	0.48
1:A:615:G:O2'	1:A:2254:G:OP1	2.30	0.48
2:B:105:GLY:O	2:B:107:ARG:NH1	2.45	0.48
16:N:157:ALA:HB3	16:N:158:PRO:CD	2.43	0.48
26:X:15:ILE:N	26:X:51:LEU:O	2.46	0.48
33:5:346:ARG:O	39:9:65:ARG:NH2	2.46	0.48
64:UU:114:TRP:O	64:UU:133:ARG:NH2	2.43	0.48
78:aa:1039:U:O2'	78:aa:1040:A:O5'	2.32	0.48
1:A:1071:G:N3	1:A:1101:G:N2	2.61	0.48
22:T:149:GLU:OE1	22:T:152:ARG:NH2	2.47	0.48
48:EE:135:ASP:OD1	48:EE:136:ASP:N	2.46	0.48
48:EE:255:ASP:OD1	48:EE:255:ASP:N	2.47	0.48
5:E:157:ARG:NH2	5:E:183:PRO:O	2.42	0.48
33:5:89:HIS:NE2	33:5:98:ILE:O	2.46	0.48
48:EE:345:ASP:OD1	48:EE:378:ARG:NH1	2.47	0.48
72:33:227:LYS:HD3	72:33:228:ALA:N	2.29	0.48
74:66:318:ASP:OD1	74:66:318:ASP:N	2.47	0.48
1:A:577:A:N6	1:A:591:G:O2'	2.47	0.47
1:A:1221:G:HO2'	1:A:1402:A:HO2'	1.62	0.47
1:A:1333:G:OP1	38:i:202:ARG:NH1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:8:236:GLY:O	36:8:326:ILE:N	2.43	0.47
67:XX:180:ARG:C	67:XX:182:THR:H	2.21	0.47
76:88:408:ASP:OD1	76:88:409:GLU:N	2.47	0.47
78:aa:1168:A:OP2	78:aa:1642:U:O2'	2.31	0.47
1:A:3047:G:N2	1:A:3050:A:OP2	2.36	0.47
78:aa:678:A:O2'	78:aa:679:U:O5'	2.31	0.47
8:f:235:SER:OG	8:f:276:TYR:OH	2.30	0.47
30:2:326:GLU:OE2	30:2:332:ARG:NH1	2.47	0.47
33:5:106:THR:O	33:5:120:ASN:ND2	2.47	0.47
82:e:284:ASN:OD1	82:e:285:ALA:N	2.47	0.47
1:A:1307:G:OP2	9:g:65:ARG:NH1	2.47	0.47
12:J:259:ARG:NH2	12:J:277:PRO:O	2.47	0.47
21:S:157:GLU:OE2	21:S:190:ARG:NH1	2.43	0.47
39:9:165:GLU:O	39:9:189:TYR:OH	2.31	0.47
68:YY:94:LYS:NZ	78:aa:1183:U:O2	2.44	0.47
1:A:1135:G:O2'	1:A:1136:A:OP2	2.29	0.47
1:A:2793:C:O2'	1:A:2826:G:O2'	2.32	0.47
20:R:284:ARG:O	41:b:136:ARG:NH1	2.48	0.47
45:BB:189:ARG:NH2	64:UU:76:ILE:O	2.47	0.47
47:DD:448:TRP:O	47:DD:452:ARG:N	2.46	0.47
77:00:43:GLN:N	77:00:43:GLN:OE1	2.48	0.47
19:Q:301:GLU:OE2	19:Q:301:GLU:N	2.48	0.47
29:1:284:ASP:OD1	29:1:286:THR:OG1	2.33	0.47
68:YY:7:ARG:NH2	68:YY:10:GLN:OE1	2.47	0.47
73:55:44:HIS:NE2	73:55:94:LYS:O	2.47	0.47
60:QQ:80:SER:OG	60:QQ:81:LYS:N	2.45	0.47
1:A:96:G:OP2	18:P:93:ARG:NH1	2.42	0.47
1:A:2333:C:H2'	1:A:2334:G:O4'	2.14	0.47
22:T:80:GLU:O	43:d:161:ARG:NH2	2.48	0.47
1:A:541:G:N7	27:Y:135:ARG:NH1	2.51	0.46
1:A:1154:U:OP2	13:K:88:LYS:NZ	2.44	0.46
14:L:33:GLU:OE1	14:L:80:LYS:NZ	2.44	0.46
69:ZZ:78:ASP:N	69:ZZ:78:ASP:OD1	2.49	0.46
69:ZZ:97:ASP:OD1	69:ZZ:98:LEU:N	2.48	0.46
1:A:1921:A:H2'	1:A:1921:A:N3	2.31	0.46
4:D:300:VAL:HG23	4:D:300:VAL:O	2.15	0.46
52:II:197:ARG:NH1	78:aa:1631:G:O6	2.49	0.46
55:LL:153:VAL:O	55:LL:165:THR:OG1	2.33	0.46
44:AA:151:ASP:O	44:AA:153:GLN:NE2	2.48	0.46
46:CC:414:LYS:NZ	48:EE:139:GLU:OE2	2.42	0.46
76:88:501:GLU:OE2	76:88:501:GLU:N	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:DD:55:ARG:NH2	47:DD:62:ILE:O	2.42	0.46
1:A:1178:U:O2	1:A:1178:U:H2'	2.16	0.46
20:R:336:THR:O	20:R:340:GLY:N	2.48	0.46
78:aa:1803:A:N6	78:aa:1804:A:N1	2.64	0.46
78:aa:1501:G:OP2	78:aa:1606:C:N4	2.44	0.46
72:33:104:ARG:NH1	72:33:201:ASP:OD2	2.48	0.46
78:aa:301:A:N6	78:aa:303:C:O2	2.49	0.46
11:I:97:ASN:OD1	11:I:101:ASP:N	2.47	0.45
15:M:49:ARG:NH2	15:M:58:THR:OG1	2.46	0.45
54:KK:344:ASN:O	54:KK:347:ARG:NH2	2.46	0.45
74:66:67:GLN:NE2	78:aa:561:A:O4'	2.49	0.45
1:A:1991:A:N3	1:A:1991:A:H2'	2.30	0.45
18:P:79:GLN:O	18:P:80:ARG:NH2	2.49	0.45
18:P:159:THR:OG1	18:P:161:ASP:OD1	2.32	0.45
74:66:300:THR:OG1	74:66:303:PHE:O	2.32	0.45
78:aa:1600:G:N1	78:aa:1603:A:OP2	2.49	0.45
46:CC:135:ARG:NH2	69:ZZ:144:GLU:OE1	2.49	0.45
69:ZZ:59:ARG:NH1	69:ZZ:65:GLU:OE1	2.45	0.45
16:N:157:ALA:HB3	16:N:158:PRO:HD3	1.98	0.45
1:A:2402:G:H2'	1:A:2403:U:C6	2.52	0.45
16:N:137:ASP:OD2	23:U:86:ARG:NH2	2.50	0.45
46:CC:421:GLN:O	46:CC:425:ASN:ND2	2.50	0.45
1:A:3390:U:OP2	15:M:200:ARG:NH1	2.50	0.45
2:B:68:TYR:OH	2:B:80:ARG:NH1	2.50	0.45
66:WW:205:SER:O	66:WW:205:SER:OG	2.31	0.45
13:K:101:MET:O	13:K:167:ASN:N	2.47	0.45
50:GG:274:GLU:OE1	50:GG:276:ARG:NE	2.47	0.45
66:WW:193:GLU:OE1	66:WW:332:ARG:NH2	2.48	0.45
24:V:193:ASP:O	24:V:197:GLY:N	2.47	0.45
56:MM:65:ILE:O	56:MM:65:ILE:HG22	2.17	0.45
58:OO:284:GLN:NE2	58:OO:316:GLY:O	2.50	0.45
3:C:91:SER:OG	10:H:113:LYS:O	2.35	0.45
21:S:106:ASN:N	21:S:115:THR:O	2.45	0.45
1:A:826:C:O2'	1:A:859:U:OP1	2.35	0.45
22:T:107:TYR:OH	22:T:149:GLU:OE2	2.31	0.45
22:T:157:ASN:OD1	22:T:160:ARG:NH1	2.37	0.45
43:d:94:GLN:OE1	43:d:96:GLN:NE2	2.49	0.45
47:DD:22:ASN:OD1	47:DD:24:TYR:N	2.48	0.45
6:F:208:ARG:NH2	37:h:94:ASP:O	2.46	0.44
17:O:53:VAL:O	17:O:57:ASN:ND2	2.50	0.44
35:7:141:VAL:N	35:7:142:PRO:CD	2.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:KK:374:ARG:NH1	78:aa:1834:G:OP1	2.50	0.44
78:aa:870:G:H2'	78:aa:871:U:C6	2.53	0.44
1:A:2492:A:H2'	1:A:2492:A:N3	2.32	0.44
1:A:3406:U:H3'	1:A:3407:U:H5''	2.00	0.44
23:U:130:ASP:OD1	23:U:131:GLY:N	2.50	0.44
5:E:58:ALA:O	29:1:116:ARG:NH2	2.51	0.44
43:d:112:ARG:O	43:d:156:ARG:NH1	2.50	0.44
78:aa:1862:C:N4	78:aa:1863:G:O6	2.50	0.44
1:A:1388:U:H4'	1:A:1389:A:O4'	2.18	0.44
22:T:216:GLU:OE2	22:T:216:GLU:N	2.47	0.44
73:55:206:GLU:N	73:55:238:LYS:O	2.51	0.44
78:aa:1707:G:N3	78:aa:1707:G:H2'	2.32	0.44
1:A:930:U:HO2'	1:A:3063:U:HO2'	1.62	0.44
1:A:2170:G:N2	1:A:2199:G:OP1	2.51	0.44
1:A:2686:U:N3	29:1:290:PHE:O	2.49	0.44
9:g:148:GLN:O	9:g:151:SER:OG	2.31	0.44
13:K:103:ASP:OD1	13:K:103:ASP:N	2.51	0.44
36:8:228:VAL:O	36:8:228:VAL:HG12	2.18	0.44
9:g:80:THR:N	9:g:130:GLU:OE2	2.51	0.44
13:K:103:ASP:OD2	13:K:106:ARG:NH1	2.51	0.44
14:L:37:THR:OG1	14:L:38:THR:N	2.51	0.44
16:N:99:LEU:O	16:N:105:HIS:NE2	2.49	0.44
50:GG:213:ARG:NH1	50:GG:215:TYR:OH	2.51	0.44
53:JJ:83:GLU:OE1	53:JJ:83:GLU:N	2.51	0.44
1:A:1178:U:O2	1:A:1178:U:H3'	2.17	0.44
1:A:1272:A:O2'	1:A:1381:A:N6	2.50	0.44
1:A:2028:G:O2'	2:B:277:GLU:OE2	2.32	0.44
2:B:172:ASP:N	2:B:291:ILE:O	2.47	0.44
56:MM:66:GLU:O	56:MM:69:ALA:N	2.40	0.44
78:aa:753:G:O2'	78:aa:761:A:N1	2.48	0.44
17:O:61:GLU:O	17:O:65:GLN:NE2	2.51	0.44
36:8:220:ASP:OD2	36:8:224:ARG:NE	2.46	0.44
44:AA:371:ASP:OD1	44:AA:371:ASP:N	2.51	0.44
45:BB:253:GLY:N	45:BB:309:GLU:OE1	2.49	0.44
54:KK:291:LYS:O	78:aa:888:A:N6	2.51	0.44
15:M:219:VAL:HG12	15:M:219:VAL:O	2.18	0.43
58:OO:285:ARG:NH2	78:aa:952:G:OP1	2.51	0.43
67:XX:85:ARG:NH1	78:aa:1574:A:OP2	2.51	0.43
1:A:1475:G:N2	1:A:1513:U:O4	2.51	0.43
1:A:2227:G:N2	1:A:2231:C:O2'	2.52	0.43
46:CC:359:SER:O	46:CC:360:GLN:HB3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:DD:93:GLU:OE1	47:DD:93:GLU:N	2.45	0.43
65:VV:73:PRO:O	74:66:322:ARG:NH1	2.46	0.43
78:aa:1827:G:N1	78:aa:1830:A:OP2	2.50	0.43
1:A:1539:G:O2'	1:A:1540:U:OP2	2.34	0.43
3:C:322:GLU:OE2	3:C:322:GLU:N	2.51	0.43
50:GG:211:LYS:N	50:GG:229:GLN:O	2.49	0.43
65:VV:73:PRO:O	74:66:322:ARG:NH2	2.49	0.43
69:ZZ:85:GLU:HA	69:ZZ:85:GLU:OE1	2.18	0.43
73:55:50:ARG:NH2	73:55:288:ASP:OD2	2.51	0.43
4:D:181:ARG:NH1	4:D:278:THR:O	2.49	0.43
1:A:367:A:N3	1:A:367:A:H2'	2.33	0.43
1:A:909:A:O2'	1:A:910:A:P	2.77	0.43
45:BB:299:ASN:OD1	45:BB:299:ASN:N	2.51	0.43
52:II:154:HIS:O	52:II:158:LYS:N	2.50	0.43
67:XX:391:ARG:NH1	67:XX:400:ASP:OD1	2.45	0.43
4:D:246:ASP:OD1	4:D:248:ARG:NH2	2.52	0.43
8:f:72:ASP:OD1	8:f:73:THR:N	2.52	0.43
39:9:149:ILE:O	39:9:153:THR:OG1	2.28	0.43
1:A:1311:U:OP2	9:g:102:LYS:NZ	2.42	0.43
1:A:3168:U:H4'	11:I:85:VAL:HG21	2.01	0.43
9:g:13:GLU:OE1	9:g:13:GLU:N	2.52	0.43
34:6:334:ASN:HD22	34:6:334:ASN:C	2.25	0.43
44:AA:258:GLY:O	44:AA:262:ASP:N	2.51	0.43
47:DD:138:ALA:N	47:DD:139:PRO:CD	2.81	0.43
54:KK:266:ASN:OD1	54:KK:267:THR:N	2.49	0.43
60:QQ:18:GLU:O	78:aa:820:U:O2'	2.32	0.43
73:55:191:TYR:O	73:55:192:LEU:C	2.61	0.43
1:A:1082:C:O2	1:A:1092:G:N1	2.51	0.43
1:A:1221:G:O2'	1:A:1402:A:O2'	2.33	0.43
1:A:2940:G:N2	1:A:2942:U:O4	2.38	0.43
32:4:49:LEU:N	32:4:50:PRO:CD	2.81	0.43
49:FF:66:ARG:NH1	49:FF:115:GLU:OE1	2.50	0.43
78:aa:1414:U:O4	78:aa:1415:A:N6	2.52	0.43
78:aa:1654:G:H2'	78:aa:1655:G:H5'	2.01	0.43
1:A:450:G:O2'	1:A:473:G:O6	2.33	0.42
1:A:640:G:OP1	35:7:94:ARG:NH1	2.52	0.42
1:A:2040:U:OP1	21:S:118:LYS:NZ	2.51	0.42
1:A:2807:A:O2'	1:A:2808:A:OP1	2.29	0.42
7:G:90:ASN:OD1	21:S:126:LYS:NZ	2.52	0.42
44:AA:248:ASN:OD1	44:AA:249:ASP:N	2.52	0.42
78:aa:1038:U:H4'	78:aa:1039:U:OP2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:5:184:ASP:N	33:5:184:ASP:OD1	2.52	0.42
64:UU:51:ARG:NH1	64:UU:71:PHE:O	2.48	0.42
78:aa:266:A:OP2	78:aa:440:A:N6	2.46	0.42
78:aa:1715:U:N3	78:aa:1780:U:OP2	2.46	0.42
1:A:374:U:OP2	1:A:375:A:O2'	2.34	0.42
1:A:2925:A:O2'	1:A:2926:C:O4'	2.36	0.42
15:M:84:LYS:O	15:M:84:LYS:CG	2.67	0.42
24:V:62:GLN:NE2	24:V:78:MET:SD	2.87	0.42
43:d:88:ALA:O	43:d:134:LEU:N	2.45	0.42
44:AA:393:ASP:OD1	44:AA:397:ARG:N	2.52	0.42
45:BB:212:GLU:OE2	76:88:477:ARG:NH2	2.51	0.42
68:YY:15:ARG:NH1	69:ZZ:236:LYS:O	2.45	0.42
78:aa:1038:U:H3'	78:aa:1039:U:H5'	2.01	0.42
43:d:128:LYS:O	43:d:132:ARG:NH2	2.52	0.42
47:DD:407:ARG:O	74:66:152:ARG:NH1	2.44	0.42
1:A:2197:U:O2'	1:A:2199:G:OP2	2.27	0.42
78:aa:1167:A:H4'	78:aa:1168:A:H5''	2.01	0.42
1:A:342:U:OP1	31:3:16:ARG:NH1	2.52	0.42
1:A:995:U:O2'	1:A:1496:U:O2	2.30	0.42
6:F:181:VAL:O	6:F:181:VAL:HG13	2.20	0.42
54:KK:256:TYR:O	54:KK:324:GLU:N	2.50	0.42
56:MM:40:HIS:NE2	67:XX:217:GLU:OE1	2.52	0.42
66:WW:86:LYS:O	66:WW:90:HIS:ND1	2.51	0.42
73:55:254:CYS:SG	73:55:255:LEU:N	2.91	0.42
78:aa:313:G:O2'	78:aa:314:C:OP2	2.34	0.42
1:A:2481:G:N3	1:A:2481:G:H2'	2.33	0.42
20:R:354:GLU:OE2	20:R:357:ARG:NH2	2.52	0.42
61:RR:143:TYR:O	61:RR:148:ARG:NH1	2.53	0.42
72:33:78:GLU:O	72:33:82:THR:OG1	2.29	0.42
15:M:144:ARG:O	15:M:145:ARG:HG2	2.19	0.42
21:S:159:LEU:O	21:S:178:ARG:NH1	2.53	0.42
54:KK:360:THR:O	63:TT:162:ARG:NH1	2.49	0.42
73:44:191:TYR:O	73:44:192:LEU:C	2.62	0.42
78:aa:112:C:O2'	78:aa:300:A:N3	2.50	0.42
78:aa:870:G:O2'	78:aa:871:U:P	2.78	0.42
1:A:2040:U:O2'	1:A:2041:A:OP2	2.30	0.41
12:J:60:TYR:O	12:J:61:HIS:ND1	2.53	0.41
55:LL:114:PRO:O	55:LL:145:ARG:NE	2.44	0.41
1:A:30:U:O2	3:C:81:GLN:NE2	2.53	0.41
1:A:536:G:N2	1:A:539:A:OP2	2.38	0.41
3:C:78:ARG:O	3:C:81:GLN:NE2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:6:96:ARG:NH2	34:6:236:LYS:O	2.51	0.41
45:BB:322:ASP:OD1	45:BB:323:THR:N	2.48	0.41
46:CC:342:ASN:OD1	46:CC:343:ASN:N	2.53	0.41
1:A:909:A:O2'	1:A:910:A:OP1	2.37	0.41
1:A:2265:C:O2	1:A:2950:C:H5''	2.20	0.41
23:U:40:GLU:OE2	23:U:42:GLN:NE2	2.47	0.41
43:d:75:ASN:OD1	43:d:149:ARG:NH2	2.49	0.41
43:d:127:ARG:NH2	43:d:129:ASP:OD2	2.51	0.41
44:AA:54:THR:HG22	44:AA:82:PRO:O	2.20	0.41
48:EE:139:GLU:OE2	48:EE:141:GLN:NE2	2.53	0.41
66:WW:240:GLN:OE1	66:WW:248:TYR:OH	2.38	0.41
78:aa:1539:A:OP1	78:aa:1563:C:O2'	2.36	0.41
1:A:2468:A:H4'	1:A:2469:A:O5'	2.20	0.41
9:g:28:SER:O	9:g:29:PRO:C	2.64	0.41
35:7:110:THR:OG1	35:7:150:GLY:O	2.27	0.41
36:8:398:VAL:O	36:8:398:VAL:HG23	2.20	0.41
72:33:229:LEU:HD12	72:33:229:LEU:C	2.46	0.41
76:88:204:ASP:C	76:88:206:GLY:H	2.28	0.41
20:R:290:ARG:O	20:R:297:TYR:HA	2.19	0.41
1:A:1719:A:OP1	2:B:307:ARG:NH1	2.50	0.41
1:A:1863:U:OP1	22:T:57:ASN:ND2	2.53	0.41
3:C:164:GLU:OE2	3:C:164:GLU:N	2.53	0.41
50:GG:90:THR:N	50:GG:93:ASN:OD1	2.51	0.41
72:33:76:THR:OG1	72:33:77:TRP:N	2.54	0.41
1:A:975:A:OP1	27:Y:95:GLY:N	2.52	0.41
19:Q:105:VAL:O	19:Q:105:VAL:HG12	2.21	0.41
88:2:4301:NAD:O5D	88:2:4301:NAD:H2N	2.20	0.41
66:WW:211:GLU:O	66:WW:215:ALA:N	2.48	0.41
67:XX:185:SER:OG	89:XX:501:ATP:O2B	2.39	0.41
69:ZZ:241:ARG:NH1	78:aa:1554:A:O5'	2.53	0.41
74:66:122:GLU:OE1	74:66:175:ARG:NH2	2.54	0.41
3:C:243:ASN:ND2	3:C:246:ASN:O	2.52	0.41
19:Q:72:ASP:OD1	19:Q:73:GLU:N	2.44	0.41
34:6:220:GLU:OE1	34:6:220:GLU:N	2.51	0.41
44:AA:151:ASP:N	44:AA:151:ASP:OD1	2.53	0.41
52:II:186:ASP:OD1	52:II:187:GLN:N	2.49	0.41
55:LL:159:SER:OG	78:aa:729:U:OP2	2.33	0.41
78:aa:396:A:N6	78:aa:431:A:O4'	2.54	0.41
83:j:188:LYS:HD2	83:j:188:LYS:C	2.46	0.41
1:A:16:A:O3'	39:9:134:ARG:NH1	2.54	0.41
1:A:319:C:O2	19:Q:219:ARG:NH2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:A:N6	1:A:2255:A:H4'	2.36	0.41
1:A:2361:U:O3'	82:e:96:SER:OG	2.39	0.41
5:E:62:SER:OG	5:E:63:GLU:N	2.53	0.41
56:MM:22:PHE:HB3	56:MM:65:ILE:HG22	2.03	0.41
73:55:87:VAL:O	73:55:87:VAL:HG13	2.21	0.41
74:66:152:ARG:NE	74:66:199:GLU:OE1	2.46	0.41
1:A:1167:A:OP2	23:U:18:ARG:NH1	2.54	0.41
20:R:291:LEU:O	20:R:292:MET:C	2.64	0.41
51:HH:132:CYS:N	51:HH:160:VAL:O	2.53	0.41
78:aa:253:U:O2'	78:aa:530:C:OP1	2.36	0.41
47:DD:61:HIS:NE2	47:DD:145:ASP:OD2	2.50	0.40
82:e:112:PRO:O	82:e:266:LYS:NZ	2.49	0.40
1:A:1136:A:O2'	1:A:1137:U:OP2	2.30	0.40
2:B:147:ASP:OD2	2:B:150:ARG:NE	2.53	0.40
32:4:132:HIS:NE2	33:5:382:GLU:OE2	2.54	0.40
45:BB:274:ASP:OD1	45:BB:362:ARG:NH1	2.54	0.40
55:LL:90:LYS:HB2	55:LL:91:PRO:HD3	2.03	0.40
78:aa:1023:C:C2'	78:aa:1024:C:H5'	2.52	0.40
52:II:304:VAL:N	52:II:308:LYS:O	2.53	0.40
1:A:2105:A:H2'	1:A:2105:A:N3	2.36	0.40
1:A:2510:G:OP1	5:E:74:ARG:NH2	2.48	0.40
65:VV:66:GLN:NE2	74:66:236:HIS:O	2.54	0.40
73:55:237:ASN:OD1	73:55:239:LEU:N	2.54	0.40
74:66:259:GLU:OE1	74:66:259:GLU:N	2.54	0.40
78:aa:1841:A:O2'	78:aa:1844:U:O4	2.38	0.40
1:A:2828:G:N2	1:A:2831:A:OP2	2.51	0.40
38:i:117:VAL:O	38:i:118:GLN:NE2	2.54	0.40
44:AA:298:THR:OG1	64:UU:90:ASP:O	2.38	0.40
48:EE:368:LEU:O	48:EE:372:ASN:ND2	2.54	0.40
71:22:312:ILE:N	78:aa:798:A:OP2	2.54	0.40
72:33:158:VAL:O	72:33:163:ARG:NH1	2.55	0.40
78:aa:1565:A:H2'	78:aa:1566:A:H4'	2.04	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	B	311/383 (81%)	304 (98%)	7 (2%)	0	100	100
3	C	305/384 (79%)	300 (98%)	5 (2%)	0	100	100
4	D	250/325 (77%)	248 (99%)	2 (1%)	0	100	100
5	E	307/352 (87%)	303 (99%)	4 (1%)	0	100	100
6	F	199/255 (78%)	197 (99%)	2 (1%)	0	100	100
7	G	72/300 (24%)	72 (100%)	0	0	100	100
8	f	243/347 (70%)	240 (99%)	3 (1%)	0	100	100
9	g	145/158 (92%)	142 (98%)	3 (2%)	0	100	100
10	H	181/183 (99%)	180 (99%)	1 (1%)	0	100	100
11	I	115/131 (88%)	113 (98%)	2 (2%)	0	100	100
12	J	241/312 (77%)	236 (98%)	5 (2%)	0	100	100
13	K	166/249 (67%)	166 (100%)	0	0	100	100
14	L	190/193 (98%)	189 (100%)	1 (0%)	0	100	100
15	M	192/258 (74%)	188 (98%)	4 (2%)	0	100	100
16	N	131/217 (60%)	125 (95%)	6 (5%)	0	100	100
17	O	268/364 (74%)	267 (100%)	1 (0%)	0	100	100
18	P	178/228 (78%)	178 (100%)	0	0	100	100
19	Q	351/396 (89%)	350 (100%)	1 (0%)	0	100	100
20	R	245/447 (55%)	240 (98%)	5 (2%)	0	100	100
21	S	175/274 (64%)	172 (98%)	3 (2%)	0	100	100
22	T	178/263 (68%)	177 (99%)	1 (1%)	0	100	100
23	U	134/161 (83%)	134 (100%)	0	0	100	100
24	V	88/219 (40%)	88 (100%)	0	0	100	100
25	W	57/129 (44%)	56 (98%)	1 (2%)	0	100	100
26	X	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
27	Y	44/140 (31%)	44 (100%)	0	0	100	100
28	0	44/124 (36%)	43 (98%)	1 (2%)	0	100	100
29	1	365/449 (81%)	362 (99%)	3 (1%)	0	100	100
30	2	121/370 (33%)	121 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	3	93/103 (90%)	91 (98%)	2 (2%)	0	100	100
32	4	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
33	5	346/439 (79%)	342 (99%)	4 (1%)	0	100	100
34	6	267/368 (73%)	264 (99%)	3 (1%)	0	100	100
35	7	82/165 (50%)	81 (99%)	1 (1%)	0	100	100
36	8	329/443 (74%)	323 (98%)	6 (2%)	0	100	100
37	h	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
38	i	120/218 (55%)	115 (96%)	5 (4%)	0	100	100
39	9	204/267 (76%)	198 (97%)	6 (3%)	0	100	100
40	a	157/225 (70%)	156 (99%)	1 (1%)	0	100	100
41	b	159/162 (98%)	157 (99%)	2 (1%)	0	100	100
42	c	96/110 (87%)	94 (98%)	2 (2%)	0	100	100
43	d	231/292 (79%)	228 (99%)	3 (1%)	0	100	100
44	AA	360/470 (77%)	355 (99%)	5 (1%)	0	100	100
45	BB	288/428 (67%)	283 (98%)	5 (2%)	0	100	100
46	CC	432/508 (85%)	426 (99%)	6 (1%)	0	100	100
47	DD	286/453 (63%)	280 (98%)	6 (2%)	0	100	100
48	EE	363/477 (76%)	356 (98%)	7 (2%)	0	100	100
49	FF	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
50	GG	221/309 (72%)	220 (100%)	1 (0%)	0	100	100
51	HH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
52	II	245/315 (78%)	239 (98%)	6 (2%)	0	100	100
53	JJ	186/268 (69%)	182 (98%)	4 (2%)	0	100	100
54	KK	122/376 (32%)	119 (98%)	3 (2%)	0	100	100
55	LL	126/174 (72%)	120 (95%)	6 (5%)	0	100	100
56	MM	116/119 (98%)	112 (97%)	4 (3%)	0	100	100
57	NN	110/113 (97%)	110 (100%)	0	0	100	100
58	OO	272/320 (85%)	270 (99%)	2 (1%)	0	100	100
59	PP	96/107 (90%)	95 (99%)	1 (1%)	0	100	100
60	QQ	156/165 (94%)	154 (99%)	2 (1%)	0	100	100
61	RR	132/256 (52%)	130 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	SS	79/91 (87%)	77 (98%)	2 (2%)	0	100	100
63	TT	86/236 (36%)	85 (99%)	1 (1%)	0	100	100
64	UU	222/253 (88%)	219 (99%)	3 (1%)	0	100	100
65	VV	255/316 (81%)	255 (100%)	0	0	100	100
66	WW	349/396 (88%)	344 (99%)	5 (1%)	0	100	100
67	XX	404/469 (86%)	393 (97%)	8 (2%)	3 (1%)	18	45
68	YY	97/108 (90%)	96 (99%)	1 (1%)	0	100	100
69	ZZ	310/382 (81%)	308 (99%)	2 (1%)	0	100	100
70	11	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
71	22	31/344 (9%)	31 (100%)	0	0	100	100
72	33	189/236 (80%)	181 (96%)	8 (4%)	0	100	100
73	44	258/310 (83%)	253 (98%)	5 (2%)	0	100	100
73	55	228/310 (74%)	224 (98%)	4 (2%)	0	100	100
74	66	281/348 (81%)	279 (99%)	2 (1%)	0	100	100
75	77	177/414 (43%)	176 (99%)	1 (1%)	0	100	100
76	88	465/508 (92%)	449 (97%)	14 (3%)	2 (0%)	30	57
77	00	46/95 (48%)	46 (100%)	0	0	100	100
77	99	34/95 (36%)	34 (100%)	0	0	100	100
81	cc	5/7 (71%)	5 (100%)	0	0	100	100
82	e	144/303 (48%)	139 (96%)	5 (4%)	0	100	100
83	j	193/201 (96%)	187 (97%)	6 (3%)	0	100	100
All	All	15380/21346 (72%)	15140 (98%)	235 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
67	XX	181	VAL
67	XX	180	ARG
67	XX	182	THR
76	88	205	VAL
76	88	203	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	257/312 (82%)	253 (98%)	4 (2%)	55	72
3	C	242/303 (80%)	242 (100%)	0	100	100
4	D	216/274 (79%)	216 (100%)	0	100	100
5	E	267/296 (90%)	265 (99%)	2 (1%)	76	80
6	F	173/216 (80%)	172 (99%)	1 (1%)	78	81
7	G	64/254 (25%)	64 (100%)	0	100	100
8	f	206/287 (72%)	206 (100%)	0	100	100
9	g	120/124 (97%)	120 (100%)	0	100	100
10	H	149/149 (100%)	149 (100%)	0	100	100
11	I	100/105 (95%)	100 (100%)	0	100	100
12	J	198/255 (78%)	197 (100%)	1 (0%)	81	82
13	K	142/205 (69%)	142 (100%)	0	100	100
14	L	164/165 (99%)	164 (100%)	0	100	100
15	M	164/209 (78%)	164 (100%)	0	100	100
16	N	119/188 (63%)	119 (100%)	0	100	100
17	O	235/315 (75%)	233 (99%)	2 (1%)	70	78
18	P	158/196 (81%)	157 (99%)	1 (1%)	78	81
19	Q	312/347 (90%)	311 (100%)	1 (0%)	86	85
20	R	212/359 (59%)	211 (100%)	1 (0%)	81	82
21	S	159/242 (66%)	158 (99%)	1 (1%)	78	81
22	T	161/224 (72%)	160 (99%)	1 (1%)	78	81
23	U	118/138 (86%)	117 (99%)	1 (1%)	73	79
24	V	80/170 (47%)	80 (100%)	0	100	100
25	W	50/102 (49%)	50 (100%)	0	100	100
26	X	46/54 (85%)	46 (100%)	0	100	100
27	Y	38/116 (33%)	38 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	0	41/108 (38%)	41 (100%)	0	100	100
29	1	316/384 (82%)	315 (100%)	1 (0%)	86	85
30	2	109/317 (34%)	109 (100%)	0	100	100
31	3	83/91 (91%)	82 (99%)	1 (1%)	63	75
32	4	113/114 (99%)	113 (100%)	0	100	100
33	5	279/351 (80%)	277 (99%)	2 (1%)	76	80
34	6	238/310 (77%)	236 (99%)	2 (1%)	73	79
35	7	69/136 (51%)	69 (100%)	0	100	100
36	8	285/378 (75%)	284 (100%)	1 (0%)	84	84
37	h	88/88 (100%)	88 (100%)	0	100	100
38	i	101/162 (62%)	101 (100%)	0	100	100
39	9	176/225 (78%)	176 (100%)	0	100	100
40	a	146/196 (74%)	146 (100%)	0	100	100
41	b	141/141 (100%)	140 (99%)	1 (1%)	76	80
42	c	86/96 (90%)	85 (99%)	1 (1%)	63	75
43	d	201/243 (83%)	201 (100%)	0	100	100
44	AA	314/393 (80%)	314 (100%)	0	100	100
45	BB	237/347 (68%)	237 (100%)	0	100	100
46	CC	405/461 (88%)	405 (100%)	0	100	100
47	DD	242/377 (64%)	237 (98%)	5 (2%)	47	68
48	EE	308/392 (79%)	308 (100%)	0	100	100
49	FF	99/99 (100%)	96 (97%)	3 (3%)	36	62
50	GG	186/260 (72%)	185 (100%)	1 (0%)	81	82
51	HH	134/135 (99%)	132 (98%)	2 (2%)	57	73
52	II	206/263 (78%)	206 (100%)	0	100	100
53	JJ	166/227 (73%)	164 (99%)	2 (1%)	63	75
54	KK	108/324 (33%)	108 (100%)	0	100	100
55	LL	103/142 (72%)	103 (100%)	0	100	100
56	MM	98/99 (99%)	98 (100%)	0	100	100
57	NN	96/97 (99%)	96 (100%)	0	100	100
58	OO	230/265 (87%)	230 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	PP	85/92 (92%)	85 (100%)	0	100	100
60	QQ	132/138 (96%)	131 (99%)	1 (1%)	73	79
61	RR	118/218 (54%)	117 (99%)	1 (1%)	73	79
62	SS	70/80 (88%)	70 (100%)	0	100	100
63	TT	75/191 (39%)	75 (100%)	0	100	100
64	UU	193/218 (88%)	192 (100%)	1 (0%)	81	82
65	VV	224/268 (84%)	224 (100%)	0	100	100
66	WW	300/333 (90%)	299 (100%)	1 (0%)	86	85
67	XX	345/391 (88%)	345 (100%)	0	100	100
68	YY	83/89 (93%)	81 (98%)	2 (2%)	43	66
69	ZZ	278/328 (85%)	278 (100%)	0	100	100
70	11	73/75 (97%)	73 (100%)	0	100	100
71	22	33/293 (11%)	32 (97%)	1 (3%)	36	62
72	33	162/195 (83%)	160 (99%)	2 (1%)	63	75
73	44	215/250 (86%)	215 (100%)	0	100	100
73	55	195/250 (78%)	195 (100%)	0	100	100
74	66	245/303 (81%)	244 (100%)	1 (0%)	84	84
75	77	153/304 (50%)	151 (99%)	2 (1%)	61	74
76	88	388/419 (93%)	388 (100%)	0	100	100
77	00	43/78 (55%)	43 (100%)	0	100	100
77	99	34/78 (44%)	34 (100%)	0	100	100
82	e	132/256 (52%)	131 (99%)	1 (1%)	73	79
83	j	168/171 (98%)	167 (99%)	1 (1%)	78	81
All	All	13298/17844 (74%)	13246 (100%)	52 (0%)	81	84

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	67	THR
2	B	109	HIS
2	B	298	HIS
2	B	326	ASP
5	E	143	ILE
5	E	333	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	167	ASP
12	J	103	ILE
17	O	168	THR
17	O	317	THR
18	P	53	PHE
19	Q	78	ASN
20	R	345	LYS
21	S	126	LYS
22	T	50	THR
23	U	68	LEU
29	1	244	VAL
31	3	65	THR
33	5	212	LEU
33	5	371	VAL
34	6	230	LEU
34	6	334	ASN
36	8	273	LEU
41	b	85	VAL
42	c	79	THR
47	DD	35	GLU
47	DD	102	LEU
47	DD	123	ASN
47	DD	170	THR
47	DD	411	VAL
49	FF	87	VAL
49	FF	93	VAL
49	FF	103	LEU
50	GG	135	ARG
51	HH	95	LEU
51	HH	132	CYS
53	JJ	121	ILE
53	JJ	153	GLU
60	QQ	29	ILE
61	RR	202	ILE
64	UU	80	GLU
66	WW	192	ASN
68	YY	52	ASN
68	YY	70	ASP
71	22	322	ILE
72	33	138	SER
72	33	229	LEU
74	66	296	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	77	246	THR
75	77	274	GLU
82	e	64	PHE
83	j	82	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	363	ASN
4	D	64	ASN
5	E	95	ASN
6	F	179	GLN
8	f	295	GLN
9	g	119	HIS
10	H	85	HIS
10	H	114	HIS
13	K	167	ASN
16	N	112	HIS
17	O	203	HIS
18	P	78	ASN
18	P	98	GLN
19	Q	78	ASN
19	Q	161	GLN
20	R	193	HIS
20	R	266	ASN
21	S	90	GLN
22	T	46	HIS
22	T	140	HIS
23	U	83	GLN
25	W	105	HIS
28	0	119	GLN
29	1	365	ASN
30	2	311	ASN
32	4	30	HIS
33	5	189	GLN
34	6	297	HIS
35	7	111	GLN
35	7	151	HIS
38	i	88	ASN
40	a	82	HIS
40	a	141	ASN
41	b	156	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	d	90	HIS
43	d	114	GLN
43	d	189	ASN
44	AA	32	ASN
44	AA	325	HIS
46	CC	134	ASN
46	CC	230	ASN
46	CC	257	ASN
47	DD	423	HIS
47	DD	447	ASN
48	EE	259	GLN
48	EE	372	ASN
49	FF	57	HIS
52	II	303	HIS
53	JJ	161	HIS
54	KK	318	ASN
55	LL	48	ASN
55	LL	122	GLN
58	OO	58	GLN
58	OO	271	ASN
59	PP	24	HIS
59	PP	30	ASN
61	RR	229	ASN
62	SS	56	HIS
63	TT	234	GLN
64	UU	56	GLN
65	VV	66	GLN
65	VV	72	HIS
65	VV	78	HIS
67	XX	114	ASN
67	XX	194	HIS
67	XX	314	HIS
67	XX	364	ASN
68	YY	52	ASN
69	ZZ	93	GLN
75	77	290	ASN
75	77	389	ASN
76	88	76	ASN
76	88	180	HIS
76	88	365	HIS
77	99	75	HIS
82	e	234	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2826/3464 (81%)	350 (12%)	6 (0%)
78	aa	1430/1864 (76%)	183 (12%)	0
79	bb	71/73 (97%)	13 (18%)	0
80	ee	10/11 (90%)	0	0
All	All	4337/5412 (80%)	546 (12%)	6 (0%)

All (546) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	18	A
1	A	19	G
1	A	29	A
1	A	46	U
1	A	47	A
1	A	52	U
1	A	58	G
1	A	79	A
1	A	90	A
1	A	98	A
1	A	99	U
1	A	104	U
1	A	106	A
1	A	107	U
1	A	118	G
1	A	311	G
1	A	317	A
1	A	319	C
1	A	334	U
1	A	347	U
1	A	348	A
1	A	350	U
1	A	351	A
1	A	353	A
1	A	367	A
1	A	370	A
1	A	376	U
1	A	387	A
1	A	392	A
1	A	393	A
1	A	395	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	414	U
1	A	419	U
1	A	433	G
1	A	435	A
1	A	440	A
1	A	441	U
1	A	443	A
1	A	462	U
1	A	477	A
1	A	478	U
1	A	486	A
1	A	522	C
1	A	525	A
1	A	569	G
1	A	571	A
1	A	583	A
1	A	584	A
1	A	587	A
1	A	599	A
1	A	608	A
1	A	609	U
1	A	611	A
1	A	639	A
1	A	829	A
1	A	839	A
1	A	840	U
1	A	845	A
1	A	846	A
1	A	849	U
1	A	888	U
1	A	910	A
1	A	914	U
1	A	931	U
1	A	958	A
1	A	960	C
1	A	967	A
1	A	969	G
1	A	977	U
1	A	988	G
1	A	994	U
1	A	995	U
1	A	1010	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1011	A
1	A	1042	G
1	A	1070	A
1	A	1071	G
1	A	1081	C
1	A	1107	U
1	A	1108	U
1	A	1109	U
1	A	1118	C
1	A	1119	A
1	A	1125	G
1	A	1134	A
1	A	1136	A
1	A	1137	U
1	A	1141	A
1	A	1160	C
1	A	1190	A
1	A	1191	G
1	A	1206	G
1	A	1219	A
1	A	1235	A
1	A	1242	G
1	A	1248	G
1	A	1257	U
1	A	1258	U
1	A	1267	G
1	A	1271	A
1	A	1280	A
1	A	1307	G
1	A	1316	A
1	A	1331	A
1	A	1333	G
1	A	1334	A
1	A	1358	A
1	A	1376	A
1	A	1377	U
1	A	1379	U
1	A	1380	A
1	A	1381	A
1	A	1382	C
1	A	1389	A
1	A	1417	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1431	A
1	A	1452	G
1	A	1453	A
1	A	1457	G
1	A	1487	U
1	A	1494	U
1	A	1495	A
1	A	1496	U
1	A	1497	A
1	A	1509	A
1	A	1522	U
1	A	1526	A
1	A	1528	U
1	A	1529	G
1	A	1565	A
1	A	1566	A
1	A	1567	A
1	A	1568	A
1	A	1578	G
1	A	1589	A
1	A	1590	A
1	A	1591	A
1	A	1604	G
1	A	1605	U
1	A	1613	C
1	A	1620	U
1	A	1626	U
1	A	1627	A
1	A	1634	G
1	A	1648	U
1	A	1703	A
1	A	1719	A
1	A	1722	A
1	A	1726	A
1	A	1842	A
1	A	1844	U
1	A	1880	U
1	A	1881	G
1	A	1882	A
1	A	1884	U
1	A	1910	G
1	A	1921	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1922	C
1	A	1951	A
1	A	1970	A
1	A	1971	A
1	A	1985	U
1	A	1988	A
1	A	1991	A
1	A	1993	U
1	A	2002	A
1	A	2029	C
1	A	2030	A
1	A	2032	A
1	A	2039	A
1	A	2041	A
1	A	2048	A
1	A	2051	A
1	A	2052	U
1	A	2091	U
1	A	2105	A
1	A	2108	A
1	A	2136	A
1	A	2142	G
1	A	2145	C
1	A	2148	A
1	A	2149	G
1	A	2150	C
1	A	2158	U
1	A	2164	G
1	A	2165	G
1	A	2172	A
1	A	2173	A
1	A	2189	A
1	A	2190	U
1	A	2198	U
1	A	2199	G
1	A	2202	U
1	A	2205	A
1	A	2206	U
1	A	2207	G
1	A	2226	U
1	A	2228	U
1	A	2256	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2258	A
1	A	2265	C
1	A	2266	A
1	A	2268	A
1	A	2278	C
1	A	2287	A
1	A	2290	C
1	A	2291	G
1	A	2295	A
1	A	2296	G
1	A	2297	A
1	A	2304	G
1	A	2328	G
1	A	2330	A
1	A	2332	A
1	A	2333	C
1	A	2337	U
1	A	2347	U
1	A	2367	A
1	A	2370	A
1	A	2371	G
1	A	2384	C
1	A	2402	G
1	A	2409	U
1	A	2411	A
1	A	2418	A
1	A	2419	A
1	A	2420	U
1	A	2427	A
1	A	2439	A
1	A	2440	G
1	A	2441	A
1	A	2477	A
1	A	2486	U
1	A	2491	A
1	A	2509	U
1	A	2511	C
1	A	2541	A
1	A	2543	C
1	A	2547	A
1	A	2548	U
1	A	2558	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2559	G
1	A	2581	G
1	A	2582	G
1	A	2592	A
1	A	2595	A
1	A	2596	A
1	A	2611	A
1	A	2612	U
1	A	2621	A
1	A	2626	U
1	A	2631	A
1	A	2632	G
1	A	2636	U
1	A	2637	U
1	A	2638	A
1	A	2656	A
1	A	2658	A
1	A	2659	G
1	A	2685	A
1	A	2686	U
1	A	2690	G
1	A	2694	G
1	A	2706	C
1	A	2710	U
1	A	2711	U
1	A	2719	U
1	A	2720	U
1	A	2721	U
1	A	2722	U
1	A	2723	U
1	A	2757	G
1	A	2758	U
1	A	2775	U
1	A	2784	U
1	A	2786	A
1	A	2795	U
1	A	2797	C
1	A	2806	U
1	A	2808	A
1	A	2810	A
1	A	2811	A
1	A	2836	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2838	C
1	A	2843	G
1	A	2852	A
1	A	2858	A
1	A	2875	U
1	A	2881	G
1	A	2882	A
1	A	2883	A
1	A	2884	A
1	A	2891	G
1	A	2897	G
1	A	2898	A
1	A	2909	A
1	A	2912	U
1	A	2927	A
1	A	2942	U
1	A	2945	G
1	A	2953	G
1	A	2955	U
1	A	2956	G
1	A	2957	U
1	A	2958	C
1	A	2969	A
1	A	2971	C
1	A	2980	U
1	A	2981	G
1	A	3006	U
1	A	3018	A
1	A	3019	A
1	A	3025	C
1	A	3030	G
1	A	3034	G
1	A	3038	A
1	A	3054	A
1	A	3061	U
1	A	3065	U
1	A	3067	U
1	A	3081	U
1	A	3082	U
1	A	3124	G
1	A	3125	G
1	A	3156	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3166	U
1	A	3259	A
1	A	3260	C
1	A	3261	A
1	A	3262	A
1	A	3263	U
1	A	3276	G
1	A	3288	A
1	A	3296	A
1	A	3310	A
1	A	3349	A
1	A	3359	A
1	A	3391	A
1	A	3399	A
1	A	3407	U
1	A	3408	A
1	A	3413	A
1	A	3420	A
1	A	3424	A
1	A	3425	U
1	A	3428	U
1	A	3429	A
1	A	3447	A
1	A	3449	U
78	aa	51	G
78	aa	52	A
78	aa	54	G
78	aa	77	A
78	aa	84	U
78	aa	90	U
78	aa	92	C
78	aa	93	U
78	aa	96	A
78	aa	106	A
78	aa	113	G
78	aa	115	U
78	aa	118	A
78	aa	122	U
78	aa	242	A
78	aa	255	U
78	aa	256	A
78	aa	266	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	aa	268	A
78	aa	269	A
78	aa	270	U
78	aa	271	A
78	aa	273	U
78	aa	278	C
78	aa	282	U
78	aa	302	U
78	aa	314	C
78	aa	318	A
78	aa	376	A
78	aa	380	G
78	aa	388	U
78	aa	389	C
78	aa	390	A
78	aa	401	G
78	aa	416	G
78	aa	417	C
78	aa	430	U
78	aa	431	A
78	aa	441	G
78	aa	445	A
78	aa	446	A
78	aa	454	A
78	aa	455	G
78	aa	482	A
78	aa	483	A
78	aa	497	U
78	aa	518	U
78	aa	540	A
78	aa	556	G
78	aa	561	A
78	aa	669	C
78	aa	670	G
78	aa	675	U
78	aa	676	U
78	aa	677	U
78	aa	680	C
78	aa	684	U
78	aa	722	A
78	aa	725	U
78	aa	737	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	aa	744	C
78	aa	756	G
78	aa	759	A
78	aa	773	A
78	aa	790	A
78	aa	799	A
78	aa	802	G
78	aa	803	G
78	aa	811	A
78	aa	828	A
78	aa	830	U
78	aa	838	A
78	aa	849	A
78	aa	856	U
78	aa	861	A
78	aa	862	A
78	aa	867	G
78	aa	871	U
78	aa	879	A
78	aa	880	G
78	aa	911	G
78	aa	913	C
78	aa	921	G
78	aa	924	G
78	aa	944	A
78	aa	945	A
78	aa	952	G
78	aa	978	A
78	aa	990	U
78	aa	991	A
78	aa	1012	A
78	aa	1014	U
78	aa	1024	C
78	aa	1038	U
78	aa	1039	U
78	aa	1040	A
78	aa	1063	U
78	aa	1064	A
78	aa	1106	A
78	aa	1118	G
78	aa	1119	U
78	aa	1126	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	aa	1127	A
78	aa	1138	A
78	aa	1152	U
78	aa	1158	G
78	aa	1161	C
78	aa	1164	C
78	aa	1167	A
78	aa	1168	A
78	aa	1169	A
78	aa	1184	U
78	aa	1185	G
78	aa	1348	C
78	aa	1357	U
78	aa	1358	C
78	aa	1385	U
78	aa	1386	U
78	aa	1392	G
78	aa	1417	U
78	aa	1425	A
78	aa	1426	U
78	aa	1437	U
78	aa	1445	U
78	aa	1450	A
78	aa	1457	G
78	aa	1475	A
78	aa	1476	A
78	aa	1480	A
78	aa	1492	A
78	aa	1493	U
78	aa	1504	A
78	aa	1505	U
78	aa	1506	A
78	aa	1511	U
78	aa	1518	U
78	aa	1526	A
78	aa	1527	A
78	aa	1529	A
78	aa	1537	G
78	aa	1553	U
78	aa	1559	A
78	aa	1566	A
78	aa	1579	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	aa	1580	A
78	aa	1581	U
78	aa	1582	A
78	aa	1583	U
78	aa	1584	A
78	aa	1585	C
78	aa	1601	A
78	aa	1630	A
78	aa	1643	C
78	aa	1654	G
78	aa	1655	G
78	aa	1658	A
78	aa	1664	C
78	aa	1677	A
78	aa	1680	A
78	aa	1707	G
78	aa	1731	U
78	aa	1735	A
78	aa	1741	G
78	aa	1751	A
78	aa	1753	G
78	aa	1758	G
78	aa	1803	A
78	aa	1805	G
78	aa	1810	A
78	aa	1817	U
78	aa	1818	U
78	aa	1828	G
78	aa	1840	G
78	aa	1841	A
78	aa	1843	U
78	aa	1844	U
78	aa	1845	A
78	aa	1847	C
78	aa	1848	A
78	aa	1849	A
78	aa	1853	U
78	aa	1854	G
78	aa	1864	A
79	bb	12	U
79	bb	13	C
79	bb	14	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	bb	19	G
79	bb	20	U
79	bb	21	A
79	bb	45	U
79	bb	47	A
79	bb	49	U
79	bb	65	C
79	bb	68	A
79	bb	73	C
79	bb	75	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	909	A
1	A	1205	A
1	A	2051	A
1	A	2332	A
1	A	2720	U
1	A	2883	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 304 ligands modelled in this entry, 301 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	ATP	XX	501	84	32,33,33	2.47	6 (18%)	48,52,52	1.83	8 (16%)
85	SPM	A	3645	-	13,13,13	0.33	0	12,12,12	0.77	0
88	NAD	2	4301	86	46,48,48	0.89	1 (2%)	64,73,73	1.35	7 (10%)

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
89	ATP	XX	501	84	-	2/22/38/38	0/3/3/3
85	SPM	A	3645	-	-	3/11/11/11	-
88	NAD	2	4301	86	-	1/30/62/62	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	XX	501	ATP	C2'-C1'	-8.07	1.28	1.53
89	XX	501	ATP	PB-O3A	5.85	1.65	1.59
89	XX	501	ATP	PA-O3A	5.78	1.65	1.59
89	XX	501	ATP	PB-O3B	5.19	1.65	1.59
88	2	4301	NAD	C2N-N1N	-2.67	1.32	1.35
89	XX	501	ATP	C8-N9	-2.45	1.33	1.37
89	XX	501	ATP	C5-N7	-2.06	1.35	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	XX	501	ATP	C4-N9-C8	6.05	112.09	105.74
88	2	4301	NAD	C5A-C4A-N3A	-5.58	119.04	126.72
89	XX	501	ATP	N9-C8-N7	-4.96	106.90	113.94
89	XX	501	ATP	N3-C4-N9	4.39	134.64	127.17
89	XX	501	ATP	C5-C4-N3	-4.29	120.81	126.72
88	2	4301	NAD	N3A-C4A-N9A	4.19	134.30	127.17
89	XX	501	ATP	C3'-C2'-C1'	3.53	108.14	101.46
89	XX	501	ATP	C5-N7-C8	3.19	108.47	103.45
88	2	4301	NAD	C5A-N7A-C8A	3.11	108.33	103.45
88	2	4301	NAD	C2A-N3A-C4A	2.98	119.10	111.83
88	2	4301	NAD	N9A-C8A-N7A	-2.91	109.81	113.94
89	XX	501	ATP	C1'-N9-C8	-2.75	121.00	127.09
88	2	4301	NAD	N3A-C2A-N1A	-2.70	124.50	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	2	4301	NAD	C4A-C5A-N7A	-2.65	107.55	110.58
89	XX	501	ATP	C4-C5-N7	-2.26	108.00	110.58

There are no chirality outliers.

All (6) torsion outliers are listed below:

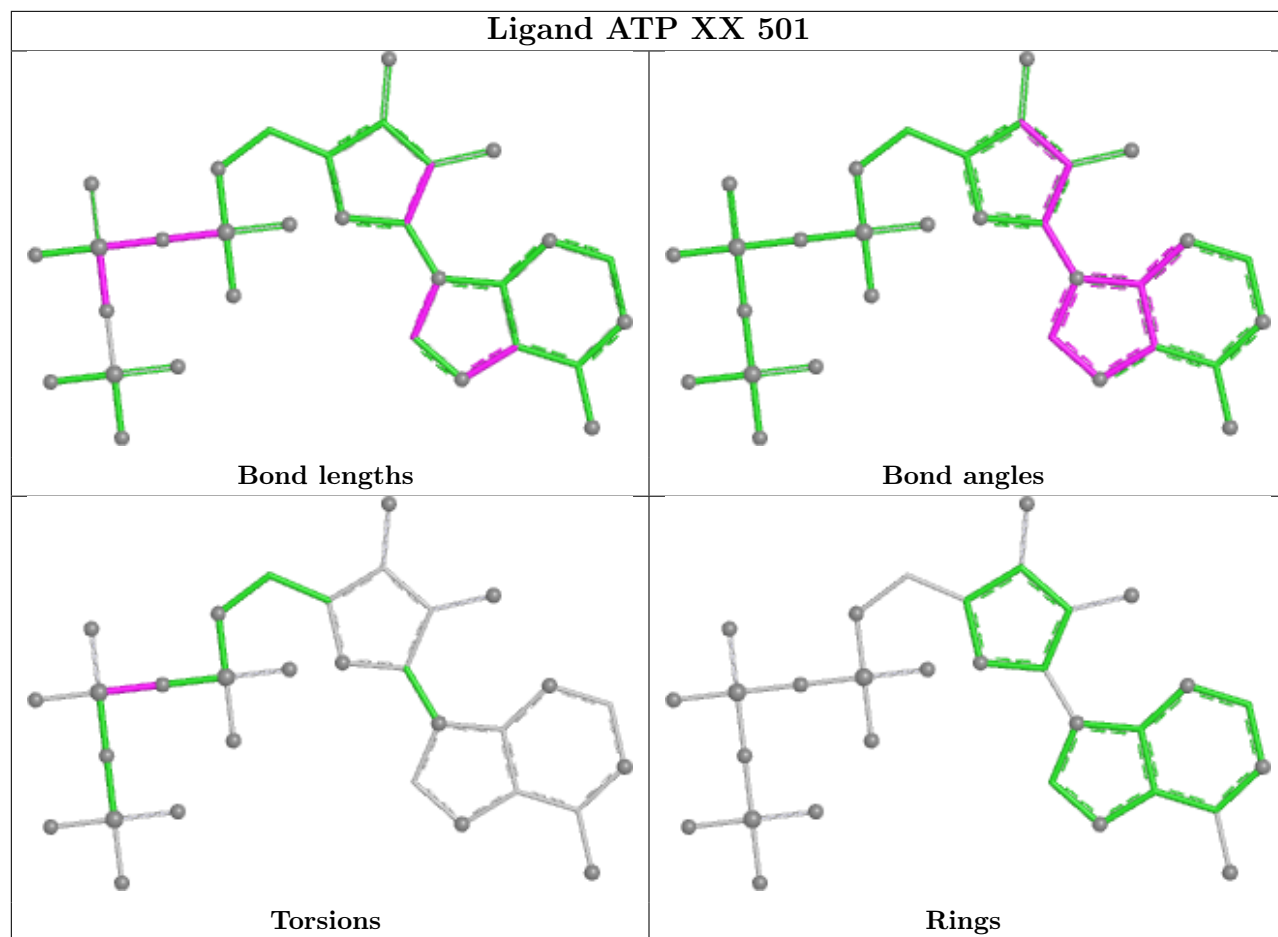
Mol	Chain	Res	Type	Atoms
85	A	3645	SPM	N5-C6-C7-C8
85	A	3645	SPM	N10-C11-C12-C13
89	XX	501	ATP	PA-O3A-PB-O2B
88	2	4301	NAD	O4D-C4D-C5D-O5D
89	XX	501	ATP	PA-O3A-PB-O1B
85	A	3645	SPM	C3-C4-N5-C6

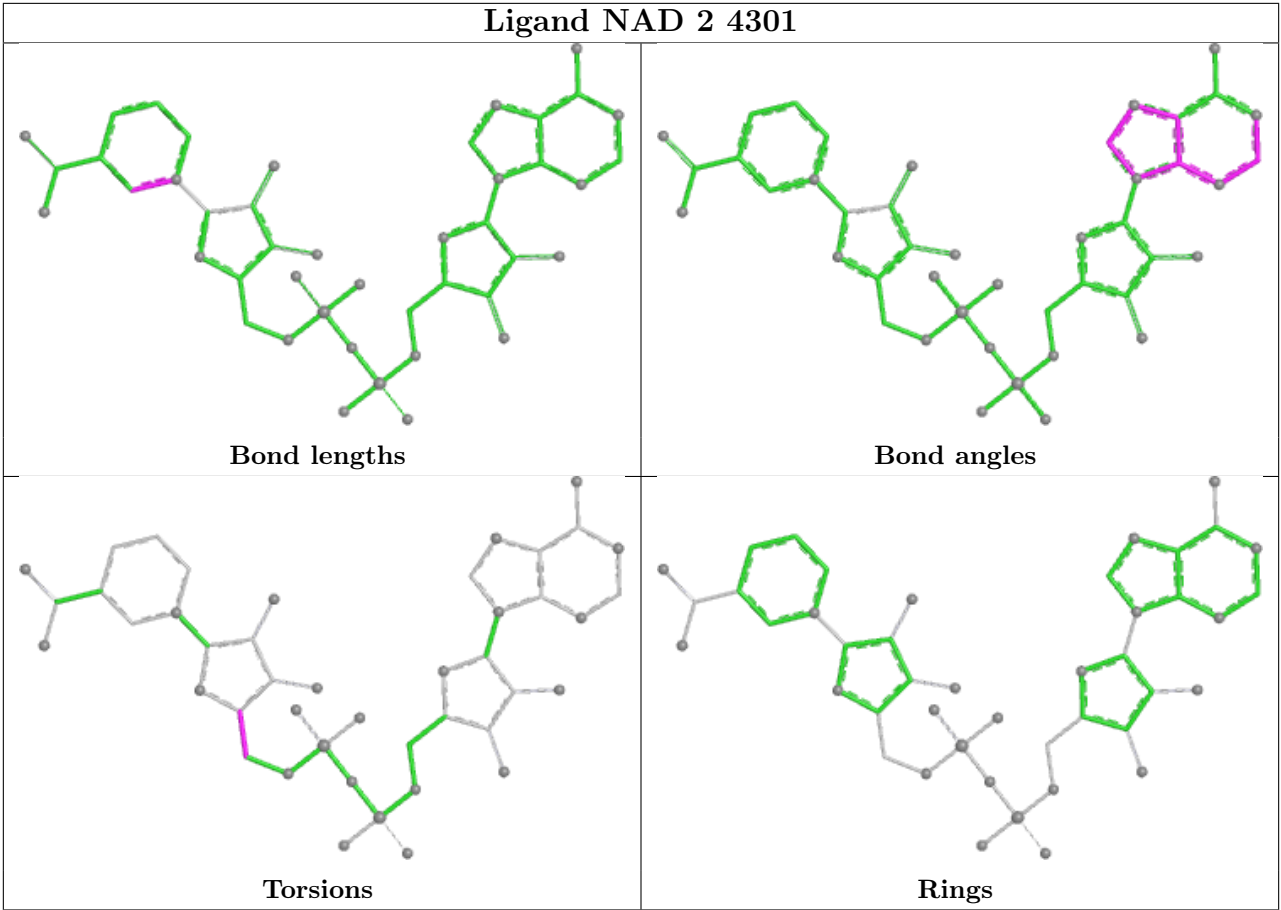
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	XX	501	ATP	2	0
88	2	4301	NAD	3	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
79	bb	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	bb	15:A	O3'	18:A	P	9.12

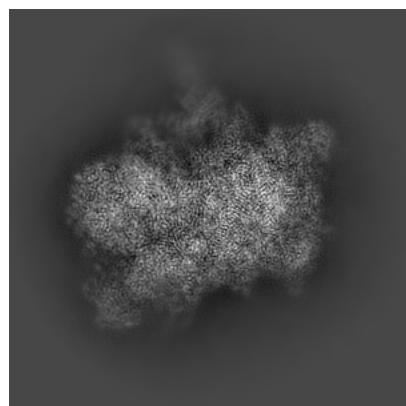
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10985. These allow visual inspection of the internal detail of the map and identification of artifacts.

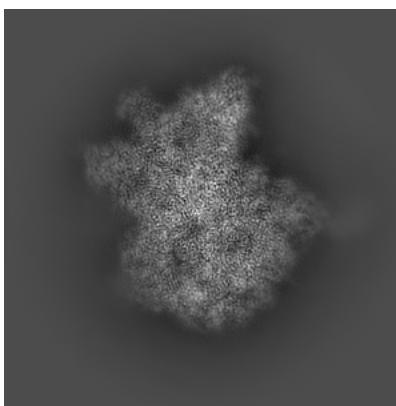
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

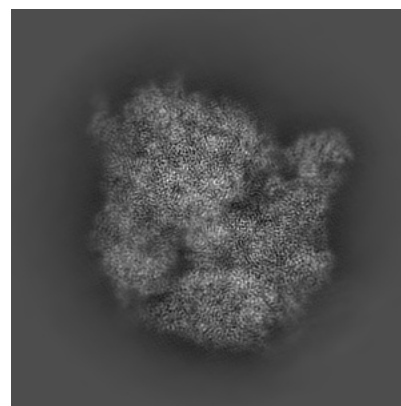
6.1.1 Primary map



X

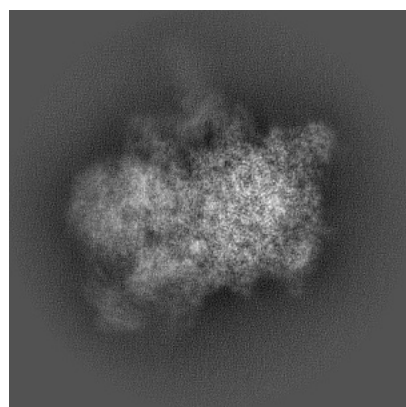


Y

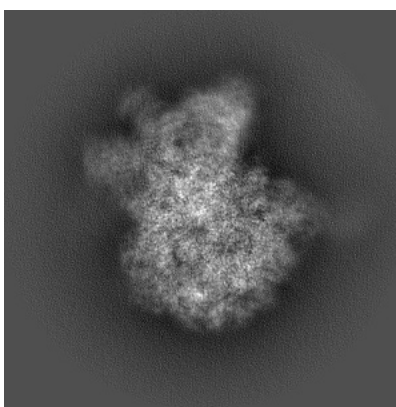


Z

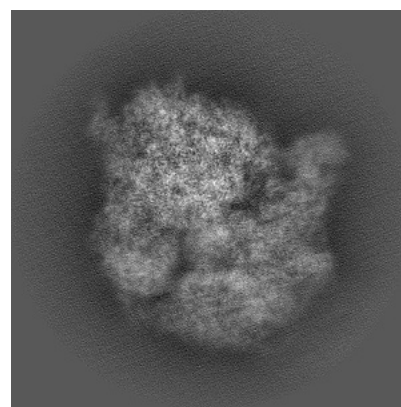
6.1.2 Raw map



X



Y

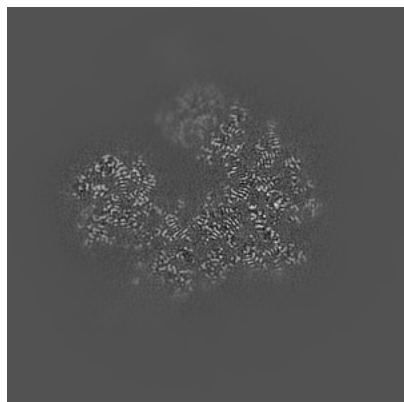


Z

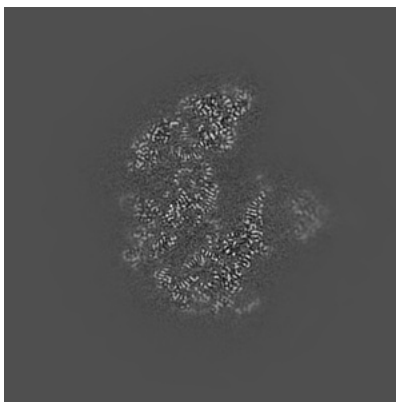
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

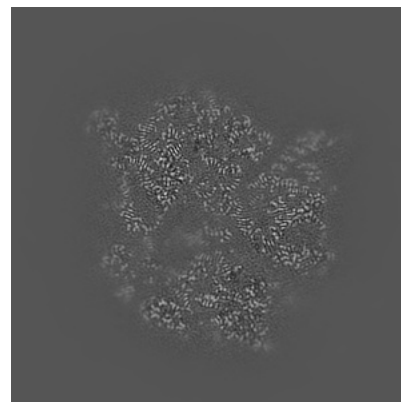
6.2.1 Primary map



X Index: 200

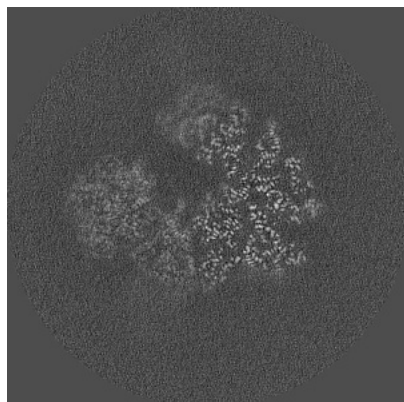


Y Index: 200

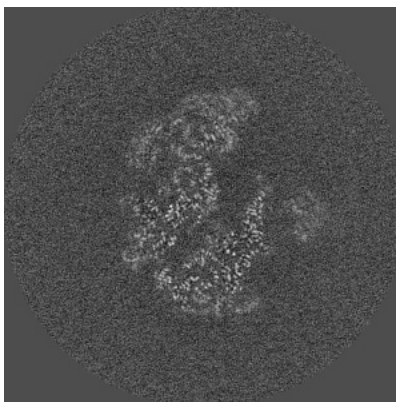


Z Index: 200

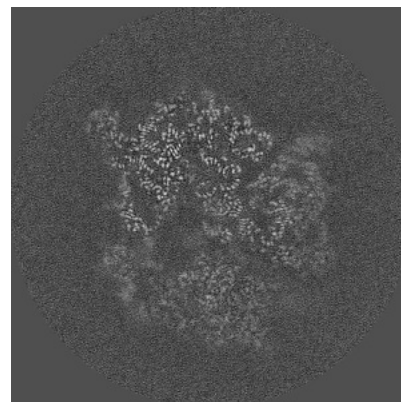
6.2.2 Raw map



X Index: 200



Y Index: 200

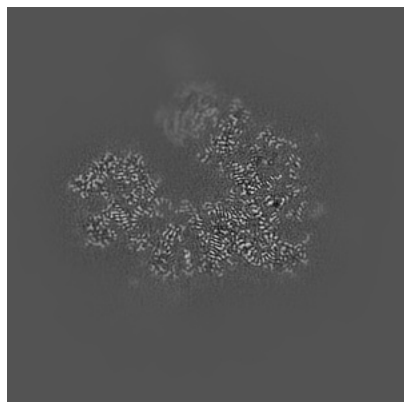


Z Index: 200

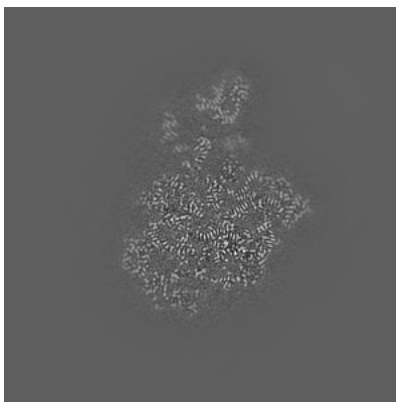
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

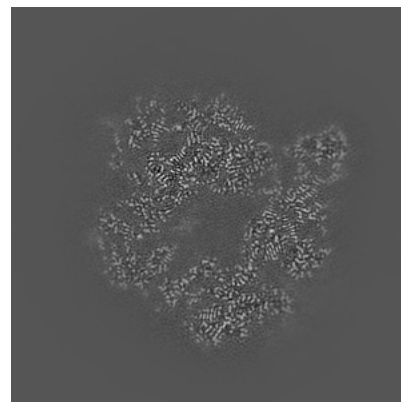
6.3.1 Primary map



X Index: 195

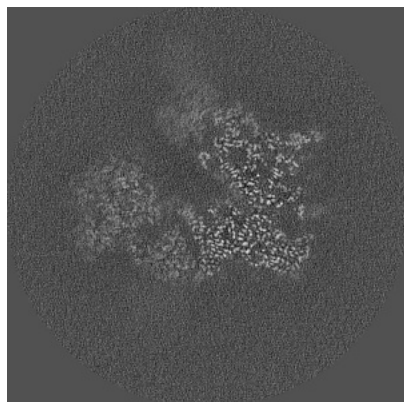


Y Index: 228

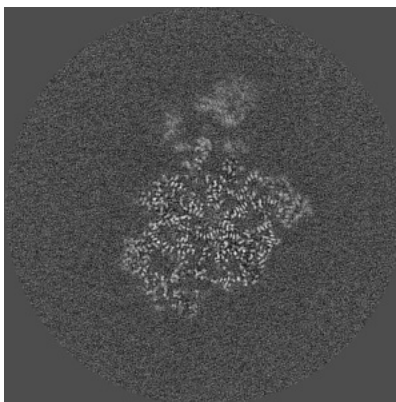


Z Index: 219

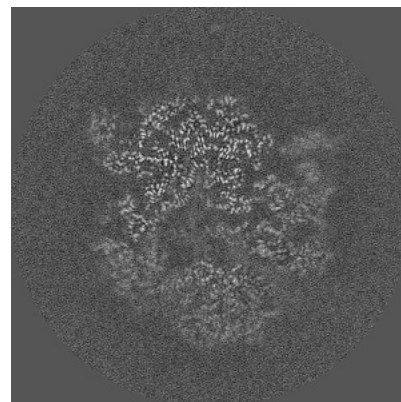
6.3.2 Raw map



X Index: 192



Y Index: 228

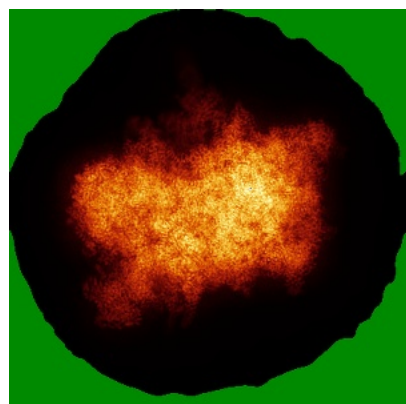


Z Index: 206

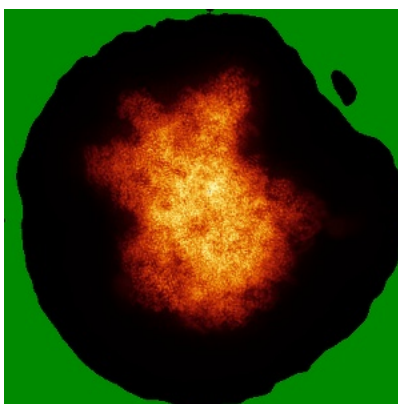
The images above show the largest variance slices of the map in three orthogonal directions.

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

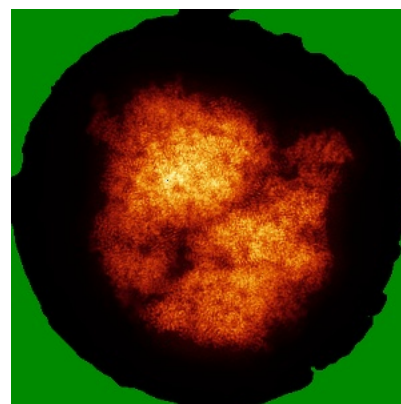
6.4.1 Primary map



X

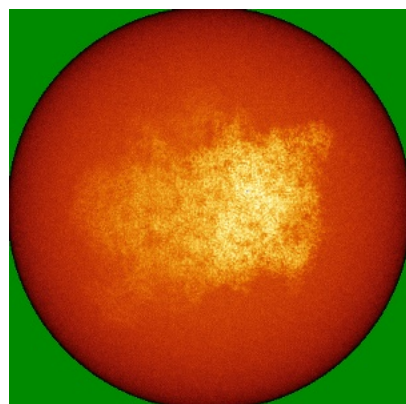


Y

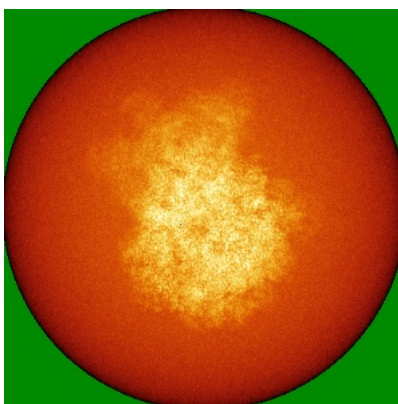


Z

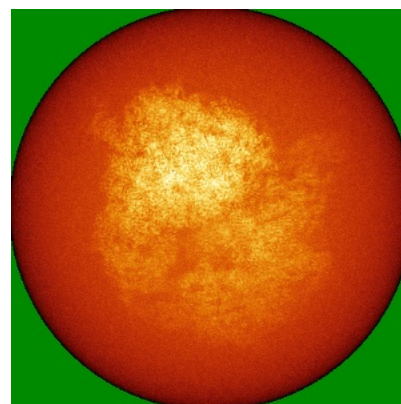
6.4.2 Raw map



X



Y

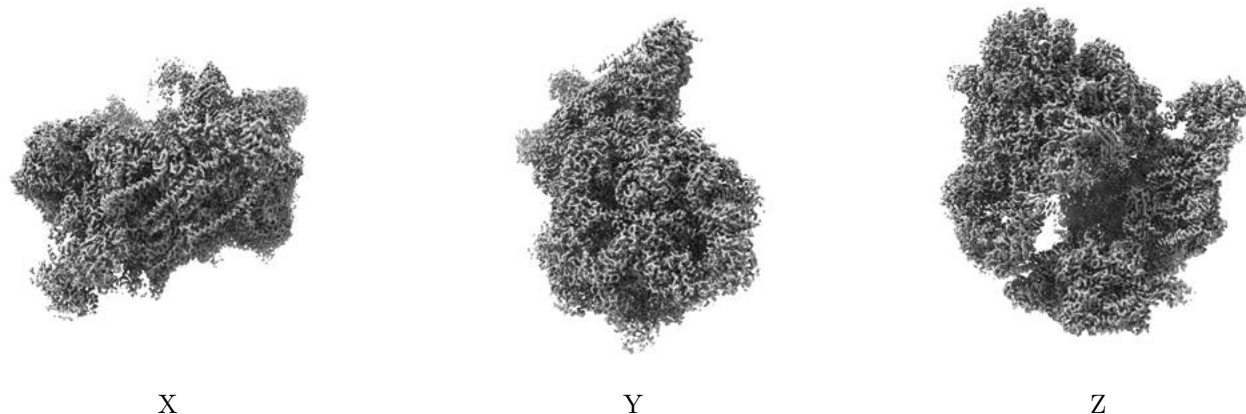


Z

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

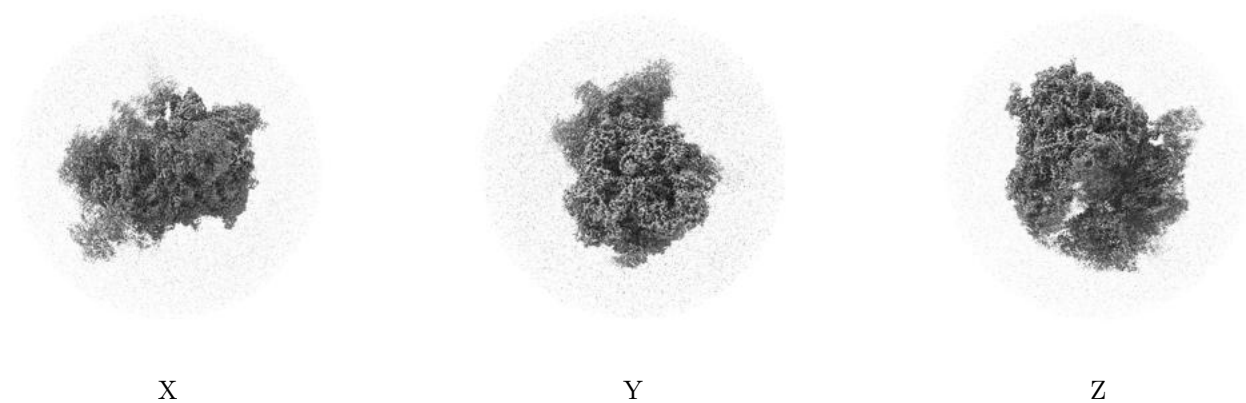
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.77. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

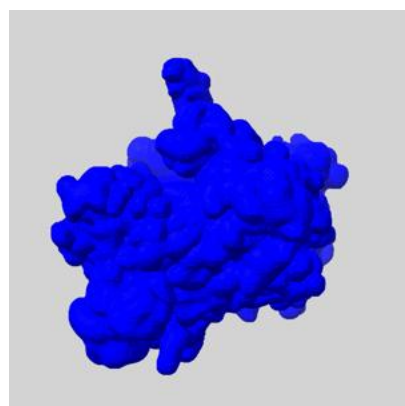
6.6 Mask visualisation [i](#)

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

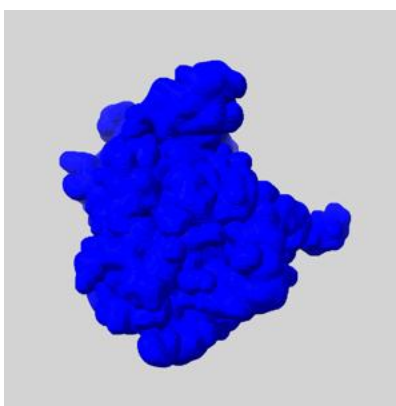
A mask typically either:

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

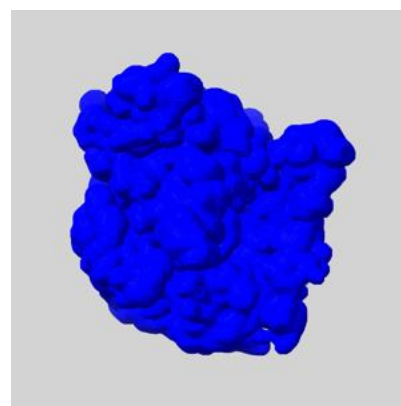
6.6.1 emd_10985_msk_1.map [i](#)



X



Y

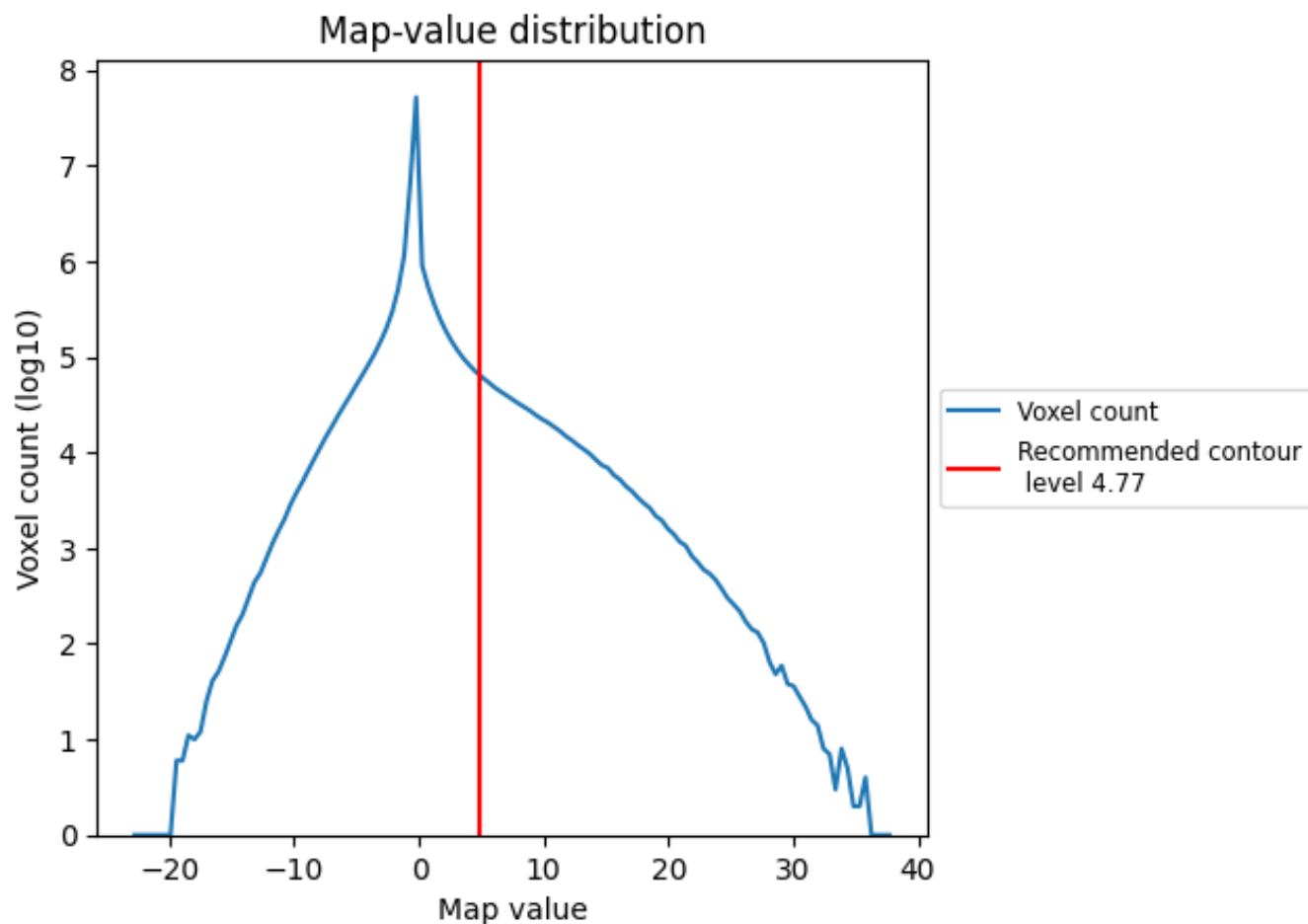


Z

7 Map analysis [i](#)

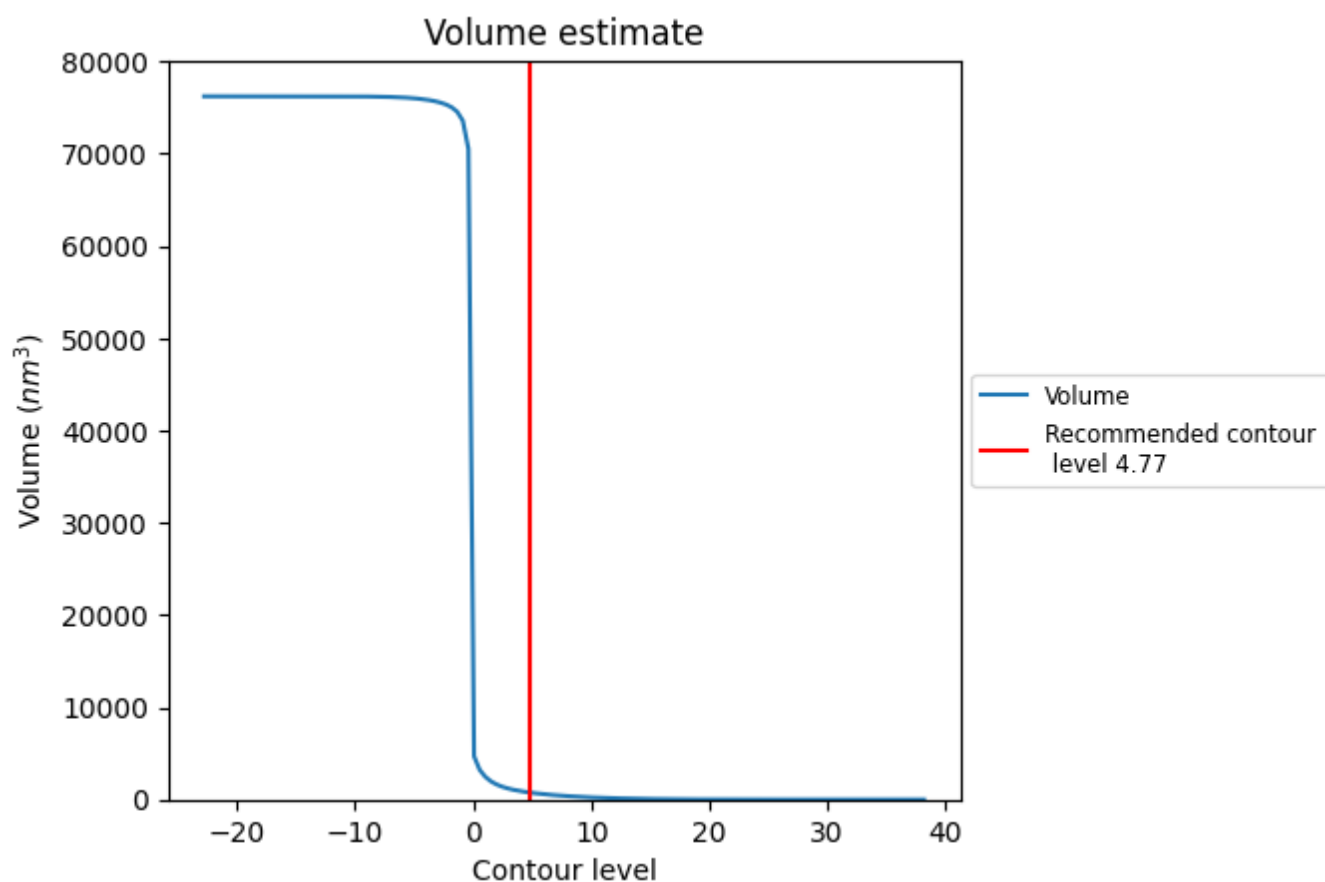
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

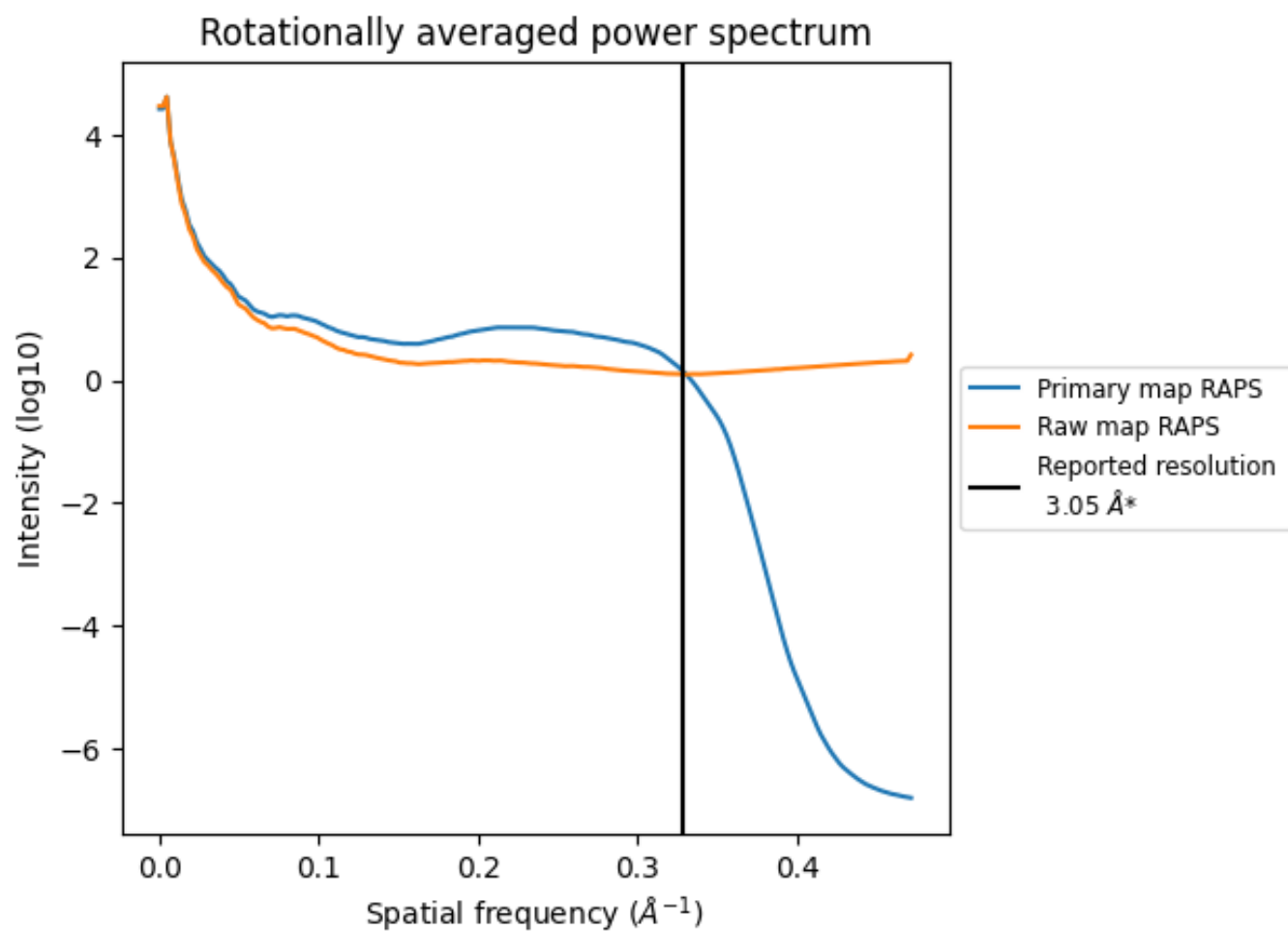
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 765 nm³; this corresponds to an approximate mass of 691 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 ⓘ

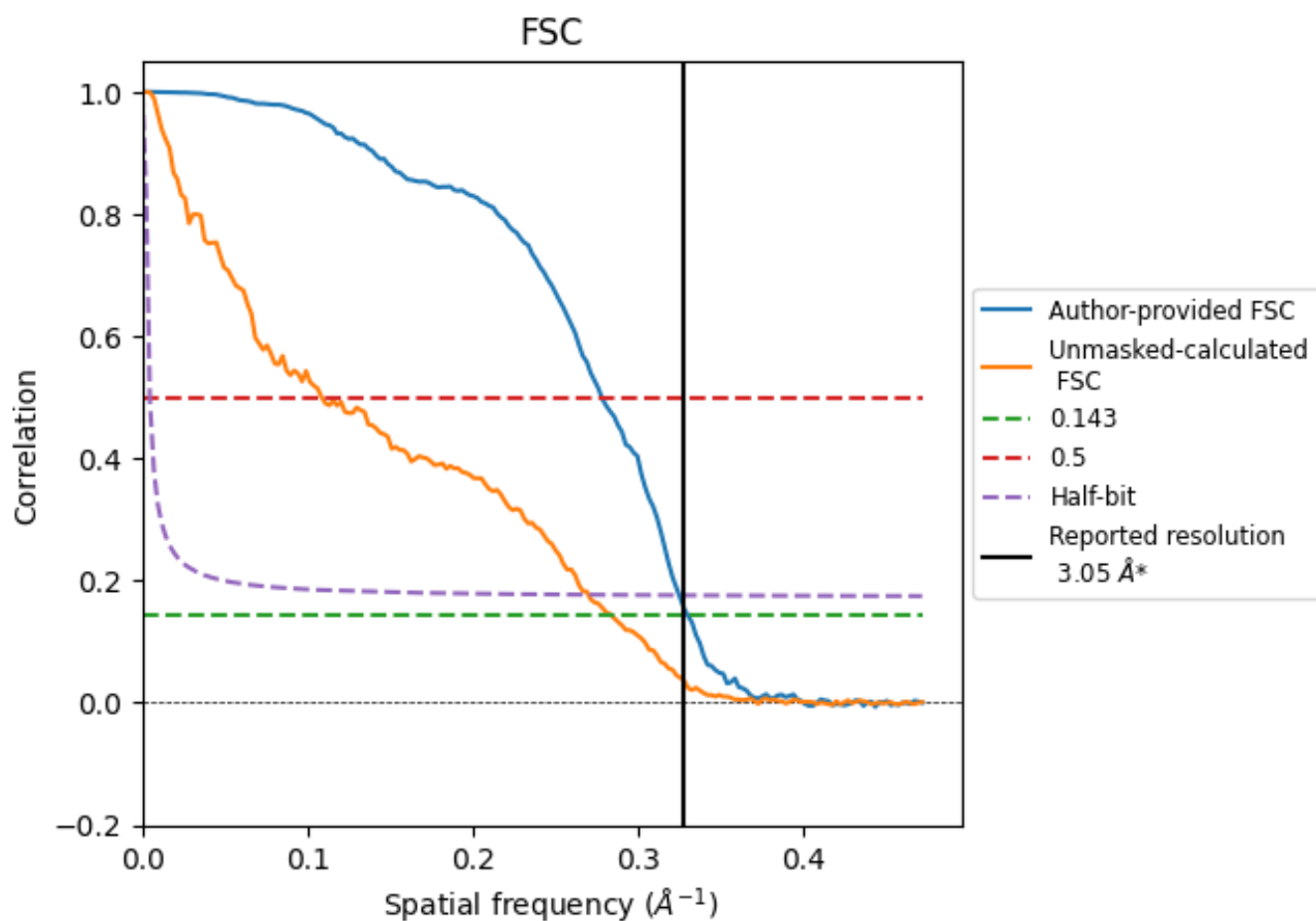


*Reported resolution corresponds to spatial frequency of 0.328 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.328 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

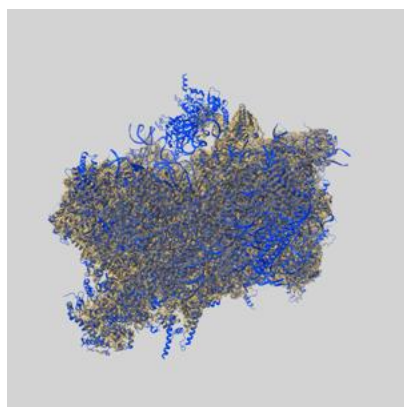
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.03	3.60	3.08
Unmasked-calculated*	3.52	9.22	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.52 differs from the reported value 3.05 by more than 10 %

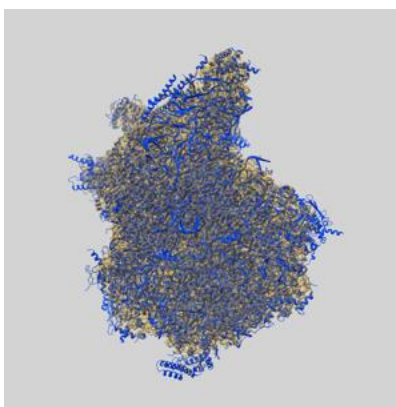
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10985 and PDB model 6YWY. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

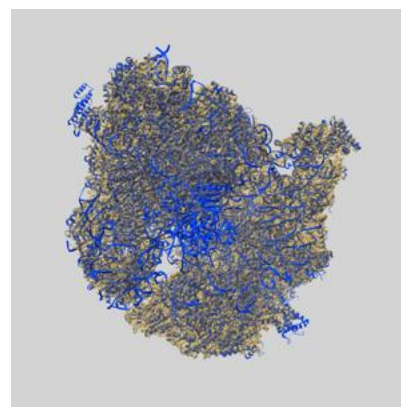
9.1 Map-model overlay [i](#)



X



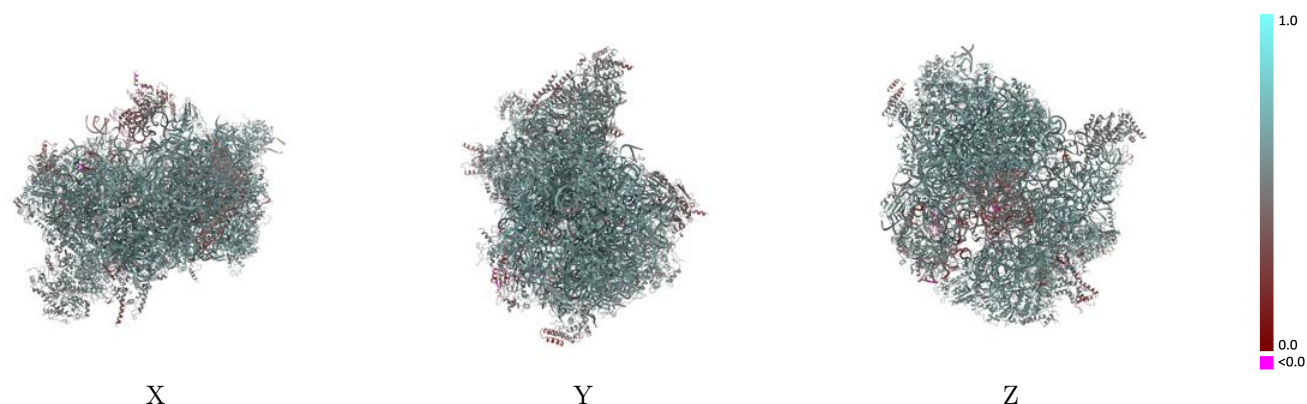
Y



Z

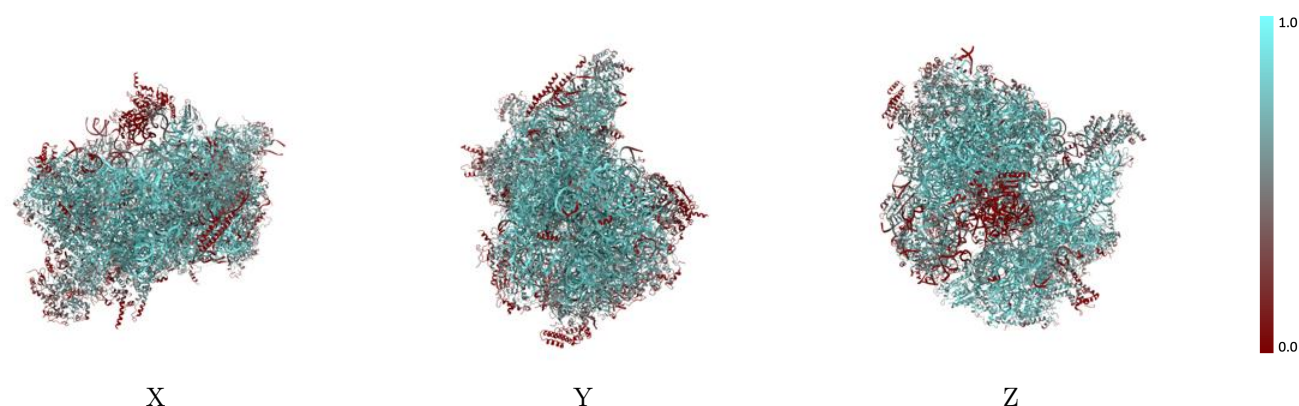
The images above show the 3D surface view of the map at the recommended contour level 4.77 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



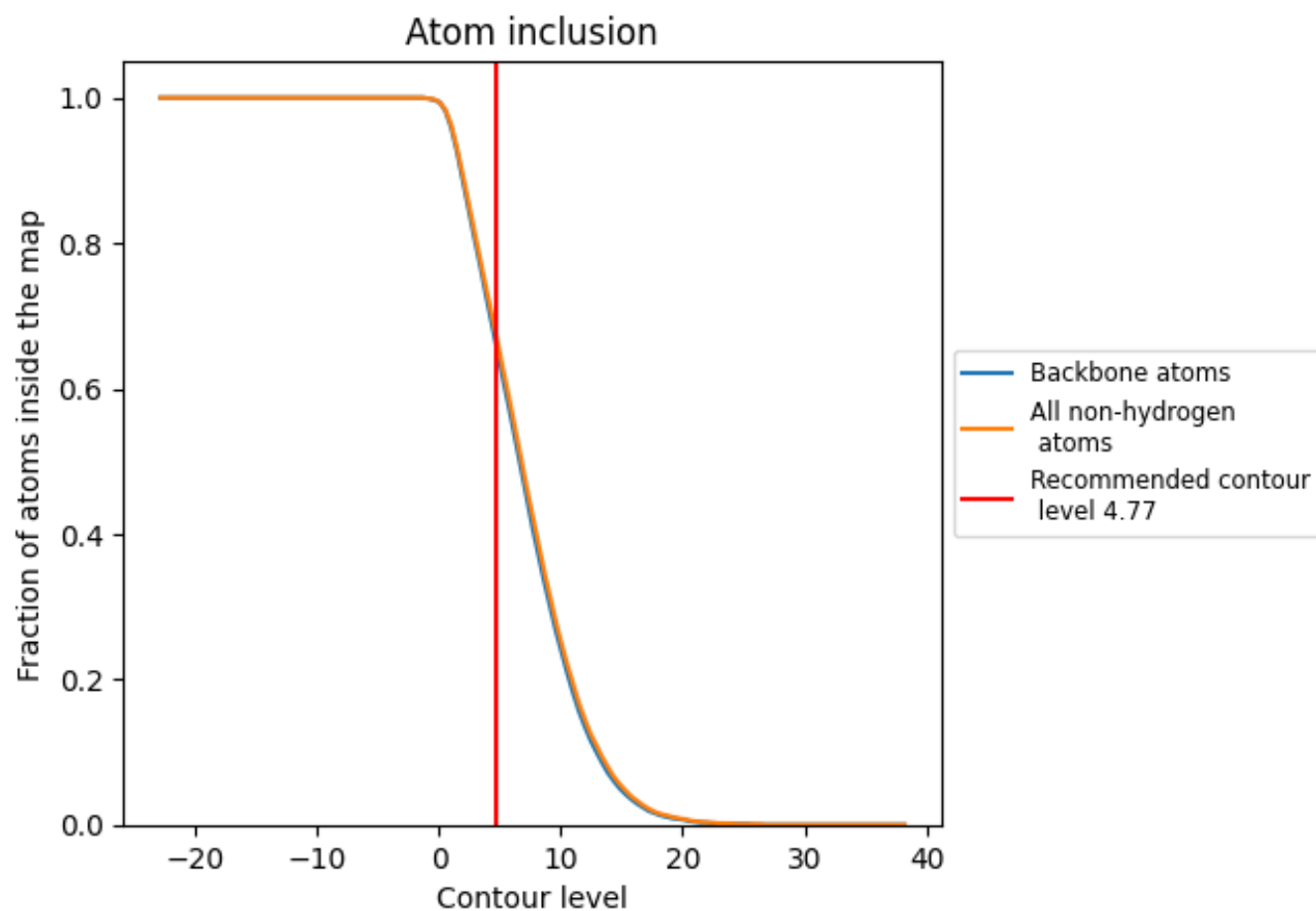
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.77).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 67% 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 (4.77) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6690	 0.5600
0	 0.8740	 0.6280
00	 0.1530	 0.4280
1	 0.5980	 0.5660
11	 0.6010	 0.5560
2	 0.6720	 0.5730
22	 0.7430	 0.6000
3	 0.6520	 0.5870
33	 0.6350	 0.5300
4	 0.7630	 0.6160
44	 0.3840	 0.4940
5	 0.6070	 0.5690
55	 0.3470	 0.4860
6	 0.5430	 0.5520
66	 0.6570	 0.5580
7	 0.6460	 0.5870
77	 0.6840	 0.5550
8	 0.2850	 0.4850
88	 0.5400	 0.5310
9	 0.4170	 0.5350
99	 0.0230	 0.3550
A	 0.7650	 0.5840
AA	 0.4310	 0.4980
B	 0.7380	 0.6060
BB	 0.6690	 0.5670
C	 0.7700	 0.6150
CC	 0.6450	 0.5490
D	 0.6420	 0.5810
DD	 0.7290	 0.5680
E	 0.6250	 0.5700
EE	 0.6580	 0.5600
F	 0.5750	 0.5490
FF	 0.6860	 0.5750
G	 0.4430	 0.5350
GG	 0.6570	 0.5660



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
H	 0.8080	 0.6240
HH	 0.7510	 0.5890
I	 0.6980	 0.6070
II	 0.6480	 0.5690
J	 0.6940	 0.5940
JJ	 0.7980	 0.5820
K	 0.7630	 0.6080
KK	 0.7140	 0.5880
L	 0.7150	 0.6000
LL	 0.7560	 0.5890
M	 0.5700	 0.5710
MM	 0.6920	 0.5760
N	 0.6910	 0.5960
NN	 0.8470	 0.6150
O	 0.6230	 0.5780
OO	 0.6230	 0.5590
P	 0.6990	 0.5990
PP	 0.7920	 0.5940
Q	 0.5460	 0.5660
QQ	 0.5910	 0.5470
R	 0.5590	 0.5380
RR	 0.5670	 0.5420
S	 0.6370	 0.5780
SS	 0.6380	 0.5540
T	 0.6400	 0.5770
TT	 0.7220	 0.5910
U	 0.6200	 0.5850
UU	 0.6280	 0.5520
V	 0.4930	 0.5350
VV	 0.5290	 0.5220
W	 0.7720	 0.6120
WW	 0.5410	 0.4850
X	 0.7370	 0.6060
XX	 0.7220	 0.5600
Y	 0.8390	 0.6320
YY	 0.7370	 0.5840
ZZ	 0.5560	 0.5220
a	 0.5680	 0.5580
aa	 0.8230	 0.5910
b	 0.5680	 0.5650
bb	 0.2730	 0.4660
c	 0.8160	 0.6300

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
cc	 0.2570	 0.4310
d	 0.6360	 0.5850
e	 0.0000	 0.0850
ee	 0.6390	 0.5470
f	 0.0710	 0.3810
g	 0.0000	 0.3280
h	 0.0030	 0.3720
i	 0.0240	 0.3210
j	 0.0000	 0.1270