



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 06:46 PM UTC

PDB ID : 9PRD / pdb\_00009prd  
EMDB ID : EMD-71809  
Title : In situ structure of the human mitoribosome in the P state from TACO1-knockout cells  
Authors : Wang, S.; Xiong, Y.; Zhang, Y.  
Deposited on : 2025-07-23  
Resolution : 3.31 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](mailto: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>.

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

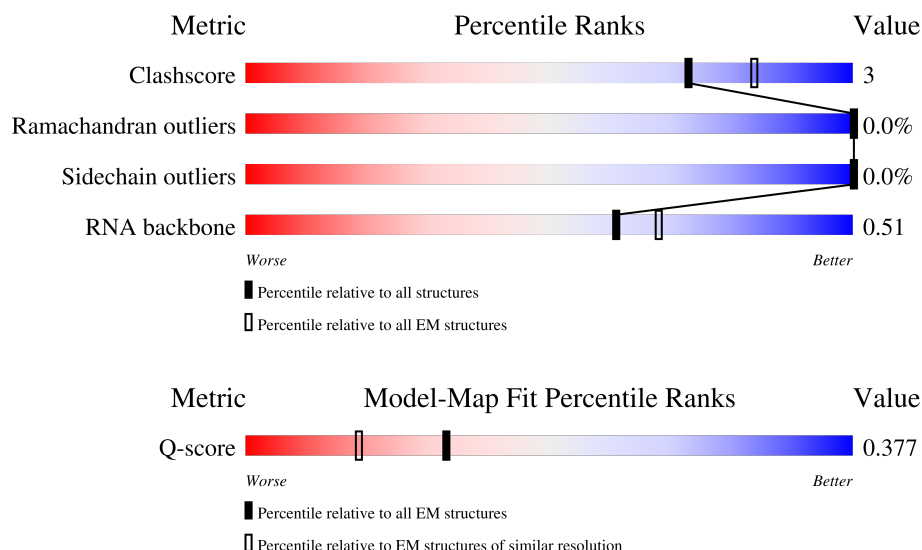
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.31 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.






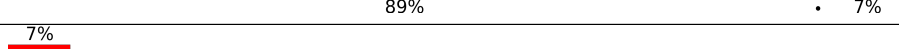

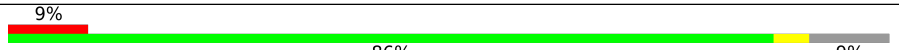



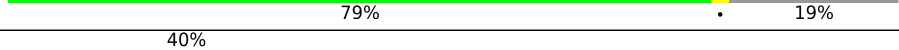

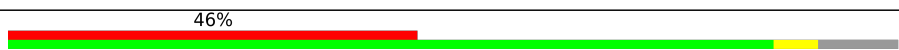
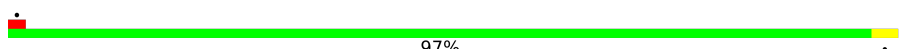

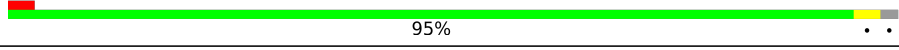

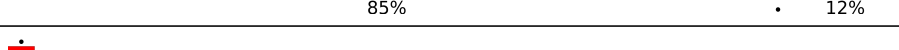

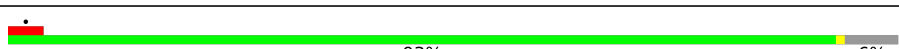


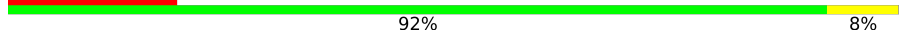



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14550 ( 2.81 - 3.81 )

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  $\geq 3$ , 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	0	188	
2	1	65	
3	2	92	

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Mol	Chain	Length	Quality of chain
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	A	1558	
12	D	305	
13	E	348	
14	F	311	
15	H	267	
16	I	261	
17	J	192	
18	K	178	
19	L	145	
20	M	296	
21	N	251	
22	O	175	
23	P	180	
24	Q	292	
25	R	149	
26	S	205	
27	T	206	
28	U	153	

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Mol	Chain	Length	Quality of chain
29	W	148	
30	X	256	
31	Y	250	
32	Z	161	
33	V	216	
34	b	215	
35	d	306	
36	e	279	
37	g	166	
38	h	158	
39	i	128	
40	j	123	
41	k	112	
42	l	138	
43	m	128	
44	n	43	
45	o	102	
46	q	222	
47	r	196	
48	t	198	
48	u	198	
49	c	332	
50	f	212	
51	p	206	
52	s	439	

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Mol	Chain	Length	Quality of chain
53	AB	296	
54	AC	167	
55	AD	430	
56	AE	125	
57	AF	242	
58	AG	396	
59	AH	201	
60	AJ	138	
61	AK	128	
62	AL	257	
63	AM	137	
64	AN	130	
65	AO	258	
66	AP	142	
67	AR	360	
68	AS	190	
69	AT	173	
70	AU	205	
71	AV	414	
72	AW	187	
73	AZ	106	
74	A0	217	
75	A1	323	
76	A3	199	
77	Az	34	

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Mol	Chain	Length	Quality of chain
78	AY	395	
79	AA	954	
80	AI	194	
81	OX	435	
82	a	142	
83	Ax	71	
84	A4	689	
85	AX	398	
86	A2	118	
87	AQ	87	
88	B	72	

## 2 Entry composition

There are 99 unique types of molecules in this entry. The entry contains 176450 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	56	Total	C	N	O	S	0	0
			464	296	89	77	2		

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	157	Total	C	N	O	S	0	0
			1327	844	235	246	2		

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 11 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1558	Total	C	N	O	P	0	0
			33070	14843	5963	10706	1558		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	A	deletion	GB 2756414513
A	?	-	C	deletion	GB 2756414513
A	?	-	U	deletion	GB 2756414513

- Molecule 12 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	238	Total	C	N	O	S	0	0
			1859	1157	376	317	9		

- Molecule 13 is a protein called 39S ribosomal protein L3, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	305	Total	C	N	O	S	0	0
			2406	1545	418	432	11		

- Molecule 14 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	252	Total	C	N	O	S	0	0
			2031	1305	370	350	6		

- Molecule 15 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	202	Total	C	N	O	S	0	0
			1661	1067	304	286	4		

- Molecule 16 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	181	Total	C	N	O	S	0	0
			1446	932	260	244	10		

- Molecule 17 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	175	Total	C	N	O	S	0	0
			1330	847	237	244	2		

- Molecule 18 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	178	Total	C	N	O	S	0	0
			1455	936	259	253	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ACE	-	acetylation	UNP H2QWN0
K	132	TYR	ASP	conflict	UNP H2QWN0

- Molecule 19 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	115	Total	C	N	O	S	0	0
			890	559	171	155	5		

- Molecule 20 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	291	Total	C	N	O	S	0	0
			2327	1483	430	408	6		

- Molecule 21 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	222	Total	C	N	O	S	0	0
			1786	1143	326	307	10		

- Molecule 22 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	154	Total	C	N	O	S	0	0
			1259	792	241	219	7		

- Molecule 23 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	144	Total	C	N	O	S	0	0
			1173	733	224	211	5		

- Molecule 24 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	239	Total	C	N	O	S	0	0
			1990	1277	353	351	9		

- Molecule 25 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	140	Total	C	N	O	S	0	0
			1154	732	231	187	4		

- Molecule 26 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	161	Total	C	N	O	S	0	0
			1293	835	227	227	4		

- Molecule 27 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	166	Total	C	N	O	S	0	0
			1369	875	254	233	7		

- Molecule 28 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	152	Total	C	N	O	S	0	0
			1248	786	234	225	3		

- Molecule 29 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	116	Total	C	N	O	S	0	0
			904	577	171	153	3		

- Molecule 30 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	244	Total	C	N	O	S	0	0
			2044	1322	352	365	5		

- Molecule 31 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	181	Total	C	N	O	S	0	0
			1556	995	298	259	4		

- Molecule 32 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	122	Total	C	N	O	S	0	0
			996	636	186	171	3		

- Molecule 33 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V	205	Total	C	N	O	S	0	0
			1676	1068	298	302	8		

- Molecule 34 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	150	Total	C	N	O	S	0	0
			1193	742	231	217	3		

- Molecule 35 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	259	Total	C	N	O	S	0	0
			2124	1357	369	384	14		

- Molecule 36 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	238	Total	C	N	O	S	0	0
			1931	1222	339	364	6		

- Molecule 37 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	134	Total	C	N	O	S	0	0
			1113	719	193	199	2		

- Molecule 38 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	110	Total	C	N	O	S	0	0
			895	568	156	168	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	97	Total	C	N	O	S	0	0
			828	532	165	127	4		

- Molecule 40 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	94	Total	C	N	O	S	0	0
			745	463	144	136	2		

- Molecule 41 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	102	Total	C	N	O	S	0	0
			774	479	148	142	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	1	ACE	-	acetylation	UNP Q96EL3

- Molecule 42 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	82	Total	C	N	O	S	0	0
			688	437	120	128	3		

- Molecule 43 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	92	Total	C	N	O	S	0	0
			791	488	159	142	2		

- Molecule 44 is a protein called Nascent polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	n	43	Total	C	N	O	0	0
			215	129	43	43		

- Molecule 45 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	94	Total	C	N	O	S	0	0
			798	501	165	129	3		

- Molecule 46 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	177	Total	C	N	O	S	0	0
			1495	929	292	269	5		

- Molecule 47 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	162	Total	C	N	O	S	0	0
			1322	839	252	223	8		

- Molecule 48 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	t	46	Total	C	N	O	0	0
			354	228	56	70		
48	u	32	Total	C	N	O	0	0
			257	168	40	49		

- Molecule 49 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	c	286	Total	C	N	O	S	0	0
			2299	1470	397	423	9		

- Molecule 50 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	f	157	Total	C	N	O	S	0	0
			1252	799	207	242	4		

- Molecule 51 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	p	147	Total	C	N	O	S	0	0
			1205	748	228	225	4		

- Molecule 52 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	385	Total	C	N	O	S	0	0
			3148	2018	558	558	14		

- Molecule 53 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AB	225	Total	C	N	O	S	0	0
			1828	1164	331	323	10		

- Molecule 54 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AC	132	Total	C	N	O	S	0	0
			1083	699	195	185	4		

- Molecule 55 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AD	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

- Molecule 56 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AE	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 57 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AF	208	Total	C	N	O	S	0	0
			1725	1104	312	298	11		

- Molecule 58 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AG	327	Total	C	N	O	S	0	0
			2688	1710	477	487	14		

- Molecule 59 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AH	140	Total	C	N	O	S	0	0
			1152	745	194	210	3		

- Molecule 60 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AJ	108	Total	C	N	O	S	0	0
			839	521	169	143	6		

- Molecule 61 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AK	101	Total	C	N	O	S	0	0
			862	537	179	141	5		

- Molecule 62 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AL	174	Total	C	N	O	S	0	0
			1453	925	270	251	7		

- Molecule 63 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AM	119	Total	C	N	O	S	0	0
			942	594	185	157	6		

- Molecule 64 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AN	110	Total	C	N	O	S	0	0
			868	562	156	147	3		

- Molecule 65 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AO	193	Total	C	N	O	S	0	0
			1592	1014	294	277	7		

- Molecule 66 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AP	97	Total	C	N	O	S	0	0
			781	501	134	138	8		

- Molecule 67 is a protein called 28S ribosomal protein S22, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace
67	AR	295	Total	C	N	O	S	0	0
			2409	1533	413	455	8		

- Molecule 68 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AS	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

- Molecule 69 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AT	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 70 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AU	176	Total	C	N	O	S	0	0
			1488	916	301	267	4		

- Molecule 71 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AV	362	Total	C	N	O	S	0	0
			2969	1904	495	558	12		

- Molecule 72 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AW	100	Total	C	N	O	S	0	0
			789	498	141	146	4		

- Molecule 73 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AZ	100	Total	C	N	O	S	0	0
			839	534	153	148	4		

- Molecule 74 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	A0	215	Total	C	N	O	S	0	0
			1787	1130	339	313	5		

- Molecule 75 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	A1	279	Total	C	N	O	S	0	0
			2265	1435	387	432	11		

- Molecule 76 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	A3	70	Total	C	N	O	S	0	0
			625	401	134	89	1		

- Molecule 77 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Az	34	Total	C	N	O	P	0	0
			719	324	123	238	34		

- Molecule 78 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AY	119	Total	C	N	O	S	0	0
			1010	654	166	188	2		

- Molecule 79 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AA	954	Total	C	N	O	P	0	0
			20260	9088	3647	6571	954		

- Molecule 80 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AI	137	Total	C	N	O	S	0	0
			1019	641	193	181	4		

- Molecule 81 is a protein called Mitochondrial inner membrane protein OXA1L.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	OX	55	Total	C	N	O	S	0	0
			468	292	93	81	2		

- Molecule 82 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	a	103	Total	C	N	O	S	0	0
			865	543	155	162	5		

- Molecule 83 is a RNA chain called P/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Ax	71	Total	C	N	O	P	0	0
			1498	673	264	491	70		

- Molecule 84 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	A4	588	Total	C	N	O	S	0	0
			4768	3053	808	879	28		

- Molecule 85 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	AX	352	Total	C	N	O	S	0	0
			2849	1822	499	517	11		

- Molecule 86 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	A2	118	Total	C	N	O	S	0	0
			935	579	182	166	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1	ACE	-	acetylation	UNP Q96BP2

- Molecule 87 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	AQ	87	Total	C	N	O	S	0	0
			744	460	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	1	ACE	-	acetylation	UNP P82921
AQ	50	ARG	CYS	variant	UNP P82921

- Molecule 88 is a RNA chain called mitochondrial tRNA<sup>Val</sup>.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	B	72	Total	C	N	O	P	0	0
			1524	685	269	498	72		

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	0	1	Total	Zn	0
			1	1	
89	4	1	Total	Zn	0
			1	1	
89	AO	1	Total	Zn	0
			1	1	

- Molecule 90 is POTASSIUM ION (CCD ID: K) (formula: K).

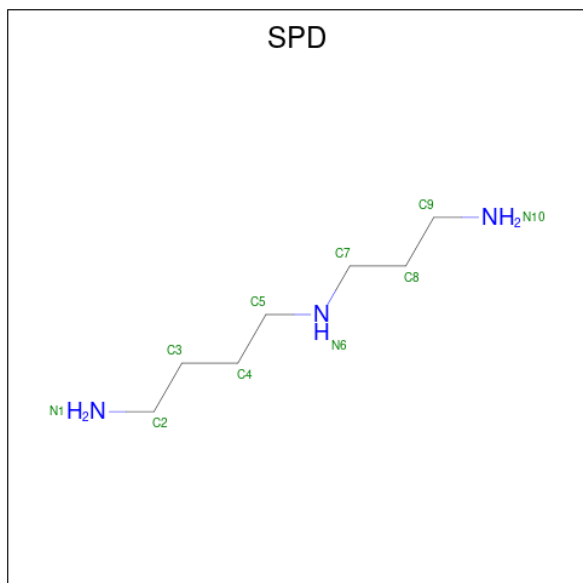
Mol	Chain	Residues	Atoms		AltConf
90	3	1	Total	K	0
			1	1	
90	6	1	Total	K	0
			1	1	
90	A	29	Total	K	0
			29	29	
90	D	1	Total	K	0
			1	1	
90	M	1	Total	K	0
			1	1	
90	N	1	Total	K	0
			1	1	
90	W	1	Total	K	0
			1	1	

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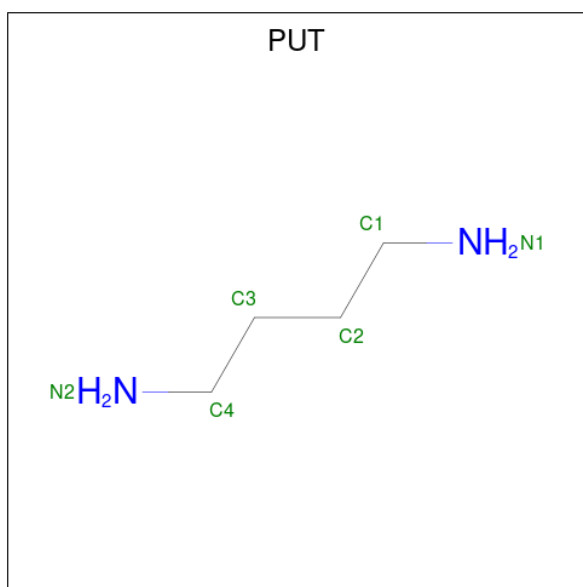
Mol	Chain	Residues	Atoms		AltConf
90	o	1	Total	K	0
			1	1	
90	AA	18	Total	K	0
			18	18	

- Molecule 91 is SPERMIDINE (CCD ID: SPD) (formula:  $C_7H_{19}N_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
91	A	1	Total	C	N	0
			10	7	3	
91	A	1	Total	C	N	0
			10	7	3	
91	A	1	Total	C	N	0
			10	7	3	
91	A	1	Total	C	N	0
			10	7	3	
91	O	1	Total	C	N	0
			10	7	3	
91	AA	1	Total	C	N	0
			10	7	3	
91	AA	1	Total	C	N	0
			10	7	3	

- Molecule 92 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula:  $C_4H_{12}N_2$ ).

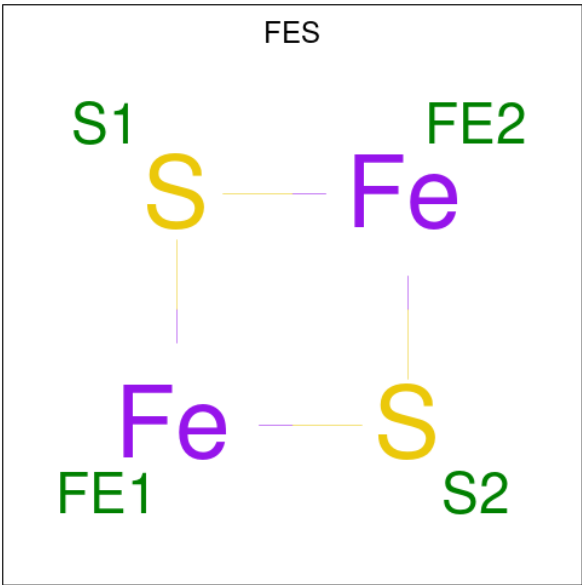


Mol	Chain	Residues	Atoms			AltConf
92	A	1	Total	C	N	0
			6	4	2	

- Molecule 93 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

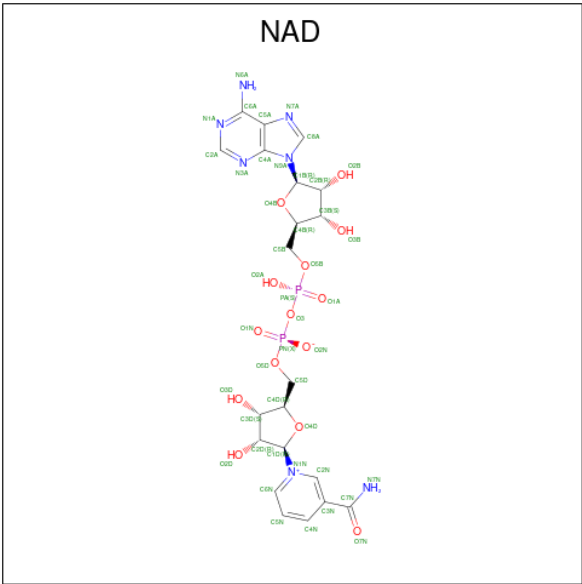
Mol	Chain	Residues	Atoms		AltConf
93	A	137	Total	Mg	0
			137	137	
93	D	2	Total	Mg	0
			2	2	
93	E	1	Total	Mg	0
			1	1	
93	g	1	Total	Mg	0
			1	1	
93	AB	1	Total	Mg	0
			1	1	
93	A3	1	Total	Mg	0
			1	1	
93	Az	1	Total	Mg	0
			1	1	
93	AA	59	Total	Mg	0
			59	59	
93	AX	1	Total	Mg	0
			1	1	

- Molecule 94 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



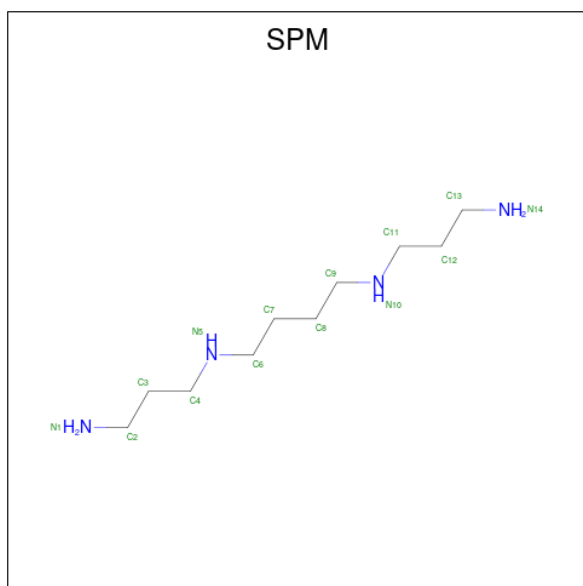
Mol	Chain	Residues	Atoms			AltConf
94	r	1	Total	Fe	S	0
			4	2	2	
94	AP	1	Total	Fe	S	0
			4	2	2	
94	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 95 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

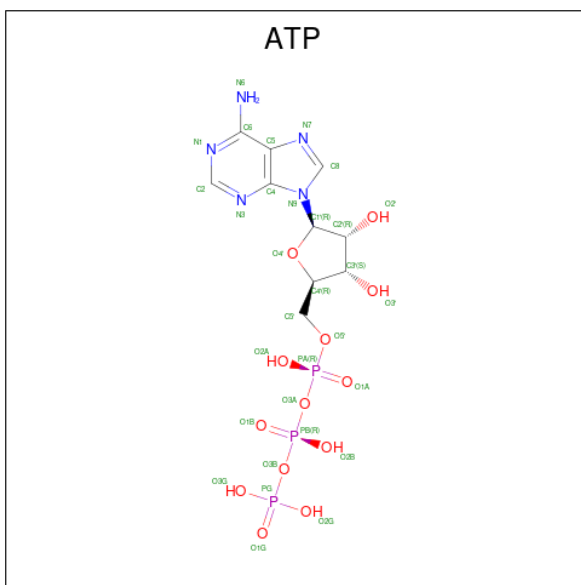
- Molecule 96 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
96	AA	1	Total	C	N		0
			14	10	4		
96	AA	1	Total	C	N		0
			14	10	4		

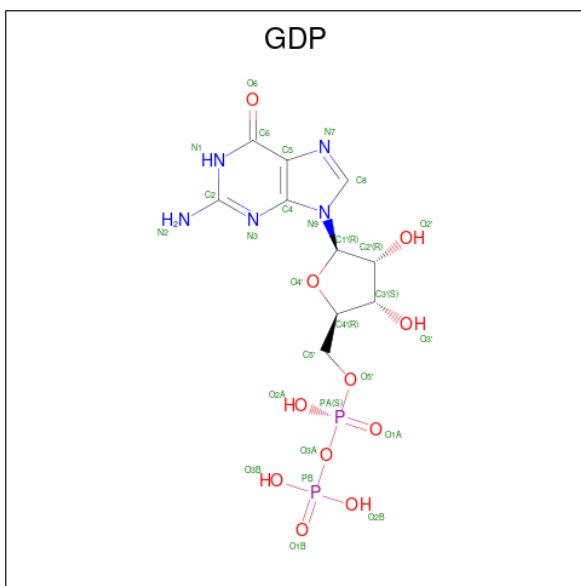
- Molecule 97 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).





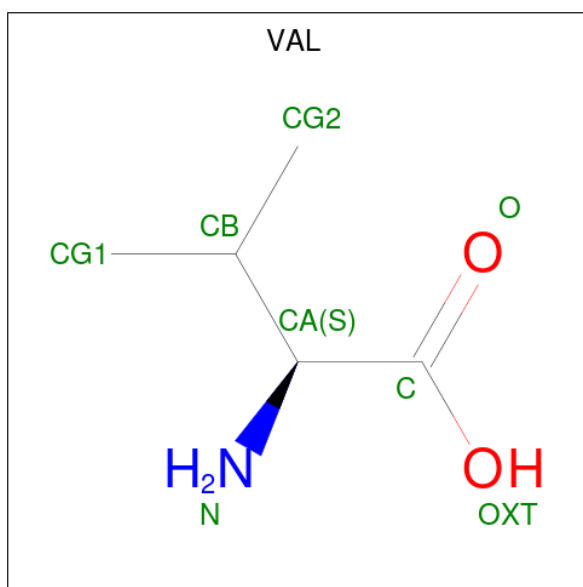
Mol	Chain	Residues	Atoms					AltConf
97	AX	1	Total	C	N	O	P	0
			31	10	5	13	3	

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



Mol	Chain	Residues	Atoms					AltConf
98	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 99 is VALINE (CCD ID: VAL) (formula:  $C_5H_{11}NO_2$ ).

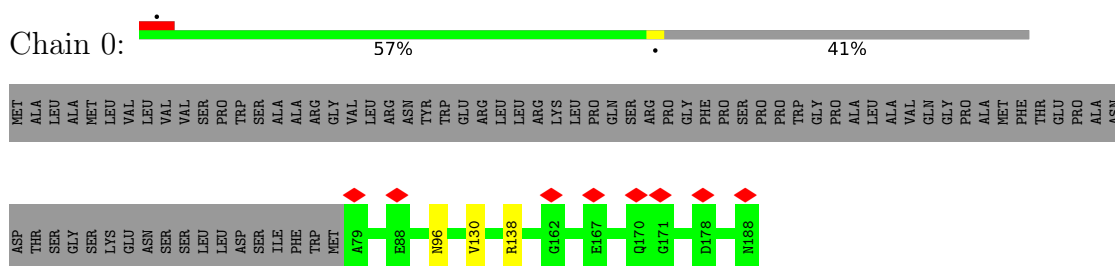


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
99	B	1	7	5	1	1	0

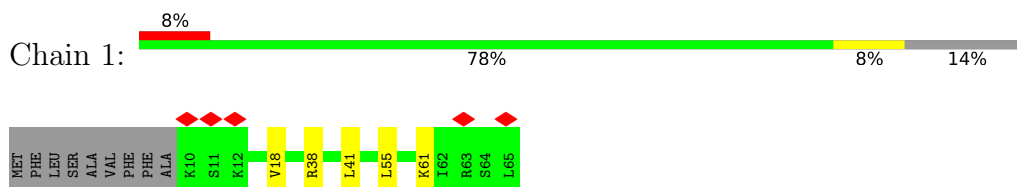
### 3 Residue-property plots [i](#)

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.

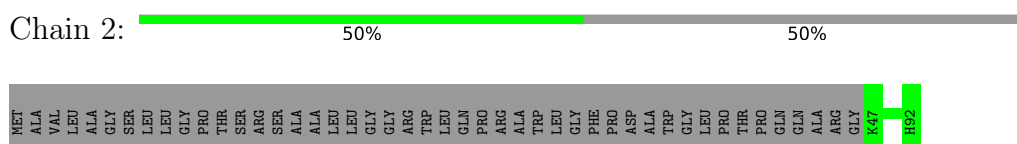
- Molecule 1: 39S ribosomal protein L32, mitochondrial



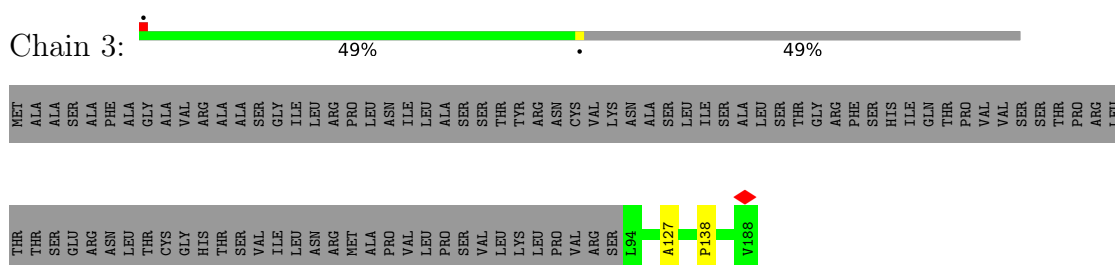
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial



- Molecule 4: 39S ribosomal protein L35, mitochondrial




- Molecule 5: 39S ribosomal protein L36, mitochondrial



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

LEU PRO ALA ALA GLY F66 K63 W88 M103

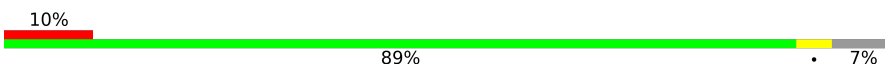
- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:  88% 5% 7%

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

T232 R242 E243 E244 I245 L253 D272 D295 L327 N331 L336 E337 Q338 D343 T362 L364 R395 Y418 A423


- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:  10% 89% 7%

MET ALA PRO TRP ARG ALA ALA CYS GLU CYS ARG TRP ARG GLY THR SER ALA VAL LEU GLY R27 D39 L42 Q63 E64 G79 E80 K81 T82 D83 P84 K85 E86 K87 K88 R106 R124 A128 R141 L173 H174 V175 V179

G180 E181 D182 D183 V187 E197 V204 E207 A208 E209 E210 G211 S212 T219 E227 L233 H234 E247 L255 P256 P257 F273 D276 F281 S282 E283 D284 Y304 E309 T310 M311 P313 F319 D336 K353 D371 S372 H373 Y380

- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7:  7% 81% 6% 13%

MET GLU ALA LEU MET GLY SER ARG ALA LEU ARG LEU TRP LEU VAL PRO GLY GLY ILE LYS TRP GLN ARG PHE ILE ALA THR SER ALA Q34 N45 L56 S57 L58 R61 K72 T77 D109 P112 W113 D114 K117 N139 M148 K159

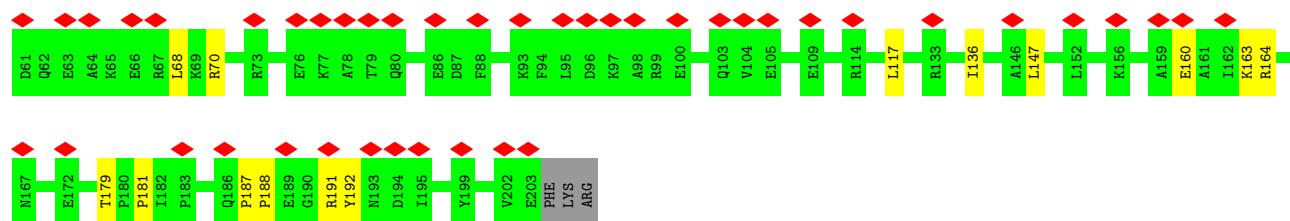
D160 E161 Y162 M163 V174 D186 D190 E191 F202 T203 K204 L209 K212 E220 E228 H232 E249 L257 Q258 D259 P267 Q277 V280 Q287 P288 T289 Q290 L293 S301 R307 K315 E326 D327 G328 SER LYS ALA THR GLU

CYS THR THR

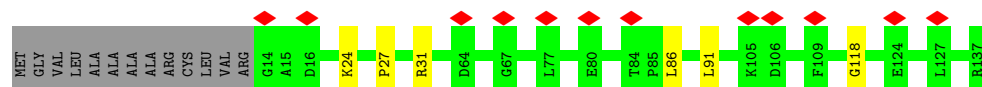
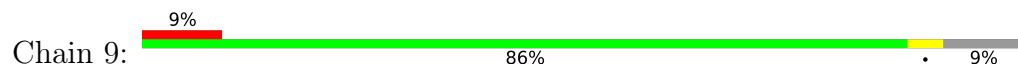
- Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8:  28% 69% 7% 24%

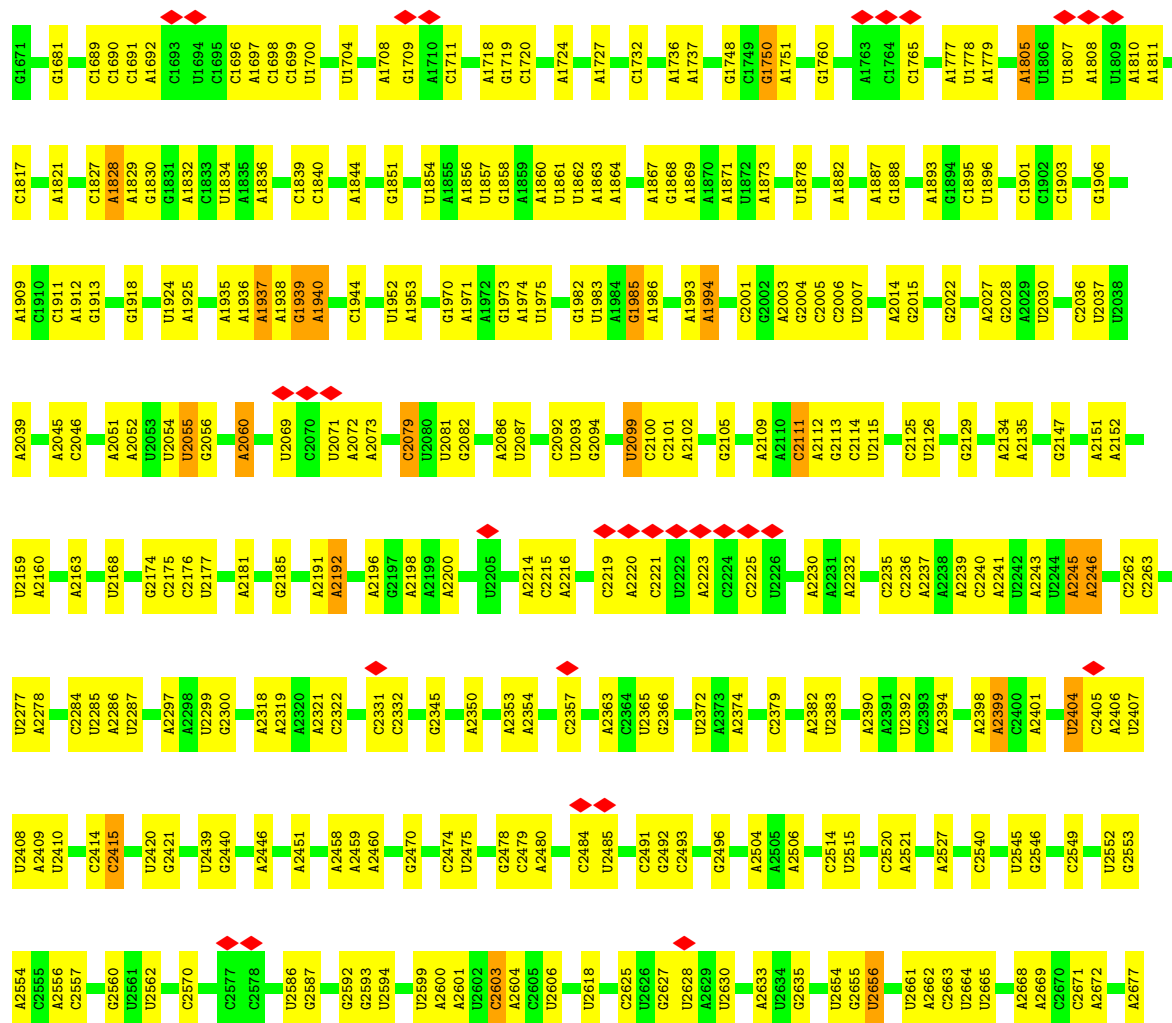
MET THR ALA SER LEU VAL ARG SER ILE SER SER LEU ALA ALA ARG PRO THR THR SER GLY LEU LEU GLY THR TRP GLN THR GLN ARG ALA ALA SER SER LEU LEU SER PHE TRP GLU LEU ILE PRO MET ARG S47 E48 P49 L50 R51 K52 K53 K54 K55 V56 D57 P58 K59 K60

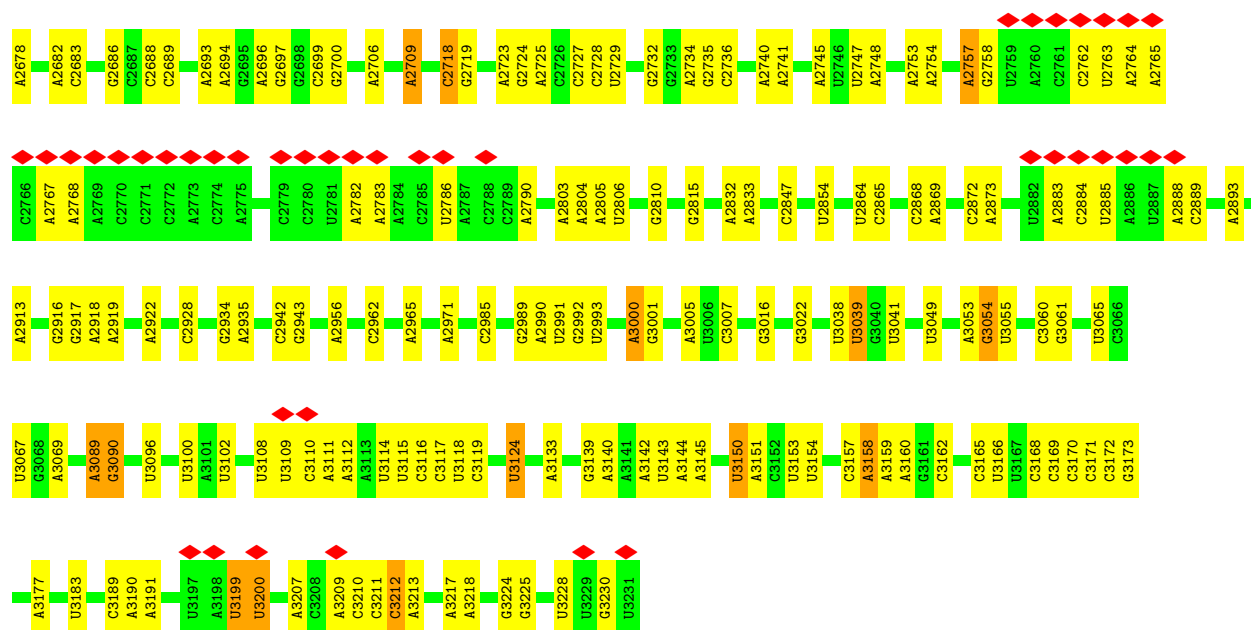


- Molecule 10: 39S ribosomal protein L41, mitochondrial

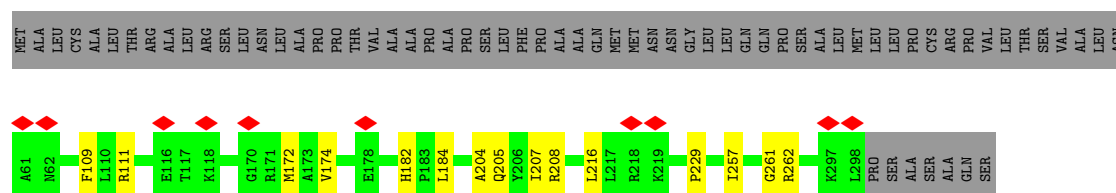


- Molecule 11: 16S mitochondrial rRNA

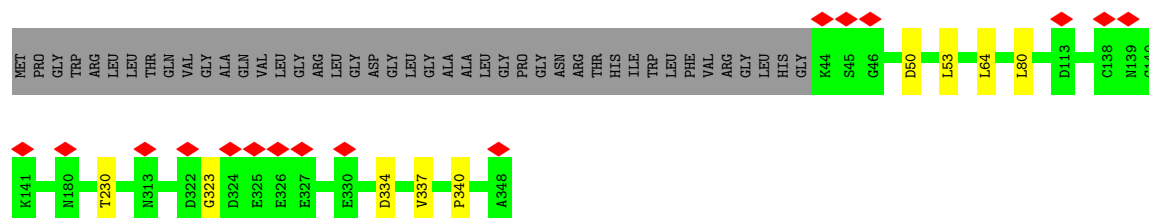
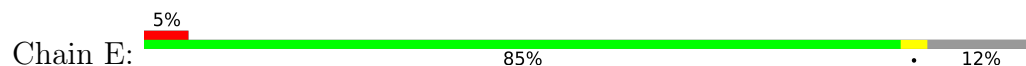




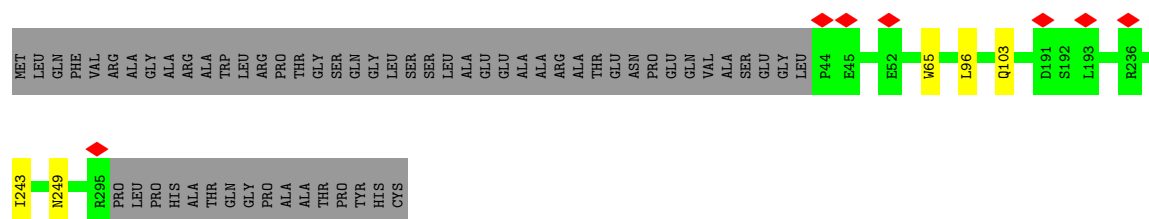
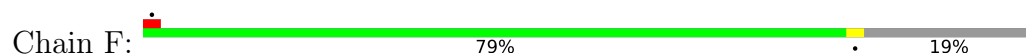
- Molecule 12: 39S ribosomal protein L2, mitochondrial



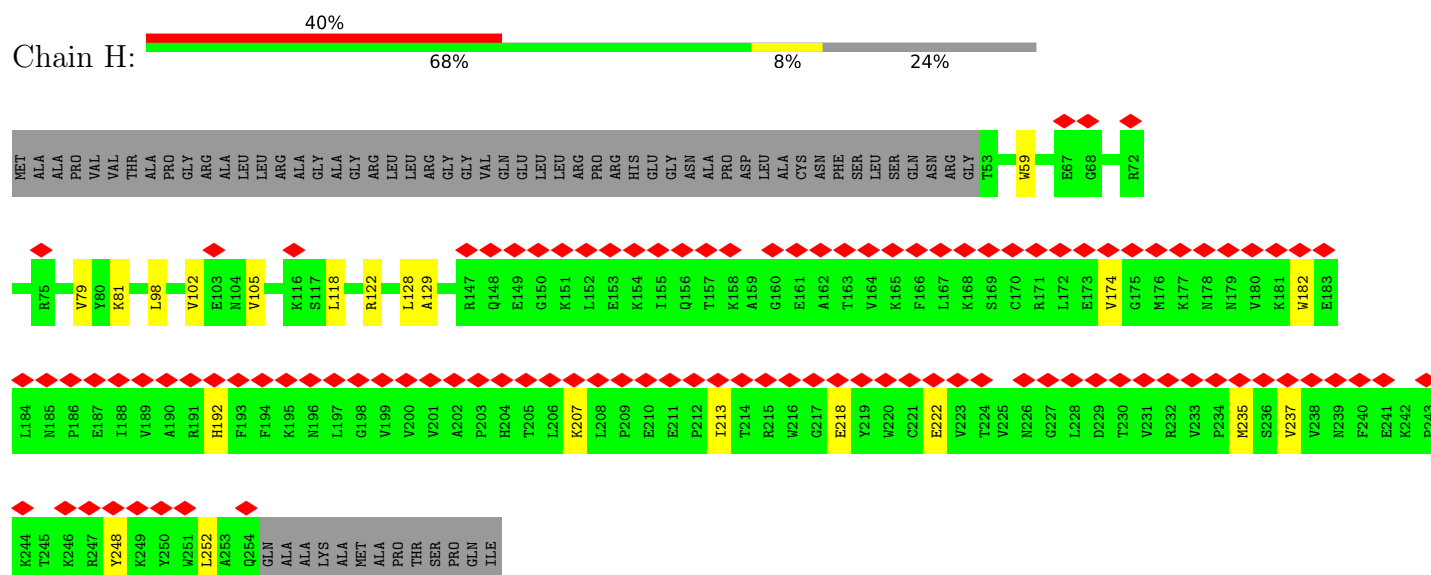
- Molecule 13: 39S ribosomal protein L3, mitochondrial



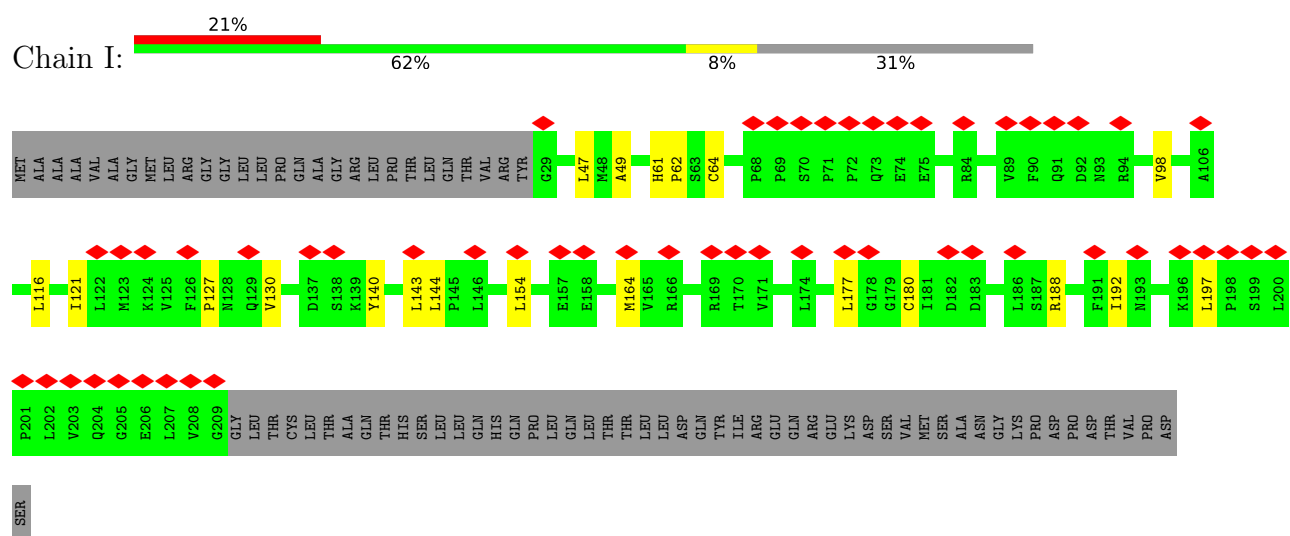
- Molecule 14: 39S ribosomal protein L4, mitochondrial



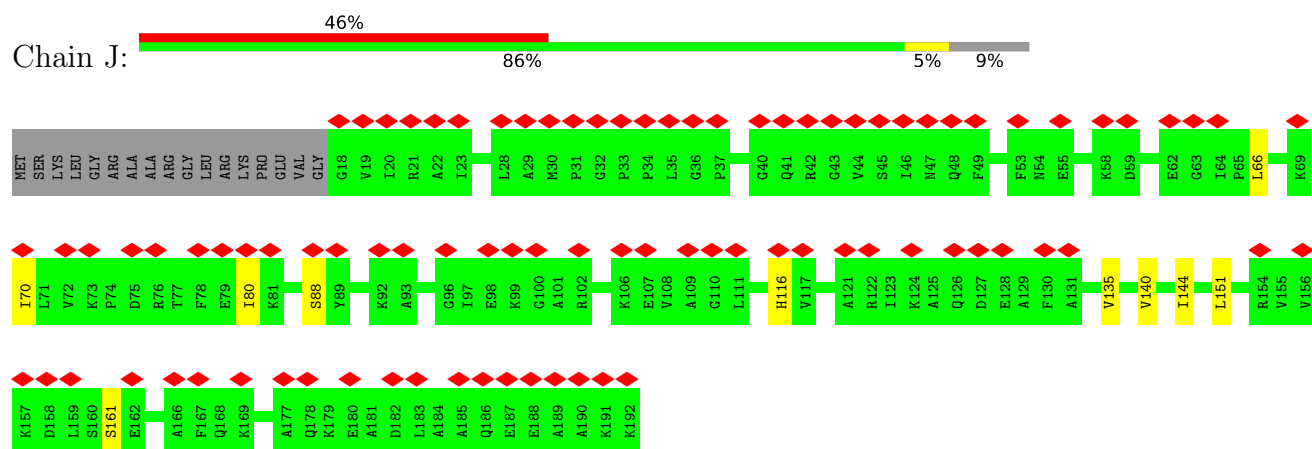
- Molecule 15: 39S ribosomal protein L9, mitochondrial



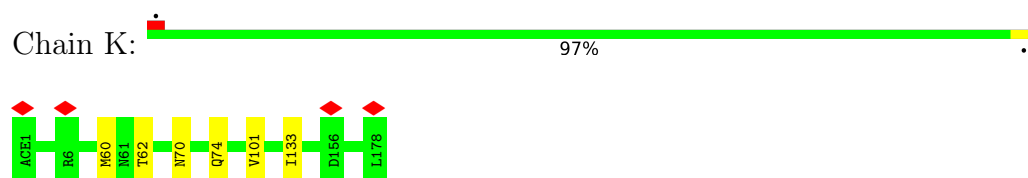
- Molecule 16: 39S ribosomal protein L10, mitochondrial



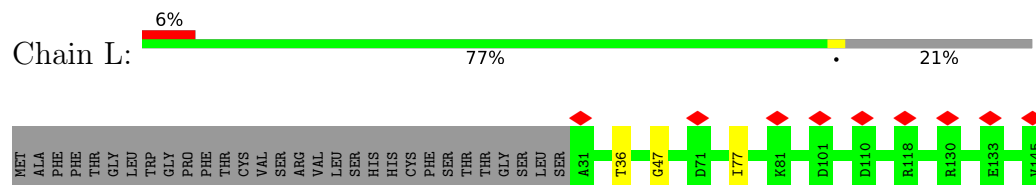
- Molecule 17: 39S ribosomal protein L11, mitochondrial



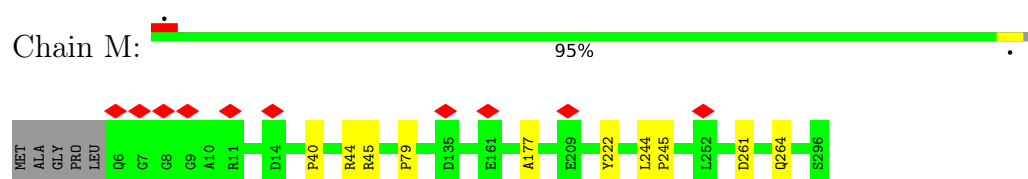
- Molecule 18: Large ribosomal subunit protein uL13m



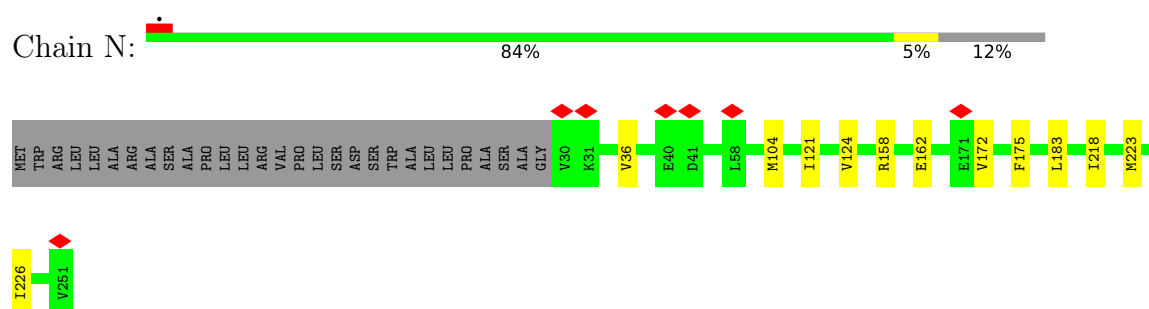
- Molecule 19: 39S ribosomal protein L14, mitochondrial



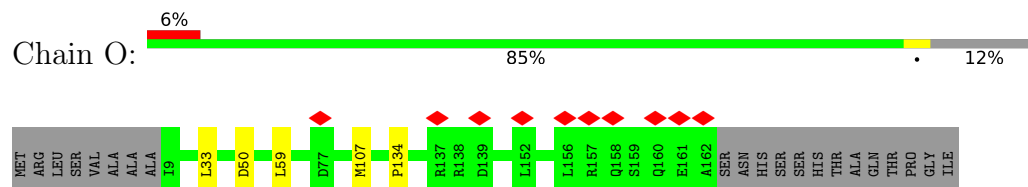
- Molecule 20: 39S ribosomal protein L15, mitochondrial



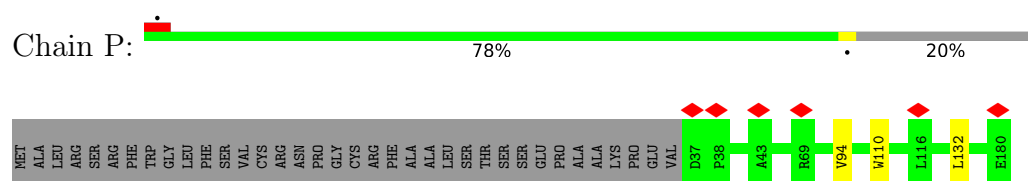
- Molecule 21: 39S ribosomal protein L16, mitochondrial



- Molecule 22: 39S ribosomal protein L17, mitochondrial

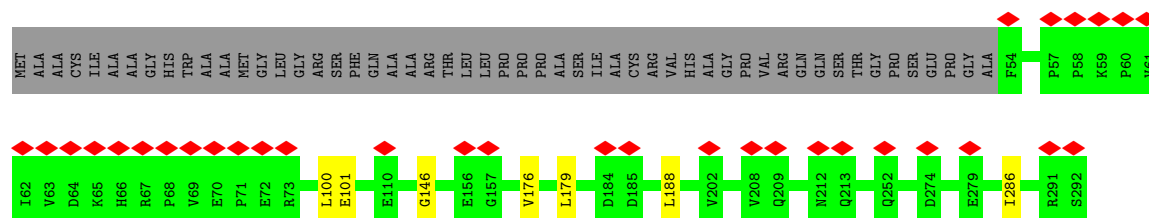
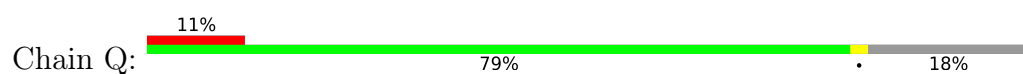


- Molecule 23: 39S ribosomal protein L18, mitochondrial

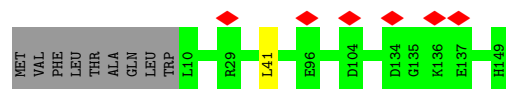


- Molecule 24: 39S ribosomal protein L19, mitochondrial

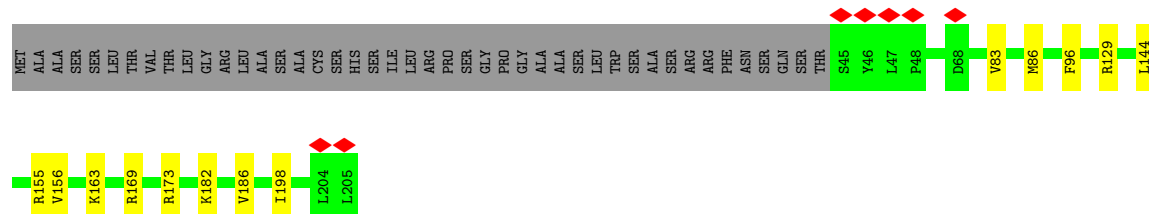




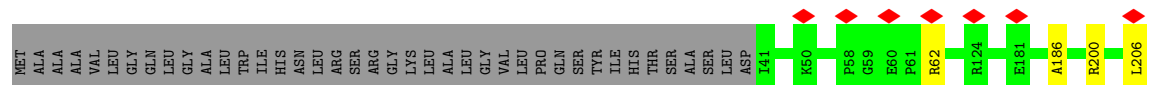
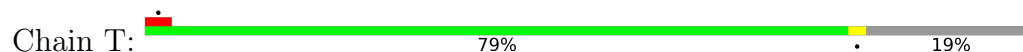
- Molecule 25: 39S ribosomal protein L20, mitochondrial



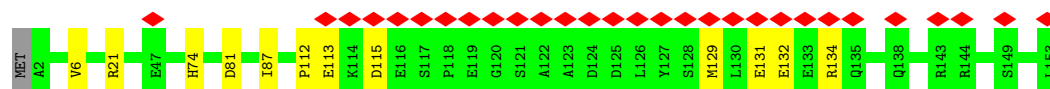
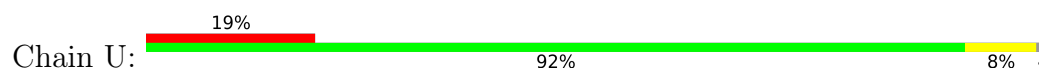
- Molecule 26: 39S ribosomal protein L21, mitochondrial



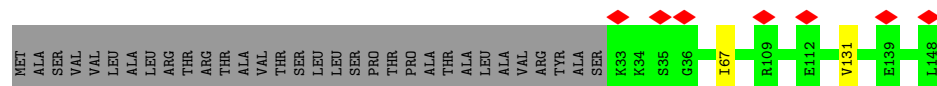
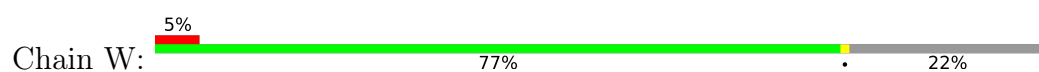
- Molecule 27: 39S ribosomal protein L22, mitochondrial



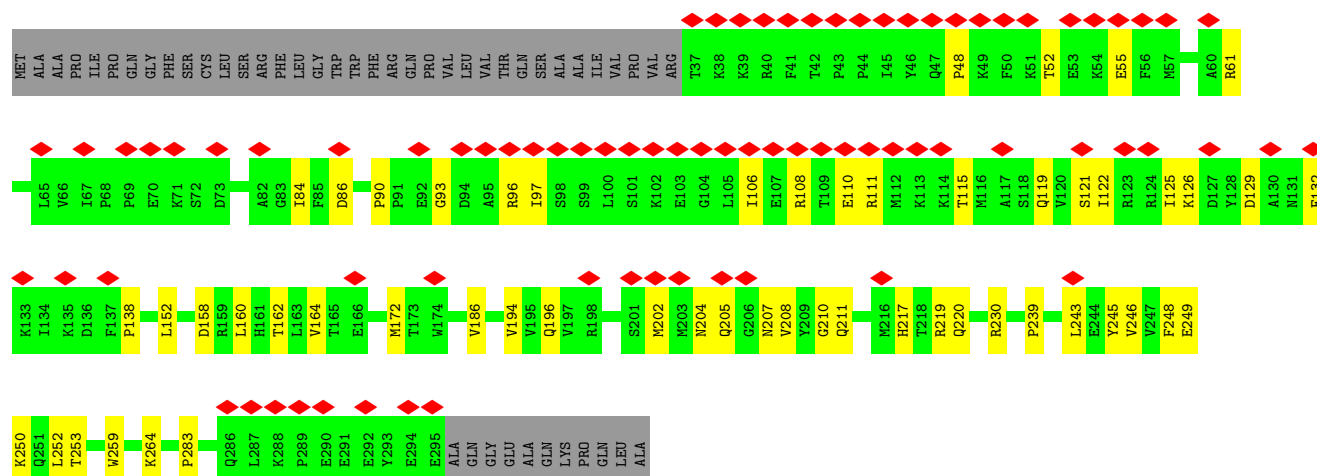
- Molecule 28: 39S ribosomal protein L23, mitochondrial



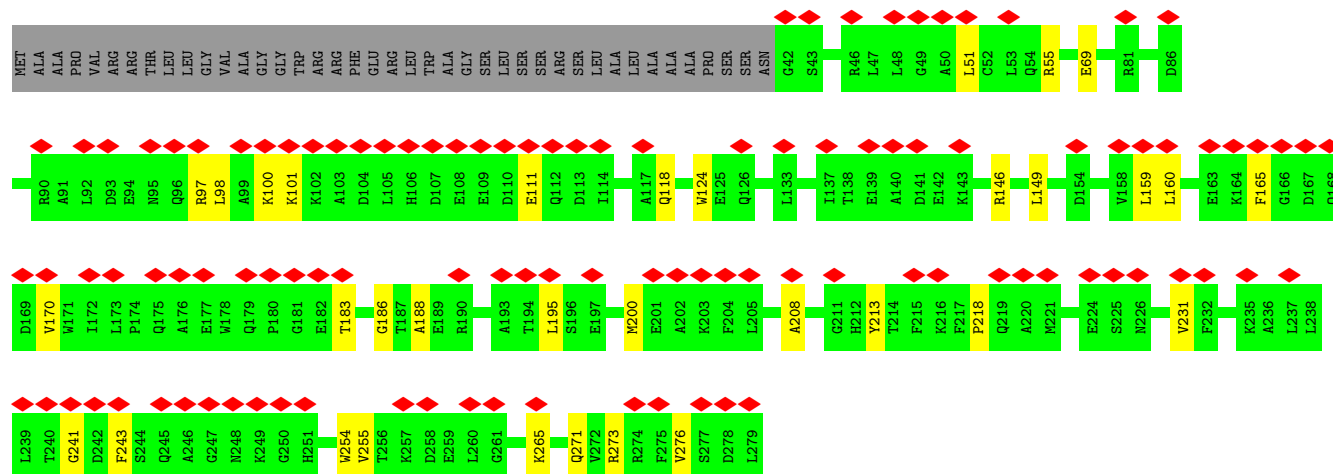
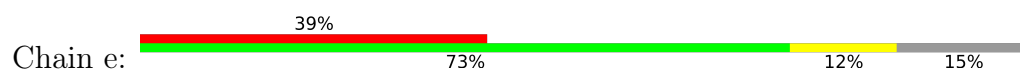
- Molecule 29: 39S ribosomal protein L27, mitochondrial



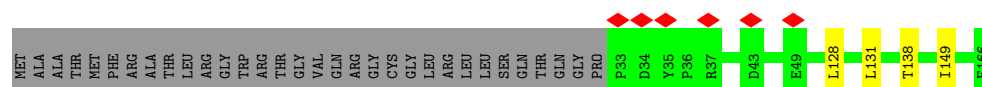
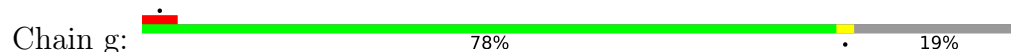
- Chain d: 



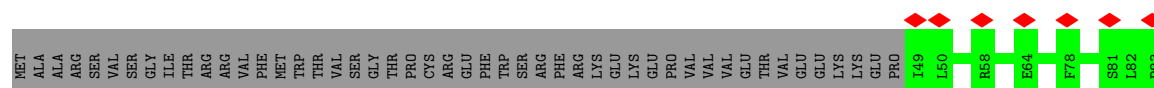
- Molecule 36: 39S ribosomal protein L46, mitochondrial

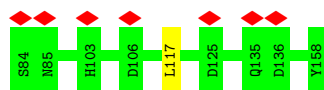


- Molecule 37: 39S ribosomal protein L49, mitochondrial

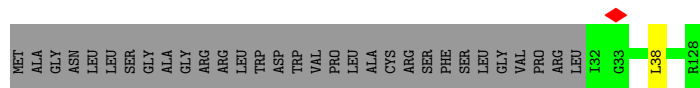
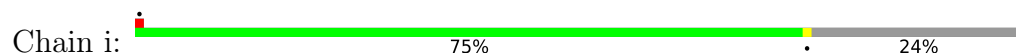


- Molecule 38: 39S ribosomal protein L50, mitochondrial

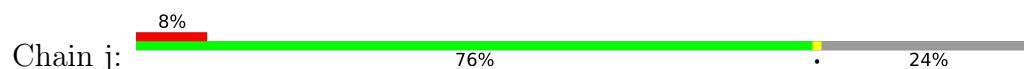




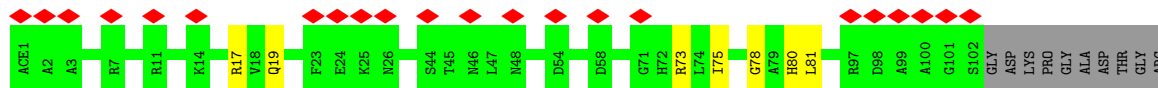
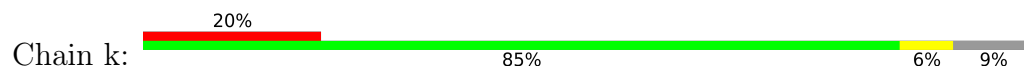
- Molecule 39: 39S ribosomal protein L51, mitochondrial



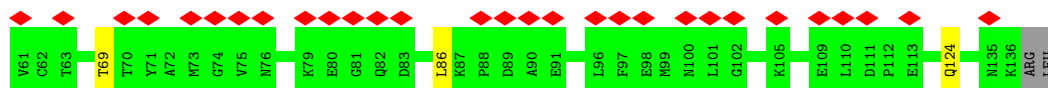
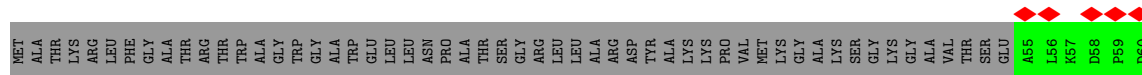
- Molecule 40: 39S ribosomal protein L52, mitochondrial



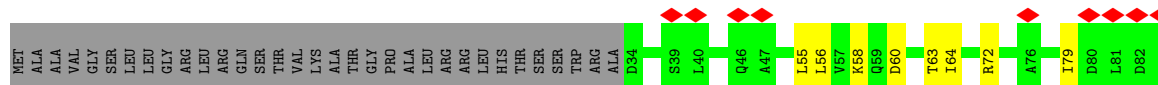
- Molecule 41: Large ribosomal subunit protein mL53



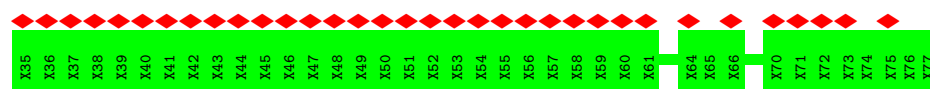
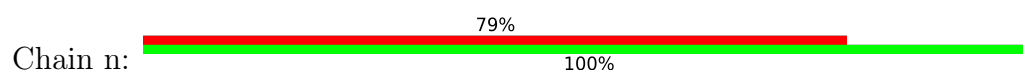
- Molecule 42: 39S ribosomal protein L54, mitochondrial



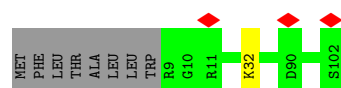
- Molecule 43: 39S ribosomal protein L55, mitochondrial



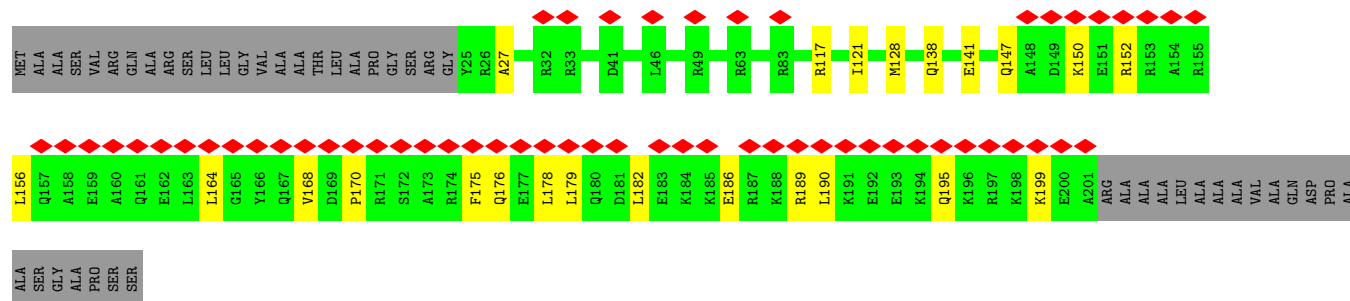
- Molecule 44: Nascent polypeptide



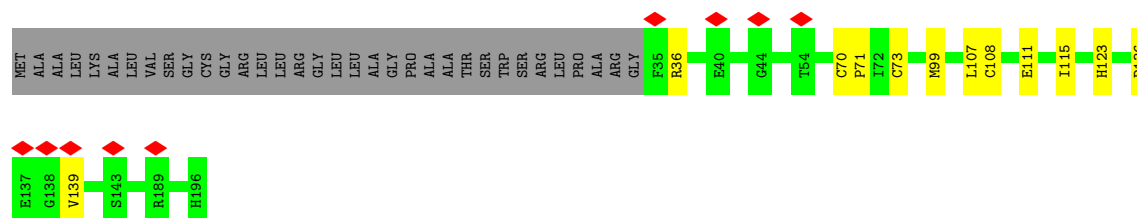
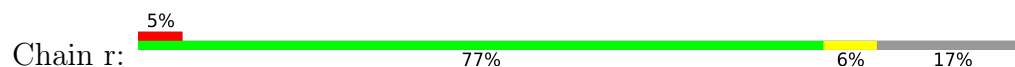
• Molecule 45: Ribosomal protein 63, mitochondrial



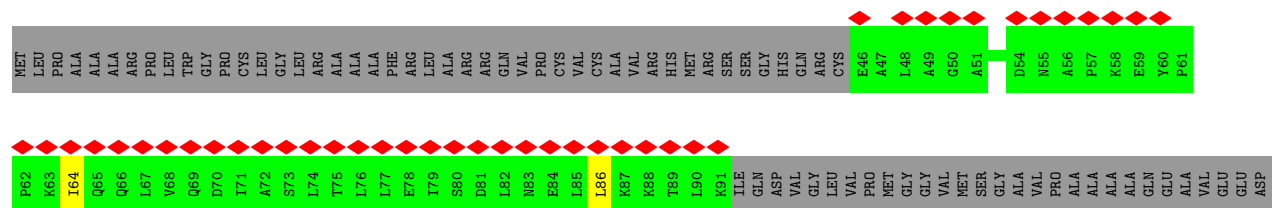
• Molecule 46: Growth arrest and DNA damage-inducible proteins-interacting protein 1

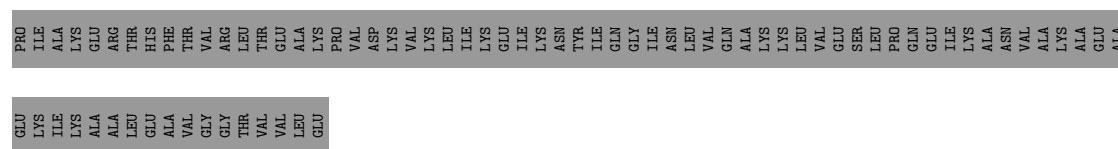


• Molecule 47: 39S ribosomal protein S18a, mitochondrial

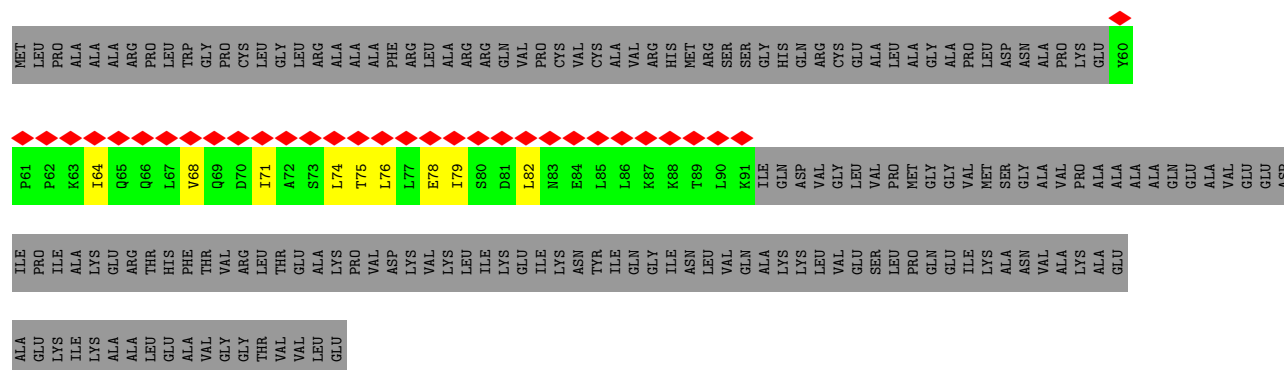


• Molecule 48: 39S ribosomal protein L12, mitochondrial

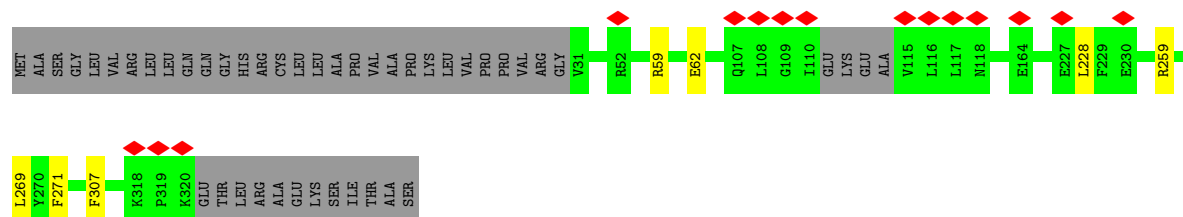
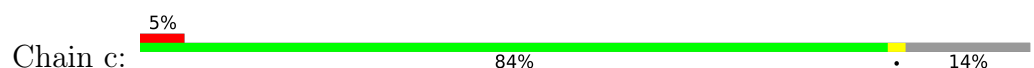




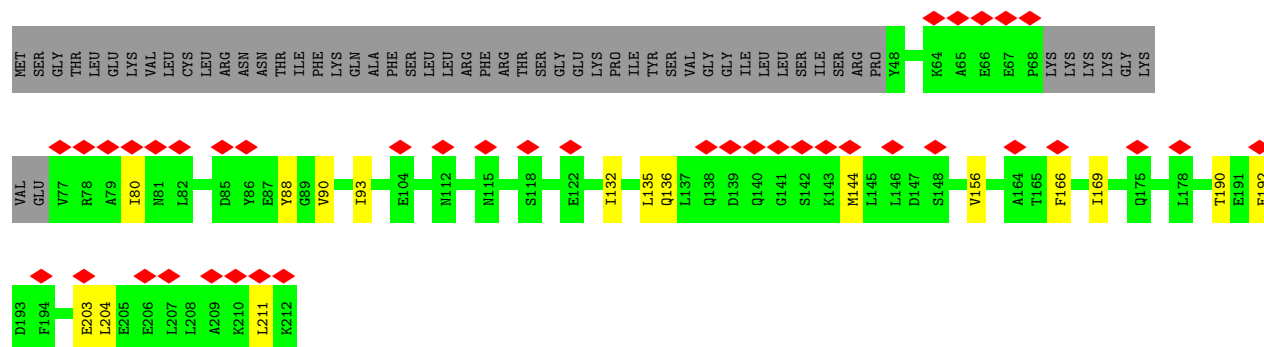
- Molecule 48: 39S ribosomal protein L12, mitochondrial



- Molecule 49: 39S ribosomal protein L44, mitochondrial

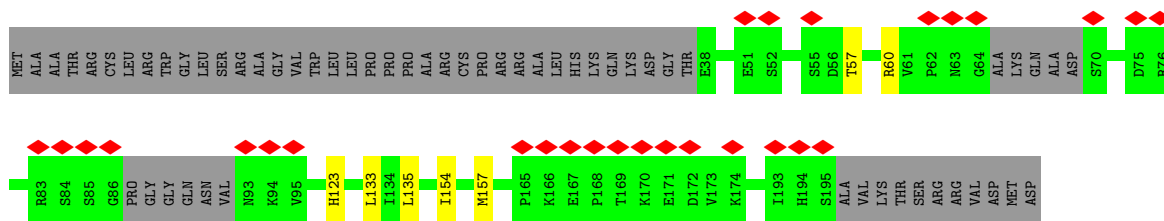


- Molecule 50: 39S ribosomal protein L48, mitochondrial

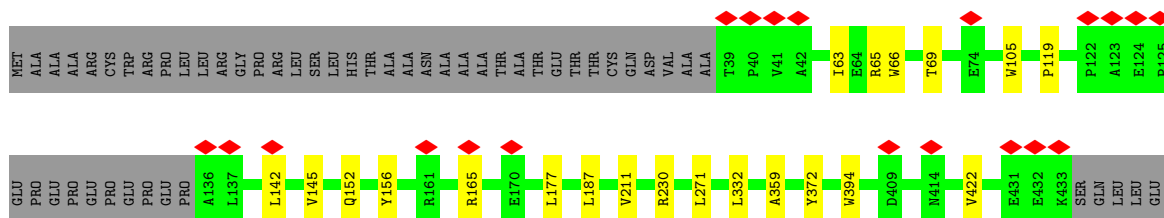
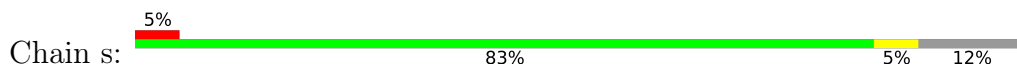


- Molecule 51: Peptidyl-tRNA hydrolase ICT1, mitochondrial

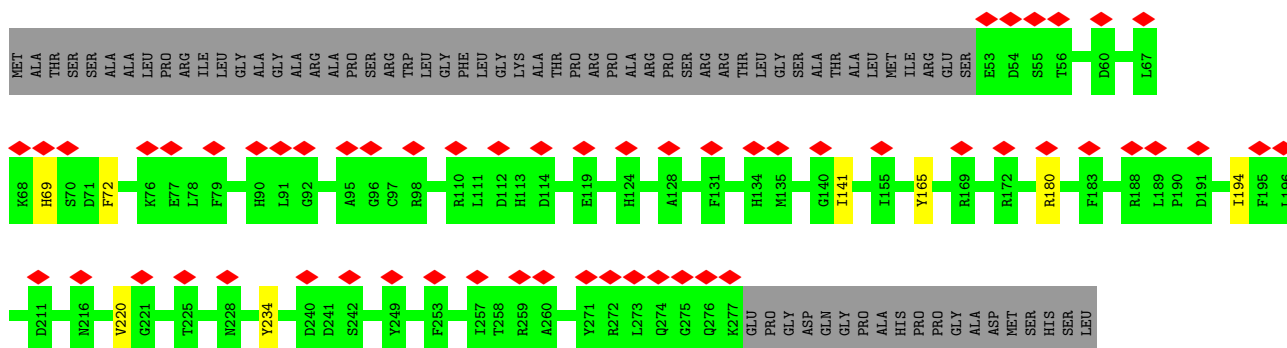
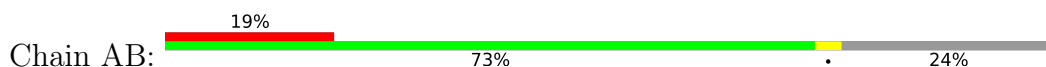




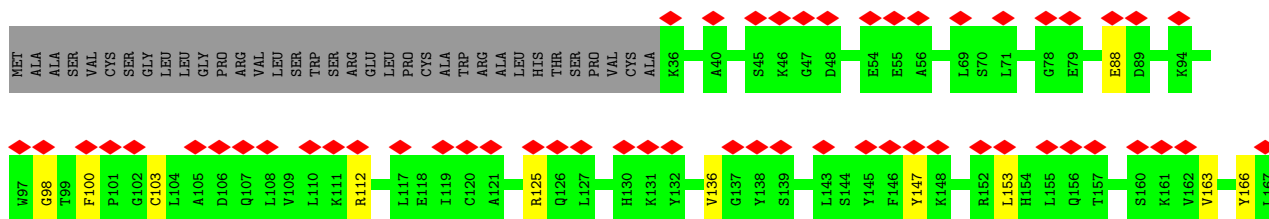
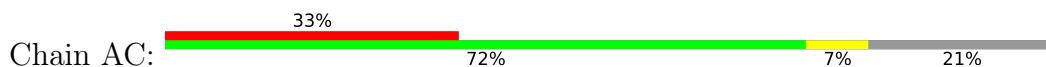
- Molecule 52: 39S ribosomal protein S30, mitochondrial



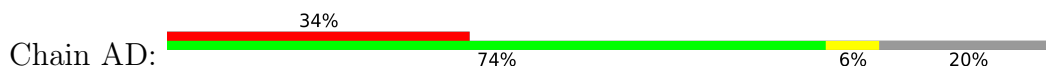
- Molecule 53: 28S ribosomal protein S2, mitochondrial

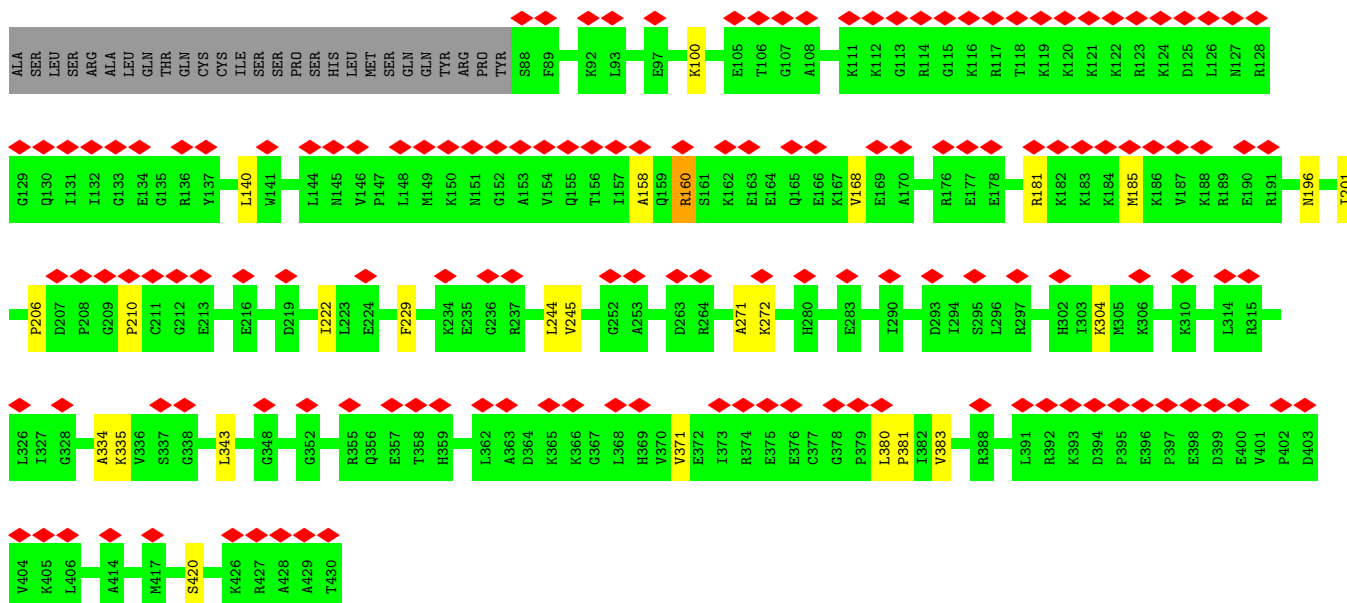


- Molecule 54: 28S ribosomal protein S24, mitochondrial

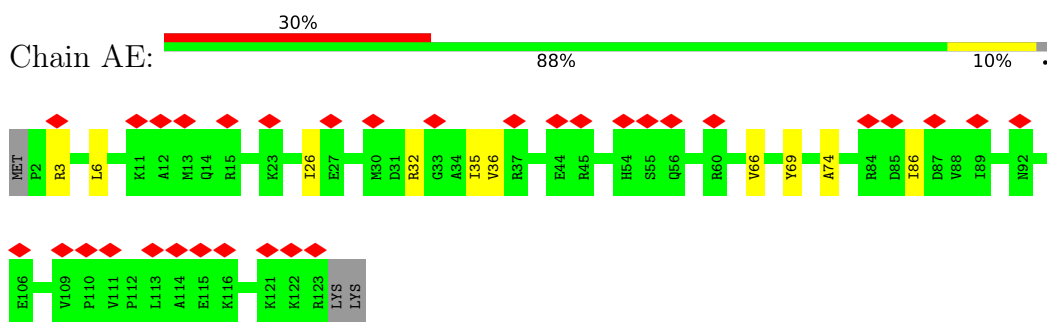


- Molecule 55: 28S ribosomal protein S5, mitochondrial

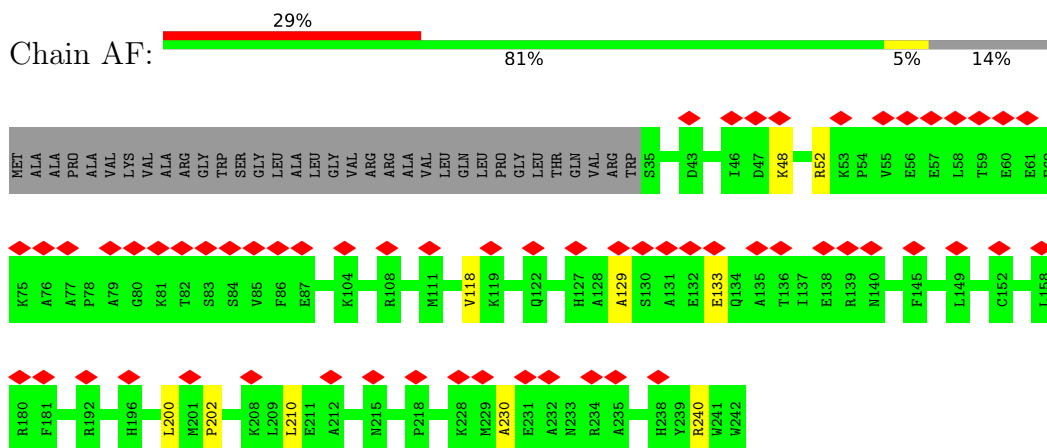




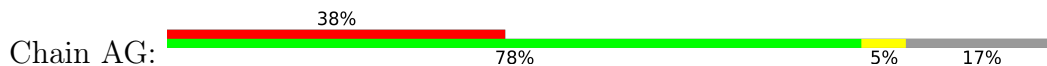
- Molecule 56: 28S ribosomal protein S6, mitochondrial



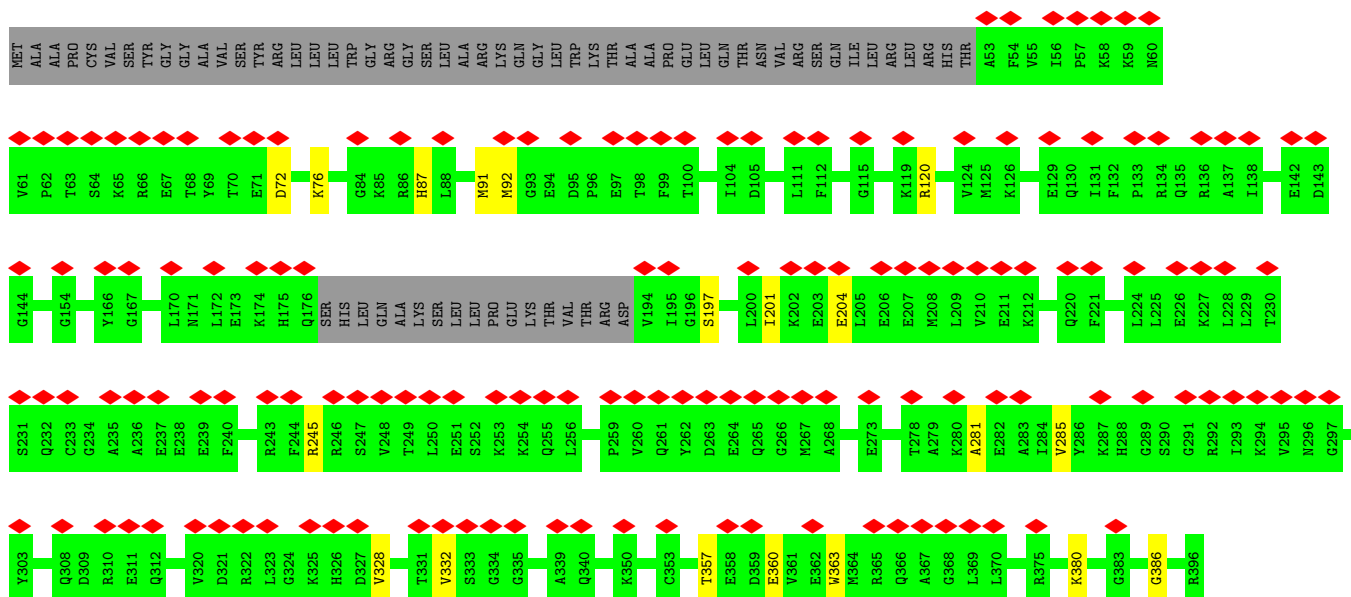
- Molecule 57: 28S ribosomal protein S7, mitochondrial



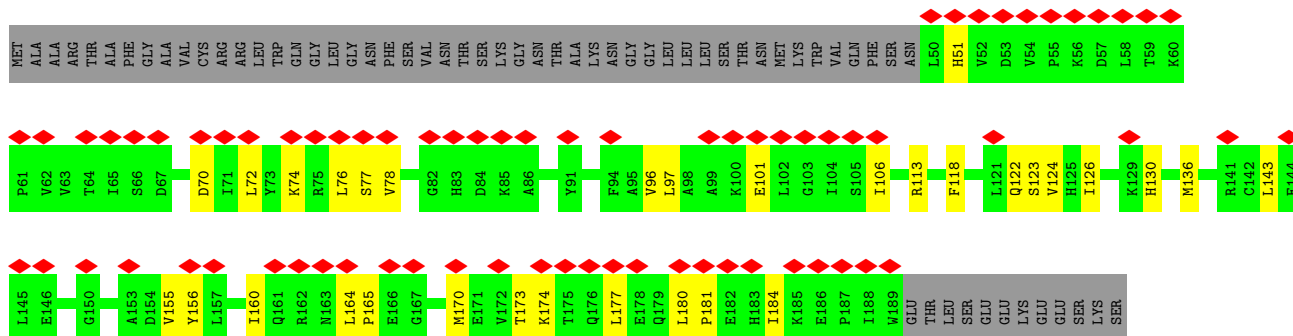
- Molecule 58: 28S ribosomal protein S9, mitochondrial



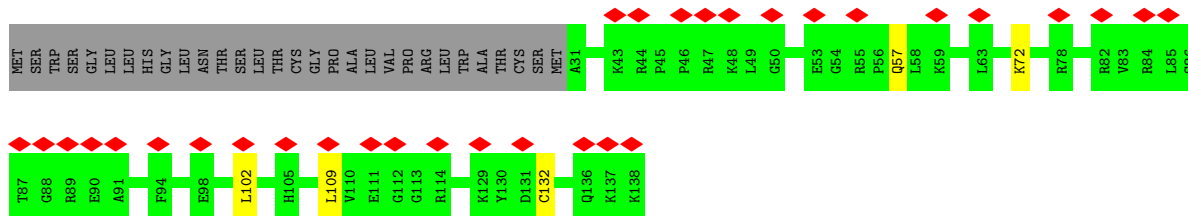
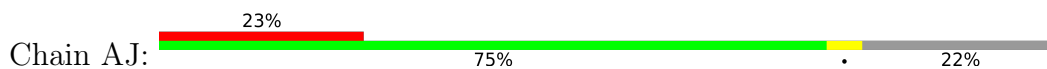




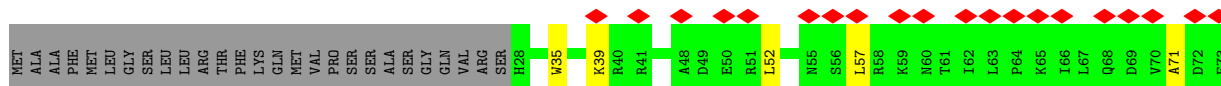
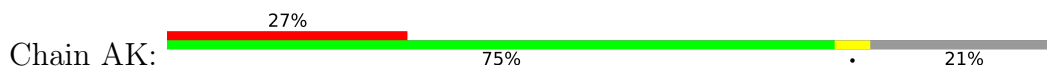
- Molecule 59: 28S ribosomal protein S10, mitochondrial

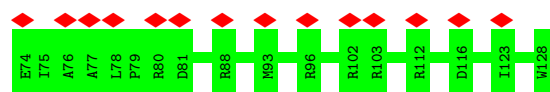


- Molecule 60: 28S ribosomal protein S12, mitochondrial

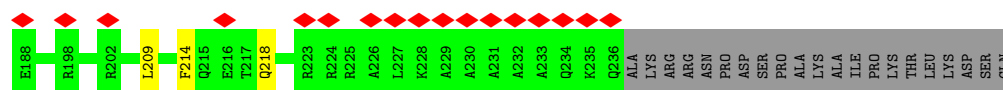
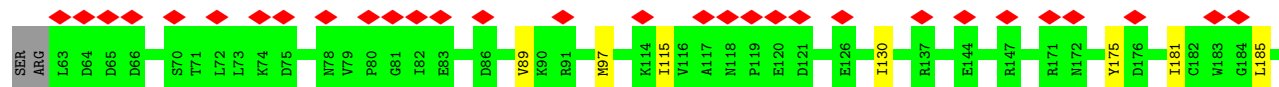
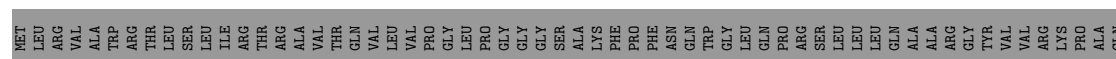


- Molecule 61: 28S ribosomal protein S14, mitochondrial

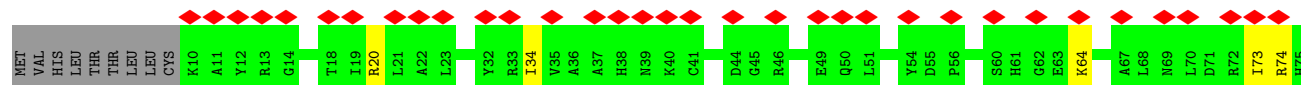
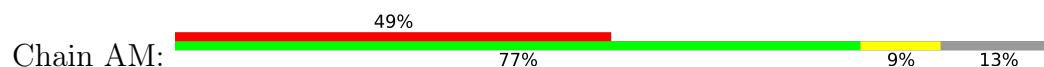




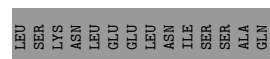
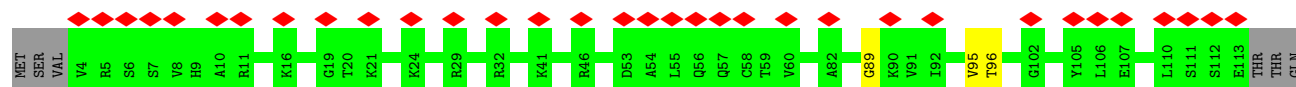
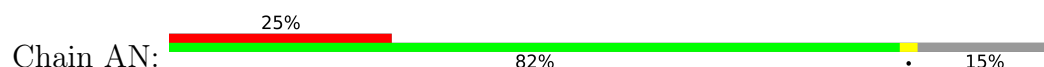
- Molecule 62: 28S ribosomal protein S15, mitochondrial



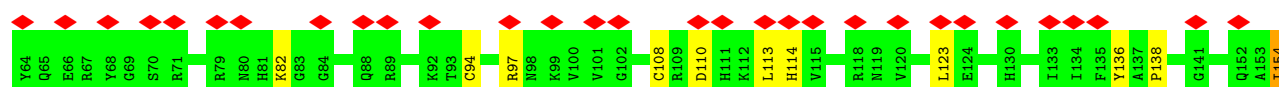
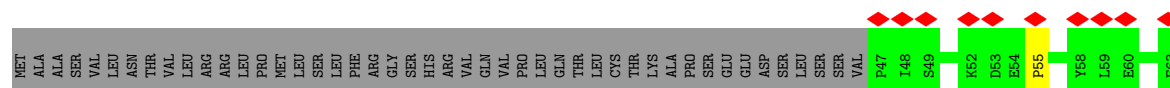
- Molecule 63: 28S ribosomal protein S16, mitochondrial

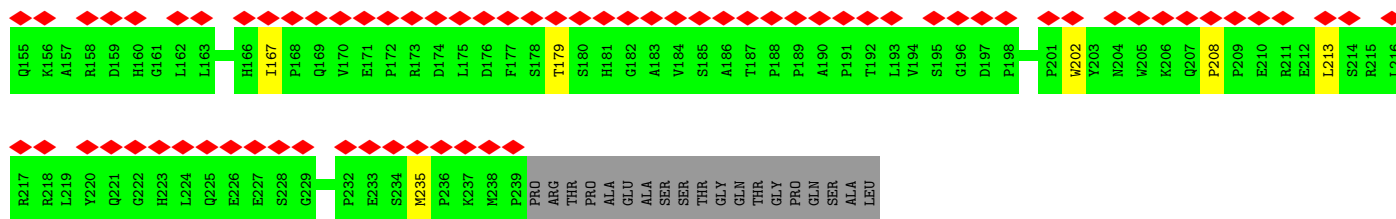


- Molecule 64: 28S ribosomal protein S17, mitochondrial

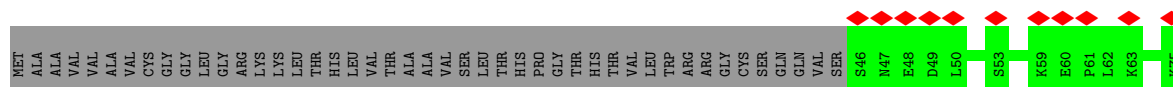


- Molecule 65: 28S ribosomal protein S18b, mitochondrial

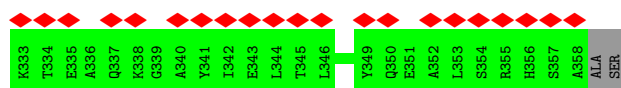
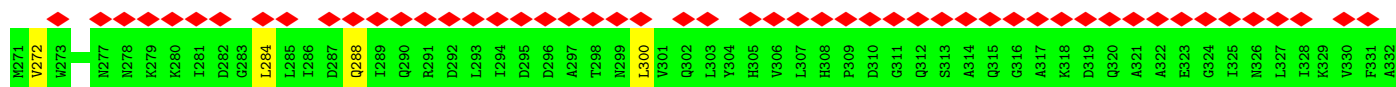
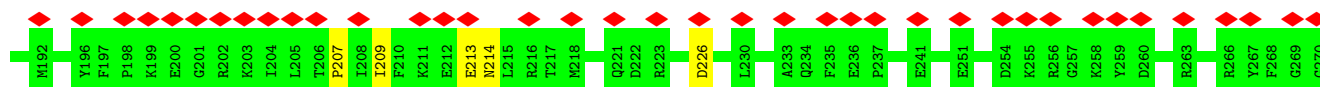
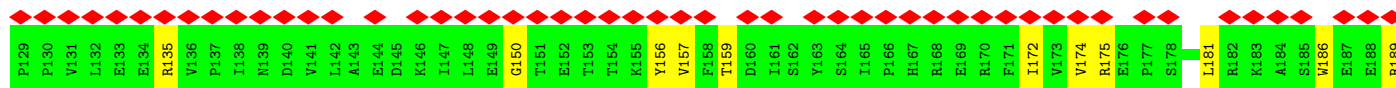
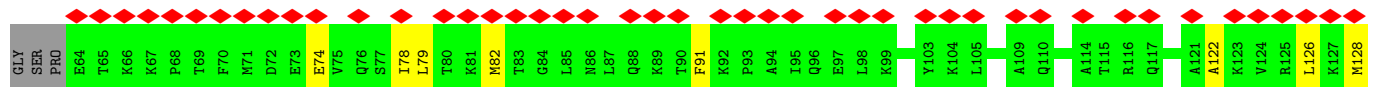
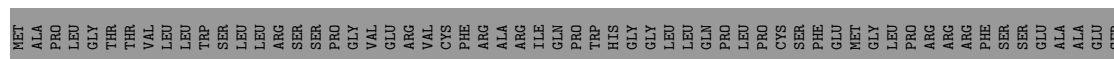
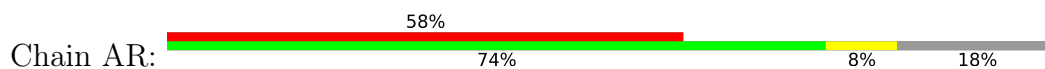




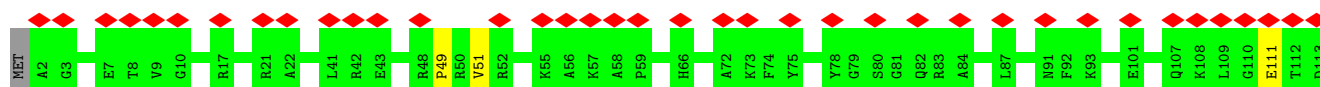
- Molecule 66: 28S ribosomal protein S18c, mitochondrial

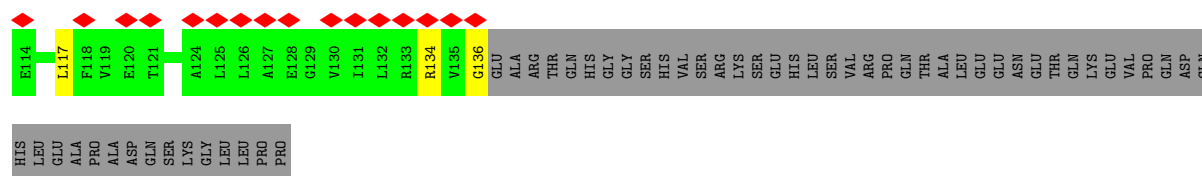


- Molecule 67: 28S ribosomal protein S22, mitochondrial

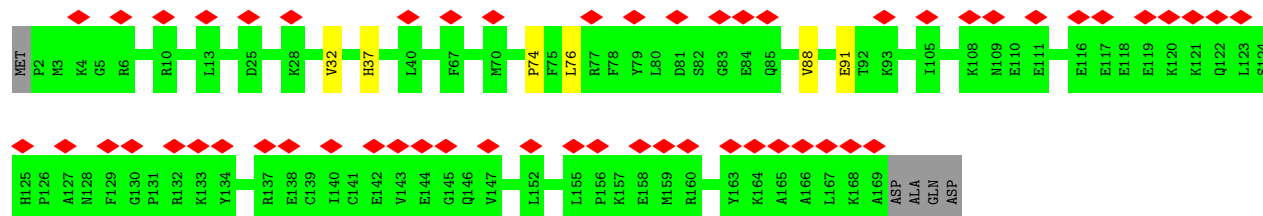


- Molecule 68: 28S ribosomal protein S23, mitochondrial

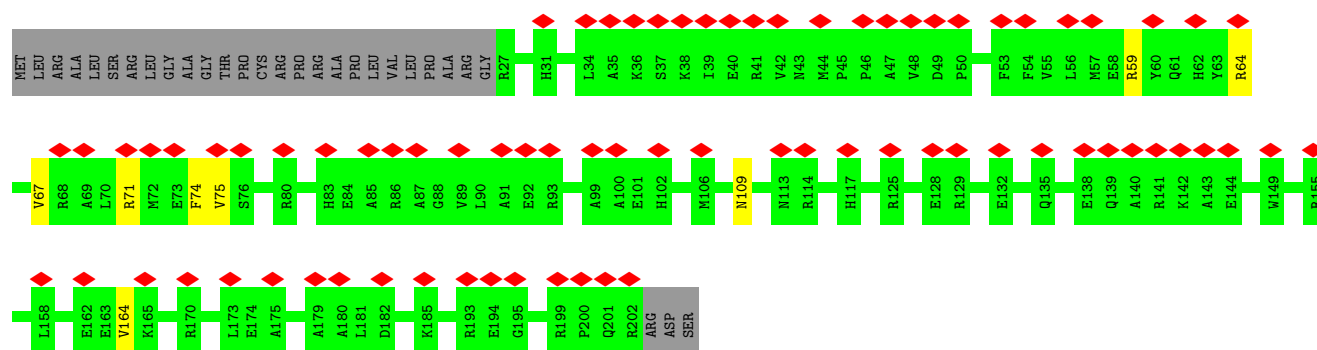
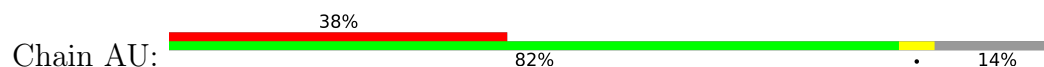




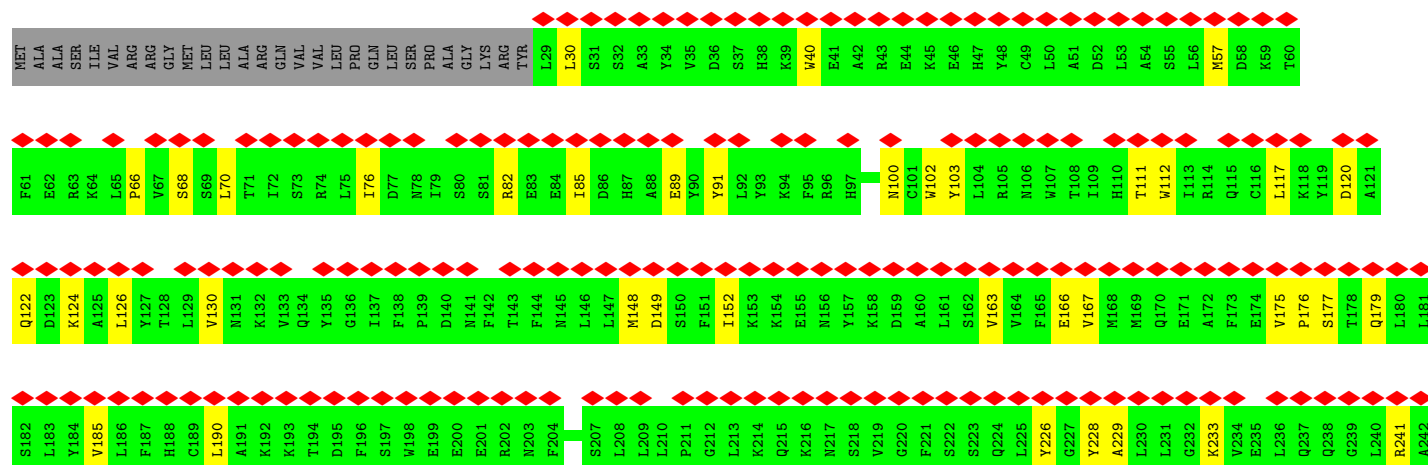
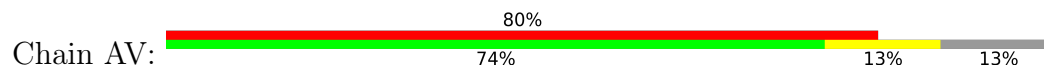
- Molecule 69: 28S ribosomal protein S25, mitochondrial



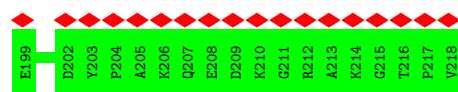
- Molecule 70: 28S ribosomal protein S26, mitochondrial



- Molecule 71: 28S ribosomal protein S27, mitochondrial

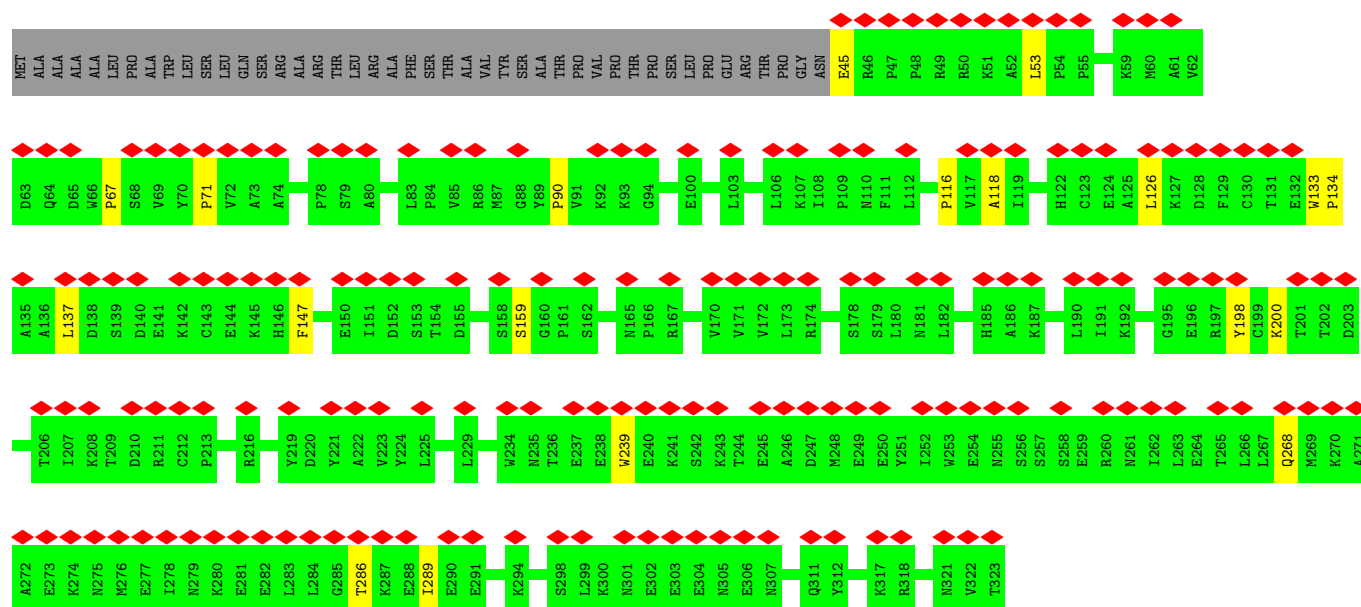






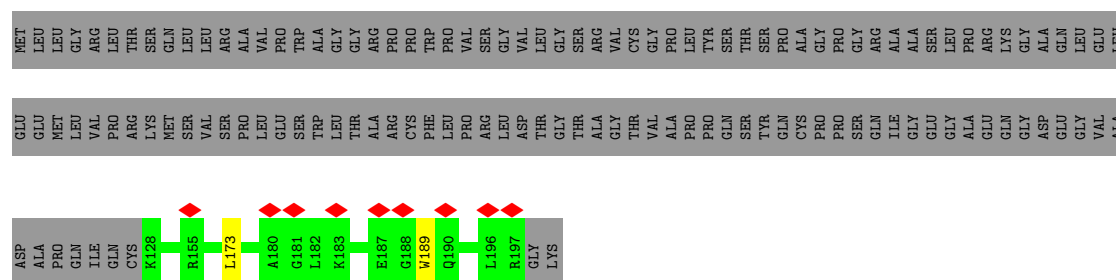
- Molecule 75: 28S ribosomal protein S35, mitochondrial

Chain A1:



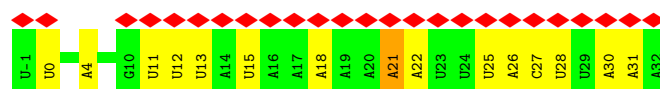
- Molecule 76: Aurora kinase A-interacting protein

Chain A3:



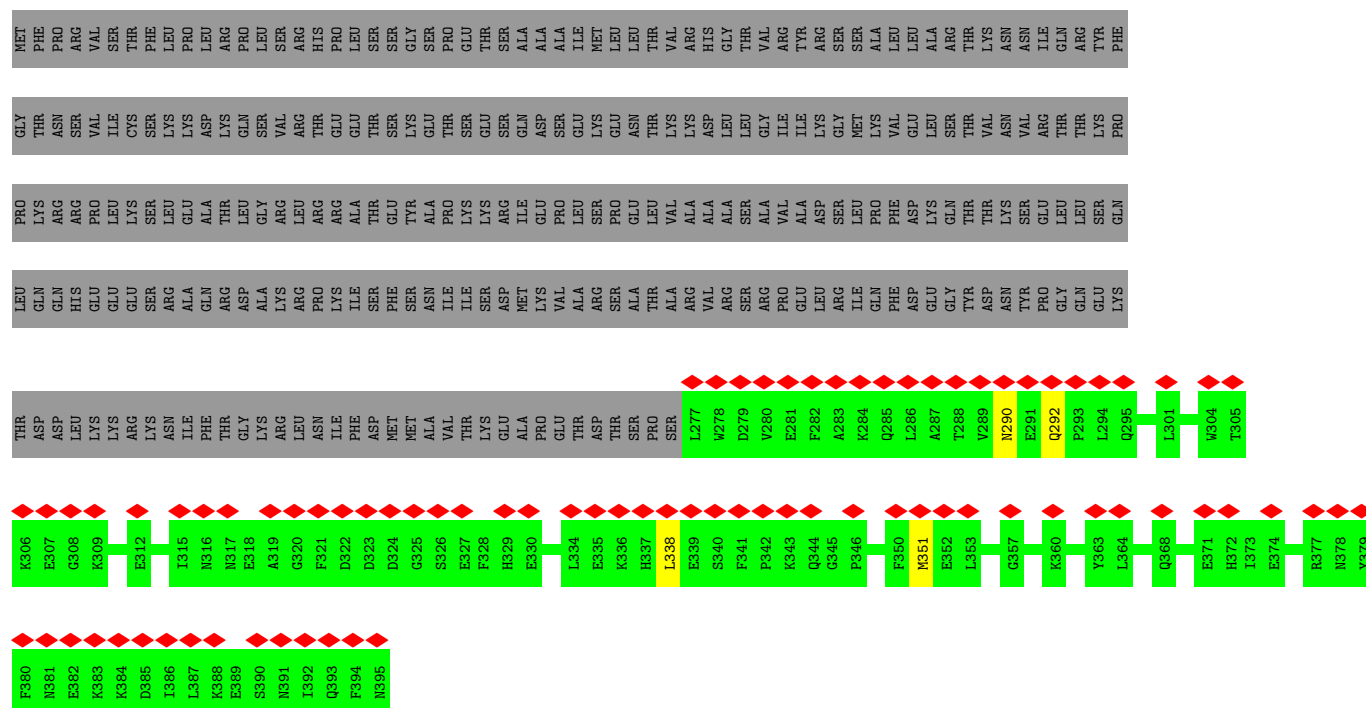
- Molecule 77: mRNA

Chain Az:

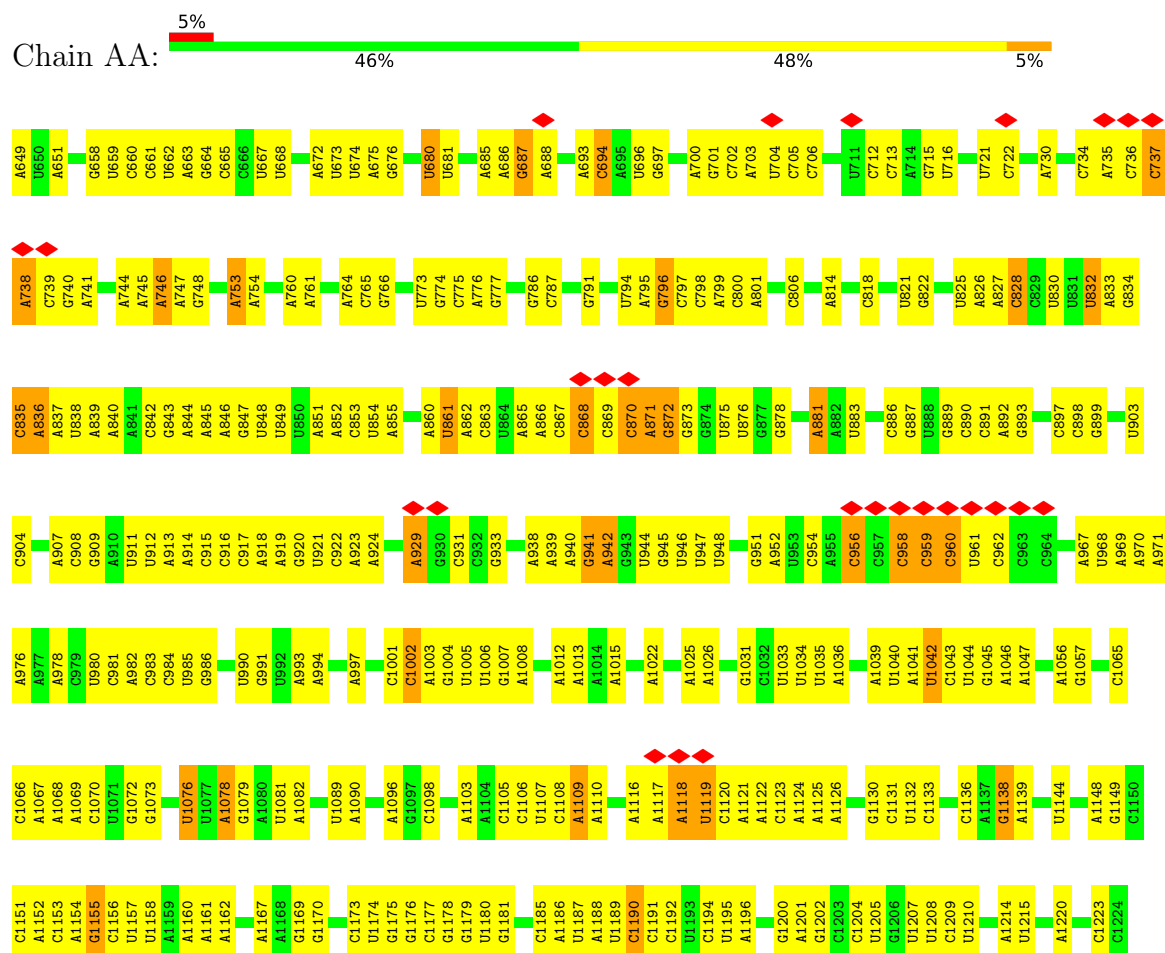


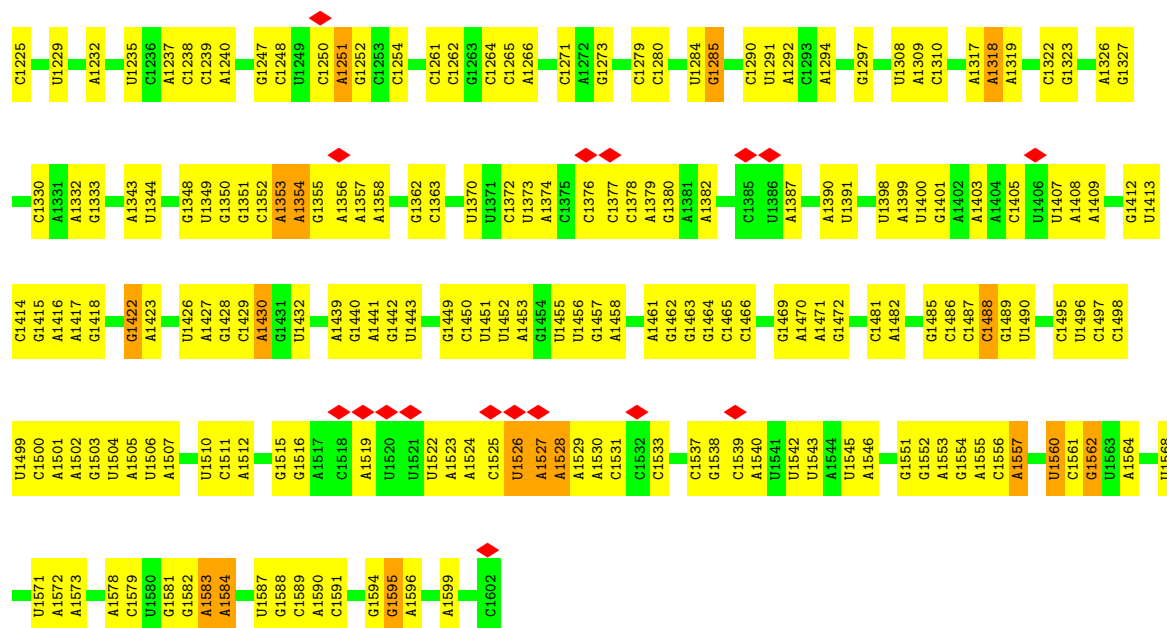
- Molecule 78: 28S ribosomal protein S31, mitochondrial

Chain AY:

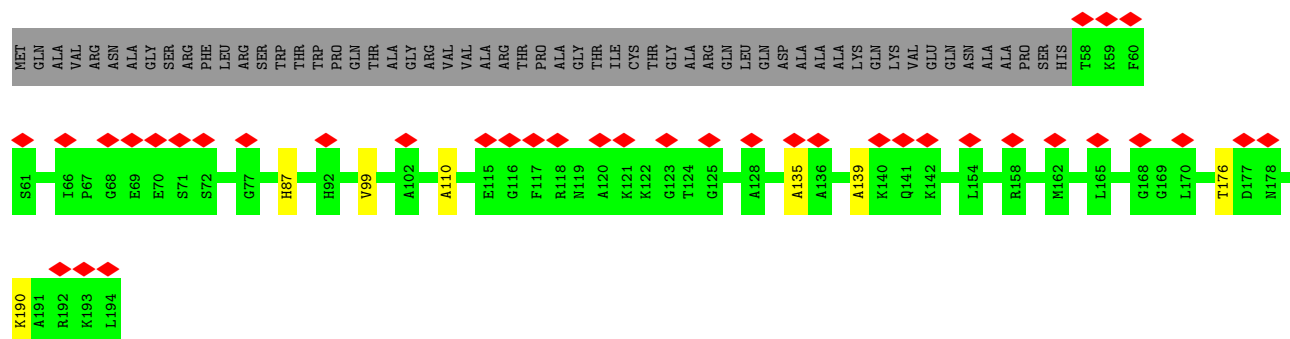


• Molecule 79: 12S mitochondrial rRNA

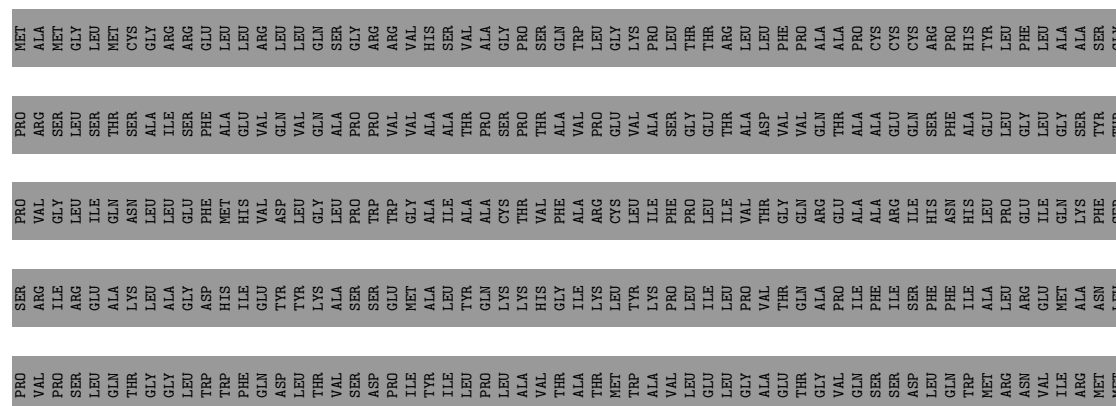




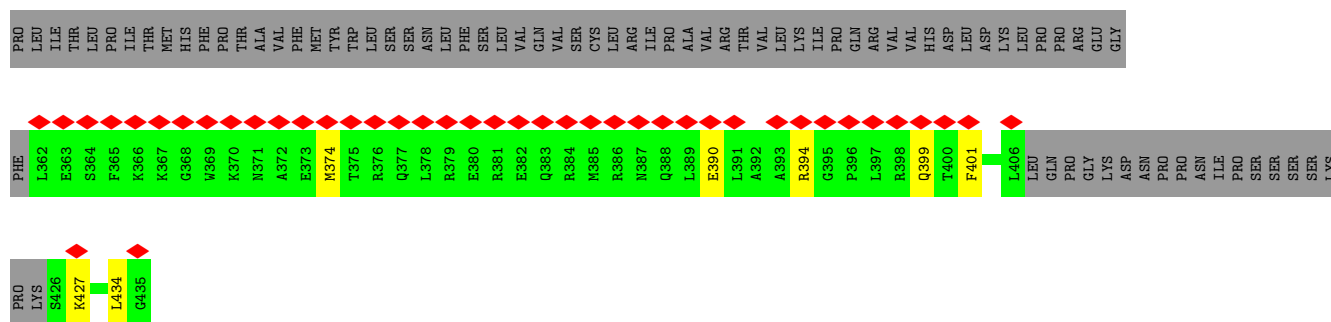
- Molecule 80: 28S ribosomal protein S11, mitochondrial



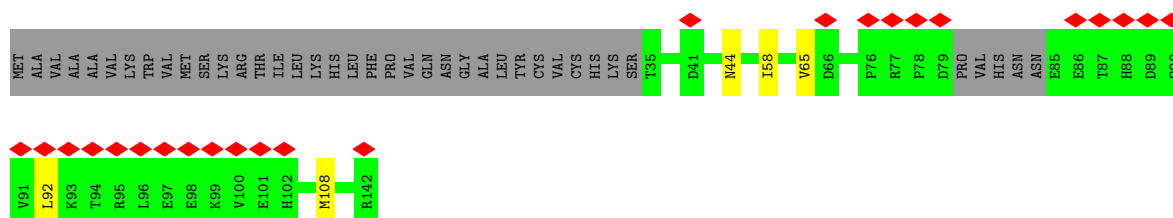
- Molecule 81: Mitochondrial inner membrane protein OXA1L



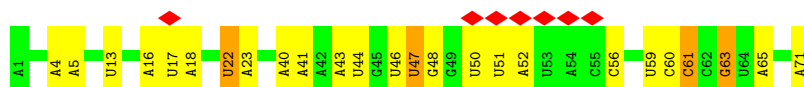




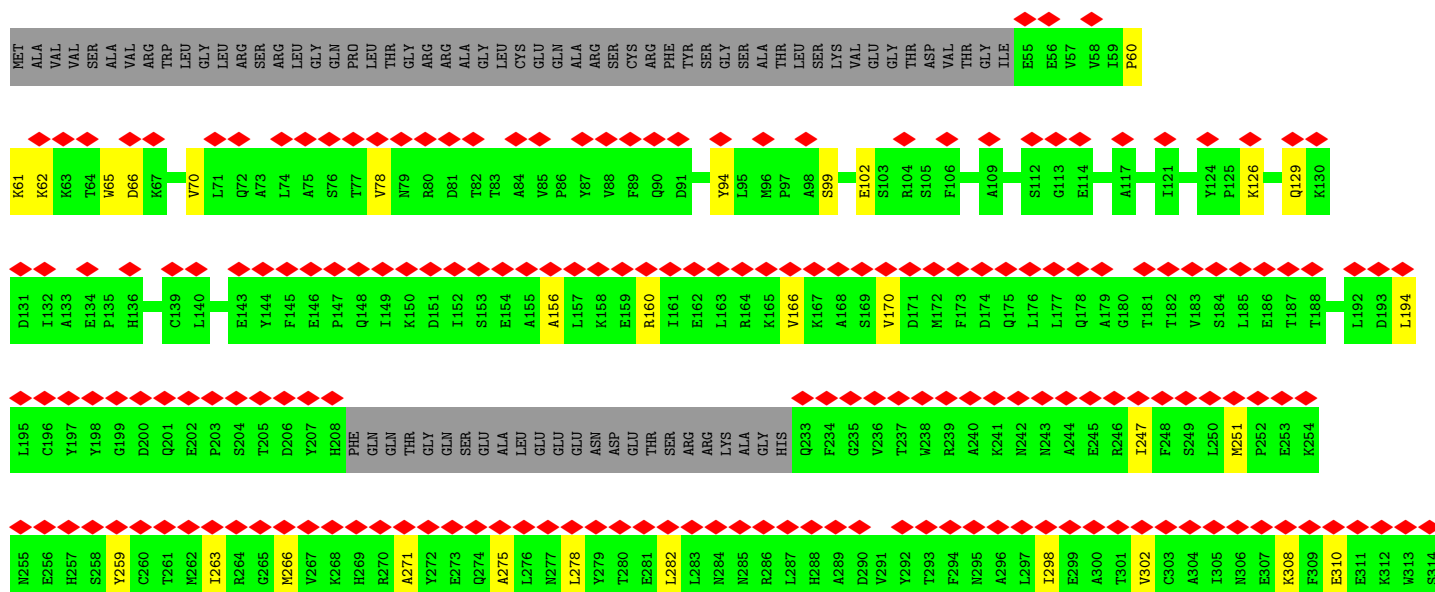
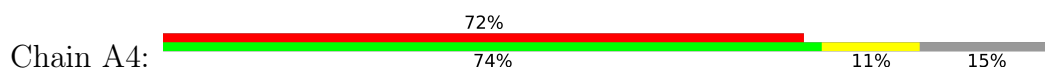
- Molecule 82: 39S ribosomal protein L42, mitochondrial

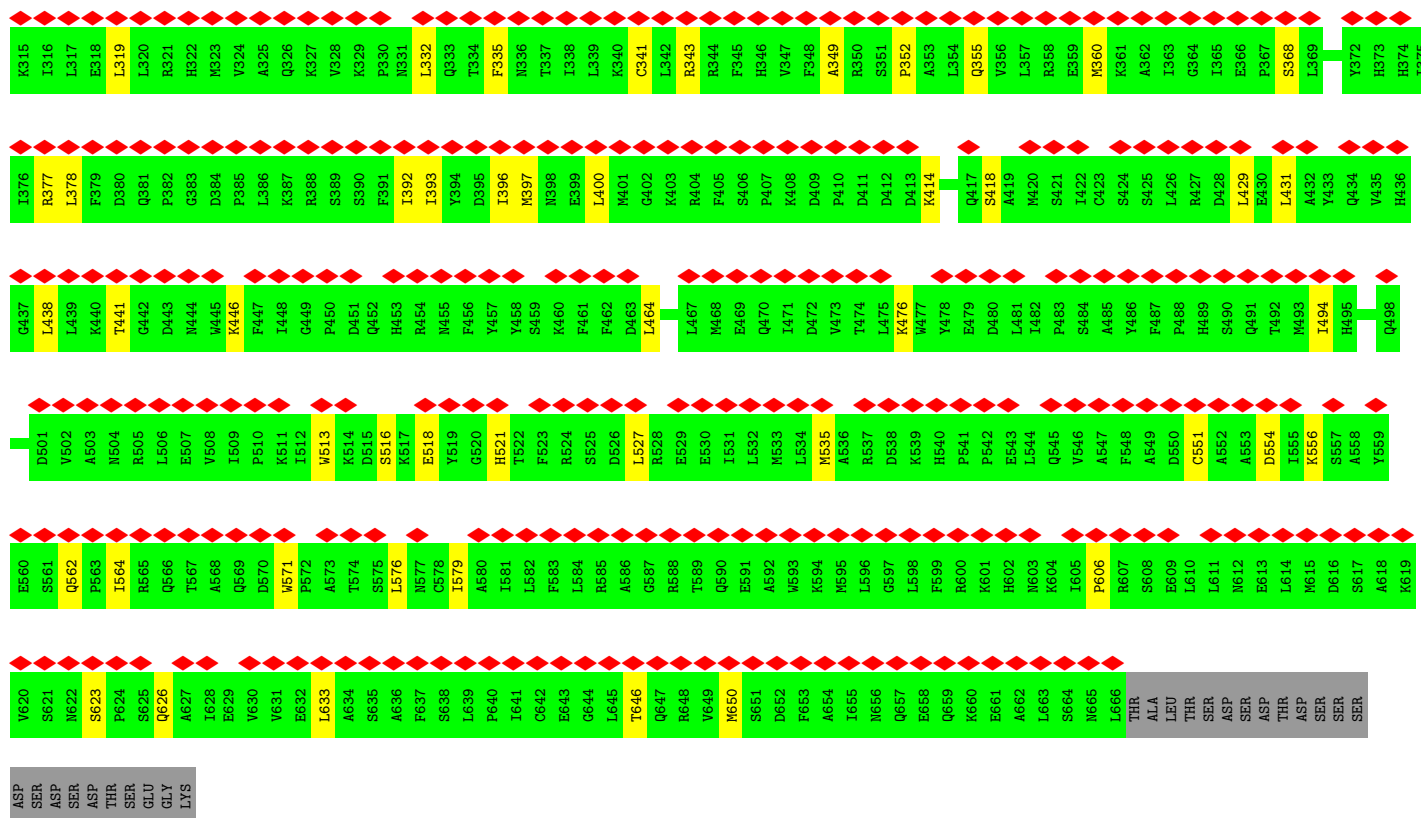


- Molecule 83: P/P-tRNA

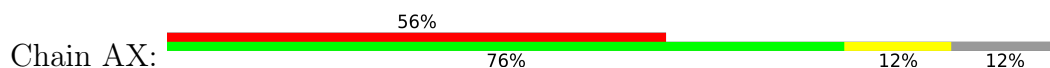


- Molecule 84: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

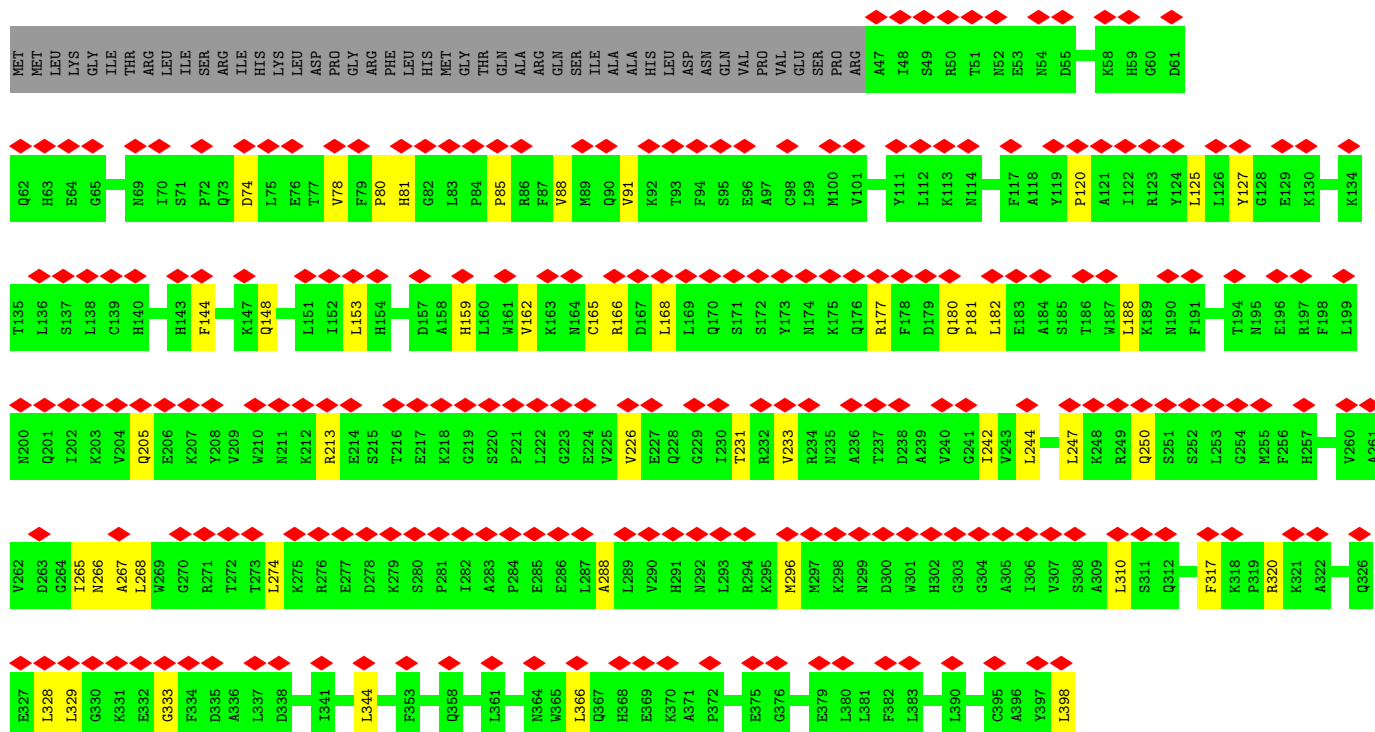




- Molecule 85: 28S ribosomal protein S29, mitochondrial

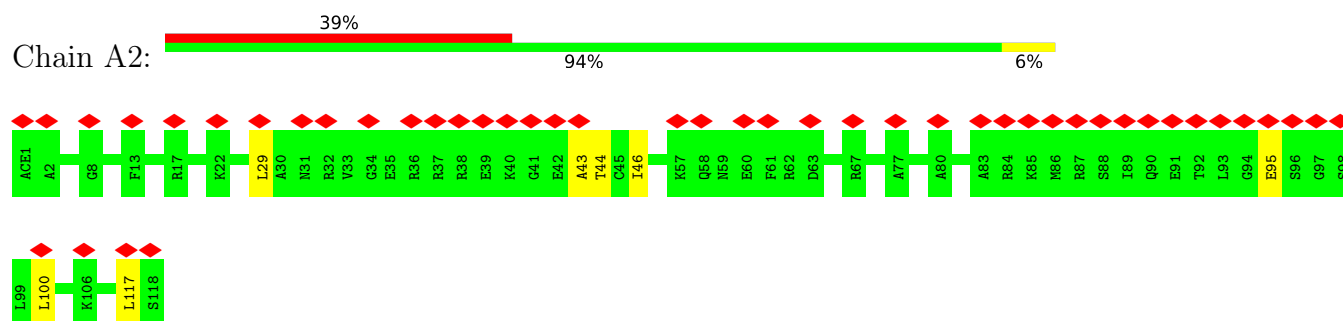


Chain AX:



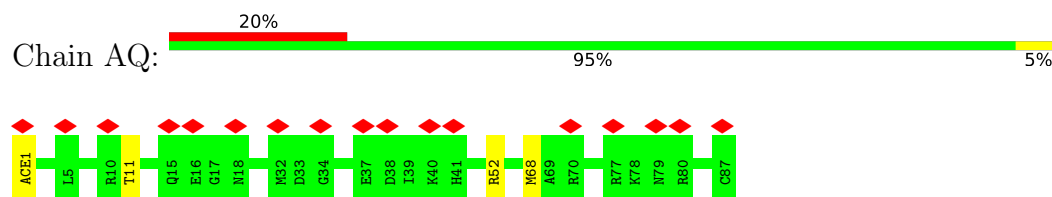
- Molecule 86: Small ribosomal subunit protein mS37

Chain A2:



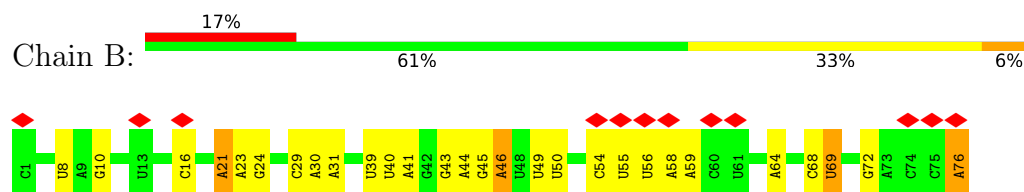
- Molecule 87: Small ribosomal subunit protein bS21m

Chain AQ:



- Molecule 88: mitochondrial tRNA<sup>Val</sup>

Chain B:



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12939	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.142	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size ( $\text{\AA}$ )	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.068, 1.068, 1.068	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0	0.22	0/913	0.27	0/1224
2	1	0.22	0/469	0.32	0/621
3	2	0.24	0/383	0.30	0/507
4	3	0.26	0/853	0.32	0/1136
5	4	0.24	0/350	0.29	0/461
6	5	0.21	0/3305	0.33	0/4502
7	6	0.20	0/3043	0.33	0/4140
8	7	0.20	0/2447	0.33	0/3310
9	8	0.17	0/1354	0.35	0/1819
10	9	0.20	0/1025	0.28	0/1379
11	A	0.26	0/36876	0.31	0/57402
12	D	0.23	0/1896	0.32	0/2549
13	E	0.23	0/2475	0.33	0/3355
14	F	0.24	0/2090	0.33	0/2842
15	H	0.18	0/1698	0.32	0/2292
16	I	0.20	0/1478	0.38	0/1999
17	J	0.18	0/1348	0.33	0/1813
18	K	0.25	0/1497	0.32	0/2031
19	L	0.20	0/905	0.29	0/1218
20	M	0.24	0/2381	0.32	0/3212
21	N	0.22	0/1833	0.30	0/2468
22	O	0.22	0/1283	0.32	0/1727
23	P	0.21	0/1199	0.31	0/1623
24	Q	0.20	0/2039	0.30	0/2750
25	R	0.25	0/1175	0.29	0/1572
26	S	0.25	0/1320	0.35	0/1789
27	T	0.23	0/1403	0.29	0/1886
28	U	0.23	0/1279	0.36	0/1730
29	W	0.24	0/926	0.30	0/1244
30	X	0.21	0/2099	0.27	0/2837
31	Y	0.22	0/1593	0.27	0/2136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Z	0.25	0/1021	0.33	0/1378
33	V	0.20	0/1721	0.29	0/2333
34	b	0.23	0/1218	0.33	0/1649
35	d	0.20	0/2181	0.36	0/2949
36	e	0.16	0/1970	0.32	0/2658
37	g	0.23	0/1151	0.31	0/1569
38	h	0.19	0/918	0.29	0/1249
39	i	0.24	0/850	0.30	0/1135
40	j	0.20	0/760	0.24	0/1023
41	k	0.17	0/783	0.29	0/1057
42	l	0.16	0/707	0.30	0/960
43	m	0.16	0/805	0.35	0/1081
45	o	0.25	0/819	0.33	0/1097
46	q	0.18	0/1529	0.33	0/2055
47	r	0.23	0/1362	0.31	0/1846
48	t	0.17	0/358	0.31	0/486
48	u	0.25	0/259	0.45	0/350
49	c	0.22	0/2347	0.29	0/3171
50	f	0.20	0/1273	0.37	0/1716
51	p	0.19	0/1223	0.30	0/1641
52	s	0.23	0/3231	0.32	0/4389
53	AB	0.18	0/1871	0.30	0/2531
54	AC	0.18	0/1113	0.33	0/1505
55	AD	0.18	0/2783	0.31	0/3724
56	AE	0.19	0/989	0.34	0/1335
57	AF	0.17	0/1767	0.31	0/2373
58	AG	0.17	0/2746	0.31	0/3681
59	AH	0.19	0/1178	0.36	0/1598
60	AJ	0.17	0/855	0.31	0/1148
61	AK	0.18	0/880	0.31	0/1182
62	AL	0.16	0/1477	0.25	0/1974
63	AM	0.17	0/963	0.33	0/1295
64	AN	0.16	0/886	0.28	0/1199
65	AO	0.15	0/1648	0.31	0/2243
66	AP	0.18	0/798	0.27	0/1070
67	AR	0.15	0/2456	0.30	0/3317
68	AS	0.15	0/1138	0.25	0/1533
69	AT	0.17	0/1402	0.35	0/1883
70	AU	0.14	0/1510	0.28	0/2025
71	AV	0.18	0/3030	0.37	0/4093
72	AW	0.16	0/801	0.32	0/1079
73	AZ	0.16	0/857	0.31	0/1141
74	A0	0.15	0/1834	0.32	0/2484

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	A1	0.15	0/2313	0.32	0/3129
76	A3	0.20	0/636	0.29	0/839
77	Az	0.17	0/804	0.34	0/1248
78	AY	0.16	0/1040	0.29	0/1402
79	AA	0.20	0/22537	0.29	0/35085
80	AI	0.18	0/1039	0.30	0/1400
81	OX	0.18	0/478	0.49	0/639
82	a	0.21	0/891	0.33	0/1208
83	Ax	0.19	0/1673	0.37	0/2602
84	A4	0.15	0/4877	0.34	0/6598
85	AX	0.16	0/2921	0.35	0/3954
86	A2	0.18	0/947	0.31	0/1266
87	AQ	0.18	0/754	0.28	0/1003
88	B	0.18	0/1626	0.27	0/2523
All	All	0.21	0/184939	0.31	0/262675

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

Mol	Chain	#Chirality outliers	#Planarity outliers
55	AD	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
55	AD	160	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	898	0	916	3	0
2	1	464	0	511	3	0
3	2	377	0	406	0	0
4	3	832	0	883	2	0
5	4	342	0	361	1	0
6	5	3210	0	3206	12	0
7	6	2948	0	2841	9	0
8	7	2390	0	2397	12	0
9	8	1327	0	1368	14	0
10	9	997	0	987	4	0
11	A	33070	0	16794	174	0
12	D	1859	0	1920	10	0
13	E	2406	0	2415	6	0
14	F	2031	0	2065	4	0
15	H	1661	0	1734	14	0
16	I	1446	0	1532	13	0
17	J	1330	0	1407	8	0
18	K	1455	0	1452	3	0
19	L	890	0	941	2	0
20	M	2327	0	2395	6	0
21	N	1786	0	1817	8	0
22	O	1259	0	1294	3	0
23	P	1173	0	1165	2	0
24	Q	1990	0	2031	5	0
25	R	1154	0	1214	1	0
26	S	1293	0	1365	8	0
27	T	1369	0	1410	6	0
28	U	1248	0	1228	8	0
29	W	904	0	934	1	0
30	X	2044	0	2060	6	0
31	Y	1556	0	1597	2	0
32	Z	996	0	1044	2	0
33	V	1676	0	1687	9	0
34	b	1193	0	1191	5	0
35	d	2124	0	2125	35	0
36	e	1931	0	1916	27	0
37	g	1113	0	1097	2	0
38	h	895	0	881	1	0
39	i	828	0	857	1	0
40	j	745	0	746	1	0
41	k	774	0	784	5	0
42	l	688	0	674	3	0
43	m	791	0	796	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	n	215	0	52	0	0
45	o	798	0	804	1	0
46	q	1495	0	1492	17	0
47	r	1322	0	1348	8	0
48	t	354	0	377	3	0
48	u	257	0	283	7	0
49	c	2299	0	2320	5	0
50	f	1252	0	1269	12	0
51	p	1205	0	1223	4	0
52	s	3148	0	3131	13	0
53	AB	1828	0	1815	5	0
54	AC	1083	0	1088	7	0
55	AD	2731	0	2804	20	0
56	AE	972	0	1000	7	0
57	AF	1725	0	1769	8	0
58	AG	2688	0	2687	12	0
59	AH	1152	0	1183	23	0
60	AJ	839	0	887	3	0
61	AK	862	0	885	3	0
62	AL	1453	0	1540	8	0
63	AM	942	0	965	9	0
64	AN	868	0	928	2	0
65	AO	1592	0	1557	13	0
66	AP	781	0	806	2	0
67	AR	2409	0	2428	21	0
68	AS	1111	0	1115	4	0
69	AT	1371	0	1393	4	0
70	AU	1488	0	1499	7	0
71	AV	2969	0	2961	34	0
72	AW	789	0	802	4	0
73	AZ	839	0	858	5	0
74	A0	1787	0	1796	15	0
75	A1	2265	0	2294	17	0
76	A3	625	0	699	2	0
77	Az	719	0	359	2	0
78	AY	1010	0	957	3	0
79	AA	20260	0	10286	345	0
80	AI	1019	0	1059	5	0
81	OX	468	0	464	7	0
82	a	865	0	829	4	0
83	Ax	1498	0	766	9	0
84	A4	4768	0	4766	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	AX	2849	0	2844	31	0
86	A2	935	0	971	6	0
87	AQ	744	0	758	4	0
88	B	1524	0	779	14	0
89	0	1	0	0	0	0
89	4	1	0	0	0	0
89	AO	1	0	0	0	0
90	3	1	0	0	0	0
90	6	1	0	0	0	0
90	A	29	0	0	0	0
90	AA	18	0	0	0	0
90	D	1	0	0	0	0
90	M	1	0	0	0	0
90	N	1	0	0	0	0
90	W	1	0	0	0	0
90	o	1	0	0	0	0
91	A	40	0	76	2	0
91	AA	20	0	38	0	0
91	O	10	0	19	0	0
92	A	6	0	12	0	0
93	A	137	0	0	0	0
93	A3	1	0	0	0	0
93	AA	59	0	0	1	0
93	AB	1	0	0	0	0
93	AX	1	0	0	0	0
93	Az	1	0	0	0	0
93	D	2	0	0	0	0
93	E	1	0	0	0	0
93	g	1	0	0	0	0
94	AP	4	0	0	0	0
94	AT	4	0	0	0	0
94	r	4	0	0	0	0
95	AA	44	0	26	1	0
96	AA	28	0	52	1	0
97	AX	31	0	12	0	0
98	AX	28	0	12	1	0
99	B	7	0	8	3	0
All	All	176450	0	149595	1075	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 3.

All (1075) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:208:VAL:HG22	35:d:253:THR:HG23	1.64	0.80
79:AA:941:G:H4'	79:AA:942:A:H5''	1.64	0.79
79:AA:745:A:H3'	79:AA:746:A:H8	1.47	0.79
55:AD:140:LEU:HD11	55:AD:160:ARG:HG3	1.65	0.79
79:AA:1562:G:H1'	79:AA:1583:MA6:H2	1.63	0.77
12:D:205:GLN:HA	12:D:208:ARG:HH21	1.50	0.77
14:F:103:GLN:HE22	14:F:249:ASN:HD22	1.33	0.77
79:AA:1528:A:H2'	79:AA:1529:A:H8	1.52	0.75
36:e:183:THR:HG23	36:e:186:GLY:H	1.51	0.73
84:A4:556:LYS:HE3	84:A4:579:ILE:HD13	1.70	0.73
35:d:186:VAL:HG21	35:d:239:PRO:HB3	1.70	0.73
79:AA:1414:C:H3'	79:AA:1415:G:H21	1.53	0.73
36:e:231:VAL:HG21	88:B:76:A:H61	1.54	0.72
33:V:79:VAL:HG12	33:V:86:VAL:HG12	1.71	0.72
79:AA:1002:C:H2'	79:AA:1003:A:H8	1.54	0.70
79:AA:1440:G:H2'	79:AA:1441:A:C8	2.26	0.70
71:AV:66:PRO:HD3	79:AA:1529:A:H1'	1.75	0.68
49:c:228:LEU:HB2	49:c:307:PHE:CD2	2.29	0.68
79:AA:918:A:H4'	79:AA:920:G:H4'	1.75	0.68
30:X:20:ILE:HG22	81:OX:434:LEU:HD23	1.76	0.67
15:H:98:LEU:HD11	15:H:105:VAL:HG23	1.77	0.66
46:q:164:LEU:HB3	46:q:168:VAL:HG21	1.77	0.66
79:AA:1068:A:H5''	80:AI:190:LYS:HD3	1.76	0.66
79:AA:1201:A:H2'	79:AA:1202:G:H8	1.60	0.66
27:T:62:ARG:HE	35:d:230:ARG:HD2	1.61	0.66
79:AA:773:U:H2'	79:AA:774:G:H8	1.61	0.66
6:5:201:ARG:HB3	6:5:232:THR:HG22	1.79	0.65
79:AA:873:G:H1'	79:AA:921:U:H1'	1.78	0.65
21:N:218:ILE:HG23	21:N:223:MET:HB2	1.78	0.64
75:A1:126:LEU:HD11	84:A4:70:VAL:HG13	1.79	0.64
79:AA:838:U:H2'	79:AA:839:A:C8	2.32	0.64
84:A4:397:MET:HG3	84:A4:431:LEU:HD11	1.78	0.64
79:AA:821:U:H2'	79:AA:822:G:H8	1.63	0.64
79:AA:990:U:H3	79:AA:997:A:H61	1.43	0.64
35:d:52:THR:HG23	35:d:55:GLU:H	1.63	0.63
35:d:208:VAL:HG23	35:d:252:LEU:HB2	1.80	0.63
55:AD:196:ASN:HD22	79:AA:878:G:H4'	1.63	0.63
36:e:165:PHE:HB3	99:B:101:VAL:HG12	1.79	0.63
12:D:172:MET:HE1	56:AE:86:ILE:HG12	1.79	0.63
9:8:68:LEU:HD21	50:f:211:LEU:HB2	1.81	0.63
79:AA:1452:U:H2'	79:AA:1453:A:H8	1.63	0.63
79:AA:1201:A:H2'	79:AA:1202:G:C8	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:1002:C:H2'	79:AA:1003:A:C8	2.35	0.62
79:AA:740:G:H2'	79:AA:741:A:H8	1.63	0.62
79:AA:1131:C:H2'	79:AA:1132:U:C6	2.35	0.62
65:AO:208:PRO:HG2	65:AO:213:LEU:HD21	1.80	0.62
63:AM:93:LEU:HD13	67:AR:156:TYR:HE2	1.65	0.62
65:AO:235:MET:HE3	67:AR:150:GLY:HA3	1.81	0.61
78:AY:290:ASN:HA	84:A4:446:LYS:HD3	1.82	0.61
11:A:2006:C:H2'	11:A:2007:U:C6	2.35	0.61
35:d:93:GLY:HA3	35:d:96:ARG:HB3	1.82	0.61
79:AA:746:A:H2'	79:AA:747:A:H8	1.65	0.61
85:AX:153:LEU:HD21	85:AX:247:LEU:HD13	1.81	0.61
79:AA:838:U:H2'	79:AA:839:A:H8	1.65	0.61
79:AA:1239:C:H2'	79:AA:1240:A:H8	1.65	0.61
11:A:2055:U:H2'	11:A:2056:G:H8	1.66	0.60
79:AA:1470:A:H2'	79:AA:1471:A:H8	1.66	0.60
62:AL:209:LEU:HD13	76:A3:173:LEU:HD12	1.83	0.60
71:AV:70:LEU:HD22	71:AV:389:LEU:HG	1.84	0.60
84:A4:302:VAL:HG21	84:A4:341:CYS:HB3	1.82	0.60
79:AA:740:G:H2'	79:AA:741:A:C8	2.37	0.60
69:AT:37:HIS:HB3	79:AA:956:C:C4	2.37	0.60
79:AA:1161:A:H2'	79:AA:1162:A:H8	1.67	0.60
84:A4:343:ARG:HA	84:A4:378:LEU:HD13	1.84	0.60
84:A4:494:ILE:HD11	84:A4:527:LEU:HA	1.83	0.60
79:AA:1398:U:H2'	79:AA:1399:A:H8	1.65	0.60
79:AA:1308:U:H2'	79:AA:1309:A:H8	1.67	0.60
75:A1:134:PRO:HB2	75:A1:137:LEU:HD23	1.84	0.59
79:AA:1132:U:H2'	79:AA:1133:C:C6	2.37	0.59
51:p:133:LEU:HD21	51:p:157:MET:HE1	1.85	0.59
63:AM:20:ARG:HB2	79:AA:839:A:H5''	1.83	0.59
54:AC:112:ARG:HB3	75:A1:159:SER:HB2	1.84	0.59
79:AA:1239:C:H2'	79:AA:1240:A:C8	2.38	0.59
78:AY:338:LEU:HD11	78:AY:351:MET:HB3	1.85	0.59
79:AA:1515:G:H2'	79:AA:1516:G:H8	1.67	0.59
79:AA:1554:G:H2'	79:AA:1555:A:C8	2.37	0.59
88:B:30:A:H2'	88:B:31:A:H8	1.67	0.59
55:AD:140:LEU:HD11	55:AD:160:ARG:HE	1.68	0.59
67:AR:207:PRO:HB2	67:AR:209:ILE:HG22	1.85	0.59
79:AA:839:A:H2'	79:AA:840:A:H8	1.66	0.59
79:AA:1515:G:H2'	79:AA:1516:G:C8	2.38	0.58
71:AV:229:ALA:HB1	71:AV:286:VAL:HG11	1.85	0.58
79:AA:1317:A:H3'	79:AA:1318:A:H8	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:872:G:H2'	79:AA:873:G:C8	2.39	0.58
79:AA:1161:A:H2'	79:AA:1162:A:C8	2.39	0.58
11:A:2545:U:H5''	11:A:2546:G:H5'	1.85	0.58
79:AA:1587:U:H2'	79:AA:1588:G:H8	1.69	0.58
67:AR:79:LEU:HB3	67:AR:128:MET:HE1	1.85	0.58
59:AH:155:VAL:HG13	75:A1:126:LEU:HD12	1.86	0.58
47:r:99:MET:HE1	47:r:115:ILE:HG22	1.86	0.57
79:AA:1528:A:H2'	79:AA:1529:A:C8	2.37	0.57
85:AX:181:PRO:HB2	85:AX:233:VAL:HG22	1.85	0.57
79:AA:1006:U:H2'	79:AA:1007:G:H8	1.69	0.57
8:7:112:PRO:HB2	8:7:267:PRO:HG2	1.87	0.57
11:A:2174:G:H4'	17:J:151:LEU:HD23	1.86	0.57
20:M:261:ASP:HB3	20:M:264:GLN:HB2	1.86	0.57
84:A4:170:VAL:HG23	84:A4:247:ILE:HD11	1.87	0.57
79:AA:872:G:H2'	79:AA:873:G:H8	1.69	0.57
84:A4:266:MET:HG2	84:A4:271:ALA:HB3	1.87	0.57
11:A:2740:A:H2'	11:A:2741:A:C8	2.39	0.57
59:AH:164:LEU:HD12	59:AH:165:PRO:HD2	1.86	0.57
54:AC:136:VAL:HG22	54:AC:153:LEU:HD22	1.86	0.57
79:AA:818:C:H1'	79:AA:851:A:H1'	1.85	0.57
11:A:1857:U:H2'	11:A:1858:G:C8	2.41	0.56
79:AA:908:C:H2'	79:AA:909:G:C8	2.40	0.56
11:A:1862:U:H2'	11:A:1863:A:H8	1.70	0.56
53:AB:220:VAL:HG22	53:AB:234:TYR:HB2	1.86	0.56
36:e:165:PHE:O	99:B:101:VAL:N	2.39	0.56
60:AJ:102:LEU:HD21	60:AJ:132:CYS:HB2	1.87	0.56
75:A1:134:PRO:HG3	84:A4:60:PRO:HD3	1.88	0.56
79:AA:861:U:H2'	79:AA:862:A:H8	1.69	0.56
9:8:187:PRO:HG2	43:m:79:ILE:HD11	1.87	0.56
79:AA:871:A:H1'	79:AA:872:G:C8	2.40	0.56
79:AA:1109:A:H2'	79:AA:1110:A:H8	1.71	0.56
79:AA:1175:G:H2'	79:AA:1176:G:C8	2.41	0.56
79:AA:1175:G:H2'	79:AA:1176:G:H8	1.70	0.56
79:AA:920:G:H2'	79:AA:921:U:C6	2.41	0.56
60:AJ:57:GLN:HB3	60:AJ:109:LEU:HD11	1.88	0.56
79:AA:836:A:H2'	79:AA:837:A:H8	1.70	0.56
79:AA:1066:C:H2'	79:AA:1067:A:C8	2.40	0.56
79:AA:1578:A:H2'	79:AA:1579:C:C6	2.41	0.56
71:AV:76:ILE:HD12	71:AV:112:TRP:HD1	1.71	0.56
79:AA:663:A:H2'	79:AA:664:G:C8	2.40	0.56
11:A:3211:C:H4'	11:A:3212:C:H5	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:160:GLU:HA	9:8:163:LYS:HE3	1.88	0.55
11:A:2086:A:H2'	11:A:2087:U:C6	2.42	0.55
13:E:50:ASP:HA	13:E:53:LEU:HG	1.87	0.55
8:7:77:THR:HG23	35:d:283:PRO:HA	1.88	0.55
11:A:1952:U:H2'	11:A:1953:A:H8	1.72	0.55
79:AA:1471:A:H2'	79:AA:1472:G:H8	1.71	0.55
79:AA:702:C:H2'	79:AA:703:A:C8	2.42	0.55
79:AA:672:A:H2'	79:AA:673:U:C6	2.42	0.55
79:AA:1552:G:H2'	79:AA:1553:A:H8	1.72	0.55
11:A:1829:A:H2'	11:A:1830:G:H8	1.72	0.55
79:AA:773:U:H2'	79:AA:774:G:C8	2.41	0.55
59:AH:118:PHE:HE1	59:AH:136:MET:HE2	1.72	0.54
61:AK:52:LEU:HD22	73:AZ:41:PRO:HG3	1.89	0.54
4:3:138:PRO:HG2	11:A:2854:U:H4'	1.89	0.54
58:AG:197:SER:HB2	58:AG:245:ARG:HB3	1.89	0.54
79:AA:1439:A:H2'	79:AA:1440:G:C8	2.43	0.54
79:AA:1488:5MC:H2'	79:AA:1489:G:C8	2.43	0.54
8:7:114:ASP:HB2	8:7:117:LYS:HB2	1.90	0.54
79:AA:1025:A:H2'	79:AA:1026:A:C8	2.41	0.54
79:AA:1214:A:H2'	79:AA:1352:C:O2	2.07	0.54
88:B:23:A:H2'	88:B:24:G:C8	2.43	0.54
21:N:124:VAL:HG12	21:N:158:ARG:HE	1.72	0.54
73:AZ:10:ARG:HH12	75:A1:239:TRP:CD1	2.26	0.54
79:AA:745:A:H3'	79:AA:746:A:C8	2.36	0.54
79:AA:1452:U:H2'	79:AA:1453:A:C8	2.41	0.54
58:AG:281:ALA:HB2	58:AG:332:VAL:HG23	1.90	0.54
59:AH:122:GLN:HG3	79:AA:1265:C:H4'	1.90	0.54
8:7:159:LYS:HE2	8:7:162:TYR:HE2	1.73	0.54
11:A:2151:A:H2'	11:A:2152:A:C8	2.43	0.54
64:AN:95:VAL:HG23	64:AN:96:THR:HG23	1.88	0.54
84:A4:308:LYS:HE3	84:A4:310:GLU:HB2	1.90	0.54
47:r:70:CYS:HB2	47:r:107:LEU:HA	1.89	0.54
79:AA:970:A:H2'	79:AA:971:A:C8	2.43	0.54
79:AA:1173:C:H2'	79:AA:1174:U:C6	2.43	0.54
79:AA:660:C:H1'	79:AA:1285:G:H21	1.73	0.54
79:AA:867:C:H2'	79:AA:870:C:N4	2.23	0.54
75:A1:53:LEU:HD12	84:A4:518:GLU:HG2	1.89	0.53
79:AA:1461:A:H4'	79:AA:1462:G:C8	2.44	0.53
36:e:218:PRO:HD2	99:B:101:VAL:HG22	1.89	0.53
48:t:64:ILE:HD11	48:u:82:LEU:HB2	1.90	0.53
79:AA:1042:U:H2'	79:AA:1043:C:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2134:A:H62	11:A:2135:A:H62	1.57	0.53
35:d:138:PRO:HG3	35:d:194:VAL:HG23	1.90	0.53
11:A:1696:C:H5''	28:U:6:VAL:HG23	1.90	0.53
15:H:98:LEU:HD23	15:H:129:ALA:HB2	1.89	0.53
48:u:64:ILE:O	48:u:68:VAL:HG23	2.09	0.53
79:AA:1119:U:H2'	79:AA:1120:C:O4'	2.09	0.53
7:6:187:VAL:HG13	7:6:319:PHE:HB3	1.90	0.53
14:F:243:ILE:HG22	46:q:27:ALA:HB2	1.91	0.53
47:r:71:PRO:HD2	47:r:107:LEU:HD23	1.90	0.53
74:A0:99:ARG:HD3	79:AA:1526:U:H2'	1.89	0.53
79:AA:799:A:H2'	79:AA:800:C:C6	2.43	0.53
79:AA:976:A:H5''	87:AQ:1:ACE:H1	1.90	0.53
79:AA:1007:G:H2'	79:AA:1008:A:H8	1.73	0.53
11:A:3150:U:H2'	11:A:3151:A:H8	1.73	0.53
13:E:80:LEU:HD12	13:E:323:GLY:HA3	1.91	0.53
59:AH:77:SER:HB2	59:AH:173:THR:HB	1.90	0.53
79:AA:1033:U:H2'	79:AA:1034:U:C6	2.44	0.53
55:AD:371:VAL:HG22	55:AD:383:VAL:HG22	1.91	0.53
71:AV:233:LYS:HD3	71:AV:286:VAL:HG23	1.91	0.53
79:AA:1552:G:H2'	79:AA:1553:A:C8	2.43	0.53
16:I:197:LEU:HD22	48:u:76:LEU:HD12	1.90	0.53
55:AD:380:LEU:HD12	55:AD:381:PRO:HD2	1.91	0.53
56:AE:26:ILE:HG23	56:AE:36:VAL:HG21	1.90	0.53
11:A:2093:U:H2'	11:A:2094:G:C8	2.44	0.53
79:AA:746:A:H2'	79:AA:747:A:C8	2.43	0.53
79:AA:1007:G:H2'	79:AA:1008:A:C8	2.44	0.53
79:AA:1416:A:H2'	79:AA:1417:A:C8	2.44	0.53
55:AD:244:LEU:HD22	55:AD:343:LEU:HD23	1.91	0.52
84:A4:562:GLN:HB3	84:A4:564:ILE:HG22	1.90	0.52
86:A2:95:GLU:HB3	86:A2:100:LEU:HG	1.91	0.52
8:7:204:LYS:HE3	82:a:92:LEU:HD13	1.91	0.52
79:AA:1078:A:H2'	79:AA:1079:G:C8	2.45	0.52
79:AA:1439:A:H2'	79:AA:1440:G:H8	1.74	0.52
16:I:116:LEU:HG	16:I:121:ILE:HB	1.90	0.52
26:S:129:ARG:HE	26:S:155:ARG:HG3	1.74	0.52
67:AR:272:VAL:HG22	67:AR:284:LEU:HD21	1.92	0.52
79:AA:852:A:H3'	79:AA:853:C:H6	1.73	0.52
11:A:3144:A:H2'	11:A:3145:A:H8	1.74	0.52
79:AA:839:A:H2'	79:AA:840:A:C8	2.44	0.52
79:AA:916:C:H2'	79:AA:917:C:C6	2.44	0.52
79:AA:1504:U:H2'	79:AA:1505:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:165:GLN:NE2	6:5:175:THR:HG22	2.25	0.52
36:e:55:ARG:HG3	36:e:149:LEU:HD22	1.92	0.52
68:AS:51:VAL:HG13	86:A2:117:LEU:HD11	1.91	0.52
46:q:168:VAL:HG12	46:q:175:PHE:HB2	1.91	0.52
49:c:259:ARG:HB2	49:c:271:PHE:HB2	1.92	0.52
59:AH:164:LEU:HD13	59:AH:170:MET:HE3	1.92	0.52
79:AA:1455:U:H2'	79:AA:1456:U:C6	2.45	0.52
11:A:1952:U:H2'	11:A:1953:A:C8	2.45	0.52
18:K:60:MET:HE2	18:K:133:ILE:HD11	1.92	0.52
11:A:2111:C:H2'	11:A:2112:A:C8	2.45	0.52
56:AE:35:ILE:HD12	62:AL:97:MET:HE2	1.91	0.52
36:e:111:GLU:HG3	85:AX:182:LEU:HD11	1.92	0.52
46:q:164:LEU:HG	46:q:178:LEU:HD23	1.91	0.52
71:AV:148:MET:HE2	71:AV:185:VAL:HG21	1.92	0.52
79:AA:696:U:H2'	79:AA:697:G:C8	2.45	0.52
79:AA:1578:A:H2'	79:AA:1579:C:H6	1.74	0.52
86:A2:43:ALA:HB1	86:A2:46:ILE:HD11	1.91	0.52
8:7:315:LYS:HD2	13:E:64:LEU:HD21	1.91	0.51
59:AH:96:VAL:HA	59:AH:106:ILE:HD13	1.91	0.51
79:AA:1238:C:H2'	79:AA:1239:C:C6	2.44	0.51
55:AD:229:PHE:H	79:AA:658:G:H4'	1.75	0.51
59:AH:76:LEU:HD23	59:AH:174:LYS:HA	1.93	0.51
79:AA:848:U:H2'	79:AA:849:U:C6	2.45	0.51
79:AA:1005:U:H4'	80:AI:87:HIS:CE1	2.45	0.51
79:AA:1169:G:H2'	79:AA:1170:G:H8	1.74	0.51
6:5:336:LEU:HD21	6:5:362:THR:HG23	1.92	0.51
11:A:2005:C:H2'	11:A:2006:C:C6	2.45	0.51
11:A:2409:A:H2'	11:A:2410:U:C6	2.46	0.51
79:AA:970:A:H2'	79:AA:971:A:H8	1.76	0.51
88:B:29:C:H2'	88:B:30:A:H8	1.75	0.51
1:0:138:ARG:HB3	11:A:2321:A:C8	2.45	0.51
71:AV:89:GLU:HG3	71:AV:124:LYS:HD2	1.91	0.51
75:A1:268:GLN:HE22	85:AX:120:PRO:HG3	1.75	0.51
35:d:219:ARG:HD3	35:d:239:PRO:HB2	1.93	0.51
74:A0:68:LEU:HD21	74:A0:80:VAL:HG21	1.91	0.51
48:t:64:ILE:HD12	48:u:78:GLU:HG3	1.91	0.51
55:AD:335:LYS:HE2	79:AA:649:A:H3'	1.92	0.51
65:AO:82:LYS:HB3	79:AA:881:A:N6	2.25	0.51
71:AV:175:VAL:HG12	71:AV:177:SER:H	1.75	0.51
79:AA:753:A:H2'	79:AA:754:A:H8	1.76	0.51
79:AA:832:U:H2'	79:AA:833:A:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:192:TYR:HB3	50:f:132:ILE:HD11	1.93	0.51
36:e:51:LEU:HD13	36:e:188:ALA:HB1	1.93	0.51
11:A:2081:U:H2'	11:A:2082:G:C8	2.45	0.51
11:A:2408:U:H2'	11:A:2409:A:H8	1.76	0.51
59:AH:97:LEU:O	59:AH:101:GLU:HG3	2.11	0.51
79:AA:1400:U:H2'	79:AA:1401:G:C8	2.46	0.51
11:A:1974:A:H5'	12:D:261:GLY:HA2	1.94	0.50
36:e:195:LEU:HD12	36:e:243:PHE:HZ	1.76	0.50
79:AA:798:C:H2'	79:AA:799:A:C8	2.46	0.50
54:AC:100:PHE:HB3	54:AC:103:CYS:HB2	1.93	0.50
70:AU:64:ARG:HA	70:AU:67:VAL:HG12	1.93	0.50
79:AA:867:C:H2'	79:AA:870:C:H42	1.76	0.50
79:AA:1374:A:H5''	85:AX:317:PHE:CE1	2.46	0.50
79:AA:1430:A:N1	79:AA:1458:A:H5''	2.27	0.50
85:AX:266:ASN:HA	85:AX:329:LEU:HD23	1.93	0.50
71:AV:68:SER:N	79:AA:1523:A:H5''	2.26	0.50
79:AA:1042:U:H2'	79:AA:1043:C:H6	1.75	0.50
35:d:96:ARG:HG2	35:d:97:ILE:H	1.77	0.50
35:d:106:ILE:O	35:d:110:GLU:HG2	2.12	0.50
55:AD:201:ILE:HB	55:AD:222:ILE:HD12	1.93	0.50
79:AA:1195:U:H2'	79:AA:1196:A:C8	2.46	0.50
11:A:1868:G:H2'	20:M:40:PRO:HG3	1.93	0.50
11:A:1939:G:O2'	11:A:1973:G:H4'	2.12	0.50
11:A:2586:U:H2'	11:A:2587:G:H8	1.77	0.50
65:AO:202:TRP:HD1	70:AU:59:ARG:HG2	1.76	0.50
79:AA:1427:A:H2'	79:AA:1428:G:C8	2.46	0.50
79:AA:1470:A:H2'	79:AA:1471:A:C8	2.47	0.50
10:9:24:LYS:HE3	28:U:74:HIS:HB2	1.93	0.50
22:O:33:LEU:HD21	22:O:59:LEU:HD22	1.94	0.50
23:P:94:VAL:HG23	23:P:132:LEU:HD21	1.93	0.50
47:r:108:CYS:SG	47:r:111:GLU:HG2	2.52	0.50
79:AA:1025:A:H2'	79:AA:1026:A:H8	1.77	0.50
85:AX:159:HIS:HA	85:AX:162:VAL:HG12	1.93	0.50
85:AX:242:ILE:HD11	98:AX:503:GDP:C5	2.46	0.50
12:D:109:PHE:CE1	12:D:208:ARG:HD3	2.47	0.50
35:d:210:GLY:O	35:d:249:GLU:HA	2.11	0.50
36:e:159:LEU:HD12	36:e:254:TRP:CH2	2.47	0.50
79:AA:1412:G:H2'	79:AA:1413:U:O4'	2.12	0.50
79:AA:1589:C:H2'	79:AA:1590:A:C8	2.47	0.50
84:A4:263:ILE:HG13	84:A4:278:LEU:HD23	1.94	0.50
17:J:140:VAL:O	17:J:144:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:A0:65:LEU:HD23	74:A0:68:LEU:HB2	1.93	0.50
79:AA:1035:U:H2'	79:AA:1036:A:H8	1.76	0.50
79:AA:1495:C:H2'	79:AA:1496:U:C6	2.46	0.50
6:5:143:PRO:HA	6:5:146:HIS:HD1	1.76	0.50
11:A:1924:U:H2'	11:A:1925:A:C8	2.47	0.50
88:B:21:A:H61	88:B:46:A:H2'	1.77	0.50
11:A:1936:A:H4'	11:A:1937:A:C8	2.47	0.49
11:A:2553:G:H2'	11:A:2554:A:H8	1.77	0.49
20:M:44:ARG:HG3	20:M:45:ARG:HG3	1.93	0.49
56:AE:32:ARG:HB3	56:AE:74:ALA:HB1	1.94	0.49
71:AV:163:VAL:O	71:AV:167:VAL:HG23	2.12	0.49
84:A4:156:ALA:O	84:A4:160:ARG:HG2	2.12	0.49
11:A:2006:C:H2'	11:A:2007:U:H6	1.73	0.49
35:d:211:GLN:HA	35:d:248:PHE:O	2.12	0.49
79:AA:833:A:H2'	79:AA:834:G:H8	1.77	0.49
79:AA:944:U:H2'	79:AA:945:G:H8	1.77	0.49
80:AI:99:VAL:HG11	80:AI:139:ALA:HB2	1.93	0.49
46:q:147:GLN:O	46:q:150:LYS:HG3	2.12	0.49
67:AR:157:VAL:HG22	67:AR:174:VAL:HG22	1.94	0.49
79:AA:686:A:H2'	79:AA:687:G:C8	2.47	0.49
79:AA:922:C:H2'	79:AA:923:A:C8	2.48	0.49
79:AA:969:A:H2'	79:AA:970:A:H8	1.77	0.49
79:AA:1401:G:N2	79:AA:1403:A:H3'	2.26	0.49
84:A4:332:LEU:HD23	84:A4:368:SER:HB3	1.94	0.49
85:AX:205:GLN:HG2	85:AX:250:GLN:HE21	1.76	0.49
9:8:147:LEU:HD21	36:e:208:ALA:HB1	1.94	0.49
11:A:1750:G:H2'	11:A:1751:A:C8	2.46	0.49
11:A:2727:C:H2'	11:A:2728:C:C6	2.47	0.49
11:A:2757:A:H2'	11:A:2758:G:O4'	2.12	0.49
11:A:3115:U:H2'	11:A:3116:C:C6	2.47	0.49
79:AA:871:A:H4'	79:AA:872:G:H5'	1.93	0.49
11:A:2420:U:H2'	11:A:2421:G:H8	1.76	0.49
59:AH:70:ASP:HA	84:A4:62:LYS:HE3	1.94	0.49
79:AA:944:U:H2'	79:AA:945:G:C8	2.48	0.49
11:A:3199:U:H5''	11:A:3200:U:H4'	1.93	0.49
12:D:207:ILE:HG12	12:D:229:PRO:HD3	1.94	0.49
17:J:88:SER:HA	17:J:151:LEU:HD11	1.94	0.49
58:AG:380:LYS:HG3	58:AG:386:GLY:HA2	1.95	0.49
79:AA:847:G:H2'	79:AA:848:U:C6	2.48	0.49
79:AA:923:A:H2'	79:AA:924:A:C8	2.48	0.49
79:AA:990:U:H2'	79:AA:991:G:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:1065:C:H2'	79:AA:1066:C:O4'	2.12	0.49
79:AA:1209:C:H2'	79:AA:1210:U:C6	2.48	0.49
35:d:250:LYS:HB2	35:d:259:TRP:HA	1.94	0.49
55:AD:140:LEU:CD1	55:AD:160:ARG:HG3	2.38	0.49
79:AA:1006:U:H2'	79:AA:1007:G:C8	2.46	0.49
79:AA:1353:A:H5'	79:AA:1354:A:H5'	1.95	0.49
85:AX:366:LEU:HD22	85:AX:398:LEU:HD22	1.95	0.49
11:A:2382:A:H2'	11:A:2383:U:C6	2.47	0.49
11:A:2662:A:H2'	11:A:2663:C:C6	2.48	0.49
11:A:2734:A:H2'	11:A:2735:G:H8	1.78	0.49
74:A0:165:PRO:HG3	74:A0:190:MET:HE2	1.94	0.49
79:AA:1047:A:C6	79:AA:1158:U:H4'	2.47	0.49
79:AA:1469:G:H2'	79:AA:1470:A:H8	1.77	0.49
84:A4:516:SER:HB2	84:A4:521:HIS:HB2	1.95	0.49
11:A:2740:A:H2'	11:A:2741:A:H8	1.77	0.49
11:A:3124:U:O2	11:A:3133:A:N7	2.46	0.49
36:e:273:ARG:HA	36:e:276:VAL:HG12	1.95	0.49
61:AK:57:LEU:HD23	61:AK:71:ALA:HB2	1.94	0.49
11:A:2764:A:C4	15:H:252:LEU:HD21	2.48	0.48
11:A:3224:G:H2'	11:A:3225:G:H8	1.78	0.48
71:AV:103:TYR:CZ	79:AA:1524:A:H4'	2.48	0.48
79:AA:715:G:H2'	79:AA:716:U:C6	2.47	0.48
11:A:2392:U:H2'	11:A:2394:A:H62	1.78	0.48
30:X:7:PRO:HD2	30:X:10:LEU:HD12	1.95	0.48
54:AC:163:VAL:HG11	54:AC:166:TYR:CE1	2.48	0.48
79:AA:663:A:H2'	79:AA:664:G:H8	1.78	0.48
79:AA:798:C:H2'	79:AA:799:A:H8	1.78	0.48
79:AA:1180:U:H2'	79:AA:1181:G:H8	1.78	0.48
9:8:191:ARG:NH2	50:f:144:MET:HG3	2.28	0.48
11:A:2727:C:H2'	11:A:2728:C:H6	1.78	0.48
32:Z:99:VAL:HG21	40:j:77:VAL:HG22	1.95	0.48
43:m:55:LEU:HD23	43:m:63:THR:HG21	1.94	0.48
55:AD:420:SER:HA	79:AA:929:A:H4'	1.95	0.48
63:AM:64:LYS:HD2	67:AR:156:TYR:CE1	2.49	0.48
79:AA:661:C:H2'	79:AA:662:U:H6	1.78	0.48
79:AA:673:U:H2'	79:AA:674:U:C6	2.48	0.48
79:AA:1265:C:H2'	79:AA:1266:A:H8	1.78	0.48
79:AA:1408:A:H2'	79:AA:1409:A:H8	1.78	0.48
84:A4:396:ILE:HG12	84:A4:400:LEU:HD23	1.96	0.48
11:A:2101:C:H2'	11:A:2102:A:H8	1.77	0.48
11:A:3151:A:H4'	24:Q:146:GLY:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:112:ARG:HH11	11:A:2406:A:H61	1.62	0.48
11:A:2099:U:H2'	11:A:2100:C:C6	2.48	0.48
79:AA:861:U:H2'	79:AA:862:A:C8	2.48	0.48
79:AA:1497:C:H2'	79:AA:1498:C:C6	2.48	0.48
11:A:2803:A:H2'	11:A:2804:A:O4'	2.13	0.48
26:S:83:VAL:HA	26:S:86:MET:HE2	1.95	0.48
79:AA:686:A:H2'	79:AA:687:G:H8	1.78	0.48
79:AA:951:G:H2'	79:AA:952:A:H8	1.78	0.48
5:4:83:LYS:HE3	5:4:88:TRP:NE1	2.29	0.48
11:A:2365:U:H2'	11:A:2366:G:C8	2.49	0.48
21:N:36:VAL:HG11	42:I:124:GLN:HB3	1.95	0.48
67:AR:159:THR:HG23	67:AR:172:ILE:HG12	1.96	0.48
79:AA:821:U:H2'	79:AA:822:G:C8	2.45	0.48
79:AA:912:U:H2'	79:AA:913:A:C8	2.48	0.48
79:AA:1560:U:H2'	79:AA:1561:C:C6	2.48	0.48
11:A:2872:C:H2'	11:A:2873:A:O4'	2.14	0.48
79:AA:833:A:H2'	79:AA:834:G:C8	2.49	0.48
57:AF:172:VAL:HG12	57:AF:240:ARG:HD3	1.96	0.48
58:AG:87:HIS:O	58:AG:91:MET:HG2	2.14	0.48
79:AA:659:U:H2'	79:AA:660:C:H6	1.79	0.48
79:AA:685:A:H2'	79:AA:686:A:C8	2.48	0.48
6:5:98:LEU:HD22	6:5:272:ASP:HB3	1.96	0.48
11:A:2408:U:H2'	11:A:2409:A:C8	2.48	0.48
15:H:118:LEU:HD11	15:H:122:ARG:HE	1.78	0.48
17:J:70:ILE:HG12	17:J:80:ILE:HG22	1.96	0.48
27:T:62:ARG:NE	35:d:230:ARG:HD2	2.29	0.48
36:e:231:VAL:HG21	88:B:76:A:N6	2.26	0.48
52:s:63:ILE:HA	52:s:66:TRP:CD1	2.48	0.48
79:AA:1471:A:H2'	79:AA:1472:G:C8	2.48	0.48
11:A:1994:A:H61	11:A:2736:C:H4'	1.79	0.47
29:W:67:ILE:HG21	29:W:131:VAL:HG21	1.95	0.47
79:AA:774:G:H2'	79:AA:775:C:C6	2.49	0.47
79:AA:940:A:N3	79:AA:1136:C:H1'	2.29	0.47
79:AA:959:C:H3'	79:AA:960:C:O4'	2.13	0.47
79:AA:1504:U:H2'	79:AA:1505:A:H8	1.78	0.47
11:A:3089:A:H3'	11:A:3090:G:C5'	2.44	0.47
15:H:207:LYS:HB3	15:H:222:GLU:HB3	1.96	0.47
35:d:217:HIS:HB2	35:d:243:LEU:HD13	1.96	0.47
36:e:200:MET:HA	36:e:241:GLY:HA3	1.95	0.47
83:Ax:4:A:H2'	83:Ax:5:A:C8	2.49	0.47
11:A:2662:A:H2'	11:A:2663:C:H6	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AR:172:ILE:HD12	67:AR:189:ARG:HG2	1.96	0.47
79:AA:827:A:H5'	79:AA:828:C:C5	2.48	0.47
79:AA:1422:G:H2'	79:AA:1423:A:C8	2.49	0.47
88:B:68:C:H2'	88:B:69:U:C6	2.50	0.47
11:A:2668:A:H2'	11:A:2669:A:C8	2.50	0.47
16:I:64:CYS:HB3	47:r:73:CYS:SG	2.54	0.47
79:AA:738:A:H3'	79:AA:739:C:C6	2.50	0.47
79:AA:1399:A:H2'	79:AA:1400:U:C6	2.50	0.47
83:Ax:47:U:H2'	83:Ax:48:G:C8	2.49	0.47
33:V:136:ARG:HD3	81:OX:401:PHE:CZ	2.50	0.47
79:AA:1238:C:H2'	79:AA:1239:C:H6	1.79	0.47
79:AA:1506:U:H2'	79:AA:1507:A:H8	1.79	0.47
83:Ax:40:A:H2'	83:Ax:41:A:C8	2.49	0.47
11:A:1911:C:H2'	11:A:1912:A:H8	1.77	0.47
11:A:2318:A:H2'	11:A:2319:A:C8	2.49	0.47
11:A:3139:G:H2'	11:A:3140:A:C8	2.49	0.47
11:A:3158:A:H2'	11:A:3159:A:H8	1.79	0.47
35:d:204:ASN:O	35:d:205:GLN:HG2	2.15	0.47
84:A4:166:VAL:HG12	84:A4:194:LEU:HG	1.97	0.47
8:7:139:ASN:HB3	8:7:174:VAL:HG21	1.96	0.47
11:A:1936:A:H4'	11:A:1937:A:N7	2.30	0.47
11:A:2134:A:N6	11:A:2135:A:H62	2.12	0.47
24:Q:176:VAL:HG11	24:Q:179:LEU:HB2	1.97	0.47
27:T:206:LEU:HA	34:b:119:PHE:CE2	2.50	0.47
35:d:158:ASP:O	35:d:162:THR:HG23	2.14	0.47
79:AA:1502:A:H2'	79:AA:1503:G:O4'	2.15	0.47
84:A4:335:PHE:CG	84:A4:360:MET:HE2	2.50	0.47
84:A4:513:TRP:HE1	84:A4:554:ASP:HB2	1.80	0.47
85:AX:244:LEU:HD22	85:AX:296:MET:HG3	1.95	0.47
79:AA:981:C:H2'	79:AA:982:A:H8	1.79	0.47
11:A:1829:A:H2'	11:A:1830:G:C8	2.50	0.47
67:AR:288:GLN:HE22	67:AR:300:LEU:HD22	1.80	0.47
71:AV:322:THR:HG23	71:AV:325:SER:H	1.79	0.47
71:AV:331:LEU:O	71:AV:335:LYS:HG2	2.15	0.47
79:AA:738:A:H3'	79:AA:739:C:H6	1.79	0.47
7:6:175:VAL:HG22	7:6:204:VAL:HG22	1.97	0.47
11:A:3115:U:H2'	11:A:3116:C:H6	1.80	0.47
35:d:202:MET:HB2	35:d:207:ASN:O	2.15	0.47
43:m:90:ARG:HE	43:m:94:ARG:HG3	1.79	0.47
71:AV:340:LYS:HB3	71:AV:340:LYS:HE3	1.73	0.47
74:A0:64:LEU:HD12	74:A0:139:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:1089:U:H2'	79:AA:1090:A:H8	1.80	0.46
85:AX:177:ARG:HD3	85:AX:288:ALA:HA	1.97	0.46
85:AX:265:ILE:HA	85:AX:268:LEU:HD23	1.97	0.46
10:9:86:LEU:HD21	10:9:91:LEU:HD12	1.96	0.46
11:A:1828:A:H4'	11:A:1829:A:C8	2.49	0.46
11:A:1839:C:H2'	11:A:1840:C:C6	2.50	0.46
46:q:170:PRO:HA	46:q:175:PHE:CD1	2.50	0.46
63:AM:114:ARG:HA	63:AM:117:GLU:HB3	1.96	0.46
79:AA:661:C:H2'	79:AA:662:U:C6	2.50	0.46
79:AA:747:A:H2'	79:AA:748:G:H8	1.80	0.46
79:AA:913:A:H2'	79:AA:914:A:C8	2.50	0.46
11:A:2277:U:H2'	11:A:2278:A:H8	1.79	0.46
16:I:47:LEU:HD22	21:N:226:ILE:HG12	1.97	0.46
79:AA:1440:G:H2'	79:AA:1441:A:H8	1.72	0.46
53:AB:194:ILE:HA	53:AB:220:VAL:O	2.15	0.46
79:AA:786:G:H2'	79:AA:787:C:C6	2.51	0.46
79:AA:1118:A:H3'	79:AA:1119:U:H5''	1.98	0.46
11:A:1911:C:H2'	11:A:1912:A:C8	2.51	0.46
15:H:102:VAL:HG22	15:H:128:LEU:HD23	1.96	0.46
17:J:116:HIS:CE1	42:l:86:LEU:HD11	2.51	0.46
36:e:111:GLU:HG2	85:AX:182:LEU:HD21	1.98	0.46
63:AM:73:ILE:O	63:AM:77:ILE:HG12	2.15	0.46
63:AM:110:LEU:O	63:AM:114:ARG:HG3	2.16	0.46
71:AV:70:LEU:HD21	71:AV:390:ILE:HD13	1.97	0.46
79:AA:1372:C:H2'	79:AA:1373:U:C6	2.51	0.46
85:AX:88:VAL:HA	85:AX:91:VAL:HG22	1.97	0.46
11:A:1697:A:H2'	11:A:1698:C:C6	2.50	0.46
11:A:3114:U:H2'	11:A:3115:U:C6	2.50	0.46
13:E:334:ASP:HB3	13:E:337:VAL:HG23	1.97	0.46
33:V:102:MET:HE3	35:d:48:PRO:HG2	1.97	0.46
79:AA:776:A:O3'	79:AA:777:G:H8	1.97	0.46
79:AA:916:C:H2'	79:AA:917:C:H6	1.81	0.46
79:AA:1496:U:H2'	79:AA:1497:C:C6	2.51	0.46
80:AI:110:ALA:HB3	80:AI:135:ALA:HB2	1.97	0.46
11:A:2235:C:H2'	11:A:2236:C:O4'	2.15	0.46
41:k:17:ARG:NH1	41:k:19:GLN:HB2	2.30	0.46
49:c:59:ARG:HB2	49:c:62:GLU:HG2	1.98	0.46
79:AA:747:A:H2'	79:AA:748:G:C8	2.51	0.46
79:AA:980:U:H2'	79:AA:981:C:C6	2.50	0.46
79:AA:1382:A:H5''	85:AX:166:ARG:HH21	1.79	0.46
79:AA:1497:C:H2'	79:AA:1498:C:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:148:MET:HE2	8:7:257:ILE:HG12	1.97	0.46
14:F:65:TRP:CD1	38:h:117:LEU:HD11	2.51	0.46
55:AD:160:ARG:NH1	55:AD:168:VAL:HG21	2.31	0.46
55:AD:181:ARG:HD2	55:AD:185:MET:HE3	1.98	0.46
79:AA:1308:U:H2'	79:AA:1309:A:C8	2.50	0.46
79:AA:1426:U:H2'	79:AA:1427:A:C8	2.50	0.46
26:S:144:LEU:HB2	82:a:58:ILE:HB	1.97	0.46
57:AF:166:ARG:NH2	79:AA:994:A:H1'	2.31	0.46
79:AA:852:A:H3'	79:AA:853:C:C6	2.51	0.46
79:AA:1523:A:H1'	79:AA:1528:A:C2	2.51	0.46
15:H:174:VAL:HG12	15:H:192:HIS:CB	2.46	0.46
35:d:152:LEU:HD11	35:d:172:MET:HE2	1.97	0.46
51:p:135:LEU:HD22	51:p:154:ILE:HG13	1.98	0.46
79:AA:875:U:H2'	79:AA:876:U:C6	2.51	0.46
79:AA:945:G:OP2	96:AA:1702:SPM:H71	2.16	0.46
79:AA:1455:U:H2'	79:AA:1456:U:H6	1.81	0.46
79:AA:1456:U:H2'	79:AA:1457:G:O4'	2.17	0.46
83:Ax:22:U:C2	83:Ax:23:A:C8	3.04	0.46
11:A:1924:U:H2'	11:A:1925:A:H8	1.81	0.45
33:V:168:GLU:HB3	81:OX:374:MET:HE1	1.98	0.45
65:AO:55:PRO:HB3	65:AO:114:HIS:HB2	1.97	0.45
79:AA:1542:U:H2'	79:AA:1543:U:C6	2.52	0.45
84:A4:393:ILE:HA	84:A4:396:ILE:HG22	1.99	0.45
7:6:234:HIS:CE1	7:6:257:PRO:HA	2.50	0.45
9:8:117:LEU:HD11	36:e:69:GLU:HB3	1.99	0.45
11:A:2661:U:H2'	11:A:2662:A:C8	2.51	0.45
11:A:2718:C:H2'	11:A:2991:U:H4'	1.97	0.45
16:I:98:VAL:HG12	16:I:177:LEU:HD12	1.97	0.45
46:q:175:PHE:CD1	46:q:179:LEU:HD23	2.51	0.45
79:AA:832:U:H2'	79:AA:833:A:C8	2.50	0.45
79:AA:985:U:H2'	79:AA:986:G:C8	2.52	0.45
79:AA:1417:A:H2'	79:AA:1418:G:O4'	2.17	0.45
28:U:113:GLU:HG2	28:U:115:ASP:OD1	2.17	0.45
59:AH:177:LEU:HB3	75:A1:147:PHE:HB2	1.98	0.45
71:AV:102:TRP:HE1	74:A0:76:LEU:HD11	1.81	0.45
73:AZ:10:ARG:HA	73:AZ:13:ARG:HB3	1.99	0.45
79:AA:969:A:H2'	79:AA:970:A:C8	2.51	0.45
79:AA:1560:U:H2'	79:AA:1561:C:H6	1.81	0.45
11:A:2491:C:H2'	11:A:2492:G:C8	2.51	0.45
11:A:2868:C:H2'	11:A:2869:A:O4'	2.17	0.45
24:Q:100:LEU:HD21	24:Q:286:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Y:124:LEU:HD21	35:d:61:ARG:HD2	1.99	0.45
35:d:90:PRO:HB3	35:d:245:TYR:CE2	2.52	0.45
41:k:17:ARG:HH12	41:k:19:GLN:HB2	1.82	0.45
48:t:86:LEU:HG	48:u:71:ILE:HD11	1.98	0.45
62:AL:89:VAL:HG22	70:AU:164:VAL:HG21	1.97	0.45
67:AR:175:ARG:CZ	67:AR:181:LEU:HB2	2.47	0.45
71:AV:117:LEU:HA	71:AV:122:GLN:HE22	1.82	0.45
79:AA:1398:U:H2'	79:AA:1399:A:C8	2.48	0.45
84:A4:392:ILE:HG13	84:A4:393:ILE:N	2.32	0.45
11:A:2175:C:H2'	11:A:2176:C:H6	1.81	0.45
51:p:123:HIS:CE1	51:p:157:MET:HG2	2.52	0.45
52:s:145:VAL:HG21	52:s:187:LEU:HD11	1.98	0.45
53:AB:141:ILE:HG23	53:AB:165:TYR:CE1	2.52	0.45
79:AA:897:C:H2'	79:AA:898:C:C6	2.52	0.45
79:AA:1044:U:H2'	79:AA:1045:G:O4'	2.16	0.45
79:AA:1154:A:O2'	79:AA:1155:G:H5'	2.17	0.45
79:AA:1190:C:H2'	79:AA:1191:C:H6	1.82	0.45
79:AA:1191:C:H2'	79:AA:1192:C:H6	1.82	0.45
79:AA:1350:G:H2'	79:AA:1351:G:C8	2.52	0.45
85:AX:266:ASN:HD22	85:AX:328:LEU:HB3	1.81	0.45
11:A:1863:A:H2'	11:A:1864:A:H8	1.81	0.45
11:A:2549:C:N4	11:A:2562:U:H2'	2.31	0.45
74:A0:21:LEU:O	74:A0:25:LEU:HG	2.17	0.45
79:AA:800:C:H2'	79:AA:801:A:C8	2.51	0.45
79:AA:1124:A:H2'	79:AA:1125:A:H2'	1.99	0.45
79:AA:1348:G:H2'	79:AA:1349:U:C6	2.52	0.45
83:Ax:4:A:H2'	83:Ax:5:A:H8	1.81	0.45
85:AX:80:PRO:HG2	85:AX:81:HIS:HD2	1.82	0.45
11:A:2051:A:H2'	11:A:2052:A:H8	1.82	0.45
17:J:161:SER:HA	42:l:69:THR:HG21	1.98	0.45
79:AA:774:G:H2'	79:AA:775:C:H6	1.81	0.45
79:AA:914:A:H2'	79:AA:915:C:C6	2.52	0.45
79:AA:945:G:H2'	79:AA:946:U:C6	2.51	0.45
79:AA:1012:A:H2'	79:AA:1013:A:C8	2.52	0.45
79:AA:1194:C:H2'	79:AA:1195:U:C6	2.51	0.45
79:AA:1588:G:H2'	79:AA:1589:C:C6	2.52	0.45
1:O:130:VAL:HG21	22:O:134:PRO:HD3	1.98	0.45
11:A:2439:U:H2'	11:A:2440:G:H8	1.80	0.45
11:A:3000:A:H2'	11:A:3001:G:C8	2.52	0.45
11:A:3000:A:H2'	11:A:3001:G:H8	1.82	0.45
36:e:146:ARG:HH21	36:e:255:VAL:HG12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:80:HIS:O	47:r:36:ARG:HD2	2.16	0.45
74:A0:64:LEU:HD12	74:A0:139:TRP:CD2	2.51	0.45
79:AA:947:U:H2'	79:AA:948:U:H6	1.81	0.45
85:AX:85:PRO:HA	85:AX:88:VAL:HG12	1.98	0.45
11:A:2439:U:H2'	11:A:2440:G:C8	2.52	0.45
35:d:108:ARG:HA	35:d:111:ARG:HD2	1.99	0.45
52:s:332:LEU:HD21	52:s:359:ALA:HB2	1.98	0.45
59:AH:156:TYR:O	59:AH:160:ILE:HG12	2.16	0.45
74:A0:118:LEU:HB3	74:A0:125:GLU:HB2	1.98	0.45
79:AA:705:C:H3'	79:AA:706:C:H6	1.82	0.45
79:AA:891:C:H2'	79:AA:892:A:O4'	2.16	0.45
79:AA:968:U:H2'	79:AA:969:A:C8	2.52	0.45
79:AA:1464:G:H2'	79:AA:1465:C:C6	2.52	0.45
85:AX:188:LEU:HD22	85:AX:226:VAL:HG23	1.99	0.45
11:A:3054:G:H2'	11:A:3055:U:C6	2.52	0.45
11:A:3158:A:H2'	11:A:3159:A:C8	2.52	0.45
30:X:40:PRO:HB3	30:X:43:TYR:CZ	2.52	0.45
50:f:80:ILE:HG23	50:f:90:VAL:HG12	1.99	0.45
52:s:211:VAL:HG22	52:s:230:ARG:HG2	1.99	0.45
71:AV:57:MET:HE1	71:AV:91:TYR:HB3	1.98	0.45
71:AV:176:PRO:HA	71:AV:179:GLN:NE2	2.31	0.45
79:AA:712:C:H2'	79:AA:713:C:O4'	2.17	0.45
79:AA:1034:U:H2'	79:AA:1035:U:C6	2.52	0.45
79:AA:1441:A:H2	79:AA:1449:G:H22	1.65	0.45
11:A:2082:G:H21	32:Z:88:MET:HG2	1.82	0.44
71:AV:82:ARG:O	71:AV:85:ILE:HG22	2.17	0.44
79:AA:705:C:H3'	79:AA:706:C:C6	2.52	0.44
79:AA:862:A:H2'	79:AA:863:C:C6	2.52	0.44
79:AA:1200:G:C2	79:AA:1201:A:C8	3.05	0.44
79:AA:1462:G:H2'	79:AA:1463:G:H8	1.82	0.44
95:AA:1701:NAD:N7A	95:AA:1701:NAD:H51N	2.31	0.44
11:A:1862:U:H2'	11:A:1863:A:C8	2.51	0.44
11:A:3144:A:H2'	11:A:3145:A:C8	2.50	0.44
27:T:206:LEU:HA	34:b:119:PHE:HE2	1.82	0.44
35:d:84:ILE:HA	35:d:211:GLN:HE22	1.81	0.44
62:AL:130:ILE:HG12	62:AL:185:LEU:HD11	1.99	0.44
79:AA:1413:U:H2'	79:AA:1414:C:O4'	2.17	0.44
80:AI:176:THR:HB	87:AQ:11:THR:HG23	1.99	0.44
36:e:101:LYS:HD3	85:AX:231:THR:OG1	2.18	0.44
37:g:128:LEU:HD23	37:g:131:LEU:HD12	1.99	0.44
79:AA:1176:G:H2'	79:AA:1177:C:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:A4:571:TRP:HE3	84:A4:576:LEU:HD21	1.81	0.44
7:6:179:VAL:HG23	7:6:183:ASP:HB2	1.99	0.44
11:A:1851:G:H2'	11:A:2693:A:N7	2.33	0.44
11:A:2060:A:C8	11:A:2079:C:C4	3.05	0.44
58:AG:120:ARG:HH21	75:A1:90:PRO:HG2	1.81	0.44
65:AO:167:ILE:HD12	67:AR:226:ASP:HB3	1.98	0.44
67:AR:74:GLU:HG2	67:AR:78:ILE:HD13	2.00	0.44
79:AA:739:C:H2'	79:AA:740:G:O4'	2.17	0.44
79:AA:1072:G:H2'	79:AA:1073:G:H8	1.82	0.44
79:AA:1174:U:H2'	79:AA:1175:G:H8	1.81	0.44
84:A4:535:MET:HE1	84:A4:551:CYS:HB3	1.99	0.44
6:5:242:ARG:HA	6:5:245:ILE:HD12	1.98	0.44
9:8:188:PRO:HG2	50:f:136:GLN:HE22	1.83	0.44
11:A:2552:U:C2	11:A:2553:G:C8	3.05	0.44
15:H:182:TRP:CH2	15:H:237:VAL:HG11	2.52	0.44
26:S:169:ARG:HB2	26:S:186:VAL:HG23	1.99	0.44
46:q:170:PRO:HA	46:q:175:PHE:CG	2.52	0.44
74:A0:11:ILE:HB	79:AA:806:C:C2	2.53	0.44
79:AA:1138:G:H2'	79:AA:1139:A:H8	1.81	0.44
79:AA:1450:C:H2'	79:AA:1451:U:C6	2.52	0.44
79:AA:1498:C:H2'	79:AA:1499:U:H6	1.83	0.44
83:Ax:46:U:H3	83:Ax:59:U:H3	1.64	0.44
86:A2:29:LEU:HD22	87:AQ:68:MET:HE2	1.99	0.44
11:A:2553:G:H2'	11:A:2554:A:C8	2.51	0.44
11:A:2942:C:H2'	11:A:2943:G:H8	1.82	0.44
43:m:56:LEU:O	43:m:63:THR:HA	2.18	0.44
48:u:75:THR:O	48:u:79:ILE:HG13	2.17	0.44
71:AV:30:LEU:HD23	71:AV:149:ASP:HB2	1.99	0.44
79:AA:1109:A:H2'	79:AA:1110:A:C8	2.52	0.44
79:AA:1174:U:H2'	79:AA:1175:G:C8	2.53	0.44
79:AA:1495:C:H2'	79:AA:1496:U:H6	1.83	0.44
36:e:170:VAL:HG11	88:B:76:A:O4'	2.17	0.44
50:f:93:ILE:O	50:f:156:VAL:HA	2.17	0.44
52:s:142:LEU:HD13	52:s:422:VAL:HG21	1.99	0.44
53:AB:69:HIS:HB2	53:AB:72:PHE:HB2	1.99	0.44
62:AL:175:TYR:HB2	64:AN:89:GLY:HA3	1.98	0.44
63:AM:74:ARG:HG3	70:AU:74:PHE:CD1	2.53	0.44
67:AR:122:ALA:O	67:AR:126:LEU:HG	2.17	0.44
79:AA:960:C:H42	79:AA:1041:A:H2	1.65	0.44
79:AA:1379:A:H2'	79:AA:1380:G:C8	2.53	0.44
7:6:255:LEU:HD12	7:6:256:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2682:A:H4'	25:R:41:LEU:HD13	1.99	0.44
15:H:79:VAL:HG22	30:X:89:GLN:HB2	1.99	0.44
65:AO:123:LEU:HD13	65:AO:154:ILE:HA	2.00	0.44
79:AA:985:U:H2'	79:AA:986:G:H8	1.83	0.44
11:A:1737:A:H61	11:A:1760:G:H1'	1.83	0.44
78:AY:292:GLN:HG2	84:A4:446:LYS:HG2	1.99	0.44
79:AA:854:U:H2'	79:AA:855:A:C8	2.53	0.44
79:AA:1177:C:H2'	79:AA:1178:G:C8	2.52	0.44
79:AA:1318:A:H3'	79:AA:1319:A:H8	1.82	0.44
79:AA:1506:U:H2'	79:AA:1507:A:C8	2.53	0.44
84:A4:606:PRO:HG3	84:A4:633:LEU:HD21	2.00	0.44
85:AX:144:PHE:O	85:AX:148:GLN:HG2	2.17	0.44
11:A:2005:C:H2'	11:A:2006:C:H6	1.83	0.43
11:A:2661:U:H2'	11:A:2662:A:H8	1.83	0.43
11:A:3153:U:H2'	11:A:3154:U:H6	1.83	0.43
69:AT:74:PRO:HD2	69:AT:91:GLU:HG3	1.99	0.43
74:A0:99:ARG:HD2	79:AA:1527:A:H4'	1.99	0.43
88:B:43:G:H2'	88:B:44:A:C8	2.52	0.43
11:A:1938:A:O2'	11:A:1940:A:H5''	2.18	0.43
11:A:2514:C:H2'	11:A:2515:U:H6	1.83	0.43
20:M:177:ALA:HA	20:M:222:TYR:CD1	2.53	0.43
74:A0:29:ARG:HG3	74:A0:105:THR:HG21	2.00	0.43
79:AA:1003:A:H2'	79:AA:1004:G:H8	1.83	0.43
79:AA:1362:G:H2'	79:AA:1363:C:H6	1.83	0.43
11:A:1863:A:H2'	11:A:1864:A:C8	2.53	0.43
11:A:3165:C:H2'	11:A:3166:U:C6	2.52	0.43
16:I:127:PRO:HG2	16:I:130:VAL:HG22	1.99	0.43
33:V:146:VAL:HG21	81:OX:401:PHE:CE1	2.54	0.43
36:e:213:TYR:HD1	36:e:271:GLN:HG2	1.83	0.43
58:AG:201:ILE:HG13	58:AG:204:GLU:H	1.82	0.43
10:9:27:PRO:O	10:9:31:ARG:HG3	2.18	0.43
18:K:62:THR:HG21	18:K:101:VAL:HA	1.99	0.43
20:M:244:LEU:HD12	20:M:245:PRO:HD2	2.01	0.43
58:AG:92:MET:HE2	58:AG:92:MET:HB2	1.86	0.43
66:AP:127:PRO:HA	66:AP:130:LEU:HG	2.00	0.43
68:AS:49:PRO:HB2	86:A2:117:LEU:HD13	2.00	0.43
71:AV:40:TRP:HZ2	71:AV:111:THR:HG23	1.84	0.43
79:AA:1251:A:H2'	79:AA:1252:G:O4'	2.19	0.43
11:A:2114:C:H2'	11:A:2115:U:H6	1.83	0.43
11:A:2470:G:H4'	19:L:36:THR:HG23	1.99	0.43
46:q:186:GLU:O	46:q:190:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:AD:304:LYS:O	55:AD:334:ALA:HA	2.18	0.43
58:AG:285:VAL:HG22	58:AG:328:VAL:HG22	2.00	0.43
71:AV:130:VAL:HG22	71:AV:166:GLU:OE2	2.18	0.43
74:A0:136:TYR:CZ	79:AA:705:C:H2'	2.53	0.43
9:8:70:ARG:NH1	83:Ax:46:U:H5'	2.33	0.43
9:8:191:ARG:NE	50:f:135:LEU:HG	2.33	0.43
11:A:3038:U:H2'	11:A:3039:OMU:H6	1.99	0.43
48:u:74:LEU:HD23	48:u:79:ILE:HG12	2.01	0.43
59:AH:124:VAL:HG13	79:AA:1264:C:H1'	2.00	0.43
71:AV:120:ASP:HA	71:AV:122:GLN:HE21	1.84	0.43
79:AA:1117:A:H2'	79:AA:1118:A:H8	1.83	0.43
79:AA:1169:G:H2'	79:AA:1170:G:C8	2.52	0.43
85:AX:165:CYS:SG	85:AX:180:GLN:HG3	2.58	0.43
85:AX:329:LEU:HB3	85:AX:333:GLY:HA3	1.99	0.43
6:5:147:ILE:HG12	6:5:191:GLN:CD	2.43	0.43
11:A:2697:G:OP2	91:A:3302:SPD:H31	2.18	0.43
11:A:2805:A:H2'	11:A:2806:U:C6	2.53	0.43
16:I:154:LEU:HD12	16:I:164:MET:HE3	2.00	0.43
36:e:265:LYS:HD2	88:B:76:A:H5'	2.01	0.43
51:p:57:THR:HA	51:p:60:ARG:HE	1.84	0.43
56:AE:96:HIS:HB3	56:AE:99:THR:HG23	2.01	0.43
69:AT:32:VAL:HG22	69:AT:76:LEU:HD22	2.01	0.43
75:A1:198:TYR:CZ	75:A1:200:LYS:HA	2.53	0.43
79:AA:1122:A:H2'	79:AA:1123:C:C6	2.53	0.43
79:AA:1237:A:H1'	79:AA:1254:C:O2	2.19	0.43
79:AA:1332:A:H2'	79:AA:1333:G:O4'	2.19	0.43
85:AX:74:ASP:O	85:AX:78:VAL:HG12	2.18	0.43
11:A:2175:C:H2'	11:A:2176:C:C6	2.53	0.43
12:D:174:VAL:HG21	12:D:182:HIS:CE1	2.54	0.43
26:S:163:LYS:HB2	34:b:106:ASP:HB3	2.01	0.43
53:AB:180:ARG:HH21	55:AD:210:PRO:HB2	1.84	0.43
75:A1:45:GLU:HG3	77:Az:21:A:N7	2.34	0.43
79:AA:659:U:H2'	79:AA:660:C:C6	2.53	0.43
79:AA:730:A:N6	79:AA:744:A:H1'	2.34	0.43
79:AA:1039:A:H2'	79:AA:1040:U:O4'	2.19	0.43
79:AA:1581:G:H2'	79:AA:1583:MA6:OP2	2.18	0.43
85:AX:162:VAL:HG11	85:AX:267:ALA:HB1	1.99	0.43
1:0:96:ASN:ND2	11:A:2709:A:H1'	2.34	0.43
7:6:273:PHE:HB3	7:6:311:MET:HG2	2.00	0.43
11:A:1778:U:H2'	11:A:1779:A:C8	2.54	0.43
11:A:1970:G:H2'	11:A:1971:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2365:U:H2'	11:A:2366:G:H8	1.84	0.43
34:b:133:PHE:HE2	49:c:269:LEU:HD23	1.83	0.43
41:k:78:GLY:HA2	41:k:81:LEU:HB2	2.00	0.43
55:AD:245:VAL:HG22	55:AD:271:ALA:HB1	2.00	0.43
62:AL:115:ILE:HG21	62:AL:181:ILE:HD13	2.01	0.43
71:AV:149:ASP:HA	71:AV:152:ILE:HG22	2.01	0.43
75:A1:286:THR:HG23	75:A1:289:ILE:H	1.83	0.43
79:AA:675:A:H2'	79:AA:676:G:H8	1.83	0.43
79:AA:685:A:H2'	79:AA:686:A:H8	1.84	0.43
79:AA:715:G:H2'	79:AA:716:U:H6	1.84	0.43
79:AA:736:C:H2'	79:AA:737:C:H5	1.84	0.43
79:AA:1362:G:H2'	79:AA:1363:C:C6	2.54	0.43
85:AX:125:LEU:HD11	85:AX:310:LEU:HG	2.00	0.43
11:A:2661:U:H4'	11:A:3160:A:O2'	2.19	0.43
35:d:207:ASN:HA	35:d:253:THR:HG21	2.00	0.43
52:s:65:ARG:O	52:s:69:THR:HG23	2.19	0.43
58:AG:360:GLU:HA	58:AG:363:TRP:CD1	2.54	0.43
79:AA:842:C:H2'	79:AA:843:G:C8	2.54	0.43
79:AA:1195:U:H2'	79:AA:1196:A:H8	1.84	0.43
79:AA:1279:C:H2'	79:AA:1280:C:H6	1.83	0.43
11:A:2245:A:H4'	11:A:2246:A:OP1	2.18	0.42
11:A:2677:A:H2'	11:A:2678:A:C8	2.54	0.42
11:A:2728:C:H2'	11:A:2729:U:H6	1.83	0.42
11:A:3153:U:H2'	11:A:3154:U:C6	2.53	0.42
26:S:173:ARG:HB2	26:S:182:LYS:HG3	2.00	0.42
35:d:122:ILE:O	35:d:126:LYS:HG2	2.19	0.42
36:e:98:LEU:HG	36:e:101:LYS:HE3	2.01	0.42
52:s:332:LEU:HD13	52:s:372:TYR:HB2	2.00	0.42
58:AG:92:MET:HG3	75:A1:116:PRO:HD2	2.00	0.42
71:AV:126:LEU:O	71:AV:130:VAL:HG23	2.19	0.42
71:AV:190:LEU:HD11	71:AV:226:TYR:CE1	2.54	0.42
79:AA:1067:A:H2'	79:AA:1068:A:O4'	2.19	0.42
79:AA:1487:C:C2	79:AA:1488:5MC:HM52	2.54	0.42
79:AA:1572:A:H2'	79:AA:1573:A:C8	2.53	0.42
11:A:3142:A:H2'	11:A:3143:U:C6	2.54	0.42
35:d:121:SER:O	35:d:125:ILE:HG13	2.19	0.42
43:m:120:ARG:HG3	43:m:123:TRP:CE2	2.54	0.42
46:q:117:ARG:O	46:q:121:ILE:HG12	2.19	0.42
66:AP:77:VAL:HG13	66:AP:120:MET:HB2	2.00	0.42
79:AA:865:A:H2'	79:AA:866:A:C8	2.55	0.42
79:AA:1591:C:H5''	87:AQ:52:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:OX:390:GLU:HB3	81:OX:394:ARG:HH21	1.84	0.42
88:B:40:U:H2'	88:B:41:A:C8	2.54	0.42
9:8:164:ARG:HG3	50:f:88:TYR:CE1	2.54	0.42
11:A:1719:G:H2'	11:A:1720:C:H6	1.83	0.42
11:A:2027:A:H2'	11:A:2028:G:O4'	2.19	0.42
11:A:2603:C:C2	11:A:2604:A:C8	3.08	0.42
13:E:340:PRO:HB2	24:Q:101:GLU:HB3	2.00	0.42
15:H:59:TRP:HE1	15:H:81:LYS:HB3	1.83	0.42
16:I:143:LEU:HD11	16:I:180:CYS:HB2	2.02	0.42
36:e:265:LYS:CD	88:B:76:A:H5'	2.50	0.42
46:q:176:GLN:HA	46:q:179:LEU:HG	2.00	0.42
55:AD:380:LEU:HD22	67:AR:91:PHE:HB2	2.01	0.42
60:AJ:72:LYS:HG3	79:AA:1557:A:H5''	2.01	0.42
75:A1:67:PRO:HG3	75:A1:118:ALA:HB2	2.01	0.42
79:AA:844:A:H2'	79:AA:845:A:O4'	2.20	0.42
84:A4:438:LEU:O	84:A4:441:THR:HG22	2.20	0.42
84:A4:646:THR:HG23	84:A4:650:MET:HE3	2.01	0.42
9:8:136:ILE:HD11	50:f:169:ILE:CG2	2.49	0.42
11:A:1805:A:H5'	33:V:96:ARG:HD2	2.01	0.42
15:H:207:LYS:HB3	15:H:222:GLU:O	2.20	0.42
21:N:104:MET:HE3	21:N:104:MET:HB3	1.94	0.42
35:d:86:ASP:HB3	35:d:196:GLN:HE22	1.84	0.42
54:AC:88:GLU:HG2	54:AC:147:TYR:CE1	2.54	0.42
57:AF:200:LEU:HB3	57:AF:202:PRO:HD2	2.01	0.42
72:AW:149:LEU:HD11	72:AW:166:ASN:HB2	2.00	0.42
73:AZ:14:LEU:O	73:AZ:18:LEU:HG	2.20	0.42
79:AA:983:C:H2'	79:AA:984:C:C6	2.54	0.42
79:AA:1510:U:H2'	79:AA:1511:C:C6	2.53	0.42
84:A4:259:TYR:CG	84:A4:282:LEU:HD13	2.54	0.42
2:1:18:VAL:HG12	2:1:61:LYS:HA	2.00	0.42
4:3:127:ALA:HA	20:M:79:PRO:HD3	2.02	0.42
8:7:163:MET:H	8:7:186:ASP:HB2	1.85	0.42
9:8:181:PRO:HB3	43:m:60:ASP:HB2	2.01	0.42
12:D:257:ILE:O	12:D:262:ARG:HD2	2.20	0.42
15:H:248:TYR:CD2	15:H:252:LEU:HD23	2.53	0.42
67:AR:79:LEU:HD23	67:AR:79:LEU:HA	1.92	0.42
71:AV:278:GLU:CD	71:AV:352:LEU:HD23	2.45	0.42
79:AA:1047:A:C5	79:AA:1158:U:H4'	2.54	0.42
79:AA:1057:G:H4'	79:AA:1578:A:H4'	2.01	0.42
79:AA:1408:A:H2'	79:AA:1409:A:C8	2.53	0.42
79:AA:1555:A:H2'	79:AA:1556:C:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2072:A:H2'	11:A:2073:A:C8	2.54	0.42
36:e:118:GLN:HG2	85:AX:213:ARG:HH12	1.83	0.42
36:e:124:TRP:CE2	43:m:72:ARG:HG2	2.54	0.42
46:q:186:GLU:HA	46:q:189:ARG:HD2	2.01	0.42
61:AK:35:TRP:CE2	61:AK:39:LYS:HD2	2.55	0.42
79:AA:1076:5MU:H2'	79:AA:1076:5MU:O2	2.19	0.42
79:AA:1204:C:H2'	79:AA:1205:U:O4'	2.19	0.42
79:AA:1207:U:H2'	79:AA:1208:U:H6	1.85	0.42
11:A:1861:U:H2'	11:A:1862:U:C6	2.54	0.42
35:d:246:VAL:HG12	35:d:264:LYS:HG2	2.00	0.42
63:AM:115:ALA:HA	63:AM:118:VAL:HG12	2.02	0.42
68:AS:134:ARG:HG2	68:AS:136:GLY:H	1.84	0.42
72:AW:145:LEU:HD11	72:AW:168:VAL:HG23	2.02	0.42
74:A0:11:ILE:HD12	79:AA:806:C:C4	2.54	0.42
74:A0:167:PRO:HG2	74:A0:170:LEU:HB2	2.02	0.42
79:AA:667:U:H2'	79:AA:668:U:C6	2.55	0.42
79:AA:1191:C:H2'	79:AA:1192:C:C6	2.55	0.42
82:a:44:ASN:O	82:a:65:VAL:HG22	2.20	0.42
84:A4:61:LYS:HA	84:A4:61:LYS:HD3	1.77	0.42
84:A4:247:ILE:O	84:A4:251:MET:HG2	2.19	0.42
84:A4:377:ARG:NH2	84:A4:418:SER:HA	2.35	0.42
88:B:29:C:C2	88:B:30:A:C8	3.07	0.42
11:A:1718:A:H2'	11:A:1719:G:O4'	2.19	0.42
11:A:1982:G:H2'	11:A:1983:U:C6	2.54	0.42
11:A:2286:A:H2'	11:A:2287:U:C6	2.55	0.42
11:A:2398:A:H2'	11:A:2399:A:O4'	2.20	0.42
11:A:2699:C:H2'	11:A:2700:G:H8	1.83	0.42
35:d:93:GLY:CA	35:d:96:ARG:HB3	2.50	0.42
50:f:166:PHE:O	50:f:169:ILE:HB	2.19	0.42
52:s:105:TRP:CD2	52:s:271:LEU:HD13	2.55	0.42
79:AA:958:C:H4'	79:AA:959:C:O4'	2.19	0.42
83:Ax:5:A:H2	83:Ax:63:G:H22	1.68	0.42
11:A:2045:A:H2'	11:A:2046:C:H6	1.85	0.42
12:D:184:LEU:HD22	12:D:216:LEU:HD13	2.01	0.42
27:T:186:ALA:HB2	82:a:108:MET:HG3	2.02	0.42
55:AD:140:LEU:HB2	55:AD:158:ALA:HB3	2.02	0.42
57:AF:171:PRO:HB3	57:AF:230:ALA:HB1	2.02	0.42
59:AH:74:LYS:HB2	59:AH:177:LEU:HG	2.02	0.42
62:AL:209:LEU:HD12	76:A3:189:TRP:CE2	2.55	0.42
65:AO:110:ASP:HB3	65:AO:113:LEU:HD12	2.01	0.42
65:AO:123:LEU:HD13	65:AO:154:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:1156:C:H2'	79:AA:1157:U:C6	2.55	0.42
79:AA:1180:U:H2'	79:AA:1181:G:C8	2.54	0.42
81:OX:427:LYS:HD2	81:OX:427:LYS:HA	1.91	0.42
11:A:1895:C:H2'	11:A:1896:U:C6	2.54	0.42
11:A:3191:A:H4'	47:r:123:HIS:HB3	2.01	0.42
14:F:96:LEU:HD23	14:F:96:LEU:HA	1.89	0.42
33:V:93:THR:HG22	33:V:112:GLU:HG3	2.02	0.42
36:e:160:LEU:HD23	36:e:160:LEU:HA	1.91	0.42
58:AG:72:ASP:O	58:AG:76:LYS:HG2	2.20	0.42
67:AR:78:ILE:O	67:AR:82:MET:HG3	2.20	0.42
70:AU:64:ARG:NH2	79:AA:845:A:H5'	2.35	0.42
71:AV:263:MET:HE1	71:AV:334:PHE:CD1	2.55	0.42
79:AA:693:A:H2'	79:AA:694:C:O4'	2.20	0.42
79:AA:746:A:H3'	93:AA:1727:MG:MG	1.45	0.42
79:AA:797:C:H2'	79:AA:798:C:C6	2.55	0.42
79:AA:1188:A:H5''	79:AA:1429:C:OP2	2.20	0.42
79:AA:1503:G:H2'	79:AA:1504:U:C6	2.54	0.42
84:A4:65:TRP:HD1	84:A4:66:ASP:O	2.03	0.42
8:7:202:PHE:HB3	8:7:280:VAL:HG21	2.02	0.41
9:8:179:THR:OG1	43:m:63:THR:HG22	2.20	0.41
11:A:1690:C:H2'	11:A:1691:C:C6	2.55	0.41
11:A:1810:A:H2'	11:A:1811:A:O4'	2.20	0.41
11:A:2415:C:H3'	52:s:165:ARG:NH2	2.35	0.41
15:H:218:GLU:HA	15:H:235:MET:O	2.19	0.41
59:AH:123:SER:HB2	79:AA:1265:C:O2'	2.20	0.41
62:AL:214:PHE:O	62:AL:218:GLN:HG2	2.20	0.41
71:AV:228:TYR:HB3	71:AV:259:ALA:HB2	2.02	0.41
79:AA:694:C:OP2	79:AA:814:A:H4'	2.20	0.41
79:AA:1035:U:H2'	79:AA:1036:A:C8	2.54	0.41
79:AA:1209:C:H2'	79:AA:1210:U:H6	1.84	0.41
83:Ax:60:C:H2'	83:Ax:61:C:C6	2.55	0.41
84:A4:298:ILE:HA	84:A4:319:LEU:HD13	2.02	0.41
7:6:219:THR:HG22	7:6:233:LEU:HA	2.02	0.41
7:6:304:TYR:CE1	7:6:313:PRO:HD3	2.55	0.41
21:N:183:LEU:HD23	21:N:183:LEU:HA	1.83	0.41
36:e:97:ARG:HA	36:e:100:LYS:HG2	2.01	0.41
41:k:73:ARG:HH21	41:k:75:ILE:HD11	1.85	0.41
54:AC:125:ARG:NH1	84:A4:94:TYR:HB2	2.35	0.41
59:AH:113:ARG:NH2	79:AA:1310:C:H5''	2.35	0.41
63:AM:34:ILE:HG12	63:AM:87:MET:HE1	2.01	0.41
67:AR:135:ARG:CZ	67:AR:186:TRP:HB3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:1527:A:H2'	79:AA:1528:A:O4'	2.20	0.41
11:A:3118:U:H2'	11:A:3119:C:H6	1.85	0.41
11:A:3143:U:H2'	11:A:3144:A:C8	2.55	0.41
26:S:156:VAL:HG22	26:S:198:ILE:HG12	2.02	0.41
52:s:119:PRO:HG3	52:s:394:TRP:CD2	2.55	0.41
59:AH:78:VAL:HB	59:AH:143:LEU:HB2	2.02	0.41
59:AH:113:ARG:HH22	79:AA:1310:C:H5''	1.85	0.41
72:AW:110:ASN:O	72:AW:126:ARG:HB2	2.21	0.41
79:AA:795:A:H3'	79:AA:796:G:O4'	2.20	0.41
79:AA:834:G:H2'	79:AA:835:C:O4'	2.20	0.41
79:AA:1185:C:H2'	79:AA:1186:A:C8	2.55	0.41
6:5:115:GLU:HB2	6:5:119:GLN:HB2	2.02	0.41
11:A:1860:A:H2'	11:A:1861:U:C6	2.55	0.41
11:A:1906:G:H2'	11:A:2014:A:H61	1.84	0.41
46:q:138:GLN:O	46:q:141:GLU:HG3	2.21	0.41
69:AT:88:VAL:HG22	70:AU:109:ASN:HD21	1.84	0.41
79:AA:825:U:H2'	79:AA:827:A:OP2	2.20	0.41
79:AA:862:A:H2'	79:AA:863:C:H6	1.85	0.41
79:AA:1279:C:H2'	79:AA:1280:C:C6	2.55	0.41
85:AX:168:LEU:HD21	85:AX:274:LEU:HD12	2.02	0.41
11:A:1985:G:C5	11:A:2004:G:C8	3.09	0.41
11:A:2109:A:C6	11:A:2111:C:C2	3.08	0.41
11:A:2176:C:H2'	11:A:2177:U:O4'	2.20	0.41
11:A:2239:A:H2'	11:A:2240:C:C6	2.55	0.41
11:A:2656:U:H4'	13:E:230:THR:OG1	2.20	0.41
11:A:3117:C:H2'	11:A:3118:U:H6	1.84	0.41
35:d:129:ASP:OD2	35:d:132:PHE:HB2	2.20	0.41
46:q:195:GLN:HB3	46:q:199:LYS:NZ	2.36	0.41
55:AD:100:LYS:HG2	79:AA:1262:C:H4'	2.03	0.41
67:AR:284:LEU:HG	67:AR:288:GLN:NE2	2.35	0.41
71:AV:241:ARG:O	71:AV:245:HIS:HB2	2.20	0.41
79:AA:680:U:H2'	79:AA:681:U:C6	2.55	0.41
79:AA:1322:C:H2'	79:AA:1323:G:O4'	2.19	0.41
2:1:38:ARG:HH12	2:1:41:LEU:HD11	1.86	0.41
6:5:165:GLN:NE2	6:5:179:VAL:HG21	2.35	0.41
8:7:277:GLN:O	8:7:301:SER:HA	2.20	0.41
11:A:2092:C:H2'	11:A:2093:U:C6	2.56	0.41
11:A:2215:C:H2'	11:A:2216:A:O4'	2.20	0.41
11:A:2664:U:H2'	11:A:2665:U:H6	1.86	0.41
11:A:3170:C:N4	11:A:3171:C:H41	2.18	0.41
16:I:140:TYR:HB3	16:I:143:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:47:GLY:HA2	19:L:77:ILE:HD11	2.03	0.41
28:U:129:MET:O	28:U:132:GLU:HG3	2.21	0.41
49:c:228:LEU:HB2	49:c:307:PHE:HD2	1.79	0.41
57:AF:48:LYS:O	57:AF:52:ARG:HG2	2.20	0.41
59:AH:51:HIS:HE1	84:A4:476:LYS:HG3	1.86	0.41
59:AH:180:LEU:HD12	59:AH:184:ILE:HG21	2.03	0.41
72:AW:131:GLY:HA2	72:AW:134:TYR:HD1	1.86	0.41
77:Az:28:U:H1'	84:A4:414:LYS:HG2	2.02	0.41
79:AA:734:C:O5'	79:AA:735:A:H5''	2.20	0.41
79:AA:1530:A:H2'	79:AA:1531:C:O4'	2.21	0.41
11:A:1834:U:C4	27:T:200:ARG:HA	2.55	0.41
91:A:3471:SPD:H22	91:A:3471:SPD:H51	1.88	0.41
33:V:138:THR:HG23	33:V:140:ALA:N	2.36	0.41
46:q:152:ARG:O	46:q:156:LEU:HG	2.20	0.41
55:AD:206:PRO:HA	55:AD:272:LYS:HD2	2.02	0.41
71:AV:100:ASN:OD1	79:AA:1523:A:H4'	2.21	0.41
71:AV:152:ILE:HD12	71:AV:185:VAL:HG22	2.02	0.41
79:AA:753:A:H2'	79:AA:754:A:C8	2.54	0.41
79:AA:1148:A:H2'	79:AA:1149:G:C8	2.55	0.41
79:AA:1489:G:H2'	79:AA:1490:U:H6	1.85	0.41
79:AA:1500:C:H2'	79:AA:1501:A:O4'	2.21	0.41
79:AA:1523:A:H2'	79:AA:1524:A:C8	2.55	0.41
88:B:49:U:H2'	88:B:50:U:C6	2.55	0.41
6:5:125:LYS:HA	6:5:253:LEU:HD11	2.03	0.41
11:A:2671:C:H2'	11:A:2672:A:H8	1.85	0.41
11:A:2688:C:H2'	11:A:2689:C:C6	2.55	0.41
16:I:49:ALA:HB1	45:o:32:LYS:HE3	2.02	0.41
16:I:61:HIS:CD2	16:I:62:PRO:HD2	2.56	0.41
22:O:50:ASP:HB2	22:O:107:MET:HE1	2.03	0.41
56:AE:3:ARG:HB2	56:AE:69:TYR:CE2	2.55	0.41
59:AH:72:LEU:HD12	75:A1:133:TRP:CZ3	2.55	0.41
65:AO:94:CYS:HB2	65:AO:108:CYS:SG	2.61	0.41
67:AR:213:GLU:HG2	67:AR:214:ASN:N	2.36	0.41
70:AU:71:ARG:O	70:AU:75:VAL:HG23	2.21	0.41
79:AA:700:A:H4'	79:AA:701:G:O5'	2.20	0.41
79:AA:1595:G:H2'	79:AA:1596:A:C8	2.56	0.41
81:OX:399:GLN:NE2	81:OX:401:PHE:HD1	2.18	0.41
2:l:55:LEU:H	46:q:128:MET:HE2	1.86	0.41
11:A:1935:A:H2'	11:A:1936:A:O4'	2.20	0.41
11:A:2192:A:O2'	17:J:135:VAL:HG11	2.21	0.41
11:A:2664:U:H2'	11:A:2665:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2747:U:H2'	11:A:2748:A:H8	1.85	0.41
12:D:109:PHE:HB3	12:D:204:ALA:HB3	2.03	0.41
15:H:182:TRP:HZ3	15:H:213:ILE:HG22	1.86	0.41
30:X:166:LEU:HD13	30:X:196:ILE:HD11	2.03	0.41
35:d:160:LEU:O	35:d:164:VAL:HG22	2.21	0.41
39:i:38:LEU:HD23	39:i:38:LEU:HA	1.96	0.41
59:AH:181:PRO:HD2	59:AH:184:ILE:HG21	2.03	0.41
75:A1:71:PRO:HB3	84:A4:78:VAL:HG21	2.02	0.41
79:AA:702:C:H1'	79:AA:842:C:H1'	2.02	0.41
79:AA:1056:A:H4'	79:AA:1588:G:N2	2.36	0.41
84:A4:429:LEU:HA	84:A4:464:LEU:HD21	2.03	0.41
84:A4:623:SER:OG	84:A4:626:GLN:HB2	2.21	0.41
11:A:2129:G:O4'	11:A:2152:A:H2	2.05	0.41
11:A:2404:U:H2'	11:A:2405:C:C6	2.56	0.41
11:A:2459:A:C4	11:A:2460:A:C8	3.09	0.41
11:A:2474:C:H2'	11:A:2475:U:O4'	2.21	0.41
11:A:3212:C:H2'	11:A:3213:A:O4'	2.21	0.41
21:N:121:ILE:HG13	21:N:162:GLU:HB3	2.02	0.41
24:Q:188:LEU:HD23	24:Q:188:LEU:HA	1.91	0.41
26:S:96:PHE:HB3	34:b:126:ILE:HD13	2.03	0.41
28:U:21:ARG:NH1	31:Y:146:VAL:HG11	2.36	0.41
47:r:136:PRO:HG2	47:r:139:VAL:HG21	2.02	0.41
57:AF:129:ALA:HB1	57:AF:133:GLU:HB2	2.02	0.41
79:AA:886:C:H2'	79:AA:887:G:C8	2.56	0.41
79:AA:982:A:H2'	79:AA:983:C:C6	2.56	0.41
6:5:215:ARG:HD2	6:5:364:LEU:O	2.21	0.40
11:A:2815:OMG:H1'	11:A:2815:OMG:HM23	1.79	0.40
28:U:131:GLU:O	28:U:134:ARG:HG3	2.20	0.40
35:d:115:THR:O	35:d:119:GLN:HG2	2.22	0.40
43:m:58:LYS:HZ1	43:m:64:ILE:HG23	1.85	0.40
50:f:190:THR:HG23	50:f:192:GLU:HG3	2.02	0.40
54:AC:98:GLY:HA3	73:AZ:71:TYR:CE1	2.56	0.40
56:AE:6:LEU:HB3	56:AE:66:VAL:HB	2.03	0.40
57:AF:240:ARG:NH1	86:A2:44:THR:H	2.19	0.40
65:AO:179:THR:HG23	67:AR:186:TRP:HZ2	1.86	0.40
68:AS:111:GLU:HG3	68:AS:117:LEU:HD13	2.03	0.40
79:AA:664:G:H2'	79:AA:665:C:C6	2.56	0.40
79:AA:764:A:H4'	79:AA:765:C:O4'	2.21	0.40
79:AA:917:C:H2'	79:AA:918:A:C8	2.56	0.40
79:AA:1130:G:H2'	79:AA:1131:C:C6	2.56	0.40
84:A4:99:SER:H	84:A4:102:GLU:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:A4:266:MET:HB3	84:A4:275:ALA:HB2	2.03	0.40
11:A:2753:A:C4	11:A:2754:A:C8	3.10	0.40
16:I:188:ARG:O	16:I:192:ILE:HD12	2.21	0.40
17:J:66:LEU:HD12	17:J:66:LEU:HA	1.95	0.40
21:N:172:VAL:HA	21:N:175:PHE:CE2	2.57	0.40
46:q:178:LEU:O	46:q:182:LEU:HG	2.21	0.40
65:AO:97:ARG:HH12	79:AA:870:C:H3'	1.86	0.40
79:AA:845:A:H2'	79:AA:846:A:C8	2.55	0.40
79:AA:868:C:H2'	79:AA:869:C:C6	2.56	0.40
79:AA:1377:C:H5''	85:AX:320:ARG:HD3	2.01	0.40
84:A4:126:LYS:HA	84:A4:129:GLN:HG2	2.03	0.40
85:AX:127:TYR:CZ	85:AX:344:LEU:HB2	2.55	0.40
7:6:106:ARG:HG2	23:P:110:TRP:CE2	2.57	0.40
11:A:2051:A:H2'	11:A:2052:A:C8	2.57	0.40
11:A:2479:C:C2	11:A:2480:A:C8	3.10	0.40
11:A:2728:C:H2'	11:A:2729:U:C6	2.56	0.40
12:D:111:ARG:HD2	12:D:111:ARG:HA	1.97	0.40
35:d:186:VAL:HG23	35:d:220:GLN:HA	2.04	0.40
52:s:105:TRP:CG	52:s:271:LEU:HD13	2.56	0.40
52:s:177:LEU:HD12	52:s:177:LEU:HA	1.92	0.40
57:AF:118:VAL:HG13	57:AF:210:LEU:HD21	2.02	0.40
58:AG:357:THR:HG23	58:AG:360:GLU:H	1.86	0.40
79:AA:1485:G:H2'	79:AA:1486:B8T:O4'	2.21	0.40
84:A4:646:THR:O	84:A4:650:MET:HG2	2.21	0.40
8:7:209:LEU:HD12	8:7:212:LYS:HE3	2.02	0.40
10:9:118:GLY:HA3	33:V:191:LEU:HD12	2.04	0.40
11:A:1912:A:H2'	11:A:1913:G:C8	2.56	0.40
11:A:2556:A:C2	11:A:2560:G:C6	3.09	0.40
11:A:3150:U:C2	11:A:3151:A:C8	3.09	0.40
16:I:144:LEU:HD12	16:I:144:LEU:HA	1.91	0.40
28:U:112:PRO:N	28:U:113:GLU:HA	2.36	0.40
37:g:138:THR:HG22	37:g:149:ILE:HG12	2.03	0.40
59:AH:130:HIS:CG	79:AA:1266:A:H5''	2.56	0.40
65:AO:136:TYR:HD1	65:AO:138:PRO:HD2	1.86	0.40
79:AA:1148:A:H2'	79:AA:1149:G:H8	1.86	0.40
79:AA:1441:A:H2'	79:AA:1442:G:O4'	2.21	0.40
79:AA:1462:G:H2'	79:AA:1463:G:C8	2.55	0.40
84:A4:352:PRO:O	84:A4:355:GLN:HG3	2.20	0.40
18:K:70:ASN:O	18:K:74:GLN:HG3	2.22	0.40
28:U:81:ASP:HB3	28:U:87:ILE:HD11	2.02	0.40
30:X:42:HIS:CG	30:X:86:ILE:HD11	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:f:203:GLU:HG2	50:f:204:LEU:N	2.36	0.40
52:s:152:GLN:HA	52:s:156:TYR:HB2	2.02	0.40
71:AV:364:LEU:HA	71:AV:367:CYS:SG	2.62	0.40
79:AA:776:A:H4'	79:AA:777:G:H5'	2.03	0.40
79:AA:1069:A:H3'	79:AA:1070:C:H6	1.86	0.40
79:AA:1357:A:H2'	79:AA:1358:A:C8	2.57	0.40
79:AA:1545:U:H2'	79:AA:1546:A:C8	2.56	0.40
84:A4:349:ALA:HB3	84:A4:378:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
2	1	54/65 (83%)	54 (100%)	0	0	100	100
3	2	44/92 (48%)	44 (100%)	0	0	100	100
4	3	93/188 (50%)	93 (100%)	0	0	100	100
5	4	36/103 (35%)	36 (100%)	0	0	100	100
6	5	392/423 (93%)	385 (98%)	7 (2%)	0	100	100
7	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
8	7	292/338 (86%)	284 (97%)	8 (3%)	0	100	100
9	8	155/206 (75%)	153 (99%)	2 (1%)	0	100	100
10	9	122/137 (89%)	117 (96%)	5 (4%)	0	100	100
12	D	236/305 (77%)	228 (97%)	8 (3%)	0	100	100
13	E	303/348 (87%)	296 (98%)	7 (2%)	0	100	100
14	F	250/311 (80%)	246 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	H	200/267 (75%)	194 (97%)	6 (3%)	0	100	100
16	I	179/261 (69%)	176 (98%)	3 (2%)	0	100	100
17	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
18	K	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
19	L	113/145 (78%)	110 (97%)	3 (3%)	0	100	100
20	M	289/296 (98%)	284 (98%)	5 (2%)	0	100	100
21	N	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
22	O	152/175 (87%)	148 (97%)	4 (3%)	0	100	100
23	P	142/180 (79%)	141 (99%)	1 (1%)	0	100	100
24	Q	237/292 (81%)	233 (98%)	4 (2%)	0	100	100
25	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
26	S	159/205 (78%)	159 (100%)	0	0	100	100
27	T	164/206 (80%)	161 (98%)	3 (2%)	0	100	100
28	U	150/153 (98%)	146 (97%)	4 (3%)	0	100	100
29	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
30	X	242/256 (94%)	239 (99%)	3 (1%)	0	100	100
31	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
32	Z	120/161 (74%)	118 (98%)	2 (2%)	0	100	100
33	V	203/216 (94%)	203 (100%)	0	0	100	100
34	b	148/215 (69%)	142 (96%)	6 (4%)	0	100	100
35	d	257/306 (84%)	238 (93%)	19 (7%)	0	100	100
36	e	236/279 (85%)	229 (97%)	7 (3%)	0	100	100
37	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
38	h	108/158 (68%)	102 (94%)	6 (6%)	0	100	100
39	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
40	j	92/123 (75%)	89 (97%)	3 (3%)	0	100	100
41	k	100/112 (89%)	99 (99%)	1 (1%)	0	100	100
42	l	80/138 (58%)	78 (98%)	2 (2%)	0	100	100
43	m	90/128 (70%)	87 (97%)	3 (3%)	0	100	100
45	o	92/102 (90%)	91 (99%)	1 (1%)	0	100	100
46	q	175/222 (79%)	175 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	r	160/196 (82%)	157 (98%)	3 (2%)	0	100	100
48	t	44/198 (22%)	44 (100%)	0	0	100	100
48	u	30/198 (15%)	30 (100%)	0	0	100	100
49	c	282/332 (85%)	278 (99%)	4 (1%)	0	100	100
50	f	153/212 (72%)	147 (96%)	6 (4%)	0	100	100
51	p	141/206 (68%)	137 (97%)	4 (3%)	0	100	100
52	s	381/439 (87%)	375 (98%)	6 (2%)	0	100	100
53	AB	223/296 (75%)	218 (98%)	5 (2%)	0	100	100
54	AC	130/167 (78%)	128 (98%)	2 (2%)	0	100	100
55	AD	341/430 (79%)	334 (98%)	7 (2%)	0	100	100
56	AE	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
57	AF	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
58	AG	323/396 (82%)	315 (98%)	8 (2%)	0	100	100
59	AH	138/201 (69%)	133 (96%)	4 (3%)	1 (1%)	18	49
60	AJ	106/138 (77%)	103 (97%)	3 (3%)	0	100	100
61	AK	99/128 (77%)	99 (100%)	0	0	100	100
62	AL	172/257 (67%)	169 (98%)	3 (2%)	0	100	100
63	AM	117/137 (85%)	115 (98%)	2 (2%)	0	100	100
64	AN	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
65	AO	191/258 (74%)	186 (97%)	5 (3%)	0	100	100
66	AP	95/142 (67%)	95 (100%)	0	0	100	100
67	AR	293/360 (81%)	285 (97%)	8 (3%)	0	100	100
68	AS	133/190 (70%)	133 (100%)	0	0	100	100
69	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
70	AU	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
71	AV	358/414 (86%)	346 (97%)	12 (3%)	0	100	100
72	AW	98/187 (52%)	96 (98%)	2 (2%)	0	100	100
73	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
74	A0	213/217 (98%)	208 (98%)	5 (2%)	0	100	100
75	A1	277/323 (86%)	264 (95%)	13 (5%)	0	100	100
76	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	AY	117/395 (30%)	115 (98%)	2 (2%)	0	100	100
80	AI	135/194 (70%)	128 (95%)	7 (5%)	0	100	100
81	OX	51/435 (12%)	47 (92%)	4 (8%)	0	100	100
82	a	99/142 (70%)	97 (98%)	2 (2%)	0	100	100
84	A4	584/689 (85%)	566 (97%)	18 (3%)	0	100	100
85	AX	350/398 (88%)	336 (96%)	14 (4%)	0	100	100
86	A2	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
87	AQ	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
All	All	14367/18802 (76%)	14047 (98%)	319 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
59	AH	126	ILE

### 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	
1	0	99/164 (60%)	99 (100%)	0	100	100
2	1	53/60 (88%)	53 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	270/303 (89%)	270 (100%)	0	100	100
9	8	146/190 (77%)	146 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	D	192/245 (78%)	192 (100%)	0	100	100
13	E	260/290 (90%)	260 (100%)	0	100	100
14	F	219/262 (84%)	219 (100%)	0	100	100
15	H	182/228 (80%)	182 (100%)	0	100	100
16	I	165/232 (71%)	165 (100%)	0	100	100
17	J	138/150 (92%)	138 (100%)	0	100	100
18	K	155/155 (100%)	155 (100%)	0	100	100
19	L	98/124 (79%)	98 (100%)	0	100	100
20	M	246/249 (99%)	246 (100%)	0	100	100
21	N	189/211 (90%)	189 (100%)	0	100	100
22	O	134/150 (89%)	134 (100%)	0	100	100
23	P	126/155 (81%)	126 (100%)	0	100	100
24	Q	221/256 (86%)	221 (100%)	0	100	100
25	R	118/126 (94%)	118 (100%)	0	100	100
26	S	146/180 (81%)	146 (100%)	0	100	100
27	T	146/176 (83%)	146 (100%)	0	100	100
28	U	134/135 (99%)	134 (100%)	0	100	100
29	W	94/119 (79%)	94 (100%)	0	100	100
30	X	220/229 (96%)	220 (100%)	0	100	100
31	Y	163/223 (73%)	163 (100%)	0	100	100
32	Z	113/147 (77%)	113 (100%)	0	100	100
33	V	183/191 (96%)	183 (100%)	0	100	100
34	b	132/186 (71%)	132 (100%)	0	100	100
35	d	237/274 (86%)	237 (100%)	0	100	100
36	e	207/236 (88%)	207 (100%)	0	100	100
37	g	124/148 (84%)	124 (100%)	0	100	100
38	h	104/148 (70%)	104 (100%)	0	100	100
39	i	86/110 (78%)	86 (100%)	0	100	100
40	j	74/97 (76%)	74 (100%)	0	100	100
41	k	83/89 (93%)	83 (100%)	0	100	100
42	l	76/116 (66%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	m	85/113 (75%)	85 (100%)	0	100	100
45	o	80/87 (92%)	80 (100%)	0	100	100
46	q	153/178 (86%)	153 (100%)	0	100	100
47	r	147/169 (87%)	147 (100%)	0	100	100
48	t	40/158 (25%)	40 (100%)	0	100	100
48	u	31/158 (20%)	31 (100%)	0	100	100
49	c	251/288 (87%)	251 (100%)	0	100	100
50	f	139/188 (74%)	139 (100%)	0	100	100
51	p	135/181 (75%)	135 (100%)	0	100	100
52	s	339/381 (89%)	339 (100%)	0	100	100
53	AB	198/249 (80%)	198 (100%)	0	100	100
54	AC	115/143 (80%)	115 (100%)	0	100	100
55	AD	286/357 (80%)	286 (100%)	0	100	100
56	AE	104/107 (97%)	104 (100%)	0	100	100
57	AF	185/209 (88%)	185 (100%)	0	100	100
58	AG	285/342 (83%)	285 (100%)	0	100	100
59	AH	130/180 (72%)	130 (100%)	0	100	100
60	AJ	93/118 (79%)	93 (100%)	0	100	100
61	AK	91/113 (80%)	91 (100%)	0	100	100
62	AL	158/226 (70%)	158 (100%)	0	100	100
63	AM	97/113 (86%)	97 (100%)	0	100	100
64	AN	96/115 (84%)	96 (100%)	0	100	100
65	AO	174/230 (76%)	173 (99%)	1 (1%)	78	80
66	AP	88/123 (72%)	88 (100%)	0	100	100
67	AR	264/318 (83%)	264 (100%)	0	100	100
68	AS	116/164 (71%)	116 (100%)	0	100	100
69	AT	153/157 (98%)	153 (100%)	0	100	100
70	AU	152/174 (87%)	152 (100%)	0	100	100
71	AV	325/364 (89%)	325 (100%)	0	100	100
72	AW	87/158 (55%)	87 (100%)	0	100	100
73	AZ	90/95 (95%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	A0	188/189 (100%)	188 (100%)	0	100	100
75	A1	257/291 (88%)	257 (100%)	0	100	100
76	A3	65/166 (39%)	65 (100%)	0	100	100
78	AY	110/357 (31%)	110 (100%)	0	100	100
80	AI	105/147 (71%)	105 (100%)	0	100	100
81	OX	49/372 (13%)	49 (100%)	0	100	100
82	a	99/133 (74%)	99 (100%)	0	100	100
84	A4	526/609 (86%)	526 (100%)	0	100	100
85	AX	311/351 (89%)	311 (100%)	0	100	100
86	A2	100/100 (100%)	100 (100%)	0	100	100
87	AQ	78/78 (100%)	78 (100%)	0	100	100
All	All	12843/16242 (79%)	12842 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
65	AO	154	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	170	ASN
6	5	186	GLN
6	5	195	HIS
6	5	251	HIS
7	6	332	HIS
8	7	111	GLN
8	7	231	GLN
8	7	287	GLN
9	8	103	GLN
9	8	186	GLN
13	E	88	HIS
13	E	123	GLN
14	F	103	GLN
16	I	36	HIS
16	I	119	HIS
17	J	186	GLN

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Mol	Chain	Res	Type
18	K	94	GLN
19	L	33	GLN
19	L	103	ASN
20	M	30	ASN
21	N	117	ASN
25	R	27	HIS
25	R	149	HIS
26	S	84	ASN
27	T	133	ASN
28	U	62	ASN
30	X	93	ASN
31	Y	88	GLN
31	Y	225	ASN
32	Z	100	HIS
34	b	123	ASN
35	d	59	HIS
35	d	77	HIS
35	d	205	GLN
36	e	248	ASN
36	e	251	HIS
37	g	155	GLN
38	h	118	HIS
39	i	120	HIS
41	k	93	HIS
42	l	125	ASN
46	q	139	GLN
46	q	167	GLN
47	r	109	GLN
49	c	192	GLN
50	f	136	GLN
52	s	107	GLN
52	s	152	GLN
52	s	387	ASN
52	s	420	GLN
53	AB	201	ASN
55	AD	130	GLN
55	AD	151	ASN
55	AD	196	ASN
55	AD	360	GLN
56	AE	56	GLN
58	AG	261	GLN
59	AH	163	ASN

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Mol	Chain	Res	Type
61	AK	55	ASN
61	AK	124	GLN
62	AL	77	GLN
62	AL	172	ASN
63	AM	28	ASN
65	AO	207	GLN
66	AP	71	HIS
66	AP	95	HIS
67	AR	224	HIS
67	AR	356	HIS
70	AU	65	GLN
71	AV	179	GLN
71	AV	238	GLN
71	AV	394	GLN
72	AW	135	GLN
74	A0	26	ASN
74	A0	145	HIS
75	A1	64	GLN
76	A3	139	ASN
76	A3	140	HIS
78	AY	378	ASN
80	AI	146	HIS
82	a	46	ASN
84	A4	233	GLN
84	A4	453	HIS
84	A4	656	ASN
85	AX	140	HIS
85	AX	190	ASN
85	AX	205	GLN
85	AX	291	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1556/1558 (99%)	254 (16%)	2 (0%)
77	Az	33/34 (97%)	14 (42%)	0
79	AA	953/954 (99%)	163 (17%)	2 (0%)
83	Ax	70/71 (98%)	16 (22%)	0
88	B	70/72 (97%)	15 (21%)	0
All	All	2682/2689 (99%)	462 (17%)	4 (0%)

All (462) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1681	G
11	A	1689	C
11	A	1692	A
11	A	1699	C
11	A	1700	U
11	A	1704	U
11	A	1708	A
11	A	1709	G
11	A	1711	C
11	A	1724	A
11	A	1727	A
11	A	1732	C
11	A	1736	A
11	A	1748	G
11	A	1750	G
11	A	1765	C
11	A	1777	A
11	A	1805	A
11	A	1807	U
11	A	1808	A
11	A	1817	C
11	A	1821	A
11	A	1827	C
11	A	1828	A
11	A	1832	A
11	A	1836	A
11	A	1844	A
11	A	1854	U
11	A	1856	A
11	A	1867	A
11	A	1869	A
11	A	1871	A
11	A	1873	A
11	A	1878	U
11	A	1882	A
11	A	1887	A
11	A	1888	G
11	A	1893	A
11	A	1901	C
11	A	1903	C
11	A	1909	A
11	A	1918	G
11	A	1937	A

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Mol	Chain	Res	Type
11	A	1939	G
11	A	1940	A
11	A	1944	C
11	A	1975	U
11	A	1985	G
11	A	1986	A
11	A	1993	A
11	A	1994	A
11	A	2001	C
11	A	2003	A
11	A	2015	G
11	A	2022	G
11	A	2030	U
11	A	2036	C
11	A	2037	U
11	A	2039	A
11	A	2054	U
11	A	2055	U
11	A	2060	A
11	A	2069	U
11	A	2071	U
11	A	2079	C
11	A	2099	U
11	A	2105	G
11	A	2111	C
11	A	2113	G
11	A	2125	C
11	A	2126	U
11	A	2147	G
11	A	2159	U
11	A	2160	A
11	A	2163	A
11	A	2168	U
11	A	2181	A
11	A	2185	G
11	A	2191	A
11	A	2192	A
11	A	2196	A
11	A	2198	A
11	A	2200	A
11	A	2214	A
11	A	2219	C

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Mol	Chain	Res	Type
11	A	2220	A
11	A	2221	C
11	A	2223	A
11	A	2225	C
11	A	2230	A
11	A	2232	A
11	A	2237	A
11	A	2241	A
11	A	2243	A
11	A	2245	A
11	A	2246	A
11	A	2262	C
11	A	2263	C
11	A	2284	C
11	A	2285	U
11	A	2297	A
11	A	2299	U
11	A	2300	G
11	A	2322	C
11	A	2331	C
11	A	2332	C
11	A	2345	G
11	A	2350	A
11	A	2353	A
11	A	2354	A
11	A	2357	C
11	A	2363	A
11	A	2372	U
11	A	2374	A
11	A	2379	C
11	A	2390	A
11	A	2399	A
11	A	2401	A
11	A	2404	U
11	A	2407	U
11	A	2414	C
11	A	2415	C
11	A	2446	A
11	A	2451	A
11	A	2458	A
11	A	2478	G
11	A	2485	U

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Mol	Chain	Res	Type
11	A	2493	C
11	A	2496	G
11	A	2504	A
11	A	2506	A
11	A	2520	C
11	A	2521	A
11	A	2527	A
11	A	2540	C
11	A	2557	C
11	A	2570	C
11	A	2592	G
11	A	2593	G
11	A	2594	U
11	A	2599	U
11	A	2600	A
11	A	2601	A
11	A	2603	C
11	A	2606	U
11	A	2618	U
11	A	2625	C
11	A	2627	G
11	A	2628	U
11	A	2630	U
11	A	2633	A
11	A	2635	G
11	A	2654	U
11	A	2655	G
11	A	2656	U
11	A	2683	C
11	A	2686	G
11	A	2694	A
11	A	2696	A
11	A	2706	A
11	A	2709	A
11	A	2718	C
11	A	2719	G
11	A	2723	A
11	A	2724	G
11	A	2725	A
11	A	2732	G
11	A	2745	A
11	A	2757	A

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Mol	Chain	Res	Type
11	A	2762	C
11	A	2763	U
11	A	2765	A
11	A	2767	A
11	A	2768	A
11	A	2782	A
11	A	2783	A
11	A	2786	U
11	A	2790	A
11	A	2810	G
11	A	2832	A
11	A	2833	A
11	A	2847	C
11	A	2864	U
11	A	2865	C
11	A	2883	A
11	A	2884	C
11	A	2885	U
11	A	2888	A
11	A	2889	C
11	A	2893	A
11	A	2913	A
11	A	2916	G
11	A	2917	G
11	A	2918	A
11	A	2919	A
11	A	2922	A
11	A	2928	C
11	A	2934	G
11	A	2935	A
11	A	2956	A
11	A	2962	C
11	A	2965	A
11	A	2971	A
11	A	2985	C
11	A	2989	G
11	A	2990	A
11	A	2992	G
11	A	2993	U
11	A	3000	A
11	A	3005	A
11	A	3007	C

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Mol	Chain	Res	Type
11	A	3016	G
11	A	3022	G
11	A	3041	U
11	A	3049	U
11	A	3053	A
11	A	3054	G
11	A	3060	C
11	A	3061	G
11	A	3065	U
11	A	3069	A
11	A	3089	A
11	A	3090	G
11	A	3096	U
11	A	3100	U
11	A	3102	U
11	A	3108	U
11	A	3109	U
11	A	3110	C
11	A	3111	A
11	A	3112	A
11	A	3124	U
11	A	3150	U
11	A	3157	C
11	A	3158	A
11	A	3162	C
11	A	3168	C
11	A	3169	C
11	A	3172	C
11	A	3173	G
11	A	3177	A
11	A	3183	U
11	A	3189	C
11	A	3190	A
11	A	3199	U
11	A	3200	U
11	A	3207	A
11	A	3209	A
11	A	3210	C
11	A	3212	C
11	A	3217	A
11	A	3218	A
11	A	3228	U

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Mol	Chain	Res	Type
11	A	3230	G
77	Az	0	U
77	Az	4	A
77	Az	11	U
77	Az	12	U
77	Az	13	U
77	Az	15	U
77	Az	18	A
77	Az	21	A
77	Az	22	A
77	Az	25	U
77	Az	26	A
77	Az	27	C
77	Az	30	A
77	Az	31	A
79	AA	651	A
79	AA	680	U
79	AA	687	G
79	AA	688	A
79	AA	694	C
79	AA	704	U
79	AA	721	U
79	AA	722	C
79	AA	737	C
79	AA	738	A
79	AA	746	A
79	AA	753	A
79	AA	760	A
79	AA	761	A
79	AA	766	G
79	AA	791	G
79	AA	794	U
79	AA	796	G
79	AA	826	A
79	AA	828	C
79	AA	830	U
79	AA	832	U
79	AA	835	C
79	AA	836	A
79	AA	860	A
79	AA	861	U
79	AA	868	C

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Mol	Chain	Res	Type
79	AA	870	C
79	AA	871	A
79	AA	872	G
79	AA	881	A
79	AA	883	U
79	AA	889	G
79	AA	890	C
79	AA	893	G
79	AA	899	G
79	AA	903	U
79	AA	904	C
79	AA	907	A
79	AA	911	U
79	AA	919	A
79	AA	929	A
79	AA	931	C
79	AA	933	G
79	AA	938	A
79	AA	939	A
79	AA	941	G
79	AA	942	A
79	AA	954	C
79	AA	956	C
79	AA	958	C
79	AA	959	C
79	AA	960	C
79	AA	961	U
79	AA	962	C
79	AA	967	A
79	AA	978	A
79	AA	993	A
79	AA	1001	C
79	AA	1002	C
79	AA	1015	A
79	AA	1022	A
79	AA	1031	G
79	AA	1042	U
79	AA	1046	A
79	AA	1076	5MU
79	AA	1078	A
79	AA	1081	U
79	AA	1082	A

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Mol	Chain	Res	Type
79	AA	1096	A
79	AA	1098	C
79	AA	1103	A
79	AA	1105	C
79	AA	1106	C
79	AA	1107	U
79	AA	1109	A
79	AA	1116	A
79	AA	1118	A
79	AA	1119	U
79	AA	1121	A
79	AA	1126	A
79	AA	1138	G
79	AA	1144	U
79	AA	1151	C
79	AA	1152	A
79	AA	1153	C
79	AA	1155	G
79	AA	1160	A
79	AA	1167	A
79	AA	1179	G
79	AA	1187	U
79	AA	1189	U
79	AA	1190	C
79	AA	1215	U
79	AA	1220	A
79	AA	1223	C
79	AA	1225	C
79	AA	1229	U
79	AA	1232	A
79	AA	1235	U
79	AA	1247	G
79	AA	1248	C
79	AA	1250	C
79	AA	1251	A
79	AA	1261	C
79	AA	1271	C
79	AA	1273	G
79	AA	1284	U
79	AA	1285	G
79	AA	1290	C
79	AA	1291	U

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Mol	Chain	Res	Type
79	AA	1292	A
79	AA	1294	A
79	AA	1297	G
79	AA	1318	A
79	AA	1326	A
79	AA	1327	G
79	AA	1330	C
79	AA	1343	A
79	AA	1344	U
79	AA	1353	A
79	AA	1354	A
79	AA	1355	G
79	AA	1356	A
79	AA	1370	U
79	AA	1376	C
79	AA	1378	C
79	AA	1387	A
79	AA	1390	A
79	AA	1391	U
79	AA	1405	C
79	AA	1407	U
79	AA	1422	G
79	AA	1430	A
79	AA	1432	U
79	AA	1443	U
79	AA	1466	C
79	AA	1481	C
79	AA	1482	A
79	AA	1512	A
79	AA	1519	A
79	AA	1522	U
79	AA	1525	C
79	AA	1526	U
79	AA	1527	A
79	AA	1528	A
79	AA	1533	C
79	AA	1537	C
79	AA	1538	G
79	AA	1539	C
79	AA	1540	A
79	AA	1551	G
79	AA	1557	A

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Mol	Chain	Res	Type
79	AA	1560	U
79	AA	1562	G
79	AA	1564	A
79	AA	1568	U
79	AA	1571	U
79	AA	1582	G
79	AA	1584	MA6
79	AA	1594	G
79	AA	1595	G
79	AA	1599	A
83	Ax	13	U
83	Ax	16	A
83	Ax	17	U
83	Ax	18	A
83	Ax	22	U
83	Ax	43	A
83	Ax	44	U
83	Ax	47	U
83	Ax	50	U
83	Ax	51	U
83	Ax	52	A
83	Ax	56	C
83	Ax	61	C
83	Ax	63	G
83	Ax	65	A
83	Ax	71	A
88	B	8	U
88	B	10	2MG
88	B	16	C
88	B	21	A
88	B	45	G
88	B	46	A
88	B	54	C
88	B	55	U
88	B	56	U
88	B	58	A
88	B	59	A
88	B	64	A
88	B	69	U
88	B	72	G
88	B	76	A

All (4) RNA pucker outliers are listed below:



Mol	Chain	Res	Type
11	A	2245	A
11	A	2484	C
79	AA	1108	C
79	AA	1390	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
11	PSU	A	3067	11	18,21,22	1.08	2 (11%)	21,30,33	0.79	1 (4%)
11	1MA	A	2617	11	21,25,26	0.42	0	30,37,40	0.60	0
11	OMU	A	3039	90,11	19,22,23	0.31	0	25,31,34	0.79	1 (4%)
88	1MA	B	9	88	21,25,26	0.39	0	30,37,40	0.67	0
11	OMG	A	3040	11	23,26,27	0.35	0	32,38,41	0.46	0
79	5MC	AA	1488	79	19,22,23	0.82	1 (5%)	26,32,35	0.50	0
88	PSU	B	39	88	18,21,22	1.01	1 (5%)	21,30,33	0.73	0
79	MA6	AA	1583	79	23,26,27	0.36	0	33,38,41	0.73	1 (3%)
11	OMG	A	2815	83,90,11	23,26,27	0.37	0	32,38,41	0.43	0
88	2MG	B	10	88	23,26,27	0.36	0	33,38,41	0.42	0
79	MA6	AA	1584	79	23,26,27	0.31	0	33,38,41	0.73	1 (3%)
79	5MU	AA	1076	79	19,22,23	0.38	0	27,32,35	0.66	0
79	B8T	AA	1486	79	19,22,23	0.40	0	25,31,34	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PSU	A	3067	11	-	1/7/25/26	0/2/2/2
11	1MA	A	2617	11	-	0/7/25/26	0/3/3/3
11	OMU	A	3039	90,11	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	1MA	B	9	88	-	1/7/25/26	0/3/3/3
11	OMG	A	3040	11	-	0/9/27/28	0/3/3/3
79	5MC	AA	1488	79	-	0/7/25/26	0/2/2/2
88	PSU	B	39	88	-	0/7/25/26	0/2/2/2
79	MA6	AA	1583	79	-	0/11/29/30	0/3/3/3
11	OMG	A	2815	83,90,11	-	0/9/27/28	0/3/3/3
88	2MG	B	10	88	-	0/9/27/28	0/3/3/3
79	MA6	AA	1584	79	-	2/11/29/30	0/3/3/3
79	5MU	AA	1076	79	-	5/7/25/26	0/2/2/2
79	B8T	AA	1486	79	-	0/7/27/28	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	B	39	PSU	C6-C5	3.50	1.39	1.35
11	A	3067	PSU	C6-C5	3.46	1.39	1.35
79	AA	1488	5MC	C5-C4	-3.23	1.41	1.44
11	A	3067	PSU	O4'-C1'	-2.46	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	3039	OMU	C2'-C1'-N1	-2.99	108.57	114.24
79	AA	1583	MA6	C2-N1-C6	2.93	118.99	111.83
79	AA	1584	MA6	C2-N1-C6	2.91	118.94	111.83
11	A	3067	PSU	O4'-C1'-C2'	2.34	108.39	105.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
79	AA	1076	5MU	O4'-C4'-C5'-O5'
79	AA	1076	5MU	C3'-C4'-C5'-O5'
79	AA	1076	5MU	C4'-C5'-O5'-P
79	AA	1584	MA6	C4'-C5'-O5'-P
79	AA	1076	5MU	C2'-C1'-N1-C2
79	AA	1076	5MU	C2'-C1'-N1-C6
11	A	3067	PSU	O4'-C4'-C5'-O5'
79	AA	1584	MA6	C3'-C4'-C5'-O5'
88	B	9	1MA	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	3039	OMU	1	0
79	AA	1488	5MC	2	0
79	AA	1583	MA6	2	0
11	A	2815	OMG	1	0
79	AA	1076	5MU	1	0
79	AA	1486	B8T	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 278 ligands modelled in this entry, 261 are monoatomic - leaving 17 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	$\# Z  > 2$
91	SPD	O	301	-	9,9,9	0.17	0	8,8,8	0.19	0
94	FES	AP	201	56,66	0,4,4	-	-	-		
94	FES	r	201	16,47	0,4,4	-	-	-		
91	SPD	A	3471	-	9,9,9	0.15	0	8,8,8	0.25	0
91	SPD	AA	1782	-	9,9,9	0.16	0	8,8,8	0.16	0
96	SPM	AA	1702	-	13,13,13	0.15	0	12,12,12	0.23	0
99	VAL	B	101	88	4,6,7	0.80	0	6,7,9	0.91	1 (16%)
91	SPD	A	3470	-	9,9,9	0.15	0	8,8,8	0.17	0
95	NAD	AA	1701	93	46,48,48	1.24	3 (6%)	64,73,73	0.82	1 (1%)
91	SPD	A	3302	-	9,9,9	0.16	0	8,8,8	0.22	0
91	SPD	AA	1703	-	9,9,9	0.16	0	8,8,8	0.32	0
92	PUT	A	3303	-	5,5,5	0.14	0	4,4,4	0.24	0
91	SPD	A	3301	93	9,9,9	0.15	0	8,8,8	0.17	0
94	FES	AT	201	69,63	0,4,4	-	-	-		
96	SPM	AA	1780	-	13,13,13	0.16	0	12,12,12	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
97	ATP	AX	501	93	32,33,33	0.49	1 (3%)	48,52,52	0.34	0
98	GDP	AX	503	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	8 (17%)

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
91	SPD	O	301	-	-	2/7/7/7	-
94	FES	AP	201	56,66	-	-	0/1/1/1
94	FES	r	201	16,47	-	-	0/1/1/1
91	SPD	A	3471	-	-	1/7/7/7	-
91	SPD	AA	1782	-	-	0/7/7/7	-
96	SPM	AA	1702	-	-	0/11/11/11	-
99	VAL	B	101	88	-	4/5/6/8	-
91	SPD	A	3470	-	-	0/7/7/7	-
95	NAD	AA	1701	93	-	4/30/62/62	0/5/5/5
91	SPD	A	3302	-	-	1/7/7/7	-
91	SPD	AA	1703	-	-	0/7/7/7	-
92	PUT	A	3303	-	-	0/3/3/3	-
91	SPD	A	3301	93	-	0/7/7/7	-
96	SPM	AA	1780	-	-	2/11/11/11	-
97	ATP	AX	501	93	-	0/22/38/38	0/3/3/3
98	GDP	AX	503	-	-	5/16/32/32	0/3/3/3
94	FES	AT	201	69,63	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
95	AA	1701	NAD	PA-O3	5.30	1.65	1.59
95	AA	1701	NAD	PN-O3	3.45	1.63	1.59
98	AX	503	GDP	C5-C4	3.09	1.47	1.38
95	AA	1701	NAD	O4D-C1D	-2.60	1.37	1.40
98	AX	503	GDP	C6-N1	-2.49	1.34	1.38
97	AX	501	ATP	PB-O3B	-2.05	1.57	1.59
98	AX	503	GDP	C5-N7	-2.00	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
98	AX	503	GDP	C5-C4-N3	-5.97	118.89	128.39
98	AX	503	GDP	C2-N3-C4	4.87	120.70	112.30
98	AX	503	GDP	N9-C4-N3	4.43	134.81	125.95
98	AX	503	GDP	C6-C5-N7	3.28	136.26	130.29
98	AX	503	GDP	C4-C5-N7	-2.60	106.54	110.67
98	AX	503	GDP	C3'-C2'-C1'	2.41	106.03	101.46
99	B	101	VAL	O-C-CA	-2.17	119.19	124.77
95	AA	1701	NAD	O2A-PA-O1A	2.12	122.30	112.44
98	AX	503	GDP	C2'-C1'-N9	-2.10	107.40	113.25
98	AX	503	GDP	O6-C6-C5	-2.08	121.04	126.53

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
99	B	101	VAL	O-C-CA-CB
99	B	101	VAL	C-CA-CB-CG1
99	B	101	VAL	C-CA-CB-CG2
91	O	301	SPD	C8-C7-N6-C5
96	AA	1780	SPM	C6-C7-C8-C9
95	AA	1701	NAD	C2N-C3N-C7N-O7N
95	AA	1701	NAD	C4N-C3N-C7N-O7N
95	AA	1701	NAD	C4N-C3N-C7N-N7N
95	AA	1701	NAD	C2N-C3N-C7N-N7N
91	O	301	SPD	N6-C7-C8-C9
98	AX	503	GDP	PA-O3A-PB-O3B
91	A	3302	SPD	C4-C5-N6-C7
98	AX	503	GDP	C5'-O5'-PA-O3A
98	AX	503	GDP	C5'-O5'-PA-O1A
98	AX	503	GDP	C5'-O5'-PA-O2A
91	A	3471	SPD	C2-C3-C4-C5
98	AX	503	GDP	PA-O3A-PB-O2B
99	B	101	VAL	N-CA-CB-CG1
96	AA	1780	SPM	C12-C11-N10-C9

There are no ring outliers.

6 monomers are involved in 8 short contacts:

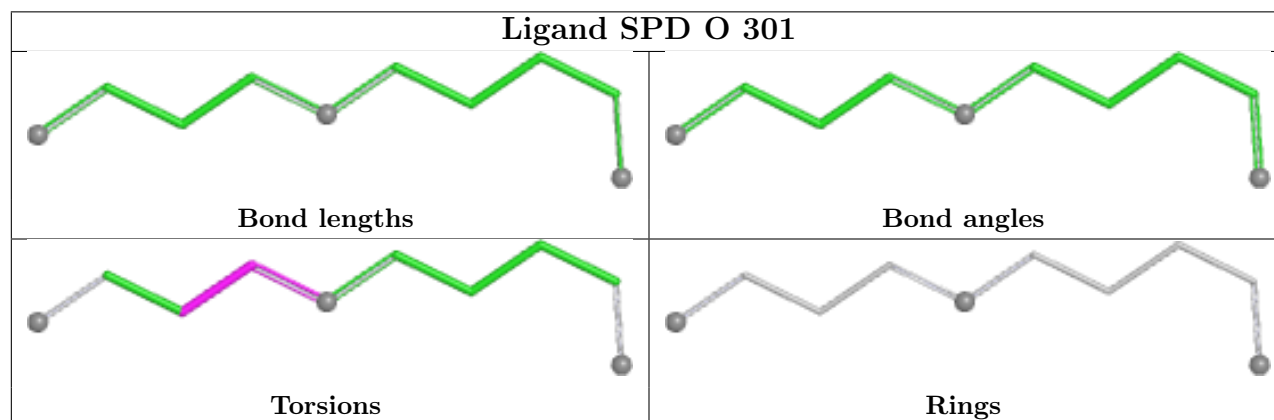
Mol	Chain	Res	Type	Clashes	Symm-Clashes
91	A	3471	SPD	1	0
96	AA	1702	SPM	1	0
99	B	101	VAL	3	0

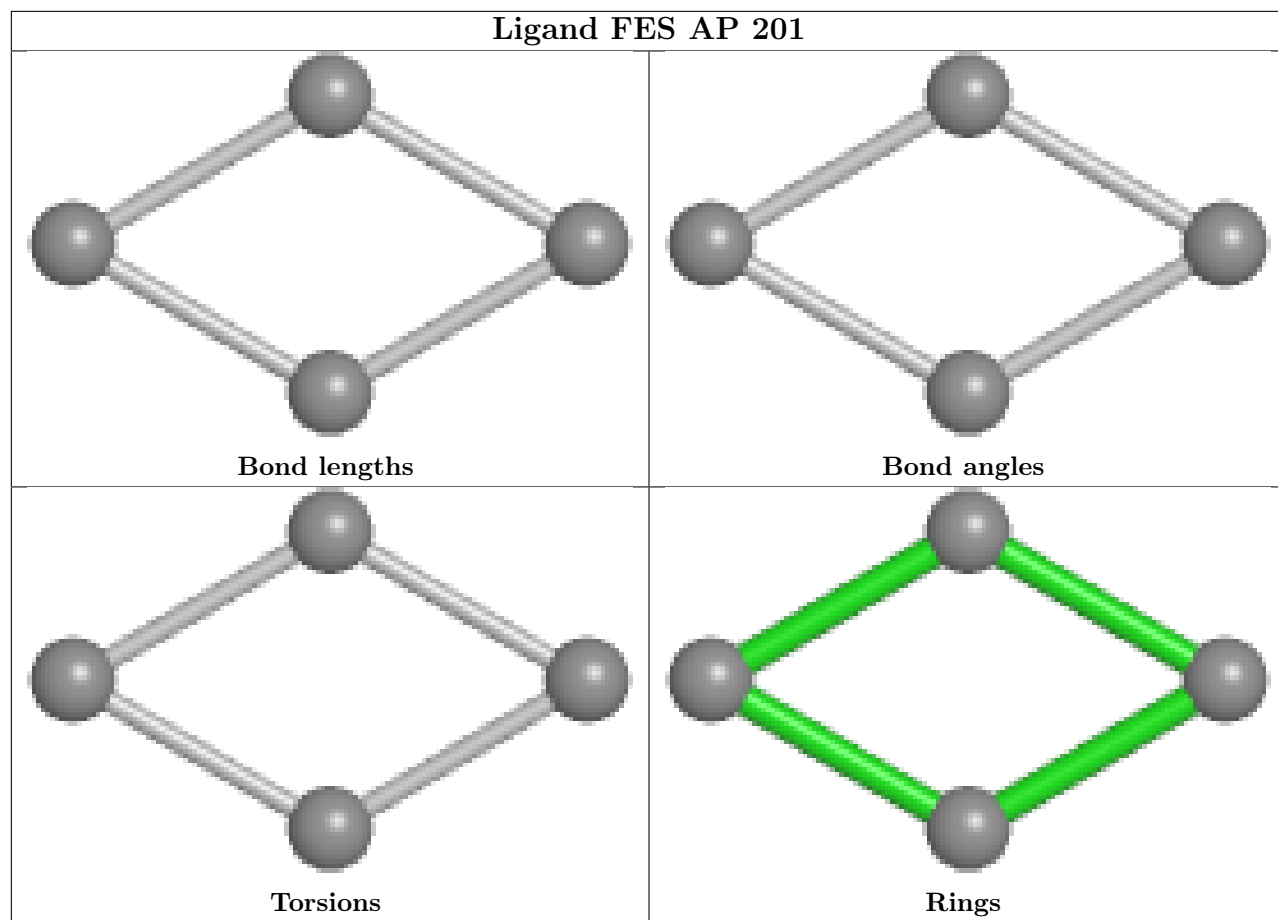
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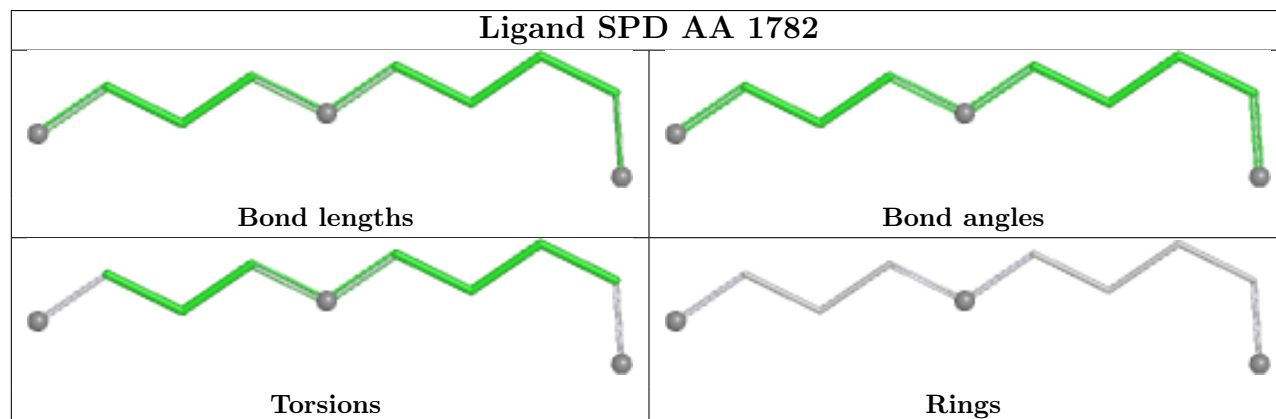
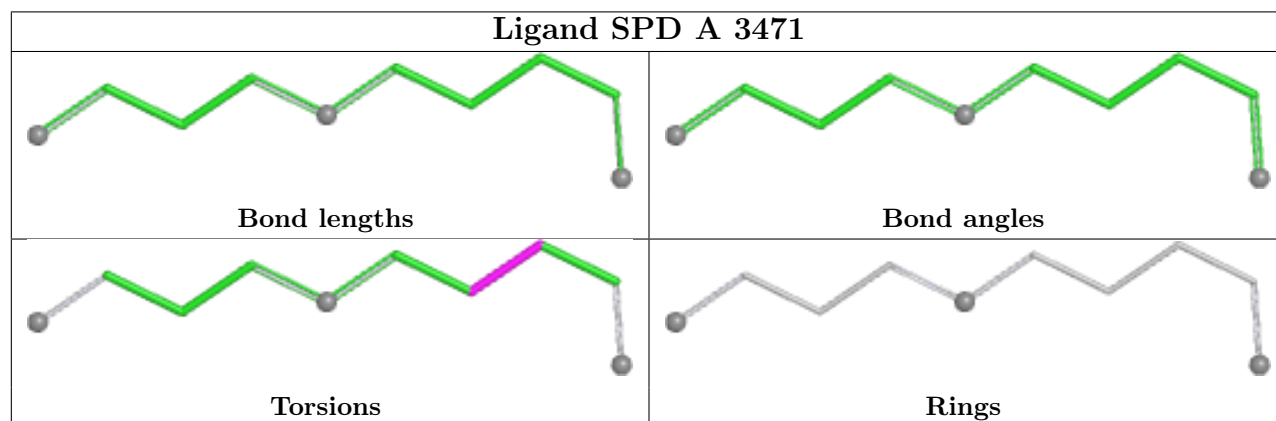
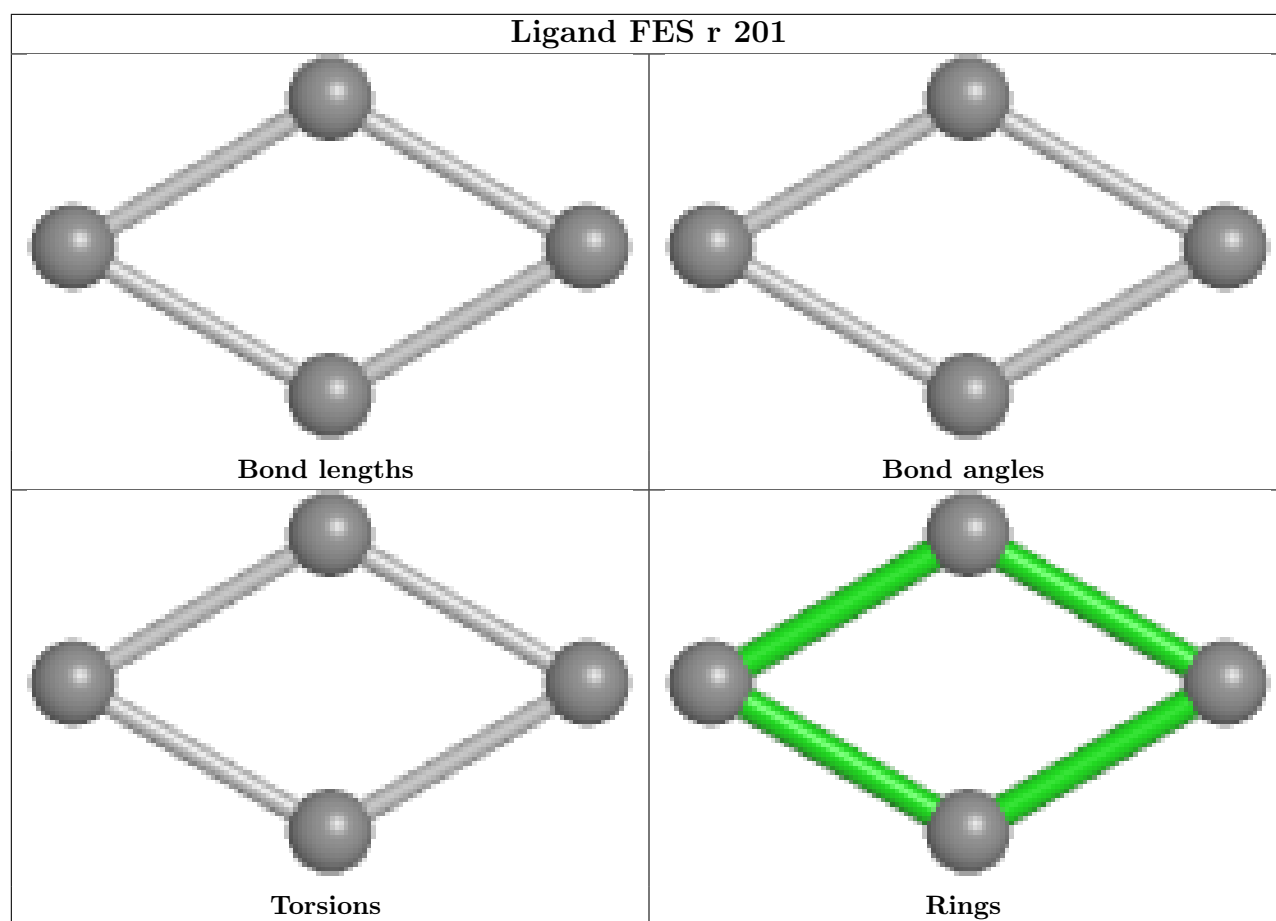
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
95	AA	1701	NAD	1	0
91	A	3302	SPD	1	0
98	AX	503	GDP	1	0

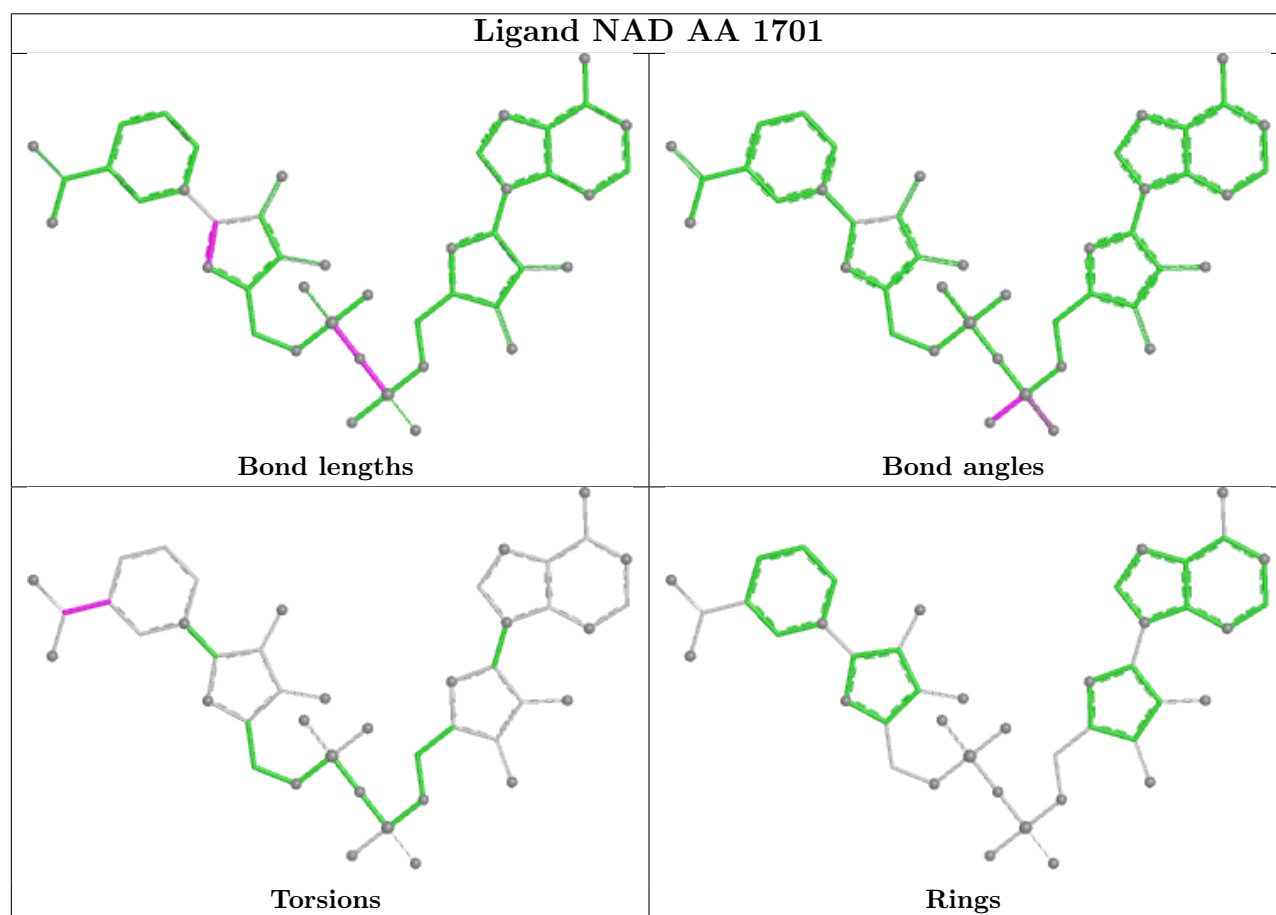
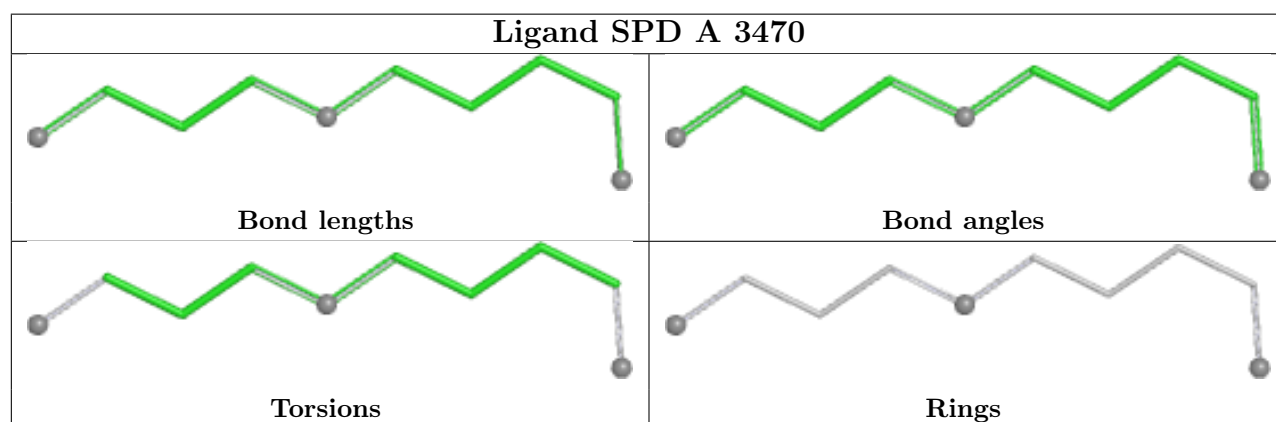
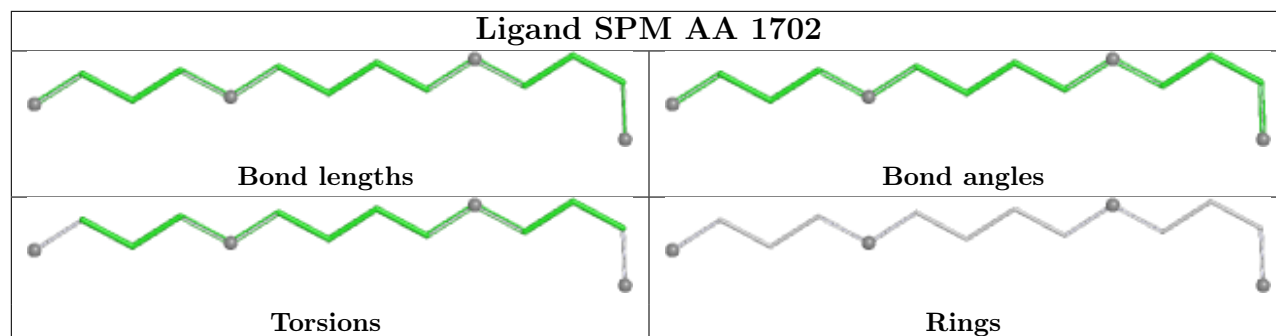
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

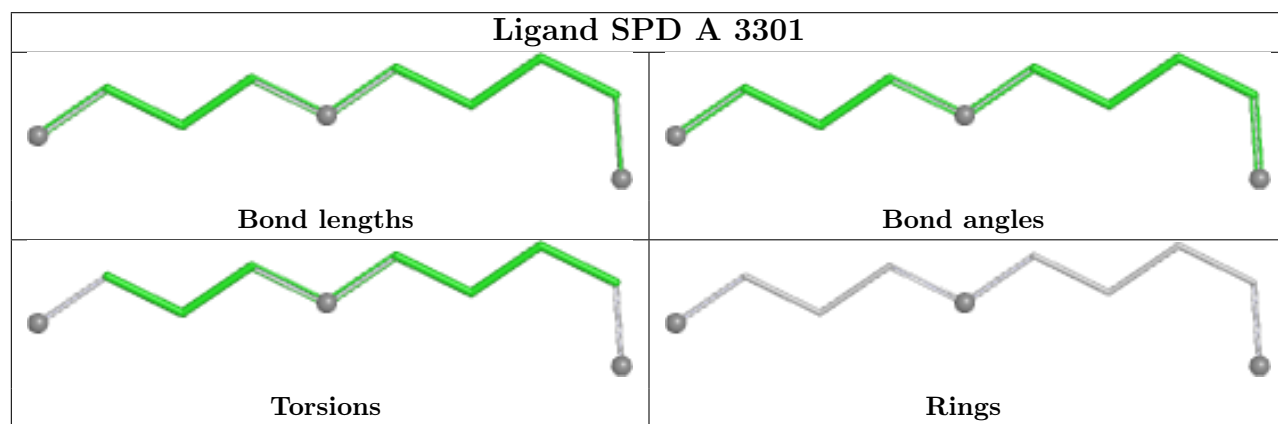
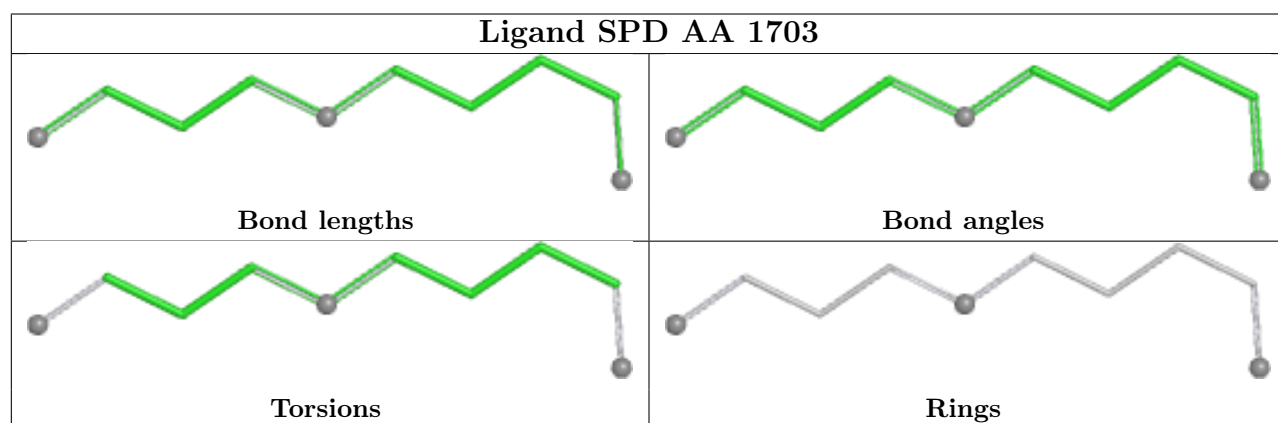
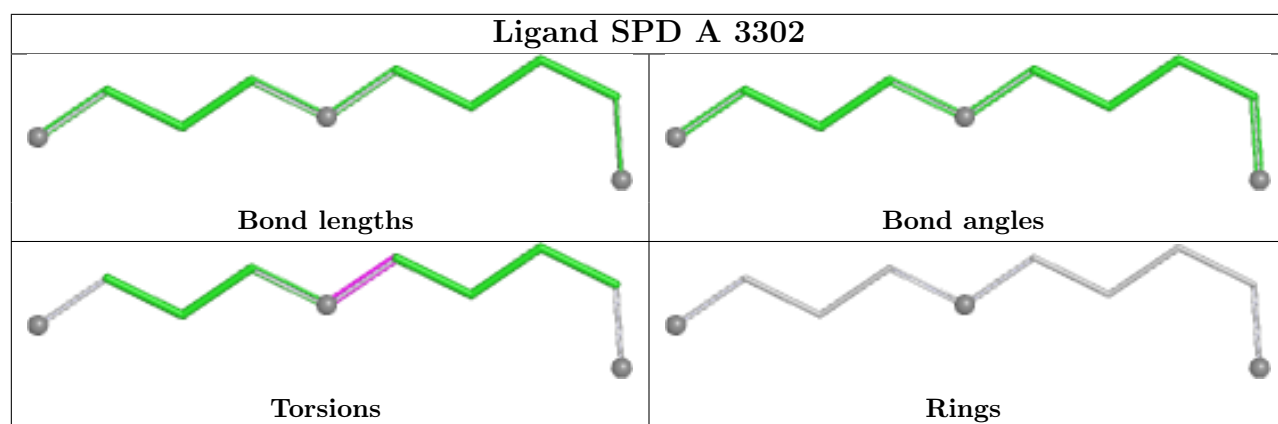


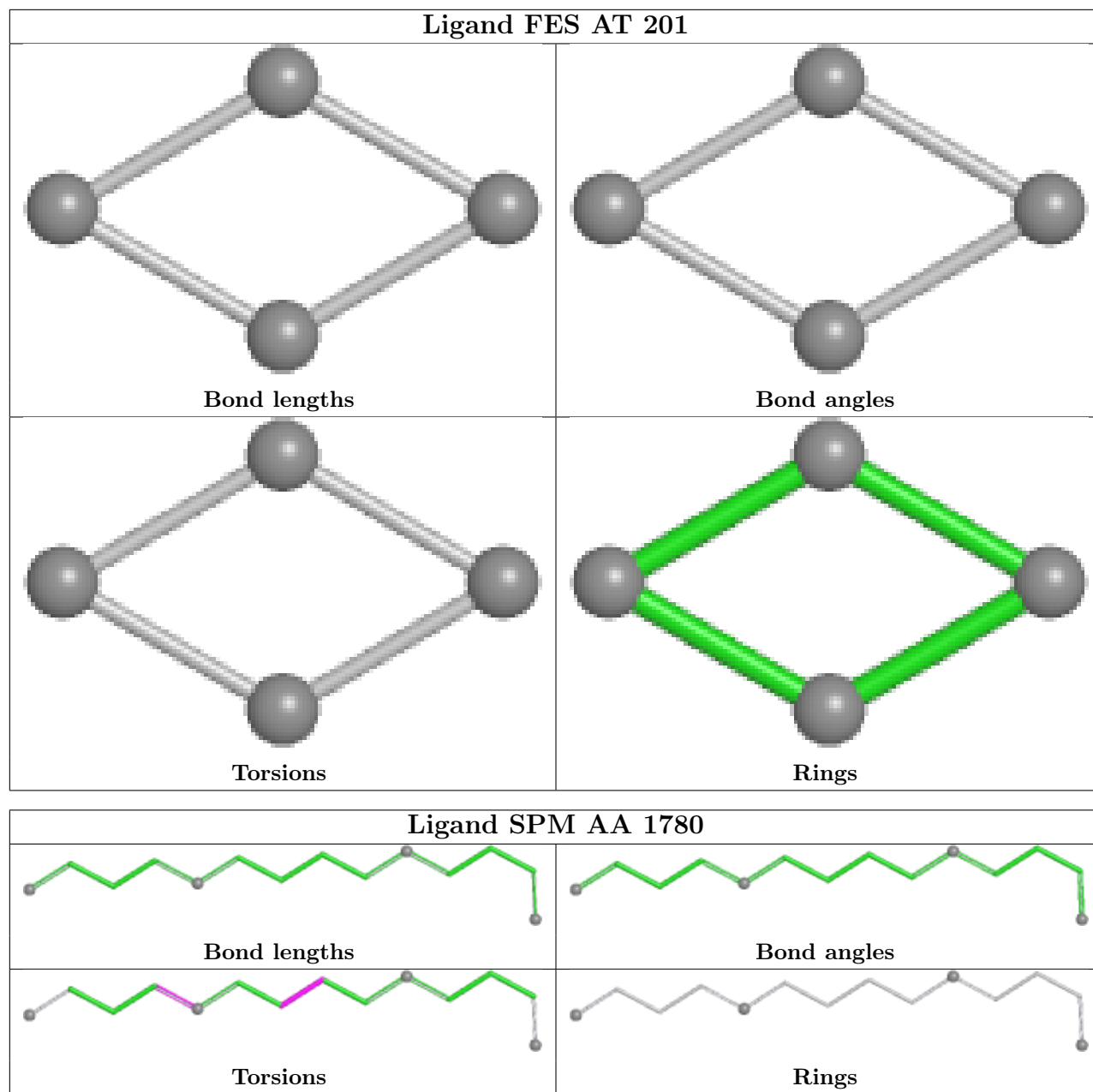




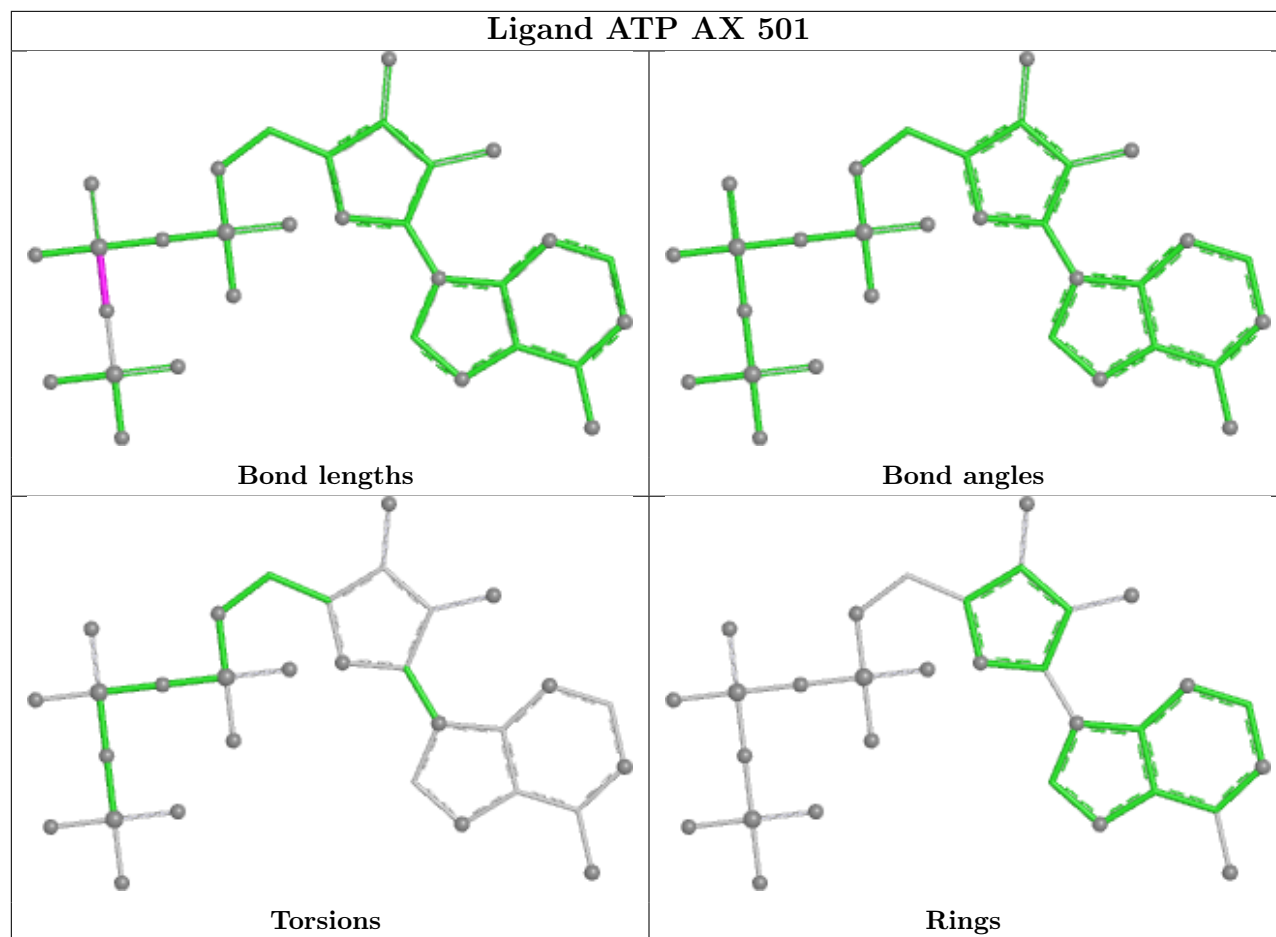




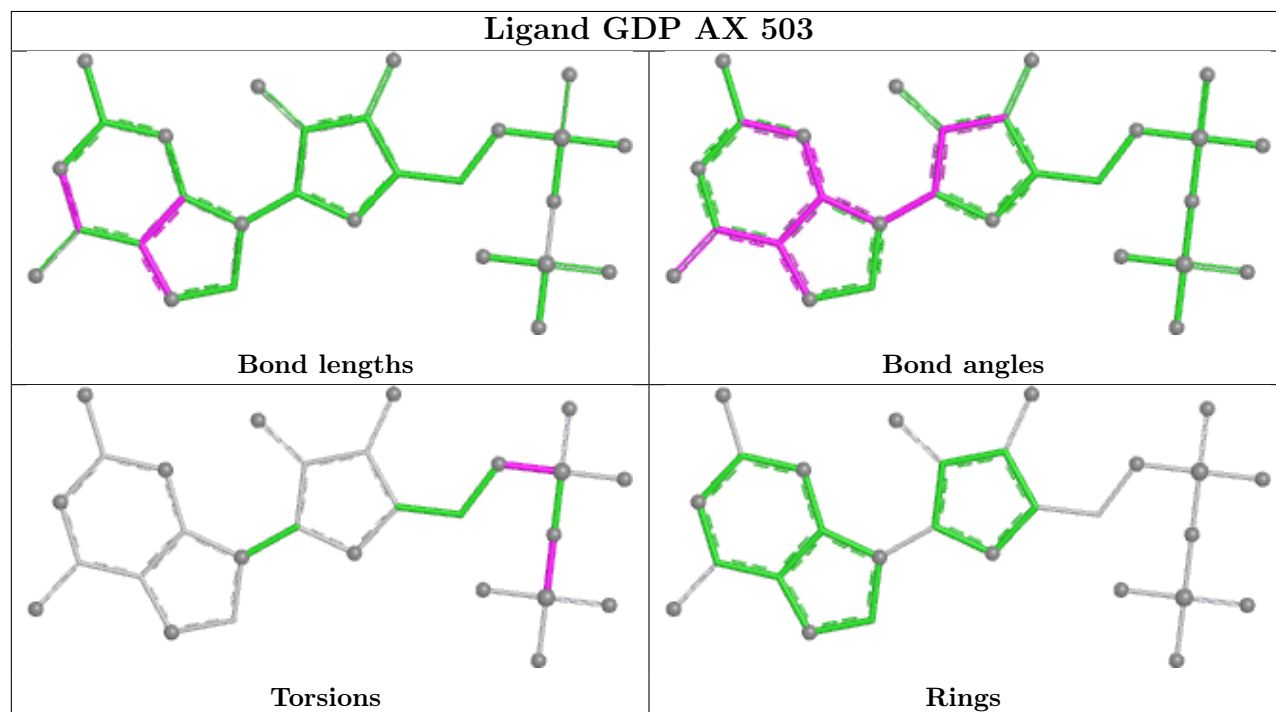




## Ligand ATP AX 501



## Ligand GDP AX 503



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	A	1
88	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2357:C	O3'	2361:G	P	8.72
1	B	46:A	O3'	48:U	P	4.54

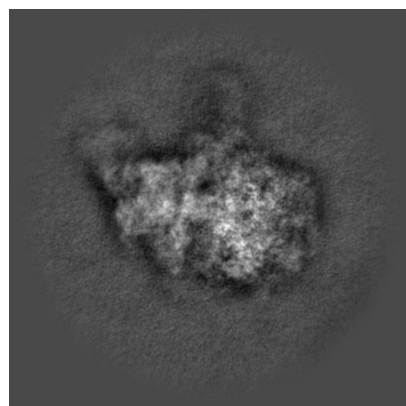
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71809. These allow visual inspection of the internal detail of the map and identification of artifacts.

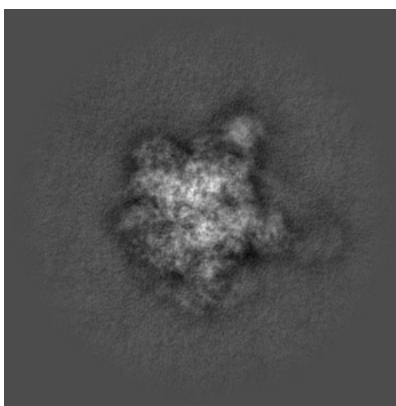
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

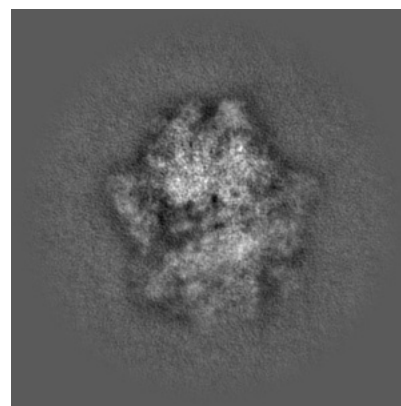
#### 6.1.1 Primary map



X

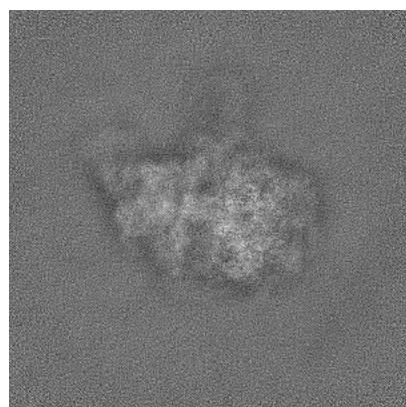


Y

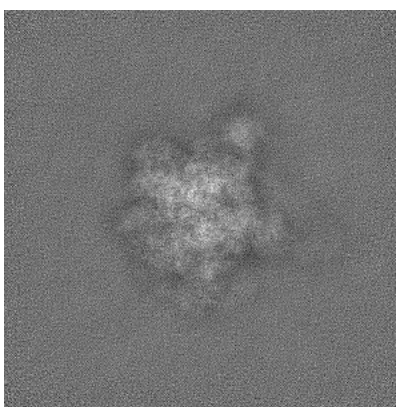


Z

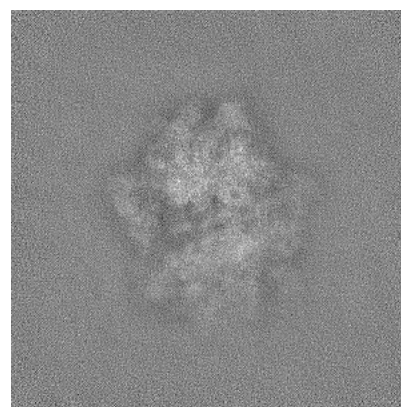
#### 6.1.2 Raw map



X



Y

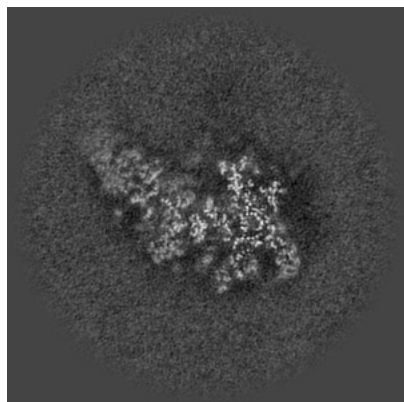


Z

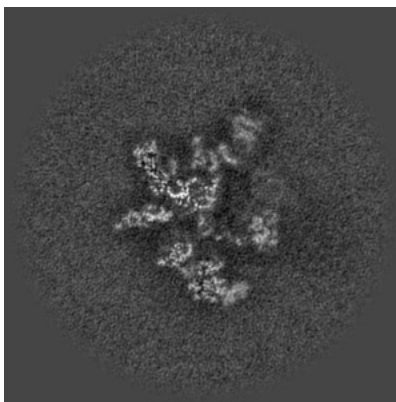
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

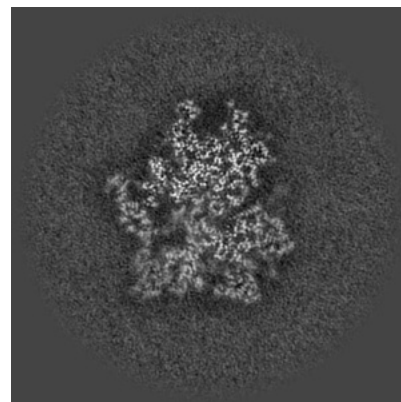
### 6.2.1 Primary map



X Index: 240

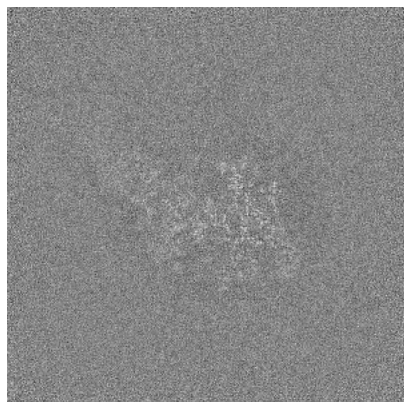


Y Index: 240

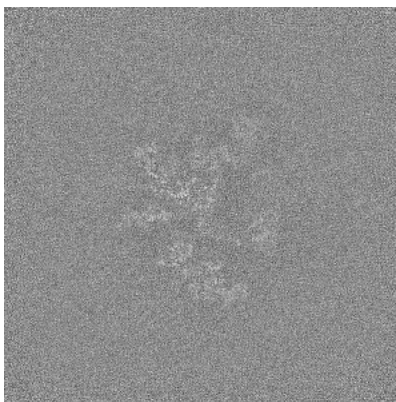


Z Index: 240

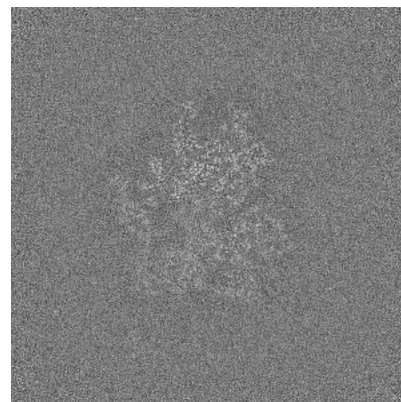
### 6.2.2 Raw map



X Index: 240



Y Index: 240



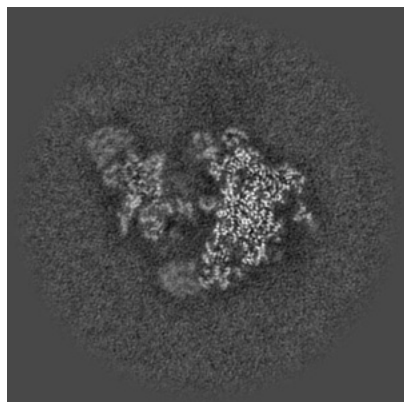
Z Index: 240

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

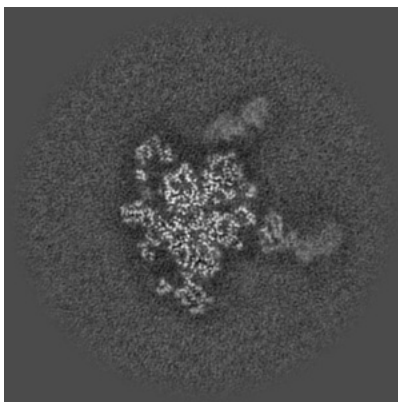


## 6.3 Largest variance slices [i](#)

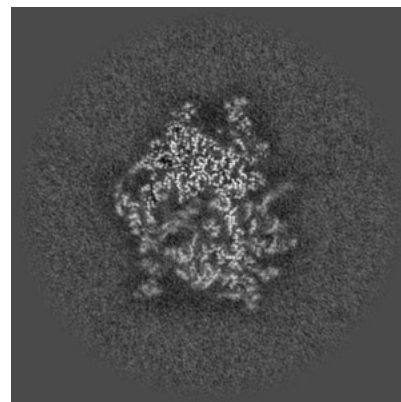
### 6.3.1 Primary map



X Index: 224

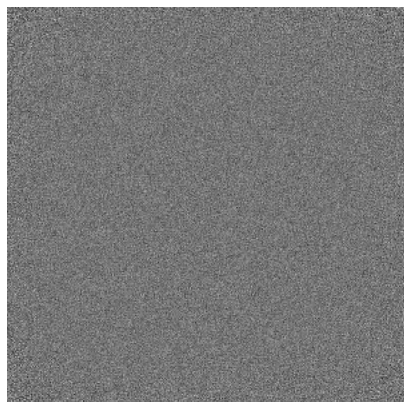


Y Index: 263

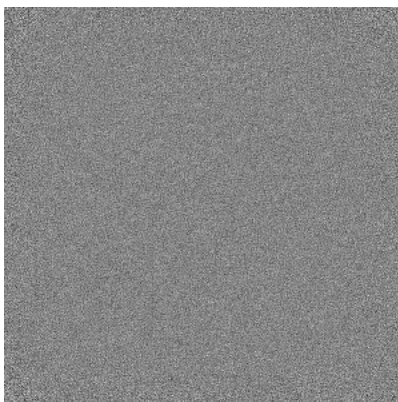


Z Index: 249

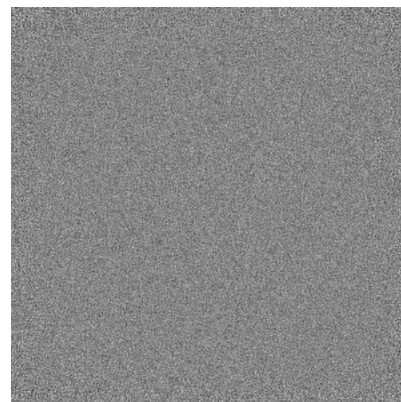
### 6.3.2 Raw map



X Index: 0



Y Index: 0



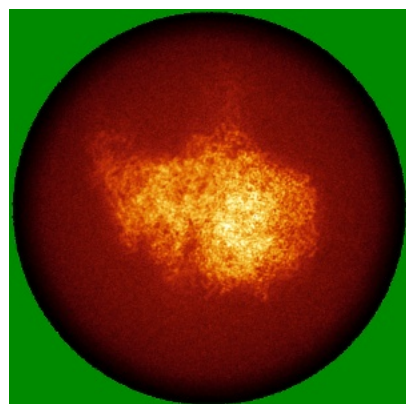
Z Index: 0

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

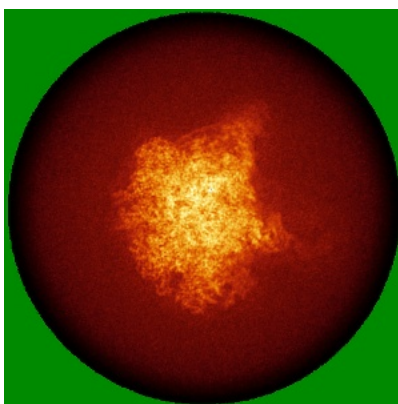


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

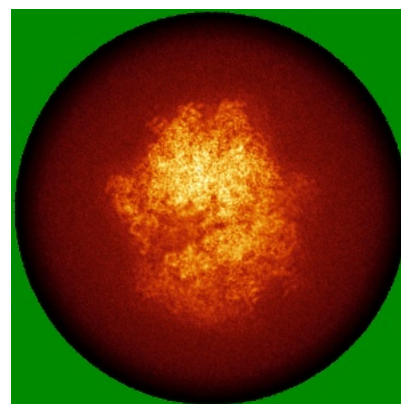
### 6.4.1 Primary map



X

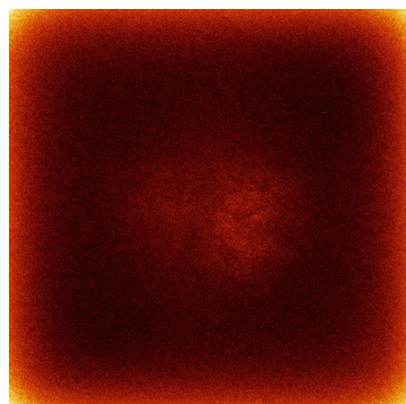


Y

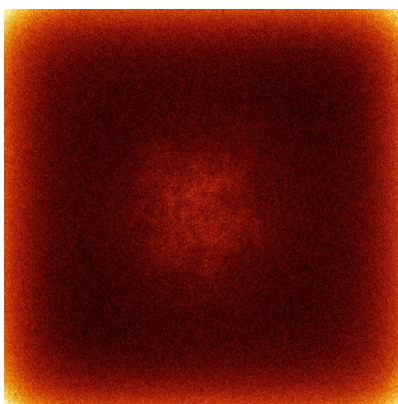


Z

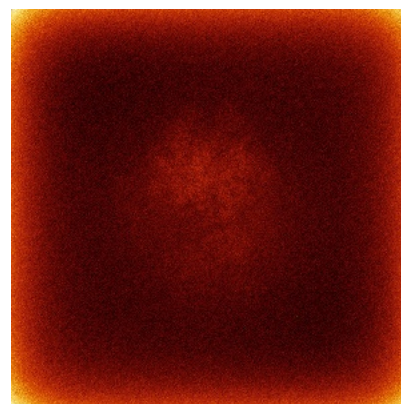
### 6.4.2 Raw map



X



Y



Z

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

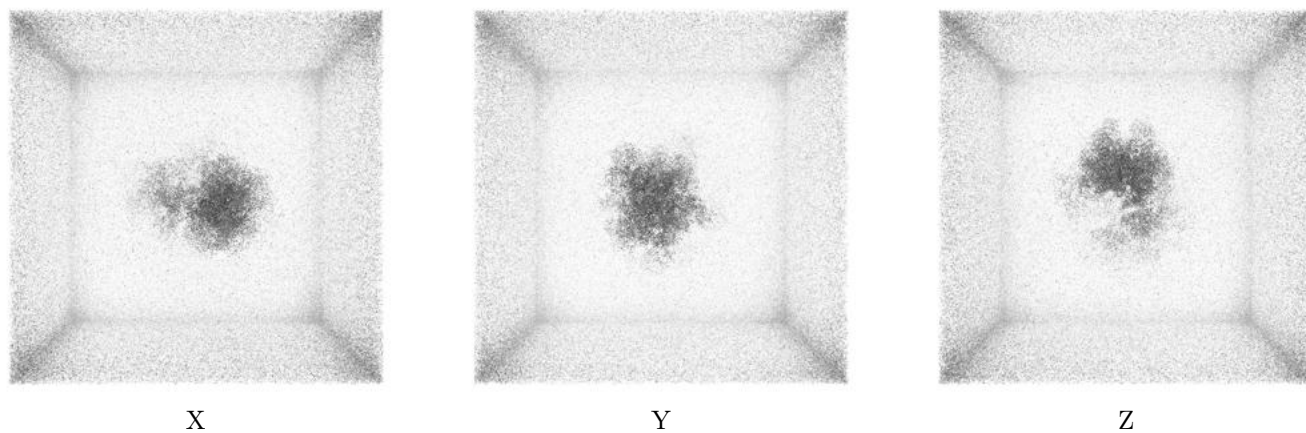
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

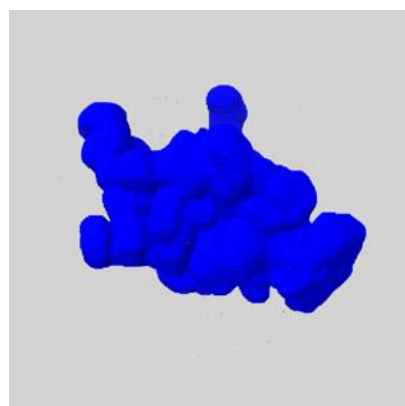
## 6.6 Mask visualisation [i](#)

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

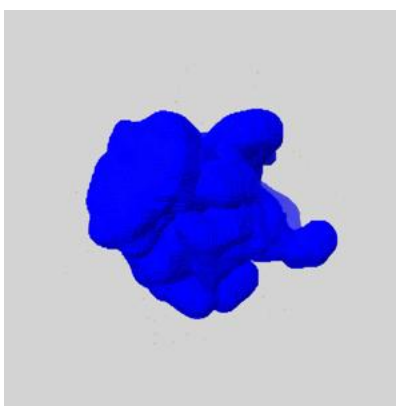
A mask typically either:

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

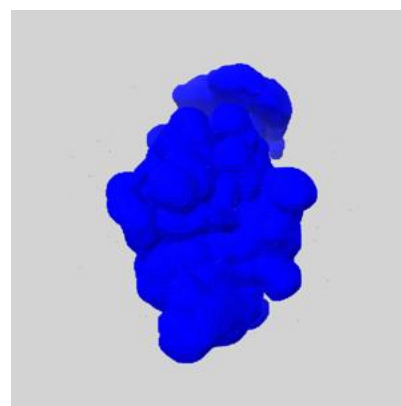
### 6.6.1 emd\_71809\_msk\_1.map [i](#)



X



Y

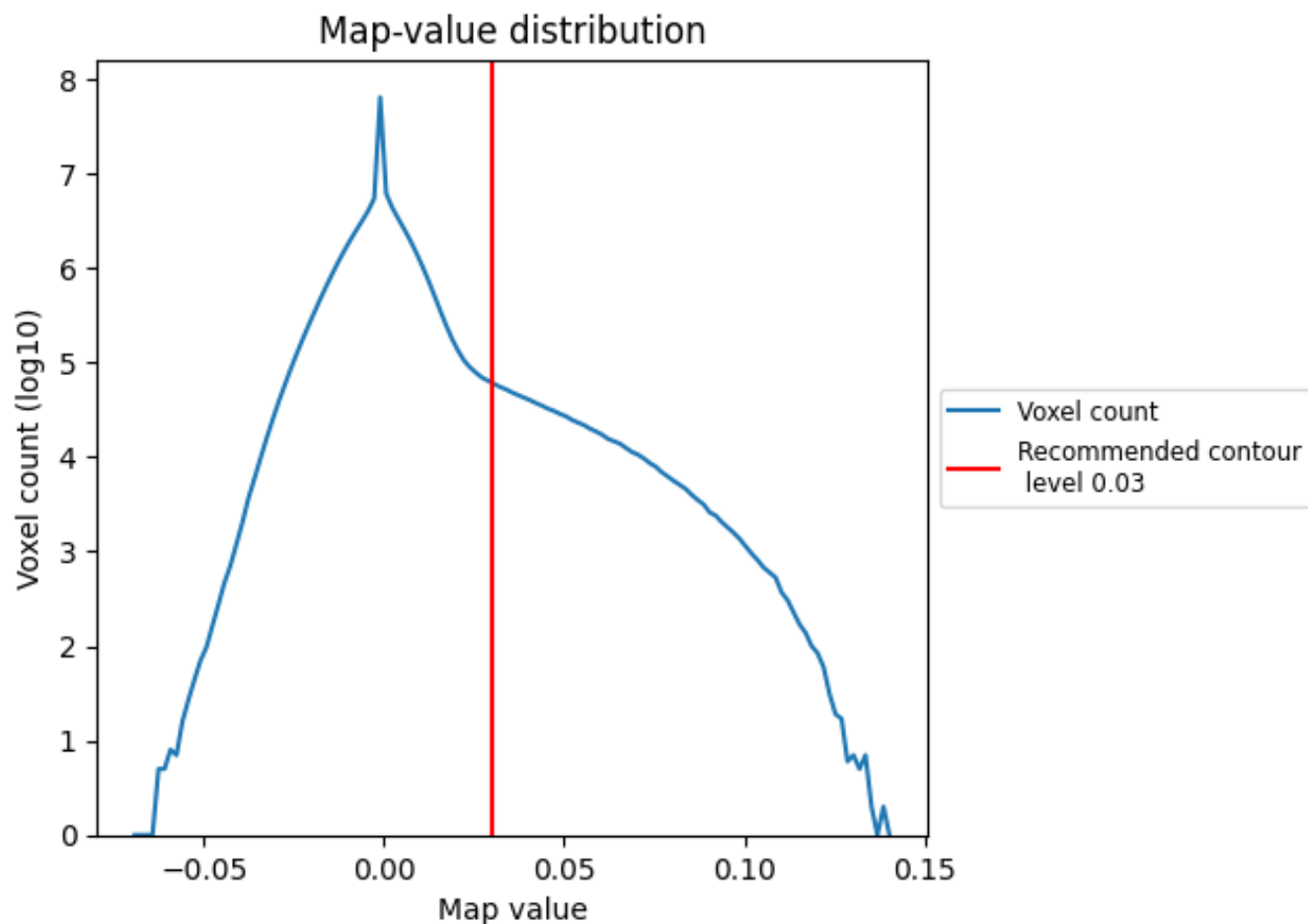


Z

## 7 Map analysis [i](#)

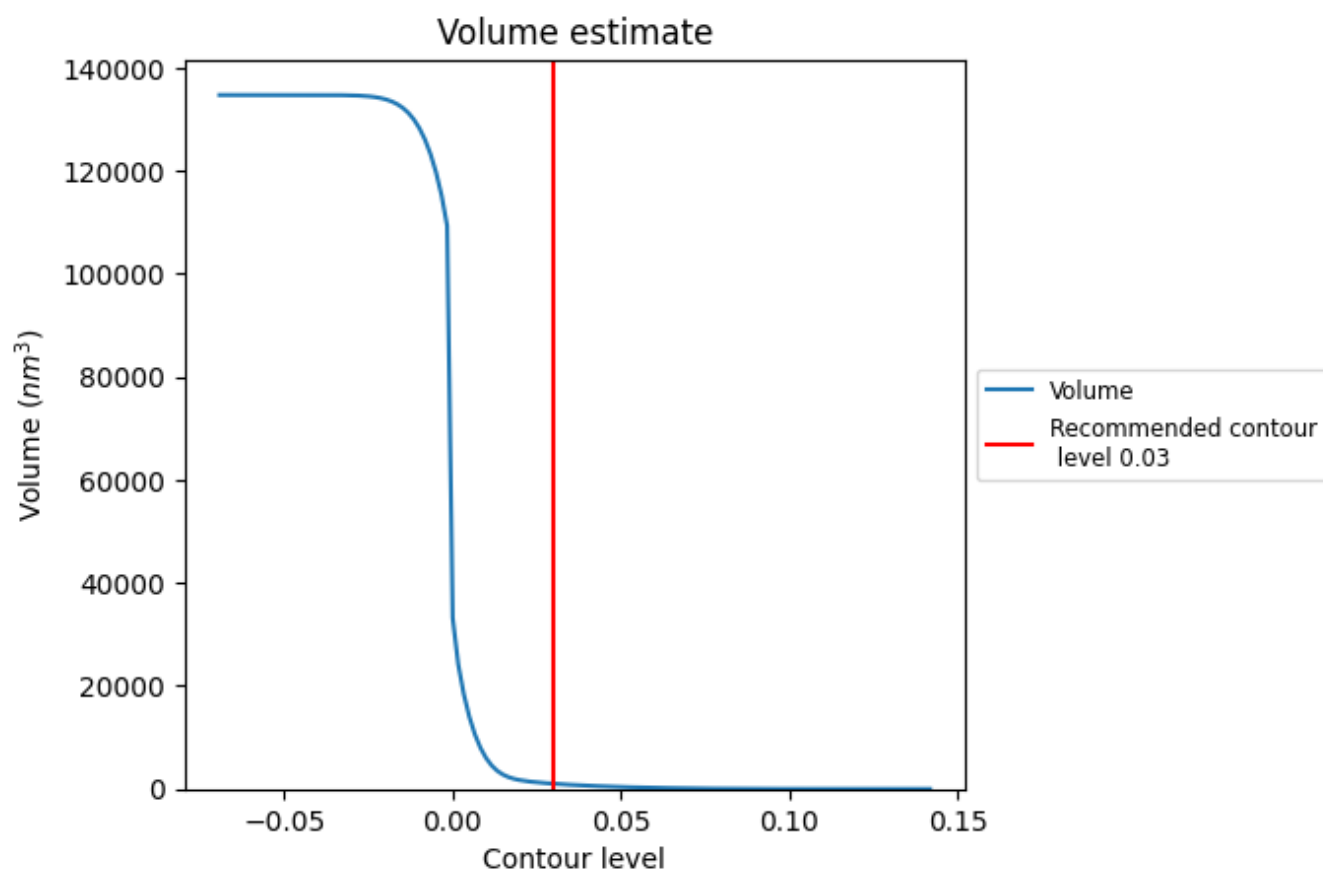
This section contains the results of statistical analysis of the map.

### 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.

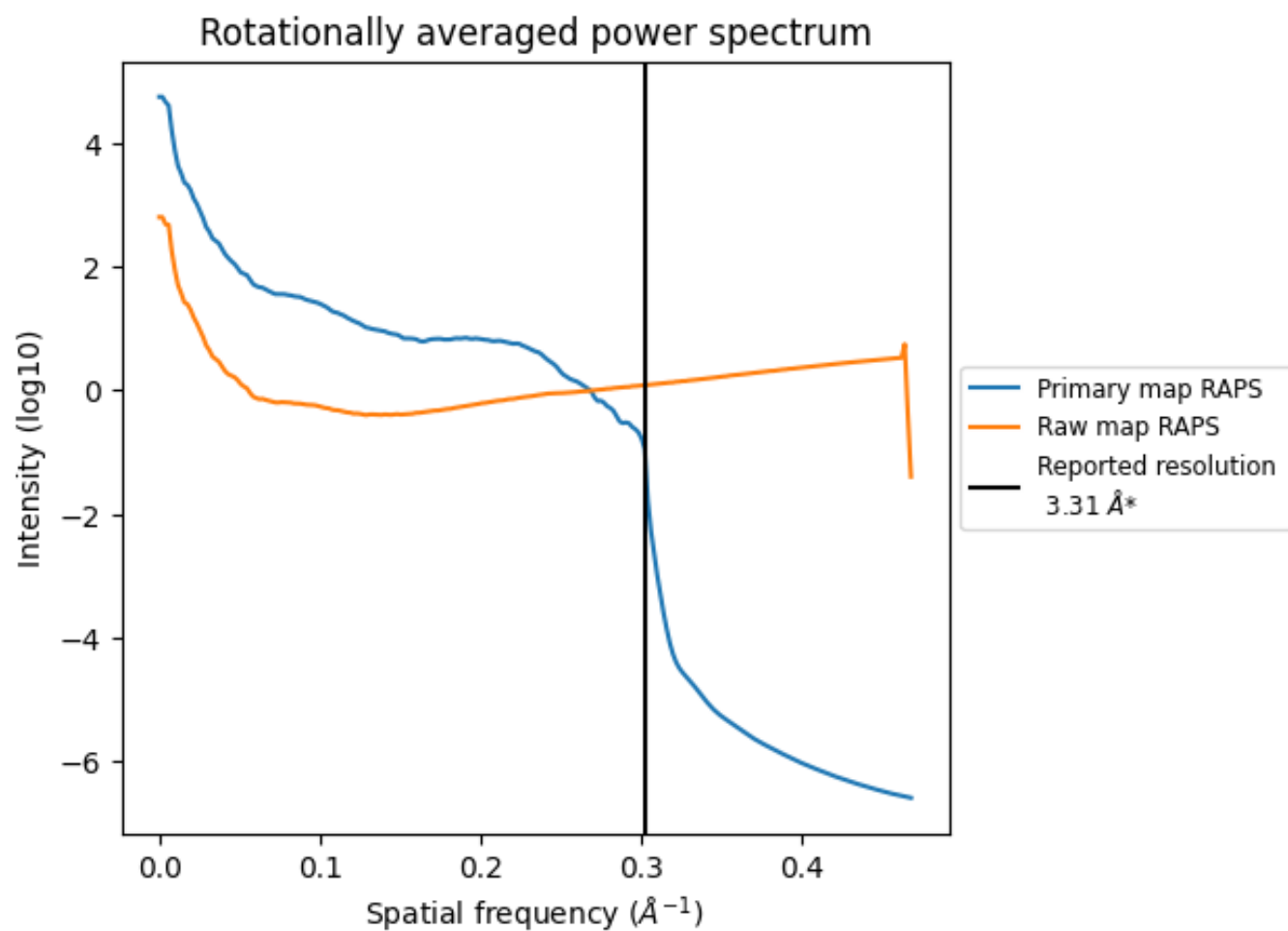
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1021 nm<sup>3</sup>; this corresponds to an approximate mass of 922 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 ⓘ

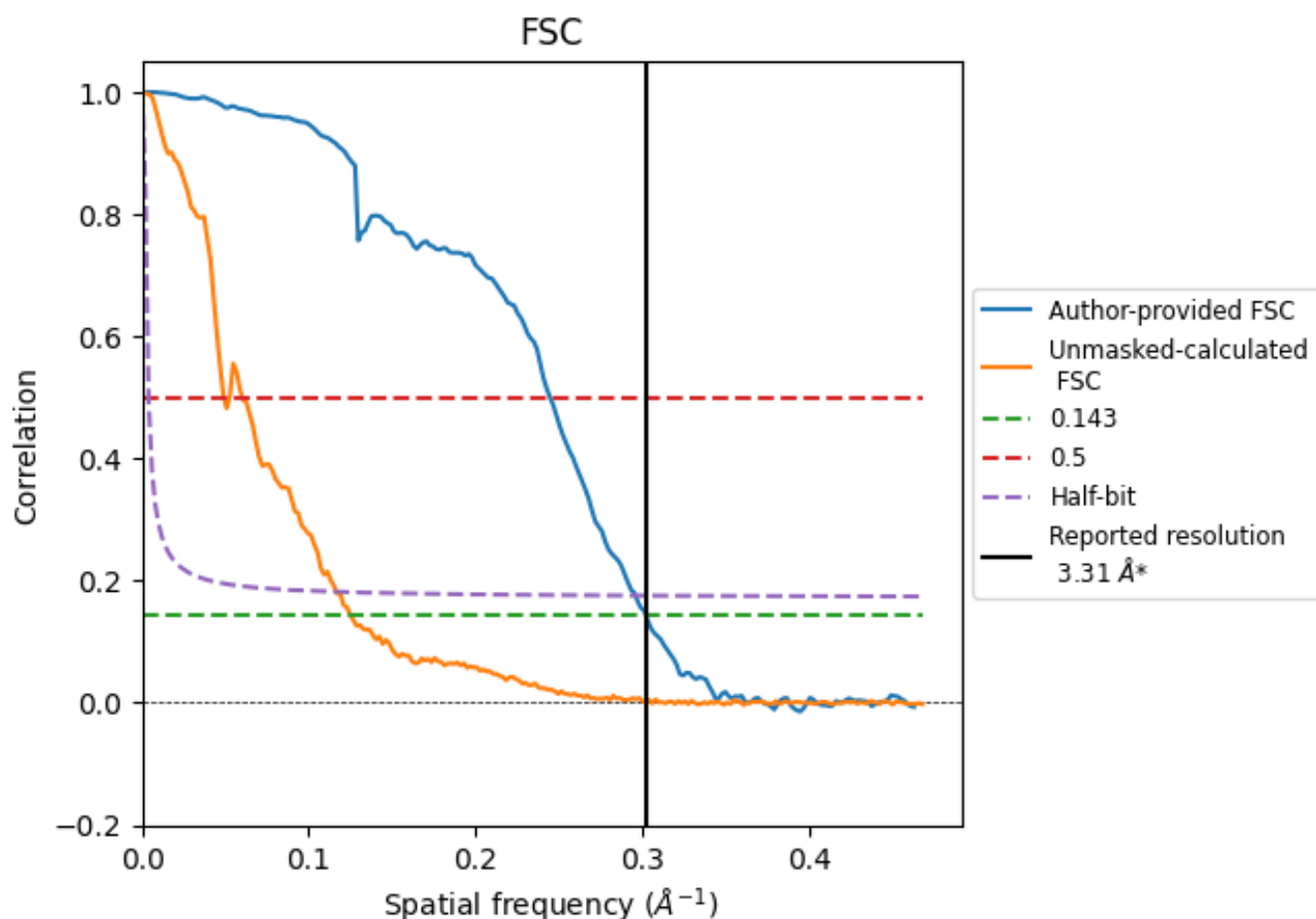


\*Reported resolution corresponds to spatial frequency of 0.302  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.302  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	3.31	4.08	3.38
Unmasked-calculated*	7.99	20.41	8.58

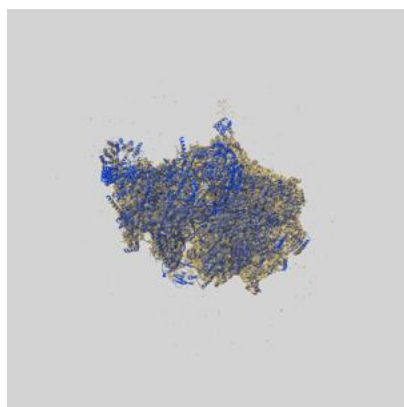
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.99 differs from the reported value 3.31 by more than 10 %



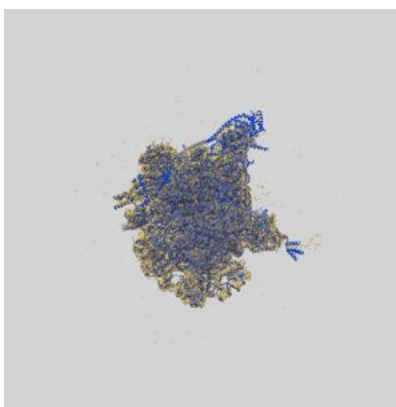
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71809 and PDB model 9PRD. Per-residue inclusion information can be found in section [3](#) on page [27](#).

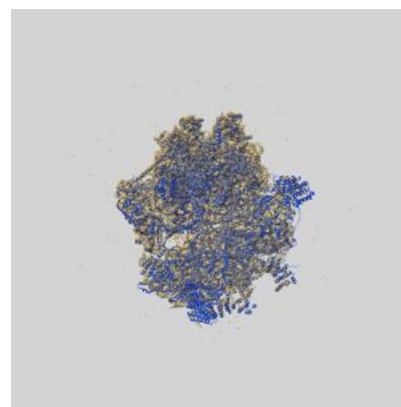
### 9.1 Map-model overlay [i](#)



X



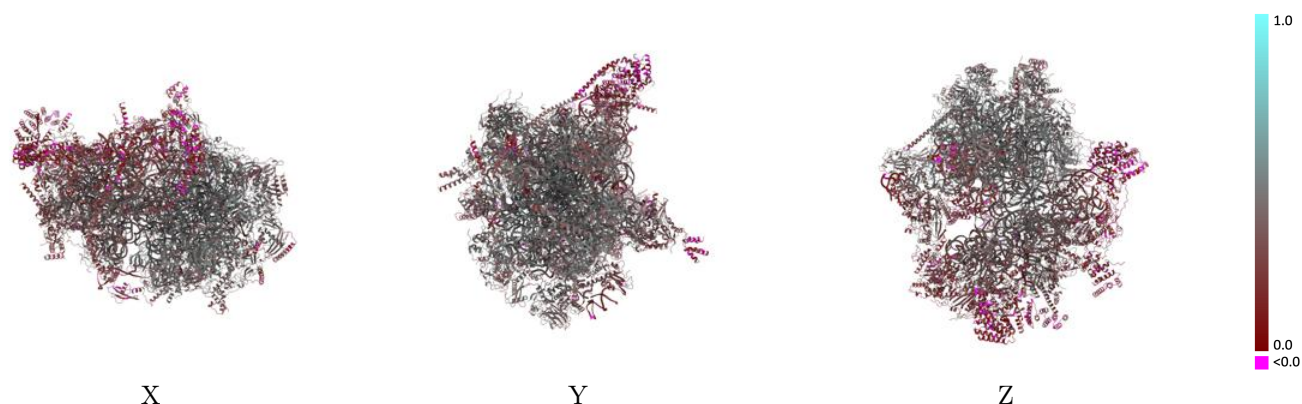
Y



Z

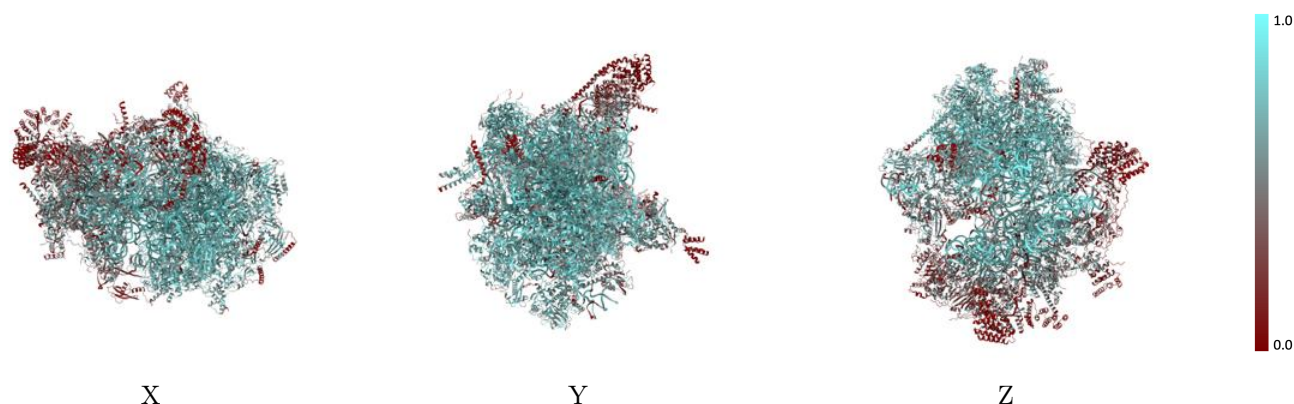
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



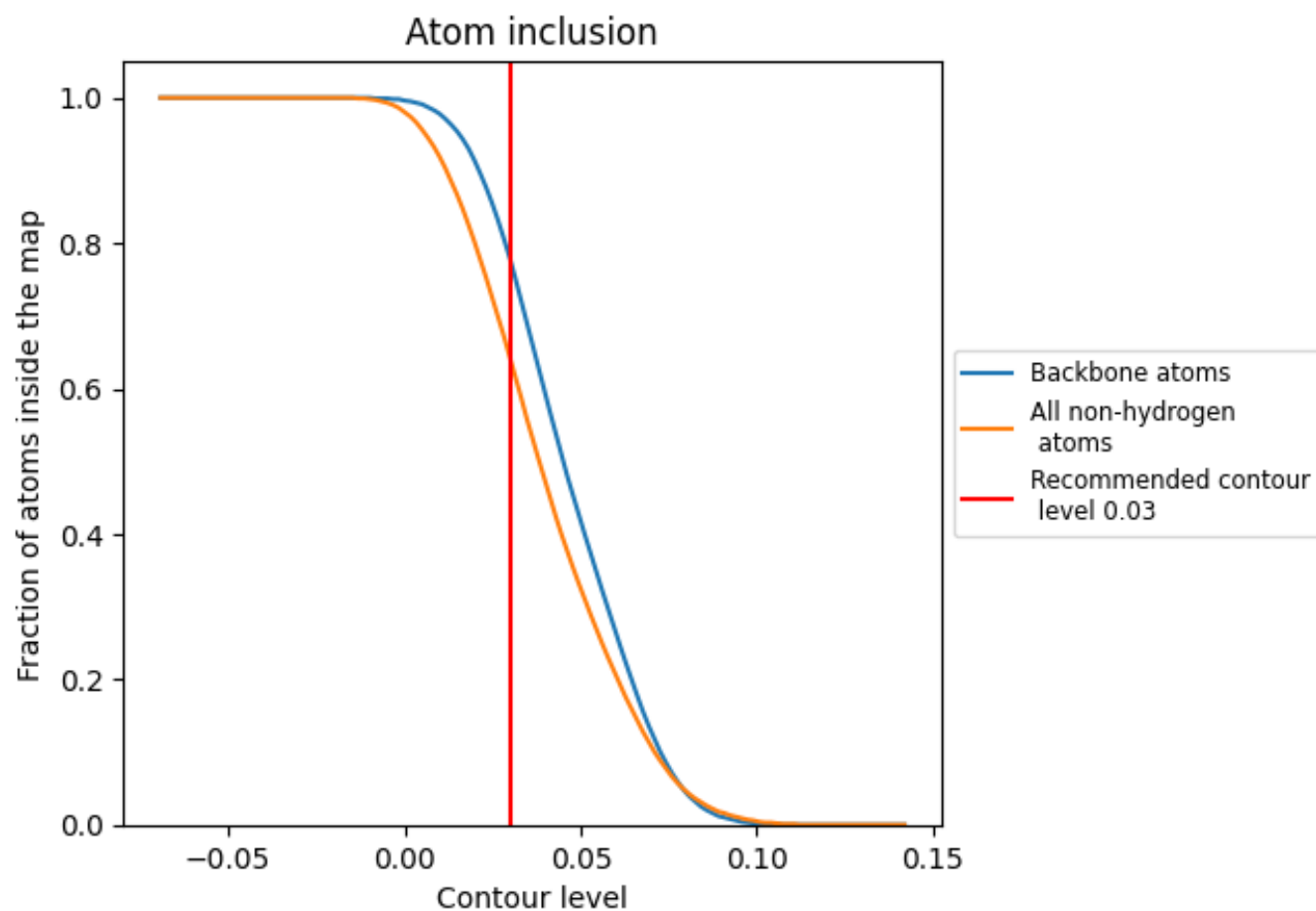
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6420	 0.3770
0	 0.7080	 0.4570
1	 0.6810	 0.4220
2	 0.7780	 0.4930
3	 0.7810	 0.4870
4	 0.7950	 0.4690
5	 0.7020	 0.4420
6	 0.6640	 0.4050
7	 0.6420	 0.4040
8	 0.4570	 0.3020
9	 0.6710	 0.4300
A	 0.8850	 0.4430
A0	 0.2450	 0.1780
A1	 0.3340	 0.2500
A2	 0.4700	 0.3380
A3	 0.6260	 0.4170
A4	 0.1720	 0.1670
AA	 0.8430	 0.3890
AB	 0.5390	 0.3490
AC	 0.4510	 0.3430
AD	 0.4410	 0.3390
AE	 0.5100	 0.3940
AF	 0.4850	 0.3280
AG	 0.4290	 0.3110
AH	 0.3750	 0.3070
AI	 0.5230	 0.3890
AJ	 0.5120	 0.3900
AK	 0.5050	 0.3340
AL	 0.5410	 0.3550
AM	 0.3690	 0.2440
AN	 0.5280	 0.3600
AO	 0.3510	 0.2590
AP	 0.5460	 0.3940
AQ	 0.5610	 0.3990
AR	 0.2740	 0.2040





























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Chain	Atom inclusion	Q-score
AS	 0.4440	 0.3080
AT	 0.4830	 0.3210
AU	 0.4350	 0.2500
AV	 0.1160	 0.1280
AW	 0.4440	 0.3320
AX	 0.3410	 0.2500
AY	 0.2850	 0.2400
AZ	 0.4050	 0.2770
Ax	 0.6920	 0.3300
Az	 0.2750	 0.2240
B	 0.7040	 0.2870
D	 0.7420	 0.4740
E	 0.7340	 0.4680
F	 0.7420	 0.4750
H	 0.3470	 0.2650
I	 0.5140	 0.3360
J	 0.3870	 0.2480
K	 0.7510	 0.4700
L	 0.6780	 0.4620
M	 0.7320	 0.4640
N	 0.7280	 0.4650
O	 0.7280	 0.4630
OX	 0.2590	 0.2500
P	 0.7030	 0.4290
Q	 0.6250	 0.4260
R	 0.7570	 0.4630
S	 0.6980	 0.4690
T	 0.7430	 0.4740
U	 0.6180	 0.4270
V	 0.6380	 0.4160
W	 0.7320	 0.4820
X	 0.6800	 0.4350
Y	 0.7250	 0.4430
Z	 0.7220	 0.4710
a	 0.5950	 0.4050
b	 0.7220	 0.4670
c	 0.6700	 0.4260
d	 0.5090	 0.3760
e	 0.4280	 0.2600
f	 0.5170	 0.3430
g	 0.7160	 0.4530
h	 0.6360	 0.3990

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Chain	Atom inclusion	Q-score
i	 0.7730	 0.4790
j	 0.6880	 0.4220
k	 0.5540	 0.3630
l	 0.4410	 0.2970
m	 0.4190	 0.2700
n	 0.2190	 0.3370
o	 0.7700	 0.4710
p	 0.5590	 0.3670
q	 0.4900	 0.3040
r	 0.7310	 0.4530
s	 0.7080	 0.4400
t	 0.1330	 0.1960
u	 0.0350	 0.1120