



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 09:05 AM EDT

PDB ID : 9PSI / pdb_00009psi
EMDB ID : EMD-71828
Title : In situ structure of the human mitoribosome in the A-P-E state from TACO1-knockout cells
Authors : Wang, S.; Xiong, Y.; Zhang, Y.
Deposited on : 2025-07-25
Resolution : 3.12 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
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) : 2.50

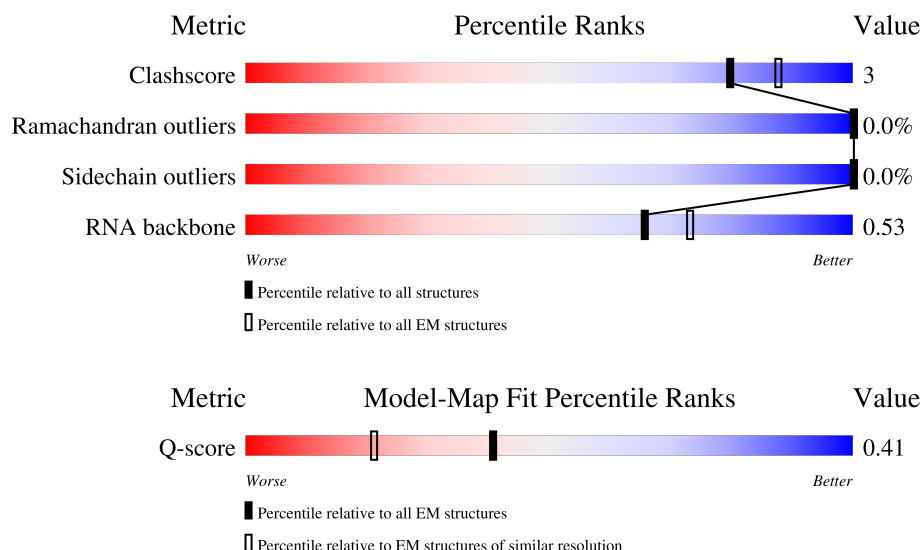
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.12 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.



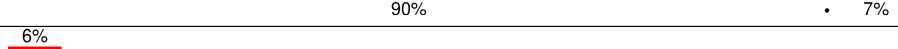
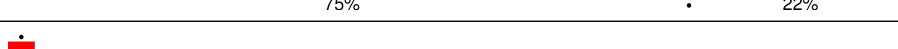
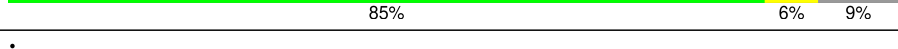
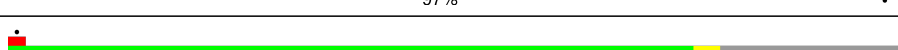
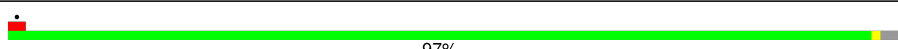
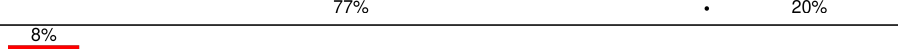
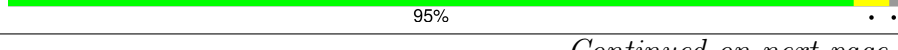
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14478 (2.62 - 3.62)

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

Mol	Chain	Length	Quality of chain
1	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	

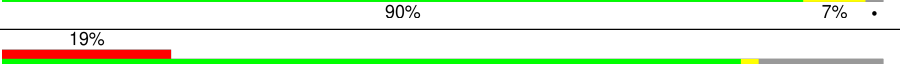
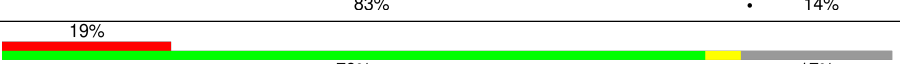
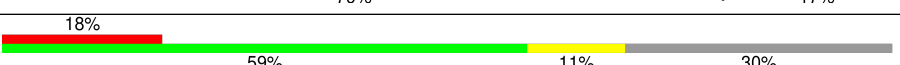
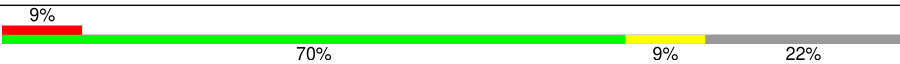
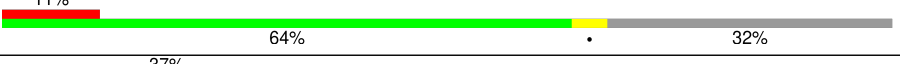
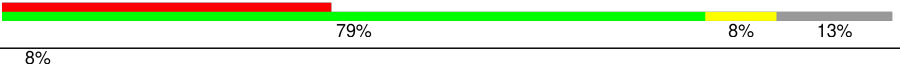
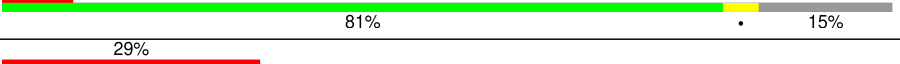
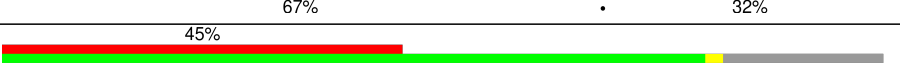
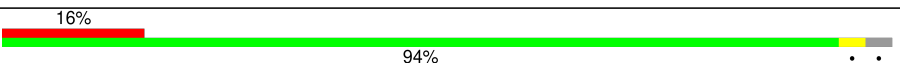
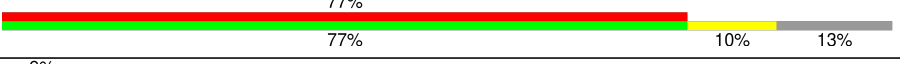
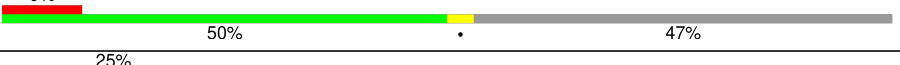
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Mol	Chain	Length	Quality of chain
29	W	148	
30	X	256	
31	Y	250	
32	Z	161	
33	z	325	
34	V	216	
35	b	215	
36	d	306	
37	e	279	
38	g	166	
39	h	158	
40	i	128	
41	j	123	
42	k	112	
43	l	138	
44	m	128	
45	n	43	
46	o	102	
47	q	222	
48	r	196	
49	t	198	
49	u	198	
50	c	332	
51	f	212	
52	p	206	

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Mol	Chain	Length	Quality of chain
53	s	439	
54	AB	296	
55	AC	167	
56	AD	430	
57	AE	125	
58	AF	242	
59	AG	396	
60	AH	201	
61	AJ	138	
62	AK	128	
63	AL	257	
64	AM	137	
65	AN	130	
66	AO	258	
67	AP	142	
68	AR	360	
69	AS	190	
70	AT	173	
71	AU	205	
72	AV	414	
73	AW	187	
74	AZ	106	
75	A0	217	
76	A1	323	
77	A3	199	

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Mol	Chain	Length	Quality of chain
78	Az	34	
79	AY	395	
80	AA	954	
81	AI	194	
82	OX	435	
83	a	142	
84	Ax	71	
85	Ay	76	
86	Aw	76	
87	A4	689	
88	AX	398	
89	A2	118	
90	AQ	87	
91	B	72	

2 Entry composition

There are 102 unique types of molecules in this entry. The entry contains 181394 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 Large ribosomal subunit protein uL1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	252	Total	C	N	O	S	0	0
			2027	1304	336	381	6		

- Molecule 34 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L45, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L49, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 42 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	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 43 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 45 is a protein called Nascent polypeptide.

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

- Molecule 46 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 47 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 48 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 49 is a protein called 39S ribosomal protein L12, mitochondrial.

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

- Molecule 50 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 51 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 52 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 53 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 54 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 55 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 56 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 57 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 58 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 59 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 60 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 61 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 62 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 63 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 64 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 65 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 66 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 67 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 68 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 69 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 70 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 71 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 72 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 73 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 74 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 75 is a protein called Small ribosomal subunit protein mS34.

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

- Molecule 76 is a protein called 28S ribosomal protein S35, mitochondrial.

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

- Molecule 77 is a protein called Aurora kinase A-interacting protein.

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

- Molecule 78 is a RNA chain called mRNA.

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

- Molecule 79 is a protein called 28S ribosomal protein S31, mitochondrial.

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

- Molecule 80 is a RNA chain called 12S mitochondrial rRNA.

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

- Molecule 81 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 82 is a protein called Mitochondrial inner membrane protein OXA1L.

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

- Molecule 83 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 84 is a RNA chain called P/P-tRNA.

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

- Molecule 85 is a RNA chain called E/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Ay	70	Total	C	N	O	P	0	0
			1483	665	261	487	70		

- Molecule 86 is a RNA chain called A/A-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Aw	68	Total	C	N	O	P	0	0
			1434	646	248	472	68		

- Molecule 87 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 88 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 89 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	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 90 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	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 91 is a RNA chain called mitochondrial tRNAVal.

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

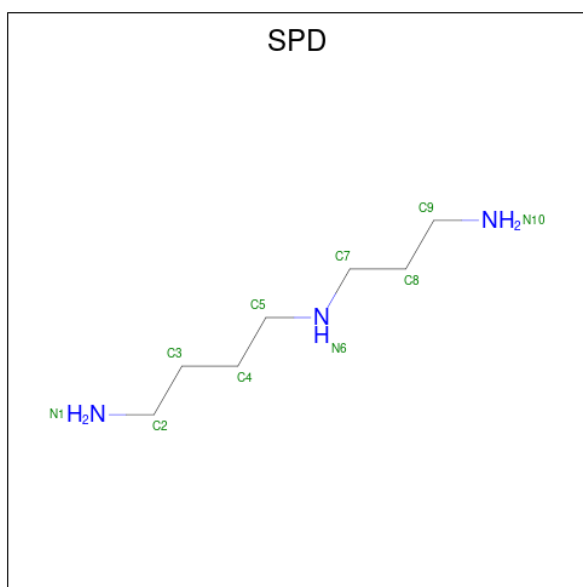
- Molecule 92 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
92	0	1	Total	Zn	0
			1	1	
92	4	1	Total	Zn	0
			1	1	
92	AO	1	Total	Zn	0
			1	1	

- Molecule 93 is POTASSIUM ION (CCD ID: K) (formula: K).

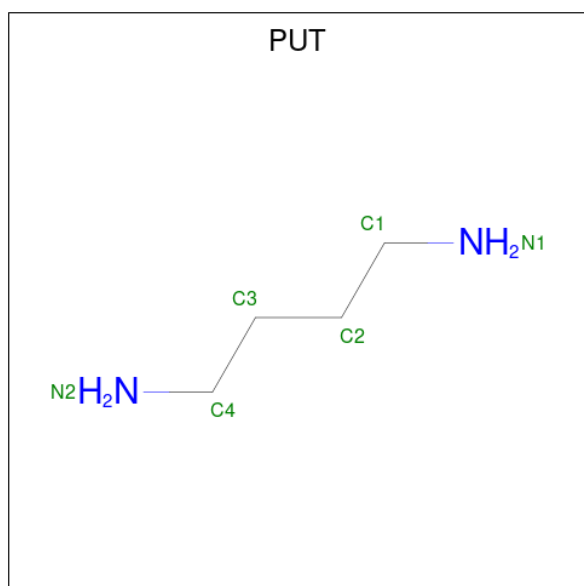
Mol	Chain	Residues	Atoms	AltConf
93	3	1	Total K 1 1	0
93	A	29	Total K 29 29	0
93	D	1	Total K 1 1	0
93	M	1	Total K 1 1	0
93	N	1	Total K 1 1	0
93	P	1	Total K 1 1	0
93	W	1	Total K 1 1	0
93	o	1	Total K 1 1	0
93	AJ	1	Total K 1 1	0
93	Az	1	Total K 1 1	0
93	AA	16	Total K 16 16	0

- Molecule 94 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 95 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



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

- Molecule 96 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

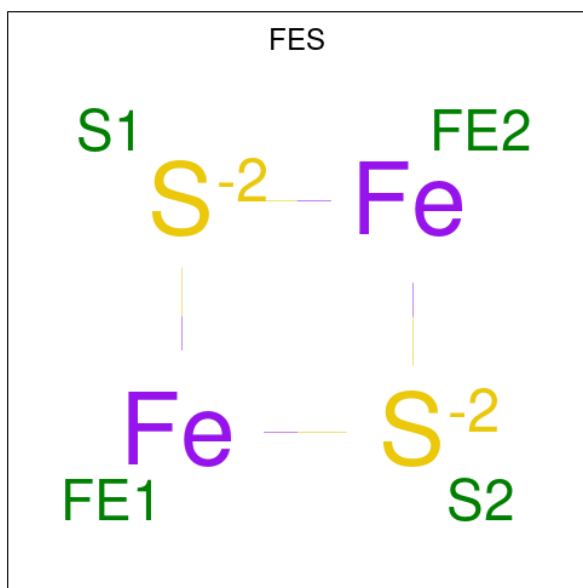
Mol	Chain	Residues	Atoms		AltConf
96	A	137	Total	Mg	0
			137	137	
96	D	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
96	E	1	Total 1	Mg 1	0
96	g	1	Total 1	Mg 1	0
96	AB	1	Total 1	Mg 1	0
96	AK	1	Total 1	Mg 1	0
96	A3	1	Total 1	Mg 1	0
96	AA	59	Total 59	Mg 59	0
96	AX	1	Total 1	Mg 1	0

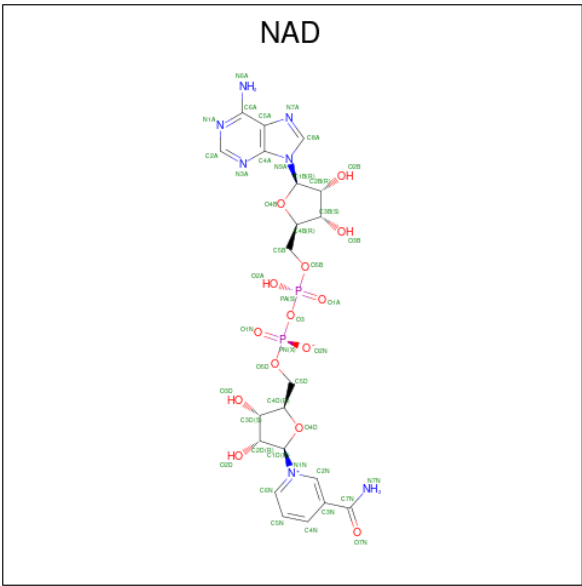
- Molecule 97 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

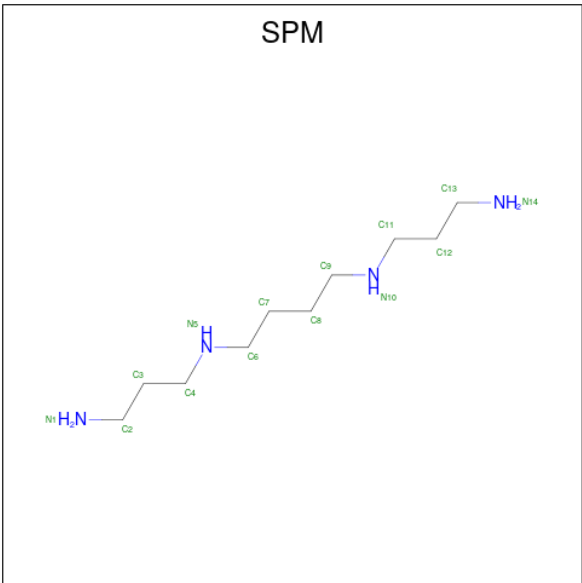
- Molecule 98 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:

C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 99 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



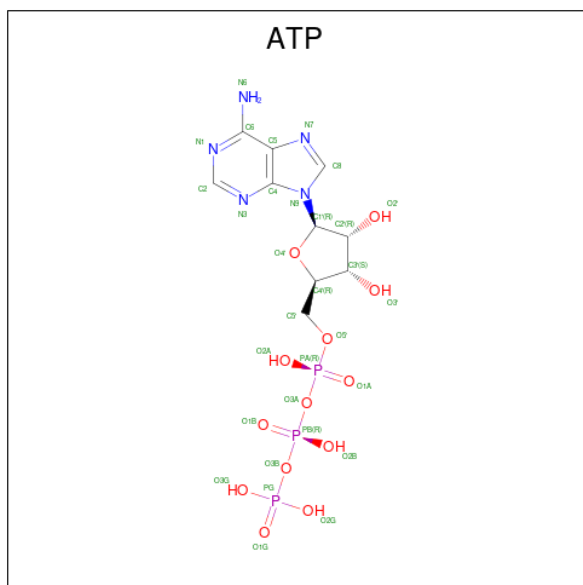
Mol	Chain	Residues	Atoms			AltConf
99	AA	1	Total	C	N	0
			14	10	4	

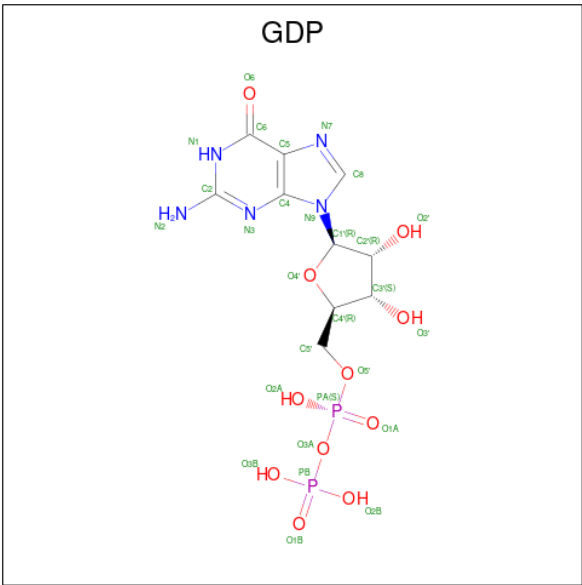
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Mol	Chain	Residues	Atoms			AltConf
99	AA	1	Total	C	N	0
			14	10	4	

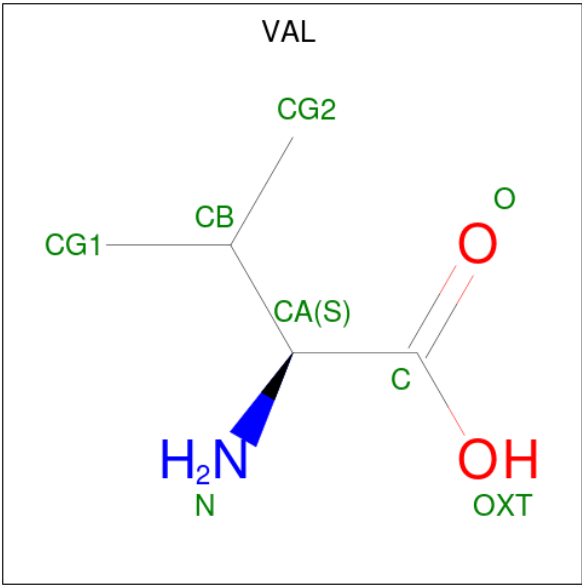
- Molecule 100 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 102 is VALINE (CCD ID: VAL) (formula: C₅H₁₁NO₂).

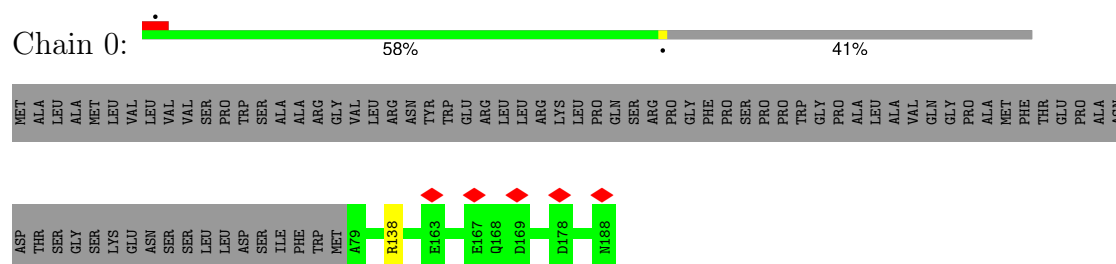


Mol	Chain	Residues	Atoms				AltConf
102	B	1	Total	C	N	O	0
			7	5	1	1	

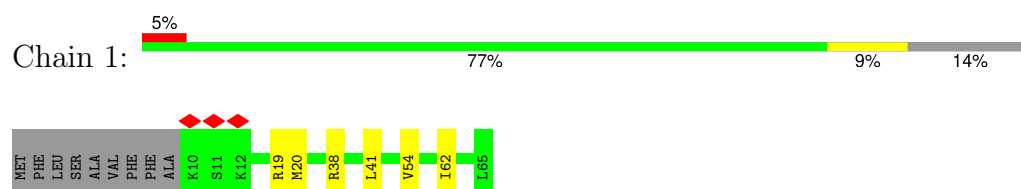
3 Residue-property plots [i](#)

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.

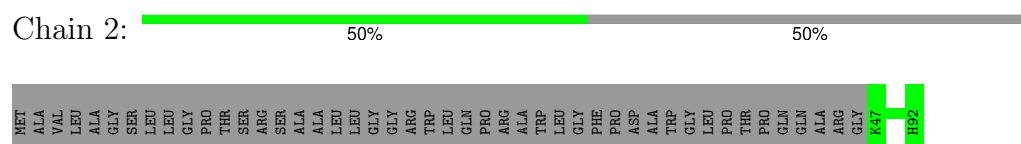
- Molecule 1: 39S ribosomal protein L32, mitochondrial



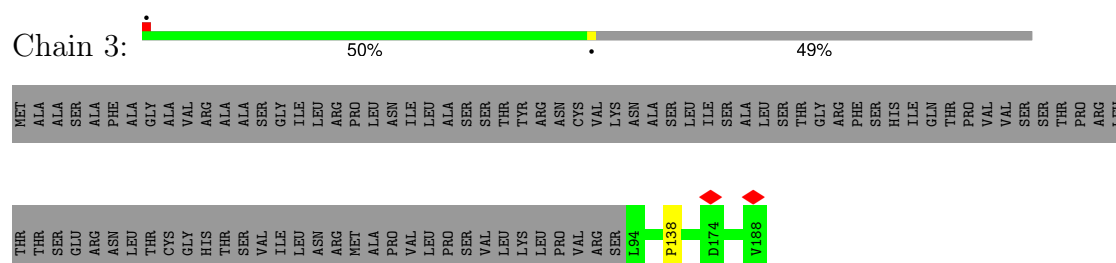
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial



- Molecule 4: 39S ribosomal protein L35, mitochondrial



- Molecule 5: 39S ribosomal protein L36, mitochondrial



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

LEU PRO ALA LEU GLY P66 M103

- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:  90% 7%

MET ALA LEU ALA SER GLY PRO ALA ARG ALA LEU CYS ALA GLY SER GLN LEU ARG GLY LEU VAL PHE GLY ARG ALA PRO ARG ARG GLY A30 E115 G116 Q119 I147 Q165 E169 T175 Q191 R201 T232 R242 H289 D307 L336 Q343

T362 K394 L417 A423

- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:  90% 6% 7%

MET ALA PRO TRP ARG ALA ALA CYS GLU CYS ARG TRP ARG GLY PHE THR SER ALA VAL LEU GLY R27 D39 E80 K81 T82 D83 P84 K85 E86 I90 R106 A115 L161 G180 E181 D182 D183 L184 V187 E207 A208 E209 E210 L217

H234 V235 L236 R244 E247 T251 P257 D276 Q277 D284 T300 E309 F319 Y380

- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7:  81% 6% 13%

MET GLU ALA LEU ALA MET GLY SER ARG ALA LEU LEU TRP VAL ALA PRO GLY GLY ILE LYS TRP ARG PHE ILE THR SER SER ALA SER Q34 L35 T59 P60 R61 K102 D109 P112 W113 D114 K117 N139 W143 M150 G151 C152 V153 I154

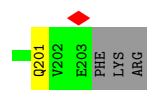
E161 V172 P173 V174 K204 L219 E220 F260 P267 F276 L286 Q287 Q290 P291 S292 R296 V304 H309 L317 E326 D327 G1N SER LYS ALA THR GLU GLU CYS THR

- Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8:  70% 19% 6% 24%

MET THR ALA SER VAL LEU ARG SER ILE LEU LEU ALA LEU ARG PRO THR THR GLY LEU LEU GLY THR TRP GLN THR GLN LEU ARG THR HIS GLN ARG ALA SER LEU LEU SER PHE TRP LEU LEU ILE PRO MET ARG S47 E48 R51 K52 K53 K54 K55 V56 D57 P58 K59 K60 D61

Q62 P63 A64 K65 L68 K69 R73 E76 K77 Q80 E86 L92 K93 F94 L95 D96 K97 A98 R99 E105 L106 E109 L117 K125 I136 E148 L152 E153 K156 A161 R164 N167 M184 Y185 Q186 P187 P188 Y192 M193 D194 I195



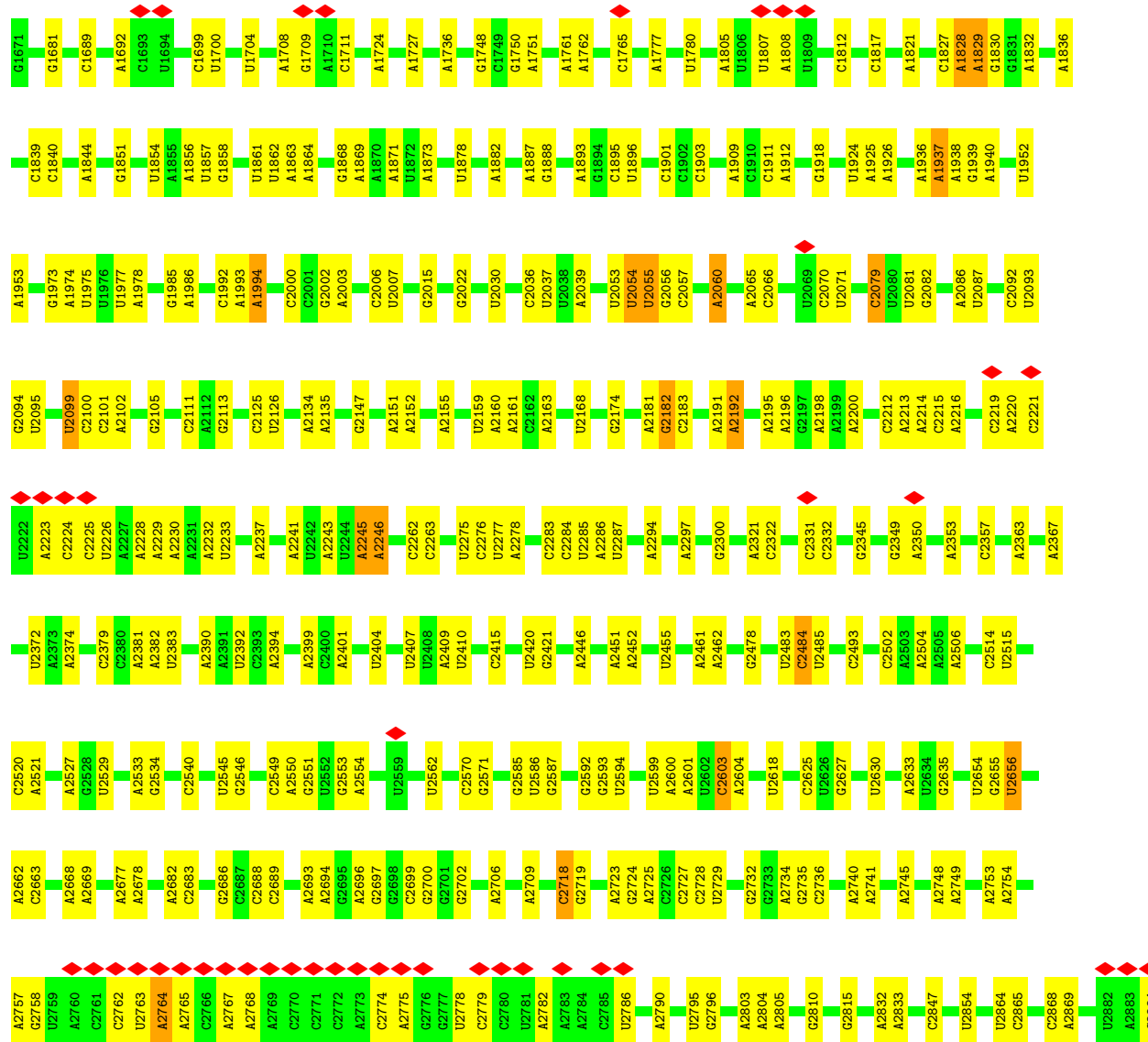
- Molecule 10: 39S ribosomal protein L41, mitochondrial

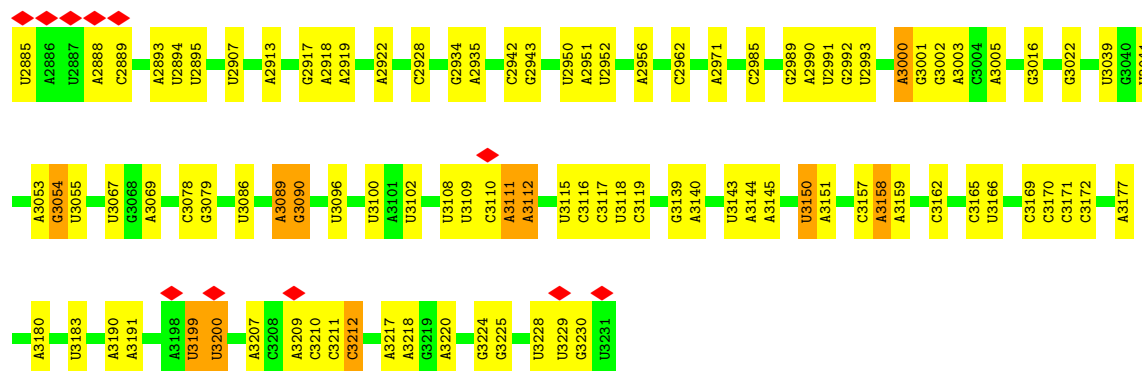
Chain 9: 88% 9%



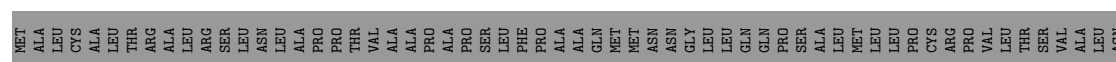
- Molecule 11: 16S mitochondrial rRNA

Chain A: 73% 26%

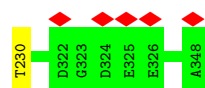
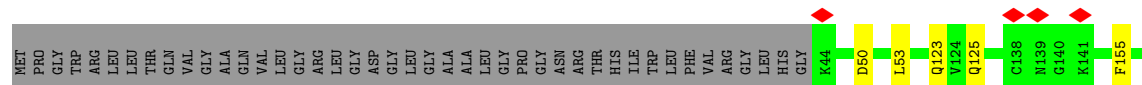
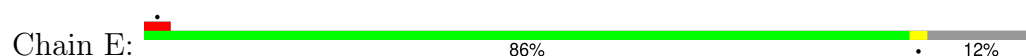




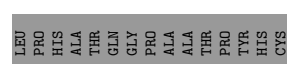
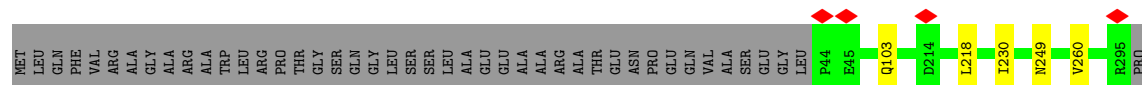
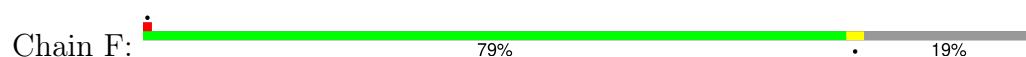
- Molecule 12: 39S ribosomal protein L2, mitochondrial



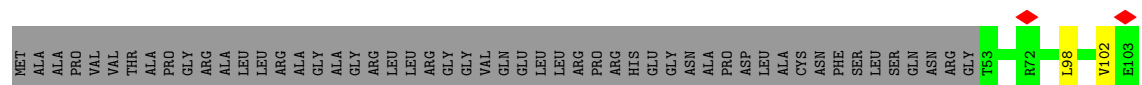
- Molecule 13: 39S ribosomal protein L3, mitochondrial

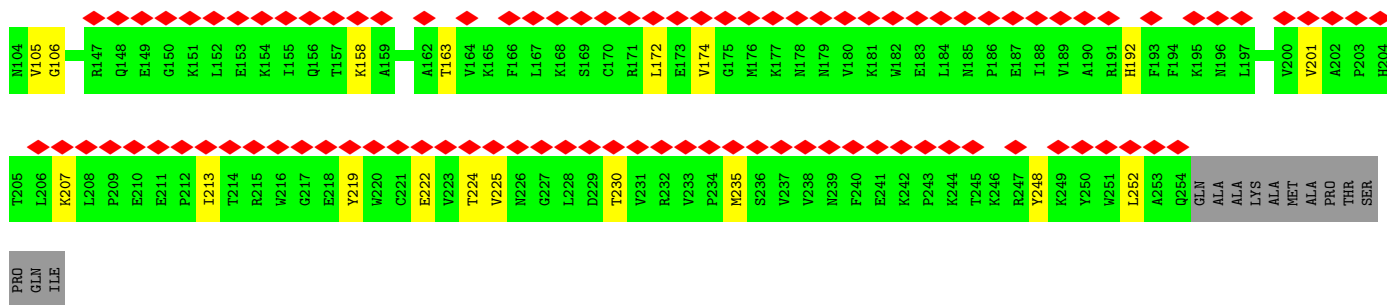


- Molecule 14: 39S ribosomal protein L4, mitochondrial

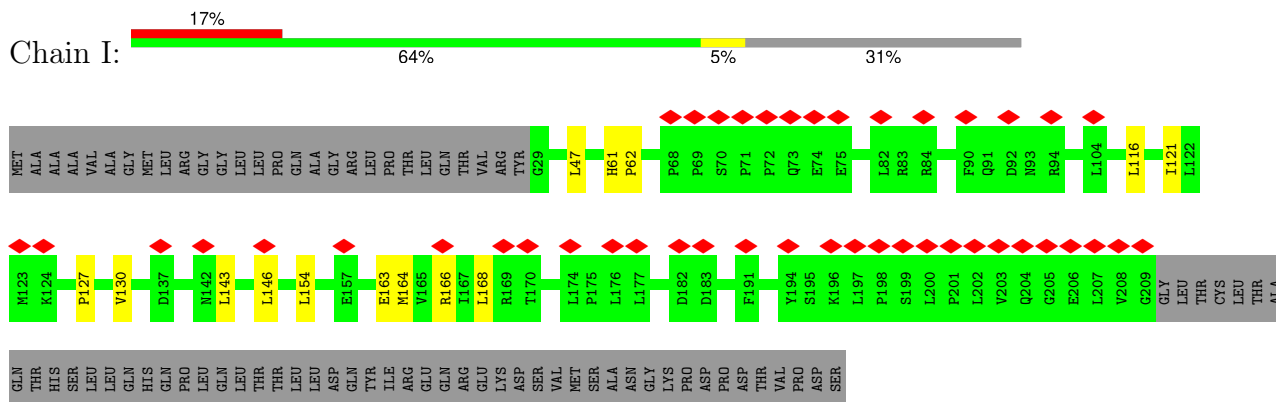


- Molecule 15: 39S ribosomal protein L9, mitochondrial

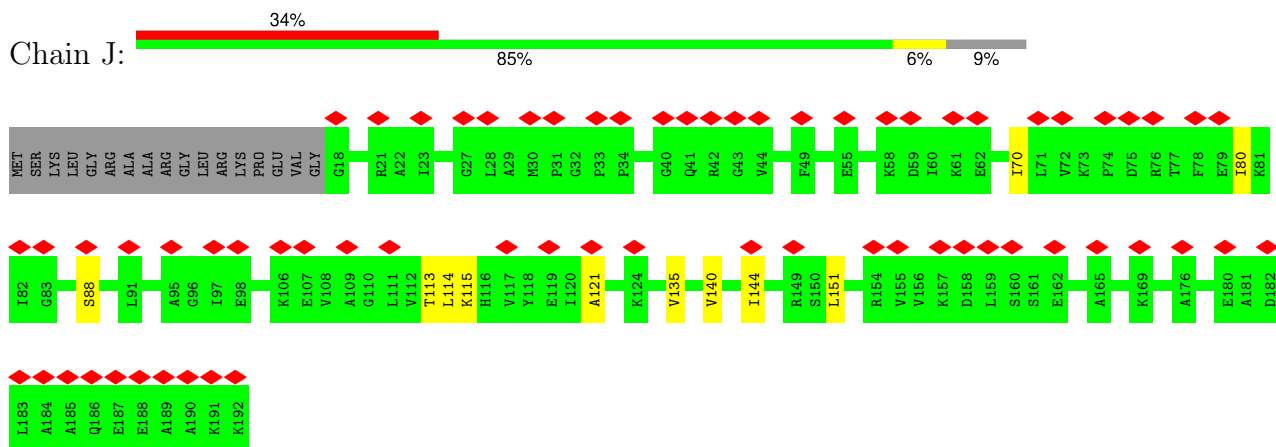




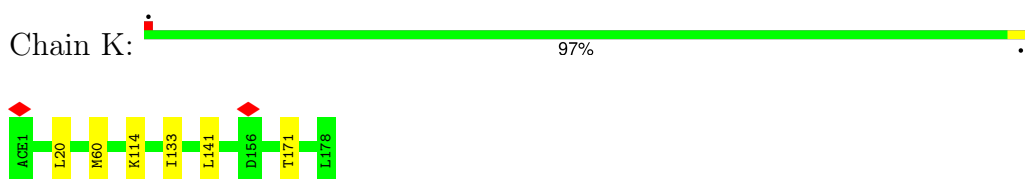
- Molecule 16: 39S ribosomal protein L10, mitochondrial



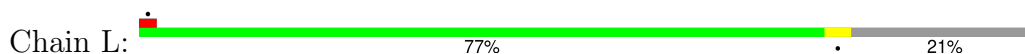
- Molecule 17: 39S ribosomal protein L11, mitochondrial



- Molecule 18: Large ribosomal subunit protein uL13m

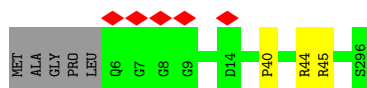


- Molecule 19: 39S ribosomal protein L14, mitochondrial

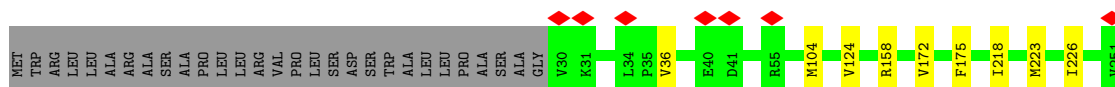
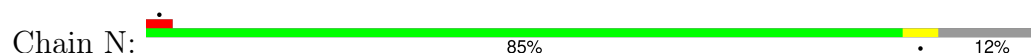




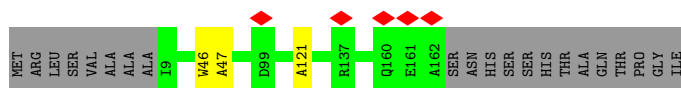
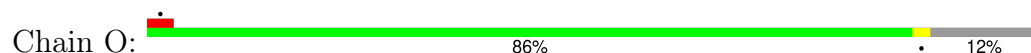
- Molecule 20: 39S ribosomal protein L15, mitochondrial



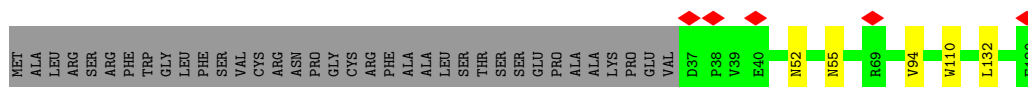
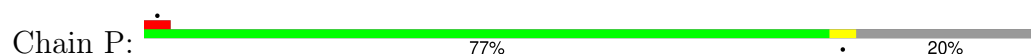
- Molecule 21: 39S ribosomal protein L16, mitochondrial



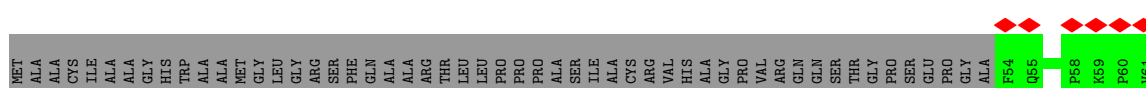
- Molecule 22: 39S ribosomal protein L17, mitochondrial



- Molecule 23: 39S ribosomal protein L18, mitochondrial



- Molecule 24: 39S ribosomal protein L19, mitochondrial

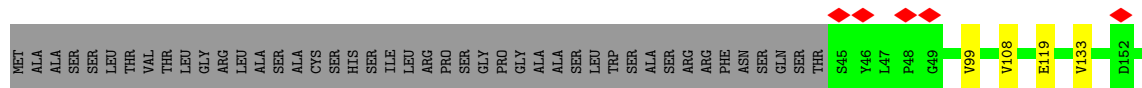


- Molecule 25: 39S ribosomal protein L20, mitochondrial

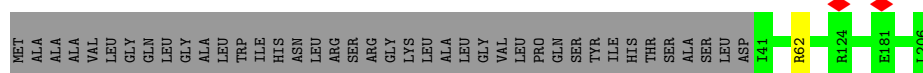
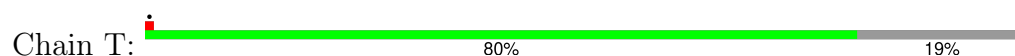




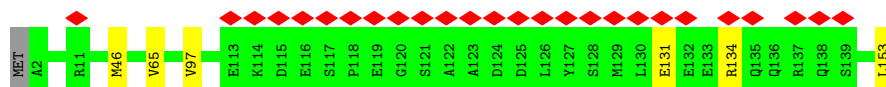
- Molecule 26: 39S ribosomal protein L21, mitochondrial



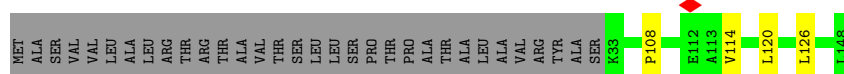
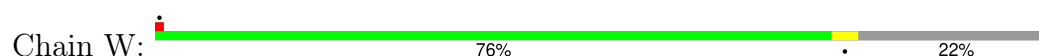
- Molecule 27: 39S ribosomal protein L22, mitochondrial



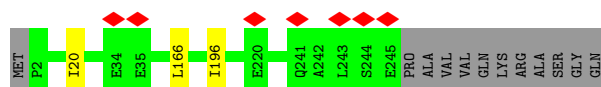
- Molecule 28: 39S ribosomal protein L23, mitochondrial



- Molecule 29: 39S ribosomal protein L27, mitochondrial

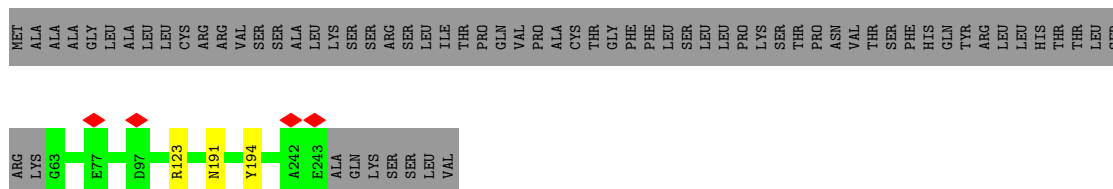


- Molecule 30: 39S ribosomal protein L28, mitochondrial

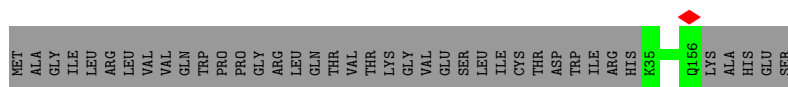
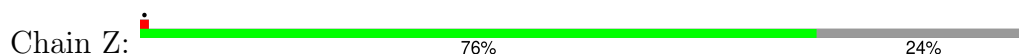


- Molecule 31: 39S ribosomal protein L47, mitochondrial

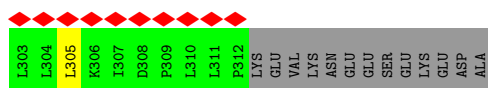
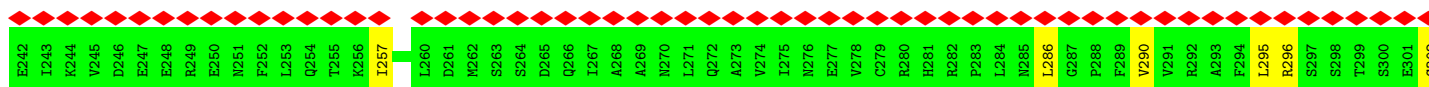
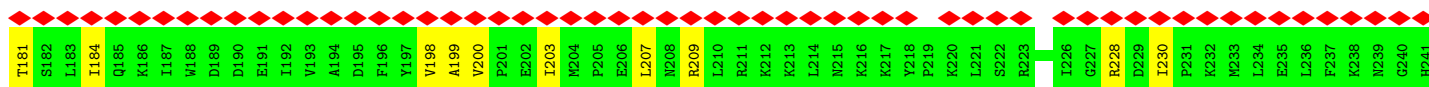
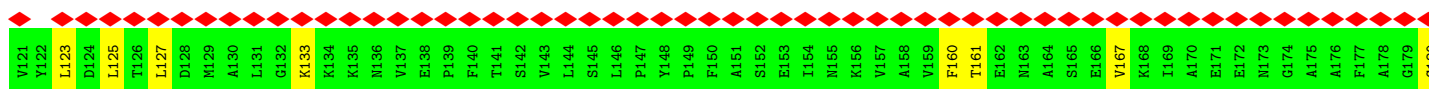
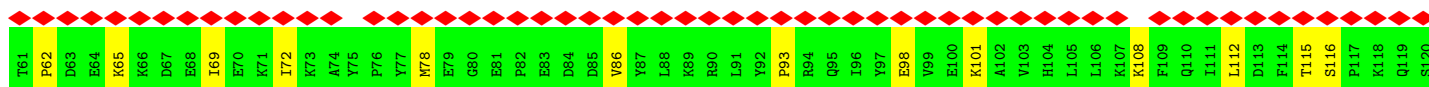
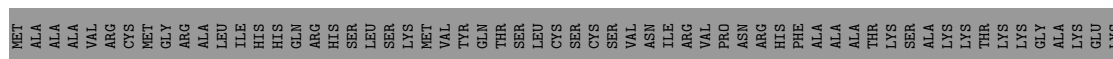
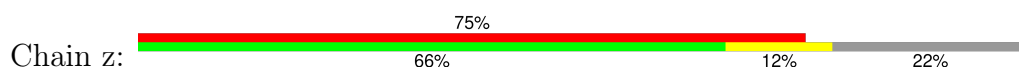




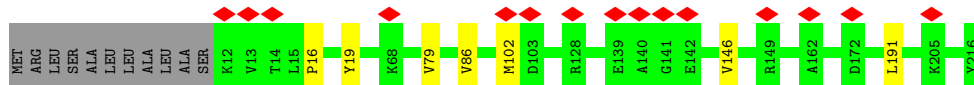
- Molecule 32: 39S ribosomal protein L30, mitochondrial



- Molecule 33: Large ribosomal subunit protein uL1m

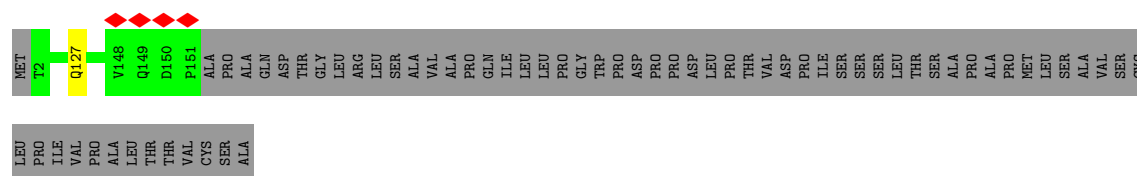


- Molecule 34: 39S ribosomal protein L24, mitochondrial

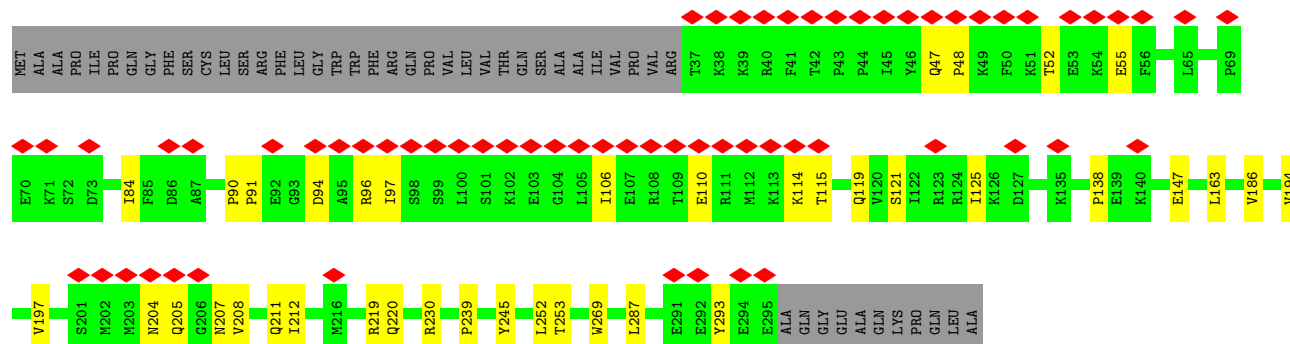


- Molecule 35: 39S ribosomal protein L43, mitochondrial

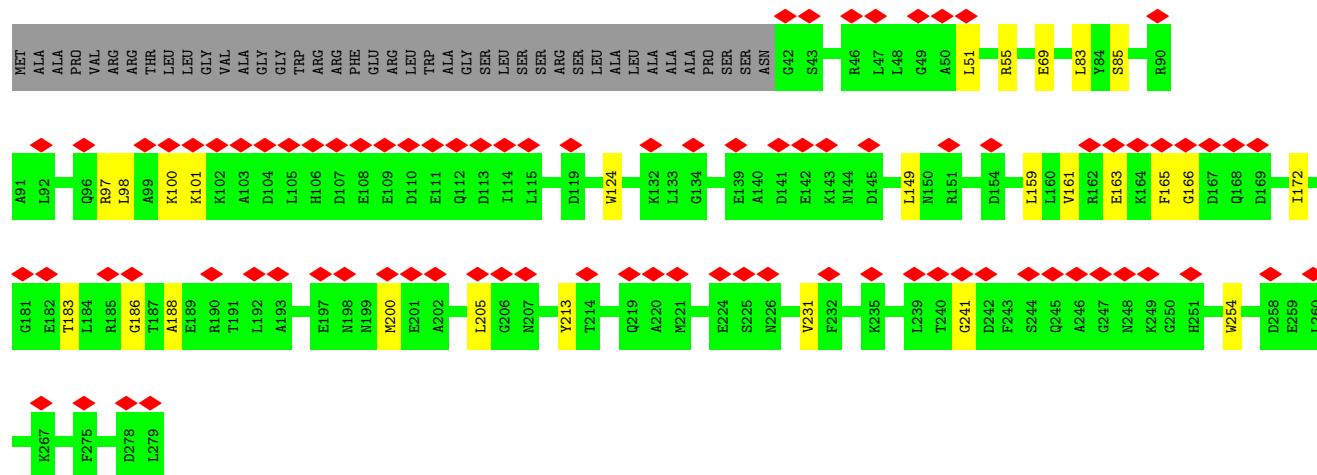
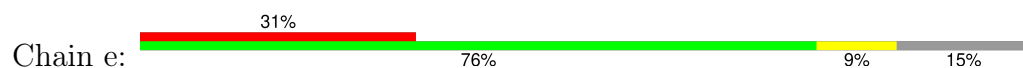




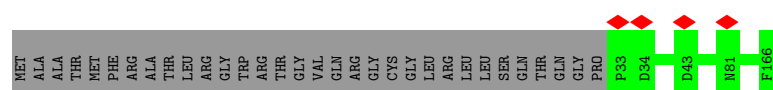
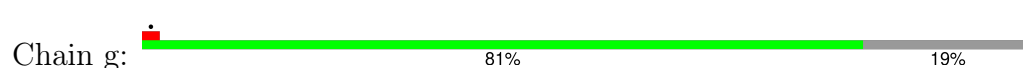
- Molecule 36: 39S ribosomal protein L45, mitochondrial



- Molecule 37: 39S ribosomal protein L46, mitochondrial

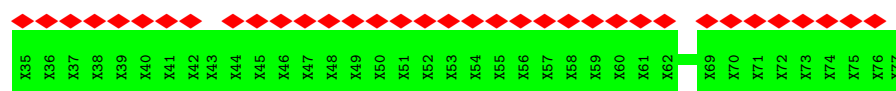


- Molecule 38: 39S ribosomal protein L49, mitochondrial

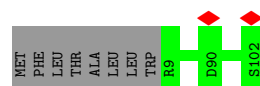


- Molecule 39: 39S ribosomal protein L50, mitochondrial

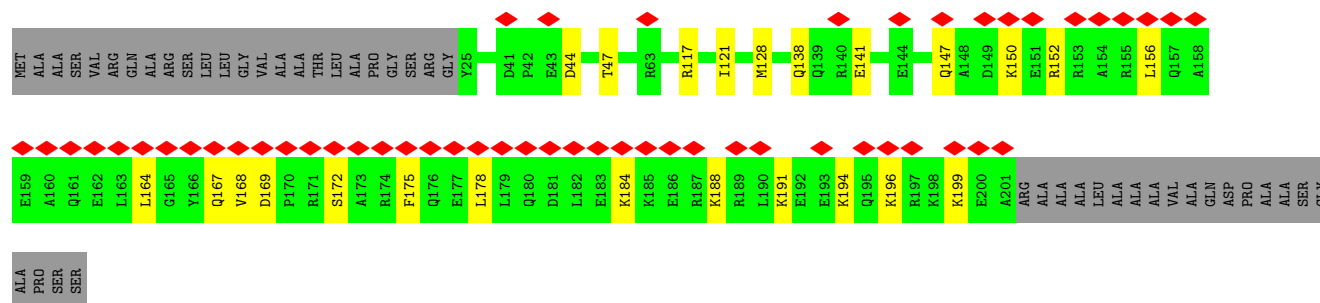




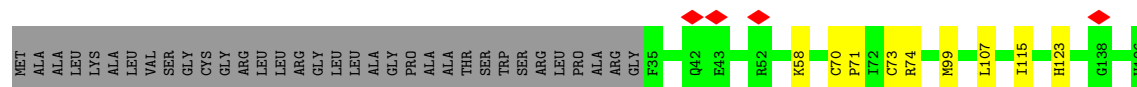
Chain o: 92% 8%



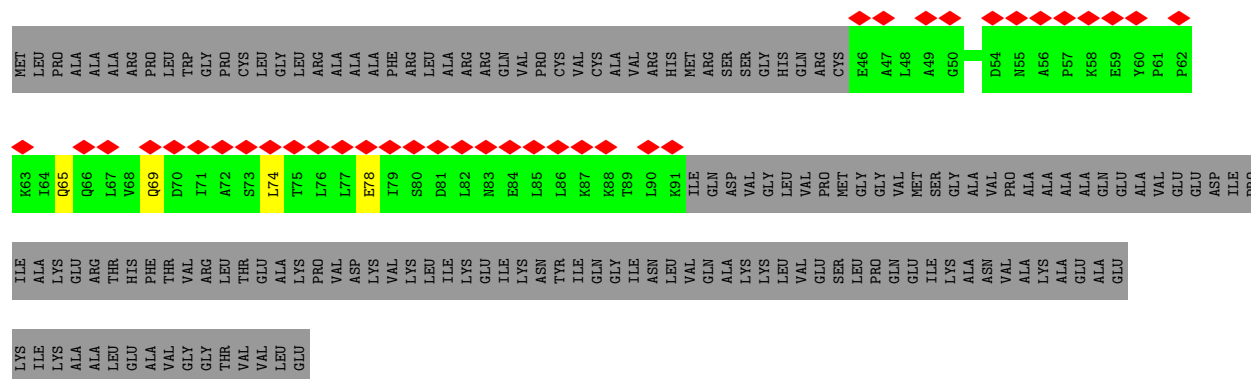
Chain g:



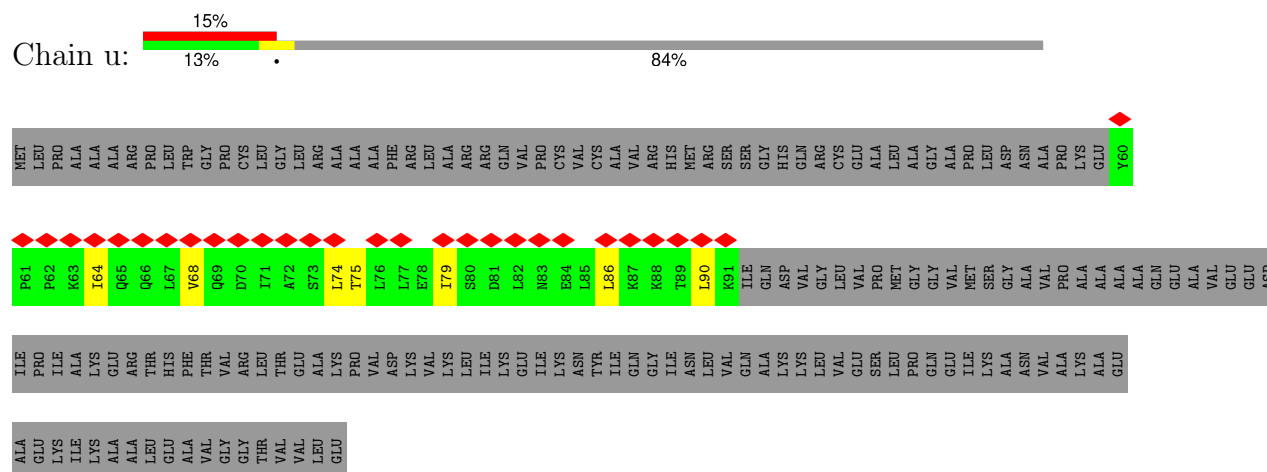
Chain r:



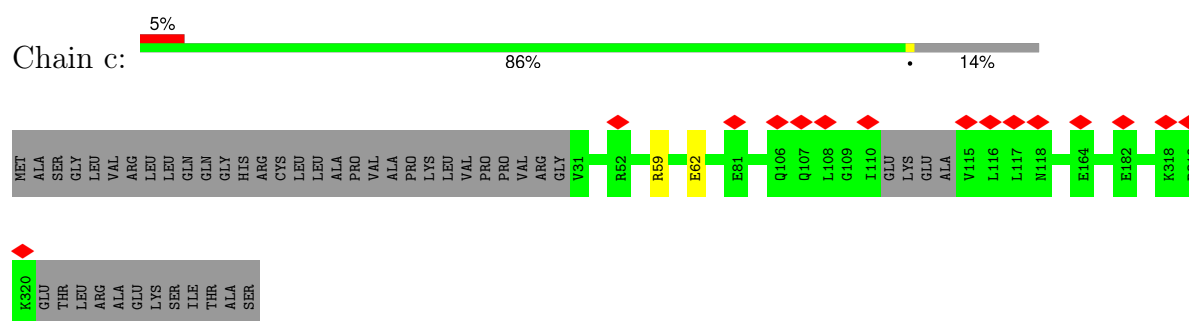
Chain t:



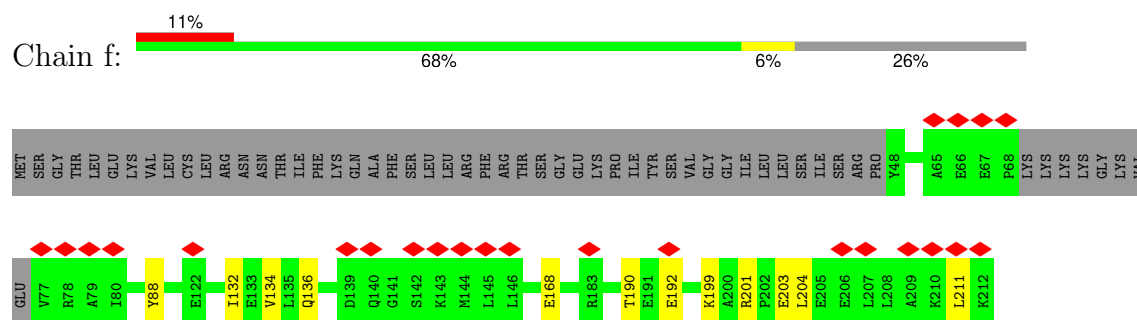
- Molecule 49: 39S ribosomal protein L12, mitochondrial



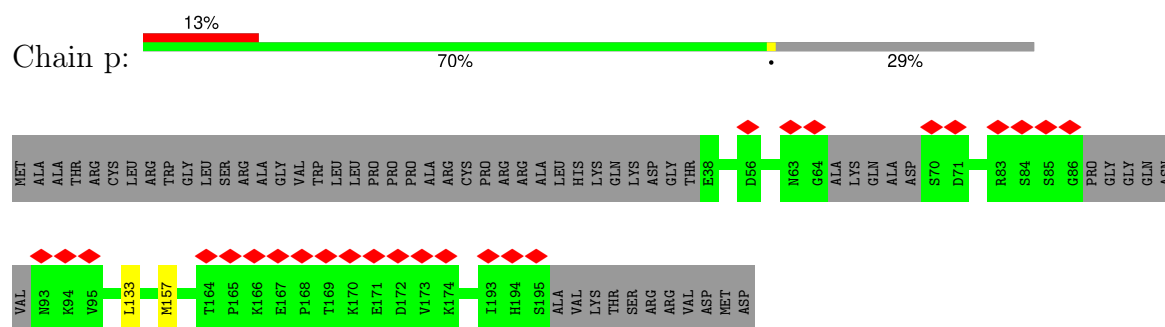
- Molecule 50: 39S ribosomal protein L44, mitochondrial



- Molecule 51: 39S ribosomal protein L48, mitochondrial

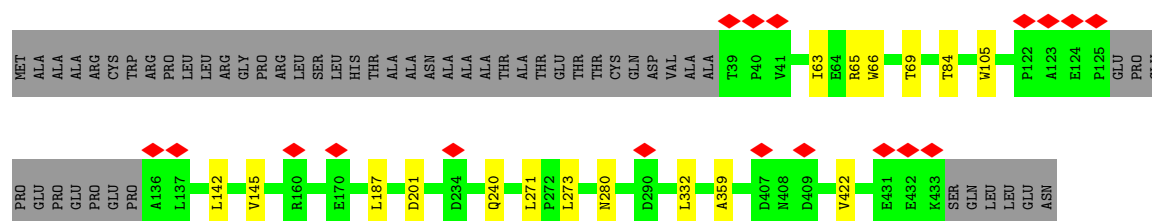


- Molecule 52: Peptidyl-tRNA hydrolase ICT1, mitochondrial



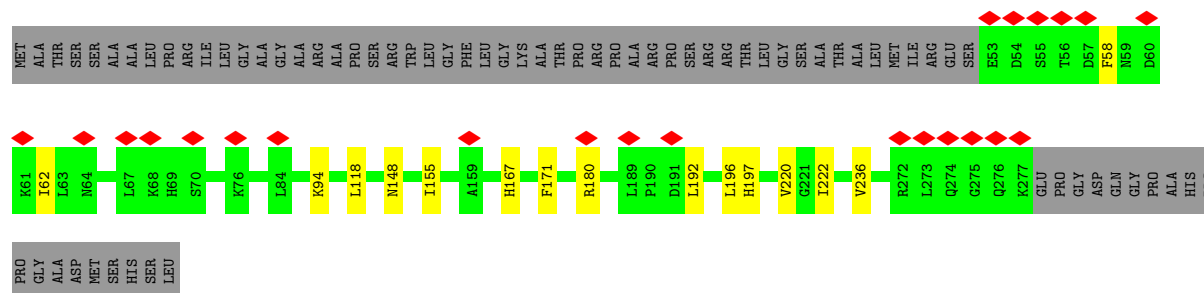
- Molecule 53: 39S ribosomal protein S30, mitochondrial

Chain s: 



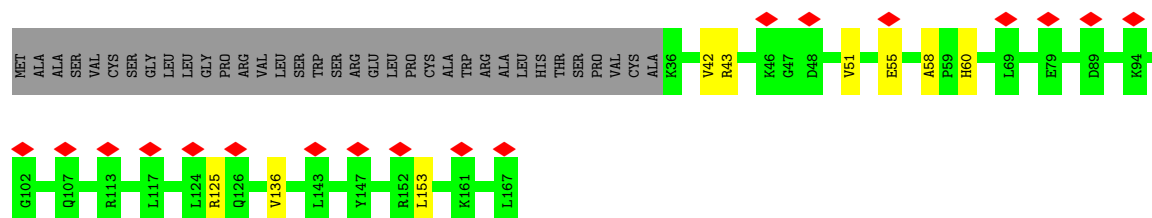
- Molecule 54: 28S ribosomal protein S2, mitochondrial

Chain AB: 



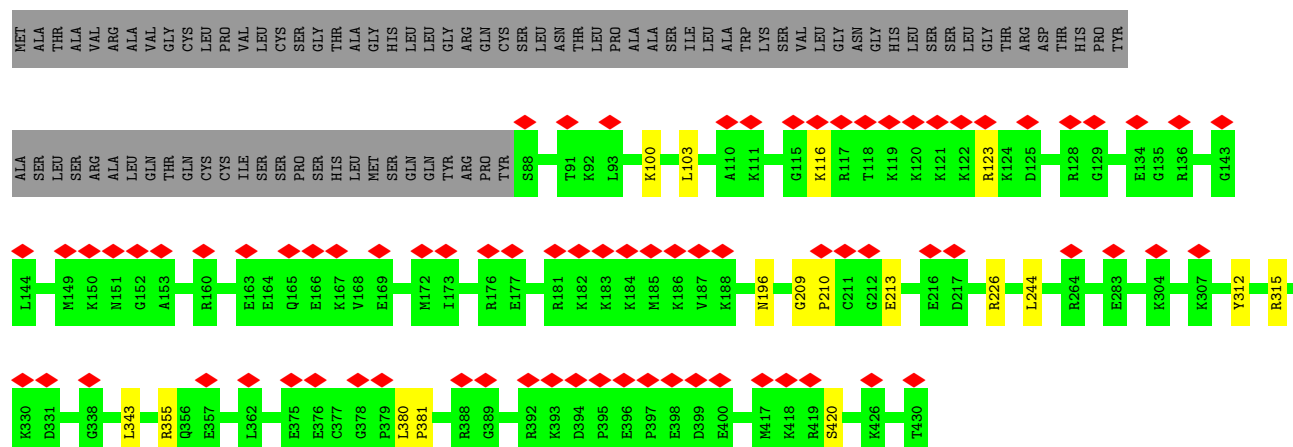
- Molecule 55: 28S ribosomal protein S24, mitochondrial

Chain AC: 

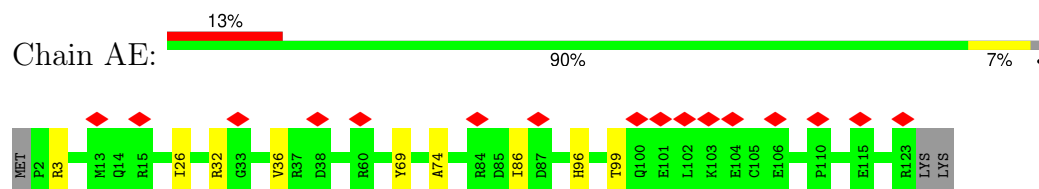


- Molecule 56: 28S ribosomal protein S5, mitochondrial

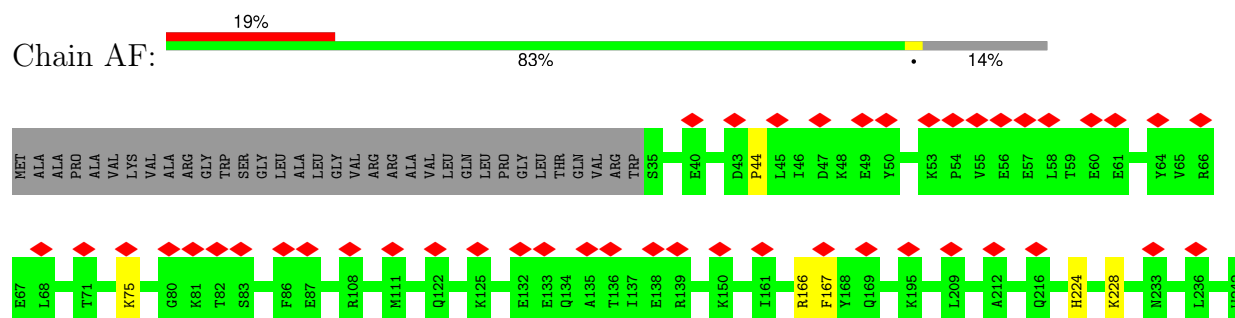
Chain AD: 



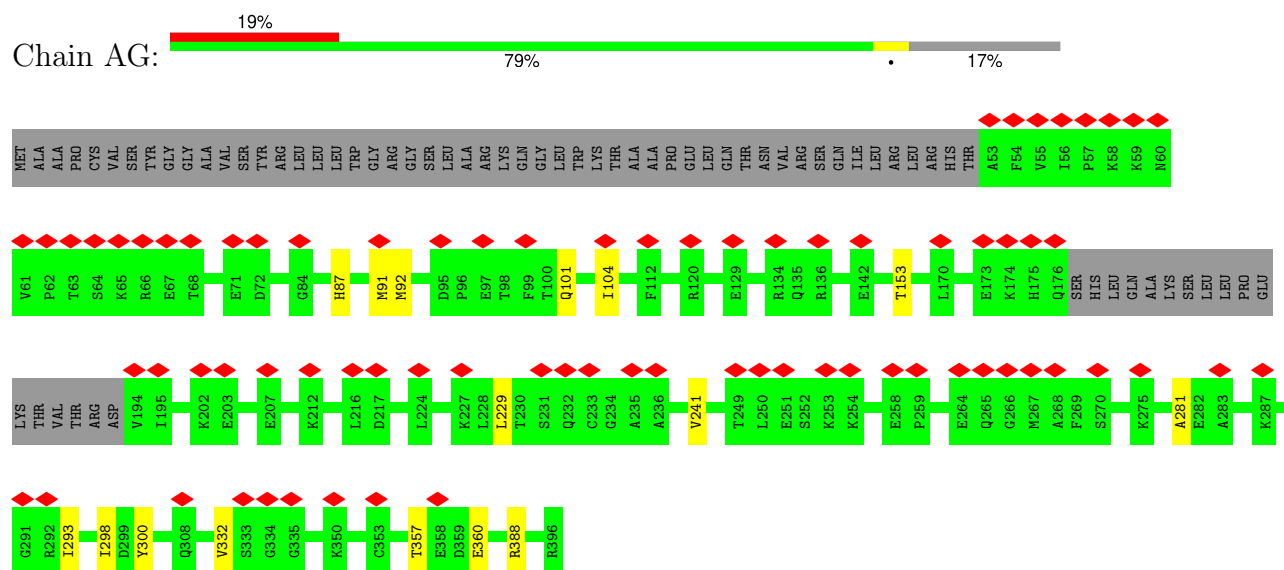
- Molecule 57: 28S ribosomal protein S6, mitochondrial



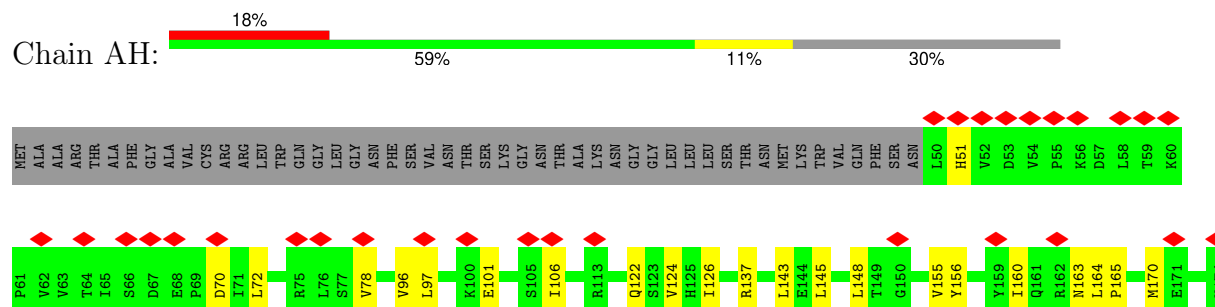
- Molecule 58: 28S ribosomal protein S7, mitochondrial

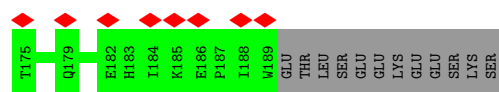


- Molecule 59: 28S ribosomal protein S9, mitochondrial

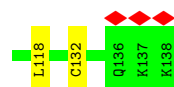
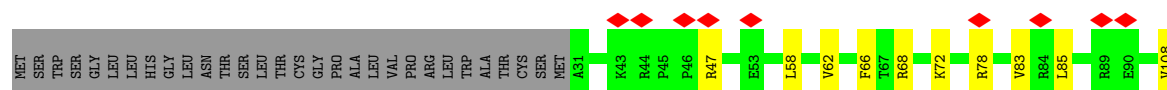


- Molecule 60: 28S ribosomal protein S10, mitochondrial

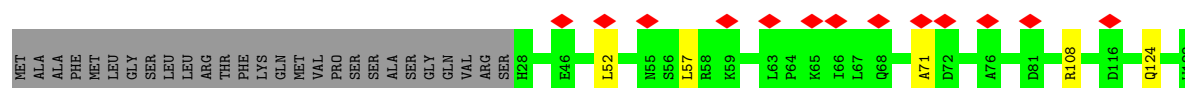
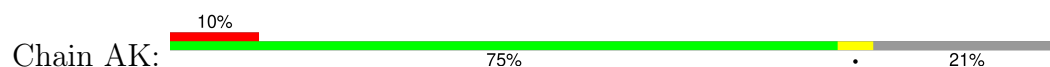




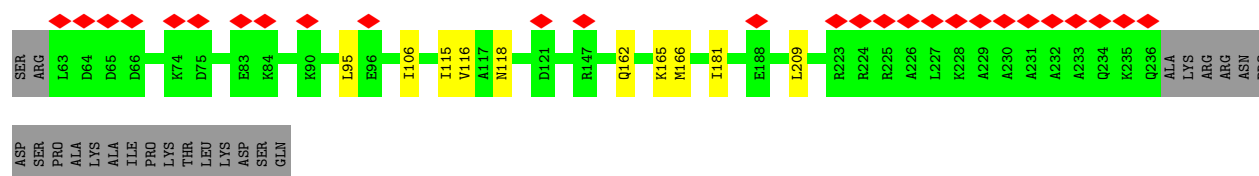
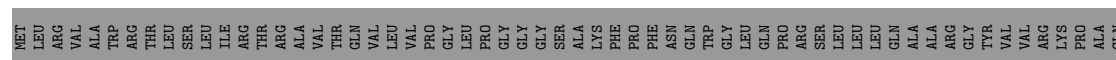
- Molecule 61: 28S ribosomal protein S12, mitochondrial



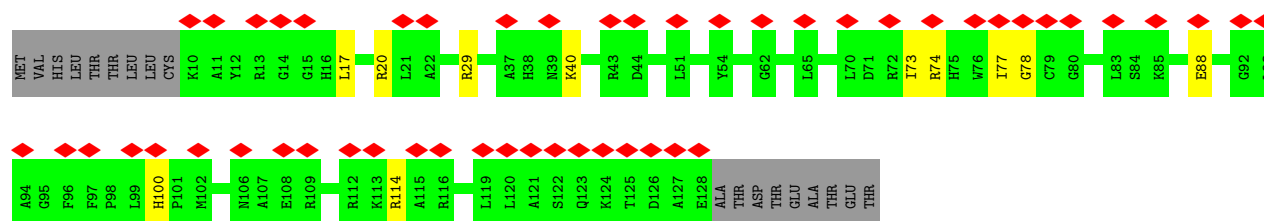
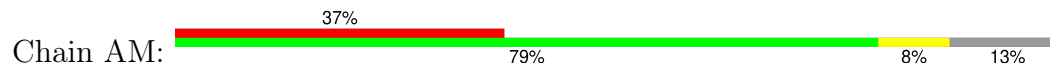
- Molecule 62: 28S ribosomal protein S14, mitochondrial



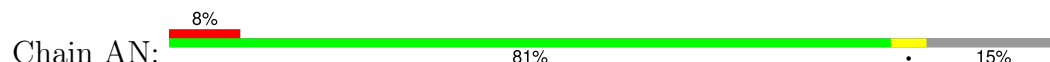
- Molecule 63: 28S ribosomal protein S15, mitochondrial

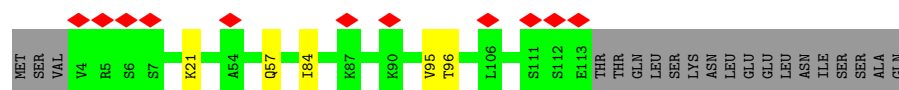


- Molecule 64: 28S ribosomal protein S16, mitochondrial



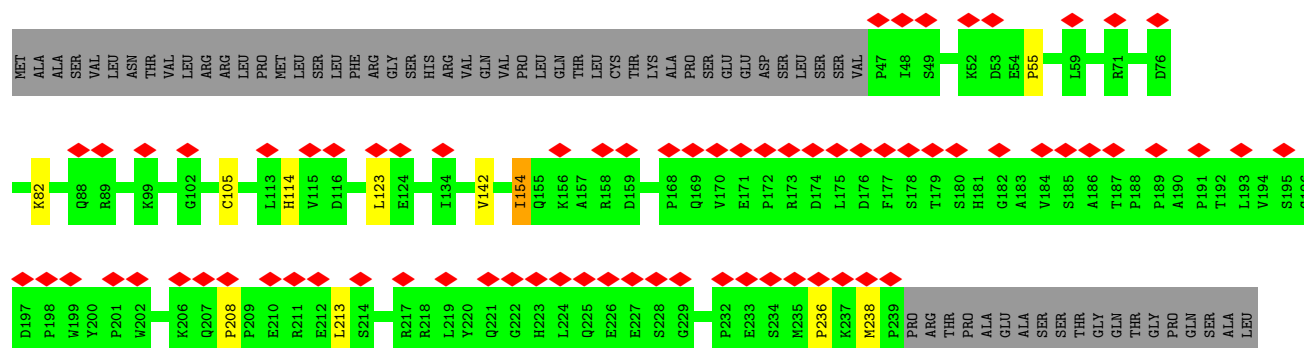
- Molecule 65: 28S ribosomal protein S17, mitochondrial





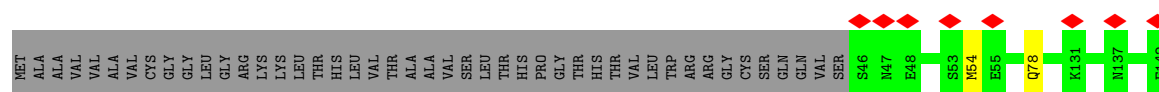
- Molecule 66: 28S ribosomal protein S18b, mitochondrial

Chain AO: 29% 71% 25%



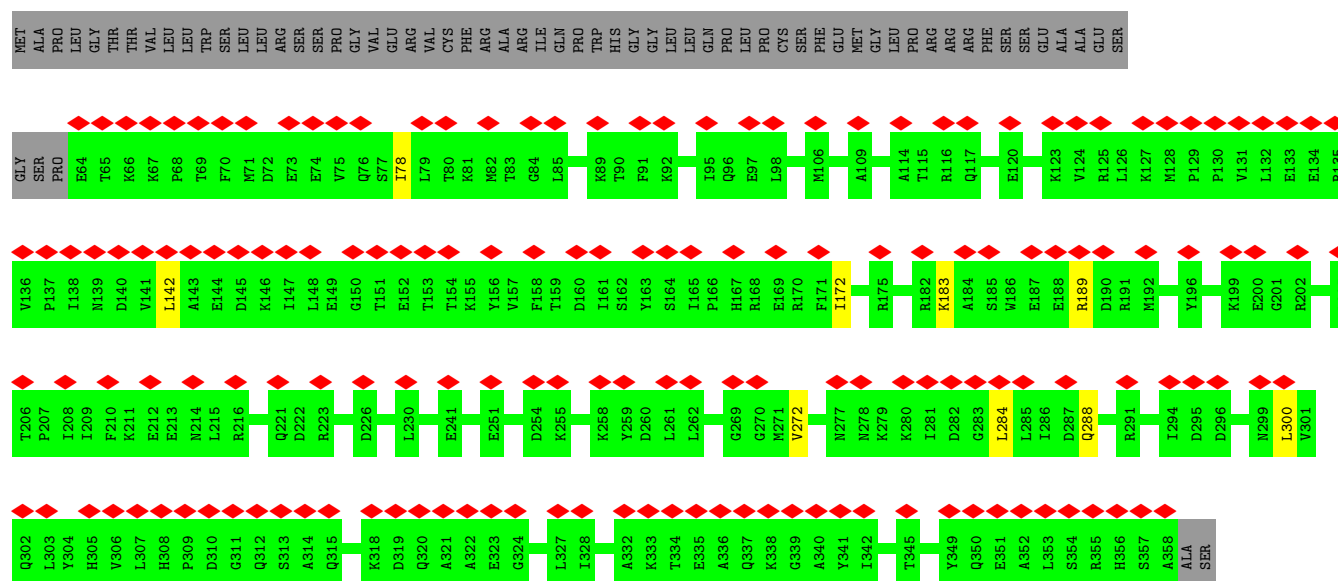
- Molecule 67: 28S ribosomal protein S18c, mitochondrial

Chain AP: 6% 67% 32%



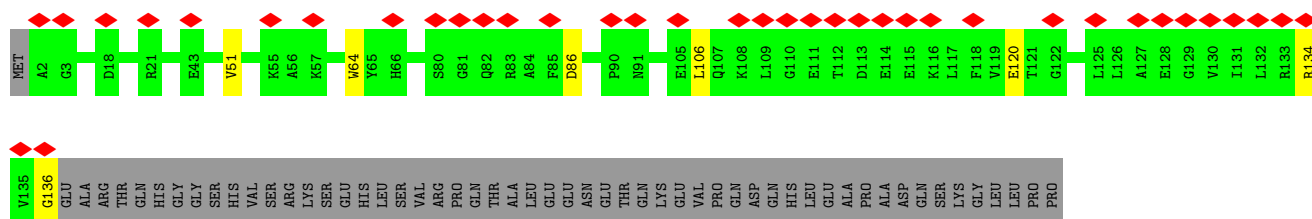
- Molecule 68: 28S ribosomal protein S22, mitochondrial

Chain AR: 45% 79% 18%

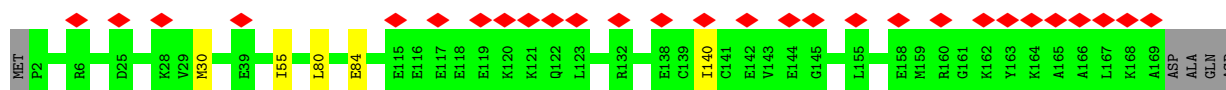


- Molecule 69: 28S ribosomal protein S23, mitochondrial

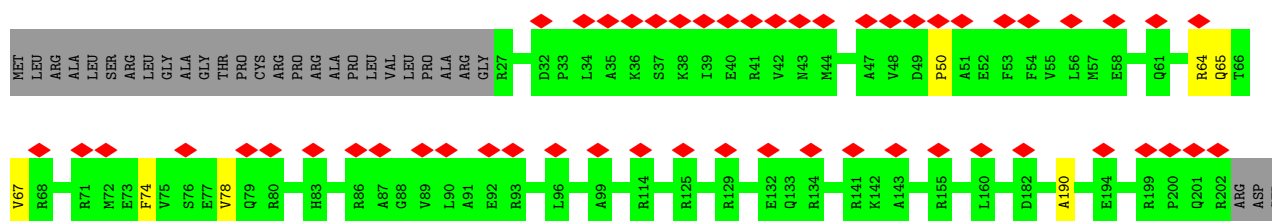
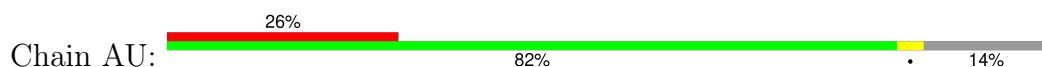
Chain AS: 20% 67% 29%



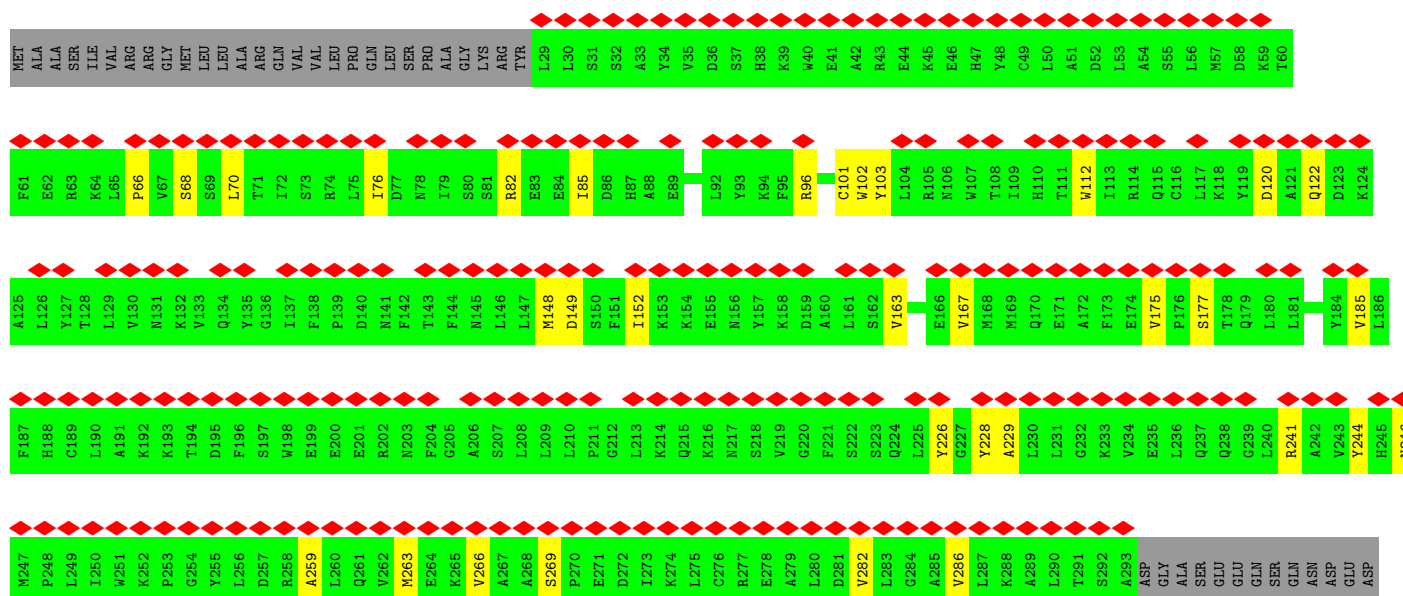
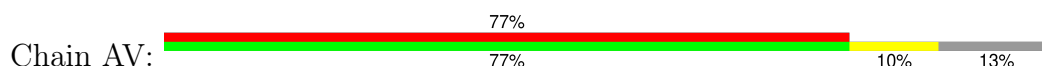
- Molecule 70: 28S ribosomal protein S25, mitochondrial

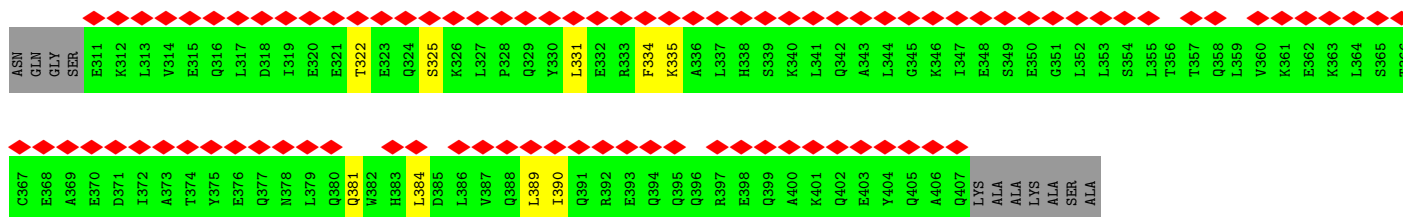


- Molecule 71: 28S ribosomal protein S26, mitochondrial

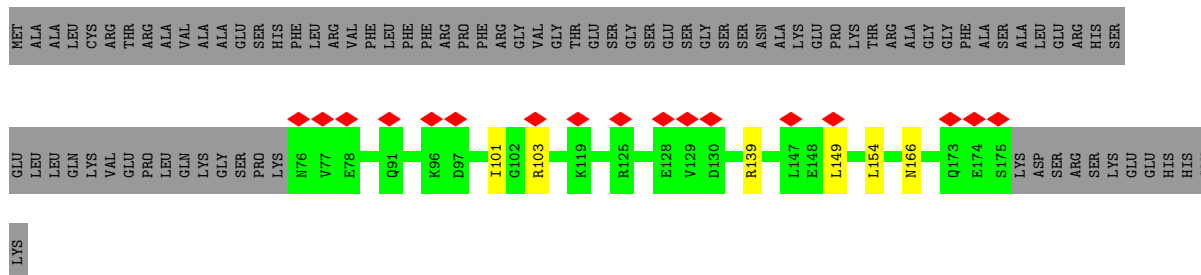


- Molecule 72: 28S ribosomal protein S27, mitochondrial

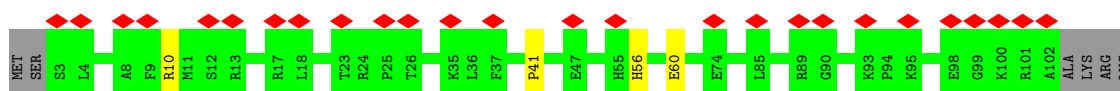
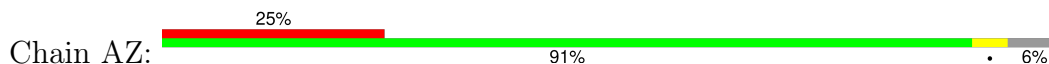




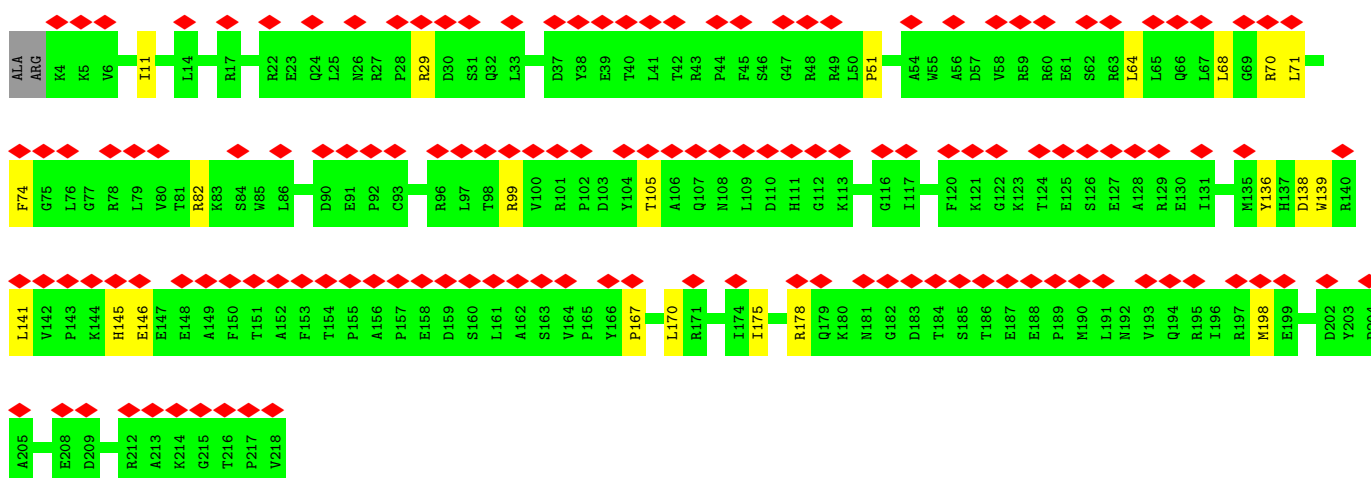
- Molecule 73: 28S ribosomal protein S28, mitochondrial



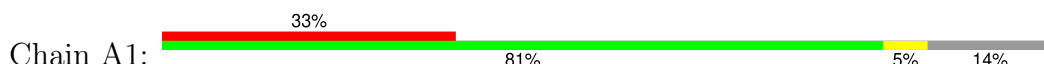
- Molecule 74: 28S ribosomal protein S33, mitochondrial

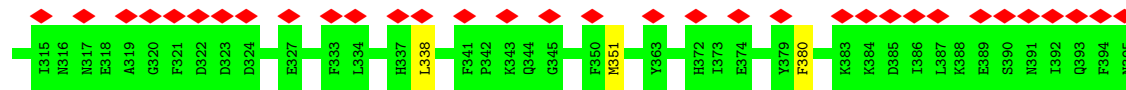
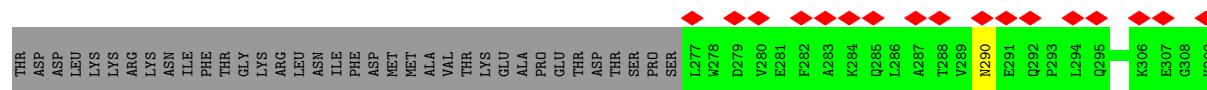


- Molecule 75: Small ribosomal subunit protein mS34



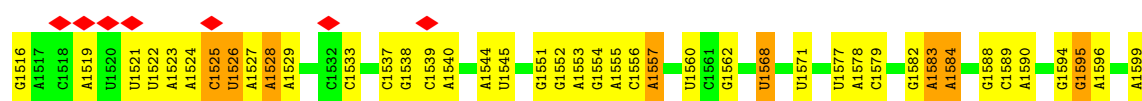
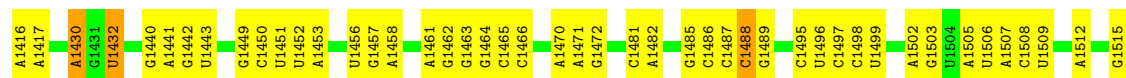
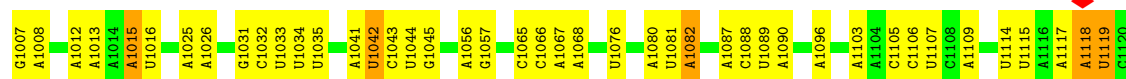
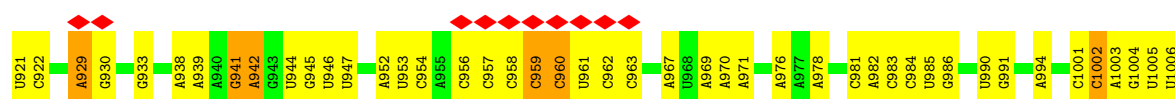
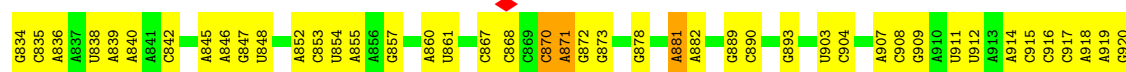
- Molecule 76: 28S ribosomal protein S35, mitochondrial

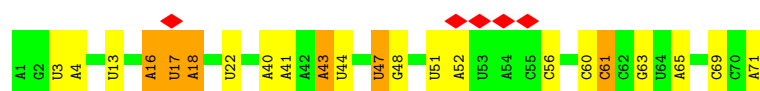




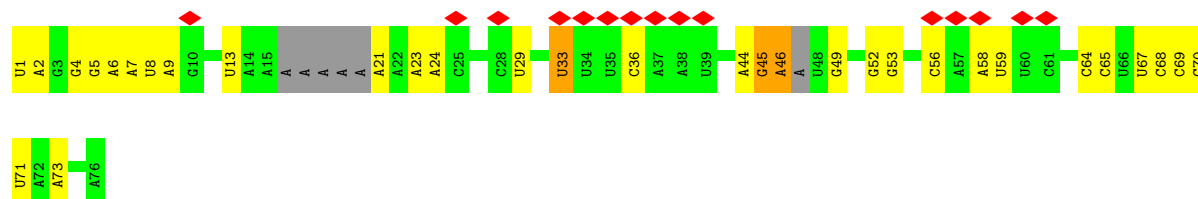
• Molecule 80: 12S mitochondrial rRNA

Chain AA: 55% 42%

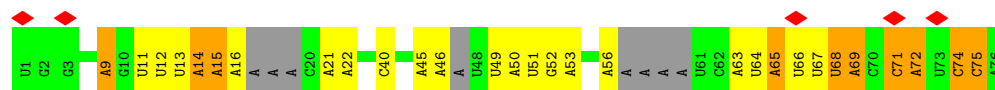




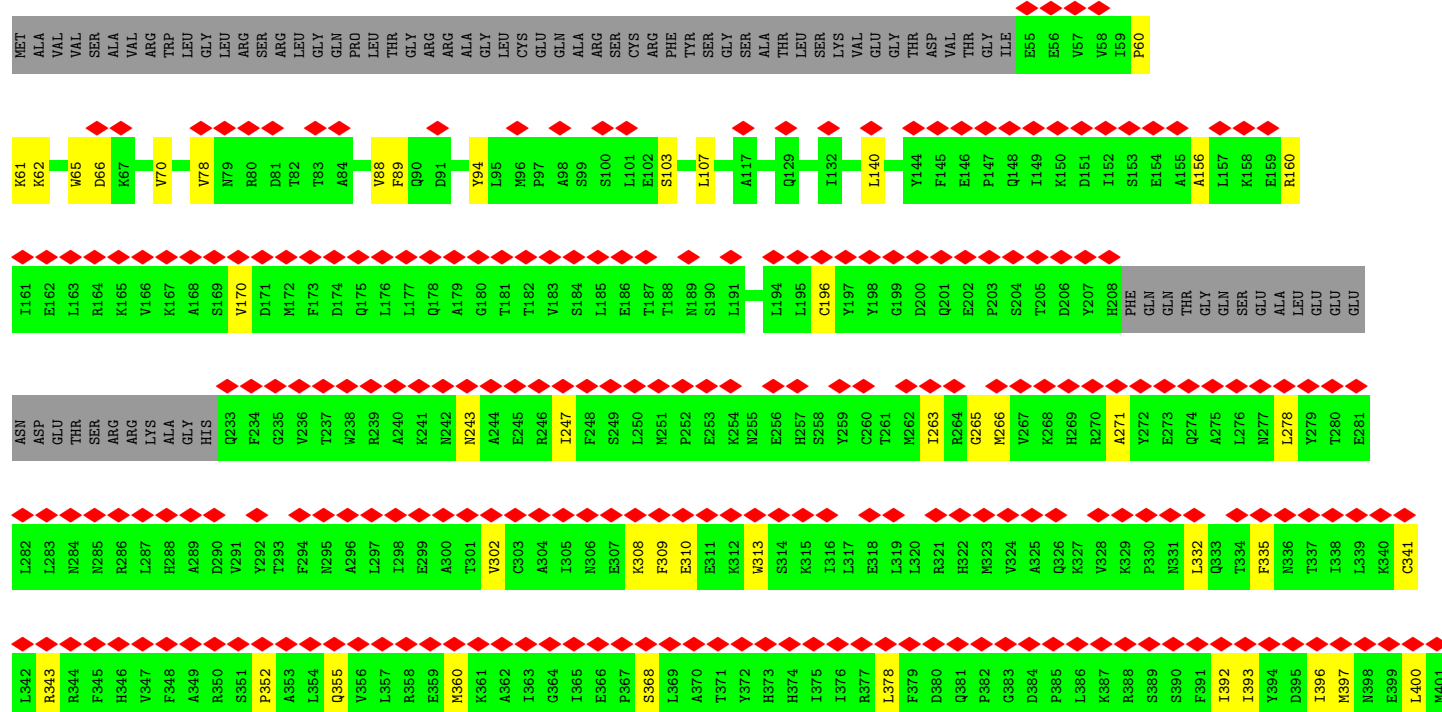
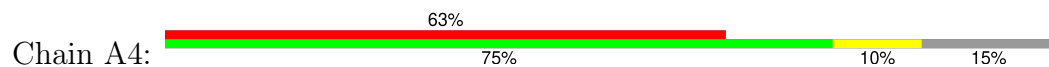
• Molecule 85: E/E-tRNA

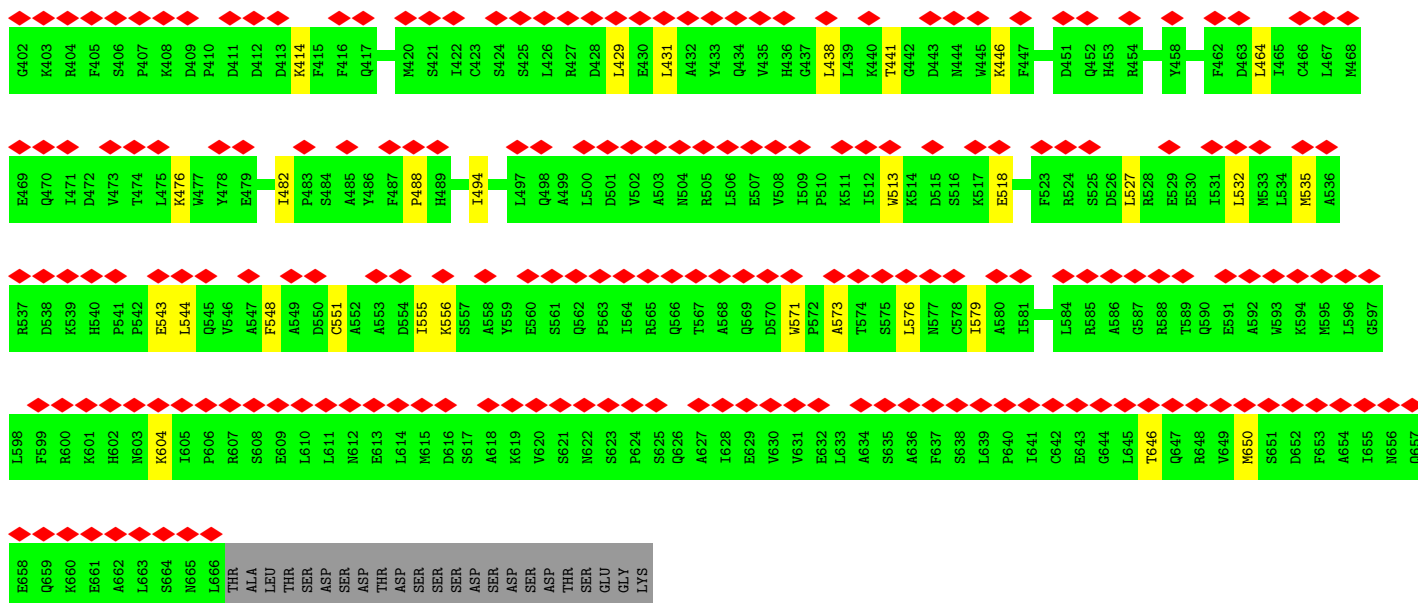


• Molecule 86: A/A-tRNA

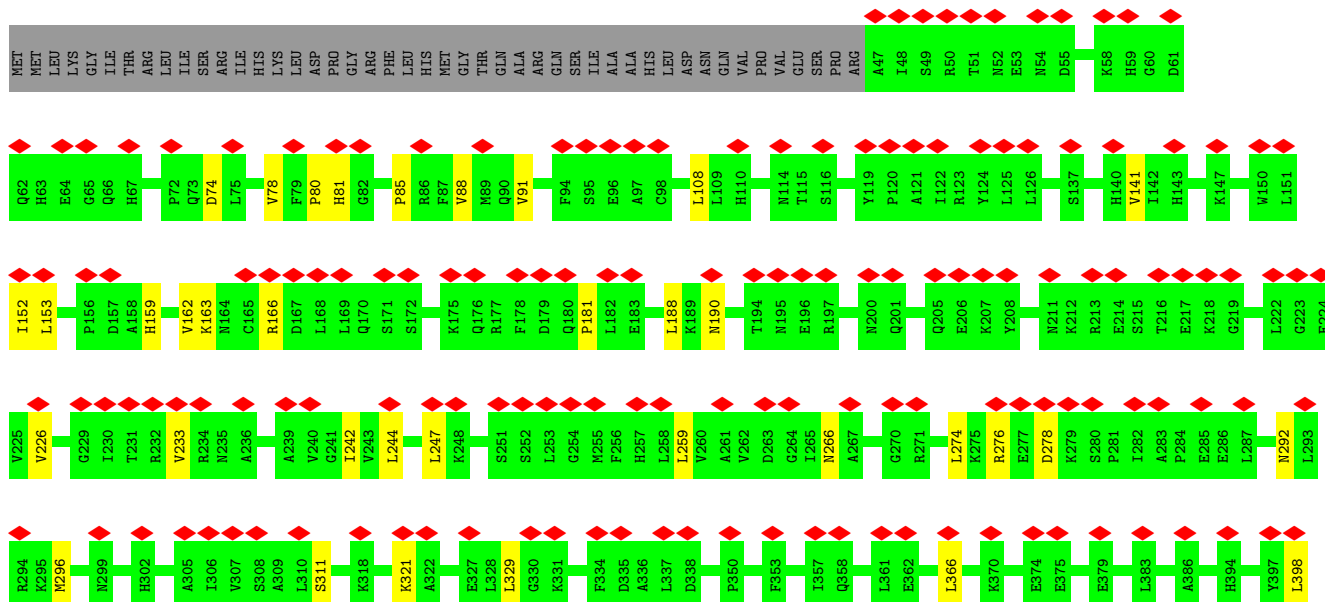
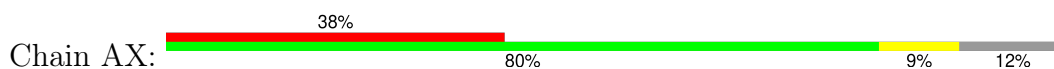


• Molecule 87: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

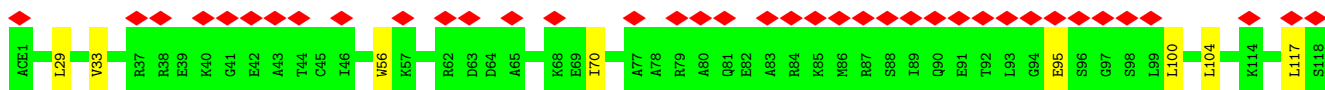




- Molecule 88: 28S ribosomal protein S29, mitochondrial



- Molecule 89: Small ribosomal subunit protein mS37



- Molecule 90: Small ribosomal subunit protein bS21m



• Molecule 91: mitochondrial tRNAVal



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27408	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	0.171	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/913	0.26	0/1224
2	1	0.23	0/469	0.28	0/621
3	2	0.30	0/383	0.29	0/507
4	3	0.29	0/853	0.28	0/1136
5	4	0.27	0/350	0.23	0/461
6	5	0.23	0/3305	0.28	0/4502
7	6	0.21	0/3043	0.29	0/4140
8	7	0.21	0/2447	0.27	0/3310
9	8	0.17	0/1354	0.32	0/1819
10	9	0.23	0/1025	0.26	0/1379
11	A	0.30	0/36876	0.30	0/57402
12	D	0.26	0/1896	0.30	0/2549
13	E	0.26	0/2475	0.30	0/3355
14	F	0.27	0/2090	0.29	0/2842
15	H	0.17	0/1698	0.29	0/2292
16	I	0.19	0/1478	0.33	0/1999
17	J	0.15	0/1348	0.29	0/1813
18	K	0.28	0/1497	0.28	0/2031
19	L	0.24	0/905	0.27	0/1218
20	M	0.27	0/2381	0.31	0/3212
21	N	0.25	0/1833	0.28	0/2468
22	O	0.25	0/1283	0.30	0/1727
23	P	0.23	0/1199	0.27	0/1623
24	Q	0.23	0/2039	0.27	0/2750
25	R	0.28	0/1175	0.27	0/1572
26	S	0.27	0/1320	0.30	0/1789
27	T	0.26	0/1403	0.27	0/1886
28	U	0.25	0/1279	0.34	0/1730
29	W	0.29	0/926	0.27	0/1244
30	X	0.23	0/2099	0.25	0/2837
31	Y	0.25	0/1593	0.26	0/2136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.26	0/1021	0.27	0/1378
33	z	0.15	0/2067	0.37	0/2793
34	V	0.22	0/1721	0.26	0/2333
35	b	0.26	0/1218	0.29	0/1649
36	d	0.20	0/2181	0.34	0/2949
37	e	0.16	0/1970	0.30	0/2658
38	g	0.24	0/1151	0.28	0/1569
39	h	0.19	0/918	0.24	0/1249
40	i	0.29	0/850	0.28	0/1135
41	j	0.22	0/760	0.23	0/1023
42	k	0.17	0/783	0.25	0/1057
43	l	0.16	0/707	0.29	0/960
44	m	0.15	0/805	0.32	0/1081
46	o	0.27	0/819	0.32	0/1097
47	q	0.19	0/1529	0.30	0/2055
48	r	0.29	0/1362	0.36	0/1846
49	t	0.14	0/358	0.29	0/486
49	u	0.19	0/259	0.40	0/350
50	c	0.23	0/2347	0.27	0/3171
51	f	0.20	0/1273	0.33	0/1716
52	p	0.20	0/1223	0.27	0/1641
53	s	0.25	0/3231	0.29	0/4389
54	AB	0.18	0/1871	0.27	0/2531
55	AC	0.18	0/1113	0.29	0/1505
56	AD	0.17	0/2783	0.26	0/3724
57	AE	0.19	0/989	0.28	0/1335
58	AF	0.16	0/1767	0.25	0/2373
59	AG	0.16	0/2746	0.28	0/3681
60	AH	0.19	0/1178	0.31	0/1598
61	AJ	0.18	0/855	0.27	0/1148
62	AK	0.19	0/880	0.26	0/1182
63	AL	0.18	0/1477	0.23	0/1974
64	AM	0.16	0/963	0.30	0/1295
65	AN	0.17	0/886	0.27	0/1199
66	AO	0.16	0/1648	0.29	0/2243
67	AP	0.19	0/798	0.30	0/1070
68	AR	0.13	0/2456	0.28	0/3317
69	AS	0.15	0/1138	0.23	0/1533
70	AT	0.17	0/1402	0.29	0/1883
71	AU	0.15	0/1510	0.27	0/2025
72	AV	0.15	0/3030	0.33	0/4093
73	AW	0.16	0/801	0.26	0/1079
74	AZ	0.16	0/857	0.30	0/1141

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	A0	0.13	0/1834	0.29	0/2484
76	A1	0.15	0/2313	0.27	0/3129
77	A3	0.21	0/636	0.26	0/839
78	Az	0.18	0/804	0.34	0/1248
79	AY	0.15	0/1040	0.24	0/1402
80	AA	0.23	0/22537	0.28	0/35085
81	AI	0.20	0/1039	0.29	0/1400
82	OX	0.17	0/478	0.41	0/639
83	a	0.23	0/891	0.34	0/1208
84	Ax	0.20	0/1673	0.35	0/2602
85	Ay	0.15	0/1655	0.26	0/2567
86	Aw	0.16	0/1600	0.29	0/2476
87	A4	0.15	0/4877	0.31	0/6598
88	AX	0.16	0/2921	0.32	0/3954
89	A2	0.18	0/947	0.30	0/1266
90	AQ	0.19	0/754	0.24	0/1003
91	B	0.20	0/1626	0.30	0/2523
All	All	0.23	0/190261	0.29	0/270511

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
48	r	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
48	r	74	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	1	0
2	1	464	0	511	4	0
3	2	377	0	406	0	0
4	3	832	0	883	1	0
5	4	342	0	361	1	0
6	5	3210	0	3206	8	0
7	6	2948	0	2841	7	0
8	7	2390	0	2397	13	0
9	8	1327	0	1368	14	0
10	9	997	0	987	3	0
11	A	33070	0	16792	137	0
12	D	1859	0	1920	8	0
13	E	2406	0	2415	4	0
14	F	2031	0	2065	3	0
15	H	1661	0	1734	15	0
16	I	1446	0	1532	8	0
17	J	1330	0	1407	8	0
18	K	1455	0	1452	4	0
19	L	890	0	941	2	0
20	M	2327	0	2395	2	0
21	N	1786	0	1817	8	0
22	O	1259	0	1294	2	0
23	P	1173	0	1165	3	0
24	Q	1990	0	2031	3	0
25	R	1154	0	1214	3	0
26	S	1293	0	1365	4	0
27	T	1369	0	1410	2	0
28	U	1248	0	1228	4	0
29	W	904	0	935	2	0
30	X	2044	0	2060	2	0
31	Y	1556	0	1597	2	0
32	Z	996	0	1044	0	0
33	z	2027	0	2076	25	0
34	V	1676	0	1687	5	0
35	b	1193	0	1191	1	0
36	d	2124	0	2125	25	0
37	e	1931	0	1916	19	0
38	g	1113	0	1097	0	0
39	h	895	0	881	0	0
40	i	828	0	857	0	0
41	j	745	0	746	2	0
42	k	774	0	784	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	l	688	0	673	5	0
44	m	791	0	796	8	0
45	n	215	0	51	0	0
46	o	798	0	804	0	0
47	q	1495	0	1492	15	0
48	r	1322	0	1348	7	0
49	t	354	0	377	2	0
49	u	257	0	283	4	0
50	c	2299	0	2320	1	0
51	f	1252	0	1269	11	0
52	p	1205	0	1223	1	0
53	s	3148	0	3131	9	0
54	AB	1828	0	1815	11	0
55	AC	1083	0	1088	7	0
56	AD	2731	0	2804	12	0
57	AE	972	0	1000	5	0
58	AF	1725	0	1769	4	0
59	AG	2688	0	2687	10	0
60	AH	1152	0	1183	17	0
61	AJ	839	0	887	8	0
62	AK	862	0	885	4	0
63	AL	1453	0	1540	7	0
64	AM	942	0	965	10	0
65	AN	868	0	928	3	0
66	AO	1592	0	1557	10	0
67	AP	781	0	806	2	0
68	AR	2409	0	2428	5	0
69	AS	1111	0	1115	5	0
70	AT	1371	0	1393	3	0
71	AU	1488	0	1499	6	0
72	AV	2969	0	2961	25	0
73	AW	789	0	802	5	0
74	AZ	839	0	858	3	0
75	A0	1787	0	1796	15	0
76	A1	2265	0	2294	15	0
77	A3	625	0	698	3	0
78	Az	719	0	359	2	0
79	AY	1010	0	957	3	0
80	AA	20260	0	10285	286	0
81	AI	1019	0	1059	5	0
82	OX	468	0	464	2	0
83	a	865	0	829	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	Ax	1498	0	766	7	0
85	Ay	1483	0	754	20	0
86	Aw	1434	0	728	11	0
87	A4	4768	0	4766	50	0
88	AX	2849	0	2844	23	0
89	A2	935	0	971	6	0
90	AQ	744	0	758	3	0
91	B	1524	0	779	11	0
92	0	1	0	0	0	0
92	4	1	0	0	0	0
92	AO	1	0	0	0	0
93	3	1	0	0	0	0
93	A	29	0	0	0	0
93	AA	16	0	0	0	0
93	AJ	1	0	0	0	0
93	Az	1	0	0	0	0
93	D	1	0	0	0	0
93	M	1	0	0	0	0
93	N	1	0	0	0	0
93	P	1	0	0	0	0
93	W	1	0	0	0	0
93	o	1	0	0	0	0
94	A	50	0	95	1	0
94	AA	20	0	38	0	0
95	A	6	0	12	0	0
96	A	137	0	0	0	0
96	A3	1	0	0	0	0
96	AA	59	0	0	0	0
96	AB	1	0	0	0	0
96	AK	1	0	0	0	0
96	AX	1	0	0	0	0
96	D	2	0	0	0	0
96	E	1	0	0	0	0
96	g	1	0	0	0	0
97	AP	4	0	0	0	0
97	AT	4	0	0	0	0
97	r	4	0	0	0	0
98	AA	44	0	26	0	0
99	AA	28	0	52	0	0
100	AX	31	0	12	0	0
101	AX	28	0	12	1	0
102	B	7	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	181394	0	153148	908	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 (908) 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)
37:e:183:THR:HG23	37:e:186:GLY:H	1.46	0.81
80:AA:941:G:H4'	80:AA:942:A:H5''	1.68	0.75
14:F:103:GLN:HE22	14:F:249:ASN:HD22	1.34	0.75
85:Ay:33:U:H2'	85:Ay:36:C:H41	1.54	0.73
9:8:187:PRO:HG2	44:m:79:ILE:HD11	1.71	0.72
79:AY:338:LEU:HD11	79:AY:351:MET:HB3	1.71	0.72
80:AA:1365:A:H4'	80:AA:1389:G:H4'	1.72	0.72
47:q:164:LEU:HB3	47:q:168:VAL:HG21	1.72	0.71
75:A0:99:ARG:HD3	80:AA:1526:U:H2'	1.73	0.71
27:T:62:ARG:HE	36:d:230:ARG:HD2	1.56	0.69
33:z:181:THR:HA	33:z:184:ILE:HD12	1.75	0.69
36:d:90:PRO:HB3	36:d:245:TYR:HE2	1.57	0.68
86:Aw:71:C:HO2'	86:Aw:72:A:H8	1.40	0.68
34:V:79:VAL:HG12	34:V:86:VAL:HG12	1.76	0.67
80:AA:1440:G:H2'	80:AA:1441:A:H8	1.58	0.67
80:AA:1440:G:H2'	80:AA:1441:A:C8	2.30	0.66
9:8:68:LEU:HD21	51:f:211:LEU:HB2	1.77	0.66
72:AV:66:PRO:HD3	80:AA:1529:A:H1'	1.78	0.65
36:d:208:VAL:HG23	36:d:252:LEU:HB2	1.76	0.65
80:AA:1528:A:H2'	80:AA:1529:A:H8	1.60	0.65
36:d:91:PRO:HB2	36:d:94:ASP:HB2	1.77	0.65
33:z:69:ILE:HD12	33:z:72:ILE:HD11	1.78	0.65
63:AL:209:LEU:HD13	77:A3:173:LEU:HD12	1.79	0.65
63:AL:165:LYS:HE3	80:AA:947:U:H5''	1.80	0.64
80:AA:976:A:H5''	90:AQ:1:ACE:H1	1.78	0.64
80:AA:1562:G:H1'	80:AA:1583:MA6:H2	1.80	0.63
87:A4:556:LYS:HE3	87:A4:579:ILE:HD13	1.79	0.63
76:A1:45:GLU:HG2	76:A1:47:PRO:HD2	1.81	0.63
80:AA:1201:A:H2'	80:AA:1202:G:H8	1.64	0.62
36:d:52:THR:HG23	36:d:55:GLU:H	1.65	0.62
56:AD:196:ASN:HD22	80:AA:878:G:H4'	1.64	0.62
80:AA:838:U:H2'	80:AA:839:A:H8	1.65	0.62
72:AV:70:LEU:HD21	72:AV:390:ILE:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:187:VAL:HG13	7:6:319:PHE:HB3	1.82	0.62
80:AA:1002:C:H2'	80:AA:1003:A:H8	1.64	0.62
72:AV:70:LEU:HD22	72:AV:389:LEU:HG	1.80	0.61
9:8:192:TYR:HE1	51:f:134:VAL:HG22	1.65	0.61
80:AA:773:U:H2'	80:AA:774:G:H8	1.65	0.61
59:AG:229:LEU:HD21	59:AG:241:VAL:HG11	1.82	0.61
33:z:198:VAL:HB	33:z:230:ILE:HG23	1.81	0.60
33:z:127:LEU:HD22	33:z:290:VAL:HG13	1.84	0.60
87:A4:397:MET:HG3	87:A4:431:LEU:HD11	1.83	0.60
61:AJ:72:LYS:HG3	80:AA:1557:A:H5''	1.83	0.60
80:AA:839:A:H2'	80:AA:840:A:H8	1.67	0.59
87:A4:494:ILE:HD11	87:A4:527:LEU:HA	1.84	0.59
80:AA:663:A:H2'	80:AA:664:G:C8	2.38	0.59
80:AA:847:G:H2'	80:AA:848:U:C6	2.38	0.59
80:AA:1398:U:H2'	80:AA:1399:A:H8	1.67	0.59
88:AX:153:LEU:HD21	88:AX:247:LEU:HD13	1.84	0.59
80:AA:1470:A:H2'	80:AA:1471:A:H8	1.68	0.58
70:AT:80:LEU:HD12	70:AT:84:GLU:HB3	1.85	0.58
12:D:205:GLN:HA	12:D:208:ARG:HH21	1.67	0.58
60:AH:137:ARG:HG3	62:AK:124:GLN:NE2	2.18	0.58
65:AN:95:VAL:HG23	65:AN:96:THR:HG23	1.84	0.58
80:AA:1578:A:H2'	80:AA:1579:C:C6	2.38	0.58
80:AA:829:C:H1'	80:AA:857:G:H22	1.68	0.58
80:AA:1007:G:H2'	80:AA:1008:A:H8	1.69	0.58
80:AA:1025:A:H2'	80:AA:1026:A:C8	2.38	0.58
11:A:2778:U:H5''	33:z:115:THR:HG22	1.86	0.58
88:AX:242:ILE:HD11	101:AX:503:GDP:C5	2.39	0.58
21:N:124:VAL:HG12	21:N:158:ARG:HE	1.67	0.58
36:d:208:VAL:HG22	36:d:253:THR:HG23	1.86	0.57
76:A1:134:PRO:HB2	76:A1:137:LEU:HD23	1.86	0.57
80:AA:918:A:H4'	80:AA:920:G:H4'	1.85	0.57
33:z:184:ILE:HG22	33:z:209:ARG:HH21	1.69	0.57
87:A4:302:VAL:HG21	87:A4:341:CYS:HB3	1.86	0.57
33:z:108:LYS:O	33:z:112:LEU:HB2	2.05	0.57
72:AV:229:ALA:HB1	72:AV:286:VAL:HG11	1.86	0.57
4:3:138:PRO:HG2	11:A:2854:U:H4'	1.87	0.57
63:AL:116:VAL:HG12	63:AL:118:ASN:H	1.70	0.57
37:e:205:LEU:HB3	51:f:168:GLU:HB2	1.86	0.57
11:A:2740:A:H2'	11:A:2741:A:C8	2.39	0.57
78:Az:28:U:H1'	87:A4:414:LYS:HG2	1.85	0.57
72:AV:148:MET:HE2	72:AV:185:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:672:A:H2'	80:AA:673:U:C6	2.40	0.56
80:AA:799:A:H2'	80:AA:800:C:C6	2.40	0.56
80:AA:1239:C:H2'	80:AA:1240:A:H8	1.69	0.56
80:AA:1382:A:H5''	88:AX:166:ARG:HH21	1.69	0.56
11:A:2174:G:H4'	17:J:151:LEU:HD23	1.87	0.56
69:AS:106:LEU:HD13	69:AS:120:GLU:HG3	1.87	0.56
80:AA:1089:U:H2'	80:AA:1090:A:H8	1.69	0.56
80:AA:1201:A:H2'	80:AA:1202:G:C8	2.39	0.56
80:AA:1452:U:H2'	80:AA:1453:A:H8	1.70	0.56
11:A:2086:A:H2'	11:A:2087:U:C6	2.40	0.56
8:7:143:TRP:HE1	8:7:172:VAL:HG23	1.70	0.56
76:A1:126:LEU:HD11	87:A4:70:VAL:HG13	1.87	0.56
11:A:2545:U:H5''	11:A:2546:G:H5'	1.86	0.56
12:D:207:ILE:HG12	12:D:229:PRO:HD3	1.88	0.56
80:AA:1042:U:H2'	80:AA:1043:C:C6	2.40	0.56
2:1:19:ARG:HB2	2:1:62:ILE:HD11	1.88	0.56
58:AF:167:PHE:HB2	85:Ay:33:U:H4'	1.87	0.56
76:A1:53:LEU:HD12	87:A4:518:GLU:HG2	1.87	0.56
80:AA:872:G:H2'	80:AA:873:G:C8	2.41	0.56
11:A:2718:C:H2'	11:A:2991:U:H4'	1.88	0.55
60:AH:70:ASP:HA	87:A4:62:LYS:HE3	1.87	0.55
87:A4:308:LYS:HE3	87:A4:310:GLU:HB2	1.89	0.55
17:J:140:VAL:O	17:J:144:ILE:HG12	2.06	0.55
80:AA:1589:C:H2'	80:AA:1590:A:C8	2.41	0.55
80:AA:852:A:H3'	80:AA:853:C:H6	1.72	0.55
60:AH:78:VAL:HB	60:AH:143:LEU:HB2	1.89	0.55
80:AA:960:C:H42	80:AA:1041:A:H2	1.55	0.54
11:A:3211:C:H4'	11:A:3212:C:H5	1.71	0.54
80:AA:1007:G:H2'	80:AA:1008:A:C8	2.42	0.54
80:AA:1033:U:H2'	80:AA:1034:U:C6	2.42	0.54
10:9:86:LEU:HD21	10:9:91:LEU:HD12	1.88	0.54
12:D:109:PHE:CE1	12:D:208:ARG:HD3	2.42	0.54
80:AA:776:A:H4'	80:AA:777:G:H5'	1.90	0.54
80:AA:845:A:H2'	80:AA:846:A:H8	1.72	0.54
86:Aw:68:U:H2'	86:Aw:69:A:C8	2.42	0.54
7:6:161:LEU:HD23	7:6:300:THR:HG21	1.89	0.54
80:AA:867:C:H2'	80:AA:870:C:N4	2.23	0.54
80:AA:1131:C:H2'	80:AA:1132:U:C6	2.42	0.54
8:7:286:LEU:HD11	8:7:296:ARG:HB2	1.90	0.54
80:AA:838:U:H2'	80:AA:839:A:C8	2.41	0.54
87:A4:513:TRP:CD1	87:A4:551:CYS:HG	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:201:ARG:HB3	6:5:232:THR:HG22	1.90	0.54
11:A:1857:U:H2'	11:A:1858:G:C8	2.43	0.54
52:p:133:LEU:HD21	52:p:157:MET:HE1	1.90	0.54
80:AA:872:G:H2'	80:AA:873:G:H8	1.72	0.54
80:AA:911:U:H2'	80:AA:912:U:C6	2.42	0.54
9:8:117:LEU:HD11	37:e:69:GLU:HB3	1.90	0.54
53:s:271:LEU:HD23	53:s:273:LEU:HD13	1.90	0.54
80:AA:738:A:H3'	80:AA:739:C:H6	1.74	0.54
80:AA:916:C:H2'	80:AA:917:C:C6	2.43	0.54
1:0:138:ARG:HB3	11:A:2321:A:C8	2.43	0.53
79:AY:290:ASN:HA	87:A4:446:LYS:HD3	1.90	0.53
80:AA:1595:G:H2'	80:AA:1596:A:C8	2.43	0.53
11:A:1994:A:H61	11:A:2736:C:H4'	1.73	0.53
21:N:124:VAL:HA	21:N:158:ARG:HH21	1.73	0.53
80:AA:663:A:H2'	80:AA:664:G:H8	1.72	0.53
80:AA:1042:U:H2'	80:AA:1043:C:H6	1.72	0.53
80:AA:1462:G:H2'	80:AA:1463:G:H8	1.71	0.53
91:B:23:A:H2'	91:B:24:G:C8	2.44	0.53
11:A:2055:U:H2'	11:A:2056:G:H8	1.74	0.53
49:t:74:LEU:HD12	49:t:78:GLU:HB2	1.89	0.53
80:AA:832:U:H2'	80:AA:833:A:H8	1.73	0.53
91:B:30:A:H2'	91:B:31:A:H8	1.72	0.53
15:H:174:VAL:HG12	15:H:192:HIS:HB3	1.89	0.53
76:A1:134:PRO:HG3	87:A4:60:PRO:HD3	1.90	0.53
80:AA:1003:A:H2'	80:AA:1004:G:H8	1.73	0.53
80:AA:914:A:H2'	80:AA:915:C:C6	2.44	0.53
80:AA:1124:A:H2'	80:AA:1125:A:H2'	1.91	0.53
12:D:109:PHE:HB3	12:D:204:ALA:HB3	1.90	0.53
33:z:78:MET:HE1	33:z:93:PRO:HD2	1.91	0.53
36:d:90:PRO:HB3	36:d:245:TYR:CE2	2.43	0.53
69:AS:51:VAL:HG13	89:A2:117:LEU:HD11	1.90	0.53
80:AA:1066:C:H2'	80:AA:1067:A:C8	2.44	0.53
11:A:2006:C:H2'	11:A:2007:U:C6	2.45	0.52
48:r:71:PRO:HD2	48:r:107:LEU:HD23	1.90	0.52
80:AA:1177:C:H2'	80:AA:1178:G:H8	1.74	0.52
80:AA:1191:C:H2'	80:AA:1192:C:C6	2.44	0.52
8:7:112:PRO:HB2	8:7:267:PRO:HG2	1.91	0.52
11:A:2093:U:H2'	11:A:2094:G:C8	2.45	0.52
11:A:2134:A:H62	11:A:2135:A:H62	1.57	0.52
60:AH:96:VAL:HA	60:AH:106:ILE:HD13	1.91	0.52
80:AA:970:A:H2'	80:AA:971:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:1006:U:H2'	80:AA:1007:G:H8	1.73	0.52
80:AA:1265:C:H2'	80:AA:1266:A:H8	1.74	0.52
80:AA:1353:A:H5'	80:AA:1354:A:H5'	1.91	0.52
80:AA:1515:G:H2'	80:AA:1516:G:C8	2.43	0.52
11:A:2529:U:OP2	12:D:208:ARG:HD2	2.10	0.52
15:H:163:THR:HG21	33:z:86:VAL:HG23	1.90	0.52
56:AD:209:GLY:HA3	56:AD:213:GLU:HB2	1.92	0.52
11:A:2099:U:H2'	11:A:2100:C:C6	2.43	0.52
24:Q:100:LEU:HD21	24:Q:286:ILE:HG12	1.90	0.52
84:Ax:40:A:H2'	84:Ax:41:A:C8	2.44	0.52
87:A4:429:LEU:HA	87:A4:464:LEU:HD21	1.91	0.52
88:AX:80:PRO:HG2	88:AX:81:HIS:HD2	1.73	0.52
11:A:1895:C:H2'	11:A:1896:U:H6	1.73	0.52
66:AO:82:LYS:HB3	80:AA:881:A:N6	2.25	0.52
80:AA:773:U:H2'	80:AA:774:G:C8	2.43	0.52
80:AA:1578:A:H2'	80:AA:1579:C:H6	1.74	0.52
16:I:154:LEU:HD12	16:I:164:MET:HE3	1.91	0.52
33:z:184:ILE:HG12	33:z:207:LEU:HD13	1.91	0.52
53:s:145:VAL:HG21	53:s:187:LEU:HD11	1.90	0.52
80:AA:673:U:H2'	80:AA:674:U:C6	2.45	0.52
87:A4:170:VAL:HG23	87:A4:247:ILE:HD11	1.92	0.52
37:e:183:THR:HG23	37:e:186:GLY:N	2.20	0.52
80:AA:1496:U:H2'	80:AA:1497:C:C6	2.45	0.52
84:Ax:47:U:H2'	84:Ax:48:G:C8	2.45	0.52
66:AO:105:CYS:HB2	66:AO:142:VAL:HA	1.90	0.52
80:AA:1376:C:H4'	80:AA:1377:C:H5'	1.91	0.52
17:J:88:SER:HA	17:J:151:LEU:HD11	1.92	0.51
34:V:102:MET:HE3	36:d:48:PRO:HG2	1.92	0.51
80:AA:920:G:H2'	80:AA:921:U:C6	2.45	0.51
80:AA:1414:C:H3'	80:AA:1415:G:H21	1.75	0.51
56:AD:244:LEU:HD22	56:AD:343:LEU:HD23	1.92	0.51
80:AA:1175:G:H2'	80:AA:1176:G:C8	2.45	0.51
85:Ay:1:U:H2'	85:Ay:2:A:C8	2.45	0.51
15:H:201:VAL:HA	33:z:86:VAL:HG12	1.92	0.51
80:AA:839:A:H2'	80:AA:840:A:C8	2.43	0.51
80:AA:1175:G:H2'	80:AA:1176:G:H8	1.76	0.51
80:AA:1239:C:H2'	80:AA:1240:A:C8	2.45	0.51
25:R:35:LYS:HD2	25:R:45:THR:HG21	1.93	0.51
66:AO:123:LEU:HD13	66:AO:154:ILE:HG13	1.93	0.51
87:A4:343:ARG:HA	87:A4:378:LEU:HD13	1.92	0.51
36:d:96:ARG:HG2	36:d:97:ILE:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:99:MET:HE1	48:r:115:ILE:HG22	1.92	0.51
54:AB:192:LEU:HD11	54:AB:220:VAL:HG23	1.93	0.51
85:Ay:1:U:H2'	85:Ay:2:A:H8	1.75	0.51
91:B:29:C:H2'	91:B:30:A:H8	1.76	0.51
56:AD:100:LYS:HG2	80:AA:1262:C:H4'	1.91	0.51
80:AA:1430:A:N1	80:AA:1458:A:H5''	2.25	0.51
54:AB:167:HIS:HE1	54:AB:171:PHE:HA	1.75	0.51
56:AD:116:LYS:HE2	78:Az:13:U:H5'	1.92	0.51
88:AX:159:HIS:HE1	88:AX:311:SER:HB3	1.76	0.51
6:5:165:GLN:NE2	6:5:175:THR:HG22	2.26	0.51
18:K:60:MET:HE2	18:K:133:ILE:HD11	1.93	0.51
36:d:115:THR:O	36:d:119:GLN:HG2	2.11	0.51
47:q:138:GLN:O	47:q:141:GLU:HG3	2.11	0.51
80:AA:740:G:H2'	80:AA:741:A:H8	1.76	0.51
80:AA:944:U:H2'	80:AA:945:G:C8	2.46	0.51
80:AA:1399:A:H2'	80:AA:1400:U:C6	2.45	0.51
56:AD:420:SER:HA	80:AA:929:A:H4'	1.93	0.51
64:AM:17:LEU:HD11	80:AA:743:C:H5'	1.92	0.51
60:AH:155:VAL:HG13	76:A1:126:LEU:HD12	1.93	0.50
80:AA:684:U:H2'	80:AA:685:A:H8	1.76	0.50
80:AA:1348:G:H2'	80:AA:1349:U:C6	2.46	0.50
72:AV:149:ASP:HA	72:AV:152:ILE:HG22	1.93	0.50
80:AA:682:A:H2'	80:AA:683:G:H8	1.77	0.50
11:A:1895:C:H2'	11:A:1896:U:C6	2.47	0.50
11:A:3089:A:H3'	11:A:3090:G:C5'	2.42	0.50
64:AM:114:ARG:HH22	66:AO:236:PRO:HD2	1.76	0.50
11:A:2586:U:H2'	11:A:2587:G:H8	1.77	0.50
37:e:166:GLY:HA3	102:B:101:VAL:HG11	1.94	0.50
80:AA:1033:U:H2'	80:AA:1034:U:H6	1.76	0.50
17:J:114:LEU:HB3	43:l:96:LEU:HD21	1.94	0.50
66:AO:208:PRO:HG2	66:AO:213:LEU:HD21	1.94	0.50
88:AX:244:LEU:HD12	88:AX:292:ASN:HB3	1.93	0.50
14:F:218:LEU:HD13	14:F:230:ILE:HD11	1.93	0.50
80:AA:1132:U:H2'	80:AA:1133:C:C6	2.47	0.50
80:AA:1416:A:H2'	80:AA:1417:A:C8	2.47	0.50
36:d:106:ILE:O	36:d:110:GLU:HG2	2.12	0.50
59:AG:293:ILE:HB	59:AG:300:TYR:HB3	1.94	0.50
64:AM:20:ARG:HB2	80:AA:839:A:H5''	1.92	0.50
80:AA:832:U:H2'	80:AA:833:A:C8	2.46	0.50
80:AA:944:U:H2'	80:AA:945:G:H8	1.76	0.50
80:AA:1461:A:H4'	80:AA:1462:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:A4:573:ALA:HB2	87:A4:604:LYS:HD3	1.94	0.50
80:AA:845:A:H2'	80:AA:846:A:C8	2.46	0.50
41:j:112:LYS:HG2	41:j:113:GLY:H	1.76	0.50
72:AV:226:TYR:CZ	72:AV:282:VAL:HG11	2.47	0.50
75:A0:64:LEU:HD12	75:A0:139:TRP:CD2	2.47	0.50
2:1:38:ARG:HH12	2:1:41:LEU:HD11	1.76	0.49
55:AC:42:VAL:HG11	55:AC:51:VAL:HG11	1.94	0.49
60:AH:122:GLN:HG3	80:AA:1265:C:H4'	1.94	0.49
61:AJ:62:VAL:HA	61:AJ:83:VAL:HG12	1.93	0.49
80:AA:1194:C:H2'	80:AA:1195:U:C6	2.47	0.49
80:AA:1308:U:H2'	80:AA:1309:A:H8	1.76	0.49
37:e:124:TRP:CE2	44:m:72:ARG:HG2	2.46	0.49
57:AE:26:ILE:HG23	57:AE:36:VAL:HG21	1.93	0.49
72:AV:322:THR:HG23	72:AV:325:SER:H	1.78	0.49
80:AA:743:C:H2'	80:AA:744:A:O4'	2.12	0.49
80:AA:1012:A:H2'	80:AA:1013:A:C8	2.47	0.49
72:AV:175:VAL:HG12	72:AV:177:SER:H	1.77	0.49
73:AW:103:ARG:HE	73:AW:139:ARG:HH21	1.59	0.49
88:AX:85:PRO:HA	88:AX:88:VAL:HG12	1.93	0.49
28:U:153:LEU:HD21	36:d:220:GLN:HB2	1.93	0.49
80:AA:1452:U:H2'	80:AA:1453:A:C8	2.47	0.49
11:A:3054:G:H2'	11:A:3055:U:C6	2.47	0.49
19:L:75:LEU:HD11	19:L:105:VAL:HG21	1.95	0.49
36:d:204:ASN:O	36:d:205:GLN:HG2	2.12	0.49
75:A0:11:ILE:HB	80:AA:806:C:C2	2.47	0.49
72:AV:163:VAL:O	72:AV:167:VAL:HG23	2.13	0.49
88:AX:366:LEU:HD22	88:AX:398:LEU:HD22	1.95	0.49
89:A2:56:TRP:HE1	89:A2:70:ILE:HD11	1.77	0.49
23:P:94:VAL:HG23	23:P:132:LEU:HD21	1.94	0.49
61:AJ:66:PHE:HE2	61:AJ:68:ARG:HE	1.61	0.49
80:AA:1002:C:H2'	80:AA:1003:A:C8	2.47	0.49
80:AA:1515:G:H2'	80:AA:1516:G:H8	1.77	0.49
80:AA:1554:G:H2'	80:AA:1555:A:C8	2.47	0.49
87:A4:571:TRP:HE3	87:A4:576:LEU:HD21	1.78	0.49
53:s:142:LEU:HD13	53:s:422:VAL:HG21	1.94	0.49
49:u:75:THR:O	49:u:79:ILE:HG13	2.13	0.49
53:s:63:ILE:HA	53:s:66:TRP:CD1	2.47	0.49
80:AA:1507:A:H2'	80:AA:1508:C:H6	1.77	0.49
87:A4:309:PHE:HB2	87:A4:313:TRP:HZ3	1.78	0.49
11:A:1974:A:H5'	12:D:261:GLY:HA2	1.95	0.48
11:A:2151:A:H2'	11:A:2152:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:116:LEU:HG	16:I:121:ILE:HB	1.95	0.48
47:q:191:LYS:HA	47:q:194:LYS:HG2	1.95	0.48
87:A4:335:PHE:CG	87:A4:360:MET:HE2	2.48	0.48
91:B:68:C:H2'	91:B:69:U:C6	2.48	0.48
30:X:20:ILE:HG22	82:OX:434:LEU:HD23	1.95	0.48
37:e:51:LEU:HD13	37:e:188:ALA:HB1	1.95	0.48
80:AA:908:C:H2'	80:AA:909:G:C8	2.49	0.48
80:AA:1317:A:H3'	80:AA:1318:A:H8	1.78	0.48
80:AA:1555:A:H2'	80:AA:1556:C:O4'	2.13	0.48
85:Ay:6:A:H2'	85:Ay:7:A:C8	2.48	0.48
11:A:2699:C:H2'	11:A:2700:G:H8	1.78	0.48
74:AZ:10:ARG:HH12	76:A1:239:TRP:CD1	2.31	0.48
80:AA:1401:G:N2	80:AA:1403:A:H3'	2.28	0.48
91:B:43:G:H2'	91:B:44:A:C8	2.47	0.48
11:A:1952:U:H2'	11:A:1953:A:C8	2.49	0.48
11:A:2727:C:H2'	11:A:2728:C:C6	2.49	0.48
33:z:180:GLY:HA2	33:z:203:ILE:HD12	1.95	0.48
37:e:213:TYR:HB3	37:e:231:VAL:HB	1.95	0.48
80:AA:1080:A:H1'	80:AA:1082:A:N7	2.28	0.48
80:AA:1244:C:H2'	80:AA:1245:U:C6	2.49	0.48
80:AA:1495:C:H2'	80:AA:1496:U:C6	2.49	0.48
11:A:1936:A:H4'	11:A:1937:A:N7	2.28	0.48
11:A:2740:A:H2'	11:A:2741:A:H8	1.77	0.48
11:A:3224:G:H2'	11:A:3225:G:H8	1.78	0.48
33:z:160:PHE:HD2	33:z:199:ALA:HB2	1.78	0.48
65:AN:21:LYS:HB3	80:AA:777:G:H5''	1.94	0.48
80:AA:659:U:H2'	80:AA:660:C:H6	1.77	0.48
80:AA:958:C:H4'	80:AA:959:C:O4'	2.13	0.48
80:AA:1588:G:H2'	80:AA:1589:C:C6	2.48	0.48
80:AA:1595:G:H2'	80:AA:1596:A:H8	1.78	0.48
88:AX:181:PRO:HB2	88:AX:233:VAL:HG22	1.95	0.48
11:A:2392:U:H2'	11:A:2394:A:H62	1.78	0.48
37:e:55:ARG:HG3	37:e:149:LEU:HD22	1.94	0.48
72:AV:68:SER:N	80:AA:1523:A:H5''	2.28	0.48
80:AA:672:A:H2'	80:AA:673:U:H6	1.78	0.48
80:AA:914:A:H2'	80:AA:915:C:H6	1.77	0.48
80:AA:661:C:H2'	80:AA:662:U:C6	2.48	0.48
86:Aw:64:U:H2'	86:Aw:65:A:H8	1.79	0.48
88:AX:244:LEU:HD22	88:AX:296:MET:HG3	1.95	0.48
11:A:1761:A:H2'	11:A:1762:A:C8	2.48	0.48
11:A:2081:U:H2'	11:A:2082:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:AU:64:ARG:HA	71:AU:67:VAL:HG12	1.95	0.48
11:A:1862:U:H2'	11:A:1863:A:H8	1.79	0.48
11:A:3158:A:H2'	11:A:3159:A:C8	2.49	0.48
80:AA:1177:C:H2'	80:AA:1178:G:C8	2.48	0.48
80:AA:705:C:H3'	80:AA:706:C:C6	2.49	0.47
80:AA:1462:G:H2'	80:AA:1463:G:C8	2.49	0.47
89:A2:95:GLU:HB3	89:A2:100:LEU:HG	1.96	0.47
11:A:1851:G:H2'	11:A:2693:A:N7	2.29	0.47
11:A:2275:U:H2'	11:A:2276:C:C6	2.50	0.47
15:H:106:GLY:HA2	15:H:158:LYS:HB2	1.95	0.47
58:AF:166:ARG:NH2	80:AA:994:A:H1'	2.29	0.47
80:AA:970:A:H2'	80:AA:971:A:H8	1.79	0.47
85:Ay:69:C:H2'	85:Ay:70:C:C6	2.49	0.47
11:A:3143:U:H2'	11:A:3144:A:H8	1.79	0.47
63:AL:209:LEU:HD12	77:A3:189:TRP:CE2	2.49	0.47
6:5:336:LEU:HD21	6:5:362:THR:HG23	1.96	0.47
11:A:2727:C:H2'	11:A:2728:C:H6	1.78	0.47
49:u:86:LEU:O	49:u:90:LEU:HB2	2.15	0.47
80:AA:659:U:H2'	80:AA:660:C:C6	2.49	0.47
80:AA:798:C:H2'	80:AA:799:A:C8	2.49	0.47
87:A4:266:MET:HG2	87:A4:271:ALA:HB3	1.97	0.47
16:I:61:HIS:CD2	16:I:62:PRO:HD2	2.49	0.47
60:AH:164:LEU:HD12	60:AH:165:PRO:HD2	1.95	0.47
80:AA:740:G:H2'	80:AA:741:A:C8	2.50	0.47
80:AA:821:U:H2'	80:AA:822:G:H8	1.80	0.47
80:AA:1348:G:H2'	80:AA:1349:U:H6	1.79	0.47
80:AA:1507:A:H2'	80:AA:1508:C:C6	2.50	0.47
91:B:21:A:H61	91:B:46:A:H2'	1.79	0.47
6:5:289:HIS:O	6:5:343:GLN:HG2	2.15	0.47
9:8:201:GLN:HB3	51:f:201:ARG:HG3	1.96	0.47
11:A:1939:G:O2'	11:A:1973:G:H4'	2.15	0.47
11:A:2275:U:H2'	11:A:2276:C:H6	1.78	0.47
11:A:2409:A:H2'	11:A:2410:U:C6	2.50	0.47
11:A:2702:G:H5'	18:K:114:LYS:HE2	1.96	0.47
26:S:99:VAL:HG12	26:S:133:VAL:HG22	1.96	0.47
54:AB:155:ILE:HG12	54:AB:196:LEU:HD13	1.96	0.47
59:AG:101:GLN:HA	59:AG:104:ILE:HD12	1.95	0.47
80:AA:1114:U:H2'	80:AA:1115:U:C6	2.50	0.47
80:AA:1161:A:H2'	80:AA:1162:A:H8	1.80	0.47
80:AA:1471:A:H2'	80:AA:1472:G:H8	1.80	0.47
86:Aw:64:U:H2'	86:Aw:65:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
91:B:74:C:H2'	91:B:75:C:O4'	2.14	0.47
11:A:2662:A:H2'	11:A:2663:C:C6	2.50	0.47
36:d:197:VAL:HG22	36:d:212:ILE:HG23	1.97	0.47
48:r:70:CYS:O	48:r:73:CYS:SG	2.73	0.47
60:AH:164:LEU:HD13	60:AH:170:MET:HE3	1.97	0.47
75:A0:136:TYR:CZ	80:AA:705:C:H2'	2.50	0.47
80:AA:711:U:H5'	80:AA:712:C:C5	2.49	0.47
11:A:1925:A:H2'	11:A:1926:A:C8	2.50	0.47
36:d:84:ILE:HA	36:d:211:GLN:HE22	1.80	0.47
47:q:164:LEU:HG	47:q:178:LEU:HD23	1.96	0.47
49:u:64:ILE:O	49:u:68:VAL:HG23	2.13	0.47
55:AC:125:ARG:NH1	87:A4:94:TYR:HB2	2.30	0.47
65:AN:57:GLN:HG3	65:AN:84:ILE:HD11	1.97	0.47
80:AA:1552:G:H2'	80:AA:1553:A:C8	2.50	0.47
11:A:2286:A:H2'	11:A:2287:U:C6	2.50	0.46
36:d:147:GLU:HG3	36:d:163:LEU:HD11	1.97	0.46
36:d:269:TRP:CD1	36:d:269:TRP:H	2.33	0.46
80:AA:915:C:H2'	80:AA:916:C:C6	2.50	0.46
80:AA:1089:U:H2'	80:AA:1090:A:C8	2.49	0.46
86:Aw:9:A:H1'	86:Aw:45:A:H2'	1.96	0.46
9:8:188:PRO:HG2	51:f:136:GLN:HE22	1.80	0.46
11:A:3150:U:C2	11:A:3151:A:C8	3.03	0.46
11:A:3165:C:H2'	11:A:3166:U:C6	2.49	0.46
47:q:168:VAL:HG12	47:q:175:PHE:HB2	1.96	0.46
53:s:332:LEU:HD21	53:s:359:ALA:HB2	1.96	0.46
64:AM:29:ARG:HH22	70:AT:140:ILE:HG23	1.81	0.46
76:A1:67:PRO:HG3	76:A1:118:ALA:HB2	1.95	0.46
80:AA:747:A:H2'	80:AA:748:G:H8	1.81	0.46
80:AA:1502:A:H2'	80:AA:1503:G:O4'	2.15	0.46
21:N:36:VAL:HG11	43:l:124:GLN:HB3	1.97	0.46
33:z:133:LYS:HE3	33:z:286:LEU:HD13	1.98	0.46
9:8:53:LYS:NZ	86:Aw:40:C:H5''	2.31	0.46
11:A:1839:C:H2'	11:A:1840:C:C6	2.50	0.46
11:A:1952:U:H2'	11:A:1953:A:H8	1.80	0.46
53:s:84:THR:HB	53:s:280:ASN:HB2	1.96	0.46
80:AA:738:A:H3'	80:AA:739:C:C6	2.51	0.46
87:A4:535:MET:HE1	87:A4:551:CYS:HB3	1.96	0.46
11:A:2101:C:H2'	11:A:2102:A:H8	1.80	0.46
18:K:171:THR:HG23	48:r:58:LYS:HA	1.98	0.46
24:Q:69:VAL:HG12	24:Q:71:PRO:HD3	1.97	0.46
47:q:152:ARG:O	47:q:156:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:983:C:H2'	80:AA:984:C:C6	2.51	0.46
87:A4:646:THR:HG23	87:A4:650:MET:HE3	1.97	0.46
54:AB:180:ARG:HH21	56:AD:210:PRO:HB2	1.80	0.46
62:AK:57:LEU:HD23	62:AK:71:ALA:HB2	1.97	0.46
80:AA:1488:5MC:H2'	80:AA:1489:G:C8	2.51	0.46
11:A:1829:A:H2'	11:A:1830:G:H8	1.80	0.46
60:AH:124:VAL:HG13	80:AA:1264:C:H1'	1.98	0.46
72:AV:263:MET:HE1	72:AV:334:PHE:HD1	1.80	0.46
80:AA:800:C:H2'	80:AA:801:A:C8	2.51	0.46
11:A:2734:A:H2'	11:A:2735:G:H8	1.79	0.46
50:c:59:ARG:HB2	50:c:62:GLU:HG2	1.98	0.46
80:AA:745:A:H3'	80:AA:746:A:H8	1.81	0.46
80:AA:985:U:H2'	80:AA:986:G:C8	2.51	0.46
80:AA:1068:A:H5''	81:AI:190:LYS:HD3	1.96	0.46
80:AA:1589:C:H2'	80:AA:1590:A:H8	1.80	0.46
87:A4:532:LEU:HD11	87:A4:555:ILE:HG21	1.98	0.46
7:6:90:ILE:HA	41:j:112:LYS:HB3	1.96	0.46
9:8:201:GLN:HB2	51:f:199:LYS:HE2	1.98	0.46
17:J:113:THR:HG23	17:J:115:LYS:H	1.79	0.46
80:AA:682:A:H2'	80:AA:683:G:C8	2.50	0.46
80:AA:1349:U:H2'	80:AA:1350:G:C8	2.49	0.46
80:AA:1485:G:H2'	80:AA:1486:B8T:O4'	2.16	0.46
80:AA:1577:U:H2'	80:AA:1578:A:C8	2.50	0.46
84:Ax:16:A:H4'	84:Ax:17:U:H5''	1.98	0.46
11:A:1977:U:H2'	11:A:1978:A:H8	1.80	0.46
11:A:2682:A:H4'	25:R:41:LEU:HD13	1.97	0.46
11:A:2868:C:H2'	11:A:2869:A:O4'	2.16	0.46
11:A:2894:U:H5''	11:A:2895:U:O4'	2.15	0.46
80:AA:1065:C:H2'	80:AA:1066:C:O4'	2.15	0.46
87:A4:196:CYS:HB3	87:A4:265:GLY:HA3	1.98	0.46
87:A4:482:ILE:HD12	87:A4:488:PRO:HD3	1.98	0.46
87:A4:646:THR:O	87:A4:650:MET:HG2	2.16	0.46
8:7:114:ASP:HB2	8:7:117:LYS:HB2	1.98	0.45
22:O:46:TRP:CD1	22:O:121:ALA:HB2	2.51	0.45
43:l:87:LYS:HB3	43:l:91:GLU:OE2	2.16	0.45
53:s:201:ASP:HB2	53:s:240:GLN:HG2	1.97	0.45
59:AG:87:HIS:O	59:AG:91:MET:HG2	2.16	0.45
61:AJ:47:ARG:HH21	80:AA:930:G:H1	1.64	0.45
70:AT:30:MET:HE1	70:AT:55:ILE:HG21	1.96	0.45
75:A0:82:ARG:HH21	75:A0:138:ASP:HB3	1.81	0.45
79:AY:351:MET:HE3	79:AY:380:PHE:HE2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Ay:64:C:H2'	85:Ay:65:C:H6	1.81	0.45
9:8:99:ARG:HG2	37:e:83:LEU:HB3	1.97	0.45
76:A1:71:PRO:HB3	87:A4:78:VAL:HG21	1.98	0.45
80:AA:1056:A:H4'	80:AA:1588:G:N2	2.31	0.45
84:Ax:3:U:H2'	84:Ax:4:A:C8	2.50	0.45
11:A:1828:A:H4'	11:A:1829:A:C8	2.51	0.45
64:AM:73:ILE:O	64:AM:77:ILE:HG12	2.16	0.45
80:AA:1408:A:H2'	80:AA:1409:A:H8	1.81	0.45
81:Al:176:THR:HB	90:AQ:11:THR:HG23	1.98	0.45
11:A:2056:G:H2'	11:A:2057:C:H6	1.82	0.45
11:A:2757:A:H2'	11:A:2758:G:O4'	2.15	0.45
11:A:3118:U:H2'	11:A:3119:C:H6	1.82	0.45
47:q:169:ASP:HB3	47:q:172:SER:HB3	1.97	0.45
57:AE:3:ARG:HD3	57:AE:69:TYR:CZ	2.51	0.45
68:AR:272:VAL:HG22	68:AR:284:LEU:HD21	1.98	0.45
72:AV:76:ILE:HD12	72:AV:112:TRP:HD1	1.82	0.45
80:AA:1373:U:H2'	80:AA:1374:A:H8	1.80	0.45
9:8:192:TYR:HB3	51:f:132:ILE:HD11	1.97	0.45
11:A:1861:U:H2'	11:A:1862:U:C6	2.51	0.45
80:AA:946:U:H2'	80:AA:947:U:C6	2.52	0.45
80:AA:1032:C:H2'	80:AA:1033:U:H6	1.82	0.45
85:Ay:52:G:H2'	85:Ay:53:G:C8	2.52	0.45
15:H:98:LEU:HD11	15:H:105:VAL:HG23	1.97	0.45
55:AC:43:ARG:HD2	80:AA:1322:C:OP1	2.16	0.45
66:AO:213:LEU:HD13	71:AU:50:PRO:HB2	1.99	0.45
80:AA:715:G:H2'	80:AA:716:U:C6	2.52	0.45
80:AA:1129:U:H2'	80:AA:1130:G:H8	1.81	0.45
80:AA:1528:A:H2'	80:AA:1529:A:C8	2.48	0.45
87:A4:352:PRO:O	87:A4:355:GLN:HG3	2.17	0.45
91:B:76:A:H4'	102:B:101:VAL:N	2.31	0.45
17:J:121:ALA:HB2	17:J:144:ILE:HG13	1.99	0.45
64:AM:88:GLU:HB3	64:AM:100:HIS:HD2	1.81	0.45
80:AA:1174:U:H2'	80:AA:1175:G:C8	2.52	0.45
80:AA:1496:U:H2'	80:AA:1497:C:H6	1.81	0.45
85:Ay:24:A:N6	85:Ay:45:G:H22	2.15	0.45
47:q:196:LYS:HA	47:q:199:LYS:HD2	1.98	0.45
55:AC:125:ARG:HH11	87:A4:94:TYR:HB2	1.82	0.45
68:AR:172:ILE:HD12	68:AR:189:ARG:HG2	1.97	0.45
75:A0:68:LEU:HD13	75:A0:71:LEU:HD12	1.98	0.45
80:AA:1146:C:H2'	80:AA:1147:G:H8	1.82	0.45
33:z:161:THR:HB	33:z:167:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AL:95:LEU:HD21	63:AL:106:ILE:HG13	1.97	0.45
72:AV:82:ARG:O	72:AV:85:ILE:HG22	2.17	0.45
72:AV:228:TYR:HB3	72:AV:259:ALA:HB2	1.99	0.45
80:AA:1066:C:H2'	80:AA:1067:A:H8	1.81	0.45
80:AA:1552:G:H2'	80:AA:1553:A:H8	1.82	0.45
87:A4:332:LEU:HD23	87:A4:368:SER:HB3	1.99	0.45
88:AX:159:HIS:HA	88:AX:162:VAL:HG12	1.99	0.45
11:A:3115:U:H2'	11:A:3116:C:C6	2.52	0.45
37:e:163:GLU:HB3	37:e:165:PHE:CE2	2.52	0.45
80:AA:798:C:H2'	80:AA:799:A:H8	1.81	0.45
80:AA:1173:C:H2'	80:AA:1174:U:C6	2.52	0.45
11:A:2779:C:H5'	33:z:116:SER:HB3	1.98	0.44
44:m:58:LYS:HB2	44:m:58:LYS:HE2	1.86	0.44
48:r:70:CYS:HB2	48:r:107:LEU:HA	1.99	0.44
80:AA:952:A:H2'	80:AA:953:U:C6	2.52	0.44
80:AA:1044:U:H2'	80:AA:1045:G:O4'	2.17	0.44
61:AJ:58:LEU:HB3	61:AJ:85:LEU:HD12	1.99	0.44
64:AM:114:ARG:HH12	66:AO:236:PRO:HD2	1.82	0.44
73:AW:154:LEU:HB3	89:A2:29:LEU:HG	1.98	0.44
80:AA:1487:C:H2'	80:AA:1488:5MC:HM53	1.99	0.44
80:AA:1498:C:H2'	80:AA:1499:U:H6	1.82	0.44
6:5:147:ILE:HG12	6:5:191:GLN:CD	2.42	0.44
12:D:205:GLN:HA	12:D:208:ARG:NH2	2.30	0.44
36:d:186:VAL:HG21	36:d:239:PRO:HB3	1.98	0.44
80:AA:696:U:H2'	80:AA:697:G:C8	2.52	0.44
80:AA:1174:U:H2'	80:AA:1175:G:H8	1.83	0.44
11:A:2367:A:H2	31:Y:123:ARG:HH22	1.65	0.44
11:A:2662:A:H2'	11:A:2663:C:H6	1.82	0.44
11:A:2803:A:H2'	11:A:2804:A:O4'	2.17	0.44
55:AC:58:ALA:HB3	55:AC:60:HIS:CE1	2.52	0.44
80:AA:911:U:H2'	80:AA:912:U:H6	1.83	0.44
86:Aw:66:U:H2'	86:Aw:67:U:C6	2.52	0.44
11:A:2585:G:H2'	11:A:2586:U:C6	2.53	0.44
61:AJ:108:VAL:HG12	61:AJ:132:CYS:HB2	1.99	0.44
80:AA:661:C:H2'	80:AA:662:U:H6	1.82	0.44
86:Aw:11:U:H2'	86:Aw:12:U:C6	2.53	0.44
88:AX:188:LEU:HD22	88:AX:226:VAL:HG23	2.00	0.44
8:7:204:LYS:HE3	83:a:92:LEU:HD13	1.99	0.44
11:A:2382:A:H2'	11:A:2383:U:C6	2.52	0.44
11:A:2778:U:O2'	33:z:116:SER:HB2	2.18	0.44
11:A:3117:C:H2'	11:A:3118:U:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:z:296:ARG:HB3	33:z:302:GLY:HA2	1.99	0.44
53:s:65:ARG:O	53:s:69:THR:HG23	2.17	0.44
54:AB:167:HIS:CE1	54:AB:171:PHE:HA	2.50	0.44
54:AB:222:ILE:HD13	54:AB:236:VAL:HB	2.00	0.44
60:AH:124:VAL:HA	62:AK:108:ARG:HH12	1.83	0.44
60:AH:145:LEU:HB3	60:AH:148:LEU:HD11	1.99	0.44
75:A0:71:LEU:HD11	75:A0:141:LEU:HD11	1.99	0.44
80:AA:867:C:H2'	80:AA:870:C:H42	1.80	0.44
80:AA:1003:A:H2'	80:AA:1004:G:C8	2.50	0.44
8:7:150:MET:O	8:7:154:ILE:HG12	2.17	0.44
11:A:1868:G:H2'	20:M:40:PRO:HG3	1.99	0.44
11:A:2514:C:H2'	11:A:2515:U:H6	1.83	0.44
11:A:2804:A:H2'	11:A:2805:A:H8	1.83	0.44
44:m:90:ARG:HE	44:m:94:ARG:HG3	1.82	0.44
61:AJ:78:ARG:HG3	61:AJ:118:LEU:HD21	1.99	0.44
62:AK:52:LEU:HD22	74:AZ:41:PRO:HG3	2.00	0.44
87:A4:392:ILE:HG13	87:A4:393:ILE:N	2.33	0.44
11:A:2245:A:H4'	11:A:2246:A:OP1	2.18	0.44
76:A1:194:VAL:HB	76:A1:197:ARG:HB2	1.99	0.44
80:AA:985:U:H2'	80:AA:986:G:H8	1.82	0.44
80:AA:1553:A:H2'	80:AA:1554:G:C8	2.53	0.44
87:A4:88:VAL:HG11	87:A4:107:LEU:HD11	1.99	0.44
8:7:139:ASN:HB3	8:7:174:VAL:HG21	1.98	0.44
56:AD:103:LEU:HD11	56:AD:123:ARG:HB2	1.99	0.44
63:AL:162:GLN:O	63:AL:166:MET:HG3	2.17	0.44
80:AA:739:C:H2'	80:AA:740:G:O4'	2.18	0.44
80:AA:1349:U:H2'	80:AA:1350:G:H8	1.82	0.44
87:A4:446:LYS:HE3	87:A4:446:LYS:HB3	1.84	0.44
7:6:217:LEU:HB3	7:6:236:LEU:HD13	1.99	0.43
11:A:2764:A:C4	15:H:252:LEU:HD21	2.52	0.43
11:A:3078:C:H2'	11:A:3079:G:C8	2.53	0.43
11:A:3144:A:H2'	11:A:3145:A:H8	1.83	0.43
15:H:174:VAL:HG12	15:H:192:HIS:CB	2.47	0.43
33:z:123:LEU:HD23	33:z:257:ILE:HD11	1.99	0.43
73:AW:149:LEU:HD11	73:AW:166:ASN:HB2	1.99	0.43
80:AA:1347:G:H2'	80:AA:1348:G:H8	1.83	0.43
81:AI:75:TRP:HB3	81:AI:146:HIS:CD2	2.53	0.43
11:A:2094:G:H2'	11:A:2095:U:H6	1.84	0.43
33:z:62:PRO:HG2	33:z:65:LYS:HB2	2.00	0.43
34:V:146:VAL:HG21	82:OX:401:PHE:CE1	2.53	0.43
55:AC:136:VAL:HG22	55:AC:153:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AP:78:GLN:HE21	71:AU:190:ALA:HB2	1.82	0.43
88:AX:81:HIS:CD2	88:AX:190:ASN:HB3	2.53	0.43
11:A:1750:G:H2'	11:A:1751:A:C8	2.53	0.43
11:A:3078:C:H2'	11:A:3079:G:H8	1.83	0.43
37:e:159:LEU:HD21	37:e:161:VAL:HG13	2.01	0.43
44:m:55:LEU:HD23	44:m:63:THR:HG21	2.01	0.43
57:AE:96:HIS:HB3	57:AE:99:THR:HG23	1.99	0.43
80:AA:1087:A:H2'	80:AA:1088:C:C6	2.52	0.43
80:AA:1456:U:H2'	80:AA:1457:G:O4'	2.18	0.43
88:AX:108:LEU:HD23	88:AX:141:VAL:HG11	2.01	0.43
11:A:2212:C:H2'	11:A:2213:A:H8	1.83	0.43
11:A:3139:G:H2'	11:A:3140:A:C8	2.54	0.43
27:T:62:ARG:NE	36:d:230:ARG:HD2	2.30	0.43
56:AD:312:TYR:CZ	56:AD:315:ARG:HD3	2.53	0.43
72:AV:103:TYR:CZ	80:AA:1524:A:H4'	2.54	0.43
80:AA:705:C:H3'	80:AA:706:C:H6	1.84	0.43
80:AA:1005:U:H4'	81:AI:87:HIS:CE1	2.54	0.43
80:AA:1260:A:C6	80:AA:1336:G:C5	3.06	0.43
80:AA:1495:C:H2'	80:AA:1496:U:H6	1.83	0.43
37:e:159:LEU:HD12	37:e:254:TRP:CZ2	2.53	0.43
42:k:66:VAL:HB	42:k:74:LEU:HB3	2.01	0.43
60:AH:97:LEU:O	60:AH:101:GLU:HG3	2.19	0.43
80:AA:1034:U:H2'	80:AA:1035:U:H6	1.84	0.43
80:AA:1162:A:H2'	80:AA:1163:C:H6	1.82	0.43
80:AA:1588:G:H2'	80:AA:1589:C:H6	1.82	0.43
5:4:103:MET:HE1	11:A:2952:U:H5'	2.00	0.43
11:A:1863:A:H2'	11:A:1864:A:C8	2.54	0.43
11:A:1911:C:H2'	11:A:1912:A:H8	1.82	0.43
11:A:2483:U:H2'	11:A:2484:C:O4'	2.18	0.43
28:U:131:GLU:O	28:U:134:ARG:HG3	2.19	0.43
72:AV:103:TYR:HA	80:AA:1525:C:H5	1.83	0.43
80:AA:1076:5MU:O2	80:AA:1076:5MU:H2'	2.18	0.43
85:Ay:23:A:H2'	85:Ay:24:A:H8	1.84	0.43
11:A:2420:U:H2'	11:A:2421:G:H8	1.84	0.43
16:I:143:LEU:HD23	16:I:146:LEU:HD13	2.00	0.43
30:X:166:LEU:HD13	30:X:196:ILE:HD11	1.99	0.43
33:z:200:VAL:HG12	33:z:228:ARG:HA	1.99	0.43
64:AM:78:GLY:HA3	71:AU:78:VAL:HG21	1.99	0.43
80:AA:871:A:H4'	80:AA:872:G:H5'	1.99	0.43
80:AA:908:C:H2'	80:AA:909:G:H8	1.82	0.43
80:AA:982:A:H2'	80:AA:983:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:983:C:H2'	80:AA:984:C:H6	1.84	0.43
80:AA:1117:A:H2'	80:AA:1118:A:H8	1.84	0.43
85:Ay:64:C:H2'	85:Ay:65:C:C6	2.53	0.43
11:A:2060:A:C8	11:A:2079:C:C4	3.06	0.43
11:A:2697:G:OP2	94:A:3302:SPD:H31	2.19	0.43
11:A:2728:C:H2'	11:A:2729:U:H6	1.82	0.43
15:H:225:VAL:HG22	33:z:86:VAL:HG21	2.01	0.43
16:I:164:MET:HE2	16:I:168:LEU:HD11	2.00	0.43
21:N:104:MET:HE3	21:N:104:MET:HB3	1.94	0.43
47:q:117:ARG:O	47:q:121:ILE:HG12	2.19	0.43
59:AG:298:ILE:HD13	88:AX:321:LYS:HE2	2.01	0.43
61:AJ:47:ARG:NH2	80:AA:930:G:H1	2.17	0.43
64:AM:74:ARG:HG3	71:AU:74:PHE:CD1	2.53	0.43
80:AA:747:A:H2'	80:AA:748:G:C8	2.53	0.43
80:AA:1470:A:H2'	80:AA:1471:A:C8	2.49	0.43
80:AA:1523:A:H2'	80:AA:1524:A:C8	2.54	0.43
11:A:2192:A:O2'	17:J:135:VAL:HG11	2.18	0.43
72:AV:96:ARG:HD2	72:AV:101:CYS:SG	2.59	0.43
75:A0:51:PRO:HG3	80:AA:705:C:H5'	2.01	0.43
80:AA:982:A:H2'	80:AA:983:C:H6	1.84	0.43
80:AA:1577:U:H2'	80:AA:1578:A:H8	1.83	0.43
85:Ay:68:C:H2'	85:Ay:69:C:H6	1.83	0.43
8:7:276:PHE:HB2	8:7:304:VAL:HG22	2.00	0.43
11:A:2668:A:H2'	11:A:2669:A:C8	2.54	0.43
11:A:2688:C:H2'	11:A:2689:C:C6	2.54	0.43
11:A:3115:U:H2'	11:A:3116:C:H6	1.84	0.43
29:W:120:LEU:HD21	29:W:126:LEU:HD21	2.00	0.43
59:AG:357:THR:HG23	59:AG:360:GLU:H	1.84	0.43
80:AA:664:G:H2'	80:AA:665:C:C6	2.54	0.43
85:Ay:68:C:H2'	85:Ay:69:C:C6	2.54	0.43
91:B:40:U:H2'	91:B:41:A:C8	2.54	0.43
36:d:205:GLN:NE2	36:d:207:ASN:HD21	2.16	0.42
80:AA:673:U:H2'	80:AA:674:U:H6	1.84	0.42
80:AA:787:C:H2'	80:AA:788:U:C6	2.54	0.42
80:AA:1412:G:H2'	80:AA:1413:U:O4'	2.19	0.42
80:AA:1544:A:H2'	80:AA:1545:U:C6	2.54	0.42
86:Aw:14:A:C2	86:Aw:15:A:H1'	2.53	0.42
7:6:234:HIS:CE1	7:6:257:PRO:HA	2.54	0.42
10:9:36:ARG:HD2	28:U:46:MET:SD	2.59	0.42
11:A:2053:U:HO2'	11:A:2054:U:H6	1.67	0.42
23:P:52:ASN:HB3	23:P:55:ASN:HB2	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:z:295:LEU:HB2	33:z:305:LEU:HD11	2.01	0.42
11:A:1924:U:H2'	11:A:1925:A:C8	2.54	0.42
26:S:119:GLU:HG2	26:S:189:PRO:HB2	2.01	0.42
54:AB:118:LEU:HD23	54:AB:118:LEU:HA	1.87	0.42
55:AC:42:VAL:HG21	55:AC:55:GLU:HB3	2.02	0.42
56:AD:355:ARG:NH1	80:AA:1118:A:H4'	2.34	0.42
60:AH:163:ASN:HB3	76:A1:114:LEU:HD11	2.02	0.42
68:AR:284:LEU:HG	68:AR:288:GLN:NE2	2.34	0.42
84:Ax:18:A:H61	84:Ax:43:A:H2'	1.85	0.42
36:d:219:ARG:HD3	36:d:239:PRO:HB2	2.00	0.42
75:A0:167:PRO:HG2	75:A0:170:LEU:HB2	2.02	0.42
76:A1:241:LYS:HE2	76:A1:241:LYS:HB2	1.87	0.42
80:AA:1043:C:H2'	80:AA:1044:U:C6	2.55	0.42
87:A4:89:PHE:HZ	87:A4:103:SER:HB2	1.84	0.42
11:A:1911:C:H2'	11:A:1912:A:C8	2.55	0.42
11:A:3000:A:H2'	11:A:3001:G:C8	2.55	0.42
11:A:3089:A:O4'	84:Ax:69:C:H5''	2.20	0.42
19:L:46:LEU:HD12	19:L:78:LYS:HD3	2.01	0.42
37:e:98:LEU:HG	37:e:101:LYS:HE3	2.01	0.42
47:q:178:LEU:HD12	47:q:178:LEU:HA	1.83	0.42
66:AO:123:LEU:HB3	66:AO:154:ILE:HG13	2.01	0.42
68:AR:288:GLN:HE22	68:AR:300:LEU:HD22	1.85	0.42
80:AA:1190:C:H2'	80:AA:1191:C:H6	1.84	0.42
80:AA:1204:C:H2'	80:AA:1205:U:O4'	2.19	0.42
85:Ay:4:G:H2'	85:Ay:5:G:H8	1.83	0.42
87:A4:65:TRP:HD1	87:A4:66:ASP:O	2.02	0.42
87:A4:543:GLU:HG2	87:A4:544:LEU:N	2.34	0.42
88:AX:152:ILE:HG12	88:AX:259:LEU:HD23	2.01	0.42
6:5:116:GLY:HA3	6:5:307:ASP:OD2	2.19	0.42
8:7:219:LEU:HD12	8:7:219:LEU:HA	1.91	0.42
15:H:224:THR:HG23	15:H:230:THR:HG22	2.01	0.42
47:q:147:GLN:O	47:q:150:LYS:HG3	2.19	0.42
56:AD:380:LEU:HD12	56:AD:381:PRO:HD2	2.01	0.42
72:AV:246:ASN:HB2	75:A0:70:ARG:HH12	1.84	0.42
75:A0:29:ARG:HG3	75:A0:105:THR:HG21	2.01	0.42
80:AA:686:A:H2'	80:AA:687:G:C8	2.55	0.42
80:AA:1441:A:H2	80:AA:1449:G:H22	1.67	0.42
80:AA:1450:C:H2'	80:AA:1451:U:C6	2.54	0.42
80:AA:1505:A:H2'	80:AA:1506:U:C6	2.55	0.42
85:Ay:70:C:H2'	85:Ay:71:U:C6	2.55	0.42
7:6:236:LEU:HG	7:6:251:THR:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:108:VAL:HB	26:S:195:ILE:HG13	2.01	0.42
80:AA:818:C:C2	80:AA:819:A:C8	3.08	0.42
80:AA:1407:U:H2'	80:AA:1408:A:C8	2.54	0.42
87:A4:393:ILE:HA	87:A4:396:ILE:HG22	2.01	0.42
2:1:20:MET:HE3	2:1:20:MET:HB3	1.96	0.42
9:8:125:LYS:HD3	91:B:29:C:H5''	2.01	0.42
11:A:1863:A:H2'	11:A:1864:A:H8	1.83	0.42
15:H:102:VAL:HB	15:H:105:VAL:HG22	2.02	0.42
16:I:163:GLU:HG3	16:I:166:ARG:HH22	1.84	0.42
18:K:20:LEU:HD22	18:K:141:LEU:HD13	2.02	0.42
69:AS:134:ARG:HG2	69:AS:136:GLY:H	1.85	0.42
72:AV:102:TRP:HD1	75:A0:74:PHE:HD2	1.68	0.42
73:AW:103:ARG:HE	73:AW:139:ARG:NH2	2.18	0.42
80:AA:730:A:C4	80:AA:731:A:C8	3.08	0.42
80:AA:771:A:H2'	80:AA:772:A:C8	2.55	0.42
80:AA:870:C:O5'	80:AA:870:C:H6	2.03	0.42
80:AA:1015:A:H3'	80:AA:1016:U:H6	1.85	0.42
80:AA:1337:U:H2'	80:AA:1338:A:H8	1.85	0.42
86:Aw:14:A:C6	86:Aw:22:A:C5	3.08	0.42
8:7:152:CYS:HB2	8:7:260:PHE:CD2	2.55	0.42
10:9:118:GLY:HA3	34:V:191:LEU:HD12	2.01	0.42
11:A:2182:G:H2'	11:A:2183:C:C6	2.54	0.42
47:q:184:LYS:O	47:q:188:LYS:HG2	2.19	0.42
51:f:190:THR:HG23	51:f:192:GLU:HG3	2.02	0.42
54:AB:167:HIS:CD2	59:AG:153:THR:HG22	2.55	0.42
80:AA:852:A:H3'	80:AA:853:C:C6	2.52	0.42
80:AA:881:A:H2'	80:AA:882:A:C4	2.55	0.42
80:AA:1181:G:H5'	80:AA:1568:U:O4	2.19	0.42
7:6:106:ARG:HG2	23:P:110:TRP:CE2	2.55	0.42
11:A:2215:C:H2'	11:A:2216:A:O4'	2.20	0.42
11:A:2950:U:H2'	11:A:2951:A:H8	1.84	0.42
17:J:70:ILE:HG12	17:J:80:ILE:HG22	2.02	0.42
37:e:97:ARG:HA	37:e:100:LYS:HG2	2.00	0.42
49:t:65:GLN:O	49:t:69:GLN:HG2	2.20	0.42
54:AB:94:LYS:HE3	54:AB:94:LYS:HB3	1.94	0.42
68:AR:142:LEU:HD21	68:AR:183:LYS:HE3	2.01	0.42
80:AA:675:A:H2'	80:AA:676:G:H8	1.84	0.42
80:AA:969:A:H2'	80:AA:970:A:H8	1.84	0.42
80:AA:1057:G:H4'	80:AA:1578:A:H4'	2.02	0.42
80:AA:1562:G:H1'	80:AA:1583:MA6:C2	2.49	0.42
87:A4:397:MET:HA	87:A4:400:LEU:HG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:AX:88:VAL:HA	88:AX:91:VAL:HG22	2.01	0.42
8:7:317:LEU:HA	8:7:317:LEU:HD23	1.84	0.41
11:A:2092:C:H2'	11:A:2093:U:H6	1.85	0.41
36:d:121:SER:O	36:d:125:ILE:HG13	2.19	0.41
53:s:105:TRP:CG	53:s:271:LEU:HD13	2.55	0.41
60:AH:51:HIS:HE1	87:A4:476:LYS:HG3	1.85	0.41
80:AA:1034:U:H2'	80:AA:1035:U:C6	2.55	0.41
87:A4:170:VAL:HG21	87:A4:243:ASN:HB3	2.02	0.41
87:A4:263:ILE:HG13	87:A4:278:LEU:HD23	2.01	0.41
88:AX:266:ASN:HA	88:AX:329:LEU:HD23	2.01	0.41
11:A:2533:A:H2'	11:A:2534:G:C8	2.55	0.41
11:A:2677:A:H2'	11:A:2678:A:C8	2.54	0.41
37:e:200:MET:HA	37:e:241:GLY:HA3	2.02	0.41
60:AH:72:LEU:HD12	76:A1:133:TRP:CZ3	2.55	0.41
66:AO:238:MET:HE3	66:AO:238:MET:HB3	1.98	0.41
80:AA:1171:A:H2'	80:AA:1172:C:O4'	2.20	0.41
80:AA:1240:A:H2'	80:AA:1241:C:C6	2.56	0.41
80:AA:1400:U:H2'	80:AA:1401:G:C8	2.55	0.41
87:A4:438:LEU:O	87:A4:441:THR:HG22	2.19	0.41
88:AX:74:ASP:O	88:AX:78:VAL:HG12	2.20	0.41
9:8:164:ARG:HG3	51:f:88:TYR:CE1	2.55	0.41
11:A:2533:A:H2'	11:A:2534:G:H8	1.85	0.41
11:A:2753:A:C4	11:A:2754:A:C8	3.07	0.41
15:H:213:ILE:HG12	15:H:219:TYR:CZ	2.55	0.41
15:H:248:TYR:CD1	15:H:252:LEU:HD23	2.55	0.41
44:m:81:LEU:HA	44:m:84:LEU:HD23	2.02	0.41
60:AH:156:TYR:O	60:AH:160:ILE:HG12	2.20	0.41
75:A0:145:HIS:ND1	75:A0:146:GLU:HG3	2.36	0.41
80:AA:757:A:H4'	80:AA:758:U:H5''	2.02	0.41
80:AA:833:A:H2'	80:AA:834:G:C8	2.56	0.41
80:AA:921:U:H2'	80:AA:922:C:O4'	2.21	0.41
80:AA:1461:A:O3'	80:AA:1462:G:H8	2.03	0.41
80:AA:1497:C:H2'	80:AA:1498:C:H6	1.86	0.41
80:AA:1508:C:H2'	80:AA:1509:U:H6	1.85	0.41
89:A2:29:LEU:HD22	90:AQ:68:MET:HE2	2.02	0.41
11:A:2212:C:H2'	11:A:2213:A:C8	2.56	0.41
11:A:2550:A:C2	11:A:2551:G:C8	3.09	0.41
11:A:2748:A:H2'	11:A:2749:A:H8	1.85	0.41
11:A:2815:OMG:H1'	11:A:2815:OMG:HM23	1.80	0.41
11:A:3199:U:H5''	11:A:3200:U:H4'	2.02	0.41
12:D:172:MET:HE1	57:AE:86:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:218:ILE:HG23	21:N:223:MET:HB2	2.02	0.41
37:e:124:TRP:CD2	44:m:72:ARG:HG2	2.55	0.41
80:AA:695:A:H2'	80:AA:696:U:O4'	2.20	0.41
80:AA:727:U:H2'	80:AA:728:C:O4'	2.21	0.41
80:AA:990:U:H2'	80:AA:991:G:O4'	2.20	0.41
80:AA:1006:U:H2'	80:AA:1007:G:C8	2.54	0.41
80:AA:1400:U:H2'	80:AA:1401:G:O4'	2.21	0.41
81:AI:100:VAL:HG12	81:AI:106:PRO:HA	2.03	0.41
87:A4:156:ALA:O	87:A4:160:ARG:HG2	2.19	0.41
88:AX:242:ILE:HD13	88:AX:242:ILE:HA	1.85	0.41
8:7:102:LYS:HB2	8:7:102:LYS:HE3	1.94	0.41
11:A:2553:G:H2'	11:A:2554:A:H8	1.85	0.41
11:A:2795:U:H2'	11:A:2796:G:H8	1.85	0.41
11:A:3111:A:H2'	11:A:3112:A:H5''	2.03	0.41
14:F:218:LEU:HD23	14:F:260:VAL:HB	2.03	0.41
15:H:172:LEU:HD23	15:H:235:MET:HE1	2.03	0.41
20:M:44:ARG:HG3	20:M:45:ARG:HG3	2.02	0.41
26:S:183:LYS:HE2	26:S:185:ILE:HD11	2.01	0.41
43:l:96:LEU:HA	43:l:99:MET:HE3	2.03	0.41
72:AV:331:LEU:O	72:AV:335:LYS:HG2	2.20	0.41
80:AA:1328:G:H2'	80:AA:1329:U:C6	2.56	0.41
84:Ax:60:C:H2'	84:Ax:61:C:C6	2.55	0.41
85:Ay:67:U:H2'	85:Ay:68:C:C6	2.56	0.41
11:A:2285:U:H2'	11:A:2286:A:H8	1.86	0.41
11:A:2942:C:H2'	11:A:2943:G:H8	1.85	0.41
13:E:123:GLN:HG2	13:E:125:GLN:HG3	2.01	0.41
21:N:36:VAL:HG23	43:l:128:ARG:HD2	2.02	0.41
21:N:172:VAL:HA	21:N:175:PHE:CE2	2.56	0.41
58:AF:44:PRO:HD3	58:AF:75:LYS:HB2	2.02	0.41
80:AA:658:G:H2'	80:AA:659:U:H6	1.84	0.41
80:AA:1362:G:H2'	80:AA:1363:C:C6	2.56	0.41
80:AA:1382:A:H2'	80:AA:1383:A:O4'	2.21	0.41
85:Ay:67:U:H2'	85:Ay:68:C:H6	1.86	0.41
11:A:2549:C:N4	11:A:2562:U:H2'	2.35	0.41
11:A:3117:C:H2'	11:A:3118:U:C6	2.56	0.41
11:A:3151:A:H4'	24:Q:146:GLY:O	2.21	0.41
16:I:127:PRO:HG2	16:I:130:VAL:HG22	2.03	0.41
33:z:123:LEU:HD21	33:z:125:LEU:HD21	2.03	0.41
58:AF:224:HIS:O	58:AF:228:LYS:HG2	2.21	0.41
80:AA:738:A:H5'	80:AA:739:C:OP2	2.21	0.41
80:AA:1441:A:H3'	80:AA:1442:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:115:GLU:HB2	6:5:119:GLN:HB2	2.03	0.41
9:8:136:ILE:HD12	9:8:136:ILE:HA	1.87	0.41
11:A:2455:U:H5''	22:O:47:ALA:HB3	2.02	0.41
15:H:207:LYS:HB3	15:H:222:GLU:HB3	2.02	0.41
28:U:65:VAL:HG13	28:U:97:VAL:HG13	2.03	0.41
29:W:108:PRO:HA	29:W:114:VAL:HG21	2.03	0.41
36:d:287:LEU:HD11	36:d:293:TYR:HA	2.03	0.41
47:q:167:GLN:HB2	51:f:199:LYS:NZ	2.36	0.41
59:AG:281:ALA:HB2	59:AG:332:VAL:HG23	2.02	0.41
59:AG:388:ARG:HG3	80:AA:1432:U:H4'	2.03	0.41
72:AV:266:VAL:HA	72:AV:269:SER:HB2	2.02	0.41
75:A0:175:ILE:HG22	75:A0:178:ARG:NH1	2.36	0.41
80:AA:821:U:H2'	80:AA:822:G:C8	2.55	0.41
80:AA:1464:G:H2'	80:AA:1465:C:C6	2.56	0.41
85:Ay:33:U:C2'	85:Ay:36:C:H41	2.26	0.41
87:A4:61:LYS:HA	87:A4:61:LYS:HD3	1.89	0.41
87:A4:535:MET:HE2	87:A4:548:PHE:CG	2.54	0.41
8:7:309:HIS:CE1	13:E:155:PHE:HA	2.56	0.41
11:A:2277:U:H2'	11:A:2278:A:H8	1.84	0.41
11:A:2656:U:H4'	13:E:230:THR:OG1	2.20	0.41
11:A:2764:A:C6	15:H:252:LEU:HD11	2.55	0.41
11:A:3150:U:H2'	11:A:3151:A:H8	1.86	0.41
33:z:98:GLU:HB3	33:z:101:LYS:HB2	2.03	0.41
37:e:172:ILE:HD13	91:B:76:A:C2	2.55	0.41
56:AD:226:ARG:HD3	80:AA:659:U:OP1	2.21	0.41
67:AP:54:MET:HE2	69:AS:64:TRP:HB3	2.03	0.41
72:AV:120:ASP:HA	72:AV:122:GLN:HE21	1.86	0.41
77:A3:165:LYS:HG2	77:A3:195:TYR:CE2	2.55	0.41
80:AA:799:A:H2'	80:AA:800:C:H6	1.86	0.41
80:AA:854:U:H2'	80:AA:855:A:C8	2.55	0.41
80:AA:1118:A:H3'	80:AA:1119:U:H5''	2.03	0.41
80:AA:1380:G:H1'	88:AX:163:LYS:HE2	2.03	0.41
11:A:1829:A:H2'	11:A:1830:G:C8	2.55	0.41
34:V:16:PRO:HD2	34:V:19:TYR:HB2	2.02	0.41
36:d:138:PRO:HD3	36:d:194:VAL:HG23	2.03	0.41
48:r:70:CYS:SG	48:r:73:CYS:SG	3.19	0.41
54:AB:148:ASN:HD22	54:AB:197:HIS:CD2	2.39	0.41
57:AE:32:ARG:HB3	57:AE:74:ALA:HB1	2.03	0.41
60:AH:155:VAL:HG21	76:A1:129:PHE:HB2	2.03	0.41
80:AA:680:U:H2'	80:AA:681:U:C6	2.56	0.41
80:AA:824:U:H2'	80:AA:825:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:1162:A:H2'	80:AA:1163:C:C6	2.56	0.41
80:AA:1309:A:H2'	80:AA:1310:C:C6	2.56	0.41
89:A2:33:VAL:HG21	89:A2:104:LEU:HD23	2.03	0.41
6:5:417:LEU:HA	6:5:417:LEU:HD23	1.88	0.40
11:A:1862:U:H2'	11:A:1863:A:C8	2.56	0.40
11:A:2603:C:C2	11:A:2604:A:C8	3.09	0.40
11:A:3170:C:N4	11:A:3171:C:H41	2.19	0.40
11:A:3191:A:H4'	48:r:123:HIS:HB3	2.03	0.40
13:E:50:ASP:HA	13:E:53:LEU:HG	2.03	0.40
16:I:47:LEU:HD22	21:N:226:ILE:HG12	2.03	0.40
31:Y:191:ASN:HB3	31:Y:194:TYR:HB3	2.03	0.40
66:AO:55:PRO:HB3	66:AO:114:HIS:HB2	2.03	0.40
80:AA:702:C:H1'	80:AA:842:C:H1'	2.03	0.40
80:AA:1180:U:H2'	80:AA:1181:G:H8	1.86	0.40
87:A4:89:PHE:CZ	87:A4:103:SER:HB2	2.56	0.40
88:AX:274:LEU:HD13	88:AX:274:LEU:HA	1.90	0.40
11:A:2065:A:C4	11:A:2066:C:C5	3.09	0.40
11:A:2461:A:H2'	11:A:2462:A:H8	1.85	0.40
11:A:2774:C:H2'	11:A:2775:A:C4	2.56	0.40
11:A:3002:G:H2'	11:A:3003:A:H8	1.87	0.40
51:f:203:GLU:HG2	51:f:204:LEU:N	2.36	0.40
63:AL:115:ILE:HG21	63:AL:181:ILE:HD13	2.04	0.40
71:AU:65:GLN:HB2	75:A0:198:MET:HE1	2.02	0.40
72:AV:241:ARG:HA	72:AV:244:TYR:CE2	2.56	0.40
72:AV:381:GLN:O	72:AV:384:LEU:HG	2.21	0.40
80:AA:684:U:H2'	80:AA:685:A:C8	2.55	0.40
80:AA:1238:C:H2'	80:AA:1239:C:C6	2.56	0.40
80:AA:1471:A:H2'	80:AA:1472:G:C8	2.55	0.40
85:Ay:21:A:H61	85:Ay:46:A:H2'	1.87	0.40
2:1:54:VAL:HG13	47:q:128:MET:HE2	2.03	0.40
11:A:2228:A:H2'	11:A:2229:A:C8	2.56	0.40
47:q:44:ASP:O	47:q:47:THR:HG22	2.22	0.40
76:A1:131:THR:HG21	87:A4:61:LYS:O	2.21	0.40
80:AA:956:C:H2'	80:AA:957:C:O4'	2.21	0.40
80:AA:1154:A:O2'	80:AA:1155:G:H5'	2.21	0.40
86:Aw:74:C:H3'	86:Aw:75:C:C6	2.55	0.40
87:A4:140:LEU:HD12	87:A4:140:LEU:HA	1.86	0.40
9:8:65:LYS:O	9:8:69:LYS:HG2	2.22	0.40
25:R:111:LYS:HD3	35:b:127:GLN:HB3	2.03	0.40
36:d:110:GLU:O	36:d:114:LYS:HG2	2.21	0.40
37:e:85:SER:HB3	44:m:50:ARG:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:AB:58:PHE:CE1	54:AB:62:ILE:HG13	2.57	0.40
59:AG:92:MET:HE2	59:AG:92:MET:HB2	1.80	0.40
64:AM:40:LYS:HB3	80:AA:712:C:H4'	2.03	0.40
69:AS:86:ASP:HB2	73:AW:101:ILE:HD13	2.01	0.40
80:AA:715:G:H2'	80:AA:716:U:H6	1.87	0.40
80:AA:853:C:H2'	80:AA:854:U:C6	2.57	0.40
80:AA:871:A:H1'	80:AA:872:G:C8	2.56	0.40
87:A4:309:PHE:HB2	87:A4:313:TRP:CZ3	2.56	0.40
49:u:74:LEU:HD23	49:u:79:ILE:HG12	2.03	0.40
74:AZ:56:HIS:O	74:AZ:60:GLU:HG3	2.21	0.40
80:AA:811:G:H2'	80:AA:812:A:O4'	2.22	0.40
80:AA:981:C:H2'	80:AA:982:A:H8	1.86	0.40
85:Ay:69:C:H2'	85:Ay:70:C:H6	1.86	0.40
88:AX:276:ARG:HB3	88:AX:278:ASP:OD1	2.22	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%)	108 (100%)	0	0	100	100
2	1	54/65 (83%)	54 (100%)	0	0	100	100
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	36/103 (35%)	36 (100%)	0	0	100	100
6	5	392/423 (93%)	384 (98%)	8 (2%)	0	100	100
7	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
8	7	292/338 (86%)	282 (97%)	10 (3%)	0	100	100
9	8	155/206 (75%)	152 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	9	122/137 (89%)	118 (97%)	4 (3%)	0	100	100
12	D	236/305 (77%)	228 (97%)	8 (3%)	0	100	100
13	E	303/348 (87%)	295 (97%)	8 (3%)	0	100	100
14	F	250/311 (80%)	246 (98%)	4 (2%)	0	100	100
15	H	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
16	I	179/261 (69%)	177 (99%)	2 (1%)	0	100	100
17	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
18	K	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
19	L	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
20	M	289/296 (98%)	281 (97%)	8 (3%)	0	100	100
21	N	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
22	O	152/175 (87%)	146 (96%)	6 (4%)	0	100	100
23	P	142/180 (79%)	137 (96%)	5 (4%)	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%)	155 (98%)	4 (2%)	0	100	100
27	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
28	U	150/153 (98%)	147 (98%)	3 (2%)	0	100	100
29	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
30	X	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
31	Y	179/250 (72%)	175 (98%)	4 (2%)	0	100	100
32	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
33	z	250/325 (77%)	235 (94%)	15 (6%)	0	100	100
34	V	203/216 (94%)	202 (100%)	1 (0%)	0	100	100
35	b	148/215 (69%)	143 (97%)	5 (3%)	0	100	100
36	d	257/306 (84%)	240 (93%)	16 (6%)	1 (0%)	30	60
37	e	236/279 (85%)	227 (96%)	9 (4%)	0	100	100
38	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
39	h	108/158 (68%)	104 (96%)	4 (4%)	0	100	100
40	i	95/128 (74%)	95 (100%)	0	0	100	100
41	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	k	100/112 (89%)	100 (100%)	0	0	100	100
43	l	80/138 (58%)	79 (99%)	1 (1%)	0	100	100
44	m	90/128 (70%)	88 (98%)	2 (2%)	0	100	100
46	o	92/102 (90%)	92 (100%)	0	0	100	100
47	q	175/222 (79%)	175 (100%)	0	0	100	100
48	r	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
49	t	44/198 (22%)	44 (100%)	0	0	100	100
49	u	30/198 (15%)	30 (100%)	0	0	100	100
50	c	282/332 (85%)	277 (98%)	5 (2%)	0	100	100
51	f	153/212 (72%)	146 (95%)	7 (5%)	0	100	100
52	p	141/206 (68%)	137 (97%)	4 (3%)	0	100	100
53	s	381/439 (87%)	375 (98%)	6 (2%)	0	100	100
54	AB	223/296 (75%)	216 (97%)	7 (3%)	0	100	100
55	AC	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
56	AD	341/430 (79%)	330 (97%)	11 (3%)	0	100	100
57	AE	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
58	AF	206/242 (85%)	205 (100%)	1 (0%)	0	100	100
59	AG	323/396 (82%)	316 (98%)	7 (2%)	0	100	100
60	AH	138/201 (69%)	133 (96%)	4 (3%)	1 (1%)	18	47
61	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
62	AK	99/128 (77%)	99 (100%)	0	0	100	100
63	AL	172/257 (67%)	171 (99%)	1 (1%)	0	100	100
64	AM	117/137 (85%)	114 (97%)	3 (3%)	0	100	100
65	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100
66	AO	191/258 (74%)	186 (97%)	5 (3%)	0	100	100
67	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
68	AR	293/360 (81%)	284 (97%)	9 (3%)	0	100	100
69	AS	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
70	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
71	AU	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
72	AV	358/414 (86%)	346 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	AW	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
74	AZ	98/106 (92%)	97 (99%)	1 (1%)	0	100	100
75	A0	213/217 (98%)	208 (98%)	5 (2%)	0	100	100
76	A1	277/323 (86%)	268 (97%)	9 (3%)	0	100	100
77	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
79	AY	117/395 (30%)	116 (99%)	1 (1%)	0	100	100
81	AI	135/194 (70%)	130 (96%)	5 (4%)	0	100	100
82	OX	51/435 (12%)	47 (92%)	4 (8%)	0	100	100
83	a	99/142 (70%)	96 (97%)	3 (3%)	0	100	100
87	A4	584/689 (85%)	569 (97%)	15 (3%)	0	100	100
88	AX	350/398 (88%)	337 (96%)	13 (4%)	0	100	100
89	A2	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
90	AQ	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
All	All	14617/19127 (76%)	14283 (98%)	332 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
60	AH	126	ILE
36	d	47	GLN

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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	z	226/287 (79%)	226 (100%)	0	100	100
34	V	183/191 (96%)	183 (100%)	0	100	100
35	b	132/186 (71%)	132 (100%)	0	100	100
36	d	237/274 (86%)	237 (100%)	0	100	100
37	e	207/236 (88%)	207 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	g	124/148 (84%)	124 (100%)	0	100	100
39	h	104/148 (70%)	104 (100%)	0	100	100
40	i	86/110 (78%)	86 (100%)	0	100	100
41	j	74/97 (76%)	74 (100%)	0	100	100
42	k	83/89 (93%)	83 (100%)	0	100	100
43	l	76/116 (66%)	76 (100%)	0	100	100
44	m	85/113 (75%)	85 (100%)	0	100	100
46	o	80/87 (92%)	80 (100%)	0	100	100
47	q	153/178 (86%)	153 (100%)	0	100	100
48	r	147/169 (87%)	147 (100%)	0	100	100
49	t	40/158 (25%)	40 (100%)	0	100	100
49	u	31/158 (20%)	31 (100%)	0	100	100
50	c	251/288 (87%)	251 (100%)	0	100	100
51	f	139/188 (74%)	139 (100%)	0	100	100
52	p	135/181 (75%)	135 (100%)	0	100	100
53	s	339/381 (89%)	339 (100%)	0	100	100
54	AB	198/249 (80%)	198 (100%)	0	100	100
55	AC	115/143 (80%)	115 (100%)	0	100	100
56	AD	286/357 (80%)	286 (100%)	0	100	100
57	AE	104/107 (97%)	104 (100%)	0	100	100
58	AF	185/209 (88%)	185 (100%)	0	100	100
59	AG	285/342 (83%)	285 (100%)	0	100	100
60	AH	130/180 (72%)	130 (100%)	0	100	100
61	AJ	93/118 (79%)	93 (100%)	0	100	100
62	AK	91/113 (80%)	91 (100%)	0	100	100
63	AL	158/226 (70%)	158 (100%)	0	100	100
64	AM	97/113 (86%)	97 (100%)	0	100	100
65	AN	96/115 (84%)	96 (100%)	0	100	100
66	AO	174/230 (76%)	173 (99%)	1 (1%)	78	81
67	AP	88/123 (72%)	88 (100%)	0	100	100
68	AR	264/318 (83%)	263 (100%)	1 (0%)	84	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	AS	116/164 (71%)	116 (100%)	0	100	100
70	AT	153/157 (98%)	153 (100%)	0	100	100
71	AU	152/174 (87%)	152 (100%)	0	100	100
72	AV	325/364 (89%)	325 (100%)	0	100	100
73	AW	87/158 (55%)	87 (100%)	0	100	100
74	AZ	90/95 (95%)	90 (100%)	0	100	100
75	A0	188/189 (100%)	188 (100%)	0	100	100
76	A1	257/291 (88%)	257 (100%)	0	100	100
77	A3	65/166 (39%)	65 (100%)	0	100	100
79	AY	110/357 (31%)	110 (100%)	0	100	100
81	AI	105/147 (71%)	105 (100%)	0	100	100
82	OX	49/372 (13%)	49 (100%)	0	100	100
83	a	99/133 (74%)	99 (100%)	0	100	100
87	A4	526/609 (86%)	526 (100%)	0	100	100
88	AX	311/351 (89%)	311 (100%)	0	100	100
89	A2	100/100 (100%)	100 (100%)	0	100	100
90	AQ	78/78 (100%)	78 (100%)	0	100	100
All	All	13069/16529 (79%)	13067 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
66	AO	154	ILE
68	AR	78	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	98	GLN
6	5	150	GLN
6	5	214	ASN
6	5	251	HIS
6	5	343	GLN
7	6	163	HIS
7	6	292	GLN

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Mol	Chain	Res	Type
8	7	231	GLN
8	7	287	GLN
9	8	186	GLN
14	F	208	HIS
14	F	249	ASN
16	I	36	HIS
16	I	114	HIS
18	K	94	GLN
18	K	117	HIS
19	L	59	HIS
21	N	138	HIS
21	N	210	GLN
21	N	237	HIS
22	O	150	GLN
22	O	154	GLN
24	Q	107	HIS
24	Q	261	ASN
25	R	89	ASN
26	S	84	ASN
26	S	140	ASN
27	T	103	ASN
30	X	93	ASN
32	Z	150	HIS
35	b	123	ASN
36	d	77	HIS
36	d	193	HIS
36	d	207	ASN
36	d	251	GLN
36	d	286	GLN
37	e	252	HIS
38	g	73	GLN
38	g	141	ASN
39	h	118	HIS
40	i	120	HIS
40	i	124	HIS
41	j	92	GLN
42	k	72	HIS
43	l	100	ASN
43	l	125	ASN
44	m	44	HIS
48	r	79	HIS
48	r	109	GLN

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Mol	Chain	Res	Type
50	c	168	HIS
50	c	192	GLN
53	s	420	GLN
54	AB	148	ASN
54	AB	167	HIS
55	AC	107	GLN
56	AD	130	GLN
56	AD	155	GLN
56	AD	196	ASN
56	AD	415	GLN
56	AD	424	ASN
57	AE	92	ASN
58	AF	214	HIS
59	AG	175	HIS
62	AK	113	HIS
62	AK	117	HIS
63	AL	77	GLN
63	AL	108	GLN
63	AL	172	ASN
64	AM	28	ASN
66	AO	65	GLN
66	AO	103	ASN
67	AP	137	ASN
68	AR	326	ASN
69	AS	66	HIS
73	AW	135	GLN
77	A3	140	HIS
77	A3	158	GLN
77	A3	190	GLN
79	AY	285	GLN
79	AY	295	GLN
81	AI	96	GLN
81	AI	183	HIS
83	a	126	HIS
87	A4	90	GLN
87	A4	122	ASN
87	A4	626	GLN
87	A4	656	ASN
88	AX	81	HIS
88	AX	180	GLN
88	AX	190	ASN
88	AX	201	GLN

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Mol	Chain	Res	Type
88	AX	326	GLN
90	AQ	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1556/1558 (99%)	251 (16%)	2 (0%)
78	Az	33/34 (97%)	12 (36%)	0
80	AA	953/954 (99%)	135 (14%)	1 (0%)
84	Ax	70/71 (98%)	15 (21%)	0
85	Ay	67/76 (88%)	13 (19%)	0
86	Aw	64/76 (84%)	21 (32%)	0
91	B	70/72 (97%)	16 (22%)	0
All	All	2813/2841 (99%)	463 (16%)	3 (0%)

All (463) 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	1736	A
11	A	1748	G
11	A	1765	C
11	A	1777	A
11	A	1780	U
11	A	1805	A
11	A	1807	U
11	A	1808	A
11	A	1812	C
11	A	1817	C
11	A	1821	A
11	A	1827	C

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Mol	Chain	Res	Type
11	A	1828	A
11	A	1829	A
11	A	1832	A
11	A	1836	A
11	A	1844	A
11	A	1854	U
11	A	1856	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
11	A	1938	A
11	A	1940	A
11	A	1975	U
11	A	1985	G
11	A	1986	A
11	A	1992	C
11	A	1993	A
11	A	1994	A
11	A	2000	C
11	A	2002	G
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	2070	C
11	A	2071	U

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Mol	Chain	Res	Type
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	2155	A
11	A	2159	U
11	A	2160	A
11	A	2161	A
11	A	2163	A
11	A	2168	U
11	A	2181	A
11	A	2182	G
11	A	2191	A
11	A	2192	A
11	A	2195	A
11	A	2196	A
11	A	2198	A
11	A	2200	A
11	A	2214	A
11	A	2219	C
11	A	2220	A
11	A	2221	C
11	A	2223	A
11	A	2224	C
11	A	2225	C
11	A	2226	U
11	A	2230	A
11	A	2232	A
11	A	2233	U
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	2283	C
11	A	2284	C

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Mol	Chain	Res	Type
11	A	2294	A
11	A	2297	A
11	A	2300	G
11	A	2322	C
11	A	2331	C
11	A	2332	C
11	A	2345	G
11	A	2349	G
11	A	2350	A
11	A	2353	A
11	A	2357	C
11	A	2363	A
11	A	2372	U
11	A	2374	A
11	A	2379	C
11	A	2381	A
11	A	2390	A
11	A	2399	A
11	A	2401	A
11	A	2404	U
11	A	2407	U
11	A	2415	C
11	A	2446	A
11	A	2451	A
11	A	2452	A
11	A	2478	G
11	A	2485	U
11	A	2493	C
11	A	2502	C
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	2570	C
11	A	2571	G
11	A	2592	G
11	A	2593	G
11	A	2594	U
11	A	2599	U
11	A	2600	A

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Mol	Chain	Res	Type
11	A	2601	A
11	A	2603	C
11	A	2618	U
11	A	2625	C
11	A	2627	G
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	2762	C
11	A	2763	U
11	A	2764	A
11	A	2765	A
11	A	2767	A
11	A	2768	A
11	A	2782	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	2884	C
11	A	2885	U
11	A	2888	A

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Mol	Chain	Res	Type
11	A	2889	C
11	A	2893	A
11	A	2907	U
11	A	2913	A
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	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	3016	G
11	A	3022	G
11	A	3041	U
11	A	3053	A
11	A	3054	G
11	A	3069	A
11	A	3086	U
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	3150	U
11	A	3157	C
11	A	3158	A
11	A	3162	C

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Mol	Chain	Res	Type
11	A	3169	C
11	A	3172	C
11	A	3177	A
11	A	3180	A
11	A	3183	U
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	3220	A
11	A	3228	U
11	A	3229	U
11	A	3230	G
78	Az	0	U
78	Az	4	A
78	Az	11	U
78	Az	12	U
78	Az	13	U
78	Az	18	A
78	Az	21	A
78	Az	22	A
78	Az	25	U
78	Az	26	A
78	Az	27	C
78	Az	31	A
80	AA	651	A
80	AA	680	U
80	AA	688	A
80	AA	704	U
80	AA	721	U
80	AA	722	C
80	AA	737	C
80	AA	738	A
80	AA	753	A
80	AA	761	A
80	AA	766	G
80	AA	791	G

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Mol	Chain	Res	Type
80	AA	794	U
80	AA	796	G
80	AA	828	C
80	AA	829	C
80	AA	830	U
80	AA	832	U
80	AA	835	C
80	AA	836	A
80	AA	860	A
80	AA	861	U
80	AA	868	C
80	AA	870	C
80	AA	871	A
80	AA	881	A
80	AA	889	G
80	AA	890	C
80	AA	893	G
80	AA	903	U
80	AA	904	C
80	AA	907	A
80	AA	919	A
80	AA	929	A
80	AA	933	G
80	AA	938	A
80	AA	939	A
80	AA	941	G
80	AA	942	A
80	AA	954	C
80	AA	959	C
80	AA	960	C
80	AA	961	U
80	AA	962	C
80	AA	963	C
80	AA	967	A
80	AA	978	A
80	AA	1001	C
80	AA	1002	C
80	AA	1015	A
80	AA	1031	G
80	AA	1042	U
80	AA	1081	U
80	AA	1082	A

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Mol	Chain	Res	Type
80	AA	1096	A
80	AA	1103	A
80	AA	1105	C
80	AA	1106	C
80	AA	1107	U
80	AA	1109	A
80	AA	1118	A
80	AA	1119	U
80	AA	1121	A
80	AA	1126	A
80	AA	1137	A
80	AA	1138	G
80	AA	1151	C
80	AA	1153	C
80	AA	1160	A
80	AA	1167	A
80	AA	1187	U
80	AA	1188	A
80	AA	1189	U
80	AA	1190	C
80	AA	1215	U
80	AA	1220	A
80	AA	1223	C
80	AA	1225	C
80	AA	1232	A
80	AA	1235	U
80	AA	1247	G
80	AA	1248	C
80	AA	1250	C
80	AA	1251	A
80	AA	1254	C
80	AA	1261	C
80	AA	1271	C
80	AA	1284	U
80	AA	1285	G
80	AA	1290	C
80	AA	1291	U
80	AA	1292	A
80	AA	1294	A
80	AA	1297	G
80	AA	1326	A
80	AA	1327	G

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Mol	Chain	Res	Type
80	AA	1343	A
80	AA	1344	U
80	AA	1353	A
80	AA	1354	A
80	AA	1356	A
80	AA	1378	C
80	AA	1387	A
80	AA	1390	A
80	AA	1405	C
80	AA	1407	U
80	AA	1430	A
80	AA	1432	U
80	AA	1443	U
80	AA	1466	C
80	AA	1481	C
80	AA	1482	A
80	AA	1512	A
80	AA	1519	A
80	AA	1521	U
80	AA	1522	U
80	AA	1525	C
80	AA	1526	U
80	AA	1527	A
80	AA	1528	A
80	AA	1533	C
80	AA	1537	C
80	AA	1538	G
80	AA	1539	C
80	AA	1540	A
80	AA	1551	G
80	AA	1557	A
80	AA	1560	U
80	AA	1568	U
80	AA	1571	U
80	AA	1582	G
80	AA	1584	MA6
80	AA	1594	G
80	AA	1595	G
80	AA	1599	A
84	Ax	13	U
84	Ax	16	A
84	Ax	17	U

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Mol	Chain	Res	Type
84	Ax	18	A
84	Ax	22	U
84	Ax	43	A
84	Ax	44	U
84	Ax	47	U
84	Ax	51	U
84	Ax	52	A
84	Ax	56	C
84	Ax	61	C
84	Ax	63	G
84	Ax	65	A
84	Ax	71	A
85	Ay	8	U
85	Ay	9	A
85	Ay	13	U
85	Ay	29	U
85	Ay	33	U
85	Ay	44	A
85	Ay	45	G
85	Ay	46	A
85	Ay	49	G
85	Ay	56	C
85	Ay	58	A
85	Ay	59	U
85	Ay	73	A
86	Aw	9	A
86	Aw	13	U
86	Aw	14	A
86	Aw	15	A
86	Aw	16	A
86	Aw	21	A
86	Aw	46	A
86	Aw	49	U
86	Aw	50	A
86	Aw	51	U
86	Aw	52	G
86	Aw	53	A
86	Aw	56	A
86	Aw	63	A
86	Aw	65	A
86	Aw	68	U
86	Aw	69	A

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Mol	Chain	Res	Type
86	Aw	71	C
86	Aw	72	A
86	Aw	74	C
86	Aw	75	C
91	B	8	U
91	B	10	2MG
91	B	16	C
91	B	19	C
91	B	21	A
91	B	45	G
91	B	46	A
91	B	54	C
91	B	55	U
91	B	56	U
91	B	58	A
91	B	59	A
91	B	64	A
91	B	69	U
91	B	72	G
91	B	76	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	2245	A
11	A	2484	C
80	AA	828	C

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	1MA	A	2617	11	21,25,26	0.41	0	30,37,40	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	OMG	A	2815	84,11,93	23,26,27	0.36	0	32,38,41	0.43	0
80	MA6	AA	1583	80	23,26,27	0.34	0	33,38,41	0.73	1 (3%)
91	1MA	B	9	91	21,25,26	0.41	0	30,37,40	0.66	0
91	PSU	B	39	91	18,21,22	1.03	1 (5%)	21,30,33	0.71	0
80	B8T	AA	1486	80	19,22,23	0.40	0	25,31,34	0.30	0
80	5MC	AA	1488	80	19,22,23	0.85	1 (5%)	26,32,35	0.51	0
91	2MG	B	10	91	23,26,27	0.36	0	33,38,41	0.41	0
11	OMG	A	3040	86,11	23,26,27	0.35	0	32,38,41	0.38	0
80	MA6	AA	1584	80	23,26,27	0.31	0	33,38,41	0.74	1 (3%)
11	OMU	A	3039	11,93	19,22,23	0.31	0	25,31,34	0.71	1 (4%)
80	5MU	AA	1076	80	19,22,23	0.38	0	27,32,35	0.66	0
11	PSU	A	3067	11	18,21,22	1.12	2 (11%)	21,30,33	0.79	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	1MA	A	2617	11	-	0/7/25/26	0/3/3/3
11	OMG	A	2815	84,11,93	-	0/9/27/28	0/3/3/3
80	MA6	AA	1583	80	-	0/11/29/30	0/3/3/3
91	1MA	B	9	91	-	0/7/25/26	0/3/3/3
91	PSU	B	39	91	-	0/7/25/26	0/2/2/2
80	B8T	AA	1486	80	-	0/7/27/28	0/2/2/2
80	5MC	AA	1488	80	-	0/7/25/26	0/2/2/2
91	2MG	B	10	91	-	0/9/27/28	0/3/3/3
11	OMG	A	3040	86,11	-	2/9/27/28	0/3/3/3
80	MA6	AA	1584	80	-	1/11/29/30	0/3/3/3
11	OMU	A	3039	11,93	-	0/9/27/28	0/2/2/2
80	5MU	AA	1076	80	-	5/7/25/26	0/2/2/2
11	PSU	A	3067	11	-	0/7/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	3067	PSU	C6-C5	3.61	1.39	1.35
91	B	39	PSU	C6-C5	3.50	1.39	1.35
80	AA	1488	5MC	C5-C4	-3.33	1.41	1.44
11	A	3067	PSU	O4'-C1'	-2.48	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	AA	1584	MA6	C2-N1-C6	2.94	119.01	111.83
80	AA	1583	MA6	C2-N1-C6	2.92	118.97	111.83
11	A	3039	OMU	C2'-C1'-N1	-2.67	109.17	114.24
11	A	3067	PSU	O4'-C1'-C2'	2.34	108.38	105.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	AA	1076	5MU	O4'-C4'-C5'-O5'
80	AA	1076	5MU	C3'-C4'-C5'-O5'
80	AA	1584	MA6	C4'-C5'-O5'-P
80	AA	1076	5MU	C4'-C5'-O5'-P
11	A	3040	OMG	C3'-C4'-C5'-O5'
80	AA	1076	5MU	C2'-C1'-N1-C2
80	AA	1076	5MU	C2'-C1'-N1-C6
11	A	3040	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	2815	OMG	1	0
80	AA	1583	MA6	2	0
80	AA	1486	B8T	1	0
80	AA	1488	5MC	2	0
80	AA	1076	5MU	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
94	SPD	A	3301	96	9,9,9	0.15	0	8,8,8	0.16	0
99	SPM	AA	1702	-	13,13,13	0.17	0	12,12,12	0.25	0
99	SPM	AA	1778	-	13,13,13	0.16	0	12,12,12	0.27	0
94	SPD	A	3302	-	9,9,9	0.15	0	8,8,8	0.25	0
97	FES	r	201	48,16	0,4,4	-	-	-	-	-
98	NAD	AA	1701	96	46,48,48	1.18	3 (6%)	64,73,73	0.81	2 (3%)
94	SPD	AA	1703	-	9,9,9	0.16	0	8,8,8	0.25	0
97	FES	AP	201	67,57	0,4,4	-	-	-	-	-
100	ATP	AX	501	96	32,33,33	0.58	1 (3%)	48,52,52	0.33	0
102	VAL	B	101	91	4,6,7	0.71	0	6,7,9	1.19	1 (16%)
94	SPD	A	3472	-	9,9,9	0.17	0	8,8,8	0.23	0
97	FES	AT	201	70,64	0,4,4	-	-	-	-	-
101	GDP	AX	503	-	29,30,30	1.18	3 (10%)	45,47,47	1.76	6 (13%)
95	PUT	A	3303	-	5,5,5	0.14	0	4,4,4	0.23	0
94	SPD	A	3471	-	9,9,9	0.15	0	8,8,8	0.33	0
94	SPD	AA	1780	-	9,9,9	0.16	0	8,8,8	0.21	0
94	SPD	A	3470	-	9,9,9	0.16	0	8,8,8	0.34	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
94	SPD	A	3301	96	-	0/7/7/7	-
99	SPM	AA	1702	-	-	0/11/11/11	-
99	SPM	AA	1778	-	-	1/11/11/11	-
94	SPD	A	3302	-	-	2/7/7/7	-
98	NAD	AA	1701	96	-	2/30/62/62	0/5/5/5
100	ATP	AX	501	96	-	0/22/38/38	0/3/3/3
94	SPD	AA	1703	-	-	0/7/7/7	-
102	VAL	B	101	91	-	1/5/6/8	-
97	FES	r	201	48,16	-	-	0/1/1/1
97	FES	AP	201	67,57	-	-	0/1/1/1
94	SPD	A	3472	-	-	1/7/7/7	-
97	FES	AT	201	70,64	-	-	0/1/1/1
101	GDP	AX	503	-	-	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
95	PUT	A	3303	-	-	0/3/3/3	-
94	SPD	A	3471	-	-	1/7/7/7	-
94	SPD	AA	1780	-	-	0/7/7/7	-
94	SPD	A	3470	-	-	0/7/7/7	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
98	AA	1701	NAD	PA-O3	4.87	1.64	1.59
101	AX	503	GDP	C5-C4	3.10	1.47	1.38
98	AA	1701	NAD	PN-O3	3.01	1.62	1.59
98	AA	1701	NAD	O4D-C1D	-2.71	1.37	1.40
101	AX	503	GDP	C6-N1	-2.52	1.34	1.38
100	AX	501	ATP	PB-O3B	-2.23	1.57	1.59
101	AX	503	GDP	C5-N7	-2.12	1.34	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
101	AX	503	GDP	C5-C4-N3	-5.92	118.97	128.39
101	AX	503	GDP	C2-N3-C4	4.90	120.74	112.30
101	AX	503	GDP	N9-C4-N3	4.46	134.87	125.95
101	AX	503	GDP	C6-C5-N7	3.28	136.25	130.29
102	B	101	VAL	O-C-CA	-2.61	118.06	124.77
98	AA	1701	NAD	O3-PA-O1A	-2.59	102.91	110.70
101	AX	503	GDP	C4-C5-N7	-2.48	106.74	110.67
101	AX	503	GDP	C3'-C2'-C1'	2.31	105.83	101.46
98	AA	1701	NAD	O2A-PA-O1A	2.27	123.01	112.44

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
101	AX	503	GDP	PA-O3A-PB-O2B
101	AX	503	GDP	PA-O3A-PB-O3B
102	B	101	VAL	C-CA-CB-CG1
94	A	3472	SPD	C7-C8-C9-N10
94	A	3302	SPD	C2-C3-C4-C5
94	A	3302	SPD	C4-C5-N6-C7
94	A	3471	SPD	C2-C3-C4-C5
99	AA	1778	SPM	C12-C11-N10-C9

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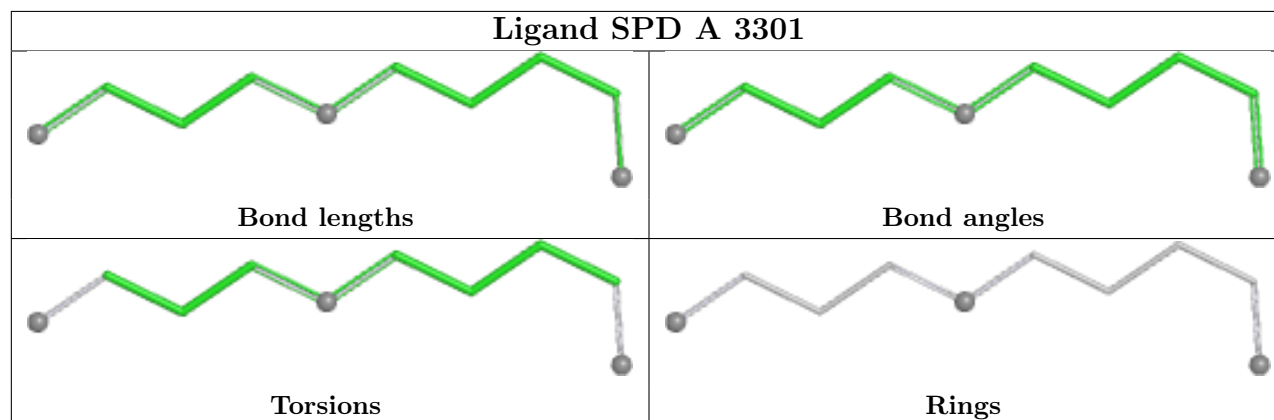
Mol	Chain	Res	Type	Atoms
101	AX	503	GDP	C5'-O5'-PA-O3A
101	AX	503	GDP	C5'-O5'-PA-O1A
101	AX	503	GDP	C5'-O5'-PA-O2A
98	AA	1701	NAD	O4D-C4D-C5D-O5D
101	AX	503	GDP	PA-O3A-PB-O1B
98	AA	1701	NAD	C4N-C3N-C7N-N7N

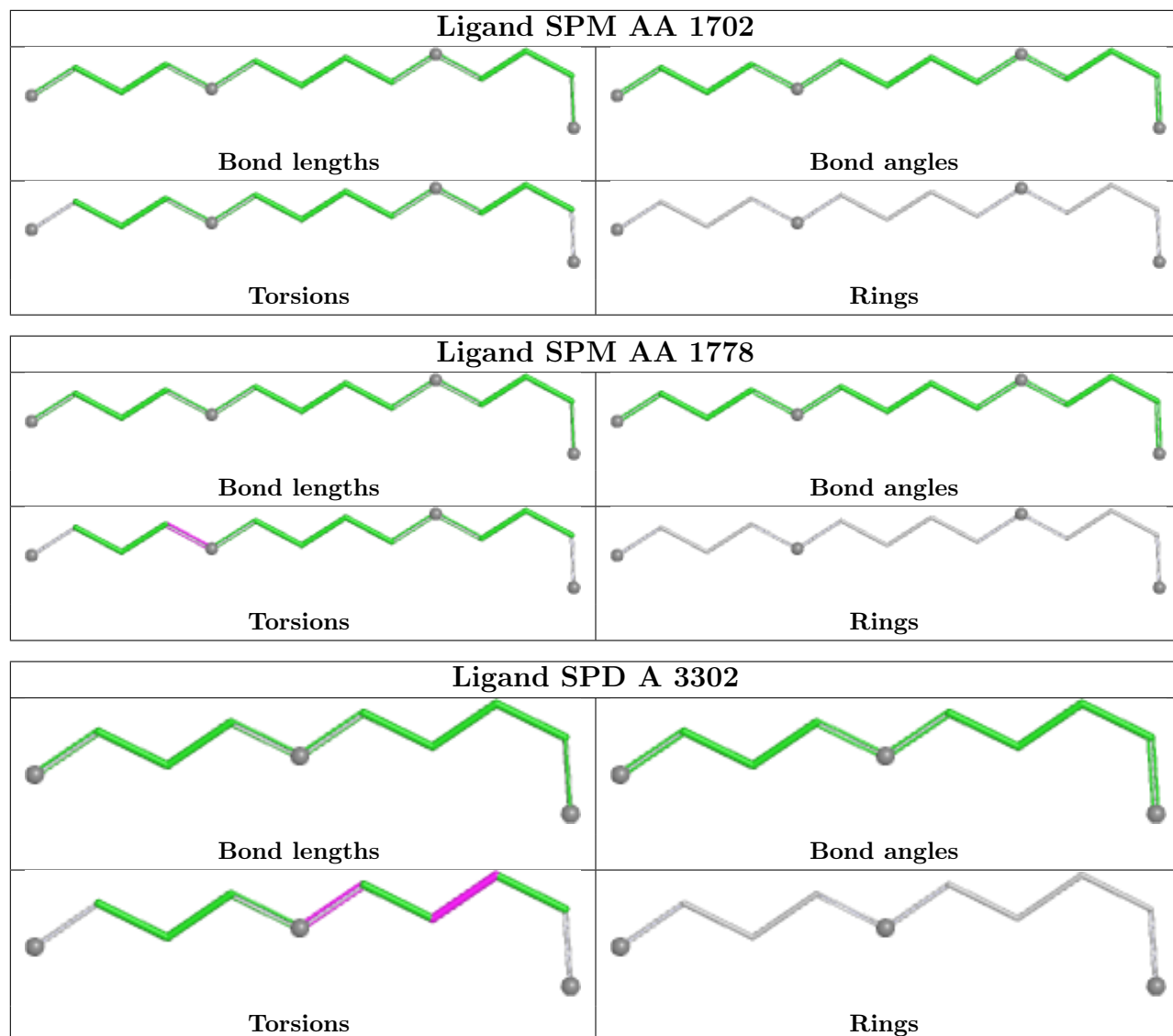
There are no ring outliers.

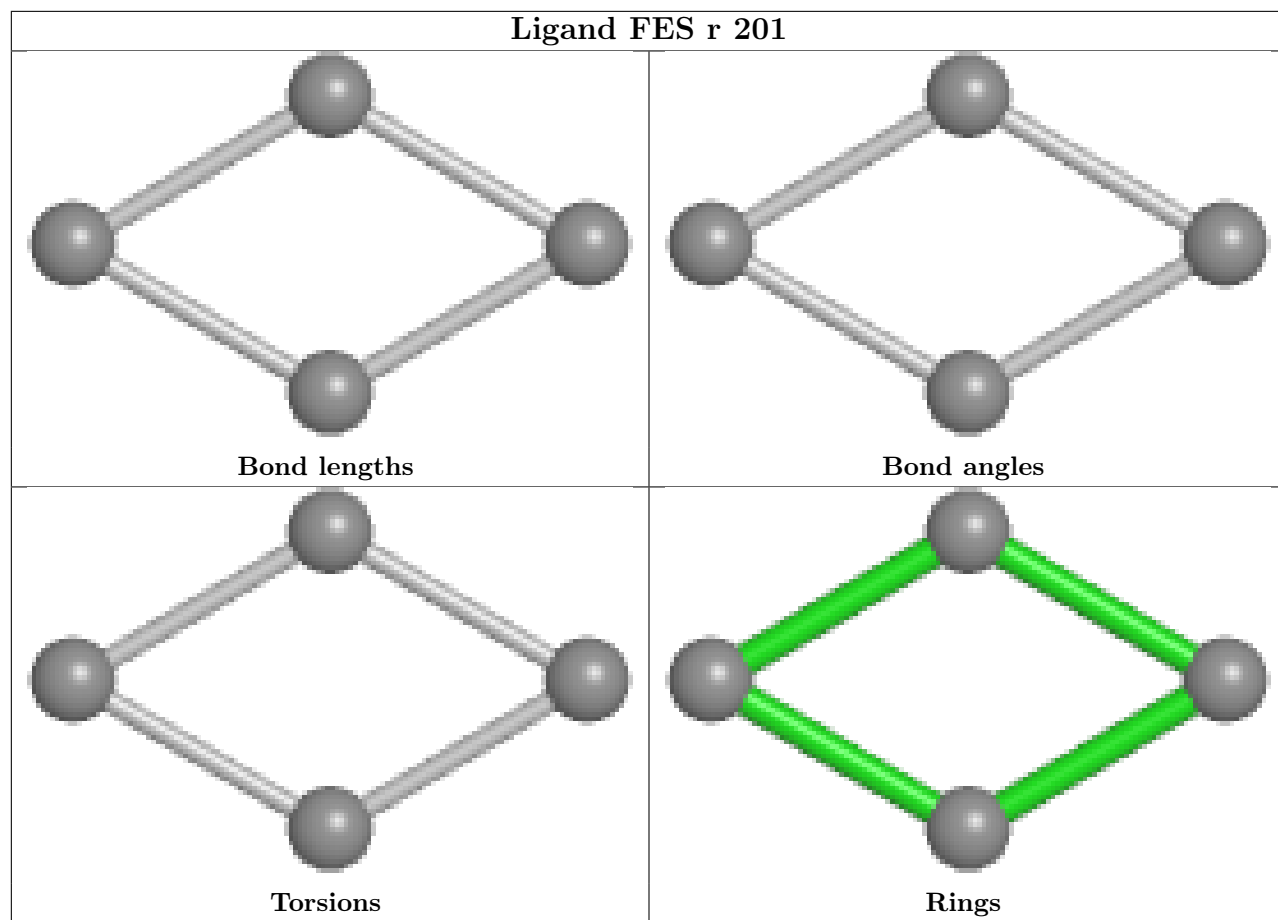
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
94	A	3302	SPD	1	0
102	B	101	VAL	2	0
101	AX	503	GDP	1	0

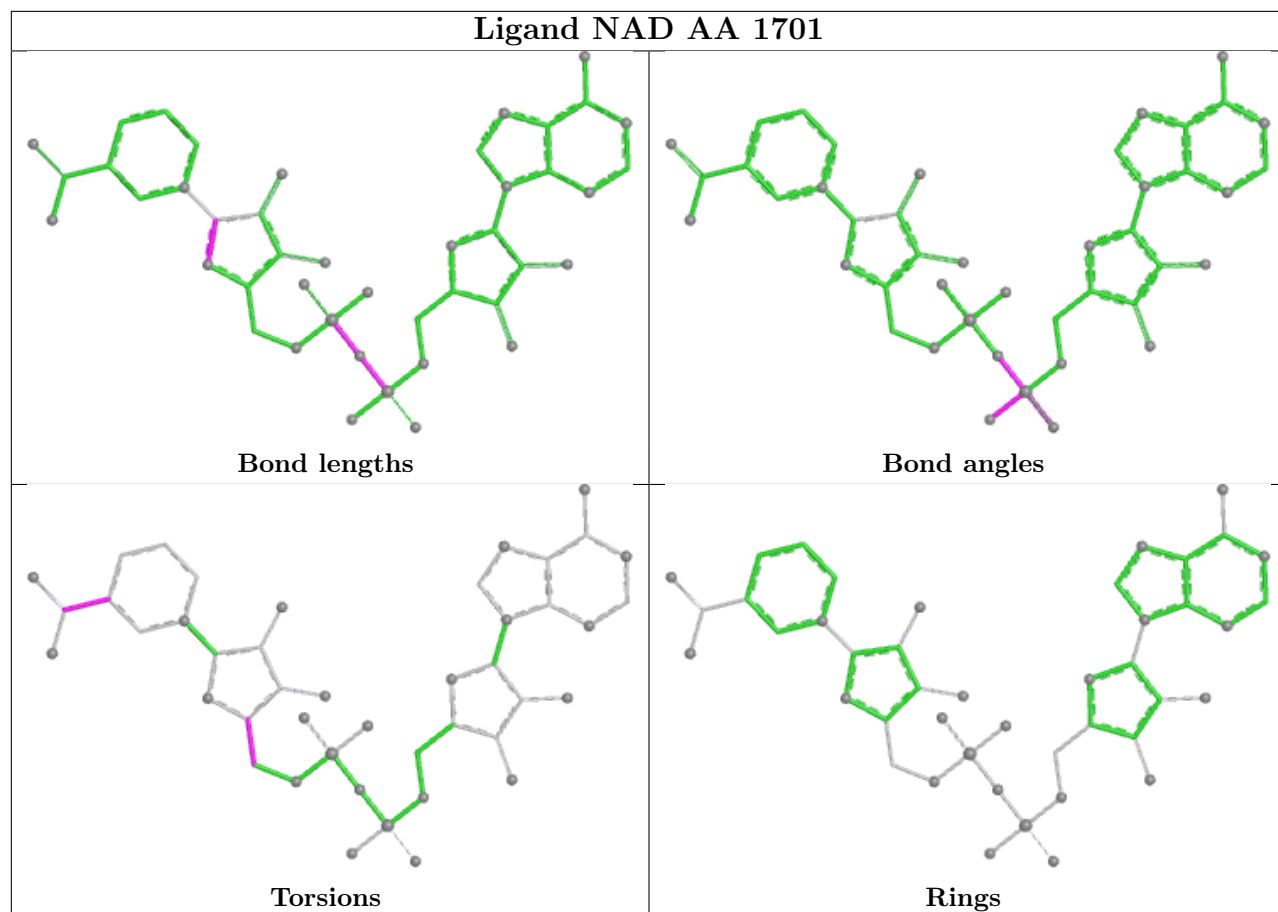
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



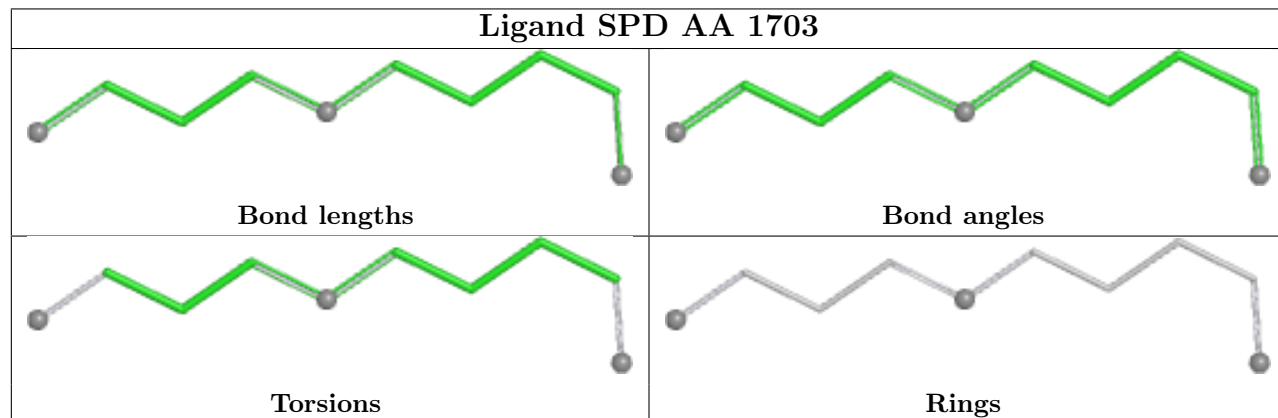


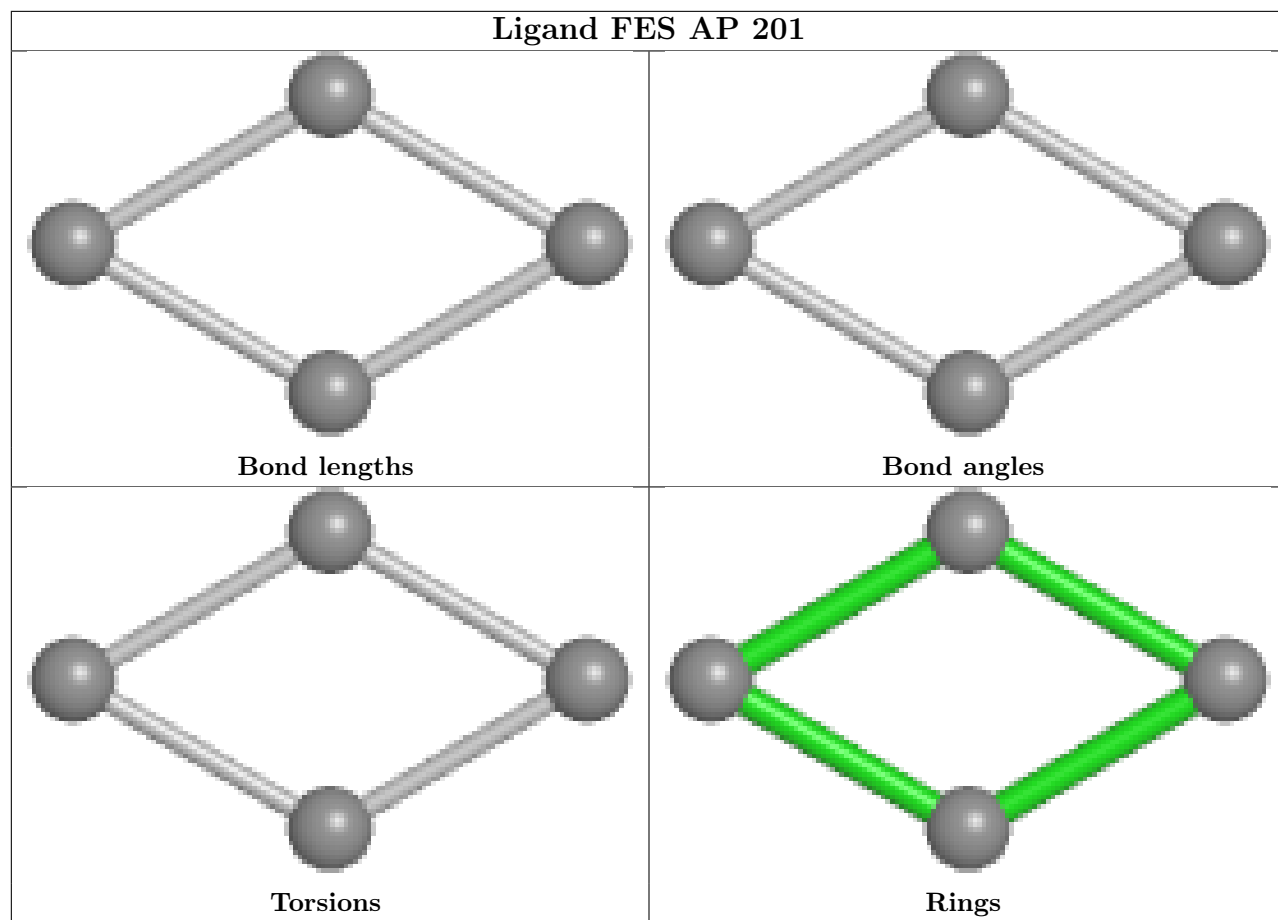


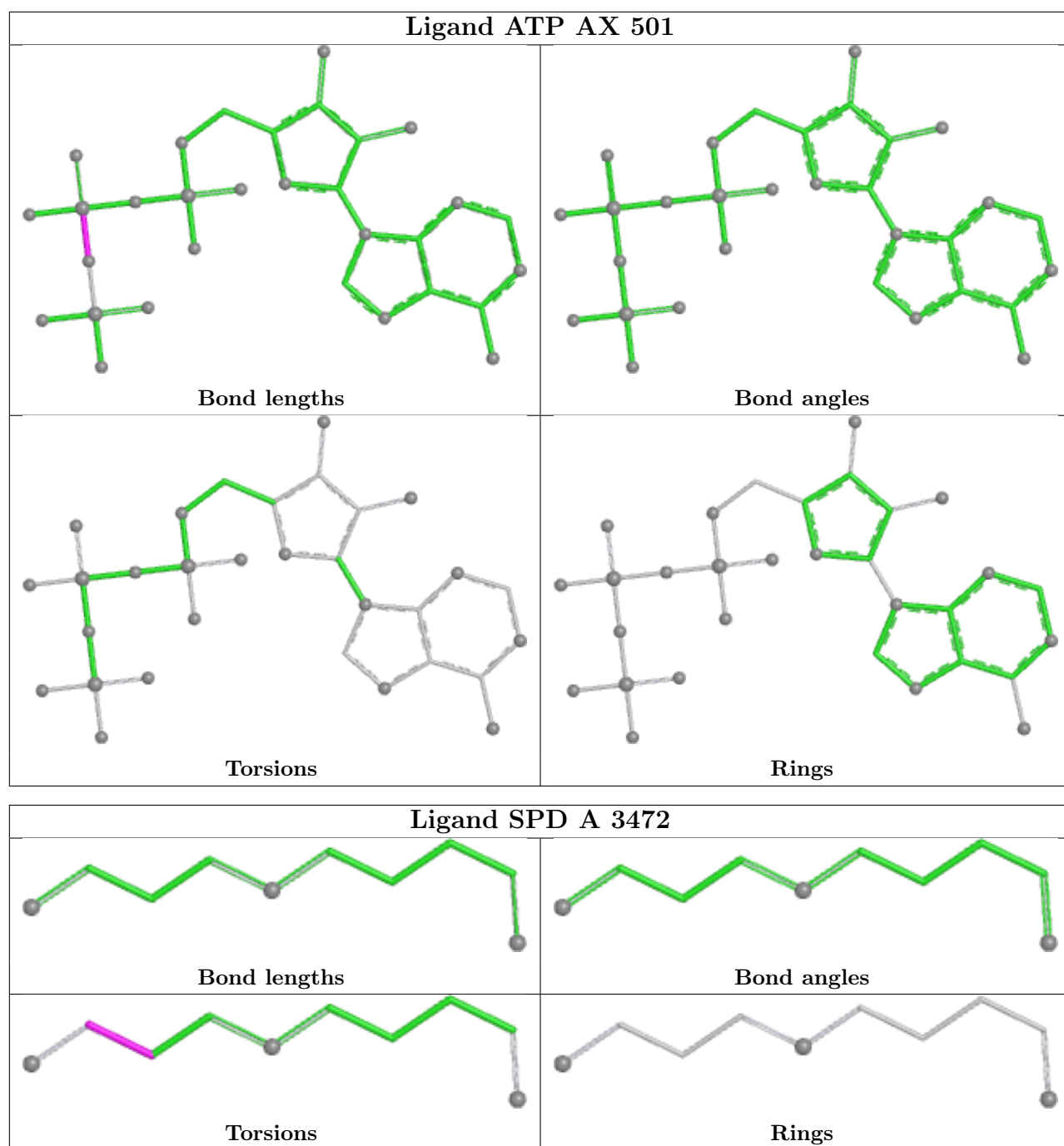
Ligand NAD AA 1701

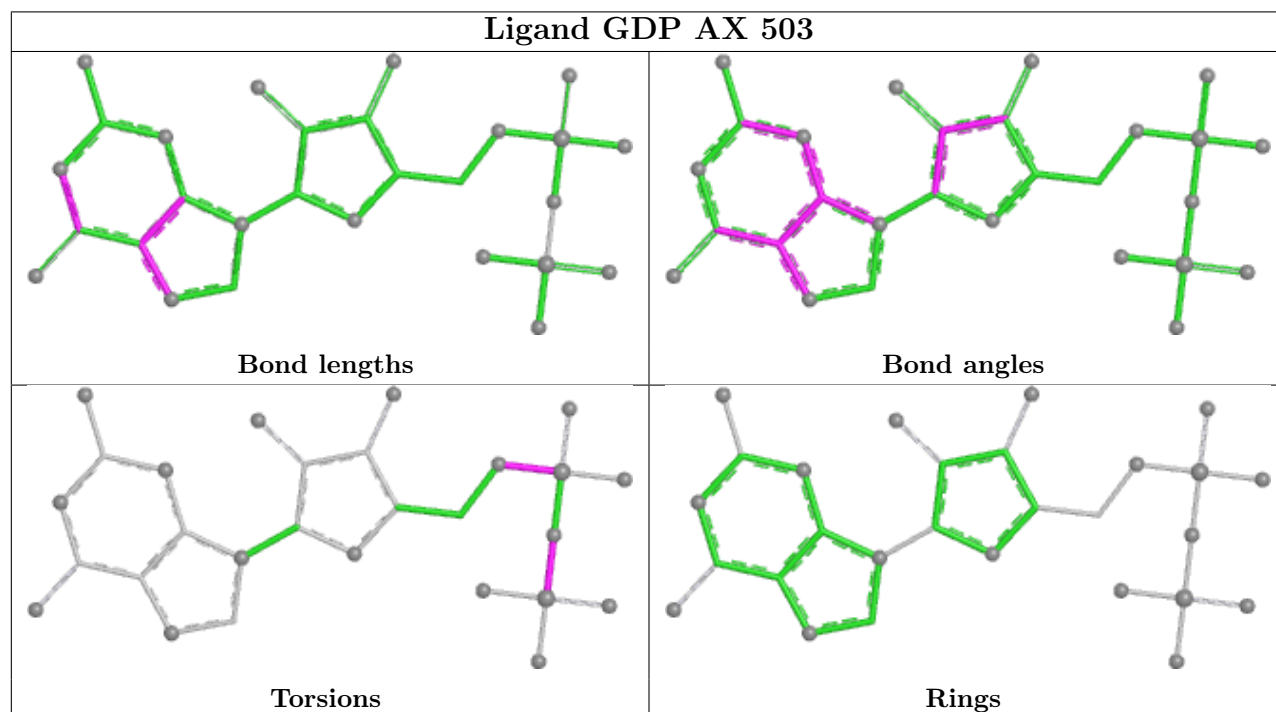
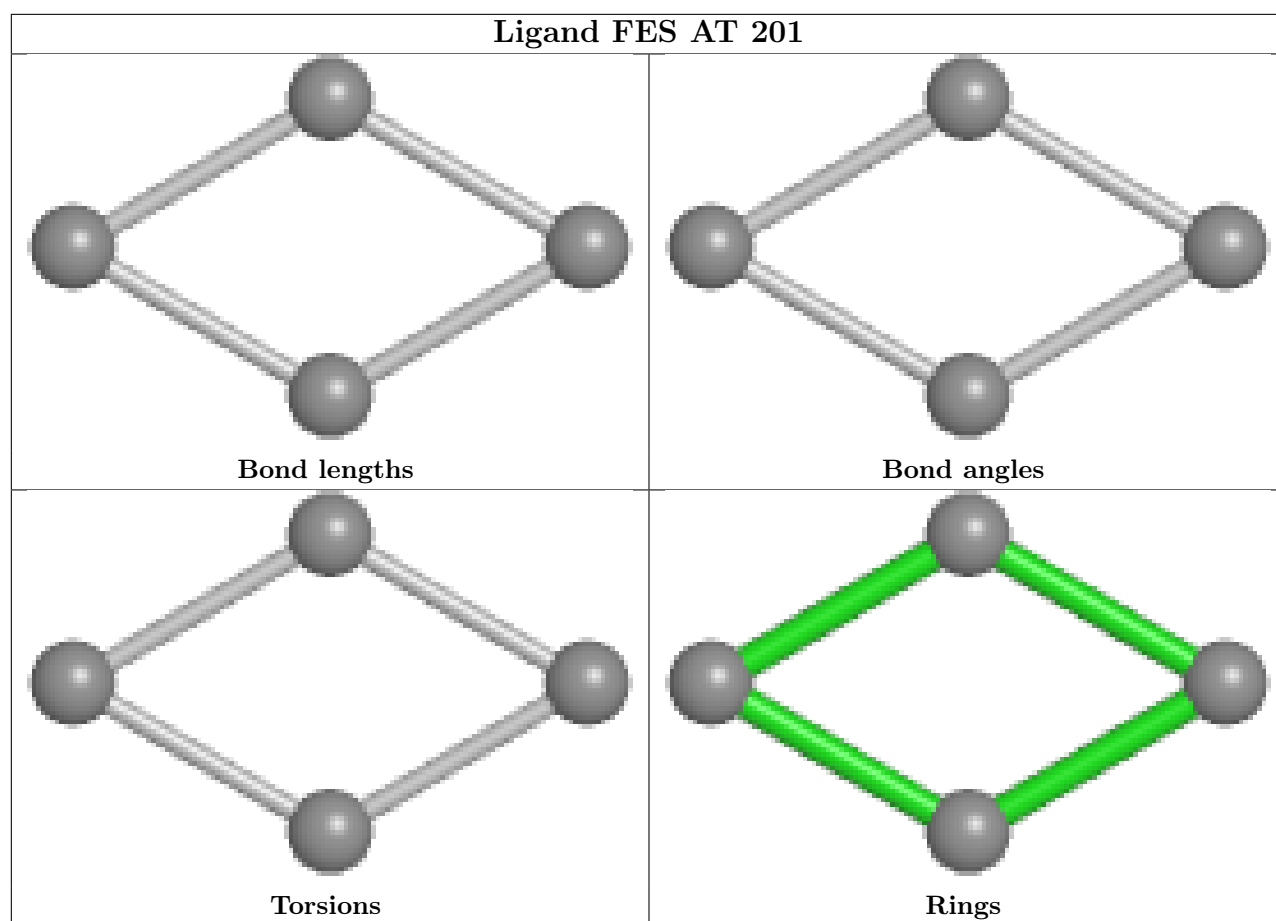


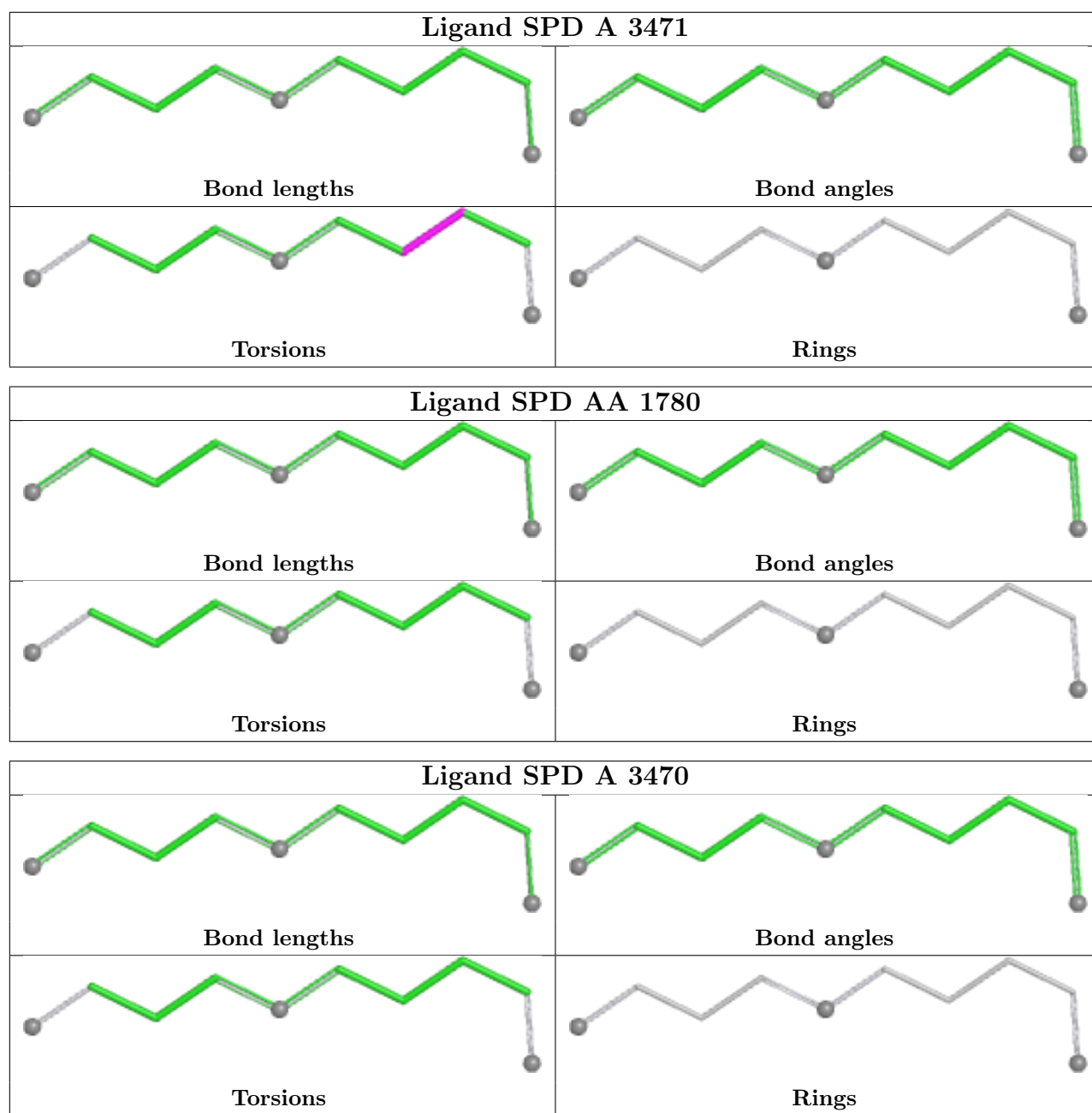
Ligand SPD AA 1703











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

Continued on next page...

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Mol	Chain	Number of breaks
91	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	8.81
1	B	46:A	O3'	48:U	P	4.51

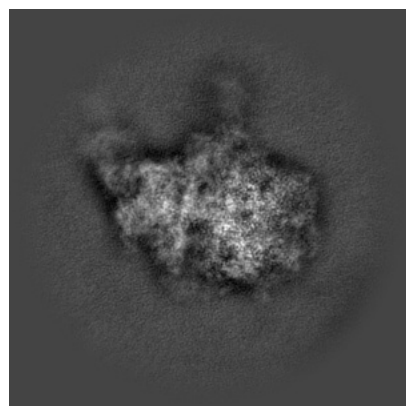
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71828. These allow visual inspection of the internal detail of the map and identification of artifacts.

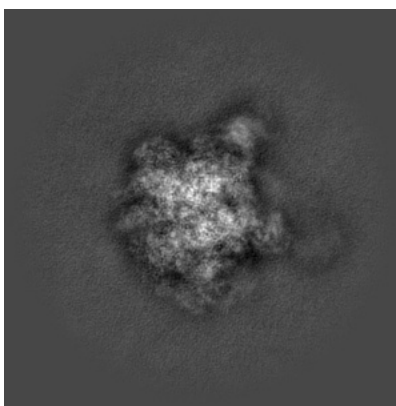
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

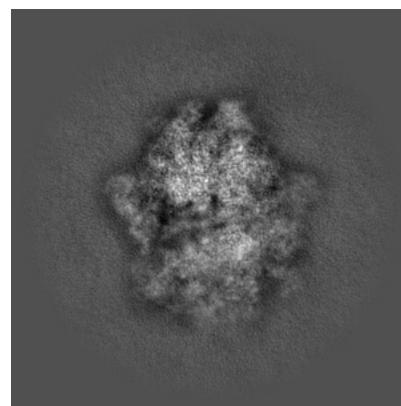
6.1.1 Primary map



X

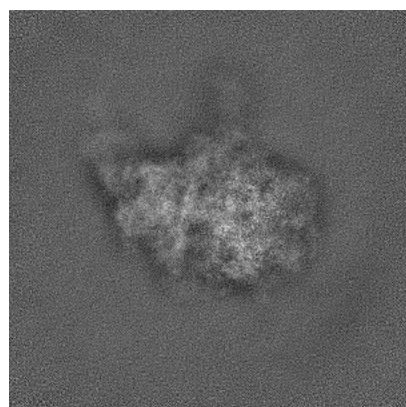


Y

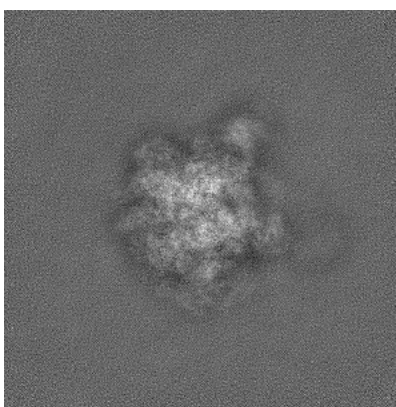


Z

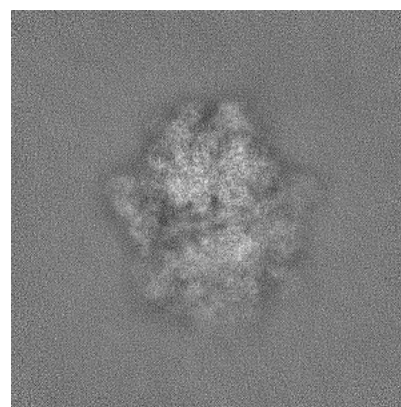
6.1.2 Raw map



X



Y

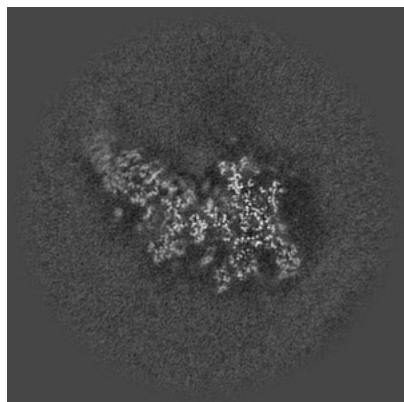


Z

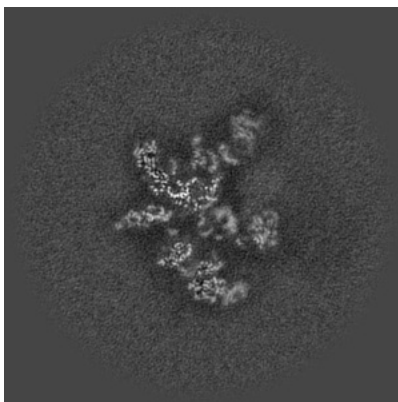
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

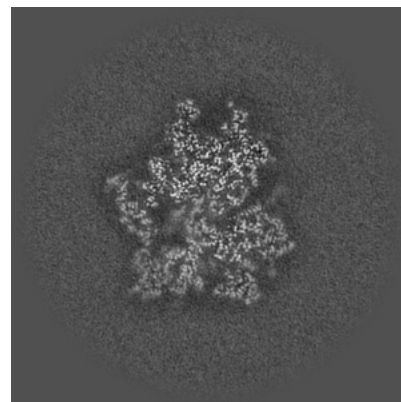
6.2.1 Primary map



X Index: 240

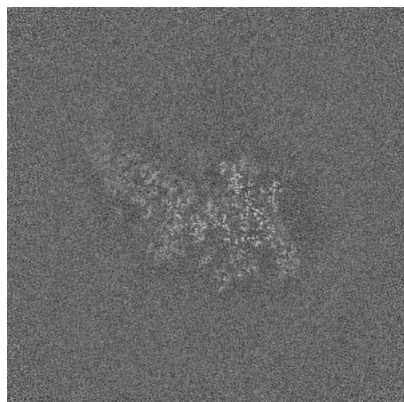


Y Index: 240

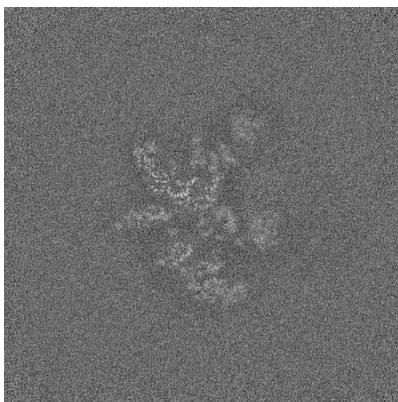


Z Index: 240

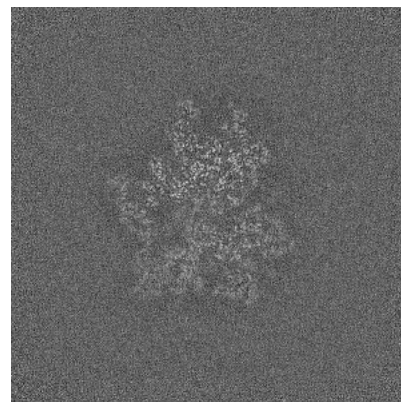
6.2.2 Raw map



X Index: 240



Y Index: 240

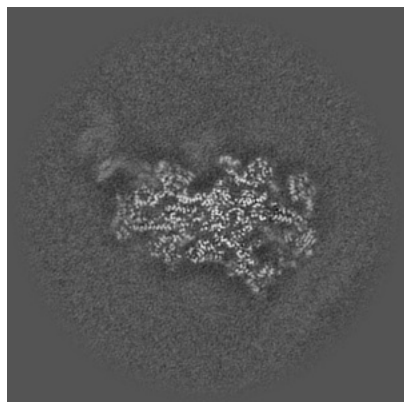


Z Index: 240

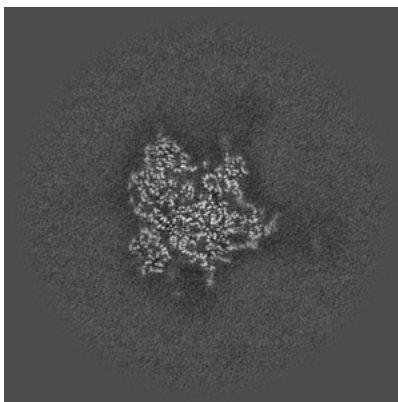
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

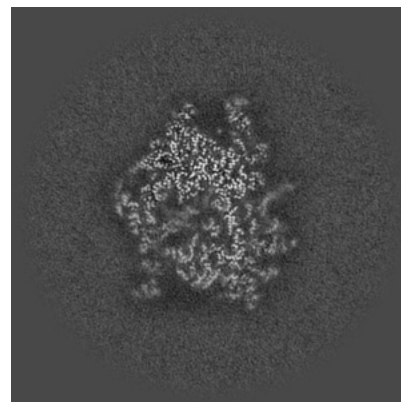
6.3.1 Primary map



X Index: 262

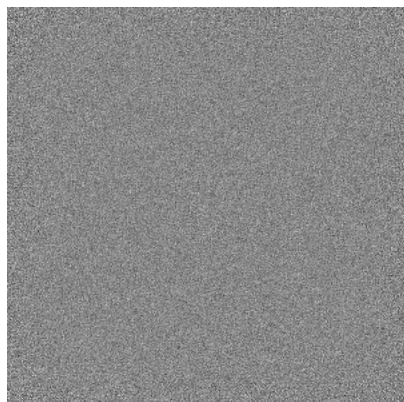


Y Index: 287

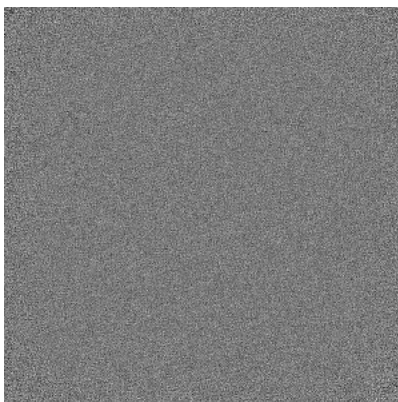


Z Index: 249

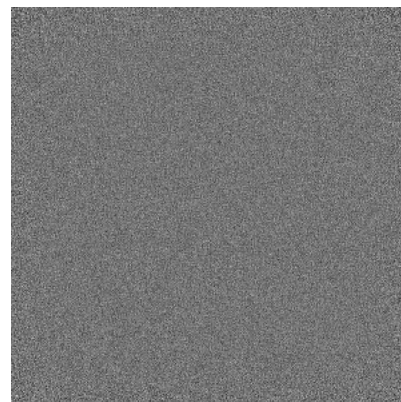
6.3.2 Raw map



X Index: 0



Y Index: 0

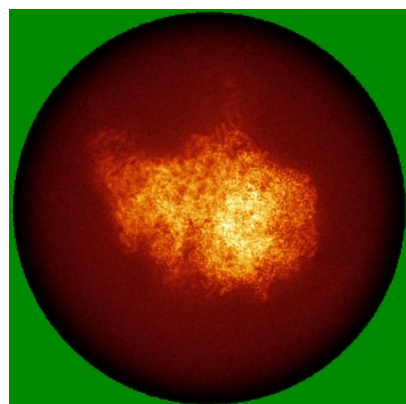


Z Index: 0

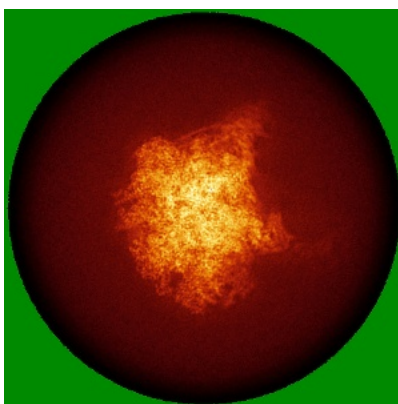
The images above show the largest variance slices of the map in three orthogonal directions.

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

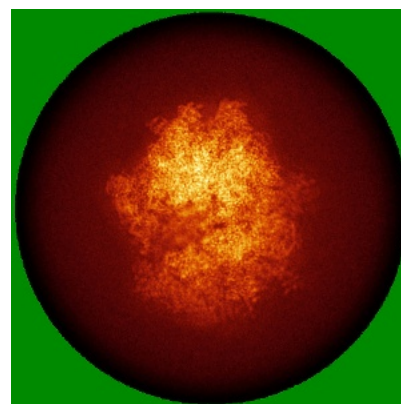
6.4.1 Primary map



X

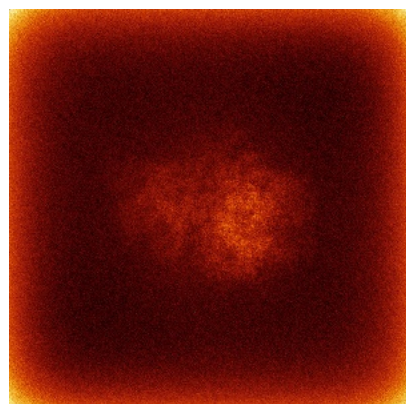


Y

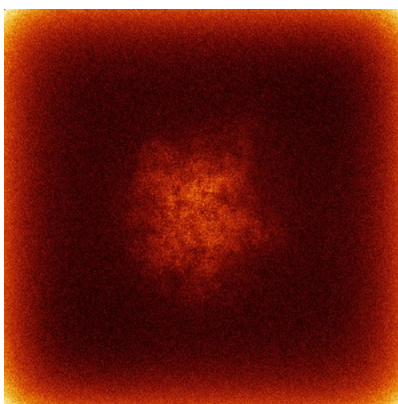


Z

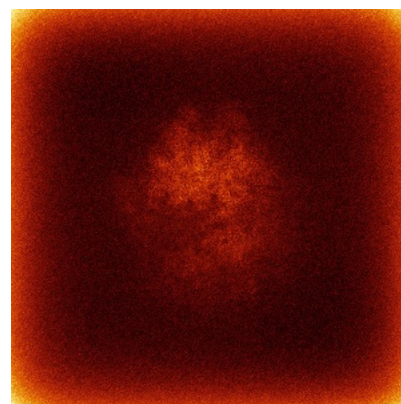
6.4.2 Raw map



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.

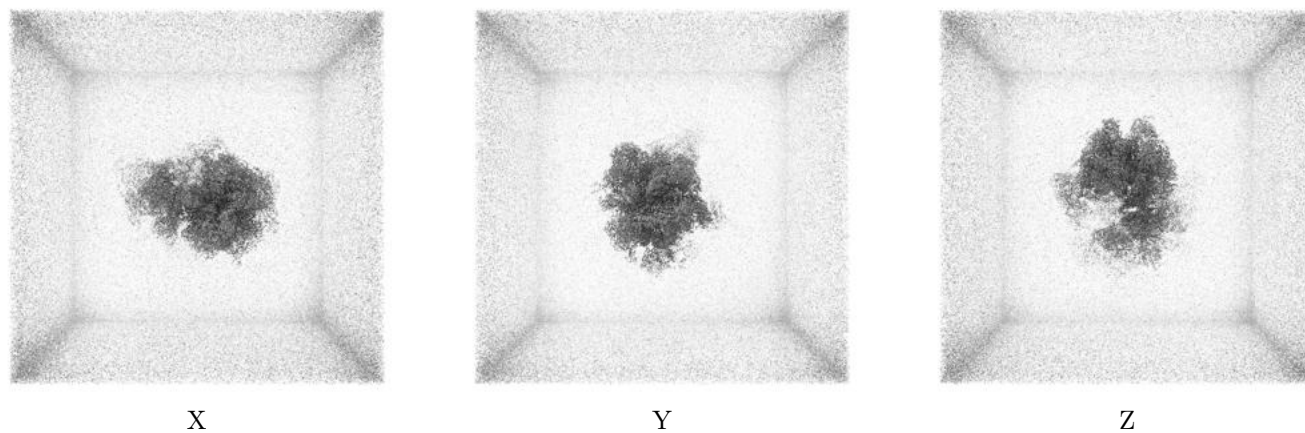
6.5 Orthogonal surface views [i](#)

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.

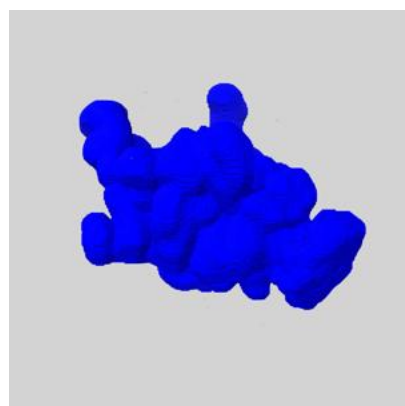
6.6 Mask visualisation [i](#)

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

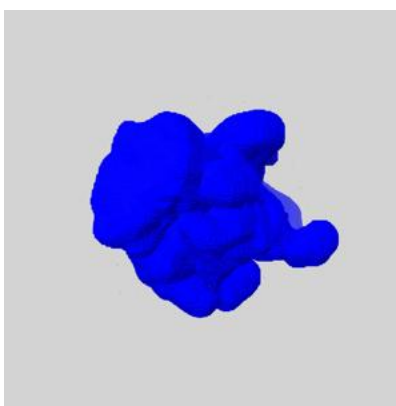
A mask typically either:

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

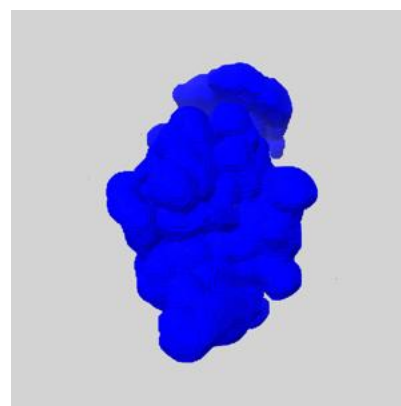
6.6.1 emd_71828_msk_1.map [i](#)



X



Y

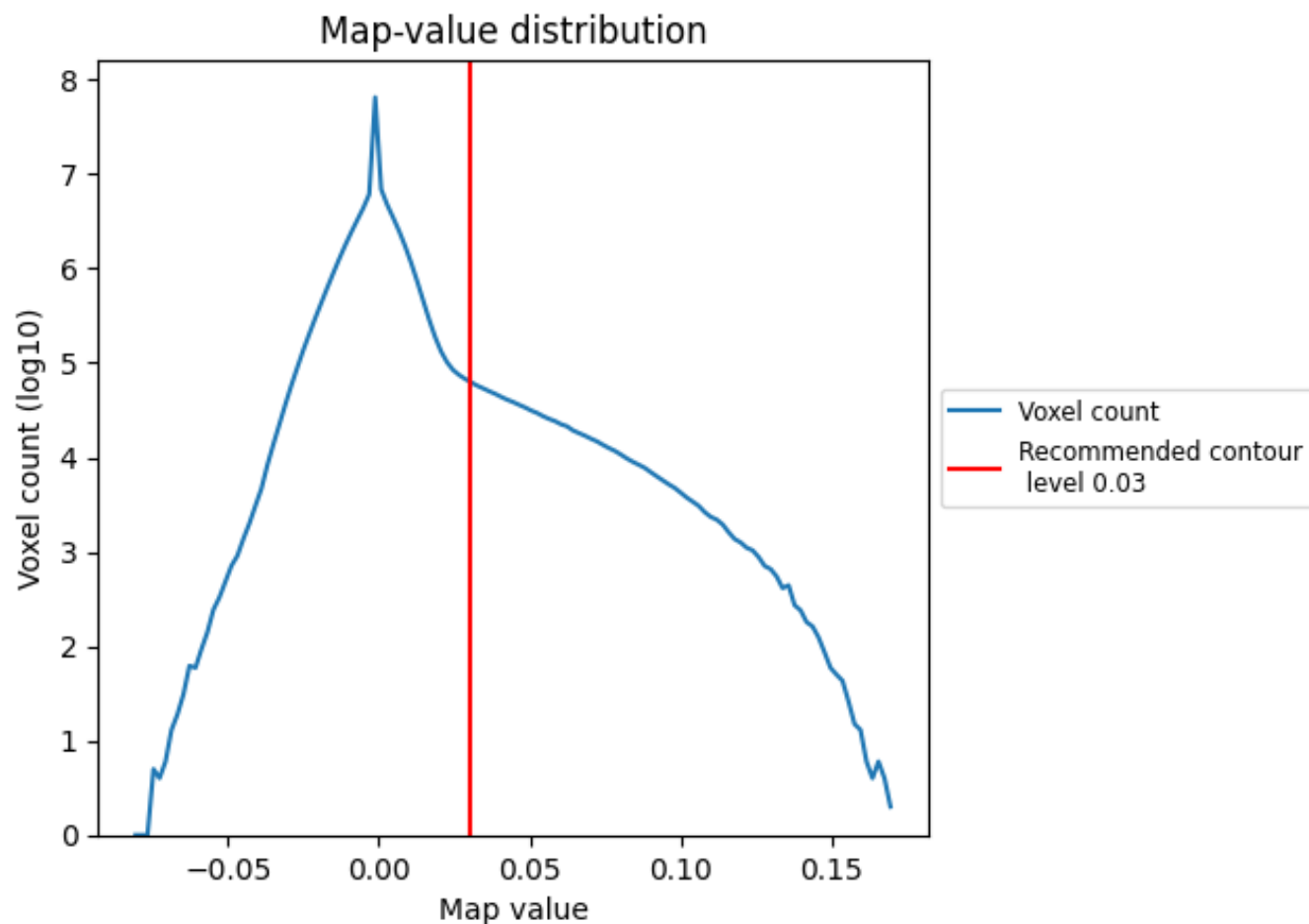


Z

7 Map analysis [i](#)

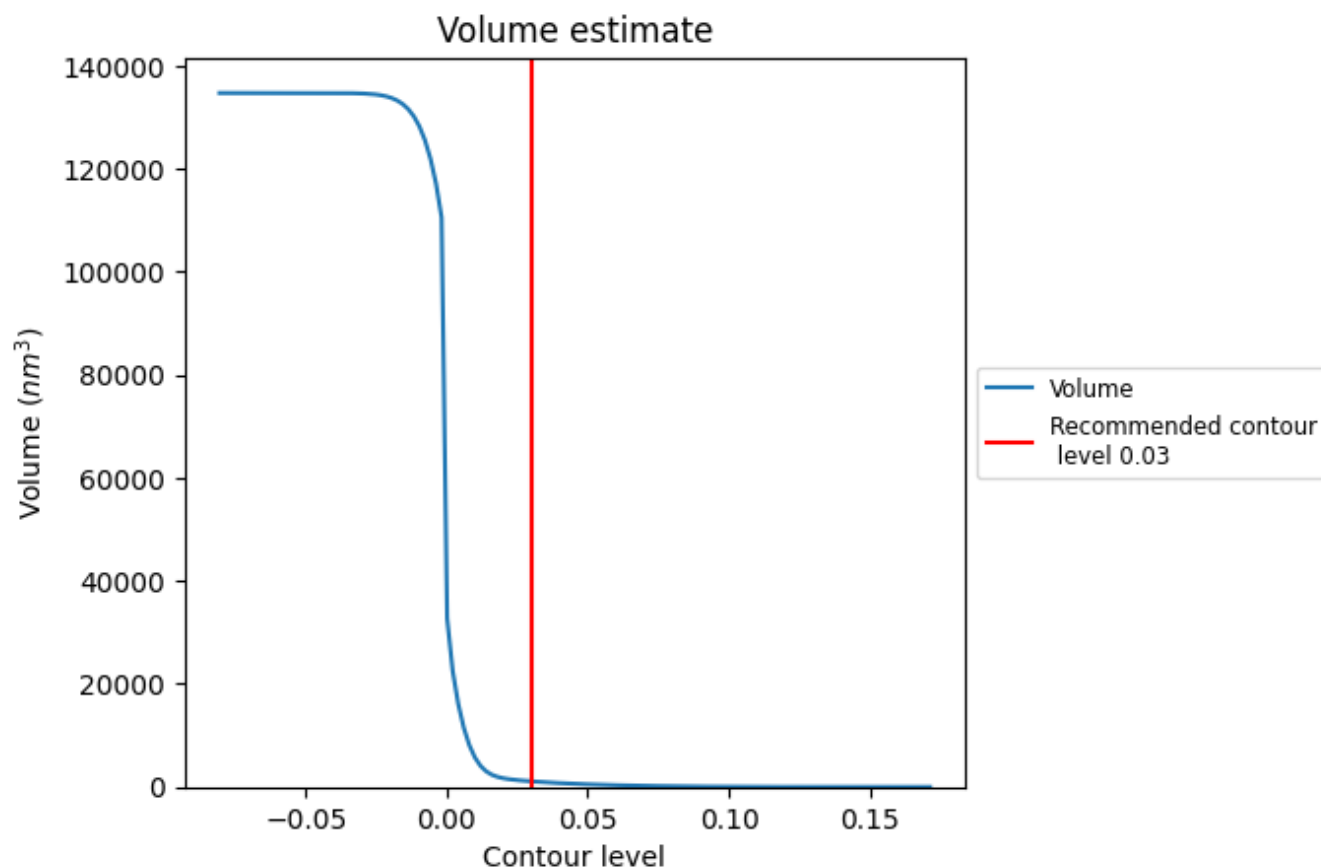
This section contains the results of statistical analysis of the map.

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.

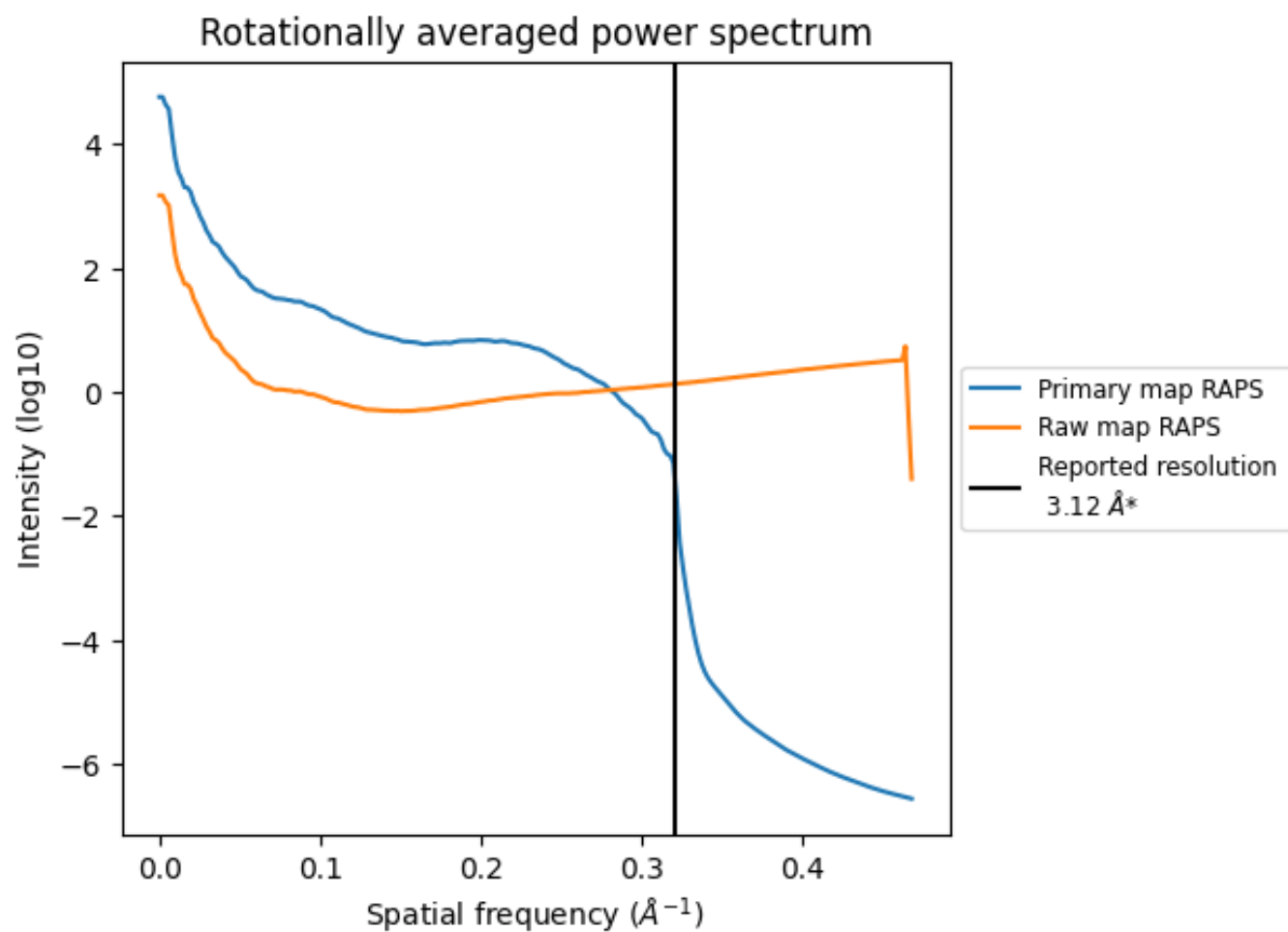
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1091 nm³; this corresponds to an approximate mass of 986 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 ⓘ

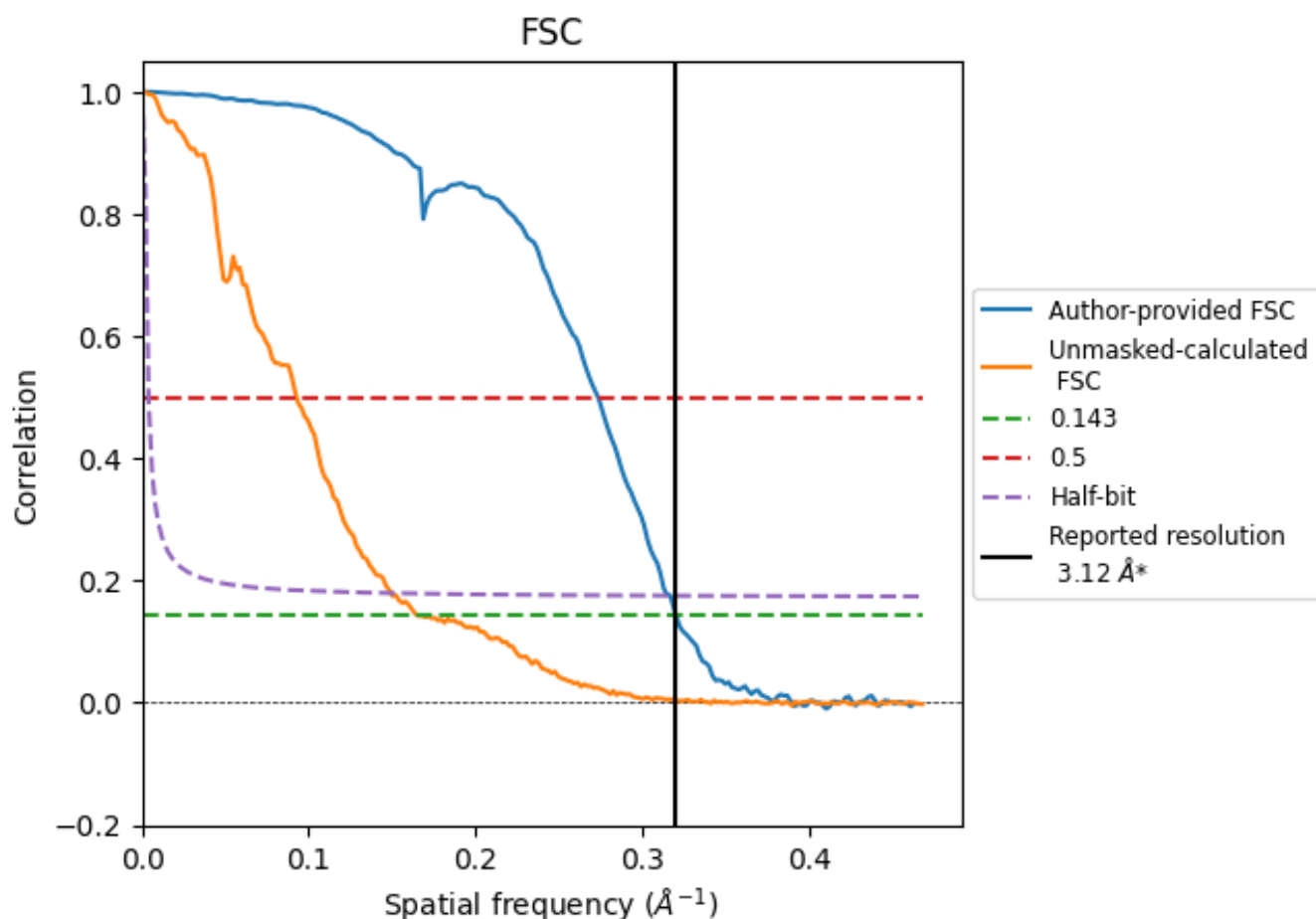


*Reported resolution corresponds to spatial frequency of 0.321 $\text{\AA}^{-1}$

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 0.321 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

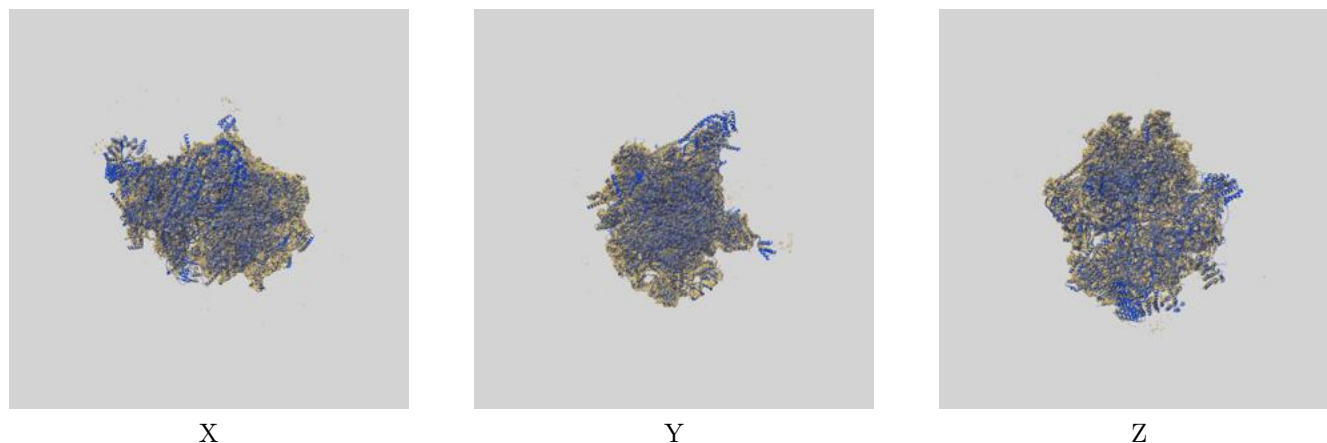
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.12	-	-
Author-provided FSC curve	3.12	3.65	3.15
Unmasked-calculated*	6.06	10.79	6.70

*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 6.06 differs from the reported value 3.12 by more than 10 %

9 Map-model fit [i](#)

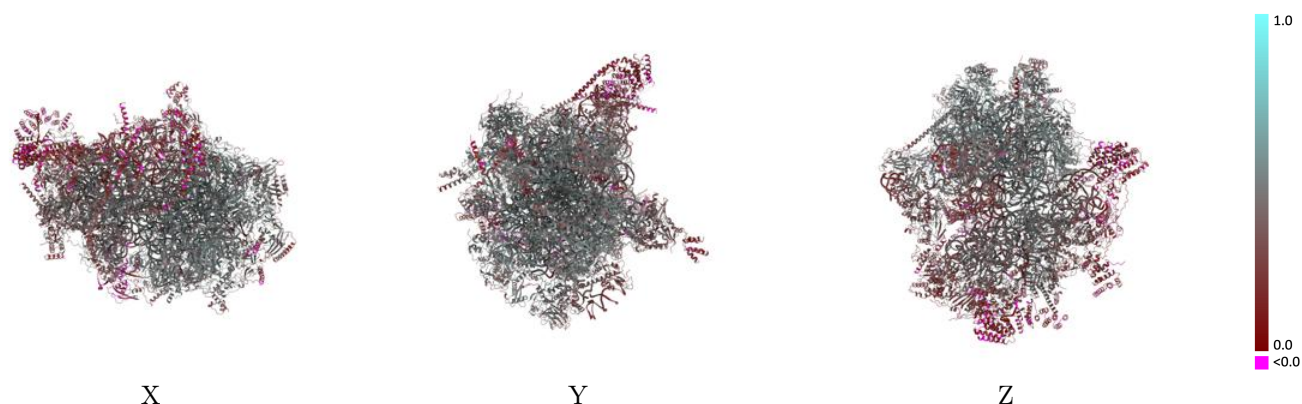
This section contains information regarding the fit between EMDB map EMD-71828 and PDB model 9PSI. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



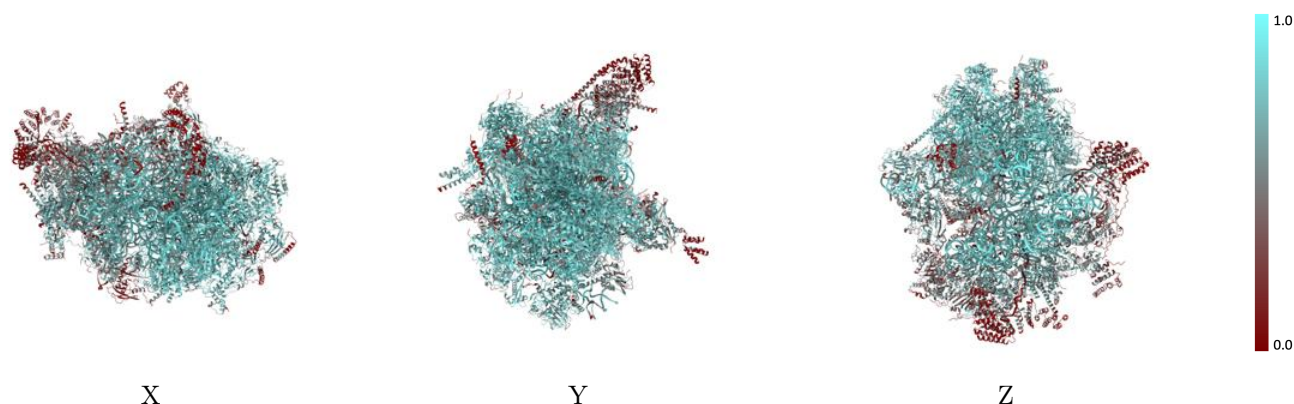
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



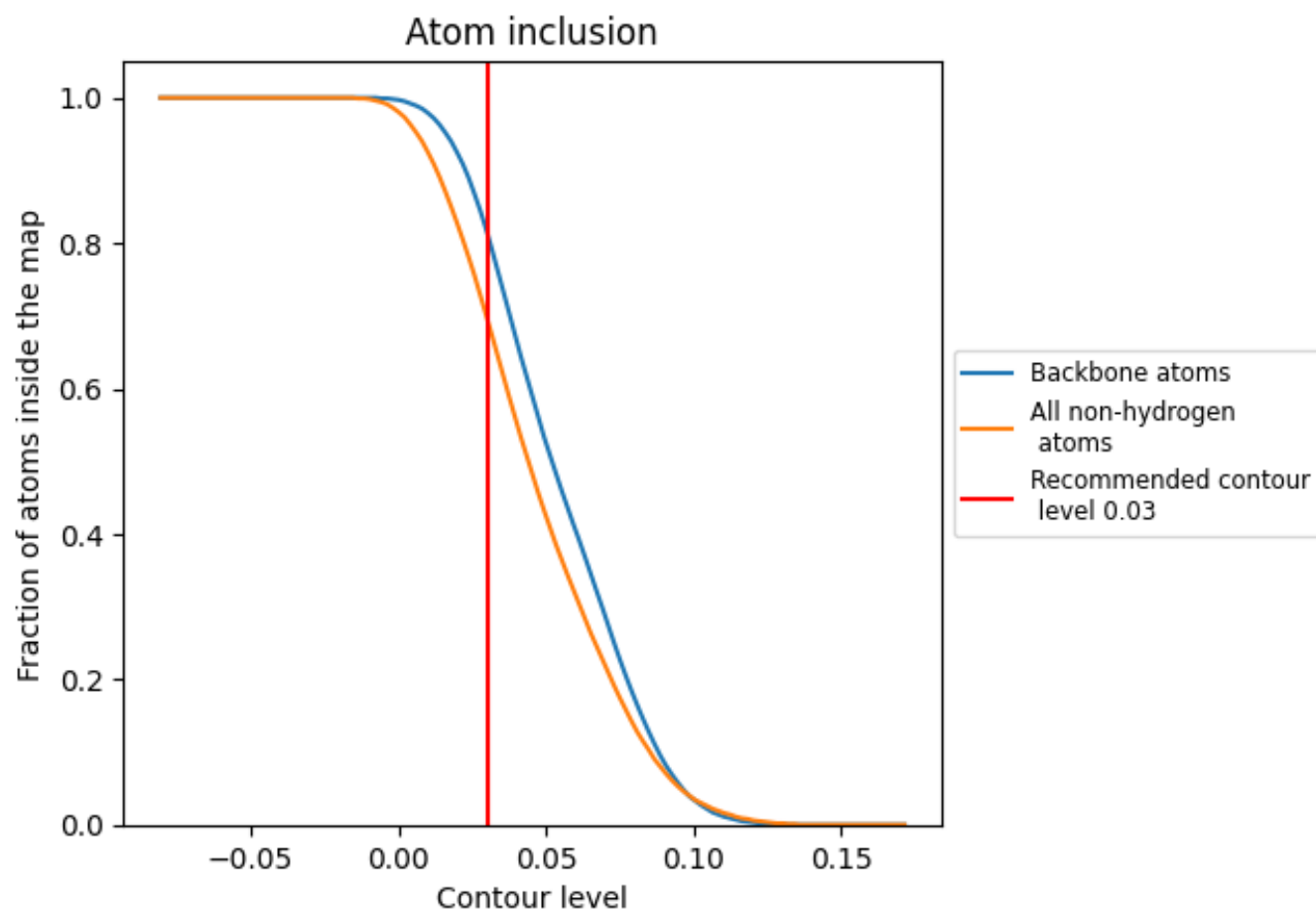
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 82% of all backbone atoms, 70% 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	 0.6970	 0.4100
0	 0.7600	 0.4990
1	 0.7120	 0.4760
2	 0.8730	 0.5350
3	 0.8430	 0.5300
4	 0.8260	 0.5210
5	 0.7720	 0.4820
6	 0.7280	 0.4430
7	 0.7130	 0.4430
8	 0.5220	 0.3330
9	 0.7460	 0.4660
A	 0.9070	 0.4790
A0	 0.3240	 0.2160
A1	 0.4610	 0.3000
A2	 0.5140	 0.3690
A3	 0.7000	 0.4610
A4	 0.2340	 0.1840
AA	 0.8860	 0.4360
AB	 0.6450	 0.3990
AC	 0.6040	 0.4170
AD	 0.5690	 0.3810
AE	 0.6480	 0.4490
AF	 0.5480	 0.3670
AG	 0.5470	 0.3530
AH	 0.5120	 0.3480
AI	 0.6370	 0.4340
AJ	 0.6340	 0.4270
AK	 0.6550	 0.4000
AL	 0.6240	 0.3970
AM	 0.4700	 0.2700
AN	 0.6440	 0.4270
AO	 0.4740	 0.3040
AP	 0.6760	 0.4360
AQ	 0.7020	 0.4470
AR	 0.3680	 0.2210



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Chain	Atom inclusion	Q-score
AS	 0.5410	 0.3340
AT	 0.5910	 0.3790
AU	 0.5060	 0.2780
AV	 0.1700	 0.1560
AW	 0.5840	 0.3760
AX	 0.4570	 0.2880
AY	 0.4220	 0.2950
AZ	 0.5280	 0.3430
Aw	 0.7110	 0.2370
Ax	 0.7730	 0.3540
Ay	 0.5820	 0.2190
Az	 0.3310	 0.2450
B	 0.7620	 0.3420
D	 0.8140	 0.5200
E	 0.7900	 0.5030
F	 0.8180	 0.5130
H	 0.3980	 0.2810
I	 0.5550	 0.3690
J	 0.4610	 0.2830
K	 0.8120	 0.5090
L	 0.7760	 0.5110
M	 0.7980	 0.5080
N	 0.7790	 0.5070
O	 0.7870	 0.5040
OX	 0.3060	 0.2480
P	 0.7530	 0.4780
Q	 0.6980	 0.4650
R	 0.8020	 0.5120
S	 0.7670	 0.5080
T	 0.8160	 0.5260
U	 0.6970	 0.4480
V	 0.7100	 0.4590
W	 0.8070	 0.5170
X	 0.7530	 0.4810
Y	 0.7940	 0.4860
Z	 0.8040	 0.5100
a	 0.6500	 0.4280
b	 0.7900	 0.5070
c	 0.7330	 0.4670
d	 0.5730	 0.4070
e	 0.4730	 0.2980
f	 0.6040	 0.3880

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Chain	Atom inclusion	Q-score
g	 0.7720	 0.4960
h	 0.6860	 0.4370
i	 0.8510	 0.5200
j	 0.7340	 0.4480
k	 0.5920	 0.3930
l	 0.4990	 0.3320
m	 0.4820	 0.3070
n	 0.2230	 0.3210
o	 0.8400	 0.5190
p	 0.6120	 0.4120
q	 0.5410	 0.3480
r	 0.7930	 0.4930
s	 0.7650	 0.4830
t	 0.1670	 0.2120
u	 0.1050	 0.1960
z	 0.0640	 0.0730