



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 01:43 PM EDT

PDB ID : 9PRQ / pdb_00009prq
EMDB ID : EMD-71811
Title : In situ structure of human mitoribosome in the A/T-P state from TACO1-knockout cells
Authors : Wang, S.; Xiong, Y.; Zhang, Y.
Deposited on : 2025-07-24
Resolution : 3.34 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:

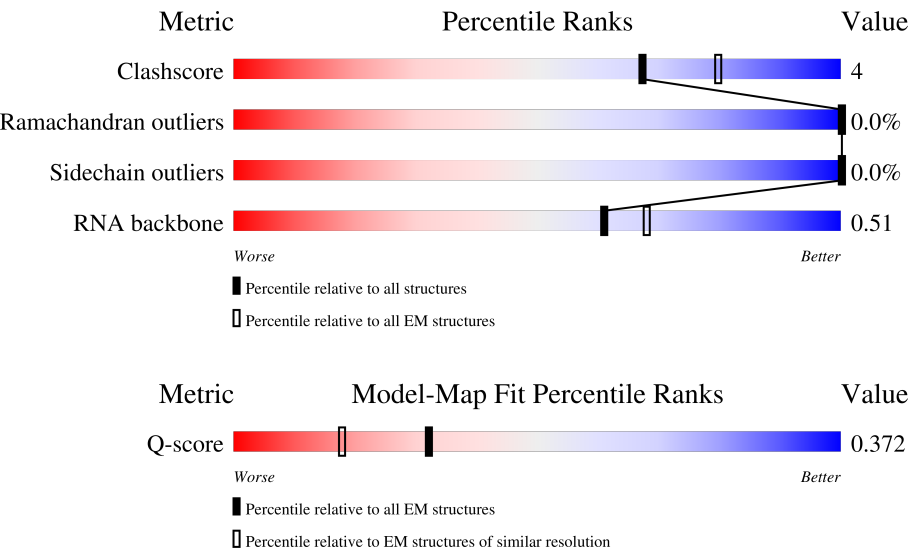
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.34 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	14446 (2.84 - 3.84)

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	57% 41%
2	1	65	6% 75% 11% 14%
3	2	92	48% 50%

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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	g	166	
34	V	216	
35	b	215	
36	d	306	
37	e	279	
38	h	158	
39	i	128	
40	j	123	
41	k	112	
42	l	138	
43	m	128	
44	n	43	
45	o	102	
46	q	222	
47	r	196	
48	t	198	
48	u	198	
49	c	332	
50	f	212	
51	p	206	
52	s	439	

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

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Mol	Chain	Length	Quality of chain
78	AY	395	
79	AA	954	
80	AI	194	
81	OX	435	
82	a	142	
83	A4	689	
84	AX	398	
85	A2	118	
86	AQ	87	
87	Ah	77	
88	Ag	455	
89	Ax	71	
90	B	72	

2 Entry composition

There are 101 unique types of molecules in this entry. The entry contains 181108 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 33 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- 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 L50, mitochondrial.

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

- Molecule 44 is a protein called Nascent polypeptide.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 77 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 83 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 84 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 85 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	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 86 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	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 87 is a RNA chain called A/T-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Ah	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 88 is a protein called Elongation factor Tu, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Ag	394	Total	C	N	O	S	0	0
			3042	1923	538	566	15		

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

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

- Molecule 90 is a RNA chain called mitochondrial tRNAVal.

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

- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
91	0	1	Total	Zn	0
			1	1	
91	4	1	Total	Zn	0
			1	1	
91	AO	1	Total	Zn	0
			1	1	

- Molecule 92 is POTASSIUM ION (CCD ID: K) (formula: K).

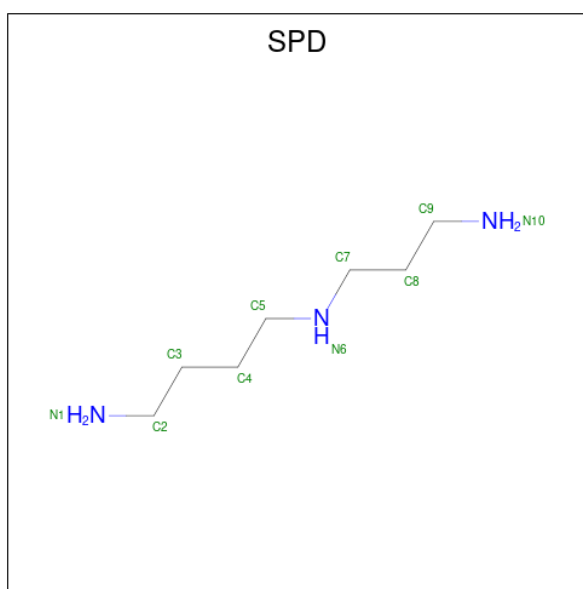
Mol	Chain	Residues	Atoms		AltConf
92	6	1	Total	K	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
92	A	28	Total	K	0
			28	28	
92	D	1	Total	K	0
			1	1	
92	M	2	Total	K	0
			2	2	
92	N	1	Total	K	0
			1	1	
92	W	1	Total	K	0
			1	1	
92	i	1	Total	K	0
			1	1	
92	o	1	Total	K	0
			1	1	
92	AA	18	Total	K	0
			18	18	

- Molecule 93 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



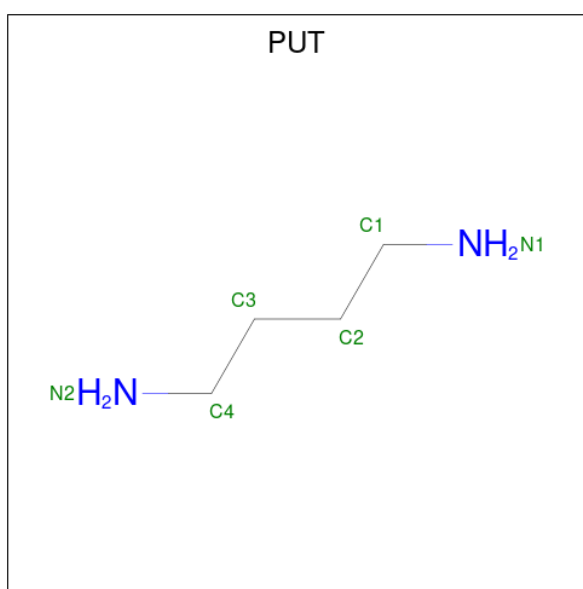
Mol	Chain	Residues	Atoms			AltConf
93	A	1	Total	C	N	0
			10	7	3	
93	A	1	Total	C	N	0
			10	7	3	
93	A	1	Total	C	N	0
			10	7	3	

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

- Molecule 94 is 1,4-DIAMINO BUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



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

- Molecule 95 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

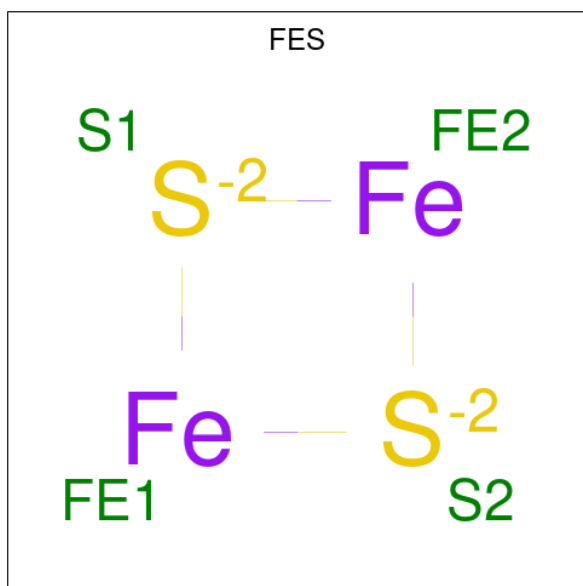
Mol	Chain	Residues	Atoms		AltConf
95	A	138	Total	Mg	0
			138	138	
95	D	2	Total	Mg	0
			2	2	
95	g	1	Total	Mg	0
			1	1	
95	AB	1	Total	Mg	0
			1	1	

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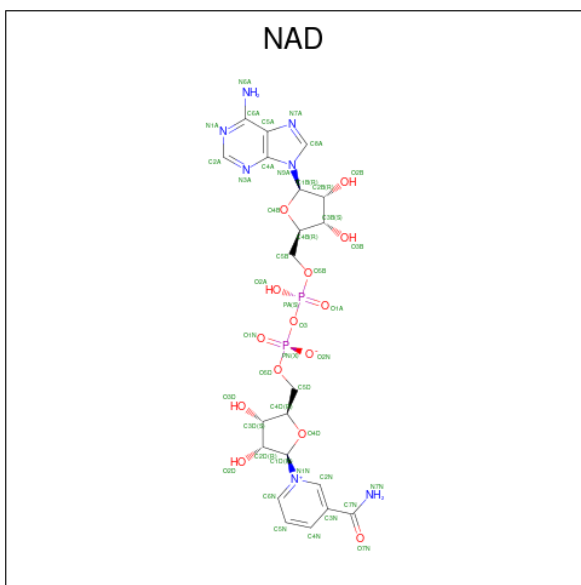
Mol	Chain	Residues	Atoms		AltConf
95	A3	1	Total	Mg	0
			1	1	
95	Az	1	Total	Mg	0
			1	1	
95	AA	59	Total	Mg	0
			59	59	
95	AX	1	Total	Mg	0
			1	1	

- Molecule 96 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



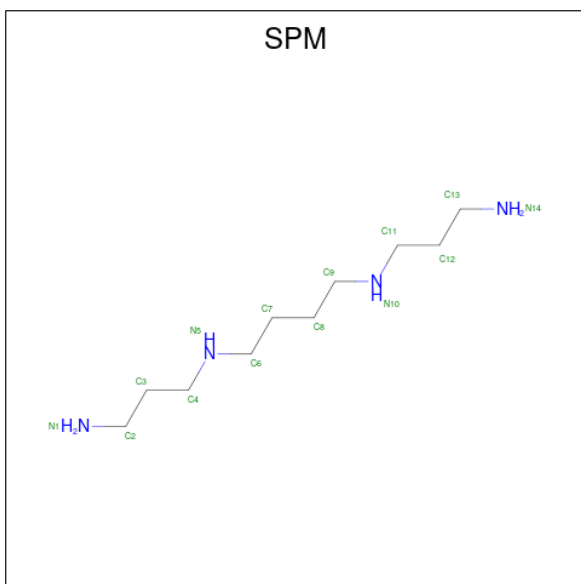
Mol	Chain	Residues	Atoms			AltConf
96	r	1	Total	Fe	S	0
			4	2	2	
96	AP	1	Total	Fe	S	0
			4	2	2	
96	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 97 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



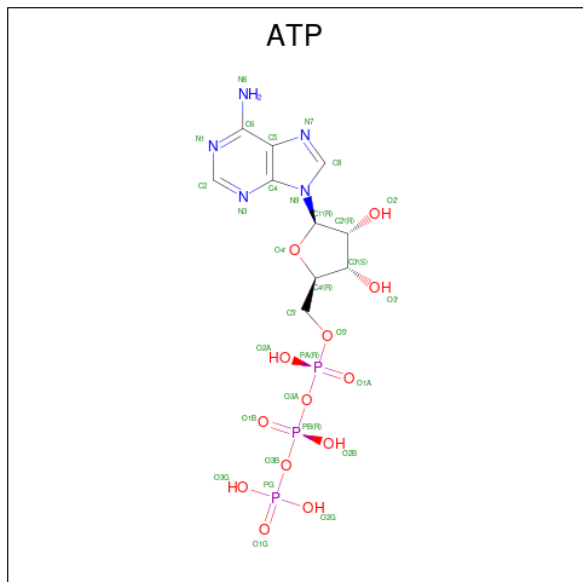
Mol	Chain	Residues	Atoms					AltConf
97	AA	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 98 is SPERMINE (CCD ID: SPM) (formula: $\text{C}_{10}\text{H}_{26}\text{N}_4$) (labeled as "Ligand of Interest" by depositor).



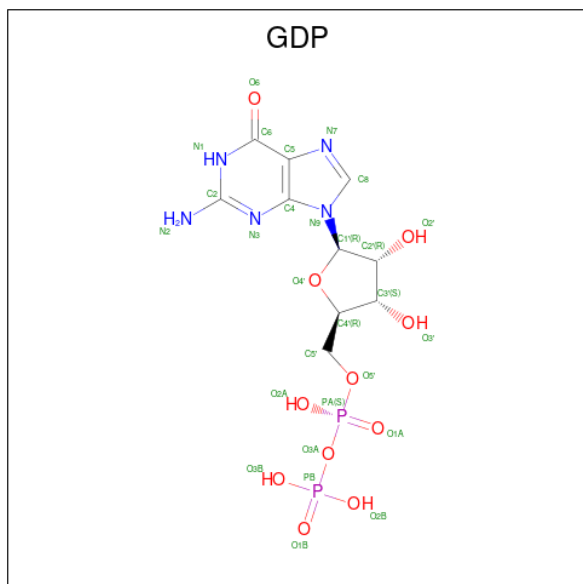
Mol	Chain	Residues	Atoms			AltConf
98	AA	1	Total 14	C 10	N 4	0
98	AA	1	Total 14	C 10	N 4	0

- Molecule 99 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



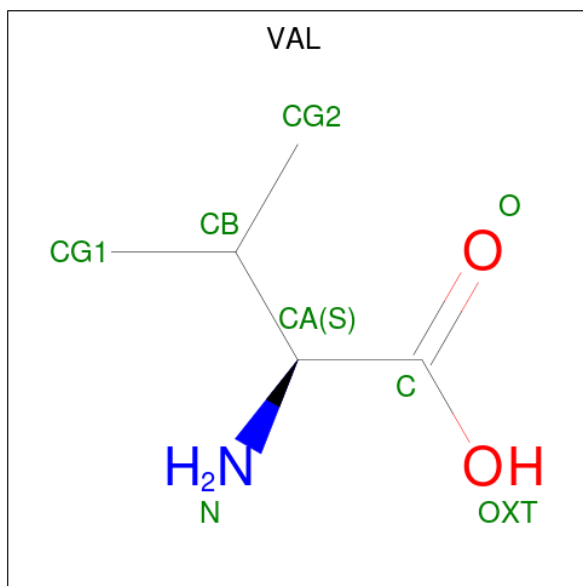
Mol	Chain	Residues	Atoms					AltConf
99	AX	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 100 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 101 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).

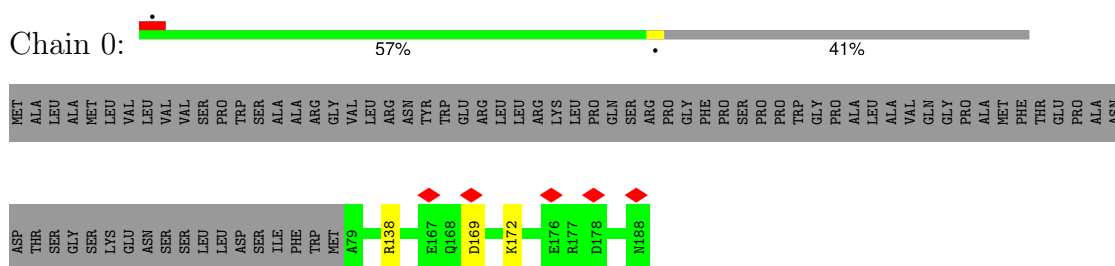


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
101	B	1	7	5	1	1	0

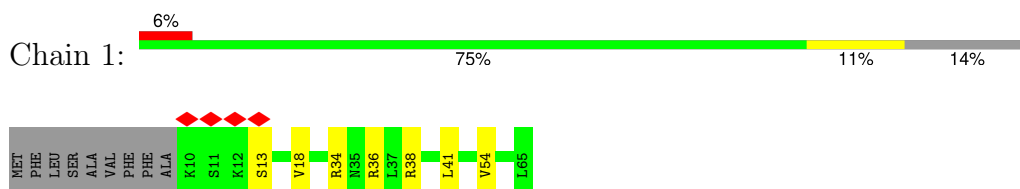
3 Residue-property plots [i](#)

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

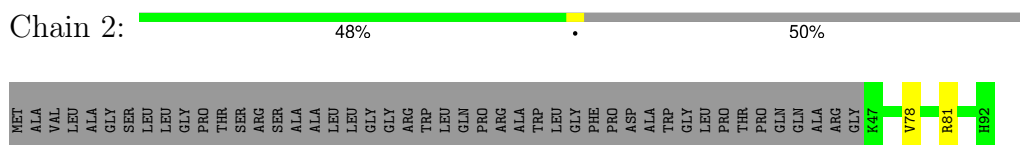
- Molecule 1: 39S ribosomal protein L32, mitochondrial



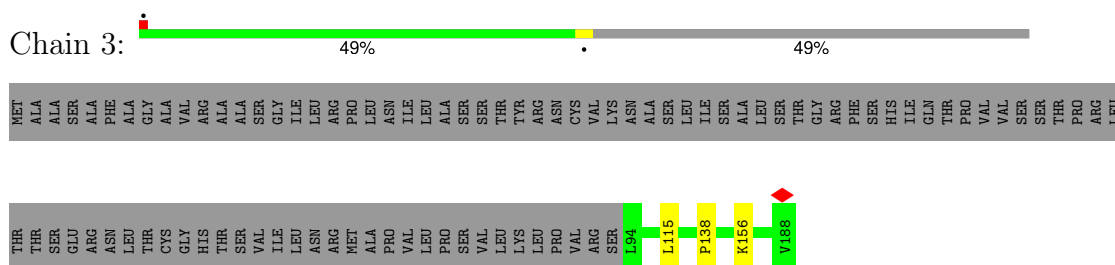
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial



- Molecule 4: 39S ribosomal protein L35, mitochondrial



- Molecule 5: 39S ribosomal protein L36, mitochondrial



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

LEU PRO ALA LEU GLY F66 M103

- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:  90% 7%

MET ALA LEU ALA SER GLY PRO ARG ALA ARG ALA LEU ALA LEU GLY SER GLN LEU LEU THR VAL GLY GLY PHE GLY ARG PRO ALA LEU SER ARG GLY A30 S41 E42 R48 L55 D101 I147 T167 Q191 R201 T232 E254 N275 H289 P301 N331

L336 E337 Q343 F354 T362 D379 R395 E409 R412 L417 A423

- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:  89% 7%

MET ALA ALA PRO TRP ARG ALA ALA LEU CYS GLU CYS ARG TRP ARG TRP GLY R27 I40 D41 L42 S43 E80 K81 T82 D83 P84 K85 E86 R106 A123 W139 C143 V179 G180 E181 D182 D183 V187 Q200 E203

E207 E210 G211 L217 H234 W235 L236 E247 L255 P256 P257 L272 D276 D280 E283 D284 E309 G315 F319 D371 Y380

- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7:  84% 13%

MET GLU ALA LEU MET GLY SER ARG ALA LEU ARG LEU TRP VAL ALA PRO GLY GLY ILE LYS TRP ARG PHE ILE ALA THR SER SER ALA SER Q34 L35 K52 L56 R61 T62 K72 P112 W113 D114 K117 D132 M149 E191 K204 L209

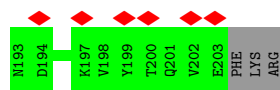
E220 K243 G258 E265 G266 P267 E279 L286 Q290 P291 S292 R296 L302 E326 D327 GLN SER LYS ALA THR GLU CYS THR THR

- Molecule 9: 39S ribosomal protein L40, mitochondrial

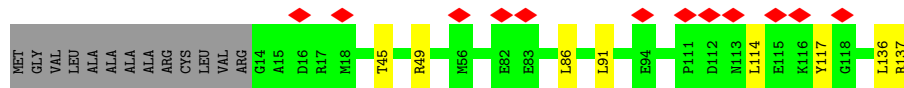
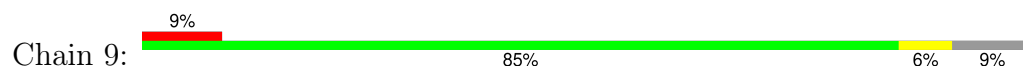
Chain 8:  69% 7% 24%

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

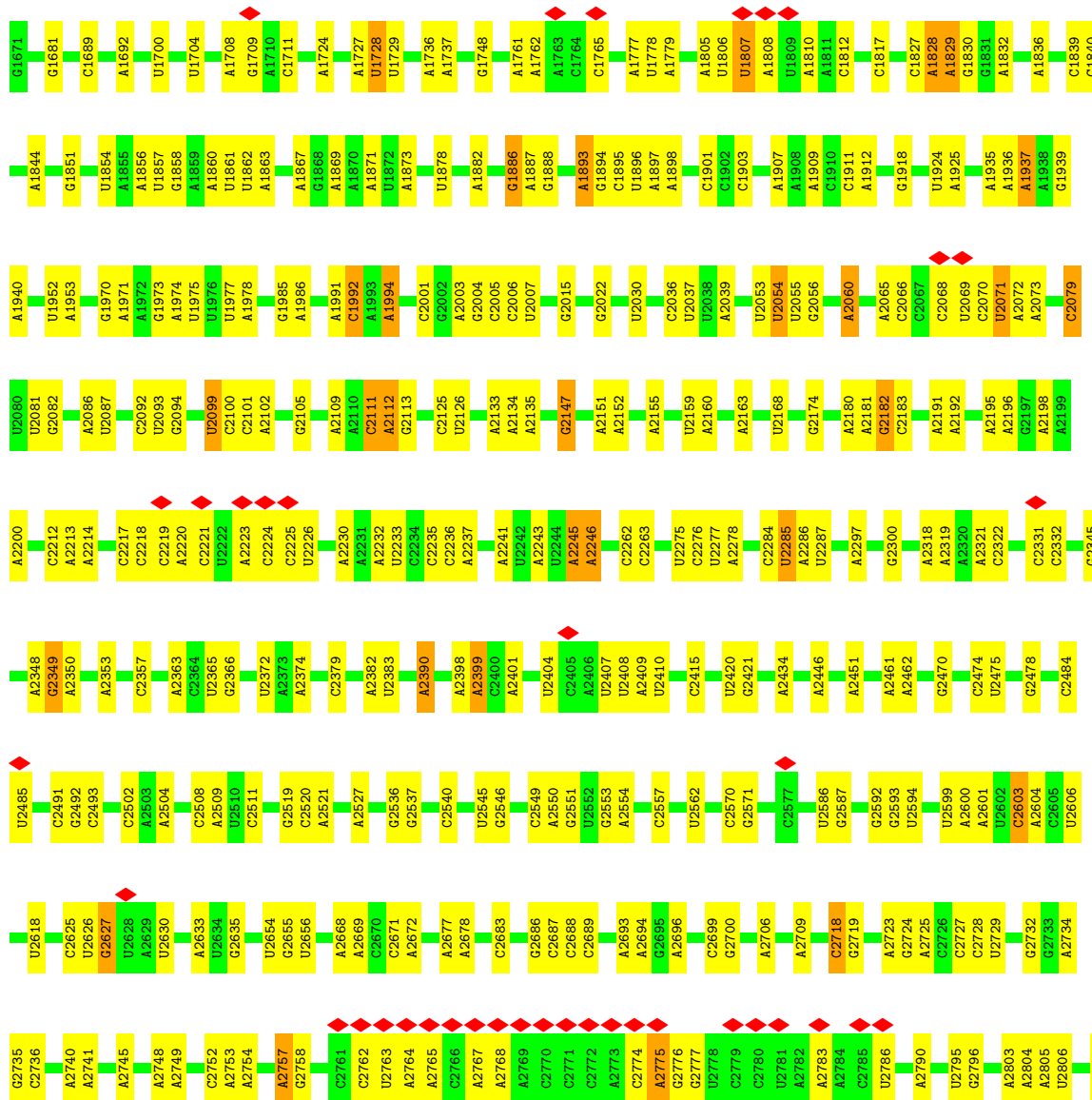
D61 Q62 E63 E66 R67 L68 R69 R70 L75 E76 K77 A78 T79 Q80 Q81 L92 K93 F94 L95 L96 D96 K97 A98 R99 E100 Q103 V104 E105 L117 K125 R129 R133 L147 L152 E153 K156 E160 A161 I162 K163 R164 E174 Q186 P187 R191 Y192

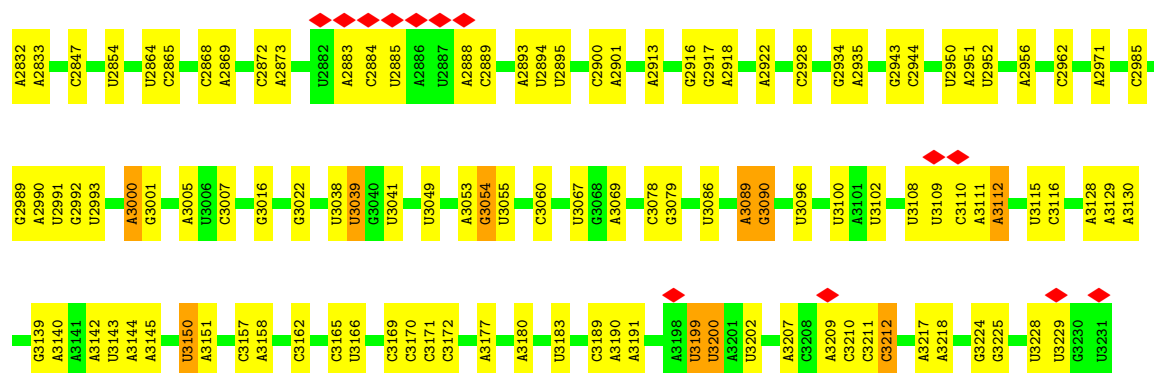


- Molecule 10: 39S ribosomal protein L41, mitochondrial

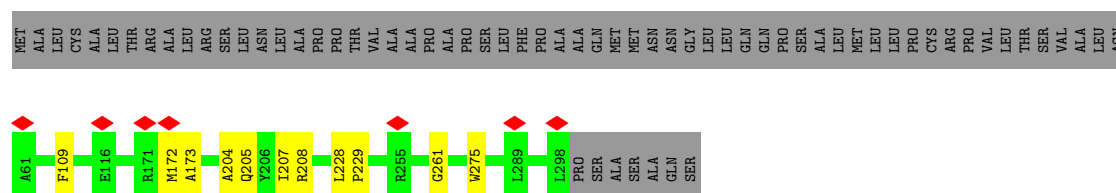
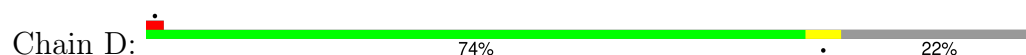


- Molecule 11: 16S mitochondrial rRNA

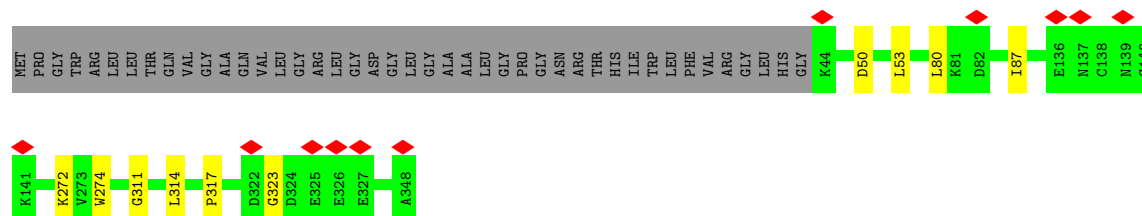
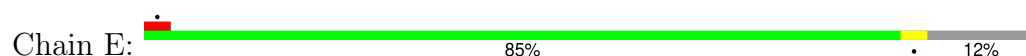




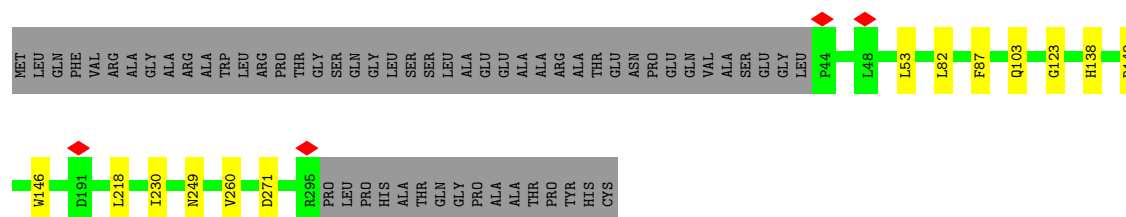
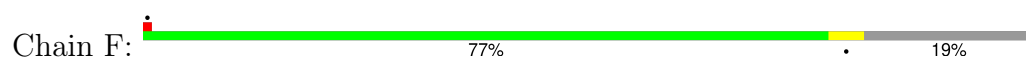
- Molecule 12: 39S ribosomal protein L2, mitochondrial



- Molecule 13: 39S ribosomal protein L3, mitochondrial

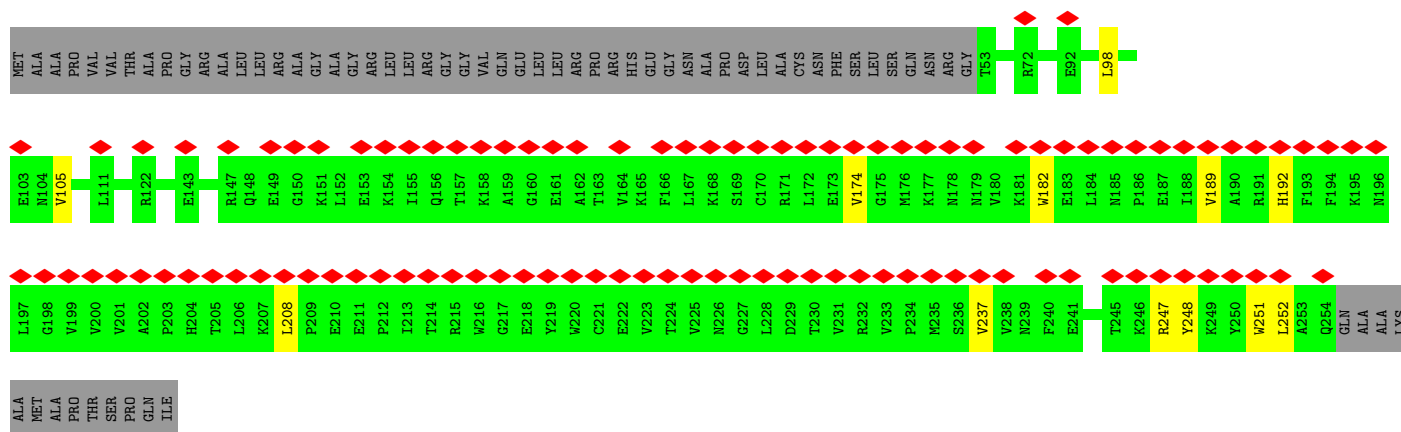


- Molecule 14: 39S ribosomal protein L4, mitochondrial

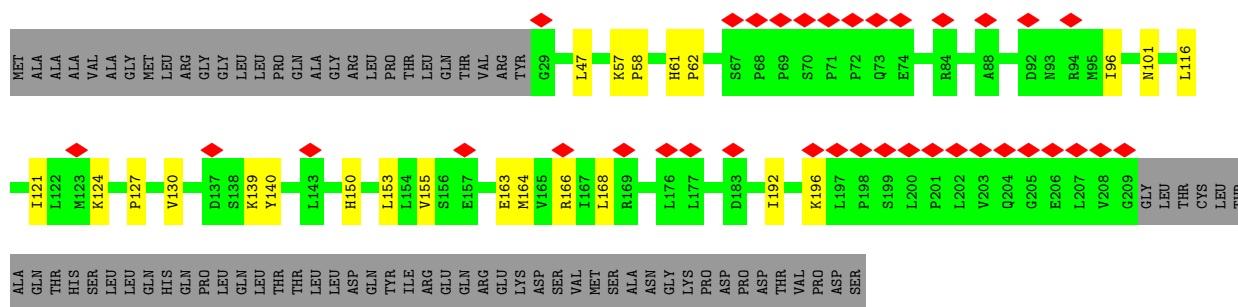


- Molecule 15: 39S ribosomal protein L9, mitochondrial

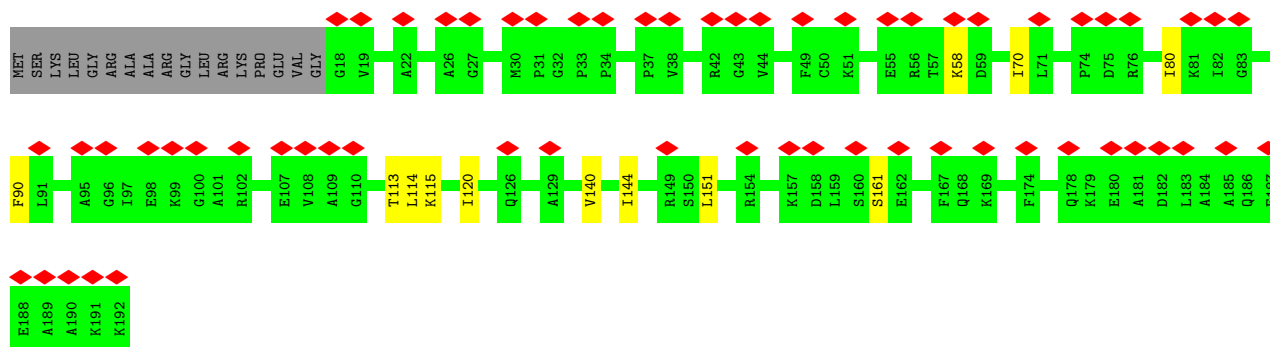
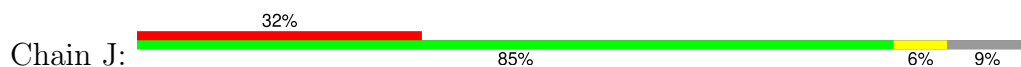




- Molecule 16: 39S ribosomal protein L10, mitochondrial



- Molecule 17: 39S ribosomal protein L11, mitochondrial

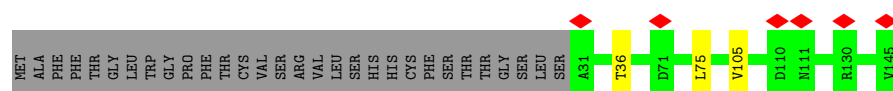


- Molecule 18: Large ribosomal subunit protein uL13m

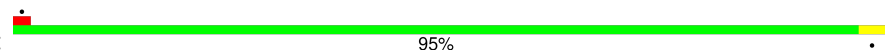


- Molecule 19: 39S ribosomal protein L14, mitochondrial

Chain L:  77% 21%



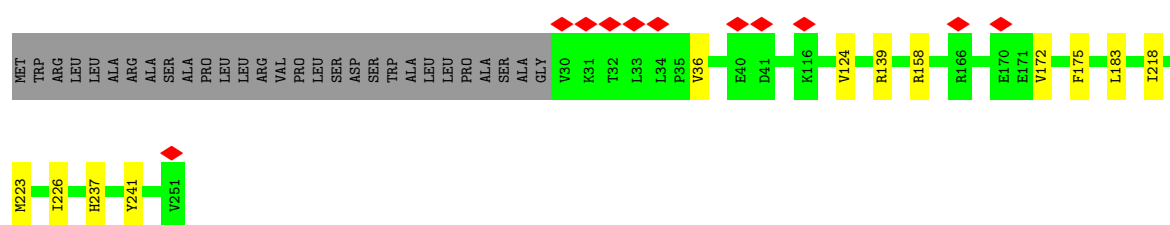
- Molecule 20: 39S ribosomal protein L15, mitochondrial

Chain M:  95% 5%



- Molecule 21: 39S ribosomal protein L16, mitochondrial

Chain N:  84% 5% 12%



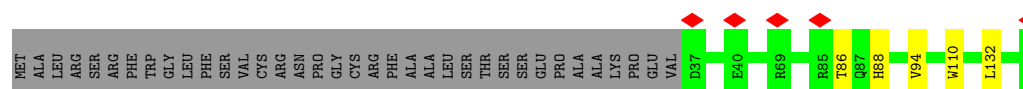
- Molecule 22: 39S ribosomal protein L17, mitochondrial

Chain O:  85% 12%



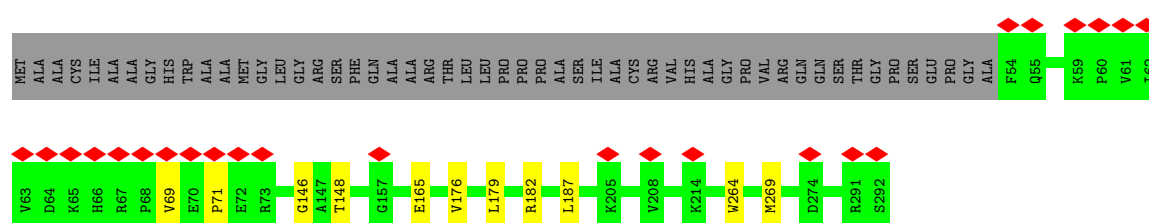
- Molecule 23: 39S ribosomal protein L18, mitochondrial

Chain P:  77% 20%

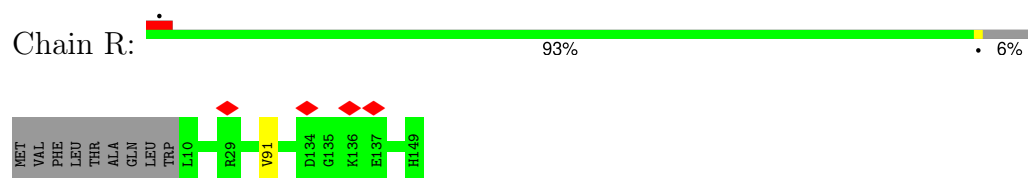


- Molecule 24: 39S ribosomal protein L19, mitochondrial

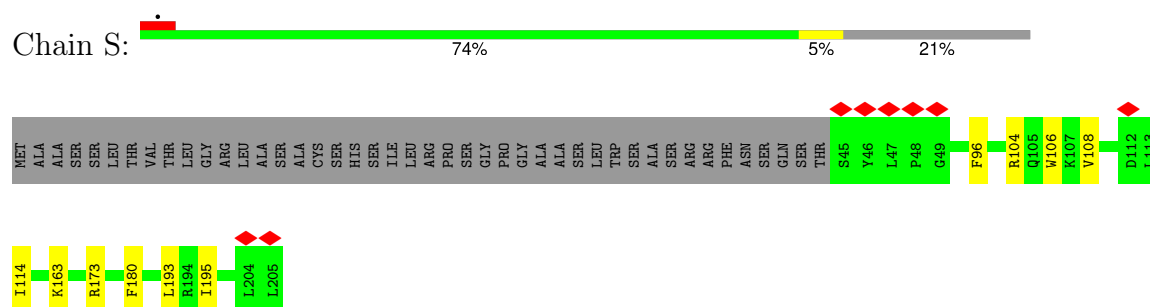
Chain Q:  8% 78% 18%



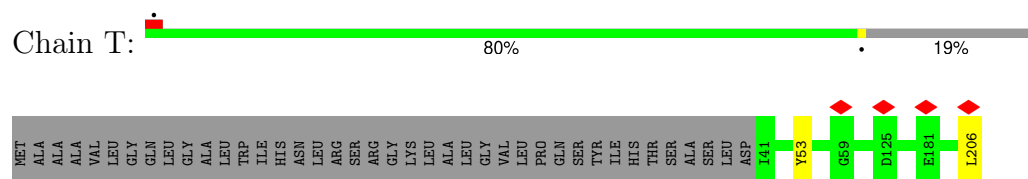
- Molecule 25: 39S ribosomal protein L20, mitochondrial



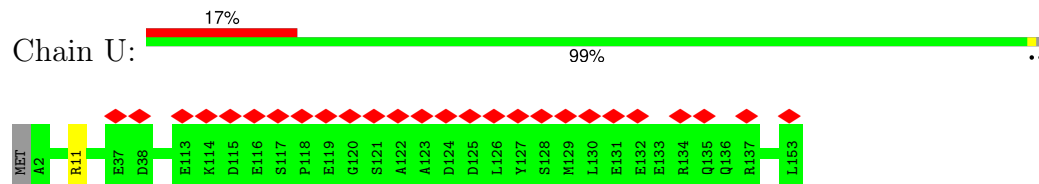
- Molecule 26: 39S ribosomal protein L21, mitochondrial



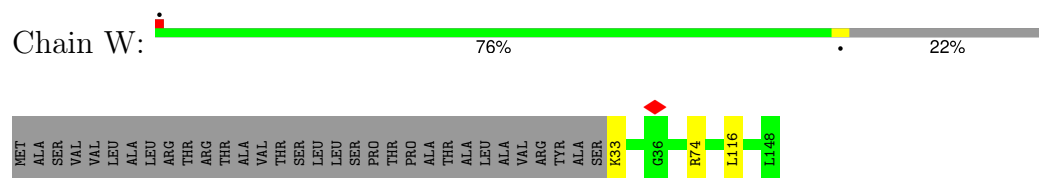
- Molecule 27: 39S ribosomal protein L22, mitochondrial



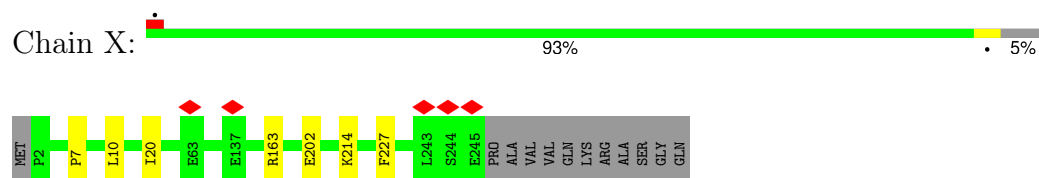
- Molecule 28: 39S ribosomal protein L23, mitochondrial



- Molecule 29: 39S ribosomal protein L27, mitochondrial

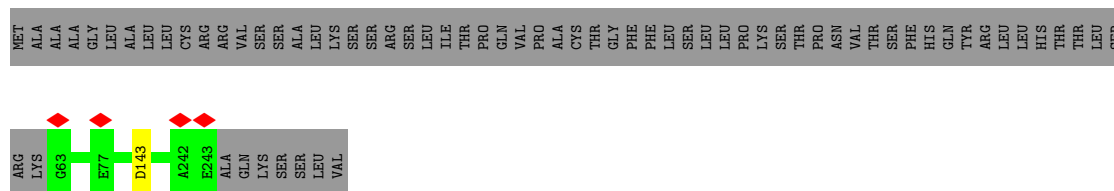


- Molecule 30: 39S ribosomal protein L28, mitochondrial



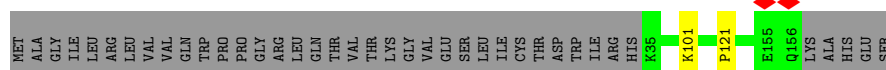
- Molecule 31: 39S ribosomal protein L47, mitochondrial

Chain Y:  72% 28%



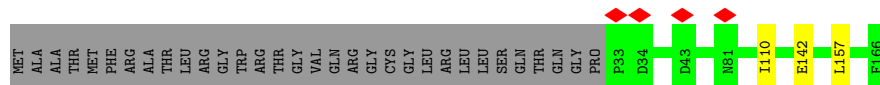
- Molecule 32: 39S ribosomal protein L30, mitochondrial

Chain Z:  75% 24%



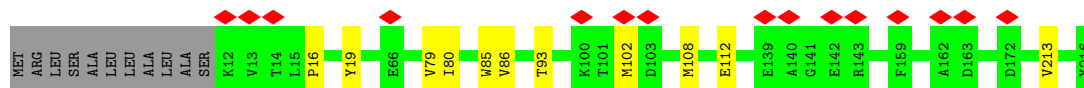
- Molecule 33: 39S ribosomal protein L49, mitochondrial

Chain g:  79% 19%



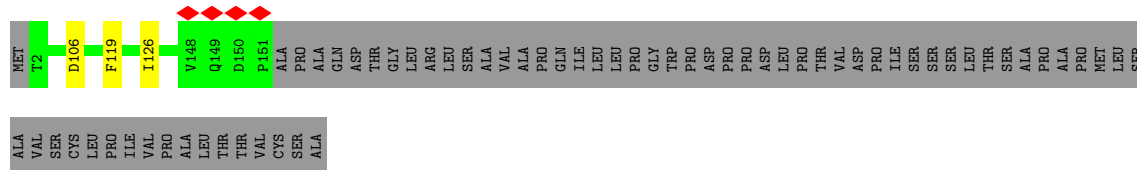
- Molecule 34: 39S ribosomal protein L24, mitochondrial

Chain V:  7% 90% 5% 5%



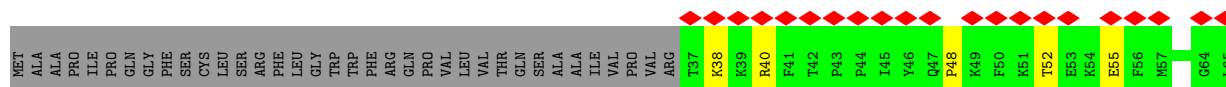
- Molecule 35: 39S ribosomal protein L43, mitochondrial

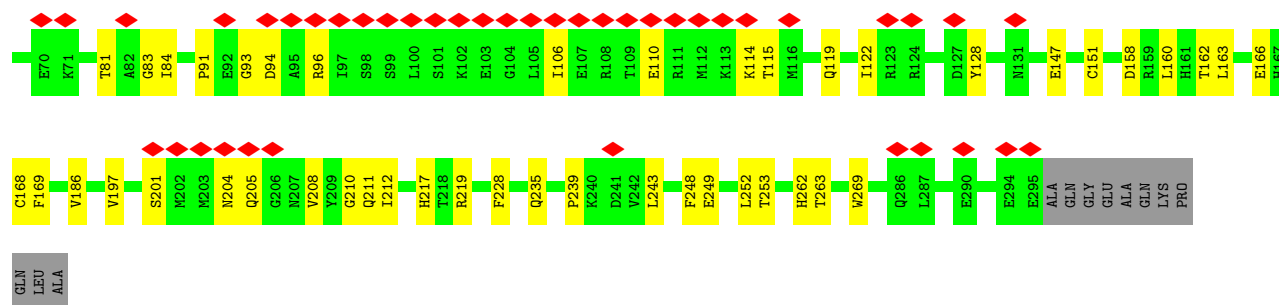
Chain b:  68% 30%



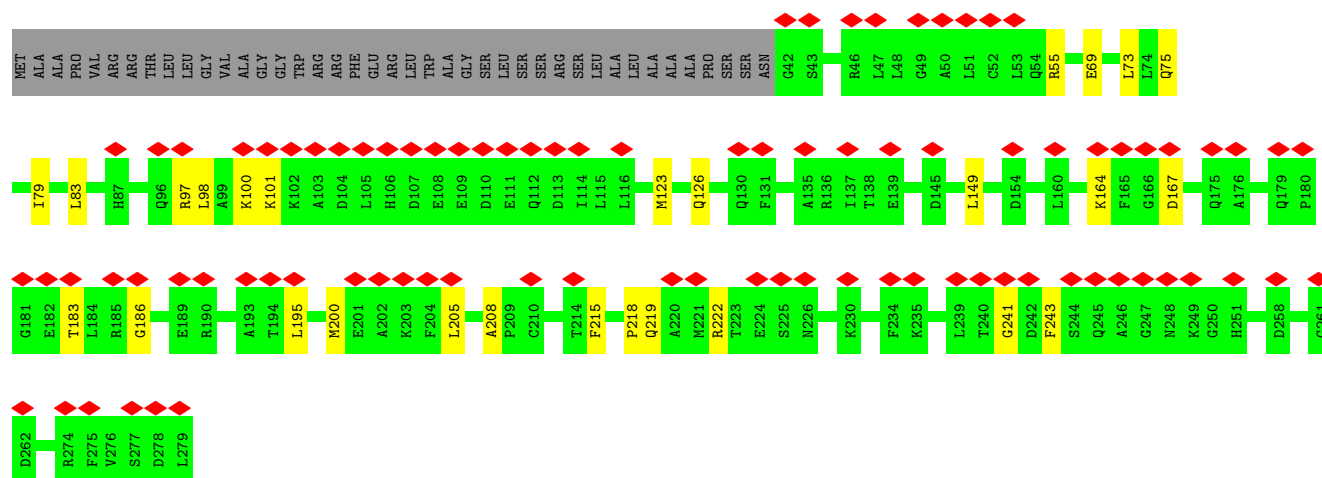
- Molecule 36: 39S ribosomal protein L45, mitochondrial

Chain d:  21% 68% 16% 15%

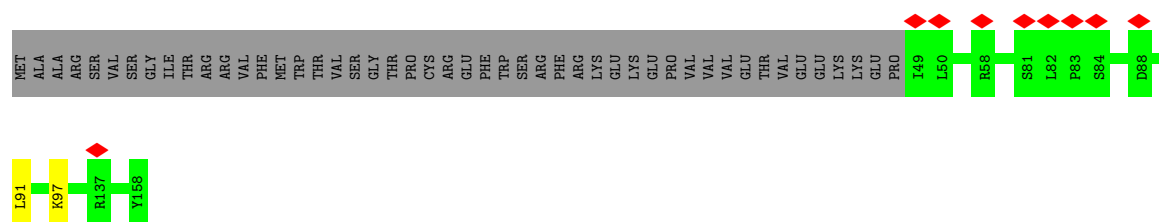




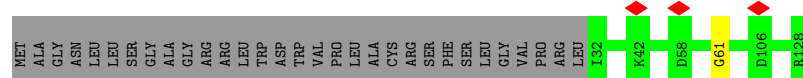
- Molecule 37: 39S ribosomal protein L46, mitochondrial



- Molecule 38: 39S ribosomal protein L50, mitochondrial



- Molecule 39: 39S ribosomal protein L51, mitochondrial

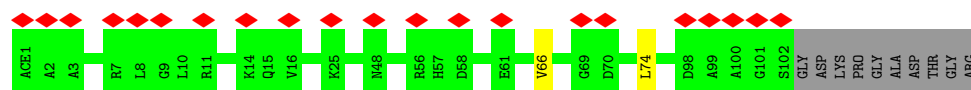
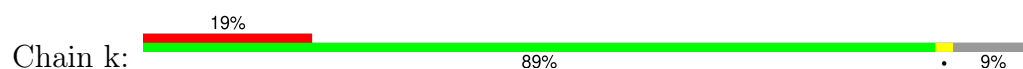


- Molecule 40: 39S ribosomal protein L52, mitochondrial

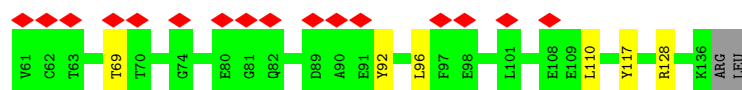
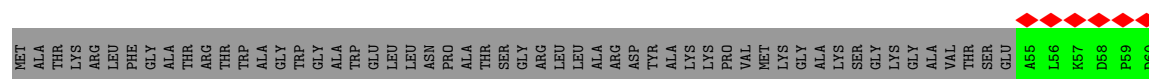




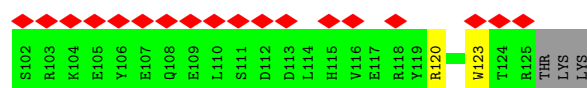
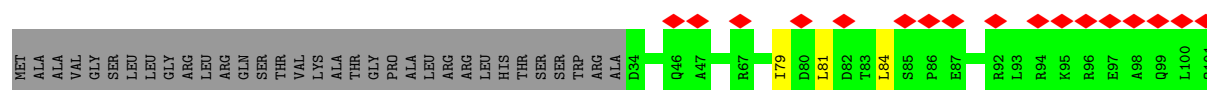
- Molecule 41: Large ribosomal subunit protein mL53



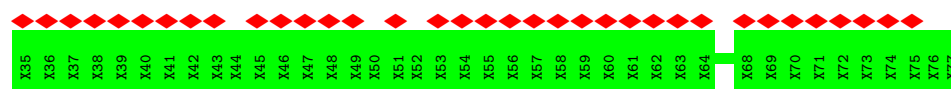
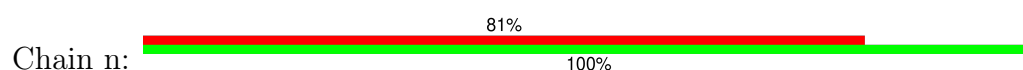
- Molecule 42: 39S ribosomal protein L54, mitochondrial



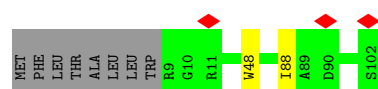
- Molecule 43: 39S ribosomal protein L55, mitochondrial



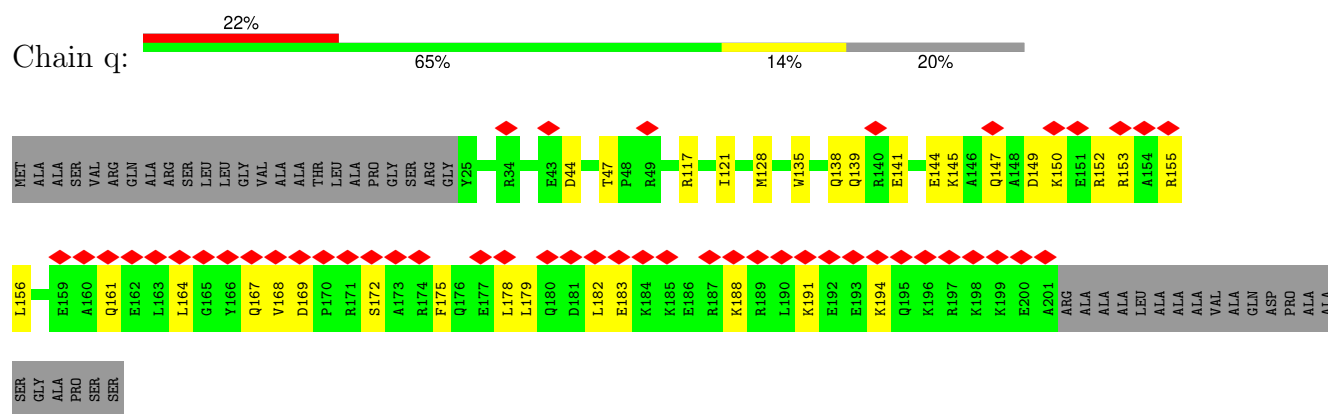
- Molecule 44: Nascent polypeptide



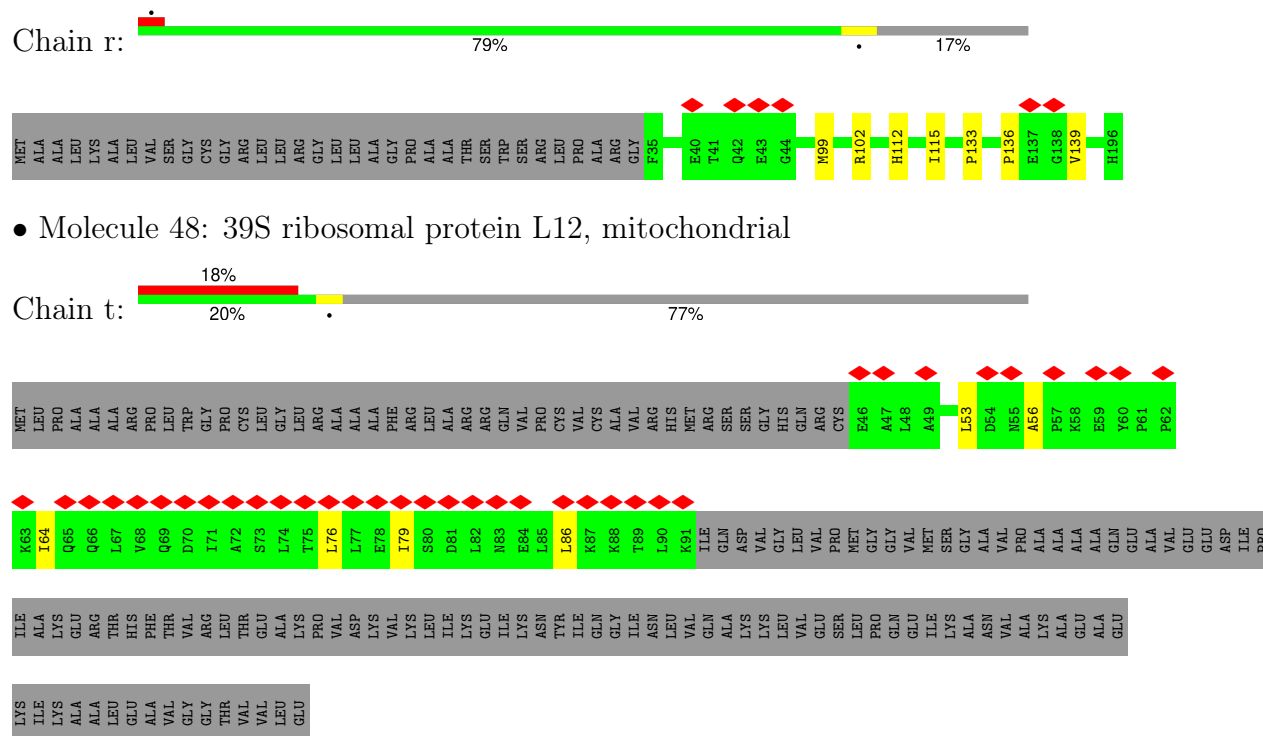
- Molecule 45: Ribosomal protein 63, mitochondrial



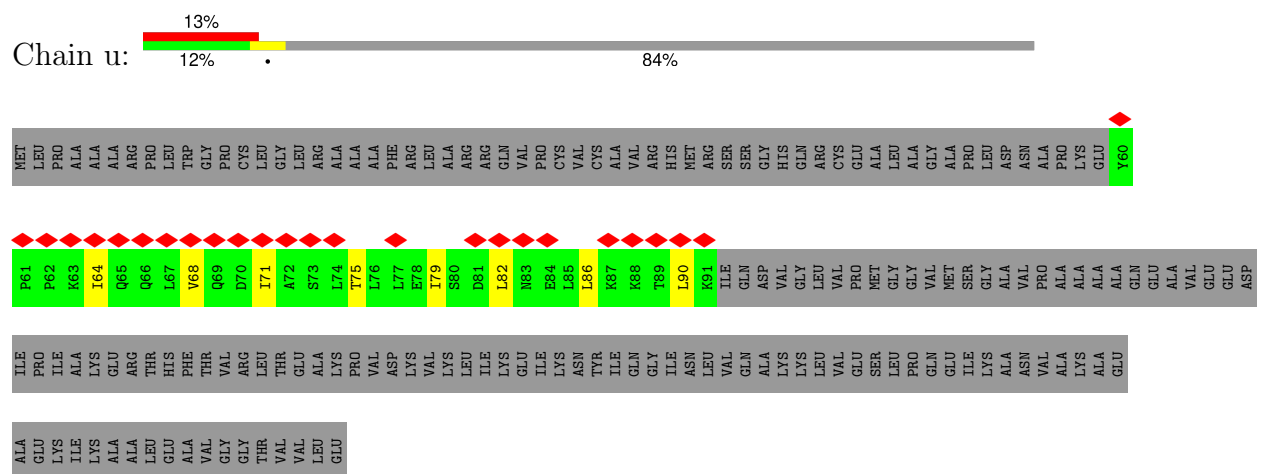
- Molecule 46: Growth arrest and DNA damage-inducible proteins-interacting protein 1



- Molecule 47: 39S ribosomal protein S18a, mitochondrial

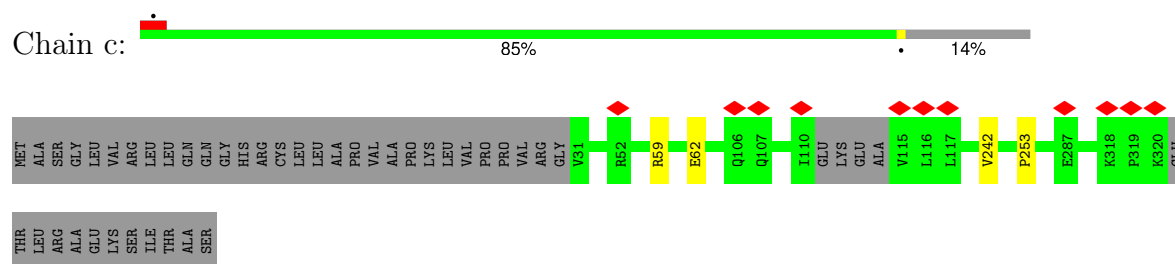


- Molecule 48: 39S ribosomal protein L12, mitochondrial



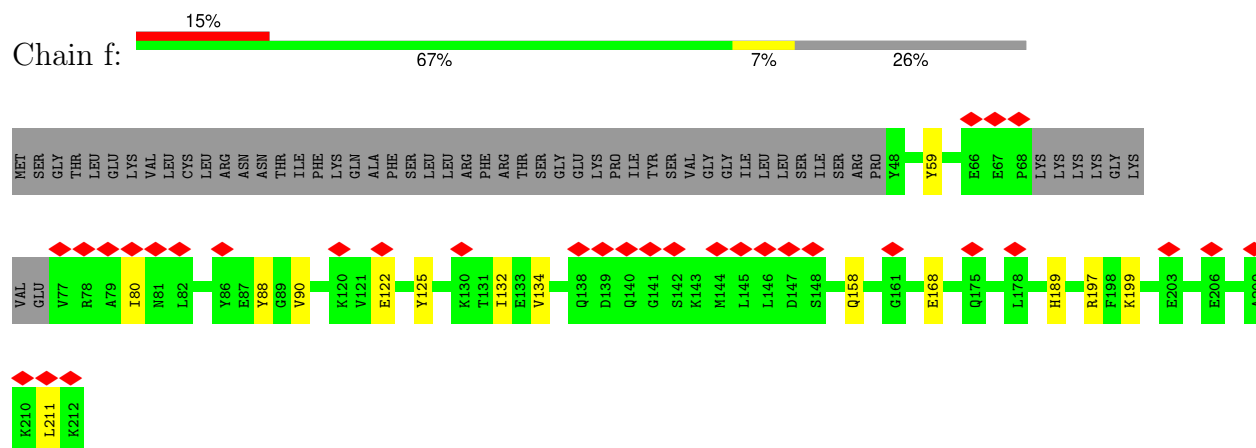
- Molecule 49: 39S ribosomal protein L44, mitochondrial

Chain c:



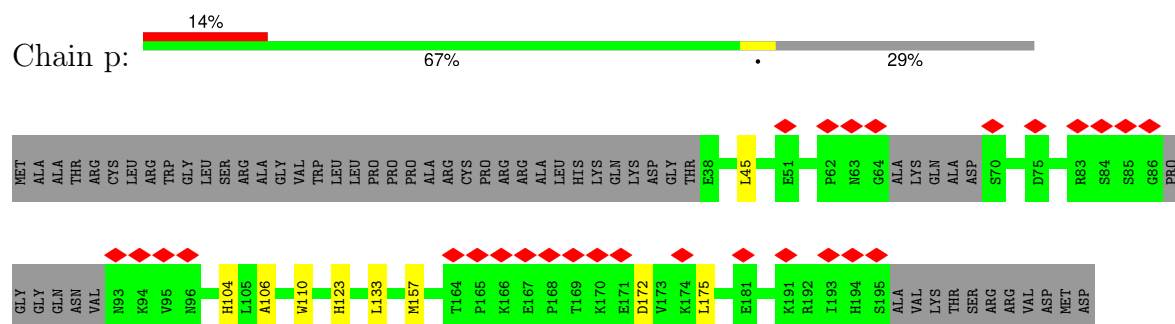
- Molecule 50: 39S ribosomal protein L48, mitochondrial

Chain f:



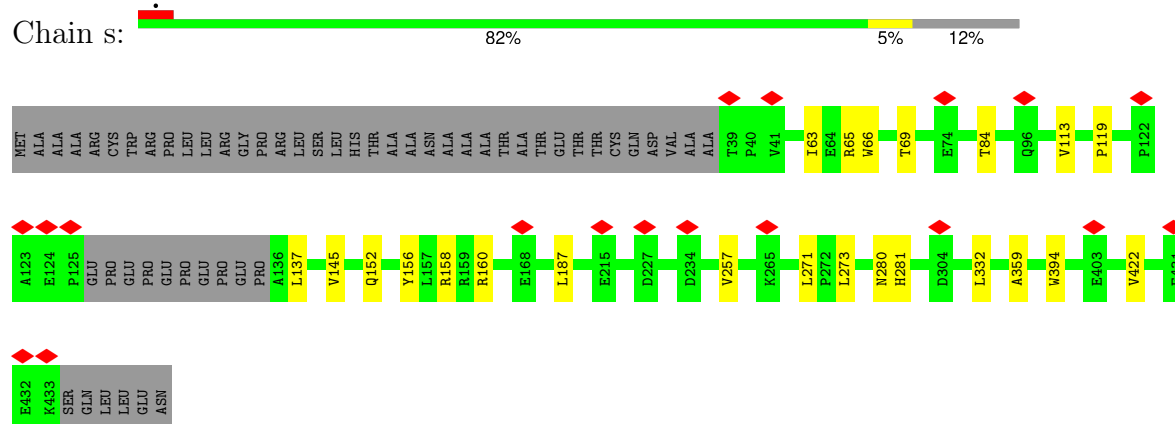
- Molecule 51: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:

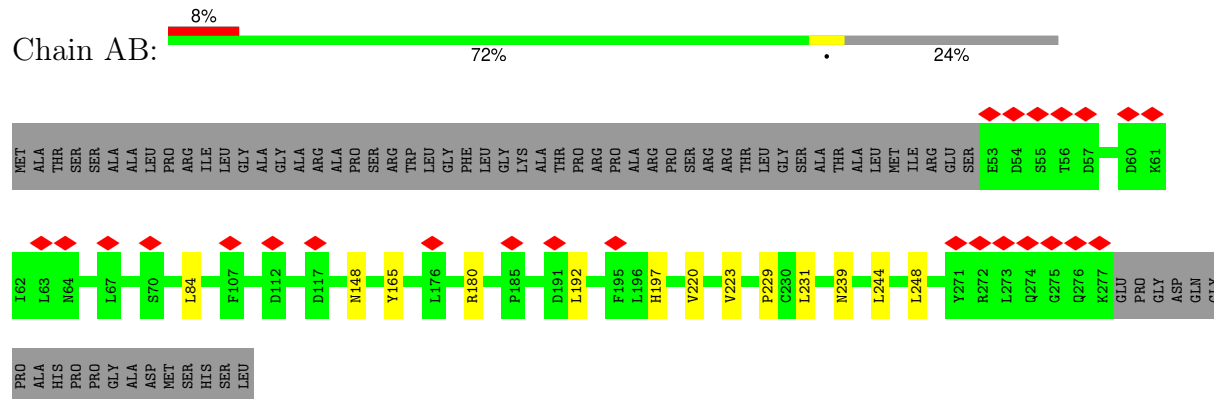


- Molecule 52: 39S ribosomal protein S30, mitochondrial

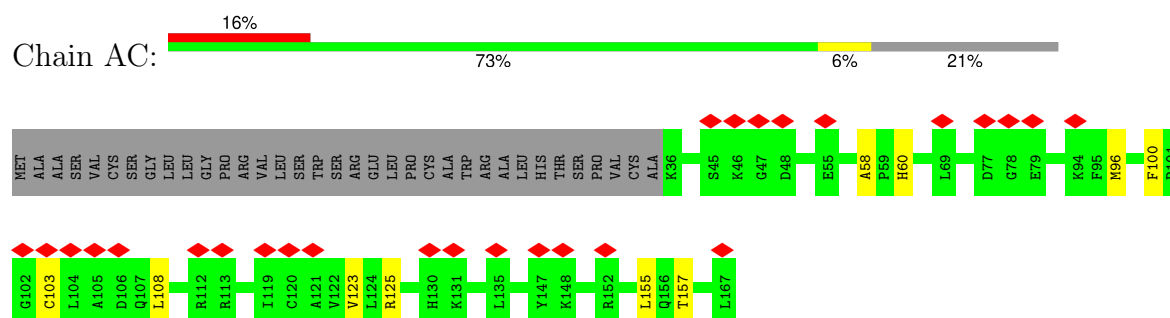
Chain s:



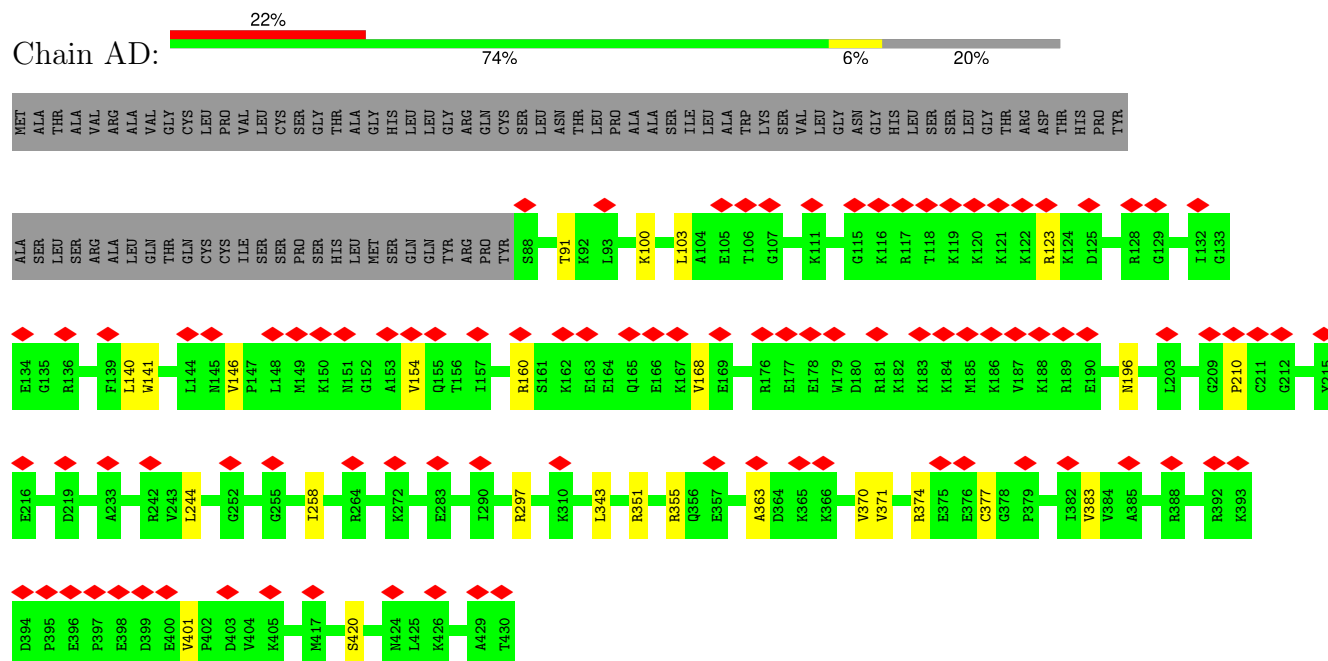
• Molecule 53: 28S ribosomal protein S2, mitochondrial



• Molecule 54: 28S ribosomal protein S24, mitochondrial

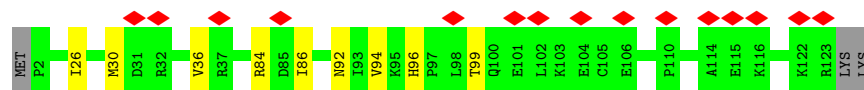


• Molecule 55: 28S ribosomal protein S5, mitochondrial

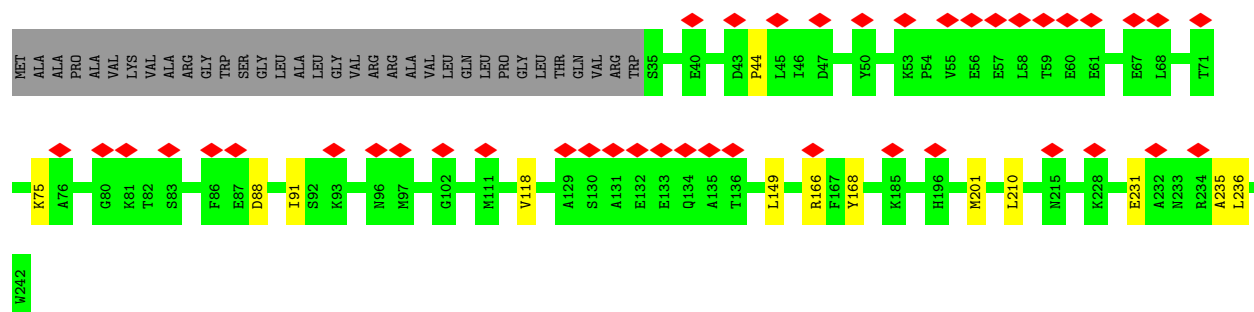
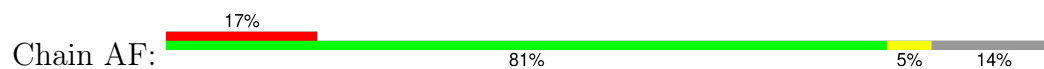


• Molecule 56: 28S ribosomal protein S6, mitochondrial

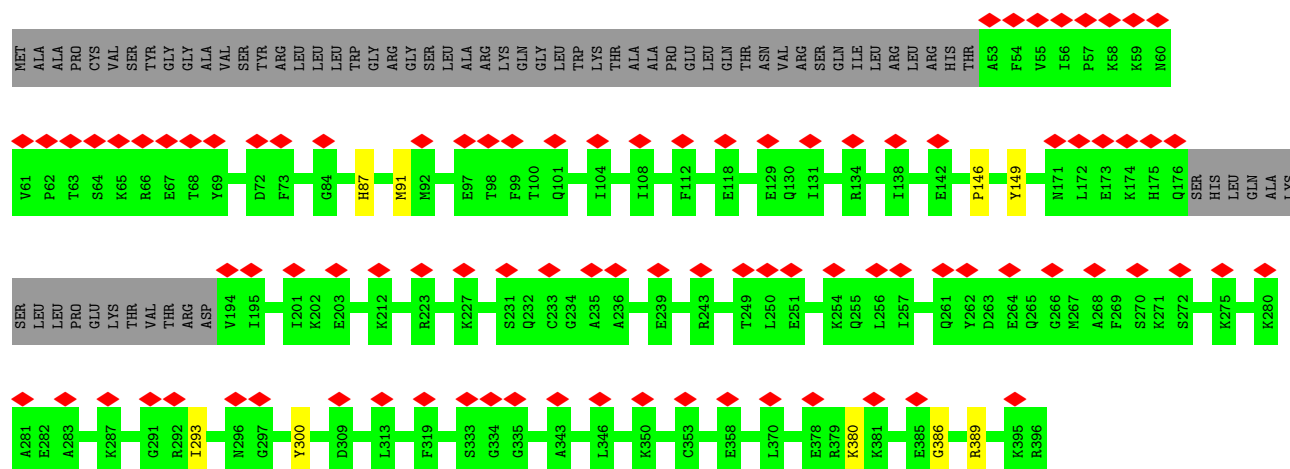
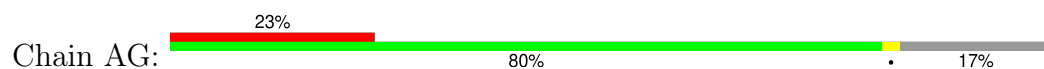




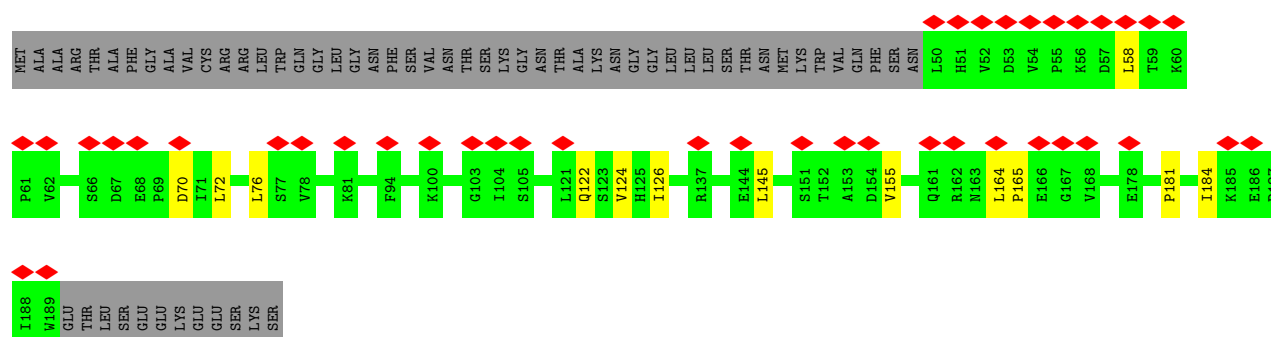
- Molecule 57: 28S ribosomal protein S7, mitochondrial



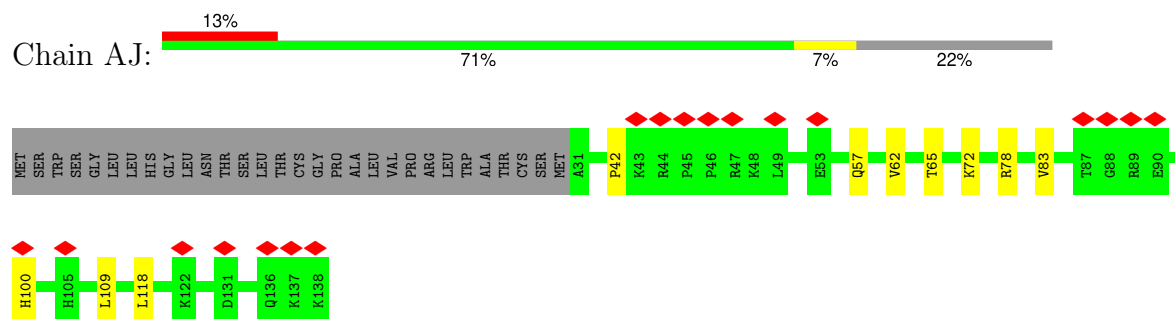
- Molecule 58: 28S ribosomal protein S9, mitochondrial



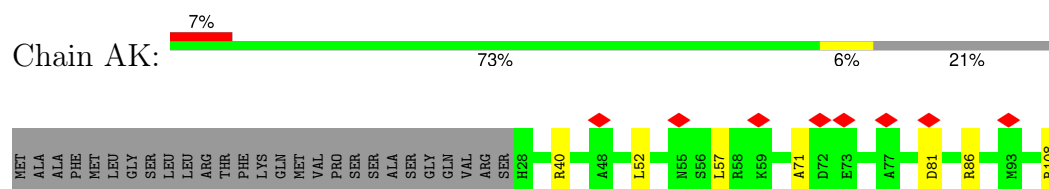
- Molecule 59: 28S ribosomal protein S10, mitochondrial



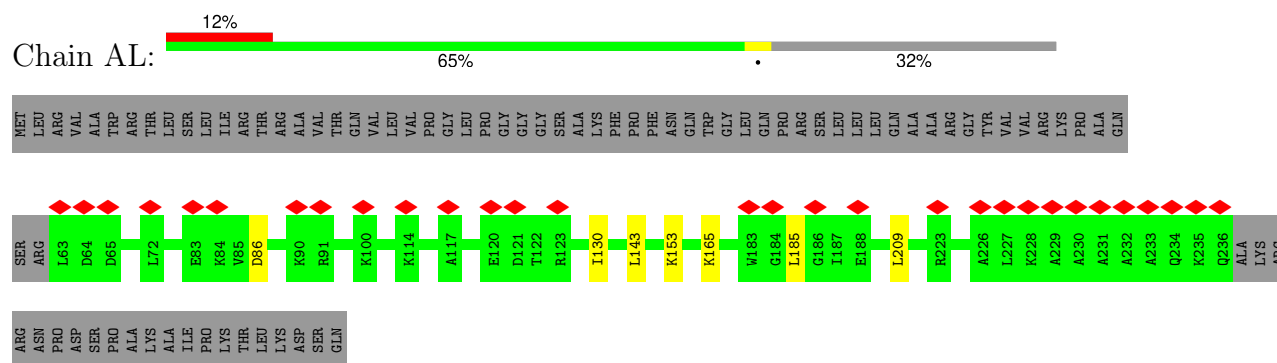
- Molecule 60: 28S ribosomal protein S12, mitochondrial



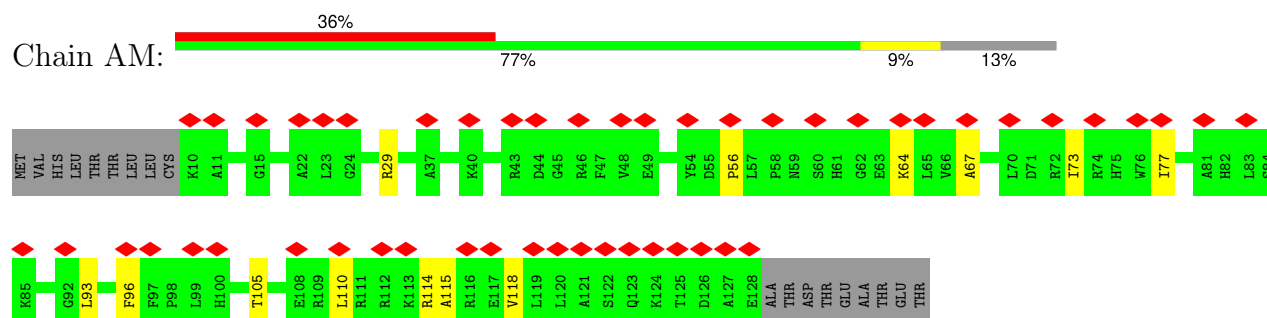
- Molecule 61: 28S ribosomal protein S14, mitochondrial



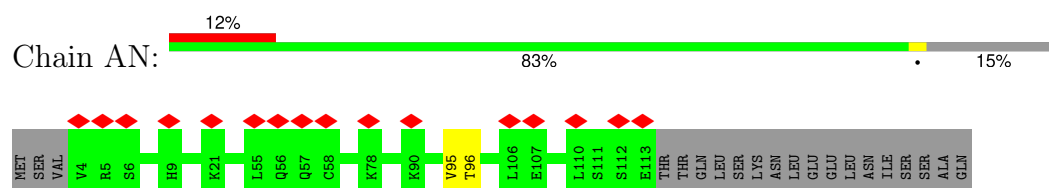
- Molecule 62: 28S ribosomal protein S15, mitochondrial



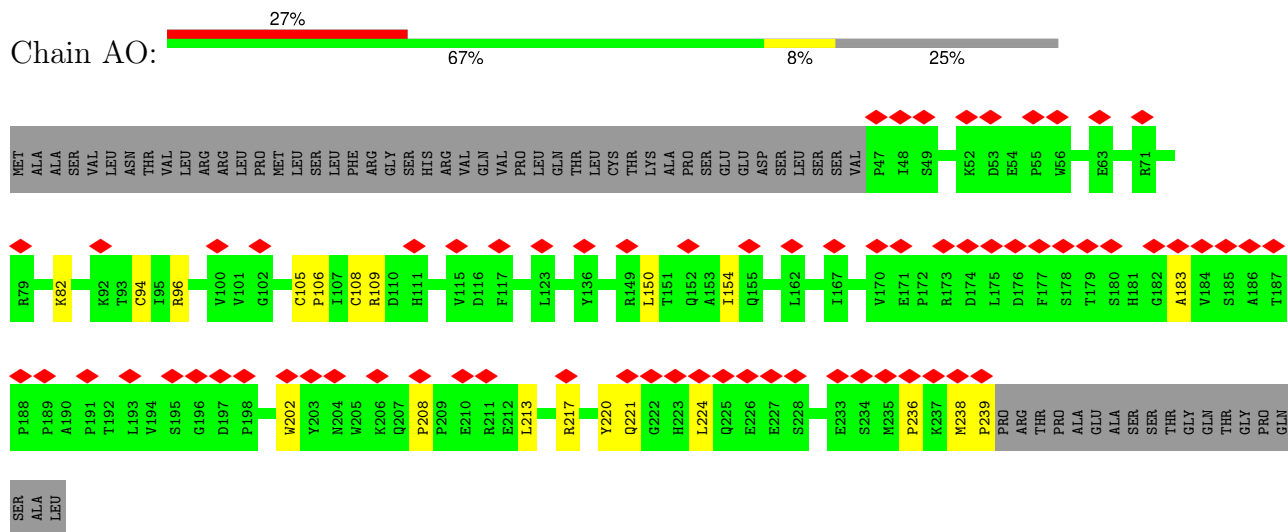
- Molecule 63: 28S ribosomal protein S16, mitochondrial



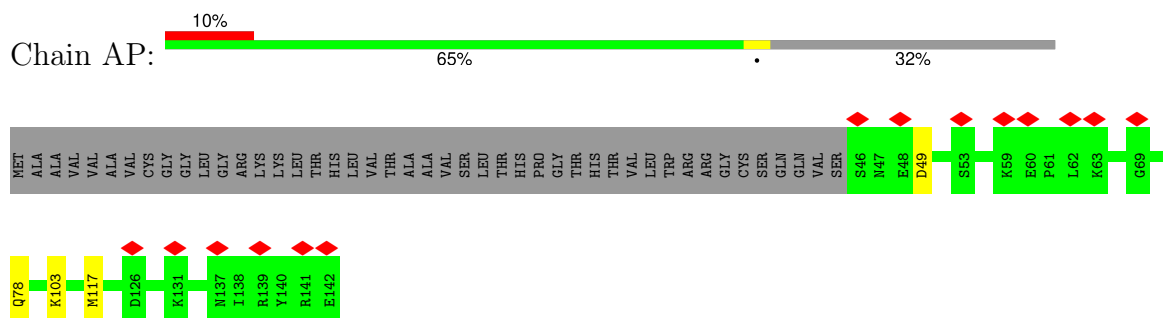
- Molecule 64: 28S ribosomal protein S17, mitochondrial



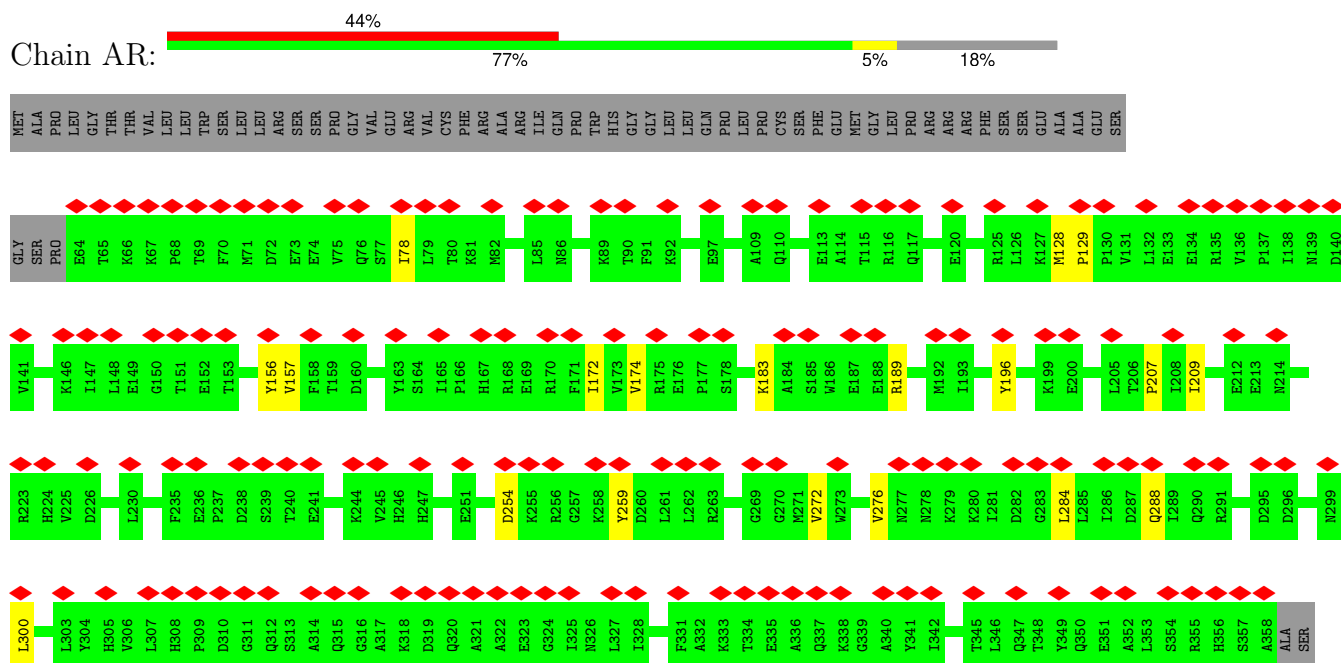
- Molecule 65: 28S ribosomal protein S18b, mitochondrial



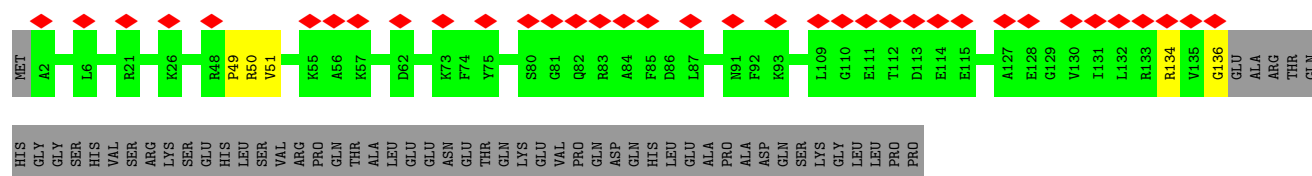
- Molecule 66: 28S ribosomal protein S18c, mitochondrial



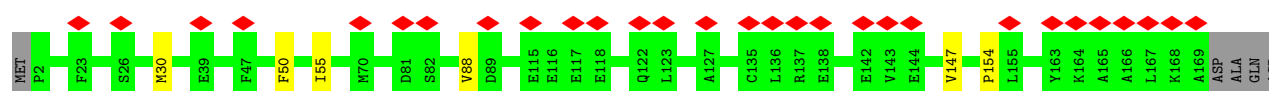
- Molecule 67: 28S ribosomal protein S22, mitochondrial



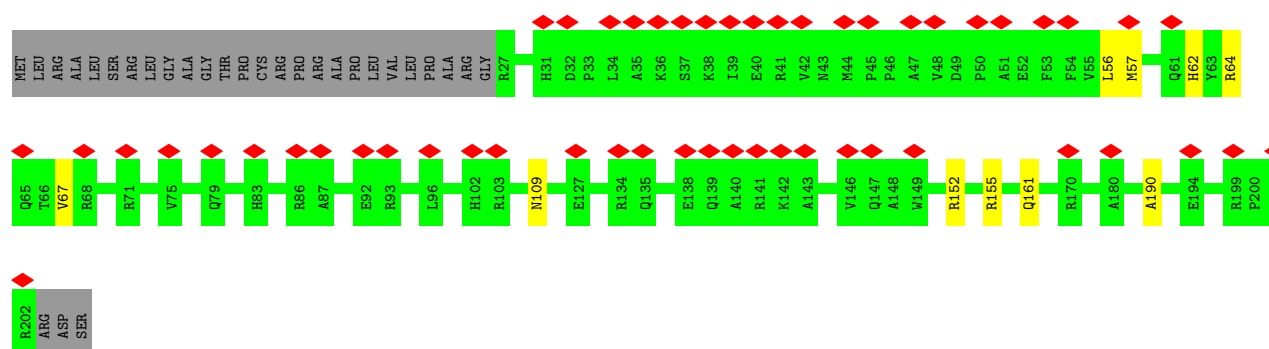
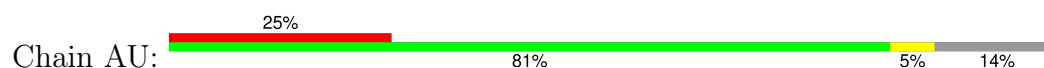
- Molecule 68: 28S ribosomal protein S23, mitochondrial



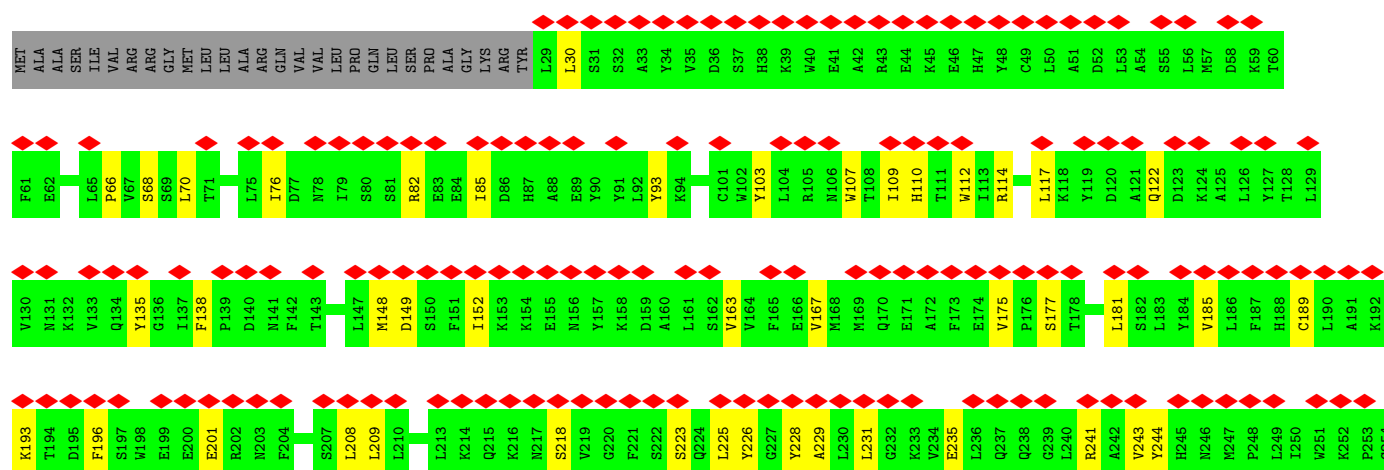
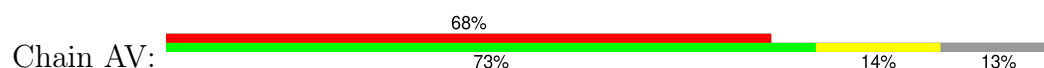
- Molecule 69: 28S ribosomal protein S25, mitochondrial

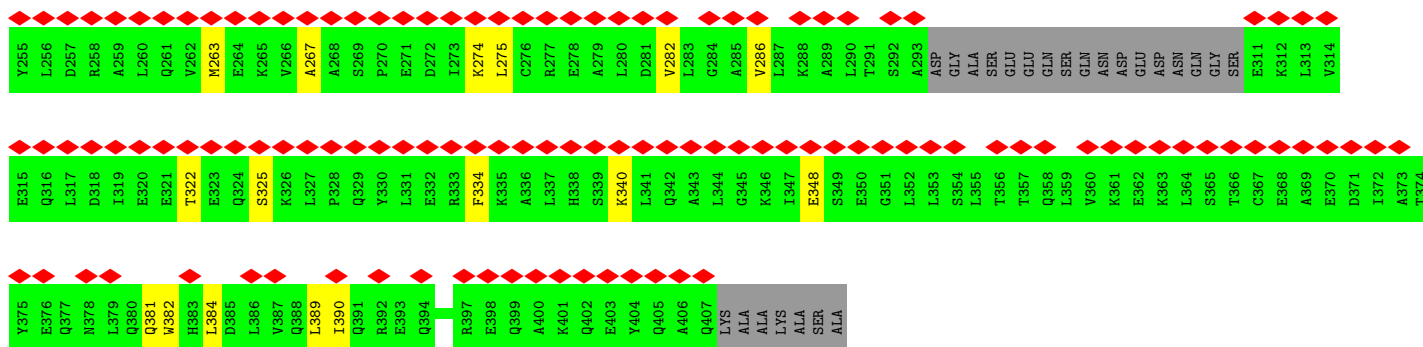


- Molecule 70: 28S ribosomal protein S26, mitochondrial

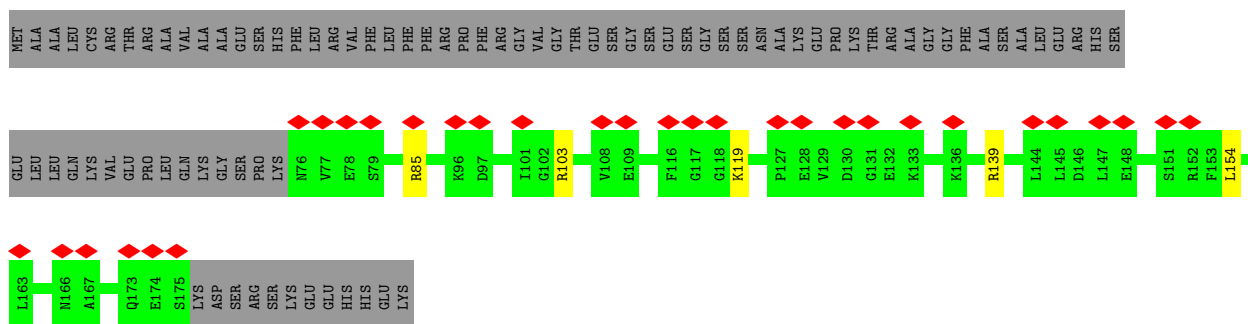


- Molecule 71: 28S ribosomal protein S27, mitochondrial

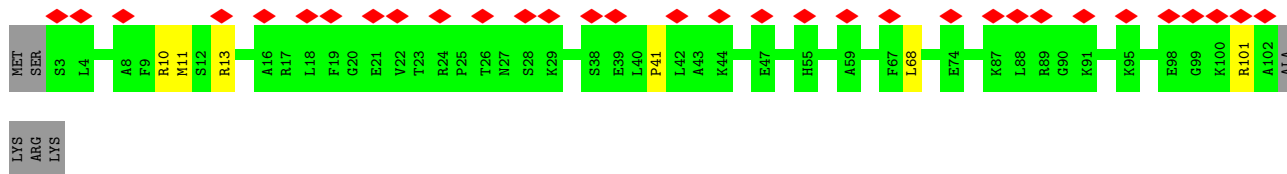
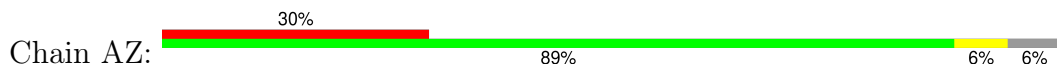




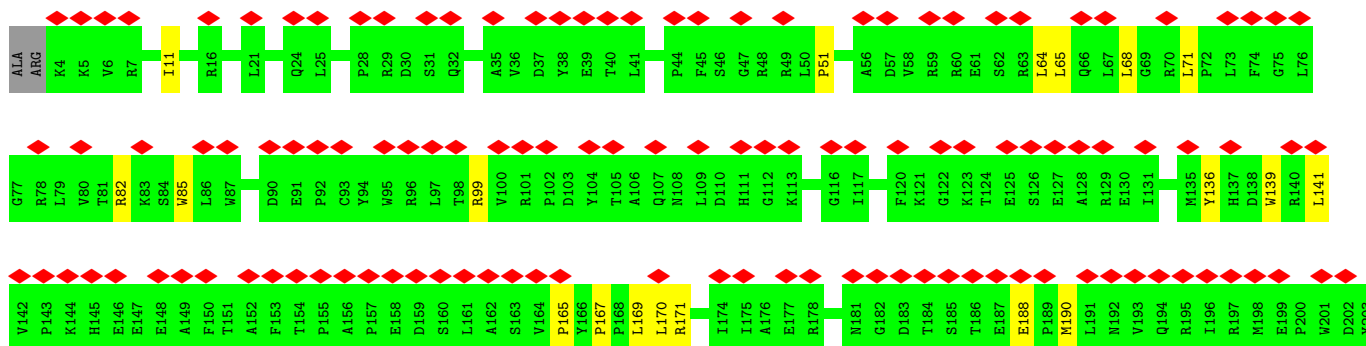
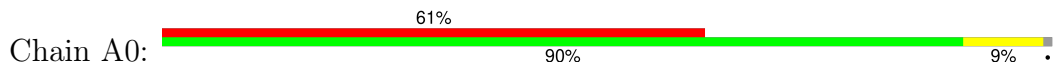
- Molecule 72: 28S ribosomal protein S28, mitochondrial

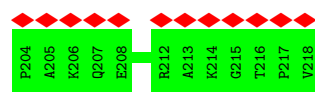


- Molecule 73: 28S ribosomal protein S33, mitochondrial



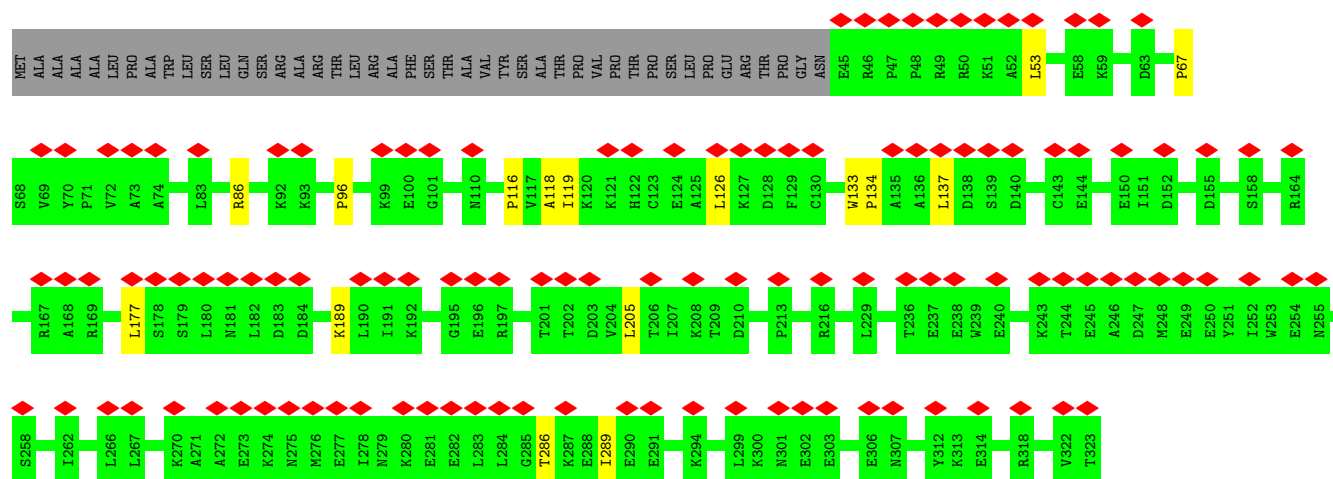
- Molecule 74: Small ribosomal subunit protein mS34





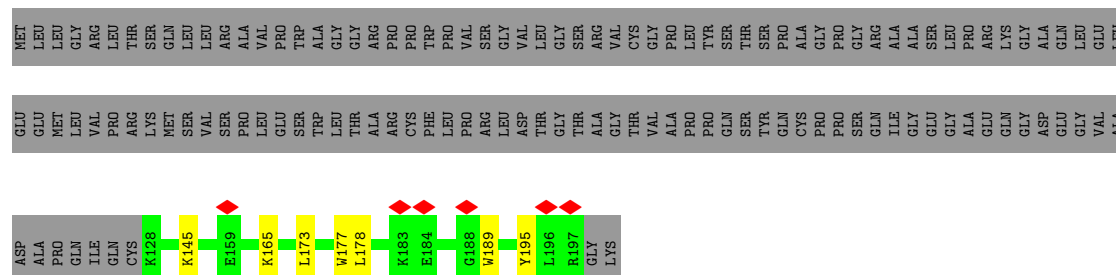
- Molecule 75: 28S ribosomal protein S35, mitochondrial

Chain A1: 37% 81% 5% 14%



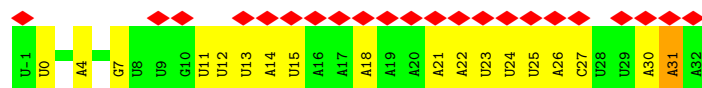
- Molecule 76: Aurora kinase A-interacting protein

Chain A3: 32% 65%



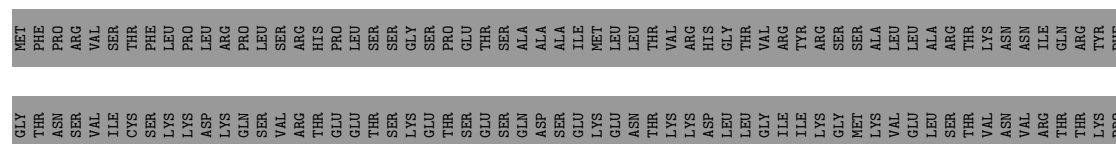
- Molecule 77: mRNA

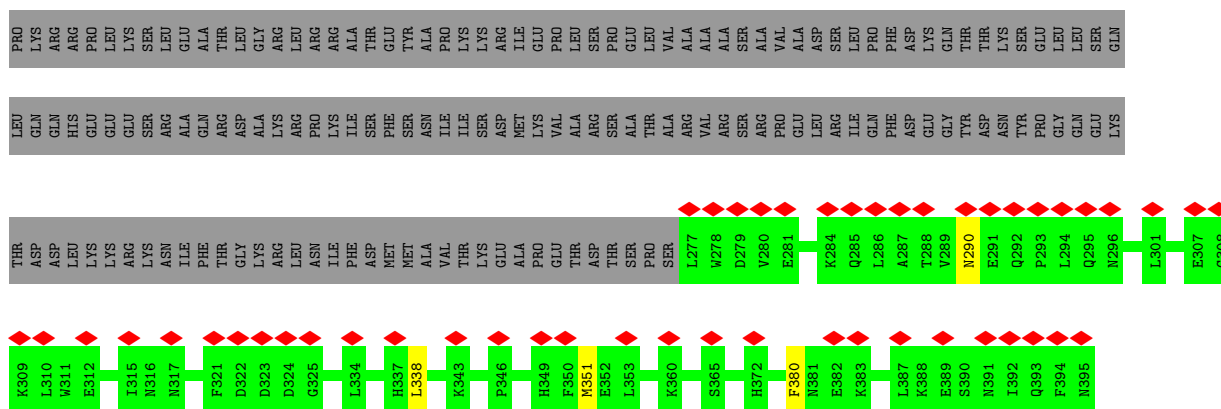
Chain Az: 65% 47% 50%



- Molecule 78: 28S ribosomal protein S31, mitochondrial

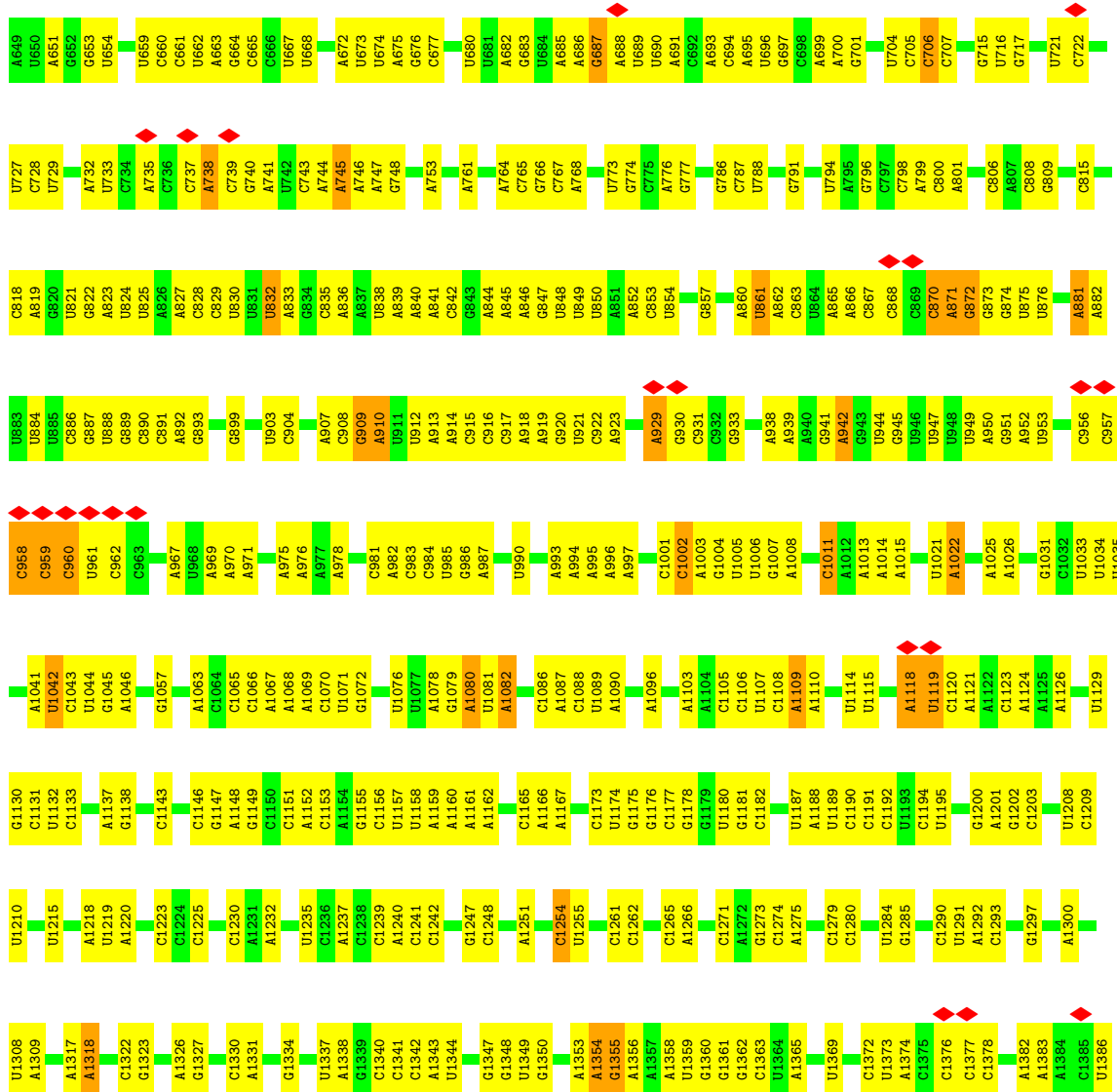
Chain AY: 12% 29% 70%

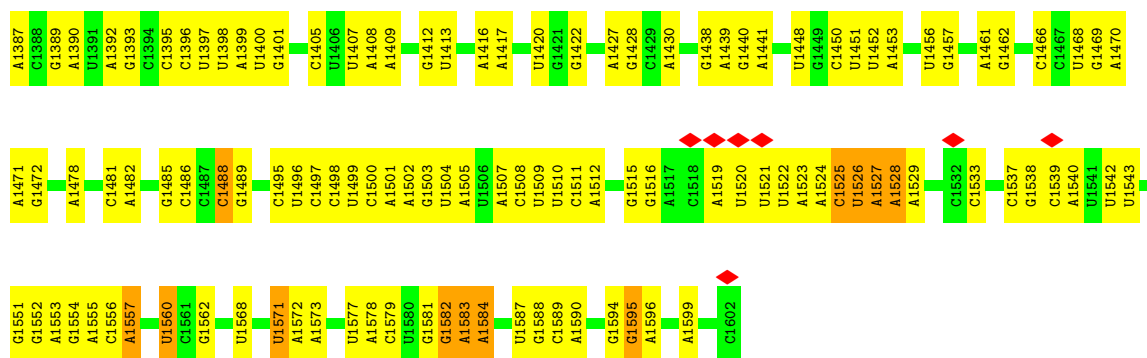




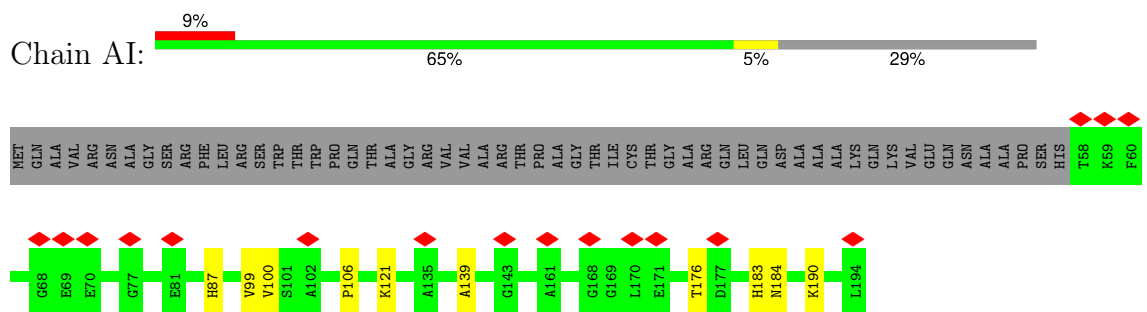
• Molecule 79: 12S mitochondrial rRNA

Chain AA: 46% 50%

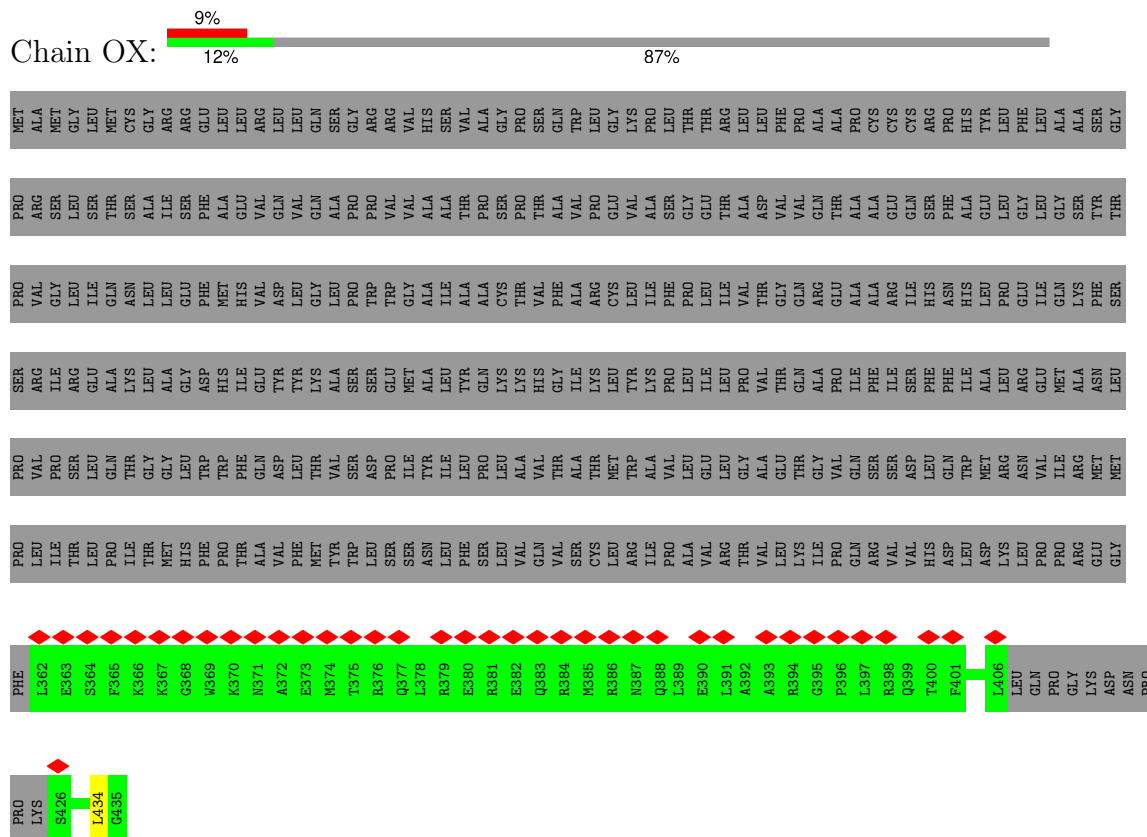




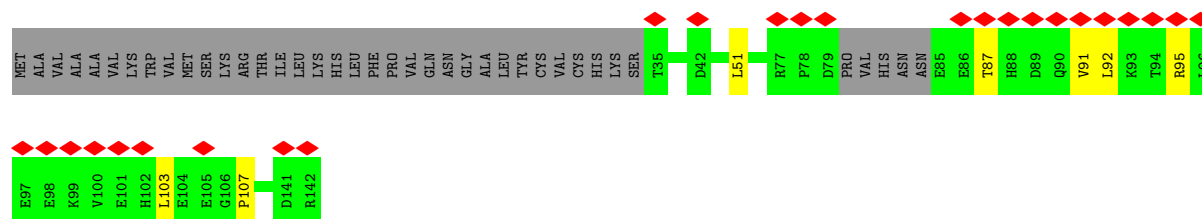
- Molecule 80: 28S ribosomal protein S11, mitochondrial



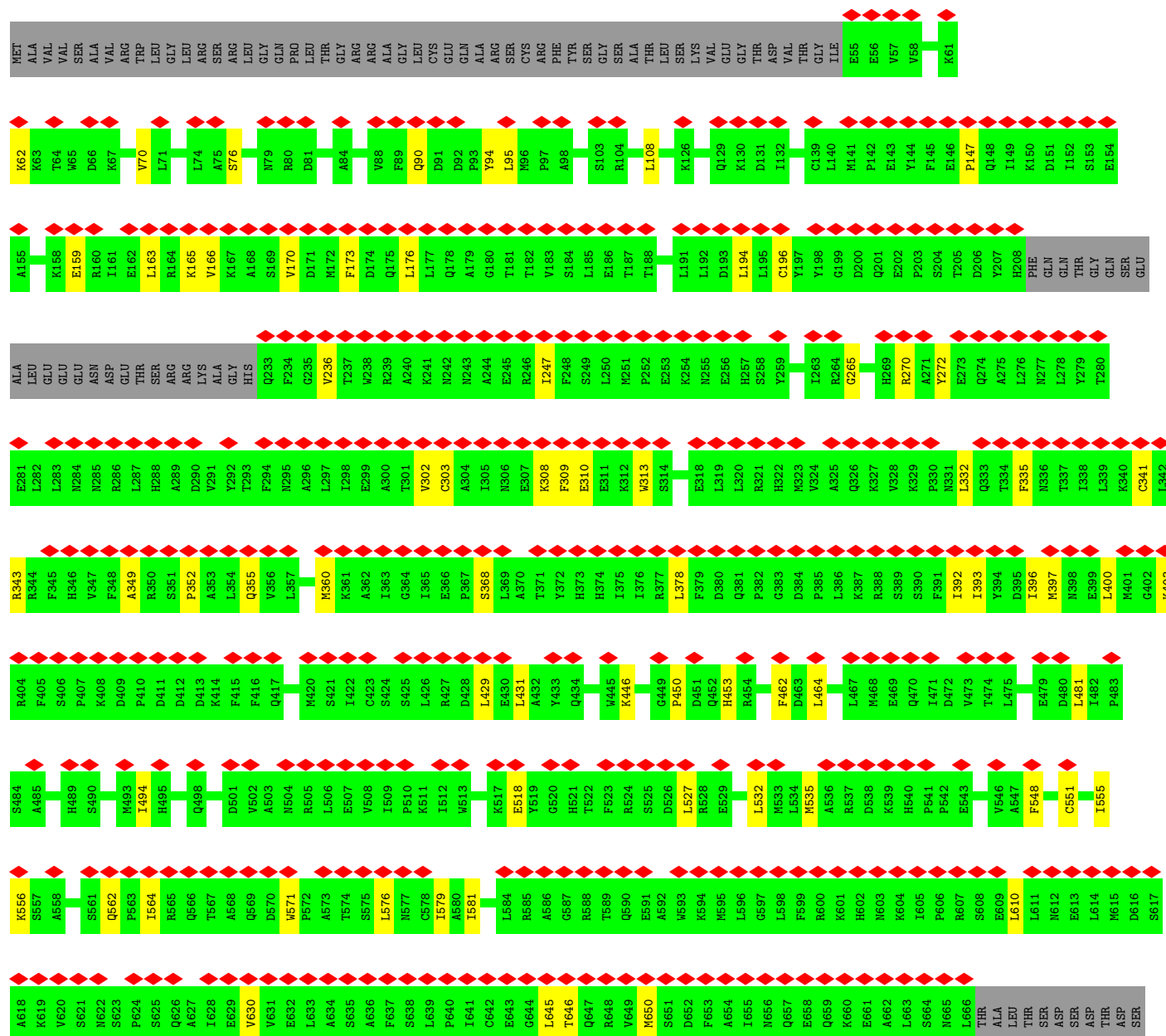
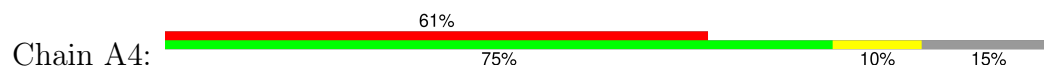
- Molecule 81: Mitochondrial inner membrane protein OXA1L



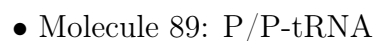
- Molecule 82: 39S ribosomal protein L42, mitochondrial



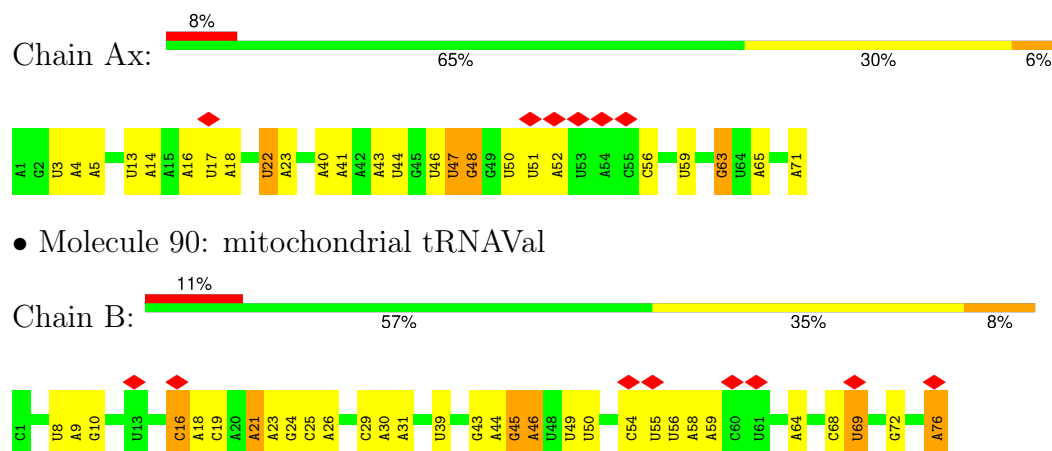
- Molecule 83: Pentatricopeptide repeat domain-containing protein 3, mitochondrial



Chain Ag:

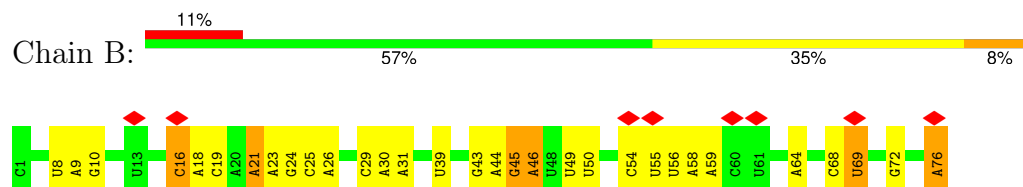


Chain Ax:



- Molecule 90: mitochondrial tRNA^{Val}

Chain B:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12962	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	0.140	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.027	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

5.1 Standard geometry

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

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	0.22	0/469	0.29	0/621
3	2	0.28	0/383	0.27	0/507
4	3	0.27	0/853	0.28	0/1136
5	4	0.24	0/350	0.24	0/461
6	5	0.22	0/3305	0.29	0/4502
7	6	0.20	0/3043	0.28	0/4140
8	7	0.21	0/2447	0.29	0/3310
9	8	0.18	0/1354	0.32	0/1819
10	9	0.23	0/1025	0.28	0/1379
11	A	0.29	0/36876	0.30	0/57402
12	D	0.23	0/1896	0.28	0/2549
13	E	0.24	0/2475	0.30	0/3355
14	F	0.26	0/2090	0.29	0/2842
15	H	0.17	0/1698	0.29	0/2292
16	I	0.19	0/1478	0.35	0/1999
17	J	0.17	0/1348	0.29	0/1813
18	K	0.26	0/1497	0.28	0/2031
19	L	0.23	0/905	0.28	0/1218
20	M	0.25	0/2381	0.30	0/3212
21	N	0.24	0/1833	0.27	0/2468
22	O	0.23	0/1283	0.27	0/1727
23	P	0.21	0/1199	0.28	0/1623
24	Q	0.22	0/2039	0.27	0/2750
25	R	0.27	0/1175	0.27	0/1572
26	S	0.25	0/1320	0.30	0/1789
27	T	0.25	0/1403	0.27	0/1886
28	U	0.24	0/1279	0.34	0/1730
29	W	0.26	0/926	0.26	0/1244
30	X	0.23	0/2099	0.25	0/2837
31	Y	0.24	0/1593	0.26	0/2136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.25	0/1021	0.29	0/1378
33	g	0.23	0/1151	0.28	0/1569
34	V	0.21	0/1721	0.26	0/2333
35	b	0.25	0/1218	0.30	0/1649
36	d	0.20	0/2181	0.34	0/2949
37	e	0.17	0/1970	0.33	0/2658
38	h	0.19	0/918	0.27	0/1249
39	i	0.27	0/850	0.29	0/1135
40	j	0.21	0/760	0.26	0/1023
41	k	0.16	0/783	0.25	0/1057
42	l	0.16	0/707	0.28	0/960
43	m	0.15	0/805	0.31	0/1081
45	o	0.26	0/819	0.29	0/1097
46	q	0.19	0/1529	0.31	0/2055
47	r	0.23	0/1362	0.30	0/1846
48	t	0.15	0/358	0.30	0/486
48	u	0.20	0/259	0.40	0/350
49	c	0.22	0/2347	0.27	0/3171
50	f	0.21	0/1273	0.33	0/1716
51	p	0.19	0/1223	0.28	0/1641
52	s	0.24	0/3231	0.30	0/4389
53	AB	0.19	0/1871	0.27	0/2531
54	AC	0.18	0/1113	0.29	0/1505
55	AD	0.18	0/2783	0.28	0/3724
56	AE	0.19	0/989	0.30	0/1335
57	AF	0.16	0/1767	0.26	0/2373
58	AG	0.16	0/2746	0.28	0/3681
59	AH	0.18	0/1178	0.30	0/1598
60	AJ	0.18	0/855	0.27	0/1148
61	AK	0.18	0/880	0.26	0/1182
62	AL	0.18	0/1477	0.23	0/1974
63	AM	0.17	0/963	0.31	0/1295
64	AN	0.18	0/886	0.29	0/1199
65	AO	0.18	0/1648	0.32	0/2243
66	AP	0.19	0/798	0.28	0/1070
67	AR	0.14	0/2456	0.28	0/3317
68	AS	0.15	0/1138	0.23	0/1533
69	AT	0.16	0/1402	0.26	0/1883
70	AU	0.16	0/1510	0.28	0/2025
71	AV	0.16	0/3030	0.34	0/4093
72	AW	0.17	0/801	0.26	0/1079
73	AZ	0.16	0/857	0.31	0/1141
74	A0	0.15	0/1834	0.30	0/2484

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	A1	0.15	0/2313	0.28	0/3129
76	A3	0.21	0/636	0.27	0/839
77	Az	0.18	0/804	0.36	0/1248
78	AY	0.14	0/1040	0.26	0/1402
79	AA	0.23	0/22537	0.29	0/35085
80	AI	0.19	0/1039	0.27	0/1400
81	OX	0.18	0/478	0.42	0/639
82	a	0.23	0/891	0.34	0/1208
83	A4	0.16	0/4877	0.33	0/6598
84	AX	0.16	0/2921	0.32	0/3954
85	A2	0.19	0/947	0.28	0/1266
86	AQ	0.19	0/754	0.27	0/1003
87	Ah	0.19	0/1805	0.41	0/2809
88	Ag	0.19	0/3097	0.43	0/4190
89	Ax	0.20	0/1673	0.37	0/2602
90	B	0.20	0/1626	0.28	0/2523
All	All	0.22	0/189841	0.30	0/269674

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2	0
2	1	464	0	511	4	0
3	2	377	0	406	1	0
4	3	832	0	883	3	0
5	4	342	0	361	1	0
6	5	3210	0	3206	9	0
7	6	2948	0	2841	8	0
8	7	2390	0	2397	7	0
9	8	1327	0	1368	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	9	997	0	987	7	0
11	A	33070	0	16794	157	0
12	D	1859	0	1920	8	0
13	E	2406	0	2415	5	0
14	F	2031	0	2065	8	0
15	H	1661	0	1734	7	0
16	I	1446	0	1532	12	0
17	J	1330	0	1407	8	0
18	K	1455	0	1452	3	0
19	L	890	0	941	2	0
20	M	2327	0	2393	6	0
21	N	1786	0	1817	8	0
22	O	1259	0	1294	6	0
23	P	1173	0	1165	4	0
24	Q	1990	0	2031	7	0
25	R	1154	0	1214	1	0
26	S	1293	0	1365	7	0
27	T	1369	0	1410	4	0
28	U	1248	0	1228	1	0
29	W	904	0	934	3	0
30	X	2044	0	2060	5	0
31	Y	1556	0	1597	1	0
32	Z	996	0	1044	2	0
33	g	1113	0	1097	2	0
34	V	1676	0	1687	8	0
35	b	1193	0	1191	4	0
36	d	2124	0	2125	38	0
37	e	1931	0	1916	18	0
38	h	895	0	881	1	0
39	i	828	0	857	1	0
40	j	745	0	746	4	0
41	k	774	0	784	1	0
42	l	688	0	674	5	0
43	m	791	0	796	3	0
44	n	215	0	51	0	0
45	o	798	0	804	2	0
46	q	1495	0	1492	23	0
47	r	1322	0	1348	4	0
48	t	354	0	377	4	0
48	u	257	0	283	6	0
49	c	2299	0	2320	2	0
50	f	1252	0	1269	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	p	1205	0	1223	6	0
52	s	3148	0	3131	13	0
53	AB	1828	0	1815	10	0
54	AC	1083	0	1088	7	0
55	AD	2731	0	2804	22	0
56	AE	972	0	1000	7	0
57	AF	1725	0	1769	9	0
58	AG	2688	0	2687	6	0
59	AH	1152	0	1183	10	0
60	AJ	839	0	887	6	0
61	AK	862	0	885	6	0
62	AL	1453	0	1540	6	0
63	AM	942	0	965	10	0
64	AN	868	0	928	1	0
65	AO	1592	0	1557	14	0
66	AP	781	0	806	4	0
67	AR	2409	0	2428	11	0
68	AS	1111	0	1115	4	0
69	AT	1371	0	1393	5	0
70	AU	1488	0	1499	9	0
71	AV	2969	0	2961	38	0
72	AW	789	0	802	5	0
73	AZ	839	0	858	5	0
74	A0	1787	0	1796	14	0
75	A1	2265	0	2294	11	0
76	A3	625	0	699	5	0
77	Az	719	0	360	3	0
78	AY	1010	0	957	3	0
79	AA	20260	0	10286	373	0
80	AI	1019	0	1059	8	0
81	OX	468	0	464	1	0
82	a	865	0	829	5	0
83	A4	4768	0	4766	47	0
84	AX	2849	0	2844	25	0
85	A2	935	0	971	7	0
86	AQ	744	0	758	3	0
87	Ah	1616	0	824	45	0
88	Ag	3042	0	3112	166	0
89	Ax	1498	0	766	9	0
90	B	1524	0	779	16	0
91	0	1	0	0	0	0
91	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	AO	1	0	0	0	0
92	6	1	0	0	0	0
92	A	28	0	0	0	0
92	AA	18	0	0	0	0
92	D	1	0	0	0	0
92	M	2	0	0	0	0
92	N	1	0	0	0	0
92	W	1	0	0	0	0
92	i	1	0	0	0	0
92	o	1	0	0	0	0
93	A	50	0	95	3	0
93	AA	20	0	38	1	0
94	A	6	0	12	0	0
95	A	138	0	0	0	0
95	A3	1	0	0	0	0
95	AA	59	0	0	0	0
95	AB	1	0	0	0	0
95	AX	1	0	0	0	0
95	Az	1	0	0	0	0
95	D	2	0	0	0	0
95	g	1	0	0	0	0
96	AP	4	0	0	0	0
96	AT	4	0	0	0	0
96	r	4	0	0	0	0
97	AA	44	0	26	1	0
98	AA	28	0	52	1	0
99	AX	31	0	12	0	0
100	AX	28	0	12	3	0
101	B	7	0	8	1	0
All	All	181108	0	153529	1256	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 4.

All (1256) 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)
88:Ag:136:ASN:HA	88:Ag:336:ARG:HH22	1.39	0.87
79:AA:1562:G:H1'	79:AA:1583:MA6:H2	1.59	0.84
88:Ag:260:LEU:HB2	88:Ag:340:MET:HB2	1.65	0.78
88:Ag:61:GLY:HA2	88:Ag:125:THR:H	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:d:93:GLY:HA2	36:d:96:ARG:HB3	1.67	0.77
88:Ag:188:ASP:HB3	88:Ag:191:MET:HB2	1.67	0.77
88:Ag:180:VAL:HB	88:Ag:217:VAL:HA	1.67	0.76
79:AA:941:G:H4'	79:AA:942:A:H5''	1.68	0.76
88:Ag:77:ILE:HD11	88:Ag:239:LEU:HD23	1.68	0.76
88:Ag:188:ASP:HB2	88:Ag:192:VAL:HG13	1.68	0.76
79:AA:1002:C:H2'	79:AA:1003:A:H8	1.51	0.75
88:Ag:63:ILE:HB	88:Ag:164:HIS:HB3	1.68	0.75
37:e:183:THR:HG23	37:e:186:GLY:H	1.51	0.74
87:Ah:51:U:H3	87:Ah:65:G:H1	1.36	0.74
88:Ag:259:LEU:HD23	88:Ag:261:PRO:HD3	1.68	0.73
79:AA:1365:A:H4'	79:AA:1389:G:H4'	1.69	0.73
79:AA:773:U:H2'	79:AA:774:G:H8	1.51	0.72
9:8:187:PRO:HG2	43:m:79:ILE:HD11	1.72	0.72
79:AA:829:C:H1'	79:AA:857:G:H22	1.54	0.72
88:Ag:73:LEU:HD13	88:Ag:150:VAL:HG12	1.71	0.72
8:7:204:LYS:HE2	82:a:92:LEU:HD22	1.70	0.72
83:A4:556:LYS:HE3	83:A4:579:ILE:HD13	1.71	0.72
88:Ag:339:VAL:HG11	88:Ag:415:ILE:HG13	1.73	0.71
88:Ag:73:LEU:HD12	88:Ag:181:ASN:HD21	1.56	0.70
46:q:168:VAL:HG12	46:q:175:PHE:HB2	1.72	0.70
87:Ah:76:C:H1'	88:Ag:266:TYR:HB3	1.74	0.70
83:A4:147:PRO:HD3	83:A4:165:LYS:HE3	1.72	0.70
79:AA:1201:A:H2'	79:AA:1202:G:H8	1.57	0.70
69:AT:88:VAL:HG22	70:AU:109:ASN:HD21	1.55	0.70
79:AA:1528:A:H2'	79:AA:1529:A:H8	1.55	0.69
46:q:164:LEU:HB3	46:q:168:VAL:HG21	1.74	0.69
88:Ag:353:GLU:HB3	88:Ag:438:ASN:HB3	1.74	0.69
88:Ag:178:VAL:HB	88:Ag:215:VAL:HG22	1.75	0.69
79:AA:918:A:H4'	79:AA:920:G:H4'	1.75	0.69
87:Ah:12:G:H1	87:Ah:23:U:H3	1.38	0.69
88:Ag:289:GLU:HG3	88:Ag:300:ARG:HH22	1.57	0.69
46:q:169:ASP:HB3	46:q:172:SER:HB3	1.74	0.69
14:F:103:GLN:HE22	14:F:249:ASN:HD22	1.39	0.68
88:Ag:425:ARG:HA	88:Ag:431:ILE:H	1.58	0.68
55:AD:140:LEU:HD11	55:AD:160:ARG:HE	1.58	0.68
87:Ah:54:G:H4'	88:Ag:368:LYS:HD3	1.75	0.67
88:Ag:170:GLN:HG3	88:Ag:423:THR:HG22	1.75	0.67
21:N:124:VAL:HG12	21:N:158:ARG:HE	1.60	0.67
83:A4:397:MET:HG3	83:A4:431:LEU:HD11	1.77	0.66
60:AJ:72:LYS:HG3	79:AA:1557:A:H5''	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:832:U:H2'	79:AA:833:A:H8	1.60	0.66
88:Ag:261:PRO:HA	88:Ag:339:VAL:HA	1.78	0.66
79:AA:1021:U:H4'	79:AA:1022:A:H5'	1.78	0.65
83:A4:400:LEU:HA	83:A4:403:LYS:HD3	1.78	0.65
79:AA:773:U:H2'	79:AA:774:G:C8	2.31	0.65
79:AA:1440:G:H2'	79:AA:1441:A:C8	2.32	0.65
11:A:2174:G:H4'	17:J:151:LEU:HD23	1.79	0.64
34:V:79:VAL:HG12	34:V:86:VAL:HG12	1.79	0.64
88:Ag:259:LEU:HD22	88:Ag:280:GLU:HB2	1.78	0.64
88:Ag:169:ARG:HD3	88:Ag:207:GLY:HA3	1.78	0.64
88:Ag:53:ARG:HE	88:Ag:57:HIS:H	1.46	0.64
88:Ag:356:VAL:HG22	88:Ag:434:GLY:HA2	1.80	0.64
79:AA:909:G:H2'	79:AA:910:A:H8	1.63	0.64
62:AL:209:LEU:HD13	76:A3:173:LEU:HD12	1.78	0.64
88:Ag:351:LYS:HB3	88:Ag:440:LEU:HB2	1.80	0.64
79:AA:976:A:H5''	86:AQ:1:ACE:H1	1.79	0.63
79:AA:663:A:H2'	79:AA:664:G:C8	2.33	0.63
79:AA:1398:U:H2'	79:AA:1399:A:H8	1.62	0.63
74:A0:171:ARG:HE	74:A0:188:GLU:HG2	1.63	0.63
79:AA:838:U:H2'	79:AA:839:A:H8	1.64	0.63
88:Ag:114:GLU:HA	88:Ag:123:ALA:HA	1.79	0.63
79:AA:847:G:H2'	79:AA:848:U:C6	2.34	0.62
79:AA:975:A:H2	80:AI:183:HIS:HB2	1.64	0.62
88:Ag:389:ILE:HD12	88:Ag:408:LEU:HB3	1.81	0.62
88:Ag:268:VAL:HG13	88:Ag:271:ARG:HB2	1.81	0.62
88:Ag:259:LEU:HB2	88:Ag:281:ARG:HG2	1.81	0.62
52:s:271:LEU:HD23	52:s:273:LEU:HD13	1.81	0.62
79:AA:1201:A:H2'	79:AA:1202:G:C8	2.34	0.62
12:D:205:GLN:HA	12:D:208:ARG:HH21	1.64	0.61
79:AA:1239:C:H2'	79:AA:1240:A:H8	1.66	0.61
36:d:52:THR:HG23	36:d:55:GLU:H	1.65	0.61
15:H:98:LEU:HD11	15:H:105:VAL:HG23	1.81	0.61
88:Ag:80:ILE:HD13	88:Ag:240:LEU:HD13	1.83	0.61
90:B:30:A:H2'	90:B:31:A:H8	1.65	0.61
88:Ag:165:LEU:HD21	88:Ag:203:LEU:HA	1.82	0.61
87:Ah:53:G:H2'	87:Ah:54:G:H8	1.66	0.60
79:AA:1347:G:H2'	79:AA:1348:G:H8	1.65	0.60
75:A1:126:LEU:HD11	83:A4:70:VAL:HG13	1.82	0.60
79:AA:1002:C:H2'	79:AA:1003:A:C8	2.35	0.60
79:AA:1025:A:H2'	79:AA:1026:A:C8	2.36	0.60
78:AY:338:LEU:HD11	78:AY:351:MET:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:867:C:H2'	79:AA:870:C:H42	1.67	0.60
88:Ag:359:LEU:HG	88:Ag:432:GLY:HA2	1.82	0.60
88:Ag:70:LYS:HG2	88:Ag:150:VAL:HG21	1.84	0.60
74:A0:99:ARG:HD3	79:AA:1526:U:H2'	1.84	0.60
7:6:255:LEU:HD12	7:6:256:PRO:HD2	1.84	0.60
30:X:20:ILE:HG22	81:OX:434:LEU:HD23	1.84	0.60
88:Ag:174:GLU:HA	88:Ag:208:TYR:HE1	1.67	0.60
50:f:90:VAL:HG13	50:f:189:HIS:HB3	1.84	0.60
79:AA:695:A:C4	88:Ag:270:GLY:HA3	2.37	0.60
79:AA:881:A:H2'	79:AA:882:A:C4	2.37	0.60
79:AA:1089:U:H2'	79:AA:1090:A:H8	1.66	0.60
88:Ag:313:LEU:HD22	88:Ag:316:ALA:HB2	1.83	0.59
71:AV:229:ALA:HB1	71:AV:286:VAL:HG11	1.83	0.59
46:q:156:LEU:HD13	46:q:183:GLU:HG2	1.84	0.59
55:AD:244:LEU:HD22	55:AD:343:LEU:HD23	1.85	0.59
11:A:3211:C:H4'	11:A:3212:C:H5	1.67	0.59
59:AH:124:VAL:HA	61:AK:108:ARG:HH12	1.67	0.59
79:AA:1175:G:H2'	79:AA:1176:G:H8	1.68	0.59
2:1:54:VAL:HG13	46:q:128:MET:HE2	1.85	0.59
79:AA:990:U:H3	79:AA:997:A:H61	1.49	0.59
83:A4:494:ILE:HD11	83:A4:527:LEU:HA	1.85	0.58
60:AJ:57:GLN:HB3	60:AJ:109:LEU:HD11	1.85	0.58
79:AA:1161:A:H2'	79:AA:1162:A:C8	2.38	0.58
83:A4:332:LEU:HD23	83:A4:368:SER:HB3	1.84	0.58
36:d:208:VAL:HG22	36:d:253:THR:HG23	1.85	0.58
79:AA:871:A:H4'	79:AA:872:G:H5'	1.84	0.58
79:AA:1408:A:H2'	79:AA:1409:A:H8	1.68	0.58
36:d:186:VAL:HG21	36:d:239:PRO:HB3	1.85	0.58
88:Ag:219:SER:HB3	88:Ag:222:CYS:HB3	1.86	0.58
11:A:1862:U:H2'	11:A:1863:A:H8	1.68	0.58
72:AW:154:LEU:HB3	85:A2:29:LEU:HG	1.85	0.58
79:AA:1006:U:H2'	79:AA:1007:G:H8	1.69	0.58
88:Ag:292:LEU:HD11	88:Ag:338:LEU:HD23	1.86	0.58
79:AA:832:U:H2'	79:AA:833:A:C8	2.38	0.58
46:q:164:LEU:HG	46:q:178:LEU:HD23	1.84	0.58
79:AA:799:A:H2'	79:AA:800:C:C6	2.38	0.58
79:AA:852:A:H3'	79:AA:853:C:H6	1.67	0.58
79:AA:1175:G:H2'	79:AA:1176:G:C8	2.39	0.58
41:k:66:VAL:HB	41:k:74:LEU:HB3	1.86	0.58
87:Ah:51:U:H2'	87:Ah:52:C:C6	2.39	0.58
88:Ag:357:TYR:HD1	88:Ag:403:ASP:HB2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:201:ARG:HB3	6:5:232:THR:HG22	1.86	0.57
10:9:86:LEU:HD21	10:9:91:LEU:HD12	1.86	0.57
70:AU:64:ARG:HH12	79:AA:844:A:H4'	1.69	0.57
71:AV:30:LEU:HD23	71:AV:149:ASP:HB2	1.87	0.57
73:AZ:101:ARG:HH21	79:AA:1340:C:H4'	1.68	0.57
88:Ag:392:PRO:HD2	88:Ag:395:LYS:HD3	1.86	0.57
79:AA:1003:A:H2'	79:AA:1004:G:H8	1.70	0.57
79:AA:1239:C:H2'	79:AA:1240:A:C8	2.39	0.57
64:AN:95:VAL:HG23	64:AN:96:THR:HG23	1.85	0.57
79:AA:1407:U:H2'	79:AA:1408:A:C8	2.39	0.57
11:A:2586:U:H2'	11:A:2587:G:H8	1.70	0.57
37:e:195:LEU:HD12	37:e:243:PHE:HZ	1.69	0.57
54:AC:125:ARG:HH11	83:A4:94:TYR:HB2	1.68	0.57
53:AB:239:ASN:HD21	72:AW:119:LYS:HG3	1.70	0.57
70:AU:64:ARG:HA	70:AU:67:VAL:HG12	1.87	0.57
6:5:409:GLU:HG3	6:5:412:ARG:HH21	1.69	0.57
11:A:2081:U:H2'	11:A:2082:G:C8	2.40	0.57
11:A:2740:A:H2'	11:A:2741:A:H8	1.68	0.57
16:I:124:LYS:HB2	16:I:153:LEU:HB2	1.86	0.57
71:AV:66:PRO:HD3	79:AA:1529:A:H1'	1.87	0.57
36:d:115:THR:O	36:d:119:GLN:HG2	2.05	0.57
71:AV:70:LEU:HD22	71:AV:389:LEU:HG	1.87	0.57
79:AA:1033:U:H2'	79:AA:1034:U:C6	2.39	0.57
83:A4:343:ARG:HA	83:A4:378:LEU:HD13	1.86	0.57
83:A4:170:VAL:HG23	83:A4:247:ILE:HD11	1.87	0.56
12:D:172:MET:HE1	56:AE:86:ILE:HG12	1.86	0.56
79:AA:1007:G:H2'	79:AA:1008:A:C8	2.39	0.56
84:AX:244:LEU:HD22	84:AX:296:MET:HG3	1.87	0.56
79:AA:705:C:H3'	79:AA:706:C:C6	2.40	0.56
79:AA:861:U:H2'	79:AA:862:A:H8	1.70	0.56
80:AI:176:THR:HB	86:AQ:11:THR:HG23	1.88	0.56
88:Ag:138:ILE:HD11	88:Ag:423:THR:HG21	1.87	0.56
88:Ag:200:ARG:HD3	88:Ag:211:GLU:HA	1.88	0.56
9:8:99:ARG:HG2	37:e:83:LEU:HB3	1.87	0.56
79:AA:908:C:H2'	79:AA:909:G:C8	2.41	0.56
11:A:2006:C:H2'	11:A:2007:U:C6	2.40	0.56
74:A0:136:TYR:CZ	79:AA:705:C:H2'	2.41	0.56
87:Ah:69:G:H2'	87:Ah:70:A:C8	2.41	0.56
9:8:192:TYR:HE1	50:f:134:VAL:HG22	1.71	0.56
11:A:1857:U:H2'	11:A:1858:G:C8	2.40	0.56
65:AO:150:LEU:O	65:AO:154:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:695:A:H61	88:Ag:271:ARG:HH21	1.54	0.56
87:Ah:6:C:H2'	87:Ah:7:G:C8	2.41	0.56
87:Ah:7:G:H2'	87:Ah:50:C:O4'	2.04	0.56
88:Ag:348:PRO:HB2	88:Ag:413:PRO:HB2	1.88	0.56
17:J:140:VAL:O	17:J:144:ILE:HG12	2.06	0.56
55:AD:160:ARG:NH1	55:AD:168:VAL:HG21	2.21	0.56
71:AV:175:VAL:HG12	71:AV:177:SER:H	1.70	0.56
79:AA:1174:U:H2'	79:AA:1175:G:H8	1.70	0.56
79:AA:1407:U:H2'	79:AA:1408:A:H8	1.71	0.56
79:AA:1578:A:H2'	79:AA:1579:C:C6	2.41	0.56
79:AA:673:U:H2'	79:AA:674:U:C6	2.41	0.56
79:AA:1408:A:H2'	79:AA:1409:A:C8	2.41	0.56
71:AV:76:ILE:HD12	71:AV:112:TRP:HD1	1.71	0.56
79:AA:1042:U:H2'	79:AA:1043:C:C6	2.41	0.56
79:AA:1132:U:H2'	79:AA:1133:C:C6	2.40	0.56
79:AA:1440:G:H2'	79:AA:1441:A:H8	1.68	0.56
79:AA:1523:A:H2'	79:AA:1524:A:C8	2.41	0.56
71:AV:149:ASP:HA	71:AV:152:ILE:HG22	1.88	0.55
73:AZ:11:MET:HE1	75:A1:189:LYS:HG3	1.87	0.55
87:Ah:50:C:H2'	87:Ah:51:U:C6	2.41	0.55
79:AA:1317:A:H3'	79:AA:1318:A:H8	1.71	0.55
83:A4:532:LEU:HD11	83:A4:555:ILE:HG21	1.88	0.55
11:A:3150:U:H2'	11:A:3151:A:H8	1.71	0.55
71:AV:103:TYR:CZ	79:AA:1524:A:H4'	2.41	0.55
79:AA:838:U:H2'	79:AA:839:A:C8	2.41	0.55
79:AA:840:A:H2'	79:AA:841:A:C8	2.41	0.55
79:AA:873:G:H2'	79:AA:874:G:C8	2.41	0.55
88:Ag:276:THR:HA	88:Ag:323:GLY:HA2	1.87	0.55
90:B:23:A:H2'	90:B:24:G:C8	2.42	0.55
11:A:2740:A:H2'	11:A:2741:A:C8	2.41	0.55
79:AA:1400:U:H2'	79:AA:1401:G:C8	2.41	0.55
84:AX:181:PRO:HB2	84:AX:233:VAL:HG22	1.88	0.55
88:Ag:59:ASN:HB2	88:Ag:145:ASP:H	1.71	0.55
36:d:197:VAL:HG13	36:d:212:ILE:HG12	1.89	0.55
79:AA:958:C:H4'	79:AA:959:C:O4'	2.06	0.55
79:AA:1555:A:H2'	79:AA:1556:C:O4'	2.07	0.55
87:Ah:69:G:H2'	87:Ah:70:A:H8	1.71	0.55
88:Ag:256:LYS:HB2	88:Ag:281:ARG:HB2	1.87	0.55
11:A:2099:U:H2'	11:A:2100:C:C6	2.41	0.55
36:d:81:THR:HG22	36:d:83:GLY:H	1.71	0.55
79:AA:1416:A:H2'	79:AA:1417:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:AV:322:THR:HG23	71:AV:325:SER:H	1.72	0.55
79:AA:873:G:H2'	79:AA:874:G:H8	1.72	0.55
79:AA:663:A:H2'	79:AA:664:G:H8	1.71	0.55
79:AA:745:A:H3'	79:AA:746:A:H8	1.71	0.55
87:Ah:67:C:H2'	87:Ah:68:G:C8	2.42	0.55
79:AA:705:C:H3'	79:AA:706:C:H6	1.71	0.54
79:AA:909:G:H2'	79:AA:910:A:C8	2.40	0.54
88:Ag:128:PRO:HG2	88:Ag:136:ASN:HB2	1.89	0.54
9:8:147:LEU:HD21	37:e:208:ALA:HB1	1.88	0.54
53:AB:180:ARG:HH21	55:AD:210:PRO:HB2	1.72	0.54
62:AL:165:LYS:HE3	79:AA:947:U:H5''	1.89	0.54
82:a:91:VAL:HG12	82:a:95:ARG:HE	1.70	0.54
87:Ah:53:G:H2'	87:Ah:54:G:C8	2.41	0.54
11:A:3143:U:H2'	11:A:3144:A:H8	1.71	0.54
11:A:3224:G:H2'	11:A:3225:G:H8	1.73	0.54
87:Ah:3:C:H42	87:Ah:71:A:H61	1.54	0.54
85:A2:95:GLU:HB3	85:A2:100:LEU:HG	1.89	0.54
6:5:55:LEU:HD11	30:X:163:ARG:HE	1.72	0.54
46:q:152:ARG:HH11	46:q:153:ARG:HH12	1.56	0.54
88:Ag:283:ILE:HD12	88:Ag:317:GLU:HG2	1.89	0.54
79:AA:845:A:H2'	79:AA:846:A:H8	1.73	0.54
79:AA:1042:U:H2'	79:AA:1043:C:H6	1.73	0.54
88:Ag:286:LYS:HG2	88:Ag:306:ILE:H	1.71	0.54
79:AA:1469:G:H2'	79:AA:1470:A:H8	1.73	0.54
7:6:139:TRP:CD1	7:6:143:CYS:HG	2.26	0.54
11:A:2545:U:H5''	11:A:2546:G:H5'	1.88	0.54
88:Ag:293:LEU:HG	88:Ag:298:ASN:HA	1.90	0.54
11:A:1895:C:H2'	11:A:1896:U:H6	1.72	0.54
55:AD:420:SER:HA	79:AA:929:A:H4'	1.90	0.54
83:A4:308:LYS:HE3	83:A4:310:GLU:HB2	1.89	0.54
59:AH:70:ASP:HA	83:A4:62:LYS:HE3	1.90	0.53
88:Ag:179:TYR:CG	88:Ag:239:LEU:HD22	2.43	0.53
79:AA:1308:U:H2'	79:AA:1309:A:H8	1.73	0.53
83:A4:562:GLN:HG3	83:A4:564:ILE:HG22	1.90	0.53
11:A:2365:U:H2'	11:A:2366:G:H8	1.74	0.53
79:AA:1347:G:H2'	79:AA:1348:G:C8	2.44	0.53
87:Ah:37:C:H3'	87:Ah:38:A:H8	1.74	0.53
21:N:218:ILE:HG23	21:N:223:MET:HB2	1.90	0.53
79:AA:1174:U:H2'	79:AA:1175:G:C8	2.43	0.53
47:r:102:ARG:HB2	47:r:112:HIS:CD2	2.44	0.53
79:AA:1006:U:H2'	79:AA:1007:G:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:1006:U:H5''	86:AQ:6:LYS:HZ3	1.73	0.53
79:AA:1399:A:H2'	79:AA:1400:U:C6	2.43	0.53
87:Ah:45:A:H3'	87:Ah:46:G:H8	1.72	0.53
88:Ag:111:ALA:HB3	88:Ag:126:ASP:HB3	1.89	0.53
16:I:116:LEU:HG	16:I:121:ILE:HB	1.89	0.53
65:AO:94:CYS:HB2	65:AO:108:CYS:SG	2.47	0.53
79:AA:1173:C:H2'	79:AA:1174:U:C6	2.43	0.53
2:1:38:ARG:HH12	2:1:41:LEU:HD11	1.74	0.53
65:AO:183:ALA:HA	67:AR:183:LYS:HE2	1.91	0.53
65:AO:217:ARG:O	65:AO:221:GLN:HG3	2.07	0.53
79:AA:1011:C:C4	79:AA:1063:A:H4'	2.44	0.53
88:Ag:216:ILE:HG21	88:Ag:238:LYS:HB2	1.90	0.53
71:AV:218:SER:HB2	71:AV:274:LYS:H	1.73	0.53
71:AV:267:ALA:HB2	71:AV:340:LYS:HZ3	1.73	0.53
75:A1:67:PRO:HG3	75:A1:118:ALA:HB2	1.90	0.53
79:AA:1577:U:H2'	79:AA:1578:A:H8	1.74	0.53
74:A0:68:LEU:HD13	74:A0:71:LEU:HD12	1.91	0.53
79:AA:944:U:H2'	79:AA:945:G:C8	2.44	0.53
87:Ah:68:G:H2'	87:Ah:69:G:C8	2.44	0.53
26:S:108:VAL:HB	26:S:195:ILE:HG13	1.90	0.52
88:Ag:389:ILE:HD11	88:Ag:406:PHE:CE1	2.45	0.52
16:I:47:LEU:HD22	21:N:226:ILE:HG12	1.92	0.52
79:AA:871:A:H1'	79:AA:872:G:C8	2.45	0.52
79:AA:1504:U:H2'	79:AA:1505:A:H8	1.74	0.52
88:Ag:81:LEU:HD13	88:Ag:88:LYS:H	1.74	0.52
71:AV:109:ILE:HD13	71:AV:138:PHE:H	1.75	0.52
79:AA:1470:A:H2'	79:AA:1471:A:H8	1.72	0.52
88:Ag:279:LEU:HG	88:Ag:318:ALA:HA	1.90	0.52
10:9:114:LEU:HD22	30:X:227:PHE:HE1	1.72	0.52
4:3:138:PRO:HG2	11:A:2854:U:H4'	1.92	0.52
79:AA:922:C:H2'	79:AA:923:A:C8	2.45	0.52
79:AA:1523:A:H1'	79:AA:1528:A:C2	2.45	0.52
88:Ag:63:ILE:HD11	88:Ag:149:LEU:HD12	1.92	0.52
88:Ag:383:TRP:NE1	88:Ag:385:MET:HB2	2.24	0.52
11:A:1952:U:H2'	11:A:1953:A:H8	1.75	0.52
36:d:219:ARG:HD3	36:d:239:PRO:HB2	1.91	0.52
79:AA:1504:U:H2'	79:AA:1505:A:C8	2.45	0.52
11:A:2055:U:H2'	11:A:2056:G:H8	1.73	0.52
79:AA:914:A:H2'	79:AA:915:C:C6	2.45	0.52
79:AA:1065:C:H2'	79:AA:1066:C:O4'	2.10	0.52
88:Ag:352:VAL:HB	88:Ag:408:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:e:98:LEU:HG	37:e:101:LYS:HE3	1.92	0.52
79:AA:660:C:H1'	79:AA:1285:G:H21	1.74	0.52
79:AA:738:A:H3'	79:AA:739:C:H6	1.74	0.52
79:AA:944:U:H2'	79:AA:945:G:H8	1.74	0.52
88:Ag:110:ALA:H	88:Ag:136:ASN:HB3	1.75	0.52
37:e:200:MET:HA	37:e:241:GLY:HA3	1.91	0.52
79:AA:715:G:H2'	79:AA:716:U:C6	2.45	0.52
88:Ag:342:LYS:HB3	88:Ag:345:SER:HB2	1.92	0.52
9:8:51:ARG:HH12	79:AA:1560:U:H5''	1.75	0.52
16:I:61:HIS:CD2	16:I:62:PRO:HD2	2.45	0.52
67:AR:172:ILE:HD12	67:AR:189:ARG:HG2	1.90	0.52
3:2:78:VAL:HG22	3:2:81:ARG:HH22	1.74	0.51
79:AA:1007:G:H2'	79:AA:1008:A:H8	1.75	0.51
79:AA:1033:U:H2'	79:AA:1034:U:H6	1.74	0.51
79:AA:1578:A:H2'	79:AA:1579:C:H6	1.74	0.51
80:AI:100:VAL:HG12	80:AI:106:PRO:HA	1.92	0.51
23:P:94:VAL:HG23	23:P:132:LEU:HD21	1.92	0.51
37:e:55:ARG:HG3	37:e:149:LEU:HD22	1.92	0.51
88:Ag:342:LYS:HD3	88:Ag:343:PRO:HD2	1.91	0.51
6:5:336:LEU:HD21	6:5:362:THR:HG23	1.92	0.51
11:A:2409:A:H2'	11:A:2410:U:C6	2.45	0.51
20:M:226:PRO:HG3	51:p:45:LEU:HD23	1.92	0.51
37:e:218:PRO:HG2	101:B:101:VAL:HG22	1.92	0.51
79:AA:1034:U:H2'	79:AA:1035:U:C6	2.46	0.51
79:AA:1177:C:H2'	79:AA:1178:G:C8	2.45	0.51
9:8:117:LEU:HD11	37:e:69:GLU:HB3	1.92	0.51
52:s:152:GLN:HA	52:s:156:TYR:HB2	1.92	0.51
67:AR:157:VAL:HG22	67:AR:174:VAL:HG22	1.92	0.51
79:AA:672:A:H2'	79:AA:673:U:C6	2.45	0.51
11:A:1761:A:H2'	11:A:1762:A:C8	2.45	0.51
79:AA:845:A:H2'	79:AA:846:A:C8	2.45	0.51
79:AA:916:C:H2'	79:AA:917:C:C6	2.45	0.51
79:AA:1071:U:H2'	79:AA:1072:G:C8	2.45	0.51
11:A:2070:C:H3'	11:A:2071:U:H4'	1.92	0.51
42:l:92:TYR:HB3	42:l:96:LEU:HD13	1.93	0.51
79:AA:686:A:H2'	79:AA:687:G:C8	2.45	0.51
36:d:38:LYS:HE2	36:d:40:ARG:HH12	1.76	0.51
75:A1:53:LEU:HD12	83:A4:518:GLU:HG2	1.93	0.51
79:AA:747:A:H2'	79:AA:748:G:C8	2.45	0.51
79:AA:1438:G:H1	79:AA:1452:U:H3	1.57	0.51
83:A4:236:VAL:HG22	83:A4:270:ARG:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ag:360:SER:HA	88:Ag:400:PRO:HB3	1.92	0.51
11:A:2006:C:H2'	11:A:2007:U:H6	1.75	0.51
14:F:218:LEU:HD13	14:F:230:ILE:HD11	1.93	0.51
79:AA:686:A:H2'	79:AA:687:G:H8	1.76	0.51
46:q:147:GLN:O	46:q:150:LYS:HG3	2.10	0.51
79:AA:1161:A:H2'	79:AA:1162:A:H8	1.73	0.51
79:AA:1554:G:H2'	79:AA:1555:A:C8	2.45	0.51
11:A:2668:A:H2'	11:A:2669:A:C8	2.46	0.50
20:M:244:LEU:HD12	20:M:245:PRO:HD2	1.92	0.50
36:d:204:ASN:O	36:d:205:GLN:HG2	2.11	0.50
71:AV:226:TYR:CZ	71:AV:282:VAL:HG11	2.46	0.50
84:AX:159:HIS:HA	84:AX:162:VAL:HG12	1.94	0.50
87:Ah:49:C:H3'	87:Ah:60:A:H1'	1.92	0.50
11:A:1862:U:H2'	11:A:1863:A:C8	2.46	0.50
18:K:20:LEU:HD22	18:K:141:LEU:HD13	1.93	0.50
52:s:113:VAL:HG11	52:s:257:VAL:HG11	1.93	0.50
87:Ah:24:C:H2'	87:Ah:25:A:C8	2.45	0.50
88:Ag:108:ILE:HG13	88:Ag:133:TYR:CZ	2.46	0.50
90:B:29:C:H2'	90:B:30:A:H8	1.76	0.50
79:AA:1003:A:H2'	79:AA:1004:G:C8	2.45	0.50
79:AA:1086:C:H2'	79:AA:1087:A:H8	1.77	0.50
79:AA:1412:G:H2'	79:AA:1413:U:O4'	2.12	0.50
87:Ah:54:G:H2'	87:Ah:55:U:C6	2.46	0.50
88:Ag:63:ILE:HG12	88:Ag:149:LEU:HA	1.92	0.50
88:Ag:273:THR:HG21	88:Ag:331:ARG:N	2.27	0.50
88:Ag:351:LYS:HD3	88:Ag:409:ILE:HG22	1.93	0.50
7:6:187:VAL:HG13	7:6:319:PHE:HB3	1.92	0.50
11:A:1806:U:H4'	11:A:1807:U:H5'	1.94	0.50
79:AA:798:C:H2'	79:AA:799:A:C8	2.47	0.50
79:AA:1177:C:H2'	79:AA:1178:G:H8	1.77	0.50
79:AA:1471:A:H2'	79:AA:1472:G:C8	2.46	0.50
88:Ag:308:MET:HB2	88:Ag:313:LEU:HD11	1.93	0.50
8:7:286:LEU:HD11	8:7:296:ARG:HB2	1.94	0.50
9:8:160:GLU:HA	9:8:163:LYS:HE3	1.93	0.50
11:A:1952:U:H2'	11:A:1953:A:C8	2.47	0.50
11:A:2950:U:H2'	11:A:2951:A:H8	1.75	0.50
93:A:3472:SPD:H21	22:O:16:ARG:HH12	1.76	0.50
75:A1:116:PRO:HA	75:A1:119:ILE:HD12	1.94	0.50
79:AA:776:A:H4'	79:AA:777:G:H5'	1.94	0.50
83:A4:335:PHE:CG	83:A4:360:MET:HE2	2.46	0.50
88:Ag:147:CYS:H	88:Ag:176:VAL:HG12	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ag:308:MET:HE1	88:Ag:322:LEU:HA	1.94	0.50
89:Ax:40:A:H2'	89:Ax:41:A:C8	2.46	0.50
11:A:1935:A:C2	11:A:1936:A:H1'	2.47	0.50
79:AA:1066:C:H2'	79:AA:1067:A:C8	2.47	0.50
79:AA:1078:A:H2'	79:AA:1079:G:C8	2.47	0.50
79:AA:1542:U:H2'	79:AA:1543:U:C6	2.47	0.50
88:Ag:204:THR:HB	88:Ag:210:GLY:HA3	1.93	0.50
89:Ax:47:U:H2'	89:Ax:48:G:C8	2.47	0.50
1:O:138:ARG:HB3	11:A:2321:A:C8	2.47	0.50
46:q:152:ARG:HG3	46:q:155:ARG:NH2	2.27	0.50
79:AA:798:C:H2'	79:AA:799:A:H8	1.76	0.50
79:AA:1129:U:H2'	79:AA:1130:G:H8	1.76	0.50
79:AA:1265:C:H2'	79:AA:1266:A:H8	1.77	0.50
79:AA:1372:C:H2'	79:AA:1373:U:H6	1.77	0.50
88:Ag:171:ILE:HD11	88:Ag:379:PHE:HE2	1.76	0.50
13:E:80:LEU:HD12	13:E:323:GLY:HA3	1.94	0.50
36:d:208:VAL:HG23	36:d:252:LEU:HB2	1.94	0.50
71:AV:163:VAL:O	71:AV:167:VAL:HG23	2.12	0.50
74:A0:71:LEU:HD11	74:A0:141:LEU:HD11	1.94	0.50
88:Ag:179:TYR:HB2	88:Ag:239:LEU:HD13	1.94	0.50
90:B:43:G:H2'	90:B:44:A:C8	2.45	0.50
15:H:247:ARG:HG2	15:H:251:TRP:HE1	1.77	0.50
46:q:167:GLN:HB2	50:f:199:LYS:NZ	2.27	0.50
53:AB:223:VAL:HG11	53:AB:229:PRO:HB3	1.94	0.50
79:AA:840:A:H2'	79:AA:841:A:H8	1.75	0.50
79:AA:1071:U:H2'	79:AA:1072:G:H8	1.77	0.50
79:AA:1148:A:H2'	79:AA:1149:G:C8	2.47	0.50
88:Ag:88:LYS:HG3	88:Ag:90:LYS:HD2	1.94	0.50
88:Ag:138:ILE:HD13	88:Ag:167:LEU:HD12	1.93	0.50
11:A:3089:A:H3'	11:A:3090:G:C5'	2.42	0.49
18:K:78:SER:HB2	18:K:89:GLN:HG2	1.93	0.49
46:q:138:GLN:O	46:q:141:GLU:HG3	2.12	0.49
79:AA:839:A:H2'	79:AA:840:A:H8	1.77	0.49
83:A4:397:MET:HA	83:A4:400:LEU:HG	1.94	0.49
6:5:289:HIS:O	6:5:343:GLN:HG2	2.12	0.49
11:A:3128:A:H2'	11:A:3129:A:C8	2.47	0.49
93:A:3301:SPD:H32	12:D:275:TRP:CE2	2.47	0.49
74:A0:11:ILE:HB	79:AA:806:C:C2	2.48	0.49
79:AA:685:A:H2'	79:AA:686:A:C8	2.47	0.49
79:AA:1086:C:H2'	79:AA:1087:A:C8	2.47	0.49
79:AA:1146:C:H2'	79:AA:1147:G:H8	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:1577:U:H2'	79:AA:1578:A:C8	2.48	0.49
83:A4:429:LEU:HA	83:A4:464:LEU:HD21	1.94	0.49
88:Ag:395:LYS:HD2	88:Ag:404:LEU:HD12	1.94	0.49
11:A:2285:U:H2'	11:A:2286:A:H8	1.77	0.49
21:N:36:VAL:HG23	42:l:128:ARG:HD2	1.95	0.49
46:q:191:LYS:HA	46:q:194:LYS:HG2	1.94	0.49
52:s:137:LEU:HD21	52:s:422:VAL:HG11	1.94	0.49
60:AJ:78:ARG:HG3	60:AJ:118:LEU:HD21	1.94	0.49
69:AT:154:PRO:HG3	79:AA:683:G:H1'	1.94	0.49
75:A1:86:ARG:HB3	75:A1:96:PRO:HB2	1.94	0.49
79:AA:1181:G:H2'	79:AA:1182:C:C6	2.47	0.49
79:AA:1349:U:H2'	79:AA:1350:G:C8	2.47	0.49
82:a:103:LEU:HD12	82:a:107:PRO:HB2	1.93	0.49
88:Ag:253:ASP:OD1	88:Ag:281:ARG:HA	2.12	0.49
18:K:60:MET:HE2	18:K:133:ILE:HD11	1.94	0.49
46:q:179:LEU:O	46:q:183:GLU:HG3	2.12	0.49
56:AE:96:HIS:HB3	56:AE:99:THR:HG23	1.94	0.49
11:A:1895:C:H2'	11:A:1896:U:C6	2.48	0.49
11:A:2727:C:H2'	11:A:2728:C:C6	2.48	0.49
11:A:3054:G:H2'	11:A:3055:U:C6	2.48	0.49
88:Ag:330:LYS:HG3	88:Ag:331:ARG:H	1.78	0.49
17:J:70:ILE:HG12	17:J:80:ILE:HG22	1.95	0.49
63:AM:67:ALA:HB2	67:AR:196:TYR:CZ	2.48	0.49
30:X:202:GLU:HB3	30:X:214:LYS:NZ	2.27	0.49
54:AC:125:ARG:NH1	83:A4:94:TYR:HB2	2.28	0.49
83:A4:309:PHE:HB2	83:A4:313:TRP:HZ3	1.77	0.49
84:AX:85:PRO:HA	84:AX:88:VAL:HG12	1.94	0.49
87:Ah:39:C:H2'	87:Ah:40:G:O4'	2.13	0.49
88:Ag:72:THR:HA	88:Ag:224:LEU:HD22	1.94	0.49
14:F:138:HIS:CD2	14:F:146:TRP:HE1	2.30	0.49
57:AF:88:ASP:HB3	57:AF:91:ILE:HB	1.94	0.49
63:AM:96:PHE:HD1	74:A0:169:LEU:HD22	1.78	0.49
79:AA:870:C:H5''	79:AA:871:A:OP1	2.12	0.49
79:AA:986:G:H2'	79:AA:987:A:C8	2.48	0.49
36:d:197:VAL:HG22	36:d:212:ILE:HG23	1.93	0.49
46:q:161:GLN:HG3	46:q:175:PHE:HE1	1.78	0.49
88:Ag:101:GLU:HB2	88:Ag:108:ILE:HG22	1.93	0.49
88:Ag:138:ILE:HA	88:Ag:141:THR:HG22	1.95	0.49
11:A:2803:A:H2'	11:A:2804:A:O4'	2.13	0.49
11:A:3078:C:H2'	11:A:3079:G:H8	1.76	0.49
75:A1:134:PRO:HB2	75:A1:137:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:676:G:H2'	79:AA:677:C:C6	2.46	0.49
79:AA:875:U:H2'	79:AA:876:U:C6	2.48	0.49
79:AA:1495:C:H2'	79:AA:1496:U:C6	2.48	0.49
83:A4:196:CYS:HB3	83:A4:265:GLY:HA3	1.95	0.49
11:A:1829:A:H2'	11:A:1830:G:H8	1.77	0.48
11:A:3144:A:H2'	11:A:3145:A:H8	1.78	0.48
53:AB:84:LEU:HD23	53:AB:248:LEU:HD21	1.95	0.48
87:Ah:21:U:H4'	87:Ah:22:A:C8	2.48	0.48
90:B:68:C:H2'	90:B:69:U:C6	2.48	0.48
37:e:219:GLN:HA	37:e:222:ARG:HB2	1.95	0.48
79:AA:1194:C:H2'	79:AA:1195:U:C6	2.48	0.48
8:7:112:PRO:HB2	8:7:267:PRO:HG2	1.96	0.48
11:A:3199:U:H5''	11:A:3200:U:H4'	1.95	0.48
60:AJ:42:PRO:HD3	79:AA:931:C:C2	2.48	0.48
79:AA:839:A:H2'	79:AA:840:A:C8	2.47	0.48
88:Ag:356:VAL:HB	88:Ag:406:PHE:HZ	1.78	0.48
88:Ag:425:ARG:HG2	88:Ag:430:THR:HA	1.96	0.48
36:d:217:HIS:HB2	36:d:243:LEU:HD13	1.95	0.48
79:AA:1360:G:H2'	79:AA:1361:G:C8	2.47	0.48
90:B:21:A:H61	90:B:46:A:H2'	1.78	0.48
9:8:125:LYS:HD3	90:B:29:C:H5''	1.95	0.48
11:A:2086:A:H2'	11:A:2087:U:C6	2.48	0.48
16:I:163:GLU:HG3	16:I:166:ARG:HH22	1.79	0.48
79:AA:1014:A:H4'	80:AI:184:ASN:HD22	1.78	0.48
79:AA:1044:U:H2'	79:AA:1045:G:O4'	2.13	0.48
88:Ag:80:ILE:HD12	88:Ag:83:GLU:HB2	1.95	0.48
88:Ag:243:VAL:HG23	88:Ag:247:ILE:HD12	1.94	0.48
66:AP:49:ASP:HA	72:AW:85:ARG:HH11	1.79	0.48
79:AA:1552:G:H2'	79:AA:1553:A:C8	2.48	0.48
87:Ah:55:U:H2'	87:Ah:56:U:O4'	2.14	0.48
88:Ag:201:GLU:HG2	88:Ag:202:LEU:HD22	1.95	0.48
11:A:3078:C:H2'	11:A:3079:G:C8	2.49	0.48
61:AK:52:LEU:HD22	73:AZ:41:PRO:HG3	1.95	0.48
79:AA:1398:U:H2'	79:AA:1399:A:C8	2.46	0.48
79:AA:1528:A:H2'	79:AA:1529:A:C8	2.42	0.48
79:AA:1587:U:H2'	79:AA:1588:G:H8	1.78	0.48
80:AI:99:VAL:HG11	80:AI:139:ALA:HB2	1.94	0.48
83:A4:630:VAL:HG12	83:A4:645:LEU:HD21	1.96	0.48
87:Ah:51:U:H2'	87:Ah:52:C:H6	1.78	0.48
11:A:1974:A:H5'	12:D:261:GLY:HA2	1.96	0.48
11:A:2382:A:H2'	11:A:2383:U:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:3165:C:H2'	11:A:3166:U:C6	2.48	0.48
36:d:84:ILE:HA	36:d:211:GLN:HE22	1.77	0.48
48:u:75:THR:O	48:u:79:ILE:HG13	2.13	0.48
67:AR:207:PRO:HB2	67:AR:209:ILE:HG22	1.96	0.48
74:A0:167:PRO:HG2	74:A0:170:LEU:HB2	1.96	0.48
79:AA:1382:A:H5''	84:AX:166:ARG:HH21	1.79	0.48
79:AA:1552:G:H2'	79:AA:1553:A:H8	1.78	0.48
27:T:206:LEU:HA	35:b:119:PHE:CE1	2.49	0.48
37:e:183:THR:HG23	37:e:186:GLY:N	2.25	0.48
66:AP:78:GLN:HE21	70:AU:190:ALA:HB2	1.79	0.48
71:AV:148:MET:HE2	71:AV:185:VAL:HG21	1.94	0.48
79:AA:983:C:H2'	79:AA:984:C:C6	2.48	0.48
79:AA:1181:G:H2'	79:AA:1182:C:H6	1.78	0.48
88:Ag:369:PRO:HG2	88:Ag:397:LEU:HD12	1.94	0.48
11:A:2151:A:H2'	11:A:2152:A:C8	2.49	0.48
52:s:63:ILE:HA	52:s:66:TRP:CD1	2.48	0.48
59:AH:76:LEU:HB2	59:AH:145:LEU:HD12	1.95	0.48
11:A:1911:C:H2'	11:A:1912:A:H8	1.78	0.47
51:p:172:ASP:HB3	51:p:175:LEU:HG	1.96	0.47
59:AH:164:LEU:HD12	59:AH:165:PRO:HD2	1.96	0.47
71:AV:103:TYR:HA	79:AA:1525:C:H5	1.79	0.47
79:AA:699:A:O3'	79:AA:850:U:H4'	2.13	0.47
79:AA:914:A:H2'	79:AA:915:C:H6	1.78	0.47
11:A:2053:U:HO2'	11:A:2054:U:H6	1.59	0.47
11:A:2286:A:H2'	11:A:2287:U:C6	2.49	0.47
34:V:16:PRO:HD2	34:V:19:TYR:HB2	1.96	0.47
51:p:133:LEU:HD21	51:p:157:MET:HE1	1.95	0.47
55:AD:371:VAL:HG22	55:AD:383:VAL:HG22	1.96	0.47
87:Ah:54:G:H2'	87:Ah:55:U:H6	1.79	0.47
88:Ag:367:HIS:NE2	88:Ag:368:LYS:HE3	2.30	0.47
63:AM:115:ALA:HA	63:AM:118:VAL:HG12	1.96	0.47
79:AA:861:U:H2'	79:AA:862:A:C8	2.49	0.47
79:AA:1043:C:H2'	79:AA:1044:U:C6	2.49	0.47
79:AA:1156:C:H2'	79:AA:1157:U:C6	2.50	0.47
79:AA:1362:G:H2'	79:AA:1363:C:C6	2.49	0.47
79:AA:1503:G:H2'	79:AA:1504:U:C6	2.49	0.47
88:Ag:128:PRO:HB2	88:Ag:133:TYR:HB3	1.95	0.47
11:A:2718:C:H2'	11:A:2991:U:H4'	1.96	0.47
79:AA:872:G:H2'	79:AA:873:G:C8	2.49	0.47
79:AA:981:C:H2'	79:AA:982:A:H8	1.78	0.47
79:AA:1360:G:H2'	79:AA:1361:G:H8	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:3143:U:H2'	11:A:3144:A:C8	2.48	0.47
79:AA:1123:C:H2'	79:AA:1124:A:O4'	2.15	0.47
79:AA:1148:A:H2'	79:AA:1149:G:H8	1.80	0.47
79:AA:1331:A:H5''	93:AA:1703:SPD:H81	1.97	0.47
87:Ah:5:C:H2'	87:Ah:6:C:C6	2.49	0.47
12:D:109:PHE:HB3	12:D:204:ALA:HB3	1.96	0.47
79:AA:818:C:H2'	79:AA:819:A:H8	1.79	0.47
79:AA:1470:A:H2'	79:AA:1471:A:C8	2.49	0.47
11:A:2134:A:H62	11:A:2135:A:H62	1.62	0.47
11:A:2275:U:H2'	11:A:2276:C:C6	2.49	0.47
11:A:2277:U:H2'	11:A:2278:A:H8	1.79	0.47
11:A:2727:C:H2'	11:A:2728:C:H6	1.79	0.47
11:A:2776:G:H2'	11:A:2777:G:H8	1.80	0.47
48:t:53:LEU:HB2	48:t:56:ALA:HB2	1.97	0.47
53:AB:192:LEU:HD11	53:AB:220:VAL:HG23	1.96	0.47
59:AH:122:GLN:HG3	79:AA:1265:C:H4'	1.96	0.47
60:AJ:62:VAL:HA	60:AJ:83:VAL:HG12	1.96	0.47
75:A1:177:LEU:HD11	75:A1:205:LEU:HB2	1.96	0.47
79:AA:872:G:H2'	79:AA:873:G:H8	1.80	0.47
83:A4:562:GLN:CG	83:A4:564:ILE:HG22	2.44	0.47
87:Ah:37:C:C2	87:Ah:38:A:C8	3.03	0.47
88:Ag:337:GLY:HA3	88:Ag:383:TRP:HB2	1.97	0.47
11:A:2060:A:C8	11:A:2079:C:C4	3.03	0.47
16:I:96:ILE:HA	16:I:155:VAL:HG12	1.97	0.47
74:A0:64:LEU:HD12	74:A0:139:TRP:CD2	2.50	0.47
79:AA:1427:A:H2'	79:AA:1428:G:C8	2.50	0.47
84:AX:56:PRO:HA	84:AX:59:HIS:CE1	2.50	0.47
87:Ah:8:U:H1'	87:Ah:49:C:H1'	1.97	0.47
88:Ag:388:ARG:HB2	88:Ag:409:ILE:HG13	1.97	0.47
34:V:102:MET:HE3	36:d:48:PRO:HG2	1.97	0.47
37:e:97:ARG:HA	37:e:100:LYS:HG2	1.97	0.47
71:AV:231:LEU:HD12	71:AV:243:VAL:HG13	1.97	0.47
79:AA:942:A:C2	98:AA:1780:SPM:H62	2.50	0.47
83:A4:571:TRP:HE3	83:A4:576:LEU:HD21	1.80	0.47
11:A:2671:C:H2'	11:A:2672:A:H8	1.79	0.47
11:A:2943:G:H2'	11:A:2944:C:C6	2.50	0.47
27:T:206:LEU:HA	35:b:119:PHE:HE1	1.79	0.47
37:e:123:MET:HG2	37:e:126:GLN:HE21	1.80	0.47
79:AA:661:C:H2'	79:AA:662:U:C6	2.50	0.47
79:AA:673:U:H2'	79:AA:674:U:H6	1.78	0.47
79:AA:1114:U:H2'	79:AA:1115:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:1359:U:H2'	79:AA:1360:G:H8	1.79	0.47
83:A4:90:GLN:HG2	83:A4:95:LEU:HD12	1.96	0.47
88:Ag:90:LYS:HB3	88:Ag:94:GLU:HB2	1.95	0.47
88:Ag:254:LEU:HB2	88:Ag:283:ILE:HB	1.97	0.47
11:A:1939:G:O2'	11:A:1973:G:H4'	2.15	0.46
71:AV:263:MET:HE1	71:AV:334:PHE:HD1	1.80	0.46
71:AV:274:LYS:HE3	71:AV:348:GLU:HA	1.97	0.46
79:AA:847:G:H2'	79:AA:848:U:H6	1.79	0.46
79:AA:1013:A:H2'	79:AA:1014:A:C8	2.50	0.46
79:AA:1131:C:H2'	79:AA:1132:U:C6	2.50	0.46
84:AX:242:ILE:HD11	100:AX:503:GDP:C5	2.51	0.46
84:AX:329:LEU:HB3	84:AX:333:GLY:HA3	1.96	0.46
11:A:1839:C:H2'	11:A:1840:C:C6	2.50	0.46
12:D:207:ILE:HG12	12:D:229:PRO:HD3	1.96	0.46
15:H:248:TYR:CD1	15:H:252:LEU:HD23	2.51	0.46
72:AW:103:ARG:HE	72:AW:139:ARG:NH2	2.13	0.46
79:AA:822:G:H2'	79:AA:823:A:H8	1.79	0.46
79:AA:915:C:H2'	79:AA:916:C:C6	2.50	0.46
79:AA:1452:U:H2'	79:AA:1453:A:H8	1.81	0.46
79:AA:1526:U:C5	79:AA:1527:A:H1'	2.50	0.46
84:AX:366:LEU:HD22	84:AX:398:LEU:HD22	1.97	0.46
88:Ag:361:LYS:HE3	88:Ag:367:HIS:HA	1.97	0.46
7:6:217:LEU:HB3	7:6:236:LEU:HD13	1.97	0.46
79:AA:818:C:H2'	79:AA:819:A:C8	2.50	0.46
79:AA:1507:A:H2'	79:AA:1508:C:C6	2.50	0.46
79:AA:1553:A:H2'	79:AA:1554:G:C8	2.51	0.46
87:Ah:2:U:H2'	87:Ah:3:C:C6	2.51	0.46
11:A:2065:A:C4	11:A:2066:C:C5	3.03	0.46
71:AV:189:CYS:O	71:AV:193:LYS:HD3	2.16	0.46
79:AA:659:U:H2'	79:AA:660:C:H6	1.80	0.46
83:A4:349:ALA:HB3	83:A4:378:LEU:HD11	1.97	0.46
89:Ax:3:U:H2'	89:Ax:4:A:C8	2.50	0.46
23:P:86:THR:HG21	90:B:24:G:H5''	1.97	0.46
51:p:123:HIS:CG	51:p:157:MET:HE3	2.50	0.46
63:AM:110:LEU:O	63:AM:114:ARG:HG3	2.16	0.46
79:AA:1515:G:H2'	79:AA:1516:G:C8	2.51	0.46
83:A4:302:VAL:HG21	83:A4:341:CYS:HB3	1.97	0.46
83:A4:535:MET:HE1	83:A4:551:CYS:HB3	1.97	0.46
84:AX:153:LEU:HD21	84:AX:247:LEU:HD13	1.98	0.46
89:Ax:5:A:H2	89:Ax:63:G:H22	1.64	0.46
11:A:3139:G:H2'	11:A:3140:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:AD:91:THR:HB	79:AA:1334:G:H5'	1.98	0.46
61:AK:57:LEU:HD23	61:AK:71:ALA:HB2	1.98	0.46
63:AM:29:ARG:HE	69:AT:147:VAL:HB	1.81	0.46
78:AY:351:MET:HE3	78:AY:380:PHE:HE2	1.80	0.46
11:A:1994:A:H61	11:A:2736:C:H4'	1.80	0.46
11:A:2804:A:H2'	11:A:2805:A:H8	1.81	0.46
13:E:50:ASP:HA	13:E:53:LEU:HG	1.97	0.46
36:d:217:HIS:HD2	36:d:243:LEU:HB2	1.79	0.46
55:AD:140:LEU:HD13	55:AD:160:ARG:HG3	1.98	0.46
55:AD:297:ARG:HH21	79:AA:1120:C:H5'	1.81	0.46
70:AU:152:ARG:HG2	70:AU:155:ARG:HH22	1.80	0.46
79:AA:727:U:H2'	79:AA:728:C:O4'	2.15	0.46
79:AA:969:A:H2'	79:AA:970:A:H8	1.80	0.46
83:A4:446:LYS:HE3	83:A4:446:LYS:HB3	1.79	0.46
84:AX:88:VAL:HA	84:AX:91:VAL:HG22	1.97	0.46
85:A2:33:VAL:HG21	85:A2:104:LEU:HD23	1.97	0.46
87:Ah:50:C:H2'	87:Ah:51:U:H6	1.81	0.46
11:A:3112:A:N7	11:A:3200:U:O2	2.49	0.46
13:E:311:GLY:HA2	13:E:314:LEU:HD12	1.97	0.46
49:c:59:ARG:HB2	49:c:62:GLU:HG2	1.97	0.46
53:AB:165:TYR:CD1	58:AG:149:TYR:HA	2.50	0.46
63:AM:105:THR:OG1	70:AU:56:LEU:HD13	2.16	0.46
79:AA:747:A:H2'	79:AA:748:G:H8	1.81	0.46
79:AA:1089:U:H2'	79:AA:1090:A:C8	2.48	0.46
79:AA:1209:C:H2'	79:AA:1210:U:C6	2.51	0.46
79:AA:1240:A:H2'	79:AA:1241:C:C6	2.51	0.46
88:Ag:286:LYS:HG2	88:Ag:305:GLY:HA2	1.98	0.46
88:Ag:410:LEU:HD23	88:Ag:414:MET:HG2	1.98	0.46
34:V:108:MET:HE1	36:d:169:PHE:HB3	1.97	0.46
79:AA:920:G:H2'	79:AA:921:U:C6	2.51	0.46
79:AA:1165:C:H2'	79:AA:1166:A:C8	2.51	0.46
84:AX:188:LEU:HD22	84:AX:226:VAL:HG23	1.97	0.46
88:Ag:65:HIS:HB3	88:Ag:68:HIS:CG	2.51	0.46
7:6:179:VAL:HG23	7:6:183:ASP:HB2	1.97	0.45
11:A:2470:G:H4'	19:L:36:THR:HG23	1.98	0.45
11:A:2699:C:H2'	11:A:2700:G:H8	1.81	0.45
16:I:57:LYS:HD3	16:I:58:PRO:HD2	1.97	0.45
17:J:161:SER:HA	42:I:69:THR:HG21	1.96	0.45
36:d:269:TRP:CD1	36:d:269:TRP:H	2.34	0.45
56:AE:92:ASN:HB2	66:AP:117:MET:HE3	1.97	0.45
58:AG:293:ILE:HB	58:AG:300:TYR:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:740:G:H2'	79:AA:741:A:H8	1.82	0.45
11:A:3129:A:H2'	11:A:3130:A:C8	2.51	0.45
36:d:110:GLU:O	36:d:114:LYS:HG2	2.17	0.45
50:f:80:ILE:HG23	50:f:90:VAL:HG12	1.99	0.45
55:AD:140:LEU:HG	55:AD:146:VAL:HG11	1.98	0.45
79:AA:685:A:H2'	79:AA:686:A:H8	1.81	0.45
79:AA:693:A:H2'	79:AA:694:C:O4'	2.16	0.45
79:AA:1191:C:H2'	79:AA:1192:C:C6	2.51	0.45
79:AA:1508:C:H2'	79:AA:1509:U:H6	1.81	0.45
83:A4:352:PRO:O	83:A4:355:GLN:HG3	2.16	0.45
88:Ag:61:GLY:HA3	88:Ag:144:LEU:HD13	1.98	0.45
11:A:3112:A:N7	11:A:3200:U:C2	2.85	0.45
33:g:110:ILE:HD11	33:g:157:LEU:HD13	1.98	0.45
71:AV:209:LEU:HD11	71:AV:228:TYR:CE1	2.51	0.45
79:AA:1471:A:H2'	79:AA:1472:G:H8	1.80	0.45
79:AA:1515:G:H2'	79:AA:1516:G:H8	1.80	0.45
8:7:114:ASP:HB2	8:7:117:LYS:HB2	1.98	0.45
11:A:1911:C:H2'	11:A:1912:A:C8	2.52	0.45
26:S:173:ARG:HB3	26:S:180:PHE:HE2	1.81	0.45
36:d:168:CYS:HB2	36:d:262:HIS:O	2.16	0.45
79:AA:852:A:H3'	79:AA:853:C:C6	2.50	0.45
84:AX:265:ILE:HD12	84:AX:268:LEU:HD23	1.99	0.45
88:Ag:257:PRO:HD2	88:Ag:281:ARG:HD2	1.99	0.45
28:U:11:ARG:HH11	34:V:213:VAL:HG12	1.82	0.45
43:m:81:LEU:HA	43:m:84:LEU:HD23	1.98	0.45
52:s:145:VAL:HG21	52:s:187:LEU:HD11	1.98	0.45
62:AL:143:LEU:HD11	62:AL:153:LYS:HA	1.99	0.45
71:AV:148:MET:HG2	71:AV:181:LEU:HG	1.98	0.45
72:AW:103:ARG:HE	72:AW:139:ARG:HH21	1.64	0.45
79:AA:767:C:H2'	79:AA:768:A:H8	1.81	0.45
79:AA:776:A:O3'	79:AA:777:G:H8	2.00	0.45
79:AA:1358:A:H2'	79:AA:1359:U:C6	2.52	0.45
88:Ag:201:GLU:HA	88:Ag:204:THR:HG22	1.99	0.45
11:A:2245:A:H4'	11:A:2246:A:OP1	2.16	0.45
47:r:99:MET:HE1	47:r:115:ILE:HG22	1.98	0.45
59:AH:155:VAL:HG13	75:A1:126:LEU:HD12	1.98	0.45
79:AA:1109:A:H2'	79:AA:1110:A:H8	1.81	0.45
79:AA:1382:A:H2'	79:AA:1383:A:O4'	2.17	0.45
79:AA:1396:C:H2'	79:AA:1397:U:C6	2.51	0.45
79:AA:1485:G:H2'	79:AA:1486:B8T:O4'	2.17	0.45
88:Ag:63:ILE:O	88:Ag:150:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ag:152:ALA:HB3	88:Ag:155:ASP:HB2	1.98	0.45
88:Ag:286:LYS:HE2	88:Ag:314:GLU:HA	1.98	0.45
88:Ag:292:LEU:HB2	88:Ag:340:MET:HG2	1.98	0.45
36:d:91:PRO:HB2	36:d:94:ASP:HB2	1.98	0.45
62:AL:209:LEU:HD12	76:A3:189:TRP:CE2	2.51	0.45
71:AV:68:SER:N	79:AA:1523:A:H5''	2.32	0.45
83:A4:556:LYS:HZ3	83:A4:571:TRP:HZ3	1.65	0.45
87:Ah:48:U:C5	87:Ah:51:U:H5''	2.52	0.45
88:Ag:55:LYS:HB2	88:Ag:121:HIS:ND1	2.32	0.45
88:Ag:357:TYR:CD1	88:Ag:403:ASP:HB2	2.51	0.45
10:9:137:ARG:HH22	31:Y:143:ASP:CG	2.24	0.45
19:L:75:LEU:HD11	19:L:105:VAL:HG21	1.98	0.45
26:S:163:LYS:HB2	35:b:106:ASP:HB3	1.97	0.45
37:e:164:LYS:HE2	37:e:167:ASP:HA	1.99	0.45
79:AA:986:G:H2'	79:AA:987:A:H8	1.81	0.45
79:AA:1202:G:H2'	79:AA:1203:C:H6	1.82	0.45
88:Ag:292:LEU:HB3	88:Ag:299:ILE:O	2.17	0.45
11:A:2872:C:H2'	11:A:2873:A:O4'	2.17	0.45
79:AA:1068:A:H5''	80:AI:190:LYS:HD3	1.99	0.45
88:Ag:68:HIS:CE1	88:Ag:151:VAL:HA	2.52	0.45
11:A:1897:A:H2'	11:A:1898:A:H8	1.82	0.45
11:A:2092:C:H2'	11:A:2093:U:C6	2.52	0.45
43:m:120:ARG:HG2	43:m:123:TRP:CE2	2.52	0.45
46:q:141:GLU:HA	46:q:144:GLU:HG3	1.98	0.45
56:AE:26:ILE:HG23	56:AE:36:VAL:HG21	1.97	0.45
79:AA:687:G:H3'	79:AA:829:C:H41	1.82	0.45
88:Ag:55:LYS:HE2	88:Ag:118:ALA:HA	1.99	0.45
11:A:2728:C:H2'	11:A:2729:U:H6	1.82	0.44
11:A:3151:A:H4'	24:Q:146:GLY:O	2.17	0.44
79:AA:653:G:H2'	79:AA:654:U:O4'	2.18	0.44
79:AA:848:U:H2'	79:AA:849:U:C6	2.51	0.44
79:AA:950:A:H2'	79:AA:951:G:H8	1.82	0.44
84:AX:242:ILE:HD11	100:AX:503:GDP:C4	2.51	0.44
88:Ag:261:PRO:HD2	88:Ag:278:THR:O	2.17	0.44
88:Ag:371:VAL:HG23	88:Ag:373:HIS:H	1.82	0.44
88:Ag:378:MET:HE3	88:Ag:408:LEU:HD11	1.99	0.44
11:A:2005:C:H2'	11:A:2006:C:C6	2.52	0.44
11:A:2101:C:H2'	11:A:2102:A:H8	1.81	0.44
11:A:3170:C:N4	11:A:3171:C:H41	2.16	0.44
42:l:110:LEU:HB3	42:l:117:TYR:HB2	1.98	0.44
54:AC:100:PHE:HB3	54:AC:103:CYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AF:118:VAL:HG13	57:AF:210:LEU:HD21	2.00	0.44
63:AM:73:ILE:O	63:AM:77:ILE:HG12	2.17	0.44
71:AV:70:LEU:HD21	71:AV:390:ILE:HD13	2.00	0.44
79:AA:732:A:H2'	79:AA:733:U:C6	2.52	0.44
79:AA:1581:G:H2'	79:AA:1583:MA6:OP2	2.17	0.44
89:Ax:4:A:H2'	89:Ax:5:A:C8	2.52	0.44
32:Z:101:LYS:HD2	40:j:84:MET:HG3	1.98	0.44
33:g:142:GLU:HB3	45:o:88:ILE:HG13	2.00	0.44
36:d:158:ASP:O	36:d:162:THR:HG23	2.17	0.44
48:u:82:LEU:O	48:u:86:LEU:HG	2.18	0.44
51:p:110:TRP:CD1	51:p:110:TRP:H	2.35	0.44
79:AA:800:C:H2'	79:AA:801:A:C8	2.52	0.44
79:AA:1496:U:H2'	79:AA:1497:C:C6	2.53	0.44
87:Ah:47:G:H4'	87:Ah:48:U:OP2	2.17	0.44
88:Ag:80:ILE:HG23	88:Ag:87:ALA:HB1	2.00	0.44
11:A:2235:C:H2'	11:A:2236:C:O4'	2.17	0.44
11:A:2553:G:H2'	11:A:2554:A:C8	2.52	0.44
48:u:86:LEU:O	48:u:90:LEU:HB2	2.17	0.44
68:AS:49:PRO:HB2	85:A2:117:LEU:HD13	1.99	0.44
79:AA:715:G:H2'	79:AA:716:U:H6	1.83	0.44
79:AA:915:C:H2'	79:AA:916:C:H6	1.82	0.44
79:AA:1354:A:H2'	79:AA:1355:G:C8	2.53	0.44
79:AA:1595:G:H2'	79:AA:1596:A:C8	2.53	0.44
88:Ag:271:ARG:HB3	88:Ag:325:LEU:HD22	1.98	0.44
88:Ag:285:LYS:HB2	88:Ag:315:ARG:HG3	1.99	0.44
4:3:115:LEU:HB2	20:M:83:PHE:HB3	2.00	0.44
26:S:96:PHE:HB3	35:b:126:ILE:HD13	2.00	0.44
30:X:7:PRO:HD2	30:X:10:LEU:HD12	2.00	0.44
74:A0:51:PRO:HG3	79:AA:705:C:H5'	1.99	0.44
79:AA:786:G:H2'	79:AA:787:C:C6	2.52	0.44
79:AA:875:U:H2'	79:AA:876:U:H6	1.82	0.44
79:AA:1156:C:H2'	79:AA:1157:U:H6	1.82	0.44
88:Ag:289:GLU:HA	88:Ag:302:VAL:HA	1.99	0.44
11:A:2553:G:H2'	11:A:2554:A:H8	1.82	0.44
11:A:2795:U:H2'	11:A:2796:G:H8	1.82	0.44
24:Q:176:VAL:HG11	24:Q:179:LEU:HB2	1.98	0.44
26:S:114:ILE:HG13	26:S:193:LEU:HB2	2.00	0.44
34:V:93:THR:HG22	34:V:112:GLU:HG3	1.99	0.44
57:AF:168:TYR:HB3	57:AF:236:LEU:HD13	2.00	0.44
71:AV:82:ARG:O	71:AV:85:ILE:HG22	2.17	0.44
79:AA:675:A:H2'	79:AA:676:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:706:C:H2'	79:AA:707:C:O4'	2.17	0.44
79:AA:1502:A:H2'	79:AA:1503:G:O4'	2.17	0.44
88:Ag:289:GLU:HB2	88:Ag:300:ARG:HH12	1.83	0.44
11:A:3115:U:H2'	11:A:3116:C:H6	1.83	0.44
50:f:122:GLU:HB2	50:f:158:GLN:HB3	2.00	0.44
71:AV:114:ARG:HA	71:AV:117:LEU:HD12	1.99	0.44
71:AV:196:PHE:HB3	71:AV:201:GLU:HG3	1.99	0.44
74:A0:65:LEU:HD23	74:A0:68:LEU:HB2	2.00	0.44
76:A3:177:TRP:CD1	76:A3:178:LEU:HD12	2.53	0.44
79:AA:959:C:H3'	79:AA:960:C:O4'	2.18	0.44
79:AA:1034:U:H2'	79:AA:1035:U:H6	1.82	0.44
83:A4:646:THR:O	83:A4:650:MET:HG2	2.18	0.44
90:B:49:U:H2'	90:B:50:U:C6	2.52	0.44
11:A:1828:A:H4'	11:A:1829:A:C8	2.52	0.44
36:d:84:ILE:HD11	36:d:263:THR:HG21	2.00	0.44
40:j:63:GLN:HE21	40:j:67:LYS:HD2	1.83	0.44
73:AZ:10:ARG:HA	73:AZ:13:ARG:HB3	2.00	0.44
79:AA:891:C:H2'	79:AA:892:A:O4'	2.17	0.44
79:AA:952:A:H2'	79:AA:953:U:C6	2.53	0.44
79:AA:1488:5MC:H2'	79:AA:1489:G:C8	2.53	0.44
9:8:68:LEU:HD21	50:f:211:LEU:HB2	1.98	0.44
11:A:1829:A:H2'	11:A:1830:G:C8	2.52	0.44
11:A:1851:G:H2'	11:A:2693:A:N7	2.32	0.44
11:A:2805:A:H2'	11:A:2806:U:C6	2.53	0.44
11:A:3144:A:H2'	11:A:3145:A:C8	2.53	0.44
22:O:26:ILE:HG13	24:Q:264:TRP:CD1	2.52	0.44
68:AS:134:ARG:HG2	68:AS:136:GLY:H	1.83	0.44
79:AA:1132:U:H2'	79:AA:1133:C:H6	1.82	0.44
88:Ag:74:THR:HG23	88:Ag:124:HIS:CG	2.52	0.44
7:6:272:LEU:HB3	7:6:315:GLY:H	1.83	0.43
11:A:2212:C:H2'	11:A:2213:A:H8	1.83	0.43
11:A:2508:C:H2'	11:A:2509:A:C8	2.53	0.43
20:M:202:LYS:HD3	20:M:294:TYR:HA	2.00	0.43
36:d:210:GLY:O	36:d:249:GLU:HA	2.18	0.43
38:h:91:LEU:HB3	38:h:97:LYS:HB2	1.99	0.43
54:AC:123:VAL:HG23	54:AC:157:THR:HG22	2.00	0.43
79:AA:822:G:H2'	79:AA:823:A:C8	2.53	0.43
79:AA:960:C:H42	79:AA:1041:A:H2	1.66	0.43
79:AA:1110:A:H61	79:AA:1131:C:H42	1.66	0.43
79:AA:1200:G:C2	79:AA:1201:A:C8	3.06	0.43
88:Ag:157:PRO:HG3	88:Ag:198:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ag:179:TYR:CZ	88:Ag:218:GLY:HA3	2.53	0.43
10:9:114:LEU:HA	10:9:117:TYR:HD1	1.83	0.43
11:A:2408:U:H2'	11:A:2409:A:C8	2.53	0.43
56:AE:94:VAL:HG12	79:AA:1033:U:H4'	2.00	0.43
57:AF:149:LEU:HD23	57:AF:149:LEU:HA	1.87	0.43
74:A0:82:ARG:HB2	74:A0:85:TRP:CG	2.53	0.43
79:AA:659:U:H2'	79:AA:660:C:C6	2.52	0.43
79:AA:821:U:H2'	79:AA:822:G:H8	1.83	0.43
79:AA:853:C:H2'	79:AA:854:U:C6	2.53	0.43
79:AA:916:C:H2'	79:AA:917:C:H6	1.83	0.43
79:AA:995:A:H2'	79:AA:996:A:O4'	2.18	0.43
79:AA:1363:C:H1'	79:AA:1448:U:O2	2.18	0.43
83:A4:393:ILE:HA	83:A4:396:ILE:HG22	1.99	0.43
84:AX:205:GLN:HG2	84:AX:250:GLN:HE21	1.83	0.43
88:Ag:55:LYS:HB3	88:Ag:120:ARG:HA	2.00	0.43
46:q:44:ASP:O	46:q:47:THR:HG22	2.18	0.43
48:t:86:LEU:HG	48:u:71:ILE:HD11	2.00	0.43
79:AA:672:A:H2'	79:AA:673:U:H6	1.81	0.43
79:AA:821:U:H1'	88:Ag:270:GLY:HA2	1.99	0.43
79:AA:1500:C:H2'	79:AA:1501:A:O4'	2.17	0.43
88:Ag:141:THR:HG23	88:Ag:171:ILE:HG21	2.00	0.43
11:A:2147:G:OP2	26:S:104:ARG:HD3	2.18	0.43
22:O:79:TRP:CE2	24:Q:269:MET:HE2	2.53	0.43
46:q:117:ARG:O	46:q:121:ILE:HG12	2.19	0.43
79:AA:687:G:H2'	79:AA:829:C:C5	2.53	0.43
88:Ag:339:VAL:HG11	88:Ag:415:ILE:CG1	2.45	0.43
11:A:1893:A:H4'	11:A:1894:G:H5'	2.00	0.43
11:A:2072:A:H62	11:A:2831:G:H2'	1.83	0.43
11:A:2182:G:H2'	11:A:2183:C:C6	2.54	0.43
11:A:2815:OMG:H1'	11:A:2815:OMG:HM23	1.78	0.43
37:e:215:PHE:CZ	90:B:76:A:H2'	2.53	0.43
59:AH:58:LEU:HD12	83:A4:76:SER:HB2	1.99	0.43
71:AV:340:LYS:HE3	71:AV:340:LYS:HB3	1.76	0.43
79:AA:808:C:H2'	79:AA:809:G:O4'	2.19	0.43
79:AA:1202:G:H2'	79:AA:1203:C:C6	2.54	0.43
79:AA:1450:C:H2'	79:AA:1451:U:C6	2.54	0.43
79:AA:1582:G:H2'	79:AA:1583:MA6:C8	2.48	0.43
79:AA:1589:C:H2'	79:AA:1590:A:C8	2.53	0.43
88:Ag:178:VAL:HG11	88:Ag:199:ILE:HD12	2.01	0.43
8:7:149:MET:HG2	8:7:209:LEU:HD23	2.01	0.43
11:A:1778:U:H2'	11:A:1779:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:174:VAL:HG12	15:H:192:HIS:CB	2.49	0.43
23:P:88:HIS:HB2	90:B:24:G:OP2	2.19	0.43
27:T:53:TYR:HD2	36:d:228:PHE:HA	1.82	0.43
46:q:152:ARG:O	46:q:156:LEU:HG	2.18	0.43
62:AL:86:ASP:HB2	70:AU:161:GLN:HE22	1.83	0.43
65:AO:208:PRO:HG2	65:AO:213:LEU:HD21	2.01	0.43
65:AO:238:MET:HA	65:AO:239:PRO:HD3	1.89	0.43
67:AR:272:VAL:O	67:AR:276:VAL:HG23	2.19	0.43
79:AA:664:G:H2'	79:AA:665:C:C6	2.53	0.43
79:AA:764:A:H4'	79:AA:765:C:O4'	2.18	0.43
79:AA:821:U:H2'	79:AA:822:G:C8	2.53	0.43
79:AA:985:U:H2'	79:AA:986:G:C8	2.54	0.43
79:AA:1571:U:O2'	79:AA:1572:A:H5'	2.19	0.43
83:A4:166:VAL:HG12	83:A4:194:LEU:HG	2.00	0.43
83:A4:450:PRO:HD2	83:A4:453:HIS:CG	2.54	0.43
84:AX:74:ASP:O	84:AX:78:VAL:HG12	2.19	0.43
87:Ah:26:C:C2	87:Ah:27:G:C8	3.07	0.43
88:Ag:150:VAL:HB	88:Ag:181:ASN:OD1	2.19	0.43
88:Ag:335:ARG:HB3	88:Ag:338:LEU:HD13	2.01	0.43
6:5:354:PHE:HB3	6:5:417:LEU:HD11	2.00	0.43
8:7:302:LEU:HD23	22:O:144:LEU:HD23	2.00	0.43
11:A:2318:A:H2'	11:A:2319:A:C8	2.54	0.43
11:A:3000:A:H2'	11:A:3001:G:C8	2.54	0.43
34:V:80:ILE:HB	34:V:85:TRP:HB2	2.00	0.43
70:AU:57:MET:HE3	70:AU:57:MET:HB3	1.89	0.43
79:AA:865:A:H2'	79:AA:866:A:C8	2.54	0.43
79:AA:1322:C:H2'	79:AA:1323:G:O4'	2.18	0.43
79:AA:1348:G:H2'	79:AA:1349:U:C6	2.53	0.43
85:A2:43:ALA:HB1	85:A2:46:ILE:HD11	2.01	0.43
11:A:1970:G:H2'	11:A:1971:A:O4'	2.19	0.43
20:M:137:GLY:HA3	20:M:157:GLN:HG2	2.00	0.43
37:e:205:LEU:HB3	50:f:168:GLU:HB2	2.01	0.43
48:t:64:ILE:HD11	48:u:82:LEU:HB2	2.00	0.43
50:f:125:TYR:CD2	50:f:197:ARG:HD3	2.54	0.43
53:AB:148:ASN:HD22	53:AB:197:HIS:CD2	2.37	0.43
53:AB:231:LEU:HD23	53:AB:231:LEU:HA	1.88	0.43
63:AM:114:ARG:HH22	65:AO:236:PRO:HD2	1.84	0.43
71:AV:175:VAL:HG12	71:AV:177:SER:N	2.34	0.43
79:AA:950:A:H2'	79:AA:951:G:C8	2.54	0.43
79:AA:1497:C:H2'	79:AA:1498:C:C6	2.54	0.43
79:AA:1507:A:H2'	79:AA:1508:C:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:A4:173:PHE:HA	83:A4:176:LEU:HD12	2.01	0.43
88:Ag:106:ILE:HB	88:Ag:130:HIS:NE2	2.34	0.43
88:Ag:107:THR:HB	88:Ag:128:PRO:HA	1.99	0.43
11:A:1924:U:H2'	11:A:1925:A:C8	2.54	0.43
11:A:2688:C:H2'	11:A:2689:C:C6	2.53	0.43
36:d:211:GLN:HG3	36:d:249:GLU:HG3	2.01	0.43
52:s:84:THR:HB	52:s:280:ASN:HB2	2.00	0.43
79:AA:694:C:H2'	79:AA:815:C:H41	1.84	0.43
79:AA:1396:C:H2'	79:AA:1397:U:H6	1.83	0.43
84:AX:310:LEU:HD11	84:AX:325:PRO:HA	2.00	0.43
88:Ag:289:GLU:HB2	88:Ag:300:ARG:NH1	2.34	0.43
88:Ag:299:ILE:HG21	88:Ag:329:LEU:HD11	2.01	0.43
88:Ag:393:PRO:C	88:Ag:395:LYS:H	2.27	0.43
36:d:128:TYR:CZ	36:d:208:VAL:HG21	2.53	0.43
36:d:217:HIS:CD2	36:d:243:LEU:HB2	2.54	0.43
71:AV:110:HIS:CE1	71:AV:114:ARG:HE	2.36	0.43
79:AA:689:U:H2'	79:AA:690:U:C6	2.53	0.43
79:AA:822:G:OP1	88:Ag:330:LYS:HE2	2.19	0.43
79:AA:969:A:H2'	79:AA:970:A:C8	2.53	0.43
79:AA:1180:U:H2'	79:AA:1181:G:H8	1.83	0.43
79:AA:1376:C:H4'	79:AA:1377:C:H5'	2.00	0.43
79:AA:1439:A:H2'	79:AA:1440:G:H8	1.83	0.43
79:AA:1495:C:H2'	79:AA:1496:U:H6	1.83	0.43
87:Ah:53:G:H4'	88:Ag:374:PHE:CD1	2.54	0.43
88:Ag:278:THR:HA	88:Ag:321:ASN:HA	2.00	0.43
11:A:2677:A:H2'	11:A:2678:A:C8	2.54	0.42
11:A:2894:U:H5''	11:A:2895:U:O4'	2.19	0.42
17:J:114:LEU:HB3	42:l:96:LEU:HD21	2.00	0.42
62:AL:130:ILE:HG12	62:AL:185:LEU:HD11	2.01	0.42
65:AO:96:ARG:HH22	79:AA:918:A:H3'	1.83	0.42
79:AA:912:U:H2'	79:AA:913:A:O4'	2.18	0.42
88:Ag:89:PHE:HZ	88:Ag:227:ARG:HG3	1.84	0.42
88:Ag:222:CYS:HA	88:Ag:225:GLU:CD	2.44	0.42
10:9:45:THR:HG22	10:9:49:ARG:O	2.20	0.42
11:A:2092:C:H2'	11:A:2093:U:H6	1.84	0.42
11:A:2111:C:H2'	11:A:2112:A:C8	2.54	0.42
11:A:2217:C:H2'	11:A:2218:C:O4'	2.19	0.42
17:J:113:THR:HG23	17:J:115:LYS:H	1.84	0.42
20:M:14:ASP:HB2	20:M:17:ARG:HH12	1.85	0.42
24:Q:182:ARG:HG3	24:Q:187:LEU:HD11	2.01	0.42
36:d:147:GLU:HG3	36:d:163:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:88:LEU:HD23	40:j:88:LEU:HA	1.89	0.42
54:AC:96:MET:HB2	54:AC:108:LEU:HD11	2.01	0.42
61:AK:81:ASP:HA	61:AK:86:ARG:HD3	2.01	0.42
74:A0:11:ILE:HD12	79:AA:806:C:C4	2.54	0.42
79:AA:1349:U:H2'	79:AA:1350:G:H8	1.83	0.42
90:B:25:C:H2'	90:B:26:A:H8	1.84	0.42
9:8:192:TYR:HB3	50:f:132:ILE:HD11	2.02	0.42
11:A:3115:U:H2'	11:A:3116:C:C6	2.54	0.42
52:s:273:LEU:HD12	52:s:273:LEU:HA	1.88	0.42
74:A0:165:PRO:HG3	74:A0:190:MET:HE2	2.01	0.42
79:AA:767:C:H2'	79:AA:768:A:C8	2.54	0.42
79:AA:886:C:H2'	79:AA:887:G:C8	2.54	0.42
79:AA:1208:U:H2'	79:AA:1209:C:C6	2.54	0.42
87:Ah:15:G:H2'	87:Ah:16:C:C6	2.54	0.42
88:Ag:88:LYS:O	88:Ag:90:LYS:HD3	2.20	0.42
6:5:167:THR:HG21	52:s:281:HIS:CE1	2.55	0.42
7:6:106:ARG:HG2	23:P:110:TRP:CE2	2.55	0.42
9:8:70:ARG:NH1	89:Ax:46:U:H5'	2.35	0.42
11:A:2099:U:H2'	11:A:2100:C:H6	1.82	0.42
11:A:2275:U:H2'	11:A:2276:C:H6	1.85	0.42
11:A:3038:U:H2'	11:A:3039:OMU:H6	2.01	0.42
12:D:173:ALA:O	56:AE:84:ARG:HD2	2.20	0.42
15:H:182:TRP:CH2	15:H:237:VAL:HG11	2.55	0.42
16:I:139:LYS:HE2	16:I:140:TYR:CZ	2.55	0.42
21:N:172:VAL:HA	21:N:175:PHE:CE2	2.55	0.42
59:AH:124:VAL:HG12	61:AK:109:ILE:HG12	2.00	0.42
63:AM:93:LEU:HD13	67:AR:156:TYR:HE2	1.84	0.42
79:AA:1456:U:H2'	79:AA:1457:G:O4'	2.19	0.42
87:Ah:67:C:H2'	87:Ah:68:G:H8	1.84	0.42
10:9:136:LEU:HD23	10:9:136:LEU:HA	1.89	0.42
11:A:2519:G:C5	12:D:228:LEU:HD13	2.54	0.42
16:I:127:PRO:HG2	16:I:130:VAL:HG22	2.02	0.42
46:q:188:LYS:HA	46:q:191:LYS:HG2	2.01	0.42
52:s:332:LEU:HD21	52:s:359:ALA:HB2	2.00	0.42
63:AM:56:PRO:HA	63:AM:64:LYS:HE3	2.00	0.42
71:AV:235:GLU:HB2	71:AV:243:VAL:HG21	2.00	0.42
71:AV:381:GLN:O	71:AV:384:LEU:HG	2.20	0.42
79:AA:661:C:H2'	79:AA:662:U:H6	1.85	0.42
88:Ag:225:GLU:HA	88:Ag:227:ARG:NH1	2.34	0.42
11:A:2004:G:H2'	11:A:2005:C:C6	2.54	0.42
11:A:2420:U:H2'	11:A:2421:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:189:VAL:HG21	15:H:208:LEU:HD21	2.00	0.42
36:d:151:CYS:HB2	36:d:160:LEU:HD13	2.01	0.42
61:AK:40:ARG:HD3	61:AK:86:ARG:HB3	2.01	0.42
79:AA:1076:5MU:O2	79:AA:1076:5MU:H2'	2.20	0.42
79:AA:1279:C:H2'	79:AA:1280:C:C6	2.55	0.42
79:AA:1468:U:H2'	79:AA:1469:G:O4'	2.19	0.42
79:AA:1488:5MC:HN41	79:AA:1562:G:H1	1.67	0.42
84:AX:238:ASP:HB3	100:AX:503:GDP:HN22	1.84	0.42
87:Ah:25:A:H2'	87:Ah:26:C:C6	2.54	0.42
88:Ag:56:PRO:O	88:Ag:120:ARG:HG2	2.19	0.42
88:Ag:95:ILE:HG13	88:Ag:113:VAL:HG11	2.01	0.42
88:Ag:265:VAL:HG22	88:Ag:275:VAL:HA	2.01	0.42
88:Ag:383:TRP:HE1	88:Ag:385:MET:HB2	1.84	0.42
1:0:169:ASP:HA	1:0:172:LYS:HD3	2.01	0.42
2:1:18:VAL:HG11	2:1:34:ARG:HE	1.84	0.42
7:6:234:HIS:CE1	7:6:257:PRO:HA	2.54	0.42
8:7:61:ARG:CZ	36:d:235:GLN:HE22	2.33	0.42
11:A:2065:A:O4'	29:W:74:ARG:HG3	2.20	0.42
11:A:2072:A:N6	11:A:2831:G:H2'	2.34	0.42
11:A:2550:A:C2	11:A:2551:G:C8	3.08	0.42
14:F:103:GLN:NE2	14:F:249:ASN:HD22	2.10	0.42
52:s:65:ARG:O	52:s:69:THR:HG23	2.19	0.42
54:AC:155:LEU:HD23	54:AC:155:LEU:HA	1.86	0.42
55:AD:258:ILE:HD11	55:AD:343:LEU:HD22	2.02	0.42
55:AD:374:ARG:HB2	55:AD:377:CYS:HB2	2.00	0.42
58:AG:87:HIS:O	58:AG:91:MET:HG2	2.19	0.42
58:AG:380:LYS:HG3	58:AG:386:GLY:HA2	2.02	0.42
76:A3:165:LYS:HG2	76:A3:195:TYR:CE2	2.55	0.42
79:AA:1497:C:H2'	79:AA:1498:C:H6	1.84	0.42
79:AA:1510:U:H2'	79:AA:1511:C:C6	2.54	0.42
88:Ag:341:VAL:HB	88:Ag:345:SER:HB3	2.02	0.42
90:B:29:C:C2	90:B:30:A:C8	3.07	0.42
6:5:301:PRO:HD3	11:A:2390:A:H4'	2.01	0.42
11:A:1860:A:H2'	11:A:1861:U:C6	2.55	0.42
11:A:2868:C:H2'	11:A:2869:A:O4'	2.20	0.42
36:d:106:ILE:O	36:d:110:GLU:HG2	2.19	0.42
67:AR:288:GLN:HE22	67:AR:300:LEU:HD22	1.84	0.42
68:AS:51:VAL:HG13	85:A2:117:LEU:HD11	2.01	0.42
71:AV:225:LEU:HD13	71:AV:275:LEU:HD21	2.02	0.42
79:AA:956:C:H2'	79:AA:957:C:O4'	2.20	0.42
79:AA:1583:MA6:O5'	79:AA:1583:MA6:H8	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:A4:392:ILE:HG13	83:A4:393:ILE:N	2.35	0.42
88:Ag:60:VAL:HG11	88:Ag:115:TYR:OH	2.19	0.42
6:5:147:ILE:HG12	6:5:191:GLN:CD	2.45	0.42
11:A:2626:U:H4'	11:A:2627:G:C8	2.55	0.42
36:d:201:SER:O	36:d:208:VAL:HG12	2.20	0.42
65:AO:106:PRO:HA	65:AO:109:ARG:NE	2.35	0.42
65:AO:202:TRP:CE3	70:AU:62:HIS:HB3	2.55	0.42
79:AA:985:U:H2'	79:AA:986:G:H8	1.84	0.42
79:AA:1274:C:H2'	79:AA:1275:A:O4'	2.20	0.42
88:Ag:391:LEU:HD22	88:Ag:395:LYS:HG2	2.01	0.42
11:A:2398:A:H2'	11:A:2399:A:O4'	2.20	0.42
11:A:2753:A:C4	11:A:2754:A:C8	3.07	0.42
11:A:3000:A:H2'	11:A:3001:G:H8	1.85	0.42
46:q:135:TRP:O	46:q:139:GLN:HG2	2.19	0.42
53:AB:244:LEU:HD23	53:AB:244:LEU:HA	1.91	0.42
55:AD:103:LEU:HD11	55:AD:123:ARG:HB2	2.01	0.42
65:AO:82:LYS:HB3	79:AA:881:A:H62	1.85	0.42
78:AY:290:ASN:HA	83:A4:446:LYS:HD3	2.01	0.42
79:AA:716:U:H2'	79:AA:717:G:C8	2.54	0.42
79:AA:887:G:H2'	79:AA:888:U:C6	2.55	0.42
79:AA:1087:A:H2'	79:AA:1088:C:C6	2.54	0.42
79:AA:1308:U:H2'	79:AA:1309:A:C8	2.54	0.42
84:AX:163:LYS:HG3	84:AX:164:ASN:ND2	2.34	0.42
14:F:53:LEU:HD11	14:F:271:ASP:HA	2.02	0.41
21:N:237:HIS:HD2	21:N:241:TYR:HB2	1.84	0.41
37:e:75:GLN:O	37:e:79:ILE:HG12	2.19	0.41
56:AE:26:ILE:HG22	56:AE:30:MET:HE2	2.03	0.41
79:AA:787:C:H2'	79:AA:788:U:H6	1.84	0.41
79:AA:1372:C:H2'	79:AA:1373:U:C6	2.52	0.41
79:AA:1523:A:H2'	79:AA:1524:A:H8	1.84	0.41
88:Ag:101:GLU:HG3	88:Ag:108:ILE:H	1.85	0.41
88:Ag:378:MET:HE1	88:Ag:380:SER:HB3	2.02	0.41
9:8:164:ARG:HG3	50:f:88:TYR:CE1	2.55	0.41
11:A:1886:G:H1	39:i:61:GLY:HA3	1.84	0.41
11:A:1977:U:H2'	11:A:1978:A:H8	1.85	0.41
11:A:2461:A:H2'	11:A:2462:A:H8	1.86	0.41
11:A:2687:C:H2'	11:A:2688:C:H6	1.85	0.41
11:A:2774:C:H2'	11:A:2775:A:C4	2.55	0.41
16:I:101:ASN:HB3	16:I:150:HIS:HB3	2.01	0.41
54:AC:58:ALA:HB3	54:AC:60:HIS:CE1	2.55	0.41
57:AF:166:ARG:NH2	79:AA:994:A:H1'	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AF:231:GLU:HA	85:A2:53:MET:SD	2.60	0.41
65:AO:82:LYS:HB3	79:AA:881:A:N6	2.35	0.41
68:AS:50:ARG:NH2	79:AA:1119:U:H5'	2.35	0.41
79:AA:1341:C:H4'	79:AA:1342:C:H5''	2.02	0.41
84:AX:159:HIS:HE1	84:AX:311:SER:HB3	1.85	0.41
88:Ag:166:LEU:HG	88:Ag:206:PHE:CE2	2.55	0.41
5:4:103:MET:HE1	11:A:2952:U:H5'	2.01	0.41
11:A:2549:C:N4	11:A:2562:U:H2'	2.35	0.41
93:A:3472:SPD:H21	22:O:16:ARG:NH1	2.36	0.41
16:I:164:MET:HE2	16:I:168:LEU:HD11	2.02	0.41
55:AD:100:LYS:HG2	79:AA:1262:C:H4'	2.03	0.41
60:AJ:65:THR:HG21	60:AJ:100:HIS:HE1	1.85	0.41
79:AA:1218:A:H3'	79:AA:1219:U:H6	1.84	0.41
79:AA:1337:U:H2'	79:AA:1338:A:C8	2.55	0.41
79:AA:1395:C:H2'	79:AA:1396:C:H6	1.85	0.41
83:A4:535:MET:HE2	83:A4:548:PHE:CG	2.55	0.41
84:AX:152:ILE:HG12	84:AX:259:LEU:HD23	2.02	0.41
87:Ah:1:G:H2'	87:Ah:2:U:C6	2.55	0.41
87:Ah:29:U:H2'	87:Ah:30:C:H6	1.85	0.41
88:Ag:65:HIS:CG	88:Ag:66:VAL:N	2.89	0.41
88:Ag:311:LYS:HE2	88:Ag:311:LYS:HB3	1.86	0.41
11:A:1897:A:H2'	11:A:1898:A:C8	2.55	0.41
11:A:1991:A:H5''	11:A:1992:C:OP1	2.20	0.41
11:A:2900:C:H2'	11:A:2901:A:H8	1.85	0.41
16:I:192:ILE:HG22	16:I:196:LYS:NZ	2.36	0.41
36:d:119:GLN:HA	36:d:122:ILE:HD12	2.01	0.41
46:q:149:ASP:O	46:q:153:ARG:HG2	2.21	0.41
55:AD:196:ASN:C	77:Az:14:A:H62	2.28	0.41
71:AV:93:TYR:HB2	71:AV:135:TYR:CE1	2.55	0.41
79:AA:787:C:H2'	79:AA:788:U:C6	2.55	0.41
89:Ax:22:U:C2	89:Ax:23:A:C8	3.08	0.41
4:3:156:LYS:HB2	4:3:156:LYS:HE3	1.82	0.41
11:A:3142:A:H2'	11:A:3143:U:C6	2.55	0.41
13:E:87:ILE:HG23	13:E:317:PRO:HD3	2.02	0.41
52:s:119:PRO:HG3	52:s:394:TRP:CD2	2.56	0.41
57:AF:44:PRO:HD3	57:AF:75:LYS:HB2	2.03	0.41
59:AH:181:PRO:HD2	59:AH:184:ILE:HG21	2.01	0.41
77:Az:30:A:H2'	77:Az:31:A:C4	2.55	0.41
79:AA:700:A:H4'	79:AA:701:G:O5'	2.20	0.41
79:AA:1241:C:H2'	79:AA:1242:C:C6	2.55	0.41
88:Ag:421:ARG:HD2	88:Ag:435:LEU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2748:A:H2'	11:A:2749:A:C8	2.56	0.41
22:O:33:LEU:HD21	22:O:59:LEU:HD22	2.01	0.41
52:s:158:ARG:HB3	52:s:160:ARG:HH21	1.85	0.41
58:AG:389:ARG:HD2	79:AA:1427:A:O2'	2.20	0.41
69:AT:30:MET:HE1	69:AT:55:ILE:HG21	2.02	0.41
79:AA:728:C:H2'	79:AA:729:U:O4'	2.20	0.41
82:a:51:LEU:HD23	82:a:51:LEU:HA	1.88	0.41
11:A:3224:G:H2'	11:A:3225:G:C8	2.55	0.41
14:F:123:GLY:HA3	14:F:142:ARG:HG2	2.02	0.41
14:F:218:LEU:HD23	14:F:260:VAL:HB	2.01	0.41
27:T:53:TYR:CD2	36:d:228:PHE:HA	2.55	0.41
36:d:211:GLN:HA	36:d:248:PHE:O	2.21	0.41
48:u:64:ILE:O	48:u:68:VAL:HG23	2.20	0.41
55:AD:154:VAL:HG21	83:A4:108:LEU:HD22	2.03	0.41
55:AD:160:ARG:HH11	55:AD:168:VAL:HG21	1.86	0.41
55:AD:351:ARG:HD2	55:AD:355:ARG:CZ	2.50	0.41
55:AD:355:ARG:NH1	79:AA:1118:A:H4'	2.36	0.41
55:AD:401:VAL:HG21	69:AT:50:PHE:CE1	2.55	0.41
75:A1:286:THR:HG23	75:A1:289:ILE:H	1.85	0.41
79:AA:738:A:H3'	79:AA:739:C:C6	2.54	0.41
79:AA:743:C:H2'	79:AA:744:A:O4'	2.20	0.41
79:AA:970:A:H2'	79:AA:971:A:C8	2.55	0.41
79:AA:1005:U:H4'	80:AI:87:HIS:CE1	2.55	0.41
79:AA:1572:A:H2'	79:AA:1573:A:C8	2.56	0.41
84:AX:100:MET:HE1	84:AX:356:CYS:HB2	2.03	0.41
88:Ag:369:PRO:HB2	88:Ag:397:LEU:HB3	2.02	0.41
11:A:2752:C:C2	11:A:2753:A:C8	3.09	0.41
79:AA:695:A:H2'	79:AA:696:U:O4'	2.21	0.41
79:AA:696:U:H2'	79:AA:697:G:C8	2.56	0.41
79:AA:949:U:O2	97:AA:1701:NAD:H6N	2.20	0.41
79:AA:1461:A:H4'	79:AA:1462:G:C8	2.56	0.41
79:AA:1498:C:H2'	79:AA:1499:U:H6	1.86	0.41
89:Ax:3:U:H2'	89:Ax:4:A:H8	1.85	0.41
2:1:13:SER:HB2	2:1:36:ARG:HH21	1.86	0.41
10:9:45:THR:HG21	10:9:49:ARG:NH2	2.36	0.41
11:A:1728:U:H2'	11:A:1729:U:O4'	2.21	0.41
11:A:2072:A:H2'	11:A:2073:A:C8	2.55	0.41
11:A:2536:G:H2'	11:A:2537:G:H8	1.86	0.41
14:F:82:LEU:HB3	14:F:87:PHE:CD1	2.56	0.41
48:t:76:LEU:HA	48:t:79:ILE:HD12	2.02	0.41
51:p:104:HIS:CE1	51:p:106:ALA:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AF:235:ALA:HB3	80:AI:121:LYS:HD2	2.03	0.41
79:AA:682:A:H2'	79:AA:683:G:H8	1.86	0.41
79:AA:1080:A:C4	79:AA:1082:A:C6	3.08	0.41
79:AA:1392:A:C4	79:AA:1393:G:C8	3.09	0.41
79:AA:1595:G:H2'	79:AA:1596:A:H8	1.86	0.41
83:A4:462:PHE:HZ	83:A4:481:LEU:HB3	1.85	0.41
83:A4:581:ILE:HG13	83:A4:610:LEU:HD13	2.03	0.41
87:Ah:21:U:N3	87:Ah:47:G:H1'	2.36	0.41
87:Ah:45:A:H3'	87:Ah:46:G:C8	2.55	0.41
88:Ag:283:ILE:HG13	88:Ag:316:ALA:O	2.20	0.41
11:A:1936:A:H4'	11:A:1937:A:N7	2.36	0.41
11:A:2734:A:H2'	11:A:2735:G:H8	1.85	0.41
17:J:90:PHE:HB3	17:J:120:ILE:HG12	2.03	0.41
32:Z:121:PRO:HD3	45:o:48:TRP:CE2	2.56	0.41
46:q:145:LYS:NZ	46:q:149:ASP:HB2	2.36	0.41
47:r:136:PRO:HG2	47:r:139:VAL:HG21	2.02	0.41
71:AV:117:LEU:HA	71:AV:122:GLN:HE22	1.86	0.41
79:AA:827:A:H8	79:AA:827:A:OP2	2.04	0.41
79:AA:862:A:H2'	79:AA:863:C:C6	2.56	0.41
79:AA:1439:A:H2'	79:AA:1440:G:C8	2.56	0.41
79:AA:1509:U:H2'	79:AA:1510:U:C6	2.56	0.41
83:A4:159:GLU:HG2	83:A4:163:LEU:HD12	2.01	0.41
83:A4:302:VAL:HG11	83:A4:341:CYS:HB3	2.03	0.41
87:Ah:49:C:H2'	87:Ah:60:A:N3	2.36	0.41
90:B:16:C:H2'	90:B:18:A:O4'	2.20	0.41
9:8:129:ARG:HE	9:8:133:ARG:HH21	1.69	0.40
11:A:2212:C:H2'	11:A:2213:A:C8	2.56	0.40
11:A:2757:A:H2'	11:A:2758:G:O4'	2.21	0.40
25:R:91:VAL:HG11	40:j:24:GLY:HA3	2.02	0.40
34:V:108:MET:HE3	36:d:166:GLU:HG3	2.01	0.40
65:AO:94:CYS:SG	65:AO:105:CYS:HB3	2.60	0.40
65:AO:220:TYR:O	65:AO:224:LEU:HG	2.21	0.40
66:AP:103:LYS:HA	66:AP:103:LYS:HD3	1.93	0.40
79:AA:1119:U:H2'	79:AA:1120:C:O4'	2.22	0.40
79:AA:1254:C:H4'	79:AA:1255:U:H5''	2.02	0.40
79:AA:1279:C:H2'	79:AA:1280:C:H6	1.86	0.40
88:Ag:68:HIS:ND1	88:Ag:150:VAL:HG23	2.37	0.40
88:Ag:167:LEU:HA	88:Ag:170:GLN:HG2	2.03	0.40
88:Ag:262:VAL:HG22	88:Ag:275:VAL:HG21	2.02	0.40
11:A:1861:U:H2'	11:A:1862:U:C6	2.56	0.40
11:A:2093:U:H2'	11:A:2094:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2109:A:C6	11:A:2111:C:C2	3.09	0.40
11:A:2474:C:H2'	11:A:2475:U:O4'	2.22	0.40
11:A:2603:C:C2	11:A:2604:A:C8	3.10	0.40
17:J:58:LYS:HA	17:J:58:LYS:HD2	1.86	0.40
26:S:104:ARG:HD2	26:S:106:TRP:CZ2	2.56	0.40
55:AD:141:TRP:HZ2	73:AZ:68:LEU:HB3	1.86	0.40
55:AD:363:ALA:HB2	55:AD:370:VAL:HG23	2.03	0.40
59:AH:72:LEU:HD12	75:A1:133:TRP:CZ3	2.56	0.40
77:Az:7:G:N2	87:Ah:38:A:H1'	2.36	0.40
79:AA:862:A:H2'	79:AA:863:C:H6	1.86	0.40
79:AA:1218:A:H3'	79:AA:1219:U:C6	2.56	0.40
79:AA:1373:U:H2'	79:AA:1374:A:H8	1.86	0.40
84:AX:136:LEU:HA	84:AX:136:LEU:HD23	1.85	0.40
87:Ah:1:G:H2'	87:Ah:2:U:H6	1.86	0.40
88:Ag:295:HIS:ND1	88:Ag:414:MET:HE1	2.36	0.40
90:B:30:A:H2'	90:B:31:A:C8	2.51	0.40
21:N:139:ARG:HH21	29:W:33:LYS:HD3	1.85	0.40
21:N:183:LEU:HD23	21:N:183:LEU:HA	1.91	0.40
24:Q:69:VAL:HG12	24:Q:71:PRO:HD3	2.03	0.40
29:W:116:LEU:HD11	50:f:59:TYR:CE2	2.56	0.40
57:AF:201:MET:HE3	79:AA:1369:U:H5	1.86	0.40
67:AR:128:MET:HA	67:AR:129:PRO:HD3	1.93	0.40
71:AV:208:LEU:HB3	71:AV:223:SER:O	2.21	0.40
79:AA:824:U:H2'	79:AA:825:U:C6	2.56	0.40
79:AA:984:C:H2'	79:AA:985:U:C6	2.56	0.40
79:AA:996:A:H2'	79:AA:997:A:O4'	2.21	0.40
79:AA:1057:G:H4'	79:AA:1578:A:H4'	2.03	0.40
79:AA:1069:A:H5''	79:AA:1070:C:H5	1.86	0.40
79:AA:1158:U:H2'	79:AA:1159:A:O4'	2.22	0.40
84:AX:159:HIS:CD2	84:AX:267:ALA:HB2	2.56	0.40
88:Ag:70:LYS:HE2	88:Ag:127:CYS:O	2.22	0.40
88:Ag:138:ILE:HG13	88:Ag:171:ILE:HD12	2.02	0.40
88:Ag:380:SER:OG	88:Ag:414:MET:HG3	2.21	0.40
11:A:2491:C:H2'	11:A:2492:G:C8	2.56	0.40
13:E:272:LYS:HE2	13:E:274:TRP:CZ3	2.57	0.40
15:H:174:VAL:HG12	15:H:192:HIS:HB3	2.04	0.40
24:Q:148:THR:HG22	24:Q:165:GLU:HG2	2.02	0.40
49:c:242:VAL:HG12	49:c:253:PRO:HD2	2.04	0.40
67:AR:254:ASP:HA	67:AR:259:TYR:CE1	2.56	0.40
67:AR:284:LEU:HG	67:AR:288:GLN:NE2	2.37	0.40
79:AA:667:U:H2'	79:AA:668:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AA:695:A:N6	88:Ag:271:ARG:HH21	2.17	0.40
79:AA:1176:G:H2'	79:AA:1177:C:O4'	2.22	0.40
79:AA:1374:A:H5''	84:AX:317:PHE:CE1	2.56	0.40
83:A4:272:TYR:CE2	83:A4:303:CYS:HB3	2.56	0.40
88:Ag:169:ARG:HH12	88:Ag:174:GLU:HB3	1.86	0.40
88:Ag:260:LEU:HA	88:Ag:278:THR:O	2.21	0.40
89:Ax:46:U:H3	89:Ax:59:U:H3	1.68	0.40
90:B:9:1MA:N3	90:B:45:G:H2'	2.36	0.40
9:8:117:LEU:HD22	37:e:73:LEU:HD23	2.02	0.40
11:A:2348:A:H2'	11:A:2349:G:O4'	2.21	0.40
11:A:2748:A:H2'	11:A:2749:A:H8	1.87	0.40
11:A:3191:A:C2	47:r:133:PRO:HB3	2.57	0.40
36:d:38:LYS:HE2	36:d:40:ARG:NH1	2.36	0.40
46:q:178:LEU:O	46:q:182:LEU:HG	2.22	0.40
53:AB:165:TYR:HE2	58:AG:146:PRO:HD2	1.87	0.40
71:AV:107:TRP:HB3	71:AV:382:TRP:CG	2.56	0.40
71:AV:241:ARG:HA	71:AV:244:TYR:CE2	2.57	0.40
76:A3:145:LYS:NZ	79:AA:1583:MA6:H5''	2.36	0.40
79:AA:1237:A:H1'	79:AA:1254:C:O2	2.20	0.40
82:a:87:THR:O	82:a:91:VAL:HG23	2.22	0.40
87:Ah:74:A:H2'	87:Ah:75:C:O4'	2.22	0.40
88:Ag:92:TYR:HB2	88:Ag:224:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	383 (98%)	9 (2%)	0	100	100
7	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
8	7	292/338 (86%)	283 (97%)	9 (3%)	0	100	100
9	8	155/206 (75%)	151 (97%)	4 (3%)	0	100	100
10	9	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
12	D	236/305 (77%)	229 (97%)	7 (3%)	0	100	100
13	E	303/348 (87%)	297 (98%)	6 (2%)	0	100	100
14	F	250/311 (80%)	248 (99%)	2 (1%)	0	100	100
15	H	200/267 (75%)	196 (98%)	4 (2%)	0	100	100
16	I	179/261 (69%)	174 (97%)	5 (3%)	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%)	282 (98%)	7 (2%)	0	100	100
21	N	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
22	O	152/175 (87%)	147 (97%)	5 (3%)	0	100	100
23	P	142/180 (79%)	140 (99%)	2 (1%)	0	100	100
24	Q	237/292 (81%)	236 (100%)	1 (0%)	0	100	100
25	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
26	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
27	T	164/206 (80%)	161 (98%)	3 (2%)	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%)	241 (100%)	1 (0%)	0	100	100
31	Y	179/250 (72%)	174 (97%)	5 (3%)	0	100	100
32	Z	120/161 (74%)	117 (98%)	3 (2%)	0	100	100
33	g	132/166 (80%)	129 (98%)	3 (2%)	0	100	100
34	V	203/216 (94%)	200 (98%)	3 (2%)	0	100	100
35	b	148/215 (69%)	142 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	d	257/306 (84%)	242 (94%)	15 (6%)	0	100	100
37	e	236/279 (85%)	226 (96%)	10 (4%)	0	100	100
38	h	108/158 (68%)	104 (96%)	4 (4%)	0	100	100
39	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
40	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
41	k	100/112 (89%)	100 (100%)	0	0	100	100
42	l	80/138 (58%)	78 (98%)	2 (2%)	0	100	100
43	m	90/128 (70%)	86 (96%)	4 (4%)	0	100	100
45	o	92/102 (90%)	92 (100%)	0	0	100	100
46	q	175/222 (79%)	175 (100%)	0	0	100	100
47	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
48	t	44/198 (22%)	44 (100%)	0	0	100	100
48	u	30/198 (15%)	30 (100%)	0	0	100	100
49	c	282/332 (85%)	280 (99%)	2 (1%)	0	100	100
50	f	153/212 (72%)	146 (95%)	7 (5%)	0	100	100
51	p	141/206 (68%)	137 (97%)	4 (3%)	0	100	100
52	s	381/439 (87%)	375 (98%)	6 (2%)	0	100	100
53	AB	223/296 (75%)	216 (97%)	7 (3%)	0	100	100
54	AC	130/167 (78%)	128 (98%)	2 (2%)	0	100	100
55	AD	341/430 (79%)	331 (97%)	10 (3%)	0	100	100
56	AE	120/125 (96%)	117 (98%)	3 (2%)	0	100	100
57	AF	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
58	AG	323/396 (82%)	315 (98%)	8 (2%)	0	100	100
59	AH	138/201 (69%)	131 (95%)	6 (4%)	1 (1%)	18	49
60	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
61	AK	99/128 (77%)	99 (100%)	0	0	100	100
62	AL	172/257 (67%)	169 (98%)	3 (2%)	0	100	100
63	AM	117/137 (85%)	114 (97%)	3 (3%)	0	100	100
64	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100
65	AO	191/258 (74%)	187 (98%)	4 (2%)	0	100	100
66	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	AR	293/360 (81%)	285 (97%)	8 (3%)	0	100	100
68	AS	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
69	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
70	AU	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
71	AV	358/414 (86%)	345 (96%)	13 (4%)	0	100	100
72	AW	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
73	AZ	98/106 (92%)	95 (97%)	3 (3%)	0	100	100
74	A0	213/217 (98%)	208 (98%)	5 (2%)	0	100	100
75	A1	277/323 (86%)	265 (96%)	12 (4%)	0	100	100
76	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
78	AY	117/395 (30%)	117 (100%)	0	0	100	100
80	AI	135/194 (70%)	129 (96%)	6 (4%)	0	100	100
81	OX	51/435 (12%)	47 (92%)	4 (8%)	0	100	100
82	a	99/142 (70%)	96 (97%)	3 (3%)	0	100	100
83	A4	584/689 (85%)	569 (97%)	15 (3%)	0	100	100
84	AX	350/398 (88%)	339 (97%)	11 (3%)	0	100	100
85	A2	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
86	AQ	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
88	Ag	392/455 (86%)	350 (89%)	41 (10%)	1 (0%)	36	65
All	All	14759/19257 (77%)	14396 (98%)	361 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
59	AH	126	ILE
88	Ag	246	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	99/164 (60%)	99 (100%)	0	100	100
2	1	53/60 (88%)	53 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	270/303 (89%)	270 (100%)	0	100	100
9	8	146/190 (77%)	146 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100
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	g	124/148 (84%)	124 (100%)	0	100	100

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	AO	174/230 (76%)	174 (100%)	0	100	100
66	AP	88/123 (72%)	88 (100%)	0	100	100
67	AR	264/318 (83%)	263 (100%)	1 (0%)	84	83
68	AS	116/164 (71%)	116 (100%)	0	100	100
69	AT	153/157 (98%)	153 (100%)	0	100	100
70	AU	152/174 (87%)	152 (100%)	0	100	100
71	AV	325/364 (89%)	325 (100%)	0	100	100
72	AW	87/158 (55%)	87 (100%)	0	100	100
73	AZ	90/95 (95%)	90 (100%)	0	100	100
74	A0	188/189 (100%)	188 (100%)	0	100	100
75	A1	257/291 (88%)	257 (100%)	0	100	100
76	A3	65/166 (39%)	65 (100%)	0	100	100
78	AY	110/357 (31%)	110 (100%)	0	100	100
80	AI	105/147 (71%)	105 (100%)	0	100	100
81	OX	49/372 (13%)	49 (100%)	0	100	100
82	a	99/133 (74%)	99 (100%)	0	100	100
83	A4	526/609 (86%)	526 (100%)	0	100	100
84	AX	311/351 (89%)	311 (100%)	0	100	100
85	A2	100/100 (100%)	100 (100%)	0	100	100
86	AQ	78/78 (100%)	78 (100%)	0	100	100
88	Ag	328/374 (88%)	328 (100%)	0	100	100
All	All	13171/16616 (79%)	13170 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
67	AR	78	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	98	GLN
2	1	31	ASN
6	5	214	ASN

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Mol	Chain	Res	Type
7	6	332	HIS
8	7	207	HIS
8	7	246	GLN
9	8	103	GLN
14	F	97	HIS
14	F	103	GLN
15	H	93	ASN
15	H	178	ASN
15	H	196	ASN
17	J	186	GLN
18	K	94	GLN
19	L	48	ASN
19	L	103	ASN
21	N	101	HIS
24	Q	237	ASN
25	R	22	GLN
26	S	84	ASN
26	S	190	GLN
30	X	175	GLN
31	Y	88	GLN
32	Z	148	GLN
35	b	24	GLN
35	b	120	HIS
36	d	161	HIS
36	d	193	HIS
40	j	63	GLN
41	k	80	HIS
46	q	167	GLN
47	r	109	GLN
49	c	168	HIS
51	p	194	HIS
52	s	87	GLN
52	s	107	GLN
52	s	281	HIS
52	s	358	GLN
52	s	385	GLN
52	s	420	GLN
55	AD	130	GLN
55	AD	155	GLN
55	AD	165	GLN
57	AF	113	GLN
57	AF	122	GLN

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Mol	Chain	Res	Type
61	AK	124	GLN
62	AL	172	ASN
65	AO	81	HIS
65	AO	114	HIS
65	AO	166	HIS
67	AR	76	GLN
67	AR	214	ASN
67	AR	288	GLN
69	AT	101	HIS
70	AU	109	ASN
73	AZ	82	GLN
75	A1	146	HIS
76	A3	140	HIS
76	A3	158	GLN
84	AX	176	GLN
84	AX	190	ASN
88	Ag	130	HIS
88	Ag	136	ASN
88	Ag	164	HIS
88	Ag	181	ASN
88	Ag	350	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1556/1558 (99%)	258 (16%)	3 (0%)
77	Az	33/34 (97%)	15 (45%)	0
79	AA	953/954 (99%)	157 (16%)	2 (0%)
87	Ah	74/77 (96%)	19 (25%)	0
89	Ax	70/71 (98%)	17 (24%)	0
90	B	70/72 (97%)	16 (22%)	0
All	All	2756/2766 (99%)	482 (17%)	5 (0%)

All (482) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1681	G
11	A	1689	C
11	A	1692	A
11	A	1700	U
11	A	1704	U

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Mol	Chain	Res	Type
11	A	1708	A
11	A	1709	G
11	A	1711	C
11	A	1724	A
11	A	1727	A
11	A	1728	U
11	A	1736	A
11	A	1737	A
11	A	1748	G
11	A	1765	C
11	A	1777	A
11	A	1805	A
11	A	1807	U
11	A	1808	A
11	A	1810	A
11	A	1812	C
11	A	1817	C
11	A	1827	C
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	1867	A
11	A	1869	A
11	A	1871	A
11	A	1873	A
11	A	1878	U
11	A	1882	A
11	A	1886	G
11	A	1887	A
11	A	1888	G
11	A	1893	A
11	A	1901	C
11	A	1903	C
11	A	1907	A
11	A	1909	A
11	A	1918	G
11	A	1937	A
11	A	1940	A

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Mol	Chain	Res	Type
11	A	1975	U
11	A	1985	G
11	A	1986	A
11	A	1992	C
11	A	1994	A
11	A	2001	C
11	A	2003	A
11	A	2015	G
11	A	2022	G
11	A	2030	U
11	A	2036	C
11	A	2037	U
11	A	2039	A
11	A	2054	U
11	A	2060	A
11	A	2068	C
11	A	2069	U
11	A	2071	U
11	A	2079	C
11	A	2099	U
11	A	2105	G
11	A	2111	C
11	A	2113	G
11	A	2125	C
11	A	2126	U
11	A	2133	A
11	A	2147	G
11	A	2155	A
11	A	2159	U
11	A	2160	A
11	A	2163	A
11	A	2168	U
11	A	2180	A
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

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Mol	Chain	Res	Type
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	2284	C
11	A	2285	U
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	2390	A
11	A	2399	A
11	A	2401	A
11	A	2404	U
11	A	2407	U
11	A	2415	C
11	A	2434	A
11	A	2446	A
11	A	2451	A

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Mol	Chain	Res	Type
11	A	2478	G
11	A	2484	C
11	A	2485	U
11	A	2493	C
11	A	2502	C
11	A	2504	A
11	A	2511	C
11	A	2520	C
11	A	2521	A
11	A	2527	A
11	A	2540	C
11	A	2557	C
11	A	2570	C
11	A	2571	G
11	A	2592	G
11	A	2593	G
11	A	2594	U
11	A	2599	U
11	A	2600	A
11	A	2601	A
11	A	2603	C
11	A	2606	U
11	A	2618	U
11	A	2625	C
11	A	2627	G
11	A	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

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Mol	Chain	Res	Type
11	A	2732	G
11	A	2745	A
11	A	2757	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	2775	A
11	A	2783	A
11	A	2786	U
11	A	2790	A
11	A	2810	G
11	A	2832	A
11	A	2833	A
11	A	2847	C
11	A	2864	U
11	A	2865	C
11	A	2883	A
11	A	2884	C
11	A	2885	U
11	A	2888	A
11	A	2889	C
11	A	2893	A
11	A	2913	A
11	A	2916	G
11	A	2917	G
11	A	2918	A
11	A	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

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Mol	Chain	Res	Type
11	A	3005	A
11	A	3007	C
11	A	3016	G
11	A	3022	G
11	A	3041	U
11	A	3049	U
11	A	3053	A
11	A	3054	G
11	A	3060	C
11	A	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
11	A	3169	C
11	A	3172	C
11	A	3177	A
11	A	3180	A
11	A	3183	U
11	A	3189	C
11	A	3190	A
11	A	3199	U
11	A	3200	U
11	A	3202	U
11	A	3207	A
11	A	3209	A
11	A	3210	C
11	A	3212	C
11	A	3217	A
11	A	3218	A
11	A	3228	U

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Mol	Chain	Res	Type
11	A	3229	U
77	Az	0	U
77	Az	4	A
77	Az	11	U
77	Az	12	U
77	Az	13	U
77	Az	15	U
77	Az	18	A
77	Az	21	A
77	Az	22	A
77	Az	23	U
77	Az	24	U
77	Az	25	U
77	Az	26	A
77	Az	27	C
77	Az	31	A
79	AA	651	A
79	AA	680	U
79	AA	687	G
79	AA	688	A
79	AA	691	A
79	AA	704	U
79	AA	706	C
79	AA	721	U
79	AA	722	C
79	AA	735	A
79	AA	737	C
79	AA	738	A
79	AA	745	A
79	AA	753	A
79	AA	761	A
79	AA	766	G
79	AA	791	G
79	AA	794	U
79	AA	796	G
79	AA	828	C
79	AA	830	U
79	AA	832	U
79	AA	835	C
79	AA	836	A
79	AA	842	C
79	AA	860	A

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Mol	Chain	Res	Type
79	AA	861	U
79	AA	868	C
79	AA	870	C
79	AA	871	A
79	AA	872	G
79	AA	881	A
79	AA	884	U
79	AA	889	G
79	AA	890	C
79	AA	893	G
79	AA	899	G
79	AA	903	U
79	AA	904	C
79	AA	907	A
79	AA	909	G
79	AA	910	A
79	AA	919	A
79	AA	929	A
79	AA	930	G
79	AA	933	G
79	AA	938	A
79	AA	939	A
79	AA	942	A
79	AA	958	C
79	AA	959	C
79	AA	960	C
79	AA	961	U
79	AA	962	C
79	AA	967	A
79	AA	978	A
79	AA	993	A
79	AA	1001	C
79	AA	1002	C
79	AA	1011	C
79	AA	1015	A
79	AA	1022	A
79	AA	1031	G
79	AA	1042	U
79	AA	1046	A
79	AA	1080	A
79	AA	1081	U
79	AA	1082	A

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Mol	Chain	Res	Type
79	AA	1096	A
79	AA	1103	A
79	AA	1105	C
79	AA	1106	C
79	AA	1107	U
79	AA	1109	A
79	AA	1118	A
79	AA	1119	U
79	AA	1121	A
79	AA	1126	A
79	AA	1137	A
79	AA	1138	G
79	AA	1143	C
79	AA	1151	C
79	AA	1152	A
79	AA	1153	C
79	AA	1155	G
79	AA	1160	A
79	AA	1167	A
79	AA	1187	U
79	AA	1188	A
79	AA	1189	U
79	AA	1190	C
79	AA	1215	U
79	AA	1220	A
79	AA	1223	C
79	AA	1225	C
79	AA	1230	C
79	AA	1232	A
79	AA	1235	U
79	AA	1247	G
79	AA	1248	C
79	AA	1251	A
79	AA	1254	C
79	AA	1261	C
79	AA	1271	C
79	AA	1273	G
79	AA	1284	U
79	AA	1290	C
79	AA	1291	U
79	AA	1292	A
79	AA	1293	C

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Mol	Chain	Res	Type
79	AA	1297	G
79	AA	1300	A
79	AA	1318	A
79	AA	1326	A
79	AA	1327	G
79	AA	1330	C
79	AA	1343	A
79	AA	1344	U
79	AA	1353	A
79	AA	1354	A
79	AA	1355	G
79	AA	1356	A
79	AA	1378	C
79	AA	1386	U
79	AA	1387	A
79	AA	1390	A
79	AA	1405	C
79	AA	1420	U
79	AA	1422	G
79	AA	1430	A
79	AA	1466	C
79	AA	1478	A
79	AA	1481	C
79	AA	1482	A
79	AA	1512	A
79	AA	1519	A
79	AA	1521	U
79	AA	1522	U
79	AA	1525	C
79	AA	1526	U
79	AA	1527	A
79	AA	1528	A
79	AA	1533	C
79	AA	1537	C
79	AA	1538	G
79	AA	1539	C
79	AA	1540	A
79	AA	1551	G
79	AA	1557	A
79	AA	1560	U
79	AA	1568	U
79	AA	1571	U

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Mol	Chain	Res	Type
79	AA	1582	G
79	AA	1584	MA6
79	AA	1594	G
79	AA	1595	G
79	AA	1599	A
87	Ah	8	U
87	Ah	10	G
87	Ah	13	U
87	Ah	19	G
87	Ah	20	U
87	Ah	21	U
87	Ah	22	A
87	Ah	31	G
87	Ah	32	C
87	Ah	34	U
87	Ah	37	C
87	Ah	45	A
87	Ah	47	G
87	Ah	48	U
87	Ah	50	C
87	Ah	59	A
87	Ah	71	A
87	Ah	76	C
87	Ah	77	A
89	Ax	13	U
89	Ax	14	A
89	Ax	16	A
89	Ax	17	U
89	Ax	18	A
89	Ax	22	U
89	Ax	43	A
89	Ax	44	U
89	Ax	47	U
89	Ax	48	G
89	Ax	50	U
89	Ax	51	U
89	Ax	52	A
89	Ax	56	C
89	Ax	63	G
89	Ax	65	A
89	Ax	71	A
90	B	8	U

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Mol	Chain	Res	Type
90	B	10	2MG
90	B	16	C
90	B	19	C
90	B	21	A
90	B	45	G
90	B	46	A
90	B	54	C
90	B	55	U
90	B	56	U
90	B	58	A
90	B	59	A
90	B	64	A
90	B	69	U
90	B	72	G
90	B	76	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	2112	A
11	A	2245	A
11	A	2484	C
79	AA	1108	C
79	AA	1520	U

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

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	$\# Z > 2$
79	B8T	AA	1486	79,95	19,22,23	0.41	0	25,31,34	0.32	0
90	2MG	B	10	90	23,26,27	0.35	0	33,38,41	0.41	0
79	MA6	AA	1583	79	23,26,27	0.34	0	33,38,41	0.71	1 (3%)

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	0.44	0	30,37,40	0.60	0
11	OMU	A	3039	11,92	19,22,23	0.31	0	25,31,34	0.79	1 (4%)
11	OMG	A	3040	11	23,26,27	0.35	0	32,38,41	0.40	0
79	5MU	AA	1076	79	19,22,23	0.39	0	27,32,35	0.63	0
90	PSU	B	39	90	18,21,22	1.03	1 (5%)	21,30,33	0.74	0
11	PSU	A	3067	11	18,21,22	1.14	2 (11%)	21,30,33	0.83	1 (4%)
79	5MC	AA	1488	79	19,22,23	0.85	1 (5%)	26,32,35	0.51	0
11	OMG	A	2815	11,92,89	23,26,27	0.37	0	32,38,41	0.45	0
79	MA6	AA	1584	79	23,26,27	0.32	0	33,38,41	0.72	1 (3%)
90	1MA	B	9	90	21,25,26	0.41	0	30,37,40	0.66	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
79	B8T	AA	1486	79,95	-	0/7/27/28	0/2/2/2
90	2MG	B	10	90	-	0/9/27/28	0/3/3/3
79	MA6	AA	1583	79	-	0/11/29/30	0/3/3/3
11	1MA	A	2617	11	-	0/7/25/26	0/3/3/3
11	OMU	A	3039	11,92	-	0/9/27/28	0/2/2/2
11	OMG	A	3040	11	-	2/9/27/28	0/3/3/3
79	5MU	AA	1076	79	-	5/7/25/26	0/2/2/2
90	PSU	B	39	90	-	0/7/25/26	0/2/2/2
11	PSU	A	3067	11	-	0/7/25/26	0/2/2/2
79	5MC	AA	1488	79	-	0/7/25/26	0/2/2/2
11	OMG	A	2815	11,92,89	-	0/9/27/28	0/3/3/3
79	MA6	AA	1584	79	-	1/11/29/30	0/3/3/3
90	1MA	B	9	90	-	0/7/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	B	39	PSU	C6-C5	3.52	1.39	1.35
11	A	3067	PSU	C6-C5	3.49	1.39	1.35
79	AA	1488	5MC	C5-C4	-3.38	1.41	1.44
11	A	3067	PSU	O4'-C1'	-2.75	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	3039	OMU	C2'-C1'-N1	-3.04	108.47	114.24
79	AA	1583	MA6	C2-N1-C6	2.92	118.96	111.83
79	AA	1584	MA6	C2-N1-C6	2.92	118.95	111.83
11	A	3067	PSU	O4'-C1'-C2'	2.34	108.39	105.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
79	AA	1486	B8T	1	0
79	AA	1583	MA6	5	0
11	A	3039	OMU	1	0
79	AA	1076	5MU	1	0
79	AA	1488	5MC	2	0
11	A	2815	OMG	1	0
90	B	9	1MA	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
97	NAD	AA	1701	95	46,48,48	1.19	3 (6%)	64,73,73	0.81	2 (3%)
93	SPD	AA	1782	-	9,9,9	0.15	0	8,8,8	0.17	0
93	SPD	A	3472	-	9,9,9	0.16	0	8,8,8	0.21	0
98	SPM	AA	1780	-	13,13,13	0.16	0	12,12,12	0.22	0
100	GDP	AX	503	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)
93	SPD	AA	1703	-	9,9,9	0.15	0	8,8,8	0.20	0
96	FES	r	201	16,47	0,4,4	-	-	-	-	-
101	VAL	B	101	90	4,6,7	0.81	0	6,7,9	1.06	1 (16%)
93	SPD	A	3470	-	9,9,9	0.16	0	8,8,8	0.22	0
93	SPD	A	3471	-	9,9,9	0.14	0	8,8,8	0.19	0
99	ATP	AX	501	95	32,33,33	0.66	1 (3%)	48,52,52	0.34	0
96	FES	AP	201	66,56	0,4,4	-	-	-	-	-
98	SPM	AA	1702	-	13,13,13	0.17	0	12,12,12	0.30	0
96	FES	AT	201	69,63	0,4,4	-	-	-	-	-
93	SPD	A	3302	-	9,9,9	0.16	0	8,8,8	0.23	0
93	SPD	A	3301	-	9,9,9	0.15	0	8,8,8	0.20	0
94	PUT	A	3303	-	5,5,5	0.14	0	4,4,4	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
97	NAD	AA	1701	95	-	3/30/62/62	0/5/5/5
93	SPD	AA	1782	-	-	0/7/7/7	-
93	SPD	A	3472	-	-	0/7/7/7	-
98	SPM	AA	1780	-	-	3/11/11/11	-
100	GDP	AX	503	-	-	9/16/32/32	0/3/3/3
93	SPD	AA	1703	-	-	0/7/7/7	-
96	FES	r	201	16,47	-	-	0/1/1/1
101	VAL	B	101	90	-	2/5/6/8	-
93	SPD	A	3470	-	-	0/7/7/7	-
93	SPD	A	3471	-	-	1/7/7/7	-
99	ATP	AX	501	95	-	0/22/38/38	0/3/3/3
98	SPM	AA	1702	-	-	0/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
96	FES	AP	201	66,56	-	-	0/1/1/1
96	FES	AT	201	69,63	-	-	0/1/1/1
93	SPD	A	3302	-	-	1/7/7/7	-
93	SPD	A	3301	-	-	0/7/7/7	-
94	PUT	A	3303	-	-	0/3/3/3	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	AA	1701	NAD	PA-O3	4.92	1.64	1.59
100	AX	503	GDP	C5-C4	3.06	1.47	1.38
99	AX	501	ATP	PB-O3B	-2.98	1.56	1.59
97	AA	1701	NAD	PN-O3	2.87	1.62	1.59
97	AA	1701	NAD	O4D-C1D	-2.67	1.37	1.40
100	AX	503	GDP	C6-N1	-2.57	1.34	1.38
100	AX	503	GDP	C5-N7	-2.05	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
100	AX	503	GDP	C5-C4-N3	-6.08	118.71	128.39
100	AX	503	GDP	C2-N3-C4	5.04	120.98	112.30
100	AX	503	GDP	N9-C4-N3	4.55	135.04	125.95
100	AX	503	GDP	C6-C5-N7	3.37	136.42	130.29
100	AX	503	GDP	C4-C5-N7	-2.60	106.55	110.67
101	B	101	VAL	O-C-CA	-2.33	118.78	124.77
97	AA	1701	NAD	O2A-PA-O1A	2.18	122.57	112.44
97	AA	1701	NAD	O3-PA-O1A	-2.17	104.19	110.70
100	AX	503	GDP	O6-C6-C5	-2.04	121.14	126.53
100	AX	503	GDP	C3'-C2'-C1'	2.01	105.26	101.46

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
100	AX	503	GDP	PA-O3A-PB-O3B
100	AX	503	GDP	C5'-O5'-PA-O2A
101	B	101	VAL	O-C-CA-CB
98	AA	1780	SPM	C7-C8-C9-N10
98	AA	1780	SPM	C6-C7-C8-C9
97	AA	1701	NAD	O4D-C4D-C5D-O5D

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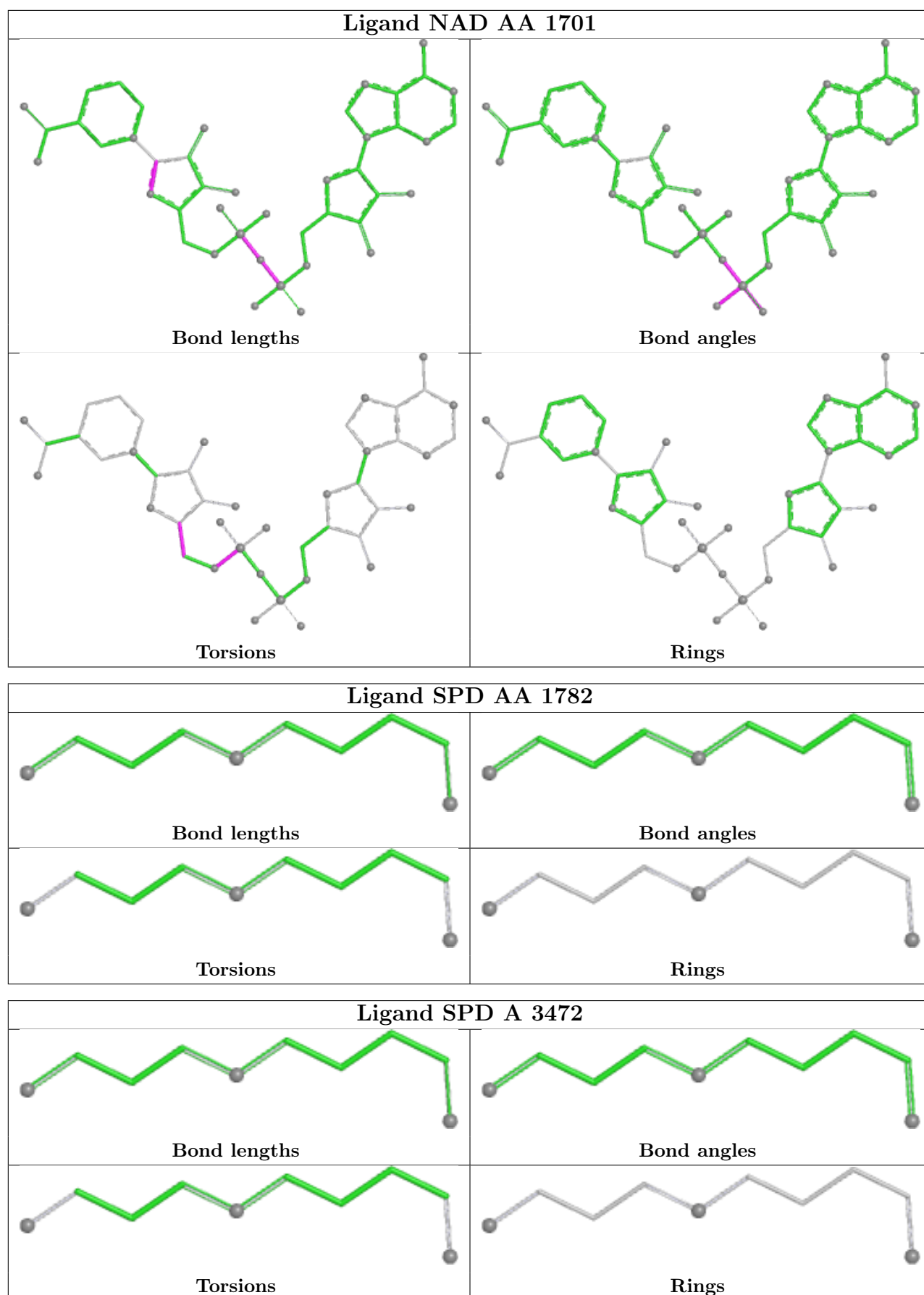
Mol	Chain	Res	Type	Atoms
97	AA	1701	NAD	C3D-C4D-C5D-O5D
100	AX	503	GDP	O4'-C4'-C5'-O5'
93	A	3302	SPD	C4-C5-N6-C7
101	B	101	VAL	C-CA-CB-CG2
97	AA	1701	NAD	C5D-O5D-PN-O1N
100	AX	503	GDP	C5'-O5'-PA-O3A
100	AX	503	GDP	C5'-O5'-PA-O1A
98	AA	1780	SPM	N5-C6-C7-C8
100	AX	503	GDP	C4'-C5'-O5'-PA
100	AX	503	GDP	PA-O3A-PB-O1B
100	AX	503	GDP	PA-O3A-PB-O2B
100	AX	503	GDP	C3'-C4'-C5'-O5'
93	A	3471	SPD	C3-C4-C5-N6

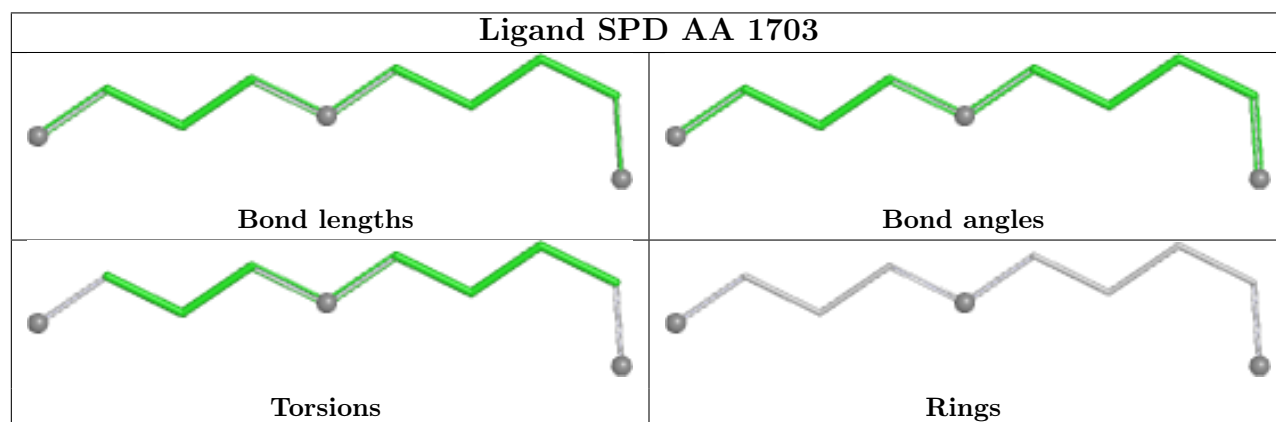
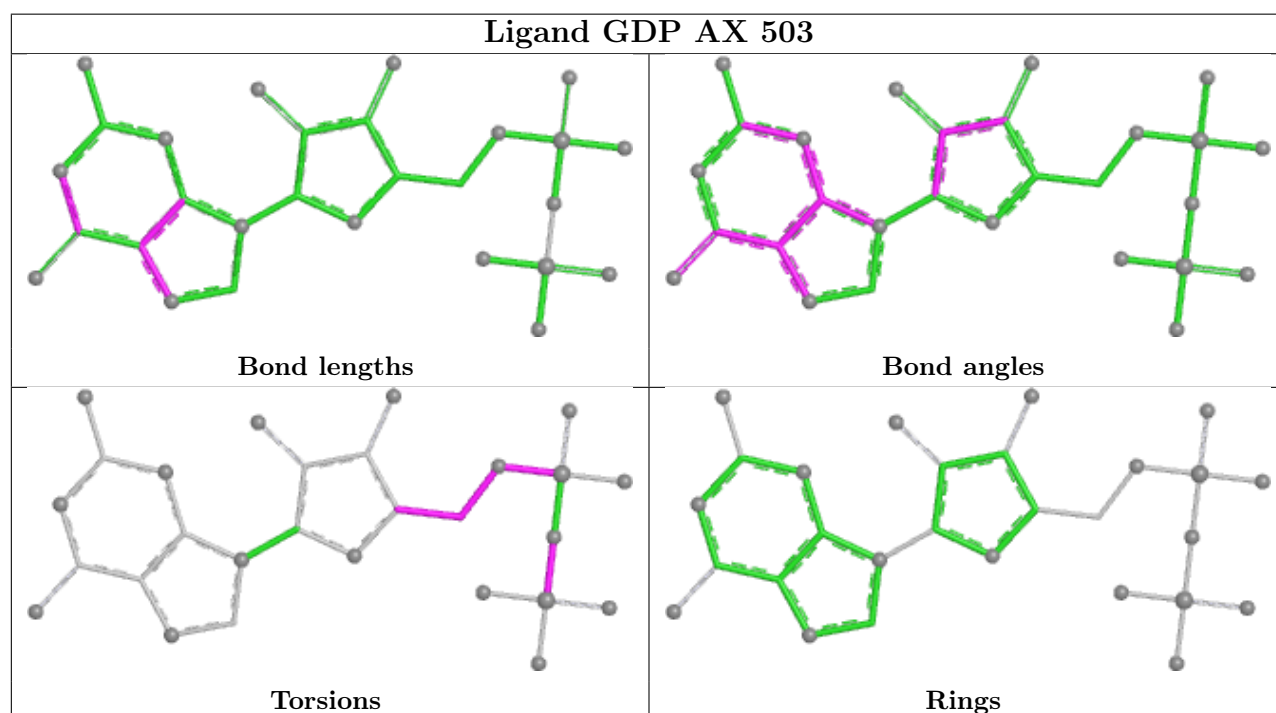
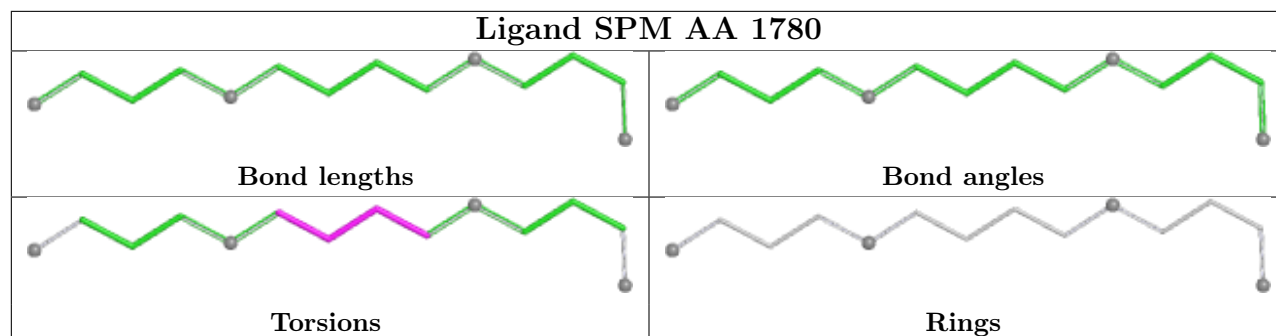
There are no ring outliers.

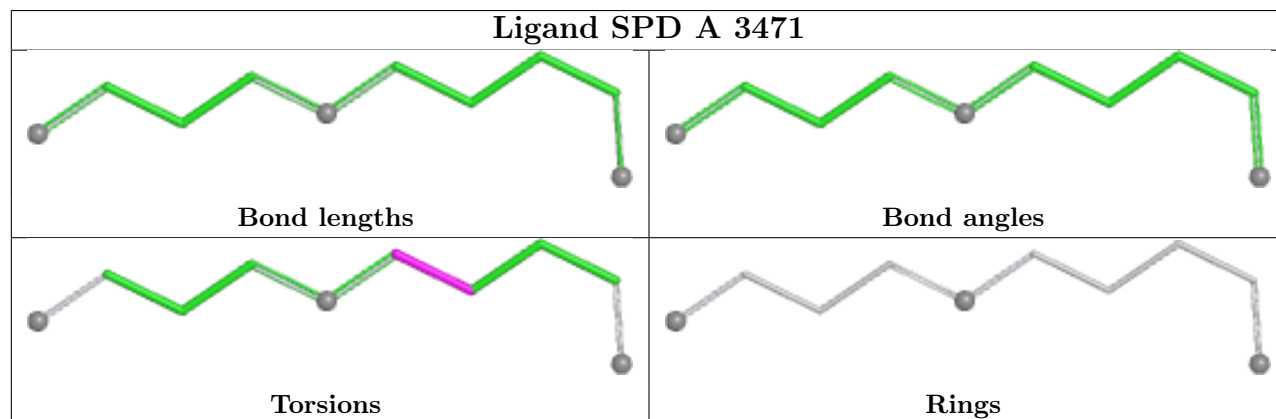
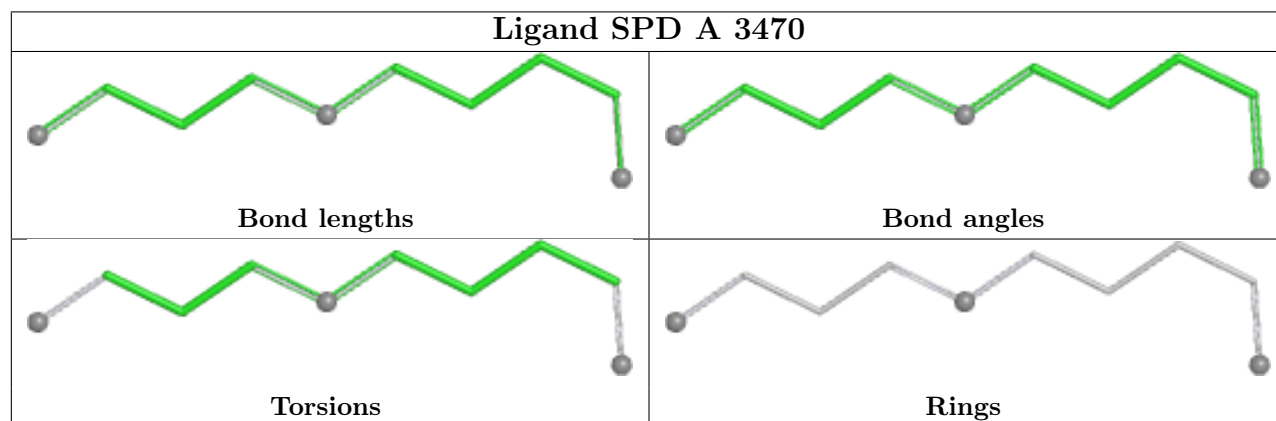
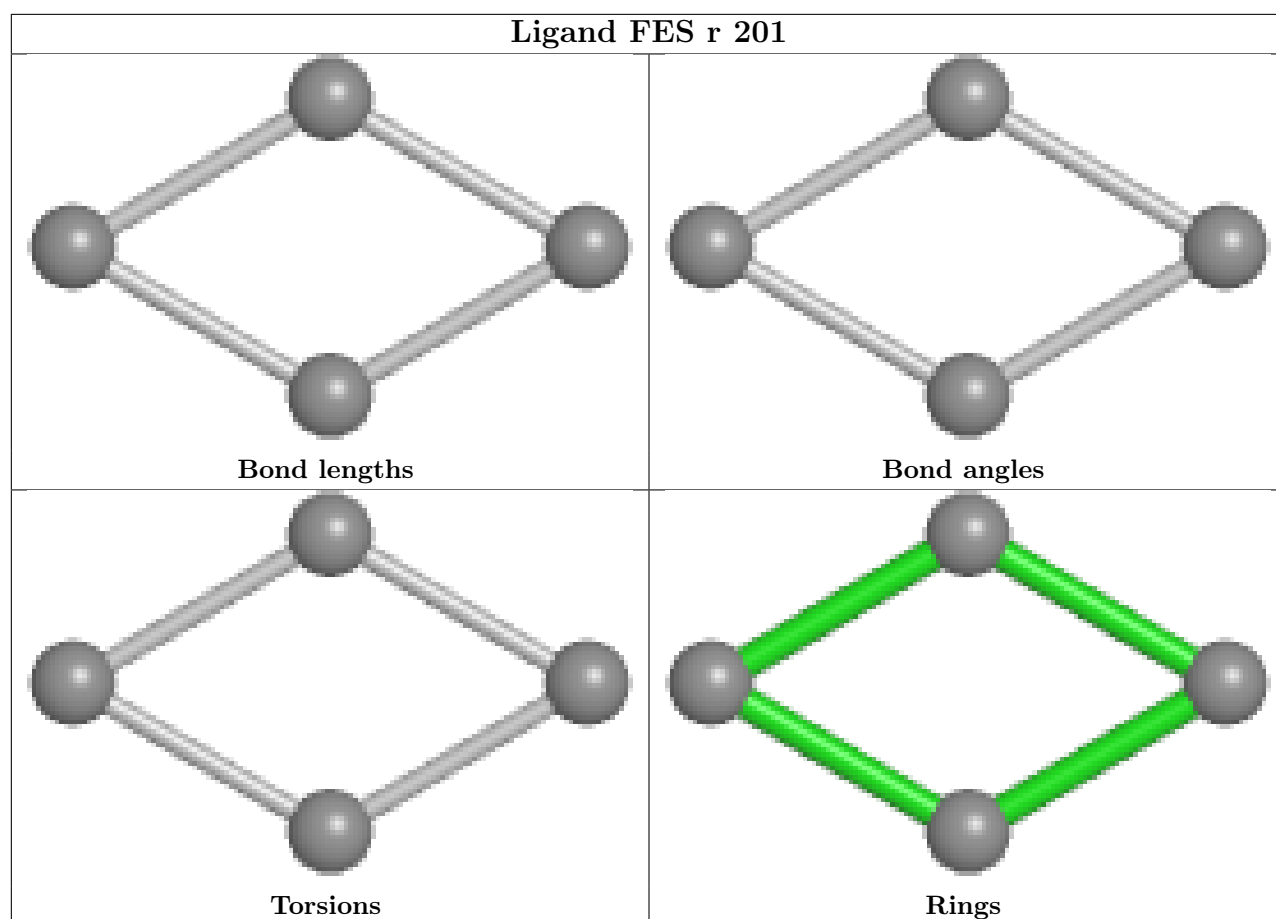
7 monomers are involved in 10 short contacts:

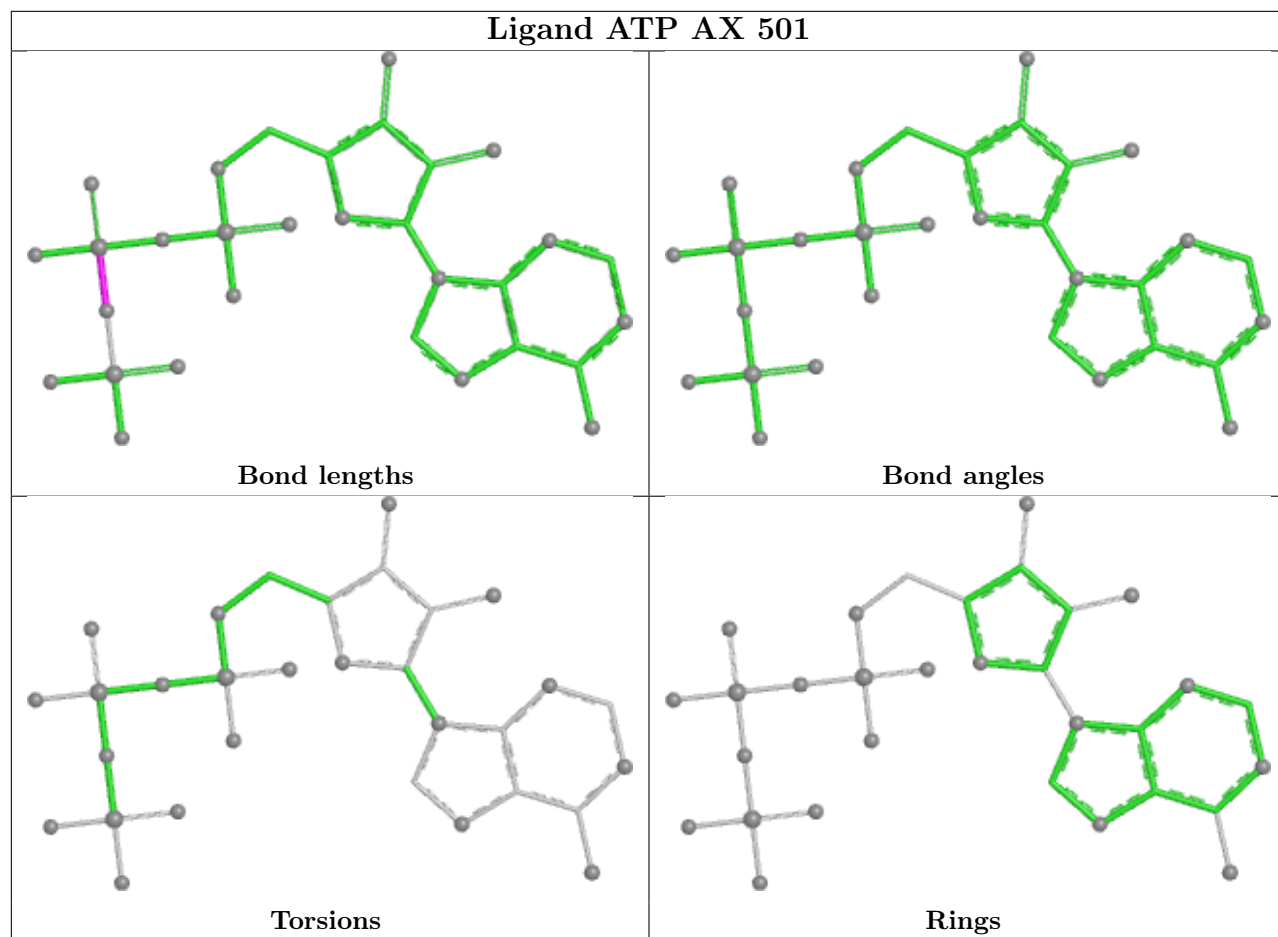
Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	AA	1701	NAD	1	0
93	A	3472	SPD	2	0
98	AA	1780	SPM	1	0
100	AX	503	GDP	3	0
93	AA	1703	SPD	1	0
101	B	101	VAL	1	0
93	A	3301	SPD	1	0

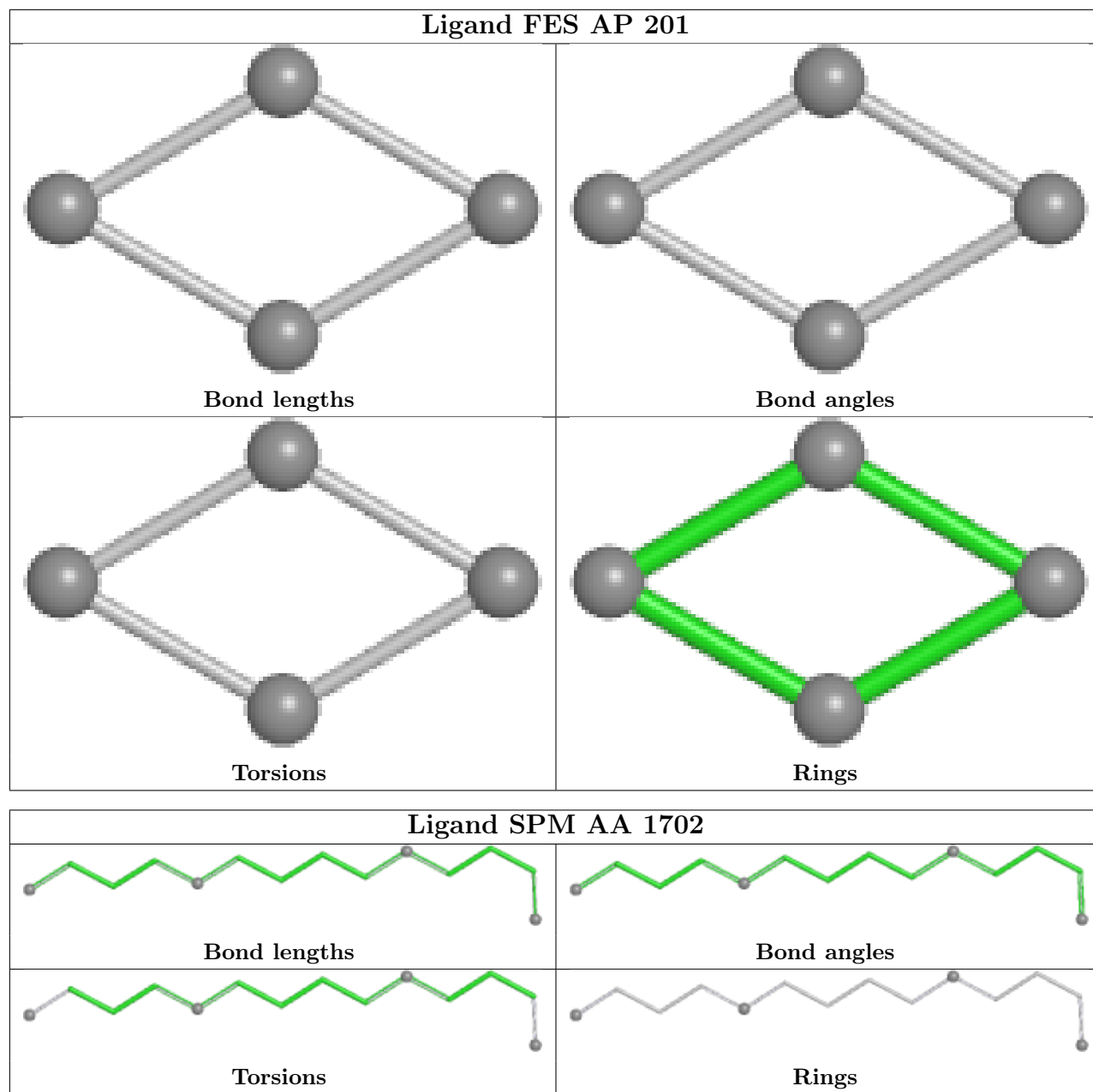
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

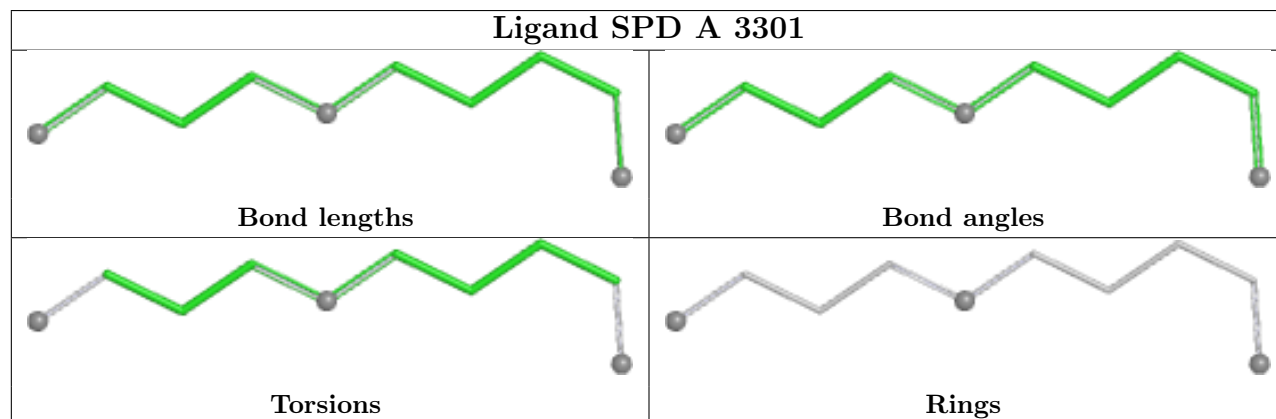
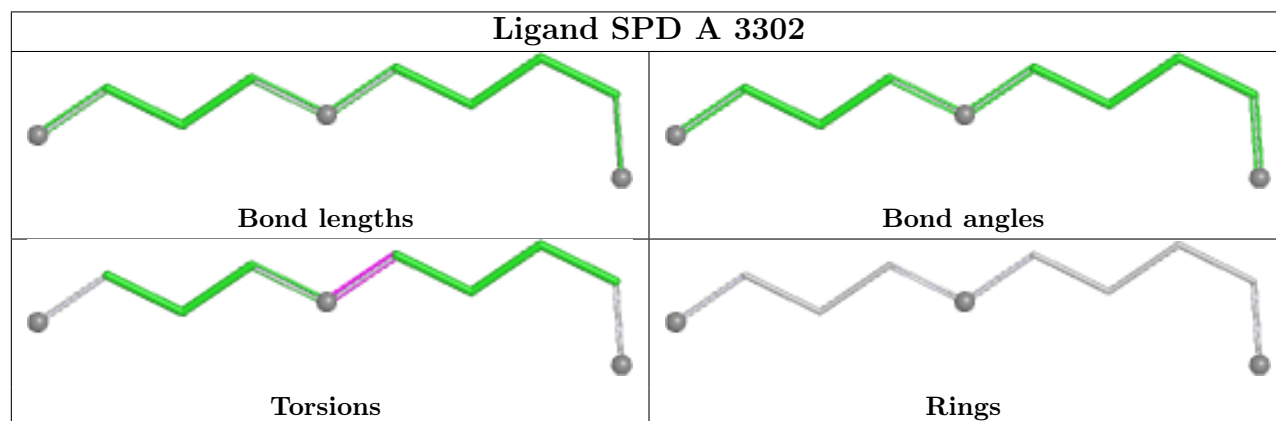
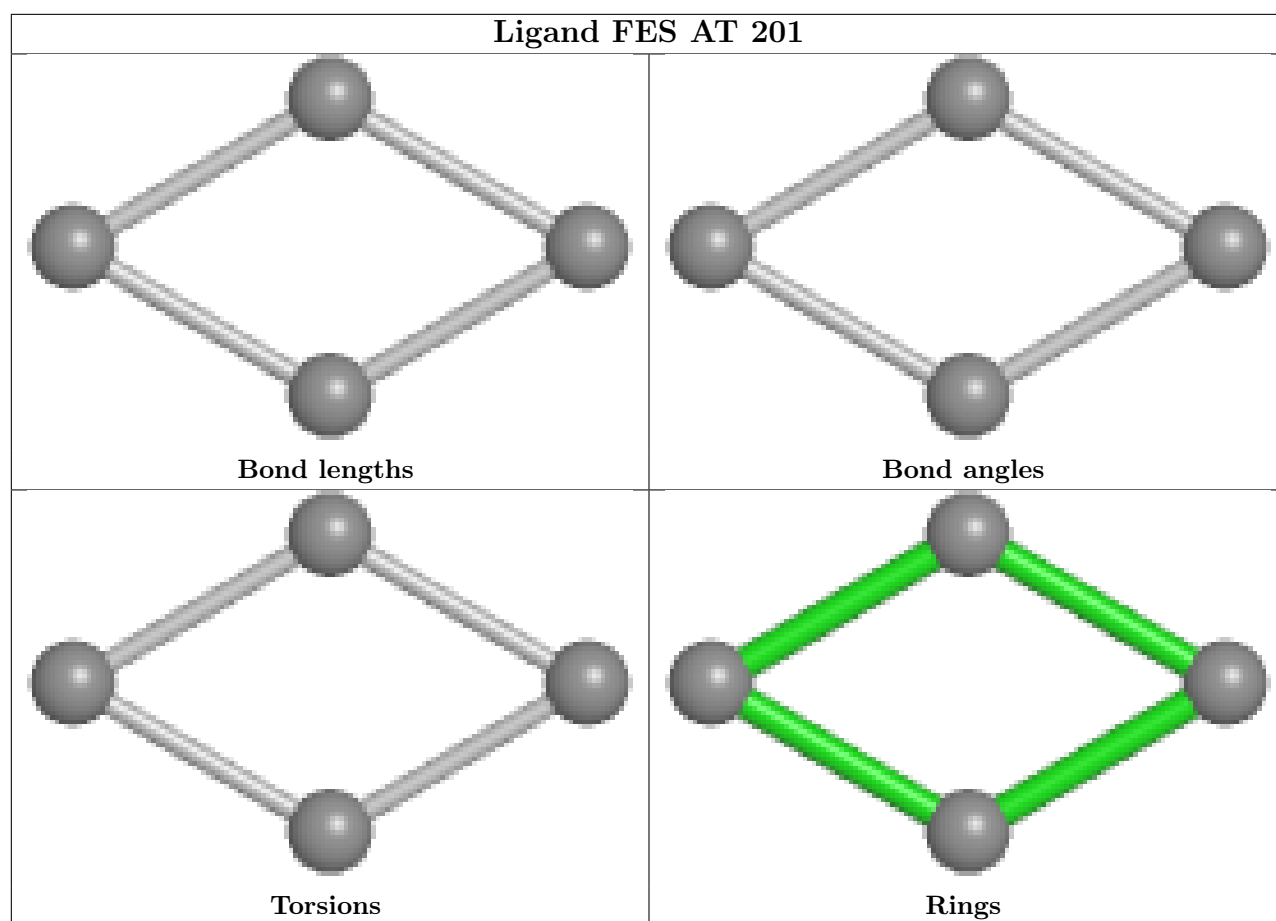












5.7 Other polymers [i](#)

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
90	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	8.56
1	B	46:A	O3'	48:U	P	4.51

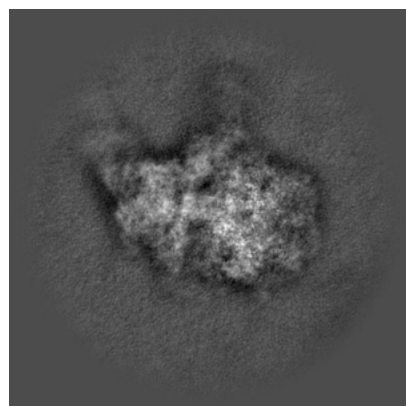
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71811. These allow visual inspection of the internal detail of the map and identification of artifacts.

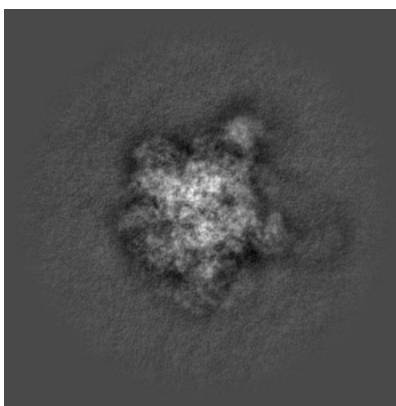
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

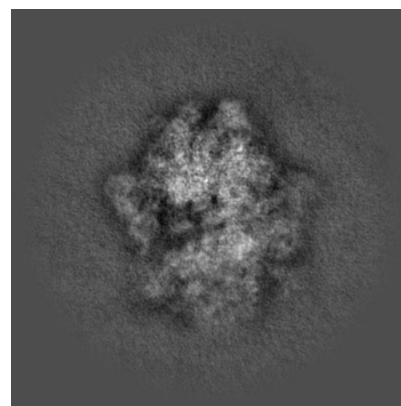
6.1.1 Primary map



X

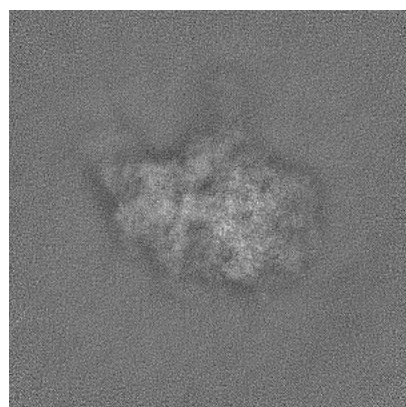


Y

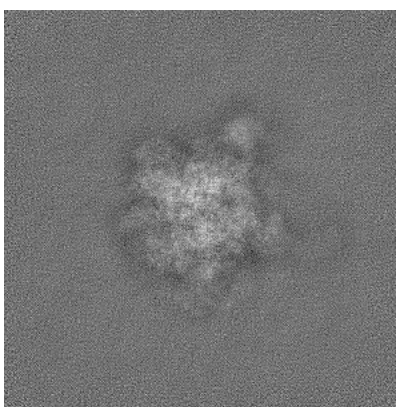


Z

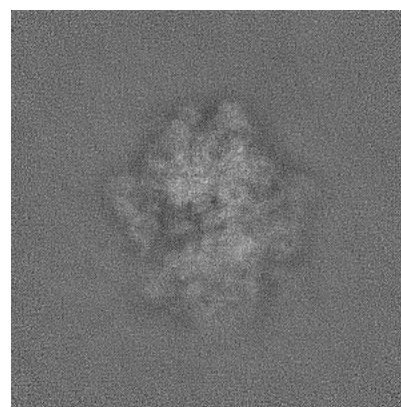
6.1.2 Raw map



X



Y

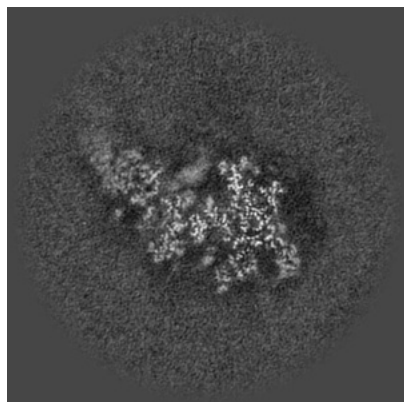


Z

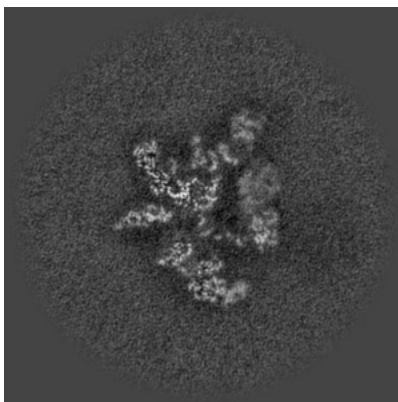
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

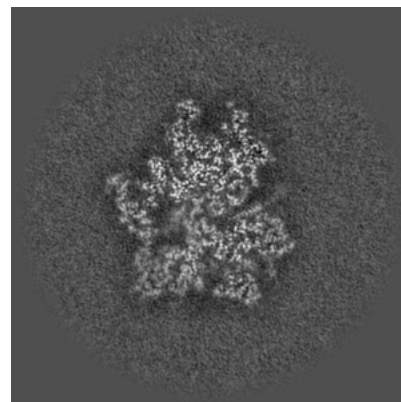
6.2.1 Primary map



X Index: 240

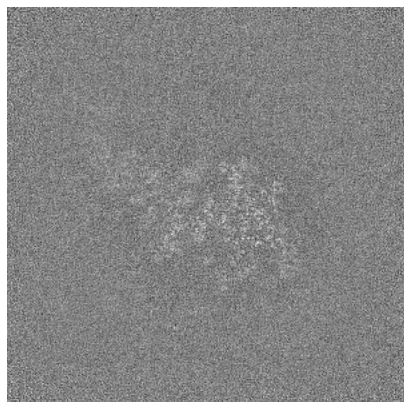


Y Index: 240

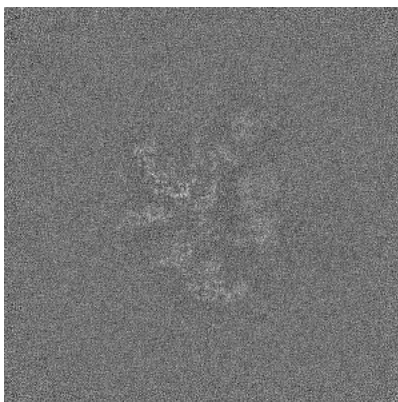


Z Index: 240

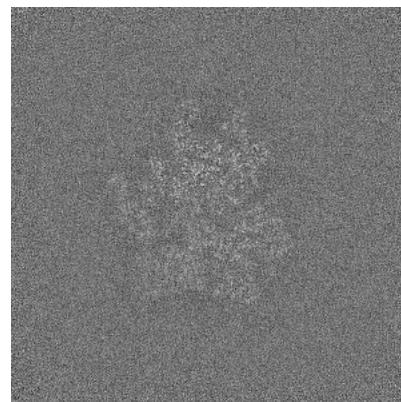
6.2.2 Raw map



X Index: 240



Y Index: 240

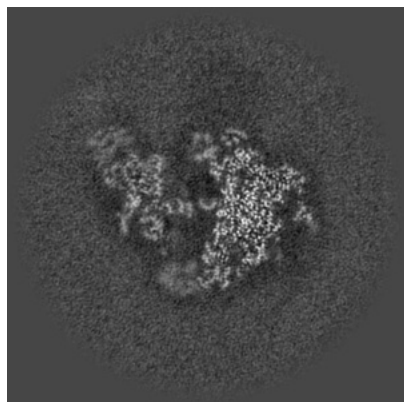


Z Index: 240

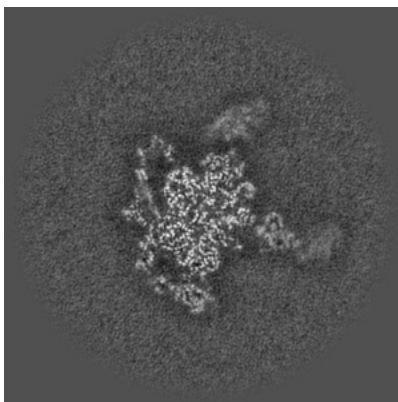
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

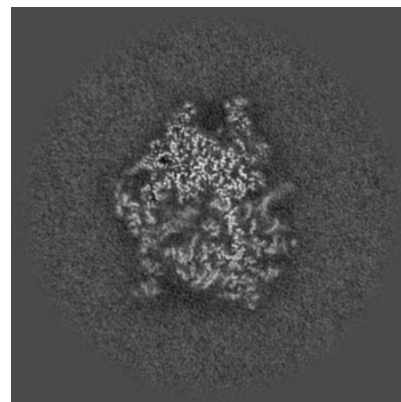
6.3.1 Primary map



X Index: 224

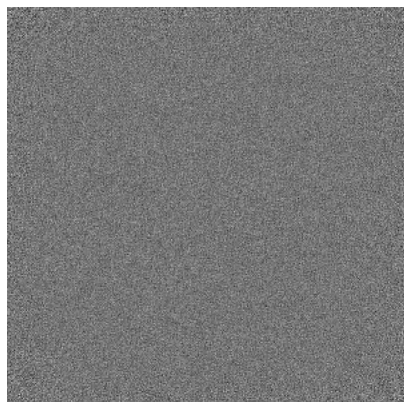


Y Index: 266

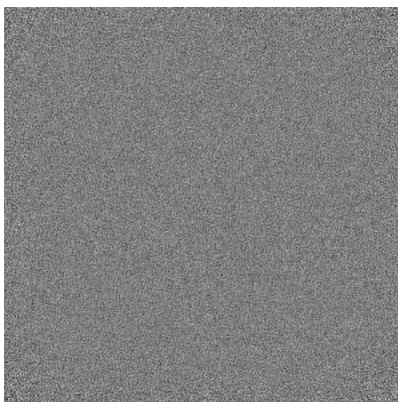


Z Index: 249

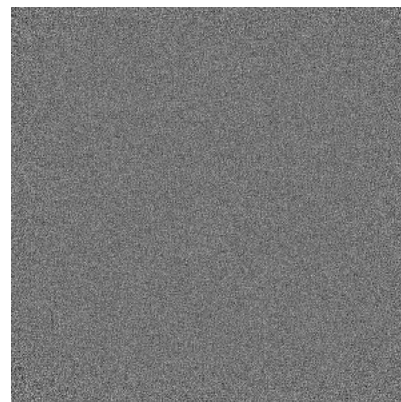
6.3.2 Raw map



X Index: 0



Y Index: 0

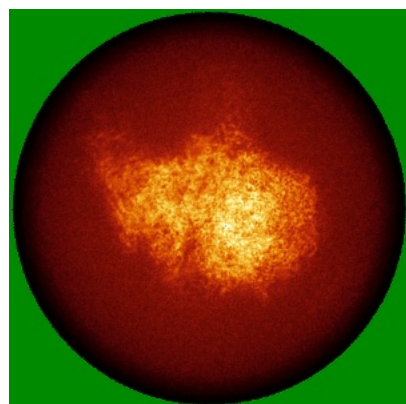


Z Index: 0

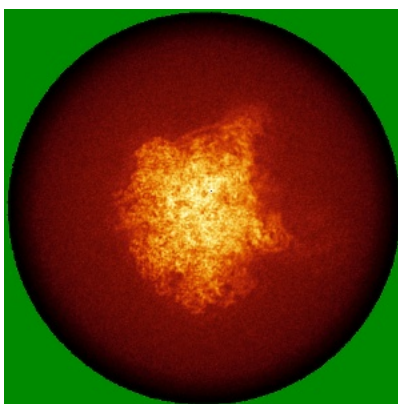
The images above show the largest variance slices of the map in three orthogonal directions.

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

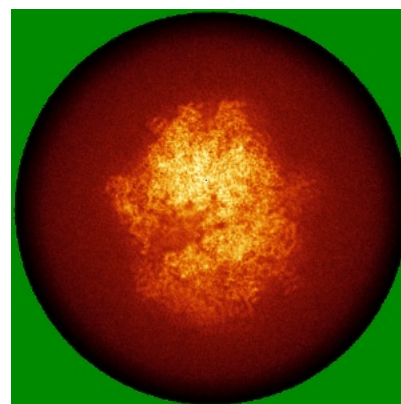
6.4.1 Primary map



X

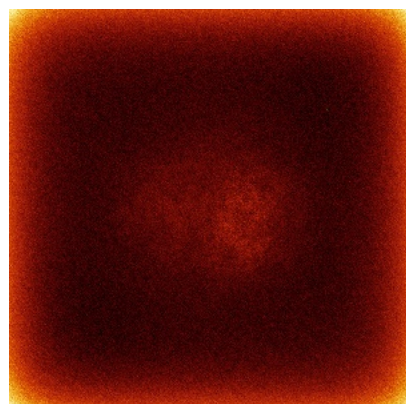


Y

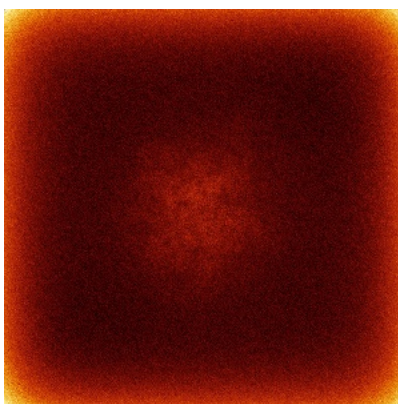


Z

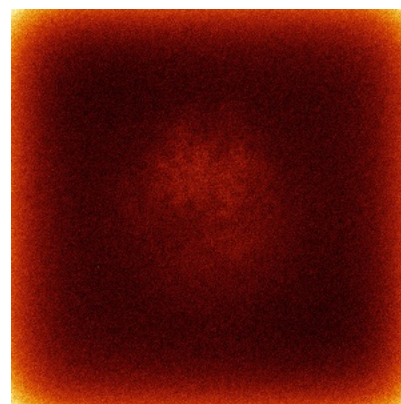
6.4.2 Raw map



X



Y



Z

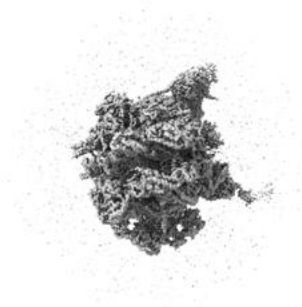
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



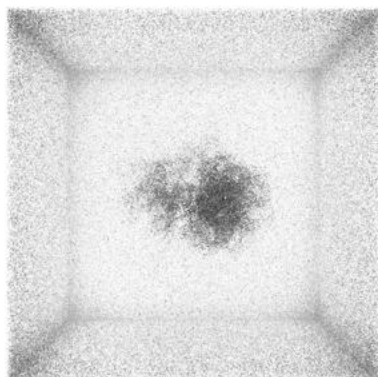
Y



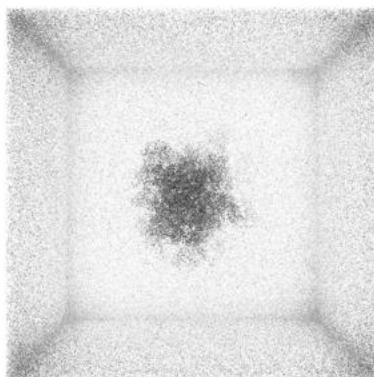
Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

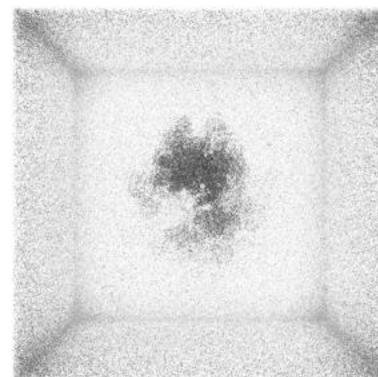
6.5.2 Raw map



X



Y



Z

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

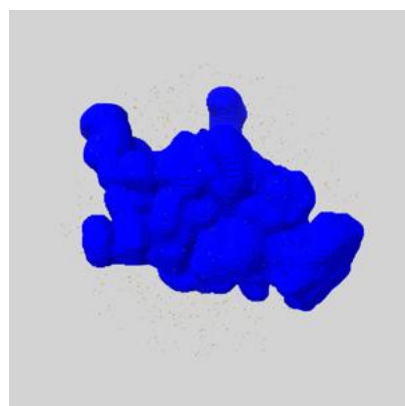
6.6 Mask visualisation [i](#)

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

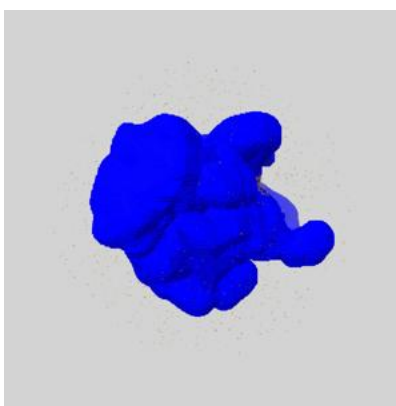
A mask typically either:

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

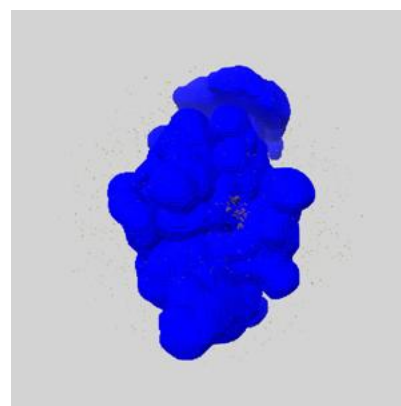
6.6.1 emd_71811_msk_1.map [i](#)



X



Y

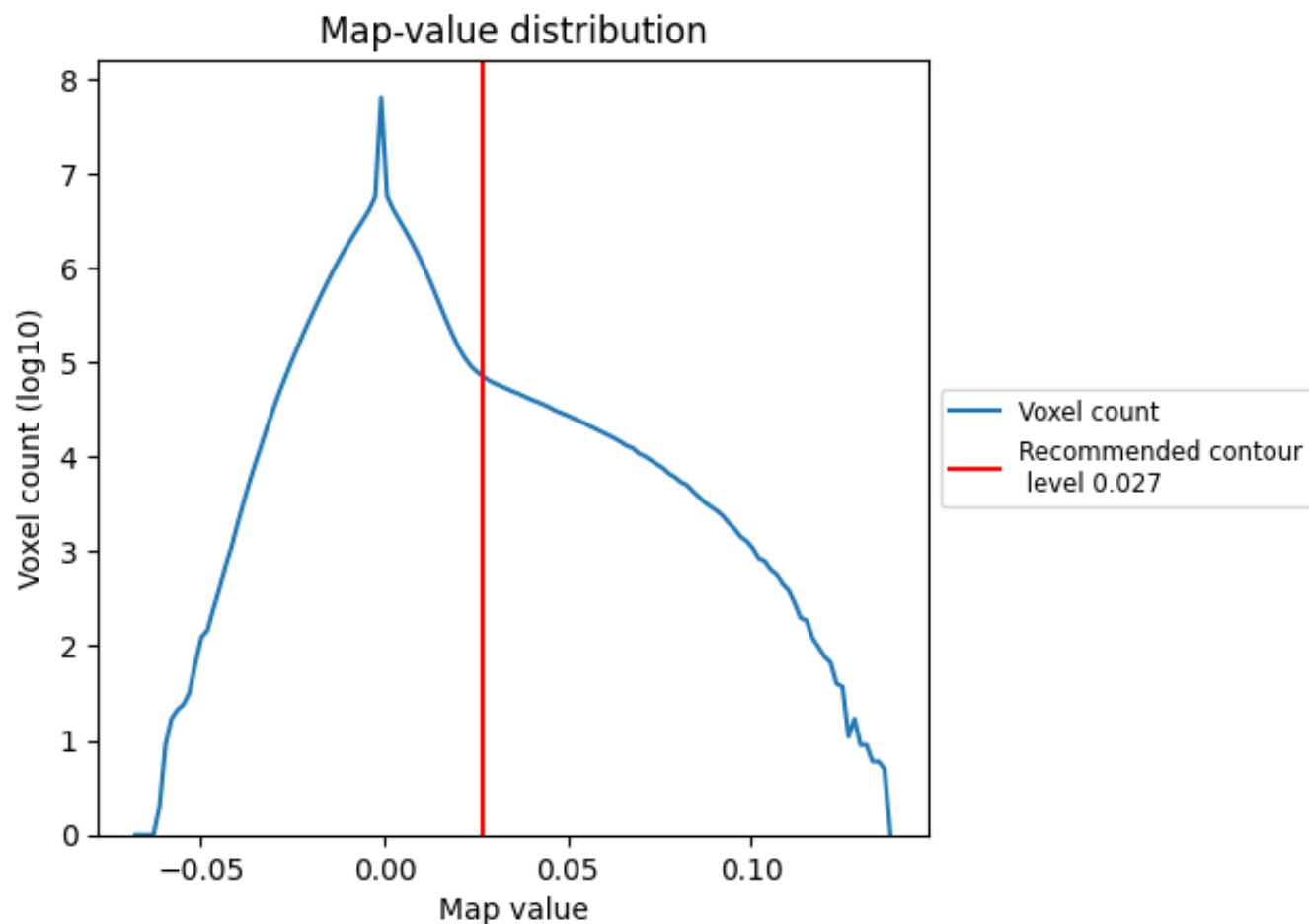


Z

7 Map analysis [i](#)

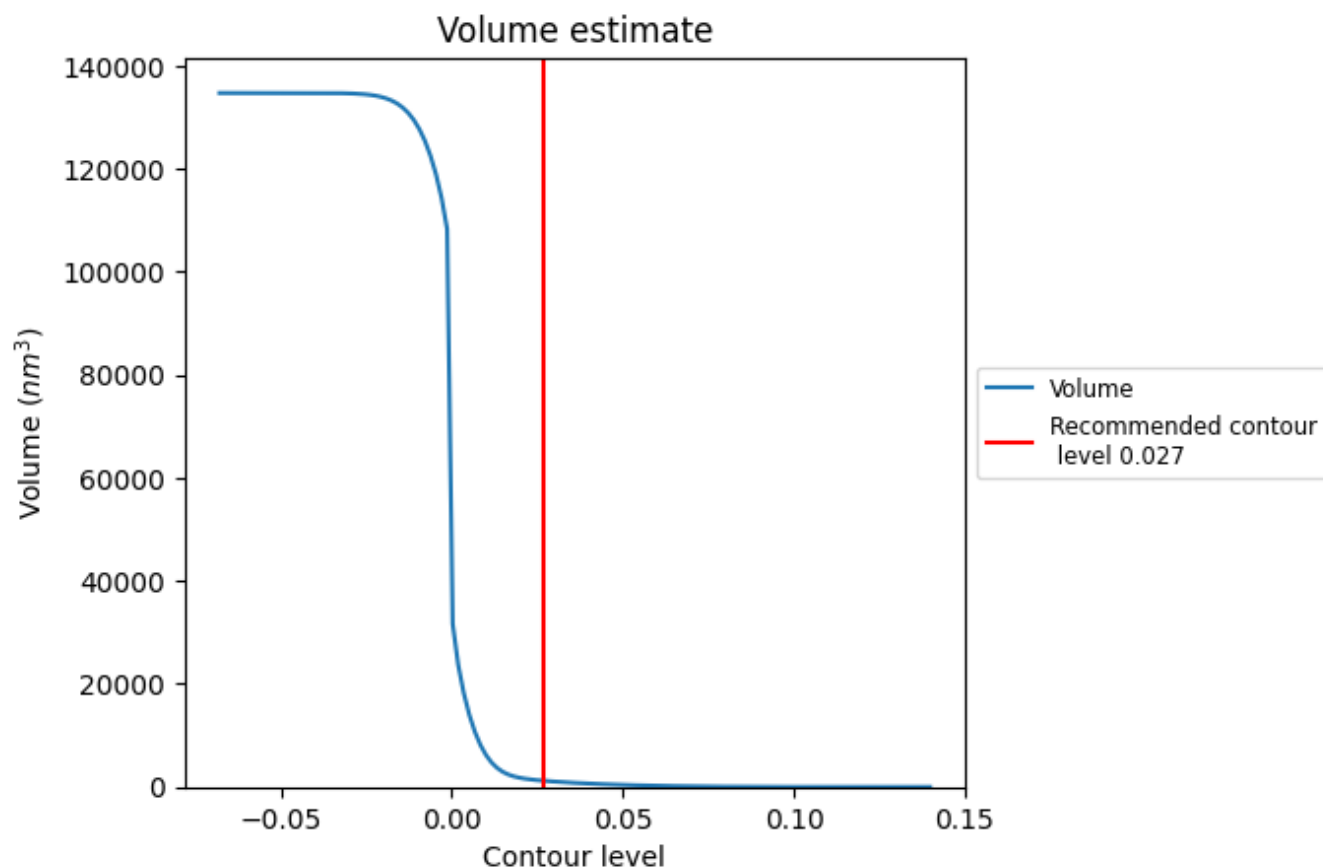
This section contains the results of statistical analysis of the map.

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.

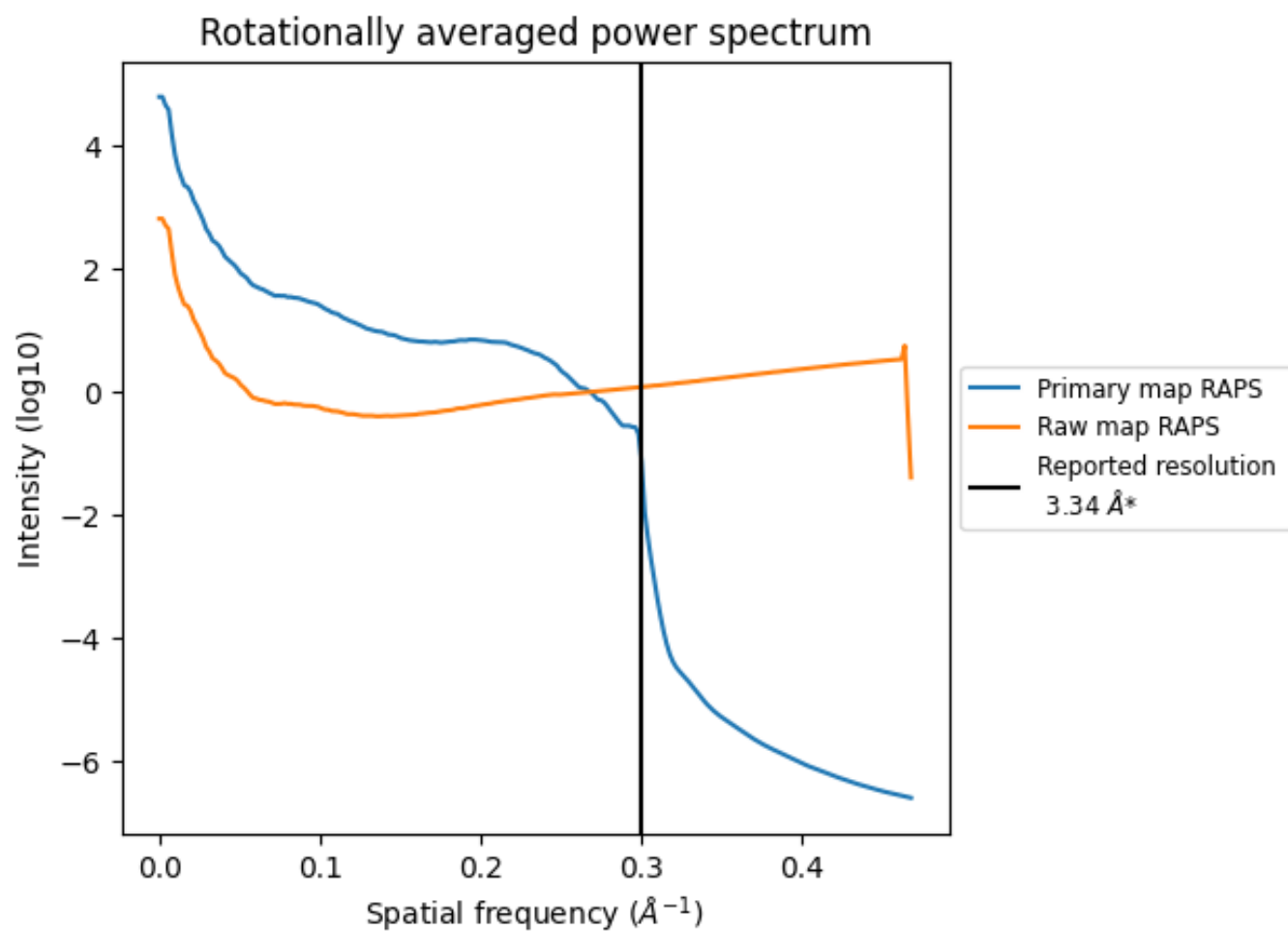
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1196 nm³; this corresponds to an approximate mass of 1080 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 ⓘ

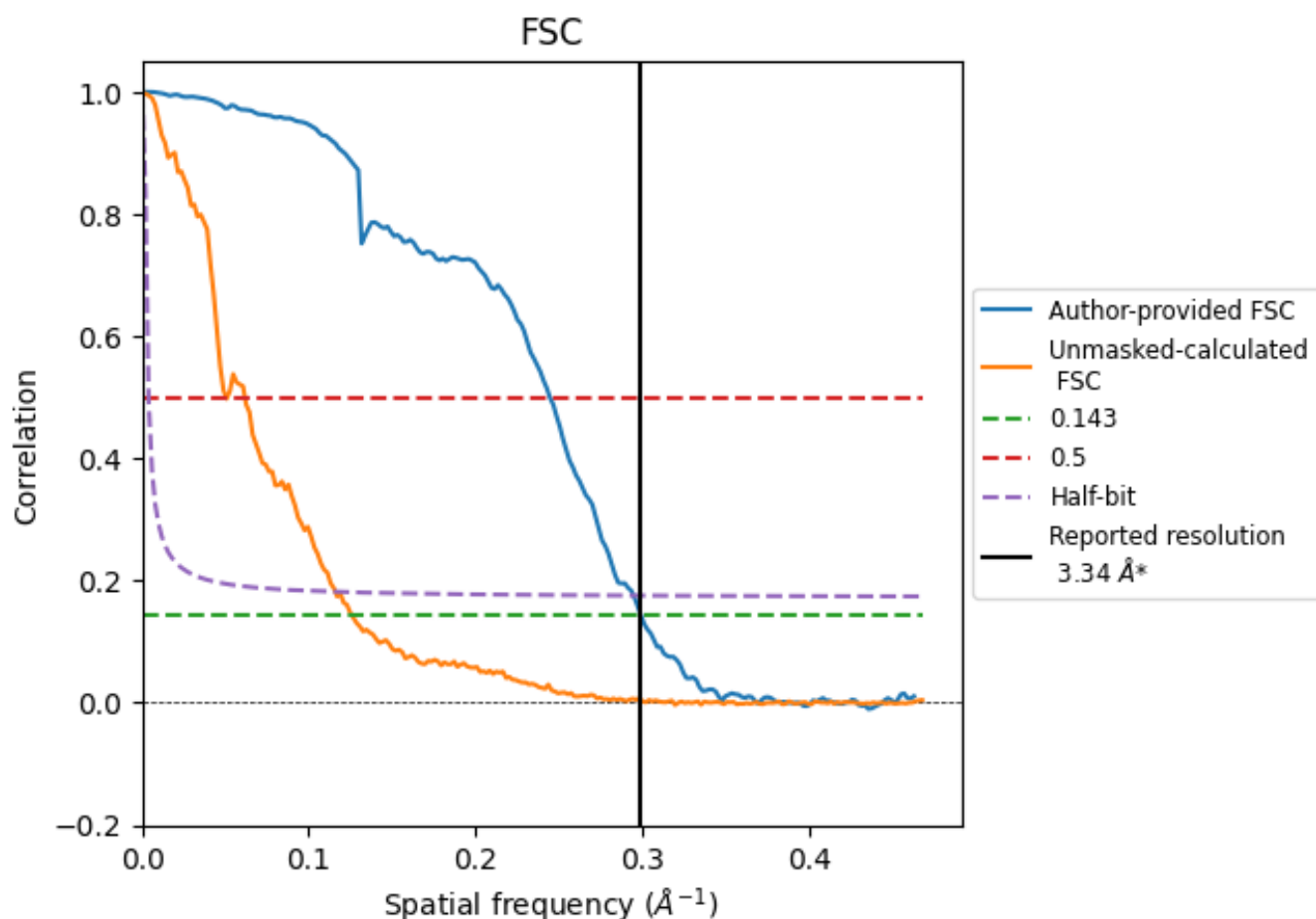


*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

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 0.299 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

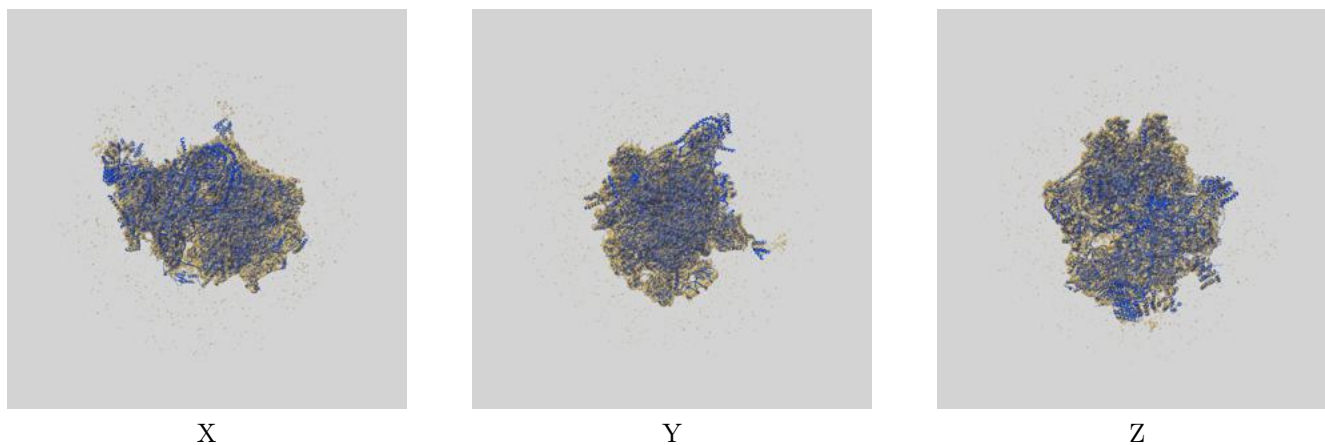
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	3.34	4.09	3.39
Unmasked-calculated*	7.94	19.84	8.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.94 differs from the reported value 3.34 by more than 10 %

9 Map-model fit [i](#)

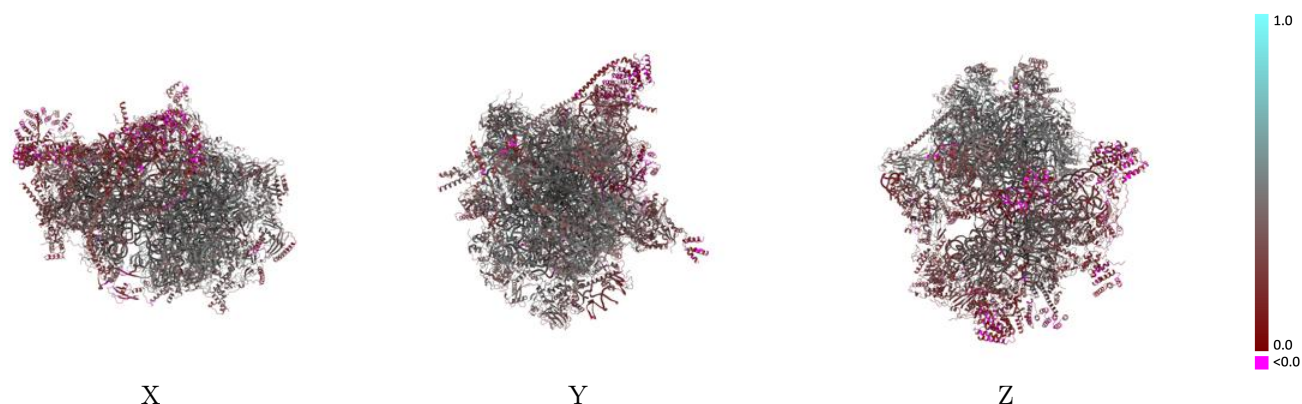
This section contains information regarding the fit between EMDB map EMD-71811 and PDB model 9PRQ. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



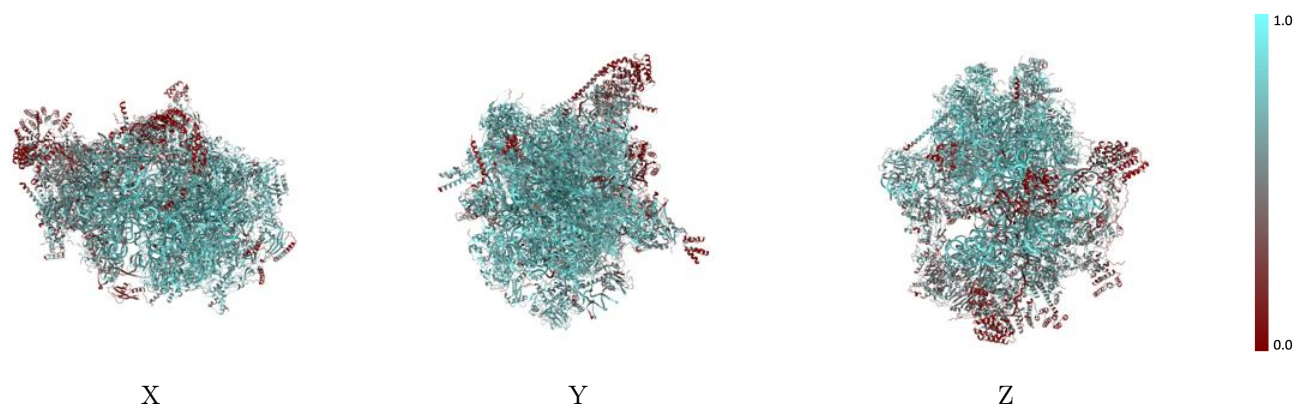
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



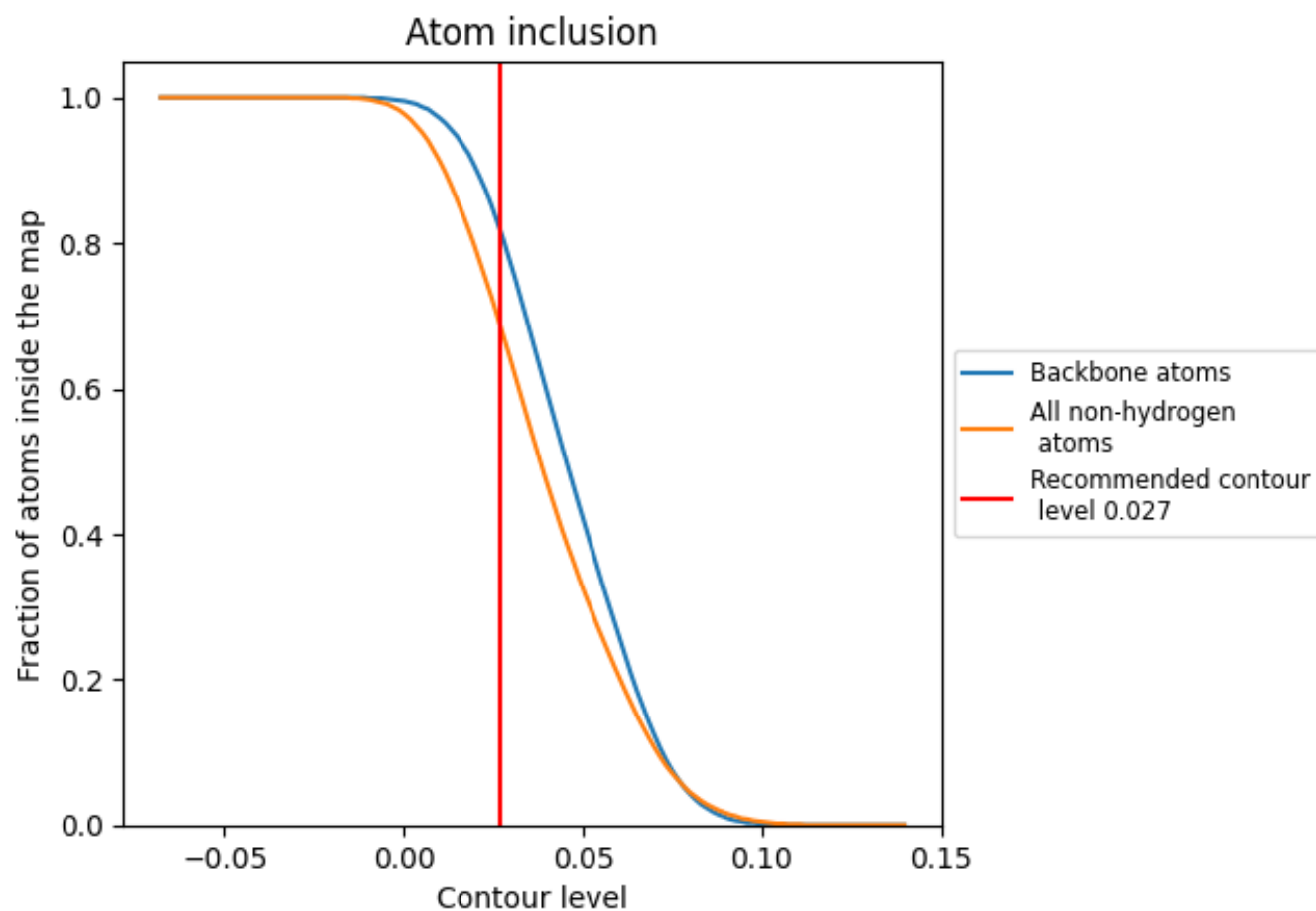
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6870	 0.3720
0	 0.7290	 0.4470
1	 0.6940	 0.4180
2	 0.8280	 0.4950
3	 0.8160	 0.4930
4	 0.8010	 0.4760
5	 0.7460	 0.4350
6	 0.7060	 0.3990
7	 0.6820	 0.4000
8	 0.5030	 0.2910
9	 0.7140	 0.4310
A	 0.9100	 0.4410
A0	 0.3540	 0.1910
A1	 0.4560	 0.2700
A2	 0.5510	 0.3450
A3	 0.6690	 0.4060
A4	 0.2670	 0.1680
AA	 0.8920	 0.3980
AB	 0.6280	 0.3500
AC	 0.5690	 0.3710
AD	 0.5430	 0.3460
AE	 0.6290	 0.4010
AF	 0.5690	 0.3250
AG	 0.5300	 0.3190
AH	 0.4900	 0.3260
AI	 0.6340	 0.3950
AJ	 0.5900	 0.3860
AK	 0.6560	 0.3650
AL	 0.6080	 0.3540
AM	 0.4650	 0.2340
AN	 0.6270	 0.3810
AO	 0.4730	 0.2460
AP	 0.6240	 0.3950
AQ	 0.6790	 0.4110
AR	 0.3750	 0.2010



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Chain	Atom inclusion	Q-score
AS	0.5200	0.3020
AT	0.5870	0.3410
AU	0.5060	0.2520
AV	0.2310	0.1360
AW	0.5200	0.3430
AX	0.4810	0.2540
AY	0.4070	0.2540
AZ	0.4990	0.2960
Ag	0.1560	0.1330
Ah	0.4050	0.1360
Ax	0.7800	0.3270
Az	0.3540	0.2230
B	0.7750	0.2940
D	0.7700	0.4770
E	0.7600	0.4620
F	0.7820	0.4660
H	0.3960	0.2620
I	0.5620	0.3300
J	0.4730	0.2510
K	0.7890	0.4700
L	0.7370	0.4660
M	0.7670	0.4600
N	0.7430	0.4600
O	0.7630	0.4600
OX	0.3150	0.2580
P	0.7410	0.4330
Q	0.6870	0.4360
R	0.7800	0.4650
S	0.7310	0.4630
T	0.7670	0.4770
U	0.6680	0.4170
V	0.6890	0.4140
W	0.7840	0.4800
X	0.7390	0.4330
Y	0.7570	0.4420
Z	0.7620	0.4730
a	0.6260	0.3970
b	0.7760	0.4670
c	0.7130	0.4240
d	0.5710	0.3650
e	0.4810	0.2480
f	0.5730	0.3490

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Chain	Atom inclusion	Q-score
g	 0.7580	 0.4580
h	 0.6950	 0.4060
i	 0.8120	 0.4790
j	 0.7110	 0.4190
k	 0.5990	 0.3580
l	 0.5310	 0.2960
m	 0.4750	 0.2950
n	 0.2700	 0.2900
o	 0.8000	 0.4640
p	 0.6040	 0.3590
q	 0.5530	 0.3070
r	 0.7630	 0.4520
s	 0.7360	 0.4410
t	 0.2180	 0.2110
u	 0.1370	 0.1330