



Full wwPDB EM Validation Report ⓘ

Aug 24, 2026 – 02:07 PM EDT

PDB ID : 9PGL / pdb_00009pgl
EMDB ID : EMD-71634
Title : In situ structure of the human mitoribosome in the A-P state with TACO1
Authors : Wang, S.; Xiong, Y.; Zhang, Y.
Deposited on : 2025-07-08
Resolution : 2.90 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:

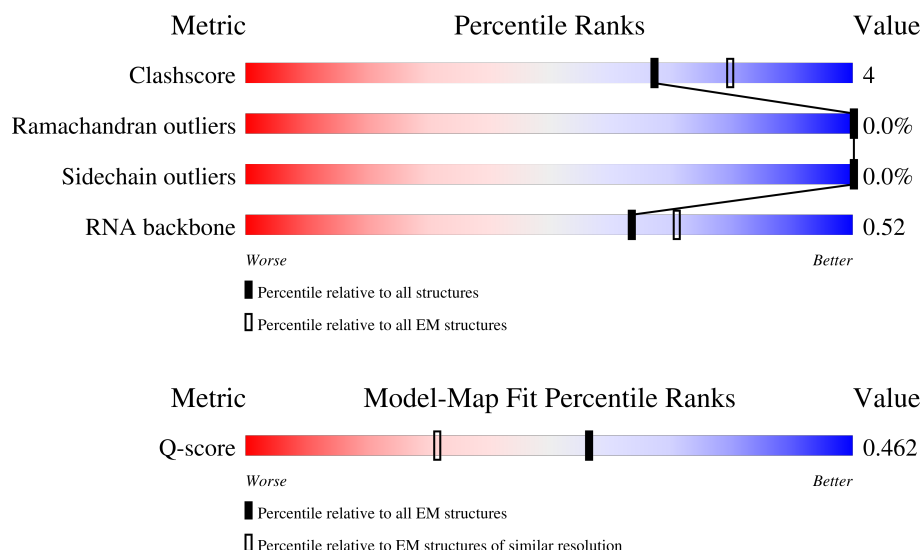
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.90 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.



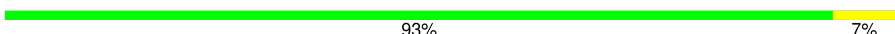
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	0	188	
2	1	65	
3	2	92	

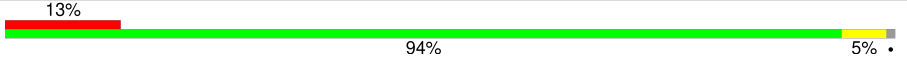
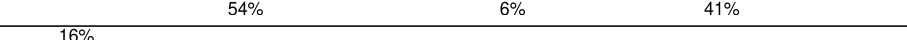
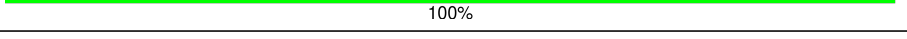
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Mol	Chain	Length	Quality of chain
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	A	1561	
12	C	297	
13	D	305	
14	E	348	
15	F	311	
16	H	267	
17	I	261	
18	J	192	
19	K	178	
20	L	145	
21	M	296	
22	N	251	
23	O	175	
24	P	180	
25	Q	292	
26	R	149	
27	S	205	
28	T	206	

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Mol	Chain	Length	Quality of chain
29	U	153	
30	W	148	
31	X	256	
32	Y	250	
33	Z	161	
34	G	198	
34	t	198	
34	u	198	
35	V	216	
36	b	215	
37	d	306	
38	e	279	
39	g	166	
40	h	158	
41	i	128	
42	j	123	
43	k	112	
44	l	138	
45	m	128	
46	n	43	
47	o	102	
48	q	222	
49	r	196	
50	c	332	
51	f	212	

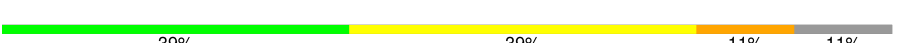
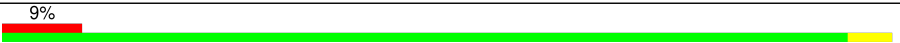
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Mol	Chain	Length	Quality of chain
52	p	206	
53	s	439	
54	AB	296	
55	AC	167	
56	AD	430	
57	AE	125	
58	AF	242	
59	AG	396	
60	AH	201	
61	AJ	138	
62	AK	128	
63	AL	257	
64	AM	137	
65	AN	130	
66	AO	258	
67	AP	142	
68	AR	360	
69	AS	190	
70	AT	173	
71	AU	205	
72	AV	414	
73	AW	187	
74	AZ	106	
75	A0	217	
76	A1	323	

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Mol	Chain	Length	Quality of chain
77	A3	199	
78	Az	34	
79	AY	395	
80	AA	954	
81	AI	194	
82	OX	435	
83	a	142	
84	Ax	71	
85	Aw	76	
86	A4	689	
87	AX	398	
88	A2	118	
89	AQ	87	
90	B	72	

2 Entry composition

There are 101 unique types of molecules in this entry. The entry contains 180184 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		

- Molecule 12 is a protein called Translational activator of cytochrome c oxidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	223	Total	C	N	O	S	0	0
			1732	1072	310	340	10		

- Molecule 13 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 17 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 19 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	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	179	ACE	-	acetylation	UNP H2QWN0
K	310	TYR	ASP	conflict	UNP H2QWN0

- Molecule 20 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 29 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 30 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 31 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 32 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	G	72	Total	C	N	O	0	0
			558	358	97	103		
34	t	46	Total	C	N	O	0	0
			354	228	56	70		
34	u	32	Total	C	N	O	0	0
			257	168	40	49		

- Molecule 35 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L45, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L46, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 43 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	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	113	ACE	-	acetylation	UNP Q96EL3

- Molecule 44 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 46 is a protein called Nascent polypeptide.

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

- Molecule 47 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 48 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 49 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 78 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 86 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 87 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 88 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	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	119	ACE	-	acetylation	UNP Q96BP2

- Molecule 89 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	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	88	ACE	-	acetylation	UNP P82921
AQ	137	ARG	CYS	variant	UNP P82921

- 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).

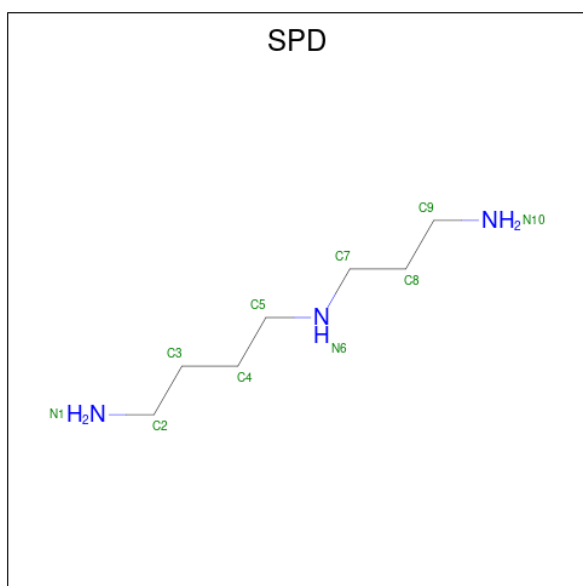
Mol	Chain	Residues	Atoms		AltConf
92	6	1	Total	K	0
			1	1	
92	A	29	Total	K	0
			29	29	
92	D	1	Total	K	0
			1	1	
92	M	2	Total	K	0
			2	2	
92	N	1	Total	K	0
			1	1	

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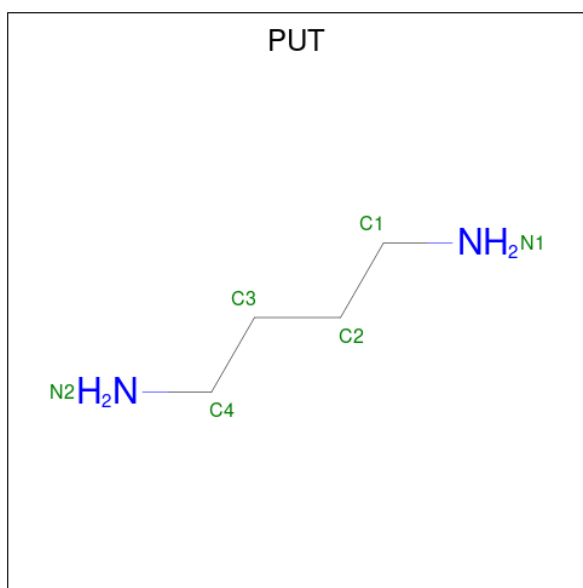
Mol	Chain	Residues	Atoms		AltConf
92	W	1	Total	K	0
			1	1	
92	o	1	Total	K	0
			1	1	
92	AA	18	Total	K	0
			18	18	

- 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	
93	A	1	Total	C	N	0
			10	7	3	
93	O	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	
93	AA	1	Total	C	N	0
			10	7	3	

- Molecule 94 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



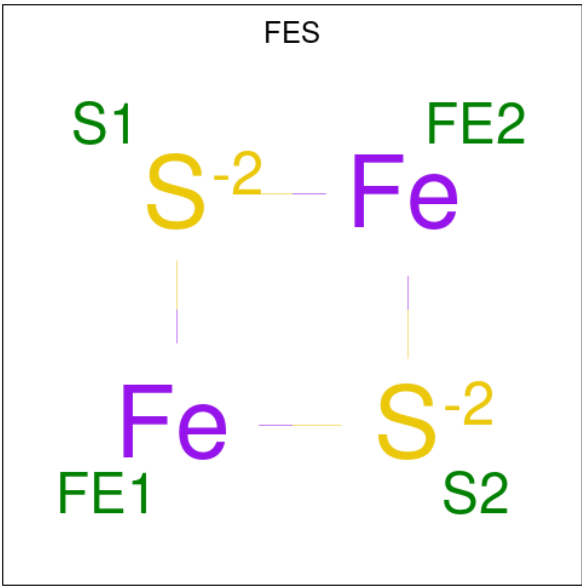
Mol	Chain	Residues	Atoms			AltConf
94	A	1	Total	C	N	0
			6	4	2	

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

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

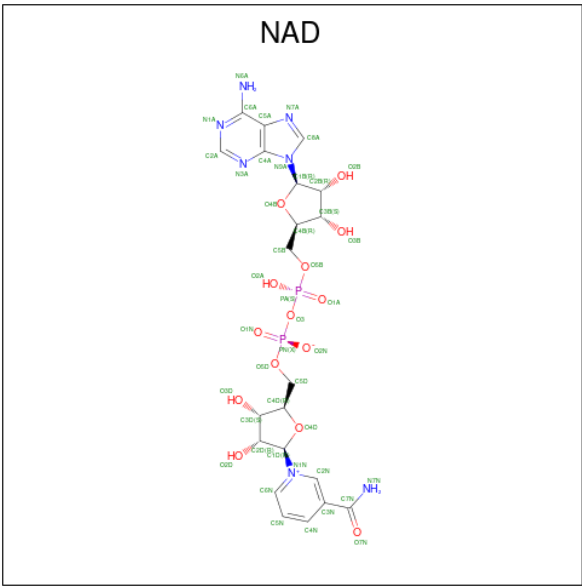
- Molecule 96 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled

as "Ligand of Interest" by depositor).



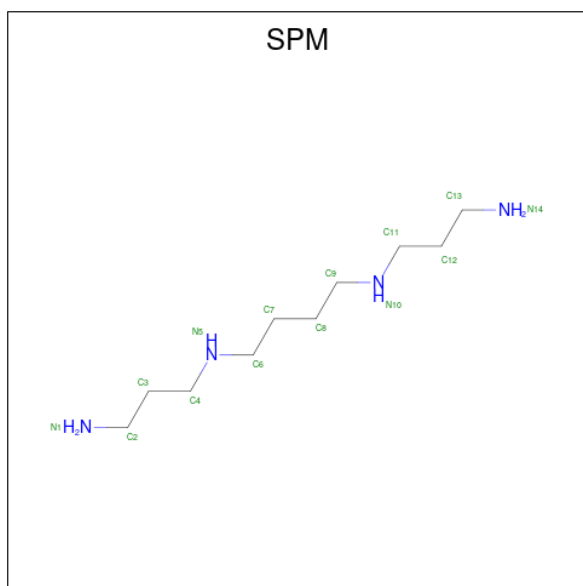
Mol	Chain	Residues	Atoms			AltConf
96	r	1	Total	Fe	S	0
			4	2	2	
96	AP	1	Total	Fe	S	0
			4	2	2	
96	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 97 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



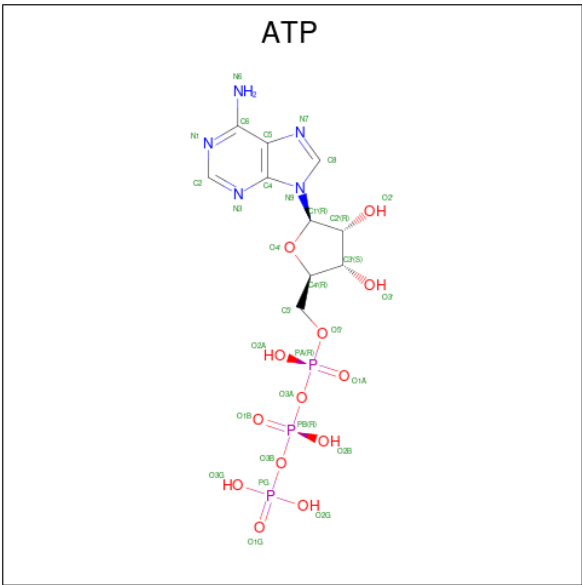
Mol	Chain	Residues	Atoms					AltConf
97	AA	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 98 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



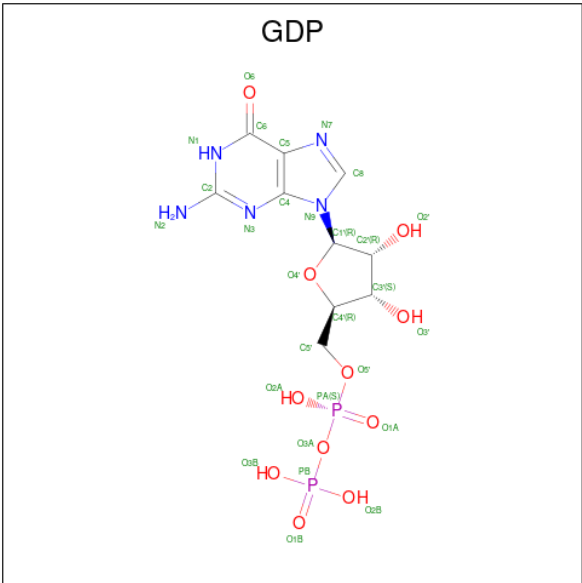
Mol	Chain	Residues	Atoms				AltConf
98	AA	1	Total	C	N		0
			14	10	4		
98	AA	1	Total	C	N		0
			14	10	4		

- 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).



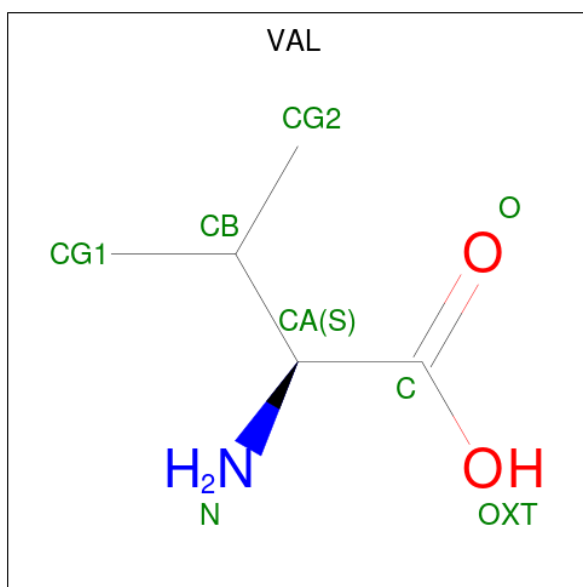
Mol	Chain	Residues	Atoms					AltConf
99	AX	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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: $C_5H_{11}NO_2$).

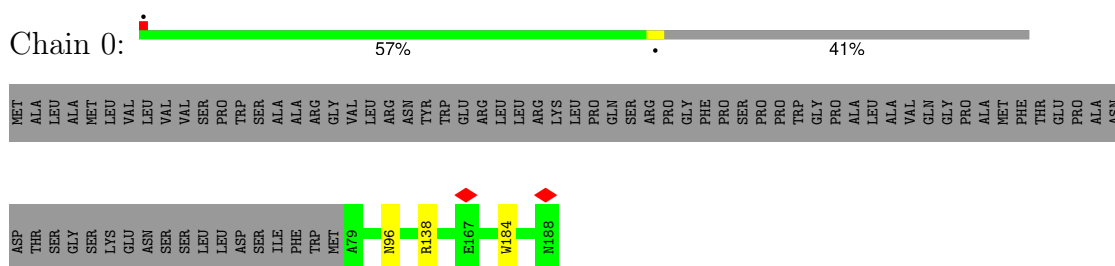


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
101	B	1	7	5	1	1	0

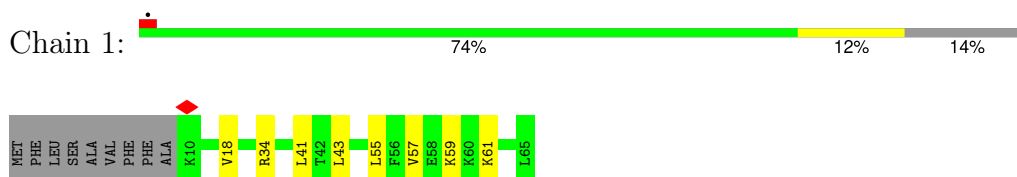
3 Residue-property plots [i](#)

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.

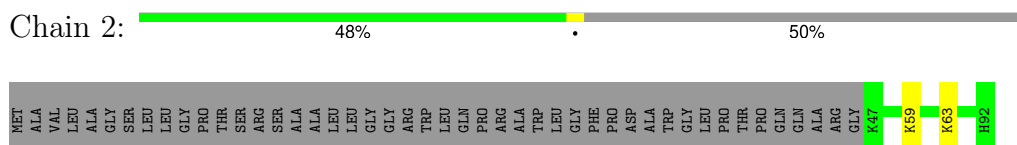
- Molecule 1: 39S ribosomal protein L32, mitochondrial



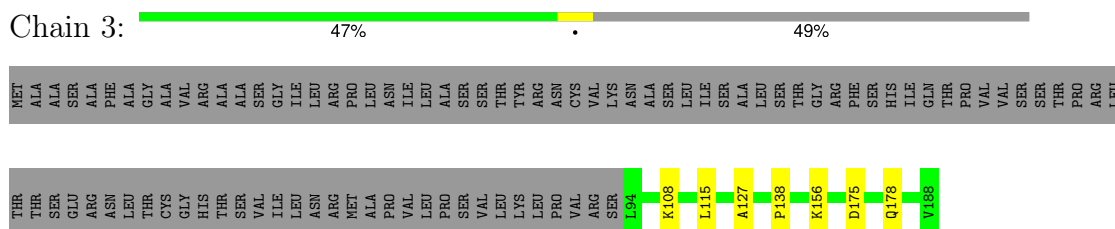
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial



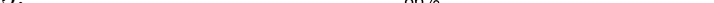
- Molecule 4: 39S ribosomal protein L35, mitochondrial

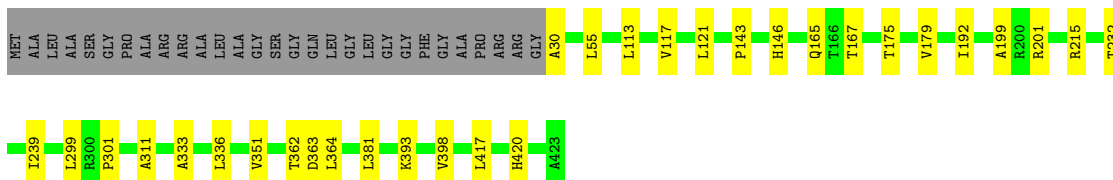


- Molecule 5: 39S ribosomal protein L36, mitochondrial

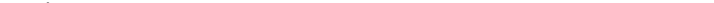


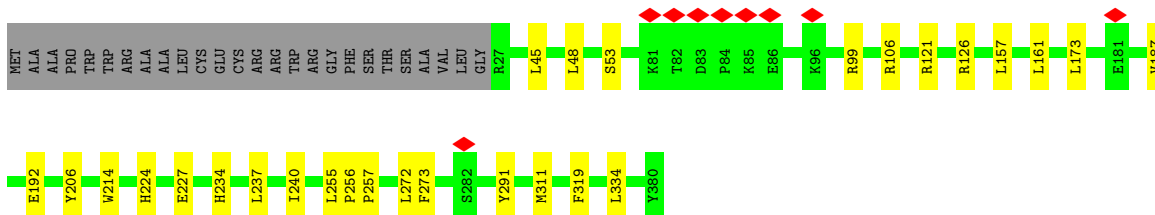
- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:  86% 7% 7%

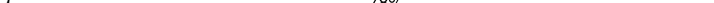


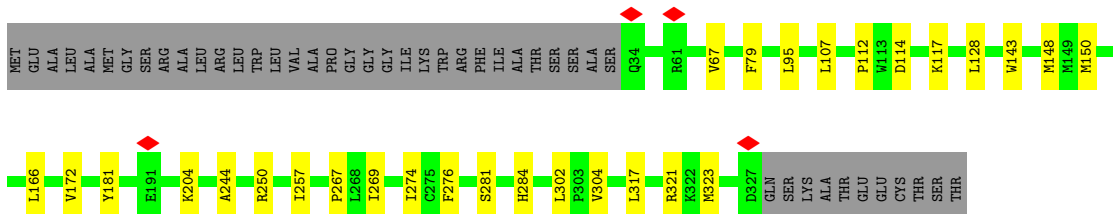
- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:  86% 7% 7%

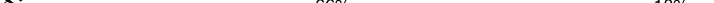


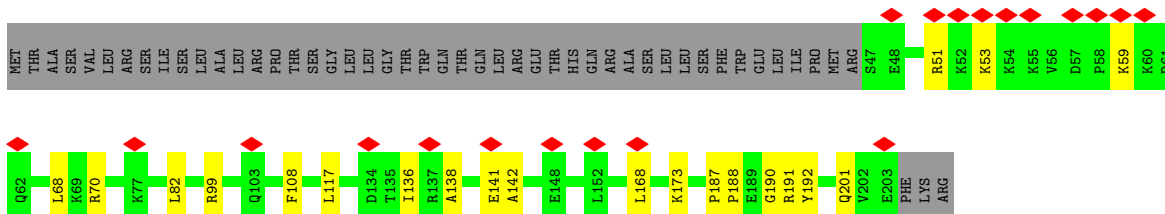
- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7:  78% 9% 13%



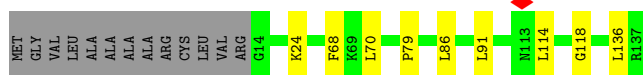
- Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8: 



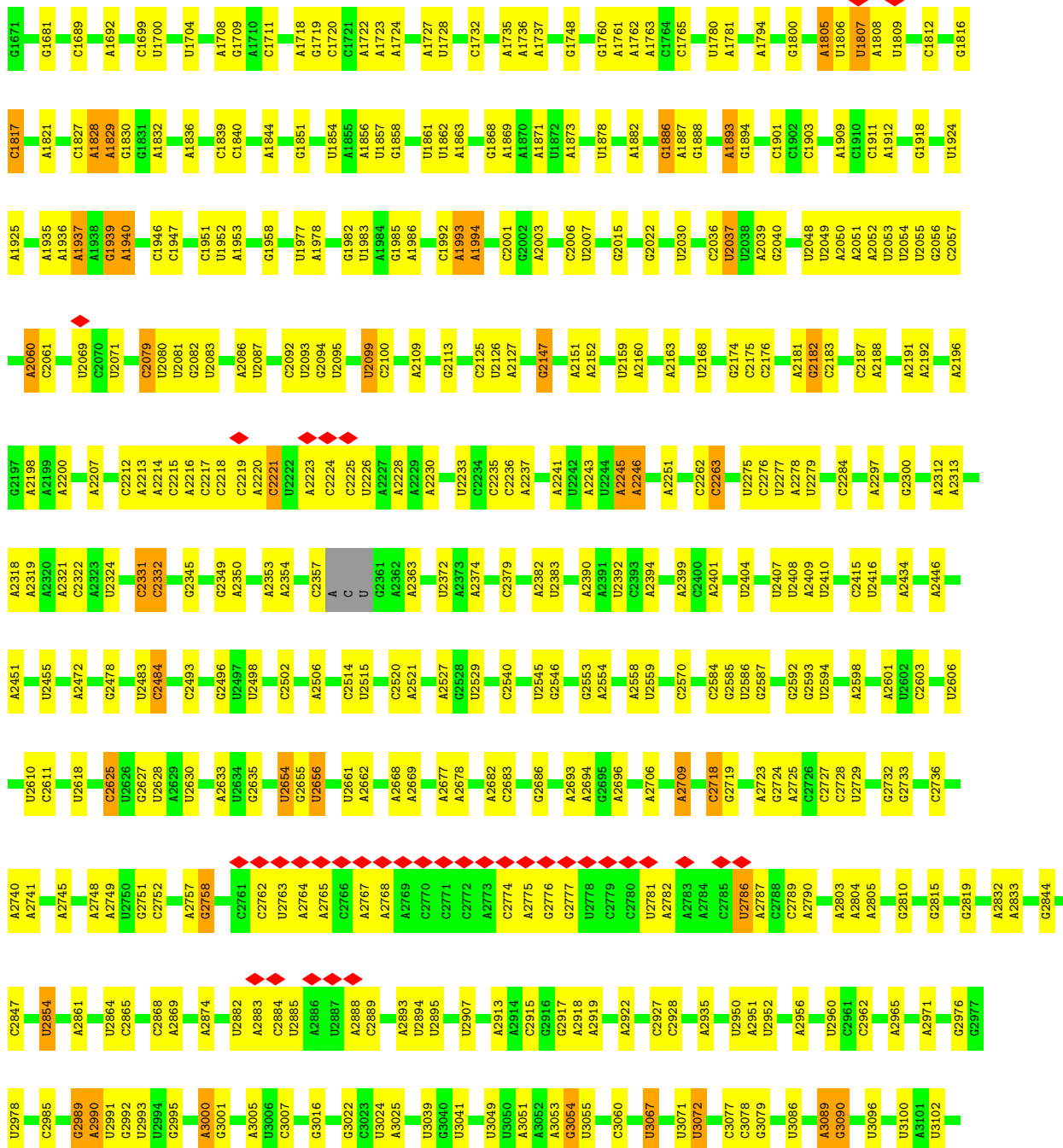
- Molecule 10: 39S ribosomal protein L41, mitochondrial

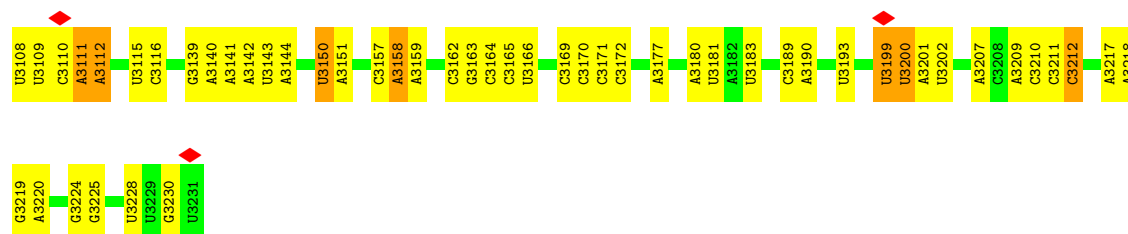
Chain 9:  84% 7% 9%



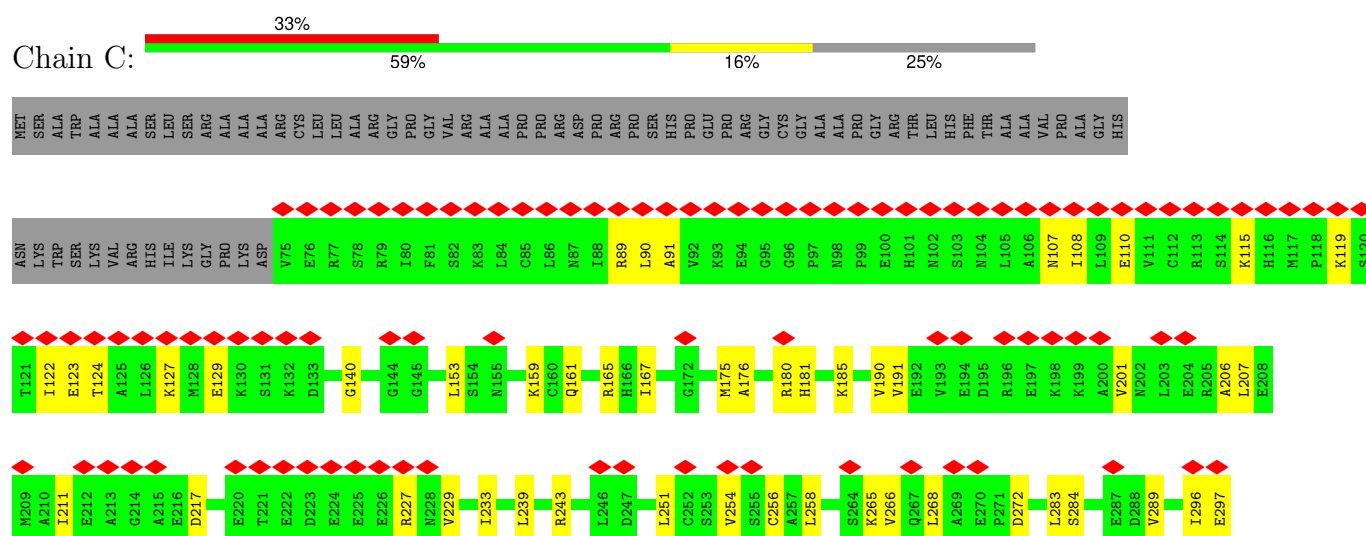
• Molecule 11: 16S mitochondrial rRNA

Chain A:  70% 26%

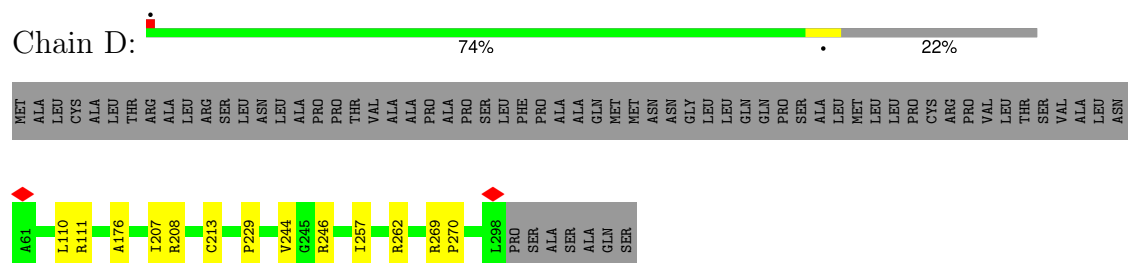




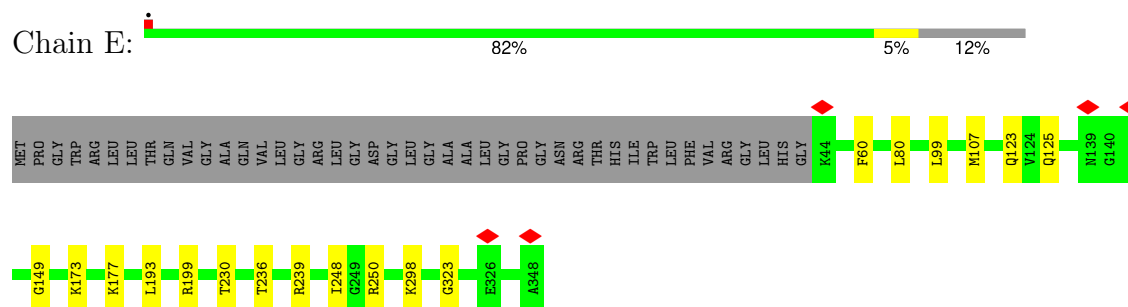
- Molecule 12: Translational activator of cytochrome c oxidase 1



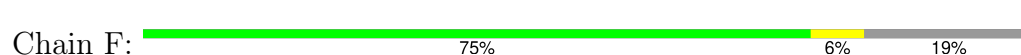
- Molecule 13: 39S ribosomal protein L2, mitochondrial

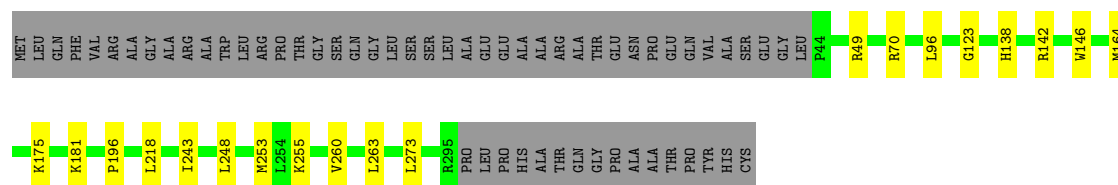


- Molecule 14: 39S ribosomal protein L3, mitochondrial

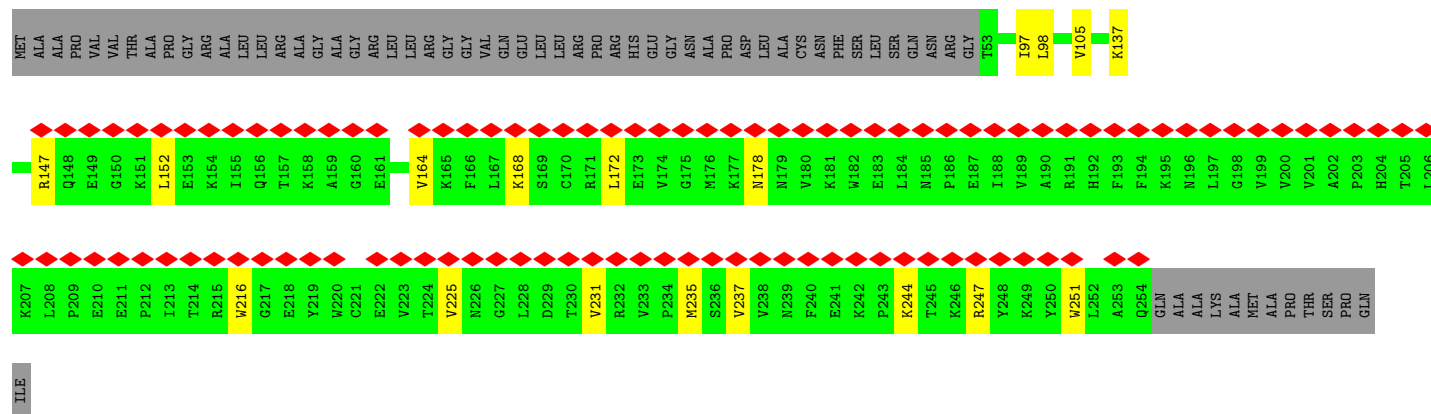
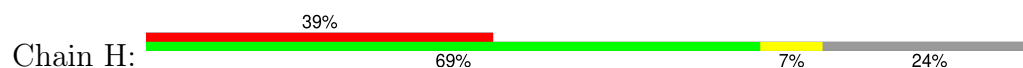


- Molecule 15: 39S ribosomal protein L4, mitochondrial





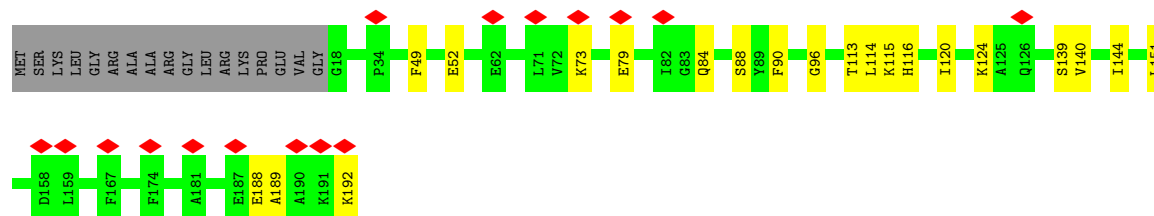
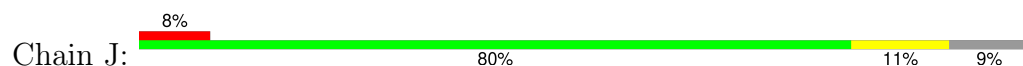
- Molecule 16: 39S ribosomal protein L9, mitochondrial



- Molecule 17: 39S ribosomal protein L10, mitochondrial



- Molecule 18: 39S ribosomal protein L11, mitochondrial



- Molecule 19: Large ribosomal subunit protein uL13m

Topic	Number of Publications
ACE179	10
K202	8
M203	8
L217	8
M238	8
N239	8
T240	8
V279	8
N293	8
M300	8
L303	8
I311	8
F344	8
L356	8

- | | |
|------|------|
| MET | ALA | PHE | PHE | THR | GLY | LEU | TRP | GLY | PRO | PHE | THR | CYS | VAL | SER | ARG | ARG | VAL | LEU | SER | SER | HIS | HIS | CYS | PHE | SER | THR | THR | GLY | SER | SER | LEU | LEU | A31 | I32 | L46 | G47 | K62 | I77 | K78 | P98 | M103 | V145 |
|------|------|

-
- | Amino Acid Type | Count (approx.) |
|-----------------|-----------------|
| MET | 50 |
| ALA | 50 |
| GLY | 50 |
| PRO | 50 |
| LEU | 50 |
| Q6 | 1000 |
| Q7 | 1000 |
| G8 | 1000 |
| G9 | 1000 |
| K28 | 250 |
| P29 | 250 |
| P40 | 250 |
| R44 | 250 |
| R45 | 250 |
| P79 | 250 |
| F83 | 250 |
| G137 | 250 |
| Q157 | 250 |
| I167 | 250 |
| V174 | 250 |
| A177 | 250 |
| F178 | 250 |
| R203 | 250 |
| P226 | 250 |
| L244 | 250 |
| P245 | 250 |
| D261 | 250 |
| Q264 | 250 |
| L285 | 250 |
| P286 | 250 |
| L289 | 250 |
| S296 | 250 |

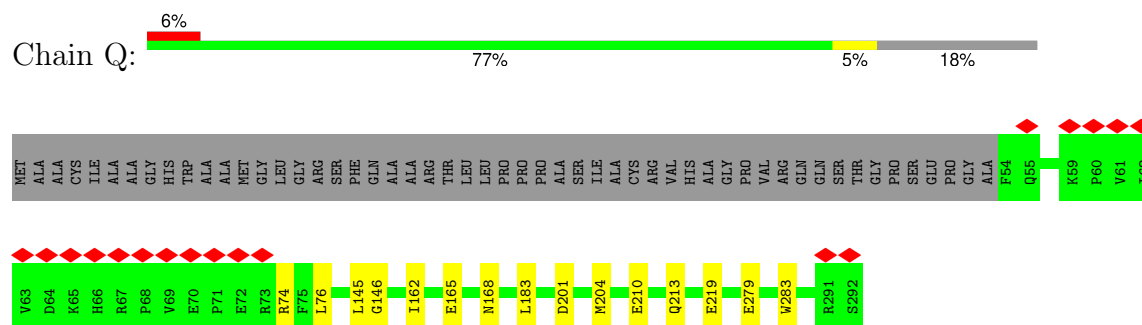
-
- Sequence logo for the 100th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis lists amino acids. The sequence is MET, TRP, ARG, LEU, LEU, ALA, ARG, ALA, SER, SER, PRO, LEU, LEU, VAL, PRO, LEU, SER, ASP, SER, TRP, ALA, ALA, LEU, PRO, ALA, SER, SER, ALA, GLY. The amino acids V90 and E40 are highlighted in red, indicating they are the most frequent at this position.

- [illegible]

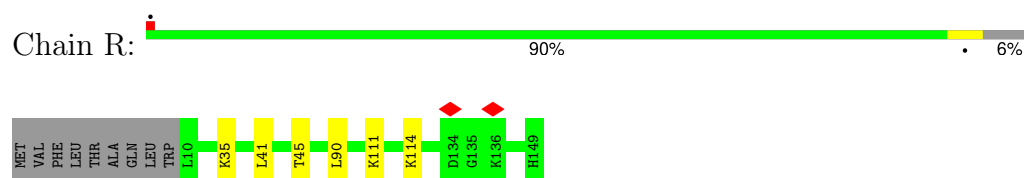
- MET
 LEU
 ALA
 ARG
 SER
 ARG
 PHE
 TRP
 GLY
 LEU
 PHE
 SER
 VAL
 CYS
 ARG
 ASN
 PRO
 GLY
 CYS
 ARG
 PHE
 ALA
 ALA
 LEU
 SER
 THR
 SER
 SER
 GLU
 PRO
 ALA
 ALA
 LYS
 PRO
 PRO
 GLU
 VAL
 D37
 P38
 N52
 N55
 F72
 R82
 R83
 R84
 R85
 T86
 H89
 R108
 E109
 W110
 M144



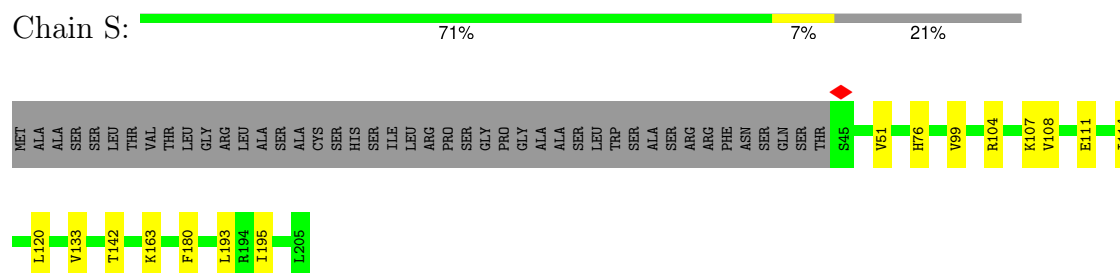
- Molecule 25: 39S ribosomal protein L19, mitochondrial



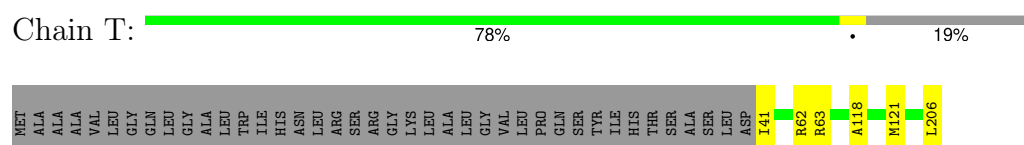
- Molecule 26: 39S ribosomal protein L20, mitochondrial



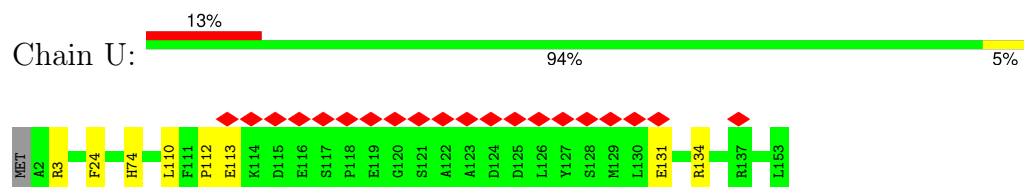
- Molecule 27: 39S ribosomal protein L21, mitochondrial



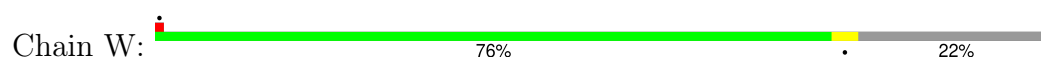
- Molecule 28: 39S ribosomal protein L22, mitochondrial

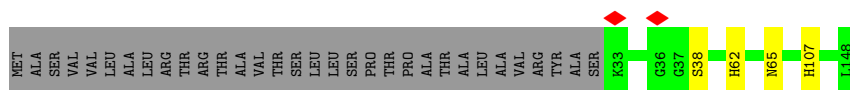


- Molecule 29: 39S ribosomal protein L23, mitochondrial

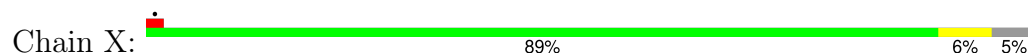


- Molecule 30: 39S ribosomal protein L27, mitochondrial





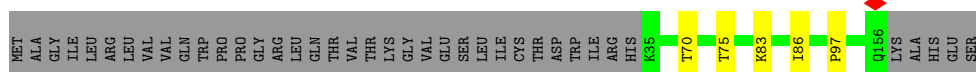
- Molecule 31: 39S ribosomal protein L28, mitochondrial



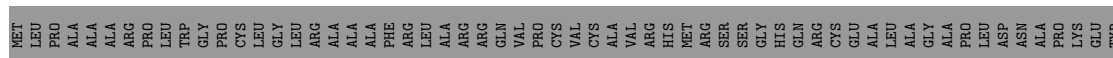
- Molecule 32: 39S ribosomal protein L47, mitochondrial



- Molecule 33: 39S ribosomal protein L30, mitochondrial

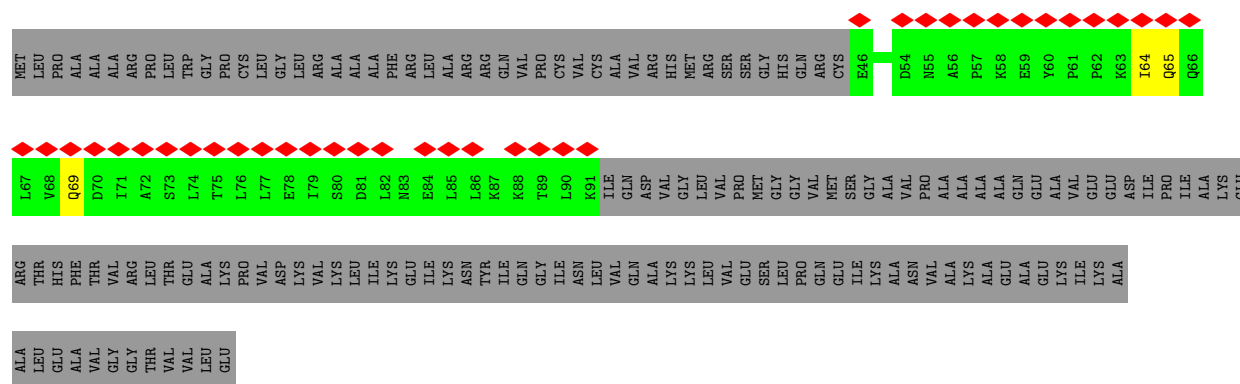


- Molecule 34: 39S ribosomal protein L12, mitochondrial

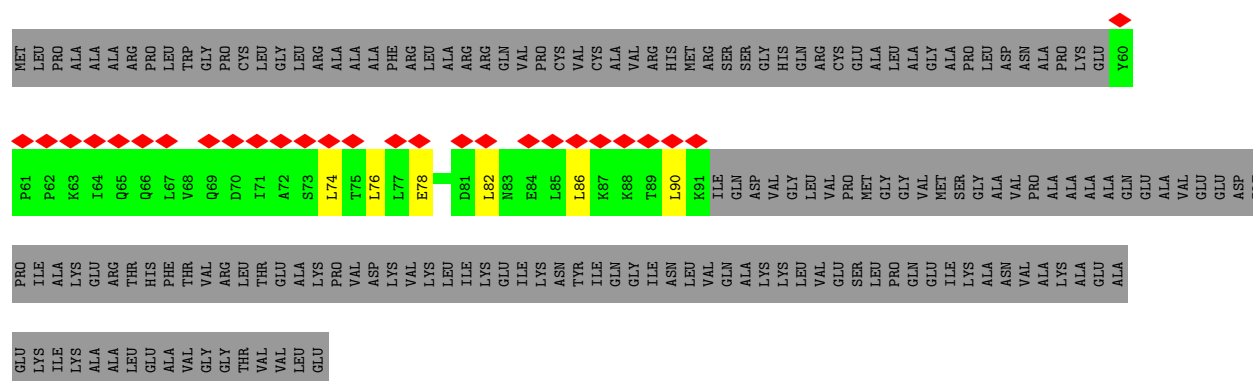


- Molecule 34: 39S ribosomal protein L12, mitochondrial

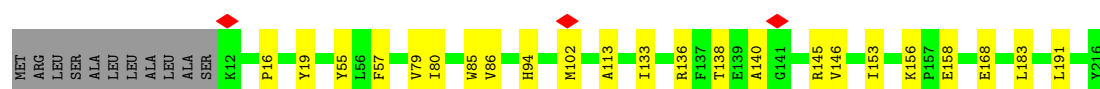
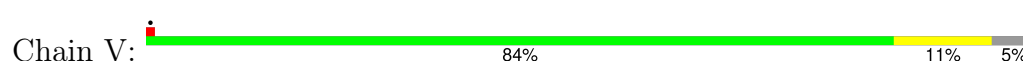




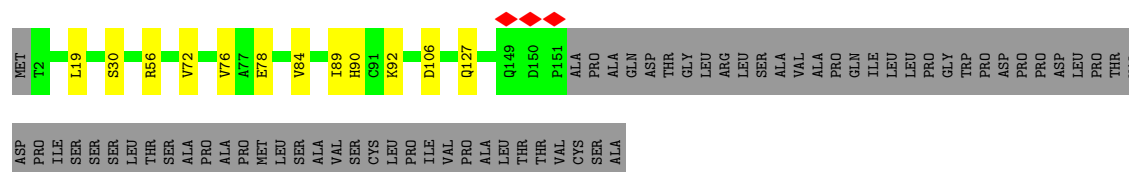
• Molecule 34: 39S ribosomal protein L12, mitochondrial



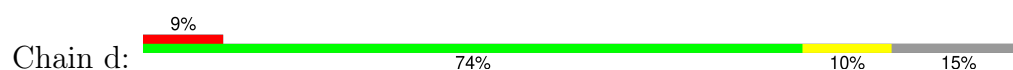
• Molecule 35: 39S ribosomal protein L24, mitochondrial

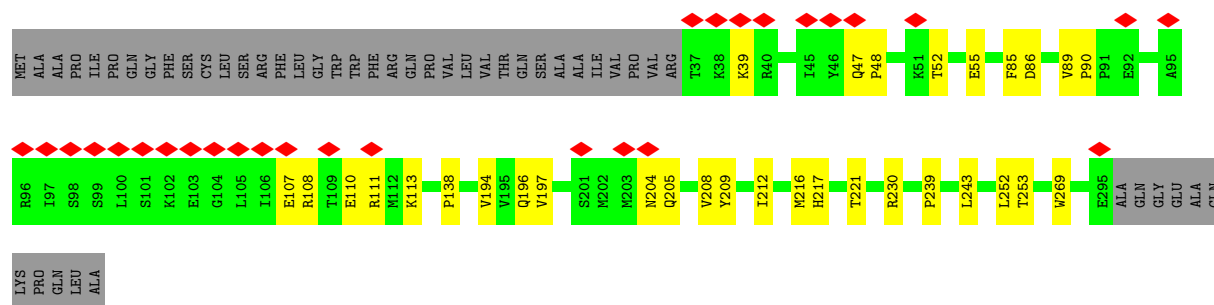


• Molecule 36: 39S ribosomal protein L43, mitochondrial



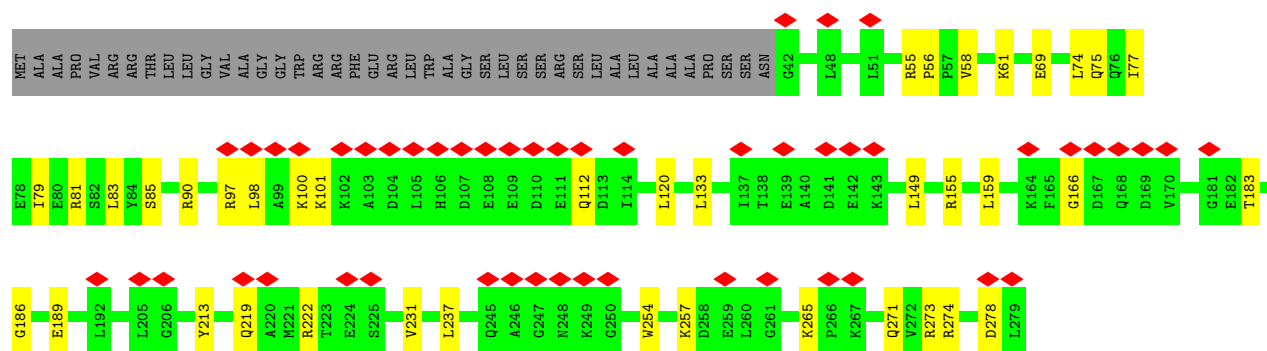
• Molecule 37: 39S ribosomal protein L45, mitochondrial





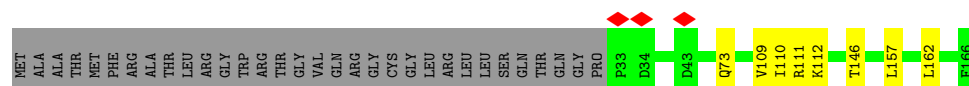
- Molecule 38: 39S ribosomal protein L46, mitochondrial

Chain e:



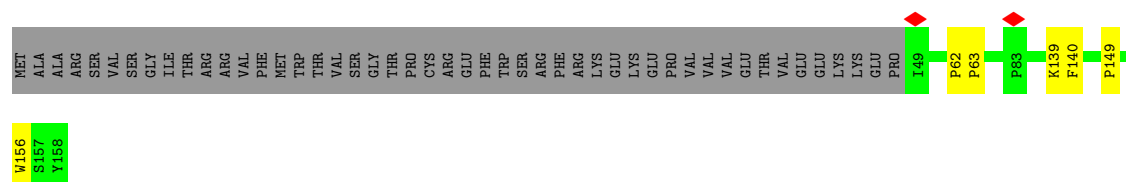
- Molecule 39: 39S ribosomal protein L49, mitochondrial

Chain g:



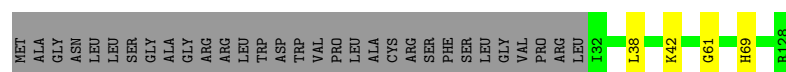
- Molecule 40: 39S ribosomal protein L50, mitochondrial

Chain h:

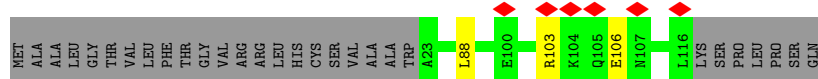
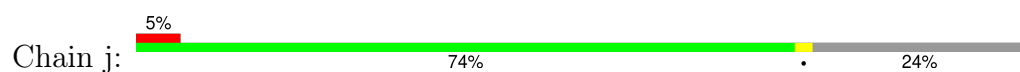


- Molecule 41: 39S ribosomal protein L51, mitochondrial

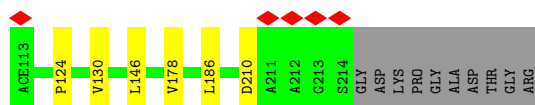
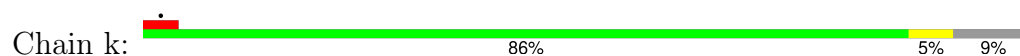
Chain i:



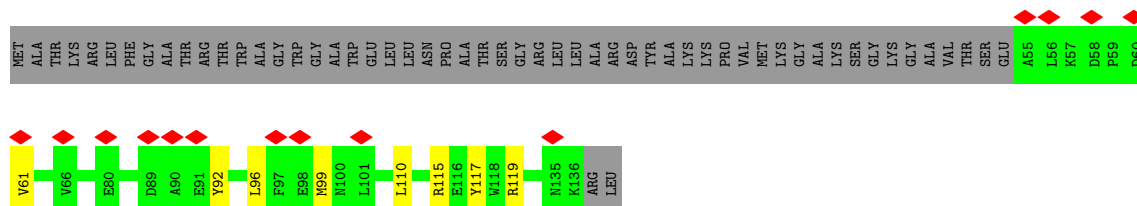
- Molecule 42: 39S ribosomal protein L52, mitochondrial



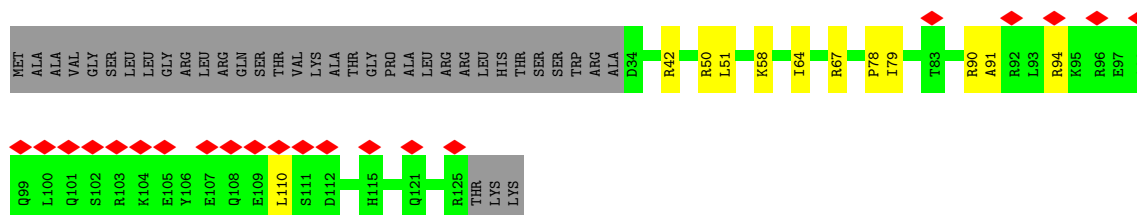
- Molecule 43: Large ribosomal subunit protein mL53



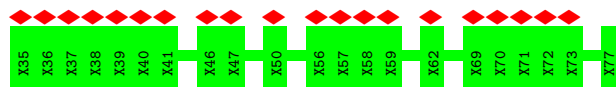
- Molecule 44: 39S ribosomal protein L54, mitochondrial



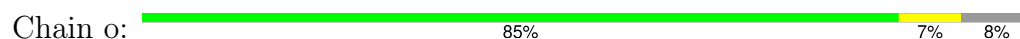
- Molecule 45: 39S ribosomal protein L55, mitochondrial



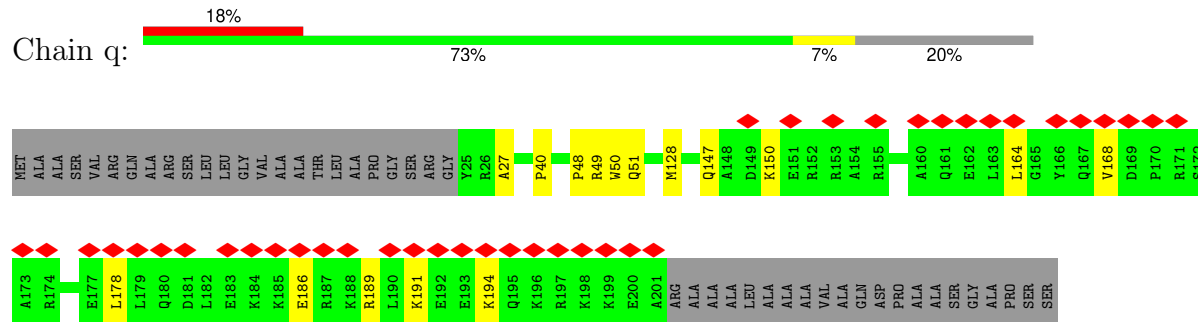
- Molecule 46: Nascent polypeptide



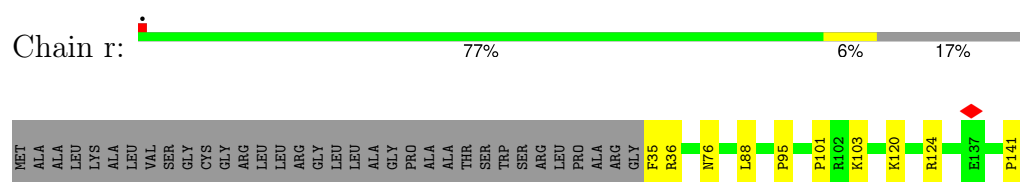
- Molecule 47: Ribosomal protein 63, mitochondrial



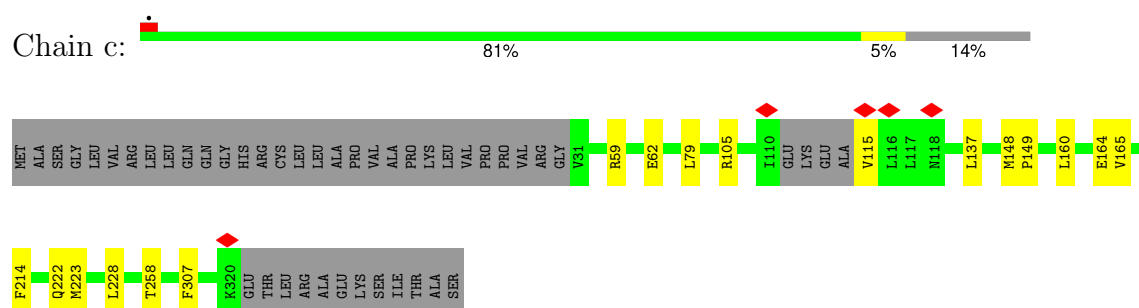
- Molecule 48: Growth arrest and DNA damage-inducible proteins-interacting protein 1



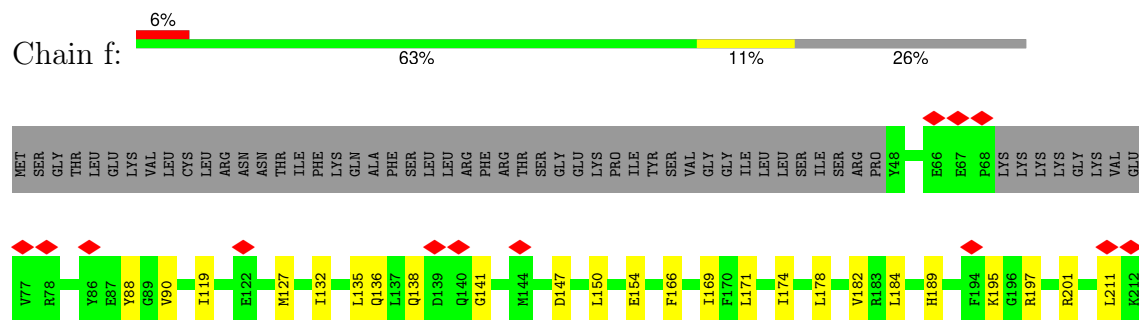
- Molecule 49: 39S ribosomal protein S18a, mitochondrial



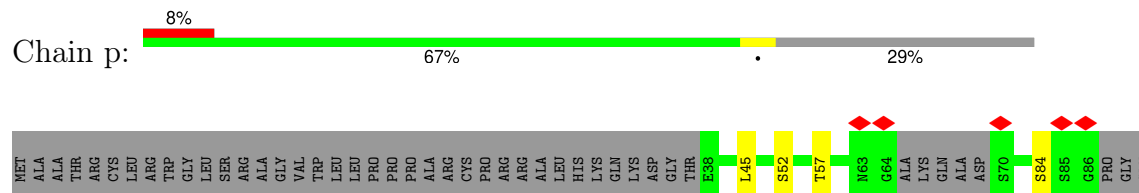
- Molecule 50: 39S ribosomal protein L44, mitochondrial

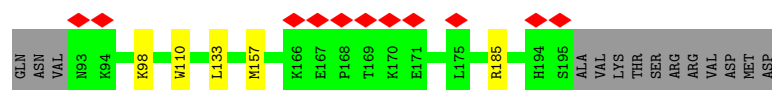


- Molecule 51: 39S ribosomal protein L48, mitochondrial

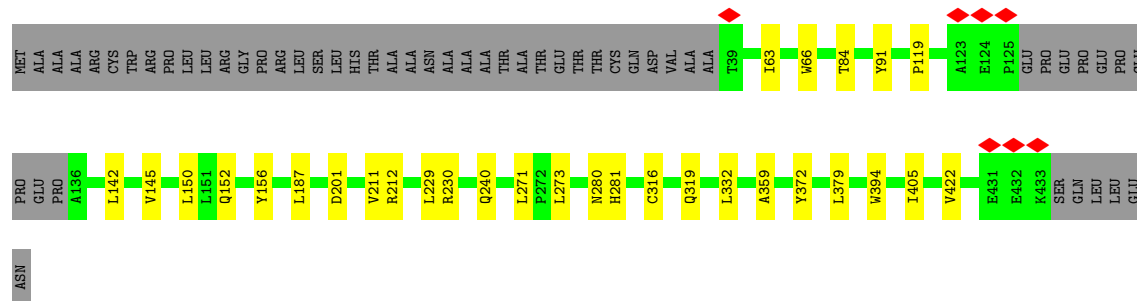
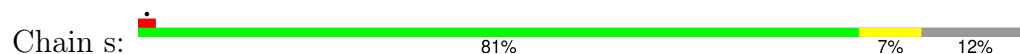


- Molecule 52: Peptidyl-tRNA hydrolase ICT1, mitochondrial

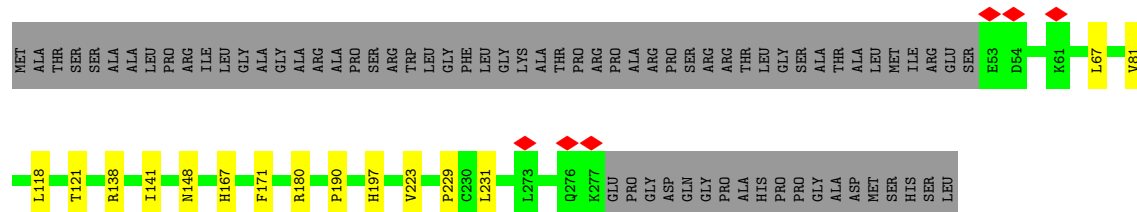




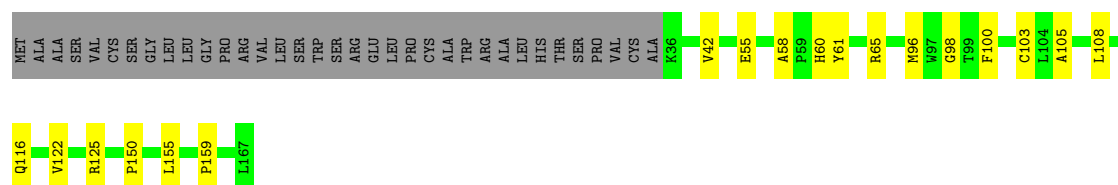
- Molecule 53: 39S ribosomal protein S30, mitochondrial



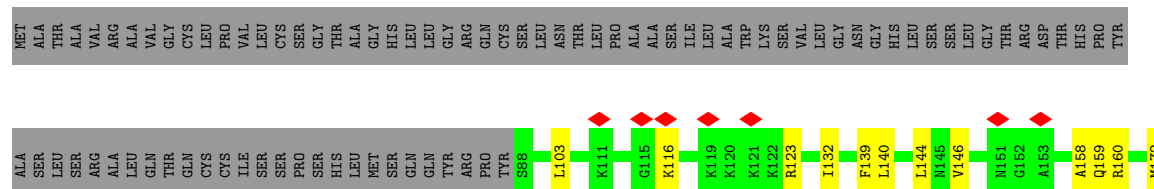
- Molecule 54: 28S ribosomal protein S2, mitochondrial



- Molecule 55: 28S ribosomal protein S24, mitochondrial

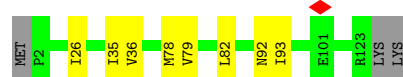


- Molecule 56: 28S ribosomal protein S5, mitochondrial

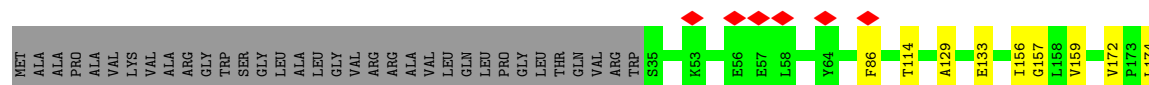
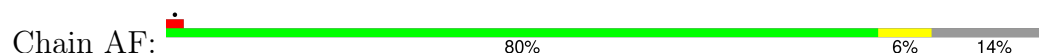




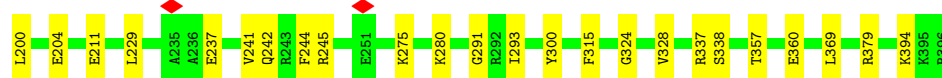
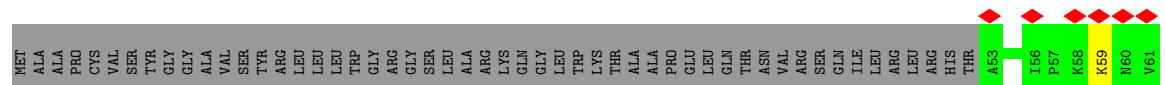
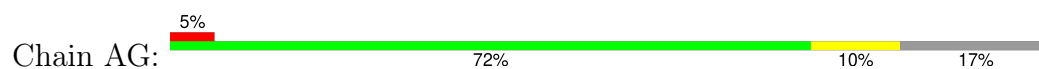
- Molecule 57: 28S ribosomal protein S6, mitochondrial



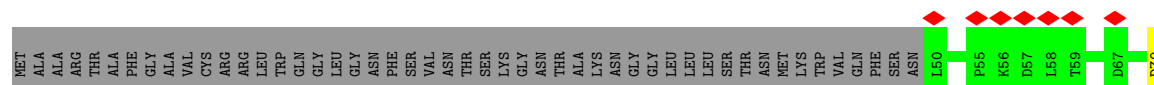
- Molecule 58: 28S ribosomal protein S7, mitochondrial



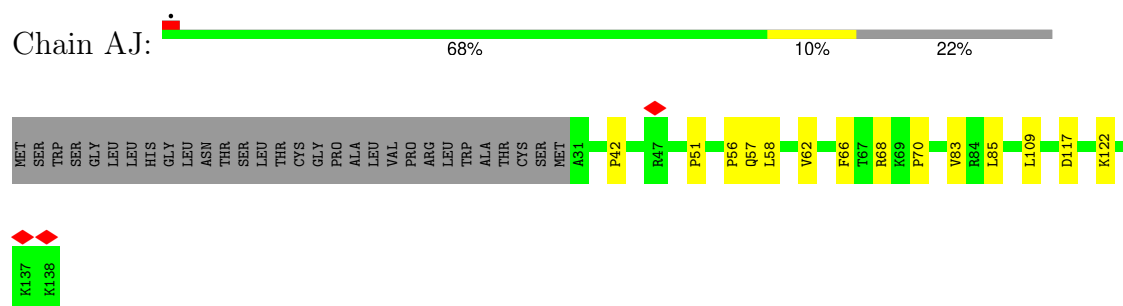
- Molecule 59: 28S ribosomal protein S9, mitochondrial



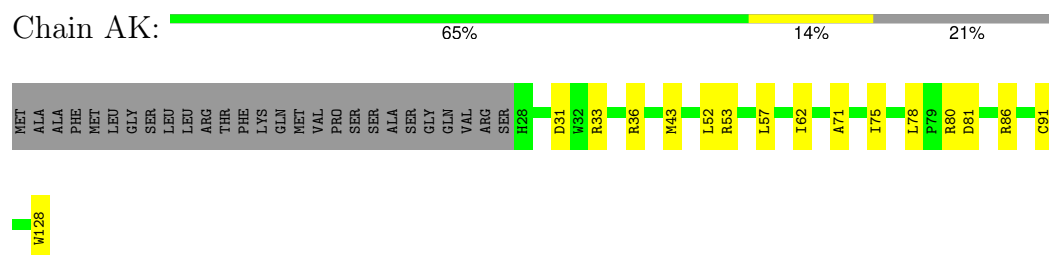
- Molecule 60: 28S ribosomal protein S10, mitochondrial



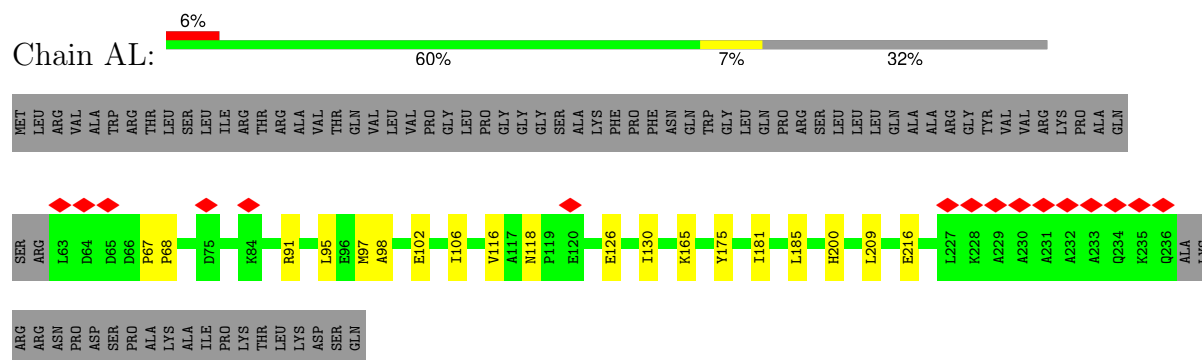
- Molecule 61: 28S ribosomal protein S12, mitochondrial



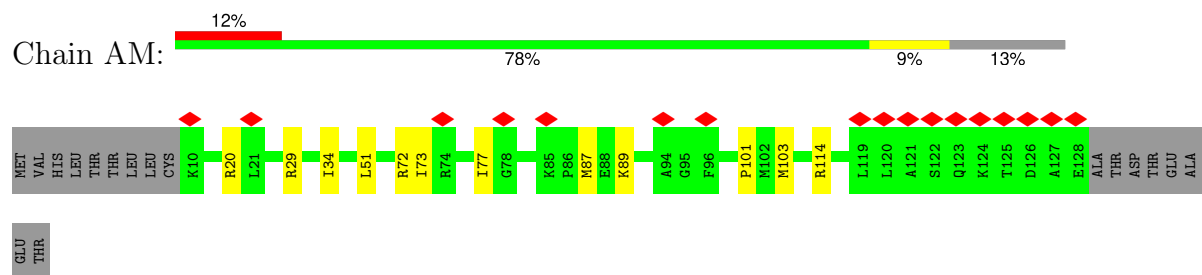
- Molecule 62: 28S ribosomal protein S14, mitochondrial



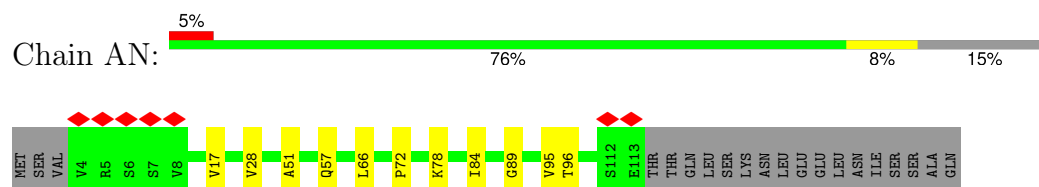
- Molecule 63: 28S ribosomal protein S15, mitochondrial



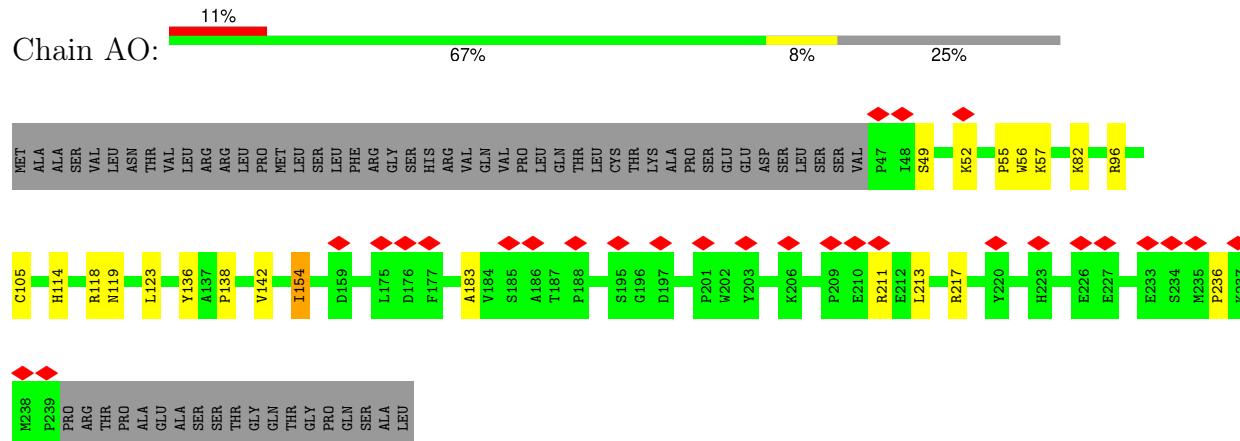
- Molecule 64: 28S ribosomal protein S16, mitochondrial



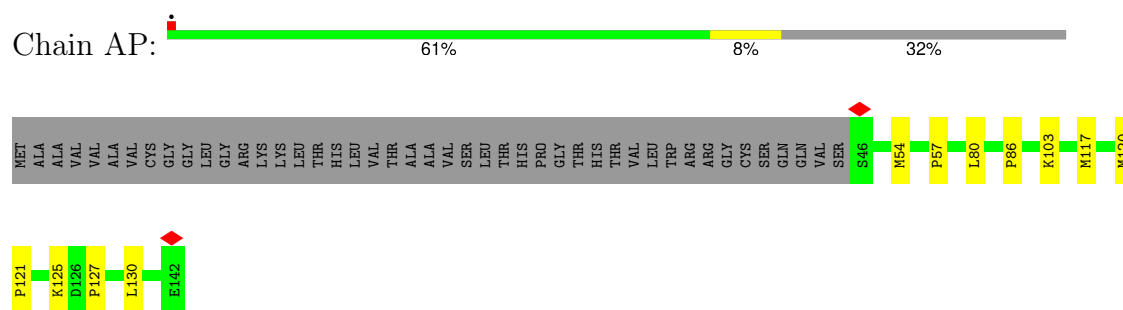
- Molecule 65: 28S ribosomal protein S17, mitochondrial



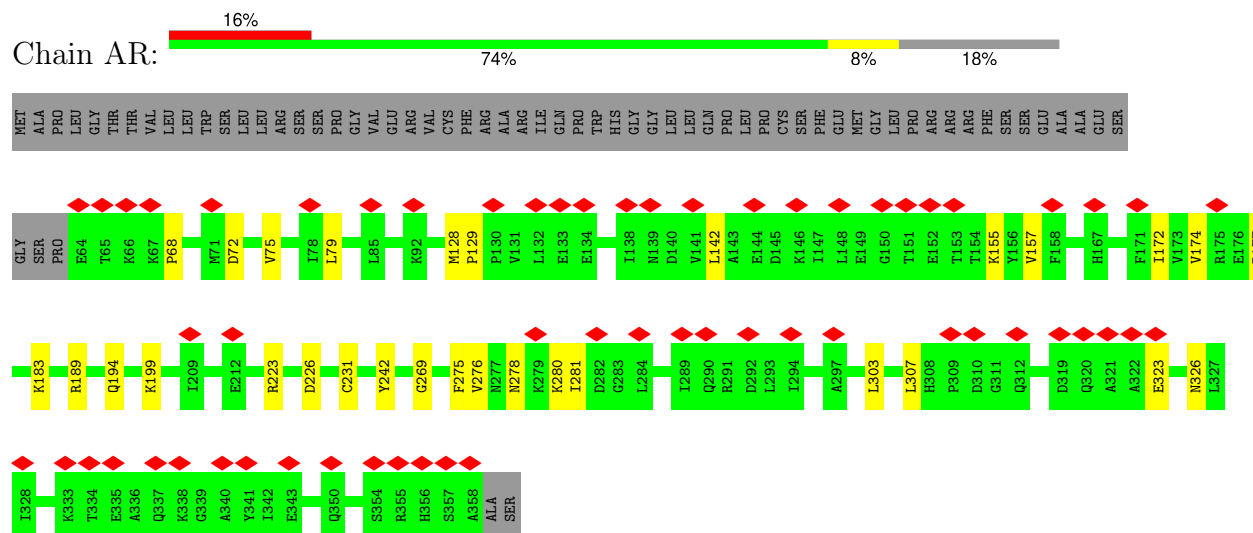
- Molecule 66: 28S ribosomal protein S18b, mitochondrial



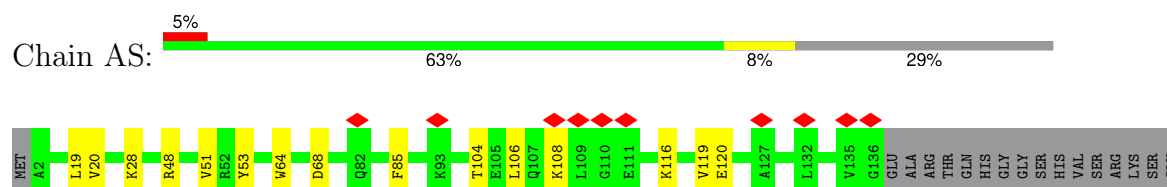
- Molecule 67: 28S ribosomal protein S18c, mitochondrial



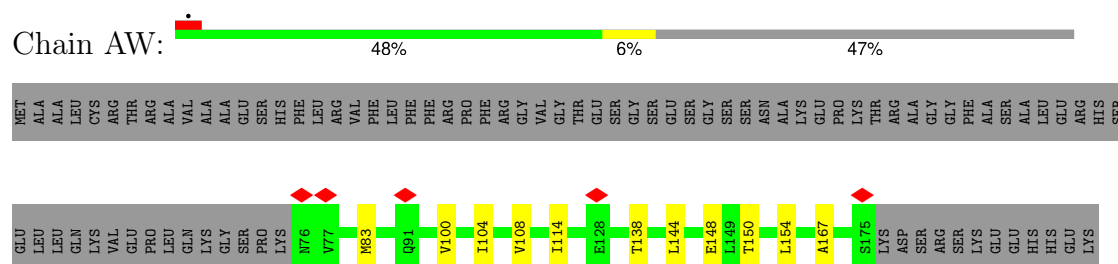
- Molecule 68: 28S ribosomal protein S22, mitochondrial



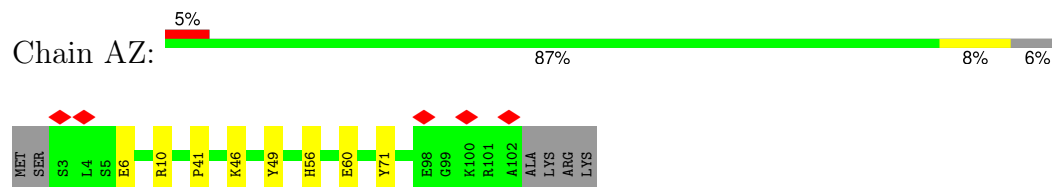
- Molecule 69: 28S ribosomal protein S23, mitochondrial



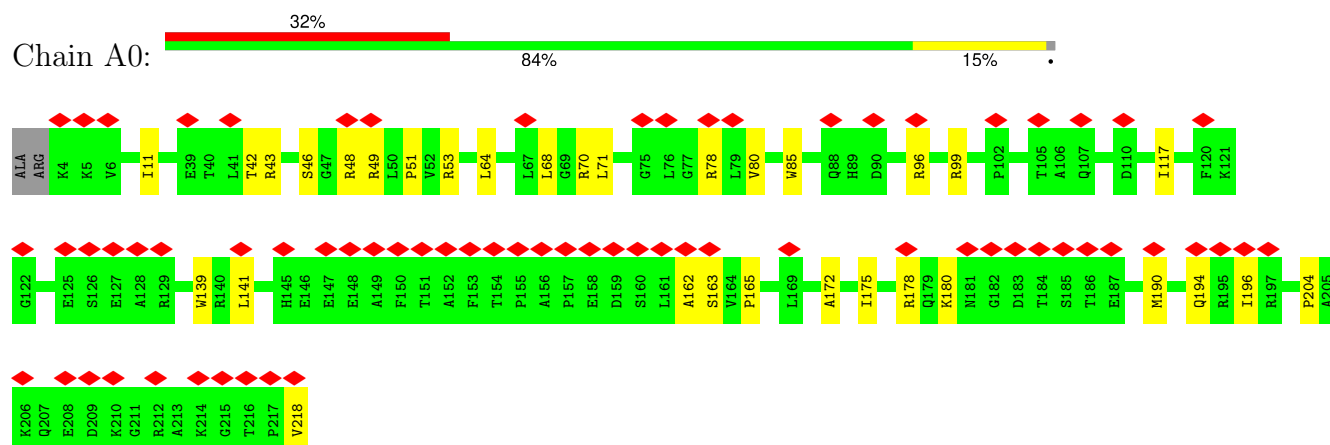
- Molecule 73: 28S ribosomal protein S28, mitochondrial



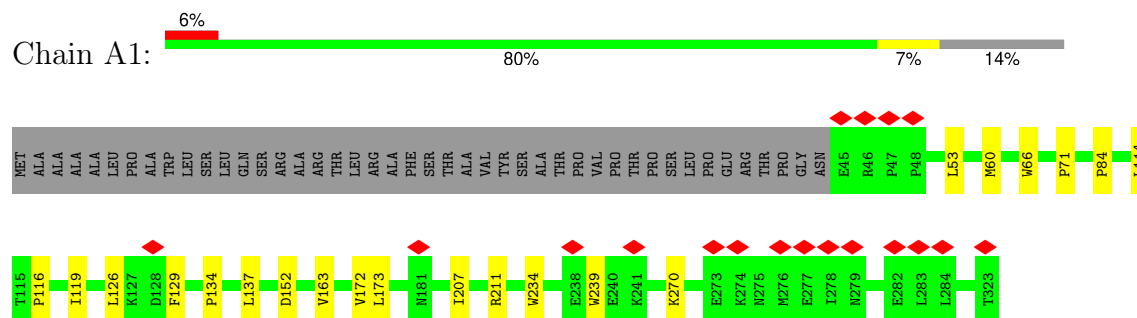
- Molecule 74: 28S ribosomal protein S33, mitochondrial



- Molecule 75: Small ribosomal subunit protein mS34



- Molecule 76: 28S ribosomal protein S35, mitochondrial

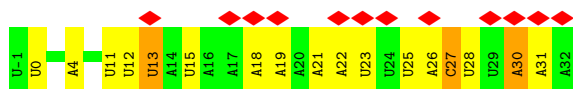


- Molecule 77: Aurora kinase A-interacting protein

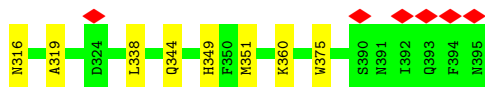
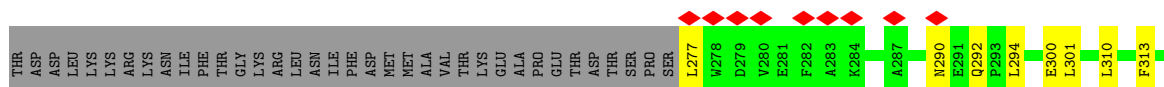
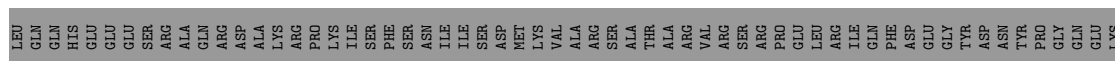




Chain Az:

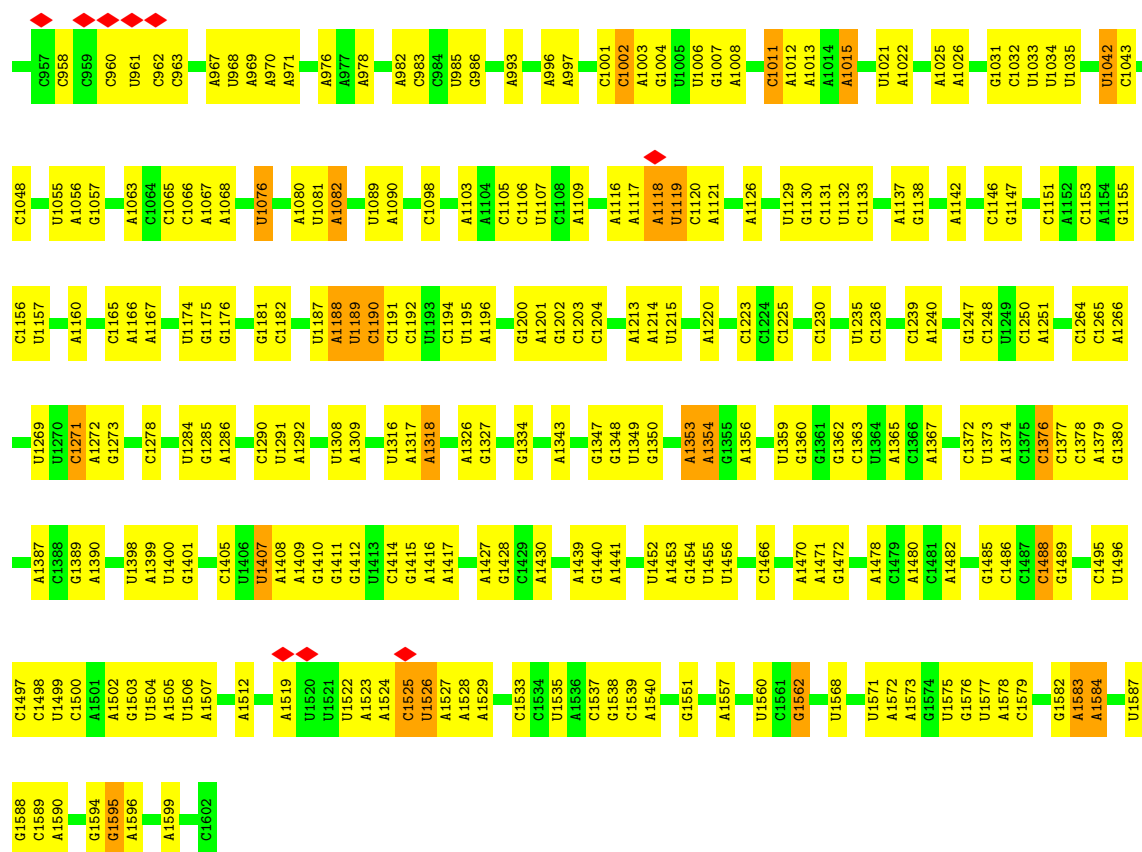


Chain AY: 26% 70%

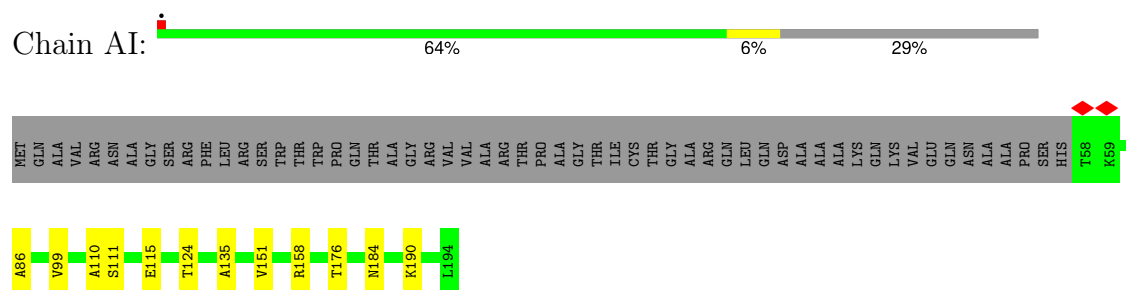


Chain AA: 59% 37%

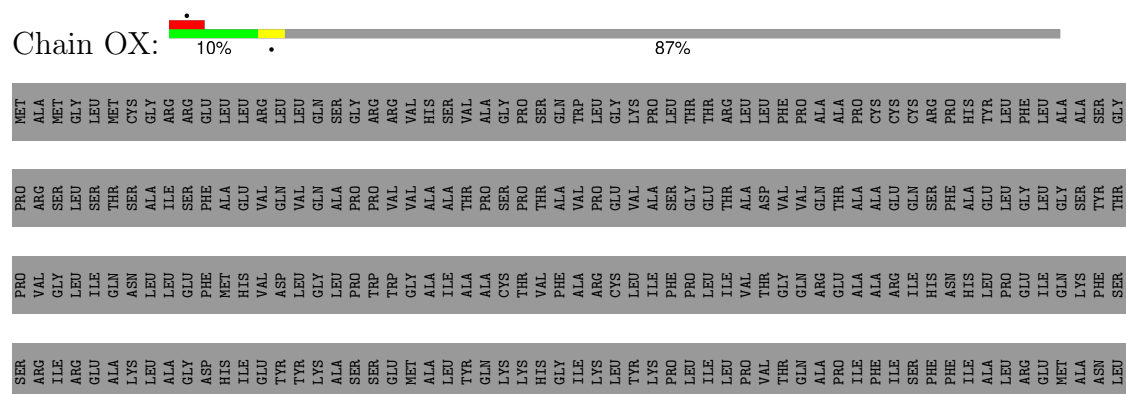


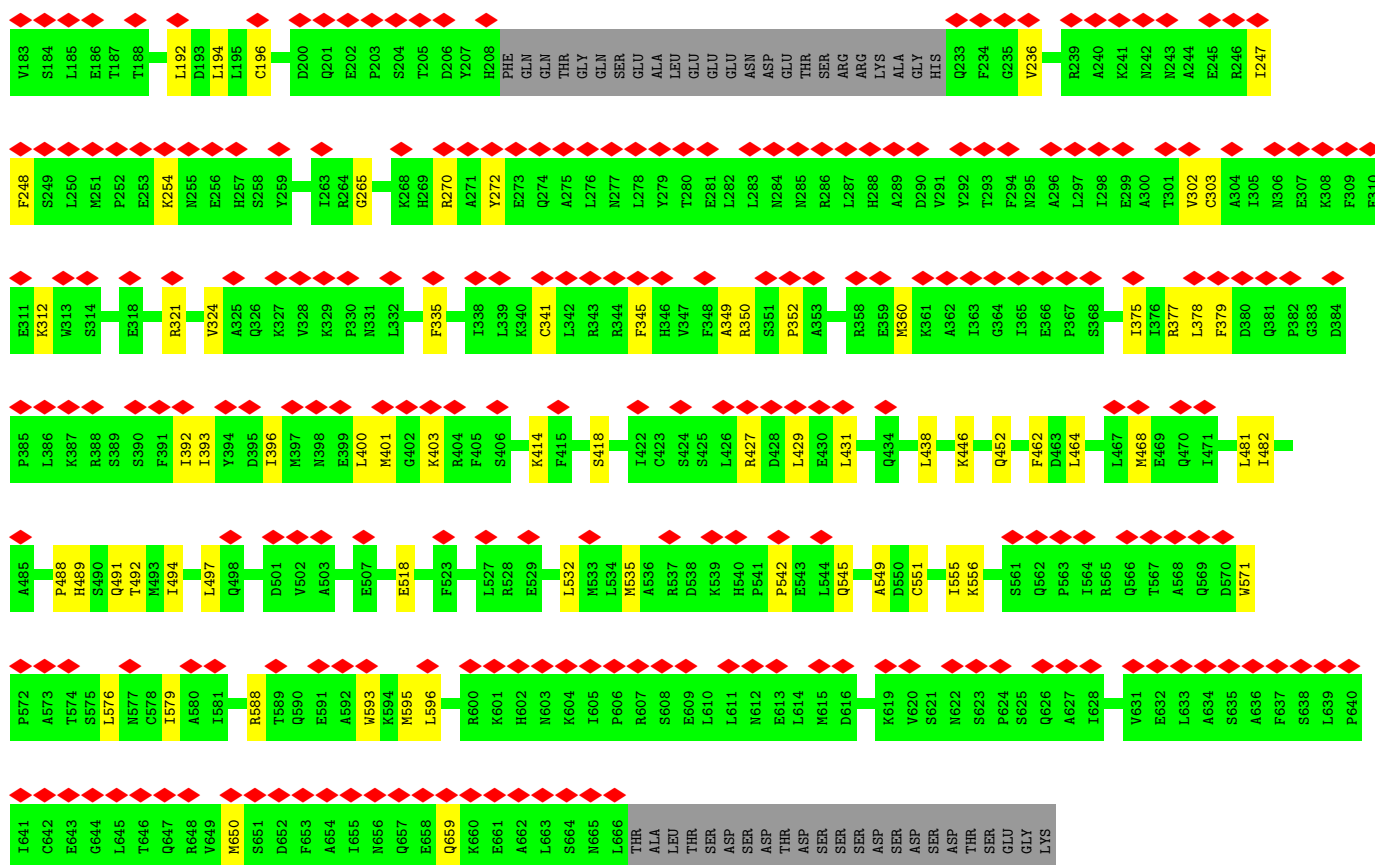


- Molecule 81: 28S ribosomal protein S11, mitochondrial



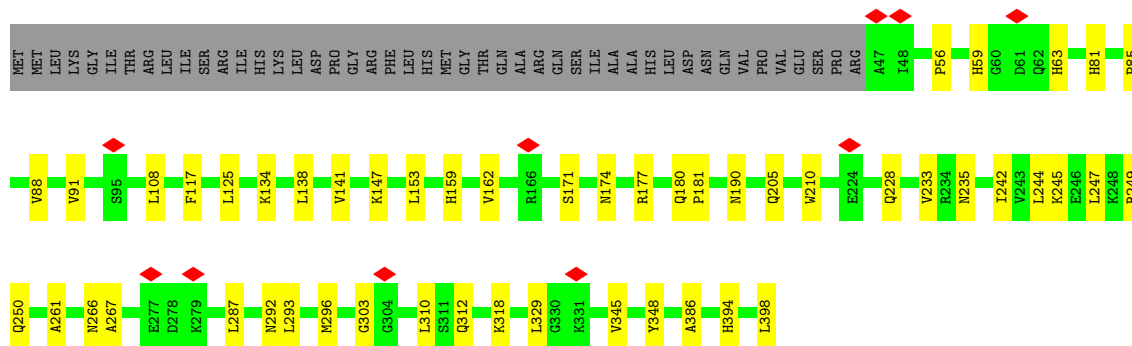
- Molecule 82: Mitochondrial inner membrane protein OXA1L





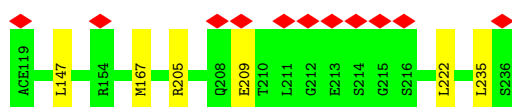
- Molecule 87: 28S ribosomal protein S29, mitochondrial

Chain AX: 76% 13% 12%



- Molecule 88: Small ribosomal subunit protein mS37

Chain A2: 95% 5% 9%



- Molecule 89: Small ribosomal subunit protein bS21m

Chain AQ:

97%



● Molecule 90: mitochondrial tRNAVal

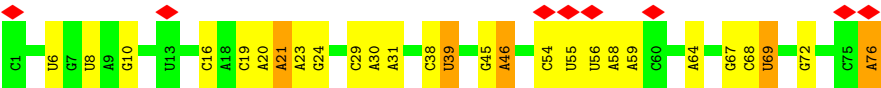
Chain B:

11%

62%

31%

7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175268	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	0.538	Depositor
Minimum map value	-0.251	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/913	0.28	0/1224
2	1	0.28	0/469	0.28	0/621
3	2	0.39	0/383	0.31	0/507
4	3	0.37	0/853	0.30	0/1136
5	4	0.33	0/350	0.29	0/461
6	5	0.29	0/3305	0.30	0/4502
7	6	0.24	0/3043	0.29	0/4140
8	7	0.25	0/2447	0.28	0/3310
9	8	0.15	0/1354	0.31	0/1819
10	9	0.29	0/1025	0.28	0/1379
11	A	0.38	0/36876	0.33	0/57402
12	C	0.14	0/1754	0.30	0/2357
13	D	0.32	0/1896	0.30	0/2549
14	E	0.32	0/2475	0.32	0/3355
15	F	0.35	0/2090	0.33	0/2842
16	H	0.18	0/1698	0.27	0/2292
17	I	0.20	0/1478	0.33	0/1999
18	J	0.16	0/1348	0.30	0/1813
19	K	0.35	0/1497	0.31	0/2031
20	L	0.30	0/905	0.31	0/1218
21	M	0.33	0/2381	0.31	0/3212
22	N	0.31	0/1833	0.30	0/2468
23	O	0.33	0/1283	0.31	0/1727
24	P	0.28	0/1199	0.29	0/1623
25	Q	0.29	0/2039	0.28	0/2750
26	R	0.37	0/1175	0.29	0/1572
27	S	0.35	0/1320	0.33	0/1789
28	T	0.35	0/1403	0.29	0/1886
29	U	0.31	0/1279	0.34	0/1730
30	W	0.33	0/926	0.28	0/1244
31	X	0.29	0/2099	0.27	0/2837

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.32	0/1593	0.27	0/2136
33	Z	0.33	0/1021	0.30	0/1378
34	G	0.14	0/562	0.47	0/754
34	t	0.12	0/358	0.26	0/486
34	u	0.17	0/259	0.35	0/350
35	V	0.25	0/1721	0.28	0/2333
36	b	0.33	0/1218	0.32	0/1649
37	d	0.21	0/2181	0.32	0/2949
38	e	0.14	0/1970	0.31	0/2658
39	g	0.32	0/1151	0.31	0/1569
40	h	0.22	0/918	0.26	0/1249
41	i	0.37	0/850	0.32	0/1135
42	j	0.29	0/760	0.26	0/1023
43	k	0.17	0/783	0.24	0/1057
44	l	0.16	0/707	0.28	0/960
45	m	0.14	0/805	0.29	0/1081
47	o	0.34	0/819	0.33	0/1097
48	q	0.21	0/1529	0.29	0/2055
49	r	0.30	0/1362	0.30	0/1846
50	c	0.28	0/2347	0.27	0/3171
51	f	0.21	0/1273	0.35	0/1716
52	p	0.22	0/1223	0.26	0/1641
53	s	0.32	0/3231	0.31	0/4389
54	AB	0.21	0/1871	0.27	0/2531
55	AC	0.20	0/1113	0.29	0/1505
56	AD	0.20	0/2783	0.27	0/3724
57	AE	0.22	0/989	0.28	0/1335
58	AF	0.18	0/1767	0.24	0/2373
59	AG	0.19	0/2746	0.27	0/3681
60	AH	0.20	0/1178	0.30	0/1598
61	AJ	0.22	0/855	0.26	0/1148
62	AK	0.20	0/880	0.27	0/1182
63	AL	0.21	0/1477	0.24	0/1974
64	AM	0.14	0/963	0.28	0/1295
65	AN	0.19	0/886	0.26	0/1199
66	AO	0.15	0/1648	0.28	0/2243
67	AP	0.23	0/798	0.27	0/1070
68	AR	0.12	0/2456	0.26	0/3317
69	AS	0.17	0/1138	0.23	0/1533
70	AT	0.17	0/1402	0.28	0/1883
71	AU	0.15	0/1510	0.26	0/2025
72	AV	0.13	0/3030	0.32	0/4093
73	AW	0.19	0/801	0.25	0/1079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	AZ	0.18	0/857	0.33	0/1141
75	A0	0.12	0/1834	0.27	0/2484
76	A1	0.16	0/2313	0.27	0/3129
77	A3	0.25	0/636	0.32	0/839
78	Az	0.18	0/804	0.32	0/1248
79	AY	0.14	0/1040	0.24	0/1402
80	AA	0.26	0/22537	0.28	0/35085
81	AI	0.24	0/1039	0.31	0/1400
82	OX	0.18	0/478	0.41	0/639
83	a	0.29	0/891	0.35	0/1208
84	Ax	0.23	0/1673	0.36	0/2602
85	Aw	0.19	0/1600	0.30	0/2476
86	A4	0.14	0/4877	0.32	0/6598
87	AX	0.16	0/2921	0.32	0/3954
88	A2	0.21	0/947	0.28	0/1266
89	AQ	0.24	0/754	0.28	0/1003
90	B	0.20	0/1626	0.29	0/2523
All	All	0.28	0/188855	0.30	0/268262

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	3	0
2	1	464	0	511	5	0
3	2	377	0	406	1	0
4	3	832	0	883	6	0
5	4	342	0	361	3	0
6	5	3210	0	3206	19	0
7	6	2948	0	2841	17	0
8	7	2390	0	2397	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	8	1327	0	1368	21	0
10	9	997	0	987	8	0
11	A	33070	0	16792	168	0
12	C	1732	0	1740	30	0
13	D	1859	0	1920	8	0
14	E	2406	0	2415	11	0
15	F	2031	0	2065	12	0
16	H	1661	0	1734	10	0
17	I	1446	0	1532	10	0
18	J	1330	0	1407	15	0
19	K	1455	0	1452	8	0
20	L	890	0	941	5	0
21	M	2327	0	2394	13	0
22	N	1786	0	1817	13	0
23	O	1259	0	1294	8	0
24	P	1173	0	1165	11	0
25	Q	1990	0	2031	9	0
26	R	1154	0	1214	5	0
27	S	1293	0	1365	12	0
28	T	1369	0	1410	6	0
29	U	1248	0	1228	5	0
30	W	904	0	934	3	0
31	X	2044	0	2060	11	0
32	Y	1556	0	1597	5	0
33	Z	996	0	1044	3	0
34	G	558	0	612	10	0
34	t	354	0	377	3	0
34	u	257	0	283	5	0
35	V	1676	0	1687	18	0
36	b	1193	0	1191	8	0
37	d	2124	0	2125	21	0
38	e	1931	0	1916	31	0
39	g	1113	0	1097	4	0
40	h	895	0	881	4	0
41	i	828	0	857	4	0
42	j	745	0	746	2	0
43	k	774	0	784	3	0
44	l	688	0	674	6	0
45	m	791	0	796	9	0
46	n	215	0	51	0	0
47	o	798	0	804	5	0
48	q	1495	0	1492	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	r	1322	0	1348	9	0
50	c	2299	0	2320	10	0
51	f	1252	0	1269	19	0
52	p	1205	0	1223	6	0
53	s	3148	0	3131	17	0
54	AB	1828	0	1815	10	0
55	AC	1083	0	1088	12	0
56	AD	2731	0	2804	23	0
57	AE	972	0	1000	6	0
58	AF	1725	0	1769	9	0
59	AG	2688	0	2687	27	0
60	AH	1152	0	1183	22	0
61	AJ	839	0	887	9	0
62	AK	862	0	885	16	0
63	AL	1453	0	1540	15	0
64	AM	942	0	965	8	0
65	AN	868	0	928	6	0
66	AO	1592	0	1557	15	0
67	AP	781	0	806	8	0
68	AR	2409	0	2428	20	0
69	AS	1111	0	1115	11	0
70	AT	1371	0	1393	12	0
71	AU	1488	0	1499	11	0
72	AV	2969	0	2961	38	0
73	AW	789	0	802	9	0
74	AZ	839	0	858	7	0
75	A0	1787	0	1796	24	0
76	A1	2265	0	2294	20	0
77	A3	625	0	698	7	0
78	Az	719	0	359	5	0
79	AY	1010	0	957	13	0
80	AA	20260	0	10284	238	0
81	AI	1019	0	1059	8	0
82	OX	468	0	464	11	0
83	a	865	0	829	6	0
84	Ax	1498	0	766	18	0
85	Aw	1434	0	728	17	0
86	A4	4768	0	4766	61	0
87	AX	2849	0	2844	31	0
88	A2	935	0	971	5	0
89	AQ	744	0	758	3	0
90	B	1524	0	779	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	0	1	0	0	0	0
91	4	1	0	0	0	0
91	AO	1	0	0	0	0
92	6	1	0	0	0	0
92	A	29	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	o	1	0	0	0	0
93	A	40	0	76	0	0
93	AA	30	0	53	2	0
93	O	10	0	19	0	0
94	A	6	0	12	0	0
95	A	137	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	AK	1	0	0	0	0
95	AX	1	0	0	0	0
95	D	2	0	0	0	0
95	E	1	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	0	0
99	AX	31	0	12	0	0
100	AX	28	0	12	1	0
101	B	7	0	8	3	0
All	All	180184	0	152683	1250	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 (1250) 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)
38:e:265:LYS:HE2	90:B:76:A:H8	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:e:166:GLY:HA3	101:B:101:VAL:HB	1.63	0.78
67:AP:80:LEU:HB2	67:AP:120:MET:HE1	1.65	0.78
38:e:183:THR:HG23	38:e:186:GLY:H	1.50	0.76
9:8:136:ILE:HD11	51:f:169:ILE:HG23	1.67	0.76
26:R:111:LYS:HB2	36:b:127:GLN:HG2	1.68	0.75
7:6:53:SER:HB3	90:B:38:C:H5''	1.70	0.73
18:J:189:ALA:HA	18:J:192:LYS:HD2	1.73	0.71
78:Az:28:U:H1'	86:A4:414:LYS:HG2	1.73	0.70
9:8:68:LEU:HD21	51:f:211:LEU:HB2	1.72	0.70
71:AU:65:GLN:HG3	75:A0:196:ILE:HD11	1.71	0.70
72:AV:66:PRO:HD3	80:AA:1529:A:H1'	1.74	0.70
80:AA:1398:U:H2'	80:AA:1399:A:H8	1.58	0.68
11:A:1886:G:H1	41:i:61:GLY:HA3	1.59	0.68
9:8:187:PRO:HG2	45:m:79:ILE:HD11	1.76	0.68
51:f:90:VAL:HG13	51:f:189:HIS:HB3	1.76	0.68
60:AH:70:ASP:HA	86:A4:62:LYS:HE3	1.74	0.67
12:C:90:LEU:HG	12:C:153:LEU:HD22	1.75	0.67
8:7:143:TRP:HE1	8:7:172:VAL:HG23	1.58	0.67
62:AK:33:ARG:HE	80:AA:1236:C:H5''	1.60	0.67
9:8:59:LYS:HB3	84:Ax:10:A:H4'	1.76	0.66
75:A0:99:ARG:HD3	80:AA:1526:U:H2'	1.76	0.66
76:A1:71:PRO:HB3	86:A4:78:VAL:HG21	1.77	0.66
6:5:143:PRO:HA	6:5:146:HIS:HD1	1.61	0.66
65:AN:72:PRO:HB3	65:AN:78:LYS:HG2	1.77	0.66
11:A:1994:A:H61	11:A:2736:C:H4'	1.61	0.66
11:A:3150:U:H2'	11:A:3151:A:H8	1.60	0.66
43:k:130:VAL:HG11	43:k:146:LEU:HB2	1.78	0.66
68:AR:155:LYS:HB3	68:AR:177:PRO:HD3	1.78	0.65
4:3:138:PRO:HG2	11:A:2854:U:H4'	1.78	0.65
80:AA:1002:C:H2'	80:AA:1003:A:H8	1.62	0.65
51:f:171:LEU:HD13	51:f:174:ILE:HD11	1.78	0.64
9:8:192:TYR:HB3	51:f:132:ILE:HD11	1.79	0.64
35:V:79:VAL:HG12	35:V:86:VAL:HG12	1.80	0.64
39:g:111:ARG:HG2	39:g:112:LYS:H	1.63	0.64
53:s:145:VAL:HG21	53:s:187:LEU:HD11	1.79	0.64
84:Ax:16:A:H4'	84:Ax:17:U:H5''	1.79	0.64
87:AX:153:LEU:HD21	87:AX:247:LEU:HD13	1.79	0.64
38:e:97:ARG:HH11	38:e:112:GLN:HE22	1.46	0.64
64:AM:20:ARG:HB2	80:AA:839:A:H5''	1.79	0.64
12:C:89:ARG:HG3	12:C:129:GLU:HG2	1.78	0.64
79:AY:338:LEU:HD11	79:AY:351:MET:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AD:140:LEU:HD11	56:AD:160:ARG:HG3	1.80	0.63
11:A:3199:U:H5''	11:A:3200:U:H4'	1.80	0.63
87:AX:108:LEU:HD23	87:AX:141:VAL:HG11	1.81	0.63
56:AD:420:SER:HA	80:AA:929:A:H4'	1.79	0.62
12:C:239:LEU:HD11	12:C:256:CYS:HB2	1.82	0.62
17:I:47:LEU:HD22	22:N:226:ILE:HG12	1.81	0.62
76:A1:126:LEU:HD11	86:A4:70:VAL:HG13	1.80	0.62
87:AX:205:GLN:HG2	87:AX:250:GLN:HE21	1.64	0.62
57:AE:35:ILE:HD11	63:AL:91:ARG:HE	1.64	0.61
12:C:211:ILE:HD12	34:G:143:VAL:HG12	1.82	0.61
59:AG:275:LYS:HG2	59:AG:280:LYS:HG2	1.80	0.61
80:AA:1003:A:H2'	80:AA:1004:G:H8	1.65	0.61
80:AA:1201:A:H2'	80:AA:1202:G:H8	1.66	0.61
80:AA:1528:A:H2'	80:AA:1529:A:H8	1.66	0.61
16:H:97:ILE:HD11	16:H:137:LYS:HG3	1.82	0.61
7:6:255:LEU:HD12	7:6:256:PRO:HD2	1.82	0.61
8:7:107:LEU:HD13	8:7:128:LEU:HD11	1.82	0.61
11:A:2055:U:H2'	11:A:2056:G:H8	1.65	0.61
67:AP:54:MET:HE2	69:AS:64:TRP:HB3	1.83	0.61
17:I:116:LEU:HG	17:I:121:ILE:HB	1.82	0.60
23:O:50:ASP:HB2	23:O:107:MET:HE1	1.83	0.60
12:C:165:ARG:HH22	85:Aw:50:A:H4'	1.66	0.60
85:Aw:68:U:H2'	85:Aw:69:A:C8	2.36	0.60
12:C:191:VAL:HG11	12:C:251:LEU:HD23	1.83	0.60
50:c:105:ARG:HH12	50:c:115:VAL:HB	1.65	0.60
86:A4:571:TRP:HE3	86:A4:576:LEU:HD21	1.65	0.60
84:Ax:8:U:H3	84:Ax:14:A:H62	1.48	0.60
21:M:244:LEU:HD12	21:M:245:PRO:HD2	1.84	0.60
34:u:86:LEU:O	34:u:90:LEU:HB2	2.02	0.60
35:V:168:GLU:HB3	82:OX:374:MET:HE1	1.84	0.60
8:7:112:PRO:HB2	8:7:267:PRO:HG2	1.84	0.59
70:AT:29:VAL:HB	70:AT:79:TYR:HB2	1.83	0.59
54:AB:180:ARG:HH21	56:AD:210:PRO:HB2	1.66	0.59
8:7:204:LYS:HE2	83:a:92:LEU:HD22	1.84	0.59
80:AA:839:A:H2'	80:AA:840:A:H8	1.66	0.59
60:AH:162:ARG:HH21	79:AY:313:PHE:HB2	1.66	0.59
60:AH:164:LEU:HD12	60:AH:165:PRO:HD2	1.84	0.59
80:AA:1347:G:H2'	80:AA:1348:G:H8	1.67	0.59
68:AR:172:ILE:HD12	68:AR:189:ARG:HG2	1.83	0.59
11:A:1952:U:H2'	11:A:1953:A:C8	2.38	0.59
22:N:218:ILE:HG23	22:N:223:MET:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:e:219:GLN:HA	38:e:222:ARG:HB2	1.85	0.59
72:AV:143:THR:HA	72:AV:146:LEU:HD12	1.85	0.59
62:AK:31:ASP:HB3	93:AA:1703:SPD:HN12	1.68	0.59
70:AT:140:ILE:HG13	70:AT:146:GLN:HG3	1.84	0.59
21:M:261:ASP:HB3	21:M:264:GLN:HB2	1.84	0.59
90:B:23:A:H2'	90:B:24:G:C8	2.38	0.59
11:A:2099:U:H2'	11:A:2100:C:C6	2.37	0.58
17:I:101:ASN:HB3	17:I:150:HIS:HB3	1.85	0.58
53:s:271:LEU:HD23	53:s:273:LEU:HD13	1.84	0.58
16:H:172:LEU:HD23	16:H:235:MET:HE1	1.85	0.58
80:AA:941:G:H4'	80:AA:942:A:H5''	1.85	0.58
10:9:86:LEU:HD21	10:9:91:LEU:HD12	1.85	0.58
47:o:12:ILE:HG13	47:o:23:ARG:HB2	1.85	0.58
18:J:88:SER:HA	18:J:151:LEU:HD11	1.86	0.58
80:AA:1201:A:H2'	80:AA:1202:G:C8	2.39	0.58
58:AF:200:LEU:HB3	58:AF:202:PRO:HD2	1.85	0.58
33:Z:75:THR:HB	33:Z:83:LYS:HG2	1.85	0.58
74:AZ:56:HIS:O	74:AZ:60:GLU:HG3	2.02	0.58
7:6:206:TYR:HH	7:6:214:TRP:CD1	2.22	0.58
11:A:2740:A:H2'	11:A:2741:A:C8	2.39	0.58
64:AM:29:ARG:HE	70:AT:147:VAL:HB	1.69	0.58
56:AD:140:LEU:HB2	56:AD:158:ALA:HB3	1.86	0.58
60:AH:76:LEU:HB2	60:AH:145:LEU:HB2	1.85	0.58
72:AV:117:LEU:HA	72:AV:122:GLN:OE1	2.04	0.58
87:AX:245:LYS:HB3	87:AX:249:ARG:HH21	1.69	0.58
90:B:30:A:H2'	90:B:31:A:H8	1.68	0.58
45:m:90:ARG:HE	45:m:94:ARG:HG3	1.69	0.57
80:AA:663:A:H2'	80:AA:664:G:C8	2.39	0.57
35:V:133:ILE:HD12	35:V:145:ARG:HB3	1.86	0.57
80:AA:686:A:H2'	80:AA:687:G:H8	1.69	0.57
13:D:213:CYS:HB3	13:D:246:ARG:HG3	1.87	0.57
51:f:119:ILE:HD11	51:f:166:PHE:HE2	1.69	0.57
80:AA:922:C:H2'	80:AA:923:A:H8	1.69	0.57
84:Ax:46:U:H3	84:Ax:59:U:H3	1.53	0.57
38:e:85:SER:HB3	45:m:50:ARG:HB3	1.87	0.57
80:AA:1440:G:H2'	80:AA:1441:A:H8	1.68	0.57
7:6:187:VAL:HG13	7:6:319:PHE:HB3	1.87	0.57
75:A0:165:PRO:HG3	75:A0:190:MET:HE2	1.85	0.57
80:AA:1025:A:H2'	80:AA:1026:A:C8	2.40	0.57
90:B:29:C:H2'	90:B:30:A:H8	1.69	0.57
35:V:136:ARG:NH2	82:OX:403:HIS:HB2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AD:140:LEU:HD23	56:AD:146:VAL:HG11	1.86	0.57
80:AA:686:A:H2'	80:AA:687:G:C8	2.40	0.57
80:AA:1440:G:H2'	80:AA:1441:A:C8	2.39	0.57
36:b:78:GLU:HG3	36:b:84:VAL:HG22	1.86	0.57
76:A1:53:LEU:HD12	86:A4:518:GLU:HG2	1.87	0.57
22:N:124:VAL:HG12	22:N:158:ARG:HE	1.69	0.57
77:A3:193:LYS:HB3	77:A3:196:LEU:HD23	1.85	0.57
31:X:20:ILE:HG22	82:OX:434:LEU:HD23	1.85	0.57
86:A4:400:LEU:HA	86:A4:403:LYS:HD3	1.86	0.57
7:6:192:GLU:HG2	52:p:185:ARG:HD3	1.87	0.56
36:b:89:ILE:HA	36:b:92:LYS:HD2	1.87	0.56
76:A1:163:VAL:H	86:A4:134:GLU:HB2	1.70	0.56
12:C:265:LYS:HB3	12:C:297:GLU:HB2	1.86	0.56
9:8:99:ARG:HG2	38:e:83:LEU:HB3	1.87	0.56
48:q:164:LEU:HG	48:q:178:LEU:HD22	1.87	0.56
11:A:3150:U:H2'	11:A:3151:A:C8	2.39	0.56
17:I:140:TYR:HB3	17:I:143:LEU:HD12	1.87	0.56
38:e:61:LYS:HE2	38:e:155:ARG:HD2	1.87	0.56
48:q:164:LEU:HB3	48:q:168:VAL:HG21	1.87	0.56
80:AA:1470:A:H2'	80:AA:1471:A:H8	1.70	0.56
31:X:168:ARG:HH11	31:X:176:LEU:HB2	1.70	0.56
59:AG:242:GLN:HA	59:AG:245:ARG:HG3	1.87	0.56
80:AA:922:C:H2'	80:AA:923:A:C8	2.41	0.56
11:A:2093:U:H2'	11:A:2094:G:C8	2.41	0.56
80:AA:1376:C:H4'	80:AA:1377:C:H5'	1.87	0.56
86:A4:482:ILE:HD12	86:A4:488:PRO:HD3	1.88	0.56
65:AN:95:VAL:HG23	65:AN:96:THR:HG23	1.88	0.55
66:AO:105:CYS:HB2	66:AO:142:VAL:HA	1.87	0.55
12:C:217:ASP:HB2	12:C:233:ILE:HB	1.88	0.55
9:8:201:GLN:HB3	51:f:201:ARG:HG3	1.88	0.55
11:A:1806:U:H4'	11:A:1807:U:H5'	1.89	0.55
37:d:138:PRO:HG3	37:d:194:VAL:HG23	1.88	0.55
80:AA:1308:U:H2'	80:AA:1309:A:H8	1.71	0.55
61:AJ:57:GLN:HB3	61:AJ:109:LEU:HD11	1.88	0.55
11:A:1851:G:H2'	11:A:2693:A:N7	2.22	0.55
21:M:177:ALA:HB1	21:M:203:ARG:HH12	1.71	0.55
38:e:55:ARG:HD3	38:e:149:LEU:HD22	1.87	0.55
11:A:1952:U:H2'	11:A:1953:A:H8	1.71	0.55
24:P:52:ASN:HB3	24:P:55:ASN:HB2	1.87	0.55
59:AG:101:GLN:HA	59:AG:104:ILE:HD12	1.88	0.55
66:AO:82:LYS:HB3	80:AA:881:A:N6	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Aw:16:A:H3'	85:Aw:20:C:H5'	1.87	0.55
80:AA:681:U:H2'	80:AA:682:A:H8	1.72	0.55
80:AA:747:A:H2'	80:AA:748:G:H8	1.72	0.55
80:AA:1002:C:H2'	80:AA:1003:A:C8	2.41	0.55
11:A:1936:A:H4'	11:A:1937:A:C8	2.42	0.55
80:AA:1400:U:H2'	80:AA:1401:G:C8	2.42	0.55
80:AA:1359:U:H2'	80:AA:1360:G:H8	1.72	0.55
9:8:51:ARG:HH22	80:AA:1560:U:H5''	1.72	0.55
11:A:1857:U:H2'	11:A:1858:G:C8	2.42	0.55
35:V:80:ILE:HB	35:V:85:TRP:HB2	1.89	0.55
62:AK:33:ARG:HG2	62:AK:36:ARG:HH22	1.72	0.55
11:A:2545:U:H5''	11:A:2546:G:H5'	1.87	0.54
59:AG:293:ILE:HG23	59:AG:328:VAL:HB	1.89	0.54
80:AA:861:U:H2'	80:AA:862:A:H8	1.72	0.54
87:AX:244:LEU:HD12	87:AX:292:ASN:HB3	1.88	0.54
72:AV:149:ASP:HA	72:AV:152:ILE:HG22	1.90	0.54
87:AX:134:LYS:HG2	87:AX:345:VAL:HG11	1.89	0.54
11:A:3211:C:H4'	11:A:3212:C:H5	1.72	0.54
15:F:243:ILE:HG22	48:q:27:ALA:HB2	1.89	0.54
25:Q:183:LEU:HD21	25:Q:219:GLU:HG3	1.89	0.54
84:Ax:4:A:H2'	84:Ax:5:A:H8	1.72	0.54
11:A:2727:C:H2'	11:A:2728:C:H6	1.72	0.54
37:d:108:ARG:HA	37:d:111:ARG:HD2	1.89	0.54
9:8:190:GLY:HA3	45:m:78:PRO:HB2	1.89	0.54
11:A:2718:C:H2'	11:A:2991:U:H4'	1.89	0.54
11:A:2727:C:H2'	11:A:2728:C:C6	2.43	0.54
11:A:2109:A:H5'	22:N:133:ARG:HD3	1.88	0.54
57:AE:92:ASN:HB2	67:AP:117:MET:HE3	1.90	0.54
72:AV:322:THR:HG23	72:AV:325:SER:H	1.72	0.54
80:AA:1068:A:H5''	81:AI:190:LYS:HD3	1.90	0.54
6:5:192:ILE:HD11	6:5:199:ALA:HB2	1.88	0.54
6:5:393:LYS:HD3	6:5:398:VAL:HG21	1.90	0.53
60:AH:162:ARG:HH12	86:A4:71:LEU:HD11	1.72	0.53
72:AV:175:VAL:HG12	72:AV:177:SER:H	1.73	0.53
80:AA:916:C:H2'	80:AA:917:C:C6	2.43	0.53
80:AA:1156:C:H2'	80:AA:1157:U:H6	1.73	0.53
87:AX:159:HIS:HA	87:AX:162:VAL:HG12	1.89	0.53
18:J:140:VAL:O	18:J:144:ILE:HG12	2.07	0.53
80:AA:842:C:H2'	80:AA:843:G:C8	2.43	0.53
80:AA:867:C:H2'	80:AA:870:C:H42	1.73	0.53
20:L:32:ILE:HD11	20:L:103:ASN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AR:79:LEU:HD22	68:AR:269:GLY:HA2	1.90	0.53
76:A1:134:PRO:HG3	86:A4:60:PRO:HD3	1.90	0.53
23:O:44:ALA:HB3	23:O:49:VAL:HG23	1.90	0.53
53:s:63:ILE:HA	53:s:66:TRP:CD1	2.43	0.53
54:AB:81:VAL:HG12	73:AW:83:MET:HE1	1.89	0.53
56:AD:116:LYS:HE2	78:Az:13:U:H5'	1.90	0.53
73:AW:104:ILE:HD13	73:AW:138:THR:HB	1.91	0.53
80:AA:1239:C:H2'	80:AA:1240:A:H8	1.72	0.53
11:A:2740:A:H2'	11:A:2741:A:H8	1.73	0.53
80:AA:976:A:H5''	89:AQ:88:ACE:H1	1.91	0.53
80:AA:1129:U:H2'	80:AA:1130:G:H8	1.73	0.53
80:AA:1589:C:H2'	80:AA:1590:A:C8	2.43	0.53
36:b:30:SER:HB2	36:b:76:VAL:HB	1.90	0.53
74:AZ:10:ARG:HH12	76:A1:239:TRP:CD1	2.27	0.53
11:A:2212:C:H2'	11:A:2213:A:H8	1.74	0.53
17:I:142:ASN:HB2	17:I:185:ILE:HD13	1.91	0.53
56:AD:317:HIS:HB3	56:AD:320:ILE:HG13	1.90	0.53
59:AG:379:ARG:HD2	62:AK:128:TRP:CE2	2.43	0.53
9:8:142:ALA:HA	38:e:274:ARG:HH21	1.74	0.53
56:AD:172:MET:O	56:AD:175:GLN:HG3	2.09	0.53
68:AR:275:PHE:HB3	68:AR:281:ILE:HG22	1.91	0.53
70:AT:118:GLU:HA	70:AT:121:LYS:HD3	1.90	0.53
80:AA:798:C:H2'	80:AA:799:A:C8	2.44	0.53
11:A:3158:A:H2'	11:A:3159:A:C8	2.44	0.53
48:q:191:LYS:HA	48:q:194:LYS:HG2	1.90	0.53
11:A:2586:U:H2'	11:A:2587:G:H8	1.73	0.53
80:AA:877:G:H2'	80:AA:878:G:H8	1.74	0.53
57:AE:26:ILE:HG23	57:AE:36:VAL:HG21	1.91	0.52
76:A1:152:ASP:HB2	76:A1:172:VAL:HB	1.91	0.52
5:4:76:CYS:HB3	5:4:98:HIS:HE1	1.74	0.52
11:A:2748:A:H2'	11:A:2749:A:C8	2.44	0.52
35:V:102:MET:HE3	37:d:48:PRO:HG2	1.90	0.52
50:c:59:ARG:HB2	50:c:62:GLU:HG2	1.92	0.52
74:AZ:10:ARG:HH12	76:A1:239:TRP:NE1	2.08	0.52
84:Ax:3:U:H2'	84:Ax:4:A:C8	2.44	0.52
12:C:140:GLY:HA2	12:C:176:ALA:H	1.73	0.52
14:E:99:LEU:HD22	14:E:193:LEU:HB3	1.92	0.52
28:T:62:ARG:HE	37:d:230:ARG:HD2	1.74	0.52
80:AA:839:A:H2'	80:AA:840:A:C8	2.44	0.52
34:t:64:ILE:HD11	34:u:82:LEU:HB2	1.92	0.52
63:AL:175:TYR:HB2	65:AN:89:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:845:A:H2'	80:AA:846:A:C8	2.45	0.52
80:AA:852:A:H3'	80:AA:853:C:H6	1.74	0.52
11:A:2668:A:H2'	11:A:2669:A:C8	2.45	0.52
16:H:247:ARG:HG2	16:H:251:TRP:HE1	1.75	0.52
22:N:98:HIS:HB3	22:N:151:VAL:HG12	1.91	0.52
58:AF:129:ALA:HB1	58:AF:133:GLU:HB2	1.92	0.52
72:AV:114:ARG:HA	72:AV:117:LEU:HD12	1.91	0.52
72:AV:116:CYS:HA	72:AV:121:ALA:HB3	1.92	0.52
72:AV:344:LEU:HD22	72:AV:346:LYS:HD3	1.91	0.52
80:AA:832:U:H2'	80:AA:833:A:C8	2.44	0.52
80:AA:1003:A:H2'	80:AA:1004:G:C8	2.43	0.52
84:Ax:40:A:H2'	84:Ax:41:A:C8	2.44	0.52
50:c:228:LEU:HB2	50:c:307:PHE:CD2	2.45	0.52
80:AA:1373:U:H2'	80:AA:1374:A:C8	2.45	0.52
80:AA:1470:A:H2'	80:AA:1471:A:C8	2.45	0.52
11:A:2514:C:H2'	11:A:2515:U:H6	1.75	0.52
64:AM:101:PRO:HB3	71:AU:59:ARG:HB3	1.90	0.52
72:AV:103:TYR:HA	80:AA:1525:C:H5	1.74	0.52
47:o:15:ARG:HB3	47:o:18:ILE:HG12	1.92	0.52
80:AA:798:C:H2'	80:AA:799:A:H8	1.75	0.52
80:AA:1042:U:H2'	80:AA:1043:C:C6	2.45	0.52
80:AA:1353:A:H5'	80:AA:1354:A:H5'	1.93	0.52
80:AA:1454:G:H2'	80:AA:1455:U:H6	1.75	0.52
86:A4:335:PHE:CG	86:A4:360:MET:HE2	2.45	0.52
11:A:2776:G:H2'	11:A:2777:G:H8	1.75	0.51
55:AC:105:ALA:HB3	55:AC:122:VAL:HG12	1.92	0.51
82:OX:376:ARG:HG2	82:OX:379:ARG:HH22	1.75	0.51
7:6:126:ARG:HB3	24:P:160:ARG:HH22	1.74	0.51
37:d:208:VAL:HG22	37:d:253:THR:HG23	1.92	0.51
69:AS:20:VAL:HG21	69:AS:28:LYS:HG2	1.91	0.51
7:6:224:HIS:CE1	7:6:227:GLU:H	2.28	0.51
52:p:84:SER:HB3	52:p:98:LYS:HB2	1.91	0.51
62:AK:52:LEU:HD22	74:AZ:41:PRO:HG3	1.93	0.51
72:AV:229:ALA:HB1	72:AV:286:VAL:HG11	1.92	0.51
1:0:138:ARG:HB3	11:A:2321:A:C8	2.46	0.51
5:4:103:MET:HE1	11:A:2952:U:H5'	1.91	0.51
11:A:1939:G:H5'	11:A:1940:A:H5''	1.92	0.51
66:AO:183:ALA:HA	68:AR:183:LYS:HE2	1.92	0.51
84:Ax:4:A:H2'	84:Ax:5:A:C8	2.45	0.51
38:e:257:LYS:HE2	38:e:273:ARG:HE	1.76	0.51
86:A4:196:CYS:HB3	86:A4:265:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2748:A:H2'	11:A:2749:A:H8	1.75	0.51
16:H:147:ARG:HG2	16:H:152:LEU:HB3	1.93	0.51
37:d:90:PRO:HB2	37:d:269:TRP:HZ2	1.76	0.51
55:AC:125:ARG:HH11	86:A4:94:TYR:HB2	1.74	0.51
65:AN:57:GLN:HG3	65:AN:84:ILE:HD11	1.93	0.51
73:AW:104:ILE:HG13	73:AW:114:ILE:HG13	1.93	0.51
10:9:79:PRO:HD2	35:V:183:LEU:HD21	1.92	0.51
55:AC:125:ARG:NH1	86:A4:94:TYR:HB2	2.26	0.51
66:AO:96:ARG:HH22	80:AA:918:A:H3'	1.76	0.51
80:AA:868:C:H2'	80:AA:869:C:H6	1.75	0.51
87:AX:181:PRO:HB2	87:AX:233:VAL:HG22	1.92	0.51
35:V:146:VAL:HG22	35:V:153:ILE:HD13	1.92	0.51
75:A0:85:TRP:HZ2	75:A0:204:PRO:HG3	1.76	0.51
11:A:2037:U:H4'	11:A:2040:G:N1	2.25	0.50
17:I:200:LEU:HD13	34:u:76:LEU:HB3	1.93	0.50
57:AE:35:ILE:HD12	63:AL:97:MET:HE2	1.93	0.50
60:AH:155:VAL:HG21	76:A1:129:PHE:HB3	1.92	0.50
69:AS:85:PHE:HB2	73:AW:100:VAL:HG12	1.92	0.50
84:Ax:8:U:O4	84:Ax:14:A:N7	2.44	0.50
11:A:2868:C:H2'	11:A:2869:A:O4'	2.11	0.50
12:C:190:VAL:HG23	12:C:254:VAL:HB	1.93	0.50
60:AH:79:LEU:HD11	60:AH:140:TYR:HB3	1.93	0.50
80:AA:915:C:H2'	80:AA:916:C:C6	2.46	0.50
11:A:3078:C:H2'	11:A:3079:G:C8	2.47	0.50
34:G:132:VAL:HG12	34:G:197:LEU:HB3	1.93	0.50
37:d:52:THR:HG23	37:d:55:GLU:H	1.77	0.50
60:AH:84:ASP:HB3	60:AH:87:VAL:HB	1.94	0.50
61:AJ:70:PRO:HB3	61:AJ:117:ASP:HB3	1.93	0.50
63:AL:216:GLU:HG3	77:A3:186:PRO:HB3	1.93	0.50
72:AV:233:LYS:HB2	72:AV:286:VAL:HG21	1.93	0.50
80:AA:1348:G:H2'	80:AA:1349:U:C6	2.46	0.50
11:A:2757:A:H2'	11:A:2758:G:O4'	2.12	0.50
56:AD:427:ARG:HD3	80:AA:650:U:C4	2.47	0.50
86:A4:429:LEU:HA	86:A4:464:LEU:HD21	1.92	0.50
26:R:114:LYS:HD3	83:a:44:ASN:HB3	1.93	0.50
63:AL:209:LEU:HD12	77:A3:189:TRP:CE2	2.45	0.50
80:AA:1165:C:H2'	80:AA:1166:A:C8	2.47	0.50
80:AA:1239:C:H2'	80:AA:1240:A:C8	2.46	0.50
11:A:2151:A:H2'	11:A:2152:A:C8	2.47	0.50
12:C:159:LYS:HE3	85:Aw:66:U:H4'	1.92	0.50
16:H:168:LYS:HD3	16:H:231:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:f:127:MET:HB2	51:f:154:GLU:HB3	1.93	0.50
55:AC:100:PHE:HB3	55:AC:103:CYS:HB2	1.94	0.50
80:AA:1007:G:H2'	80:AA:1008:A:C8	2.45	0.50
12:C:180:ARG:NH1	12:C:181:HIS:HB3	2.27	0.50
63:AL:126:GLU:HB3	63:AL:181:ILE:HD11	1.93	0.50
80:AA:749:G:H2'	80:AA:750:G:C8	2.47	0.50
80:AA:1416:A:H2'	80:AA:1417:A:C8	2.47	0.50
11:A:2392:U:H2'	11:A:2394:A:H62	1.77	0.50
11:A:1868:G:H2'	21:M:40:PRO:HG3	1.94	0.50
23:O:46:TRP:CD1	23:O:121:ALA:HB2	2.47	0.50
80:AA:1349:U:H2'	80:AA:1350:G:C8	2.45	0.50
80:AA:1578:A:H2'	80:AA:1579:C:C6	2.47	0.50
11:A:2584:C:H2'	11:A:2585:G:H8	1.77	0.49
11:A:3142:A:H2'	11:A:3143:U:C6	2.47	0.49
53:s:152:GLN:HA	53:s:156:TYR:HB2	1.93	0.49
71:AU:64:ARG:HA	71:AU:67:VAL:HG12	1.94	0.49
80:AA:799:A:H2'	80:AA:800:C:C6	2.47	0.49
6:5:201:ARG:HB3	6:5:232:THR:HG22	1.94	0.49
80:AA:872:G:H2'	80:AA:873:G:C8	2.47	0.49
80:AA:1033:U:H2'	80:AA:1034:U:C6	2.47	0.49
6:5:165:GLN:NE2	6:5:175:THR:HG22	2.27	0.49
11:A:2127:A:H4'	11:A:2251:A:C5	2.46	0.49
25:Q:201:ASP:HB3	25:Q:204:MET:HB3	1.94	0.49
38:e:183:THR:HG23	38:e:186:GLY:N	2.23	0.49
68:AR:276:VAL:HG21	68:AR:303:LEU:HD22	1.93	0.49
80:AA:914:A:H2'	80:AA:915:C:C6	2.48	0.49
34:G:160:GLN:HA	34:G:163:LYS:HE2	1.94	0.49
69:AS:51:VAL:HG13	88:A2:235:LEU:HD11	1.94	0.49
80:AA:1131:C:H2'	80:AA:1132:U:C6	2.47	0.49
80:AA:1452:U:H2'	80:AA:1453:A:H8	1.77	0.49
11:A:3077:C:H2'	11:A:3078:C:H6	1.77	0.49
14:E:123:GLN:HG2	14:E:125:GLN:HG3	1.94	0.49
56:AD:225:VAL:HG22	56:AD:243:VAL:HG22	1.95	0.49
75:A0:71:LEU:HD11	75:A0:141:LEU:HD11	1.93	0.49
79:AY:316:ASN:HB3	79:AY:319:ALA:HB2	1.95	0.49
80:AA:1057:G:H4'	80:AA:1578:A:H4'	1.95	0.49
87:AX:312:GLN:HE21	87:AX:318:LYS:HB2	1.77	0.49
62:AK:81:ASP:HA	62:AK:86:ARG:HD3	1.92	0.49
80:AA:1407:U:H2'	80:AA:1408:A:H8	1.77	0.49
35:V:57:PHE:CD1	35:V:156:LYS:HE3	2.48	0.49
76:A1:211:ARG:HG2	79:AY:360:LYS:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:1398:U:H2'	80:AA:1399:A:C8	2.44	0.49
86:A4:302:VAL:HG11	86:A4:341:CYS:HB3	1.93	0.49
6:5:55:LEU:HD11	31:X:163:ARG:HG2	1.94	0.49
6:5:113:LEU:HD12	6:5:311:ALA:HB1	1.95	0.49
8:7:114:ASP:HB2	8:7:117:LYS:HB2	1.95	0.49
22:N:124:VAL:HA	22:N:158:ARG:HH21	1.76	0.49
38:e:213:TYR:HB3	38:e:231:VAL:HB	1.94	0.49
58:AF:157:GLY:HA3	58:AF:174:LEU:HD21	1.95	0.49
80:AA:872:G:H2'	80:AA:873:G:H8	1.78	0.49
80:AA:1488:5MC:H2'	80:AA:1489:G:C8	2.48	0.49
81:AI:176:THR:HB	89:AQ:98:THR:HG23	1.94	0.49
86:A4:170:VAL:HG23	86:A4:247:ILE:HD11	1.95	0.49
87:AX:244:LEU:HD22	87:AX:296:MET:HG3	1.95	0.49
11:A:2409:A:H2'	11:A:2410:U:C6	2.47	0.49
27:S:107:LYS:HD3	28:T:206:LEU:HD11	1.95	0.49
87:AX:348:TYR:HB2	87:AX:386:ALA:HB1	1.95	0.49
10:9:24:LYS:HE3	29:U:74:HIS:HB2	1.95	0.49
18:J:113:THR:HG23	18:J:115:LYS:H	1.78	0.49
4:3:175:ASP:HB3	4:3:178:GLN:HB2	1.95	0.48
8:7:302:LEU:HD23	23:O:144:LEU:HD23	1.94	0.48
14:E:248:ILE:HG13	14:E:250:ARG:H	1.78	0.48
59:AG:87:HIS:O	59:AG:91:MET:HG2	2.13	0.48
80:AA:747:A:H2'	80:AA:748:G:C8	2.47	0.48
80:AA:1042:U:H2'	80:AA:1043:C:H6	1.76	0.48
85:Aw:9:A:H1'	85:Aw:45:A:H2'	1.95	0.48
11:A:1893:A:H4'	11:A:1894:G:H5'	1.95	0.48
15:F:49:ARG:HD2	15:F:263:LEU:HD22	1.95	0.48
64:AM:114:ARG:NH2	66:AO:236:PRO:HD2	2.28	0.48
80:AA:918:A:H4'	80:AA:920:G:H4'	1.95	0.48
87:AX:85:PRO:HA	87:AX:88:VAL:HG12	1.95	0.48
11:A:2060:A:H2'	11:A:2061:C:H6	1.78	0.48
11:A:2279:U:H5''	15:F:255:LYS:HZ3	1.78	0.48
64:AM:34:ILE:HG12	64:AM:87:MET:HE1	1.94	0.48
73:AW:144:LEU:HD23	73:AW:167:ALA:HB2	1.96	0.48
80:AA:730:A:H3'	80:AA:731:A:H8	1.78	0.48
84:Ax:47:U:H3	84:Ax:58:U:H3	1.61	0.48
11:A:1761:A:H2'	11:A:1762:A:C8	2.49	0.48
11:A:2086:A:H2'	11:A:2087:U:C6	2.49	0.48
11:A:3193:U:H5''	49:r:141:PRO:HB3	1.95	0.48
35:V:94:HIS:HE1	35:V:113:ALA:HB2	1.78	0.48
57:AE:78:MET:HE3	57:AE:82:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:AW:108:VAL:HG21	89:AQ:170:PRO:HA	1.95	0.48
86:A4:489:HIS:HB3	86:A4:492:THR:HG23	1.95	0.48
7:6:157:LEU:O	7:6:161:LEU:HB2	2.12	0.48
11:A:3089:A:H3'	11:A:3090:G:C5'	2.44	0.48
55:AC:98:GLY:HA3	74:AZ:71:TYR:CE1	2.49	0.48
59:AG:293:ILE:HB	59:AG:300:TYR:HB3	1.95	0.48
72:AV:96:ARG:HD2	72:AV:101:CYS:SG	2.53	0.48
51:f:138:GLN:HE21	51:f:141:GLY:HA3	1.78	0.48
70:AT:32:VAL:HB	70:AT:66:MET:HG2	1.96	0.48
72:AV:70:LEU:HD21	72:AV:390:ILE:HD13	1.96	0.48
80:AA:1317:A:H3'	80:AA:1318:A:H8	1.78	0.48
72:AV:68:SER:N	80:AA:1523:A:H5''	2.28	0.48
80:AA:739:C:H2'	80:AA:740:G:O4'	2.13	0.48
11:A:1862:U:H2'	11:A:1863:A:H8	1.79	0.48
15:F:123:GLY:HA3	15:F:142:ARG:HG2	1.95	0.48
27:S:51:VAL:HG22	49:r:76:ASN:HB2	1.96	0.48
45:m:51:LEU:HD12	45:m:67:ARG:HB3	1.96	0.48
6:5:239:ILE:HD11	6:5:420:HIS:CE1	2.49	0.48
7:6:234:HIS:CE1	7:6:257:PRO:HA	2.48	0.48
8:7:150:MET:O	8:7:154:ILE:HG12	2.14	0.48
60:AH:76:LEU:HD12	60:AH:148:LEU:HD22	1.95	0.48
79:AY:292:GLN:HG2	86:A4:446:LYS:HG2	1.96	0.48
86:A4:236:VAL:HG13	86:A4:270:ARG:HB3	1.96	0.48
7:6:173:LEU:HD13	7:6:272:LEU:HD22	1.96	0.48
12:C:284:SER:HA	12:C:289:VAL:HG11	1.96	0.48
59:AG:136:ARG:HD3	59:AG:139:GLN:NE2	2.28	0.48
59:AG:136:ARG:HD3	59:AG:139:GLN:HE21	1.79	0.48
68:AR:142:LEU:HD11	75:A0:172:ALA:HB2	1.96	0.48
69:AS:104:THR:O	69:AS:108:LYS:HG2	2.14	0.48
80:AA:838:U:H2'	80:AA:839:A:H8	1.79	0.48
80:AA:1089:U:H2'	80:AA:1090:A:H8	1.78	0.48
86:A4:349:ALA:HA	86:A4:352:PRO:HG2	1.96	0.48
11:A:2776:G:H1'	16:H:178:ASN:HD21	1.79	0.47
72:AV:81:SER:HB3	72:AV:84:GLU:HG3	1.96	0.47
72:AV:228:TYR:HB3	72:AV:259:ALA:HB2	1.96	0.47
75:A0:165:PRO:HA	75:A0:190:MET:HG2	1.96	0.47
80:AA:771:A:H2'	80:AA:772:A:C8	2.49	0.47
80:AA:1007:G:H2'	80:AA:1008:A:H8	1.79	0.47
80:AA:1407:U:H2'	80:AA:1408:A:C8	2.49	0.47
81:AI:111:SER:O	81:AI:115:GLU:HG2	2.14	0.47
87:AX:125:LEU:HD11	87:AX:310:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:41:LEU:HD23	2:1:43:LEU:HD11	1.95	0.47
35:V:55:TYR:HB2	35:V:133:ILE:HD11	1.95	0.47
53:s:316:CYS:HB3	53:s:319:GLN:HB2	1.96	0.47
71:AU:28:LYS:HE2	80:AA:699:A:H3'	1.96	0.47
80:AA:861:U:H2'	80:AA:862:A:C8	2.50	0.47
84:Ax:47:U:H2'	84:Ax:48:G:C8	2.49	0.47
86:A4:532:LEU:HD11	86:A4:555:ILE:HG21	1.95	0.47
67:AP:86:PRO:HA	67:AP:125:LYS:HB2	1.95	0.47
68:AR:68:PRO:HD2	68:AR:307:LEU:HD12	1.96	0.47
80:AA:832:U:H2'	80:AA:833:A:H8	1.80	0.47
86:A4:375:ILE:HA	86:A4:378:LEU:HD12	1.95	0.47
59:AG:291:GLY:HA3	59:AG:324:GLY:HA2	1.96	0.47
80:AA:833:A:H2'	80:AA:834:G:C8	2.48	0.47
9:8:138:ALA:O	9:8:141:GLU:HG3	2.15	0.47
11:A:2677:A:H2'	11:A:2678:A:C8	2.49	0.47
11:A:3054:G:H2'	11:A:3055:U:C6	2.50	0.47
11:A:3078:C:H2'	11:A:3079:G:H8	1.77	0.47
15:F:138:HIS:CD2	15:F:146:TRP:HE1	2.33	0.47
20:L:98:PRO:HA	25:Q:162:ILE:HG12	1.97	0.47
32:Y:191:ASN:HB3	32:Y:194:TYR:HB3	1.96	0.47
60:AH:122:GLN:HA	60:AH:132:VAL:HG23	1.97	0.47
70:AT:161:GLY:HA2	70:AT:164:LYS:HE2	1.96	0.47
80:AA:982:A:H2'	80:AA:983:C:C6	2.50	0.47
6:5:165:GLN:NE2	6:5:179:VAL:HG21	2.29	0.47
14:E:177:LYS:HG3	14:E:298:LYS:HB2	1.96	0.47
17:I:96:ILE:HA	17:I:155:VAL:HG12	1.96	0.47
20:L:46:LEU:HD12	20:L:78:LYS:HD3	1.96	0.47
56:AD:209:GLY:HA3	56:AD:213:GLU:HB2	1.95	0.47
63:AL:130:ILE:HG12	63:AL:185:LEU:HD11	1.97	0.47
66:AO:136:TYR:HD1	66:AO:138:PRO:HD2	1.79	0.47
68:AR:157:VAL:HG22	68:AR:174:VAL:HG22	1.95	0.47
90:B:68:C:H2'	90:B:69:U:C6	2.49	0.47
6:5:351:VAL:HG22	6:5:381:LEU:HD23	1.96	0.47
8:7:148:MET:HE2	8:7:257:ILE:HG12	1.97	0.47
50:c:258:THR:HA	83:a:72:THR:HG22	1.95	0.47
53:s:201:ASP:HB2	53:s:240:GLN:HG2	1.97	0.47
62:AK:91:CYS:HB3	62:AK:96:ARG:H	1.80	0.47
68:AR:231:CYS:SG	68:AR:242:TYR:HA	2.54	0.47
80:AA:848:U:H2'	80:AA:849:U:C6	2.50	0.47
80:AA:1175:G:H2'	80:AA:1176:G:H8	1.80	0.47
80:AA:1471:A:H2'	80:AA:1472:G:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:AI:110:ALA:HB3	81:AI:135:ALA:HB2	1.97	0.47
72:AV:133:VAL:HG23	72:AV:134:GLN:HG3	1.97	0.47
75:A0:68:LEU:HD21	75:A0:80:VAL:HG21	1.96	0.47
8:7:276:PHE:HB2	8:7:304:VAL:HG22	1.96	0.47
34:G:132:VAL:HG23	34:G:172:ILE:HB	1.97	0.47
37:d:86:ASP:HB3	37:d:196:GLN:HE22	1.80	0.47
38:e:159:LEU:HD12	38:e:254:TRP:CZ2	2.50	0.47
60:AH:163:ASN:HB3	76:A1:114:LEU:HD11	1.96	0.47
63:AL:209:LEU:HD13	77:A3:173:LEU:HD12	1.97	0.47
74:AZ:6:GLU:O	74:AZ:10:ARG:HG3	2.14	0.47
80:AA:818:C:H2'	80:AA:819:A:H8	1.79	0.47
80:AA:970:A:H2'	80:AA:971:A:C8	2.50	0.47
4:3:127:ALA:HA	21:M:79:PRO:HD3	1.97	0.47
14:E:80:LEU:HD12	14:E:323:GLY:HA3	1.96	0.47
29:U:110:LEU:HD12	32:Y:118:GLU:HG2	1.97	0.47
72:AV:340:LYS:HE3	72:AV:340:LYS:HB3	1.76	0.47
80:AA:1349:U:H2'	80:AA:1350:G:H8	1.78	0.47
11:A:2056:G:H2'	11:A:2057:C:H6	1.80	0.46
12:C:124:THR:HA	12:C:127:LYS:HG2	1.97	0.46
18:J:114:LEU:HB3	44:l:96:LEU:HD21	1.96	0.46
34:t:64:ILE:HD12	34:u:78:GLU:HG3	1.97	0.46
56:AD:139:PHE:HA	56:AD:159:GLN:HA	1.97	0.46
11:A:1862:U:H2'	11:A:1863:A:C8	2.51	0.46
11:A:2728:C:H2'	11:A:2729:U:H6	1.79	0.46
18:J:113:THR:HG22	18:J:116:HIS:ND1	2.30	0.46
59:AG:136:ARG:HH22	59:AG:211:GLU:HG2	1.80	0.46
78:Az:27:C:H4'	86:A4:452:GLN:HG3	1.96	0.46
80:AA:673:U:H2'	80:AA:674:U:C6	2.50	0.46
80:AA:911:U:H2'	80:AA:912:U:C6	2.51	0.46
81:AI:151:VAL:HG21	81:AI:158:ARG:HG3	1.97	0.46
86:A4:236:VAL:HG22	86:A4:270:ARG:HG3	1.97	0.46
11:A:2182:G:H2'	11:A:2183:C:C6	2.51	0.46
11:A:2382:A:H2'	11:A:2383:U:C6	2.50	0.46
18:J:188:GLU:HG3	18:J:192:LYS:HE3	1.96	0.46
29:U:131:GLU:O	29:U:134:ARG:HG3	2.15	0.46
45:m:58:LYS:HZ2	45:m:64:ILE:HG23	1.80	0.46
80:AA:740:G:H2'	80:AA:741:A:H8	1.79	0.46
80:AA:1365:A:H4'	80:AA:1389:G:H4'	1.97	0.46
87:AX:210:TRP:NE1	87:AX:228:GLN:HG2	2.31	0.46
87:AX:242:ILE:HD11	100:AX:503:GDP:C4	2.51	0.46
8:7:244:ALA:HB1	8:7:250:ARG:HE	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:70:LEU:HD13	32:Y:101:LEU:HD22	1.98	0.46
11:A:2277:U:H2'	11:A:2278:A:H8	1.80	0.46
11:A:2989:G:H5''	11:A:2990:A:H5''	1.98	0.46
16:H:164:VAL:HG23	16:H:225:VAL:HG11	1.97	0.46
19:K:238:MET:HE2	19:K:311:ILE:HD11	1.98	0.46
60:AH:97:LEU:O	60:AH:101:GLU:HG3	2.15	0.46
60:AH:182:GLU:HA	60:AH:185:LYS:HZ2	1.80	0.46
62:AK:57:LEU:HD23	62:AK:71:ALA:HB2	1.96	0.46
69:AS:48:ARG:HH22	80:AA:1119:U:P	2.39	0.46
80:AA:1056:A:H4'	80:AA:1588:G:N2	2.30	0.46
80:AA:1577:U:H2'	80:AA:1578:A:H8	1.81	0.46
11:A:2006:C:H2'	11:A:2007:U:C6	2.51	0.46
24:P:82:ARG:NH1	24:P:84:ILE:HD11	2.30	0.46
69:AS:116:LYS:HA	69:AS:119:VAL:HG22	1.98	0.46
75:A0:42:THR:HG22	75:A0:49:ARG:HA	1.97	0.46
84:Ax:60:C:H2'	84:Ax:61:C:C6	2.50	0.46
28:T:118:ALA:HA	28:T:121:MET:HG2	1.97	0.46
35:V:146:VAL:HG21	82:OX:401:PHE:CE1	2.51	0.46
36:b:56:ARG:HG3	40:h:149:PRO:HG3	1.98	0.46
48:q:186:GLU:HA	48:q:189:ARG:HD2	1.96	0.46
56:AD:132:ILE:HG13	56:AD:144:LEU:HD21	1.97	0.46
62:AK:62:ILE:HG21	79:AY:349:HIS:HB3	1.97	0.46
68:AR:142:LEU:HD21	68:AR:183:LYS:HE3	1.97	0.46
75:A0:162:ALA:HA	75:A0:194:GLN:HG2	1.98	0.46
80:AA:681:U:H2'	80:AA:682:A:C8	2.50	0.46
11:A:2081:U:H2'	11:A:2082:G:C8	2.50	0.46
11:A:2894:U:H5''	11:A:2895:U:O4'	2.16	0.46
12:C:167:ILE:HD11	12:C:283:LEU:HD23	1.98	0.46
21:M:226:PRO:HG3	52:p:45:LEU:HD23	1.97	0.46
53:s:84:THR:HB	53:s:280:ASN:HB2	1.96	0.46
53:s:212:ARG:HD3	53:s:379:LEU:HB3	1.98	0.46
55:AC:61:TYR:HB3	55:AC:65:ARG:HB2	1.97	0.46
56:AD:355:ARG:NH1	80:AA:1118:A:H4'	2.31	0.46
68:AR:323:GLU:H	68:AR:326:ASN:HB2	1.80	0.46
70:AT:74:PRO:HD2	70:AT:91:GLU:HG3	1.97	0.46
72:AV:165:PHE:HA	72:AV:168:MET:HE3	1.97	0.46
80:AA:854:U:H2'	80:AA:855:A:C8	2.51	0.46
80:AA:970:A:H2'	80:AA:971:A:H8	1.80	0.46
11:A:2553:G:H2'	11:A:2554:A:H8	1.81	0.46
18:J:73:LYS:NZ	18:J:79:GLU:HB2	2.31	0.46
37:d:110:GLU:O	37:d:113:LYS:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:AC:96:MET:HB2	55:AC:108:LEU:HD11	1.97	0.46
59:AG:200:LEU:HD12	59:AG:204:GLU:HB3	1.98	0.46
72:AV:360:VAL:HG13	72:AV:364:LEU:HD22	1.97	0.46
77:A3:177:TRP:CD1	77:A3:178:LEU:HD12	2.51	0.46
80:AA:1146:C:H2'	80:AA:1147:G:H8	1.81	0.46
80:AA:1452:U:H2'	80:AA:1453:A:C8	2.51	0.46
86:A4:401:MET:HA	86:A4:438:LEU:HD21	1.97	0.46
9:8:191:ARG:NE	51:f:135:LEU:HG	2.31	0.46
11:A:1861:U:H2'	11:A:1862:U:C6	2.50	0.46
12:C:119:LYS:HD3	12:C:122:ILE:HD11	1.98	0.46
17:I:143:LEU:HD23	17:I:146:LEU:HD13	1.97	0.46
32:Y:176:ILE:HG21	82:OX:430:TRP:CG	2.50	0.46
50:c:79:LEU:HD13	50:c:214:PHE:HE2	1.81	0.46
58:AF:156:ILE:HD11	88:A2:167:MET:HE2	1.98	0.46
80:AA:705:C:H3'	80:AA:706:C:H6	1.81	0.46
80:AA:1117:A:H2'	80:AA:1118:A:H8	1.80	0.46
80:AA:1174:U:H2'	80:AA:1175:G:C8	2.51	0.46
86:A4:427:ARG:HB3	86:A4:468:MET:HE2	1.98	0.46
54:AB:223:VAL:HG11	54:AB:229:PRO:HB3	1.98	0.46
59:AG:229:LEU:HD21	59:AG:241:VAL:HG11	1.98	0.46
62:AK:80:ARG:HH22	80:AA:1350:G:P	2.39	0.46
75:A0:175:ILE:HG22	75:A0:178:ARG:HH12	1.81	0.46
80:AA:1194:C:H2'	80:AA:1195:U:C6	2.51	0.46
85:Aw:71:C:HO2'	85:Aw:72:A:H8	1.64	0.46
86:A4:312:LYS:HG3	86:A4:345:PHE:HE2	1.81	0.46
11:A:2275:U:H2'	11:A:2276:C:C6	2.50	0.45
11:A:2786:U:H2'	11:A:2787:A:C8	2.51	0.45
19:K:202:LYS:HG2	19:K:203:MET:HG2	1.97	0.45
33:Z:70:THR:HG22	33:Z:97:PRO:HA	1.97	0.45
39:g:109:VAL:HG13	39:g:146:THR:HG23	1.98	0.45
44:l:92:TYR:HB3	44:l:96:LEU:HD13	1.98	0.45
62:AK:43:MET:SD	62:AK:81:ASP:HB2	2.56	0.45
67:AP:103:LYS:HA	67:AP:103:LYS:HD3	1.72	0.45
70:AT:22:VAL:HG22	70:AT:58:LYS:HB3	1.98	0.45
72:AV:30:LEU:HD23	72:AV:149:ASP:HB2	1.97	0.45
75:A0:43:ARG:HH21	80:AA:706:C:H5'	1.80	0.45
80:AA:1006:U:H2'	80:AA:1007:G:H8	1.82	0.45
86:A4:156:ALA:O	86:A4:160:ARG:HG2	2.16	0.45
87:AX:180:GLN:HE22	87:AX:287:LEU:HD12	1.81	0.45
87:AX:205:GLN:HG2	87:AX:250:GLN:NE2	2.31	0.45
13:D:257:ILE:O	13:D:262:ARG:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:216:TRP:HA	16:H:237:VAL:HB	1.97	0.45
24:P:151:TRP:CG	90:B:39:PSU:H4'	2.51	0.45
31:X:50:PHE:CG	31:X:59:ARG:HD3	2.51	0.45
35:V:158:GLU:HG2	82:OX:388:GLN:HE22	1.80	0.45
54:AB:148:ASN:HD22	54:AB:197:HIS:CD2	2.35	0.45
80:AA:1011:C:C4	80:AA:1063:A:H4'	2.51	0.45
80:AA:1347:G:H2'	80:AA:1348:G:C8	2.48	0.45
80:AA:1408:A:H2'	80:AA:1409:A:H8	1.80	0.45
86:A4:462:PHE:HZ	86:A4:481:LEU:HB3	1.81	0.45
86:A4:462:PHE:HE2	86:A4:482:ILE:HG12	1.81	0.45
86:A4:535:MET:HE1	86:A4:551:CYS:HB3	1.97	0.45
11:A:2803:A:H2'	11:A:2804:A:O4'	2.16	0.45
11:A:3071:U:H2'	11:A:3072:U:H2'	1.98	0.45
11:A:3115:U:H2'	11:A:3116:C:C6	2.51	0.45
22:N:163:MET:HE2	22:N:163:MET:HB3	1.91	0.45
29:U:3:ARG:HB3	29:U:24:PHE:HE1	1.82	0.45
60:AH:76:LEU:HD11	60:AH:153:ALA:HB1	1.98	0.45
86:A4:494:ILE:HA	86:A4:497:LEU:HD12	1.97	0.45
11:A:1828:A:H4'	11:A:1829:A:C8	2.52	0.45
11:A:1936:A:H4'	11:A:1937:A:N7	2.31	0.45
59:AG:75:LYS:HA	59:AG:78:ILE:HD12	1.98	0.45
80:AA:1132:U:H2'	80:AA:1133:C:C6	2.51	0.45
80:AA:1495:C:H2'	80:AA:1496:U:C6	2.51	0.45
80:AA:1504:U:H2'	80:AA:1505:A:C8	2.52	0.45
85:Aw:66:U:H2'	85:Aw:67:U:C6	2.51	0.45
86:A4:556:LYS:HE3	86:A4:579:ILE:HD13	1.99	0.45
87:AX:266:ASN:HA	87:AX:329:LEU:HD23	1.98	0.45
87:AX:293:LEU:HD23	87:AX:293:LEU:HA	1.79	0.45
11:A:2212:C:H2'	11:A:2213:A:C8	2.52	0.45
11:A:2758:G:H1	11:A:2789:C:H1'	1.81	0.45
14:E:199:ARG:HA	14:E:199:ARG:HD3	1.79	0.45
15:F:218:LEU:HD23	15:F:260:VAL:HB	1.98	0.45
16:H:244:LYS:HG3	16:H:247:ARG:HH21	1.81	0.45
18:J:90:PHE:HD2	18:J:120:ILE:HG12	1.81	0.45
23:O:38:ARG:HB2	23:O:85:LEU:HD11	1.98	0.45
34:G:138:LYS:HB2	34:G:141:ASP:HB2	1.99	0.45
59:AG:125:MET:HE1	76:A1:84:PRO:HD2	1.99	0.45
80:AA:1439:A:H2'	80:AA:1440:G:H8	1.82	0.45
83:a:92:LEU:HD23	83:a:95:ARG:HD2	1.98	0.45
21:M:167:ILE:HG21	21:M:174:VAL:HB	1.99	0.45
22:N:200:LYS:HA	22:N:200:LYS:HD3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:e:55:ARG:NH1	38:e:58:VAL:HG23	2.32	0.45
48:q:147:GLN:O	48:q:150:LYS:HG3	2.16	0.45
55:AC:155:LEU:HD23	55:AC:155:LEU:HA	1.84	0.45
6:5:117:VAL:O	6:5:121:LEU:HG	2.17	0.45
6:5:333:ALA:HB1	6:5:363:ASP:HA	1.99	0.45
7:6:121:ARG:HD3	9:8:108:PHE:HZ	1.81	0.45
9:8:188:PRO:HB2	51:f:136:GLN:OE1	2.16	0.45
11:A:2318:A:H2'	11:A:2319:A:C8	2.51	0.45
11:A:3224:G:H2'	11:A:3225:G:H8	1.82	0.45
14:E:236:THR:HG23	14:E:239:ARG:HD3	1.98	0.45
27:S:108:VAL:HB	27:S:195:ILE:HG13	1.99	0.45
29:U:112:PRO:N	29:U:113:GLU:HA	2.32	0.45
31:X:25:PRO:HG2	31:X:203:TRP:CE2	2.52	0.45
37:d:217:HIS:CD2	37:d:243:LEU:HB2	2.52	0.45
42:j:88:LEU:HD23	42:j:88:LEU:HA	1.79	0.45
56:AD:260:LYS:HD2	80:AA:1286:A:OP1	2.16	0.45
2:1:34:ARG:HD3	2:1:41:LEU:HD13	1.99	0.45
8:7:67:VAL:HB	8:7:79:PHE:HB2	1.99	0.45
11:A:2092:C:H2'	11:A:2093:U:C6	2.52	0.45
12:C:266:VAL:HG13	12:C:296:ILE:HD13	1.98	0.45
26:R:35:LYS:HD2	26:R:45:THR:HG21	1.99	0.45
52:p:133:LEU:HD21	52:p:157:MET:HE1	1.98	0.45
53:s:91:TYR:HE2	53:s:229:LEU:HD22	1.82	0.45
53:s:332:LEU:HD21	53:s:359:ALA:HB2	1.99	0.45
56:AD:103:LEU:HD11	56:AD:123:ARG:HB2	1.99	0.45
75:A0:46:SER:HA	75:A0:218:VAL:HB	1.97	0.45
76:A1:116:PRO:HA	76:A1:119:ILE:HD12	1.99	0.45
80:AA:1200:G:C2	80:AA:1201:A:C8	3.05	0.45
4:3:156:LYS:HE3	4:3:156:LYS:HB2	1.77	0.45
11:A:1839:C:H2'	11:A:1840:C:C6	2.52	0.45
24:P:89:HIS:HD2	90:B:24:G:P	2.40	0.45
54:AB:167:HIS:ND1	59:AG:153:THR:HA	2.32	0.45
55:AC:58:ALA:HB3	55:AC:60:HIS:CE1	2.52	0.45
80:AA:865:A:H2'	80:AA:866:A:C8	2.52	0.45
80:AA:1033:U:H2'	80:AA:1034:U:H6	1.81	0.45
85:Aw:5:A:H2'	85:Aw:6:U:H6	1.82	0.45
12:C:201:VAL:HG12	12:C:206:ALA:HB2	1.99	0.45
14:E:107:MET:HE3	25:Q:145:LEU:HD12	1.99	0.45
14:E:149:GLY:H	14:E:173:LYS:HB3	1.82	0.45
72:AV:364:LEU:HA	72:AV:367:CYS:SG	2.57	0.45
11:A:2586:U:H2'	11:A:2587:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:V:138:THR:HG23	35:V:140:ALA:H	1.82	0.44
45:m:110:LEU:HD13	79:AY:344:GLN:HE22	1.83	0.44
61:AJ:42:PRO:HD3	80:AA:931:C:C2	2.52	0.44
79:AY:290:ASN:HA	86:A4:446:LYS:HD3	1.99	0.44
86:A4:396:ILE:HG12	86:A4:400:LEU:HD23	1.98	0.44
87:AX:394:HIS:CE1	87:AX:398:LEU:HD12	2.52	0.44
39:g:73:GLN:HB2	39:g:162:LEU:HD21	1.98	0.44
53:s:332:LEU:HD13	53:s:372:TYR:HB2	1.98	0.44
68:AR:278:ASN:HB3	68:AR:280:LYS:HG2	1.99	0.44
80:AA:867:C:H2'	80:AA:870:C:N4	2.33	0.44
86:A4:593:TRP:HA	86:A4:596:LEU:HD23	1.98	0.44
90:B:21:A:H61	90:B:46:A:H2'	1.82	0.44
2:1:18:VAL:HG12	2:1:61:LYS:HA	2.00	0.44
7:6:106:ARG:HE	24:P:110:TRP:CG	2.35	0.44
10:9:114:LEU:HD21	31:X:231:VAL:HG11	1.98	0.44
11:A:2051:A:H2'	11:A:2052:A:C8	2.52	0.44
11:A:2529:U:H2'	13:D:208:ARG:HD2	1.98	0.44
11:A:2728:C:H2'	11:A:2729:U:C6	2.52	0.44
11:A:3141:A:H2'	11:A:3142:A:C8	2.52	0.44
12:C:91:ALA:HB2	12:C:108:ILE:HD12	1.98	0.44
25:Q:210:GLU:HB2	25:Q:213:GLN:HG3	1.98	0.44
32:Y:71:PRO:HA	32:Y:74:TRP:CD2	2.52	0.44
37:d:107:GLU:HB3	37:d:111:ARG:CZ	2.47	0.44
45:m:91:ALA:HA	45:m:94:ARG:HE	1.82	0.44
80:AA:1372:C:H2'	80:AA:1373:U:C6	2.52	0.44
82:OX:366:LYS:HE3	82:OX:370:LYS:HZ3	1.81	0.44
10:9:118:GLY:HA3	35:V:191:LEU:HD12	1.99	0.44
11:A:2804:A:H2'	11:A:2805:A:C8	2.52	0.44
44:l:115:ARG:NH1	44:l:119:ARG:HH11	2.15	0.44
51:f:150:LEU:HD23	51:f:150:LEU:HA	1.85	0.44
59:AG:200:LEU:HD22	59:AG:244:PHE:HB3	1.98	0.44
63:AL:98:ALA:HB1	63:AL:102:GLU:HG3	1.99	0.44
67:AP:127:PRO:HA	67:AP:130:LEU:HG	2.00	0.44
80:AA:951:G:H2'	80:AA:952:A:H8	1.82	0.44
80:AA:1065:C:H2'	80:AA:1066:C:O4'	2.18	0.44
80:AA:1411:G:H2'	80:AA:1412:G:H8	1.83	0.44
80:AA:1471:A:H2'	80:AA:1472:G:C8	2.51	0.44
12:C:243:ARG:HD2	12:C:256:CYS:HB3	1.99	0.44
18:J:84:GLN:HB2	18:J:124:LYS:HD2	1.99	0.44
21:M:137:GLY:HA3	21:M:157:GLN:HG2	1.98	0.44
24:P:108:ARG:HD3	90:B:23:A:H4'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:AC:116:GLN:HA	55:AC:150:PRO:HG2	2.00	0.44
62:AK:33:ARG:NE	80:AA:1236:C:H5'	2.30	0.44
63:AL:95:LEU:HD21	63:AL:106:ILE:HG13	1.98	0.44
68:AR:72:ASP:HB3	68:AR:75:VAL:HB	2.00	0.44
75:A0:163:SER:HB3	75:A0:190:MET:HB3	1.99	0.44
80:AA:1213:A:H2'	80:AA:1214:A:C4	2.52	0.44
80:AA:1265:C:H2'	80:AA:1266:A:H8	1.82	0.44
8:7:317:LEU:HD23	8:7:317:LEU:HA	1.74	0.44
11:A:2656:U:H4'	14:E:230:THR:OG1	2.17	0.44
11:A:2804:A:H2'	11:A:2805:A:H8	1.82	0.44
38:e:90:ARG:HH22	38:e:120:LEU:HD23	1.83	0.44
48:q:40:PRO:HG2	48:q:51:GLN:HB3	2.00	0.44
34:u:74:LEU:HG	34:u:78:GLU:HB3	2.00	0.44
72:AV:388:GLN:O	72:AV:391:GLN:HG3	2.18	0.44
80:AA:1188:A:H4'	80:AA:1189:U:H5'	2.00	0.44
80:AA:1577:U:H2'	80:AA:1578:A:C8	2.53	0.44
11:A:1829:A:H2'	11:A:1830:G:H8	1.83	0.44
11:A:1977:U:H2'	11:A:1978:A:H8	1.82	0.44
11:A:2610:U:H2'	11:A:2611:C:C6	2.53	0.44
19:K:240:THR:HG21	19:K:279:VAL:HA	1.99	0.44
25:Q:76:LEU:HD23	25:Q:279:GLU:HG2	2.00	0.44
75:A0:64:LEU:HD12	75:A0:139:TRP:CD2	2.53	0.44
76:A1:134:PRO:HB2	76:A1:137:LEU:HD23	1.99	0.44
80:AA:1012:A:H2'	80:AA:1013:A:C8	2.52	0.44
80:AA:1076:5MU:O2	80:AA:1076:5MU:H2'	2.18	0.44
80:AA:1203:C:H2'	80:AA:1204:C:H6	1.83	0.44
80:AA:1411:G:H2'	80:AA:1412:G:C8	2.53	0.44
11:A:2060:A:C8	11:A:2079:C:C4	3.06	0.44
11:A:2187:C:H2'	11:A:2188:A:C8	2.53	0.44
11:A:3024:U:H2'	11:A:3025:A:H8	1.83	0.44
27:S:114:ILE:HD11	27:S:193:LEU:HD12	1.99	0.44
38:e:97:ARG:HA	38:e:100:LYS:HG2	2.00	0.44
38:e:265:LYS:HE2	90:B:76:A:C8	2.31	0.44
44:l:96:LEU:HA	44:l:99:MET:HE3	1.99	0.44
50:c:160:LEU:HD21	50:c:223:MET:HG3	1.99	0.44
68:AR:128:MET:H	68:AR:128:MET:HG2	1.65	0.44
79:AY:301:LEU:HD12	79:AY:310:LEU:HD22	1.99	0.44
80:AA:845:A:H2'	80:AA:846:A:H8	1.82	0.44
9:8:168:LEU:HD23	51:f:88:TYR:HE2	1.83	0.44
11:A:1829:A:H2'	11:A:1830:G:C8	2.52	0.44
11:A:3077:C:H2'	11:A:3078:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:3139:G:H2'	11:A:3140:A:C8	2.53	0.44
56:AD:380:LEU:HD12	56:AD:381:PRO:HD2	1.99	0.44
66:AO:123:LEU:HD13	66:AO:154:ILE:HG13	1.98	0.44
75:A0:48:ARG:HH21	80:AA:702:C:H42	1.66	0.44
80:AA:847:G:H2'	80:AA:848:U:C6	2.52	0.44
80:AA:1399:A:H2'	80:AA:1400:U:C6	2.53	0.44
80:AA:1595:G:H2'	80:AA:1596:A:C8	2.52	0.44
86:A4:350:ARG:HD2	86:A4:379:PHE:CE2	2.52	0.44
87:AX:117:PHE:HB3	87:AX:303:GLY:HA2	1.99	0.44
11:A:2995:G:H1	11:A:3067:PSU:HN3	1.66	0.43
12:C:107:ASN:O	12:C:110:GLU:HG3	2.18	0.43
12:C:161:GLN:HG3	12:C:175:MET:HE1	2.00	0.43
27:S:99:VAL:HG12	27:S:133:VAL:HG22	2.00	0.43
54:AB:167:HIS:HE2	54:AB:171:PHE:HA	1.82	0.43
80:AA:1181:G:H2'	80:AA:1182:C:C6	2.53	0.43
80:AA:1439:A:H2'	80:AA:1440:G:C8	2.53	0.43
87:AX:174:ASN:HD22	87:AX:177:ARG:CZ	2.30	0.43
1:O:184:TRP:H	1:O:184:TRP:CD1	2.35	0.43
6:5:30:ALA:HB2	13:D:110:LEU:HD22	1.99	0.43
11:A:1800:G:H1'	11:A:1805:A:N6	2.32	0.43
11:A:3143:U:H2'	11:A:3144:A:H8	1.83	0.43
11:A:3181:U:OP1	49:r:101:PRO:HG3	2.18	0.43
13:D:176:ALA:HB1	13:D:244:VAL:HG11	2.00	0.43
38:e:166:GLY:HA3	101:B:101:VAL:CB	2.40	0.43
71:AU:45:PRO:HB2	75:A0:53:ARG:HH21	1.83	0.43
73:AW:154:LEU:HB3	88:A2:147:LEU:HG	1.99	0.43
80:AA:705:C:H3'	80:AA:706:C:C6	2.53	0.43
86:A4:335:PHE:CE2	86:A4:360:MET:HB2	2.52	0.43
6:5:165:GLN:HE22	6:5:175:THR:HG22	1.83	0.43
6:5:215:ARG:HD2	6:5:364:LEU:O	2.19	0.43
11:A:2049:U:H2'	11:A:2050:A:H8	1.84	0.43
11:A:2275:U:H2'	11:A:2276:C:H6	1.83	0.43
11:A:2682:A:H4'	26:R:41:LEU:HD13	1.99	0.43
53:s:142:LEU:HD13	53:s:422:VAL:HG21	2.00	0.43
66:AO:56:TRP:HZ3	66:AO:118:ARG:HB3	1.83	0.43
69:AS:19:LEU:HD23	69:AS:19:LEU:HA	1.86	0.43
72:AV:66:PRO:HB3	72:AV:99:PRO:HB2	1.99	0.43
80:AA:818:C:H2'	80:AA:819:A:C8	2.53	0.43
80:AA:952:A:H2'	80:AA:953:U:C6	2.53	0.43
80:AA:1528:A:H2'	80:AA:1529:A:C8	2.49	0.43
87:AX:88:VAL:HA	87:AX:91:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2483:U:H2'	11:A:2484:C:O4'	2.18	0.43
11:A:3219:G:H2'	11:A:3220:A:H5''	2.00	0.43
55:AC:42:VAL:HG21	55:AC:55:GLU:HB3	2.00	0.43
72:AV:209:LEU:HD11	72:AV:228:TYR:CZ	2.53	0.43
80:AA:1034:U:H2'	80:AA:1035:U:C6	2.53	0.43
86:A4:126:LYS:HA	86:A4:129:GLN:HG2	2.00	0.43
11:A:3151:A:H4'	25:Q:146:GLY:O	2.19	0.43
56:AD:363:ALA:HB2	56:AD:370:VAL:HG23	2.00	0.43
60:AH:124:VAL:HG13	80:AA:1264:C:H1'	2.00	0.43
72:AV:70:LEU:HD22	72:AV:389:LEU:HG	1.99	0.43
80:AA:947:U:H2'	80:AA:948:U:H6	1.83	0.43
1:O:96:ASN:ND2	11:A:2709:A:H1'	2.33	0.43
17:I:40:MET:HE1	17:I:48:MET:HE2	2.01	0.43
21:M:266:PHE:HB2	21:M:269:LEU:HB2	2.00	0.43
38:e:265:LYS:HD3	90:B:76:A:H5''	2.00	0.43
53:s:150:LEU:HD22	53:s:405:ILE:HD11	1.99	0.43
75:A0:96:ARG:HB3	75:A0:117:ILE:HG22	2.01	0.43
87:AX:210:TRP:CZ3	87:AX:235:ASN:HB3	2.54	0.43
3:2:59:LYS:HG2	3:2:63:LYS:HE2	2.01	0.43
9:8:70:ARG:NH1	84:Ax:46:U:H5'	2.33	0.43
11:A:1935:A:C2	11:A:1936:A:H1'	2.53	0.43
11:A:2147:G:OP2	27:S:104:ARG:HD3	2.18	0.43
11:A:3170:C:N4	11:A:3171:C:H41	2.17	0.43
12:C:180:ARG:HH11	12:C:181:HIS:HB3	1.83	0.43
37:d:204:ASN:O	37:d:205:GLN:HG2	2.19	0.43
55:AC:125:ARG:HH21	55:AC:159:PRO:HD3	1.83	0.43
80:AA:659:U:H2'	80:AA:660:C:C6	2.54	0.43
86:A4:89:PHE:HZ	86:A4:103:SER:HB2	1.84	0.43
86:A4:392:ILE:HG13	86:A4:393:ILE:N	2.33	0.43
6:5:167:THR:HG21	53:s:281:HIS:CE1	2.54	0.43
6:5:299:LEU:HB3	6:5:301:PRO:HD2	2.00	0.43
11:A:2331:C:H3'	11:A:2332:C:O4'	2.19	0.43
11:A:2598:A:H3'	11:A:2625:C:H42	1.83	0.43
12:C:207:LEU:HD13	34:G:158:LEU:HD13	1.99	0.43
13:D:269:ARG:HG2	13:D:270:PRO:HD2	1.99	0.43
22:N:101:HIS:CD2	22:N:184:PRO:HD3	2.54	0.43
27:S:142:THR:HG22	83:a:60:CYS:HB2	2.01	0.43
28:T:41:ILE:HG12	37:d:39:LYS:HE3	2.01	0.43
28:T:63:ARG:O	37:d:230:ARG:HD3	2.19	0.43
38:e:133:LEU:HD23	38:e:133:LEU:H	1.84	0.43
43:k:124:PRO:HG3	43:k:210:ASP:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:AV:76:ILE:HD12	72:AV:112:TRP:HD1	1.84	0.43
76:A1:173:LEU:HD22	76:A1:207:ILE:HD12	2.01	0.43
79:AY:277:LEU:HD21	86:A4:194:LEU:HA	2.01	0.43
84:Ax:3:U:H2'	84:Ax:4:A:H8	1.84	0.43
85:Aw:3:G:H2'	85:Aw:4:U:H6	1.83	0.43
85:Aw:26:U:H2'	85:Aw:27:A:C8	2.54	0.43
87:AX:59:HIS:HA	87:AX:63:HIS:ND1	2.34	0.43
11:A:1737:A:H61	11:A:1760:G:H1'	1.84	0.43
27:S:111:GLU:HG2	36:b:19:LEU:HD11	2.01	0.43
31:X:166:LEU:HD13	31:X:196:ILE:HD11	2.00	0.43
50:c:137:LEU:HD23	50:c:137:LEU:HA	1.85	0.43
59:AG:80:GLU:HG3	76:A1:84:PRO:HB3	2.01	0.43
75:A0:64:LEU:HB2	75:A0:139:TRP:CD1	2.54	0.43
80:AA:862:A:H2'	80:AA:863:C:C6	2.54	0.43
80:AA:1175:G:H2'	80:AA:1176:G:C8	2.53	0.43
87:AX:81:HIS:CD2	87:AX:190:ASN:HB3	2.54	0.43
90:B:23:A:H2'	90:B:24:G:H8	1.83	0.43
6:5:417:LEU:HD23	6:5:417:LEU:HA	1.86	0.43
11:A:1719:G:H2'	11:A:1720:C:H6	1.83	0.43
11:A:2263:C:H5'	27:S:180:PHE:CE1	2.54	0.43
11:A:2558:A:H2'	11:A:2559:U:C6	2.54	0.43
12:C:115:LYS:HA	12:C:115:LYS:HD3	1.87	0.43
15:F:181:LYS:HD3	15:F:181:LYS:HA	1.84	0.43
19:K:356:LEU:HG	49:r:95:PRO:HD3	2.01	0.43
24:P:144:MET:HE2	24:P:144:MET:HB3	1.91	0.43
31:X:212:ILE:HD13	82:OX:434:LEU:HG	2.01	0.43
57:AE:79:VAL:HG23	57:AE:93:ILE:HD12	2.01	0.43
58:AF:114:THR:HG21	58:AF:205:LEU:HG	2.00	0.43
59:AG:315:PHE:CD2	59:AG:369:LEU:HD21	2.54	0.43
71:AU:117:HIS:HA	71:AU:120:ARG:HH11	1.83	0.43
72:AV:118:LYS:HB2	72:AV:118:LYS:HE3	1.87	0.43
76:A1:60:MET:HE1	76:A1:66:TRP:HZ3	1.84	0.43
80:AA:982:A:H2'	80:AA:983:C:H6	1.83	0.43
4:3:115:LEU:HB2	21:M:83:PHE:HB3	2.00	0.42
11:A:2245:A:H4'	11:A:2246:A:OP1	2.17	0.42
18:J:96:GLY:HA2	44:l:61:VAL:HG21	2.01	0.42
27:S:163:LYS:HB2	36:b:106:ASP:HB3	2.01	0.42
35:V:16:PRO:HD2	35:V:19:TYR:HB2	2.00	0.42
49:r:35:PHE:HB3	49:r:36:ARG:H	1.73	0.42
80:AA:865:A:H2'	80:AA:866:A:H8	1.83	0.42
80:AA:877:G:H2'	80:AA:878:G:C8	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:1498:C:H2'	80:AA:1499:U:H6	1.84	0.42
86:A4:248:PHE:CE1	86:A4:254:LYS:HD2	2.54	0.42
86:A4:556:LYS:HD2	86:A4:595:MET:HE1	2.01	0.42
11:A:1982:G:H2'	11:A:1983:U:C6	2.54	0.42
11:A:2455:U:H5''	23:O:47:ALA:HB3	2.01	0.42
16:H:98:LEU:HD11	16:H:105:VAL:HG23	2.02	0.42
28:T:62:ARG:NE	37:d:230:ARG:HD2	2.34	0.42
37:d:216:MET:HE2	37:d:216:MET:HB3	1.96	0.42
63:AL:209:LEU:HD22	77:A3:173:LEU:HD12	2.00	0.42
66:AO:56:TRP:HE1	66:AO:57:LYS:HE3	1.84	0.42
67:AP:57:PRO:HG3	69:AS:68:ASP:HB3	2.00	0.42
70:AT:34:TYR:HA	70:AT:74:PRO:HB3	2.00	0.42
72:AV:82:ARG:O	72:AV:85:ILE:HG22	2.19	0.42
72:AV:246:ASN:HB2	75:A0:70:ARG:HH12	1.83	0.42
80:AA:871:A:H4'	80:AA:872:G:H5'	2.02	0.42
80:AA:996:A:H2'	80:AA:997:A:H8	1.85	0.42
80:AA:1202:G:H2'	80:AA:1203:C:C6	2.54	0.42
80:AA:1203:C:H2'	80:AA:1204:C:C6	2.54	0.42
85:Aw:64:U:H2'	85:Aw:65:A:C8	2.55	0.42
86:A4:236:VAL:HA	86:A4:270:ARG:HB3	2.00	0.42
9:8:53:LYS:HZ2	85:Aw:40:C:H5''	1.84	0.42
21:M:44:ARG:HG3	21:M:45:ARG:HG3	2.01	0.42
51:f:195:LYS:HA	51:f:195:LYS:HD2	1.85	0.42
52:p:110:TRP:CD1	52:p:110:TRP:H	2.36	0.42
58:AF:159:VAL:HG13	58:AF:172:VAL:HG21	2.01	0.42
59:AG:357:THR:HG23	59:AG:360:GLU:H	1.83	0.42
72:AV:76:ILE:HD12	72:AV:112:TRP:CD1	2.55	0.42
76:A1:270:LYS:HD2	76:A1:270:LYS:HA	1.82	0.42
80:AA:745:A:H3'	80:AA:746:A:H8	1.84	0.42
80:AA:1119:U:H2'	80:AA:1120:C:O4'	2.20	0.42
11:A:2094:G:H2'	11:A:2095:U:H6	1.85	0.42
11:A:2472:A:H62	11:A:2654:U:H3	1.65	0.42
11:A:2751:G:H2'	11:A:2752:C:C6	2.54	0.42
11:A:3115:U:H2'	11:A:3116:C:H6	1.85	0.42
20:L:47:GLY:HA2	20:L:77:ILE:HD11	2.01	0.42
40:h:139:LYS:HD2	40:h:139:LYS:HA	1.91	0.42
41:i:38:LEU:HD23	41:i:38:LEU:HA	1.88	0.42
54:AB:118:LEU:HA	54:AB:121:THR:HB	2.00	0.42
61:AJ:66:PHE:HE2	61:AJ:68:ARG:HE	1.67	0.42
63:AL:116:VAL:HG12	63:AL:118:ASN:H	1.85	0.42
64:AM:73:ILE:O	64:AM:77:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AA:664:G:H2'	80:AA:665:C:C6	2.54	0.42
80:AA:1174:U:H2'	80:AA:1175:G:H8	1.84	0.42
80:AA:1502:A:H2'	80:AA:1503:G:O4'	2.20	0.42
86:A4:377:ARG:NH2	86:A4:418:SER:HA	2.34	0.42
86:A4:542:PRO:HA	86:A4:545:GLN:HB2	2.01	0.42
7:6:237:LEU:HB2	7:6:240:ILE:HD11	2.01	0.42
7:6:291:TYR:CE1	7:6:334:LEU:HB3	2.55	0.42
11:A:2082:G:H2'	11:A:2083:U:O4'	2.18	0.42
30:W:62:HIS:H	30:W:65:ASN:ND2	2.18	0.42
38:e:77:ILE:HG23	38:e:81:ARG:HH21	1.85	0.42
49:r:120:LYS:HB3	49:r:124:ARG:NH1	2.35	0.42
53:s:273:LEU:HD12	53:s:273:LEU:HA	1.83	0.42
66:AO:55:PRO:HB3	66:AO:114:HIS:HB2	2.00	0.42
77:A3:154:ARG:HH11	77:A3:154:ARG:HB2	1.85	0.42
80:AA:702:C:H2'	80:AA:703:A:C8	2.54	0.42
80:AA:740:G:H2'	80:AA:741:A:C8	2.55	0.42
84:Ax:25:C:H2'	84:Ax:26:G:H8	1.84	0.42
22:N:109:ILE:HD13	22:N:161:VAL:HG11	2.02	0.42
37:d:89:VAL:HA	37:d:90:PRO:HD3	1.90	0.42
50:c:148:MET:HG3	50:c:149:PRO:HD2	2.02	0.42
58:AF:240:ARG:HG3	58:AF:242:TRP:CE3	2.55	0.42
59:AG:394:LYS:HD2	59:AG:394:LYS:HA	1.86	0.42
68:AR:194:GLN:HE22	68:AR:199:LYS:H	1.66	0.42
80:AA:985:U:H2'	80:AA:986:G:C8	2.54	0.42
80:AA:1032:C:H2'	80:AA:1033:U:H6	1.84	0.42
80:AA:1271:C:H3'	80:AA:1272:A:H8	1.84	0.42
80:AA:1372:C:H2'	80:AA:1373:U:H6	1.85	0.42
80:AA:1455:U:H2'	80:AA:1456:U:C6	2.55	0.42
80:AA:1572:A:H2'	80:AA:1573:A:C8	2.54	0.42
7:6:45:LEU:HD12	7:6:48:LEU:HD12	2.02	0.42
15:F:70:ARG:HA	15:F:196:PRO:HD3	2.02	0.42
19:K:217:LEU:HD11	19:K:303:LEU:HB2	2.01	0.42
37:d:197:VAL:HG13	37:d:212:ILE:HG12	2.01	0.42
53:s:211:VAL:HG22	53:s:230:ARG:HG2	2.02	0.42
56:AD:231:MET:HG3	80:AA:1480:A:C2	2.55	0.42
59:AG:92:MET:HE2	59:AG:92:MET:HB2	1.86	0.42
63:AL:200:HIS:CD2	63:AL:200:HIS:H	2.37	0.42
80:AA:672:A:H2'	80:AA:673:U:C6	2.54	0.42
82:OX:427:LYS:HD2	82:OX:427:LYS:HA	1.94	0.42
88:A2:222:LEU:HD12	88:A2:222:LEU:HA	1.92	0.42
90:B:29:C:H2'	90:B:30:A:C8	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:166:LEU:HB3	8:7:181:TYR:HE2	1.85	0.42
11:A:2080:U:O2'	47:o:60:ARG:HA	2.20	0.42
11:A:2553:G:H2'	11:A:2554:A:C8	2.54	0.42
11:A:2661:U:H2'	11:A:2662:A:C8	2.55	0.42
11:A:2976:G:H21	11:A:2978:U:H5	1.66	0.42
11:A:3201:A:H2'	11:A:3202:U:O4'	2.20	0.42
13:D:207:ILE:HG12	13:D:229:PRO:HD3	2.00	0.42
34:G:188:LEU:HA	34:G:191:VAL:HG12	2.01	0.42
35:V:146:VAL:HG21	82:OX:401:PHE:HE1	1.83	0.42
51:f:178:LEU:HD12	51:f:182:VAL:HB	2.02	0.42
60:AH:181:PRO:HD2	60:AH:184:ILE:HG21	2.02	0.42
60:AH:182:GLU:HA	60:AH:185:LYS:NZ	2.35	0.42
84:Ax:60:C:H2'	84:Ax:61:C:H6	1.85	0.42
5:4:103:MET:HB3	5:4:103:MET:HE2	1.80	0.42
11:A:2950:U:H2'	11:A:2951:A:H8	1.85	0.42
31:X:42:HIS:CG	31:X:86:ILE:HD11	2.55	0.42
66:AO:55:PRO:HB2	66:AO:119:ASN:ND2	2.34	0.42
69:AS:51:VAL:HG23	69:AS:53:TYR:CE1	2.55	0.42
80:AA:1055:U:C2	80:AA:1056:A:C8	3.08	0.42
80:AA:1575:U:H2'	80:AA:1576:G:C8	2.55	0.42
85:Aw:23:A:H2'	85:Aw:24:A:C8	2.55	0.42
86:A4:166:VAL:HG12	86:A4:194:LEU:HG	2.00	0.42
10:9:136:LEU:HD23	10:9:136:LEU:HA	1.82	0.42
11:A:2192:A:H4'	18:J:139:SER:HB3	2.02	0.42
22:N:172:VAL:HA	22:N:175:PHE:CE2	2.55	0.42
38:e:213:TYR:HD1	38:e:271:GLN:HG2	1.85	0.42
40:h:140:PHE:HB2	40:h:156:TRP:CD2	2.54	0.42
59:AG:108:ILE:HD13	59:AG:108:ILE:HA	1.89	0.42
61:AJ:56:PRO:HB3	80:AA:924:A:N3	2.35	0.42
61:AJ:62:VAL:HA	61:AJ:83:VAL:HG12	2.00	0.42
72:AV:167:VAL:HG13	72:AV:172:ALA:HB3	2.02	0.42
80:AA:685:A:H2'	80:AA:686:A:C8	2.55	0.42
80:AA:1021:U:H4'	80:AA:1022:A:H5'	2.02	0.42
80:AA:1587:U:H2'	80:AA:1588:G:H8	1.85	0.42
81:AI:86:ALA:HA	81:AI:99:VAL:HA	2.02	0.42
84:Ax:22:U:C2	84:Ax:23:A:C8	3.08	0.42
9:8:82:LEU:HD11	51:f:197:ARG:HB3	2.02	0.41
11:A:1946:C:H2'	11:A:1947:C:H6	1.85	0.41
11:A:1951:C:H2'	11:A:1952:U:C6	2.55	0.41
22:N:249:LYS:HA	22:N:249:LYS:HD3	1.87	0.41
27:S:76:HIS:ND1	83:a:50:ALA:HA	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b:72:VAL:HG13	36:b:90:HIS:HB2	2.01	0.41
38:e:98:LEU:O	38:e:101:LYS:HG3	2.20	0.41
60:AH:137:ARG:HG3	62:AK:124:GLN:NE2	2.35	0.41
80:AA:724:C:H2'	80:AA:725:C:C6	2.55	0.41
80:AA:1006:U:H2'	80:AA:1007:G:C8	2.55	0.41
80:AA:1362:G:H2'	80:AA:1363:C:C6	2.55	0.41
11:A:2215:C:H2'	11:A:2216:A:O4'	2.20	0.41
13:D:111:ARG:HA	13:D:111:ARG:HD2	1.84	0.41
15:F:164:MET:HE2	41:i:69:HIS:CE1	2.54	0.41
21:M:28:LYS:HG2	21:M:29:PRO:HD2	2.02	0.41
24:P:86:THR:HG21	90:B:24:G:H5''	2.02	0.41
38:e:56:PRO:HG3	38:e:237:LEU:HD21	2.02	0.41
38:e:186:GLY:HA2	38:e:189:GLU:OE1	2.20	0.41
38:e:257:LYS:HD3	38:e:278:ASP:HB3	2.02	0.41
54:AB:141:ILE:HB	54:AB:190:PRO:HA	2.03	0.41
61:AJ:58:LEU:HB3	61:AJ:85:LEU:HD12	2.01	0.41
73:AW:144:LEU:HD23	73:AW:144:LEU:HA	1.88	0.41
75:A0:71:LEU:HD13	75:A0:78:ARG:HG3	2.01	0.41
86:A4:321:ARG:HA	86:A4:324:VAL:HG22	2.01	0.41
4:3:108:LYS:HA	4:3:108:LYS:HD3	1.84	0.41
7:6:273:PHE:HB3	7:6:311:MET:HG2	2.03	0.41
8:7:281:SER:HB3	8:7:321:ARG:HG2	2.01	0.41
11:A:2312:A:H2'	11:A:2313:A:O4'	2.21	0.41
12:C:227:ARG:NH1	12:C:229:VAL:HG12	2.36	0.41
21:M:178:PHE:O	21:M:203:ARG:HD2	2.20	0.41
33:Z:86:ILE:HD13	33:Z:86:ILE:HA	1.92	0.41
34:G:130:PHE:HE2	34:G:178:LYS:HB2	1.84	0.41
34:t:65:GLN:O	34:t:69:GLN:HG2	2.20	0.41
56:AD:269:ARG:HH21	80:AA:1278:C:P	2.43	0.41
66:AO:49:SER:H	66:AO:52:LYS:NZ	2.18	0.41
71:AU:60:TYR:CE2	80:AA:845:A:H4'	2.55	0.41
80:AA:661:C:H2'	80:AA:662:U:C6	2.56	0.41
80:AA:1485:G:H2'	80:AA:1486:B8T:O4'	2.20	0.41
84:Ax:59:U:H2'	84:Ax:60:C:C6	2.55	0.41
9:8:53:LYS:NZ	85:Aw:40:C:H5''	2.36	0.41
9:8:117:LEU:HD11	38:e:69:GLU:HB3	2.02	0.41
11:A:1911:C:H2'	11:A:1912:A:H8	1.85	0.41
11:A:2174:G:H4'	18:J:151:LEU:HD23	2.03	0.41
11:A:2815:OMG:H1'	11:A:2815:OMG:HM23	1.64	0.41
24:P:108:ARG:HD3	90:B:23:A:H5''	2.02	0.41
25:Q:165:GLU:HB2	25:Q:168:ASN:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:d:208:VAL:HG23	37:d:252:LEU:HB2	2.03	0.41
50:c:164:GLU:HG2	50:c:165:VAL:N	2.35	0.41
54:AB:231:LEU:HD23	54:AB:231:LEU:HA	1.91	0.41
59:AG:337:ARG:HG3	59:AG:338:SER:N	2.36	0.41
60:AH:162:ARG:HD3	60:AH:162:ARG:HA	1.82	0.41
61:AJ:56:PRO:HB3	80:AA:924:A:C2	2.55	0.41
62:AK:53:ARG:HD3	79:AY:375:TRP:CE3	2.56	0.41
72:AV:120:ASP:HA	72:AV:122:GLN:HE22	1.85	0.41
80:AA:996:A:H2'	80:AA:997:A:C8	2.55	0.41
80:AA:1015:A:P	81:AI:184:ASN:HD21	2.43	0.41
80:AA:1496:U:H2'	80:AA:1497:C:C6	2.56	0.41
11:A:1762:A:H2'	11:A:1763:A:C8	2.56	0.41
11:A:2774:C:H2'	11:A:2775:A:C5	2.55	0.41
11:A:3165:C:H2'	11:A:3166:U:C6	2.56	0.41
17:I:102:VAL:HG22	17:I:174:LEU:HD13	2.03	0.41
31:X:10:LEU:HD23	31:X:10:LEU:HA	1.92	0.41
42:j:103:ARG:HA	42:j:106:GLU:CD	2.45	0.41
50:c:165:VAL:HG13	50:c:222:GLN:HG3	2.02	0.41
62:AK:53:ARG:HD3	79:AY:375:TRP:CD2	2.55	0.41
65:AN:51:ALA:HB2	65:AN:66:LEU:HD13	2.02	0.41
66:AO:213:LEU:HB3	66:AO:217:ARG:HH22	1.85	0.41
72:AV:276:CYS:SG	72:AV:352:LEU:HD21	2.60	0.41
79:AY:294:LEU:HD13	79:AY:300:GLU:HB2	2.02	0.41
80:AA:1190:C:H2'	80:AA:1191:C:H6	1.86	0.41
87:AX:138:LEU:HD11	87:AX:261:ALA:HB1	2.02	0.41
87:AX:171:SER:HB3	87:AX:177:ARG:HB2	2.02	0.41
8:7:269:ILE:HD12	8:7:274:ILE:HB	2.03	0.41
11:A:1816:G:H2'	11:A:1817:C:O4'	2.21	0.41
12:C:268:LEU:HD23	12:C:272:ASP:HB3	2.03	0.41
12:C:296:ILE:HD13	12:C:296:ILE:HA	1.91	0.41
19:K:344:PHE:HZ	49:r:88:LEU:HD12	1.86	0.41
26:R:90:LEU:HD23	26:R:90:LEU:HA	1.85	0.41
38:e:75:GLN:O	38:e:79:ILE:HG12	2.20	0.41
40:h:62:PRO:HA	40:h:63:PRO:HD3	1.98	0.41
41:i:42:LYS:HD3	41:i:42:LYS:HA	1.88	0.41
51:f:136:GLN:HB2	51:f:147:ASP:HB2	2.01	0.41
52:p:52:SER:O	52:p:57:THR:HG21	2.20	0.41
60:AH:76:LEU:HD23	60:AH:174:LYS:HA	2.02	0.41
63:AL:165:LYS:HE3	80:AA:947:U:H5''	2.02	0.41
64:AM:51:LEU:HD22	64:AM:72:ARG:HB3	2.02	0.41
70:AT:158:GLU:O	70:AT:164:LYS:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:AZ:46:LYS:HA	74:AZ:49:TYR:CE2	2.55	0.41
80:AA:732:A:H2'	80:AA:733:U:C6	2.56	0.41
80:AA:1499:U:H2'	80:AA:1500:C:H6	1.85	0.41
85:Aw:14:A:C6	85:Aw:22:A:C5	3.09	0.41
86:A4:431:LEU:HD12	86:A4:431:LEU:HA	1.83	0.41
88:A2:205:ARG:HA	88:A2:209:GLU:HB2	2.03	0.41
6:5:336:LEU:HD21	6:5:362:THR:HG23	2.01	0.41
10:9:68:PHE:CE2	10:9:70:LEU:HB2	2.56	0.41
11:A:2235:C:H2'	11:A:2236:C:O4'	2.20	0.41
11:A:2408:U:H2'	11:A:2409:A:C8	2.56	0.41
11:A:2819:G:H21	30:W:38:SER:HB3	1.85	0.41
12:C:185:LYS:HD2	12:C:258:LEU:HB3	2.02	0.41
14:E:60:PHE:CG	23:O:153:ARG:HD2	2.55	0.41
15:F:96:LEU:HD23	15:F:96:LEU:HA	1.82	0.41
15:F:248:LEU:HG	15:F:253:MET:HE2	2.03	0.41
34:G:185:LYS:NZ	34:G:195:VAL:H	2.19	0.41
59:AG:59:LYS:HE2	59:AG:62:PRO:HA	2.03	0.41
64:AM:89:LYS:HG3	64:AM:103:MET:HE2	2.03	0.41
71:AU:49:ASP:HB3	71:AU:52:GLU:HB3	2.01	0.41
80:AA:745:A:C4	80:AA:746:A:C8	3.08	0.41
80:AA:1066:C:H2'	80:AA:1067:A:C8	2.56	0.41
80:AA:1427:A:H2'	80:AA:1428:G:C8	2.55	0.41
80:AA:1506:U:H2'	80:AA:1507:A:C8	2.55	0.41
85:Aw:3:G:H2'	85:Aw:4:U:C6	2.56	0.41
86:A4:446:LYS:HE3	86:A4:446:LYS:HB3	1.91	0.41
11:A:1861:U:H2'	11:A:1862:U:H6	1.85	0.41
11:A:1993:A:H8	11:A:2498:U:O2'	2.04	0.41
11:A:2175:C:H2'	11:A:2176:C:H6	1.86	0.41
18:J:113:THR:HG23	18:J:115:LYS:N	2.36	0.41
22:N:250:ARG:HE	22:N:250:ARG:HB3	1.69	0.41
23:O:46:TRP:HD1	23:O:121:ALA:HB2	1.85	0.41
37:d:221:THR:HG22	37:d:239:PRO:HA	2.02	0.41
39:g:110:ILE:HD11	39:g:157:LEU:HD13	2.03	0.41
54:AB:67:LEU:HD11	54:AB:138:ARG:HH21	1.85	0.41
66:AO:213:LEU:HD13	71:AU:50:PRO:HB2	2.02	0.41
72:AV:169:MET:HE1	72:AV:247:MET:HG2	2.02	0.41
80:AA:696:U:H2'	80:AA:697:G:C8	2.55	0.41
86:A4:549:ALA:HB1	86:A4:588:ARG:HD2	2.03	0.41
7:6:99:ARG:HH22	90:B:20:A:H2'	1.86	0.41
9:8:173:LYS:HB3	51:f:184:LEU:HB3	2.03	0.41
11:A:1839:C:H5''	19:K:293:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2051:A:H2'	11:A:2052:A:H8	1.85	0.41
11:A:2053:U:OP2	47:o:79:THR:HG23	2.20	0.41
11:A:3000:A:H2'	11:A:3001:G:C8	2.56	0.41
12:C:119:LYS:O	12:C:123:GLU:HG2	2.21	0.41
24:P:72:PHE:HB2	30:W:107:HIS:HA	2.02	0.41
25:Q:74:ARG:HH21	25:Q:283:TRP:CG	2.39	0.41
34:G:150:LYS:HE2	34:G:157:ASN:HA	2.03	0.41
44:l:110:LEU:HB3	44:l:117:TYR:HB2	2.03	0.41
47:o:24:PRO:HG2	49:r:169:TRP:HB2	2.02	0.41
56:AD:226:ARG:HD3	80:AA:659:U:OP1	2.21	0.41
68:AR:142:LEU:HD13	68:AR:142:LEU:HA	1.96	0.41
69:AS:106:LEU:HD13	69:AS:120:GLU:HG3	2.03	0.41
70:AT:19:GLY:HA3	70:AT:54:GLN:HB3	2.03	0.41
71:AU:176:ARG:HA	71:AU:176:ARG:HD2	1.85	0.41
72:AV:103:TYR:CZ	80:AA:1524:A:H4'	2.56	0.41
78:Az:27:C:C2	78:Az:28:U:H5	2.39	0.41
80:AA:914:A:H2'	80:AA:915:C:H6	1.85	0.41
80:AA:1080:A:H1'	80:AA:1082:A:N7	2.36	0.41
80:AA:1191:C:H2'	80:AA:1192:C:C6	2.56	0.41
80:AA:1316:U:H2'	80:AA:1317:A:O4'	2.21	0.41
80:AA:1379:A:H2'	80:AA:1380:G:C8	2.56	0.41
80:AA:1523:A:H2'	80:AA:1524:A:C8	2.56	0.41
86:A4:393:ILE:HA	86:A4:396:ILE:HG22	2.02	0.41
86:A4:489:HIS:CE1	86:A4:491:GLN:HG3	2.55	0.41
2:l:55:LEU:H	48:q:128:MET:HE2	1.86	0.41
8:7:284:HIS:CD2	8:7:323:MET:HA	2.56	0.41
18:J:49:PHE:HA	18:J:52:GLU:CD	2.46	0.41
20:L:62:LYS:HE2	20:L:62:LYS:HB3	1.99	0.41
65:AN:17:VAL:HG22	65:AN:28:VAL:HG22	2.03	0.41
68:AR:128:MET:HA	68:AR:129:PRO:HD3	1.98	0.41
75:A0:11:ILE:HB	80:AA:806:C:C2	2.56	0.41
80:AA:659:U:O2'	80:AA:1285:G:H1'	2.21	0.41
80:AA:968:U:H2'	80:AA:969:A:C8	2.56	0.41
80:AA:1195:U:H2'	80:AA:1196:A:C8	2.55	0.41
80:AA:1373:U:H2'	80:AA:1374:A:H8	1.83	0.41
80:AA:1408:A:H2'	80:AA:1409:A:C8	2.56	0.41
85:Aw:40:C:H2'	85:Aw:41:A:H8	1.86	0.41
86:A4:88:VAL:HG11	86:A4:107:LEU:HD11	2.03	0.41
8:7:95:LEU:HD23	8:7:95:LEU:HA	1.92	0.40
11:A:1781:A:N1	11:A:1794:A:H5''	2.36	0.40
11:A:3163:G:H2'	11:A:3164:C:H6	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AJ:51:PRO:HG3	61:AJ:122:LYS:HB3	2.02	0.40
67:AP:120:MET:HG2	67:AP:121:PRO:O	2.21	0.40
71:AU:45:PRO:HA	71:AU:46:PRO:HD3	1.94	0.40
75:A0:180:LYS:HA	75:A0:180:LYS:HD3	1.92	0.40
93:AA:1782:SPD:H41	93:AA:1783:SPD:H52	2.04	0.40
86:A4:192:LEU:HD12	86:A4:192:LEU:HA	1.89	0.40
86:A4:650:MET:SD	86:A4:659:GLN:HG2	2.60	0.40
87:AX:159:HIS:CD2	87:AX:267:ALA:HB2	2.56	0.40
11:A:1924:U:H2'	11:A:1925:A:C8	2.57	0.40
11:A:2221:C:H5''	49:r:103:LYS:NZ	2.37	0.40
11:A:2585:G:H2'	11:A:2586:U:C6	2.56	0.40
19:K:300:MET:HE3	19:K:300:MET:HB3	1.91	0.40
48:q:48:PRO:HB2	48:q:50:TRP:CD1	2.57	0.40
51:f:136:GLN:CB	51:f:147:ASP:HB2	2.51	0.40
53:s:119:PRO:HG3	53:s:394:TRP:CE3	2.56	0.40
58:AF:86:PHE:HE2	87:AX:398:LEU:HD21	1.87	0.40
58:AF:238:HIS:CD2	81:AI:124:THR:HB	2.56	0.40
59:AG:92:MET:HG3	76:A1:116:PRO:HD2	2.03	0.40
63:AL:67:PRO:HA	63:AL:68:PRO:HD3	1.99	0.40
68:AR:79:LEU:HD13	68:AR:128:MET:HE1	2.03	0.40
68:AR:223:ARG:HB3	68:AR:226:ASP:HB2	2.04	0.40
80:AA:1409:A:H2'	80:AA:1410:G:H8	1.86	0.40
80:AA:1495:C:H2'	80:AA:1496:U:H6	1.85	0.40
90:B:6:U:H3	90:B:67:G:H1	1.69	0.40
2:1:57:VAL:HG23	2:1:59:LYS:HE3	2.03	0.40
11:A:1718:A:H2'	11:A:1719:G:O4'	2.21	0.40
35:V:138:THR:HG23	35:V:140:ALA:N	2.36	0.40
37:d:85:PHE:HZ	37:d:209:TYR:HB2	1.87	0.40
62:AK:75:ILE:HA	62:AK:78:LEU:HD12	2.03	0.40
80:AA:749:G:H2'	80:AA:750:G:H8	1.86	0.40
80:AA:1414:C:H3'	80:AA:1415:G:H21	1.86	0.40
80:AA:1505:A:H2'	80:AA:1506:U:C6	2.56	0.40
80:AA:1562:G:H1'	80:AA:1583:MA6:H2	2.02	0.40
87:AX:56:PRO:HD2	87:AX:147:LYS:HG3	2.02	0.40
11:A:1722:A:H2'	11:A:1723:A:O4'	2.22	0.40
11:A:1735:A:H3'	48:q:49:ARG:HH12	1.85	0.40
11:A:2217:C:H2'	11:A:2218:C:O4'	2.21	0.40
11:A:3111:A:H2'	11:A:3112:A:H5''	2.03	0.40
15:F:175:LYS:HG2	15:F:273:LEU:HD13	2.03	0.40
38:e:74:LEU:HD22	45:m:42:ARG:HB3	2.03	0.40
43:k:178:VAL:HB	43:k:186:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AD:203:LEU:HB2	56:AD:220:THR:HB	2.03	0.40
59:AG:168:MET:HE3	59:AG:237:GLU:HG3	2.03	0.40
60:AH:104:ILE:HG23	60:AH:148:LEU:HD11	2.04	0.40
60:AH:187:PRO:HB3	76:A1:234:TRP:CG	2.55	0.40
70:AT:77:ARG:HG2	70:AT:79:TYR:CE1	2.56	0.40
73:AW:148:GLU:HG2	73:AW:150:THR:HG23	2.02	0.40
75:A0:51:PRO:HG3	80:AA:705:C:H5'	2.04	0.40
80:AA:672:A:H2'	80:AA:673:U:H6	1.87	0.40
80:AA:949:U:O2	97:AA:1701:NAD:H6N	2.21	0.40
86:A4:92:ASP:O	86:A4:96:MET:HG2	2.22	0.40
86:A4:272:TYR:CE2	86:A4:303:CYS:HB3	2.56	0.40
11:A:2127:A:H4'	11:A:2251:A:C6	2.57	0.40
11:A:3143:U:H2'	11:A:3144:A:C8	2.56	0.40
27:S:120:LEU:HD23	27:S:120:LEU:HA	1.86	0.40
31:X:218:LEU:HD23	31:X:218:LEU:HA	1.90	0.40
38:e:166:GLY:CA	101:B:101:VAL:HB	2.44	0.40
56:AD:326:LEU:HD23	56:AD:326:LEU:HA	1.96	0.40
66:AO:211:ARG:HD2	72:AV:319:ILE:HD11	2.04	0.40
78:Az:30:A:H2'	78:Az:31:A:C4	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	108/188 (57%)	108 (100%)	0	0	100	100
2	1	54/65 (83%)	54 (100%)	0	0	100	100
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	36/103 (35%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	5	392/423 (93%)	387 (99%)	5 (1%)	0	100	100
7	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
8	7	292/338 (86%)	282 (97%)	10 (3%)	0	100	100
9	8	155/206 (75%)	152 (98%)	3 (2%)	0	100	100
10	9	122/137 (89%)	117 (96%)	5 (4%)	0	100	100
12	C	221/297 (74%)	214 (97%)	7 (3%)	0	100	100
13	D	236/305 (77%)	231 (98%)	5 (2%)	0	100	100
14	E	303/348 (87%)	294 (97%)	9 (3%)	0	100	100
15	F	250/311 (80%)	246 (98%)	4 (2%)	0	100	100
16	H	200/267 (75%)	193 (96%)	7 (4%)	0	100	100
17	I	179/261 (69%)	172 (96%)	7 (4%)	0	100	100
18	J	173/192 (90%)	170 (98%)	3 (2%)	0	100	100
19	K	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
20	L	113/145 (78%)	110 (97%)	3 (3%)	0	100	100
21	M	289/296 (98%)	283 (98%)	6 (2%)	0	100	100
22	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
23	O	152/175 (87%)	146 (96%)	6 (4%)	0	100	100
24	P	142/180 (79%)	138 (97%)	4 (3%)	0	100	100
25	Q	237/292 (81%)	232 (98%)	5 (2%)	0	100	100
26	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
27	S	159/205 (78%)	158 (99%)	1 (1%)	0	100	100
28	T	164/206 (80%)	162 (99%)	2 (1%)	0	100	100
29	U	150/153 (98%)	146 (97%)	4 (3%)	0	100	100
30	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
31	X	242/256 (94%)	239 (99%)	3 (1%)	0	100	100
32	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
33	Z	120/161 (74%)	118 (98%)	2 (2%)	0	100	100
34	G	70/198 (35%)	66 (94%)	4 (6%)	0	100	100
34	t	44/198 (22%)	44 (100%)	0	0	100	100
34	u	30/198 (15%)	30 (100%)	0	0	100	100
35	V	203/216 (94%)	199 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	b	148/215 (69%)	140 (95%)	8 (5%)	0	100	100
37	d	257/306 (84%)	239 (93%)	17 (7%)	1 (0%)	30	59
38	e	236/279 (85%)	228 (97%)	8 (3%)	0	100	100
39	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
40	h	108/158 (68%)	103 (95%)	5 (5%)	0	100	100
41	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
42	j	92/123 (75%)	89 (97%)	3 (3%)	0	100	100
43	k	100/112 (89%)	99 (99%)	1 (1%)	0	100	100
44	l	80/138 (58%)	77 (96%)	3 (4%)	0	100	100
45	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
47	o	92/102 (90%)	92 (100%)	0	0	100	100
48	q	175/222 (79%)	175 (100%)	0	0	100	100
49	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
50	c	282/332 (85%)	277 (98%)	5 (2%)	0	100	100
51	f	153/212 (72%)	150 (98%)	3 (2%)	0	100	100
52	p	141/206 (68%)	138 (98%)	3 (2%)	0	100	100
53	s	381/439 (87%)	370 (97%)	11 (3%)	0	100	100
54	AB	223/296 (75%)	220 (99%)	3 (1%)	0	100	100
55	AC	130/167 (78%)	125 (96%)	5 (4%)	0	100	100
56	AD	341/430 (79%)	332 (97%)	9 (3%)	0	100	100
57	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
58	AF	206/242 (85%)	205 (100%)	1 (0%)	0	100	100
59	AG	323/396 (82%)	319 (99%)	4 (1%)	0	100	100
60	AH	138/201 (69%)	134 (97%)	3 (2%)	1 (1%)	18	48
61	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
62	AK	99/128 (77%)	99 (100%)	0	0	100	100
63	AL	172/257 (67%)	169 (98%)	3 (2%)	0	100	100
64	AM	117/137 (85%)	115 (98%)	2 (2%)	0	100	100
65	AN	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
66	AO	191/258 (74%)	186 (97%)	5 (3%)	0	100	100
67	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	AR	293/360 (81%)	285 (97%)	8 (3%)	0	100	100
69	AS	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
70	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
71	AU	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
72	AV	358/414 (86%)	347 (97%)	11 (3%)	0	100	100
73	AW	98/187 (52%)	95 (97%)	3 (3%)	0	100	100
74	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
75	A0	213/217 (98%)	206 (97%)	7 (3%)	0	100	100
76	A1	277/323 (86%)	268 (97%)	9 (3%)	0	100	100
77	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
79	AY	117/395 (30%)	115 (98%)	2 (2%)	0	100	100
81	AI	135/194 (70%)	132 (98%)	3 (2%)	0	100	100
82	OX	51/435 (12%)	47 (92%)	4 (8%)	0	100	100
83	a	99/142 (70%)	98 (99%)	1 (1%)	0	100	100
86	A4	584/689 (85%)	568 (97%)	16 (3%)	0	100	100
87	AX	350/398 (88%)	342 (98%)	8 (2%)	0	100	100
88	A2	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
89	AQ	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
All	All	14658/19297 (76%)	14325 (98%)	331 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	99/164 (60%)	99 (100%)	0	100	100
2	1	53/60 (88%)	53 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
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	C	193/245 (79%)	193 (100%)	0	100	100
13	D	192/245 (78%)	192 (100%)	0	100	100
14	E	260/290 (90%)	260 (100%)	0	100	100
15	F	219/262 (84%)	219 (100%)	0	100	100
16	H	182/228 (80%)	182 (100%)	0	100	100
17	I	165/232 (71%)	165 (100%)	0	100	100
18	J	138/150 (92%)	138 (100%)	0	100	100
19	K	155/155 (100%)	155 (100%)	0	100	100
20	L	98/124 (79%)	98 (100%)	0	100	100
21	M	246/249 (99%)	246 (100%)	0	100	100
22	N	189/211 (90%)	189 (100%)	0	100	100
23	O	134/150 (89%)	134 (100%)	0	100	100
24	P	126/155 (81%)	126 (100%)	0	100	100
25	Q	221/256 (86%)	221 (100%)	0	100	100
26	R	118/126 (94%)	118 (100%)	0	100	100
27	S	146/180 (81%)	146 (100%)	0	100	100
28	T	146/176 (83%)	146 (100%)	0	100	100
29	U	134/135 (99%)	134 (100%)	0	100	100
30	W	94/119 (79%)	94 (100%)	0	100	100
31	X	220/229 (96%)	220 (100%)	0	100	100
32	Y	163/223 (73%)	163 (100%)	0	100	100
33	Z	113/147 (77%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	G	60/158 (38%)	60 (100%)	0	100	100
34	t	40/158 (25%)	40 (100%)	0	100	100
34	u	31/158 (20%)	31 (100%)	0	100	100
35	V	183/191 (96%)	183 (100%)	0	100	100
36	b	132/186 (71%)	132 (100%)	0	100	100
37	d	237/274 (86%)	237 (100%)	0	100	100
38	e	207/236 (88%)	207 (100%)	0	100	100
39	g	124/148 (84%)	124 (100%)	0	100	100
40	h	104/148 (70%)	104 (100%)	0	100	100
41	i	86/110 (78%)	86 (100%)	0	100	100
42	j	74/97 (76%)	74 (100%)	0	100	100
43	k	83/89 (93%)	83 (100%)	0	100	100
44	l	76/116 (66%)	76 (100%)	0	100	100
45	m	85/113 (75%)	85 (100%)	0	100	100
47	o	80/87 (92%)	80 (100%)	0	100	100
48	q	153/178 (86%)	153 (100%)	0	100	100
49	r	147/169 (87%)	147 (100%)	0	100	100
50	c	251/288 (87%)	251 (100%)	0	100	100
51	f	139/188 (74%)	139 (100%)	0	100	100
52	p	135/181 (75%)	135 (100%)	0	100	100
53	s	339/381 (89%)	339 (100%)	0	100	100
54	AB	198/249 (80%)	198 (100%)	0	100	100
55	AC	115/143 (80%)	115 (100%)	0	100	100
56	AD	286/357 (80%)	286 (100%)	0	100	100
57	AE	104/107 (97%)	104 (100%)	0	100	100
58	AF	185/209 (88%)	185 (100%)	0	100	100
59	AG	285/342 (83%)	285 (100%)	0	100	100
60	AH	130/180 (72%)	130 (100%)	0	100	100
61	AJ	93/118 (79%)	93 (100%)	0	100	100
62	AK	91/113 (80%)	91 (100%)	0	100	100
63	AL	158/226 (70%)	158 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	AM	97/113 (86%)	97 (100%)	0	100	100
65	AN	96/115 (84%)	96 (100%)	0	100	100
66	AO	174/230 (76%)	173 (99%)	1 (1%)	78	93
67	AP	88/123 (72%)	88 (100%)	0	100	100
68	AR	264/318 (83%)	264 (100%)	0	100	100
69	AS	116/164 (71%)	116 (100%)	0	100	100
70	AT	153/157 (98%)	153 (100%)	0	100	100
71	AU	152/174 (87%)	152 (100%)	0	100	100
72	AV	325/364 (89%)	325 (100%)	0	100	100
73	AW	87/158 (55%)	87 (100%)	0	100	100
74	AZ	90/95 (95%)	90 (100%)	0	100	100
75	A0	188/189 (100%)	188 (100%)	0	100	100
76	A1	257/291 (88%)	257 (100%)	0	100	100
77	A3	65/166 (39%)	65 (100%)	0	100	100
79	AY	110/357 (31%)	110 (100%)	0	100	100
81	AI	105/147 (71%)	105 (100%)	0	100	100
82	OX	49/372 (13%)	49 (100%)	0	100	100
83	a	99/133 (74%)	99 (100%)	0	100	100
86	A4	526/609 (86%)	526 (100%)	0	100	100
87	AX	311/351 (89%)	311 (100%)	0	100	100
88	A2	100/100 (100%)	100 (100%)	0	100	100
89	AQ	78/78 (100%)	78 (100%)	0	100	100
All	All	13096/16645 (79%)	13095 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
66	AO	154	ILE

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

Mol	Chain	Res	Type
4	3	178	GLN

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Mol	Chain	Res	Type
6	5	165	GLN
6	5	195	HIS
6	5	214	ASN
6	5	269	ASN
7	6	292	GLN
7	6	373	HIS
8	7	84	ASN
8	7	111	GLN
8	7	287	GLN
9	8	186	GLN
12	C	263	ASN
12	C	275	GLN
12	C	281	GLN
13	D	168	HIS
13	D	195	ASN
15	F	208	HIS
16	H	178	ASN
19	K	272	GLN
20	L	104	ASN
22	N	210	GLN
24	P	89	HIS
25	Q	158	GLN
25	Q	172	GLN
25	Q	203	ASN
25	Q	209	GLN
25	Q	237	ASN
26	R	22	GLN
26	R	149	HIS
27	S	75	HIS
27	S	196	ASN
28	T	145	GLN
30	W	80	HIS
31	X	4	HIS
31	X	27	HIS
37	d	157	HIS
37	d	161	HIS
40	h	67	GLN
40	h	110	HIS
41	i	59	ASN
41	i	120	HIS
44	l	100	ASN
47	o	21	HIS

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Mol	Chain	Res	Type
48	q	120	HIS
49	r	69	GLN
49	r	79	HIS
50	c	107	GLN
50	c	172	ASN
51	f	112	ASN
52	p	143	GLN
53	s	71	HIS
53	s	107	GLN
53	s	358	GLN
53	s	420	GLN
54	AB	201	ASN
54	AB	216	ASN
56	AD	165	GLN
56	AD	273	ASN
56	AD	360	GLN
57	AE	54	HIS
57	AE	56	GLN
57	AE	57	GLN
58	AF	196	HIS
59	AG	87	HIS
59	AG	139	GLN
59	AG	242	GLN
59	AG	288	HIS
60	AH	125	HIS
62	AK	113	HIS
63	AL	77	GLN
63	AL	146	HIS
65	AN	52	HIS
66	AO	160	HIS
67	AP	115	GLN
68	AR	312	GLN
69	AS	97	GLN
71	AU	109	ASN
72	AV	170	GLN
73	AW	106	HIS
74	AZ	82	GLN
75	A0	24	GLN
77	A3	158	GLN
81	AI	93	ASN
81	AI	184	ASN
82	OX	403	HIS

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Mol	Chain	Res	Type
86	A4	274	GLN
86	A4	491	GLN
86	A4	626	GLN
87	AX	174	ASN
87	AX	180	GLN
87	AX	205	GLN
87	AX	292	ASN
88	A2	189	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1556/1561 (99%)	262 (16%)	1 (0%)
78	Az	33/34 (97%)	15 (45%)	0
80	AA	953/954 (99%)	140 (14%)	0
84	Ax	70/71 (98%)	16 (22%)	0
85	Aw	64/76 (84%)	21 (32%)	0
90	B	70/72 (97%)	16 (22%)	0
All	All	2746/2768 (99%)	470 (17%)	1 (0%)

All (470) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1681	G
11	A	1689	C
11	A	1692	A
11	A	1699	C
11	A	1700	U
11	A	1704	U
11	A	1708	A
11	A	1709	G
11	A	1711	C
11	A	1724	A
11	A	1727	A
11	A	1728	U
11	A	1732	C
11	A	1736	A
11	A	1748	G
11	A	1765	C
11	A	1780	U
11	A	1805	A

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Mol	Chain	Res	Type
11	A	1807	U
11	A	1808	A
11	A	1809	U
11	A	1812	C
11	A	1817	C
11	A	1821	A
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	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	1909	A
11	A	1918	G
11	A	1937	A
11	A	1939	G
11	A	1940	A
11	A	1958	G
11	A	1985	G
11	A	1986	A
11	A	1992	C
11	A	1993	A
11	A	1994	A
11	A	2001	C
11	A	2003	A
11	A	2015	G
11	A	2022	G
11	A	2030	U
11	A	2036	C

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Mol	Chain	Res	Type
11	A	2037	U
11	A	2039	A
11	A	2048	U
11	A	2054	U
11	A	2060	A
11	A	2069	U
11	A	2071	U
11	A	2079	C
11	A	2099	U
11	A	2113	G
11	A	2125	C
11	A	2126	U
11	A	2147	G
11	A	2159	U
11	A	2160	A
11	A	2163	A
11	A	2168	U
11	A	2181	A
11	A	2182	G
11	A	2191	A
11	A	2196	A
11	A	2198	A
11	A	2200	A
11	A	2207	A
11	A	2214	A
11	A	2219	C
11	A	2220	A
11	A	2221	C
11	A	2223	A
11	A	2224	C
11	A	2225	C
11	A	2226	U
11	A	2228	A
11	A	2230	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

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Mol	Chain	Res	Type
11	A	2284	C
11	A	2297	A
11	A	2300	G
11	A	2322	C
11	A	2324	U
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	2354	A
11	A	2357	C
11	A	2363	A
11	A	2372	U
11	A	2374	A
11	A	2379	C
11	A	2390	A
11	A	2399	A
11	A	2401	A
11	A	2404	U
11	A	2407	U
11	A	2415	C
11	A	2416	U
11	A	2434	A
11	A	2446	A
11	A	2451	A
11	A	2478	G
11	A	2484	C
11	A	2493	C
11	A	2496	G
11	A	2502	C
11	A	2506	A
11	A	2520	C
11	A	2521	A
11	A	2527	A
11	A	2540	C
11	A	2570	C
11	A	2592	G
11	A	2593	G
11	A	2594	U
11	A	2601	A

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Mol	Chain	Res	Type
11	A	2603	C
11	A	2606	U
11	A	2618	U
11	A	2625	C
11	A	2627	G
11	A	2628	U
11	A	2630	U
11	A	2633	A
11	A	2635	G
11	A	2654	U
11	A	2655	G
11	A	2656	U
11	A	2683	C
11	A	2686	G
11	A	2694	A
11	A	2696	A
11	A	2706	A
11	A	2709	A
11	A	2718	C
11	A	2719	G
11	A	2723	A
11	A	2724	G
11	A	2725	A
11	A	2732	G
11	A	2733	G
11	A	2745	A
11	A	2758	G
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	2781	U
11	A	2782	A
11	A	2786	U
11	A	2790	A
11	A	2810	G
11	A	2832	A
11	A	2833	A
11	A	2844	G
11	A	2847	C

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Mol	Chain	Res	Type
11	A	2854	U
11	A	2861	A
11	A	2864	U
11	A	2865	C
11	A	2874	A
11	A	2882	U
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	2907	U
11	A	2913	A
11	A	2915	C
11	A	2917	G
11	A	2918	A
11	A	2919	A
11	A	2922	A
11	A	2927	C
11	A	2928	C
11	A	2935	A
11	A	2956	A
11	A	2960	U
11	A	2962	C
11	A	2965	A
11	A	2971	A
11	A	2985	C
11	A	2989	G
11	A	2990	A
11	A	2992	G
11	A	2993	U
11	A	3000	A
11	A	3005	A
11	A	3007	C
11	A	3016	G
11	A	3022	G
11	A	3041	U
11	A	3049	U
11	A	3051	A
11	A	3053	A
11	A	3054	G

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Mol	Chain	Res	Type
11	A	3060	C
11	A	3072	U
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	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
11	A	3230	G
78	Az	0	U
78	Az	4	A
78	Az	11	U
78	Az	12	U
78	Az	13	U
78	Az	15	U
78	Az	18	A
78	Az	19	A

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Mol	Chain	Res	Type
78	Az	21	A
78	Az	22	A
78	Az	23	U
78	Az	25	U
78	Az	26	A
78	Az	27	C
78	Az	30	A
80	AA	651	A
80	AA	680	U
80	AA	688	A
80	AA	704	U
80	AA	712	C
80	AA	721	U
80	AA	722	C
80	AA	735	A
80	AA	737	C
80	AA	738	A
80	AA	753	A
80	AA	760	A
80	AA	761	A
80	AA	766	G
80	AA	791	G
80	AA	794	U
80	AA	796	G
80	AA	802	C
80	AA	828	C
80	AA	829	C
80	AA	830	U
80	AA	832	U
80	AA	835	C
80	AA	860	A
80	AA	861	U
80	AA	868	C
80	AA	870	C
80	AA	871	A
80	AA	881	A
80	AA	890	C
80	AA	893	G
80	AA	903	U
80	AA	904	C
80	AA	907	A
80	AA	919	A

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Mol	Chain	Res	Type
80	AA	929	A
80	AA	938	A
80	AA	939	A
80	AA	941	G
80	AA	942	A
80	AA	954	C
80	AA	958	C
80	AA	960	C
80	AA	961	U
80	AA	962	C
80	AA	963	C
80	AA	967	A
80	AA	978	A
80	AA	993	A
80	AA	1001	C
80	AA	1002	C
80	AA	1011	C
80	AA	1015	A
80	AA	1031	G
80	AA	1042	U
80	AA	1048	C
80	AA	1076	5MU
80	AA	1081	U
80	AA	1082	A
80	AA	1098	C
80	AA	1103	A
80	AA	1105	C
80	AA	1106	C
80	AA	1107	U
80	AA	1109	A
80	AA	1116	A
80	AA	1118	A
80	AA	1119	U
80	AA	1121	A
80	AA	1126	A
80	AA	1137	A
80	AA	1138	G
80	AA	1142	A
80	AA	1151	C
80	AA	1153	C
80	AA	1155	G
80	AA	1160	A

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Mol	Chain	Res	Type
80	AA	1167	A
80	AA	1187	U
80	AA	1188	A
80	AA	1189	U
80	AA	1190	C
80	AA	1215	U
80	AA	1220	A
80	AA	1223	C
80	AA	1225	C
80	AA	1230	C
80	AA	1235	U
80	AA	1247	G
80	AA	1248	C
80	AA	1250	C
80	AA	1251	A
80	AA	1269	U
80	AA	1271	C
80	AA	1273	G
80	AA	1284	U
80	AA	1290	C
80	AA	1291	U
80	AA	1292	A
80	AA	1318	A
80	AA	1326	A
80	AA	1327	G
80	AA	1334	G
80	AA	1343	A
80	AA	1353	A
80	AA	1354	A
80	AA	1356	A
80	AA	1367	A
80	AA	1376	C
80	AA	1378	C
80	AA	1387	A
80	AA	1390	A
80	AA	1405	C
80	AA	1407	U
80	AA	1430	A
80	AA	1466	C
80	AA	1478	A
80	AA	1482	A
80	AA	1512	A

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Mol	Chain	Res	Type
80	AA	1519	A
80	AA	1522	U
80	AA	1525	C
80	AA	1526	U
80	AA	1527	A
80	AA	1533	C
80	AA	1535	U
80	AA	1537	C
80	AA	1538	G
80	AA	1539	C
80	AA	1540	A
80	AA	1551	G
80	AA	1557	A
80	AA	1562	G
80	AA	1568	U
80	AA	1571	U
80	AA	1582	G
80	AA	1584	MA6
80	AA	1594	G
80	AA	1595	G
80	AA	1599	A
84	Ax	9	C
84	Ax	13	U
84	Ax	16	A
84	Ax	17	U
84	Ax	18	A
84	Ax	22	U
84	Ax	43	A
84	Ax	44	U
84	Ax	47	U
84	Ax	50	U
84	Ax	51	U
84	Ax	52	A
84	Ax	56	C
84	Ax	63	G
84	Ax	65	A
84	Ax	71	A
85	Aw	9	A
85	Aw	13	U
85	Aw	14	A
85	Aw	15	A
85	Aw	16	A

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Mol	Chain	Res	Type
85	Aw	21	A
85	Aw	46	A
85	Aw	49	U
85	Aw	51	U
85	Aw	52	G
85	Aw	53	A
85	Aw	54	U
85	Aw	56	A
85	Aw	63	A
85	Aw	65	A
85	Aw	68	U
85	Aw	69	A
85	Aw	71	C
85	Aw	72	A
85	Aw	74	C
85	Aw	75	C
90	B	8	U
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 (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	2245	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PSU	A	3067	11	18,21,22	1.13	2 (11%)	21,30,33	0.84	1 (4%)
11	1MA	A	2617	11	21,25,26	0.44	0	30,37,40	0.64	0
80	MA6	AA	1584	80	23,26,27	0.33	0	33,38,41	0.74	1 (3%)
90	2MG	B	10	90	23,26,27	0.35	0	33,38,41	0.45	0
80	5MC	AA	1488	80	19,22,23	0.92	1 (5%)	26,32,35	0.50	0
11	OMG	A	3040	11,85	23,26,27	0.37	0	32,38,41	0.37	0
80	B8T	AA	1486	95,80	19,22,23	0.41	0	25,31,34	0.31	0
11	OMU	A	3039	11,92	19,22,23	0.32	0	25,31,34	0.62	1 (4%)
90	PSU	B	39	90	18,21,22	1.05	1 (5%)	21,30,33	0.72	0
80	MA6	AA	1583	80	23,26,27	0.35	0	33,38,41	0.78	1 (3%)
80	5MU	AA	1076	80	19,22,23	0.41	0	27,32,35	0.65	0
11	OMG	A	2815	11,84,92	23,26,27	0.39	0	32,38,41	0.41	0
90	1MA	B	9	90	21,25,26	0.40	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
11	PSU	A	3067	11	-	0/7/25/26	0/2/2/2
11	1MA	A	2617	11	-	0/7/25/26	0/3/3/3
80	MA6	AA	1584	80	-	1/11/29/30	0/3/3/3
90	2MG	B	10	90	-	0/9/27/28	0/3/3/3
80	5MC	AA	1488	80	-	0/7/25/26	0/2/2/2
11	OMG	A	3040	11,85	-	0/9/27/28	0/3/3/3
80	B8T	AA	1486	95,80	-	0/7/27/28	0/2/2/2
11	OMU	A	3039	11,92	-	0/9/27/28	0/2/2/2
90	PSU	B	39	90	-	0/7/25/26	0/2/2/2
80	MA6	AA	1583	80	-	0/11/29/30	0/3/3/3
80	5MU	AA	1076	80	-	5/7/25/26	0/2/2/2
11	OMG	A	2815	11,84,92	-	1/9/27/28	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)
80	AA	1488	5MC	C5-C4	-3.64	1.41	1.44
90	B	39	PSU	C6-C5	3.58	1.39	1.35
11	A	3067	PSU	C6-C5	3.40	1.39	1.35
11	A	3067	PSU	O4'-C1'	-2.66	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	AA	1583	MA6	C2-N1-C6	3.03	119.22	111.83
80	AA	1584	MA6	C2-N1-C6	2.92	118.97	111.83
11	A	3067	PSU	O4'-C1'-C2'	2.59	108.73	105.15
11	A	3039	OMU	C2'-C1'-N1	-2.38	109.72	114.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2815	OMG	C1'-C2'-O2'-CM2
80	AA	1076	5MU	O4'-C4'-C5'-O5'
80	AA	1076	5MU	C3'-C4'-C5'-O5'
80	AA	1584	MA6	C4'-C5'-O5'-P
80	AA	1076	5MU	C4'-C5'-O5'-P
80	AA	1076	5MU	C2'-C1'-N1-C2
80	AA	1076	5MU	C2'-C1'-N1-C6

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	3067	PSU	1	0
80	AA	1488	5MC	1	0
80	AA	1486	B8T	1	0
90	B	39	PSU	1	0
80	AA	1583	MA6	1	0
80	AA	1076	5MU	1	0
11	A	2815	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 279 ligands modelled in this entry, 261 are monoatomic - leaving 18 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
93	SPD	AA	1783	93	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	AA	1703	-	9,9,9	0.15	0	8,8,8	0.24	0
93	SPD	A	3470	-	9,9,9	0.17	0	8,8,8	0.22	0
98	SPM	AA	1780	-	13,13,13	0.17	0	12,12,12	0.22	0
93	SPD	A	3302	-	9,9,9	0.16	0	8,8,8	0.20	0
100	GDP	AX	503	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	8 (17%)
96	FES	r	201	49,17	0,4,4	-	-	-	-	-
96	FES	AT	201	64,70	0,4,4	-	-	-	-	-
101	VAL	B	101	90	4,6,7	0.83	0	6,7,9	1.03	1 (16%)
99	ATP	AX	501	95	32,33,33	0.59	1 (3%)	48,52,52	0.36	0
94	PUT	A	3303	-	5,5,5	0.13	0	4,4,4	0.25	0
93	SPD	A	3301	-	9,9,9	0.18	0	8,8,8	0.23	0
93	SPD	A	3471	-	9,9,9	0.15	0	8,8,8	0.33	0
93	SPD	AA	1782	93	9,9,9	0.15	0	8,8,8	0.17	0
96	FES	AP	201	67,57	0,4,4	-	-	-	-	-
98	SPM	AA	1702	-	13,13,13	0.18	0	12,12,12	0.27	0
93	SPD	O	301	-	9,9,9	0.17	0	8,8,8	0.20	0
97	NAD	AA	1701	95	46,48,48	1.15	3 (6%)	64,73,73	0.86	3 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	SPD	AA	1783	93	-	1/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	SPD	AA	1703	-	-	0/7/7/7	-
93	SPD	A	3470	-	-	0/7/7/7	-
98	SPM	AA	1780	-	-	0/11/11/11	-
93	SPD	A	3302	-	-	1/7/7/7	-
100	GDP	AX	503	-	-	1/16/32/32	0/3/3/3
96	FES	r	201	49,17	-	-	0/1/1/1
96	FES	AT	201	64,70	-	-	0/1/1/1
101	VAL	B	101	90	-	0/5/6/8	-
99	ATP	AX	501	95	-	4/22/38/38	0/3/3/3
94	PUT	A	3303	-	-	0/3/3/3	-
93	SPD	A	3301	-	-	0/7/7/7	-
93	SPD	A	3471	-	-	1/7/7/7	-
93	SPD	AA	1782	93	-	0/7/7/7	-
98	SPM	AA	1702	-	-	0/11/11/11	-
96	FES	AP	201	67,57	-	-	0/1/1/1
93	SPD	O	301	-	-	0/7/7/7	-
97	NAD	AA	1701	95	-	0/30/62/62	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	AA	1701	NAD	PA-O3	4.38	1.64	1.59
100	AX	503	GDP	C5-C4	3.07	1.47	1.38
97	AA	1701	NAD	O4D-C1D	-2.76	1.37	1.40
100	AX	503	GDP	C6-N1	-2.56	1.34	1.38
99	AX	501	ATP	PB-O3B	-2.50	1.56	1.59
97	AA	1701	NAD	PN-O3	2.43	1.62	1.59
100	AX	503	GDP	C5-N7	-2.13	1.34	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
100	AX	503	GDP	C5-C4-N3	-5.96	118.91	128.39
100	AX	503	GDP	C2-N3-C4	4.94	120.81	112.30
100	AX	503	GDP	N9-C4-N3	4.43	134.81	125.95
100	AX	503	GDP	C6-C5-N7	3.28	136.27	130.29
97	AA	1701	NAD	O3-PA-O1A	-2.59	102.92	110.70
100	AX	503	GDP	C4-C5-N7	-2.49	106.72	110.67
100	AX	503	GDP	C3'-C2'-C1'	2.33	105.88	101.46
97	AA	1701	NAD	O2A-PA-O1A	2.20	122.69	112.44
101	B	101	VAL	O-C-CA	-2.19	119.14	124.77
100	AX	503	GDP	O6-C6-C5	-2.13	120.92	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
100	AX	503	GDP	C2'-C1'-N9	-2.11	107.38	113.25
97	AA	1701	NAD	O7N-C7N-N7N	2.07	125.61	122.62

There are no chirality outliers.

All (8) torsion outliers are listed below:

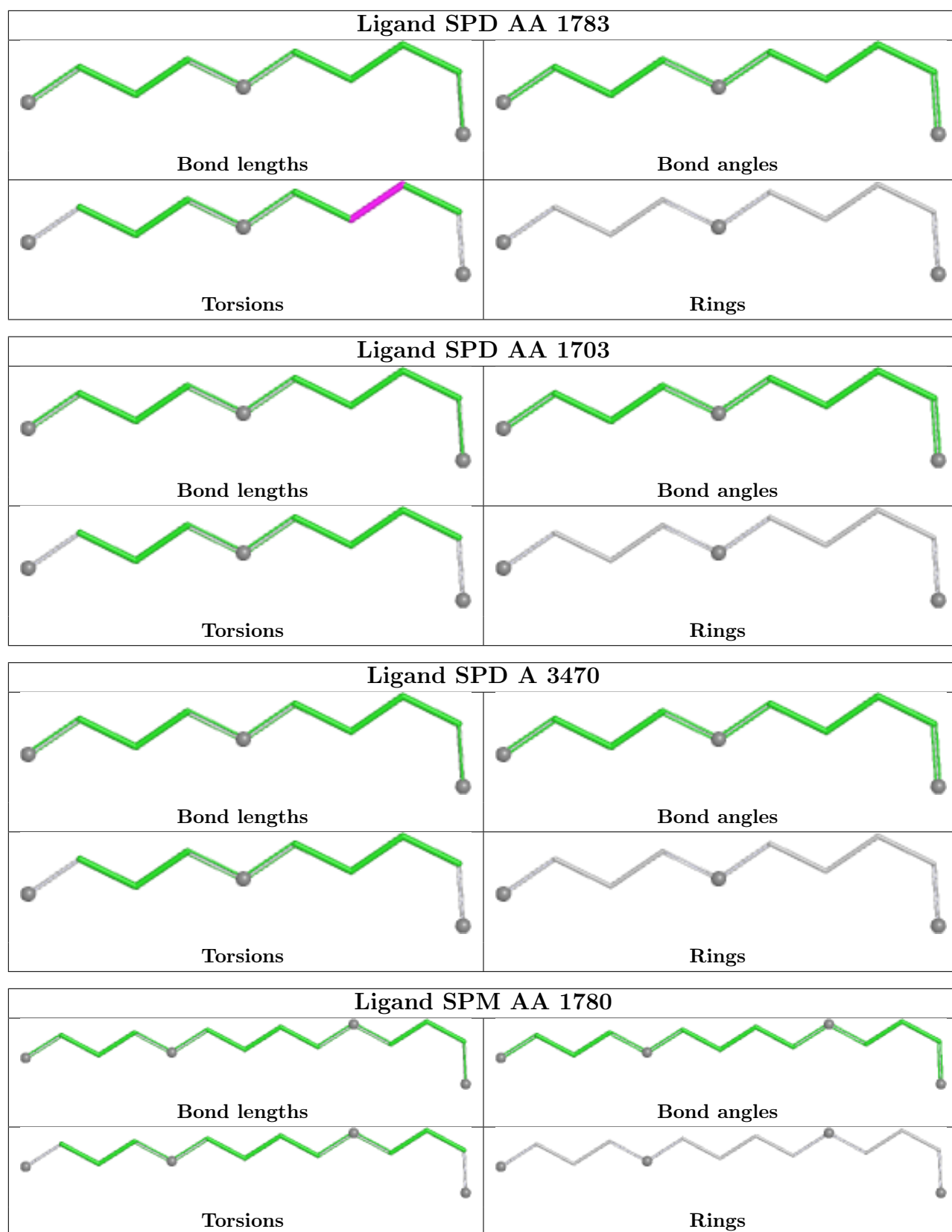
Mol	Chain	Res	Type	Atoms
99	AX	501	ATP	PB-O3B-PG-O2G
99	AX	501	ATP	PB-O3B-PG-O3G
100	AX	503	GDP	C5'-O5'-PA-O1A
93	A	3471	SPD	C2-C3-C4-C5
99	AX	501	ATP	PA-O3A-PB-O1B
93	AA	1783	SPD	C2-C3-C4-C5
93	A	3302	SPD	N1-C2-C3-C4
99	AX	501	ATP	PA-O3A-PB-O2B

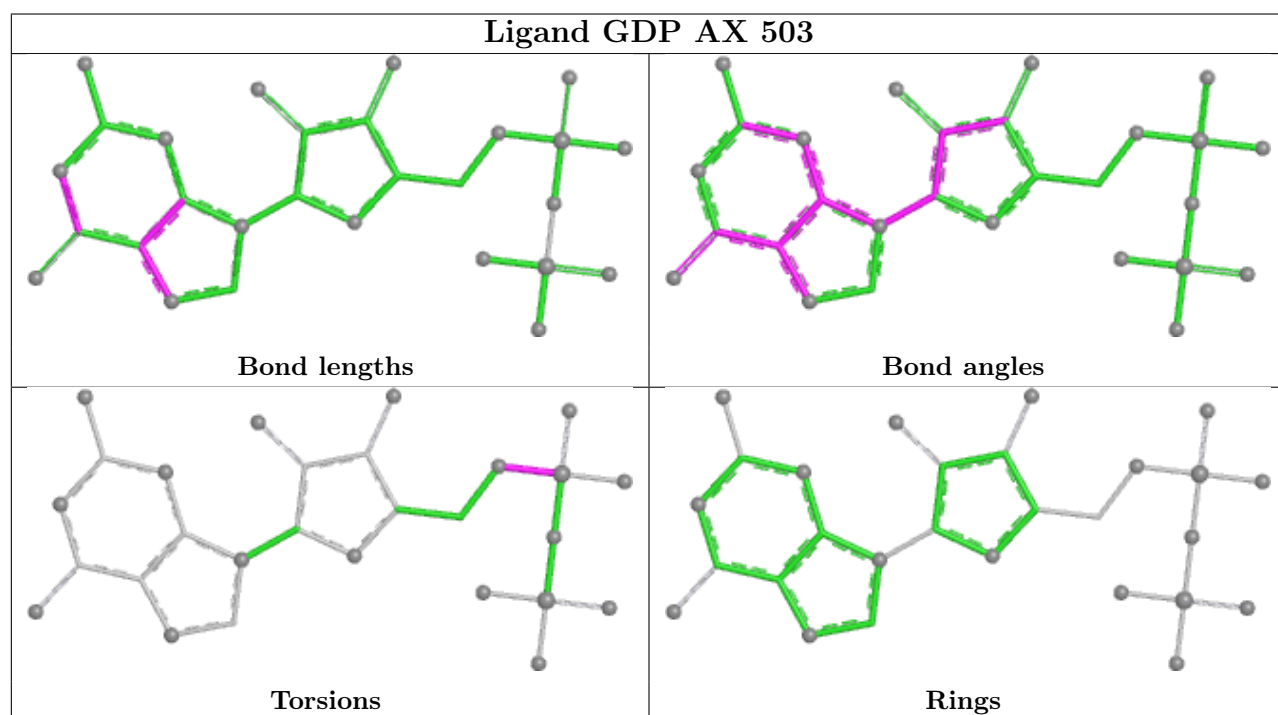
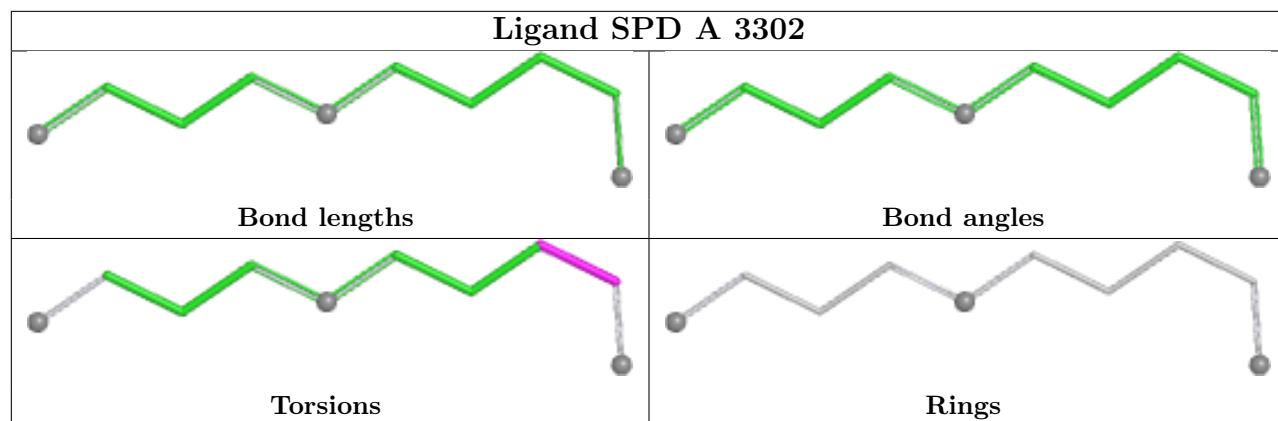
There are no ring outliers.

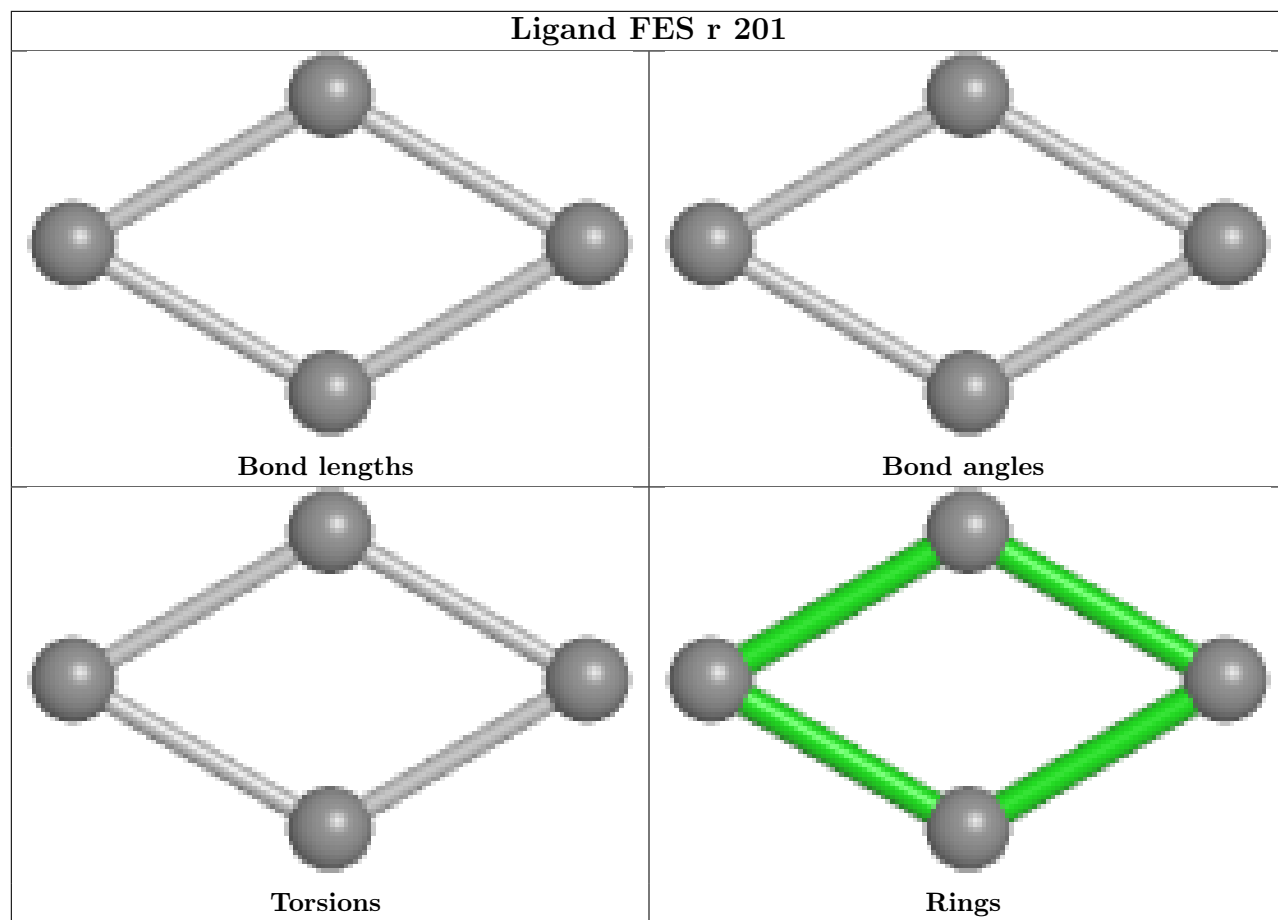
6 monomers are involved in 7 short contacts:

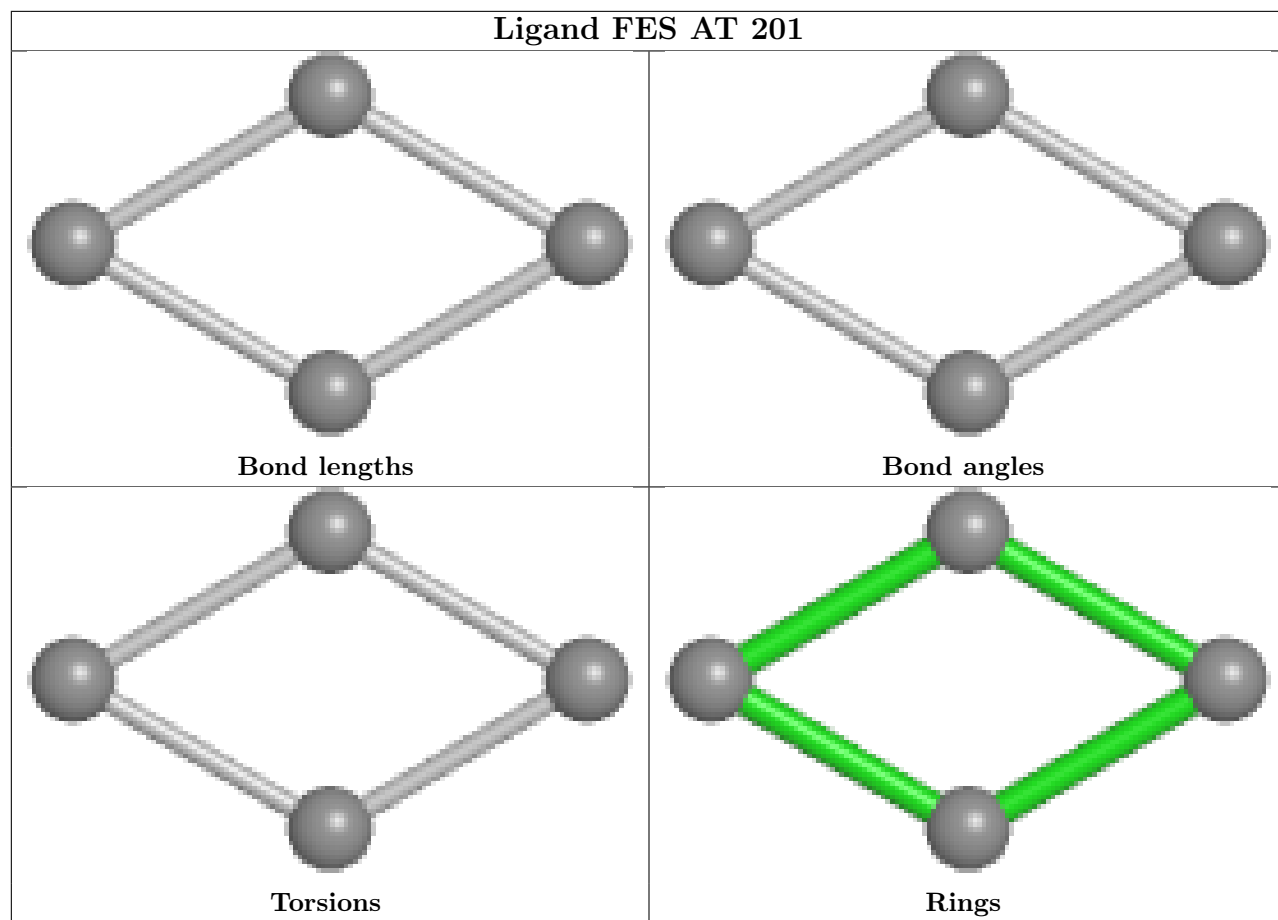
Mol	Chain	Res	Type	Clashes	Symm-Clashes
93	AA	1783	SPD	1	0
93	AA	1703	SPD	1	0
100	AX	503	GDP	1	0
101	B	101	VAL	3	0
93	AA	1782	SPD	1	0
97	AA	1701	NAD	1	0

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

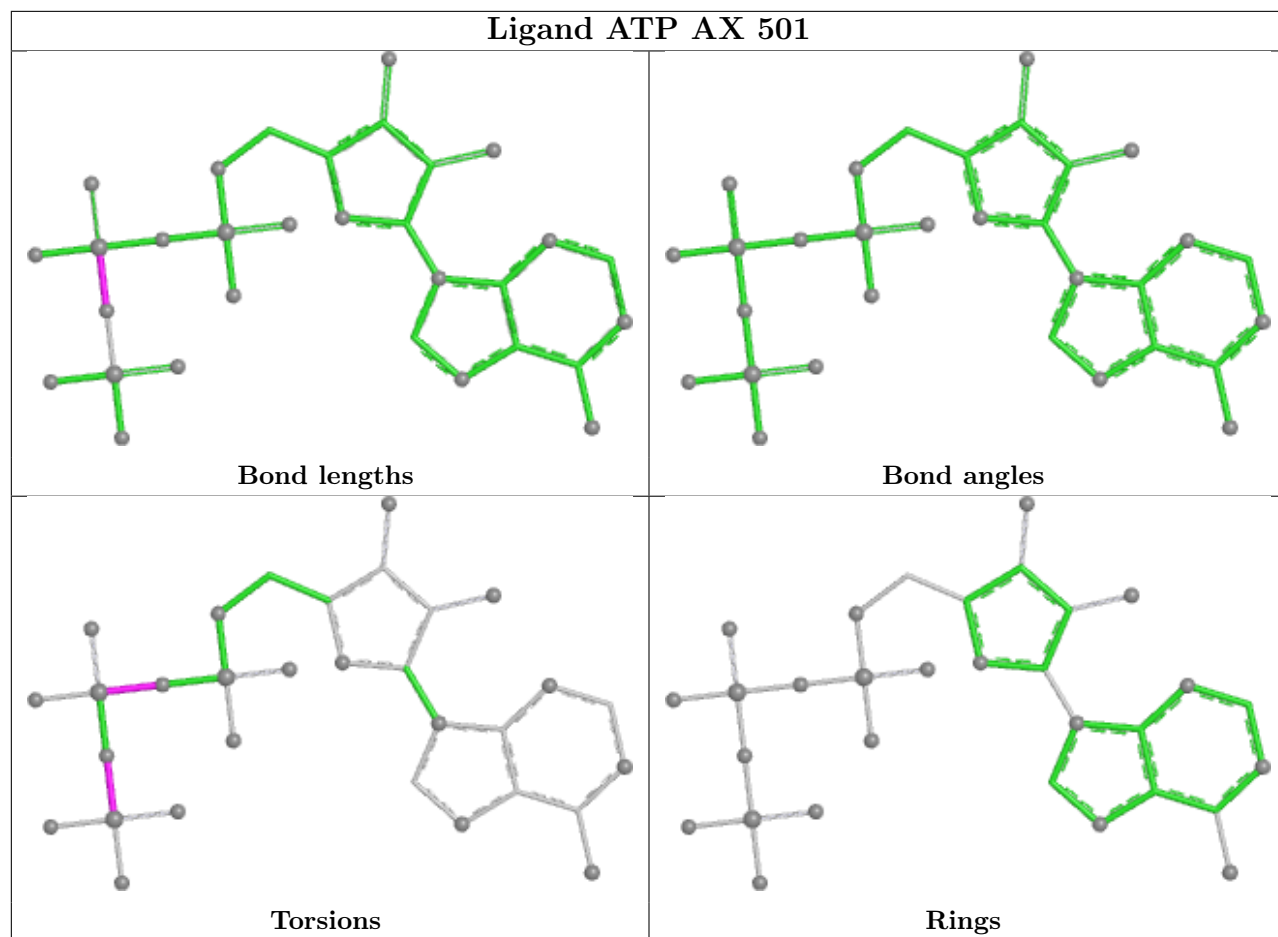




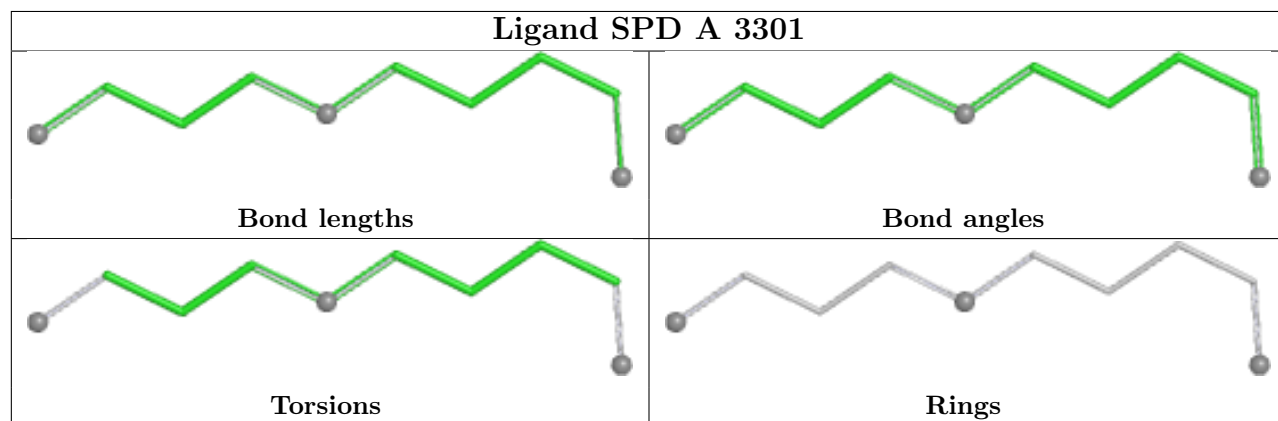




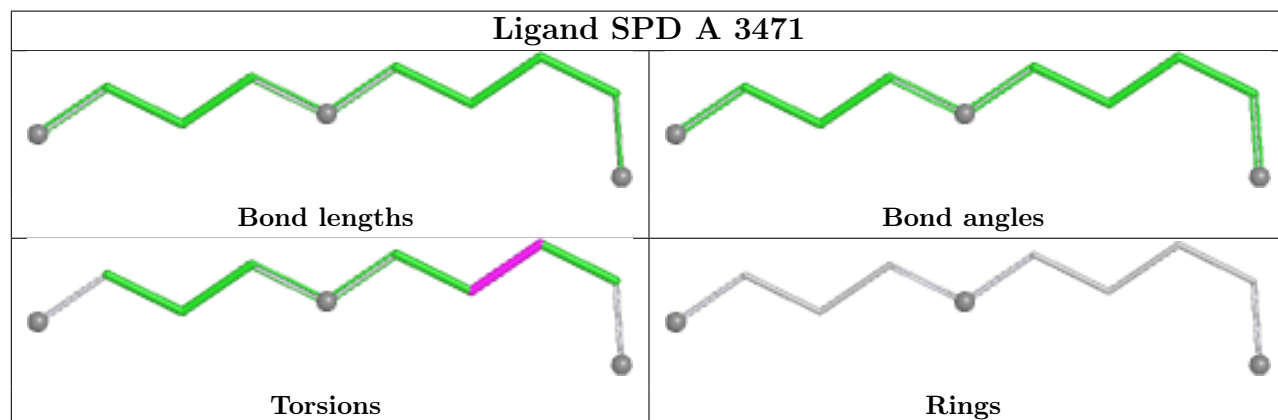
Ligand ATP AX 501

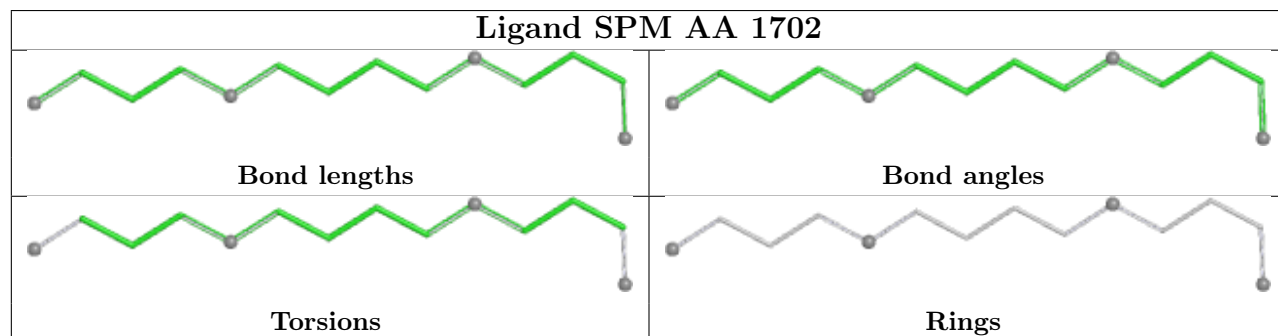
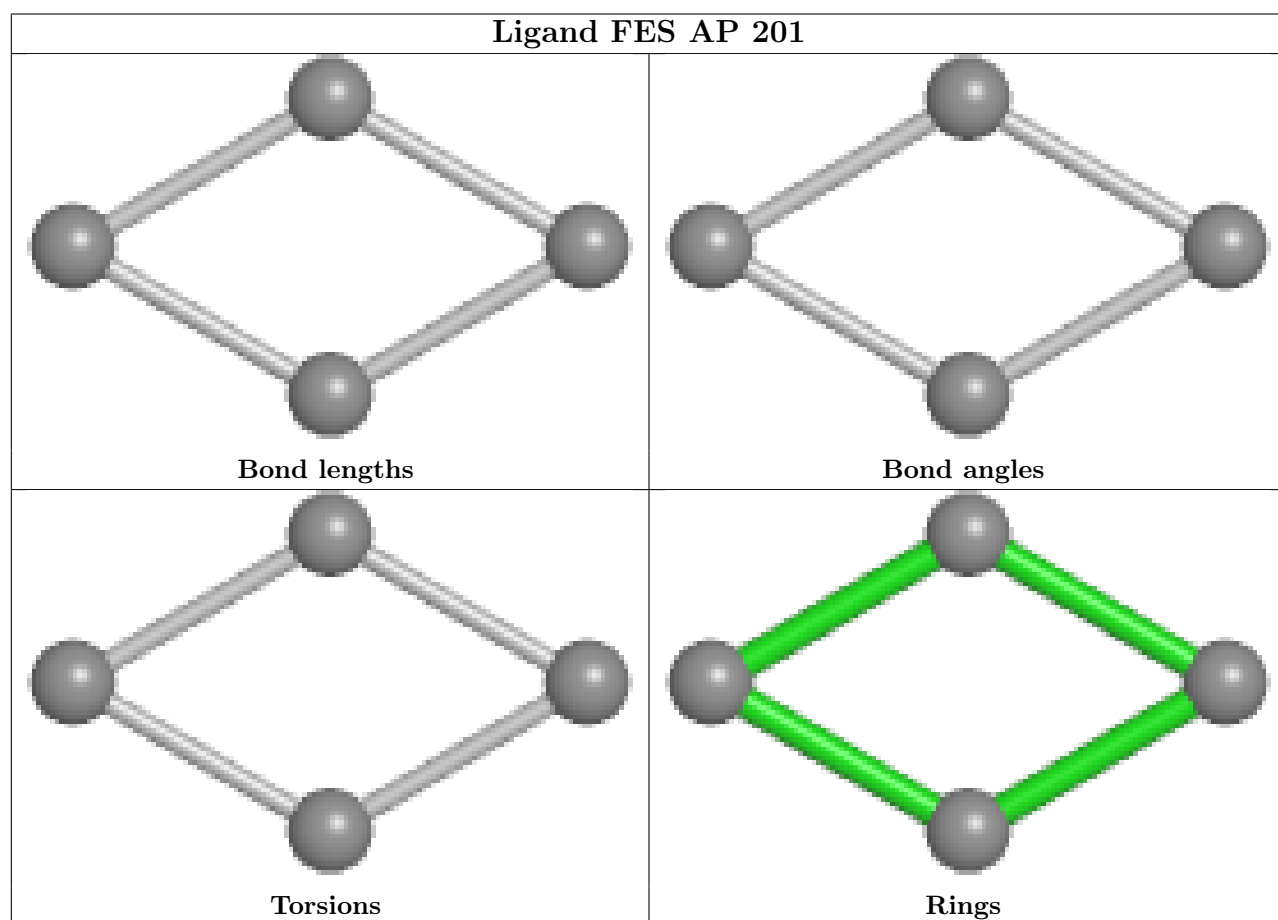
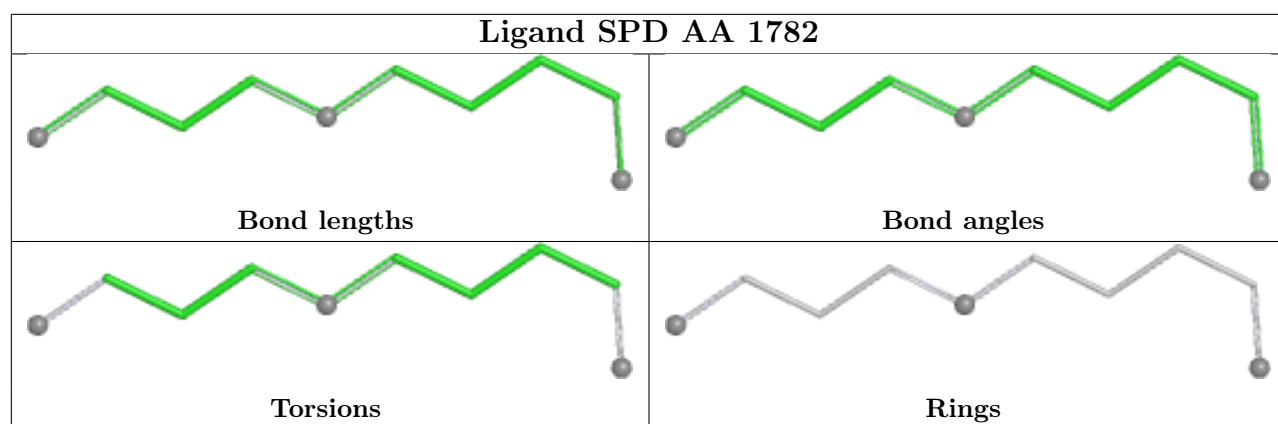


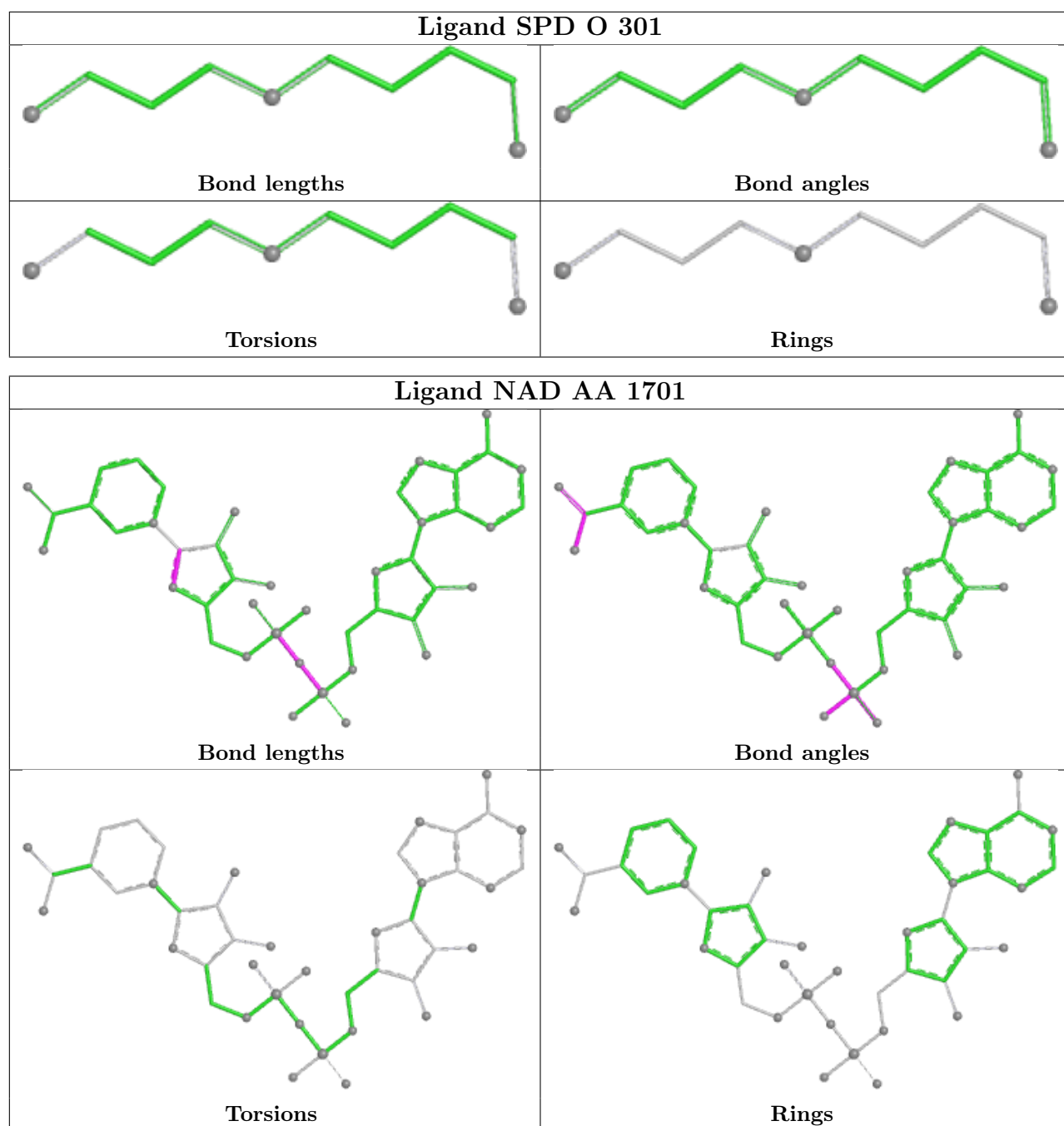
Ligand SPD A 3301



Ligand SPD A 3471







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
90	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	46:A	O3'	48:U	P	4.53

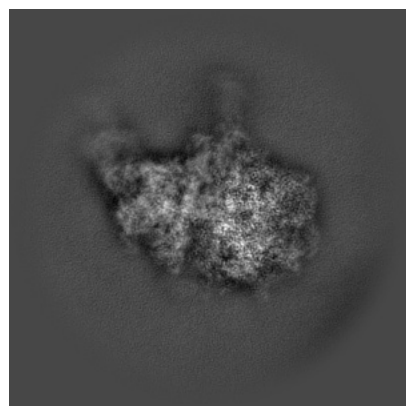
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71634. These allow visual inspection of the internal detail of the map and identification of artifacts.

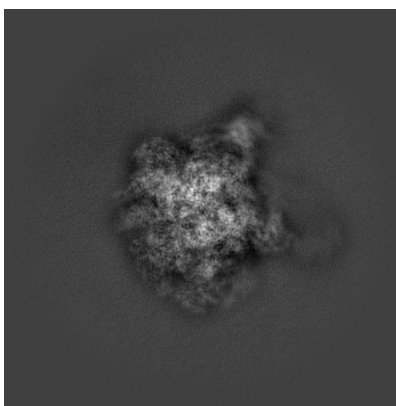
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

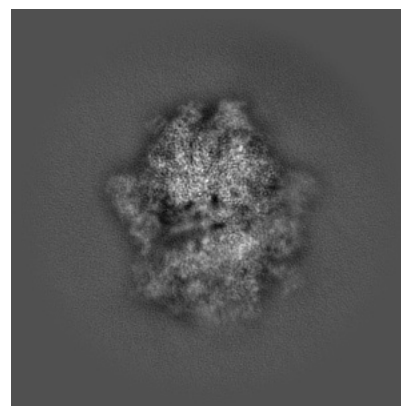
6.1.1 Primary map



X

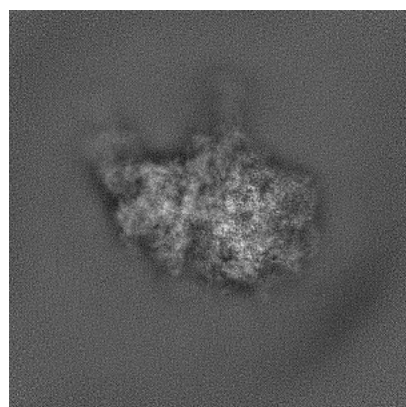


Y

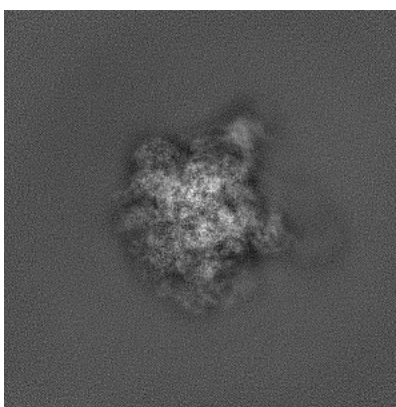


Z

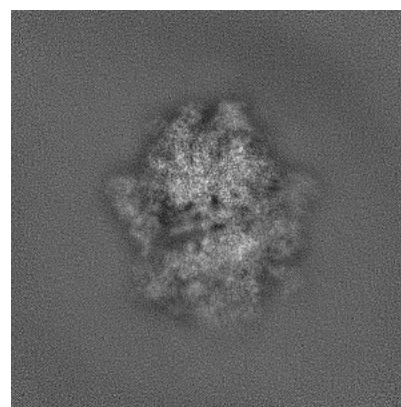
6.1.2 Raw map



X



Y

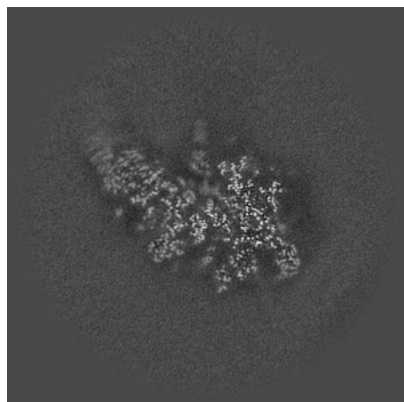


Z

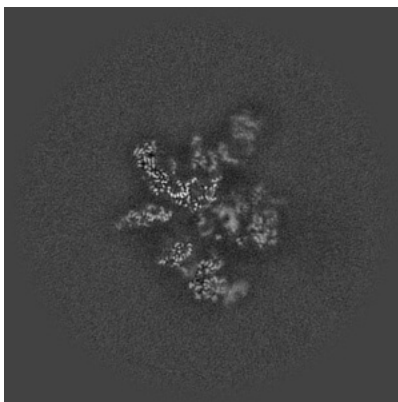
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

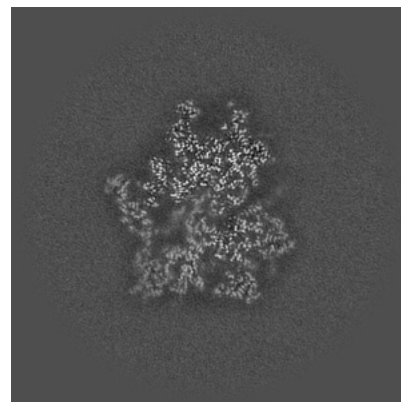
6.2.1 Primary map



X Index: 240

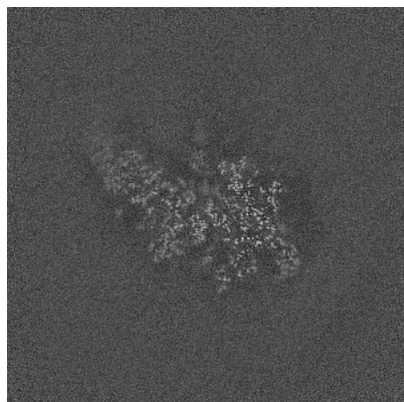


Y Index: 240



Z Index: 240

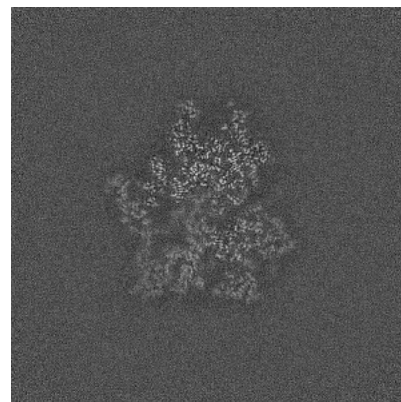
6.2.2 Raw map



X Index: 240



Y Index: 240

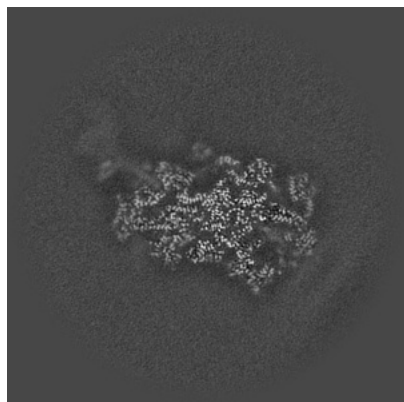


Z Index: 240

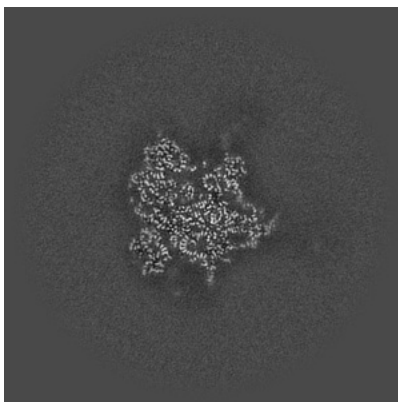
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

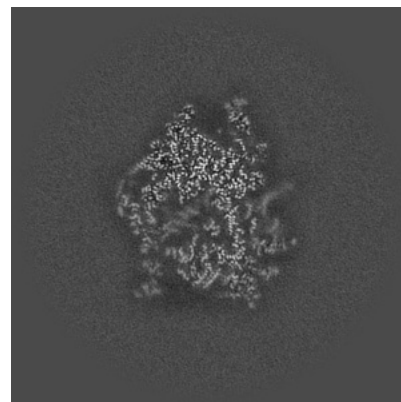
6.3.1 Primary map



X Index: 262

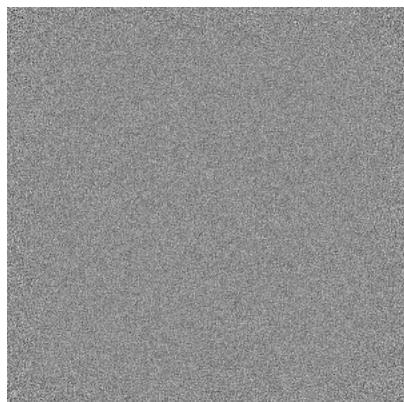


Y Index: 287

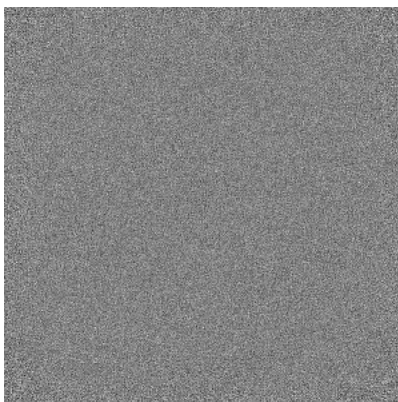


Z Index: 249

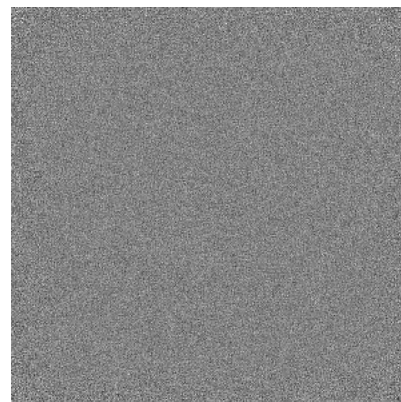
6.3.2 Raw map



X Index: 0



Y Index: 0

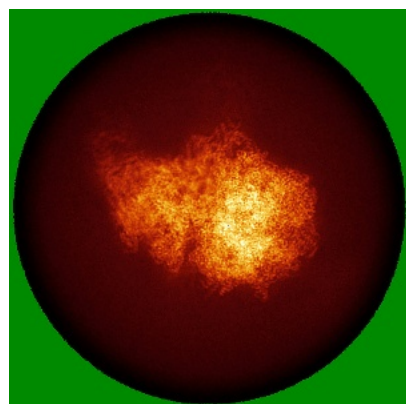


Z Index: 0

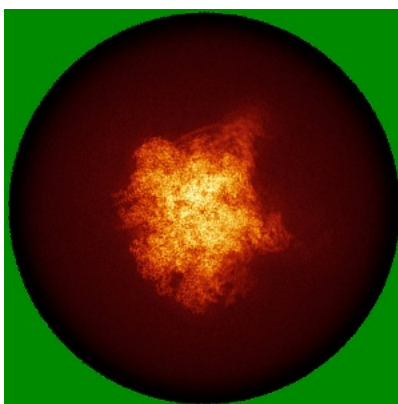
The images above show the largest variance slices of the map in three orthogonal directions.

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

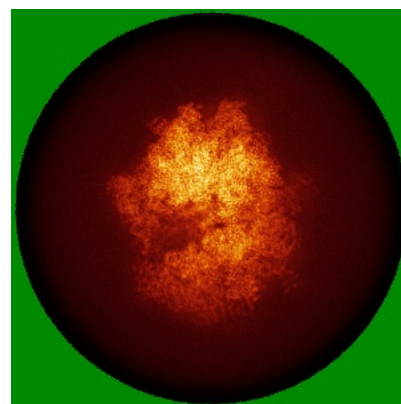
6.4.1 Primary map



X

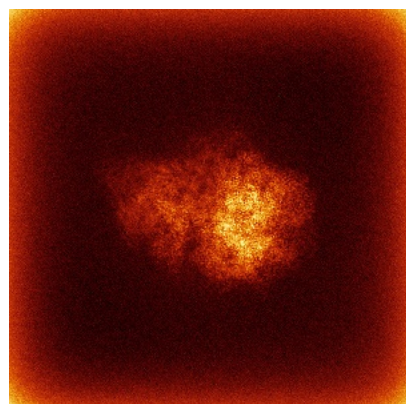


Y

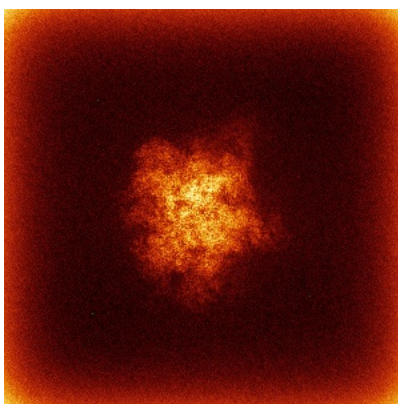


Z

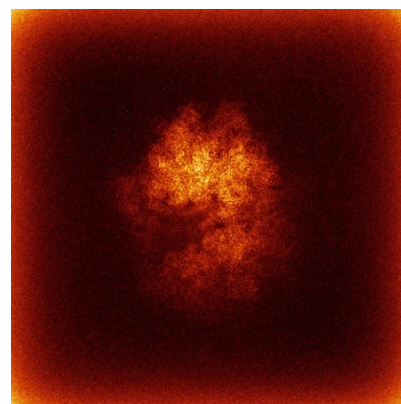
6.4.2 Raw map



X



Y

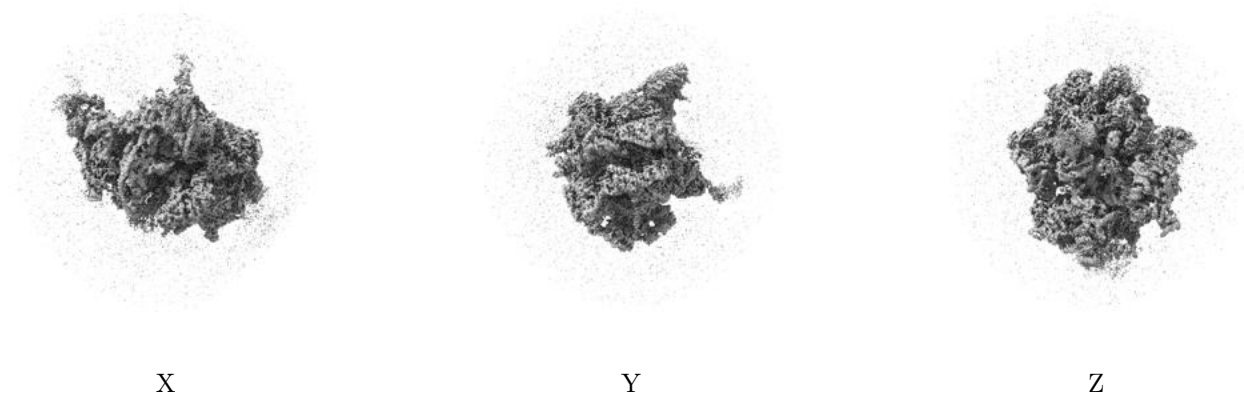


Z

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

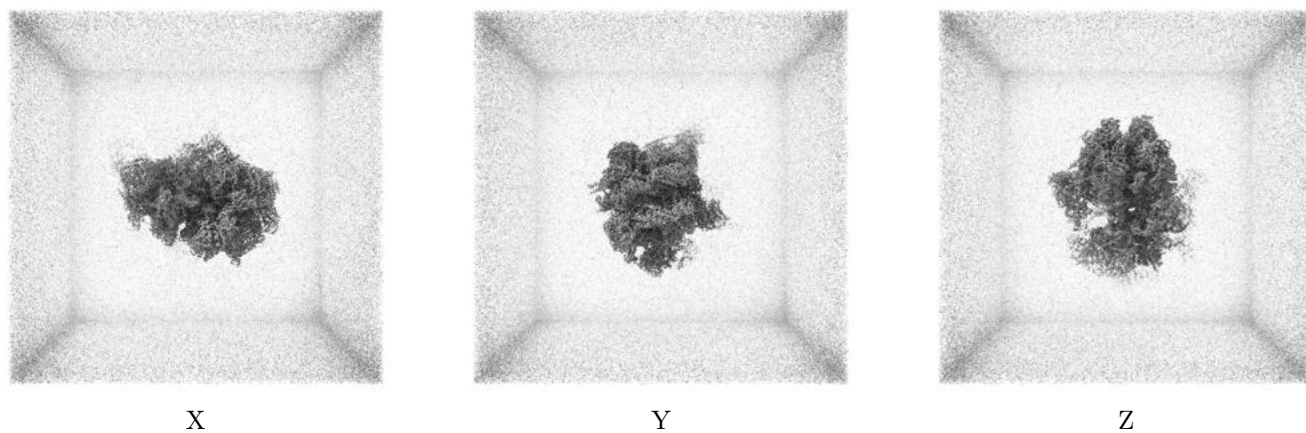
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

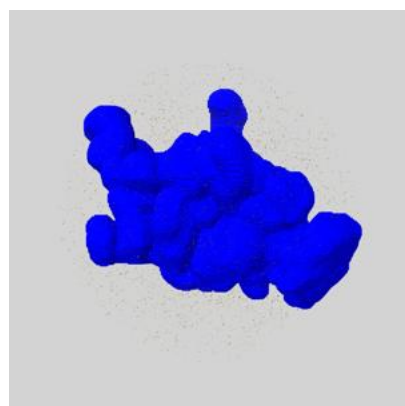
6.6 Mask visualisation [i](#)

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

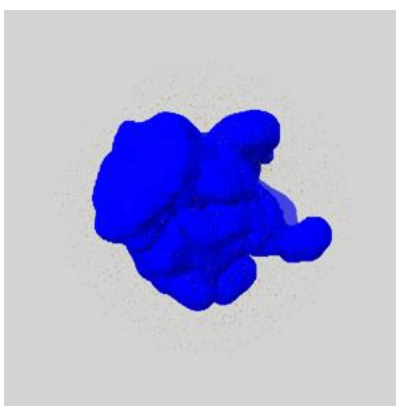
A mask typically either:

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

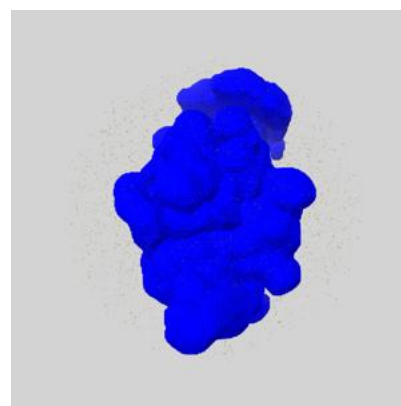
6.6.1 emd_71634_msk_1.map [i](#)



X



Y

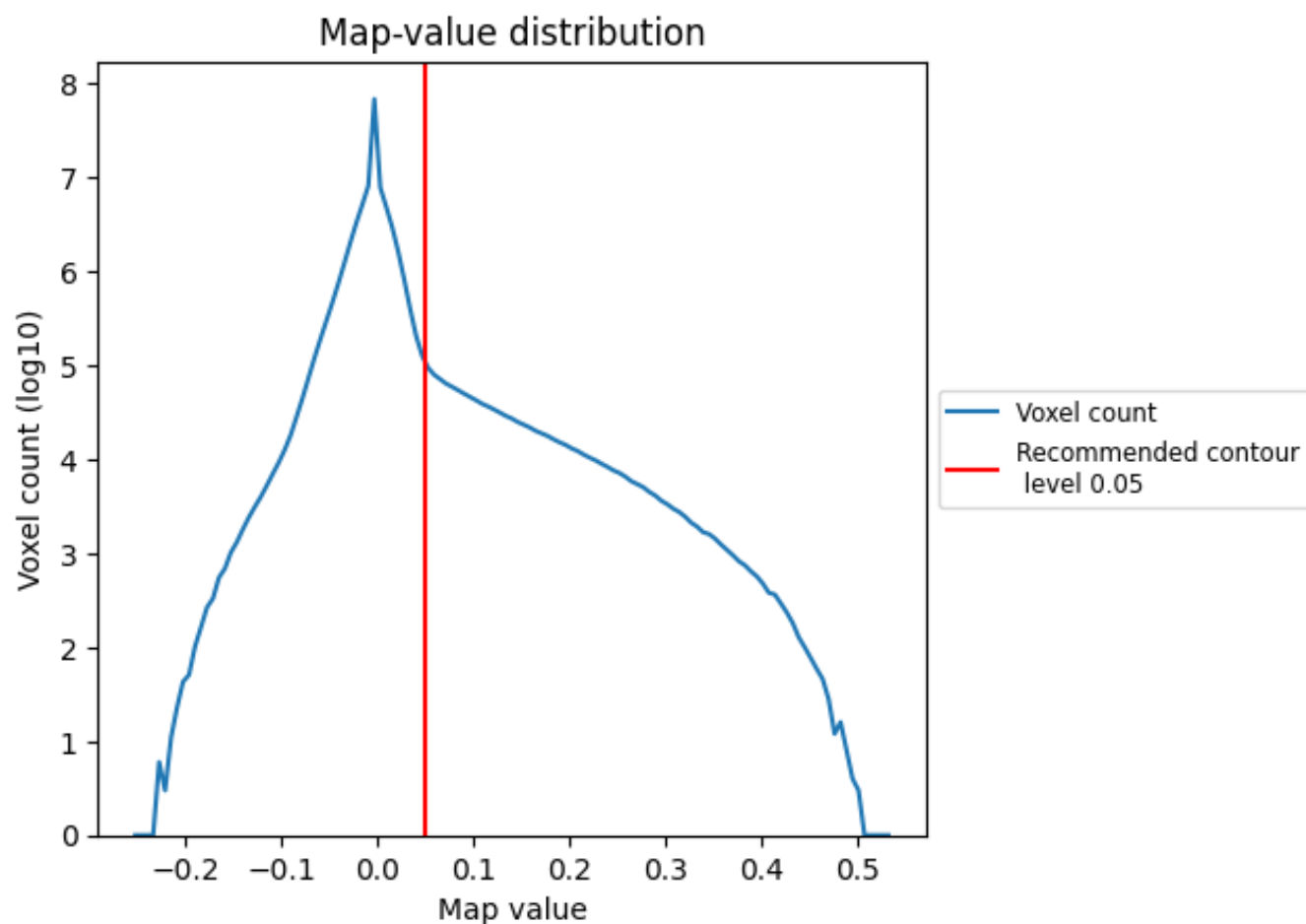


Z

7 Map analysis [i](#)

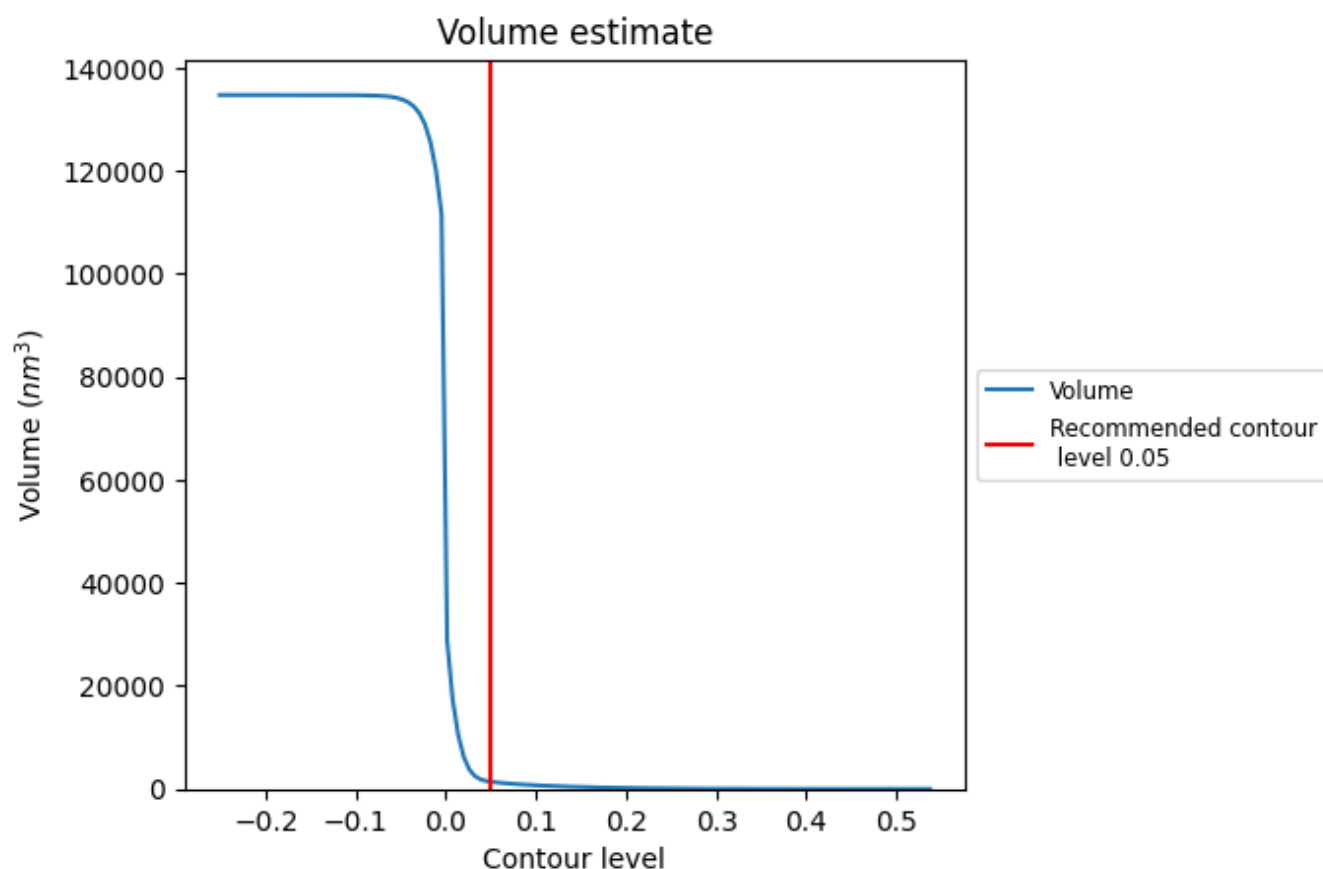
This section contains the results of statistical analysis of the map.

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.

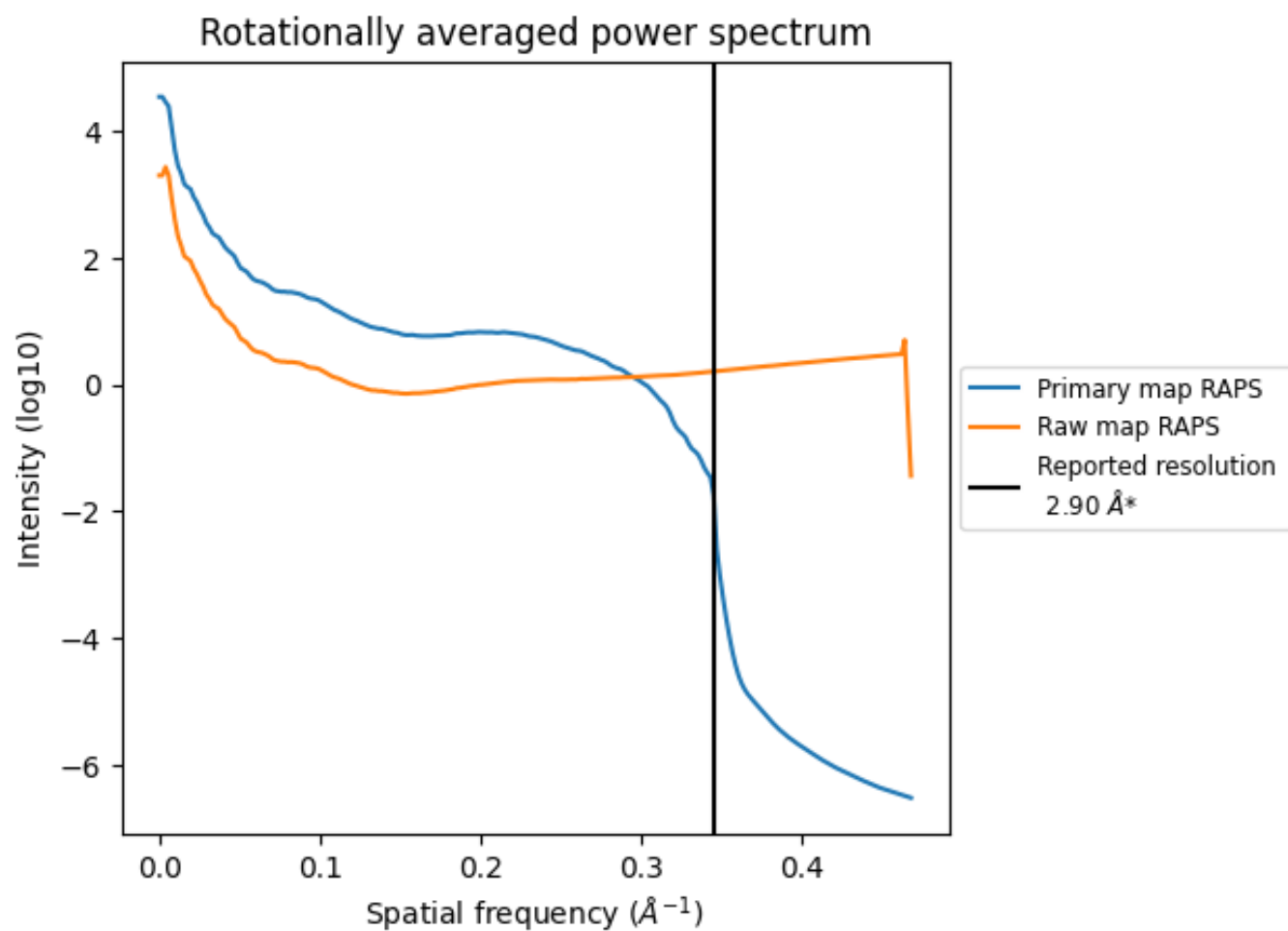
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1397 nm^3 ; this corresponds to an approximate mass of 1262 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 ⓘ

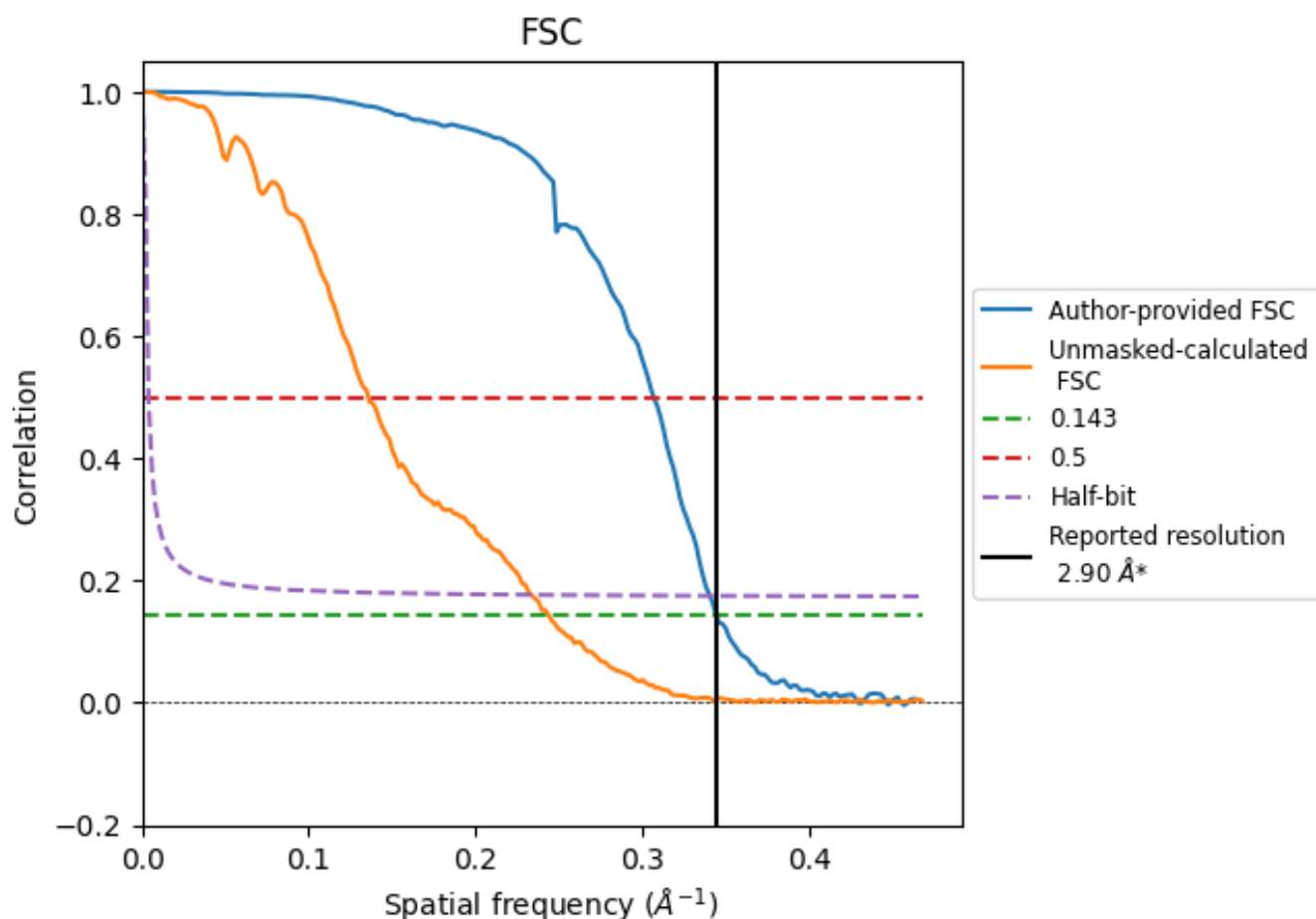


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

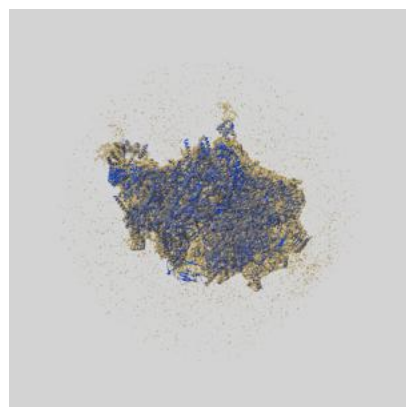
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.26	2.94
Unmasked-calculated*	4.10	7.36	4.28

*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 4.10 differs from the reported value 2.9 by more than 10 %

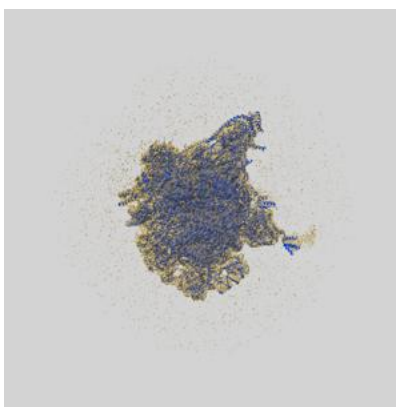
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71634 and PDB model 9PGL. Per-residue inclusion information can be found in section 3 on page 27.

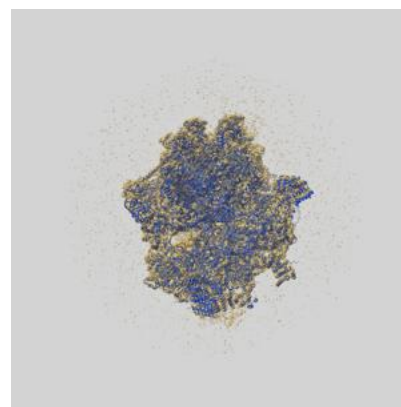
9.1 Map-model overlay [i](#)



X



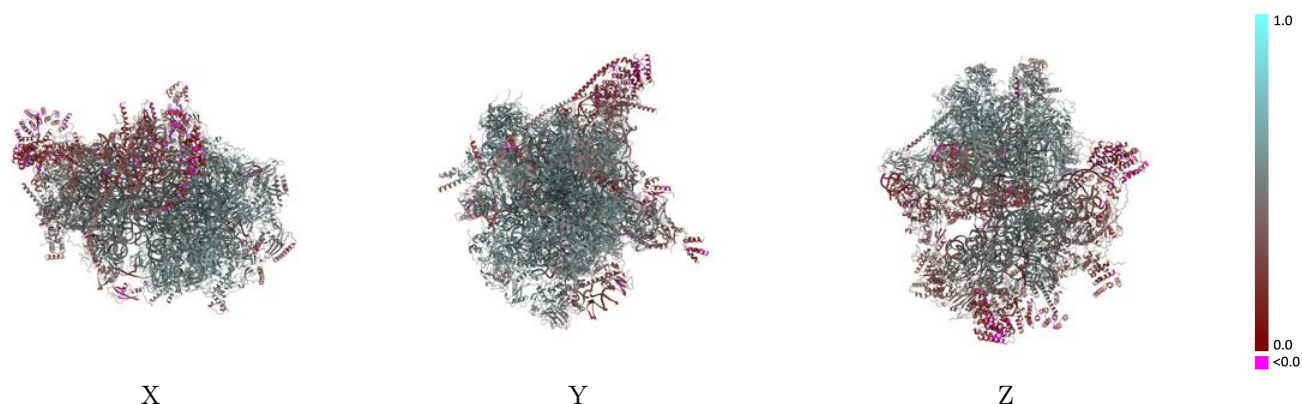
Y



Z

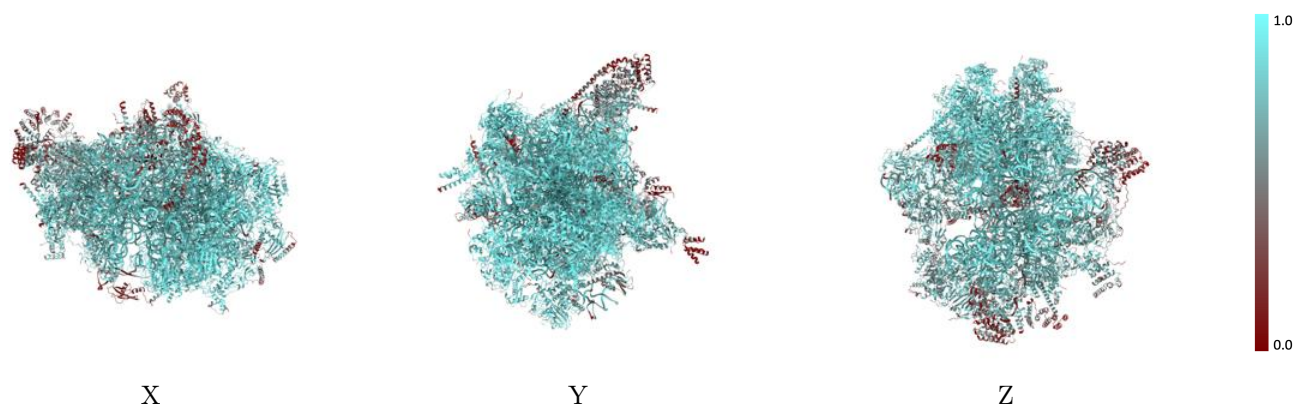
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



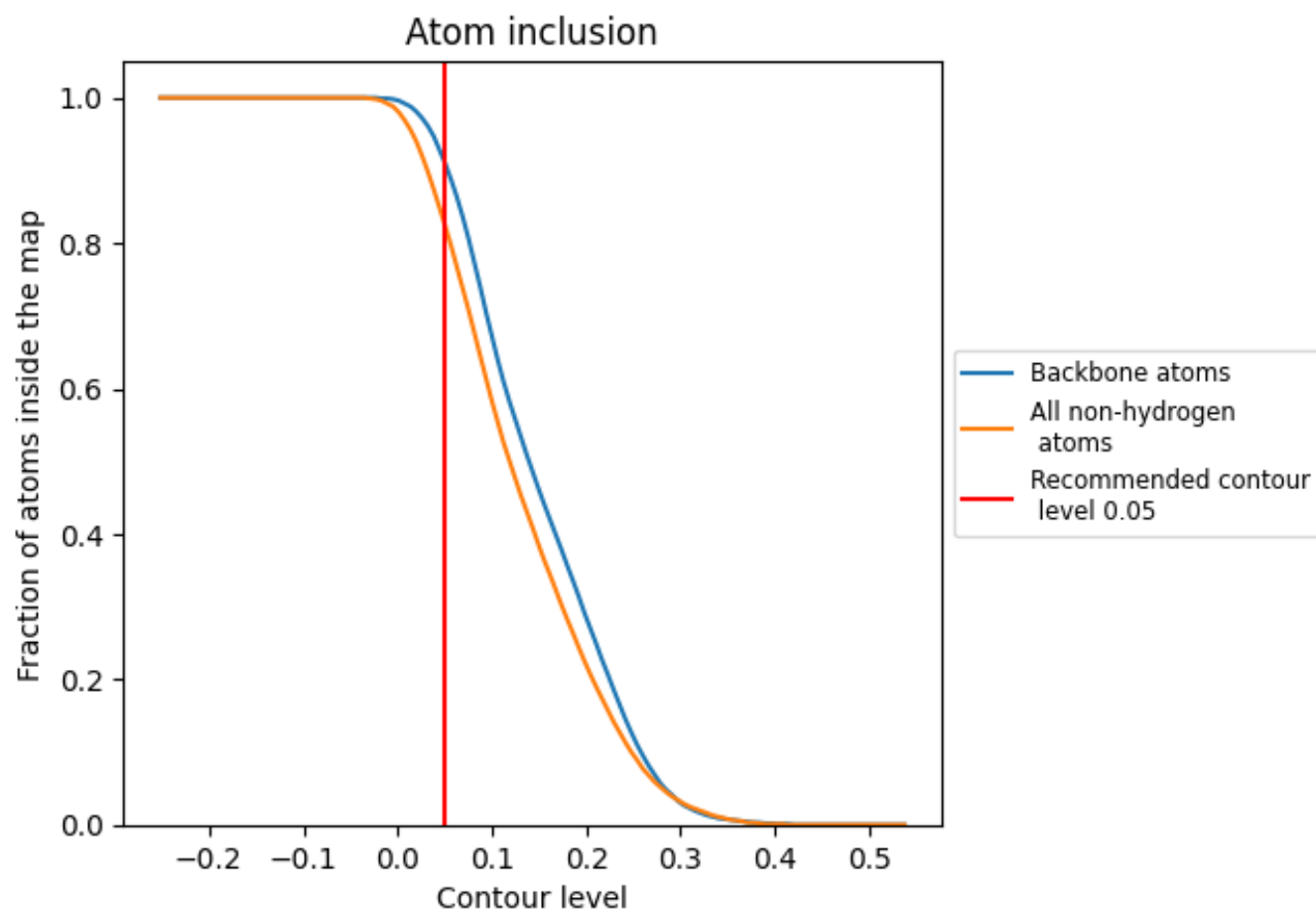
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 83% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8260	 0.4620
0	 0.9090	 0.5480
1	 0.8600	 0.5220
2	 0.9720	 0.5840
3	 0.9560	 0.5810
4	 0.9360	 0.5720
5	 0.8980	 0.5370
6	 0.8410	 0.4840
7	 0.8460	 0.4880
8	 0.6470	 0.3570
9	 0.8830	 0.5260
A	 0.9600	 0.5320
A0	 0.5230	 0.2540
A1	 0.6890	 0.3750
A2	 0.7490	 0.4560
A3	 0.8540	 0.5090
A4	 0.4260	 0.2120
AA	 0.9590	 0.4720
AB	 0.8170	 0.4690
AC	 0.7980	 0.4770
AD	 0.7580	 0.4510
AE	 0.8300	 0.5060
AF	 0.7890	 0.4410
AG	 0.7390	 0.4260
AH	 0.7130	 0.4160
AI	 0.8340	 0.5000
AJ	 0.8110	 0.5010
AK	 0.8520	 0.4630
AL	 0.7640	 0.4480
AM	 0.6530	 0.3140
AN	 0.7610	 0.4650
AO	 0.6700	 0.3470
AP	 0.8340	 0.4930
AQ	 0.8770	 0.5130
AR	 0.5990	 0.2850



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Chain	Atom inclusion	Q-score
AS	 0.7530	 0.4060
AT	 0.7680	 0.4250
AU	 0.6660	 0.3370
AV	 0.3380	 0.1480
AW	 0.7600	 0.4690
AX	 0.7210	 0.3760
AY	 0.6270	 0.3430
AZ	 0.7410	 0.3900
Aw	 0.9340	 0.3310
Ax	 0.8800	 0.3950
Az	 0.5520	 0.2860
B	 0.7790	 0.2580
C	 0.4220	 0.3210
D	 0.9360	 0.5690
E	 0.9240	 0.5550
F	 0.9420	 0.5650
G	 0.2170	 0.2090
H	 0.4320	 0.3100
I	 0.7170	 0.4020
J	 0.6580	 0.3430
K	 0.9440	 0.5630
L	 0.9250	 0.5550
M	 0.9180	 0.5530
N	 0.9030	 0.5500
O	 0.9310	 0.5530
OX	 0.5700	 0.3400
P	 0.8970	 0.5280
Q	 0.8360	 0.5200
R	 0.9360	 0.5660
S	 0.9070	 0.5570
T	 0.9340	 0.5740
U	 0.8250	 0.5090
V	 0.8640	 0.5090
W	 0.9250	 0.5670
X	 0.8790	 0.5310
Y	 0.9140	 0.5470
Z	 0.9170	 0.5620
a	 0.7810	 0.4810
b	 0.9280	 0.5620
c	 0.8840	 0.5220
d	 0.7390	 0.4570
e	 0.5990	 0.3060

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Chain	Atom inclusion	Q-score
f	 0.7060	 0.4020
g	 0.9040	 0.5480
h	 0.8470	 0.4870
i	 0.9490	 0.5760
j	 0.8570	 0.5030
k	 0.7570	 0.4200
l	 0.6730	 0.3720
m	 0.6130	 0.3380
n	 0.5260	 0.3310
o	 0.9480	 0.5750
p	 0.7660	 0.4690
q	 0.6550	 0.3880
r	 0.9130	 0.5380
s	 0.8990	 0.5410
t	 0.2270	 0.2060
u	 0.1910	 0.2060