



Full wwPDB EM Validation Report ⓘ

Sep 21, 2026 – 03:19 am BST

PDB ID : 9SL3 / pdb_00009sl3
EMDB ID : EMD-54983
Title : Human mitoribosome bound to TACO1 (domain 1 ordered), mRNA, A/A-,
P/P- and E/E-tRNAs
Authors : Singh, V.; Khawaja, A.; Rorbach, J.
Deposited on : 2025-09-02
Resolution : 4.05 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

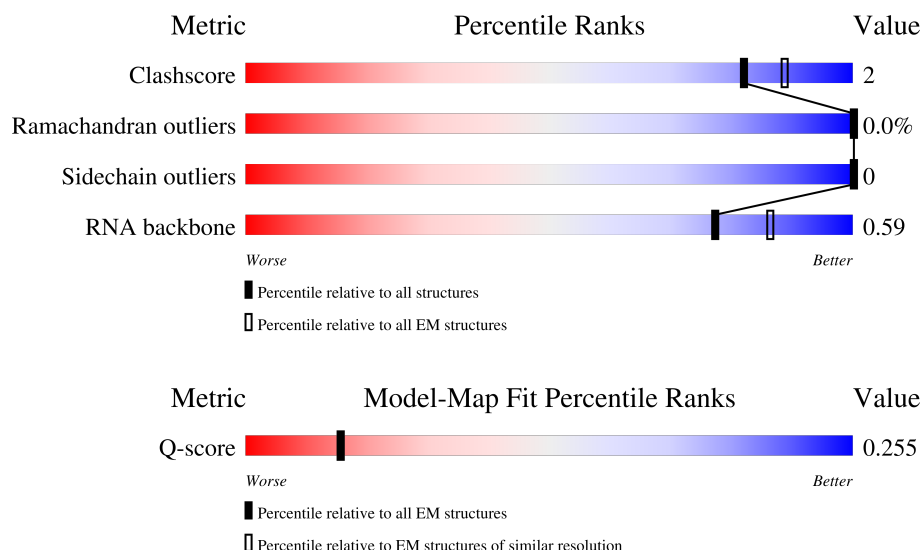
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.05 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6569 (3.55 - 4.55)

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

Mol	Chain	Length	Quality of chain
1	A5	297	
2	AA	954	
3	AB	296	

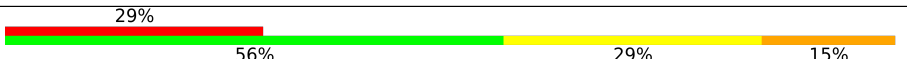
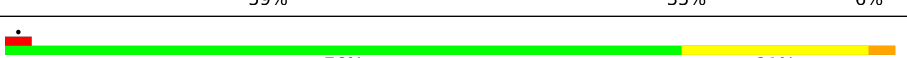
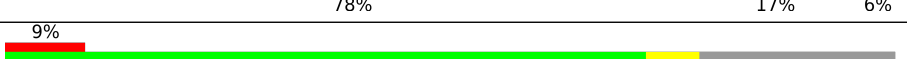
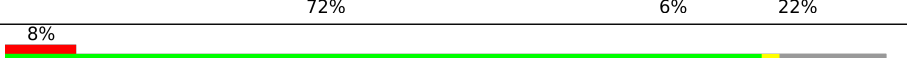
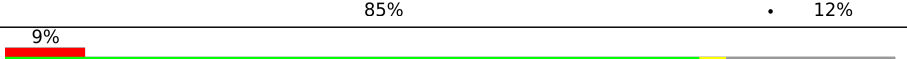
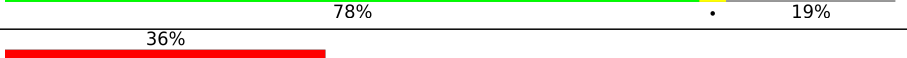
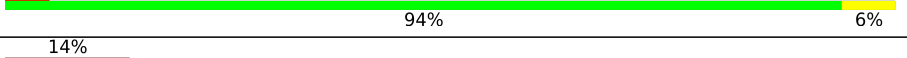
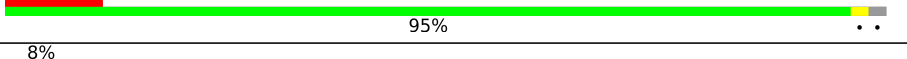
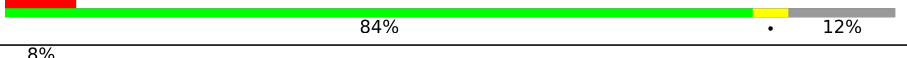
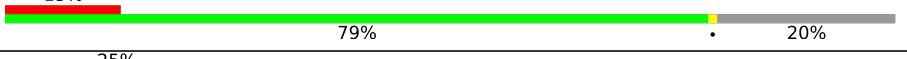
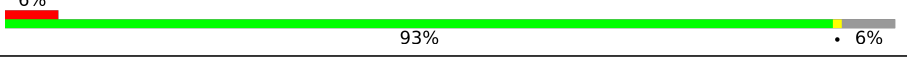
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Mol	Chain	Length	Quality of chain
4	AC	167	
5	AD	430	
6	AE	125	
7	AF	242	
8	AG	396	
9	AH	201	
10	AI	194	
11	AJ	138	
12	AK	128	
13	AL	257	
14	AM	137	
15	AN	130	
16	AO	258	
17	AP	142	
18	AQ	87	
19	AR	360	
20	AS	190	
21	AT	173	
22	AU	205	
23	AV	414	
24	AW	187	
25	AX	398	
26	AY	395	
27	AZ	106	
28	A0	217	

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Mol	Chain	Length	Quality of chain
29	A1	323	
30	A2	118	
31	A3	199	
32	A4	689	
33	Aw	68	
34	Ax	70	
35	Ay	70	
36	Az	34	
37	A	1561	
38	B	72	
39	D	305	
40	E	348	
41	F	311	
42	I	261	
43	J	192	
44	K	178	
45	L	145	
46	M	296	
47	N	251	
48	O	175	
49	P	180	
50	Q	292	
51	R	149	
52	S	205	
53	T	206	

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Mol	Chain	Length	Quality of chain
54	U	153	
55	V	216	
56	W	148	
57	X	256	
58	Y	250	
59	Z	161	
60	0	188	
61	1	65	
62	2	92	
63	3	188	
64	4	103	
65	5	423	
66	6	380	
67	7	338	
68	8	206	
69	9	137	
70	a	142	
71	b	215	
72	c	332	
73	d	306	
74	e	279	
75	f	212	
76	g	166	
77	h	158	
78	i	128	

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Mol	Chain	Length	Quality of chain
79	j	123	
80	k	112	
81	l	138	
82	m	128	
83	o	102	
84	p	206	
85	q	222	
86	r	196	
87	s	439	
88	t	198	
88	t1	198	
88	u	198	
88	v	198	
88	w	198	
88	x	198	
88	y	198	
89	H	267	
90	z	325	

2 Entry composition [i](#)

There are 99 unique types of molecules in this entry. The entry contains 339415 atoms, of which 155776 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 Translational activator of cytochrome c oxidase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A5	220	Total	C	H	N	O	S	0	0
			3423	1058	1715	306	335	9		

- Molecule 2 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AA	954	Total	C	H	N	O	P	0	0
			30518	9088	10258	3647	6571	954		

- Molecule 3 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	AB	225	Total	C	H	N	O	S	0	0
			3643	1164	1815	331	323	10		

- Molecule 4 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	AC	132	Total	C	H	N	O	S	0	0
			2171	699	1088	195	185	4		

- Molecule 5 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	AD	343	Total	C	H	N	O	S	0	0
			5535	1713	2804	518	487	13		

- Molecule 6 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	AE	122	Total	C	H	N	O	S	0	0
			1972	614	1000	177	177	4		

- Molecule 7 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	AF	208	Total	C	H	N	O	S	0	0
			3494	1104	1769	312	298	11		

- Molecule 8 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	AG	327	Total	C	H	N	O	S	0	0
			5375	1710	2687	477	487	14		

- Molecule 9 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	AH	140	Total	C	H	N	O	S	0	0
			2335	745	1183	194	210	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS11m.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	AI	137	Total	C	H	N	O	S	0	0
			2072	642	1052	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	184	5F0	ASN	conflict	UNP P82912

- Molecule 11 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AJ	108	Total	C	H	N	O	S	0	0
			1724	521	885	169	143	6		

- Molecule 12 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AK	101	Total	C	H	N	O	S	0	0
			1747	537	885	179	141	5		

- Molecule 13 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AL	174	Total	C	H	N	O	S	0	0
			2993	925	1540	270	251	7		

- Molecule 14 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AM	119	Total	C	H	N	O	S	0	0
			1907	594	965	185	157	6		

- Molecule 15 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	AN	110	Total	C	H	N	O	S	0	0
			1796	562	928	156	147	3		

- Molecule 16 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AO	193	Total	C	H	N	O	S	0	0
			3149	1014	1557	294	277	7		

- Molecule 17 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AP	97	Total	C	H	N	O	S	0	0
			1587	501	806	134	138	8		

- Molecule 18 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AQ	87	Total	C	H	N	O	S	0	0
			1502	460	758	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 19 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AR	295	Total	C	H	N	O	S	0	0
			4837	1533	2428	413	455	8		

- Molecule 20 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AS	135	Total	C	H	N	O	S	0	0
			2226	716	1115	198	196	1		

- Molecule 21 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	AT	168	Total	C	H	N	O	S	0	0
			2764	877	1393	239	244	11		

- Molecule 22 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AU	176	Total	C	H	N	O	S	0	0
			2987	916	1499	301	267	4		

- Molecule 23 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AV	362	Total	C	H	N	O	S	0	0
			5930	1904	2961	495	558	12		

- Molecule 24 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AW	100	Total	C	H	N	O	S	0	0
			1591	498	802	141	146	4		

- Molecule 25 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AX	352	Total	C	H	N	O	S	0	0
			5692	1822	2843	499	517	11		

- Molecule 26 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AY	149	Total	C	H	N	O	S	0	0
			2443	801	1197	207	234	4		

- Molecule 27 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	AZ	100	Total	C	H	N	O	S	0	0
			1697	534	858	153	148	4		

- Molecule 28 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	A0	215	Total	C	H	N	O	S	0	0
			3583	1130	1796	339	313	5		

- Molecule 29 is a protein called Small ribosomal subunit protein mS35.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	A1	278	Total	C	H	N	O	S	0	0
			4545	1430	2289	386	429	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	45	ASP	GLU	conflict	UNP P82673

- Molecule 30 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	A2	118	Total	C	H	N	O	S	0	0
			1906	579	971	182	166	8		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 31 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	A3	70	Total	C	H	N	O	S	0	0
			1324	401	699	134	89	1		

- Molecule 32 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	A4	588	Total	C	H	N	O	S	0	0
			9534	3053	4766	808	879	28		

- Molecule 33 is a RNA chain called A-site tRNA (68-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	Aw	68	Total	C	H	N	O	P	0	0
			2147	643	720	237	479	68		

- Molecule 34 is a RNA chain called P-site RNA (70-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
34	Ax	70	Total	C	H	N	O	P	0	0
			2232	665	750	259	488	70		

- Molecule 35 is a RNA chain called E-site tRNA (70-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
35	Ay	55	Total	C	H	N	O	P	0	0
			1761	524	592	209	381	55		

- Molecule 36 is a RNA chain called mRNA (34-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
36	Az	34	Total	C	H	N	O	P	0	0
			1079	324	361	124	236	34		

- Molecule 37 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	A	1557	Total	C	H	N	O	P	0	0
			49813	14833	16765	5958	10700	1557		

- Molecule 38 is a RNA chain called tRNA-Val (73-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
38	B	72	Total	C	H	N	O	P	0	0
			2295	685	771	269	498	72		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
39	D	238	Total	C	H	N	O	S	0	0
			3779	1157	1920	376	317	9		

- Molecule 40 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	E	305	Total	C	H	N	O	S	0	0
			4821	1545	2415	418	432	11		

- Molecule 41 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	F	252	Total	C	H	N	O	S	0	0
			4096	1305	2065	370	350	6		

- Molecule 42 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	I	212	Total	C	H	N	O	S	0	0
			3480	1088	1785	304	292	11		

- Molecule 43 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	J	175	Total	C	H	N	O	S	0	0
			2737	847	1407	237	244	2		

- Molecule 44 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	K	178	Total	C	H	N	O	S	0	0
			2907	936	1452	259	253	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	2	ACE	-	acetylation	UNP Q9BYD1

- Molecule 45 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	L	115	Total	C	H	N	O	S	0	0
			1832	559	942	171	155	5		

- Molecule 46 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	M	289	Total	C	H	N	O	S	0	0
			4698	1476	2384	427	405	6		

- Molecule 47 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	N	222	Total	C	H	N	O	S	0	0
			3603	1143	1817	326	307	10		

- Molecule 48 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	O	154	Total	C	H	N	O	S	0	0
			2553	792	1294	241	219	7		

- Molecule 49 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	P	144	Total	C	H	N	O	S	0	0
			2338	733	1165	224	211	5		

- Molecule 50 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	Q	238	Total	C	H	N	O	S	0	0
			4001	1268	2022	352	350	9		

- Molecule 51 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	R	140	Total	C	H	N	O	S	0	0
			2368	732	1214	231	187	4		

- Molecule 52 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	S	161	Total	C	H	N	O	S	0	0
			2658	835	1365	227	227	4		

- Molecule 53 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	T	166	Total	C	H	N	O	S	0	0
			2779	875	1410	254	233	7		

- Molecule 54 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	U	153	Total	C	H	N	O	S	0	0
			2483	788	1232	234	226	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	1	ACE	-	acetylation	UNP Q16540

- Molecule 55 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	V	205	Total	C	H	N	O	S	0	0
			3363	1068	1687	298	302	8		

- Molecule 56 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	W	116	Total	C	H	N	O	S	0	0
			1839	577	935	171	153	3		

- Molecule 57 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	X	244	Total	C	H	N	O	S	0	0
			4104	1322	2060	352	365	5		

- Molecule 58 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	Y	181	Total	C	H	N	O	S	0	0
			3153	995	1597	298	259	4		

- Molecule 59 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	Z	122	Total	C	H	N	O	S	0	0
			2040	636	1044	186	171	3		

- Molecule 60 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	0	110	Total	C	H	N	O	S	0	0
			1814	554	916	176	162	6		

- Molecule 61 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	1	56	Total	C	H	N	O	S	0	0
			975	296	511	89	77	2		

- Molecule 62 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	2	46	Total	C	H	N	O	S	0	0
			783	233	406	83	60	1		

- Molecule 63 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	3	95	Total	C	H	N	O	S	0	0
			1715	539	883	162	128	3		

- Molecule 64 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	4	38	Total	C	H	N	O	S	0	0
			703	217	361	72	49	4		

- Molecule 65 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	5	394	Total	C	H	N	O	S	0	0
			6416	2073	3206	560	566	11		

- Molecule 66 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	6	354	Total	C	H	N	O	S	0	0
			5789	1881	2841	525	533	9		

- Molecule 67 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	7	294	Total	C	H	N	O	S	0	0
			4787	1529	2397	405	438	18		

- Molecule 68 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	8	157	Total	C	H	N	O	S	0	0
			2695	844	1368	235	246	2		

- Molecule 69 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	9	124	Total	C	H	N	O	S	0	0
			1984	644	987	170	181	2		

- Molecule 70 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	a	100	Total	C	H	N	O	S	0	0
			1650	529	810	152	154	5		

- Molecule 71 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	b	150	Total	C	H	N	O	S	0	0
			2391	744	1195	231	218	3		

- Molecule 72 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	c	286	Total	C	H	N	O	S	0	0
			4619	1470	2320	397	423	9		

- Molecule 73 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	d	237	Total	C	H	N	O	S	0	0
			3879	1251	1930	331	354	13		

- Molecule 74 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	e	238	Total	C	H	N	O	S	0	0
			3847	1222	1916	339	364	6		

- Molecule 75 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	f	157	Total	C	H	N	O	S	0	0
			2521	799	1269	207	242	4		

- Molecule 76 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	g	134	Total	C	H	N	O	S	0	0
			2210	719	1097	193	199	2		

- Molecule 77 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	h	110	Total	C	H	N	O	S	0	0
			1776	568	881	156	168	3		

- Molecule 78 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	i	97	Total	C	H	N	O	S	0	0
			1685	532	857	165	127	4		

- Molecule 79 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	j	94	Total	C	H	N	O	S	0	0
			1491	463	746	144	136	2		

- Molecule 80 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	k	102	Total	C	H	N	O	S	0	0
			1558	479	784	148	142	5		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 81 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	l	82	Total	C	H	N	O	S	0	0
			1362	437	674	120	128	3		

- Molecule 82 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	m	92	Total	C	H	N	O	S	0	0
			1588	488	797	159	142	2		

- Molecule 83 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	o	94	Total	C	H	N	O	S	0	0
			1602	501	804	165	129	3		

- Molecule 84 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	p	147	Total	C	H	N	O	S	0	0
			2428	748	1223	228	225	4		

- Molecule 85 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	q	165	Total	C	H	N	O	S	0	0
			2763	865	1374	270	249	5		

- Molecule 86 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	r	162	Total	C	H	N	O	S	0	0
			2670	839	1348	252	223	8		

- Molecule 87 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	s	386	Total	C	H	N	O	S	0	0
			6294	2023	3139	559	559	14		

- Molecule 88 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	t	46	Total	C	H	N	O	0	0
			731	228	377	56	70		
88	u	32	Total	C	H	N	O	0	0
			540	168	283	40	49		
88	v	32	Total	C	H	N	O	0	0
			540	168	283	40	49		
88	w	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
88	x	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
88	y	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
88	t1	71	Total	C	H	N	O	0	0
			1145	352	599	93	101		

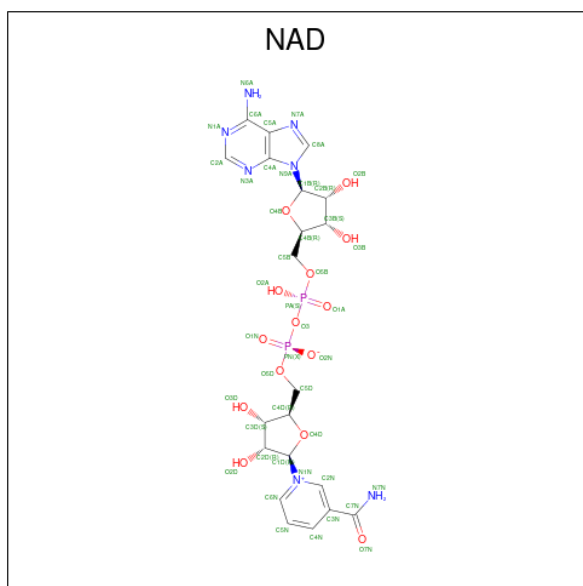
- Molecule 89 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
89	H	202	Total	C	H	N	O	S	0	0
			3395	1067	1734	304	286	4		

- Molecule 90 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
90	z	252	Total	C	H	N	O	S	0	0
			4103	1304	2076	336	381	6		

- Molecule 91 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						AltConf
91	AA	1	Total	C	H	N	O	P	0
			69	21	25	7	14	2	

- Molecule 92 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
92	AA	55	Total	Mg	0
			55	55	
92	AB	1	Total	Mg	0
			1	1	
92	AX	1	Total	Mg	0
			1	1	
92	Az	1	Total	Mg	0
			1	1	
92	A	136	Total	Mg	0
			136	136	
92	D	1	Total	Mg	0
			1	1	

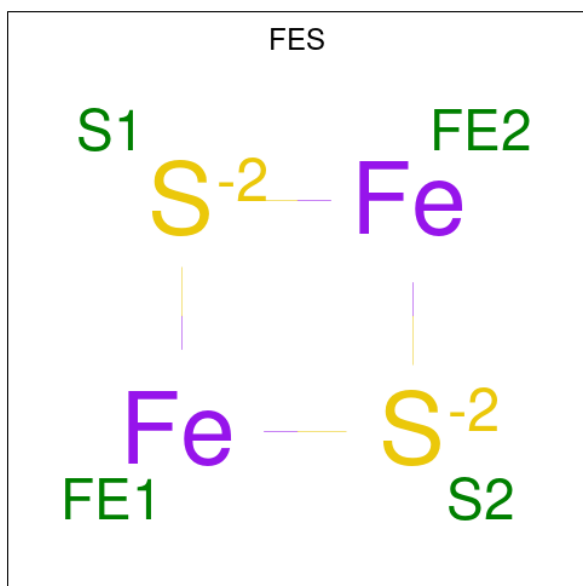
- Molecule 93 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
93	AA	13	Total 13	K 13	0
93	A	24	Total 24	K 24	0
93	D	1	Total 1	K 1	0
93	M	1	Total 1	K 1	0

- Molecule 94 is ZINC ION (CCD ID: ZN) (formula: Zn).

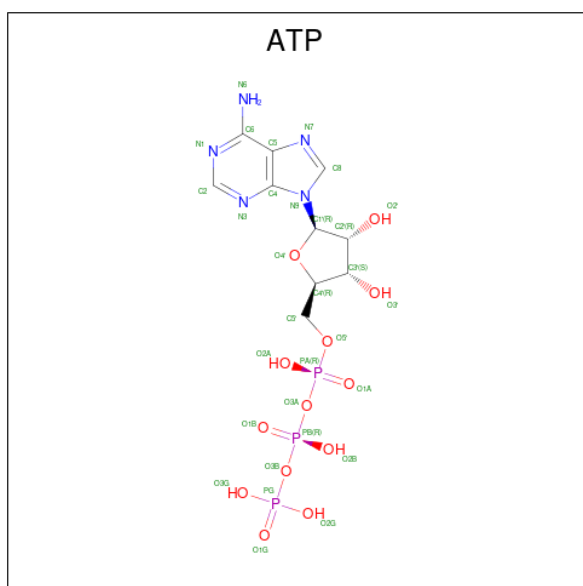
Mol	Chain	Residues	Atoms		AltConf
94	AO	1	Total 1	Zn 1	0
94	0	1	Total 1	Zn 1	0
94	4	1	Total 1	Zn 1	0

- Molecule 95 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



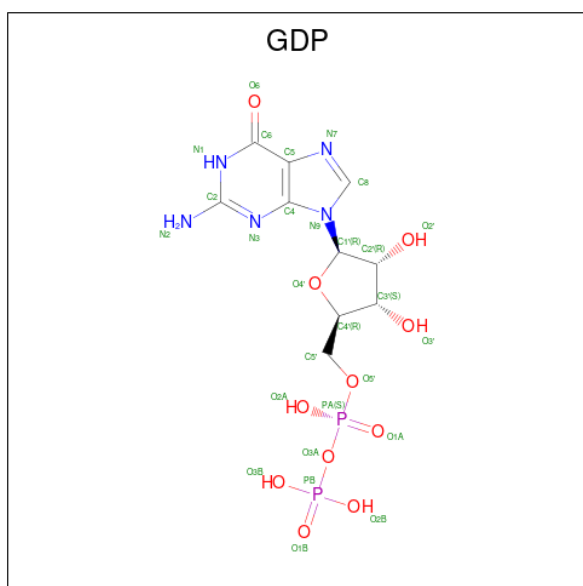
Mol	Chain	Residues	Atoms			AltConf
95	AP	1	Total 4	Fe 2	S 2	0
95	AT	1	Total 4	Fe 2	S 2	0
95	r	1	Total 4	Fe 2	S 2	0

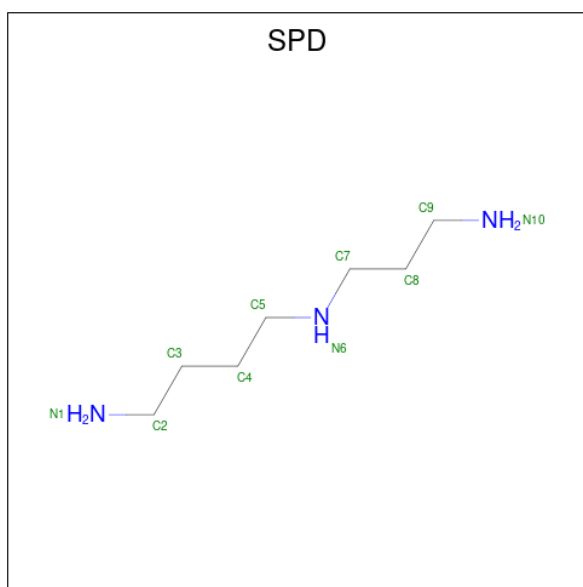
- Molecule 96 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
96	AX	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

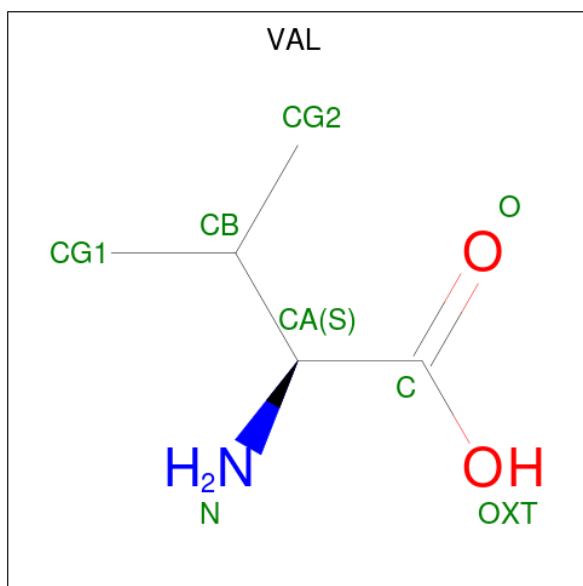
- Molecule 97 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





Mol	Chain	Residues	Atoms				AltConf
98	A	1	Total	C	H	N	0
			31	7	21	3	

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

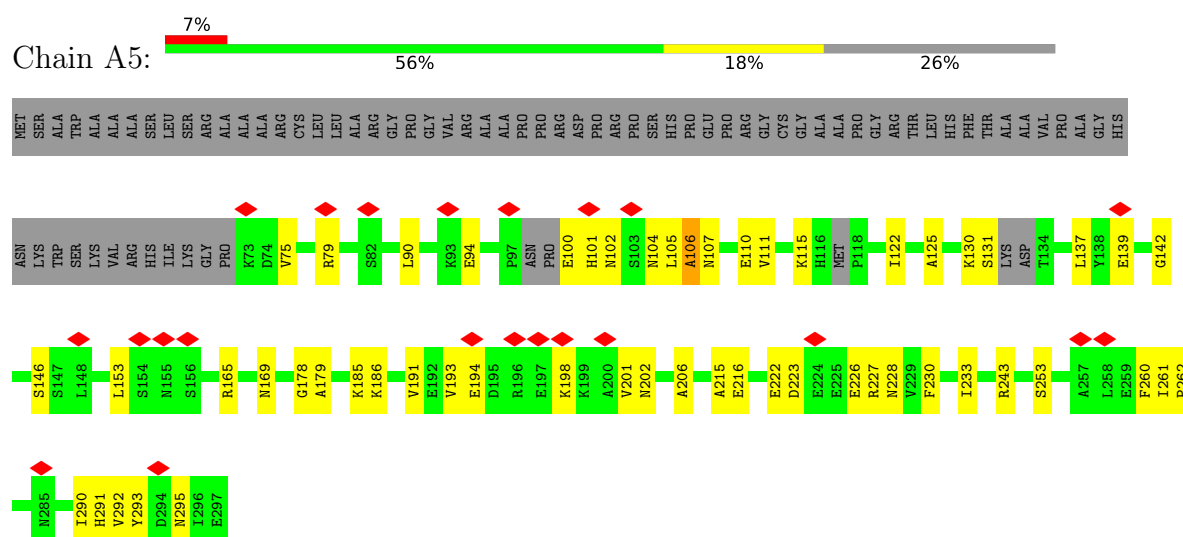


Mol	Chain	Residues	Atoms					AltConf
99	e	1	Total	C	H	N	O	0
			15	5	8	1	1	

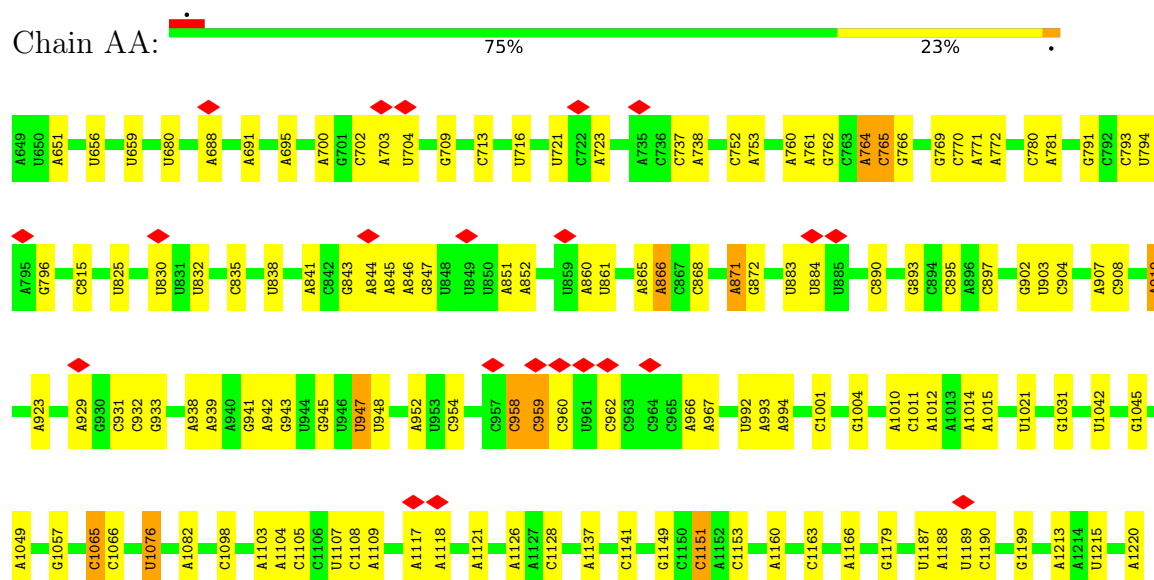
3 Residue-property plots

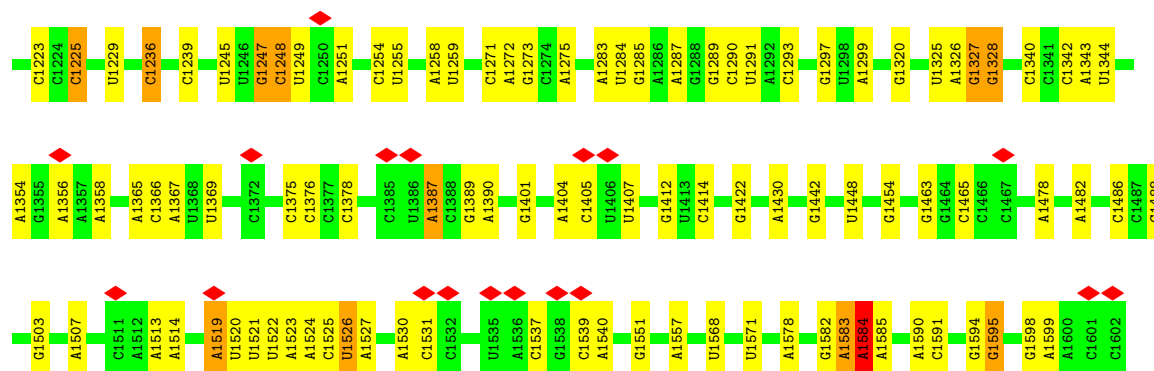
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Translational activator of cytochrome c oxidase 1

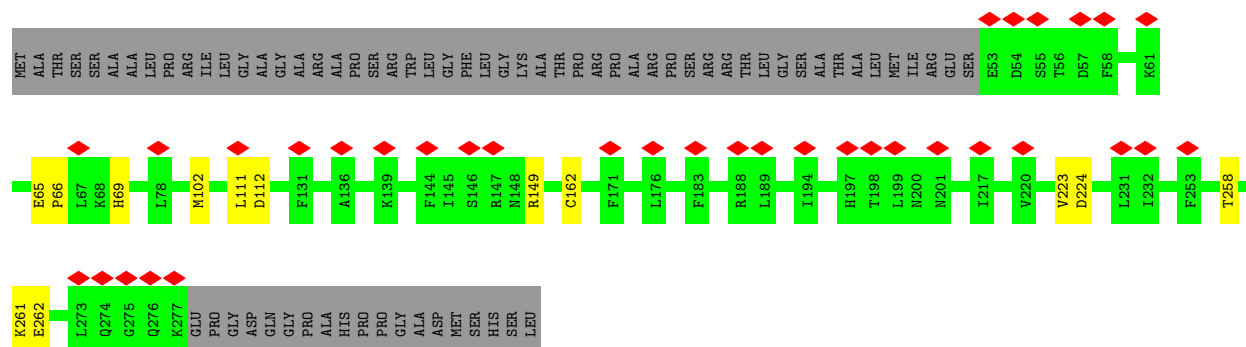
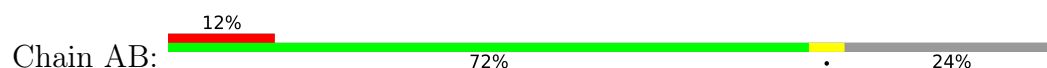


- Molecule 2: 12S mitochondrial rRNA

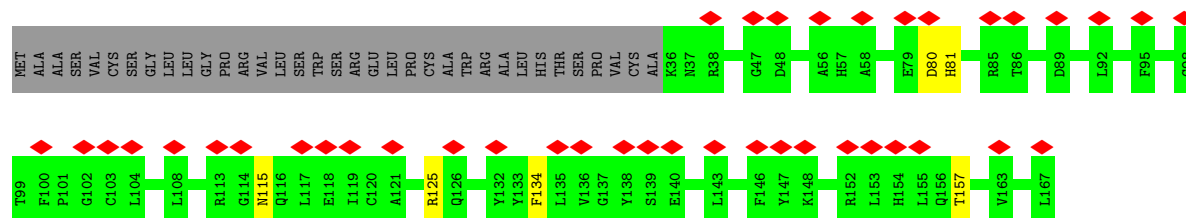
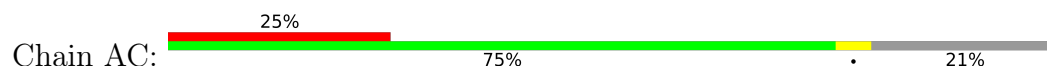




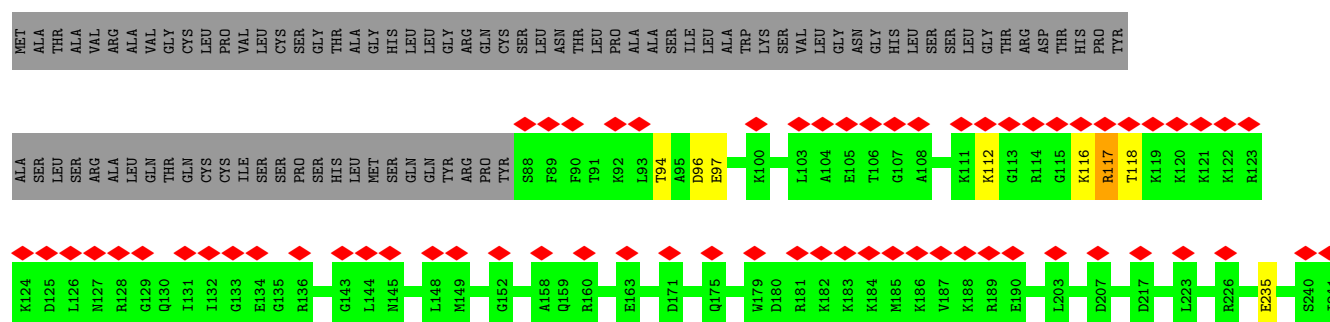
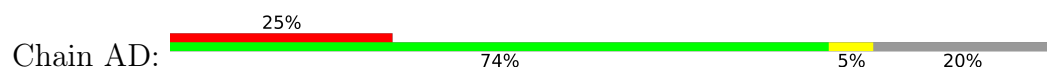
• Molecule 3: 28S ribosomal protein S2, mitochondrial

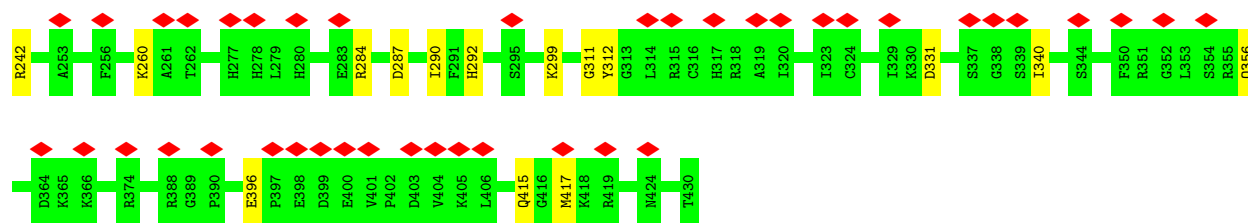


• Molecule 4: 28S ribosomal protein S24, mitochondrial



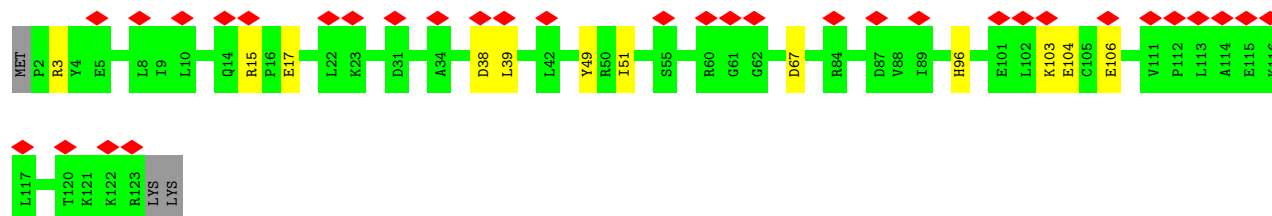
• Molecule 5: 28S ribosomal protein S5, mitochondrial





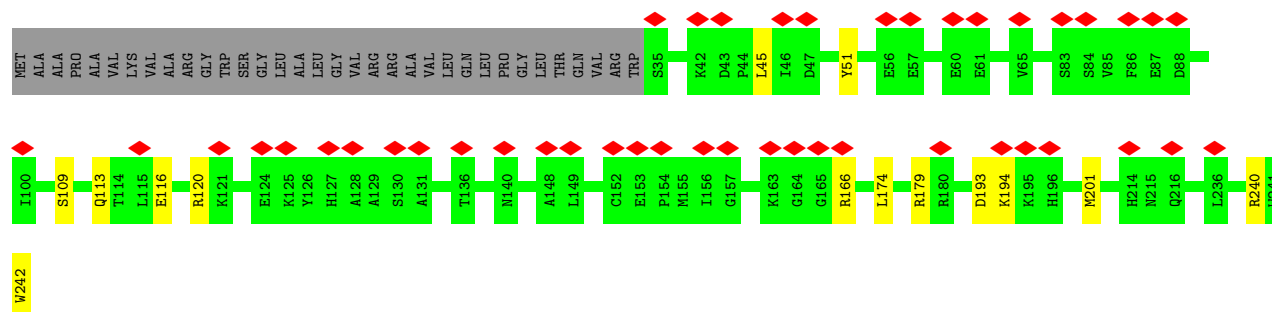
- Molecule 6: 28S ribosomal protein S6, mitochondrial

Chain AE: 26% 88% 10%



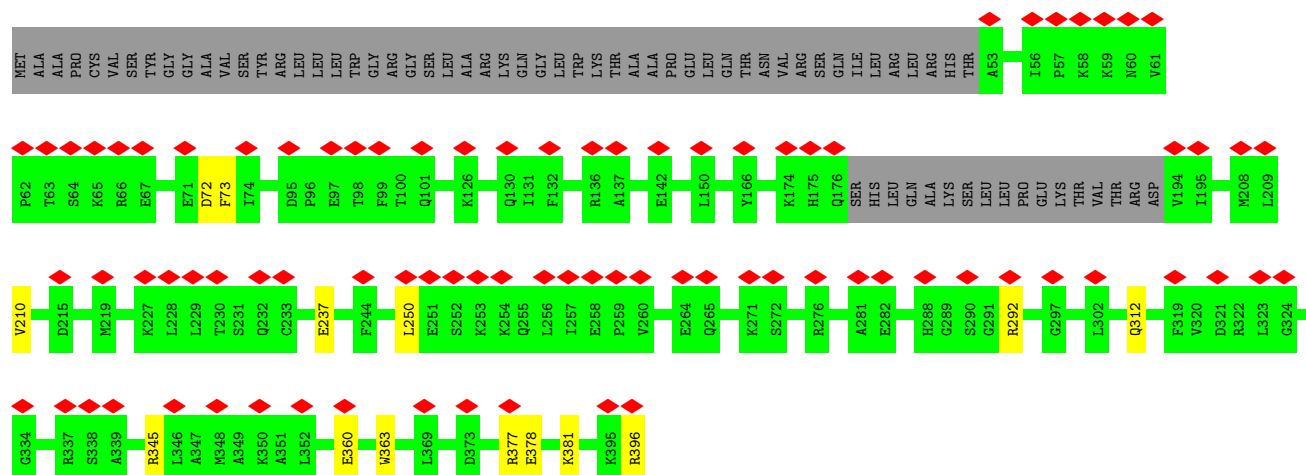
- Molecule 7: 28S ribosomal protein S7, mitochondrial

Chain AF: 18% 80% 6% 14%

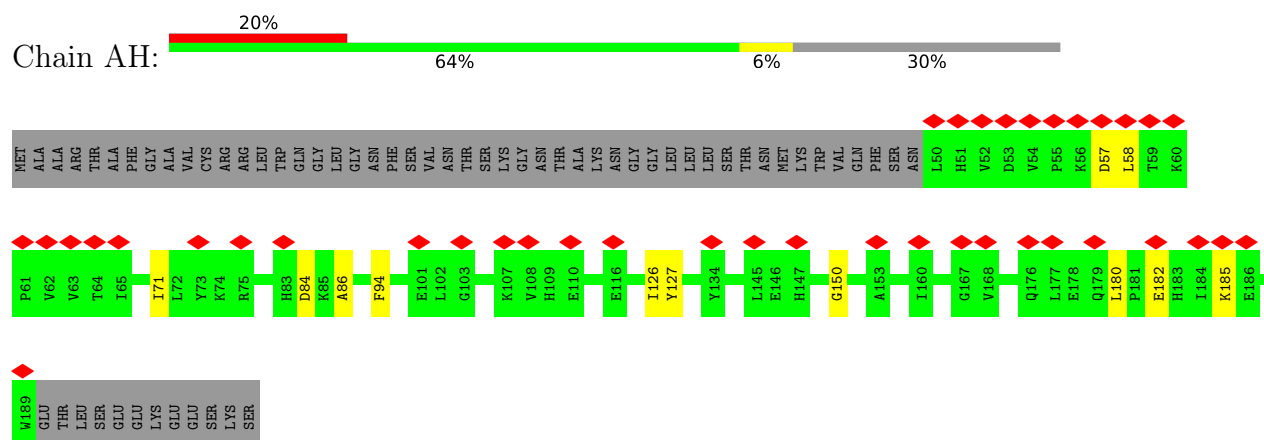


- Molecule 8: 28S ribosomal protein S9, mitochondrial

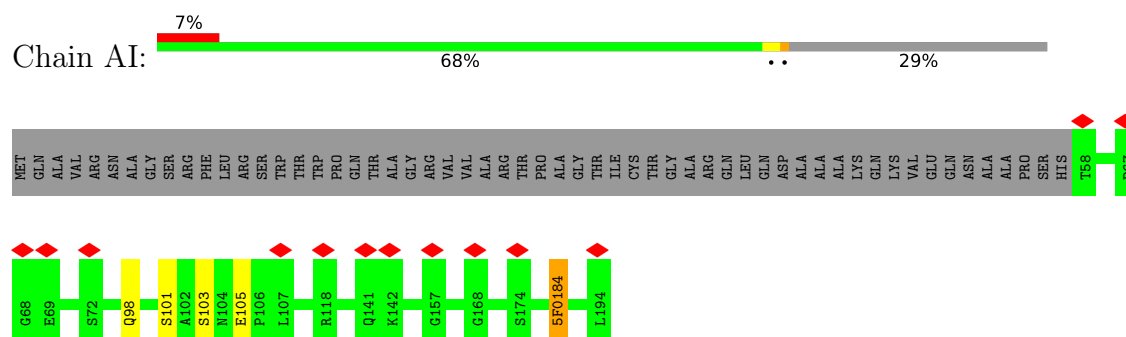
Chain AG: 21% 79% 17%



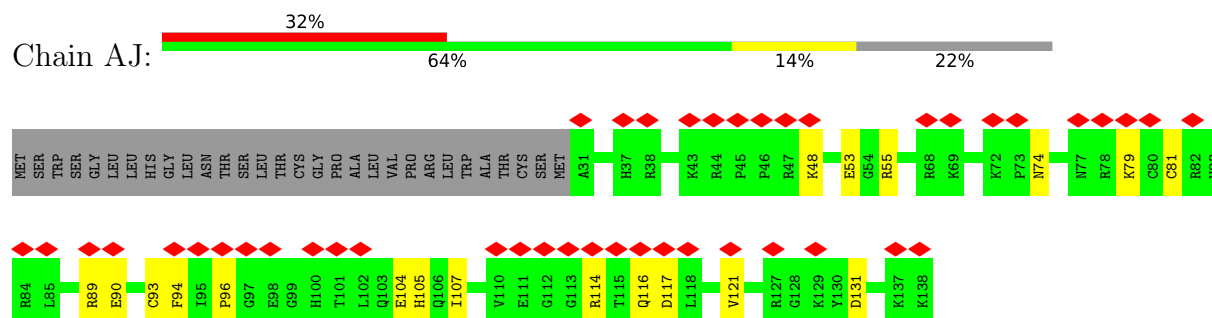
- Molecule 9: 28S ribosomal protein S10, mitochondrial



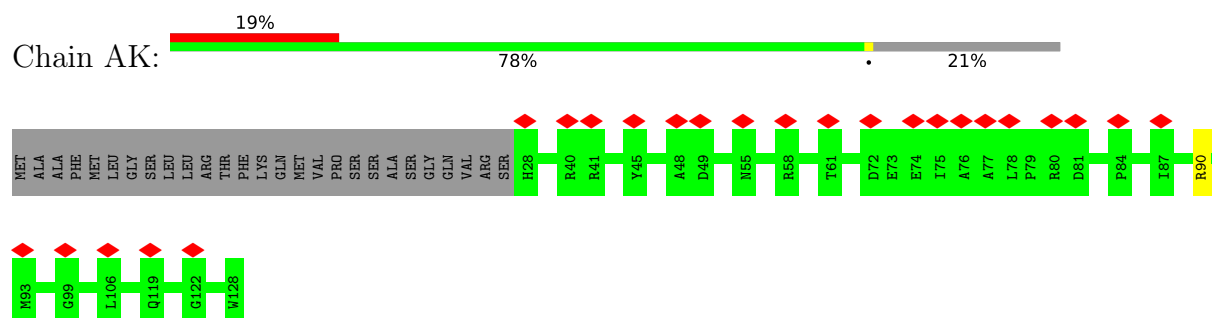
- Molecule 10: Small ribosomal subunit protein uS11m



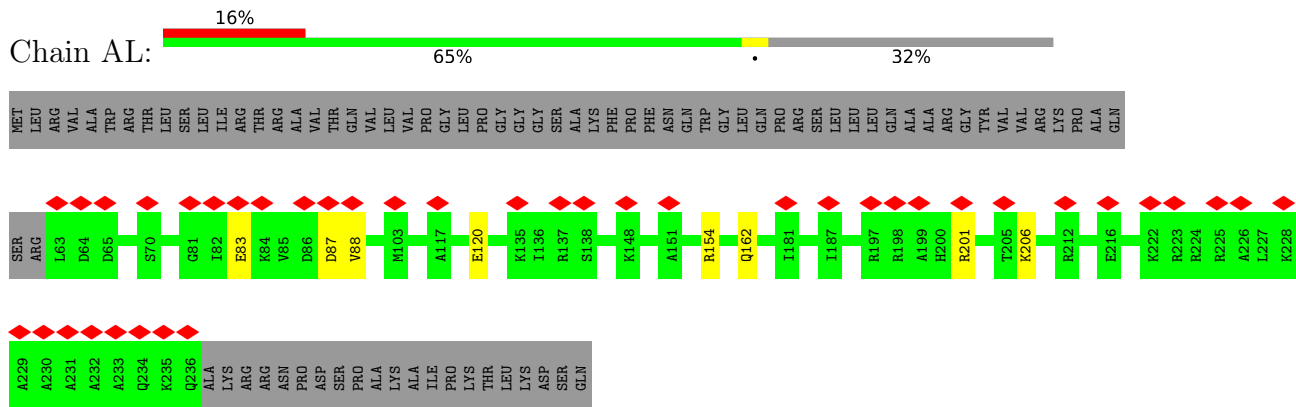
- Molecule 11: 28S ribosomal protein S12, mitochondrial



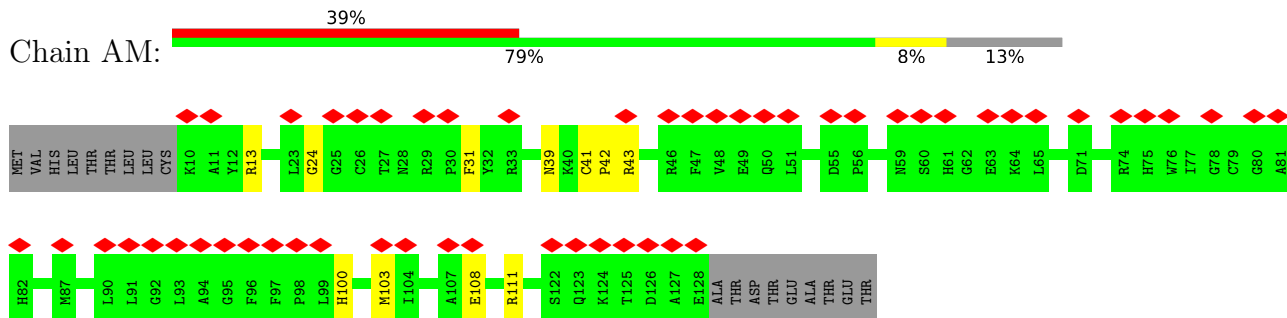
- Molecule 12: 28S ribosomal protein S14, mitochondrial



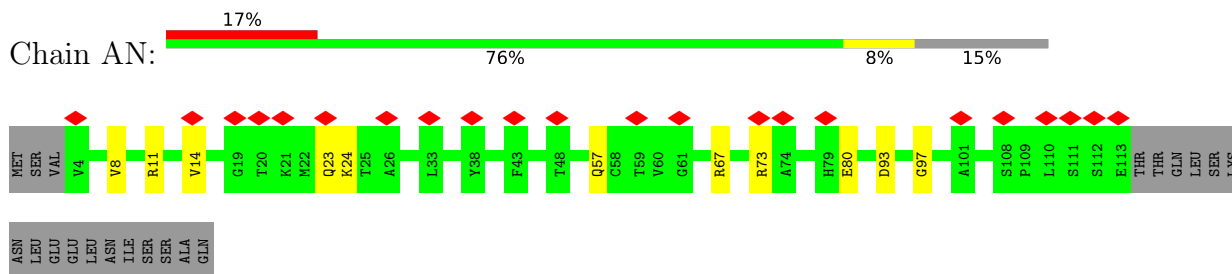
- Molecule 13: 28S ribosomal protein S15, mitochondrial



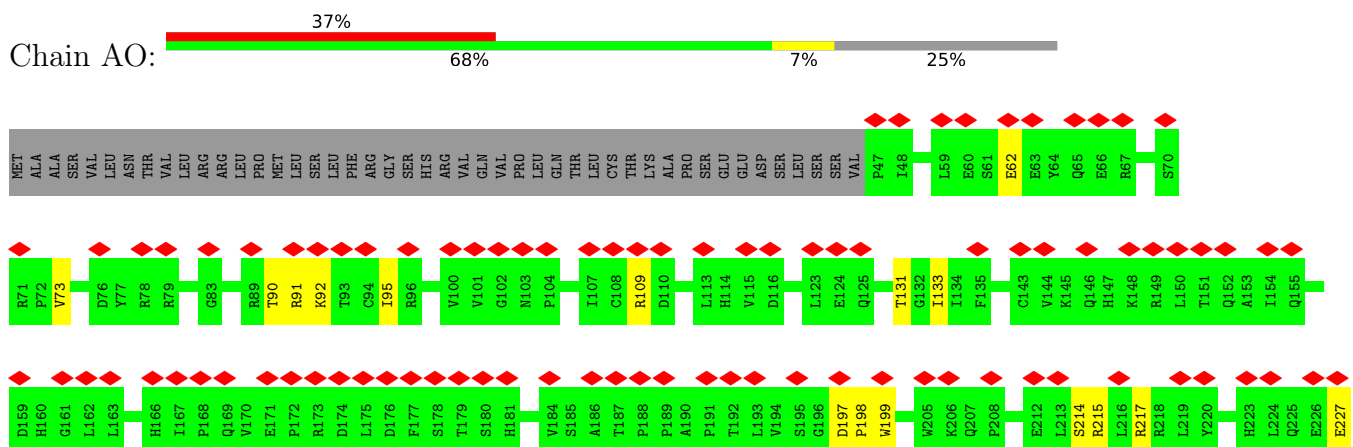
- Molecule 14: 28S ribosomal protein S16, mitochondrial

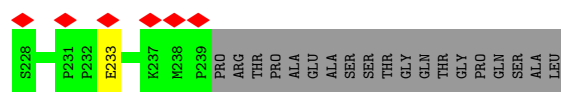


- Molecule 15: 28S ribosomal protein S17, mitochondrial

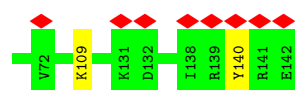
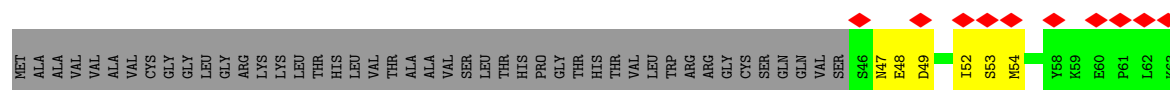


- Molecule 16: 28S ribosomal protein S18b, mitochondrial

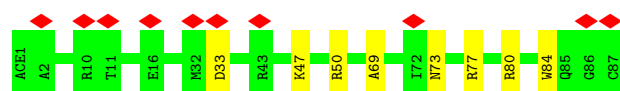
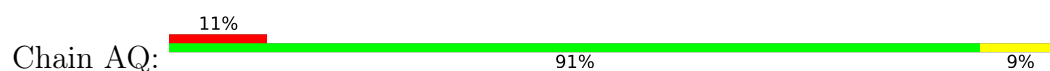




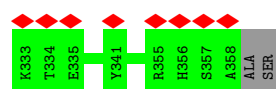
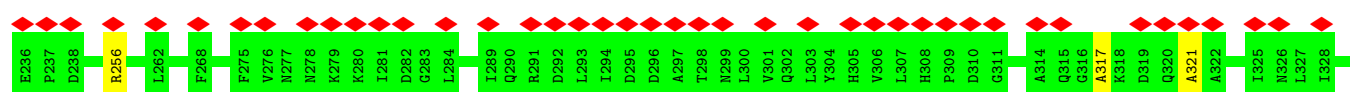
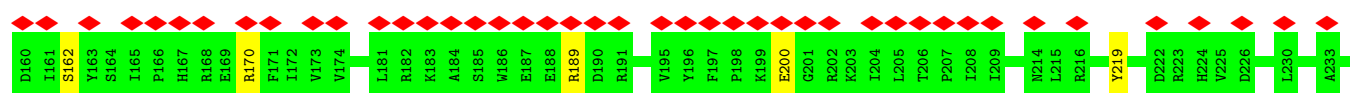
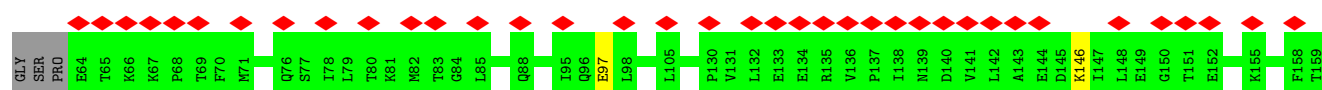
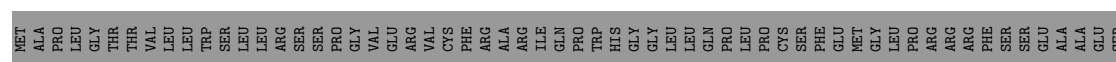
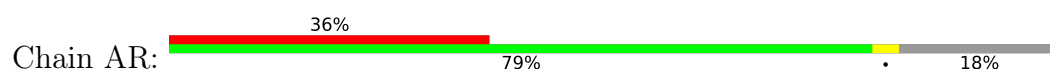
- Molecule 17: 28S ribosomal protein S18c, mitochondrial



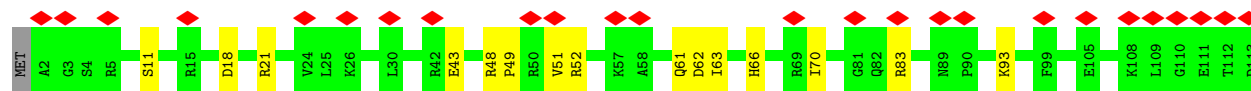
- Molecule 18: Small ribosomal subunit protein bS21m

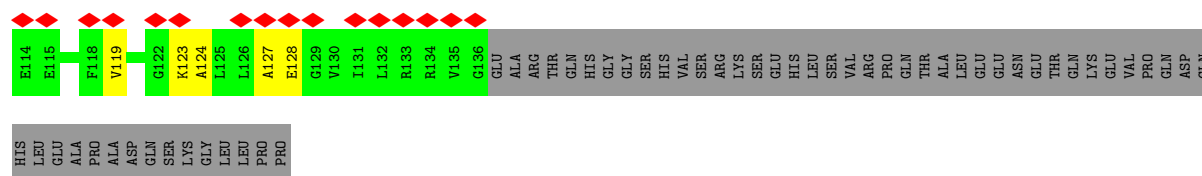


- Molecule 19: 28S ribosomal protein S22, mitochondrial

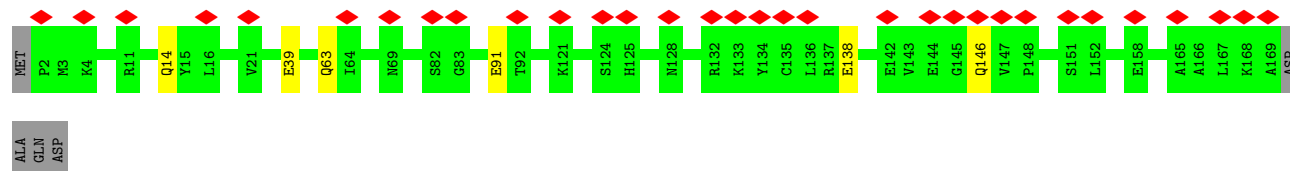


- Molecule 20: 28S ribosomal protein S23, mitochondrial

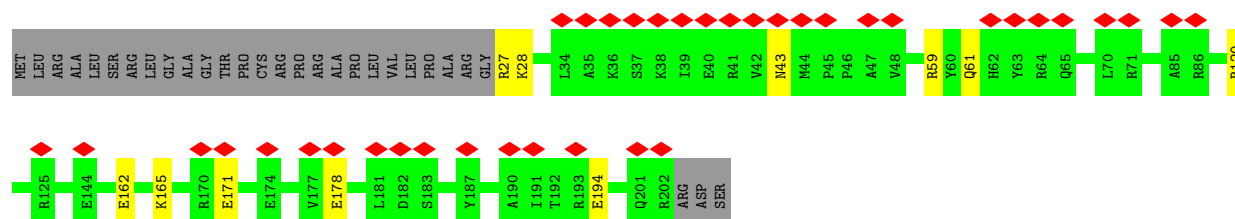
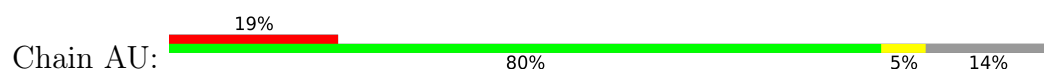




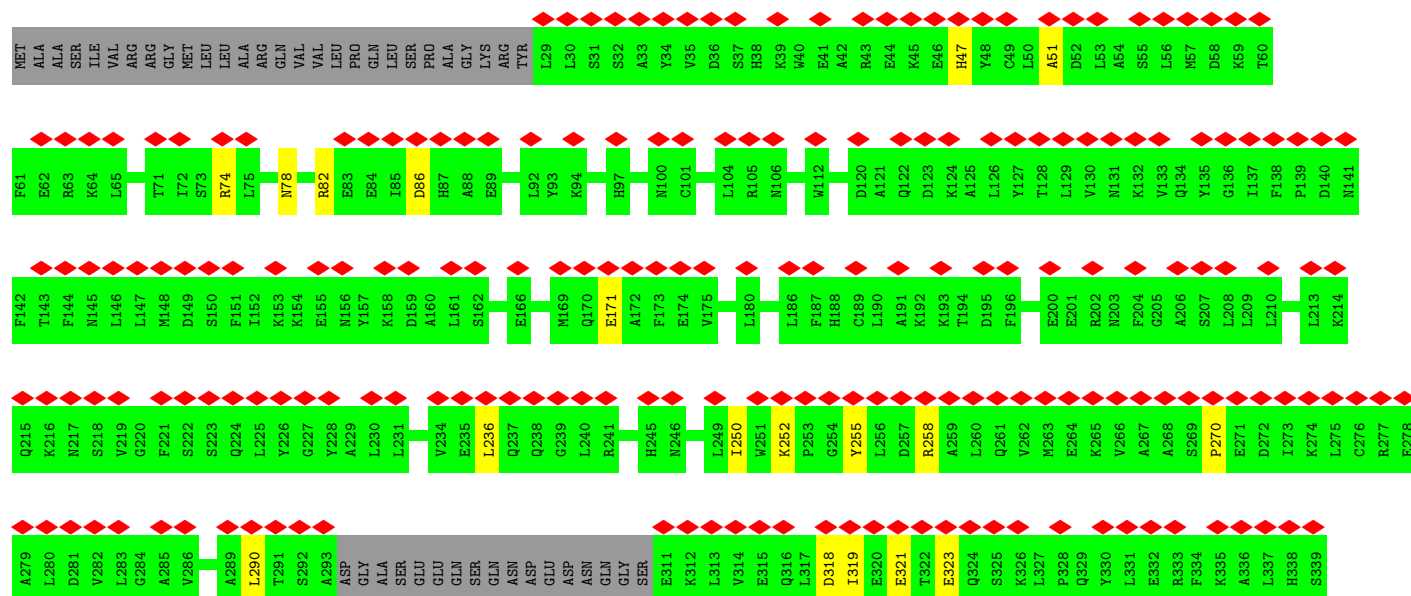
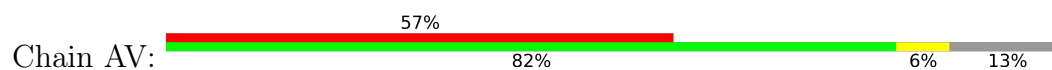
- Molecule 21: 28S ribosomal protein S25, mitochondrial



- Molecule 22: 28S ribosomal protein S26, mitochondrial

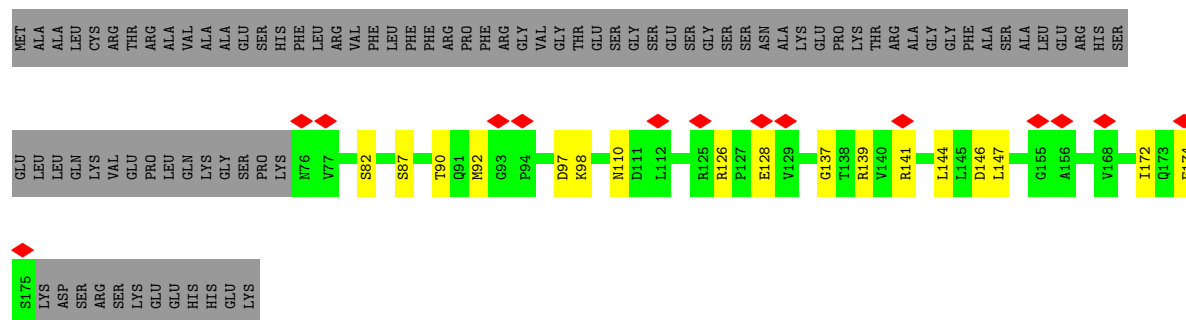


- Molecule 23: 28S ribosomal protein S27, mitochondrial

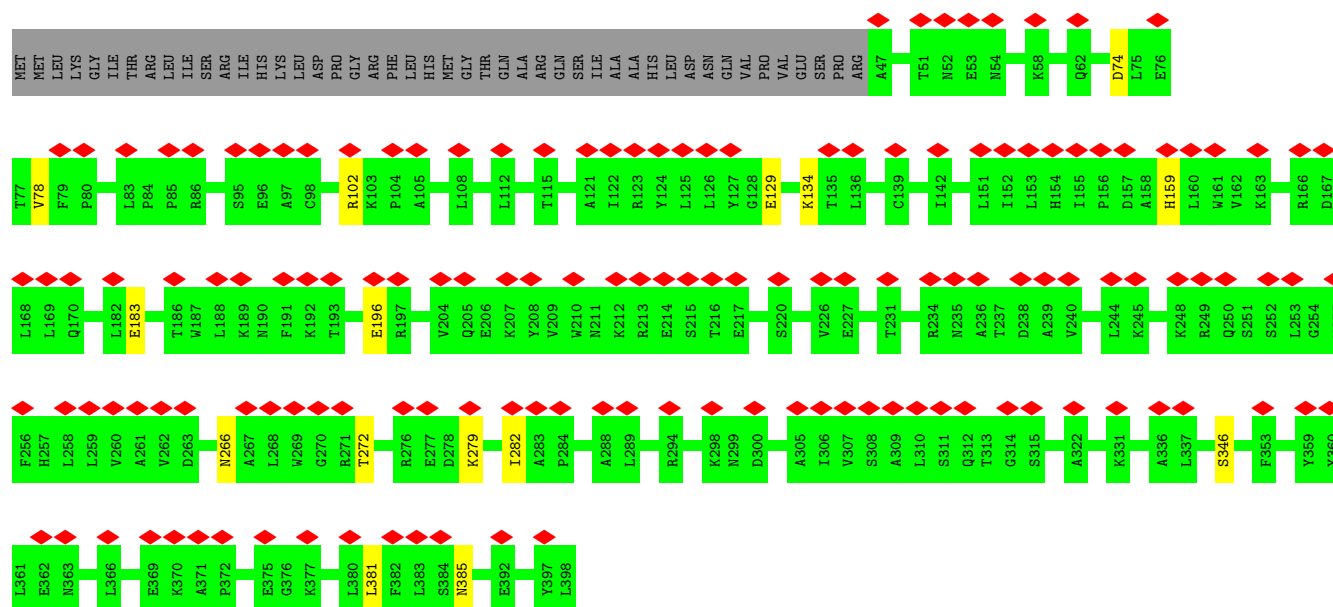
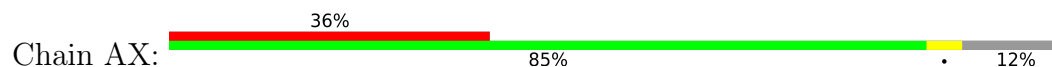




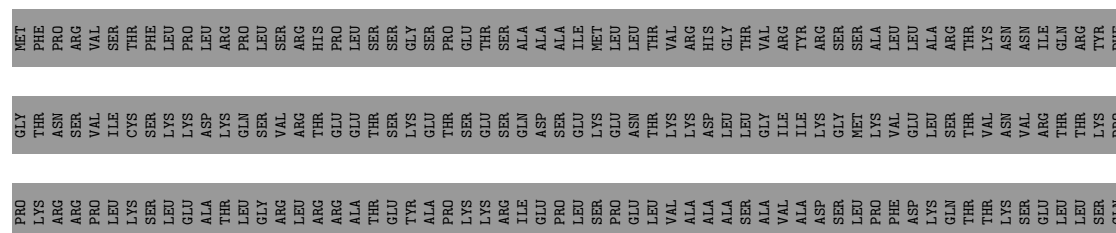
- Molecule 24: 28S ribosomal protein S28, mitochondrial

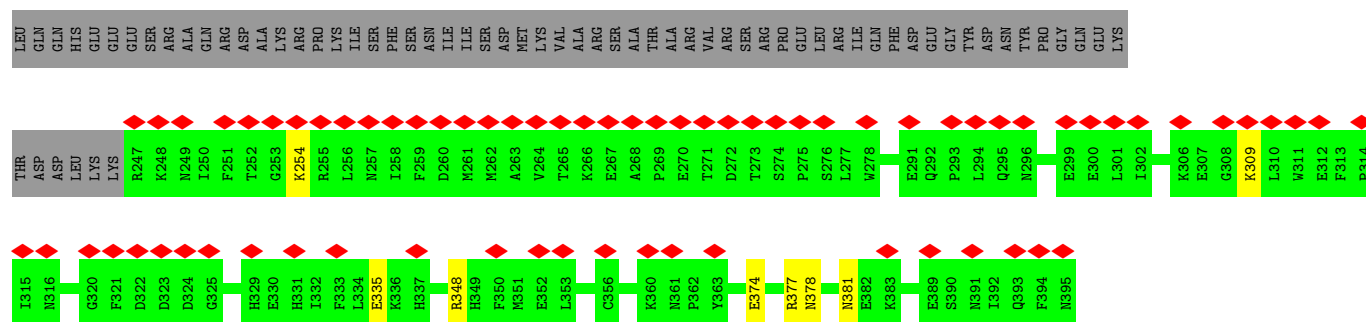


- Molecule 25: 28S ribosomal protein S29, mitochondrial

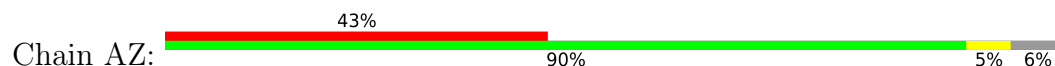


- Molecule 26: 28S ribosomal protein S31, mitochondrial

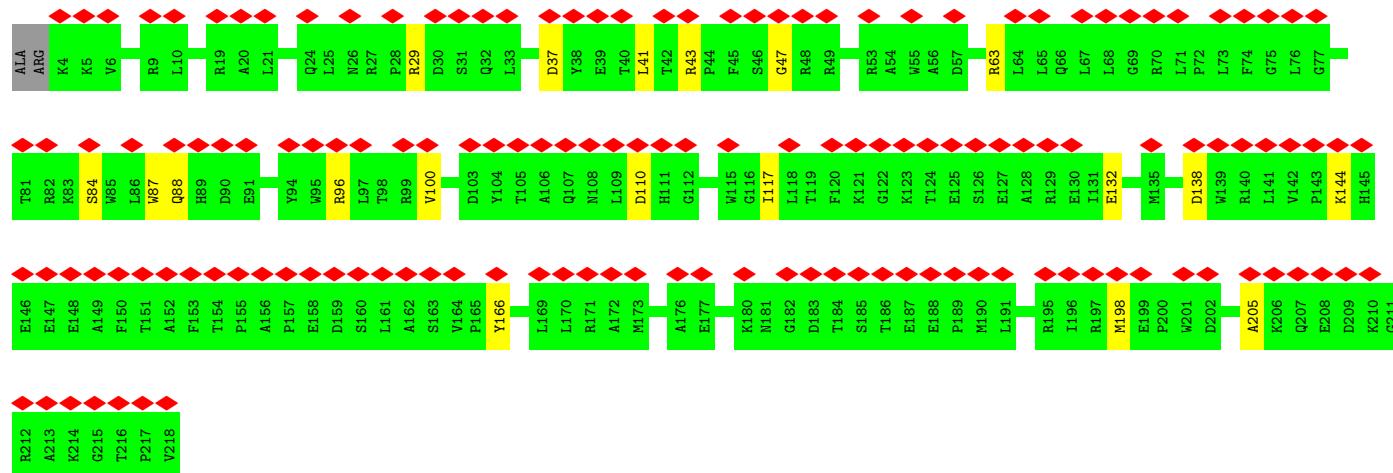
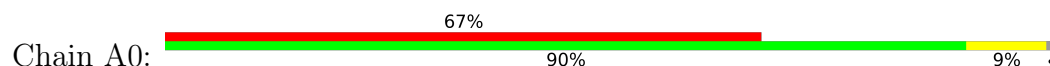




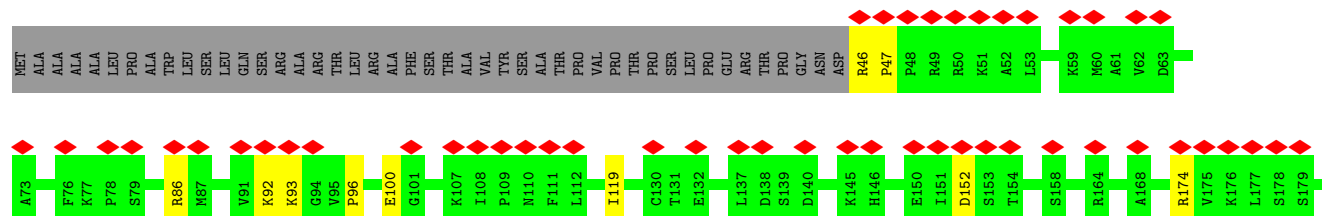
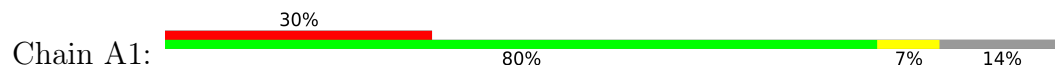
- Molecule 27: 28S ribosomal protein S33, mitochondrial

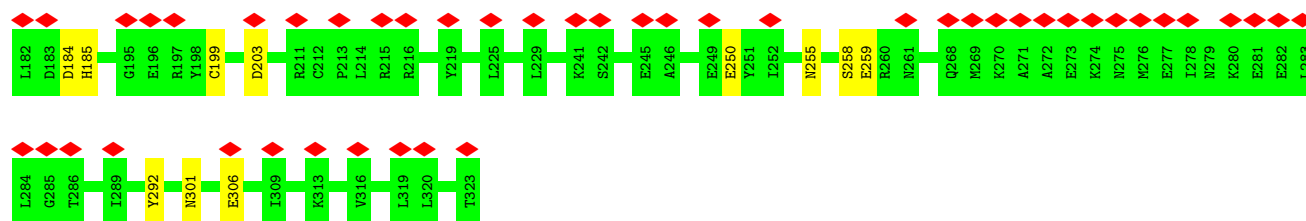


- Molecule 28: 28S ribosomal protein S34, mitochondrial

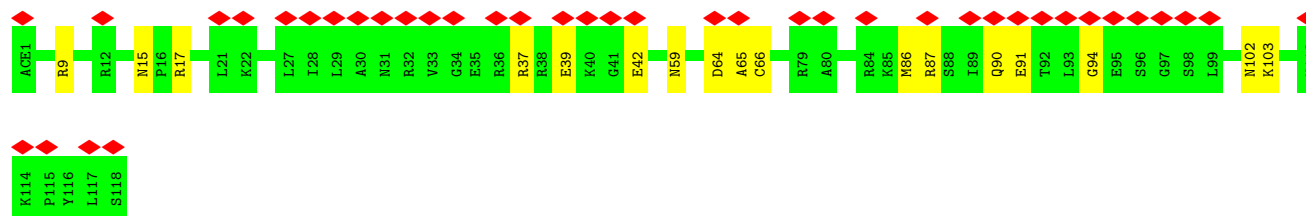
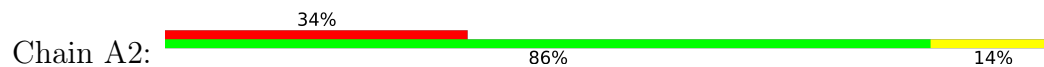


- Molecule 29: Small ribosomal subunit protein mS35

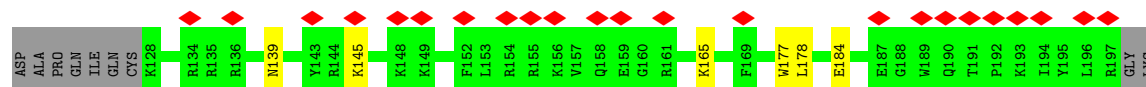
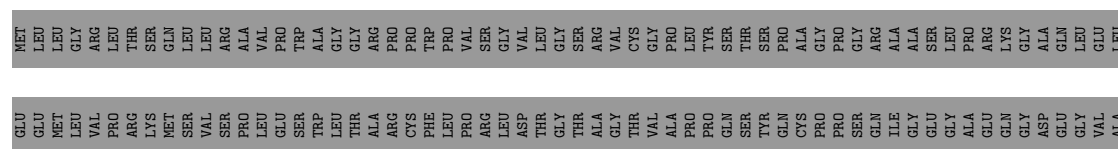




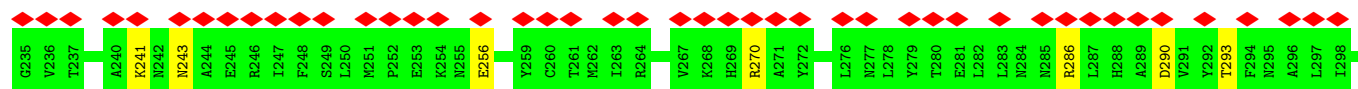
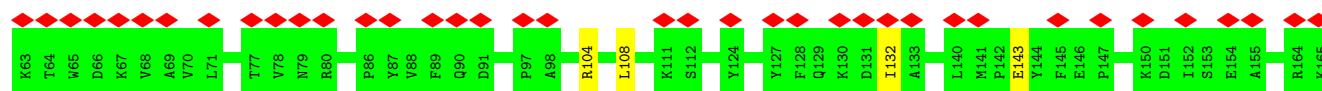
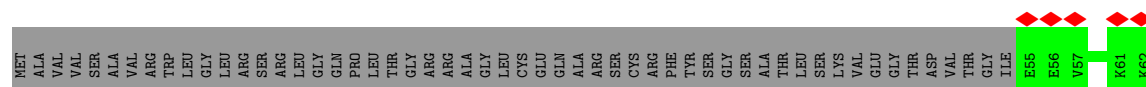
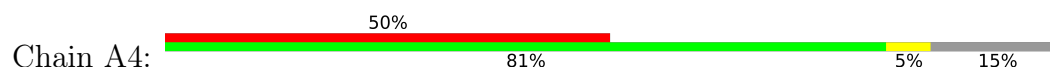
- Molecule 30: Small ribosomal subunit protein mS37

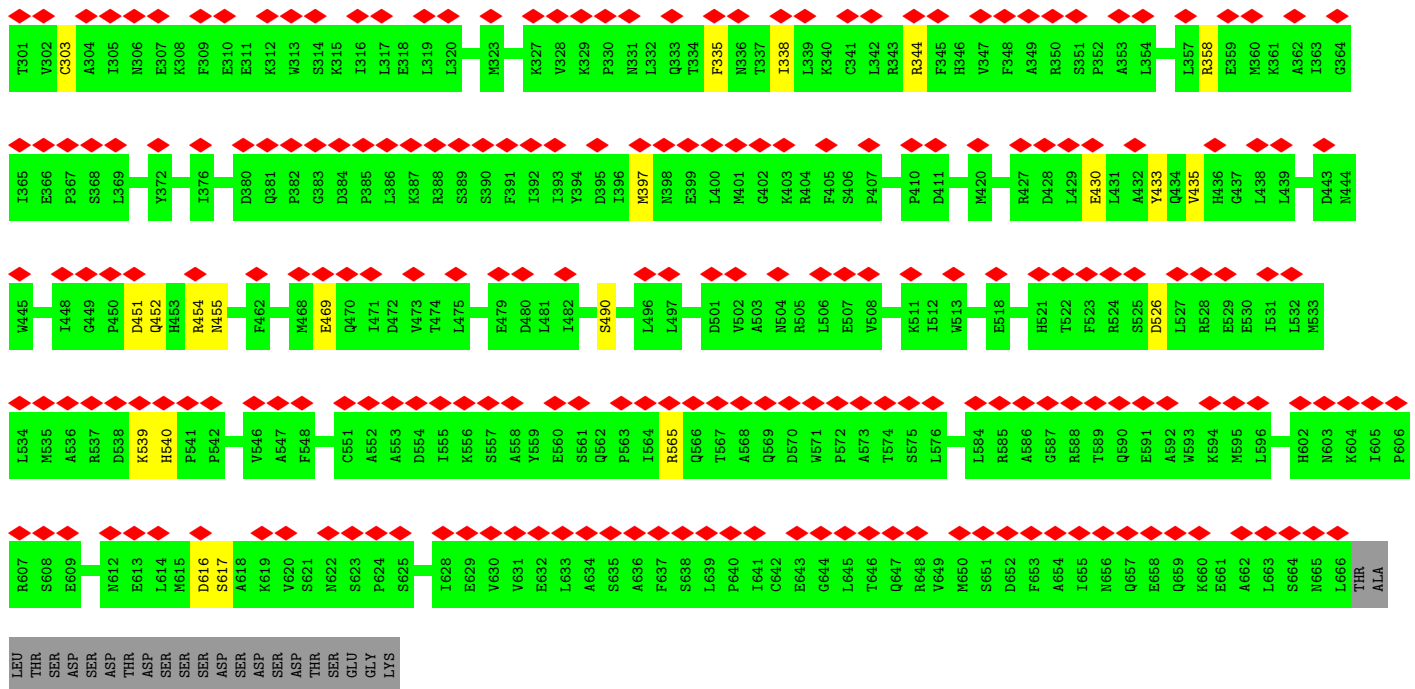


- Molecule 31: Aurora kinase A-interacting protein

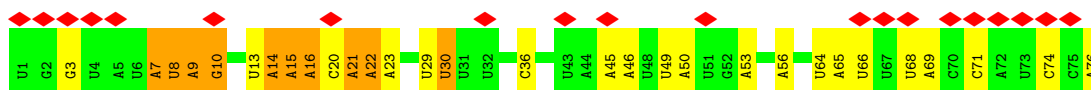


- Molecule 32: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

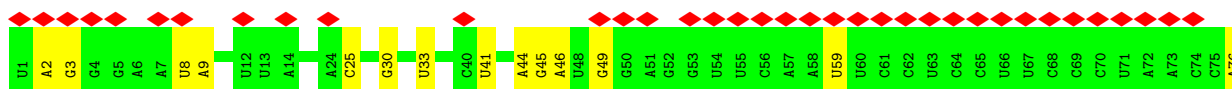
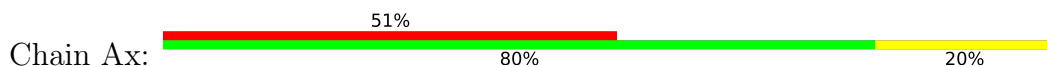




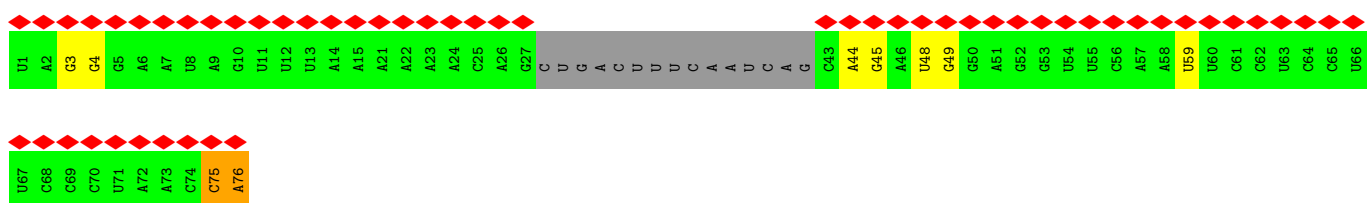
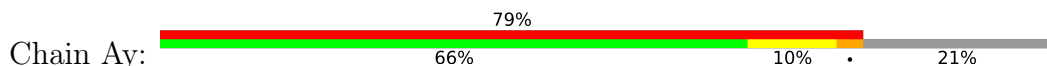
- Molecule 33: A-site tRNA (68-MER)



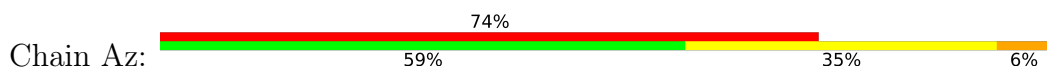
- Molecule 34: P-site RNA (70-MER)

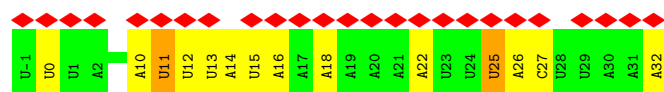


- Molecule 35: E-site tRNA (70-MER)



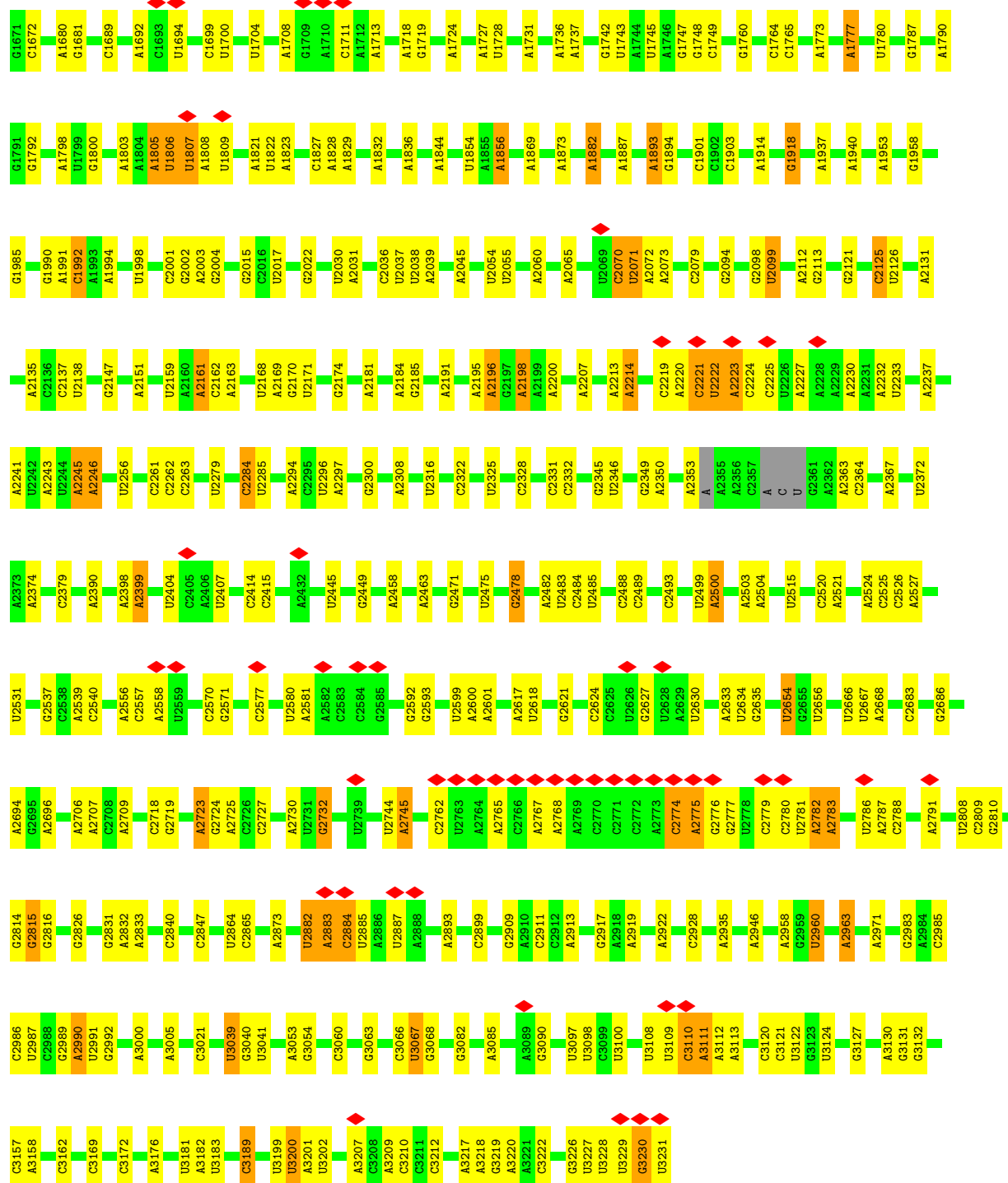
- Molecule 36: mRNA (34-MER)





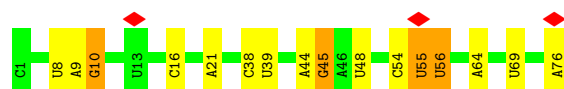
• Molecule 37: 16S mitochondrial rRNA

Chain A: 76% 21%



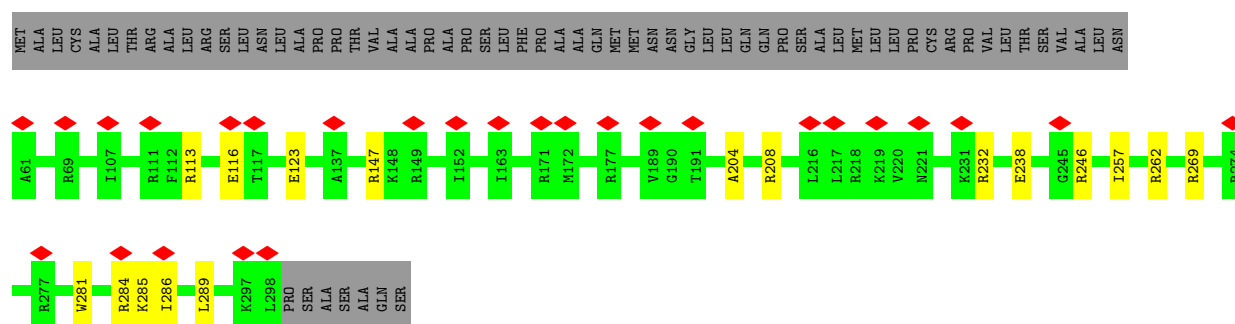
• Molecule 38: tRNA-Val (73-MER)

Chain B: 



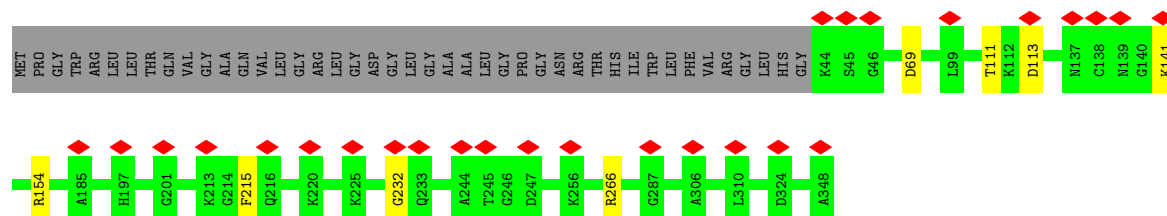
- Molecule 39: 39S ribosomal protein L2, mitochondrial

Chain D: 



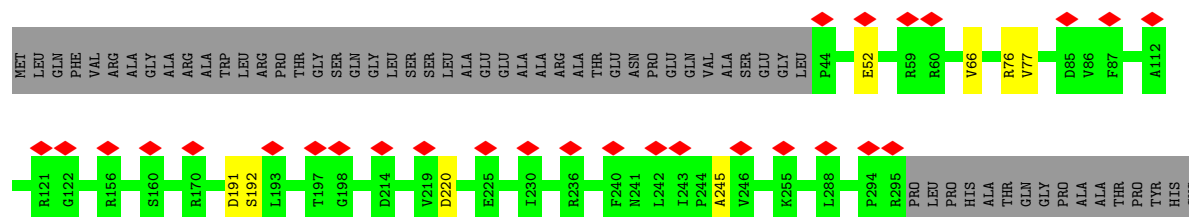
- Molecule 40: 39S ribosomal protein L3, mitochondrial

Chain E: 



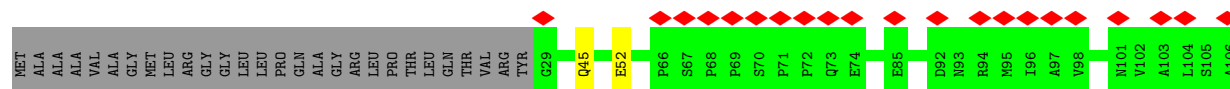
- Molecule 41: 39S ribosomal protein L4, mitochondrial

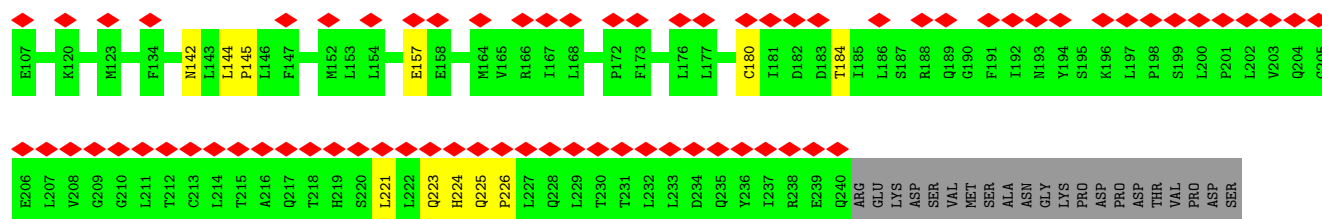
Chain F: 



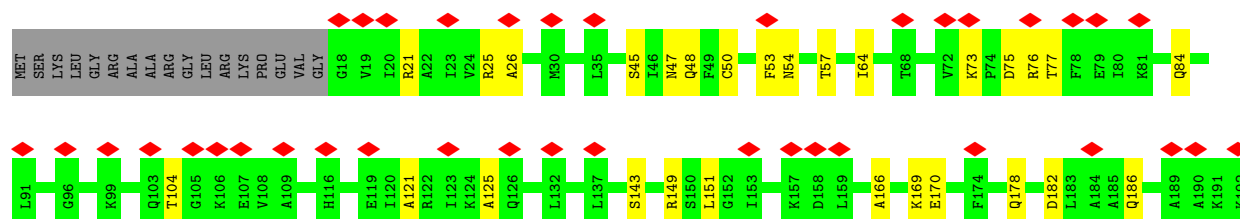
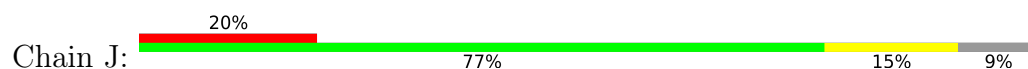
- Molecule 42: 39S ribosomal protein L10, mitochondrial

Chain I: 

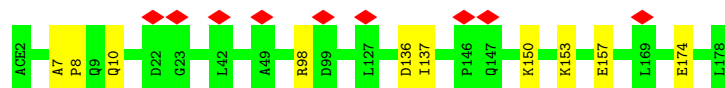




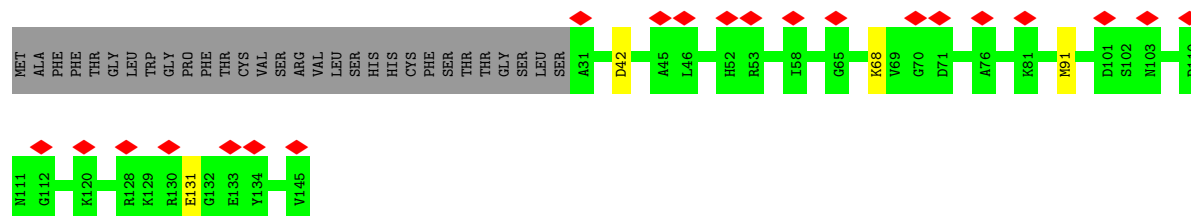
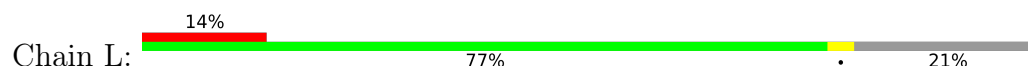
- Molecule 43: 39S ribosomal protein L11, mitochondrial



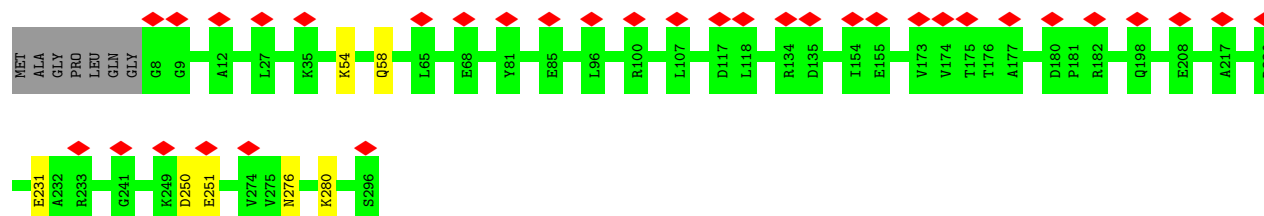
- Molecule 44: Large ribosomal subunit protein uL13m



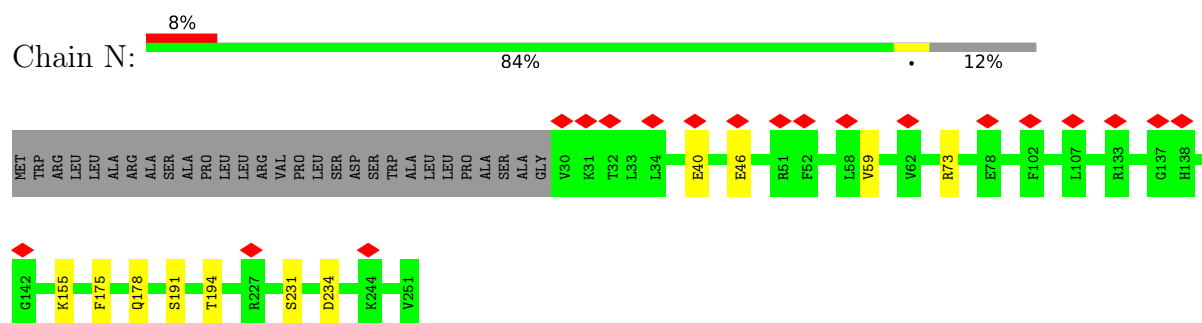
- Molecule 45: 39S ribosomal protein L14, mitochondrial



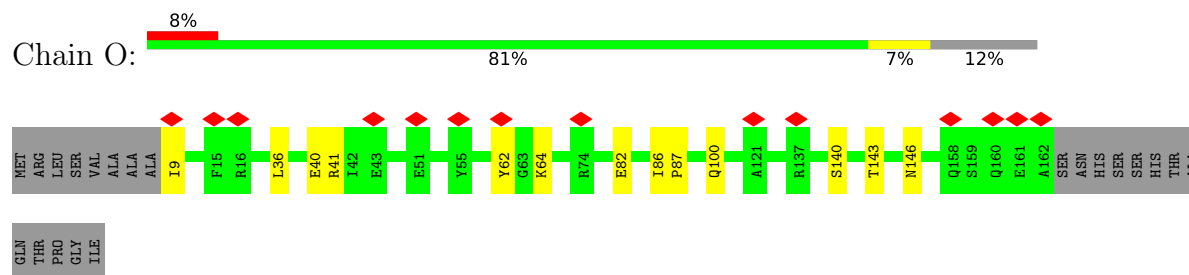
- Molecule 46: 39S ribosomal protein L15, mitochondrial



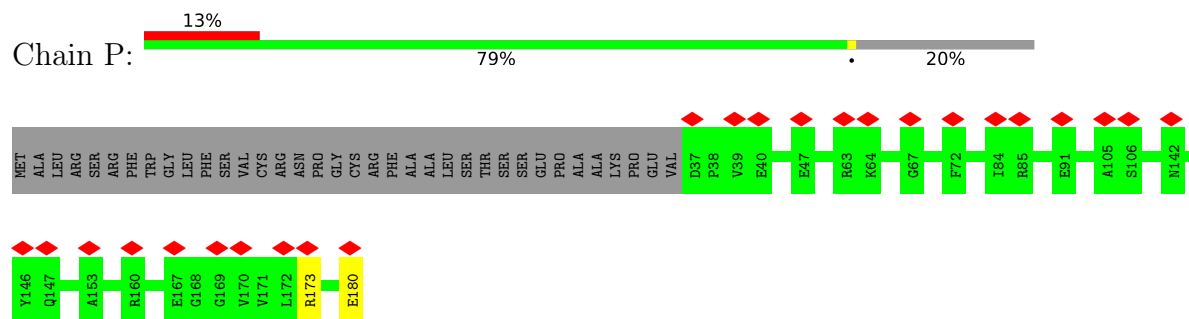
- Molecule 47: 39S ribosomal protein L16, mitochondrial



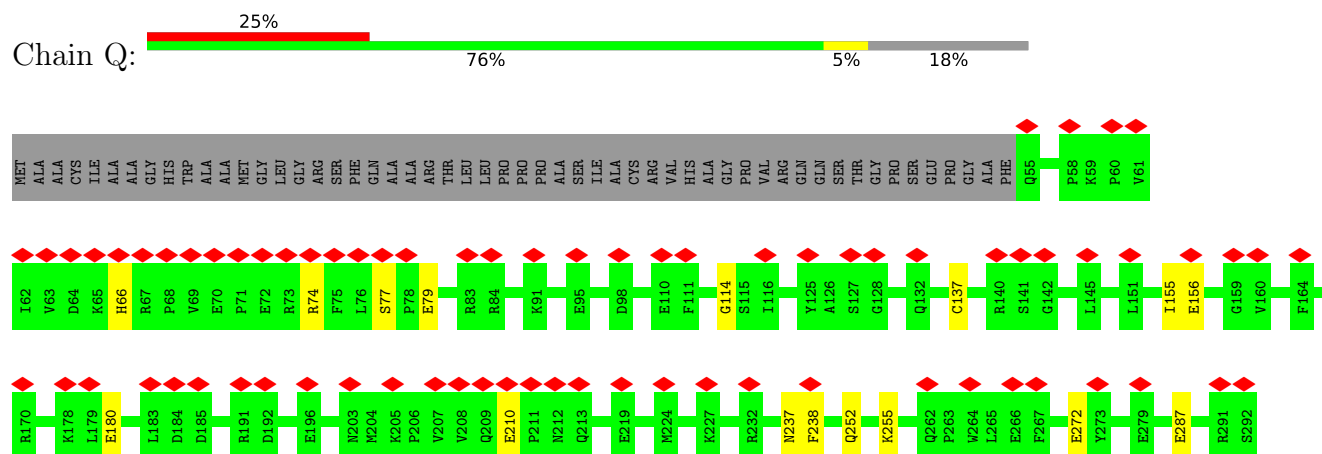
- Molecule 48: 39S ribosomal protein L17, mitochondrial



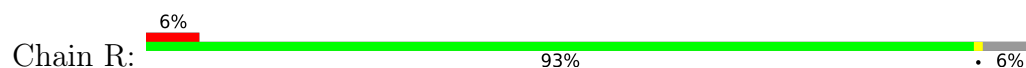
- Molecule 49: 39S ribosomal protein L18, mitochondrial

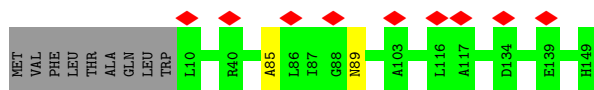


- Molecule 50: 39S ribosomal protein L19, mitochondrial



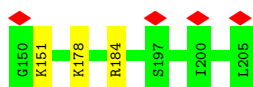
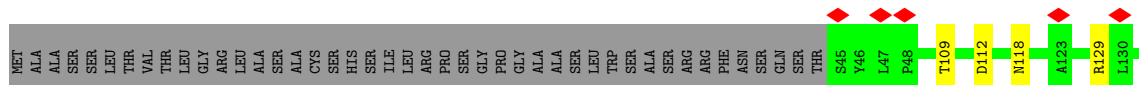
- Molecule 51: 39S ribosomal protein L20, mitochondrial





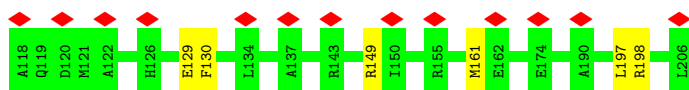
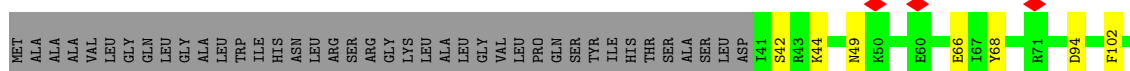
- Molecule 52: 39S ribosomal protein L21, mitochondrial

Chain S: 75% 21%



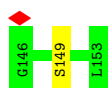
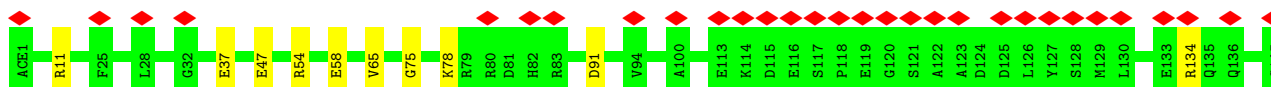
- Molecule 53: 39S ribosomal protein L22, mitochondrial

Chain T: 8% 74% 6% 19%



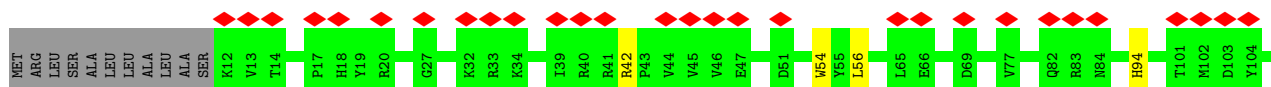
- Molecule 54: Large ribosomal subunit protein uL23m

Chain U: 20% 93% 7%

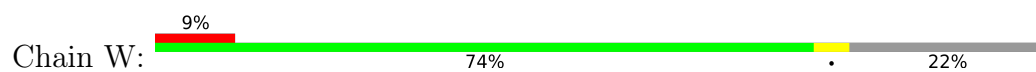


- Molecule 55: 39S ribosomal protein L24, mitochondrial

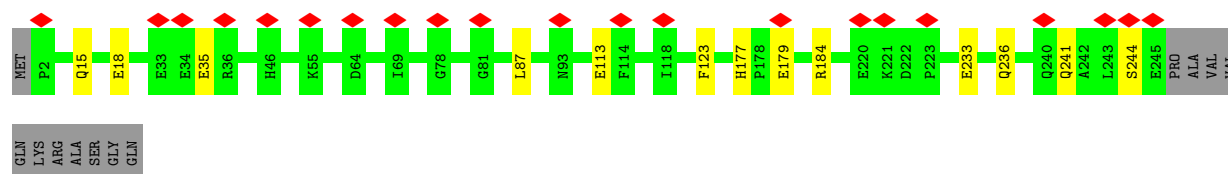
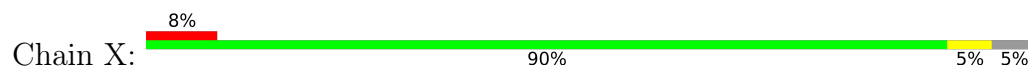
Chain V: 21% 88% 6% 5%



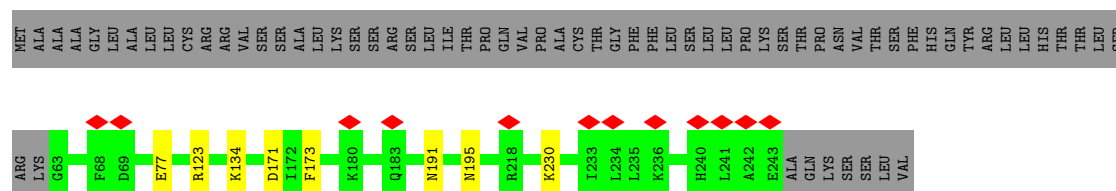
- Molecule 56: 39S ribosomal protein L27, mitochondrial



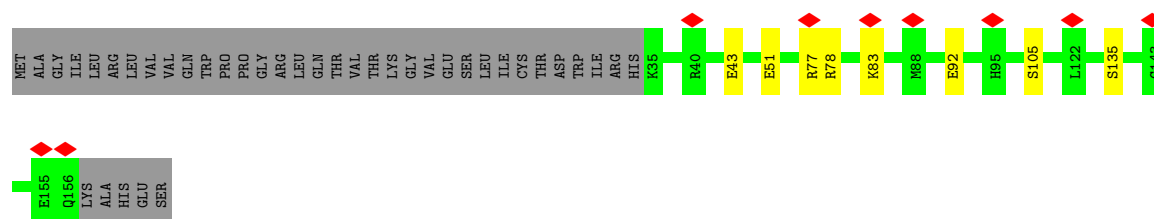
- Molecule 57: 39S ribosomal protein L28, mitochondrial



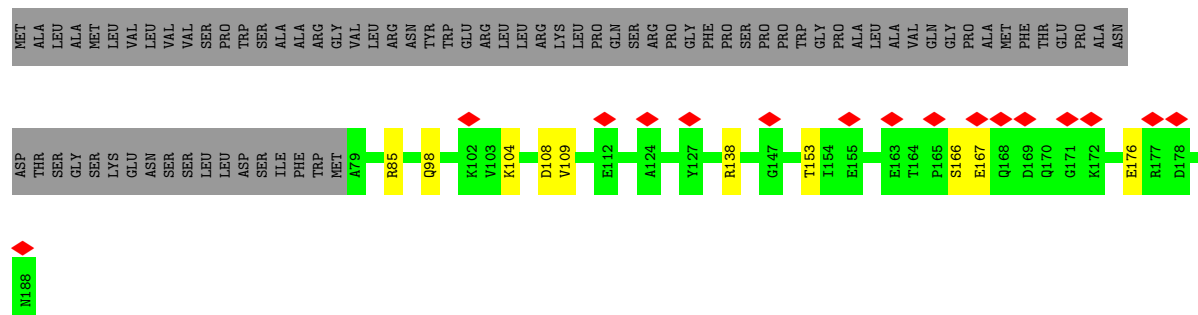
- Molecule 58: 39S ribosomal protein L47, mitochondrial



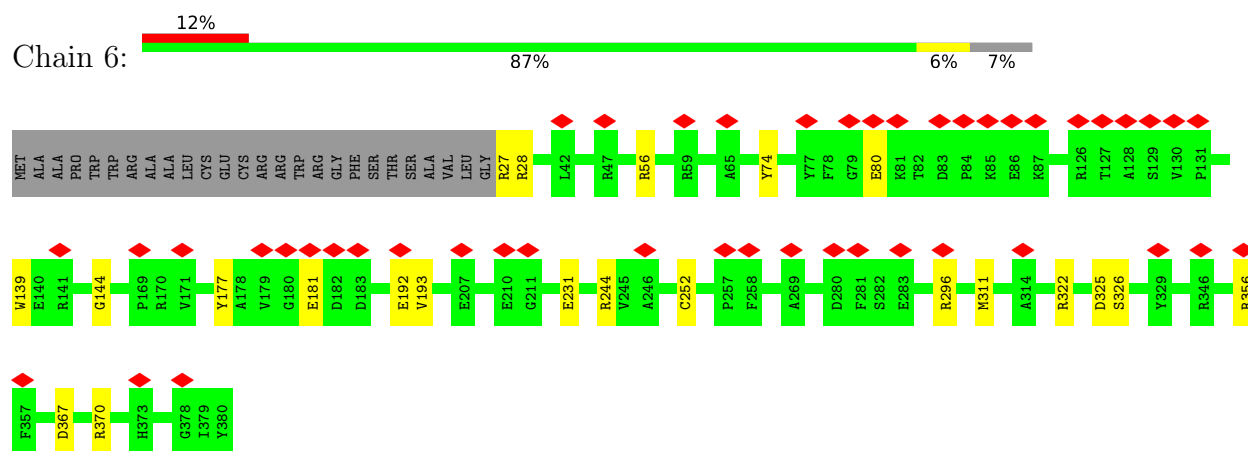
- Molecule 59: 39S ribosomal protein L30, mitochondrial



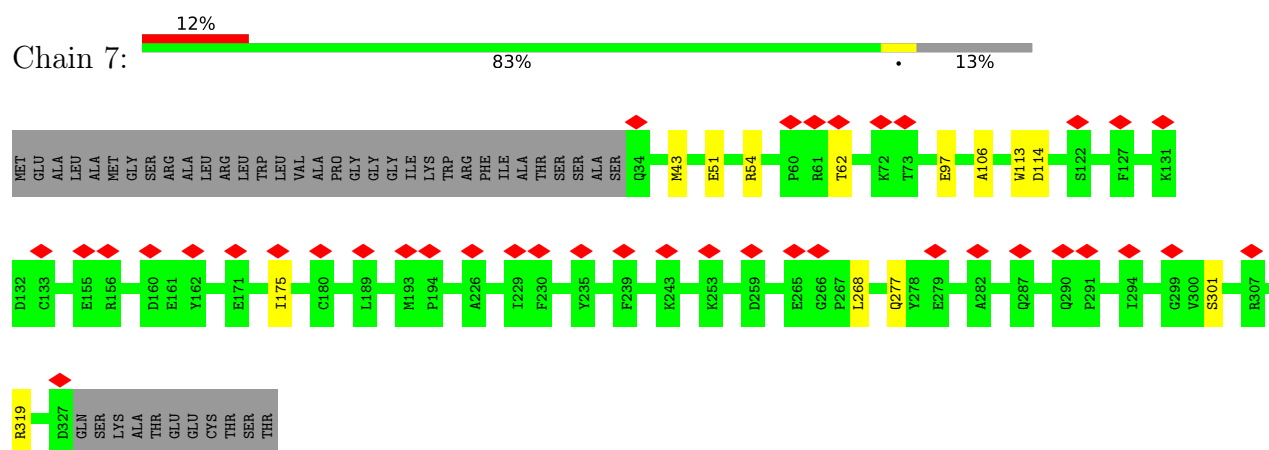
- Molecule 60: 39S ribosomal protein L32, mitochondrial



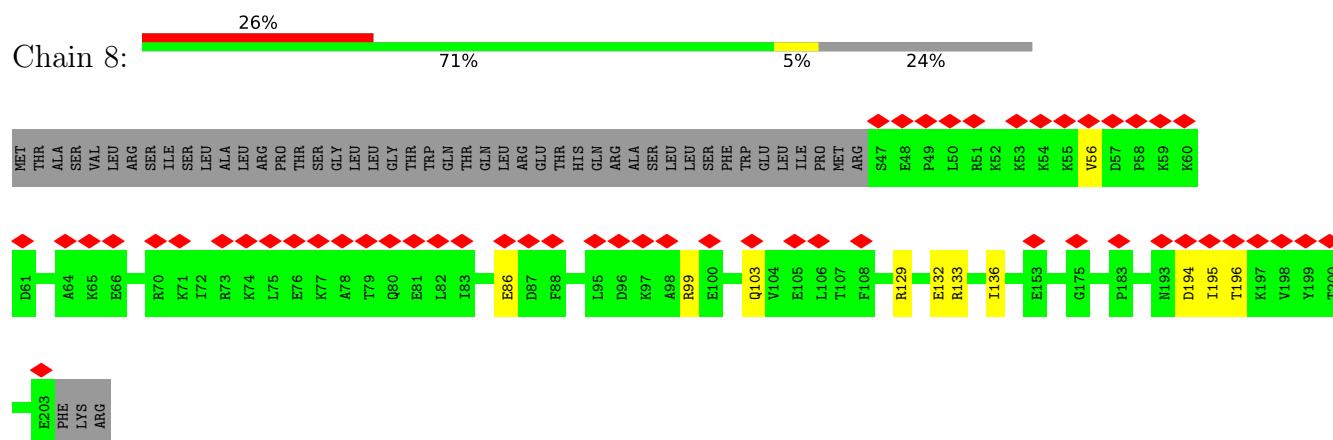
- Molecule 66: 39S ribosomal protein L38, mitochondrial



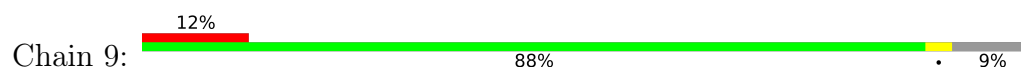
- Molecule 67: 39S ribosomal protein L39, mitochondrial

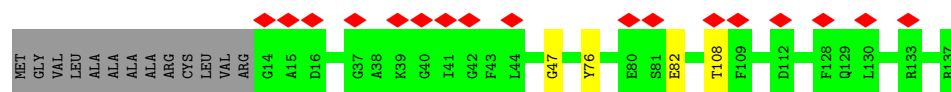


- Molecule 68: 39S ribosomal protein L40, mitochondrial

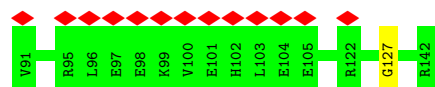
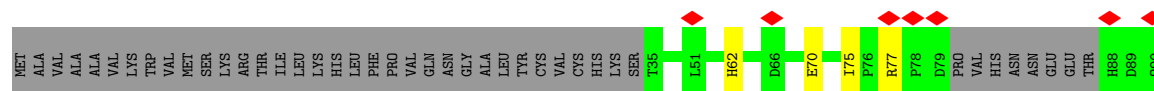


- Molecule 69: 39S ribosomal protein L41, mitochondrial

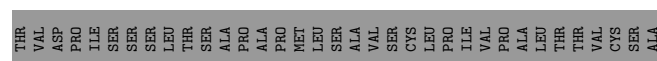
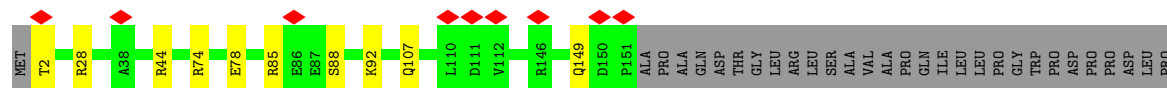




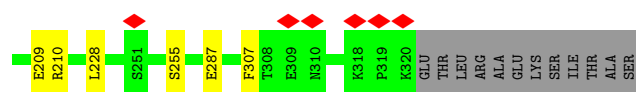
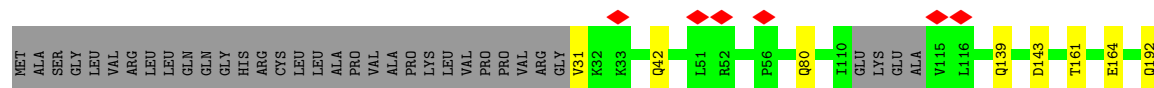
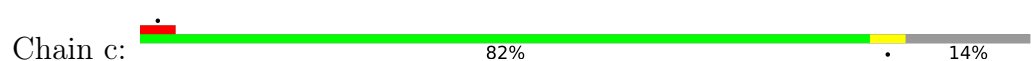
- Molecule 70: 39S ribosomal protein L42, mitochondrial



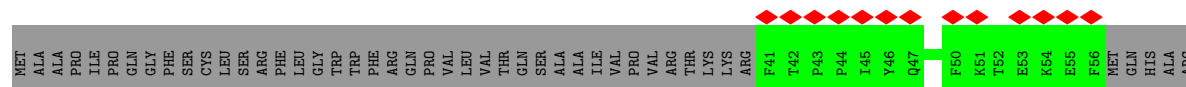
- Molecule 71: 39S ribosomal protein L43, mitochondrial



- Molecule 72: 39S ribosomal protein L44, mitochondrial

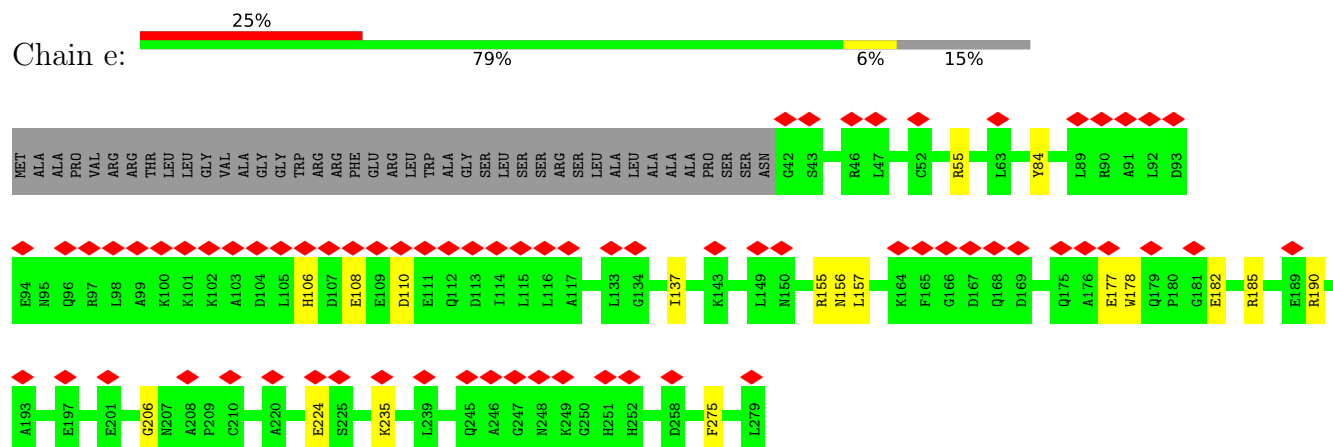


- Molecule 73: 39S ribosomal protein L45, mitochondrial

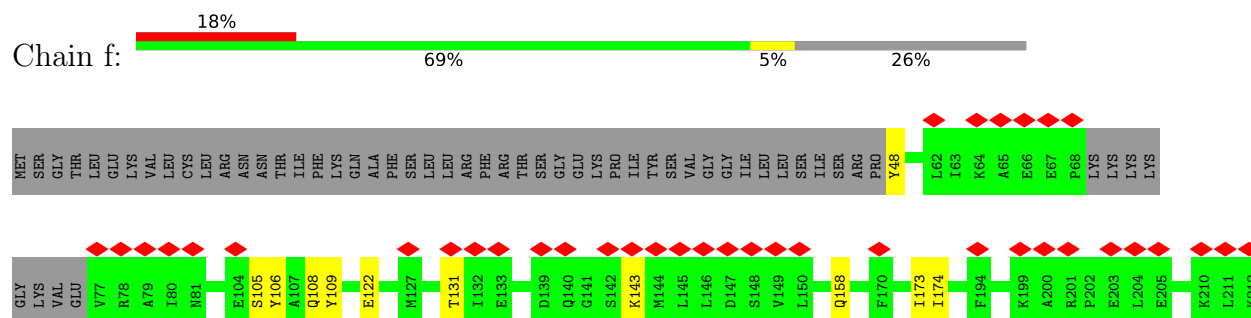


ALA
GLN
LYS
PRO
GLN
LEU
ALA

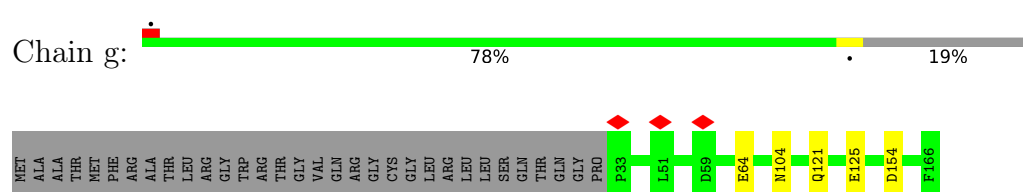
- Molecule 74: 39S ribosomal protein L46, mitochondrial



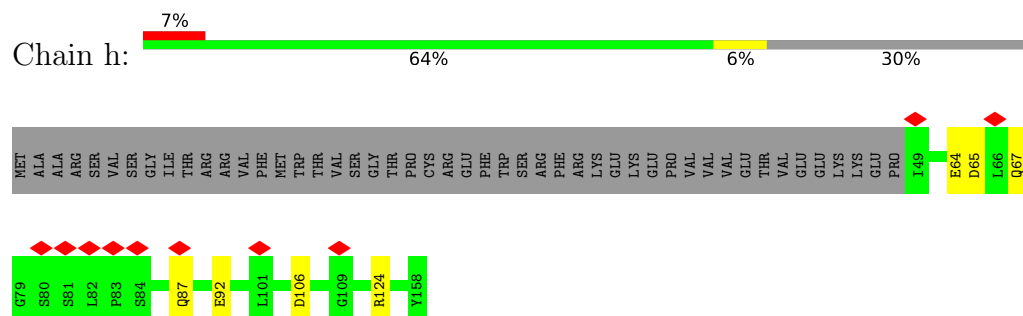
- Molecule 75: 39S ribosomal protein L48, mitochondrial



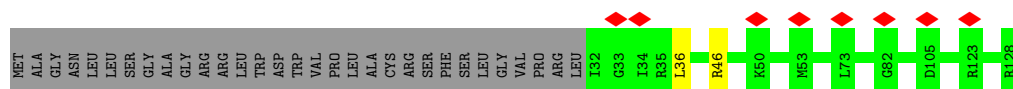
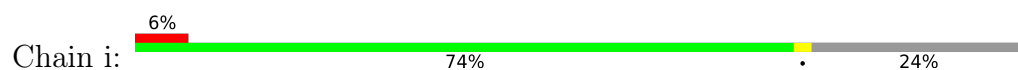
- Molecule 76: 39S ribosomal protein L49, mitochondrial



- Molecule 77: 39S ribosomal protein L50, mitochondrial



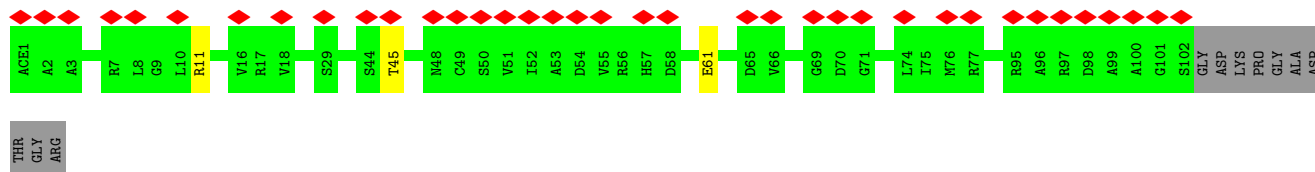
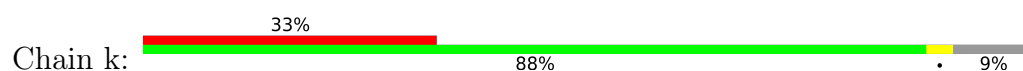
- Molecule 78: 39S ribosomal protein L51, mitochondrial



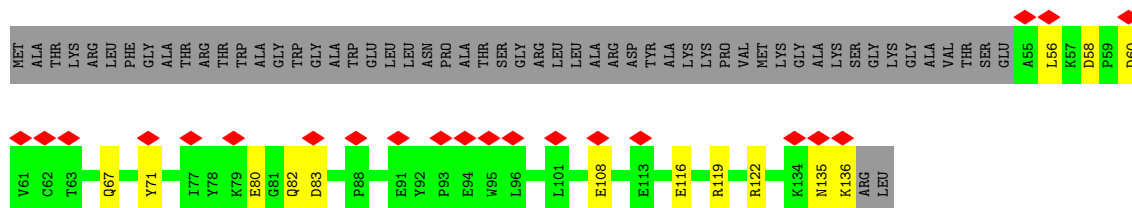
- Molecule 79: 39S ribosomal protein L52, mitochondrial



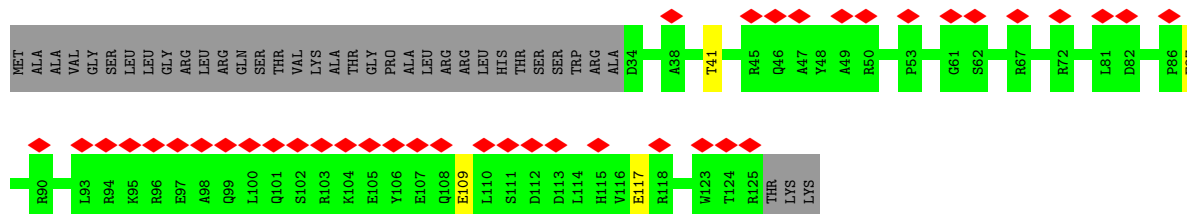
- Molecule 80: Large ribosomal subunit protein mL53



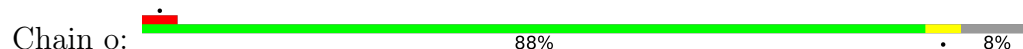
- Molecule 81: 39S ribosomal protein L54, mitochondrial

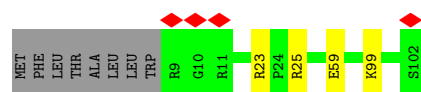


- Molecule 82: 39S ribosomal protein L55, mitochondrial

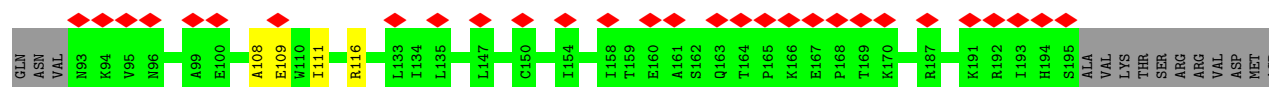
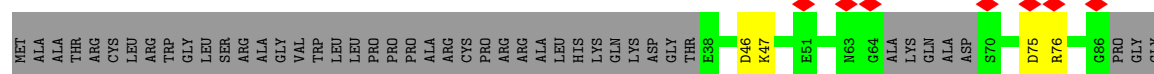


- Molecule 83: Ribosomal protein 63, mitochondrial

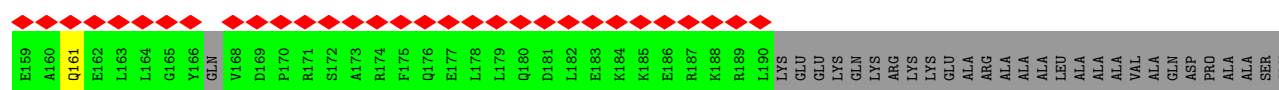
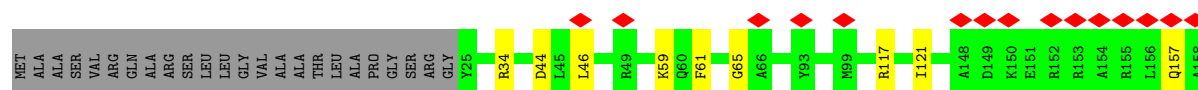




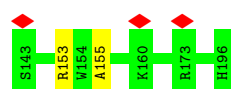
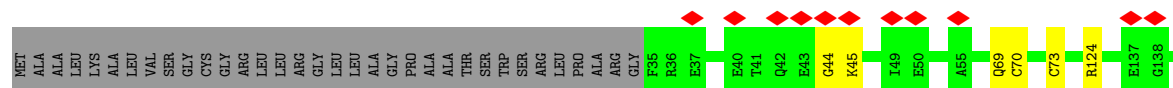
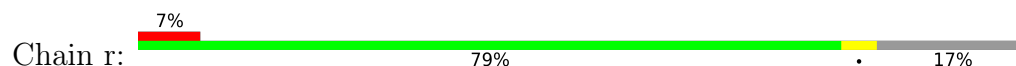
- Molecule 84: Peptidyl-tRNA hydrolase ICT1, mitochondrial



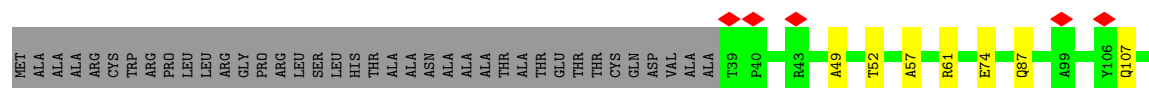
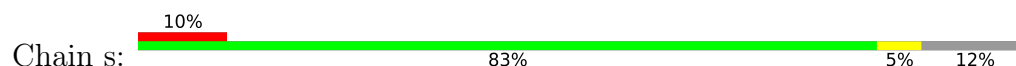
- Molecule 85: Growth arrest and DNA damage-inducible proteins-interacting protein 1



- Molecule 86: 39S ribosomal protein S18a, mitochondrial

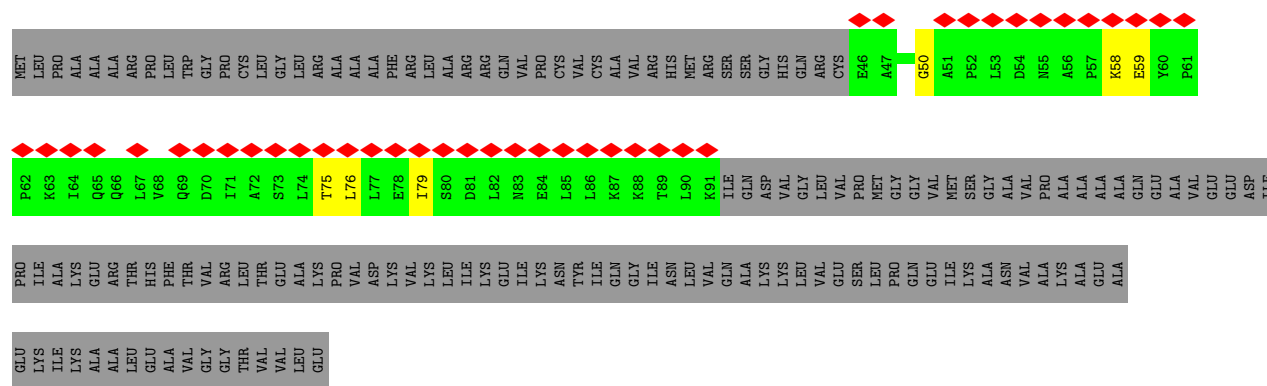


- Molecule 87: 39S ribosomal protein S30, mitochondrial

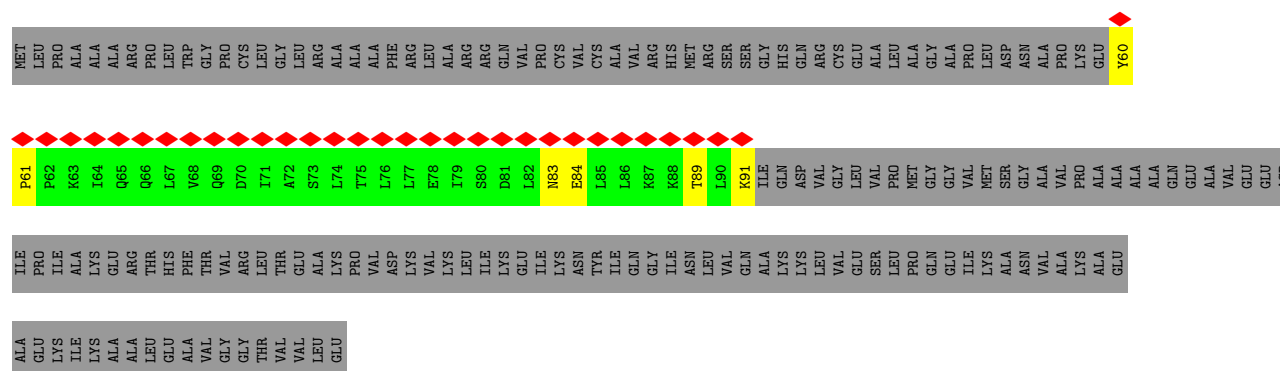




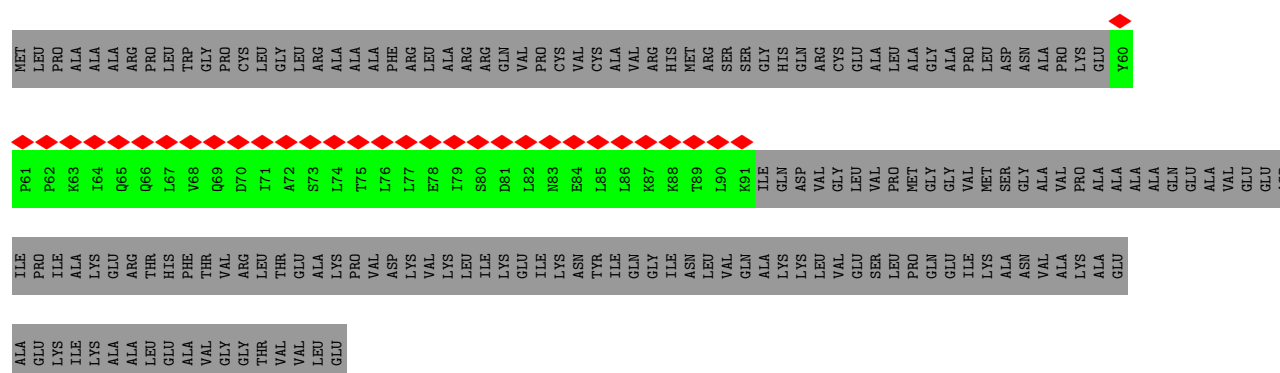
- Molecule 88: 39S ribosomal protein L12, mitochondrial



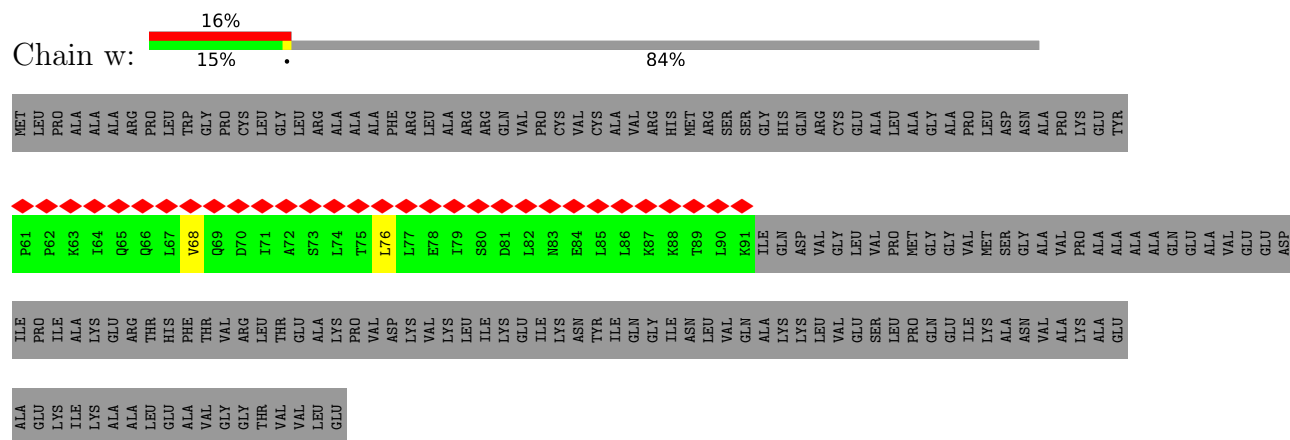
- Molecule 88: 39S ribosomal protein L12, mitochondrial



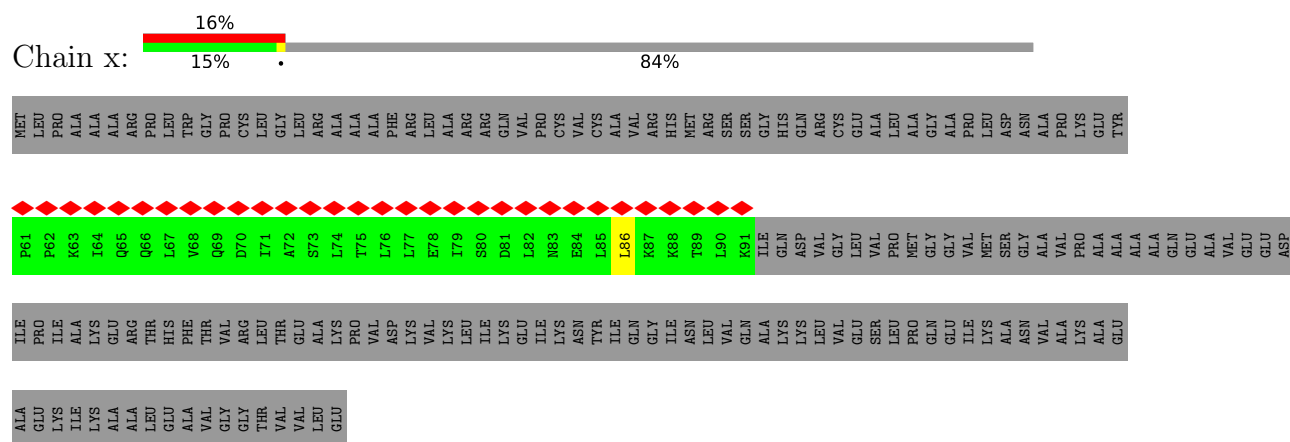
- Molecule 88: 39S ribosomal protein L12, mitochondrial



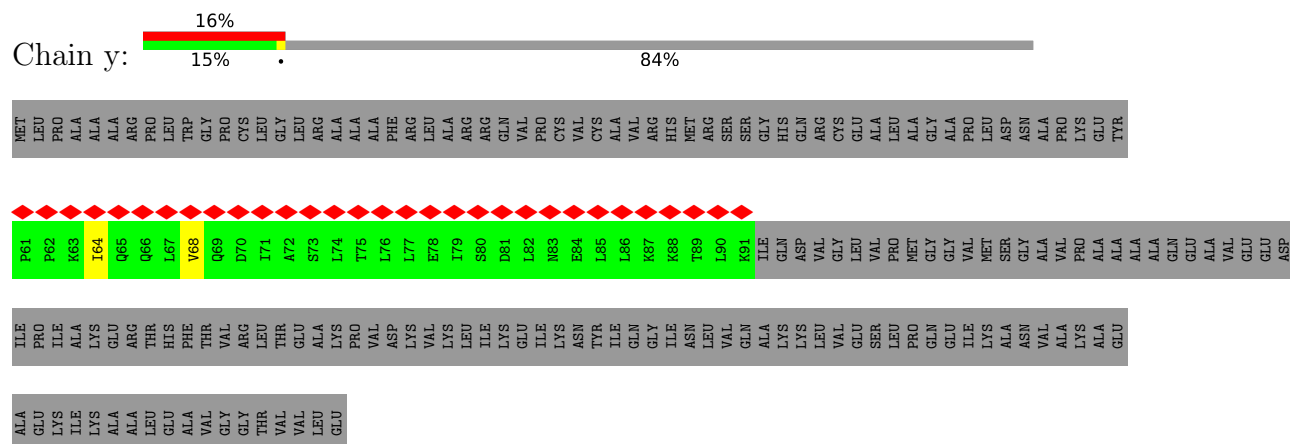
• Molecule 88: 39S ribosomal protein L12, mitochondrial



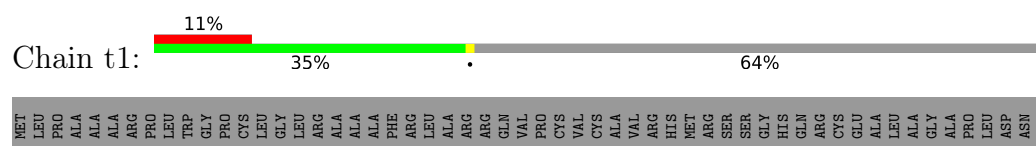
• Molecule 88: 39S ribosomal protein L12, mitochondrial



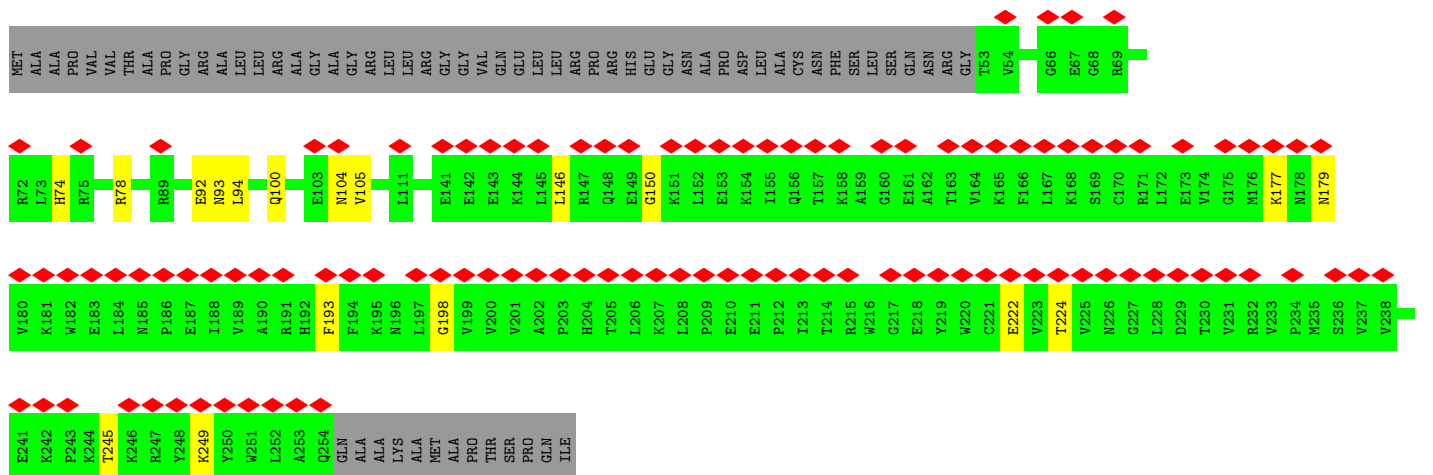
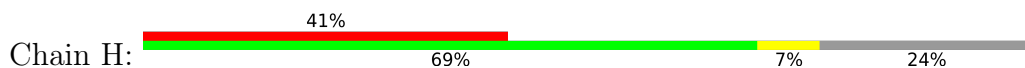
• Molecule 88: 39S ribosomal protein L12, mitochondrial



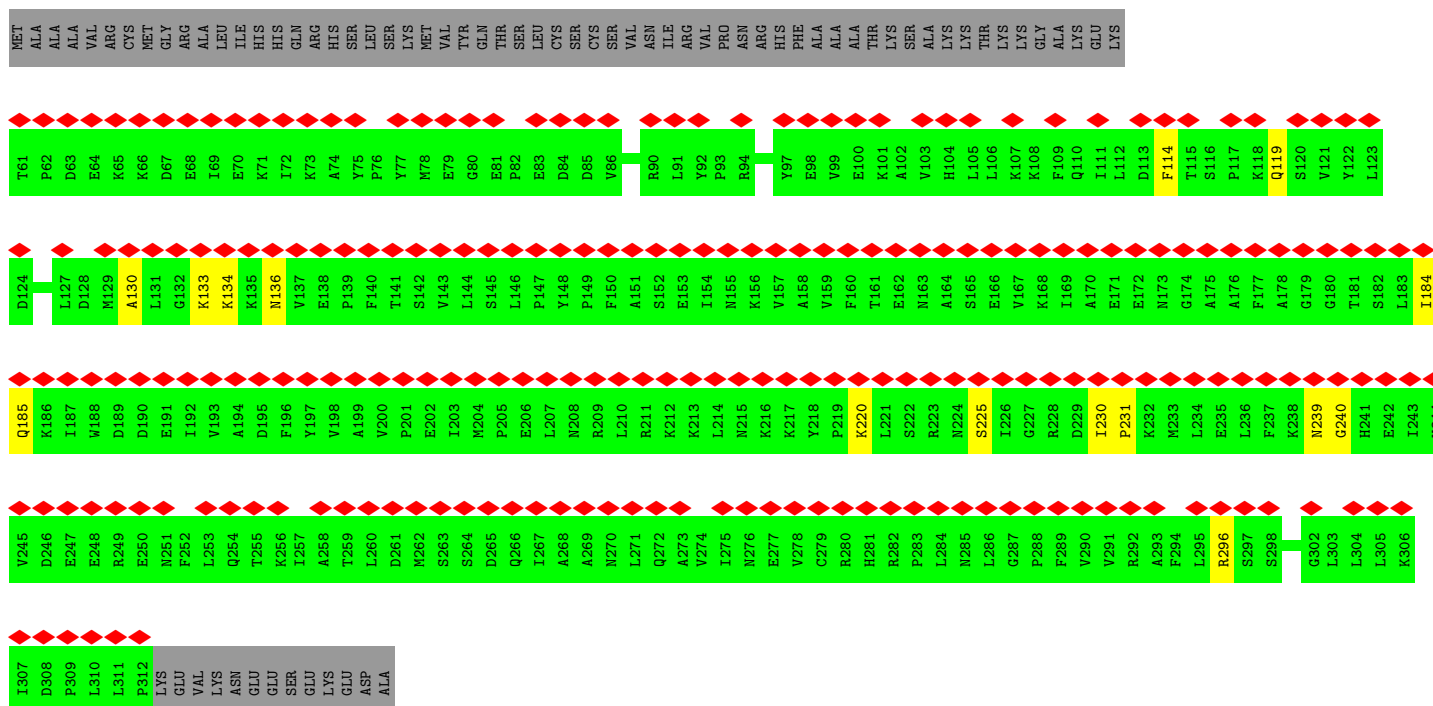
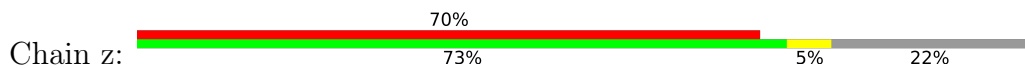
• Molecule 88: 39S ribosomal protein L12, mitochondrial



- Molecule 89: 39S ribosomal protein L9, mitochondrial



- Molecule 90: 39S ribosomal protein L1, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7024	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.648	Depositor
Minimum map value	-0.235	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.164	Depositor
Map size (Å)	528.128, 528.128, 528.128	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82519996, 0.82519996, 0.82519996	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, ACE, ZN, SPD, 5MU, K, B8T, GDP, THC, OMG, 1MA, MG, 2MG, ATP, OMU, 5F0, 5MC, PSU, FES, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A5	0.13	0/1726	0.34	0/2314
2	AA	0.08	0/22537	0.19	0/35085
3	AB	0.08	0/1871	0.23	0/2531
4	AC	0.15	0/1113	0.27	0/1505
5	AD	0.09	0/2783	0.23	0/3724
6	AE	0.08	0/989	0.23	0/1335
7	AF	0.08	0/1767	0.21	0/2373
8	AG	0.08	0/2746	0.22	0/3681
9	AH	0.08	0/1178	0.23	0/1598
10	AI	0.08	0/1030	0.21	0/1386
11	AJ	0.11	0/855	0.29	0/1148
12	AK	0.07	0/880	0.20	0/1182
13	AL	0.08	0/1477	0.20	0/1974
14	AM	0.08	0/963	0.24	0/1295
15	AN	0.08	0/886	0.23	0/1199
16	AO	0.08	0/1648	0.23	0/2243
17	AP	0.10	0/798	0.24	0/1070
18	AQ	0.14	0/754	0.24	0/1003
19	AR	0.07	0/2456	0.20	0/3317
20	AS	0.11	0/1138	0.25	0/1533
21	AT	0.08	0/1402	0.22	0/1883
22	AU	0.07	0/1510	0.19	0/2025
23	AV	0.07	0/3030	0.20	0/4093
24	AW	0.08	0/801	0.23	0/1079
25	AX	0.07	0/2921	0.21	0/3954
26	AY	0.08	0/1280	0.20	0/1725
27	AZ	0.08	0/857	0.22	0/1141
28	A0	0.08	0/1834	0.23	0/2484
29	A1	0.08	0/2304	0.22	0/3117
30	A2	0.14	0/947	0.27	0/1266
31	A3	0.09	0/636	0.25	0/839

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	A4	0.08	0/4877	0.22	0/6598
33	Aw	0.11	0/1590	0.23	0/2459
34	Ax	0.06	0/1654	0.14	0/2565
35	Ay	0.06	0/1305	0.16	0/2023
36	Az	0.07	0/803	0.19	0/1246
37	A	0.10	0/36850	0.21	0/57359
38	B	0.06	0/1626	0.15	0/2523
39	D	0.08	0/1896	0.22	0/2549
40	E	0.10	0/2475	0.24	0/3355
41	F	0.08	0/2090	0.23	0/2842
42	I	0.12	0/1731	0.28	0/2345
43	J	0.11	0/1348	0.28	0/1813
44	K	0.11	0/1497	0.25	0/2031
45	L	0.09	0/905	0.25	0/1218
46	M	0.08	0/2368	0.23	0/3195
47	N	0.08	0/1833	0.23	0/2468
48	O	0.07	0/1283	0.23	0/1727
49	P	0.07	0/1199	0.21	0/1623
50	Q	0.08	0/2027	0.22	0/2734
51	R	0.08	0/1175	0.19	0/1572
52	S	0.08	0/1320	0.23	0/1789
53	T	0.08	0/1403	0.22	0/1886
54	U	0.12	0/1280	0.23	0/1732
55	V	0.10	0/1721	0.23	0/2333
56	W	0.09	0/926	0.22	0/1244
57	X	0.08	0/2099	0.20	0/2837
58	Y	0.08	0/1593	0.19	0/2136
59	Z	0.09	0/1021	0.23	0/1378
60	0	0.09	0/913	0.22	0/1224
61	1	0.08	0/469	0.23	0/621
62	2	0.09	0/383	0.22	0/507
63	3	0.08	0/853	0.22	0/1136
64	4	0.09	0/350	0.22	0/461
65	5	0.08	0/3305	0.22	0/4502
66	6	0.12	0/3043	0.24	0/4140
67	7	0.08	0/2447	0.22	0/3310
68	8	0.10	0/1354	0.26	0/1819
69	9	0.08	0/1025	0.22	0/1379
70	a	0.09	0/866	0.23	0/1174
71	b	0.17	0/1211	0.22	0/1639
72	c	0.08	0/2347	0.21	0/3171
73	d	0.09	0/2003	0.24	0/2713
74	e	0.07	0/1970	0.21	0/2658

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	f	0.08	0/1273	0.20	0/1716
76	g	0.08	0/1151	0.22	0/1569
77	h	0.12	0/918	0.23	0/1249
78	i	0.10	0/850	0.23	0/1135
79	j	0.09	0/760	0.22	0/1023
80	k	0.14	0/783	0.24	0/1057
81	l	0.10	0/707	0.26	0/960
82	m	0.07	0/805	0.21	0/1081
83	o	0.09	0/819	0.23	0/1097
84	p	0.08	0/1223	0.21	0/1641
85	q	0.08	0/1422	0.19	0/1916
86	r	0.08	0/1362	0.24	0/1846
87	s	0.08	0/3239	0.22	0/4400
88	t	0.11	0/358	0.30	0/486
88	t1	0.10	0/550	0.27	0/740
88	u	0.10	0/259	0.23	0/350
88	v	0.06	0/259	0.16	0/350
88	w	0.08	0/246	0.22	0/331
88	x	0.07	0/246	0.18	0/331
88	y	0.14	0/246	0.26	0/331
89	H	0.09	0/1698	0.24	0/2292
90	z	0.09	0/2067	0.27	0/2793
All	All	0.09	0/192792	0.22	0/273830

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	AI	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	AI	184	5F0	Mainchain

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	A5	1708	1715	1716	38	0
2	AA	20260	10258	10287	98	0
3	AB	1828	1815	1815	8	0
4	AC	1083	1088	1088	5	0
5	AD	2731	2804	2804	15	0
6	AE	972	1000	1000	8	0
7	AF	1725	1769	1769	8	0
8	AG	2688	2687	2687	10	0
9	AH	1152	1183	1183	7	0
10	AI	1020	1052	1053	3	0
11	AJ	839	885	885	15	0
12	AK	862	885	885	1	0
13	AL	1453	1540	1540	7	0
14	AM	942	965	965	9	0
15	AN	868	928	928	7	0
16	AO	1592	1557	1557	12	0
17	AP	781	806	806	8	0
18	AQ	744	758	758	7	0
19	AR	2409	2428	2428	7	0
20	AS	1111	1115	1115	13	0
21	AT	1371	1393	1393	6	0
22	AU	1488	1499	1499	10	0
23	AV	2969	2961	2961	15	0
24	AW	789	802	802	10	0
25	AX	2849	2843	2843	9	0
26	AY	1246	1197	1197	5	0
27	AZ	839	858	858	6	0
28	A0	1787	1796	1796	13	0
29	A1	2256	2289	2288	13	0
30	A2	935	971	971	11	0
31	A3	625	699	699	5	0
32	A4	4768	4766	4766	23	0
33	Aw	1427	720	723	12	0
34	Ax	1482	750	752	3	0
35	Ay	1169	592	594	4	0
36	Az	718	361	360	4	0
37	A	33048	16765	16787	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	B	1524	771	780	3	0
39	D	1859	1920	1919	12	0
40	E	2406	2415	2415	6	0
41	F	2031	2065	2065	5	0
42	I	1695	1785	1785	13	0
43	J	1330	1407	1407	19	0
44	K	1455	1452	1452	7	0
45	L	890	942	941	3	0
46	M	2314	2384	2384	4	0
47	N	1786	1817	1817	7	0
48	O	1259	1294	1294	9	0
49	P	1173	1165	1165	2	0
50	Q	1979	2022	2022	10	0
51	R	1154	1214	1214	1	0
52	S	1293	1365	1365	5	0
53	T	1369	1410	1410	10	0
54	U	1251	1232	1232	9	0
55	V	1676	1687	1687	11	0
56	W	904	935	935	6	0
57	X	2044	2060	2060	9	0
58	Y	1556	1597	1597	7	0
59	Z	996	1044	1044	8	0
60	0	898	916	916	8	0
61	1	464	511	511	3	0
62	2	377	406	406	1	0
63	3	832	883	883	3	0
64	4	342	361	361	1	0
65	5	3210	3206	3206	9	0
66	6	2948	2841	2841	17	0
67	7	2390	2397	2397	8	0
68	8	1327	1368	1368	9	0
69	9	997	987	987	4	0
70	a	840	810	810	5	0
71	b	1196	1195	1190	7	0
72	c	2299	2320	2320	12	0
73	d	1949	1930	1930	19	0
74	e	1931	1916	1916	11	0
75	f	1252	1269	1269	9	0
76	g	1113	1097	1097	4	0
77	h	895	881	881	6	0
78	i	828	857	857	2	0
79	j	745	746	746	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	k	774	784	784	2	0
81	l	688	674	674	10	0
82	m	791	797	796	4	0
83	o	798	804	804	4	0
84	p	1205	1223	1223	6	0
85	q	1389	1374	1374	6	0
86	r	1322	1348	1348	5	0
87	s	3155	3139	3139	16	0
88	t	354	377	377	7	0
88	t1	546	599	599	1	0
88	u	257	283	283	4	0
88	v	257	283	283	0	0
88	w	245	275	275	5	0
88	x	245	275	275	1	0
88	y	245	275	275	3	0
89	H	1661	1734	1734	15	0
90	z	2027	2076	2076	11	0
91	AA	44	25	25	2	0
92	A	136	0	0	0	0
92	AA	55	0	0	0	0
92	AB	1	0	0	0	0
92	AX	1	0	0	0	0
92	Az	1	0	0	0	0
92	D	1	0	0	0	0
93	A	24	0	0	0	0
93	AA	13	0	0	0	0
93	D	1	0	0	0	0
93	M	1	0	0	0	0
94	0	1	0	0	0	0
94	4	1	0	0	0	0
94	AO	1	0	0	0	0
95	AP	4	0	0	0	0
95	AT	4	0	0	0	0
95	r	4	0	0	0	0
96	AX	31	12	12	0	0
97	AX	28	10	12	0	0
98	A	10	21	19	0	0
99	e	7	8	8	0	0
All	All	183639	155776	155835	813	0

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

All (813) 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)
2:AA:1076:5MU:C4	2:AA:1076:5MU:C5	1.80	1.69
54:U:11:ARG:NH1	55:V:212:LYS:O	2.05	0.89
37:A:2125:C:OP2	52:S:178:LYS:NZ	2.08	0.86
59:Z:105:SER:OG	83:o:59:GLU:OE2	1.96	0.83
37:A:1777:A:N6	37:A:1780:U:OP2	2.13	0.82
43:J:25:ARG:NH1	81:l:58:ASP:OD1	2.15	0.79
37:A:2325:U:O2'	48:O:82:GLU:OE2	2.00	0.78
2:AA:1166:A:OP2	11:AJ:114:ARG:NH2	2.16	0.78
66:6:367:ASP:OD1	66:6:370:ARG:NH1	2.16	0.78
79:j:101:GLU:OE2	79:j:105:GLN:NE2	2.16	0.78
32:A4:433:TYR:OH	32:A4:469:GLU:OE1	2.01	0.77
65:5:243:GLU:N	65:5:243:GLU:OE1	2.18	0.76
53:T:102:PHE:O	60:0:104:LYS:NZ	2.18	0.76
88:u:83:ASN:OD1	88:u:84:GLU:N	2.19	0.75
71:b:28:ARG:NH1	71:b:78:GLU:OE1	2.20	0.75
73:d:244:GLU:N	73:d:244:GLU:OE1	2.20	0.74
7:AF:174:LEU:O	7:AF:179:ARG:NH1	2.21	0.74
2:AA:1199:G:N1	2:AA:1422:G:OP2	2.21	0.74
2:AA:1583:MA6:H93	2:AA:1584:MA6:H92	1.69	0.73
32:A4:200:ASP:OD2	32:A4:243:ASN:N	2.20	0.73
23:AV:252:LYS:O	23:AV:258:ARG:NH2	2.22	0.73
73:d:86:ASP:OD2	73:d:198:ARG:NH2	2.21	0.73
24:AW:110:ASN:OD1	24:AW:126:ARG:N	2.20	0.73
28:A0:88:GLN:OE1	28:A0:88:GLN:N	2.21	0.73
74:e:235:LYS:NZ	74:e:275:PHE:O	2.19	0.72
42:I:52:GLU:N	42:I:52:GLU:OE1	2.21	0.72
21:AT:14:GLN:N	21:AT:14:GLN:OE1	2.23	0.72
59:Z:78:ARG:O	59:Z:83:LYS:NZ	2.21	0.72
89:H:104:ASN:OD1	89:H:105:VAL:N	2.22	0.72
5:AD:284:ARG:NH1	5:AD:287:ASP:OD1	2.23	0.72
2:AA:1454:G:OP2	8:AG:377:ARG:NH1	2.23	0.72
17:AP:140:TYR:OH	18:AQ:33:ASP:OD1	2.07	0.72
37:A:2256:U:O2'	52:S:118:ASN:ND2	2.21	0.72
37:A:2499:U:O2	37:A:2503:A:N6	2.23	0.71
9:AH:180:LEU:O	9:AH:185:LYS:NZ	2.22	0.71
37:A:1747:G:OP2	37:A:1749:C:N4	2.23	0.71
66:6:80:GLU:OE1	66:6:80:GLU:N	2.24	0.71
79:j:102:GLN:OE1	79:j:102:GLN:N	2.22	0.71
54:U:134:ARG:O	54:U:134:ARG:NH1	2.23	0.71
77:h:87:GLN:OE1	77:h:124:ARG:NH1	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A4:430:GLU:N	32:A4:430:GLU:OE1	2.24	0.70
32:A4:616:ASP:OD1	32:A4:617:SER:N	2.25	0.70
41:F:76:ARG:NH2	77:h:106:ASP:OD1	2.25	0.70
2:AA:1520:U:OP2	23:AV:407:GLN:NE2	2.23	0.70
37:A:2169:A:OP1	43:J:21:ARG:NH1	2.25	0.69
73:d:292:GLU:N	73:d:292:GLU:OE1	2.24	0.69
2:AA:1358:A:O2'	34:Ax:30:G:OP1	2.10	0.69
87:s:385:GLN:N	87:s:385:GLN:OE1	2.25	0.69
21:AT:138:GLU:OE1	21:AT:138:GLU:N	2.25	0.69
43:J:84:GLN:OE1	43:J:84:GLN:N	2.26	0.69
44:K:136:ASP:OD1	44:K:137:ILE:N	2.25	0.69
29:A1:100:GLU:N	29:A1:100:GLU:OE1	2.25	0.69
37:A:2499:U:OP2	37:A:2504:A:N6	2.25	0.68
11:AJ:74:ASN:ND2	11:AJ:117:ASP:OD1	2.26	0.68
23:AV:321:GLU:OE1	23:AV:321:GLU:N	2.26	0.68
33:Aw:9:A:OP1	33:Aw:21:A:N6	2.26	0.68
54:U:75:GLY:N	54:U:91:ASP:OD1	2.26	0.68
82:m:87:GLU:OE1	82:m:87:GLU:N	2.26	0.68
42:I:225:GLN:NE2	88:y:68:VAL:HG13	2.09	0.68
11:AJ:53:GLU:OE2	11:AJ:89:ARG:NH2	2.27	0.68
58:Y:134:LYS:NZ	69:9:76:TYR:OH	2.26	0.68
32:A4:241:LYS:HD2	32:A4:241:LYS:O	1.94	0.67
10:AI:103:SER:OG	10:AI:105:GLU:OE1	2.11	0.67
37:A:3068:G:OP2	37:A:3068:G:N2	2.26	0.67
16:AO:73:VAL:O	16:AO:109:ARG:NH2	2.27	0.67
26:AY:374:GLU:OE2	26:AY:378:ASN:ND2	2.27	0.67
32:A4:451:ASP:OD1	32:A4:452:GLN:N	2.27	0.67
42:I:225:GLN:HE22	88:y:68:VAL:HG13	1.60	0.67
21:AT:39:GLU:N	21:AT:39:GLU:OE1	2.25	0.67
27:AZ:6:GLU:N	27:AZ:6:GLU:OE1	2.28	0.67
55:V:139:GLU:N	55:V:139:GLU:OE1	2.28	0.67
75:f:106:TYR:OH	75:f:174:ILE:O	2.13	0.66
73:d:192:SER:OG	73:d:216:MET:SD	2.49	0.66
81:l:135:ASN:OD1	81:l:136:LYS:N	2.28	0.66
37:A:1805:A:OP2	55:V:94:HIS:NE2	2.24	0.66
2:AA:952:A:N3	2:AA:954:C:N4	2.44	0.65
8:AG:72:ASP:OD1	8:AG:73:PHE:N	2.29	0.65
20:AS:18:ASP:OD1	20:AS:21:ARG:NH2	2.29	0.65
37:A:2261:C:O2'	52:S:184:ARG:NH1	2.28	0.65
88:t:76:LEU:HA	88:t:79:ILE:HG22	1.78	0.65
19:AR:200:GLU:N	19:AR:200:GLU:OE1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Q:155:ILE:HG22	50:Q:156:GLU:OE1	1.96	0.65
2:AA:1583:MA6:OP1	31:A3:145:LYS:NZ	2.30	0.65
21:AT:146:GLN:N	21:AT:146:GLN:OE1	2.28	0.65
25:AX:272:THR:OG1	25:AX:282:ILE:O	2.13	0.65
21:AT:91:GLU:OE1	22:AU:120:ARG:NH2	2.29	0.65
1:A5:142:GLY:N	1:A5:146:SER:O	2.29	0.65
16:AO:199:TRP:NE1	28:A0:166:TYR:O	2.29	0.65
39:D:116:GLU:OE1	39:D:116:GLU:N	2.27	0.65
43:J:178:GLN:O	43:J:182:ASP:N	2.28	0.65
1:A5:216:GLU:N	1:A5:233:ILE:O	2.29	0.65
2:AA:1530:A:OP1	28:A0:29:ARG:NH2	2.30	0.65
41:F:52:GLU:N	41:F:52:GLU:OE1	2.30	0.65
6:AE:38:ASP:OD1	6:AE:39:LEU:N	2.30	0.64
1:A5:101:HIS:HA	37:A:3131:G:H5'	1.79	0.64
37:A:3063:G:O2'	37:A:3066:C:OP2	2.15	0.64
57:X:177:HIS:O	57:X:184:ARG:NH1	2.30	0.64
4:AC:125:ARG:NH2	4:AC:157:THR:O	2.30	0.64
3:AB:102:MET:HE1	3:AB:223:VAL:HG23	1.80	0.63
32:A4:303:CYS:SG	32:A4:344:ARG:NH2	2.71	0.63
13:AL:120:GLU:N	13:AL:120:GLU:OE1	2.31	0.63
50:Q:114:GLY:N	50:Q:137:CYS:O	2.29	0.63
74:e:55:ARG:NH2	74:e:155:ARG:O	2.31	0.63
76:g:64:GLU:N	76:g:64:GLU:OE1	2.31	0.63
77:h:64:GLU:OE1	77:h:64:GLU:N	2.31	0.63
28:A0:63:ARG:NH2	28:A0:110:ASP:OD2	2.31	0.63
30:A2:15:ASN:OD1	30:A2:17:ARG:NH1	2.32	0.63
2:AA:713:C:O2	22:AU:27:ARG:N	2.32	0.62
2:AA:1583:MA6:H93	2:AA:1584:MA6:C9	2.29	0.62
67:7:175:ILE:O	67:7:319:ARG:NH2	2.32	0.62
73:d:158:ASP:OD1	73:d:159:ARG:N	2.32	0.62
59:Z:43:GLU:OE1	59:Z:43:GLU:N	2.30	0.62
11:AJ:90:GLU:N	11:AJ:90:GLU:OE1	2.32	0.62
37:A:3067:PSU:H5'	40:E:232:GLY:O	2.00	0.62
68:8:136:ILE:HG22	75:f:173:ILE:HD11	1.80	0.62
22:AU:194:GLU:N	22:AU:194:GLU:OE1	2.33	0.62
29:A1:184:ASP:OD1	29:A1:185:HIS:N	2.31	0.62
88:t:75:THR:HA	88:w:68:VAL:HG11	1.82	0.62
37:A:2727:C:O2'	37:A:2815:OMG:N2	2.33	0.62
65:5:377:ASP:OD1	65:5:380:GLN:NE2	2.32	0.61
2:AA:948:U:OP2	2:AA:1045:G:N2	2.28	0.61
1:A5:90:LEU:O	1:A5:94:GLU:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:139:GLU:OE1	1:A5:178:GLY:N	2.33	0.61
65:5:254:GLU:OE1	65:5:254:GLU:N	2.31	0.61
2:AA:752:C:O2'	2:AA:793:C:N4	2.33	0.61
84:p:111:ILE:O	84:p:116:ARG:NH1	2.33	0.61
88:u:89:THR:O	88:w:76:LEU:HD13	2.01	0.61
23:AV:250:ILE:O	23:AV:255:TYR:OH	2.18	0.61
33:Aw:8:U:HO2'	33:Aw:13:U:H3	1.46	0.61
43:J:182:ASP:O	43:J:186:GLN:N	2.33	0.61
15:AN:57:GLN:N	15:AN:57:GLN:OE1	2.33	0.61
13:AL:87:ASP:OD1	13:AL:88:VAL:N	2.34	0.61
14:AM:24:GLY:N	14:AM:31:PHE:O	2.31	0.60
24:AW:137:GLY:O	24:AW:139:ARG:NH1	2.33	0.60
43:J:45:SER:OG	43:J:47:ASN:OD1	2.18	0.60
28:A0:132:GLU:OE2	28:A0:205:ALA:N	2.33	0.60
23:AV:171:GLU:O	28:A0:144:LYS:NZ	2.34	0.60
77:h:67:GLN:NE2	77:h:71:GLU:OE2	2.35	0.60
37:A:1990:G:OP1	39:D:269:ARG:NH2	2.34	0.60
24:AW:87:SER:HG	24:AW:90:THR:HG1	1.49	0.59
81:l:108:GLU:OE1	81:l:108:GLU:N	2.33	0.59
37:A:2730:A:O2'	37:A:2732:G:O4'	2.19	0.59
46:M:54:LYS:N	46:M:58:GLN:OE1	2.29	0.59
61:1:34:ARG:NH1	61:1:38:ARG:O	2.35	0.59
5:AD:94:THR:OG1	5:AD:96:ASP:OD1	2.21	0.59
32:A4:143:GLU:N	32:A4:143:GLU:OE1	2.36	0.59
58:Y:77:GLU:OE1	58:Y:77:GLU:N	2.34	0.59
2:AA:1526:U:N3	28:A0:100:VAL:O	2.36	0.59
4:AC:80:ASP:OD1	4:AC:81:HIS:ND1	2.35	0.59
11:AJ:81:CYS:N	11:AJ:93:CYS:SG	2.76	0.59
2:AA:893:G:OP2	11:AJ:79:LYS:NZ	2.36	0.58
2:AA:1524:A:N6	23:AV:396:GLN:OE1	2.34	0.58
24:AW:174:GLU:OE1	24:AW:174:GLU:N	2.36	0.58
85:q:117:ARG:O	85:q:121:ILE:HD12	2.03	0.58
9:AH:71:ILE:O	9:AH:150:GLY:N	2.35	0.58
41:F:220:ASP:O	41:F:245:ALA:N	2.37	0.58
48:O:64:LYS:NZ	48:O:100:GLN:O	2.37	0.58
37:A:1823:A:OP2	70:a:127:GLY:N	2.36	0.58
17:AP:47:ASN:ND2	17:AP:49:ASP:OD1	2.35	0.58
5:AD:312:TYR:N	5:AD:331:ASP:OD2	2.37	0.58
8:AG:378:GLU:OE2	8:AG:381:LYS:NZ	2.37	0.58
49:P:180:GLU:N	49:P:180:GLU:OE1	2.37	0.58
68:8:99:ARG:NH1	74:e:84:TYR:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AI:101:SER:OG	10:AI:105:GLU:OE1	2.22	0.58
30:A2:102:ASN:OD1	30:A2:103:LYS:N	2.36	0.58
84:p:109:GLU:OE1	84:p:109:GLU:N	2.33	0.58
89:H:146:LEU:O	89:H:150:GLY:N	2.37	0.58
2:AA:1104:A:OP1	2:AA:1591:C:O2'	2.22	0.57
42:I:157:GLU:OE1	42:I:157:GLU:N	2.34	0.57
65:5:368:GLU:OE1	65:5:368:GLU:N	2.37	0.57
2:AA:1583:MA6:H102	2:AA:1584:MA6:H103	1.84	0.57
25:AX:196:GLU:OE1	25:AX:196:GLU:N	2.34	0.57
37:A:3127:G:N2	37:A:3130:A:OP2	2.32	0.57
43:J:121:ALA:O	43:J:125:ALA:N	2.32	0.57
14:AM:108:GLU:OE2	22:AU:59:ARG:NH2	2.36	0.57
32:A4:256:GLU:OE1	32:A4:256:GLU:N	2.34	0.57
41:F:191:ASP:OD1	41:F:192:SER:N	2.37	0.57
68:8:103:GLN:OE1	68:8:103:GLN:N	2.37	0.57
47:N:175:PHE:O	47:N:178:GLN:HG2	2.03	0.57
19:AR:317:ALA:O	19:AR:321:ALA:N	2.38	0.57
8:AG:210:VAL:HG12	8:AG:210:VAL:O	2.04	0.57
60:0:176:GLU:OE1	60:0:176:GLU:N	2.31	0.57
3:AB:258:THR:O	3:AB:262:GLU:OE1	2.23	0.57
37:A:1672:C:OP1	53:T:44:LYS:N	2.37	0.57
81:l:67:GLN:O	81:l:71:TYR:N	2.33	0.57
27:AZ:74:GLU:OE1	27:AZ:74:GLU:N	2.37	0.57
37:A:2537:G:O2'	37:A:2634:U:OP2	2.21	0.57
46:M:231:GLU:OE1	46:M:231:GLU:N	2.37	0.57
44:K:174:GLU:N	44:K:174:GLU:OE1	2.38	0.56
88:t:76:LEU:HD13	88:w:68:VAL:HG13	1.87	0.56
88:u:91:LYS:C	88:w:76:LEU:HD11	2.29	0.56
2:AA:762:G:OP1	13:AL:206:LYS:NZ	2.37	0.56
8:AG:312:GLN:OE1	8:AG:345:ARG:NH1	2.38	0.56
9:AH:57:ASP:OD1	9:AH:58:LEU:N	2.38	0.56
30:A2:64:ASP:OD1	30:A2:65:ALA:N	2.37	0.56
37:A:3219:G:O2'	37:A:3222:C:N4	2.38	0.56
40:E:69:ASP:OD1	40:E:154:ARG:NH1	2.37	0.56
59:Z:92:GLU:OE1	59:Z:92:GLU:N	2.36	0.56
19:AR:97:GLU:OE1	19:AR:97:GLU:N	2.39	0.56
35:Ay:75:C:O2'	35:Ay:76:A:OP1	2.21	0.56
58:Y:191:ASN:O	58:Y:195:ASN:ND2	2.38	0.56
14:AM:111:ARG:NH1	16:AO:233:GLU:O	2.39	0.56
55:V:112:GLU:N	55:V:112:GLU:OE1	2.39	0.56
89:H:93:ASN:OD1	89:H:94:LEU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:2364:C:OP2	54:U:78:LYS:NZ	2.39	0.56
5:AD:117:ARG:NH2	36:Az:14:A:O5'	2.40	0.55
47:N:40:GLU:OE1	47:N:40:GLU:N	2.36	0.55
72:c:139:GLN:NE2	72:c:143:ASP:OD2	2.39	0.55
80:k:11:ARG:NH1	80:k:45:THR:O	2.38	0.55
84:p:75:ASP:OD1	84:p:76:ARG:N	2.39	0.55
24:AW:128:GLU:OE1	24:AW:128:GLU:N	2.38	0.55
50:Q:210:GLU:N	50:Q:210:GLU:OE1	2.38	0.55
71:b:149:GLN:OE1	71:b:149:GLN:N	2.40	0.55
85:q:44:ASP:OD1	85:q:46:LEU:N	2.37	0.55
1:A5:137:LEU:N	37:A:2960:U:O4	2.38	0.55
2:AA:1259:U:OP2	2:AA:1327:G:P	2.64	0.55
37:A:2346:U:OP1	87:s:223:ARG:NH2	2.39	0.55
66:6:311:MET:O	79:j:112:LYS:NZ	2.39	0.55
3:AB:102:MET:HE2	3:AB:224:ASP:O	2.06	0.55
6:AE:103:LYS:NZ	6:AE:104:GLU:OE2	2.40	0.55
23:AV:270:PRO:O	23:AV:346:LYS:NZ	2.40	0.55
33:Aw:14:A:H3'	33:Aw:15:A:O4'	2.06	0.55
37:A:1672:C:OP2	53:T:42:SER:OG	2.11	0.54
15:AN:8:VAL:O	15:AN:11:ARG:NH1	2.39	0.54
37:A:2328:C:N4	87:s:52:THR:O	2.40	0.54
37:A:2709:A:N3	60:0:98:GLN:NE2	2.55	0.54
63:3:104:ARG:NH1	63:3:160:LYS:O	2.40	0.54
1:A5:104:ASN:O	1:A5:105:LEU:HB2	2.07	0.54
33:Aw:15:A:H2'	33:Aw:16:A:H4'	1.89	0.54
57:X:35:GLU:O	57:X:35:GLU:HG2	2.07	0.54
77:h:92:GLU:OE1	77:h:92:GLU:N	2.35	0.54
63:3:188:VAL:O	66:6:356:ARG:NH2	2.40	0.54
42:I:225:GLN:CG	42:I:226:PRO:HD3	2.37	0.54
65:5:385:HIS:O	65:5:404:VAL:N	2.38	0.54
2:AA:1163:C:OP2	11:AJ:48:LYS:NZ	2.41	0.54
50:Q:74:ARG:NH2	50:Q:287:GLU:OE2	2.41	0.54
37:A:2220:A:H3'	37:A:2221:C:H4'	1.89	0.54
42:I:225:GLN:HG3	42:I:226:PRO:HD3	1.90	0.54
72:c:80:GLN:O	72:c:210:ARG:NH2	2.41	0.54
6:AE:106:GLU:OE1	6:AE:106:GLU:N	2.33	0.54
73:d:94:ASP:OD2	73:d:245:TYR:OH	2.22	0.54
2:AA:1225:C:N4	2:AA:1448:U:O2'	2.41	0.53
57:X:113:GLU:OE2	57:X:123:PHE:N	2.41	0.53
15:AN:93:ASP:O	15:AN:97:GLY:N	2.36	0.53
42:I:142:ASN:OD1	88:t:50:GLY:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Aw:9:A:H1'	33:Aw:45:A:H2'	1.90	0.53
72:c:209:GLU:OE1	72:c:209:GLU:N	2.36	0.53
18:AQ:69:ALA:O	18:AQ:73:ASN:ND2	2.37	0.53
33:Aw:9:A:O2'	33:Aw:10:G:N7	2.41	0.53
90:z:230:ILE:N	90:z:231:PRO:CD	2.72	0.53
2:AA:897:C:OP2	11:AJ:116:GLN:NE2	2.41	0.53
3:AB:162:CYS:O	3:AB:261:LYS:NZ	2.40	0.53
37:A:2098:G:O2'	37:A:2099:U:OP2	2.20	0.53
87:s:87:GLN:NE2	87:s:279:GLU:OE1	2.42	0.53
37:A:2458:A:OP2	48:O:9:ILE:N	2.42	0.53
1:A5:111:VAL:O	1:A5:115:LYS:HG2	2.09	0.53
72:c:42:GLN:NE2	78:i:36:LEU:O	2.41	0.53
6:AE:49:TYR:O	6:AE:51:ILE:HD12	2.09	0.53
2:AA:825:U:O2'	11:AJ:55:ARG:NH2	2.42	0.53
37:A:3039:OMU:O5'	37:A:3039:OMU:H6	2.09	0.53
47:N:46:GLU:OE1	47:N:46:GLU:N	2.38	0.53
79:j:53:ASP:OD1	79:j:54:GLY:N	2.42	0.53
20:AS:11:SER:OG	20:AS:43:GLU:OE2	2.22	0.52
37:A:1856:A:OP2	37:A:2986:C:O2'	2.27	0.52
43:J:25:ARG:NE	81:l:56:LEU:O	2.40	0.52
72:c:228:LEU:HD13	72:c:307:PHE:CD2	2.43	0.52
2:AA:947:U:OP1	13:AL:162:GLN:NE2	2.40	0.52
25:AX:183:GLU:OE1	25:AX:183:GLU:N	2.41	0.52
37:A:2379:C:O2	69:9:47:GLY:N	2.42	0.52
37:A:2776:G:N2	89:H:179:ASN:OD1	2.42	0.52
38:B:38:C:OP1	66:6:56:ARG:NH2	2.41	0.52
37:A:1787:G:N2	37:A:1790:A:OP2	2.37	0.52
47:N:231:SER:N	47:N:234:ASP:OD2	2.39	0.52
54:U:47:GLU:OE1	54:U:47:GLU:N	2.43	0.52
68:8:86:GLU:OE1	68:8:86:GLU:N	2.39	0.52
88:t:58:LYS:NZ	88:t:59:GLU:O	2.42	0.52
35:Ay:75:C:HO2'	35:Ay:76:A:P	2.32	0.52
69:9:82:GLU:OE1	69:9:82:GLU:N	2.38	0.52
5:AD:96:ASP:OD1	5:AD:97:GLU:N	2.43	0.52
37:A:2826:G:OP1	56:W:49:ARG:NH1	2.42	0.52
53:T:198:ARG:NH2	72:c:287:GLU:OE1	2.42	0.52
2:AA:764:A:H4'	2:AA:765:C:O5'	2.09	0.52
37:A:2070:C:N4	37:A:2831:G:O4'	2.43	0.52
37:A:2883:A:H4'	37:A:2884:C:OP2	2.10	0.52
43:J:47:ASN:OD1	43:J:48:GLN:N	2.42	0.52
11:AJ:104:GLU:OE1	11:AJ:105:HIS:ND1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AM:111:ARG:NH2	19:AR:146:LYS:O	2.43	0.51
57:X:35:GLU:N	57:X:35:GLU:OE1	2.44	0.51
74:e:224:GLU:OE1	74:e:224:GLU:N	2.44	0.51
79:j:45:GLU:OE2	79:j:70:ARG:NH2	2.40	0.51
2:AA:691:A:N7	2:AA:716:U:O2'	2.42	0.51
20:AS:48:ARG:HD2	20:AS:49:PRO:O	2.10	0.51
71:b:88:SER:O	71:b:92:LYS:NZ	2.43	0.51
5:AD:396:GLU:OE1	5:AD:396:GLU:N	2.41	0.51
37:A:2161:A:H5'	37:A:2162:C:OP2	2.09	0.51
43:J:50:CYS:O	43:J:54:ASN:ND2	2.43	0.51
51:R:85:ALA:O	51:R:89:ASN:ND2	2.42	0.51
68:8:129:ARG:O	68:8:133:ARG:N	2.39	0.51
74:e:106:HIS:NE2	74:e:108:GLU:OE1	2.44	0.51
90:z:130:ALA:HB1	90:z:136:ASN:HB2	1.92	0.51
43:J:73:LYS:N	43:J:77:THR:O	2.43	0.51
72:c:164:GLU:OE1	72:c:164:GLU:N	2.41	0.51
2:AA:1245:U:O2'	27:AZ:96:LYS:NZ	2.42	0.51
37:A:2882:U:O2	49:P:173:ARG:NH2	2.43	0.51
55:V:180:GLU:OE1	55:V:180:GLU:N	2.39	0.51
2:AA:838:U:O2	14:AM:43:ARG:NH1	2.42	0.51
2:AA:1401:G:N1	2:AA:1404:A:OP2	2.44	0.51
37:A:1953:A:O2'	37:A:2463:A:OP1	2.29	0.51
52:S:109:THR:N	52:S:112:ASP:OD2	2.43	0.51
2:AA:702:C:O3'	2:AA:847:G:N2	2.43	0.51
2:AA:1021:U:OP2	30:A2:9:ARG:NH2	2.43	0.51
55:V:133:ILE:HG21	55:V:145:ARG:HB3	1.91	0.51
2:AA:1004:G:O2'	10:AI:98:GLN:NE2	2.44	0.51
48:O:41:ARG:O	60:O:138:ARG:NH2	2.42	0.51
87:s:405:ILE:HG23	87:s:405:ILE:O	2.10	0.51
1:A5:111:VAL:HG13	1:A5:115:LYS:NZ	2.26	0.51
37:A:2471:G:O2'	37:A:2654:U:O4	2.24	0.51
23:AV:376:GLU:OE2	23:AV:380:GLN:NE2	2.44	0.50
84:p:76:ARG:NH1	84:p:109:GLU:OE1	2.44	0.50
6:AE:67:ASP:OD2	6:AE:96:HIS:NE2	2.44	0.50
13:AL:83:GLU:OE1	13:AL:83:GLU:N	2.42	0.50
16:AO:62:GLU:N	16:AO:62:GLU:OE1	2.43	0.50
29:A1:255:ASN:N	29:A1:259:GLU:OE1	2.42	0.50
89:H:222:GLU:OE2	89:H:224:THR:OG1	2.28	0.50
48:O:140:SER:O	48:O:146:ASN:ND2	2.41	0.50
9:AH:94:PHE:CE1	29:A1:119:ILE:HD13	2.45	0.50
37:A:1798:A:N3	55:V:42:ARG:NH2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:1014:A:O2'	2:AA:1031:G:O4'	2.30	0.50
22:AU:171:GLU:OE1	22:AU:171:GLU:N	2.42	0.50
28:A0:37:ASP:O	28:A0:41:LEU:N	2.45	0.50
37:A:2245:A:H4'	37:A:2246:A:OP1	2.10	0.50
37:A:2398:A:H2'	37:A:2399:A:O4'	2.12	0.50
47:N:73:ARG:O	47:N:155:LYS:NZ	2.45	0.50
66:6:181:GLU:OE1	66:6:181:GLU:N	2.42	0.50
6:AE:17:GLU:N	6:AE:17:GLU:OE1	2.45	0.50
9:AH:84:ASP:OD1	9:AH:86:ALA:N	2.45	0.50
57:X:87:LEU:O	89:H:78:ARG:NH1	2.44	0.50
68:8:56:VAL:HG23	68:8:56:VAL:O	2.12	0.50
1:A5:194:GLU:HB2	1:A5:198:LYS:HA	1.94	0.50
7:AF:193:ASP:OD1	7:AF:194:LYS:N	2.45	0.50
16:AO:215:ARG:NH1	28:A0:87:TRP:O	2.40	0.50
39:D:238:GLU:OE1	39:D:238:GLU:N	2.44	0.50
90:z:239:ASN:OD1	90:z:240:GLY:N	2.44	0.50
37:A:2816:G:O6	56:W:33:LYS:NZ	2.38	0.50
50:Q:237:ASN:OD1	50:Q:238:PHE:N	2.45	0.50
56:W:120:LEU:HD11	56:W:126:LEU:CD1	2.42	0.50
68:8:194:ASP:OD1	68:8:196:THR:HG23	2.12	0.50
73:d:202:MET:N	73:d:202:MET:SD	2.84	0.50
7:AF:240:ARG:NH2	7:AF:242:TRP:OXT	2.45	0.49
80:k:61:GLU:OE1	80:k:61:GLU:N	2.34	0.49
87:s:49:ALA:O	87:s:61:ARG:NH1	2.45	0.49
29:A1:152:ASP:OD2	29:A1:174:ARG:NH1	2.42	0.49
87:s:406:GLU:N	87:s:406:GLU:OE1	2.45	0.49
19:AR:170:ARG:O	19:AR:189:ARG:NH1	2.43	0.49
37:A:2191:A:N6	37:A:2198:A:OP2	2.45	0.49
60:0:153:THR:HG22	60:0:153:THR:O	2.13	0.49
70:a:70:GLU:OE1	70:a:70:GLU:N	2.40	0.49
2:AA:656:U:N3	2:AA:659:U:OP2	2.41	0.49
2:AA:1598:G:O2'	30:A2:37:ARG:NH2	2.46	0.49
6:AE:15:ARG:NH2	22:AU:178:GLU:OE1	2.43	0.49
37:A:1991:A:H5''	37:A:1992:C:OP1	2.12	0.49
5:AD:116:LYS:O	5:AD:118:THR:N	2.45	0.49
37:A:1822:U:O2	37:A:2707:A:O2'	2.30	0.49
79:j:67:LYS:O	79:j:71:GLU:HG2	2.12	0.49
2:AA:1293:C:N4	18:AQ:80:ARG:O	2.45	0.49
37:A:2783:A:O4'	90:z:296:ARG:NH1	2.46	0.49
1:A5:191:VAL:HG13	1:A5:230:PHE:HB2	1.95	0.49
15:AN:67:ARG:NH2	15:AN:80:GLU:OE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:7:106:ALA:O	67:7:113:TRP:N	2.44	0.49
2:AA:1057:G:H4'	2:AA:1578:A:H4'	1.94	0.49
29:A1:250:GLU:OE2	29:A1:301:ASN:ND2	2.45	0.49
37:A:2017:U:O2'	37:A:2723:A:N1	2.45	0.49
88:y:64:ILE:O	88:y:68:VAL:HG23	2.13	0.49
89:H:177:LYS:NZ	90:z:114:PHE:O	2.37	0.49
89:H:193:PHE:O	89:H:198:GLY:N	2.46	0.49
2:AA:1414:C:OP2	75:f:143:LYS:NZ	2.42	0.48
37:A:2213:A:H3'	37:A:2214:A:H5''	1.95	0.48
2:AA:871:A:O4'	2:AA:919:A:N6	2.47	0.48
18:AQ:77:ARG:O	18:AQ:80:ARG:NH1	2.46	0.48
74:e:108:GLU:O	74:e:110:ASP:N	2.45	0.48
22:AU:61:GLN:O	28:A0:198:MET:HE2	2.13	0.48
37:A:2539:A:H4'	37:A:2540:C:OP1	2.13	0.48
65:5:128:LEU:HD11	65:5:376:VAL:HG12	1.96	0.48
37:A:3110:C:O2'	40:E:266:ARG:NH1	2.47	0.48
54:U:37:GLU:OE1	54:U:37:GLU:N	2.34	0.48
90:z:133:LYS:HG2	90:z:134:LYS:H	1.77	0.48
2:AA:1583:MA6:C10	2:AA:1584:MA6:H103	2.44	0.48
26:AY:377:ARG:O	26:AY:381:ASN:ND2	2.46	0.48
37:A:1882:A:N6	37:A:1893:A:O4'	2.47	0.48
53:T:66:GLU:N	53:T:66:GLU:OE1	2.47	0.48
59:Z:135:SER:HA	79:j:71:GLU:OE2	2.13	0.48
1:A5:106:ALA:O	1:A5:110:GLU:N	2.36	0.48
26:AY:335:GLU:OE1	26:AY:348:ARG:NH2	2.47	0.48
37:A:2580:U:O4	37:A:2581:A:N6	2.47	0.48
37:A:2987:U:O2'	37:A:2991:U:OP1	2.30	0.48
16:AO:197:ASP:OD1	16:AO:198:PRO:HD2	2.13	0.48
37:A:2308:A:OP1	60:0:85:ARG:NH2	2.42	0.48
89:H:92:GLU:N	89:H:92:GLU:OE1	2.47	0.48
39:D:281:TRP:O	39:D:285:LYS:NZ	2.46	0.48
84:p:108:ALA:O	84:p:116:ARG:NH1	2.47	0.48
37:A:3201:A:H2'	37:A:3202:U:O4'	2.14	0.47
50:Q:180:GLU:OE1	50:Q:180:GLU:N	2.47	0.47
54:U:149:SER:O	73:d:273:LYS:NZ	2.47	0.47
66:6:325:ASP:OD1	66:6:326:SER:N	2.47	0.47
1:A5:102:ASN:N	37:A:3130:A:O2'	2.45	0.47
2:AA:994:A:O2'	7:AF:166:ARG:NH1	2.47	0.47
17:AP:48:GLU:OE1	17:AP:48:GLU:N	2.47	0.47
35:Ay:75:C:N4	37:A:2909:G:O2'	2.47	0.47
37:A:2779:C:OP1	90:z:119:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:1340:C:OP2	27:AZ:100:LYS:NZ	2.45	0.47
74:e:156:ASN:OD1	74:e:157:LEU:N	2.47	0.47
2:AA:1327:G:O2'	2:AA:1328:G:OP1	2.29	0.47
23:AV:82:ARG:NH1	23:AV:86:ASP:OD1	2.48	0.47
2:AA:1098:C:OP1	2:AA:1151:C:N4	2.47	0.47
37:A:1745:U:O4	63:3:108:LYS:NZ	2.46	0.47
43:J:26:ALA:N	43:J:64:ILE:O	2.42	0.47
73:d:81:THR:HG22	73:d:83:GLY:H	1.79	0.47
1:A5:243:ARG:NE	1:A5:253:SER:HB2	2.29	0.47
33:Aw:7:A:O2'	33:Aw:8:U:OP1	2.30	0.47
85:q:61:PHE:O	85:q:65:GLY:N	2.41	0.47
90:z:220:LYS:N	90:z:225:SER:OG	2.45	0.47
2:AA:895:C:N4	11:AJ:117:ASP:OD2	2.48	0.47
2:AA:945:G:O2'	13:AL:154:ARG:NH2	2.46	0.47
2:AA:1287:A:OP2	5:AD:260:LYS:NZ	2.41	0.47
7:AF:45:LEU:O	7:AF:51:TYR:OH	2.28	0.47
7:AF:109:SER:O	7:AF:113:GLN:HG3	2.14	0.47
37:A:2458:A:O2'	40:E:215:PHE:O	2.30	0.47
37:A:2499:U:O2'	37:A:2500:A:OP1	2.31	0.47
2:AA:1065:C:H2'	2:AA:1066:C:O4'	2.15	0.47
70:a:75:ILE:HD13	72:c:255:SER:HB2	1.96	0.47
86:r:44:GLY:O	86:r:45:LYS:HG2	2.14	0.47
33:Aw:8:U:O2'	33:Aw:13:U:N3	2.40	0.47
88:t:76:LEU:CD1	88:w:68:VAL:HG13	2.45	0.47
2:AA:841:A:OP1	14:AM:39:ASN:ND2	2.46	0.46
2:AA:843:G:N2	2:AA:846:A:OP2	2.39	0.46
23:AV:318:ASP:OD1	23:AV:319:ILE:N	2.48	0.46
30:A2:90:GLN:O	30:A2:94:GLY:N	2.39	0.46
32:A4:490:SER:OG	36:Az:25:U:N3	2.39	0.46
42:I:180:CYS:SG	42:I:184:THR:N	2.88	0.46
56:W:102:GLU:OE2	66:6:74:TYR:N	2.47	0.46
2:AA:765:C:O2	2:AA:765:C:O2'	2.27	0.46
33:Aw:20:C:OP1	33:Aw:21:A:O2'	2.33	0.46
37:A:3226:G:O2'	37:A:3229:U:O4	2.34	0.46
81:l:82:GLN:NE2	81:l:83:ASP:O	2.48	0.46
65:5:280:GLN:NE2	87:s:155:PHE:O	2.44	0.46
66:6:177:TYR:CD2	66:6:193:VAL:HG11	2.49	0.46
87:s:74:GLU:OE1	87:s:74:GLU:N	2.38	0.46
87:s:271:LEU:N	87:s:272:PRO:HA	2.31	0.46
1:A5:186:LYS:NZ	1:A5:216:GLU:OE2	2.41	0.46
2:AA:1285:G:O2'	5:AD:242:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:1327:G:N2	9:AH:127:TYR:OH	2.41	0.46
23:AV:236:LEU:HD12	23:AV:290:LEU:HD13	1.98	0.46
29:A1:258:SER:OG	29:A1:292:TYR:OH	2.33	0.46
37:A:2484:C:H5''	37:A:2485:U:OP1	2.15	0.46
37:A:2882:U:H4'	37:A:2883:A:H5''	1.97	0.46
37:A:3120:C:H2'	37:A:3121:C:O4'	2.16	0.46
53:T:49:ASN:ND2	53:T:68:TYR:O	2.49	0.46
55:V:188:VAL:O	55:V:188:VAL:HG23	2.15	0.46
2:AA:1247:G:H3'	2:AA:1249:U:OP2	2.16	0.46
5:AD:290:ILE:HB	5:AD:356:GLN:HE22	1.81	0.46
17:AP:53:SER:O	17:AP:54:MET:HG3	2.15	0.46
81:l:116:GLU:OE1	81:l:119:ARG:NH1	2.49	0.46
4:AC:115:ASN:ND2	26:AY:309:LYS:O	2.49	0.46
20:AS:124:ALA:O	20:AS:127:ALA:N	2.48	0.46
37:A:1918:G:N2	37:A:1998:U:O4	2.48	0.46
37:A:2138:U:O2'	37:A:2151:A:N3	2.49	0.46
37:A:2958:A:N6	37:A:2963:A:O2'	2.49	0.46
2:AA:958:C:H4'	2:AA:959:C:O4'	2.15	0.46
2:AA:1229:U:O2'	2:AA:1442:G:O4'	2.34	0.46
74:e:178:TRP:NE1	74:e:182:GLU:O	2.45	0.46
23:AV:47:HIS:O	23:AV:47:HIS:ND1	2.49	0.46
37:A:2135:A:N3	37:A:2135:A:H2'	2.31	0.46
37:A:2489:C:O2'	37:A:2621:G:OP1	2.33	0.46
41:F:66:VAL:O	41:F:77:VAL:N	2.48	0.46
1:A5:139:GLU:OE1	1:A5:179:ALA:N	2.49	0.45
29:A1:46:ARG:HB2	29:A1:47:PRO:HD3	1.98	0.45
37:A:1773:A:OP2	72:c:31:VAL:N	2.50	0.45
39:D:123:GLU:N	39:D:123:GLU:OE1	2.50	0.45
65:5:165:GLN:HG2	65:5:166:THR:HG23	1.98	0.45
33:Aw:29:U:H3'	33:Aw:30:U:H5''	1.97	0.45
37:A:2777:G:O3'	89:H:177:LYS:HE3	2.16	0.45
1:A5:100:GLU:O	1:A5:101:HIS:HB2	2.16	0.45
1:A5:185:LYS:HA	1:A5:260:PHE:HA	1.98	0.45
2:AA:844:A:H2'	2:AA:845:A:O4'	2.16	0.45
2:AA:871:A:N6	2:AA:919:A:O5'	2.48	0.45
39:D:257:ILE:O	39:D:262:ARG:NH1	2.45	0.45
43:J:104:THR:OG1	43:J:149:ARG:O	2.31	0.45
1:A5:122:ILE:HA	1:A5:125:ALA:HB3	1.98	0.45
25:AX:381:LEU:O	25:AX:385:ASN:N	2.47	0.45
37:A:2531:U:O4	39:D:246:ARG:NH2	2.50	0.45
37:A:3227:U:O2'	37:A:3230:G:OP2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:2001:C:H4'	37:A:2002:G:OP1	2.16	0.45
37:A:2525:C:OP2	37:A:2526:C:O2'	2.34	0.45
37:A:2777:G:OP1	89:H:245:THR:OG1	2.33	0.45
43:J:166:ALA:O	43:J:169:LYS:HG2	2.16	0.45
75:f:105:SER:CB	82:m:41:THR:HG21	2.45	0.45
88:u:60:TYR:HB2	88:u:61:PRO:HD3	1.97	0.45
16:AO:217:ARG:NH1	16:AO:227:GLU:OE2	2.49	0.45
28:A0:84:SER:OG	28:A0:138:ASP:OD2	2.29	0.45
32:A4:290:ASP:OD1	32:A4:293:THR:OG1	2.27	0.45
37:A:2774:C:H2'	37:A:2775:A:C8	2.51	0.45
69:9:108:THR:HG23	69:9:108:THR:O	2.16	0.45
73:d:97:ILE:O	73:d:98:SER:C	2.58	0.45
1:A5:101:HIS:O	1:A5:105:LEU:N	2.49	0.45
1:A5:292:VAL:HG12	1:A5:293:TYR:N	2.32	0.45
2:AA:1236:C:OP2	12:AK:90:ARG:NH2	2.47	0.45
2:AA:1342:C:OP2	27:AZ:96:LYS:NZ	2.47	0.45
2:AA:1365:A:H4'	2:AA:1389:G:H4'	1.99	0.45
8:AG:396:ARG:NH1	34:Ax:33:U:OP2	2.44	0.45
11:AJ:107:ILE:N	11:AJ:131:ASP:OD2	2.45	0.45
1:A5:206:ALA:HB2	1:A5:230:PHE:CE2	2.52	0.45
37:A:1731:A:OP1	89:H:74:HIS:NE2	2.49	0.45
73:d:129:ASP:OD1	73:d:129:ASP:O	2.35	0.45
84:p:46:ASP:OD1	84:p:47:LYS:N	2.50	0.45
14:AM:41:CYS:SG	14:AM:42:PRO:HD2	2.57	0.45
32:A4:526:ASP:OD1	32:A4:526:ASP:N	2.50	0.45
32:A4:539:LYS:NZ	32:A4:540:HIS:O	2.45	0.45
37:A:1806:U:H4'	37:A:1807:U:H5'	1.99	0.45
37:A:1914:A:N6	37:A:2004:G:O6	2.50	0.45
60:0:108:ASP:OD1	60:0:109:VAL:N	2.49	0.45
81:l:80:GLU:OE1	81:l:80:GLU:N	2.42	0.45
89:H:177:LYS:HD2	90:z:114:PHE:O	2.17	0.45
2:AA:1327:G:HO2'	2:AA:1328:G:P	2.40	0.45
37:A:2279:U:OP2	78:i:46:ARG:NH1	2.42	0.45
14:AM:100:HIS:O	14:AM:103:MET:HG2	2.17	0.44
20:AS:119:VAL:O	20:AS:123:LYS:N	2.41	0.44
23:AV:236:LEU:HD21	23:AV:323:GLU:HB2	1.99	0.44
37:A:1800:G:N1	37:A:1803:A:OP2	2.50	0.44
37:A:2482:A:H2'	37:A:2483:U:O4'	2.15	0.44
74:e:137:ILE:HG23	74:e:137:ILE:O	2.17	0.44
79:j:98:LEU:O	79:j:102:GLN:OE1	2.36	0.44
1:A5:191:VAL:HA	1:A5:253:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AV:51:ALA:HB3	50:Q:66:HIS:HB2	2.00	0.44
37:A:2121:G:O3'	59:Z:77:ARG:HA	2.18	0.44
71:b:44:ARG:NH2	83:o:99:LYS:O	2.50	0.44
20:AS:62:ASP:OD1	20:AS:63:ILE:N	2.51	0.44
24:AW:141:ARG:NH1	24:AW:172:ILE:O	2.51	0.44
32:A4:132:ILE:O	32:A4:132:ILE:CG2	2.66	0.44
42:I:223:GLN:C	42:I:226:PRO:HD2	2.42	0.44
73:d:90:PRO:HB3	73:d:245:TYR:HE2	1.82	0.44
2:AA:966:A:OP2	17:AP:109:LYS:NZ	2.47	0.44
3:AB:65:GLU:OE2	3:AB:69:HIS:NE2	2.46	0.44
75:f:122:GLU:N	75:f:158:GLN:O	2.51	0.44
8:AG:250:LEU:HD12	8:AG:250:LEU:O	2.18	0.44
17:AP:52:ILE:HD11	20:AS:66:HIS:CD2	2.52	0.44
26:AY:254:LYS:O	32:A4:358:ARG:NH1	2.50	0.44
29:A1:92:LYS:O	29:A1:93:LYS:HG2	2.18	0.44
39:D:286:ILE:HG13	39:D:286:ILE:O	2.18	0.44
45:L:42:ASP:OD1	45:L:42:ASP:C	2.61	0.44
47:N:59:VAL:O	47:N:59:VAL:HG13	2.18	0.44
71:b:85:ARG:NH1	71:b:107:GLN:OE1	2.51	0.44
87:s:174:LEU:HB3	87:s:175:PRO:HD3	2.00	0.44
1:A5:262:PRO:HB3	1:A5:295:ASN:HA	1.99	0.44
2:AA:1151:C:OP2	13:AL:201:ARG:NH1	2.44	0.44
5:AD:112:LYS:NZ	5:AD:235:GLU:O	2.50	0.44
19:AR:162:SER:O	19:AR:170:ARG:NH1	2.50	0.44
19:AR:219:TYR:O	19:AR:256:ARG:NH2	2.50	0.44
29:A1:86:ARG:NH1	29:A1:96:PRO:O	2.49	0.44
32:A4:132:ILE:O	32:A4:132:ILE:HG22	2.17	0.44
35:Ay:75:C:O2'	35:Ay:76:A:P	2.75	0.44
2:AA:1272:A:N6	2:AA:1320:G:O2'	2.44	0.44
2:AA:1583:MA6:H2'	2:AA:1584:MA6:C1'	2.48	0.44
6:AE:3:ARG:NH2	6:AE:67:ASP:OD2	2.50	0.44
15:AN:23:GLN:NE2	15:AN:24:LYS:HG3	2.33	0.44
37:A:2599:U:OP2	37:A:2624:C:N4	2.50	0.44
46:M:250:ASP:OD1	46:M:251:GLU:N	2.51	0.44
48:O:36:LEU:O	48:O:40:GLU:N	2.48	0.44
66:6:192:GLU:OE2	66:6:322:ARG:NH1	2.50	0.44
16:AO:131:THR:HG22	16:AO:133:ILE:HG12	1.99	0.44
16:AO:214:SER:OG	16:AO:217:ARG:NH2	2.51	0.44
30:A2:42:GLU:OE1	30:A2:42:GLU:HA	2.18	0.44
37:A:1742:G:O2'	37:A:1743:U:OP2	2.36	0.44
37:A:2195:A:H5''	37:A:2196:A:OP1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:s:182:SER:OG	87:s:202:TYR:OH	2.35	0.44
29:A1:306:GLU:OE1	29:A1:306:GLU:N	2.49	0.43
37:A:2284:C:OP2	71:b:74:ARG:NH2	2.47	0.43
37:A:3082:G:N2	37:A:3085:A:OP2	2.41	0.43
45:L:68:LYS:NZ	45:L:91:MET:SD	2.91	0.43
50:Q:252:GLN:O	50:Q:255:LYS:HG2	2.18	0.43
57:X:241:GLN:OE1	57:X:244:SER:OG	2.33	0.43
2:AA:1412:G:OP1	25:AX:279:LYS:NZ	2.45	0.43
25:AX:129:GLU:O	25:AX:134:LYS:NZ	2.51	0.43
32:A4:270:ARG:O	32:A4:270:ARG:HG2	2.18	0.43
33:Aw:22:A:H2'	33:Aw:23:A:O4'	2.18	0.43
37:A:1764:C:OP1	85:q:34:ARG:NH1	2.51	0.43
37:A:2367:A:N3	58:Y:123:ARG:NH2	2.67	0.43
72:c:161:THR:O	72:c:192:GLN:NE2	2.51	0.43
1:A5:105:LEU:O	1:A5:106:ALA:C	2.61	0.43
20:AS:124:ALA:O	20:AS:128:GLU:OE1	2.36	0.43
37:A:2475:U:N3	37:A:2478:G:OP2	2.44	0.43
37:A:2744:U:H4'	37:A:2745:A:H5'	2.00	0.43
37:A:2814:G:O2'	37:A:2983:G:OP1	2.35	0.43
54:U:54:ARG:NH1	54:U:65:VAL:O	2.51	0.43
55:V:122:LEU:HB2	55:V:133:ILE:HD12	2.00	0.43
73:d:187:GLU:OE1	73:d:219:ARG:NH1	2.51	0.43
1:A5:105:LEU:O	1:A5:107:ASN:N	2.51	0.43
2:AA:1247:G:H4'	2:AA:1248:C:OP2	2.18	0.43
5:AD:292:HIS:H	5:AD:356:GLN:NE2	2.17	0.43
30:A2:91:GLU:N	30:A2:91:GLU:OE1	2.51	0.43
37:A:2065:A:OP1	75:f:48:TYR:N	2.51	0.43
37:A:2137:C:OP2	59:Z:77:ARG:NH1	2.51	0.43
48:O:62:TYR:OH	50:Q:272:GLU:OE2	2.32	0.43
66:6:231:GLU:N	66:6:231:GLU:OE1	2.52	0.43
2:AA:1366:C:H3'	2:AA:1367:A:H5'	1.99	0.43
53:T:129:GLU:HG2	53:T:130:PHE:N	2.33	0.43
70:a:62:HIS:O	70:a:62:HIS:ND1	2.51	0.43
2:AA:769:G:OP2	15:AN:73:ARG:NH2	2.52	0.43
2:AA:1213:A:N3	2:AA:1239:C:O2'	2.47	0.43
8:AG:360:GLU:HA	8:AG:363:TRP:HD1	1.84	0.43
28:A0:96:ARG:HB3	28:A0:117:ILE:HG22	1.99	0.43
32:A4:454:ARG:NH1	32:A4:455:ASN:OD1	2.52	0.43
37:A:2883:A:N3	37:A:2883:A:H2'	2.33	0.43
37:A:3131:G:H2'	37:A:3132:G:O4'	2.19	0.43
55:V:54:TRP:NE1	55:V:56:LEU:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:h:65:ASP:OD1	77:h:69:ARG:NH2	2.52	0.43
2:AA:781:A:O2'	91:AA:1701:NAD:N7N	2.52	0.43
2:AA:1595:G:O6	18:AQ:50:ARG:NH2	2.51	0.43
32:A4:286:ARG:O	32:A4:286:ARG:NE	2.52	0.43
37:A:1737:A:N6	37:A:1760:G:O2'	2.52	0.43
57:X:15:GLN:NE2	57:X:18:GLU:OE2	2.47	0.43
73:d:109:THR:OG1	73:d:110:GLU:N	2.51	0.43
37:A:1718:A:H2'	37:A:1719:G:O4'	2.18	0.43
37:A:2808:U:H2'	37:A:2809:C:O4'	2.18	0.43
73:d:215:ARG:HG3	73:d:245:TYR:CE1	2.54	0.43
30:A2:39:GLU:OE2	30:A2:87:ARG:NE	2.52	0.43
38:B:44:A:H2'	38:B:45:G:O4'	2.19	0.43
42:I:45:GLN:NE2	83:o:25:ARG:O	2.48	0.43
90:z:184:ILE:HG13	90:z:185:GLN:N	2.34	0.43
1:A5:165:ARG:O	1:A5:169:ASN:ND2	2.52	0.43
1:A5:223:ASP:OD1	1:A5:227:ARG:N	2.47	0.43
2:AA:770:C:H2'	2:AA:771:A:O4'	2.19	0.43
16:AO:95:ILE:HG13	16:AO:95:ILE:O	2.19	0.43
28:A0:43:ARG:O	28:A0:47:GLY:N	2.44	0.43
37:A:2072:A:OP2	66:6:28:ARG:NH1	2.50	0.43
43:J:75:ASP:O	43:J:76:ARG:HB2	2.19	0.43
2:AA:919:A:OP2	16:AO:92:LYS:HD3	2.19	0.42
5:AD:311:GLY:N	5:AD:331:ASP:OD2	2.52	0.42
37:A:1749:C:OP2	37:A:2899:C:O2'	2.37	0.42
37:A:2667:U:H2'	37:A:2668:A:O4'	2.18	0.42
60:0:166:SER:OG	60:0:167:GLU:N	2.52	0.42
72:c:228:LEU:HD13	72:c:307:PHE:HD2	1.83	0.42
73:d:89:VAL:O	73:d:89:VAL:HG23	2.19	0.42
76:g:121:GLN:O	76:g:125:GLU:HG3	2.18	0.42
2:AA:1369:U:OP2	7:AF:201:MET:N	2.41	0.42
33:Aw:64:U:H2'	33:Aw:65:A:O4'	2.18	0.42
53:T:149:ARG:O	53:T:161:MET:N	2.35	0.42
56:W:120:LEU:HD11	56:W:126:LEU:HD12	2.00	0.42
65:5:134:GLU:OE1	65:5:134:GLU:N	2.41	0.42
68:8:132:GLU:OE2	75:f:109:TYR:OH	2.32	0.42
68:8:195:ILE:HG13	75:f:131:THR:HG23	2.00	0.42
2:AA:1289:G:O2'	2:AA:1297:G:OP2	2.33	0.42
5:AD:415:GLN:NE2	5:AD:417:MET:SD	2.93	0.42
15:AN:14:VAL:O	21:AT:63:GLN:NE2	2.51	0.42
74:e:185:ARG:NH1	74:e:206:GLY:O	2.52	0.42
76:g:154:ASP:OD1	76:g:154:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:s:246:GLN:NE2	87:s:354:PRO:O	2.52	0.42
37:A:3202:U:P	40:E:141:LYS:HZ2	2.42	0.42
39:D:113:ARG:O	39:D:147:ARG:NH1	2.48	0.42
40:E:111:THR:OG1	40:E:113:ASP:OD1	2.33	0.42
53:T:94:ASP:OD2	67:7:97:GLU:N	2.39	0.42
66:6:139:TRP:O	66:6:144:GLY:N	2.52	0.42
67:7:62:THR:O	67:7:62:THR:HG23	2.20	0.42
1:A5:201:VAL:HG12	1:A5:202:ASN:N	2.34	0.42
2:AA:1519:A:H2'	2:AA:1519:A:N3	2.35	0.42
7:AF:116:GLU:OE2	7:AF:120:ARG:NH2	2.45	0.42
20:AS:70:ILE:HD12	20:AS:70:ILE:H	1.83	0.42
25:AX:102:ARG:NH2	25:AX:346:SER:O	2.46	0.42
37:A:1680:A:OP1	58:Y:230:LYS:NZ	2.50	0.42
37:A:2170:G:N3	43:J:143:SER:OG	2.51	0.42
37:A:2990:A:H4'	37:A:2991:U:OP1	2.19	0.42
39:D:232:ARG:HA	39:D:289:LEU:HD21	2.01	0.42
87:s:107:GLN:O	87:s:111:LYS:N	2.53	0.42
37:A:2449:G:OP2	87:s:225:ARG:NH2	2.47	0.42
73:d:92:GLU:OE1	73:d:92:GLU:HA	2.20	0.42
86:r:69:GLN:N	86:r:73:CYS:SG	2.93	0.42
86:r:70:CYS:N	86:r:73:CYS:SG	2.88	0.42
2:AA:1590:A:OP2	18:AQ:47:LYS:NZ	2.47	0.42
27:AZ:13:ARG:NH1	82:m:109:GLU:O	2.53	0.42
29:A1:258:SER:HG	29:A1:292:TYR:HH	1.65	0.42
37:A:2325:U:OP1	87:s:57:ALA:N	2.49	0.42
57:X:233:GLU:O	57:X:236:GLN:NE2	2.53	0.42
1:A5:90:LEU:HB2	1:A5:153:LEU:HD21	2.02	0.42
2:AA:883:U:H4'	2:AA:884:U:OP1	2.20	0.42
11:AJ:94:PHE:O	11:AJ:96:PRO:HD3	2.20	0.42
17:AP:49:ASP:OD2	24:AW:82:SER:N	2.52	0.42
17:AP:52:ILE:CD1	20:AS:66:HIS:CD2	3.03	0.42
37:A:3189:C:O2'	86:r:155:ALA:N	2.50	0.42
39:D:204:ALA:O	39:D:208:ARG:NH2	2.36	0.42
2:AA:1583:MA6:O5'	2:AA:1583:MA6:H8	2.19	0.42
4:AC:80:ASP:OD1	4:AC:81:HIS:N	2.52	0.42
25:AX:74:ASP:O	25:AX:78:VAL:N	2.44	0.42
37:A:1792:G:N7	62:2:87:ARG:NH2	2.55	0.42
37:A:2284:C:OP2	71:b:74:ARG:NH1	2.52	0.42
44:K:150:LYS:HD3	44:K:150:LYS:C	2.45	0.42
57:X:179:GLU:OE1	57:X:179:GLU:N	2.49	0.42
58:Y:171:ASP:OD1	58:Y:173:PHE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:7:277:GLN:O	67:7:301:SER:OG	2.36	0.42
1:A5:130:LYS:HG2	1:A5:131:SER:H	1.84	0.42
30:A2:86:MET:SD	30:A2:91:GLU:OE2	2.78	0.42
37:A:2556:A:H2'	37:A:2557:C:O4'	2.20	0.42
55:V:161:ARG:NH2	55:V:163:ASP:OD2	2.51	0.42
58:Y:171:ASP:OD1	58:Y:171:ASP:C	2.62	0.42
2:AA:703:A:OP2	22:AU:43:ASN:ND2	2.53	0.41
66:6:244:ARG:NE	66:6:244:ARG:HA	2.35	0.41
67:7:43:MET:SD	67:7:43:MET:C	3.03	0.41
67:7:114:ASP:OD1	67:7:268:LEU:N	2.52	0.41
85:q:157:GLN:NE2	85:q:161:GLN:OE1	2.53	0.41
89:H:100:GLN:OE1	89:H:100:GLN:N	2.53	0.41
29:A1:199:CYS:O	29:A1:203:ASP:N	2.52	0.41
32:A4:397:MET:HE1	32:A4:435:VAL:HG23	2.02	0.41
37:A:2174:G:H4'	43:J:151:LEU:HD13	2.01	0.41
2:AA:1108:C:H4'	2:AA:1109:A:OP2	2.21	0.41
2:AA:1367:A:N6	2:AA:1387:A:N3	2.68	0.41
37:A:2131:A:OP1	83:o:23:ARG:NH2	2.50	0.41
37:A:2515:U:OP1	39:D:284:ARG:NH2	2.53	0.41
38:B:55:U:H3'	38:B:56:U:H5''	2.02	0.41
73:d:205:GLN:O	73:d:205:GLN:CD	2.63	0.41
82:m:117:GLU:N	82:m:117:GLU:OE1	2.54	0.41
2:AA:1141:C:OP1	31:A3:139:ASN:ND2	2.50	0.41
2:AA:1522:U:H2'	2:AA:1523:A:O4'	2.21	0.41
16:AO:90:THR:HG22	16:AO:91:ARG:N	2.35	0.41
42:I:226:PRO:HA	88:x:86:LEU:HD11	2.03	0.41
43:J:53:PHE:O	43:J:57:THR:HG22	2.21	0.41
52:S:129:ARG:NH2	52:S:151:LYS:O	2.53	0.41
67:7:51:GLU:OE2	67:7:54:ARG:NH1	2.54	0.41
1:A5:222:GLU:HB3	1:A5:226:GLU:HA	2.03	0.41
2:AA:865:A:H2'	2:AA:866:A:O4'	2.20	0.41
30:A2:59:ASN:ND2	30:A2:66:CYS:SG	2.84	0.41
37:A:2776:G:H5'	89:H:249:LYS:HE3	2.02	0.41
50:Q:77:SER:OG	50:Q:79:GLU:OE1	2.37	0.41
61:1:46:TYR:HA	61:1:53:ARG:HA	2.01	0.41
70:a:75:ILE:HD12	70:a:77:ARG:HH11	1.85	0.41
1:A5:75:VAL:HG12	1:A5:79:ARG:HE	1.86	0.41
1:A5:106:ALA:O	1:A5:107:ASN:C	2.62	0.41
22:AU:162:GLU:O	22:AU:165:LYS:HG2	2.21	0.41
37:A:2045:A:N6	37:A:2094:G:O6	2.53	0.41
72:c:228:LEU:HD13	72:c:307:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:l:60:ASP:OD1	81:l:60:ASP:O	2.38	0.41
86:r:124:ARG:NH1	86:r:153:ARG:O	2.52	0.41
90:z:220:LYS:N	90:z:225:SER:HG	2.19	0.41
2:AA:1422:G:N3	34:Ax:41:U:O2'	2.49	0.41
20:AS:83:ARG:NH1	20:AS:93:LYS:O	2.53	0.41
37:A:2196:A:OP1	81:l:122:ARG:NH1	2.53	0.41
88:t:75:THR:O	88:t:79:ILE:N	2.46	0.41
31:A3:177:TRP:CD1	31:A3:178:LEU:HD12	2.55	0.41
47:N:191:SER:H	47:N:194:THR:HG1	1.66	0.41
54:U:58:GLU:OE1	54:U:58:GLU:HA	2.21	0.41
66:6:252:CYS:SG	66:6:296:ARG:NH1	2.94	0.41
1:A5:215:ALA:HB1	1:A5:233:ILE:O	2.20	0.41
2:AA:700:A:OP1	22:AU:28:LYS:N	2.36	0.41
3:AB:65:GLU:N	3:AB:66:PRO:HD2	2.36	0.41
20:AS:51:VAL:HG12	20:AS:52:ARG:N	2.36	0.41
24:AW:92:MET:O	24:AW:98:LYS:NZ	2.54	0.41
24:AW:97:ASP:N	24:AW:144:LEU:O	2.53	0.41
32:A4:335:PHE:O	32:A4:338:ILE:HG22	2.21	0.41
37:A:2073:A:OP2	66:6:27:ARG:N	2.54	0.41
37:A:3110:C:OP2	37:A:3110:C:H3'	2.20	0.41
44:K:153:LYS:HG2	44:K:157:GLU:HB2	2.02	0.41
45:L:131:GLU:OE1	45:L:131:GLU:N	2.45	0.41
1:A5:290:ILE:HG22	1:A5:291:HIS:CD2	2.56	0.41
2:AA:1149:G:OP2	31:A3:165:LYS:NZ	2.48	0.41
2:AA:1375:C:H2'	2:AA:1376:C:O4'	2.21	0.41
3:AB:149:ARG:NH2	18:AQ:84:TRP:O	2.54	0.41
8:AG:292:ARG:HA	8:AG:292:ARG:CZ	2.51	0.41
9:AH:182:GLU:HA	9:AH:185:LYS:HD3	2.03	0.41
11:AJ:94:PHE:HB2	11:AJ:121:VAL:HG11	2.03	0.41
31:A3:184:GLU:OE1	31:A3:184:GLU:N	2.54	0.41
32:A4:565:ARG:HD2	32:A4:565:ARG:C	2.45	0.41
37:A:2666:U:H2'	37:A:2667:U:O4'	2.21	0.41
44:K:10:GLN:NE2	53:T:197:LEU:O	2.52	0.41
48:O:143:THR:OG1	48:O:146:ASN:ND2	2.53	0.41
59:Z:51:GLU:H	59:Z:51:GLU:CD	2.29	0.41
64:4:90:VAL:O	64:4:99:LYS:HA	2.21	0.41
88:t1:153:ILE:HD11	88:t1:172:ILE:HG23	2.03	0.41
2:AA:709:G:OP1	14:AM:13:ARG:NH2	2.54	0.40
91:AA:1701:NAD:N7N	91:AA:1701:NAD:O4B	2.54	0.40
11:AJ:104:GLU:O	11:AJ:105:HIS:HB2	2.21	0.40
23:AV:74:ARG:O	23:AV:78:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:1760:G:H3'	85:q:59:LYS:HZ1	1.85	0.40
37:A:2873:A:OP1	56:W:85:LYS:N	2.54	0.40
37:A:3181:U:OP2	37:A:3182:A:O2'	2.35	0.40
48:O:86:ILE:HB	48:O:87:PRO:HD3	2.01	0.40
75:f:105:SER:O	75:f:108:GLN:HG2	2.21	0.40
2:AA:760:A:N1	2:AA:780:C:O2'	2.49	0.40
20:AS:61:GLN:OE1	20:AS:61:GLN:N	2.54	0.40
37:A:2071:U:O2'	66:6:28:ARG:NH2	2.54	0.40
37:A:2781:U:O3'	37:A:2782:A:H2'	2.21	0.40
37:A:3111:A:H2'	37:A:3112:A:H5''	2.03	0.40
44:K:7:ALA:HB3	44:K:8:PRO:HD3	2.02	0.40
46:M:276:ASN:O	46:M:280:LYS:N	2.54	0.40
2:AA:1254:C:H4'	2:AA:1255:U:C5'	2.52	0.40
25:AX:159:HIS:NE2	25:AX:266:ASN:OD1	2.54	0.40
36:Az:15:U:O4	36:Az:16:A:N6	2.54	0.40
37:A:3200:U:OP1	44:K:98:ARG:NE	2.54	0.40
42:I:144:LEU:N	42:I:145:PRO:HD2	2.36	0.40
42:I:221:LEU:O	42:I:224:HIS:ND1	2.49	0.40
73:d:137:PHE:N	73:d:138:PRO:HD2	2.36	0.40
2:AA:769:G:N2	2:AA:772:A:OP2	2.44	0.40
3:AB:111:LEU:O	3:AB:112:ASP:HB2	2.21	0.40
24:AW:146:ASP:OD1	24:AW:147:LEU:N	2.54	0.40
36:Az:10:A:H5'	36:Az:11:U:P	2.61	0.40
37:A:2222:U:C1'	37:A:2223:A:OP1	2.69	0.40
43:J:169:LYS:HG3	43:J:170:GLU:N	2.37	0.40
61:l:34:ARG:NH1	61:l:35:ASN:O	2.55	0.40
74:e:177:GLU:O	74:e:190:ARG:NH2	2.51	0.40
1:A5:186:LYS:HB2	1:A5:261:ILE:HG12	2.04	0.40
1:A5:193:VAL:HG21	1:A5:228:ASN:HB3	2.02	0.40
2:AA:1325:U:H2'	2:AA:1327:G:H5'	2.04	0.40
4:AC:134:PHE:CD1	4:AC:134:PHE:C	2.99	0.40
5:AD:340:ILE:O	5:AD:340:ILE:HG22	2.21	0.40
8:AG:237:GLU:OE1	8:AG:237:GLU:N	2.50	0.40
32:A4:104:ARG:O	32:A4:108:LEU:HD13	2.21	0.40
76:g:104:ASN:OD1	76:g:104:ASN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A5	212/297 (71%)	191 (90%)	20 (9%)	1 (0%)	24	61
3	AB	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
4	AC	130/167 (78%)	125 (96%)	5 (4%)	0	100	100
5	AD	341/430 (79%)	330 (97%)	9 (3%)	2 (1%)	21	58
6	AE	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
7	AF	206/242 (85%)	205 (100%)	1 (0%)	0	100	100
8	AG	323/396 (82%)	320 (99%)	3 (1%)	0	100	100
9	AH	138/201 (69%)	137 (99%)	0	1 (1%)	18	55
10	AI	134/194 (69%)	132 (98%)	2 (2%)	0	100	100
11	AJ	106/138 (77%)	98 (92%)	8 (8%)	0	100	100
12	AK	99/128 (77%)	99 (100%)	0	0	100	100
13	AL	172/257 (67%)	172 (100%)	0	0	100	100
14	AM	117/137 (85%)	117 (100%)	0	0	100	100
15	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100
16	AO	191/258 (74%)	190 (100%)	1 (0%)	0	100	100
17	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
18	AQ	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
19	AR	293/360 (81%)	286 (98%)	7 (2%)	0	100	100
20	AS	133/190 (70%)	127 (96%)	6 (4%)	0	100	100
21	AT	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
22	AU	174/205 (85%)	174 (100%)	0	0	100	100
23	AV	358/414 (86%)	355 (99%)	3 (1%)	0	100	100
24	AW	98/187 (52%)	96 (98%)	2 (2%)	0	100	100
25	AX	350/398 (88%)	346 (99%)	4 (1%)	0	100	100
26	AY	147/395 (37%)	147 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
28	A0	213/217 (98%)	209 (98%)	4 (2%)	0	100	100
29	A1	276/323 (85%)	273 (99%)	3 (1%)	0	100	100
30	A2	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
31	A3	68/199 (34%)	68 (100%)	0	0	100	100
32	A4	584/689 (85%)	579 (99%)	5 (1%)	0	100	100
39	D	236/305 (77%)	233 (99%)	3 (1%)	0	100	100
40	E	303/348 (87%)	297 (98%)	6 (2%)	0	100	100
41	F	250/311 (80%)	250 (100%)	0	0	100	100
42	I	210/261 (80%)	204 (97%)	6 (3%)	0	100	100
43	J	173/192 (90%)	165 (95%)	8 (5%)	0	100	100
44	K	176/178 (99%)	174 (99%)	2 (1%)	0	100	100
45	L	113/145 (78%)	113 (100%)	0	0	100	100
46	M	287/296 (97%)	285 (99%)	2 (1%)	0	100	100
47	N	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
48	O	152/175 (87%)	150 (99%)	2 (1%)	0	100	100
49	P	142/180 (79%)	142 (100%)	0	0	100	100
50	Q	236/292 (81%)	235 (100%)	1 (0%)	0	100	100
51	R	138/149 (93%)	138 (100%)	0	0	100	100
52	S	159/205 (78%)	157 (99%)	2 (1%)	0	100	100
53	T	164/206 (80%)	164 (100%)	0	0	100	100
54	U	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
55	V	203/216 (94%)	202 (100%)	1 (0%)	0	100	100
56	W	114/148 (77%)	114 (100%)	0	0	100	100
57	X	242/256 (94%)	242 (100%)	0	0	100	100
58	Y	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
59	Z	120/161 (74%)	120 (100%)	0	0	100	100
60	0	108/188 (57%)	108 (100%)	0	0	100	100
61	1	54/65 (83%)	54 (100%)	0	0	100	100
62	2	44/92 (48%)	44 (100%)	0	0	100	100
63	3	93/188 (50%)	93 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	4	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
65	5	392/423 (93%)	389 (99%)	3 (1%)	0	100	100
66	6	352/380 (93%)	345 (98%)	7 (2%)	0	100	100
67	7	292/338 (86%)	286 (98%)	6 (2%)	0	100	100
68	8	155/206 (75%)	153 (99%)	2 (1%)	0	100	100
69	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
70	a	96/142 (68%)	96 (100%)	0	0	100	100
71	b	148/215 (69%)	147 (99%)	1 (1%)	0	100	100
72	c	282/332 (85%)	280 (99%)	2 (1%)	0	100	100
73	d	231/306 (76%)	228 (99%)	3 (1%)	0	100	100
74	e	236/279 (85%)	227 (96%)	9 (4%)	0	100	100
75	f	153/212 (72%)	152 (99%)	1 (1%)	0	100	100
76	g	132/166 (80%)	131 (99%)	1 (1%)	0	100	100
77	h	108/158 (68%)	108 (100%)	0	0	100	100
78	i	95/128 (74%)	95 (100%)	0	0	100	100
79	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
80	k	100/112 (89%)	100 (100%)	0	0	100	100
81	l	80/138 (58%)	77 (96%)	3 (4%)	0	100	100
82	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
83	o	92/102 (90%)	92 (100%)	0	0	100	100
84	p	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
85	q	161/222 (72%)	160 (99%)	1 (1%)	0	100	100
86	r	160/196 (82%)	160 (100%)	0	0	100	100
87	s	382/439 (87%)	378 (99%)	4 (1%)	0	100	100
88	t	44/198 (22%)	44 (100%)	0	0	100	100
88	t1	69/198 (35%)	68 (99%)	1 (1%)	0	100	100
88	u	30/198 (15%)	30 (100%)	0	0	100	100
88	v	30/198 (15%)	30 (100%)	0	0	100	100
88	w	29/198 (15%)	29 (100%)	0	0	100	100
88	x	29/198 (15%)	29 (100%)	0	0	100	100
88	y	29/198 (15%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
89	H	200/267 (75%)	199 (100%)	1 (0%)	0	100	100
90	z	250/325 (77%)	244 (98%)	6 (2%)	0	100	100
All	All	14979/19979 (75%)	14787 (99%)	188 (1%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	AH	126	ILE
5	AD	117	ARG
1	A5	106	ALA
5	AD	299	LYS

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	A5	190/245 (78%)	190 (100%)	0	100	100
3	AB	198/249 (80%)	198 (100%)	0	100	100
4	AC	115/143 (80%)	115 (100%)	0	100	100
5	AD	286/357 (80%)	286 (100%)	0	100	100
6	AE	104/107 (97%)	104 (100%)	0	100	100
7	AF	185/209 (88%)	185 (100%)	0	100	100
8	AG	285/342 (83%)	285 (100%)	0	100	100
9	AH	130/180 (72%)	130 (100%)	0	100	100
10	AI	104/146 (71%)	104 (100%)	0	100	100
11	AJ	93/118 (79%)	93 (100%)	0	100	100
12	AK	91/113 (80%)	91 (100%)	0	100	100
13	AL	158/226 (70%)	158 (100%)	0	100	100
14	AM	97/113 (86%)	97 (100%)	0	100	100
15	AN	96/115 (84%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AO	174/230 (76%)	174 (100%)	0	100	100
17	AP	88/123 (72%)	88 (100%)	0	100	100
18	AQ	78/78 (100%)	78 (100%)	0	100	100
19	AR	264/318 (83%)	264 (100%)	0	100	100
20	AS	116/164 (71%)	116 (100%)	0	100	100
21	AT	153/157 (98%)	153 (100%)	0	100	100
22	AU	152/174 (87%)	152 (100%)	0	100	100
23	AV	325/364 (89%)	325 (100%)	0	100	100
24	AW	87/158 (55%)	87 (100%)	0	100	100
25	AX	311/351 (89%)	311 (100%)	0	100	100
26	AY	137/357 (38%)	137 (100%)	0	100	100
27	AZ	90/95 (95%)	90 (100%)	0	100	100
28	A0	188/189 (100%)	188 (100%)	0	100	100
29	A1	256/291 (88%)	256 (100%)	0	100	100
30	A2	100/100 (100%)	100 (100%)	0	100	100
31	A3	65/166 (39%)	65 (100%)	0	100	100
32	A4	526/609 (86%)	526 (100%)	0	100	100
39	D	192/245 (78%)	192 (100%)	0	100	100
40	E	260/290 (90%)	260 (100%)	0	100	100
41	F	219/262 (84%)	219 (100%)	0	100	100
42	I	194/232 (84%)	194 (100%)	0	100	100
43	J	138/150 (92%)	138 (100%)	0	100	100
44	K	155/155 (100%)	155 (100%)	0	100	100
45	L	98/124 (79%)	98 (100%)	0	100	100
46	M	245/249 (98%)	245 (100%)	0	100	100
47	N	189/211 (90%)	189 (100%)	0	100	100
48	O	134/150 (89%)	134 (100%)	0	100	100
49	P	126/155 (81%)	126 (100%)	0	100	100
50	Q	220/256 (86%)	220 (100%)	0	100	100
51	R	118/126 (94%)	118 (100%)	0	100	100
52	S	146/180 (81%)	146 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	T	146/176 (83%)	146 (100%)	0	100	100
54	U	134/134 (100%)	134 (100%)	0	100	100
55	V	183/191 (96%)	183 (100%)	0	100	100
56	W	94/119 (79%)	94 (100%)	0	100	100
57	X	220/229 (96%)	220 (100%)	0	100	100
58	Y	163/223 (73%)	163 (100%)	0	100	100
59	Z	113/147 (77%)	113 (100%)	0	100	100
60	0	99/164 (60%)	99 (100%)	0	100	100
61	1	53/60 (88%)	53 (100%)	0	100	100
62	2	40/72 (56%)	40 (100%)	0	100	100
63	3	88/166 (53%)	88 (100%)	0	100	100
64	4	37/89 (42%)	37 (100%)	0	100	100
65	5	353/368 (96%)	353 (100%)	0	100	100
66	6	313/332 (94%)	313 (100%)	0	100	100
67	7	270/303 (89%)	270 (100%)	0	100	100
68	8	146/190 (77%)	146 (100%)	0	100	100
69	9	104/112 (93%)	104 (100%)	0	100	100
70	a	96/133 (72%)	96 (100%)	0	100	100
71	b	131/185 (71%)	131 (100%)	0	100	100
72	c	251/288 (87%)	251 (100%)	0	100	100
73	d	219/274 (80%)	219 (100%)	0	100	100
74	e	207/236 (88%)	207 (100%)	0	100	100
75	f	139/188 (74%)	139 (100%)	0	100	100
76	g	124/148 (84%)	124 (100%)	0	100	100
77	h	104/148 (70%)	104 (100%)	0	100	100
78	i	86/110 (78%)	86 (100%)	0	100	100
79	j	74/97 (76%)	74 (100%)	0	100	100
80	k	83/89 (93%)	83 (100%)	0	100	100
81	l	76/116 (66%)	76 (100%)	0	100	100
82	m	85/113 (75%)	85 (100%)	0	100	100
83	o	80/87 (92%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	p	135/181 (75%)	135 (100%)	0	100	100
85	q	142/178 (80%)	142 (100%)	0	100	100
86	r	147/169 (87%)	147 (100%)	0	100	100
87	s	340/381 (89%)	340 (100%)	0	100	100
88	t	40/158 (25%)	40 (100%)	0	100	100
88	t1	59/158 (37%)	59 (100%)	0	100	100
88	u	31/158 (20%)	31 (100%)	0	100	100
88	v	31/158 (20%)	31 (100%)	0	100	100
88	w	30/158 (19%)	30 (100%)	0	100	100
88	x	30/158 (19%)	30 (100%)	0	100	100
88	y	30/158 (19%)	30 (100%)	0	100	100
89	H	182/228 (80%)	182 (100%)	0	100	100
90	z	226/287 (79%)	226 (100%)	0	100	100
All	All	13410/17189 (78%)	13410 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A5	169	ASN
3	AB	130	ASN
4	AC	126	GLN
5	AD	130	GLN
5	AD	356	GLN
5	AD	359	HIS
5	AD	415	GLN
7	AF	146	HIS
7	AF	147	GLN
8	AG	77	GLN
8	AG	82	ASN
8	AG	288	HIS
9	AH	130	HIS
9	AH	183	HIS
10	AI	87	HIS
14	AM	50	GLN
14	AM	75	HIS

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Mol	Chain	Res	Type
14	AM	100	HIS
15	AN	9	HIS
16	AO	103	ASN
16	AO	111	HIS
16	AO	169	GLN
18	AQ	85	GLN
19	AR	224	HIS
20	AS	66	HIS
21	AT	37	HIS
21	AT	54	GLN
22	AU	109	ASN
23	AV	87	HIS
23	AV	215	GLN
23	AV	383	HIS
23	AV	388	GLN
23	AV	391	GLN
25	AX	69	ASN
25	AX	148	GLN
25	AX	385	ASN
26	AY	381	ASN
28	A0	145	HIS
29	A1	235	ASN
29	A1	268	GLN
30	A2	113	ASN
31	A3	140	HIS
32	A4	355	GLN
32	A4	521	HIS
32	A4	590	GLN
40	E	63	GLN
40	E	202	GLN
40	E	237	HIS
40	E	280	HIS
41	F	251	HIS
42	I	43	GLN
42	I	151	ASN
42	I	225	GLN
43	J	116	HIS
44	K	89	GLN
45	L	48	ASN
45	L	59	HIS
45	L	143	ASN
46	M	71	GLN

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Mol	Chain	Res	Type
50	Q	132	GLN
52	S	118	ASN
53	T	126	HIS
55	V	18	HIS
56	W	72	HIS
57	X	27	HIS
57	X	172	GLN
58	Y	88	GLN
58	Y	99	HIS
58	Y	117	GLN
63	3	170	ASN
65	5	275	ASN
65	5	343	GLN
65	5	384	GLN
66	6	69	HIS
66	6	308	GLN
67	7	34	GLN
68	8	62	GLN
68	8	177	HIS
68	8	186	GLN
71	b	16	HIS
71	b	25	GLN
71	b	27	GLN
72	c	77	HIS
72	c	107	GLN
72	c	168	HIS
72	c	177	GLN
73	d	149	HIS
74	e	112	GLN
74	e	248	ASN
74	e	251	HIS
75	f	92	ASN
76	g	102	HIS
78	i	120	HIS
78	i	124	HIS
80	k	72	HIS
81	l	67	GLN
81	l	82	GLN
82	m	59	GLN
84	p	152	GLN
84	p	190	GLN
85	q	180	GLN

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Mol	Chain	Res	Type
86	r	79	HIS
86	r	109	GLN
87	s	107	GLN
87	s	300	HIS
87	s	423	HIS
89	H	156	GLN
90	z	276	ASN
88	t1	129	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	AA	953/954 (99%)	135 (14%)	5 (0%)
33	Aw	65/68 (95%)	23 (35%)	0
34	Ax	67/70 (95%)	11 (16%)	0
35	Ay	52/70 (74%)	9 (17%)	0
36	Az	33/34 (97%)	10 (30%)	0
37	A	1554/1561 (99%)	233 (14%)	7 (0%)
38	B	70/72 (97%)	12 (17%)	0
All	All	2794/2829 (98%)	433 (15%)	12 (0%)

All (433) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	AA	651	A
2	AA	680	U
2	AA	688	A
2	AA	695	A
2	AA	704	U
2	AA	721	U
2	AA	723	A
2	AA	737	C
2	AA	738	A
2	AA	753	A
2	AA	761	A
2	AA	764	A
2	AA	765	C
2	AA	766	G
2	AA	791	G
2	AA	794	U
2	AA	796	G

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Mol	Chain	Res	Type
2	AA	815	C
2	AA	830	U
2	AA	832	U
2	AA	835	C
2	AA	851	A
2	AA	852	A
2	AA	860	A
2	AA	861	U
2	AA	866	A
2	AA	868	C
2	AA	871	A
2	AA	872	G
2	AA	890	C
2	AA	902	G
2	AA	903	U
2	AA	904	C
2	AA	907	A
2	AA	908	C
2	AA	919	A
2	AA	923	A
2	AA	929	A
2	AA	931	C
2	AA	932	C
2	AA	933	G
2	AA	938	A
2	AA	939	A
2	AA	942	A
2	AA	943	G
2	AA	947	U
2	AA	958	C
2	AA	959	C
2	AA	960	C
2	AA	962	C
2	AA	967	A
2	AA	992	U
2	AA	993	A
2	AA	1001	C
2	AA	1010	A
2	AA	1011	C
2	AA	1012	A
2	AA	1015	A
2	AA	1042	U

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Mol	Chain	Res	Type
2	AA	1049	A
2	AA	1065	C
2	AA	1082	A
2	AA	1103	A
2	AA	1105	C
2	AA	1107	U
2	AA	1117	A
2	AA	1118	A
2	AA	1121	A
2	AA	1126	A
2	AA	1128	C
2	AA	1137	A
2	AA	1151	C
2	AA	1153	C
2	AA	1160	A
2	AA	1179	G
2	AA	1187	U
2	AA	1188	A
2	AA	1189	U
2	AA	1190	C
2	AA	1215	U
2	AA	1220	A
2	AA	1223	C
2	AA	1225	C
2	AA	1236	C
2	AA	1247	G
2	AA	1248	C
2	AA	1251	A
2	AA	1258	A
2	AA	1271	C
2	AA	1273	G
2	AA	1275	A
2	AA	1283	A
2	AA	1284	U
2	AA	1290	C
2	AA	1291	U
2	AA	1299	A
2	AA	1326	A
2	AA	1327	G
2	AA	1328	G
2	AA	1343	A
2	AA	1344	U

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Mol	Chain	Res	Type
2	AA	1354	A
2	AA	1356	A
2	AA	1378	C
2	AA	1387	A
2	AA	1390	A
2	AA	1405	C
2	AA	1407	U
2	AA	1430	A
2	AA	1463	G
2	AA	1478	A
2	AA	1482	A
2	AA	1503	G
2	AA	1507	A
2	AA	1513	A
2	AA	1514	A
2	AA	1519	A
2	AA	1521	U
2	AA	1525	C
2	AA	1526	U
2	AA	1527	A
2	AA	1531	C
2	AA	1537	C
2	AA	1539	C
2	AA	1540	A
2	AA	1551	G
2	AA	1557	A
2	AA	1568	U
2	AA	1571	U
2	AA	1582	G
2	AA	1584	MA6
2	AA	1585	A
2	AA	1594	G
2	AA	1595	G
2	AA	1599	A
33	Aw	3	G
33	Aw	7	A
33	Aw	8	U
33	Aw	9	A
33	Aw	10	G
33	Aw	14	A
33	Aw	15	A
33	Aw	16	A

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Mol	Chain	Res	Type
33	Aw	21	A
33	Aw	22	A
33	Aw	30	U
33	Aw	36	C
33	Aw	46	A
33	Aw	49	U
33	Aw	50	A
33	Aw	53	A
33	Aw	56	A
33	Aw	66	U
33	Aw	68	U
33	Aw	69	A
33	Aw	71	C
33	Aw	74	C
33	Aw	76	A
34	Ax	2	A
34	Ax	3	G
34	Ax	8	U
34	Ax	9	A
34	Ax	25	C
34	Ax	44	A
34	Ax	45	G
34	Ax	46	A
34	Ax	49	G
34	Ax	59	U
34	Ax	76	A
35	Ay	3	G
35	Ay	4	G
35	Ay	44	A
35	Ay	45	G
35	Ay	48	U
35	Ay	49	G
35	Ay	59	U
35	Ay	75	C
35	Ay	76	A
36	Az	0	U
36	Az	11	U
36	Az	12	U
36	Az	13	U
36	Az	18	A
36	Az	22	A
36	Az	25	U

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Mol	Chain	Res	Type
36	Az	26	A
36	Az	27	C
36	Az	32	A
37	A	1681	G
37	A	1689	C
37	A	1692	A
37	A	1694	U
37	A	1699	C
37	A	1700	U
37	A	1704	U
37	A	1708	A
37	A	1711	C
37	A	1713	A
37	A	1724	A
37	A	1727	A
37	A	1728	U
37	A	1736	A
37	A	1748	G
37	A	1765	C
37	A	1777	A
37	A	1805	A
37	A	1806	U
37	A	1807	U
37	A	1808	A
37	A	1809	U
37	A	1821	A
37	A	1827	C
37	A	1828	A
37	A	1829	A
37	A	1832	A
37	A	1836	A
37	A	1844	A
37	A	1854	U
37	A	1856	A
37	A	1869	A
37	A	1873	A
37	A	1882	A
37	A	1887	A
37	A	1893	A
37	A	1894	G
37	A	1901	C
37	A	1903	C

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Mol	Chain	Res	Type
37	A	1918	G
37	A	1937	A
37	A	1940	A
37	A	1958	G
37	A	1985	G
37	A	1992	C
37	A	1994	A
37	A	2003	A
37	A	2015	G
37	A	2022	G
37	A	2030	U
37	A	2031	A
37	A	2036	C
37	A	2037	U
37	A	2038	U
37	A	2039	A
37	A	2054	U
37	A	2055	U
37	A	2060	A
37	A	2070	C
37	A	2071	U
37	A	2079	C
37	A	2099	U
37	A	2113	G
37	A	2125	C
37	A	2126	U
37	A	2147	G
37	A	2159	U
37	A	2161	A
37	A	2163	A
37	A	2168	U
37	A	2171	U
37	A	2181	A
37	A	2184	A
37	A	2185	G
37	A	2196	A
37	A	2198	A
37	A	2200	A
37	A	2207	A
37	A	2214	A
37	A	2219	C
37	A	2221	C

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Mol	Chain	Res	Type
37	A	2222	U
37	A	2223	A
37	A	2224	C
37	A	2225	C
37	A	2227	A
37	A	2230	A
37	A	2232	A
37	A	2233	U
37	A	2237	A
37	A	2241	A
37	A	2243	A
37	A	2245	A
37	A	2246	A
37	A	2262	C
37	A	2263	C
37	A	2284	C
37	A	2285	U
37	A	2294	A
37	A	2296	U
37	A	2297	A
37	A	2300	G
37	A	2316	U
37	A	2322	C
37	A	2331	C
37	A	2332	C
37	A	2345	G
37	A	2349	G
37	A	2350	A
37	A	2353	A
37	A	2363	A
37	A	2372	U
37	A	2374	A
37	A	2390	A
37	A	2399	A
37	A	2404	U
37	A	2407	U
37	A	2414	C
37	A	2415	C
37	A	2445	U
37	A	2478	G
37	A	2488	C
37	A	2493	C

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Mol	Chain	Res	Type
37	A	2500	A
37	A	2520	C
37	A	2521	A
37	A	2524	A
37	A	2527	A
37	A	2558	A
37	A	2570	C
37	A	2571	G
37	A	2577	C
37	A	2592	G
37	A	2593	G
37	A	2600	A
37	A	2601	A
37	A	2618	U
37	A	2627	G
37	A	2630	U
37	A	2633	A
37	A	2635	G
37	A	2654	U
37	A	2656	U
37	A	2683	C
37	A	2686	G
37	A	2694	A
37	A	2696	A
37	A	2706	A
37	A	2718	C
37	A	2719	G
37	A	2723	A
37	A	2724	G
37	A	2725	A
37	A	2732	G
37	A	2745	A
37	A	2762	C
37	A	2765	A
37	A	2767	A
37	A	2768	A
37	A	2774	C
37	A	2775	A
37	A	2780	C
37	A	2782	A
37	A	2783	A
37	A	2786	U

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Mol	Chain	Res	Type
37	A	2787	A
37	A	2788	C
37	A	2791	A
37	A	2810	G
37	A	2832	A
37	A	2833	A
37	A	2840	C
37	A	2847	C
37	A	2864	U
37	A	2865	C
37	A	2882	U
37	A	2883	A
37	A	2884	C
37	A	2885	U
37	A	2887	U
37	A	2893	A
37	A	2911	C
37	A	2913	A
37	A	2917	G
37	A	2919	A
37	A	2922	A
37	A	2928	C
37	A	2935	A
37	A	2946	A
37	A	2960	U
37	A	2963	A
37	A	2971	A
37	A	2985	C
37	A	2989	G
37	A	2990	A
37	A	2992	G
37	A	3000	A
37	A	3005	A
37	A	3021	C
37	A	3041	U
37	A	3053	A
37	A	3054	G
37	A	3060	C
37	A	3090	G
37	A	3098	U
37	A	3100	U
37	A	3108	U

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Mol	Chain	Res	Type
37	A	3109	U
37	A	3110	C
37	A	3111	A
37	A	3113	A
37	A	3122	U
37	A	3124	U
37	A	3157	C
37	A	3158	A
37	A	3162	C
37	A	3169	C
37	A	3172	C
37	A	3176	A
37	A	3183	U
37	A	3189	C
37	A	3199	U
37	A	3200	U
37	A	3207	A
37	A	3209	A
37	A	3210	C
37	A	3212	C
37	A	3217	A
37	A	3218	A
37	A	3220	A
37	A	3228	U
37	A	3230	G
37	A	3231	U
38	B	8	U
38	B	10	2MG
38	B	16	C
38	B	21	A
38	B	45	G
38	B	48	U
38	B	54	C
38	B	55	U
38	B	56	U
38	B	64	A
38	B	69	U
38	B	76	A

All (12) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
2	AA	907	A
2	AA	941	G
2	AA	1117	A
2	AA	1327	G
2	AA	1465	C
37	A	2030	U
37	A	2112	A
37	A	2222	U
37	A	2224	C
37	A	2245	A
37	A	2883	A
37	A	3097	U

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

15 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
37	OMU	A	3039	93,37	19,22,23	3.07	8 (42%)	26,31,34	1.69	5 (19%)
38	1MA	B	9	38	21,25,26	2.88	5 (23%)	31,37,40	1.66	5 (16%)
38	2MG	B	10	38	23,26,27	2.97	9 (39%)	32,38,41	2.82	11 (34%)
38	PSU	B	39	38	18,21,22	1.10	1 (5%)	22,30,33	1.82	5 (22%)
2	MA6	AA	1584	2	23,26,27	1.44	3 (13%)	34,38,41	3.51	12 (35%)
2	B8T	AA	1486	92,2	19,22,23	3.37	8 (42%)	26,31,34	0.84	1 (3%)
2	5MC	AA	1488	2	18,22,23	3.61	7 (38%)	26,32,35	0.99	1 (3%)
37	OMG	A	2815	93,34,37	23,26,27	2.44	8 (34%)	33,38,41	2.26	10 (30%)
37	1MA	A	2617	37	21,25,26	2.86	5 (23%)	31,37,40	1.65	5 (16%)
37	PSU	A	3067	37	18,21,22	1.13	1 (5%)	22,30,33	1.92	6 (27%)
71	THC	b	2	71	8,9,10	1.05	1 (12%)	9,11,13	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	5F0	AI	184	10	8,8,9	2.21	3 (37%)	7,9,11	2.53	2 (28%)
2	5MU	AA	1076	2	19,22,23	7.26	8 (42%)	28,32,35	3.30	10 (35%)
2	MA6	AA	1583	2	23,26,27	1.44	3 (13%)	34,38,41	3.43	11 (32%)
37	OMG	A	3040	93,33,37	23,26,27	2.45	8 (34%)	33,38,41	2.27	10 (30%)

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
37	OMU	A	3039	93,37	-	0/9/27/28	0/2/2/2
38	1MA	B	9	38	-	0/7/25/26	0/3/3/3
38	2MG	B	10	38	-	1/9/27/28	0/3/3/3
38	PSU	B	39	38	-	0/7/25/26	0/2/2/2
2	MA6	AA	1584	2	-	1/11/29/30	0/3/3/3
2	B8T	AA	1486	92,2	-	0/7/27/28	0/2/2/2
2	5MC	AA	1488	2	-	0/7/25/26	0/2/2/2
37	OMG	A	2815	93,34,37	-	1/9/27/28	0/3/3/3
37	1MA	A	2617	37	-	0/7/25/26	0/3/3/3
37	PSU	A	3067	37	-	0/7/25/26	0/2/2/2
71	THC	b	2	71	-	0/8/10/12	-
10	5F0	AI	184	10	-	1/9/9/10	-
2	5MU	AA	1076	2	-	0/7/25/26	0/2/2/2
2	MA6	AA	1583	2	-	0/11/29/30	0/3/3/3
37	OMG	A	3040	93,33,37	-	0/9/27/28	0/3/3/3

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	1076	5MU	C4-C5	21.36	1.80	1.44
2	AA	1076	5MU	C6-N1	15.33	1.64	1.38
2	AA	1076	5MU	C6-C5	-11.81	1.15	1.34
2	AA	1076	5MU	C4-N3	-11.29	1.17	1.38
2	AA	1488	5MC	C6-C5	9.27	1.49	1.34
38	B	9	1MA	C2-N3	8.72	1.46	1.30
37	A	2617	1MA	C2-N3	8.66	1.46	1.30
38	B	10	2MG	C2-N3	7.80	1.46	1.31
37	A	3039	OMU	C2-N1	7.20	1.50	1.38
2	AA	1486	B8T	C4-N3	7.11	1.45	1.32
37	A	3039	OMU	C2-N3	6.92	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	B	9	1MA	C4-N3	6.68	1.49	1.35
37	A	2617	1MA	C4-N3	6.63	1.49	1.35
2	AA	1486	B8T	C2-N3	6.62	1.49	1.36
2	AA	1488	5MC	C4-N3	6.58	1.45	1.34
38	B	10	2MG	C4-N3	6.53	1.49	1.34
37	A	2815	OMG	C4-N3	6.44	1.49	1.34
37	A	3040	OMG	C4-N3	6.42	1.49	1.34
2	AA	1488	5MC	C2-N3	6.22	1.49	1.36
2	AA	1486	B8T	C6-C5	6.15	1.49	1.35
38	B	10	2MG	C2-N2	5.80	1.46	1.33
37	A	3039	OMU	C6-C5	5.74	1.48	1.35
38	B	10	2MG	C2-N1	5.71	1.45	1.36
37	A	3040	OMG	C2-N3	5.58	1.46	1.33
37	A	2815	OMG	C2-N3	5.56	1.46	1.33
2	AA	1486	B8T	C4-N4	5.31	1.46	1.35
10	AI	184	5F0	O-C	4.83	1.47	1.19
37	A	3040	OMG	C2-N2	4.82	1.45	1.34
37	A	2815	OMG	C2-N2	4.79	1.45	1.34
38	B	9	1MA	C2-N1	4.70	1.44	1.35
37	A	2617	1MA	C2-N1	4.66	1.44	1.35
2	AA	1584	MA6	C6-N6	4.64	1.50	1.36
2	AA	1583	MA6	C6-N6	4.58	1.50	1.36
2	AA	1488	5MC	C6-N1	4.55	1.45	1.38
2	AA	1488	5MC	C4-N4	4.44	1.45	1.34
2	AA	1486	B8T	C2-N1	4.39	1.49	1.40
37	A	3039	OMU	C4-N3	4.20	1.46	1.38
2	AA	1076	5MU	C2-N3	4.10	1.45	1.38
2	AA	1488	5MC	C2-N1	4.08	1.48	1.40
38	B	9	1MA	C5-C6	3.80	1.53	1.43
2	AA	1486	B8T	C5-C4	3.79	1.48	1.40
37	A	2617	1MA	C5-C6	3.72	1.53	1.43
2	AA	1076	5MU	C2-N1	3.63	1.44	1.38
38	B	39	PSU	C6-C5	3.56	1.39	1.35
2	AA	1486	B8T	C6-N1	3.55	1.46	1.38
37	A	3067	PSU	C6-C5	3.55	1.39	1.35
37	A	2815	OMG	C5-N7	-3.10	1.33	1.39
37	A	3040	OMG	C5-N7	-2.96	1.33	1.39
37	A	2617	1MA	C5-N7	-2.90	1.33	1.39
37	A	3039	OMU	C6-N1	2.88	1.44	1.38
37	A	3039	OMU	O4-C4	-2.87	1.18	1.24
38	B	9	1MA	C5-N7	-2.83	1.33	1.39
38	B	10	2MG	C6-N1	2.82	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	B	10	2MG	C5-C6	2.82	1.54	1.44
37	A	3040	OMG	C2-N1	2.70	1.44	1.37
2	AA	1486	B8T	O2-C2	-2.69	1.18	1.23
10	AI	184	5F0	OD1-C1	2.67	1.39	1.33
37	A	2815	OMG	C2-N1	2.67	1.44	1.37
2	AA	1488	5MC	O2-C2	-2.63	1.18	1.23
2	AA	1583	MA6	C5-C4	-2.57	1.34	1.39
2	AA	1076	5MU	O4-C4	-2.54	1.18	1.23
37	A	2815	OMG	C5-C6	2.53	1.53	1.44
37	A	3040	OMG	C5-C6	2.53	1.53	1.44
37	A	2815	OMG	O6-C6	-2.48	1.18	1.23
37	A	3040	OMG	O6-C6	-2.47	1.18	1.23
37	A	3040	OMG	C6-N1	2.45	1.43	1.38
2	AA	1584	MA6	C5-C4	-2.45	1.34	1.39
37	A	3039	OMU	C5-C4	2.41	1.49	1.43
37	A	2815	OMG	C6-N1	2.35	1.43	1.38
2	AA	1076	5MU	O2-C2	-2.30	1.18	1.23
38	B	10	2MG	O6-C6	-2.30	1.19	1.23
10	AI	184	5F0	CB-C	2.23	1.55	1.49
38	B	10	2MG	C5-N7	-2.20	1.34	1.39
37	A	3039	OMU	O2-C2	-2.17	1.19	1.23
2	AA	1584	MA6	C5-N7	-2.16	1.34	1.39
71	b	2	THC	CA-N1	-2.15	1.43	1.46
2	AA	1583	MA6	C5-N7	-2.14	1.35	1.39
38	B	10	2MG	C8-N7	2.04	1.38	1.32

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AA	1584	MA6	N1-C6-N6	-14.37	101.37	117.08
2	AA	1583	MA6	N1-C6-N6	-13.97	101.81	117.08
2	AA	1076	5MU	C5-C4-N3	10.35	124.15	115.31
38	B	10	2MG	C1'-N9-C8	-7.96	104.05	126.70
2	AA	1584	MA6	C5-C6-N6	7.71	138.73	125.30
2	AA	1076	5MU	C5-C6-N1	-7.61	115.51	123.34
2	AA	1583	MA6	C5-C6-N6	7.45	138.27	125.30
2	AA	1076	5MU	C4-N3-C2	-6.87	118.45	127.35
38	B	10	2MG	C1'-N9-C4	6.87	146.91	126.50
38	B	10	2MG	C2-N3-C4	6.37	119.94	112.04
37	A	3040	OMG	C1'-N9-C4	-5.82	109.21	126.50
10	AI	184	5F0	O-C-CB	-5.59	109.13	125.43
37	A	3040	OMG	C1'-N9-C8	5.54	142.48	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	A	2815	OMG	C5-C4-N3	-5.50	119.54	128.46
37	A	2815	OMG	C1'-N9-C4	-5.40	110.45	126.50
2	AA	1583	MA6	N1-C2-N3	-5.35	120.23	128.60
2	AA	1584	MA6	N1-C2-N3	-5.28	120.34	128.60
37	A	2815	OMG	C1'-N9-C8	5.27	141.70	126.70
2	AA	1584	MA6	C5-C4-N3	-5.22	119.94	126.75
37	A	3039	OMU	C4-N3-C2	-5.21	119.71	126.58
2	AA	1583	MA6	C5-C4-N3	-5.13	120.06	126.75
37	A	3040	OMG	C5-C4-N3	-5.10	120.19	128.46
38	B	9	1MA	N1-C2-N3	-5.07	119.97	126.00
37	A	2617	1MA	N1-C2-N3	-4.98	120.08	126.00
37	A	3067	PSU	N1-C2-N3	4.87	120.65	115.13
37	A	3067	PSU	C4-N3-C2	-4.82	119.40	126.34
38	B	10	2MG	C5-C4-N3	-4.78	120.70	128.46
37	A	2617	1MA	C5-C4-N3	-4.69	120.26	127.26
38	B	39	PSU	C4-N3-C2	-4.64	119.66	126.34
38	B	9	1MA	C5-C4-N3	-4.62	120.36	127.26
38	B	39	PSU	N1-C2-N3	4.53	120.27	115.13
37	A	2815	OMG	C2-N3-C4	4.50	120.33	112.30
2	AA	1076	5MU	C5M-C5-C6	-4.50	116.84	122.85
2	AA	1076	5MU	N3-C2-N1	4.46	120.81	114.89
2	AA	1584	MA6	N9-C8-N7	-4.42	107.87	113.91
2	AA	1583	MA6	N9-C8-N7	-4.42	107.87	113.91
37	A	3040	OMG	C2-N3-C4	4.36	120.07	112.30
38	B	10	2MG	C2-N1-C6	-4.15	119.70	124.48
2	AA	1076	5MU	C5M-C5-C4	4.02	123.19	118.77
38	B	9	1MA	C2-N3-C4	3.89	120.05	112.41
37	A	2617	1MA	C2-N3-C4	3.87	120.01	112.41
2	AA	1076	5MU	O4-C4-C5	-3.79	120.51	124.90
2	AA	1584	MA6	C4-C5-C6	3.67	119.99	115.88
37	A	3039	OMU	N3-C2-N1	3.67	119.76	114.89
38	B	10	2MG	N9-C8-N7	-3.66	106.51	113.39
2	AA	1583	MA6	C4-C5-C6	3.63	119.94	115.88
2	AA	1583	MA6	C2-N1-C6	3.47	119.95	111.75
2	AA	1584	MA6	C2-N1-C6	3.46	119.94	111.75
2	AA	1584	MA6	C2-N3-C4	3.45	119.90	111.75
2	AA	1583	MA6	C2-N3-C4	3.45	119.89	111.75
2	AA	1488	5MC	C5-C6-N1	-3.37	119.87	123.34
37	A	3039	OMU	C5-C4-N3	3.34	119.84	114.84
37	A	2815	OMG	N9-C4-N3	3.29	132.54	125.94
2	AA	1584	MA6	C5-N7-C8	3.21	108.07	103.51
2	AA	1583	MA6	N3-C4-N9	3.18	132.32	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	A	2815	OMG	C2-N1-C6	-3.11	119.42	125.10
10	AI	184	5F0	OD1-C1-CA	3.11	119.49	111.52
2	AA	1584	MA6	N3-C4-N9	3.11	132.21	127.08
2	AA	1583	MA6	C5-N7-C8	3.11	107.92	103.51
37	A	3040	OMG	N9-C4-N3	3.05	132.07	125.94
37	A	3040	OMG	C2-N1-C6	-2.96	119.70	125.10
37	A	3040	OMG	N9-C8-N7	-2.92	107.90	113.39
37	A	3039	OMU	O4-C4-C5	-2.89	120.08	125.16
38	B	10	2MG	N9-C4-N3	2.74	131.44	125.94
37	A	2815	OMG	N9-C8-N7	-2.74	108.24	113.39
37	A	3067	PSU	O2-C2-N1	-2.71	119.81	122.79
37	A	2815	OMG	C5-C6-N1	2.69	120.03	113.19
37	A	3040	OMG	C5-C6-N1	2.67	119.98	113.19
38	B	39	PSU	O2-C2-N1	-2.62	119.90	122.79
38	B	10	2MG	C5-C6-N1	2.61	119.81	113.19
38	B	9	1MA	N9-C8-N7	-2.58	108.54	113.39
37	A	2617	1MA	N9-C8-N7	-2.57	108.55	113.39
2	AA	1076	5MU	O4-C4-N3	-2.49	115.34	120.12
38	B	10	2MG	N1-C2-N3	-2.49	120.10	123.95
38	B	10	2MG	C8-N7-C5	2.48	108.72	104.24
38	B	10	2MG	O6-C6-C5	-2.47	120.04	126.60
2	AA	1583	MA6	C4-N9-C8	2.46	108.40	105.73
2	AA	1486	B8T	C6-C5-C4	2.46	119.97	116.96
37	A	3040	OMG	O6-C6-C5	-2.45	120.10	126.60
37	A	2815	OMG	O6-C6-C5	-2.44	120.14	126.60
38	B	39	PSU	C6-C5-C4	2.43	119.90	118.20
2	AA	1076	5MU	O2-C2-N1	-2.43	119.55	122.79
37	A	3067	PSU	C6-N1-C2	-2.40	120.23	122.68
37	A	3067	PSU	C6-C5-C4	2.39	119.87	118.20
2	AA	1584	MA6	C4-N9-C8	2.32	108.24	105.73
2	AA	1076	5MU	C6-C5-C4	2.32	119.97	118.03
37	A	3067	PSU	O4'-C1'-C2'	2.23	108.29	105.14
37	A	2617	1MA	N9-C4-N3	2.21	132.08	126.94
2	AA	1584	MA6	C4-C5-N7	-2.18	107.97	110.62
38	B	39	PSU	C6-N1-C2	-2.12	120.52	122.68
37	A	2815	OMG	C8-N7-C5	2.12	108.07	104.24
37	A	3040	OMG	C8-N7-C5	2.08	108.01	104.24
38	B	9	1MA	N9-C4-N3	2.03	131.68	126.94
37	A	3039	OMU	O2-C2-N1	-2.01	120.12	122.79

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	AI	184	5F0	N-CA-CB-C
2	AA	1584	MA6	C4'-C5'-O5'-P
37	A	2815	OMG	C4'-C5'-O5'-P
38	B	10	2MG	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	A	3039	OMU	1	0
2	AA	1584	MA6	5	0
37	A	2815	OMG	1	0
37	A	3067	PSU	1	0
2	AA	1076	5MU	1	0
2	AA	1583	MA6	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 245 ligands modelled in this entry, 237 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
91	NAD	AA	1701	92	45,48,48	3.57	19 (42%)	63,73,73	1.73	12 (19%)
99	VAL	e	301	-	4,6,7	0.52	0	6,7,9	0.95	0
97	GDP	AX	503	-	28,30,30	1.14	3 (10%)	44,47,47	1.84	7 (15%)
95	FES	r	201	42,86	0,4,4	-	-	-	-	-
95	FES	AT	201	21,14	0,4,4	-	-	-	-	-
96	ATP	AX	501	92	29,33,33	3.10	10 (34%)	44,52,52	2.89	15 (34%)
95	FES	AP	201	6,17	0,4,4	-	-	-	-	-
98	SPD	A	3301	-	9,9,9	0.33	0	8,8,8	0.86	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
91	NAD	AA	1701	92	-	1/30/62/62	0/5/5/5
97	GDP	AX	503	-	-	0/16/32/32	0/3/3/3
95	FES	r	201	42,86	-	-	0/1/1/1
95	FES	AP	201	6,17	-	-	0/1/1/1
95	FES	AT	201	21,14	-	-	0/1/1/1
96	ATP	AX	501	92	-	1/22/38/38	0/3/3/3
99	VAL	e	301	-	-	0/5/6/8	-
98	SPD	A	3301	-	-	0/7/7/7	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
96	AX	501	ATP	C2'-C3'	-10.61	1.24	1.53
91	AA	1701	NAD	C7N-N7N	9.69	1.51	1.33
91	AA	1701	NAD	O4B-C1B	8.50	1.62	1.42
91	AA	1701	NAD	C3D-C4D	-8.42	1.31	1.53
91	AA	1701	NAD	O4D-C4D	7.32	1.61	1.45
91	AA	1701	NAD	C2B-C1B	-7.08	1.30	1.53
91	AA	1701	NAD	O4D-C1D	-6.68	1.31	1.41
96	AX	501	ATP	C6-N6	6.44	1.50	1.34
91	AA	1701	NAD	O4B-C4B	-6.24	1.31	1.45
91	AA	1701	NAD	C3N-C7N	5.54	1.58	1.50
96	AX	501	ATP	O4'-C1'	-4.83	1.30	1.42
96	AX	501	ATP	C2'-C1'	4.31	1.67	1.53
91	AA	1701	NAD	O7N-C7N	-4.12	1.16	1.24
96	AX	501	ATP	C5'-C4'	-3.98	1.39	1.51
91	AA	1701	NAD	C5A-C4A	-3.75	1.32	1.39
96	AX	501	ATP	O3'-C3'	3.73	1.51	1.43
91	AA	1701	NAD	C8A-N9A	-3.39	1.31	1.37
91	AA	1701	NAD	O3D-C3D	3.21	1.50	1.43
97	AX	503	GDP	C5-C4	3.06	1.47	1.38
96	AX	501	ATP	C3'-C4'	3.05	1.60	1.53
91	AA	1701	NAD	O3B-C3B	-3.03	1.35	1.43
96	AX	501	ATP	O4'-C4'	2.99	1.51	1.45
91	AA	1701	NAD	O2B-C2B	2.81	1.49	1.43
91	AA	1701	NAD	C5N-C4N	-2.60	1.33	1.38
96	AX	501	ATP	C5-C4	-2.59	1.34	1.39
97	AX	503	GDP	C6-N1	-2.38	1.34	1.38
96	AX	501	ATP	O2'-C2'	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	AA	1701	NAD	C5A-N7A	-2.33	1.34	1.39
91	AA	1701	NAD	C6A-N6A	2.24	1.39	1.34
91	AA	1701	NAD	C4N-C3N	-2.15	1.35	1.39
97	AX	503	GDP	C5-N7	-2.15	1.34	1.39
91	AA	1701	NAD	C8A-N7A	2.03	1.35	1.31

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
96	AX	501	ATP	C1'-N9-C8	-8.38	108.21	127.14
96	AX	501	ATP	N9-C8-N7	-6.32	105.26	113.91
97	AX	503	GDP	C5-C4-N3	-6.11	118.55	128.46
96	AX	501	ATP	N6-C6-N1	-5.83	105.59	118.35
96	AX	501	ATP	C4-N9-C1'	5.73	140.25	126.59
96	AX	501	ATP	N3-C2-N1	-5.52	119.97	128.60
91	AA	1701	NAD	N3A-C2A-N1A	-5.46	120.06	128.60
96	AX	501	ATP	C4-N9-C8	5.36	111.54	105.73
91	AA	1701	NAD	C5A-C4A-N3A	-5.20	119.96	126.75
96	AX	501	ATP	C5-C6-N6	5.06	134.43	123.43
97	AX	503	GDP	C2-N3-C4	4.85	120.95	112.30
97	AX	503	GDP	N9-C4-N3	4.69	135.36	125.94
91	AA	1701	NAD	N9A-C8A-N7A	-4.65	107.55	113.91
96	AX	501	ATP	C5-C4-N3	-4.53	120.83	126.75
96	AX	501	ATP	C5-N7-C8	3.84	108.96	103.51
96	AX	501	ATP	N3-C4-N9	3.81	133.37	127.08
97	AX	503	GDP	PA-O3A-PB	-3.75	119.95	132.83
91	AA	1701	NAD	C2A-N3A-C4A	3.65	120.36	111.75
91	AA	1701	NAD	C1B-N9A-C8A	-3.55	119.11	127.14
91	AA	1701	NAD	N3A-C4A-N9A	3.46	132.78	127.08
96	AX	501	ATP	C2-N3-C4	3.29	119.53	111.75
91	AA	1701	NAD	C5A-N7A-C8A	3.18	108.02	103.51
97	AX	503	GDP	C6-C5-N7	3.13	136.06	130.25
91	AA	1701	NAD	C4A-N9A-C8A	2.77	108.73	105.73
96	AX	501	ATP	PB-O3B-PG	-2.65	123.73	132.83
97	AX	503	GDP	C4-C5-N7	-2.58	106.64	110.72
96	AX	501	ATP	C3'-C2'-C1'	2.50	106.17	101.43
96	AX	501	ATP	PA-O3A-PB	-2.45	124.43	132.83
91	AA	1701	NAD	C4A-N9A-C1B	2.34	132.16	126.59
97	AX	503	GDP	O6-C6-C5	-2.17	120.85	126.60
96	AX	501	ATP	O4'-C1'-N9	2.16	112.31	108.06
91	AA	1701	NAD	C3N-C7N-N7N	2.12	120.29	117.75
91	AA	1701	NAD	PN-O3-PA	-2.10	125.63	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	AA	1701	NAD	C6N-N1N-C2N	-2.02	120.14	121.97

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
91	AA	1701	NAD	C4B-C5B-O5B-PA
96	AX	501	ATP	PA-O3A-PB-O2B

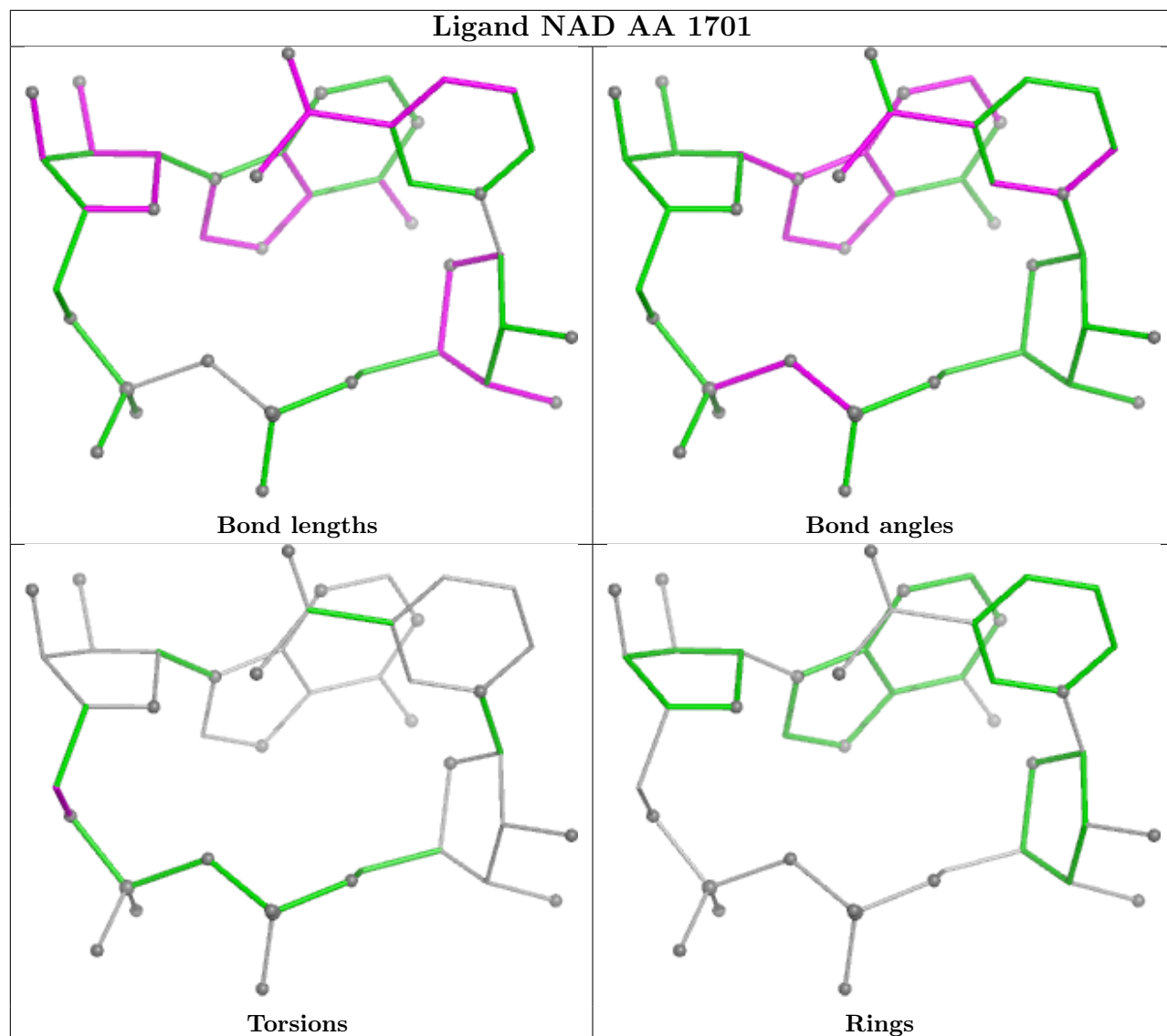
There are no ring outliers.

1 monomer is involved in 2 short contacts:

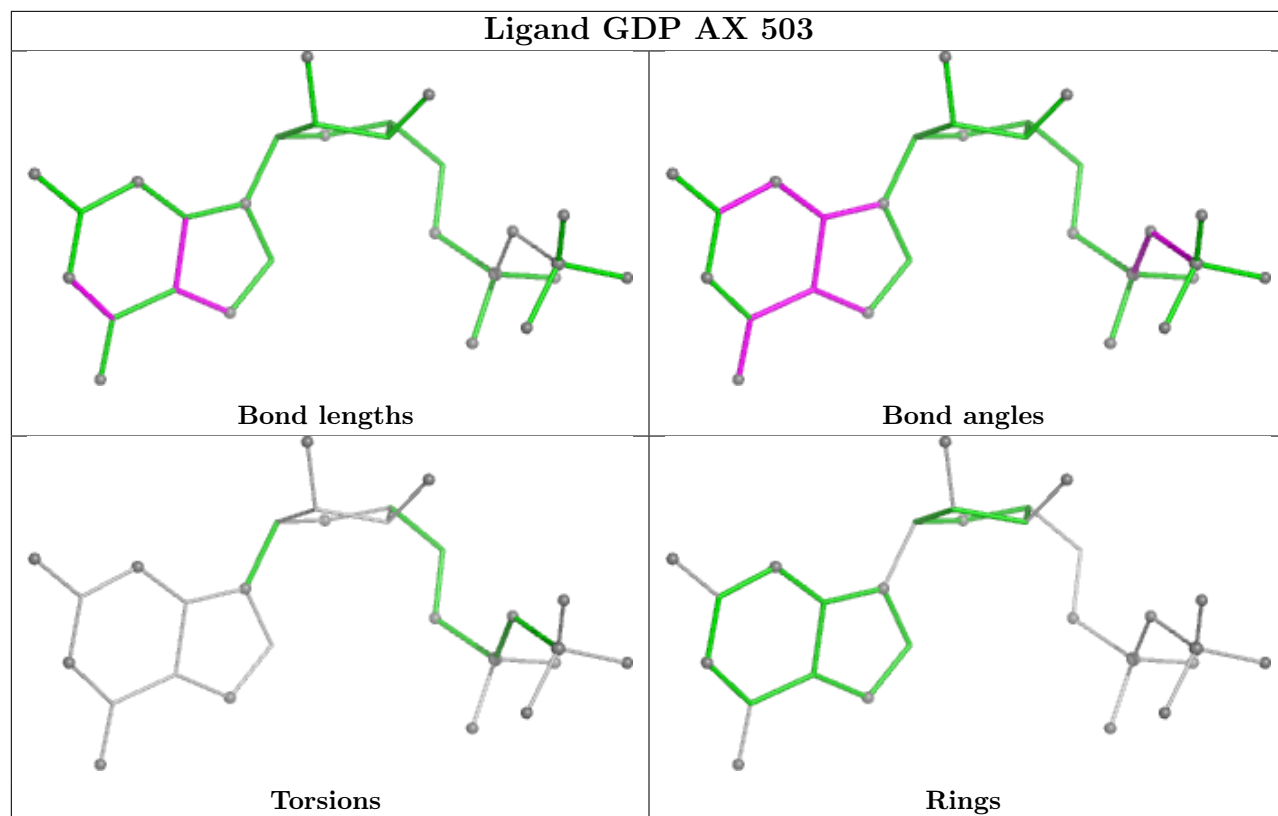
Mol	Chain	Res	Type	Clashes	Symm-Clashes
91	AA	1701	NAD	2	0

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

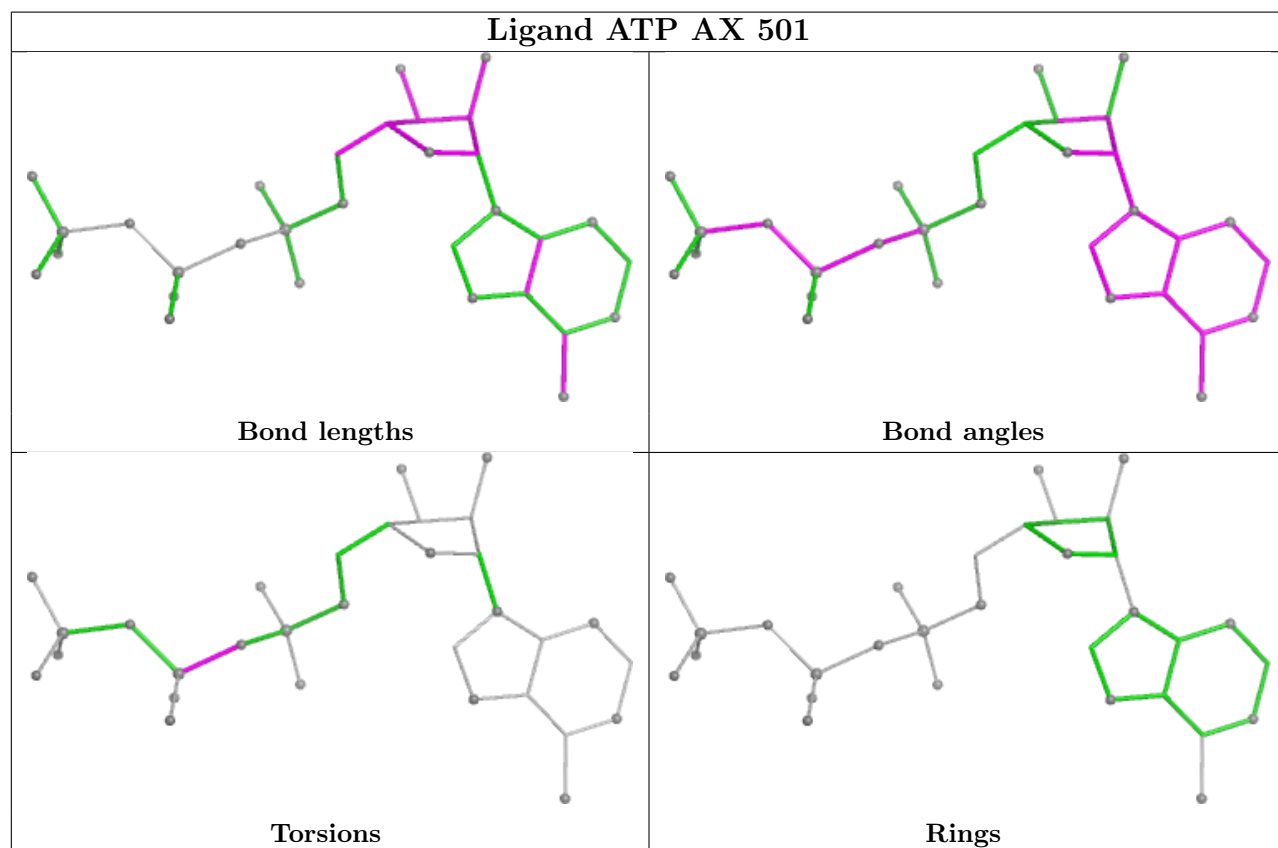
Ligand NAD AA 1701



Ligand GDP AX 503



Ligand ATP AX 501



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
33	Aw	3
34	Ax	2
35	Ay	1
38	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ay	15:A	O3'	21:A	P	9.65
1	Ax	15:A	O3'	21:A	P	8.40
1	B	56:U	O3'	58:A	P	4.51
1	Aw	56:A	O3'	61:U	P	4.08
1	Ax	46:A	O3'	48:U	P	3.84
1	Aw	46:A	O3'	48:U	P	3.67
1	Aw	16:A	O3'	20:C	P	3.08

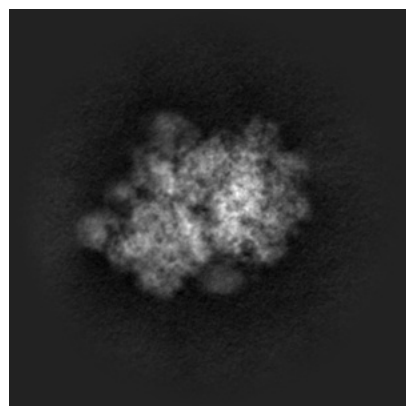
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54983. These allow visual inspection of the internal detail of the map and identification of artifacts.

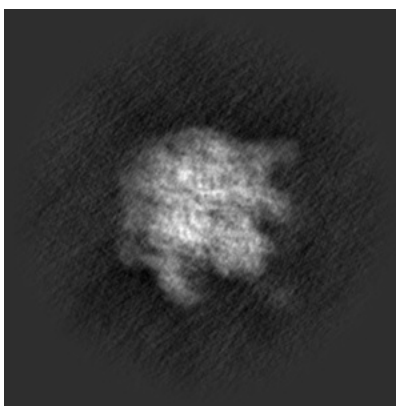
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

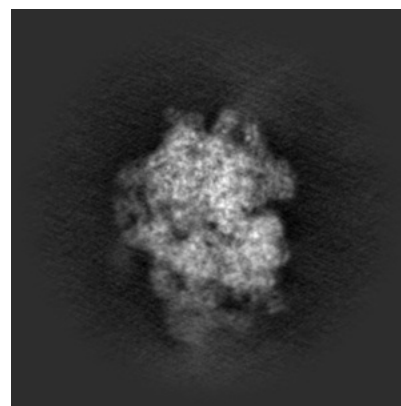
6.1.1 Primary map



X

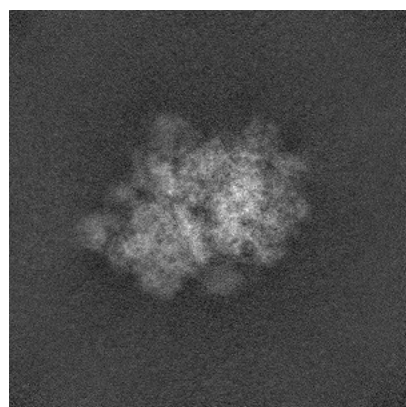


Y

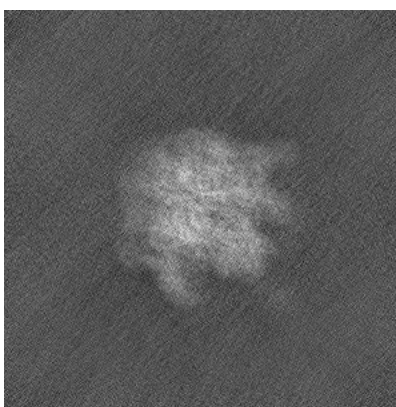


Z

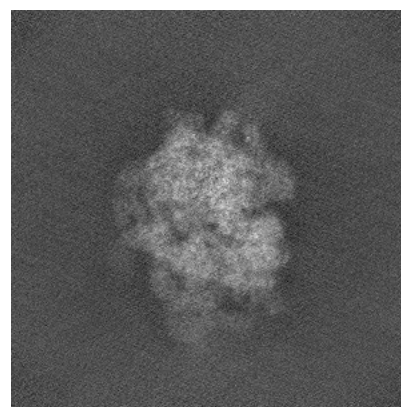
6.1.2 Raw map



X



Y

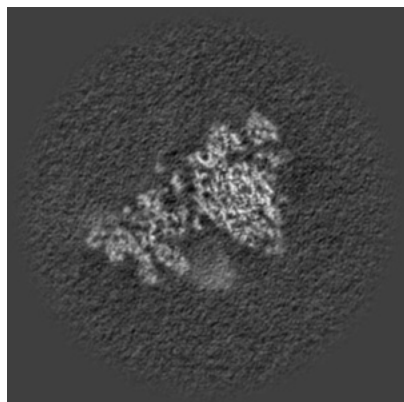


Z

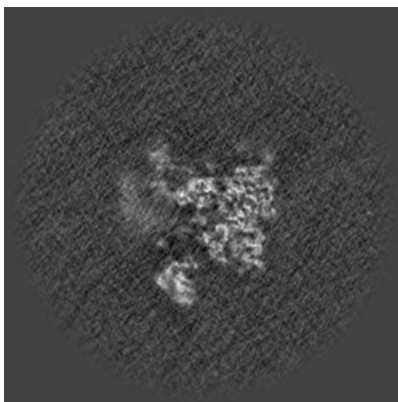
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

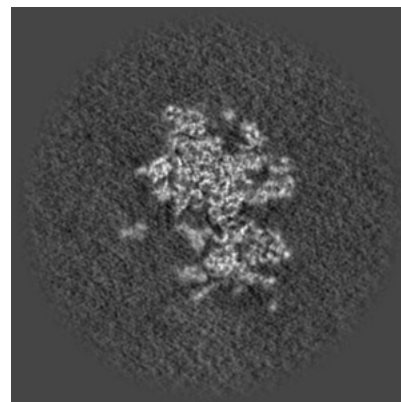
6.2.1 Primary map



X Index: 320

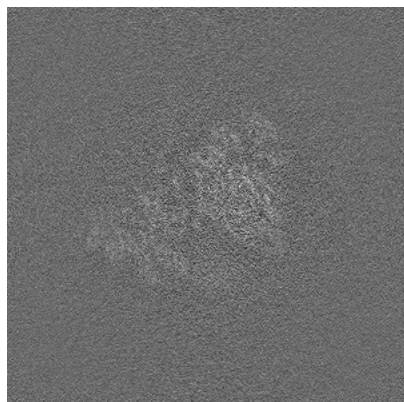


Y Index: 320

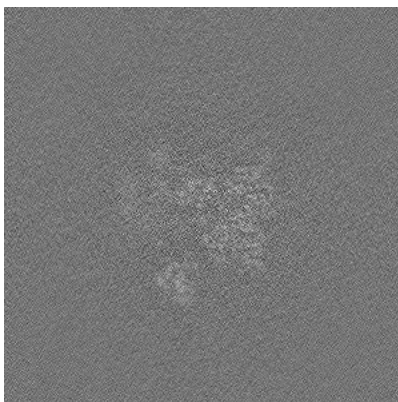


Z Index: 320

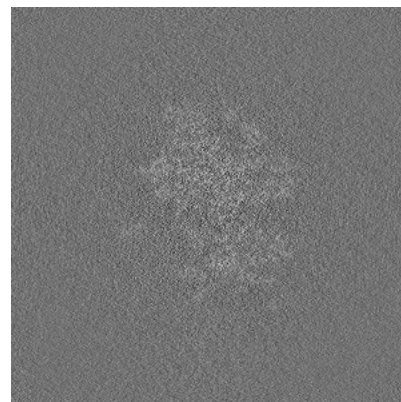
6.2.2 Raw map



X Index: 320



Y Index: 320

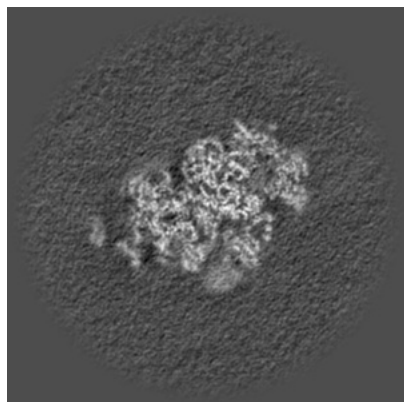


Z Index: 320

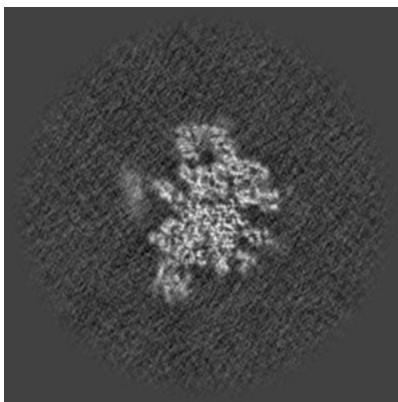
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

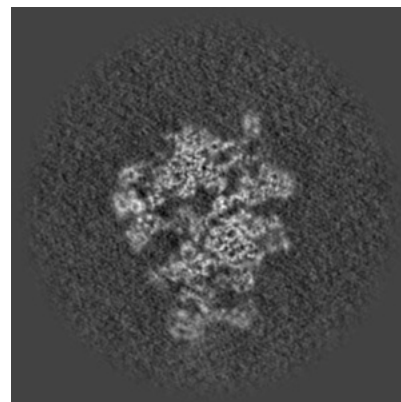
6.3.1 Primary map



X Index: 345

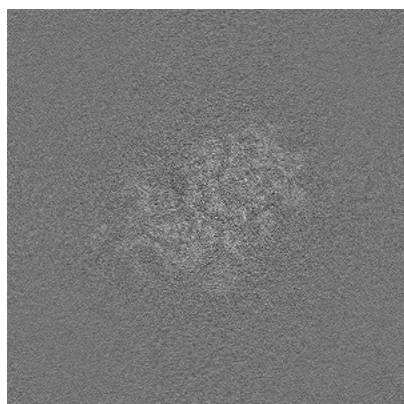


Y Index: 363

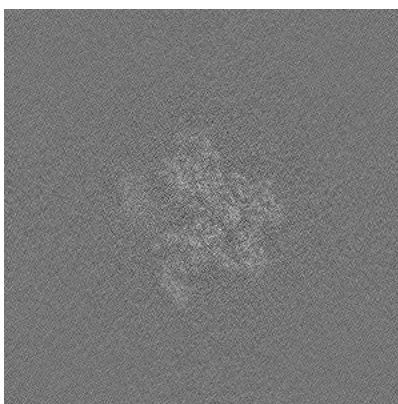


Z Index: 284

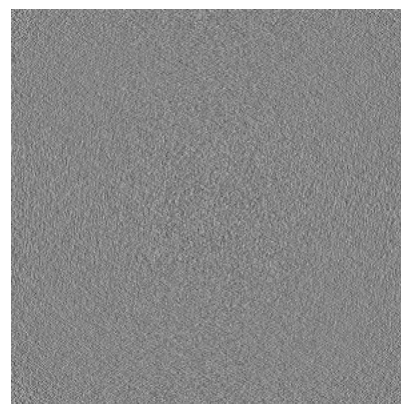
6.3.2 Raw map



X Index: 338



Y Index: 336

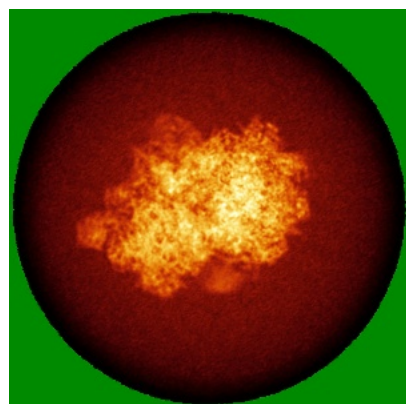


Z Index: 0

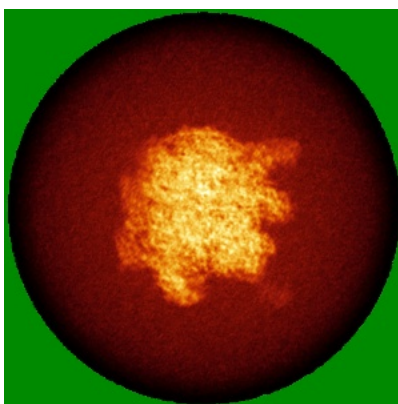
The images above show the largest variance slices of the map in three orthogonal directions.

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

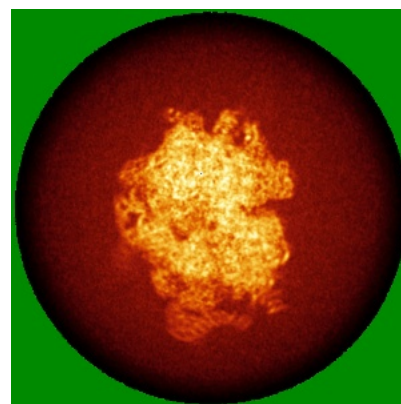
6.4.1 Primary map



X

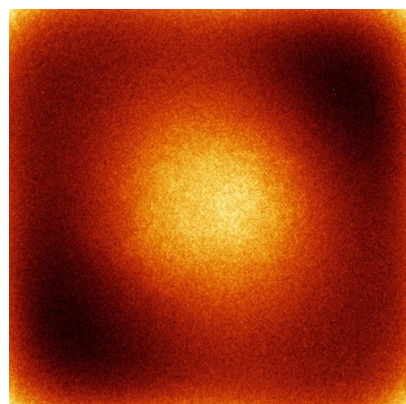


Y

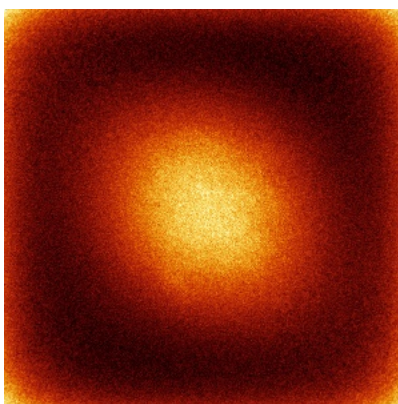


Z

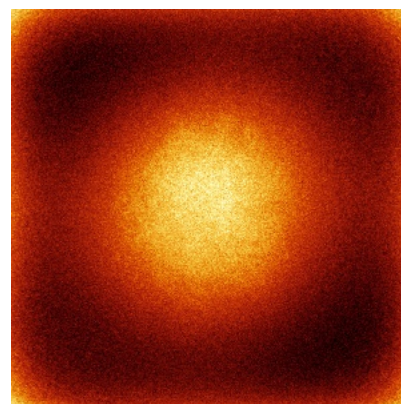
6.4.2 Raw map



X



Y

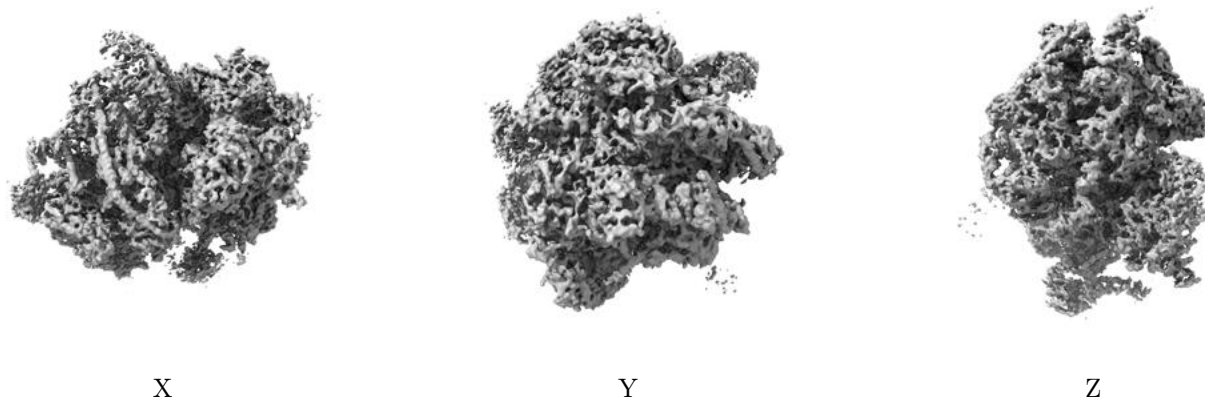


Z

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.

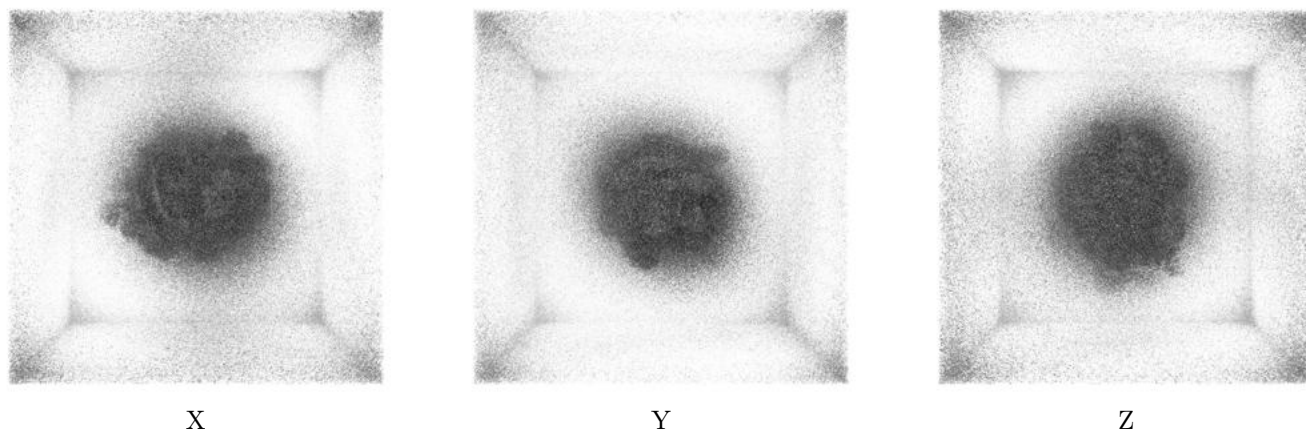
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.164. 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.

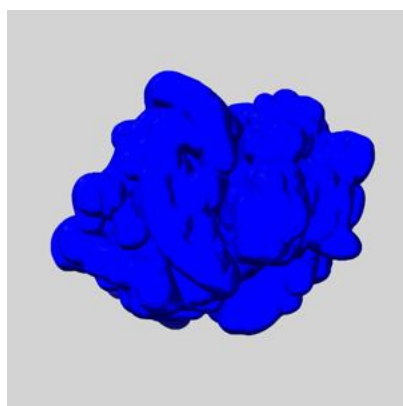
6.6 Mask visualisation [i](#)

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

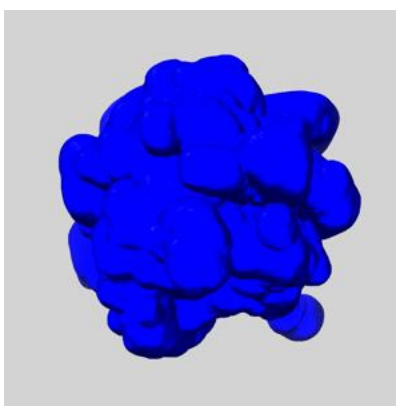
A mask typically either:

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

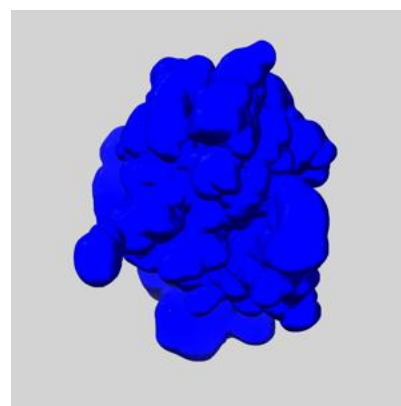
6.6.1 emd_54983_msk_1.map [i](#)



X



Y

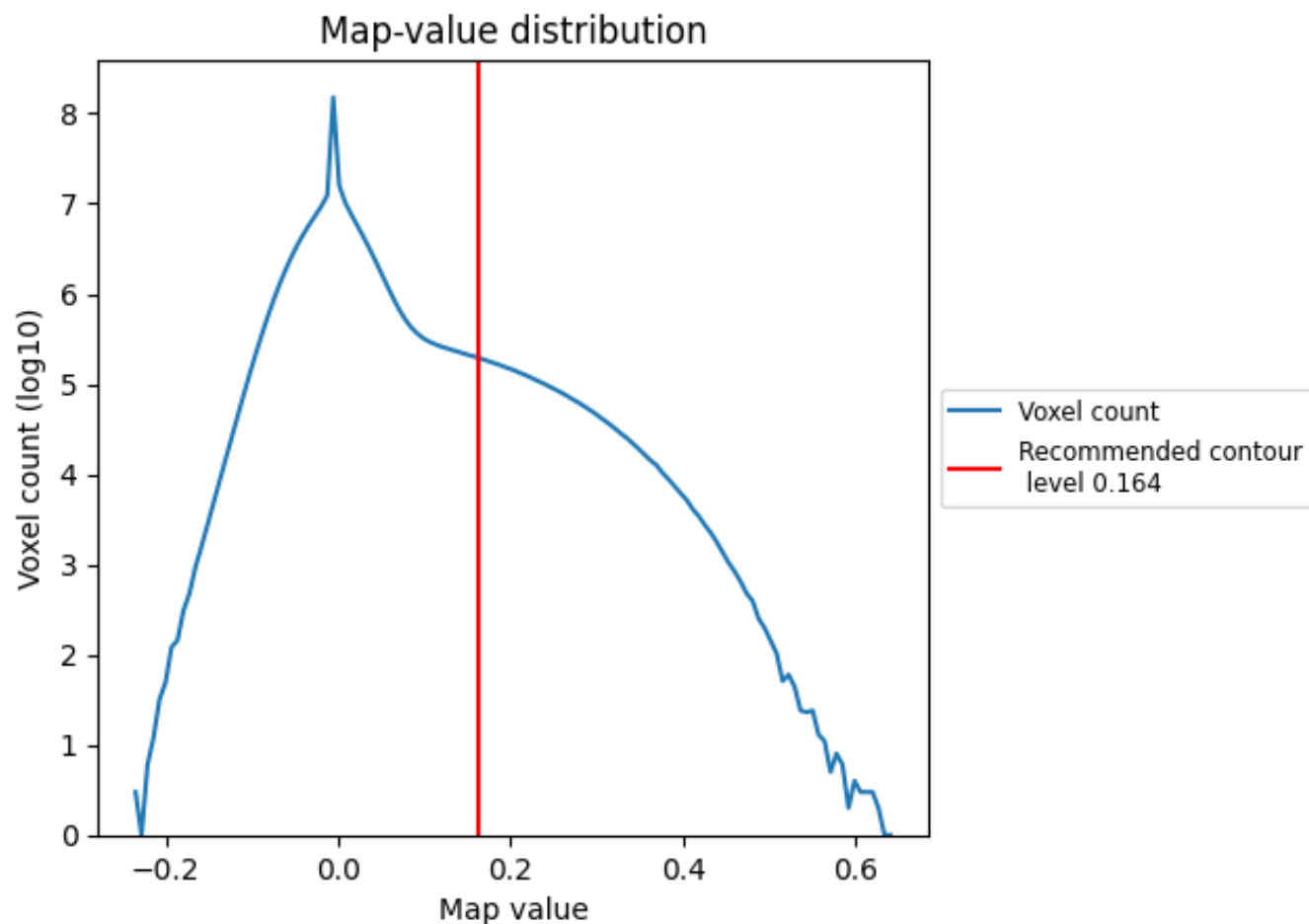


Z

7 Map analysis [i](#)

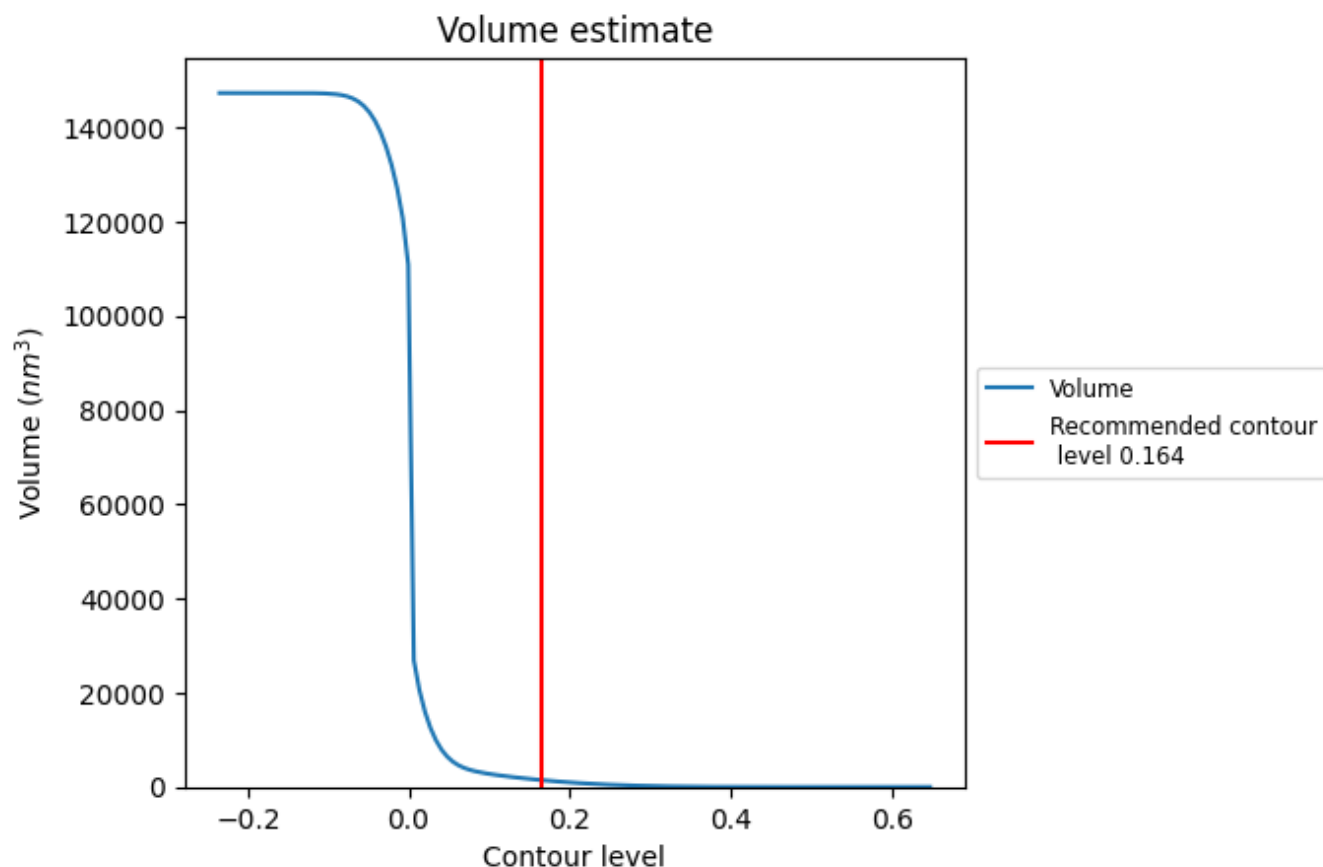
This section contains the results of statistical analysis of the map.

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.

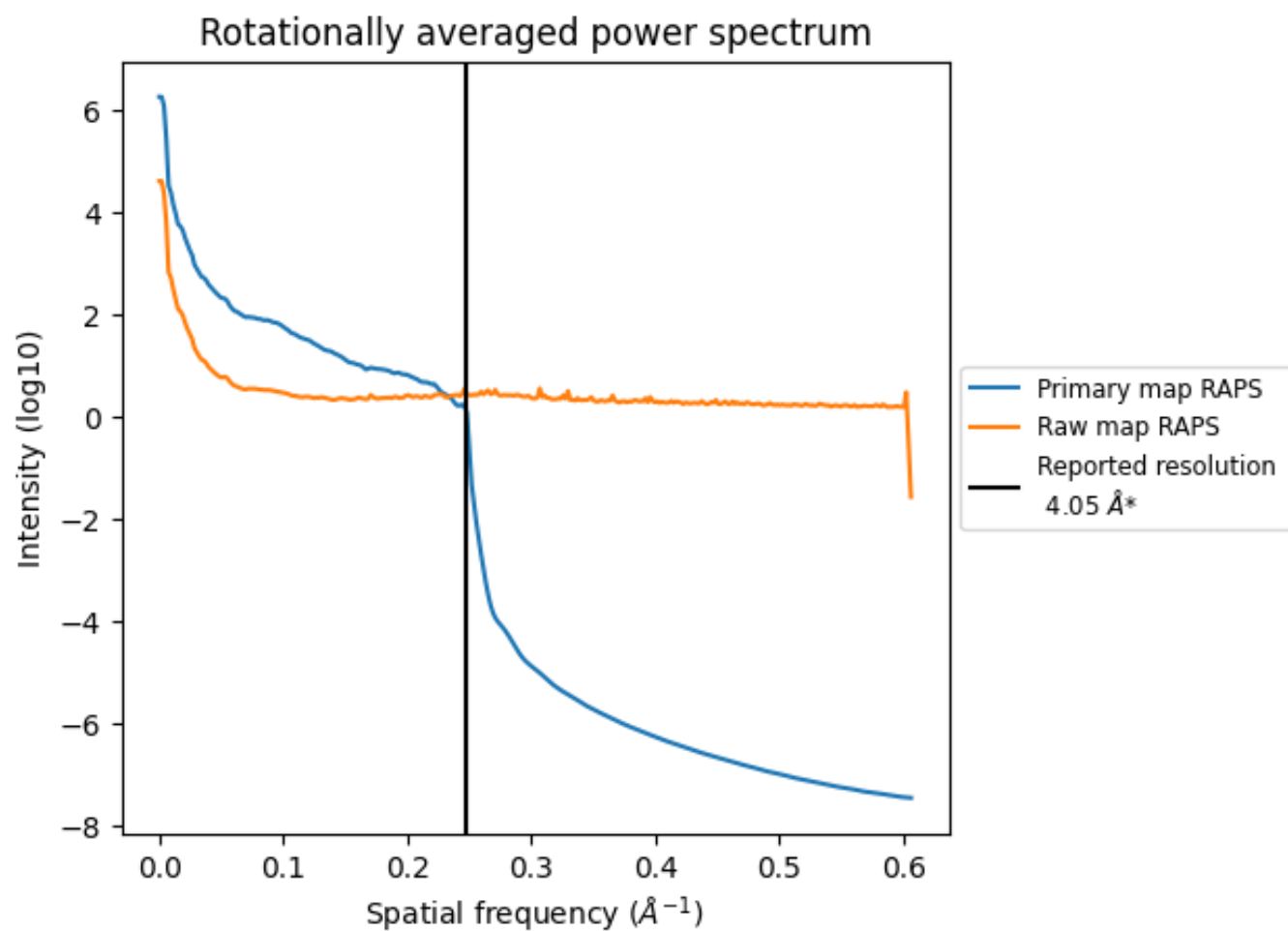
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1474 nm³; this corresponds to an approximate mass of 1332 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 ⓘ

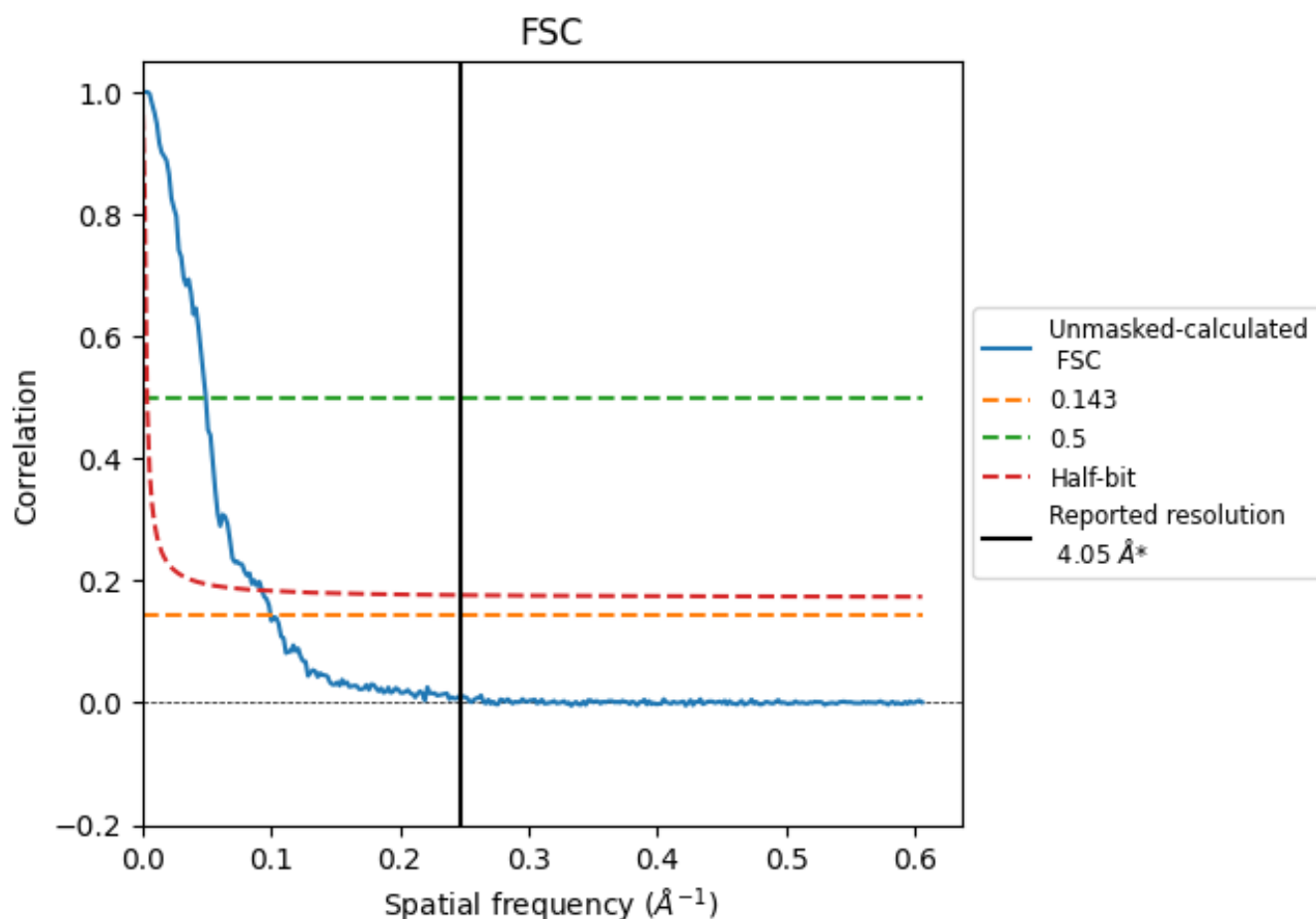


*Reported resolution corresponds to spatial frequency of 0.247 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.247 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

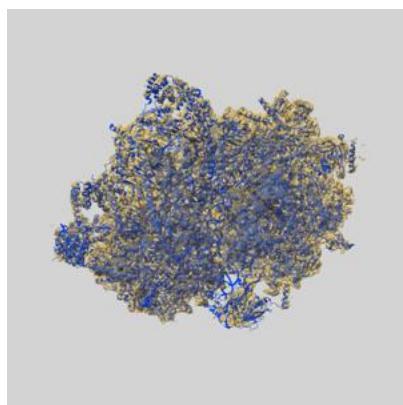
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.03	20.24	10.74

*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 10.03 differs from the reported value 4.05 by more than 10 %

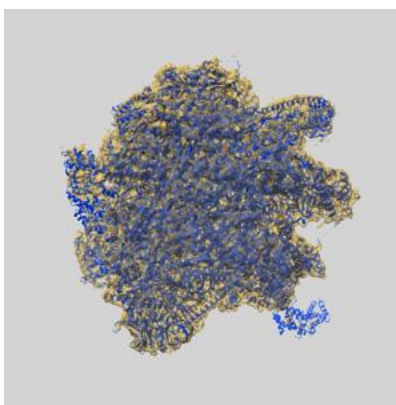
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54983 and PDB model 9SL3. Per-residue inclusion information can be found in section 3 on page 25.

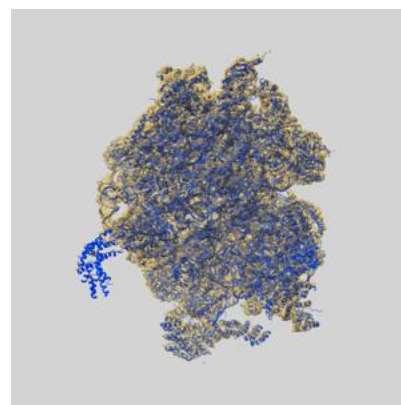
9.1 Map-model overlay [i](#)



X



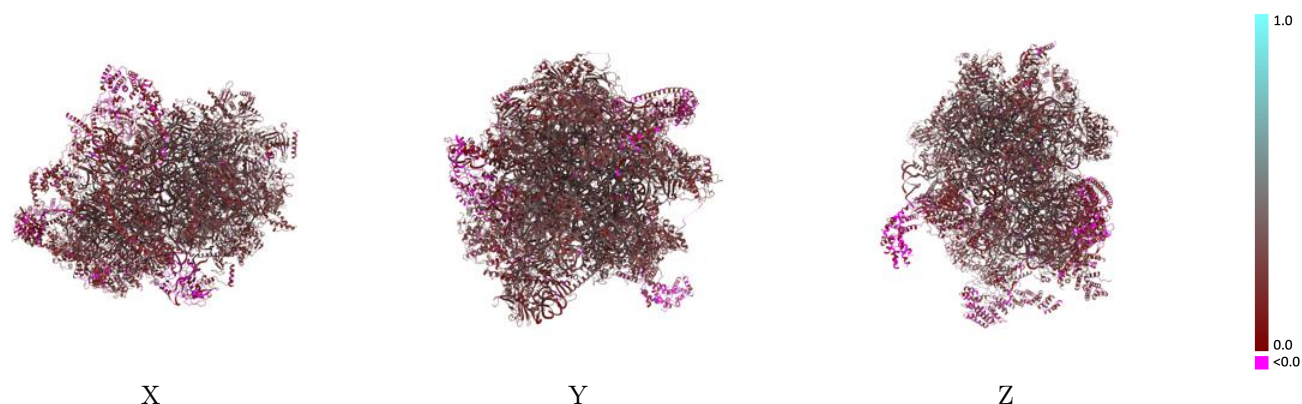
Y



Z

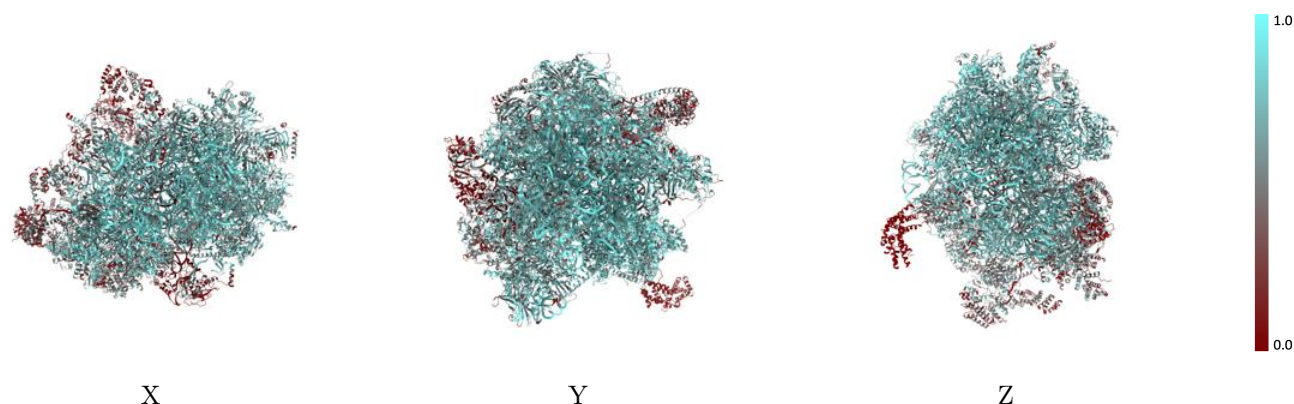
The images above show the 3D surface view of the map at the recommended contour level 0.164 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



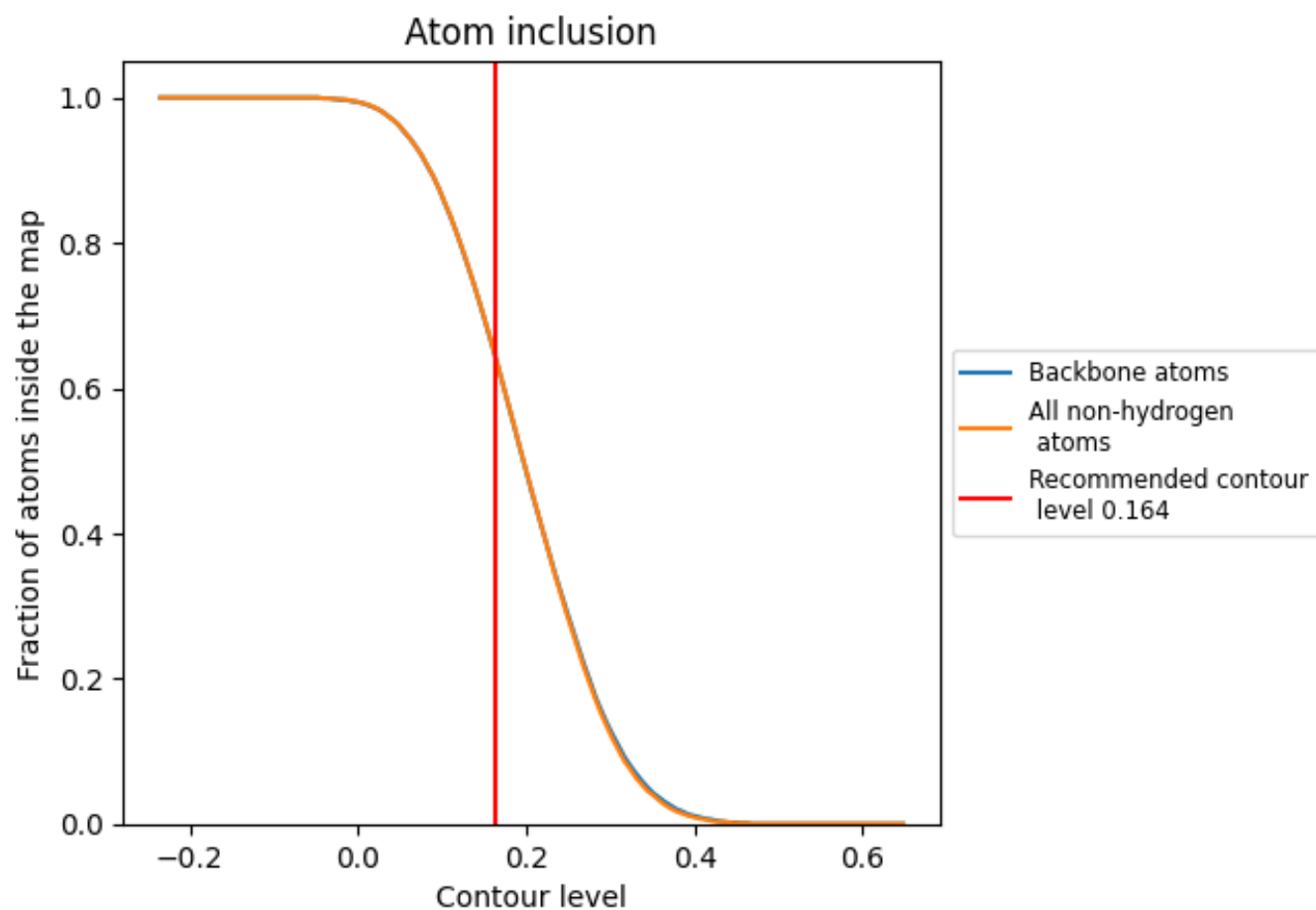
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.164).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.164) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6410	 0.2550
0	 0.6490	 0.2850
1	 0.5410	 0.2500
2	 0.7700	 0.3230
3	 0.6510	 0.3260
4	 0.7030	 0.2740
5	 0.6640	 0.2650
6	 0.6640	 0.2720
7	 0.6460	 0.2540
8	 0.5010	 0.2080
9	 0.6610	 0.2740
A	 0.8740	 0.3270
A0	 0.3060	 0.1620
A1	 0.4930	 0.2120
A2	 0.5230	 0.2260
A3	 0.5180	 0.2720
A4	 0.3550	 0.1340
A5	 0.6840	 0.1910
AA	 0.8460	 0.2870
AB	 0.6440	 0.2410
AC	 0.5230	 0.2640
AD	 0.5430	 0.2490
AE	 0.5950	 0.2280
AF	 0.5600	 0.2330
AG	 0.5460	 0.2150
AH	 0.5170	 0.2340
AI	 0.6990	 0.2480
AJ	 0.4400	 0.2440
AK	 0.5800	 0.2290
AL	 0.6140	 0.2190
AM	 0.4470	 0.1730
AN	 0.6130	 0.2410
AO	 0.4390	 0.2080
AP	 0.6240	 0.2420
AQ	 0.6790	 0.2470



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Chain	Atom inclusion	Q-score
AR	 0.4230	 0.1870
AS	 0.5440	 0.2150
AT	 0.5820	 0.2500
AU	 0.5560	 0.1800
AV	 0.3080	 0.1110
AW	 0.6500	 0.2100
AX	 0.4790	 0.2100
AY	 0.4340	 0.1780
AZ	 0.4320	 0.2050
Aw	 0.5260	 0.1890
Ax	 0.3960	 0.2120
Ay	 0.0090	 0.0410
Az	 0.2570	 0.1180
B	 0.8480	 0.2250
D	 0.6950	 0.2970
E	 0.6830	 0.2890
F	 0.6740	 0.3070
H	 0.3650	 0.1450
I	 0.4320	 0.1800
J	 0.6020	 0.1930
K	 0.7220	 0.3040
L	 0.5970	 0.2950
M	 0.6570	 0.2910
N	 0.7100	 0.3020
O	 0.6580	 0.2900
P	 0.6240	 0.2730
Q	 0.5300	 0.2700
R	 0.7120	 0.3000
S	 0.7250	 0.3270
T	 0.6770	 0.3180
U	 0.6150	 0.2830
V	 0.6010	 0.2690
W	 0.6740	 0.3070
X	 0.6690	 0.2710
Y	 0.6890	 0.2670
Z	 0.6970	 0.3360
a	 0.6160	 0.2720
b	 0.7340	 0.3200
c	 0.6990	 0.2830
d	 0.5590	 0.2450
e	 0.5570	 0.1740
f	 0.5360	 0.2250

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Chain	Atom inclusion	Q-score
g	 0.7450	 0.3110
h	 0.6950	 0.2920
i	 0.6860	 0.3170
j	 0.6900	 0.2950
k	 0.5140	 0.2010
l	 0.5670	 0.1920
m	 0.4770	 0.1790
o	 0.7610	 0.3160
p	 0.5770	 0.2470
q	 0.5170	 0.1990
r	 0.7230	 0.2790
s	 0.6860	 0.2710
t	 0.0790	 0.0720
t1	 0.5120	 0.1420
u	 0.0080	 0.0560
v	 0.0000	 0.0540
w	 0.0040	 0.0360
x	 0.0000	 0.0170
y	 0.0000	 -0.0220
z	 0.1180	 0.0430