



## Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 06:17 pm BST

PDB ID : 8RRI / pdb\_00008rri  
EMDB ID : EMD-19460  
Title : Human mitochondrial ribosome in complex with antibiotic tigecycline  
Authors : Khawaja, A.; Sing, V.; Nguyen, M.D.; Rorbach, J.  
Deposited on : 2024-01-22  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

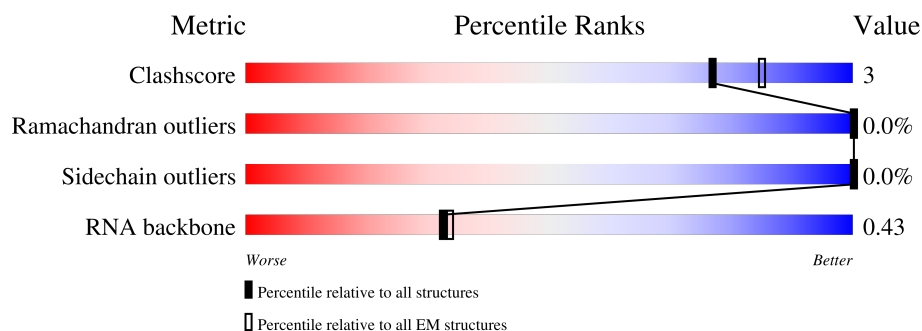
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	B	72	
2	D	305	
3	E	348	
4	F	311	
5	H	267	
6	J	192	
7	K	178	
























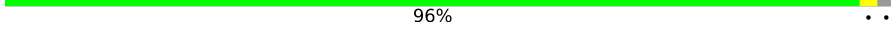

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Mol	Chain	Length	Quality of chain
8	L	145	
9	M	296	
10	N	251	
11	O	175	
12	P	180	
13	Q	292	
14	R	149	
15	S	205	
16	T	206	
17	U	153	
18	V	216	
19	W	148	
20	X	256	
21	Y	250	
22	Z	161	
23	0	188	
24	1	65	
25	2	92	
26	3	188	
27	4	103	
28	z	325	
29	5	423	
30	6	380	
31	7	338	
32	8	206	

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Mol	Chain	Length	Quality of chain
33	9	137	
34	a	142	
35	b	215	
36	c	332	
37	d	306	
38	e	279	
39	f	212	
40	g	166	
41	h	158	
42	i	128	
43	j	123	
44	k	112	
45	l	138	
46	m	128	
47	o	102	
48	p	206	
49	q	222	
50	r	196	
51	s	439	
52	AB	296	
53	AC	167	
54	AD	430	
55	AE	125	
56	AF	242	
57	AG	396	



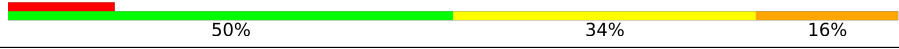

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Mol	Chain	Length	Quality of chain
58	AH	201	
59	AI	194	
60	AJ	138	
61	AK	128	
62	AL	257	
63	AM	137	
64	AN	130	
65	AO	258	
66	AP	142	
67	AQ	87	
68	AR	360	
69	AS	190	
70	AT	169	
71	AU	205	
72	AV	414	
73	AW	187	
74	AX	398	
75	AY	395	
76	AZ	106	
77	A0	217	
78	A1	323	
79	A2	118	
80	A3	199	
81	A4	689	
82	Ay	52	

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Mol	Chain	Length	Quality of chain
83	AA	954	
84	A	1558	
85	Az	32	
86	Ax	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	VAL	B	101	-	-	X	-

## 2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 323259 atoms, of which 147805 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 RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	72	Total	C	H	N	O	P	0	0
			2303	685	779	269	498	72		

- Molecule 2 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 3 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	305	Total	C	H	N	O	S	0	0
			4822	1545	2416	418	432	11		

- Molecule 4 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 5 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 6 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J	175	Total	C	H	N	O	S	0	0
			2738	847	1408	237	244	2		

- Molecule 7 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	K	178	Total	C	H	N	O	S	0	0
			2906	936	1451	259	253	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ACE	-	acetylation	UNP Q9BYD1

- Molecule 8 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	L	115	Total	C	H	N	O	S	0	0
			1831	559	941	171	155	5		

- Molecule 9 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	M	291	Total	C	H	N	O	S	0	0
			4722	1483	2395	430	408	6		

- Molecule 10 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 11 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	O	154	Total	C	H	N	O	S	0	0
			2554	792	1295	241	219	7		

- Molecule 12 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 13 is a protein called 39S ribosomal protein L19, mitochondrial.



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

- Molecule 14 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	U	153	Total	C	H	N	O	S	0	0
			2482	788	1231	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 18 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Z	122	Total	C	H	N	O	S	0	0
			2041	636	1045	186	171	3		

- Molecule 23 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	0	110	Total	C	H	N	O	S	0	0
			1818	554	920	176	162	6		

- Molecule 24 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	1	56	Total	C	H	N	O	S	0	0
			975	296	511	89	77	2		

- Molecule 25 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	2	46	Total	C	H	N	O	S	0	0
			783	233	406	83	60	1		

- Molecule 26 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	3	95	Total	C	H	N	O	S	0	0
			1715	539	883	162	128	3		

- Molecule 27 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	4	38	Total	C	H	N	O	S	0	0
			704	217	362	72	49	4		

- Molecule 28 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	z	164	Total	C	H	N	O	S	0	0
			2680	856	1353	217	250	4		

- Molecule 29 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	5	394	Total	C	H	N	O	S	0	0
			6416	2073	3206	560	566	11		

- Molecule 30 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	6	354	Total	C	H	N	O	S	0	0
			5789	1881	2841	525	533	9		

- Molecule 31 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	7	294	Total	C	H	N	O	S	0	0
			4787	1529	2397	405	438	18		

- Molecule 32 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	8	146	Total	C	H	N	O	S	0	0
			2497	786	1262	217	230	2		

- Molecule 33 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	9	124	Total	C	H	N	O	S	0	0
			1984	644	987	170	181	2		

- Molecule 34 is a protein called 39S ribosomal protein L42, mitochondrial.

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

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

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

- Molecule 36 is a protein called 39S ribosomal protein L44, mitochondrial.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
37	d	236	Total	C	H	N	O	S	0	0
			3874	1248	1928	333	352	13		

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

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 44 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	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	2	ACE	-	acetylation	UNP Q96EL3

- Molecule 45 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 46 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	m	92	Total	C	H	N	O	S	0	0
			1587	488	796	159	142	2		

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

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

- Molecule 48 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 49 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	q	161	Total	C	H	N	O	S	0	0
			2677	841	1327	260	244	5		

- Molecule 50 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	r	162	Total	C	H	N	O	S	0	0
			2672	839	1350	252	223	8		

- Molecule 51 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	s	386	Total	C	H	N	O	S	0	0
			6295	2023	3140	559	559	14		

- Molecule 52 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 53 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 54 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 55 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 56 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 57 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	AG	326	Total	C	H	N	O	S	0	0
			5359	1705	2678	476	486	14		

- Molecule 58 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 59 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	AI	137	Total	C	H	N	O	S	0	0
			2079	642	1059	192	182	4		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
60	AJ	108	Total	C	H	N	O	S	0	0
			1726	521	887	169	143	6		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
62	AL	167	Total	C	H	N	O	S	0	0
			2897	897	1491	260	242	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
65	AO	193	Total	C	H	N	O	S	0	0
			3153	1014	1561	294	277	7		

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



Mol	Chain	Residues	Atoms						AltConf	Trace
66	AP	97	Total	C	H	N	O	S	0	0
			1588	501	807	134	138	8		

- Molecule 67 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	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	2	ACE	-	acetylation	UNP P82921
AQ	50	ARG	CYS	variant	UNP P82921

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

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

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

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

- Molecule 70 is a protein called Small ribosomal subunit protein mS25.

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

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

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

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

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

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

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

- Molecule 74 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 75 is a protein called 28S ribosomal protein S31, mitochondrial.

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

- Molecule 76 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 77 is a protein called 28S ribosomal protein S34, mitochondrial.

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

- Molecule 78 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	A1	276	Total	C	H	N	O	S	0	0
			4507	1419	2269	381	427	11		

- Molecule 79 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	A2	118	Total	C	H	N	O	S	0	0
			1905	579	970	182	166	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	2	ACE	-	acetylation	UNP Q96BP2

- Molecule 80 is a protein called Aurora kinase A-interacting protein.

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

- Molecule 81 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 82 is a RNA chain called E/E-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	Ay	4	Total	C	H	N	O	P	0	0
			129	38	45	16	26	4		

- Molecule 83 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	AA	954	Total	C	H	N	O	P	0	0
			30564	9088	10304	3647	6571	954		

- Molecule 84 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	A	1551	Total	C	H	N	O	P	1	0
			49680	14786	16737	5941	10664	1552		

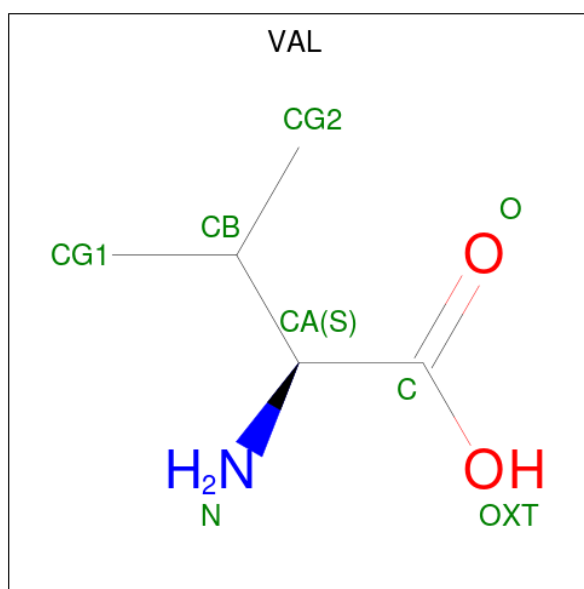
- Molecule 85 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	Az	32	Total	C	H	N	O	P	0	0
			1020	306	340	119	223	32		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
86	Ax	70	Total	C	H	N	O	P	0	0
			2234	665	752	261	486	70		

- Molecule 87 is VALINE (CCD ID: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
87	B	1	Total	C	H	N	O	0
			18	5	11	1	1	

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

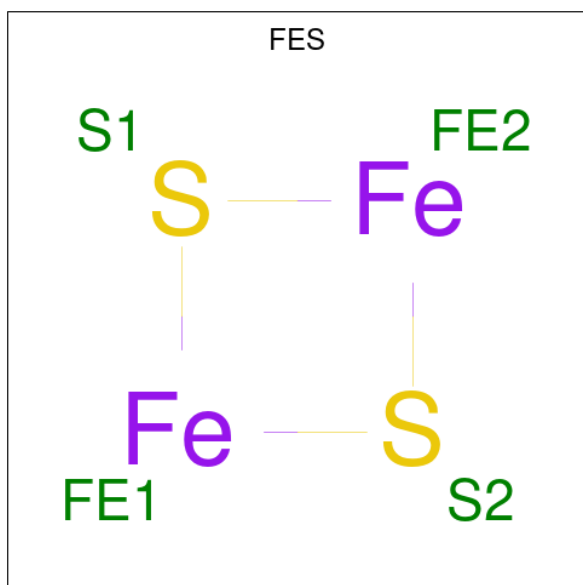
Mol	Chain	Residues	Atoms		AltConf
88	D	1	Total	Mg	0
			1	1	
88	E	1	Total	Mg	0
			1	1	
88	2	1	Total	Mg	0
			1	1	
88	AX	1	Total	Mg	0
			1	1	

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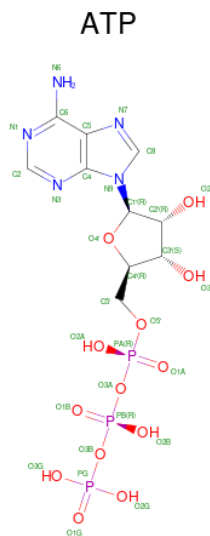
Mol	Chain	Residues	Atoms		AltConf
88	AA	23	Total 23	Mg 23	0
88	A	67	Total 67	Mg 67	0

- Molecule 89 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



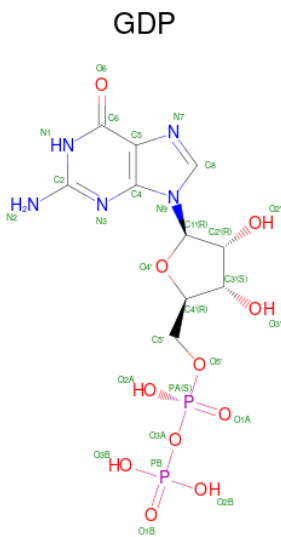
Mol	Chain	Residues	Atoms			AltConf
89	r	1	Total 4	Fe 2	S 2	0
89	AP	1	Total 4	Fe 2	S 2	0
89	AT	1	Total 4	Fe 2	S 2	0

- Molecule 90 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).



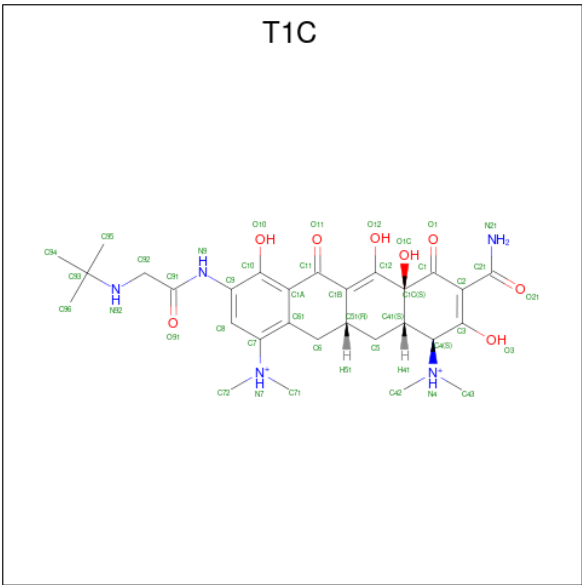
Mol	Chain	Residues	Atoms						AltConf
90	AX	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



Mol	Chain	Residues	Atoms						AltConf
91	AX	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

- Molecule 92 is TIGECYCLINE (CCD ID: T1C) (formula:  $\text{C}_{29}\text{H}_{41}\text{N}_5\text{O}_8$ ).



Mol	Chain	Residues	Atoms					AltConf
92	AA	1	Total	C	H	N	O	0
			83	29	41	5	8	
92	A	1	Total	C	H	N	O	0
			83	29	41	5	8	
92	A	1	Total	C	H	N	O	0
			83	29	41	5	8	

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

Mol	Chain	Residues	Atoms		AltConf
93	AA	2	Total	K	0
			2	2	
93	A	14	Total	K	0
			14	14	

- Molecule 94 is water.

Mol	Chain	Residues	Atoms		AltConf
94	D	9	Total	O	0
			9	9	
94	E	10	Total	O	0
			10	10	
94	F	4	Total	O	0
			4	4	
94	L	4	Total	O	0
			4	4	

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Mol	Chain	Residues	Atoms		AltConf
94	M	1	Total 1	O 1	0
94	N	2	Total 2	O 2	0
94	O	3	Total 3	O 3	0
94	2	4	Total 4	O 4	0
94	AC	4	Total 4	O 4	0
94	AD	2	Total 2	O 2	0
94	AG	7	Total 7	O 7	0
94	AH	7	Total 7	O 7	0
94	AJ	1	Total 1	O 1	0
94	AK	7	Total 7	O 7	0
94	A2	1	Total 1	O 1	0
94	A3	1	Total 1	O 1	0
94	AA	200	Total 200	O 200	0
94	A	694	Total 694	O 694	0
94	Az	7	Total 7	O 7	0
94	Ax	2	Total 2	O 2	0

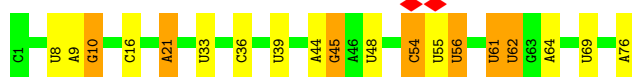


### 3 Residue-property plots [i](#)

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

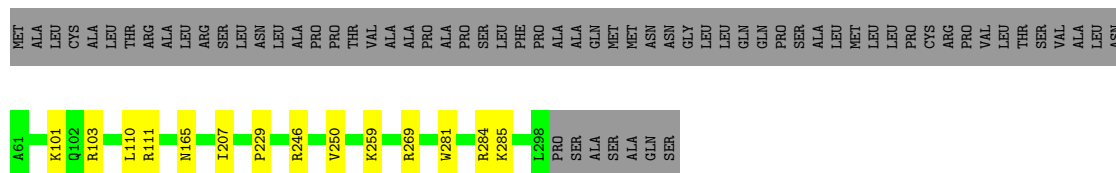
- Molecule 1: mitochondrial tRNAVal

Chain B: 




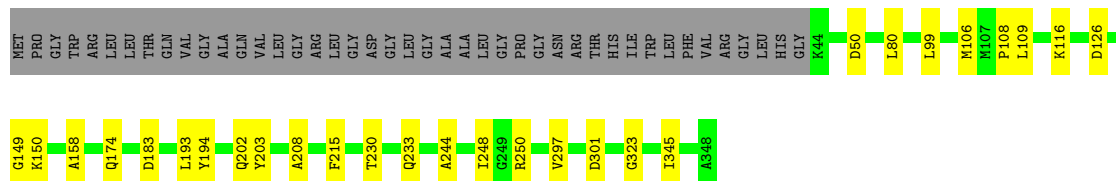
- Molecule 2: 39S ribosomal protein L2, mitochondrial

Chain D: 



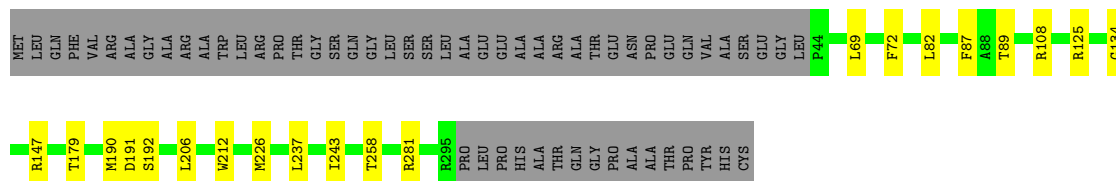
- Molecule 3: 39S ribosomal protein L3, mitochondrial

Chain E: 

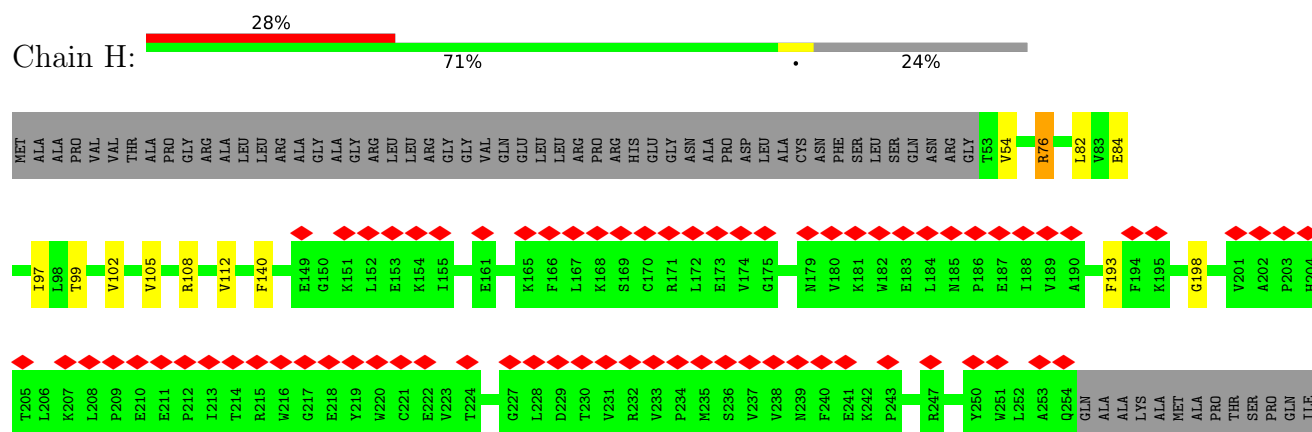


- Molecule 4: 39S ribosomal protein L4, mitochondrial

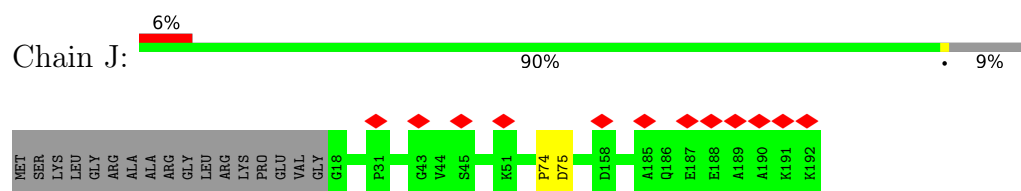
Chain F: 



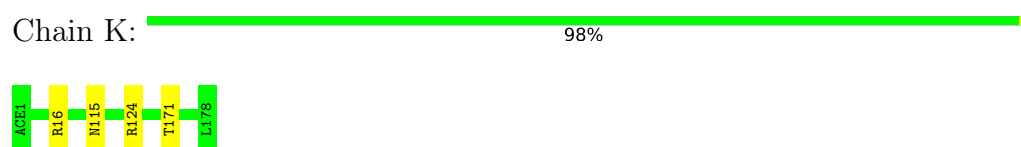
- Molecule 5: 39S ribosomal protein L9, mitochondrial



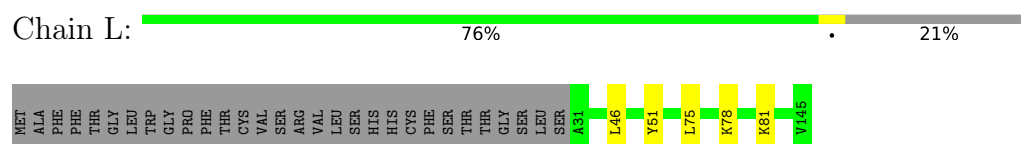
- Molecule 6: 39S ribosomal protein L11, mitochondrial



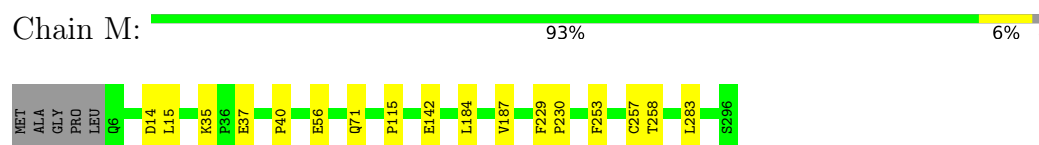
- Molecule 7: Large ribosomal subunit protein uL13m



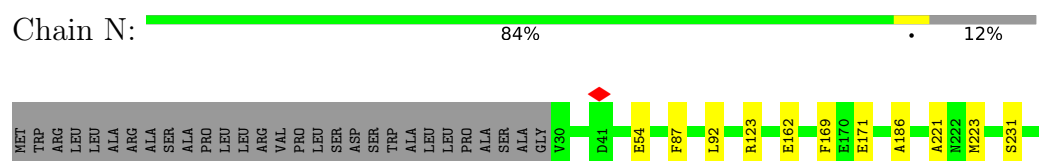
- Molecule 8: 39S ribosomal protein L14, mitochondrial




- Molecule 9: 39S ribosomal protein L15, mitochondrial

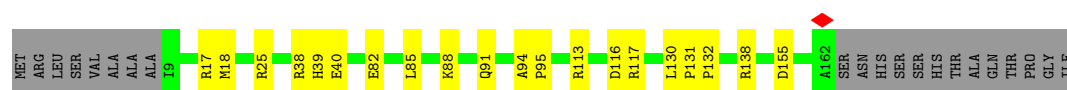


- Molecule 10: 39S ribosomal protein L16, mitochondrial




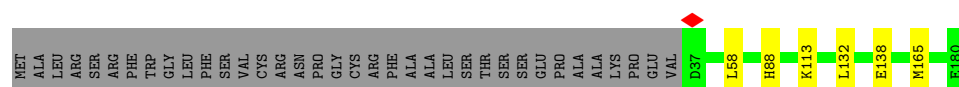
- Molecule 11: 39S ribosomal protein L17, mitochondrial

Chain O:  77% 11% 12%




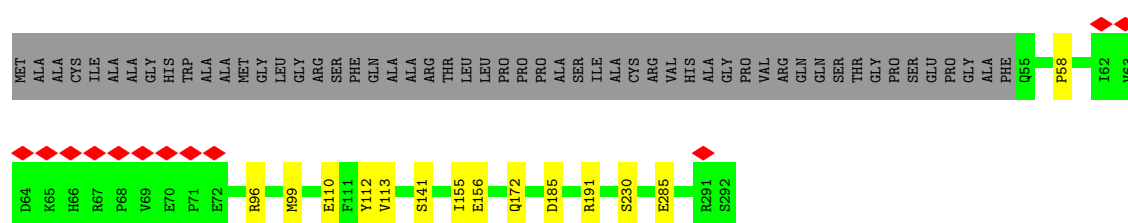
- Molecule 12: 39S ribosomal protein L18, mitochondrial

Chain P:  77% 0% 20%



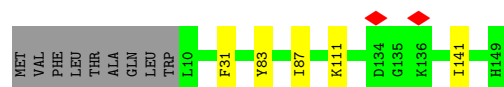
- Molecule 13: 39S ribosomal protein L19, mitochondrial

Chain Q:  77% 5% 18%



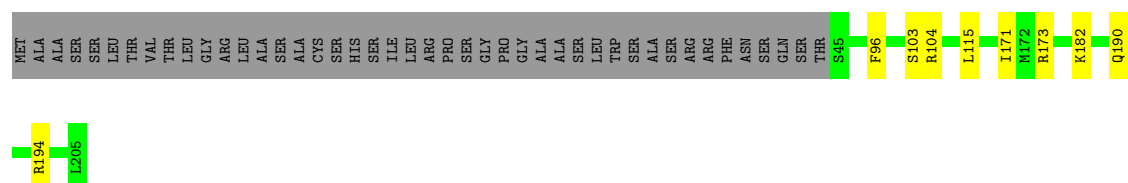
- Molecule 14: 39S ribosomal protein L20, mitochondrial

Chain R:  91% 0% 6%




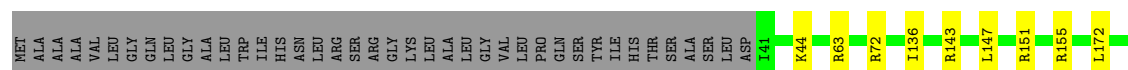
- Molecule 15: 39S ribosomal protein L21, mitochondrial

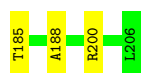
Chain S:  74% 0% 21%



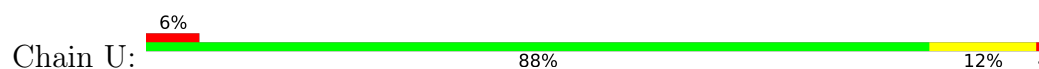
- Molecule 16: 39S ribosomal protein L22, mitochondrial

Chain T:  75% 6% 19%





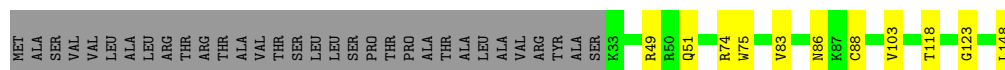
- Molecule 17: Large ribosomal subunit protein uL23m



- Molecule 18: 39S ribosomal protein L24, mitochondrial



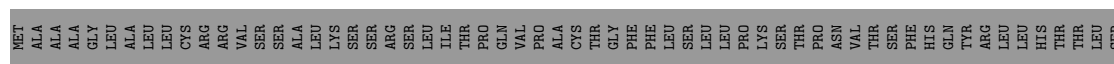
- Molecule 19: 39S ribosomal protein L27, mitochondrial



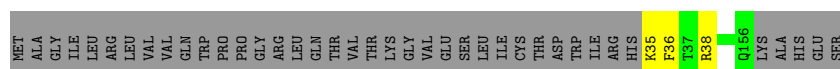
- Molecule 20: 39S ribosomal protein L28, mitochondrial



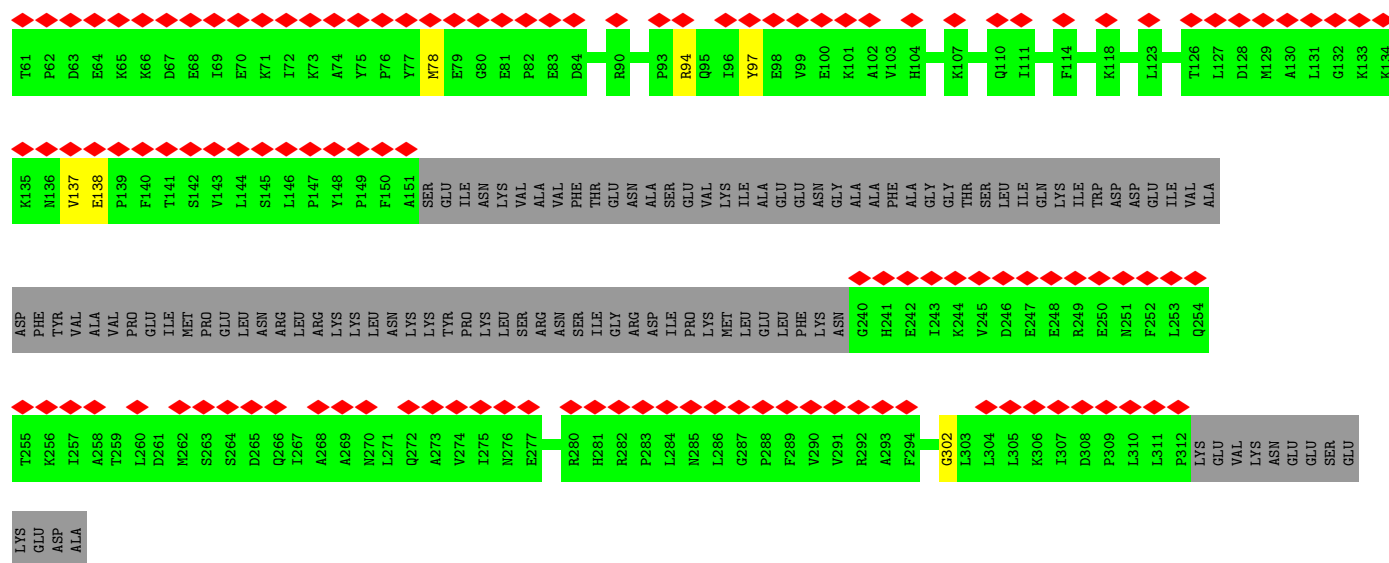
- Molecule 21: 39S ribosomal protein L47, mitochondrial



- Molecule 22: 39S ribosomal protein L30, mitochondrial

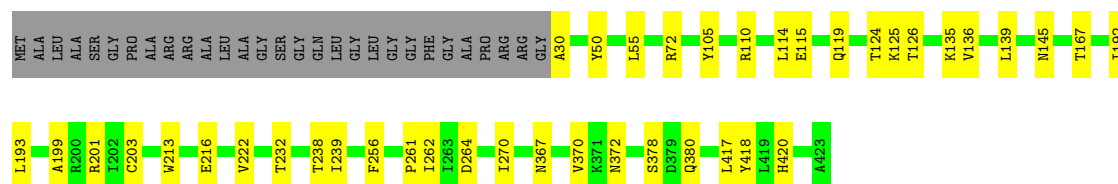


- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |   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



- Molecule 29: 39S ribosomal protein L37, mitochondrial

Chain 5: 83% 10% 7%



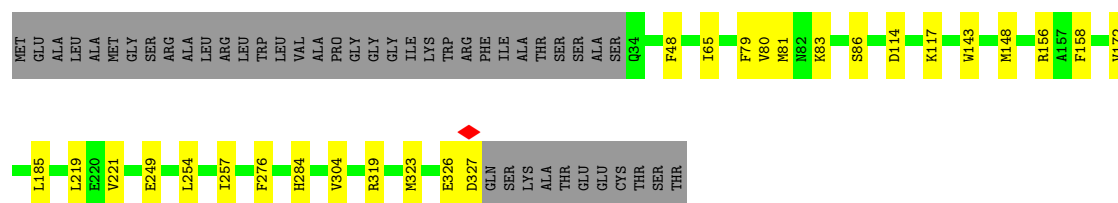
- Molecule 30: 39S ribosomal protein L38, mitochondrial

Chain 6: 90% 7%



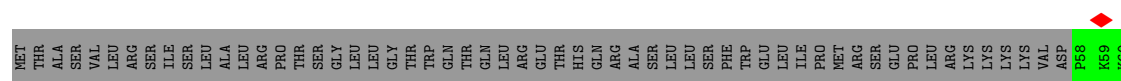
- Molecule 31: 39S ribosomal protein L39, mitochondrial

Chain 7: 79% 8% 13%



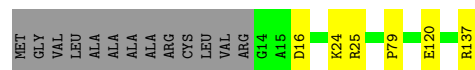
- Molecule 32: 39S ribosomal protein L40, mitochondrial

Chain 8: 67% 29%



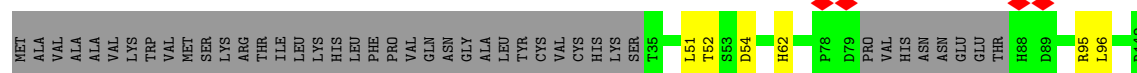
- Molecule 33: 39S ribosomal protein L41, mitochondrial

Chain 9: 86% 9%



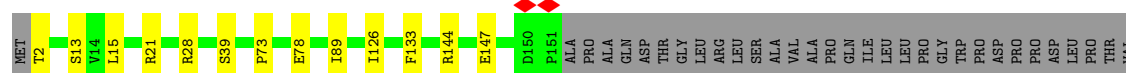
- Molecule 34: 39S ribosomal protein L42, mitochondrial

Chain a: 66% 30%



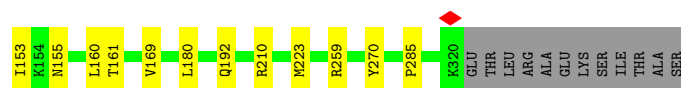
- Molecule 35: 39S ribosomal protein L43, mitochondrial

Chain b: 64% 6% 30%



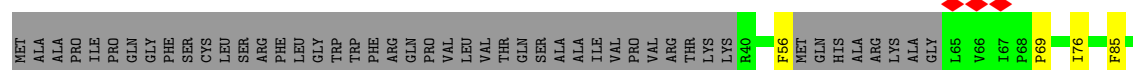
- Molecule 36: 39S ribosomal protein L44, mitochondrial

Chain c: 80% 7% 14%

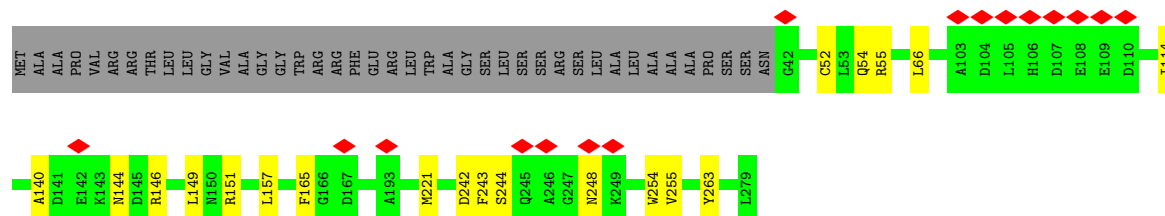
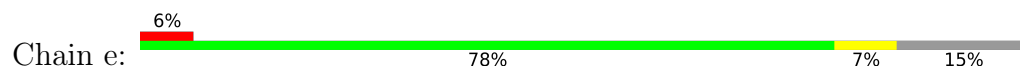


- Molecule 37: 39S ribosomal protein L45, mitochondrial

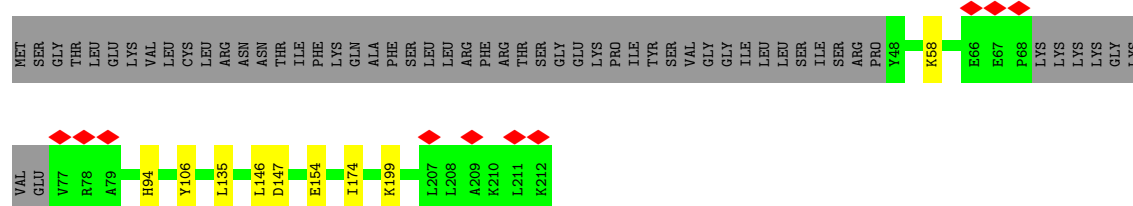
Chain d: 68% 9% 23%



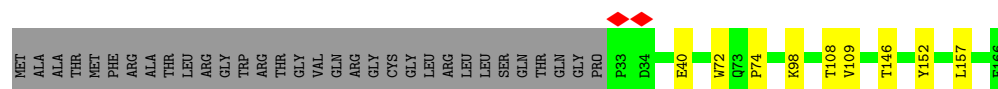
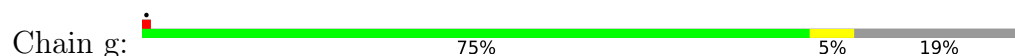
- Molecule 38: 39S ribosomal protein L46, mitochondrial



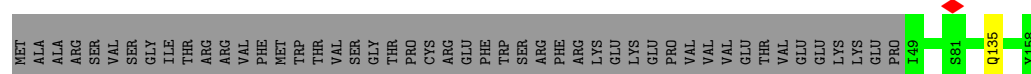
- Molecule 39: 39S ribosomal protein L48, mitochondrial



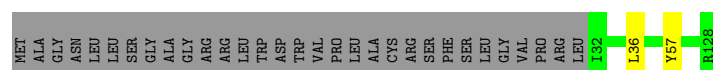
- Molecule 40: 39S ribosomal protein L49, mitochondrial



- Molecule 41: 39S ribosomal protein L50, mitochondrial



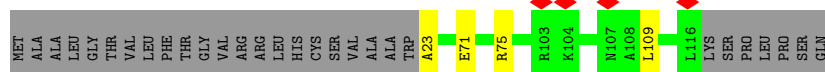
- Molecule 42: 39S ribosomal protein L51, mitochondrial






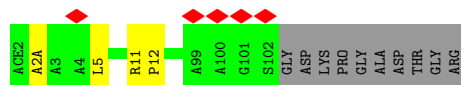
- Molecule 43: 39S ribosomal protein L52, mitochondrial

Chain j:  73% 24%



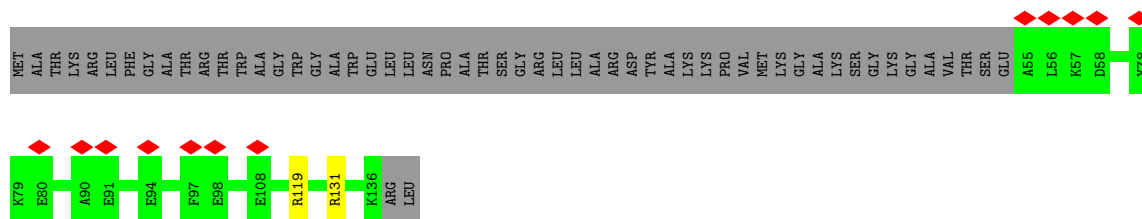
- Molecule 44: Large ribosomal subunit protein mL53

Chain k:  88% 9%



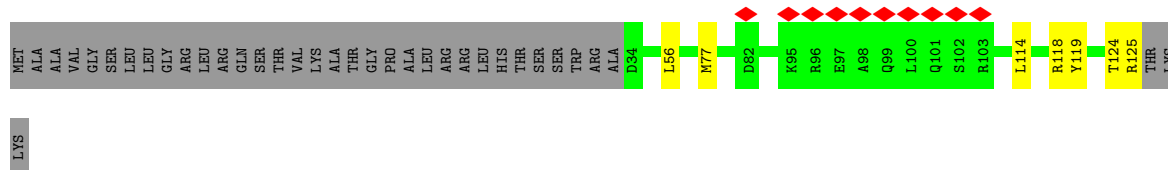
- Molecule 45: 39S ribosomal protein L54, mitochondrial

Chain l:  58% 41% 9%




- Molecule 46: 39S ribosomal protein L55, mitochondrial

Chain m:  66% 5% 28% 8%



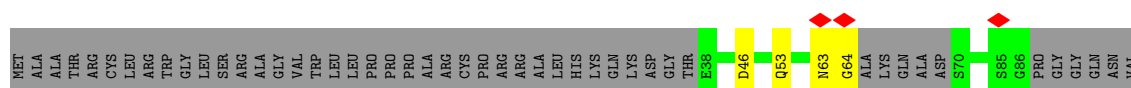
- Molecule 47: Ribosomal protein 63, mitochondrial

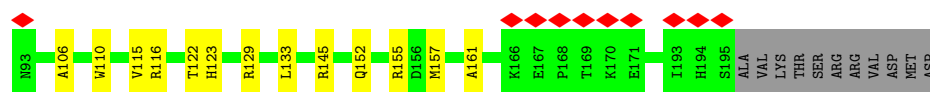
Chain o:  88% 8%



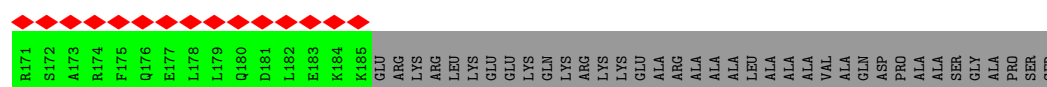
- Molecule 48: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:  63% 8% 29% 6%

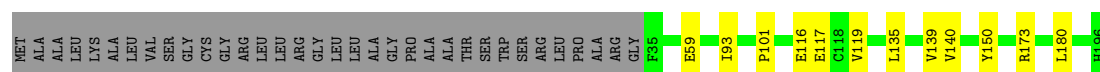
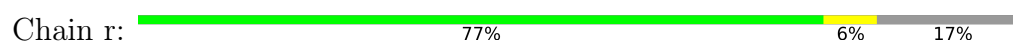




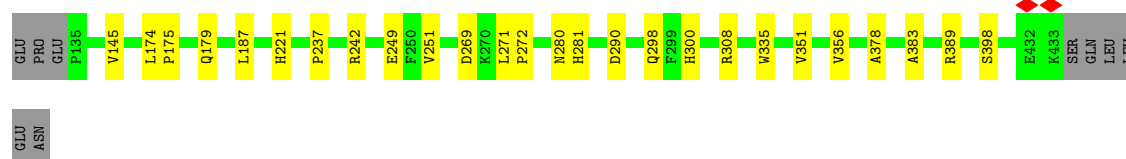
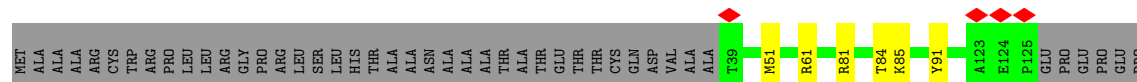
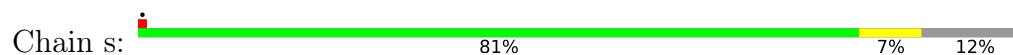
- Molecule 49: Growth arrest and DNA damage-inducible proteins-interacting protein 1



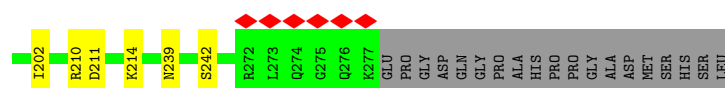
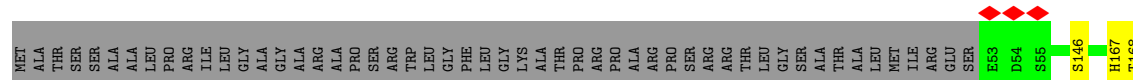
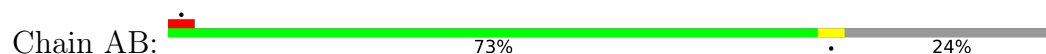
- Molecule 50: 39S ribosomal protein S18a, mitochondrial



- Molecule 51: 39S ribosomal protein S30, mitochondrial

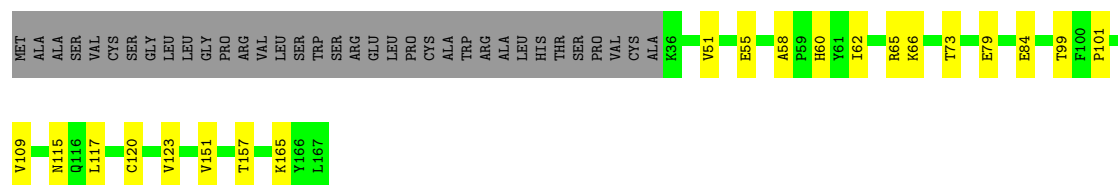


- Molecule 52: 28S ribosomal protein S2, mitochondrial



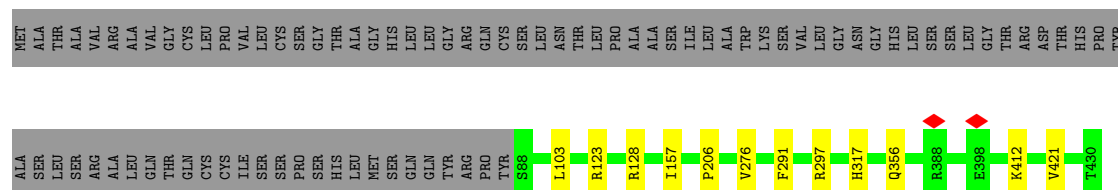
- Molecule 53: 28S ribosomal protein S24, mitochondrial





- Molecule 54: 28S ribosomal protein S5, mitochondrial

Chain AD: 77% 20%



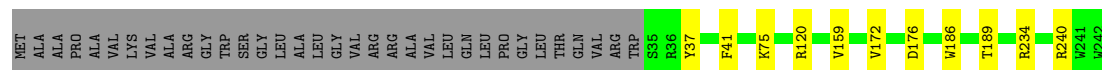
- Molecule 55: 28S ribosomal protein S6, mitochondrial

Chain AE: 96% 4%



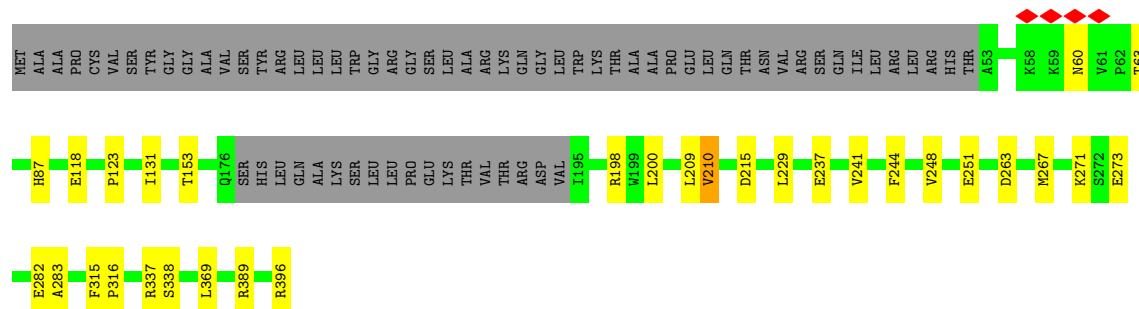
- Molecule 56: 28S ribosomal protein S7, mitochondrial

Chain AF: 81% 14%



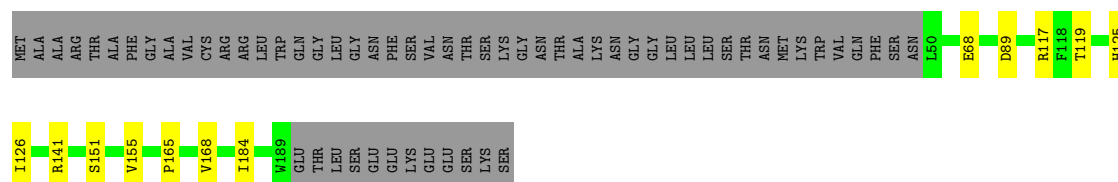
- Molecule 57: 28S ribosomal protein S9, mitochondrial

Chain AG: 74% 18%

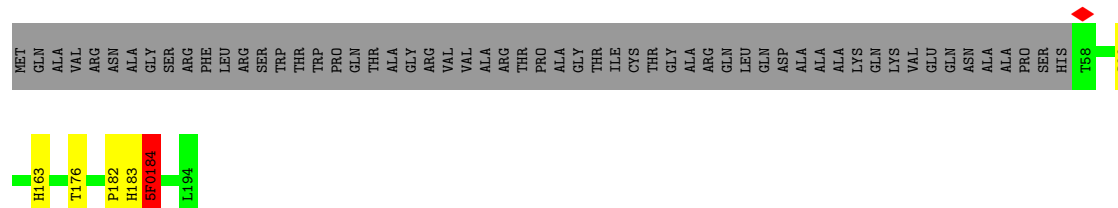


- Molecule 58: 28S ribosomal protein S10, mitochondrial

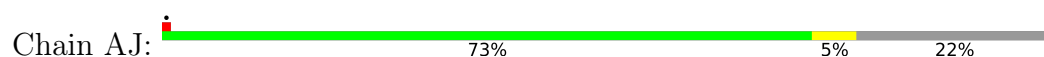
Chain AH: 64% 30%



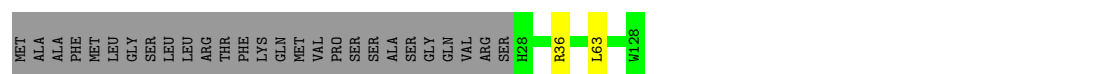
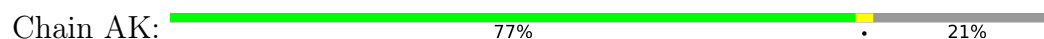
- Molecule 59: 28S ribosomal protein S11, mitochondrial



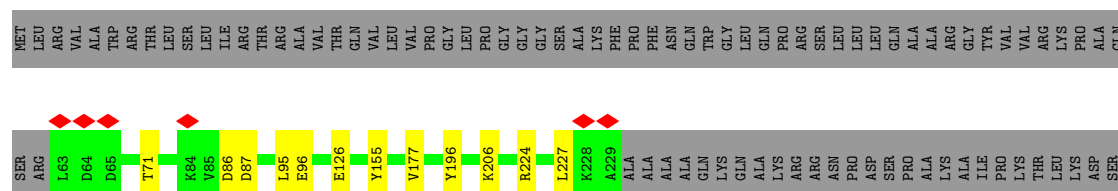
- Molecule 60: 28S ribosomal protein S12, mitochondrial



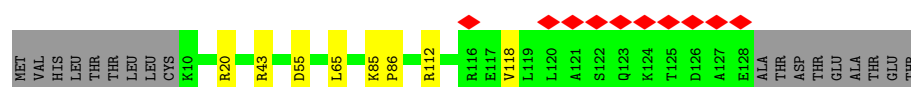
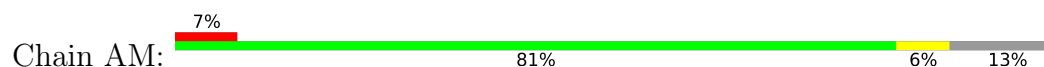
- Molecule 61: 28S ribosomal protein S14, mitochondrial




- Molecule 62: 28S ribosomal protein S15, mitochondrial



- Molecule 63: 28S ribosomal protein S16, mitochondrial




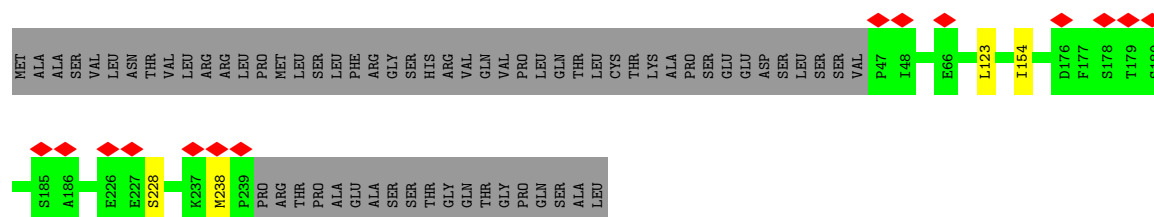
- Molecule 64: 28S ribosomal protein S17, mitochondrial

Chain AN: 



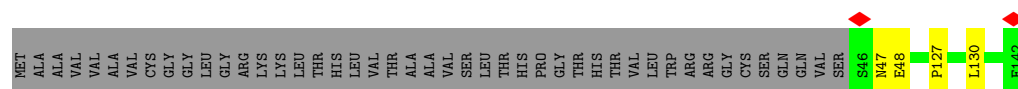
- Molecule 65: 28S ribosomal protein S18b, mitochondrial

Chain AO: 



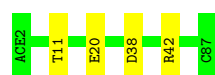
- Molecule 66: 28S ribosomal protein S18c, mitochondrial

Chain AP: 




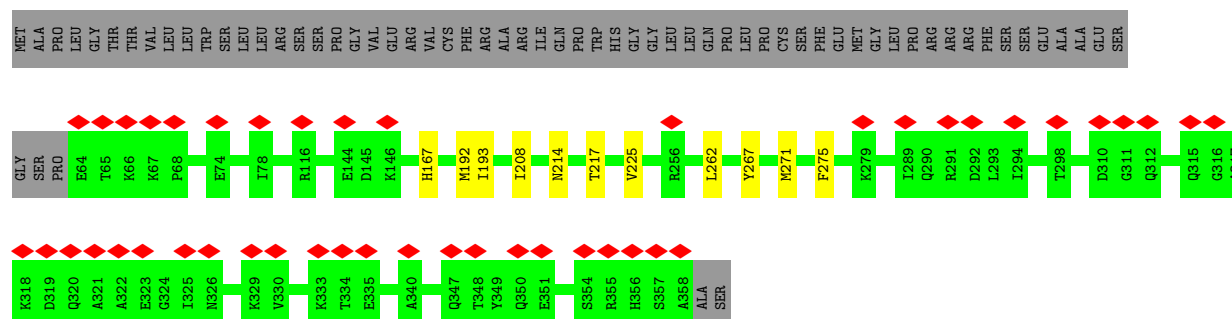
- Molecule 67: Small ribosomal subunit protein bS21m

Chain AQ: 



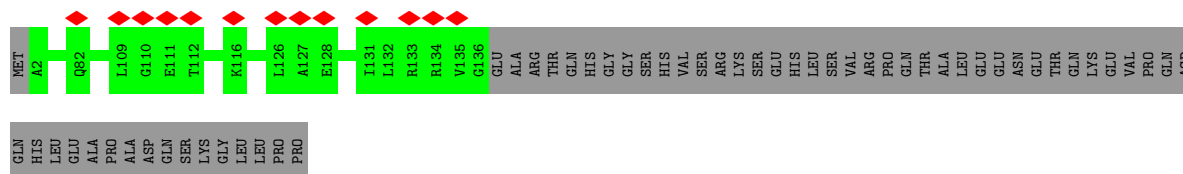
- Molecule 68: 28S ribosomal protein S22, mitochondrial

Chain AR: 



- Molecule 69: 28S ribosomal protein S23, mitochondrial

Chain AS: 



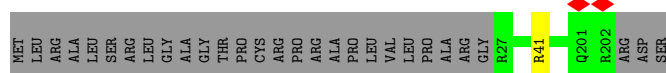
- Molecule 70: Small ribosomal subunit protein mS25

Chain AT: 95%



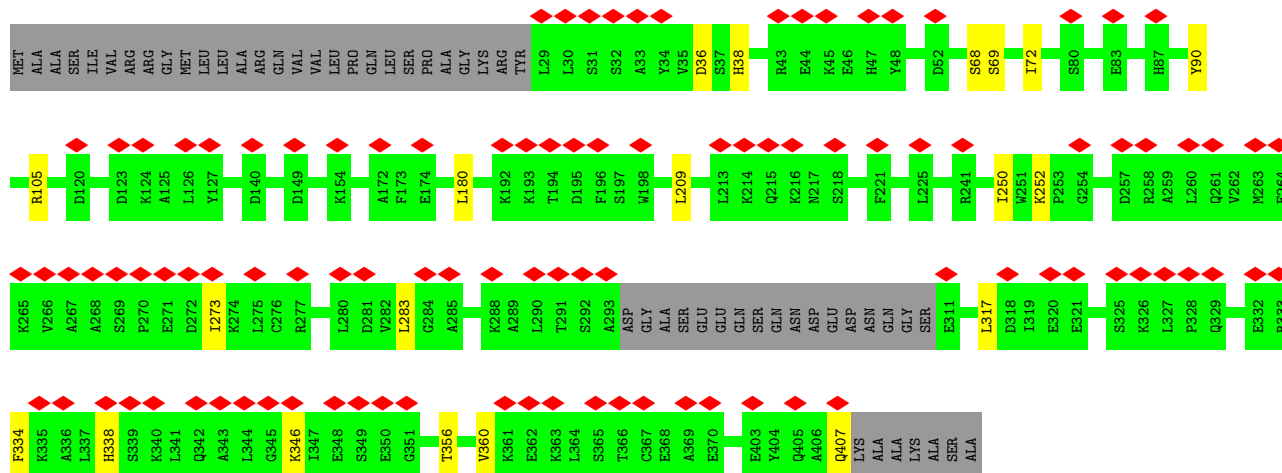
- Molecule 71: 28S ribosomal protein S26, mitochondrial

Chain AU: 85% 14%



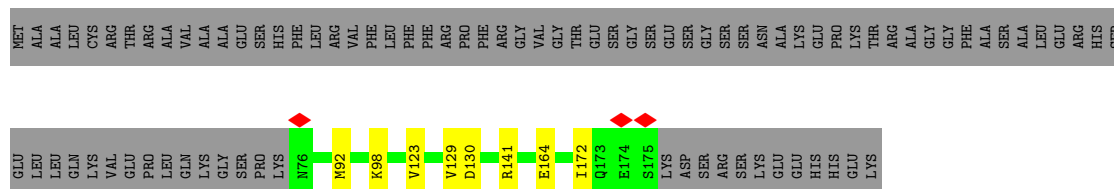
- Molecule 72: 28S ribosomal protein S27, mitochondrial

Chain AV: 25% 83% 5% 13%



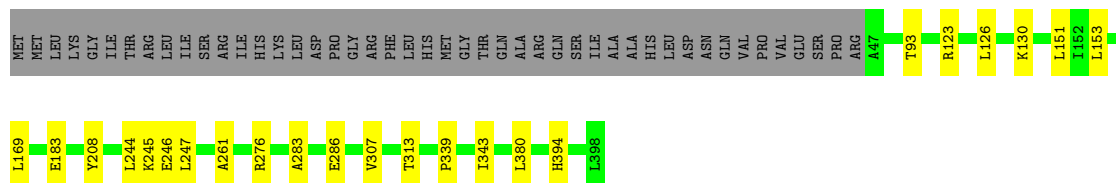
- Molecule 73: 28S ribosomal protein S28, mitochondrial

Chain AW: 49% 47%



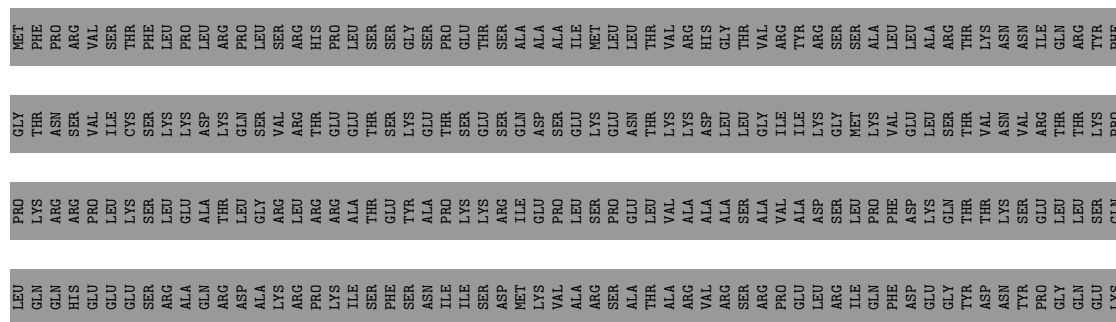
- Molecule 74: 28S ribosomal protein S29, mitochondrial

Chain AX:  83% 6% 12%



- Molecule 75: 28S ribosomal protein S31, mitochondrial

Chain AY:  37% 62%



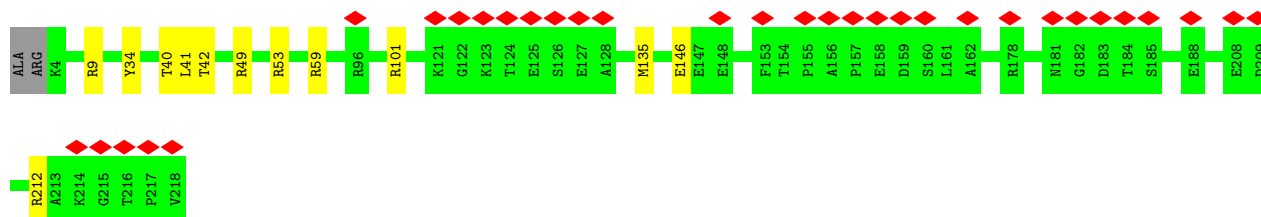
- Molecule 76: 28S ribosomal protein S33, mitochondrial

Chain AZ:  89% 6% 6%




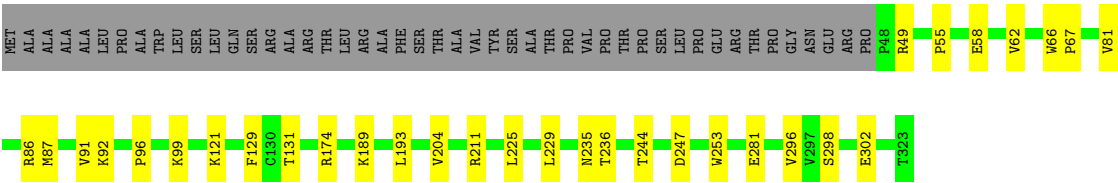
- Molecule 77: 28S ribosomal protein S34, mitochondrial

Chain A0:  15% 94% 6%



- Molecule 78: 28S ribosomal protein S35, mitochondrial

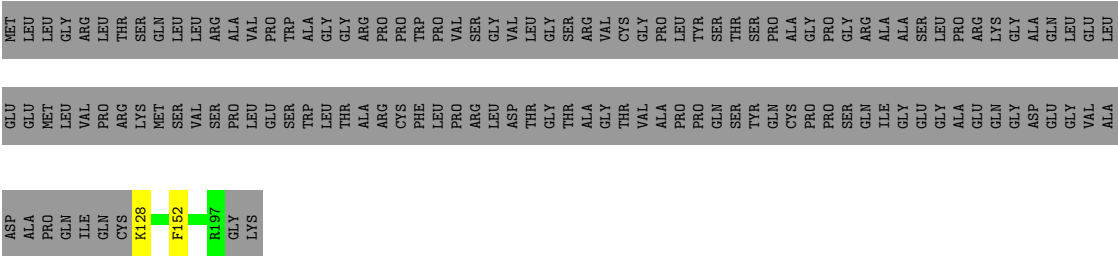
Chain A1:  76% 10% 15%



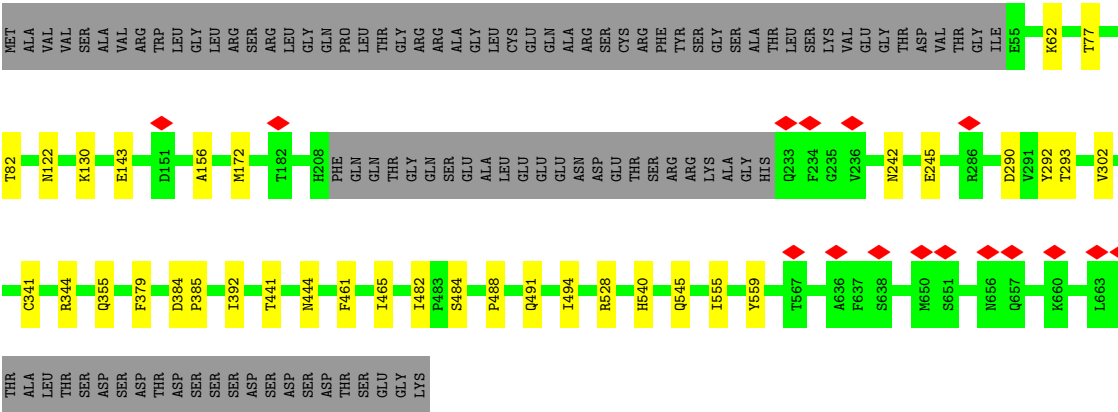
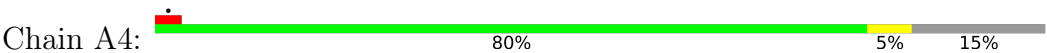
• Molecule 79: Small ribosomal subunit protein mS37



• Molecule 80: Aurora kinase A-interacting protein



• Molecule 81: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

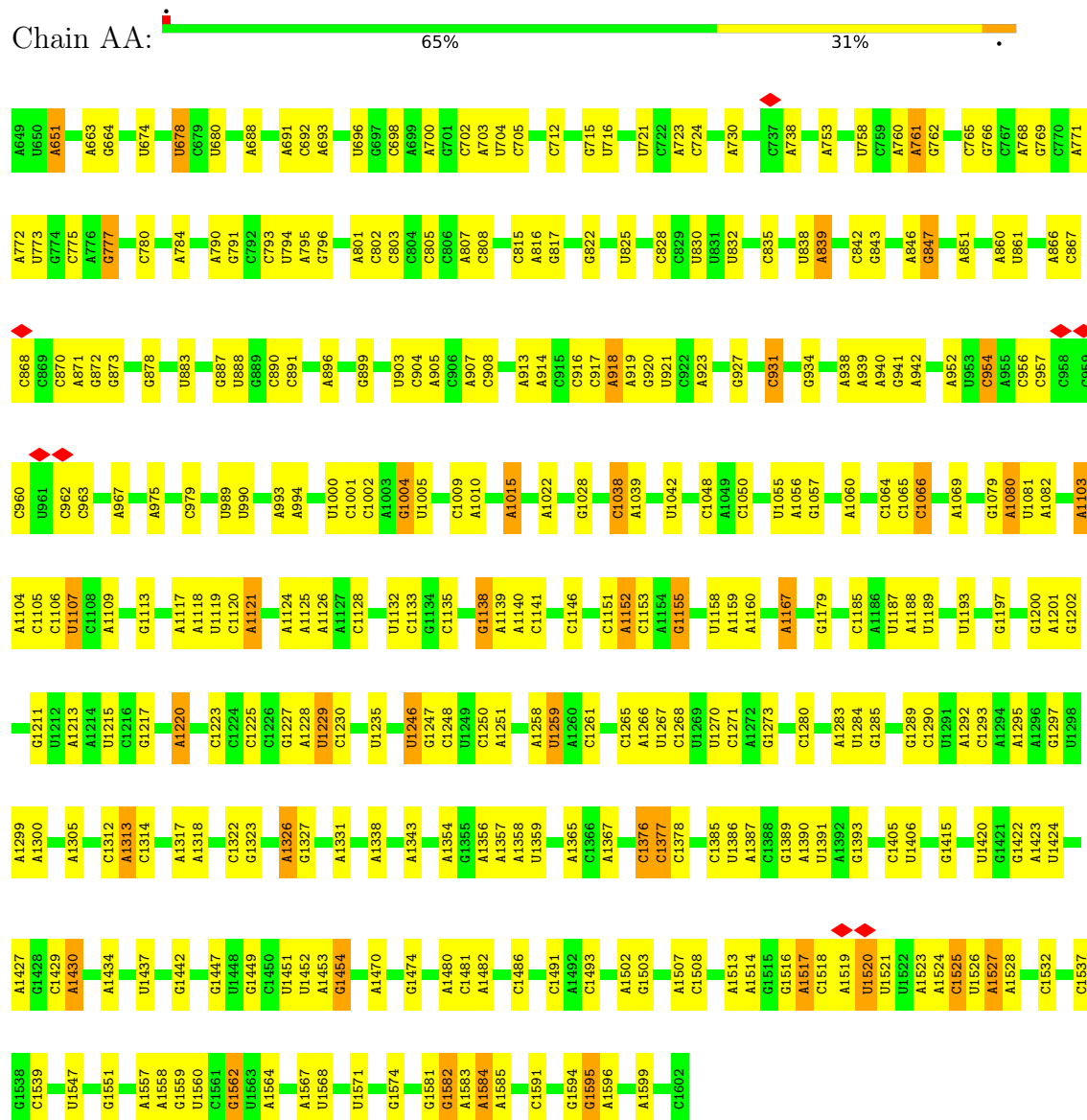


• Molecule 82: E/E-tRNA

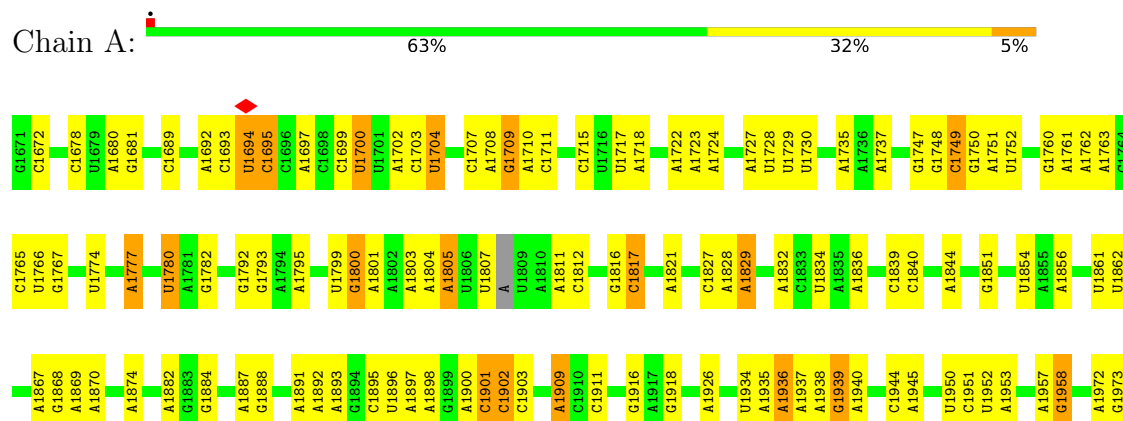


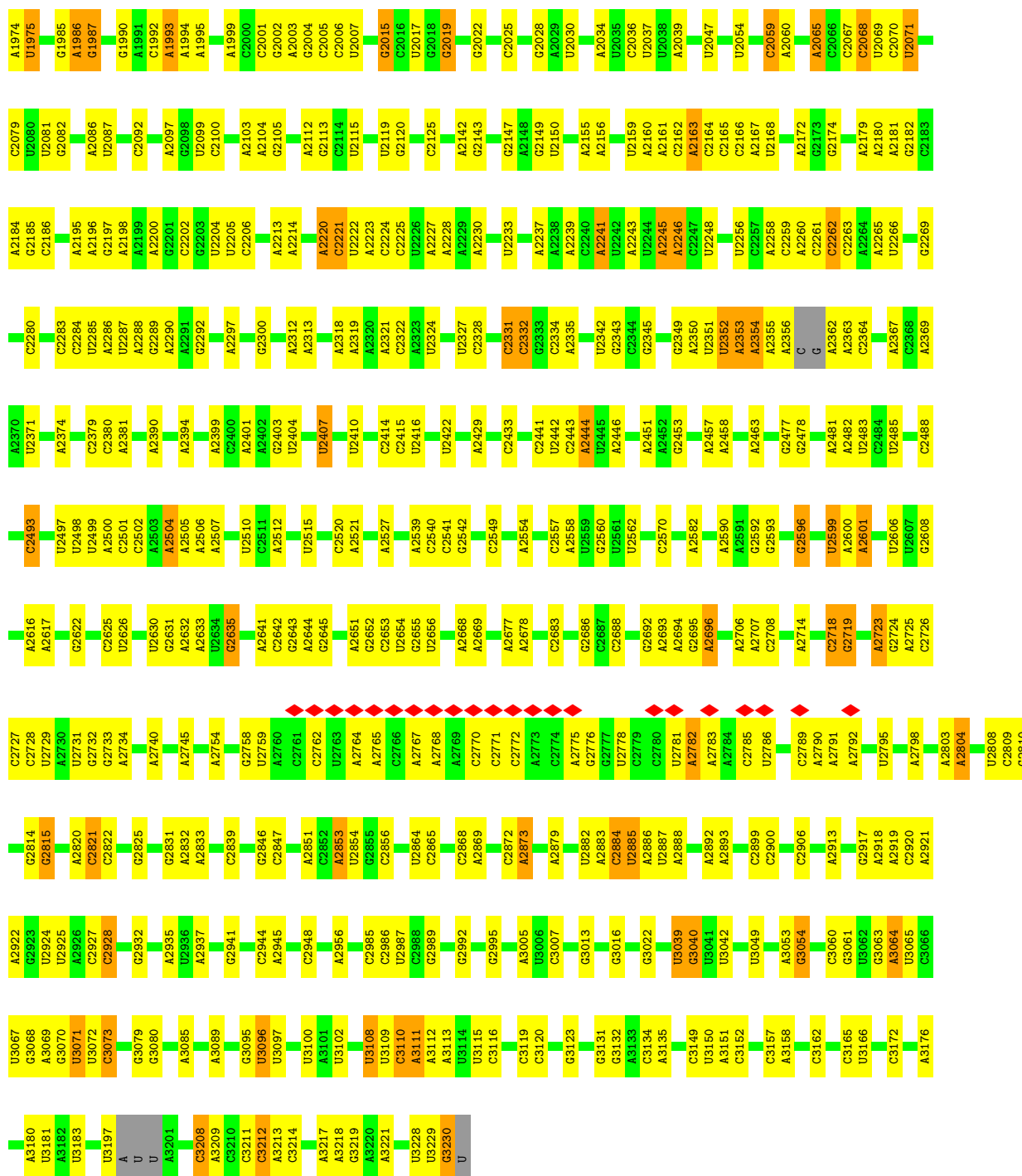


• Molecule 83: 12S mitochondrial rRNA

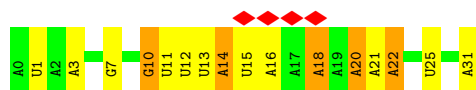


• Molecule 84: 16S mitochondrial rRNA

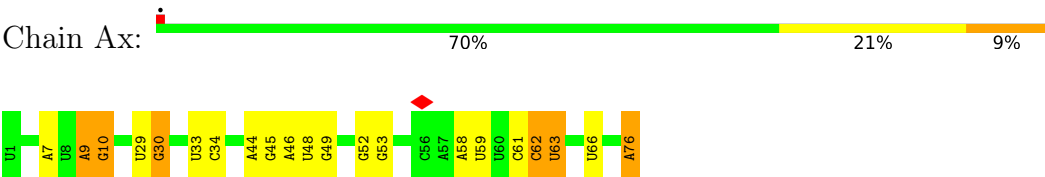




- Molecule 85: mRNA



- Molecule 86: P/P-tRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	266550	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)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	79.417	Depositor
Minimum map value	-23.844	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	1.082	Depositor
Recommended contour level	1.9	Depositor
Map size ( $\text{\AA}$ )	517.12, 517.12, 517.12	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.01, 1.01, 1.01	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, MA6, 2MG, OMG, MG, OMU, GDP, PSU, ATP, B8T, 5MC, FES, 5F0, THC, T1C, 5MU, K, ACE

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	B	0.18	0/1627	0.23	0/2527
2	D	0.29	0/1896	0.37	0/2549
3	E	0.39	0/2475	0.42	0/3355
4	F	0.40	0/2090	0.45	0/2842
5	H	0.18	0/1698	0.25	0/2292
6	J	0.08	0/1348	0.24	0/1813
7	K	0.35	0/1497	0.41	0/2031
8	L	0.30	0/905	0.41	0/1218
9	M	0.34	0/2381	0.42	0/3212
10	N	0.29	0/1833	0.34	0/2468
11	O	0.36	0/1283	0.40	0/1727
12	P	0.27	0/1199	0.31	0/1623
13	Q	0.30	0/2027	0.35	0/2734
14	R	0.36	0/1175	0.39	0/1572
15	S	0.34	0/1320	0.40	0/1789
16	T	0.43	0/1403	0.44	0/1886
17	U	0.30	0/1280	0.39	0/1732
18	V	0.24	0/1721	0.32	0/2333
19	W	0.32	0/926	0.40	0/1244
20	X	0.27	0/2099	0.29	0/2837
21	Y	0.32	0/1593	0.35	0/2136
22	Z	0.29	0/1021	0.40	0/1378
23	0	0.35	0/913	0.39	0/1224
24	1	0.24	0/469	0.33	0/621
25	2	0.42	0/383	0.47	0/507
26	3	0.39	0/853	0.46	0/1136
27	4	0.30	0/350	0.36	0/461
28	z	0.07	0/1354	0.19	0/1831
29	5	0.26	0/3305	0.35	0/4502
30	6	0.24	0/3043	0.30	0/4140
31	7	0.29	0/2447	0.35	0/3310

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	8	0.12	0/1261	0.20	0/1696
33	9	0.26	0/1025	0.31	0/1379
34	a	0.29	0/866	0.34	0/1174
35	b	0.34	0/1211	0.38	0/1639
36	c	0.26	0/2347	0.31	0/3171
37	d	0.26	0/2000	0.33	0/2708
38	e	0.11	0/1970	0.23	0/2658
39	f	0.17	0/1273	0.24	0/1716
40	g	0.34	0/1151	0.41	0/1569
41	h	0.21	0/918	0.26	0/1249
42	i	0.39	0/850	0.45	0/1135
43	j	0.28	0/760	0.35	0/1023
44	k	0.15	0/783	0.25	0/1057
45	l	0.11	0/707	0.22	0/960
46	m	0.16	0/805	0.29	0/1081
47	o	0.38	0/819	0.46	0/1097
48	p	0.20	0/1223	0.28	0/1641
49	q	0.19	0/1384	0.25	0/1869
50	r	0.27	0/1362	0.35	0/1846
51	s	0.29	0/3239	0.35	0/4400
52	AB	0.21	0/1871	0.28	0/2531
53	AC	0.52	0/1113	0.49	0/1505
54	AD	0.22	0/2783	0.29	0/3724
55	AE	0.19	0/989	0.29	0/1335
56	AF	0.41	0/1767	0.36	0/2373
57	AG	0.41	0/2739	0.38	0/3671
58	AH	0.49	0/1178	0.49	0/1598
59	AI	0.20	0/1030	0.28	0/1386
60	AJ	0.17	0/855	0.29	0/1148
61	AK	0.54	0/880	0.49	0/1182
62	AL	0.16	0/1430	0.24	0/1911
63	AM	0.13	0/963	0.26	0/1295
64	AN	0.16	0/886	0.27	0/1199
65	AO	0.12	0/1648	0.24	0/2243
66	AP	0.19	0/798	0.27	0/1070
67	AQ	0.25	0/754	0.32	0/1003
68	AR	0.10	0/2456	0.20	0/3317
69	AS	0.13	0/1138	0.19	0/1533
70	AT	0.15	0/1402	0.25	0/1883
71	AU	0.10	0/1510	0.19	0/2025
72	AV	0.08	0/3030	0.21	0/4093
73	AW	0.17	0/801	0.25	0/1079
74	AX	0.38	0/2921	0.36	0/3954

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	AY	0.38	0/1280	0.34	0/1725
76	AZ	0.44	0/857	0.41	0/1141
77	A0	0.09	0/1834	0.21	0/2484
78	A1	0.41	0/2285	0.39	0/3090
79	A2	0.23	0/947	0.93	3/1266 (0.2%)
80	A3	0.21	0/636	0.29	0/839
81	A4	0.21	0/4877	0.29	0/6598
82	Ay	0.15	0/93	0.17	0/142
83	AA	0.35	0/22537	0.31	0/35085
84	A	0.48	0/36732	0.44	0/57173
85	Az	0.15	0/761	0.23	0/1182
86	Ax	0.22	0/1655	0.25	0/2569
All	All	0.34	0/183304	0.36	3/260450 (0.0%)

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
4	F	0	1
5	H	0	1
17	U	0	1
59	AI	0	2
79	A2	0	2
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	A2	2(A)	ALA	O-C-N	-19.92	91.13	123.00
79	A2	2(A)	ALA	CA-C-N	17.00	163.27	121.80
79	A2	2(A)	ALA	C-N-CA	17.00	163.27	121.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
79	A2	2(A)	ALA	Mainchain,Peptide
59	AI	183	HIS	Mainchain

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Mol	Chain	Res	Type	Group
59	AI	184	5F0	Mainchain
4	F	108	ARG	Sidechain
5	H	76	ARG	Sidechain
17	U	2	ALA	Peptide

## 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	B	1524	779	778	9	0
2	D	1859	1920	1920	11	0
3	E	2406	2416	2415	20	0
4	F	2031	2065	2065	14	0
5	H	1661	1734	1734	9	0
6	J	1330	1408	1407	1	0
7	K	1455	1451	1452	5	0
8	L	890	941	941	3	0
9	M	2327	2395	2395	12	0
10	N	1786	1817	1817	8	0
11	O	1259	1295	1294	23	0
12	P	1173	1165	1165	6	0
13	Q	1979	2022	2022	9	0
14	R	1154	1214	1214	4	0
15	S	1293	1365	1365	7	0
16	T	1369	1410	1410	10	0
17	U	1251	1231	1232	14	0
18	V	1676	1687	1687	14	0
19	W	904	935	935	10	0
20	X	2044	2060	2060	6	0
21	Y	1556	1597	1597	9	0
22	Z	996	1045	1044	3	0
23	0	898	920	920	9	0
24	1	464	511	511	3	0
25	2	377	406	406	2	0
26	3	832	883	883	2	0
27	4	342	362	362	5	0
28	z	1327	1353	1353	3	0
29	5	3210	3206	3206	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	6	2948	2841	2841	11	0
31	7	2390	2397	2397	17	0
32	8	1235	1262	1262	6	0
33	9	997	987	987	6	0
34	a	840	810	810	5	0
35	b	1196	1195	1190	9	0
36	c	2299	2320	2320	13	0
37	d	1946	1928	1927	17	0
38	e	1931	1916	1916	28	0
39	f	1252	1269	1269	7	0
40	g	1113	1097	1097	5	0
41	h	895	881	881	1	0
42	i	828	857	857	2	0
43	j	745	746	746	5	0
44	k	774	784	784	2	0
45	l	688	674	674	2	0
46	m	791	796	796	4	0
47	o	798	804	804	5	0
48	p	1205	1223	1223	10	0
49	q	1350	1327	1327	7	0
50	r	1322	1350	1349	10	0
51	s	3155	3140	3139	19	0
52	AB	1828	1815	1815	7	0
53	AC	1083	1088	1088	14	0
54	AD	2731	2804	2804	9	0
55	AE	972	1000	1000	2	0
56	AF	1725	1769	1769	10	0
57	AG	2681	2678	2678	27	0
58	AH	1152	1183	1183	11	0
59	AI	1020	1059	1053	4	0
60	AJ	839	887	887	4	0
61	AK	862	885	885	2	0
62	AL	1406	1491	1491	8	0
63	AM	942	965	965	8	0
64	AN	868	928	928	5	0
65	AO	1592	1561	1561	3	0
66	AP	781	807	806	2	0
67	AQ	744	758	758	4	0
68	AR	2409	2428	2428	8	0
69	AS	1111	1115	1115	0	0
70	AT	1371	1393	1393	4	0
71	AU	1488	1499	1499	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	AV	2969	2961	2961	14	0
73	AW	789	802	802	4	0
74	AX	2849	2843	2843	16	0
75	AY	1246	1197	1197	4	0
76	AZ	839	858	858	6	0
77	A0	1787	1796	1796	9	0
78	A1	2238	2269	2269	25	0
79	A2	935	970	970	4	0
80	A3	625	699	699	2	0
81	A4	4768	4766	4766	22	0
82	Ay	84	45	45	0	0
83	AA	20260	10304	10291	106	0
84	A	32943	16737	16738	252	0
85	Az	680	340	340	6	0
86	Ax	1482	752	753	10	0
87	B	7	11	8	20	0
88	2	1	0	0	0	0
88	A	67	0	0	0	0
88	AA	23	0	0	1	0
88	AX	1	0	0	0	0
88	D	1	0	0	0	0
88	E	1	0	0	0	0
89	AP	4	0	0	0	0
89	AT	4	0	0	0	0
89	r	4	0	0	0	0
90	AX	31	12	12	0	0
91	AX	28	10	12	2	0
92	A	84	82	76	2	0
92	AA	42	41	38	0	0
93	A	14	0	0	0	0
93	AA	2	0	0	0	0
94	0	3	0	0	0	0
94	2	4	0	0	0	0
94	A	694	0	0	31	0
94	A2	1	0	0	0	0
94	A3	1	0	0	0	0
94	AA	200	0	0	7	0
94	AC	4	0	0	0	0
94	AD	2	0	0	0	0
94	AG	7	0	0	0	0
94	AH	7	0	0	1	0
94	AJ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
94	AK	7	0	0	0	0
94	Ax	2	0	0	1	0
94	Az	7	0	0	0	0
94	D	9	0	0	0	0
94	E	10	0	0	0	0
94	F	4	0	0	0	0
94	L	4	0	0	0	0
94	M	1	0	0	0	0
94	N	2	0	0	0	0
All	All	175454	147805	147766	869	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (869) 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)
87:B:101:VAL:CG1	38:e:165:PHE:CZ	2.24	1.21
87:B:101:VAL:HG12	38:e:165:PHE:CE1	1.76	1.20
87:B:101:VAL:CG1	38:e:165:PHE:CE1	2.25	1.20
87:B:101:VAL:C	38:e:165:PHE:HE1	1.62	1.06
87:B:101:VAL:HG12	38:e:165:PHE:CZ	1.92	1.00
87:B:101:VAL:HG13	38:e:165:PHE:CZ	1.97	0.99
87:B:101:VAL:HG13	38:e:165:PHE:CE1	1.98	0.94
83:AA:1305:A:OP2	94:AA:1802:HOH:O	1.84	0.94
87:B:101:VAL:C	38:e:165:PHE:CE1	2.49	0.90
27:4:66:PHE:N	84:A:3013:G:HO2'	1.70	0.90
84:A:2941:G:O6	94:A:3401:HOH:O	1.90	0.89
84:A:3212:C:O2	84:A:3230:G:N2	2.12	0.81
83:AA:1567:A:OP2	94:AA:1804:HOH:O	2.00	0.79
87:B:101:VAL:HA	38:e:221:MET:CE	2.11	0.79
17:U:1:ACE:O	17:U:22:THR:OG1	1.99	0.79
4:F:212:TRP:O	4:F:258:THR:OG1	2.01	0.78
84:A:2632:A:OP2	94:A:3403:HOH:O	2.01	0.78
17:U:21:ARG:NH2	21:Y:143:ASP:OD1	2.19	0.76
17:U:21:ARG:O	33:9:137:ARG:NH1	2.18	0.76
83:AA:1470:A:N3	94:AA:1811:HOH:O	2.21	0.73
84:A:2512:A:O2'	84:A:2541:C:OP1	2.04	0.73
1:B:76:A:O2'	87:B:101:VAL:O	1.90	0.73
58:AH:117:ARG:NH1	94:AH:301:HOH:O	2.22	0.73
1:B:76:A:HO2'	87:B:101:VAL:C	1.95	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:B:101:VAL:CG1	38:e:165:PHE:HZ	1.98	0.72
17:U:46:MET:HE1	17:U:72:VAL:HG13	1.71	0.72
83:AA:1331:A:OP2	94:AA:1806:HOH:O	2.08	0.72
61:AK:36:ARG:NH1	83:AA:1235:U:OP1	2.23	0.72
64:AN:31:THR:HG22	64:AN:46:ARG:HB3	1.72	0.72
63:AM:65:LEU:HD12	68:AR:192:MET:HE1	1.73	0.71
84:A:2740:A:N3	84:A:2921:A:O2'	2.23	0.71
83:AA:1389:G:O6	83:AA:1415:G:O2'	2.06	0.71
84:A:2641:A:N3	94:A:3435:HOH:O	2.24	0.69
57:AG:60:ASN:O	57:AG:63:THR:HG23	1.92	0.69
74:AX:208:TYR:OH	74:AX:246:GLU:OE2	2.11	0.69
16:T:155:ARG:NH1	84:A:1957:A:OP2	2.26	0.68
5:H:76:ARG:NH1	84:A:1730:U:OP1	2.27	0.68
43:j:23:ALA:HB2	84:A:2248:U:OP2	1.92	0.68
84:A:3212:C:N3	84:A:3230:G:N1	2.32	0.68
87:B:101:VAL:HG13	38:e:165:PHE:HZ	1.57	0.68
53:AC:115:ASN:ND2	75:AY:309:LYS:O	2.27	0.68
4:F:226:MET:SD	49:q:26:ARG:NH2	2.67	0.68
39:f:106:TYR:OH	39:f:174:ILE:O	2.11	0.68
84:A:2808:U:OP1	94:A:3407:HOH:O	2.11	0.68
83:AA:698:C:O2'	83:AA:851:A:N7	2.27	0.67
38:e:146:ARG:NH1	38:e:263:TYR:OH	2.28	0.67
48:p:46:ASP:OD1	48:p:53:GLN:NE2	2.28	0.67
43:j:23:ALA:HB3	84:A:2150:U:OP2	1.95	0.67
83:AA:678:U:O2'	83:AA:872:G:O2'	2.13	0.67
7:K:16:ARG:NH2	7:K:124:ARG:HH21	1.91	0.67
11:O:132:PRO:HD3	23:O:185:PHE:HD1	1.59	0.67
31:7:284:HIS:HB3	31:7:323:MET:HE2	1.77	0.67
84:A:2542:G:OP2	94:A:3408:HOH:O	2.12	0.67
7:K:171:THR:HG22	50:r:59:GLU:H	1.60	0.66
10:N:231:SER:OG	84:A:2104:A:OP1	2.08	0.66
84:A:1953:A:O2'	84:A:2463:A:OP1	2.13	0.66
84:A:2692:G:N1	84:A:2696:A:OP2	2.23	0.66
87:B:101:VAL:HA	38:e:221:MET:SD	2.35	0.66
57:AG:389:ARG:HD2	83:AA:1427:A:O2'	1.95	0.66
81:A4:528:ARG:O	81:A4:559:TYR:OH	2.10	0.66
84:A:2778:U:OP1	84:A:2782:A:N6	2.29	0.66
83:AA:691:A:N7	83:AA:716:U:O2'	2.28	0.66
13:Q:155:ILE:HG22	13:Q:156:GLU:OE1	1.95	0.66
22:Z:35:LYS:N	84:A:2103:A:HO2'	1.94	0.66
57:AG:210:VAL:HG12	57:AG:210:VAL:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:AA:1314:C:OP2	94:AA:1808:HOH:O	2.14	0.66
84:A:2985:C:OP1	94:A:3410:HOH:O	2.13	0.65
67:AQ:38:ASP:OD2	83:AA:1015:A:O2'	2.15	0.65
45:l:119:ARG:NH2	84:A:2195:A:OP1	2.30	0.65
92:A:3301:T1C:O1C	92:A:3301:T1C:H422	1.97	0.65
83:AA:702:C:O2'	83:AA:842:C:O2	2.14	0.65
84:A:2944:C:OP2	94:A:3411:HOH:O	2.13	0.65
84:A:1747:G:OP2	84:A:1749:C:N4	2.27	0.65
84:A:2498:U:OP1	94:A:3414:HOH:O	2.15	0.64
9:M:37:GLU:N	9:M:37:GLU:OE1	2.30	0.64
84:A:2719:G:OP2	94:A:3412:HOH:O	2.15	0.64
31:7:249:GLU:OE1	31:7:249:GLU:N	2.31	0.64
84:A:2622:G:N7	94:A:3448:HOH:O	2.30	0.64
56:AF:159:VAL:HG23	56:AF:172:VAL:HG21	1.80	0.63
84:A:3219:G:O2'	84:A:3221:A:OP2	2.13	0.63
56:AF:172:VAL:HG12	56:AF:240:ARG:HD3	1.79	0.63
26:3:94:LEU:N	84:A:1752:U:OP1	2.31	0.63
84:A:1909:A:OP1	94:A:3415:HOH:O	2.15	0.63
11:O:38:ARG:CG	11:O:85:LEU:HD11	2.29	0.63
83:AA:803:C:OP1	83:AA:816:A:N6	2.32	0.63
1:B:21:A:OP1	12:P:113:LYS:NZ	2.31	0.63
24:1:52:GLN:NE2	49:q:125:MET:SD	2.72	0.62
27:4:76:CYS:SG	27:4:79:CYS:N	2.72	0.62
71:AU:41:ARG:NH2	83:AA:702:C:OP1	2.33	0.62
76:AZ:89:ARG:NH2	83:AA:1338:A:OP2	2.31	0.62
29:5:105:TYR:CE1	29:5:262:ILE:HD12	2.34	0.62
83:AA:1289:G:O2'	83:AA:1297:G:OP2	2.17	0.62
33:9:16:ASP:OD1	33:9:25:ARG:NH2	2.33	0.61
39:f:94:HIS:ND1	39:f:154:GLU:OE2	2.33	0.61
77:A0:34:TYR:OH	77:A0:212:ARG:NH1	2.33	0.61
36:c:124:GLU:OE2	36:c:128:GLN:NE2	2.33	0.61
81:A4:122:ASN:ND2	81:A4:143:GLU:OE1	2.30	0.61
70:AT:56:GLN:HB2	70:AT:64:ILE:HD12	1.82	0.61
84:A:2652:G:O6	94:A:3413:HOH:O	2.15	0.61
88:AA:1705:MG:MG	94:AA:1944:HOH:O	1.42	0.61
7:K:16:ARG:NH1	7:K:124:ARG:HE	1.99	0.61
36:c:93:VAL:HG22	36:c:180:LEU:HD12	1.81	0.61
84:A:2616:A:OP2	94:A:3417:HOH:O	2.16	0.61
49:q:111:GLU:OE2	49:q:115:ARG:NH2	2.34	0.61
57:AG:200:LEU:HD22	57:AG:244:PHE:HB3	1.83	0.61
81:A4:302:VAL:O	81:A4:344:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:193:PHE:O	5:H:198:GLY:N	2.34	0.60
57:AG:337:ARG:HG3	57:AG:338:SER:N	2.15	0.60
84:A:2927:C:OP1	94:A:3416:HOH:O	2.16	0.60
84:A:2726:C:H4'	92:A:3302:T1C:H962	1.82	0.60
51:s:242:ARG:NH1	51:s:290:ASP:OD2	2.34	0.60
21:Y:117:GLN:NE2	84:A:2369:A:OP1	2.34	0.60
78:A1:281:GLU:OE1	78:A1:281:GLU:N	2.31	0.60
3:E:345:ILE:O	13:Q:172:GLN:NE2	2.32	0.60
11:O:132:PRO:HD3	23:O:185:PHE:CD1	2.36	0.59
84:A:1901:C:O2'	84:A:1902:C:OP1	2.14	0.59
84:A:3080:G:N7	94:A:3456:HOH:O	2.32	0.59
11:O:131:PRO:HA	23:O:185:PHE:CD1	2.37	0.59
13:Q:141:SER:OG	84:A:3152:C:OP1	2.13	0.59
2:D:284:ARG:NH2	84:A:2515:U:OP1	2.35	0.59
29:5:192:ILE:HD11	29:5:199:ALA:HB2	1.85	0.59
29:5:201:ARG:HB3	29:5:232:THR:HG22	1.82	0.59
38:e:114:ILE:HG21	74:AX:169:LEU:HD11	1.85	0.59
47:o:20:LYS:HD2	84:A:2112:A:H5'	1.84	0.59
50:r:135:LEU:HD22	50:r:139:VAL:HG13	1.84	0.59
72:AV:36:ASP:OD1	72:AV:38:HIS:ND1	2.36	0.59
83:AA:769:G:N2	83:AA:772:A:OP2	2.35	0.59
1:B:76:A:O2'	87:B:101:VAL:C	2.44	0.59
83:AA:678:U:HO2'	83:AA:872:G:HO2'	1.45	0.59
84:A:2352:U:O2'	84:A:2353:A:OP1	2.18	0.59
19:W:74:ARG:HG3	84:A:2065:A:C4	2.37	0.59
66:AP:127:PRO:HA	66:AP:130:LEU:HD13	1.85	0.59
84:A:2631:G:OP1	94:A:3419:HOH:O	2.17	0.59
84:A:2728:C:O2'	94:A:3418:HOH:O	2.16	0.59
74:AX:153:LEU:HD21	74:AX:244:LEU:CD2	2.33	0.58
77:A0:101:ARG:NH2	83:AA:1528:A:OP1	2.33	0.58
83:AA:888:U:O2'	83:AA:891:C:N3	2.36	0.58
83:AA:873:G:N3	83:AA:921:U:O2'	2.36	0.58
58:AH:119:THR:HG21	83:AA:1451:U:H4'	1.85	0.58
63:AM:118:VAL:HG12	65:AO:238:MET:HB3	1.84	0.58
87:B:101:VAL:HA	38:e:221:MET:HE1	1.86	0.58
58:AH:125:HIS:O	83:AA:1227:G:O4'	2.20	0.58
84:A:3110:C:O2'	84:A:3111:A:OP2	2.17	0.58
13:Q:110:GLU:OE2	13:Q:112:TYR:OH	2.17	0.58
72:AV:250:ILE:HG22	72:AV:252:LYS:H	1.68	0.58
84:A:1777:A:N6	84:A:1780:U:OP2	2.35	0.58
74:AX:153:LEU:HD21	74:AX:244:LEU:HD22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:163:ARG:HE	29:5:55:LEU:HD11	1.70	0.57
29:5:167:THR:HG21	51:s:281:HIS:CE1	2.39	0.57
54:AD:291:PHE:N	54:AD:356:GLN:OE1	2.35	0.57
78:A1:49:ARG:NH1	85:Az:20:A:N7	2.52	0.57
80:A3:128:LYS:NZ	83:AA:1107:U:O4	2.32	0.57
2:D:101:LYS:NZ	84:A:1926:A:OP2	2.33	0.57
3:E:202:GLN:NE2	3:E:301:ASP:OD1	2.38	0.57
16:T:200:ARG:HA	84:A:1834:U:C4	2.39	0.57
21:Y:157:GLN:NE2	33:9:120:GLU:OE1	2.37	0.57
84:A:3109:U:H3'	84:A:3110:C:H5''	1.87	0.57
62:AL:126:GLU:HG2	62:AL:177:VAL:HG11	1.86	0.57
29:5:119:GLN:NE2	29:5:261:PRO:O	2.37	0.57
2:D:284:ARG:O	84:A:2562:U:O2'	2.13	0.57
19:W:74:ARG:HD2	19:W:75:TRP:CE2	2.40	0.57
28:z:94:ARG:NH1	28:z:302:GLY:O	2.37	0.57
13:Q:96:ARG:NE	13:Q:285:GLU:OE1	2.34	0.56
74:AX:126:LEU:HD23	74:AX:343:ILE:HB	1.85	0.56
84:A:2352:U:O3'	84:A:2353:A:C8	2.58	0.56
84:A:3123:G:O2'	84:A:3132:G:O6	2.15	0.56
25:2:87:ARG:NH2	84:A:1792:G:N7	2.52	0.56
38:e:151:ARG:NH1	38:e:254:TRP:O	2.37	0.56
78:A1:81:VAL:O	78:A1:99:LYS:NZ	2.38	0.56
4:F:72:PHE:HA	4:F:206:LEU:HD13	1.87	0.56
11:O:17:ARG:NH1	84:A:2457:A:O2'	2.37	0.56
25:2:64:HIS:ND1	84:A:1916:G:OP1	2.36	0.56
37:d:147:GLU:OE1	37:d:159:ARG:NH2	2.38	0.56
12:P:58:LEU:HB2	30:6:265:ILE:HD13	1.88	0.56
52:AB:167:HIS:CD2	57:AG:153:THR:HA	2.39	0.56
60:AJ:67:THR:HG22	60:AJ:79:LYS:HD3	1.88	0.56
74:AX:151:LEU:CD2	74:AX:247:LEU:HD22	2.36	0.56
83:AA:1516:G:N2	83:AA:1517:A:H62	2.04	0.56
3:E:150:LYS:O	3:E:174:GLN:N	2.36	0.56
24:1:46:TYR:N	84:A:2853:A:OP2	2.39	0.55
50:r:140:VAL:HG23	50:r:140:VAL:O	2.06	0.55
11:O:40:GLU:OE2	11:O:88:LYS:NZ	2.40	0.55
77:A0:53:ARG:NH2	83:AA:846:A:N1	2.52	0.55
54:AD:297:ARG:NH1	83:AA:1121:A:OP2	2.39	0.55
84:A:2332:C:N4	84:A:2442:U:H3	2.03	0.55
23:0:138:ARG:HB3	84:A:2321:A:C8	2.42	0.55
54:AD:412:LYS:NZ	83:AA:931:C:OP1	2.39	0.55
19:W:49:ARG:NH1	19:W:51:GLN:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:AN:67:ARG:NH1	64:AN:80:GLU:OE2	2.39	0.55
5:H:105:VAL:HG12	5:H:112:VAL:HG11	1.89	0.54
87:B:101:VAL:CA	38:e:221:MET:SD	2.95	0.54
17:U:66:ALA:HB2	17:U:100:ALA:HA	1.89	0.54
62:AL:206:LYS:NZ	83:AA:762:G:OP1	2.40	0.54
3:E:158:ALA:CB	84:A:3208:C:O2'	2.55	0.54
84:A:2497:U:O4	94:A:3420:HOH:O	2.18	0.54
74:AX:380:LEU:HD23	74:AX:394:HIS:CD2	2.41	0.54
50:r:117:GLU:HG3	50:r:180:LEU:HD12	1.90	0.54
74:AX:130:LYS:NZ	74:AX:313:THR:OG1	2.23	0.54
19:W:103:VAL:HG11	30:6:61:ALA:HB1	1.89	0.54
9:M:35:LYS:NZ	84:A:2269:G:OP1	2.42	0.54
48:p:106:ALA:O	48:p:116:ARG:NH2	2.40	0.54
74:AX:183:GLU:N	74:AX:183:GLU:OE1	2.40	0.54
29:5:167:THR:HG21	51:s:281:HIS:NE2	2.23	0.53
32:8:81:GLU:HB2	39:f:199:LYS:HD3	1.91	0.53
84:A:2668:A:H2'	84:A:2669:A:C8	2.43	0.53
30:6:336:ASP:OD1	48:p:129:ARG:NH2	2.41	0.53
15:S:194:ARG:NH2	35:b:13:SER:OG	2.42	0.53
66:AP:47:ASN:OD1	66:AP:48:GLU:N	2.42	0.53
83:AA:760:A:O3'	83:AA:761:A:H4'	2.08	0.53
84:A:2868:C:H2'	84:A:2869:A:O4'	2.09	0.53
50:r:93:ILE:HG21	50:r:119:VAL:HG21	1.90	0.53
83:AA:760:A:N1	83:AA:780:C:O2'	2.39	0.53
83:AA:1064:C:O2'	83:AA:1065:C:OP2	2.22	0.53
29:5:216:GLU:OE2	29:5:367:ASN:ND2	2.41	0.53
83:AA:1229:U:O2'	83:AA:1442:G:O4'	2.27	0.53
87:B:101:VAL:HG23	38:e:221:MET:HB2	1.90	0.53
84:A:2115:U:H1'	84:A:2814:G:O6	2.08	0.53
72:AV:180:LEU:HB3	72:AV:360:VAL:HG22	1.90	0.53
5:H:99:THR:O	5:H:108:ARG:NH1	2.41	0.53
7:K:16:ARG:CZ	7:K:124:ARG:HE	2.21	0.53
72:AV:250:ILE:HD11	77:A0:146:GLU:HB2	1.89	0.53
76:AZ:7:TYR:OH	78:A1:189:LYS:HE3	2.09	0.53
83:AA:1227:G:OP2	83:AA:1228:A:O2'	2.23	0.53
58:AH:151:SER:O	58:AH:155:VAL:HG23	2.08	0.52
15:S:96:PHE:HB3	35:b:126:ILE:HD13	1.91	0.52
60:AJ:78:ARG:HB2	60:AJ:118:LEU:HD11	1.92	0.52
84:A:2086:A:H2'	84:A:2087:U:C6	2.44	0.52
56:AF:240:ARG:NH2	79:A2:44:THR:O	2.43	0.52
72:AV:273:ILE:O	72:AV:346:LYS:NZ	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:A:2017:U:OP1	94:A:3423:HOH:O	2.19	0.52
3:E:208:ALA:HB2	3:E:297:VAL:HG12	1.90	0.52
81:A4:290:ASP:OD1	81:A4:292:TYR:N	2.43	0.52
43:j:23:ALA:HB1	84:A:2149:G:OP1	2.09	0.52
56:AF:234:ARG:HB2	79:A2:53:MET:HE1	1.92	0.52
78:A1:298:SER:O	78:A1:302:GLU:HG2	2.10	0.52
4:F:69:LEU:HG	4:F:190:MET:HE2	1.92	0.52
4:F:281:ARG:HD2	84:A:1884:G:N7	2.25	0.52
83:AA:917:C:O2'	83:AA:921:U:OP1	2.26	0.52
16:T:185:THR:HG23	16:T:188:ALA:H	1.75	0.51
48:p:110:TRP:H	48:p:110:TRP:CD1	2.28	0.51
57:AG:237:GLU:OE1	57:AG:237:GLU:N	2.40	0.51
62:AL:96:GLU:OE1	62:AL:96:GLU:N	2.41	0.51
51:s:298:GLN:HG3	51:s:335:TRP:CZ3	2.46	0.51
81:A4:156:ALA:HB3	81:A4:172:MET:HE1	1.92	0.51
84:A:2004:G:OP1	94:A:3422:HOH:O	2.19	0.51
10:N:123:ARG:NH1	10:N:162:GLU:OE1	2.44	0.51
35:b:28:ARG:NH2	35:b:78:GLU:OE1	2.37	0.51
35:b:144:ARG:N	35:b:147:GLU:OE1	2.35	0.51
81:A4:441:THR:OG1	81:A4:444:ASN:ND2	2.44	0.51
10:N:54:GLU:OE1	10:N:54:GLU:N	2.43	0.51
23:O:142:GLY:HA3	84:A:2321:A:C2	2.46	0.51
81:A4:242:ASN:ND2	81:A4:245:GLU:OE2	2.44	0.51
84:A:2006:C:H2'	84:A:2007:U:C6	2.46	0.51
87:B:101:VAL:HG23	38:e:221:MET:CB	2.40	0.51
11:O:38:ARG:HG3	11:O:85:LEU:HD11	1.93	0.51
83:AA:1560:U:O2'	84:A:2582:A:N1	2.43	0.51
2:D:207:ILE:HG12	2:D:229:PRO:HD3	1.93	0.51
38:e:242:ASP:OD1	38:e:243:PHE:N	2.41	0.51
84:A:3108:U:H2'	84:A:3108:U:O2	2.11	0.51
3:E:244:ALA:HB1	3:E:248:ILE:HD11	1.92	0.50
31:7:276:PHE:HB2	31:7:304:VAL:HG22	1.92	0.50
84:A:2443:C:O2'	84:A:2444:A:OP1	2.17	0.50
9:M:56:GLU:HG3	84:A:2015:G:O4'	2.12	0.50
11:O:38:ARG:HD2	11:O:82:GLU:OE1	2.12	0.50
57:AG:263:ASP:OD1	57:AG:267:MET:N	2.43	0.50
86:Ax:29:U:H2'	86:Ax:30:G:O4'	2.11	0.50
10:N:171:GLU:OE2	45:l:131:ARG:NH1	2.44	0.50
18:V:133:ILE:HG21	18:V:145:ARG:HB3	1.93	0.50
21:Y:196:ARG:NH1	84:A:1700:U:OP1	2.44	0.50
58:AH:89:ASP:OD1	58:AH:141:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AH:155:VAL:HG21	78:A1:129:PHE:HB3	1.94	0.50
75:AY:256:LEU:N	81:A4:355:GLN:OE1	2.45	0.50
84:A:2510:U:OP2	94:A:3424:HOH:O	2.19	0.50
30:6:102:GLN:OE1	30:6:106:ARG:NH1	2.44	0.50
57:AG:215:ASP:OD1	57:AG:215:ASP:N	2.45	0.50
29:5:115:GLU:HB2	29:5:119:GLN:HB2	1.94	0.50
65:AO:123:LEU:HB3	65:AO:154:ILE:HD13	1.93	0.50
63:AM:65:LEU:HD12	68:AR:192:MET:CE	2.41	0.50
27:4:66:PHE:N	84:A:3013:G:O2'	2.39	0.50
62:AL:71:THR:HG23	62:AL:95:LEU:HD23	1.93	0.50
64:AN:29:ARG:HD3	64:AN:46:ARG:HD2	1.92	0.50
83:AA:663:A:H2'	83:AA:664:G:C8	2.47	0.50
84:A:2442:U:H2'	84:A:2443:C:O4'	2.11	0.50
10:N:87:PHE:CE1	10:N:169:PHE:HB2	2.46	0.50
77:A0:42:THR:HG22	77:A0:49:ARG:HG2	1.94	0.50
84:A:2162:C:N4	84:A:2222:U:OP1	2.45	0.50
13:Q:113:VAL:HG21	13:Q:185:ASP:C	2.37	0.50
20:X:42:HIS:CD2	20:X:86:ILE:HD11	2.47	0.50
37:d:263:THR:OG1	37:d:264:LYS:N	2.45	0.50
84:A:1934:U:H2'	84:A:1935:A:O4'	2.12	0.50
74:AX:380:LEU:HD23	74:AX:394:HIS:HD2	1.77	0.49
83:AA:692:C:N3	83:AA:693:A:C2	2.80	0.49
83:AA:1434:A:N7	94:AA:1822:HOH:O	2.35	0.49
27:4:88:TRP:CE2	84:A:2160:A:H2'	2.47	0.49
40:g:98:LYS:HB2	40:g:152:TYR:CE1	2.47	0.49
83:AA:1104:A:OP1	83:AA:1591:C:O2'	2.26	0.49
84:A:3212:C:H2'	84:A:3213:A:O4'	2.12	0.49
29:5:105:TYR:CZ	29:5:262:ILE:HD12	2.48	0.49
74:AX:123:ARG:NH1	74:AX:339:PRO:O	2.46	0.49
17:U:75:GLY:HA3	17:U:89:LYS:O	2.13	0.49
1:B:45:G:O6	12:P:88:HIS:NE2	2.42	0.49
54:AD:421:VAL:HG22	54:AD:421:VAL:O	2.12	0.49
12:P:132:LEU:HD23	12:P:165:MET:HE1	1.94	0.49
56:AF:159:VAL:CG2	56:AF:172:VAL:HG21	2.43	0.49
19:W:118:THR:HA	30:6:51:TYR:O	2.13	0.49
20:X:163:ARG:NE	29:5:55:LEU:HD11	2.28	0.49
38:e:52:CYS:O	38:e:54:GLN:NE2	2.46	0.49
47:o:20:LYS:HG3	84:A:2112:A:H5''	1.94	0.49
36:c:80:GLN:O	36:c:210:ARG:NH2	2.46	0.49
83:AA:1152:A:H2'	83:AA:1155:G:N3	2.28	0.49
2:D:246:ARG:NH2	2:D:250:VAL:HG13	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:81:ASP:OD1	17:U:85:VAL:HG12	2.13	0.48
18:V:122:LEU:HD23	18:V:133:ILE:HG13	1.94	0.48
31:7:143:TRP:HE1	31:7:172:VAL:HG23	1.78	0.48
84:A:2599:U:OP2	84:A:2625:C:N4	2.46	0.48
58:AH:184:ILE:O	58:AH:184:ILE:HG22	2.12	0.48
73:AW:123:VAL:HG12	73:AW:164:GLU:OE1	2.13	0.48
74:AX:245:LYS:NZ	91:AX:503:GDP:O2B	2.46	0.48
84:A:1718:A:N3	84:A:1911:C:O2'	2.43	0.48
29:5:136:VAL:HG11	29:5:417:LEU:HD23	1.95	0.48
59:AI:182:PRO:HB2	59:AI:184:5F0:O	2.13	0.48
84:A:2928:C:OP2	84:A:3073:C:O2'	2.31	0.48
1:B:44:A:H2'	1:B:45:G:O4'	2.13	0.48
19:W:148:LEU:O	30:6:339:GLU:N	2.45	0.48
28:z:78:MET:O	28:z:97:TYR:OH	2.31	0.48
29:5:203:CYS:O	51:s:179:GLN:NE2	2.46	0.48
51:s:91:TYR:HE1	51:s:269:ASP:OD1	1.96	0.48
54:AD:206:PRO:HG2	54:AD:276:VAL:HG11	1.95	0.48
74:AX:283:ALA:N	74:AX:286:GLU:OE1	2.36	0.48
35:b:133:PHE:CG	36:c:259:ARG:HD3	2.48	0.48
63:AM:112:ARG:NE	65:AO:228:SER:OG	2.46	0.48
83:AA:1429:C:H4'	83:AA:1430:A:H5'	1.95	0.48
12:P:132:LEU:HB3	12:P:165:MET:HE1	1.96	0.48
39:f:58:LYS:NZ	84:A:2068:C:O2	2.46	0.48
84:A:1935:A:H2'	84:A:1936:A:O4'	2.14	0.48
84:A:2549:C:N4	84:A:2562:U:H2'	2.28	0.48
84:A:2643:G:O2'	84:A:2645:G:OP2	2.30	0.48
29:5:124:THR:OG1	29:5:126:THR:HG22	2.12	0.48
29:5:270:ILE:HG22	84:A:2410:U:H4'	1.96	0.48
83:AA:693:A:N1	83:AA:822:G:O6	2.46	0.48
2:D:269:ARG:NH1	84:A:1990:G:OP1	2.41	0.48
76:AZ:11:MET:HE1	78:A1:189:LYS:HG3	1.95	0.48
81:A4:379:PHE:CE2	81:A4:392:ILE:HD13	2.48	0.48
83:AA:1453:A:H2'	83:AA:1454:G:O4'	2.12	0.48
84:A:1722:A:H2'	84:A:1723:A:O4'	2.13	0.48
84:A:2499:U:OP2	94:A:3426:HOH:O	2.20	0.48
18:V:64:ILE:HA	18:V:120:VAL:HG12	1.96	0.48
18:V:94:HIS:NE2	84:A:1805:A:OP2	2.30	0.48
53:AC:58:ALA:HB3	53:AC:60:HIS:CE1	2.49	0.48
78:A1:174:ARG:HG3	78:A1:204:VAL:HG11	1.95	0.48
84:A:2728:C:H4'	84:A:2815:OMG:HM22	1.96	0.48
31:7:326:GLU:O	31:7:327:ASP:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AG:389:ARG:NH1	83:AA:1427:A:H1'	2.29	0.48
83:AA:1138:G:O2'	83:AA:1167:A:N1	2.45	0.48
83:AA:1581:G:N1	83:AA:1584:MA6:OP2	2.43	0.48
4:F:89:THR:O	4:F:179:THR:HG21	2.14	0.47
14:R:141:ILE:HG22	34:a:51:LEU:HD12	1.96	0.47
41:h:135:GLN:N	41:h:135:GLN:OE1	2.47	0.47
84:A:2718:C:H5'	84:A:2719:G:O5'	2.14	0.47
84:A:2820:A:H2'	84:A:2821:C:O4'	2.13	0.47
32:8:191:ARG:O	39:f:135:LEU:N	2.41	0.47
51:s:51:MET:SD	51:s:61:ARG:HG2	2.54	0.47
83:AA:815:C:O2'	83:AA:817:G:OP1	2.18	0.47
84:A:2067:C:H3'	84:A:2068:C:O4'	2.13	0.47
34:a:52:THR:OG1	34:a:54:ASP:OD1	2.28	0.47
63:AM:85:LYS:HB2	63:AM:86:PRO:HD3	1.97	0.47
67:AQ:38:ASP:OD1	67:AQ:42:ARG:NE	2.47	0.47
78:A1:225:LEU:O	78:A1:229:LEU:HD23	2.13	0.47
83:AA:1055:U:H2'	83:AA:1056:A:O4'	2.13	0.47
84:A:2477:G:OP1	94:A:3425:HOH:O	2.20	0.47
84:A:3072[A]:U:H4'	84:A:3073:C:OP1	2.13	0.47
84:A:2825:G:O2'	84:A:2892:A:N3	2.36	0.47
84:A:3039:OMU:O3'	84:A:3039:OMU:HM22	2.14	0.47
38:e:140:ALA:O	38:e:144:ASN:N	2.46	0.47
54:AD:128:ARG:O	85:Az:18:A:N6	2.47	0.47
2:D:110:LEU:HD22	29:5:30:ALA:HB2	1.95	0.47
14:R:31:PHE:CD1	84:A:1829:A:H5''	2.50	0.47
20:X:173:ASP:O	20:X:188:TYR:OH	2.31	0.47
29:5:213:TRP:CH2	29:5:222:VAL:HG23	2.50	0.47
48:p:152:GLN:OE1	48:p:155:ARG:NH1	2.45	0.47
57:AG:87:HIS:CE1	78:A1:62:VAL:HG22	2.50	0.47
58:AH:151:SER:HB2	78:A1:131:THR:HG22	1.96	0.47
84:A:3212:C:N4	84:A:3230:G:O6	2.23	0.47
3:E:250:ARG:NE	84:A:2688:C:OP1	2.46	0.47
32:8:63:GLU:O	32:8:67:ARG:HG2	2.15	0.47
56:AF:186:TRP:HA	56:AF:189:THR:HG22	1.96	0.47
59:AI:163:HIS:NE2	67:AQ:20:GLU:OE2	2.46	0.47
62:AL:224:ARG:HG2	62:AL:227:LEU:HD12	1.96	0.47
78:A1:66:TRP:N	78:A1:67:PRO:CD	2.78	0.47
84:A:2327:U:H2'	84:A:2328:C:O4'	2.15	0.47
84:A:3063:G:N2	94:A:3434:HOH:O	2.41	0.47
84:A:3071:U:H2'	84:A:3072[A]:U:H2'	1.96	0.47
50:r:116:GLU:O	50:r:119:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:A:1693:C:C3'	84:A:1694:U:H4'	2.45	0.47
84:A:3064:A:H5''	84:A:3065:U:H5'	1.96	0.47
3:E:126:ASP:O	3:E:149:GLY:O	2.33	0.47
21:Y:112:LEU:HD13	21:Y:132:LEU:HA	1.97	0.47
31:7:158:PHE:CZ	31:7:185:LEU:HD21	2.50	0.47
84:A:2142:A:C2	84:A:2262:C:H2'	2.50	0.47
9:M:142:GLU:OE2	48:p:145:ARG:NH2	2.48	0.47
13:Q:96:ARG:HA	13:Q:99:MET:HE3	1.97	0.47
56:AF:120:ARG:HH11	74:AX:93:THR:HG21	1.80	0.47
68:AR:225:VAL:HG22	68:AR:262:LEU:HD12	1.97	0.47
29:5:239:ILE:HD11	29:5:420:HIS:CE1	2.50	0.46
57:AG:198:ARG:HG2	57:AG:248:VAL:HG23	1.97	0.46
68:AR:208:ILE:O	68:AR:214:ASN:ND2	2.41	0.46
83:AA:1139:A:H2'	83:AA:1140:A:O4'	2.15	0.46
84:A:2099:U:OP1	94:A:3427:HOH:O	2.20	0.46
4:F:147:ARG:NH1	84:A:1795:A:OP1	2.40	0.46
53:AC:65:ARG:HG2	57:AG:118:GLU:OE1	2.15	0.46
57:AG:229:LEU:HD21	57:AG:241:VAL:HG11	1.96	0.46
83:AA:1312:C:C2'	83:AA:1313:A:H5''	2.45	0.46
84:A:2539:A:OP1	94:A:3429:HOH:O	2.21	0.46
84:A:3165:C:H2'	84:A:3166:U:C6	2.50	0.46
31:7:148:MET:HE2	31:7:257:ILE:HG12	1.97	0.46
78:A1:86:ARG:HB3	78:A1:96:PRO:HB2	1.97	0.46
22:Z:38:ARG:NH2	84:A:2059:C:OP1	2.48	0.46
52:AB:214:LYS:HE3	83:AA:1280:C:H5''	1.97	0.46
55:AE:49:TYR:OH	55:AE:90:ARG:NH1	2.48	0.46
81:A4:540:HIS:O	81:A4:545:GLN:NE2	2.48	0.46
86:Ax:52:G:O6	86:Ax:62:C:N4	2.47	0.46
9:M:184:LEU:HA	9:M:187:VAL:HG12	1.98	0.46
11:O:155:ASP:OD2	31:7:319:ARG:NE	2.39	0.46
38:e:244:SER:O	38:e:248:ASN:ND2	2.48	0.46
49:q:37:PRO:HG2	49:q:68:SER:HA	1.98	0.46
53:AC:51:VAL:HG22	53:AC:55:GLU:HB2	1.98	0.46
81:A4:384:ASP:HB3	81:A4:385:PRO:HD3	1.96	0.46
84:A:1697:A:N3	84:A:1703:C:O2'	2.44	0.46
5:H:54:VAL:HG13	5:H:82:LEU:HD13	1.97	0.46
29:5:139:LEU:O	29:5:145:ASN:ND2	2.31	0.46
74:AX:261:ALA:HA	74:AX:307:VAL:O	2.16	0.46
81:A4:491:GLN:O	81:A4:494:ILE:N	2.48	0.46
84:A:2726:C:O2	84:A:2937:A:N1	2.48	0.46
36:c:161:THR:O	36:c:192:GLN:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:d:95:ALA:HA	37:d:243:LEU:HD22	1.98	0.46
37:d:186:VAL:HG21	37:d:239:PRO:HB3	1.97	0.46
46:m:124:THR:O	46:m:125:ARG:C	2.59	0.46
53:AC:65:ARG:NE	57:AG:118:GLU:OE1	2.49	0.46
85:Az:14:A:N3	85:Az:14:A:H2'	2.29	0.46
11:O:113:ARG:O	11:O:117:ARG:HA	2.15	0.46
16:T:44:LYS:NZ	84:A:1812:C:OP2	2.47	0.46
18:V:23:MET:HE2	18:V:23:MET:HA	1.97	0.46
51:s:174:LEU:HB3	51:s:175:PRO:HD3	1.98	0.46
16:T:63:ARG:O	37:d:230:ARG:HD3	2.16	0.46
17:U:18:ARG:NE	18:V:206:GLU:OE2	2.49	0.46
46:m:56:LEU:HD21	46:m:77:MET:HE2	1.98	0.46
52:AB:239:ASN:ND2	52:AB:242:SER:OG	2.47	0.46
68:AR:214:ASN:O	68:AR:217:THR:OG1	2.33	0.46
84:A:1874:A:N1	84:A:1900:A:H2	2.14	0.46
11:O:130:LEU:HD22	23:0:134:THR:HG23	1.98	0.46
29:5:135:LYS:NZ	29:5:238:THR:O	2.49	0.46
37:d:109:THR:OG1	37:d:110:GLU:N	2.45	0.46
52:AB:146:SER:O	52:AB:168:THR:HA	2.16	0.46
83:AA:1481:C:O2'	85:Az:10:G:O6	2.29	0.46
83:AA:1595:G:H2'	83:AA:1596:A:O4'	2.16	0.46
4:F:191:ASP:OD1	4:F:192:SER:N	2.47	0.45
22:Z:36:PHE:O	84:A:2119:U:O2'	2.31	0.45
78:A1:121:LYS:NZ	81:A4:77:THR:O	2.41	0.45
2:D:259:LYS:HD2	84:A:1939:G:C8	2.51	0.45
58:AH:68:GLU:OE2	81:A4:62:LYS:NZ	2.43	0.45
73:AW:92:MET:O	73:AW:98:LYS:NZ	2.49	0.45
73:AW:129:VAL:HG23	73:AW:130:ASP:N	2.31	0.45
83:AA:1267:U:H2'	83:AA:1268:C:C6	2.51	0.45
84:A:1839:C:H2'	84:A:1840:C:C6	2.51	0.45
84:A:2259:C:O2'	84:A:2261:C:OP2	2.24	0.45
84:A:3110:C:O2'	84:A:3111:A:P	2.73	0.45
3:E:50:ASP:O	11:O:138:ARG:NH2	2.50	0.45
5:H:54:VAL:HG13	5:H:82:LEU:CD1	2.46	0.45
84:A:1735:A:H2'	84:A:1735:A:N3	2.31	0.45
84:A:1851:G:H2'	84:A:2693:A:N7	2.31	0.45
84:A:2625:C:C5	84:A:2626:U:N3	2.84	0.45
11:O:116:ASP:OD2	84:A:2453:G:O2'	2.34	0.45
15:S:173:ARG:HG3	15:S:182:LYS:HD2	1.99	0.45
26:3:113:ARG:HH22	84:A:1750:G:P	2.39	0.45
51:s:378:ALA:HB1	51:s:383:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AF:37:TYR:CD2	56:AF:75:LYS:HE3	2.51	0.45
83:AA:1259:U:H5	83:AA:1326:A:HO2'	1.60	0.45
84:A:3212:C:O5'	84:A:3212:C:H6	1.99	0.45
68:AR:167:HIS:ND1	68:AR:193:ILE:HG23	2.31	0.45
84:A:1702:A:O2'	84:A:1704:U:H5	1.99	0.45
53:AC:123:VAL:HG23	53:AC:157:THR:HG22	1.98	0.45
62:AL:196:TYR:O	83:AA:1048:C:H2'	2.17	0.45
76:AZ:96:LYS:HB3	83:AA:1246:U:C5	2.52	0.45
5:H:84:GLU:OE1	20:X:44:ARG:NH2	2.49	0.45
28:z:137:VAL:HG12	28:z:138:GLU:N	2.31	0.45
50:r:117:GLU:CG	50:r:180:LEU:HD12	2.47	0.45
62:AL:86:ASP:OD1	62:AL:87:ASP:N	2.49	0.45
78:A1:49:ARG:CZ	85:Az:20:A:H62	2.30	0.45
81:A4:482:ILE:HD13	81:A4:488:PRO:HG3	1.98	0.45
83:AA:952:A:N3	83:AA:954:C:N4	2.65	0.45
84:A:1717:U:H2'	84:A:1718:A:O4'	2.16	0.45
87:B:101:VAL:CG1	38:e:165:PHE:HE1	2.00	0.45
42:i:57:TYR:OH	49:q:28:ARG:O	2.34	0.45
83:AA:1562:G:O2'	83:AA:1583:MA6:N1	2.49	0.45
84:A:1729:U:O2'	84:A:1751:A:N1	2.49	0.45
86:Ax:7:A:O2'	86:Ax:49:G:O4'	2.33	0.45
15:S:104:ARG:NH1	15:S:104:ARG:HB3	2.32	0.45
18:V:34:LYS:NZ	84:A:1800:G:O6	2.45	0.45
58:AH:184:ILE:O	58:AH:184:ILE:CG2	2.65	0.45
63:AM:43:ARG:NH1	83:AA:838:U:O2'	2.47	0.45
83:AA:765:C:H5	83:AA:777:G:H1	1.65	0.45
84:A:2808:U:H2'	84:A:2809:C:O4'	2.17	0.45
63:AM:55:ASP:HB2	70:AT:140:ILE:HD13	1.99	0.45
72:AV:407:GLN:NE2	83:AA:1520:U:O3'	2.50	0.45
14:R:111:LYS:HE2	34:a:62:HIS:O	2.17	0.44
32:8:147:LEU:C	32:8:147:LEU:HD23	2.43	0.44
32:8:173:LYS:NZ	32:8:174:GLU:O	2.41	0.44
84:A:1993:A:N7	84:A:1995:A:H1'	2.33	0.44
84:A:3040:OMG:O4'	84:A:3069:A:O2'	2.23	0.44
1:B:61:U:HO2'	1:B:62:U:H6	1.64	0.44
3:E:202:GLN:HG2	3:E:203:TYR:N	2.32	0.44
4:F:243:ILE:HG22	49:q:27:ALA:HB2	2.00	0.44
10:N:221:ALA:HB3	10:N:223:MET:HG3	1.99	0.44
18:V:41:ARG:NH2	84:A:1800:G:N7	2.66	0.44
46:m:118:ARG:NH2	46:m:119:TYR:OH	2.50	0.44
56:AF:41:PHE:HB3	56:AF:75:LYS:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:AV:334:PHE:O	72:AV:338:HIS:N	2.41	0.44
81:A4:555:ILE:HG22	81:A4:559:TYR:CE2	2.52	0.44
83:AA:1502:A:H2'	83:AA:1503:G:O4'	2.17	0.44
84:A:2028:G:H4'	84:A:2047:U:O3'	2.17	0.44
84:A:2081:U:H2'	84:A:2082:G:C8	2.51	0.44
84:A:2265:A:H2'	84:A:2266:U:O4'	2.17	0.44
84:A:2924:U:H2'	84:A:2925:U:C6	2.51	0.44
16:T:136:ILE:HD13	16:T:172:LEU:CD2	2.48	0.44
36:c:94:ASN:OD1	36:c:122:ASN:ND2	2.41	0.44
1:B:33:U:O2	1:B:36:C:H5	2.00	0.44
29:5:167:THR:O	29:5:167:THR:HG22	2.18	0.44
51:s:271:LEU:N	51:s:272:PRO:HA	2.32	0.44
57:AG:251:GLU:OE1	57:AG:251:GLU:N	2.43	0.44
83:AA:1518:C:H2'	83:AA:1519:A:O4'	2.17	0.44
11:O:38:ARG:HG2	11:O:85:LEU:HD21	1.98	0.44
11:O:38:ARG:HG2	11:O:85:LEU:HD11	1.99	0.44
21:Y:126:MET:HE3	21:Y:129:PRO:HA	2.00	0.44
33:9:24:LYS:NZ	84:A:2422:U:OP2	2.49	0.44
37:d:69:PRO:HD2	37:d:76:ILE:HD11	1.99	0.44
57:AG:337:ARG:NH1	57:AG:338:SER:HB3	2.33	0.44
73:AW:141:ARG:NH1	73:AW:172:ILE:O	2.50	0.44
75:AY:360:LYS:HA	78:A1:211:ARG:HD2	2.00	0.44
83:AA:1265:C:H2'	83:AA:1266:A:H8	1.83	0.44
84:A:2071:U:OP1	84:A:2831:G:N2	2.45	0.44
84:A:2873:A:H3'	84:A:2888:A:H62	1.83	0.44
11:O:18:MET:CG	11:O:25:ARG:HG3	2.48	0.44
13:Q:191:ARG:NH2	13:Q:230:SER:OG	2.50	0.44
31:7:156:ARG:O	34:a:95:ARG:NH2	2.51	0.44
40:g:108:THR:HG21	40:g:157:LEU:HD12	1.99	0.44
51:s:249:GLU:OE1	51:s:251:VAL:O	2.35	0.44
51:s:351:VAL:O	51:s:389:ARG:NH1	2.45	0.44
78:A1:253:TRP:CD1	78:A1:296:VAL:HG21	2.52	0.44
84:A:1957:A:C3'	84:A:1958:G:H5''	2.48	0.44
84:A:2821:C:O2'	84:A:2822:C:H5'	2.18	0.44
11:O:131:PRO:HA	23:0:185:PHE:CE1	2.53	0.44
17:U:19:VAL:O	17:U:19:VAL:HG13	2.16	0.44
31:7:172:VAL:HG12	31:7:326:GLU:HB2	1.99	0.44
84:A:2025:C:H4'	84:A:2260:A:H8	1.81	0.44
84:A:2245:A:H4'	84:A:2246:A:OP1	2.17	0.44
84:A:3213:A:H2'	84:A:3214:C:C6	2.53	0.44
10:N:92:LEU:N	10:N:186:ALA:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:d:88:TYR:CZ	37:d:195:VAL:HG21	2.52	0.44
47:o:26:PHE:CZ	84:A:2155:A:C6	3.06	0.44
84:A:2286:A:H2'	84:A:2287:U:C6	2.53	0.44
3:E:99:LEU:CD2	3:E:193:LEU:HB3	2.48	0.44
5:H:102:VAL:HG13	5:H:105:VAL:HB	1.99	0.44
18:V:148:THR:HG22	18:V:148:THR:O	2.18	0.44
21:Y:143:ASP:OD1	33:9:137:ARG:NH2	2.51	0.44
36:c:270:TYR:O	36:c:285:PRO:HA	2.17	0.44
83:AA:989:U:H2'	83:AA:990:U:O4'	2.18	0.44
84:A:1737:A:N6	84:A:1760:G:H1'	2.32	0.44
84:A:2220:A:H2'	84:A:2221:C:O2	2.18	0.44
84:A:2821:C:OP2	94:A:3430:HOH:O	2.21	0.44
3:E:99:LEU:HD11	3:E:194:TYR:O	2.17	0.43
10:N:87:PHE:HE1	10:N:169:PHE:HB2	1.83	0.43
16:T:143:ARG:O	84:A:1672:C:O2'	2.35	0.43
50:r:150:TYR:OH	84:A:2241:A:OP1	2.16	0.43
50:r:173:ARG:NH1	84:A:2156:A:N7	2.65	0.43
57:AG:273:GLU:HG3	57:AG:282:GLU:HG2	2.00	0.43
84:A:2143:G:C5	84:A:2258:A:C2	3.06	0.43
84:A:2632:A:O2'	84:A:2635:G:N3	2.40	0.43
86:Ax:30:G:N7	94:Ax:101:HOH:O	2.37	0.43
48:p:63:ASN:OD1	48:p:64:GLY:N	2.51	0.43
83:AA:1258:A:H4'	83:AA:1259:U:H3'	2.00	0.43
84:A:2005:C:H2'	84:A:2006:C:C6	2.53	0.43
43:j:109:LEU:H	43:j:109:LEU:HD23	1.83	0.43
53:AC:73:THR:O	53:AC:79:GLU:HG3	2.19	0.43
53:AC:84:GLU:OE1	53:AC:84:GLU:N	2.42	0.43
76:AZ:42:LEU:HA	76:AZ:45:LYS:HD3	1.99	0.43
84:A:1816:G:H2'	84:A:1817:C:O4'	2.18	0.43
84:A:2899:C:H2'	84:A:2900:C:O4'	2.19	0.43
29:5:114:LEU:N	29:5:264:ASP:OD2	2.51	0.43
48:p:133:LEU:HD21	48:p:157:MET:SD	2.59	0.43
80:A3:152:PHE:CD2	84:A:2596:G:H5'	2.53	0.43
83:AA:1000:U:H4'	83:AA:1002:C:O4'	2.19	0.43
84:A:1973:G:H2'	84:A:1975:U:OP2	2.18	0.43
4:F:82:LEU:HB3	4:F:87:PHE:CD2	2.53	0.43
16:T:147:LEU:HG	37:d:56:PHE:CE2	2.53	0.43
36:c:151:GLU:O	36:c:155:ASN:ND2	2.52	0.43
63:AM:20:ARG:NH2	83:AA:839:A:O2'	2.52	0.43
84:A:1895:C:H2'	84:A:1896:U:C6	2.53	0.43
84:A:2099:U:H2'	84:A:2100:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:A:2162:C:H42	84:A:2222:U:P	2.42	0.43
84:A:3070:G:C2'	84:A:3071:U:H5'	2.48	0.43
86:Ax:9:A:O2'	86:Ax:10:G:N7	2.40	0.43
11:O:39:HIS:O	11:O:40:GLU:HB2	2.18	0.43
29:5:115:GLU:HG3	29:5:256:PHE:CD2	2.53	0.43
31:7:221:VAL:HG22	31:7:254:LEU:HD23	1.99	0.43
37:d:85:PHE:CZ	37:d:209:TYR:HB2	2.54	0.43
48:p:122:THR:HG23	48:p:123:HIS:ND1	2.34	0.43
53:AC:109:VAL:HB	53:AC:120:CYS:HB2	2.00	0.43
60:AJ:51:PRO:HG3	60:AJ:122:LYS:HB3	2.01	0.43
84:A:1751:A:H2'	84:A:1752:U:O4'	2.18	0.43
84:A:2331:C:H3'	84:A:2332:C:O4'	2.17	0.43
85:Az:21:A:H1'	85:Az:22:A:C6	2.54	0.43
86:Ax:52:G:N1	86:Ax:62:C:N3	2.66	0.43
7:K:115:ASN:HB2	84:A:1839:C:OP1	2.19	0.43
29:5:125:LYS:NZ	29:5:370:VAL:O	2.52	0.43
56:AF:176:ASP:OD1	56:AF:176:ASP:N	2.48	0.43
68:AR:262:LEU:HD11	68:AR:267:TYR:HB2	2.00	0.43
84:A:2289:G:C6	84:A:2290:A:C5	3.07	0.43
84:A:2352:U:H4'	84:A:2362:A:C5	2.54	0.43
84:A:2652:G:H2'	84:A:2653:C:O4'	2.18	0.43
4:F:237:LEU:O	49:q:25:TYR:N	2.52	0.43
54:AD:157:ILE:HD12	54:AD:157:ILE:H	1.84	0.43
78:A1:55:PRO:O	78:A1:58:GLU:HG2	2.18	0.43
84:A:1749:C:OP2	84:A:2899:C:O2'	2.31	0.43
84:A:1750:G:H2'	84:A:1751:A:C8	2.53	0.43
84:A:2728:C:H2'	84:A:2729:U:C6	2.54	0.43
31:7:79:PHE:HB3	31:7:81:MET:SD	2.58	0.43
84:A:3115:U:H2'	84:A:3116:C:C6	2.54	0.43
11:O:91:GLN:OE1	23:0:153:THR:OG1	2.32	0.43
14:R:83:TYR:CZ	14:R:87:ILE:HG13	2.53	0.43
35:b:15:LEU:HD21	36:c:169:VAL:HA	2.00	0.43
51:s:221:HIS:NE2	84:A:2334:C:OP1	2.47	0.43
61:AK:63:LEU:HD11	75:AY:350:PHE:HB2	2.01	0.43
83:AA:702:C:H2'	83:AA:703:A:O4'	2.19	0.43
84:A:2163:A:H2'	84:A:2164:C:O4'	2.18	0.43
84:A:2599:U:H2'	84:A:2608:G:O6	2.18	0.43
84:A:3068:G:OP2	84:A:3068:G:N2	2.50	0.43
84:A:3119:C:H2'	84:A:3120:C:O4'	2.18	0.43
83:AA:872:G:N2	83:AA:920:G:O2'	2.52	0.42
83:AA:1124:A:H2'	83:AA:1125:A:H2'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:A:1867:A:N1	84:A:2019:G:O2'	2.49	0.42
84:A:2429:A:N1	84:A:2433:C:O2'	2.37	0.42
84:A:2733:G:H2'	84:A:2734:A:O4'	2.19	0.42
2:D:281:TRP:O	2:D:285:LYS:HE2	2.19	0.42
4:F:125:ARG:NH2	84:A:2006:C:H5''	2.34	0.42
29:5:110:ARG:HG2	84:A:2407:U:O2'	2.19	0.42
37:d:261:MET:HE2	37:d:261:MET:HB3	1.93	0.42
84:A:2352:U:H4'	84:A:2353:A:OP2	2.19	0.42
84:A:2482:A:H2'	84:A:2483:U:O4'	2.19	0.42
3:E:215:PHE:O	84:A:2458:A:O2'	2.29	0.42
11:O:38:ARG:HG2	11:O:38:ARG:HH11	1.84	0.42
11:O:38:ARG:HG2	11:O:38:ARG:NH1	2.34	0.42
11:O:94:ALA:HB3	11:O:95:PRO:HD3	2.01	0.42
84:A:2196:A:O2'	84:A:2213:A:N1	2.48	0.42
84:A:2677:A:H2'	84:A:2678:A:C8	2.54	0.42
30:6:252:CYS:SG	30:6:296:ARG:NH1	2.92	0.42
38:e:157:LEU:HA	38:e:255:VAL:O	2.19	0.42
54:AD:317:HIS:HD2	83:AA:651:A:H4'	1.84	0.42
57:AG:315:PHE:CD2	57:AG:369:LEU:HD21	2.54	0.42
72:AV:105:ARG:NH2	83:AA:1525:C:O5'	2.52	0.42
74:AX:276:ARG:NH2	74:AX:286:GLU:OE2	2.52	0.42
79:A2:110:ARG:HD2	83:AA:1293:C:O2'	2.20	0.42
84:A:3069:A:H2'	84:A:3070:G:O4'	2.18	0.42
18:V:23:MET:HE3	18:V:114:PRO:HG3	2.00	0.42
29:5:193:LEU:N	29:5:193:LEU:HD12	2.34	0.42
31:7:114:ASP:HB2	31:7:117:LYS:HB2	2.02	0.42
84:A:1803:A:H4'	84:A:1804:A:H3'	2.00	0.42
84:A:2644:A:OP1	94:A:3431:HOH:O	2.21	0.42
5:H:97:ILE:HG21	5:H:140:PHE:HD2	1.84	0.42
35:b:39:SER:OG	84:A:2285:U:O2'	2.36	0.42
37:d:250:LYS:HD3	37:d:252:LEU:HD23	2.02	0.42
38:e:55:ARG:O	38:e:55:ARG:HG3	2.19	0.42
51:s:84:THR:HB	51:s:280:ASN:HB2	2.02	0.42
83:AA:1079:G:C6	83:AA:1080:A:N7	2.88	0.42
84:A:2707:A:H2'	84:A:2708:C:C6	2.55	0.42
3:E:109:LEU:C	3:E:109:LEU:HD12	2.45	0.42
44:k:2(A):ALA:HB3	44:k:5:LEU:HB3	2.02	0.42
52:AB:211:ASP:OD1	52:AB:214:LYS:NZ	2.49	0.42
53:AC:117:LEU:HD23	53:AC:151:VAL:HG22	2.01	0.42
83:AA:1201:A:H2'	83:AA:1202:G:C8	2.55	0.42
83:AA:1447:G:C6	83:AA:1449:G:C2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:71:GLN:HB2	84:A:2034:A:O2'	2.19	0.42
16:T:72:ARG:NH2	84:A:1672:C:OP1	2.40	0.42
16:T:151:ARG:HG3	84:A:2354:A:C6	2.55	0.42
17:U:143:ARG:HG2	31:7:80:VAL:HG21	2.01	0.42
24:1:19:ARG:HB2	24:1:62:ILE:HD11	2.01	0.42
29:5:50:TYR:OH	29:5:72:ARG:O	2.27	0.42
44:k:11:ARG:HB2	44:k:12:PRO:HD3	2.02	0.42
51:s:308:ARG:NH2	51:s:398:SER:OG	2.53	0.42
72:AV:68:SER:N	83:AA:1523:A:H5'	2.34	0.42
72:AV:356:THR:O	72:AV:360:VAL:HG23	2.20	0.42
83:AA:1507:A:H2'	83:AA:1508:C:O4'	2.19	0.42
84:A:1782:G:O2'	84:A:1793:G:O6	2.32	0.42
84:A:2651:A:H2'	84:A:2652:G:O4'	2.19	0.42
19:W:86:ASN:OD1	84:A:2872:C:H4'	2.20	0.42
37:d:91:PRO:HD2	37:d:94:ASP:OD2	2.19	0.42
46:m:114:LEU:O	46:m:119:TYR:CD2	2.73	0.42
48:p:115:VAL:HG13	48:p:161:ALA:HB3	2.02	0.42
83:AA:703:A:P	83:AA:847:G:H21	2.43	0.42
84:A:2505:A:H2'	84:A:2507:A:N7	2.35	0.42
84:A:2693:A:N3	84:A:2986:C:H5''	2.35	0.42
84:A:2937:A:O2'	86:Ax:76:A:N1	2.50	0.42
9:M:40:PRO:HG3	84:A:1868:G:H2'	2.02	0.42
36:c:42:GLN:NE2	42:i:36:LEU:O	2.53	0.42
70:AT:33:ASN:O	70:AT:74:PRO:HA	2.20	0.42
72:AV:283:LEU:HD23	72:AV:334:PHE:CD1	2.55	0.42
83:AA:916:C:H2'	83:AA:917:C:O4'	2.20	0.42
83:AA:1523:A:H2	83:AA:1527:A:H61	1.67	0.42
84:A:1761:A:H2'	84:A:1762:A:O4'	2.20	0.42
3:E:106:MET:SD	84:A:3149:C:H5'	2.59	0.41
29:5:201:ARG:NH1	29:5:418:TYR:O	2.47	0.41
51:s:249:GLU:HA	51:s:356:VAL:HG11	2.01	0.41
83:AA:1132:U:H2'	83:AA:1133:C:C6	2.55	0.41
86:Ax:62:C:H2'	86:Ax:63:U:C6	2.55	0.41
3:E:230:THR:O	3:E:233:GLN:HG2	2.20	0.41
35:b:21:ARG:NH1	36:c:79:LEU:O	2.53	0.41
43:j:71:GLU:O	43:j:75:ARG:HG3	2.21	0.41
78:A1:91:VAL:HG12	78:A1:92:LYS:N	2.34	0.41
79:A2:49:MET:HG2	79:A2:53:MET:HE2	2.01	0.41
81:A4:461:PHE:O	81:A4:465:ILE:HG12	2.20	0.41
83:AA:758:U:O4	83:AA:1159:A:H1'	2.20	0.41
83:AA:1065:C:H2'	83:AA:1066:C:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:108:PRO:HB3	3:E:116:LYS:HE2	2.02	0.41
8:L:46:LEU:HD12	8:L:78:LYS:HD3	2.02	0.41
52:AB:210:ARG:HG2	52:AB:214:LYS:NZ	2.34	0.41
53:AC:51:VAL:HG12	53:AC:165:LYS:O	2.20	0.41
57:AG:210:VAL:O	57:AG:210:VAL:CG1	2.65	0.41
91:AX:503:GDP:H5'	91:AX:503:GDP:H8	1.85	0.41
83:AA:1259:U:C6	83:AA:1326:A:O2'	2.72	0.41
83:AA:1582:G:H1'	84:A:2582:A:O3'	2.20	0.41
84:A:1694:U:O2'	84:A:1695:C:P	2.78	0.41
84:A:2019:G:H8	84:A:2019:G:H5''	1.85	0.41
8:L:75:LEU:O	8:L:81:LYS:HA	2.20	0.41
15:S:171:ILE:HD13	84:A:2143:G:H4'	2.03	0.41
29:5:378:SER:O	29:5:380:GLN:NE2	2.49	0.41
31:7:65:ILE:HG23	31:7:83:LYS:HB2	2.02	0.41
40:g:109:VAL:HG13	40:g:146:THR:HG23	2.01	0.41
51:s:145:VAL:HG11	51:s:187:LEU:HD11	2.03	0.41
53:AC:99:THR:C	53:AC:101:PRO:HD3	2.45	0.41
68:AR:271:MET:HE2	68:AR:275:PHE:HE2	1.85	0.41
72:AV:69:SER:O	72:AV:72:ILE:HG22	2.20	0.41
2:D:103:ARG:NH2	84:A:2403:G:OP2	2.53	0.41
17:U:64:PRO:HB2	17:U:100:ALA:HB3	2.02	0.41
18:V:144:VAL:HG21	18:V:153:ILE:HD13	2.01	0.41
57:AG:271:LYS:HA	57:AG:283:ALA:O	2.20	0.41
57:AG:315:PHE:HB3	57:AG:316:PRO:HD3	2.02	0.41
83:AA:1103:A:N7	83:AA:1574:G:O2'	2.53	0.41
83:AA:1376:C:H4'	83:AA:1377:C:OP1	2.21	0.41
84:A:3068:G:N3	84:A:3068:G:H2'	2.36	0.41
84:A:3095:G:H5'	84:A:3096:U:OP1	2.21	0.41
3:E:158:ALA:HB1	84:A:3208:C:O2'	2.21	0.41
3:E:183:ASP:OD1	3:E:183:ASP:N	2.53	0.41
4:F:89:THR:HG22	4:F:179:THR:OG1	2.21	0.41
6:J:74:PRO:HA	6:J:75:ASP:HA	1.82	0.41
9:M:115:PRO:HG3	9:M:258:THR:OG1	2.20	0.41
17:U:28:LEU:O	21:Y:114:THR:HG23	2.20	0.41
32:8:86:GLU:HA	32:8:89:ILE:HG22	2.03	0.41
37:d:85:PHE:HZ	37:d:209:TYR:HB2	1.85	0.41
57:AG:209:LEU:O	57:AG:210:VAL:HB	2.20	0.41
59:AI:98:GLN:HE22	83:AA:1004:G:H21	1.67	0.41
64:AN:74:ALA:HB2	83:AA:768:A:OP2	2.21	0.41
77:A0:135:MET:SD	77:A0:135:MET:N	2.86	0.41
83:AA:1317:A:H3'	83:AA:1318:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:A:1680:A:H2'	84:A:1681:G:O4'	2.21	0.41
84:A:2195:A:O2'	84:A:2214:A:O2'	2.36	0.41
84:A:2884:C:O3'	84:A:2885:U:O4'	2.39	0.41
9:M:283:LEU:HD22	40:g:40:GLU:HG2	2.01	0.41
19:W:74:ARG:HD2	19:W:75:TRP:CZ2	2.56	0.41
27:4:79:CYS:SG	27:4:98:HIS:ND1	2.89	0.41
39:f:147:ASP:OD1	39:f:147:ASP:N	2.53	0.41
51:s:237:PRO:HB3	51:s:300:HIS:CE1	2.55	0.41
57:AG:123:PRO:HD3	78:A1:87:MET:HE3	2.02	0.41
76:AZ:11:MET:HE3	78:A1:193:LEU:HG	2.03	0.41
29:5:213:TRP:CZ3	29:5:222:VAL:HG23	2.56	0.41
57:AG:131:ILE:HG21	78:A1:86:ARG:NH2	2.36	0.41
57:AG:263:ASP:OD1	57:AG:263:ASP:N	2.51	0.41
58:AH:165:PRO:HG2	58:AH:168:VAL:HG21	2.01	0.41
84:A:2318:A:H2'	84:A:2319:A:C8	2.55	0.41
84:A:2734:A:N3	94:A:3471:HOH:O	2.37	0.41
9:M:253:PHE:CE1	9:M:257:CYS:SG	3.14	0.41
15:S:103:SER:HB3	84:A:2256:U:O4'	2.21	0.41
18:V:86:VAL:HG21	18:V:120:VAL:HG21	2.02	0.41
18:V:183:LEU:HD11	33:9:79:PRO:CD	2.50	0.41
19:W:123:GLY:N	30:6:51:TYR:OH	2.53	0.41
37:d:183:TRP:HA	37:d:221:THR:O	2.21	0.41
53:AC:62:ILE:O	53:AC:66:LYS:O	2.39	0.41
55:AE:49:TYR:CE2	83:AA:975:A:H5''	2.56	0.41
59:AI:176:THR:HG23	67:AQ:11:THR:OG1	2.21	0.41
60:AJ:51:PRO:O	60:AJ:89:ARG:NH2	2.49	0.41
77:A0:41:LEU:HD21	77:A0:59:ARG:HE	1.86	0.41
78:A1:174:ARG:HG3	78:A1:204:VAL:CG1	2.51	0.41
83:AA:715:G:N3	83:AA:816:A:O2'	2.47	0.41
83:AA:1188:A:H2'	83:AA:1429:C:OP2	2.20	0.41
84:A:1861:U:H2'	84:A:1862:U:C6	2.56	0.41
84:A:1950:U:H2'	84:A:1951:C:C6	2.56	0.41
84:A:2312:A:H2'	84:A:2313:A:O4'	2.21	0.41
84:A:2441:C:H2'	84:A:2442:U:C6	2.56	0.41
84:A:2641:A:H2'	84:A:2642:C:O4'	2.21	0.41
84:A:2803:A:H2'	84:A:2804:A:O4'	2.20	0.41
84:A:3064:A:C5'	84:A:3065:U:H5'	2.51	0.41
84:A:3079:G:N7	94:A:3472:HOH:O	2.37	0.41
3:E:80:LEU:HD12	3:E:323:GLY:HA3	2.02	0.41
8:L:51:TYR:CE2	8:L:78:LYS:HA	2.55	0.41
9:M:14:ASP:OD1	9:M:15:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:115:LEU:HD11	15:S:190:GLN:HB3	2.03	0.41
31:7:81:MET:HB3	31:7:86:SER:CB	2.51	0.41
64:AN:8:VAL:HB	64:AN:68:ALA:HB1	2.02	0.41
78:A1:235:ASN:OD1	78:A1:236:THR:N	2.54	0.41
83:AA:835:C:N4	83:AA:851:A:OP2	2.51	0.41
84:A:1800:G:N1	84:A:1803:A:OP2	2.54	0.41
84:A:2343:G:H3'	84:A:2343:G:N3	2.36	0.41
21:Y:192:LYS:HG2	84:A:1709:G:H4'	2.04	0.40
35:b:73:PRO:HB2	35:b:89:ILE:HG13	2.02	0.40
36:c:160:LEU:HD21	36:c:223:MET:HG3	2.03	0.40
50:r:101:PRO:HG3	84:A:3181:U:OP1	2.20	0.40
52:AB:202:ILE:HD13	83:AA:1295:A:C4	2.56	0.40
54:AD:103:LEU:HD11	54:AD:123:ARG:HB2	2.02	0.40
57:AG:396:ARG:NH1	86:Ax:33:U:OP2	2.42	0.40
62:AL:155:TYR:HH	83:AA:1038:C:HO2'	1.65	0.40
72:AV:209:LEU:HD12	72:AV:209:LEU:C	2.46	0.40
77:A0:9:ARG:NE	83:AA:805:C:O2	2.48	0.40
81:A4:82:THR:HA	81:A4:484:SER:HB2	2.03	0.40
84:A:2504:A:C8	84:A:2504:A:H5'	2.56	0.40
84:A:2506:A:H1'	84:A:2601:A:N6	2.36	0.40
84:A:2727:C:H2'	84:A:2728:C:C6	2.56	0.40
13:Q:58:PRO:HB2	72:AV:90:TYR:HB2	2.02	0.40
17:U:150:TRP:CE2	37:d:172:MET:HG2	2.56	0.40
20:X:95:ASP:O	20:X:98:SER:OG	2.40	0.40
30:6:217:LEU:C	30:6:217:LEU:HD12	2.46	0.40
38:e:66:LEU:H	38:e:66:LEU:HD12	1.86	0.40
38:e:149:LEU:HD12	38:e:149:LEU:N	2.37	0.40
53:AC:62:ILE:O	53:AC:62:ILE:CG2	2.68	0.40
81:A4:130:LYS:HA	81:A4:130:LYS:HE2	2.03	0.40
83:AA:1220:A:N3	86:Ax:34:C:H4'	2.36	0.40
84:A:1986:A:H3'	84:A:1987:G:C5'	2.52	0.40
84:A:2352:U:H1'	84:A:2362:A:C8	2.56	0.40
84:A:3007:C:C6	84:A:3054:G:H1'	2.55	0.40
2:D:111:ARG:O	2:D:165:ASN:ND2	2.55	0.40
18:V:41:ARG:NH1	84:A:1799:U:OP2	2.54	0.40
39:f:146:LEU:HD12	39:f:146:LEU:O	2.21	0.40
77:A0:40:THR:O	77:A0:42:THR:HG23	2.21	0.40
81:A4:302:VAL:HG11	81:A4:341:CYS:HB3	2.04	0.40
83:AA:1200:G:C2	83:AA:1201:A:C8	3.09	0.40
83:AA:1322:C:H2'	83:AA:1323:G:O4'	2.21	0.40
84:A:1897:A:H2'	84:A:1898:A:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:C:H41	1:B:56:U:C1'	2.34	0.40
11:O:132:PRO:CD	23:O:185:PHE:CD1	3.04	0.40
12:P:138:GLU:OE1	30:6:136:ARG:NH1	2.55	0.40
29:5:124:THR:O	29:5:372:ASN:ND2	2.53	0.40
30:6:187:VAL:O	30:6:191:ASN:OD1	2.40	0.40
34:a:96:LEU:HD12	34:a:96:LEU:N	2.36	0.40
36:c:142:GLU:CG	36:c:153:ILE:HD13	2.52	0.40
37:d:137:PHE:O	37:d:138:PRO:C	2.62	0.40
40:g:72:TRP:CH2	40:g:74:PRO:HB3	2.56	0.40
47:o:20:LYS:HD2	84:A:2112:A:C5'	2.49	0.40
70:AT:78:PHE:O	70:AT:85:GLN:HA	2.21	0.40
78:A1:244:THR:OG1	78:A1:247:ASP:OD1	2.30	0.40
81:A4:290:ASP:OD1	81:A4:293:THR:N	2.47	0.40
81:A4:306:ASN:OD1	81:A4:344:ARG:NH2	2.54	0.40
83:AA:918:A:O2'	83:AA:920:G:O2'	2.13	0.40
84:A:1993:A:C5	84:A:1995:A:H1'	2.56	0.40
84:A:2493:C:N3	94:A:3469:HOH:O	2.36	0.40
4:F:134:GLY:HA2	84:A:2723:A:OP2	2.21	0.40
9:M:229:PHE:N	9:M:230:PRO:CD	2.85	0.40
17:U:2:ALA:HB3	17:U:24:PHE:CZ	2.57	0.40
19:W:83:VAL:HA	19:W:88:CYS:O	2.22	0.40
31:7:48:PHE:CZ	31:7:219:LEU:HG	2.57	0.40
47:o:81:LYS:O	47:o:82:PHE:HB2	2.21	0.40
51:s:81:ARG:O	51:s:85:LYS:HB2	2.22	0.40
84:A:1952:U:H2'	84:A:1953:A:C8	2.56	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	
2	D	236/305 (77%)	231 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	303/348 (87%)	298 (98%)	5 (2%)	0	100	100
4	F	250/311 (80%)	245 (98%)	5 (2%)	0	100	100
5	H	200/267 (75%)	192 (96%)	8 (4%)	0	100	100
6	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
7	K	176/178 (99%)	174 (99%)	2 (1%)	0	100	100
8	L	113/145 (78%)	110 (97%)	3 (3%)	0	100	100
9	M	289/296 (98%)	282 (98%)	7 (2%)	0	100	100
10	N	220/251 (88%)	217 (99%)	3 (1%)	0	100	100
11	O	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
12	P	142/180 (79%)	141 (99%)	1 (1%)	0	100	100
13	Q	236/292 (81%)	234 (99%)	2 (1%)	0	100	100
14	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
15	S	159/205 (78%)	157 (99%)	2 (1%)	0	100	100
16	T	164/206 (80%)	158 (96%)	6 (4%)	0	100	100
17	U	151/153 (99%)	147 (97%)	3 (2%)	1 (1%)	19	29
18	V	203/216 (94%)	199 (98%)	4 (2%)	0	100	100
19	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
20	X	242/256 (94%)	238 (98%)	4 (2%)	0	100	100
21	Y	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
22	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
23	0	108/188 (57%)	108 (100%)	0	0	100	100
24	1	54/65 (83%)	54 (100%)	0	0	100	100
25	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
26	3	93/188 (50%)	93 (100%)	0	0	100	100
27	4	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
28	z	160/325 (49%)	156 (98%)	4 (2%)	0	100	100
29	5	392/423 (93%)	380 (97%)	12 (3%)	0	100	100
30	6	352/380 (93%)	340 (97%)	12 (3%)	0	100	100
31	7	292/338 (86%)	284 (97%)	8 (3%)	0	100	100
32	8	144/206 (70%)	143 (99%)	1 (1%)	0	100	100
33	9	122/137 (89%)	120 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	a	96/142 (68%)	92 (96%)	4 (4%)	0	100	100
35	b	148/215 (69%)	143 (97%)	5 (3%)	0	100	100
36	c	282/332 (85%)	275 (98%)	7 (2%)	0	100	100
37	d	230/306 (75%)	221 (96%)	9 (4%)	0	100	100
38	e	236/279 (85%)	222 (94%)	14 (6%)	0	100	100
39	f	153/212 (72%)	150 (98%)	3 (2%)	0	100	100
40	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
41	h	108/158 (68%)	106 (98%)	2 (2%)	0	100	100
42	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
43	j	92/123 (75%)	88 (96%)	4 (4%)	0	100	100
44	k	100/112 (89%)	99 (99%)	1 (1%)	0	100	100
45	l	80/138 (58%)	79 (99%)	1 (1%)	0	100	100
46	m	90/128 (70%)	88 (98%)	2 (2%)	0	100	100
47	o	92/102 (90%)	92 (100%)	0	0	100	100
48	p	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
49	q	159/222 (72%)	158 (99%)	1 (1%)	0	100	100
50	r	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
51	s	382/439 (87%)	376 (98%)	6 (2%)	0	100	100
52	AB	223/296 (75%)	216 (97%)	7 (3%)	0	100	100
53	AC	130/167 (78%)	125 (96%)	5 (4%)	0	100	100
54	AD	341/430 (79%)	325 (95%)	16 (5%)	0	100	100
55	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
56	AF	206/242 (85%)	203 (98%)	3 (2%)	0	100	100
57	AG	322/396 (81%)	314 (98%)	7 (2%)	1 (0%)	37	51
58	AH	138/201 (69%)	133 (96%)	4 (3%)	1 (1%)	19	29
59	AI	134/194 (69%)	129 (96%)	5 (4%)	0	100	100
60	AJ	106/138 (77%)	101 (95%)	5 (5%)	0	100	100
61	AK	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
62	AL	165/257 (64%)	163 (99%)	2 (1%)	0	100	100
63	AM	117/137 (85%)	115 (98%)	2 (2%)	0	100	100
64	AN	108/130 (83%)	101 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	AO	191/258 (74%)	186 (97%)	5 (3%)	0	100	100
66	AP	95/142 (67%)	93 (98%)	2 (2%)	0	100	100
67	AQ	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
68	AR	293/360 (81%)	281 (96%)	12 (4%)	0	100	100
69	AS	133/190 (70%)	128 (96%)	5 (4%)	0	100	100
70	AT	166/169 (98%)	161 (97%)	5 (3%)	0	100	100
71	AU	174/205 (85%)	171 (98%)	3 (2%)	0	100	100
72	AV	358/414 (86%)	340 (95%)	17 (5%)	1 (0%)	37	51
73	AW	98/187 (52%)	96 (98%)	2 (2%)	0	100	100
74	AX	350/398 (88%)	343 (98%)	7 (2%)	0	100	100
75	AY	147/395 (37%)	145 (99%)	2 (1%)	0	100	100
76	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
77	A0	213/217 (98%)	204 (96%)	9 (4%)	0	100	100
78	A1	274/323 (85%)	262 (96%)	12 (4%)	0	100	100
79	A2	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
80	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
81	A4	584/689 (85%)	567 (97%)	17 (3%)	0	100	100
All	All	14185/18031 (79%)	13836 (98%)	345 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	U	2	ALA
58	AH	126	ILE
72	AV	317	LEU
57	AG	210	VAL

### 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	
2	D	192/245 (78%)	192 (100%)	0	100	100
3	E	260/290 (90%)	260 (100%)	0	100	100
4	F	219/262 (84%)	219 (100%)	0	100	100
5	H	182/228 (80%)	182 (100%)	0	100	100
6	J	138/150 (92%)	138 (100%)	0	100	100
7	K	155/155 (100%)	155 (100%)	0	100	100
8	L	98/124 (79%)	98 (100%)	0	100	100
9	M	246/249 (99%)	246 (100%)	0	100	100
10	N	189/211 (90%)	189 (100%)	0	100	100
11	O	134/150 (89%)	134 (100%)	0	100	100
12	P	126/155 (81%)	126 (100%)	0	100	100
13	Q	220/256 (86%)	220 (100%)	0	100	100
14	R	118/126 (94%)	118 (100%)	0	100	100
15	S	146/180 (81%)	146 (100%)	0	100	100
16	T	146/176 (83%)	146 (100%)	0	100	100
17	U	134/134 (100%)	134 (100%)	0	100	100
18	V	183/191 (96%)	183 (100%)	0	100	100
19	W	94/119 (79%)	94 (100%)	0	100	100
20	X	220/229 (96%)	220 (100%)	0	100	100
21	Y	163/223 (73%)	163 (100%)	0	100	100
22	Z	113/147 (77%)	113 (100%)	0	100	100
23	0	99/164 (60%)	99 (100%)	0	100	100
24	1	53/60 (88%)	53 (100%)	0	100	100
25	2	40/72 (56%)	40 (100%)	0	100	100
26	3	88/166 (53%)	88 (100%)	0	100	100
27	4	37/89 (42%)	37 (100%)	0	100	100
28	z	150/287 (52%)	150 (100%)	0	100	100
29	5	353/368 (96%)	353 (100%)	0	100	100
30	6	313/332 (94%)	313 (100%)	0	100	100
31	7	270/303 (89%)	270 (100%)	0	100	100
32	8	135/190 (71%)	135 (100%)	0	100	100
33	9	104/112 (93%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	a	96/133 (72%)	96 (100%)	0	100	100
35	b	131/185 (71%)	131 (100%)	0	100	100
36	c	251/288 (87%)	251 (100%)	0	100	100
37	d	218/274 (80%)	218 (100%)	0	100	100
38	e	207/236 (88%)	207 (100%)	0	100	100
39	f	139/188 (74%)	139 (100%)	0	100	100
40	g	124/148 (84%)	124 (100%)	0	100	100
41	h	104/148 (70%)	104 (100%)	0	100	100
42	i	86/110 (78%)	86 (100%)	0	100	100
43	j	74/97 (76%)	74 (100%)	0	100	100
44	k	83/89 (93%)	83 (100%)	0	100	100
45	l	76/116 (66%)	76 (100%)	0	100	100
46	m	85/113 (75%)	85 (100%)	0	100	100
47	o	80/87 (92%)	80 (100%)	0	100	100
48	p	135/181 (75%)	135 (100%)	0	100	100
49	q	138/178 (78%)	138 (100%)	0	100	100
50	r	147/169 (87%)	147 (100%)	0	100	100
51	s	340/381 (89%)	340 (100%)	0	100	100
52	AB	198/249 (80%)	198 (100%)	0	100	100
53	AC	115/143 (80%)	115 (100%)	0	100	100
54	AD	286/357 (80%)	286 (100%)	0	100	100
55	AE	104/107 (97%)	104 (100%)	0	100	100
56	AF	185/209 (88%)	185 (100%)	0	100	100
57	AG	284/342 (83%)	284 (100%)	0	100	100
58	AH	130/180 (72%)	130 (100%)	0	100	100
59	AI	104/146 (71%)	104 (100%)	0	100	100
60	AJ	93/118 (79%)	93 (100%)	0	100	100
61	AK	91/113 (80%)	91 (100%)	0	100	100
62	AL	155/226 (69%)	155 (100%)	0	100	100
63	AM	97/113 (86%)	97 (100%)	0	100	100
64	AN	96/115 (84%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	AO	174/230 (76%)	174 (100%)	0	100	100
66	AP	88/123 (72%)	88 (100%)	0	100	100
67	AQ	78/78 (100%)	78 (100%)	0	100	100
68	AR	264/318 (83%)	264 (100%)	0	100	100
69	AS	116/164 (71%)	116 (100%)	0	100	100
70	AT	153/154 (99%)	153 (100%)	0	100	100
71	AU	152/174 (87%)	152 (100%)	0	100	100
72	AV	325/364 (89%)	325 (100%)	0	100	100
73	AW	87/158 (55%)	87 (100%)	0	100	100
74	AX	311/351 (89%)	311 (100%)	0	100	100
75	AY	137/357 (38%)	137 (100%)	0	100	100
76	AZ	90/95 (95%)	90 (100%)	0	100	100
77	A0	188/189 (100%)	188 (100%)	0	100	100
78	A1	254/291 (87%)	254 (100%)	0	100	100
79	A2	100/100 (100%)	100 (100%)	0	100	100
80	A3	65/166 (39%)	65 (100%)	0	100	100
81	A4	526/609 (86%)	526 (100%)	0	100	100
All	All	12678/15603 (81%)	12678 (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 (87) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	235	GLN
3	E	57	ASN
3	E	123	GLN
3	E	125	GLN
4	F	58	HIS
4	F	98	GLN
4	F	257	GLN
5	H	156	GLN
5	H	178	ASN
7	K	61	ASN
7	K	94	GLN
7	K	117	HIS

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Mol	Chain	Res	Type
7	K	147	GLN
8	L	103	ASN
10	N	178	GLN
12	P	142	ASN
13	Q	107	HIS
13	Q	158	GLN
15	S	100	HIS
15	S	118	ASN
15	S	179	ASN
17	U	77	ASN
17	U	82	HIS
18	V	195	GLN
19	W	72	HIS
20	X	89	GLN
20	X	93	ASN
21	Y	99	HIS
23	0	120	HIS
28	z	251	ASN
28	z	270	ASN
29	5	165	GLN
29	5	275	ASN
29	5	343	GLN
29	5	384	GLN
30	6	307	HIS
32	8	143	GLN
32	8	184	ASN
35	b	81	ASN
35	b	123	ASN
36	c	65	ASN
36	c	128	GLN
36	c	155	ASN
37	d	207	ASN
38	e	75	GLN
42	i	59	ASN
43	j	31	GLN
44	k	15	GLN
48	p	194	HIS
49	q	60	GLN
49	q	120	HIS
51	s	191	HIS
51	s	327	ASN
51	s	358	GLN

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Mol	Chain	Res	Type
51	s	387	ASN
52	AB	93	HIS
52	AB	167	HIS
56	AF	214	HIS
57	AG	288	HIS
58	AH	147	HIS
59	AI	146	HIS
60	AJ	105	HIS
60	AJ	136	GLN
62	AL	99	ASN
62	AL	118	ASN
62	AL	162	GLN
65	AO	111	HIS
65	AO	155	GLN
66	AP	95	HIS
67	AQ	41	HIS
68	AR	108	GLN
68	AR	308	HIS
72	AV	141	ASN
72	AV	238	GLN
73	AW	86	HIS
74	AX	81	HIS
74	AX	180	GLN
74	AX	205	GLN
76	AZ	63	GLN
77	A0	137	HIS
77	A0	145	HIS
78	A1	231	HIS
78	A1	279	ASN
81	A4	79	ASN
81	A4	122	ASN
81	A4	444	ASN
81	A4	504	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	71/72 (98%)	12 (16%)	1 (1%)
82	A <sub>y</sub>	3/52 (5%)	0	0
83	AA	953/954 (99%)	218 (22%)	0
84	A	1546/1558 (99%)	333 (21%)	14 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
85	Az	31/32 (96%)	15 (48%)	0
86	Ax	68/70 (97%)	15 (22%)	0
All	All	2672/2738 (97%)	593 (22%)	15 (0%)

All (593) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	8	U
1	B	10	2MG
1	B	16	C
1	B	21	A
1	B	45	G
1	B	48	U
1	B	54	C
1	B	55	U
1	B	56	U
1	B	62	U
1	B	64	A
1	B	69	U
83	AA	651	A
83	AA	674	U
83	AA	678	U
83	AA	680	U
83	AA	688	A
83	AA	696	U
83	AA	700	A
83	AA	704	U
83	AA	705	C
83	AA	712	C
83	AA	721	U
83	AA	723	A
83	AA	724	C
83	AA	730	A
83	AA	738	A
83	AA	753	A
83	AA	761	A
83	AA	766	G
83	AA	771	A
83	AA	773	U
83	AA	775	C
83	AA	777	G
83	AA	784	A

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Mol	Chain	Res	Type
83	AA	790	A
83	AA	791	G
83	AA	793	C
83	AA	794	U
83	AA	795	A
83	AA	796	G
83	AA	801	A
83	AA	802	C
83	AA	807	A
83	AA	808	C
83	AA	825	U
83	AA	828	C
83	AA	830	U
83	AA	832	U
83	AA	839	A
83	AA	843	G
83	AA	847	G
83	AA	860	A
83	AA	861	U
83	AA	866	A
83	AA	867	C
83	AA	868	C
83	AA	870	C
83	AA	871	A
83	AA	878	G
83	AA	883	U
83	AA	887	G
83	AA	890	C
83	AA	896	A
83	AA	899	G
83	AA	903	U
83	AA	904	C
83	AA	905	A
83	AA	907	A
83	AA	908	C
83	AA	913	A
83	AA	914	A
83	AA	918	A
83	AA	919	A
83	AA	923	A
83	AA	927	G
83	AA	931	C

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Mol	Chain	Res	Type
83	AA	934	G
83	AA	938	A
83	AA	939	A
83	AA	940	A
83	AA	941	G
83	AA	942	A
83	AA	954	C
83	AA	956	C
83	AA	957	C
83	AA	960	C
83	AA	962	C
83	AA	963	C
83	AA	967	A
83	AA	979	C
83	AA	993	A
83	AA	994	A
83	AA	1001	C
83	AA	1004	G
83	AA	1005	U
83	AA	1009	C
83	AA	1010	A
83	AA	1015	A
83	AA	1022	A
83	AA	1028	G
83	AA	1038	C
83	AA	1039	A
83	AA	1042	U
83	AA	1050	C
83	AA	1057	G
83	AA	1060	A
83	AA	1066	C
83	AA	1069	A
83	AA	1080	A
83	AA	1081	U
83	AA	1082	A
83	AA	1103	A
83	AA	1105	C
83	AA	1106	C
83	AA	1107	U
83	AA	1109	A
83	AA	1113	G
83	AA	1117	A

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Mol	Chain	Res	Type
83	AA	1118	A
83	AA	1119	U
83	AA	1120	C
83	AA	1121	A
83	AA	1126	A
83	AA	1128	C
83	AA	1135	C
83	AA	1138	G
83	AA	1141	C
83	AA	1146	C
83	AA	1151	C
83	AA	1152	A
83	AA	1153	C
83	AA	1155	G
83	AA	1158	U
83	AA	1160	A
83	AA	1167	A
83	AA	1179	G
83	AA	1185	C
83	AA	1187	U
83	AA	1189	U
83	AA	1193	U
83	AA	1197	G
83	AA	1211	G
83	AA	1213	A
83	AA	1215	U
83	AA	1217	G
83	AA	1220	A
83	AA	1223	C
83	AA	1225	C
83	AA	1229	U
83	AA	1230	C
83	AA	1246	U
83	AA	1247	G
83	AA	1248	C
83	AA	1250	C
83	AA	1251	A
83	AA	1259	U
83	AA	1261	C
83	AA	1270	U
83	AA	1271	C
83	AA	1273	G

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Mol	Chain	Res	Type
83	AA	1283	A
83	AA	1284	U
83	AA	1285	G
83	AA	1290	C
83	AA	1292	A
83	AA	1299	A
83	AA	1300	A
83	AA	1313	A
83	AA	1326	A
83	AA	1327	G
83	AA	1343	A
83	AA	1354	A
83	AA	1356	A
83	AA	1357	A
83	AA	1358	A
83	AA	1359	U
83	AA	1365	A
83	AA	1367	A
83	AA	1376	C
83	AA	1377	C
83	AA	1378	C
83	AA	1385	C
83	AA	1386	U
83	AA	1387	A
83	AA	1390	A
83	AA	1391	U
83	AA	1393	G
83	AA	1405	C
83	AA	1406	U
83	AA	1420	U
83	AA	1422	G
83	AA	1423	A
83	AA	1424	U
83	AA	1430	A
83	AA	1437	U
83	AA	1452	U
83	AA	1454	G
83	AA	1474	G
83	AA	1480	A
83	AA	1482	A
83	AA	1491	C
83	AA	1493	C

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Mol	Chain	Res	Type
83	AA	1513	A
83	AA	1514	A
83	AA	1517	A
83	AA	1520	U
83	AA	1521	U
83	AA	1524	A
83	AA	1525	C
83	AA	1526	U
83	AA	1527	A
83	AA	1532	C
83	AA	1537	C
83	AA	1539	C
83	AA	1547	U
83	AA	1551	G
83	AA	1557	A
83	AA	1558	A
83	AA	1559	G
83	AA	1562	G
83	AA	1564	A
83	AA	1568	U
83	AA	1571	U
83	AA	1582	G
83	AA	1584	MA6
83	AA	1585	A
83	AA	1594	G
83	AA	1595	G
83	AA	1599	A
84	A	1678	C
84	A	1689	C
84	A	1692	A
84	A	1694	U
84	A	1695	C
84	A	1699	C
84	A	1700	U
84	A	1704	U
84	A	1707	C
84	A	1708	A
84	A	1709	G
84	A	1710	A
84	A	1711	C
84	A	1715	C
84	A	1724	A

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Mol	Chain	Res	Type
84	A	1727	A
84	A	1728	U
84	A	1748	G
84	A	1763	A
84	A	1765	C
84	A	1766	U
84	A	1767	G
84	A	1774	U
84	A	1777	A
84	A	1780	U
84	A	1800	G
84	A	1801	A
84	A	1805	A
84	A	1807	U
84	A	1811	A
84	A	1817	C
84	A	1821	A
84	A	1827	C
84	A	1828	A
84	A	1829	A
84	A	1832	A
84	A	1836	A
84	A	1844	A
84	A	1854	U
84	A	1856	A
84	A	1869	A
84	A	1870	A
84	A	1882	A
84	A	1887	A
84	A	1888	G
84	A	1891	A
84	A	1892	A
84	A	1893	A
84	A	1902	C
84	A	1903	C
84	A	1909	A
84	A	1918	G
84	A	1936	A
84	A	1937	A
84	A	1939	G
84	A	1940	A
84	A	1944	C

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Mol	Chain	Res	Type
84	A	1945	A
84	A	1958	G
84	A	1972	A
84	A	1974	A
84	A	1975	U
84	A	1985	G
84	A	1986	A
84	A	1987	G
84	A	1992	C
84	A	1993	A
84	A	1994	A
84	A	1999	A
84	A	2001	C
84	A	2002	G
84	A	2003	A
84	A	2015	G
84	A	2019	G
84	A	2022	G
84	A	2030	U
84	A	2036	C
84	A	2037	U
84	A	2039	A
84	A	2054	U
84	A	2059	C
84	A	2060	A
84	A	2065	A
84	A	2068	C
84	A	2069	U
84	A	2070	C
84	A	2071	U
84	A	2079	C
84	A	2092	C
84	A	2097	A
84	A	2105	G
84	A	2113	G
84	A	2120	G
84	A	2125	C
84	A	2147	G
84	A	2159	U
84	A	2161	A
84	A	2163	A
84	A	2165	C

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Mol	Chain	Res	Type
84	A	2166	C
84	A	2167	A
84	A	2168	U
84	A	2172	A
84	A	2174	G
84	A	2179	A
84	A	2180	A
84	A	2181	A
84	A	2182	G
84	A	2184	A
84	A	2185	G
84	A	2186	C
84	A	2197	G
84	A	2198	A
84	A	2200	A
84	A	2202	C
84	A	2204	U
84	A	2205	U
84	A	2206	C
84	A	2220	A
84	A	2221	C
84	A	2223	A
84	A	2224	C
84	A	2225	C
84	A	2227	A
84	A	2228	A
84	A	2230	A
84	A	2233	U
84	A	2237	A
84	A	2239	A
84	A	2241	A
84	A	2243	A
84	A	2245	A
84	A	2246	A
84	A	2262	C
84	A	2263	C
84	A	2280	C
84	A	2283	C
84	A	2284	C
84	A	2288	A
84	A	2292	G
84	A	2297	A

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Mol	Chain	Res	Type
84	A	2300	G
84	A	2322	C
84	A	2324	U
84	A	2331	C
84	A	2332	C
84	A	2335	A
84	A	2342	U
84	A	2345	G
84	A	2349	G
84	A	2350	A
84	A	2351	U
84	A	2352	U
84	A	2353	A
84	A	2354	A
84	A	2355	A
84	A	2356	A
84	A	2363	A
84	A	2364	C
84	A	2367	A
84	A	2371	U
84	A	2374	A
84	A	2379	C
84	A	2380	C
84	A	2381	A
84	A	2390	A
84	A	2394	A
84	A	2399	A
84	A	2401	A
84	A	2404	U
84	A	2407	U
84	A	2414	C
84	A	2415	C
84	A	2416	U
84	A	2444	A
84	A	2446	A
84	A	2451	A
84	A	2478	G
84	A	2481	A
84	A	2485	U
84	A	2488	C
84	A	2493	C
84	A	2500	A

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Mol	Chain	Res	Type
84	A	2501	C
84	A	2502	C
84	A	2504	A
84	A	2520	C
84	A	2521	A
84	A	2527	A
84	A	2540	C
84	A	2554	A
84	A	2557	C
84	A	2558	A
84	A	2560	G
84	A	2570	C
84	A	2590	A
84	A	2592	G
84	A	2593	G
84	A	2596	G
84	A	2599	U
84	A	2600	A
84	A	2601	A
84	A	2606	U
84	A	2630	U
84	A	2633	A
84	A	2635	G
84	A	2654	U
84	A	2655	G
84	A	2656	U
84	A	2683	C
84	A	2686	G
84	A	2694	A
84	A	2695	G
84	A	2696	A
84	A	2706	A
84	A	2714	A
84	A	2718	C
84	A	2719	G
84	A	2723	A
84	A	2724	G
84	A	2725	A
84	A	2731	U
84	A	2732	G
84	A	2745	A
84	A	2754	A

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Mol	Chain	Res	Type
84	A	2758	G
84	A	2759	U
84	A	2762	C
84	A	2764	A
84	A	2765	A
84	A	2767	A
84	A	2768	A
84	A	2770	C
84	A	2771	C
84	A	2772	C
84	A	2775	A
84	A	2776	G
84	A	2781	U
84	A	2782	A
84	A	2783	A
84	A	2785	C
84	A	2786	U
84	A	2789	C
84	A	2790	A
84	A	2791	A
84	A	2792	A
84	A	2795	U
84	A	2798	A
84	A	2804	A
84	A	2810	G
84	A	2821	C
84	A	2832	A
84	A	2833	A
84	A	2839	C
84	A	2846	G
84	A	2847	C
84	A	2851	A
84	A	2853	A
84	A	2854	U
84	A	2856	C
84	A	2864	U
84	A	2865	C
84	A	2873	A
84	A	2879	A
84	A	2882	U
84	A	2883	A
84	A	2884	C

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Mol	Chain	Res	Type
84	A	2885	U
84	A	2886	A
84	A	2887	U
84	A	2893	A
84	A	2906	C
84	A	2913	A
84	A	2917	G
84	A	2918	A
84	A	2919	A
84	A	2920	C
84	A	2922	A
84	A	2928	C
84	A	2932	G
84	A	2935	A
84	A	2945	A
84	A	2948	C
84	A	2956	A
84	A	2987	U
84	A	2989	G
84	A	2992	G
84	A	2995	G
84	A	3005	A
84	A	3016	G
84	A	3022	G
84	A	3042	U
84	A	3049	U
84	A	3053	A
84	A	3054	G
84	A	3060	C
84	A	3061	G
84	A	3064	A
84	A	3071	U
84	A	3073	C
84	A	3085	A
84	A	3089	A
84	A	3096	U
84	A	3097	U
84	A	3100	U
84	A	3102	U
84	A	3108	U
84	A	3110	C
84	A	3111	A

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Mol	Chain	Res	Type
84	A	3112	A
84	A	3113	A
84	A	3131	G
84	A	3134	C
84	A	3135	A
84	A	3150	U
84	A	3151	A
84	A	3157	C
84	A	3158	A
84	A	3162	C
84	A	3172	C
84	A	3176	A
84	A	3180	A
84	A	3183	U
84	A	3197	U
84	A	3208	C
84	A	3209	A
84	A	3211	C
84	A	3212	C
84	A	3217	A
84	A	3218	A
84	A	3228	U
84	A	3229	U
84	A	3230	G
85	Az	1	U
85	Az	3	A
85	Az	7	G
85	Az	10	G
85	Az	11	U
85	Az	12	U
85	Az	13	U
85	Az	14	A
85	Az	15	U
85	Az	16	A
85	Az	18	A
85	Az	20	A
85	Az	22	A
85	Az	25	U
85	Az	31	A
86	Ax	9	A
86	Ax	10	G
86	Ax	30	G

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Mol	Chain	Res	Type
86	Ax	44	A
86	Ax	45	G
86	Ax	46	A
86	Ax	48	U
86	Ax	53	G
86	Ax	58	A
86	Ax	59	U
86	Ax	61	C
86	Ax	62	C
86	Ax	63	U
86	Ax	66	U
86	Ax	76	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	61	U
84	A	1694	U
84	A	1749	C
84	A	1901	C
84	A	1938	A
84	A	1958	G
84	A	1974	A
84	A	2221	C
84	A	2245	A
84	A	2352	U
84	A	2363	A
84	A	2599	U
84	A	2919	A
84	A	3110	C
84	A	3211	C

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

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
35	THC	b	2	35	8,9,10	1.04	1 (12%)	9,11,13	0.98	0
83	5MU	AA	1076	83	19,22,23	0.57	0	28,32,35	0.49	0
83	B8T	AA	1486	83,88	19,22,23	3.11	8 (42%)	26,31,34	0.80	1 (3%)
84	1MA	A	2617	84	16,25,26	1.04	2 (12%)	18,37,40	1.33	2 (11%)
83	MA6	AA	1583	83	18,26,27	0.78	0	19,38,41	0.72	0
1	1MA	B	9	1	16,25,26	0.93	2 (12%)	18,37,40	1.18	2 (11%)
84	OMG	A	2815	86,84,93	18,26,27	1.44	3 (16%)	19,38,41	0.76	0
84	OMG	A	3040	84	18,26,27	1.16	2 (11%)	19,38,41	0.88	2 (10%)
84	PSU	A	3067	84	18,21,22	1.24	3 (16%)	22,30,33	2.16	6 (27%)
84	OMU	A	3039	84	19,22,23	2.91	8 (42%)	26,31,34	1.90	6 (23%)
59	5F0	AI	184	59	8,8,9	0.58	0	7,9,11	1.29	1 (14%)
1	2MG	B	10	1	18,26,27	1.15	2 (11%)	16,38,41	0.89	1 (6%)
83	MA6	AA	1584	83	18,26,27	0.77	0	19,38,41	0.66	0
83	5MC	AA	1488	83	18,22,23	0.74	0	26,32,35	0.57	0
1	PSU	B	39	1	18,21,22	1.09	1 (5%)	22,30,33	1.78	3 (13%)

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
35	THC	b	2	35	-	0/8/10/12	-
83	5MU	AA	1076	83	-	0/7/25/26	0/2/2/2
83	B8T	AA	1486	83,88	-	2/7/27/28	0/2/2/2
84	1MA	A	2617	84	-	0/3/25/26	0/3/3/3
83	MA6	AA	1583	83	-	0/7/29/30	0/3/3/3
1	1MA	B	9	1	-	0/3/25/26	0/3/3/3
84	OMG	A	2815	86,84,93	-	0/5/27/28	0/3/3/3
84	OMG	A	3040	84	-	0/5/27/28	0/3/3/3
84	PSU	A	3067	84	-	0/7/25/26	0/2/2/2
84	OMU	A	3039	84	-	0/9/27/28	0/2/2/2
59	5F0	AI	184	59	-	1/9/9/10	-
1	2MG	B	10	1	-	0/5/27/28	0/3/3/3
83	MA6	AA	1584	83	-	1/7/29/30	0/3/3/3
83	5MC	AA	1488	83	-	0/7/25/26	0/2/2/2
1	PSU	B	39	1	-	0/7/25/26	0/2/2/2



All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	A	3039	OMU	C2-N1	6.72	1.49	1.38
83	AA	1486	B8T	C4-N3	6.44	1.44	1.32
84	A	3039	OMU	C2-N3	6.36	1.49	1.38
83	AA	1486	B8T	C2-N3	6.02	1.48	1.36
83	AA	1486	B8T	C6-C5	5.77	1.48	1.35
84	A	3039	OMU	C6-C5	5.42	1.47	1.35
83	AA	1486	B8T	C4-N4	4.96	1.46	1.35
84	A	2815	OMG	C8-N7	-4.09	1.28	1.35
84	A	3039	OMU	C4-N3	3.86	1.45	1.38
83	AA	1486	B8T	C2-N1	3.58	1.47	1.40
83	AA	1486	B8T	O2-C2	-3.40	1.17	1.23
84	A	3067	PSU	C6-C5	3.32	1.39	1.35
83	AA	1486	B8T	C6-N1	3.31	1.46	1.38
84	A	3039	OMU	O4-C4	-3.27	1.18	1.24
1	B	39	PSU	C6-C5	3.26	1.39	1.35
83	AA	1486	B8T	C5-C4	3.24	1.47	1.40
1	B	10	2MG	C8-N7	-3.09	1.29	1.35
84	A	2617	1MA	C8-N7	-2.84	1.30	1.35
84	A	3040	OMG	C8-N7	-2.81	1.30	1.35
84	A	2815	OMG	C5-C6	-2.74	1.41	1.47
84	A	3039	OMU	C6-N1	2.71	1.44	1.38
84	A	3039	OMU	O2-C2	-2.59	1.18	1.23
1	B	10	2MG	C5-C6	-2.49	1.42	1.47
84	A	3040	OMG	C5-C6	-2.47	1.42	1.47
1	B	9	1MA	C8-N7	-2.37	1.31	1.35
1	B	9	1MA	C5-C4	-2.35	1.37	1.43
84	A	2617	1MA	C5-C4	-2.31	1.37	1.43
84	A	2815	OMG	C5-C4	-2.23	1.37	1.43
84	A	3067	PSU	O4'-C1'	-2.15	1.40	1.43
84	A	3067	PSU	C4-C5	-2.11	1.38	1.44
35	b	2	THC	CA-N1	-2.07	1.43	1.46
84	A	3039	OMU	C5-C4	2.01	1.48	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	A	3039	OMU	C4-N3-C2	-5.72	119.03	126.58
84	A	3067	PSU	N1-C2-N3	5.69	121.58	115.13
84	A	3067	PSU	C4-N3-C2	-4.80	119.42	126.34
1	B	39	PSU	C4-N3-C2	-4.77	119.47	126.34
1	B	39	PSU	N1-C2-N3	4.55	120.28	115.13
84	A	3039	OMU	N3-C2-N1	4.04	120.25	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	A	3039	OMU	C5-C4-N3	3.75	120.45	114.84
84	A	3067	PSU	C6-C5-C4	3.38	120.56	118.20
84	A	2617	1MA	N1-C6-N6	3.29	128.13	119.77
84	A	3067	PSU	C6-N1-C2	-3.27	119.34	122.68
84	A	3039	OMU	O4-C4-C5	-3.21	119.52	125.16
1	B	9	1MA	N1-C6-N6	2.92	127.21	119.77
59	AI	184	5F0	O-C-CB	-2.80	117.28	125.43
84	A	3067	PSU	O2-C2-N1	-2.70	119.81	122.79
84	A	2617	1MA	C5-C6-N1	-2.67	109.91	113.90
84	A	3039	OMU	O2-C2-N1	-2.48	119.48	122.79
83	AA	1486	B8T	C6-C5-C4	2.46	119.97	116.96
84	A	3039	OMU	C2'-C1'-N1	-2.36	109.64	114.22
84	A	3067	PSU	O4'-C1'-C2'	2.33	108.43	105.14
84	A	3040	OMG	O6-C6-C5	2.32	128.90	124.37
1	B	9	1MA	C5-C6-N1	-2.31	110.44	113.90
1	B	39	PSU	O2-C2-N1	-2.25	120.32	122.79
1	B	10	2MG	O6-C6-C5	2.19	128.65	124.37
84	A	3040	OMG	C5-C6-N1	-2.02	110.39	113.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	AA	1486	B8T	O4'-C4'-C5'-O5'
83	AA	1486	B8T	C3'-C4'-C5'-O5'
83	AA	1584	MA6	C4'-C5'-O5'-P
59	AI	184	5F0	N-CA-CB-C

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	AA	1583	MA6	1	0
84	A	2815	OMG	1	0
84	A	3040	OMG	1	0
84	A	3039	OMU	1	0
59	AI	184	5F0	1	0
83	AA	1584	MA6	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 119 ligands modelled in this entry, 110 are monoatomic - leaving 9 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	$\# Z  > 2$
87	VAL	B	101	-	4,6,7	0.70	0	6,7,9	1.22	1 (16%)
92	T1C	A	3302	88	44,45,45	0.92	3 (6%)	53,72,72	0.77	1 (1%)
90	ATP	AX	501	88	26,33,33	0.87	1 (3%)	31,52,52	1.04	2 (6%)
89	FES	r	201	50	0,4,4	-	-	-		
89	FES	AT	201	63,70	0,4,4	-	-	-		
91	GDP	AX	503	-	24,30,30	0.98	1 (4%)	30,47,47	1.20	3 (10%)
92	T1C	AA	1701	88	44,45,45	0.88	3 (6%)	53,72,72	0.68	1 (1%)
92	T1C	A	3301	88	44,45,45	0.92	3 (6%)	53,72,72	0.77	1 (1%)
89	FES	AP	201	55,66	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	VAL	B	101	-	-	4/5/6/8	-
92	T1C	A	3302	88	-	5/22/80/80	0/4/4/4
90	ATP	AX	501	88	-	1/18/38/38	0/3/3/3
89	FES	r	201	50	-	-	0/1/1/1
89	FES	AT	201	63,70	-	-	0/1/1/1
91	GDP	AX	503	-	-	2/12/32/32	0/3/3/3
92	T1C	AA	1701	88	-	0/22/80/80	0/4/4/4
92	T1C	A	3301	88	-	0/22/80/80	0/4/4/4
89	FES	AP	201	55,66	-	-	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	A	3302	T1C	C2-C3	-3.13	1.32	1.40
92	A	3301	T1C	C2-C3	-3.13	1.32	1.40
92	AA	1701	T1C	C93-N92	2.68	1.53	1.49
91	AX	503	GDP	C6-N1	-2.65	1.33	1.37
92	A	3302	T1C	C93-N92	2.63	1.53	1.49
92	A	3301	T1C	C93-N92	2.56	1.53	1.49
92	AA	1701	T1C	C7-N7	2.38	1.48	1.42
92	A	3301	T1C	C7-N7	2.37	1.48	1.42
92	A	3302	T1C	C7-N7	2.34	1.48	1.42
92	AA	1701	T1C	C2-C3	-2.21	1.34	1.40
90	AX	501	ATP	C8-N7	-2.06	1.31	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	AX	503	GDP	PA-O3A-PB	-3.83	119.69	132.83
92	A	3302	T1C	C92-N92-C93	3.01	119.62	115.84
87	B	101	VAL	O-C-CA	-2.96	117.02	124.78
92	A	3301	T1C	C92-N92-C93	2.87	119.43	115.84
91	AX	503	GDP	C5-C6-N1	2.48	118.33	113.95
91	AX	503	GDP	C8-N7-C5	2.42	107.60	102.99
90	AX	501	ATP	C5-C6-N6	2.31	123.86	120.35
90	AX	501	ATP	O2'-C2'-C1'	-2.12	103.03	110.85
92	AA	1701	T1C	C8-C7-N7	-2.00	118.22	120.91

There are no chirality outliers.

All (12) torsion outliers are listed below:

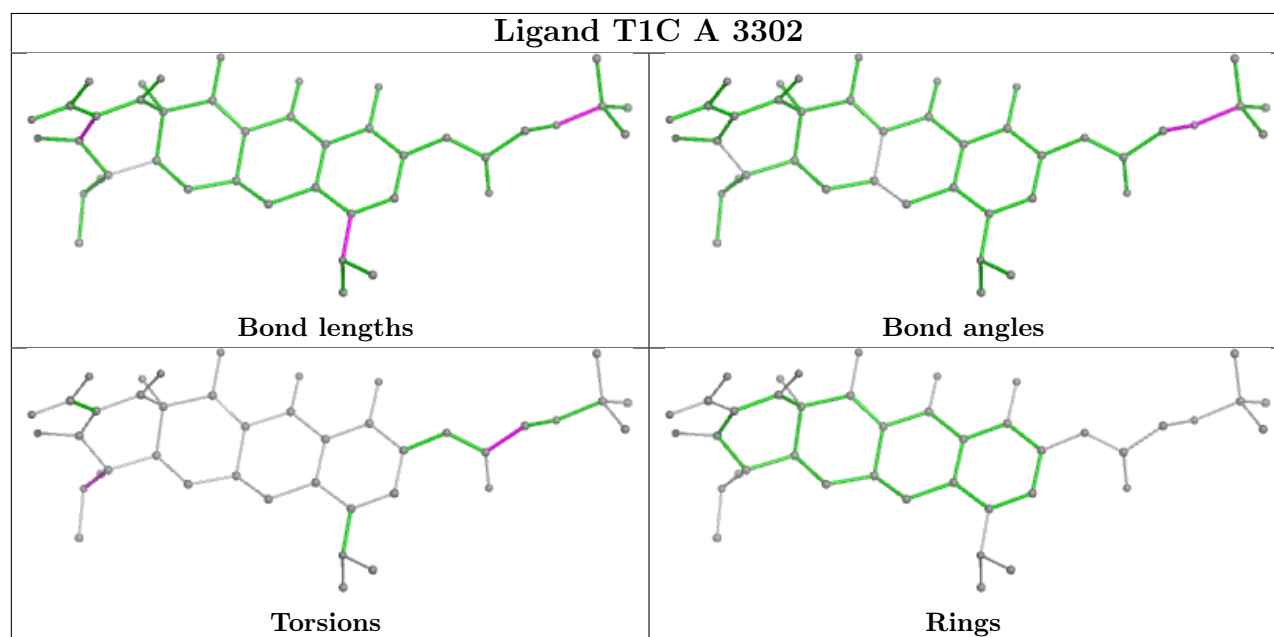
Mol	Chain	Res	Type	Atoms
87	B	101	VAL	N-CA-CB-CG1
87	B	101	VAL	C-CA-CB-CG1
87	B	101	VAL	C-CA-CB-CG2
91	AX	503	GDP	O4'-C4'-C5'-O5'
92	A	3302	T1C	C41-C4-N4-C42
92	A	3302	T1C	C3-C4-N4-C43
92	A	3302	T1C	C3-C4-N4-C42
87	B	101	VAL	N-CA-CB-CG2
90	AX	501	ATP	O4'-C4'-C5'-O5'
92	A	3302	T1C	C41-C4-N4-C43
91	AX	503	GDP	C3'-C4'-C5'-O5'
92	A	3302	T1C	N9-C91-C92-N92

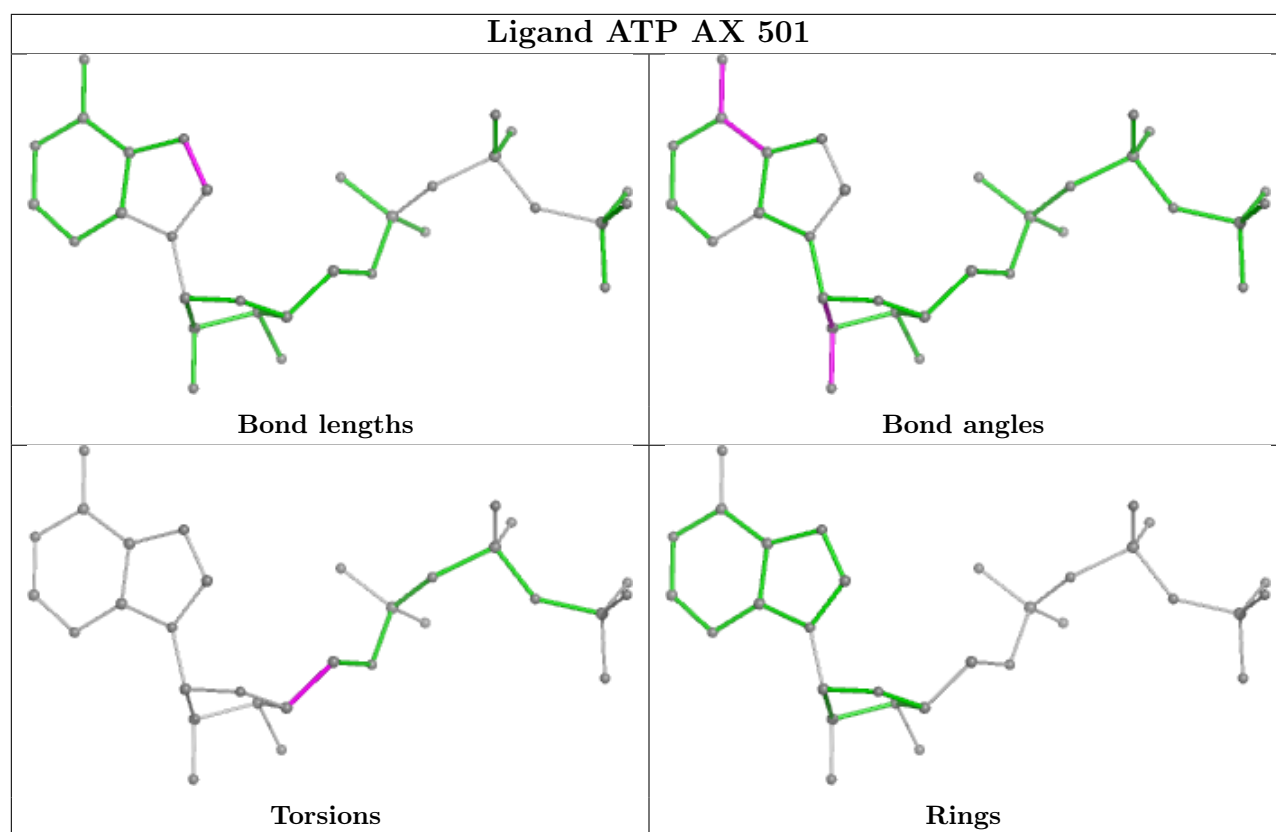
There are no ring outliers.

4 monomers are involved in 24 short contacts:

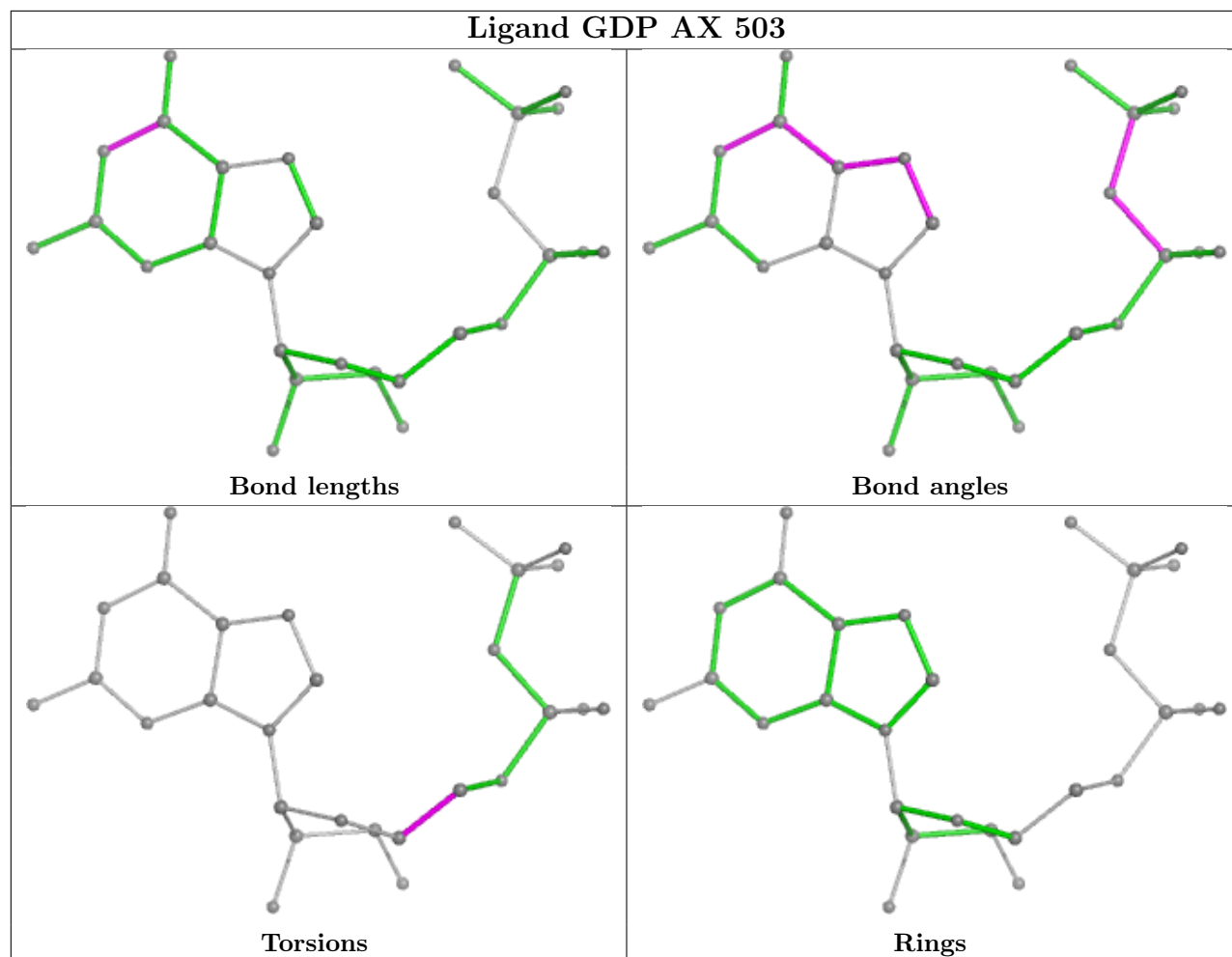
Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	B	101	VAL	20	0
92	A	3302	T1C	1	0
91	AX	503	GDP	2	0
92	A	3301	T1C	1	0

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

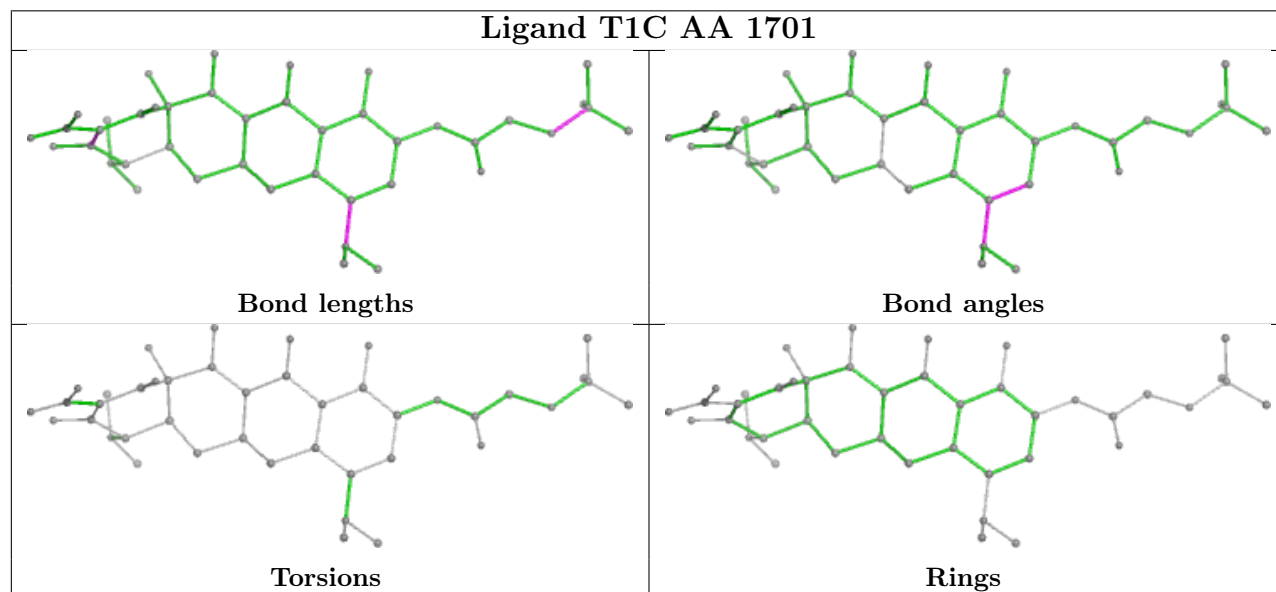


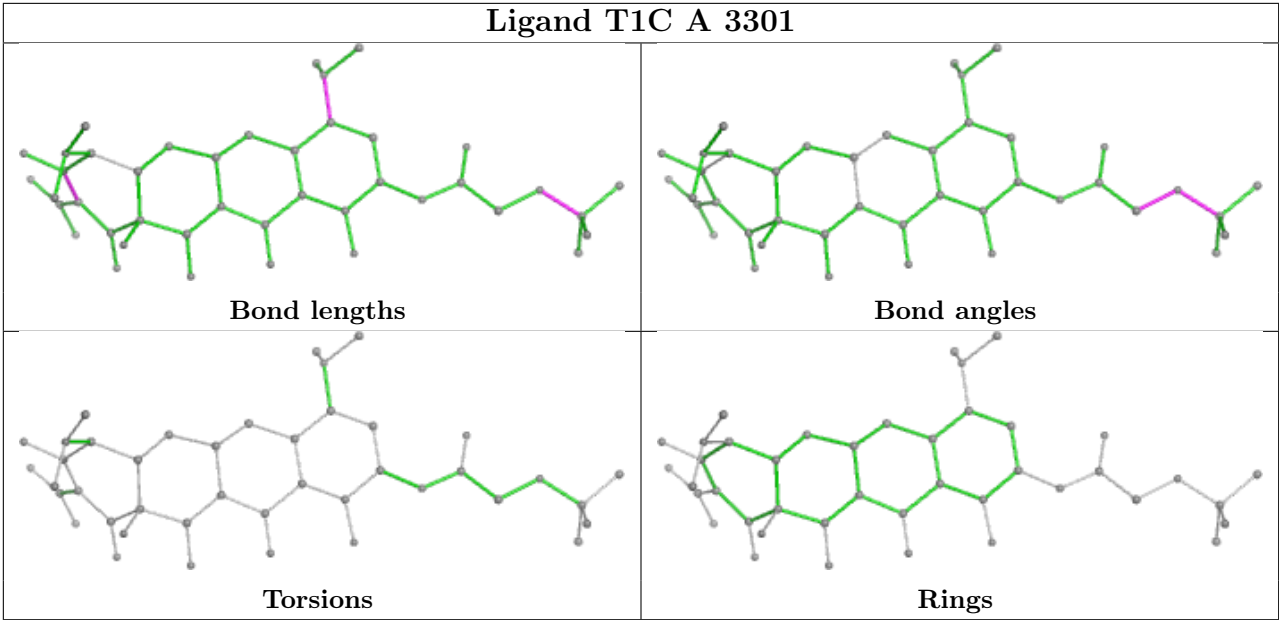


## Ligand GDP AX 503



## Ligand T1C AA 1701





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
86	Ax	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ax	15:A	O3'	21:A	P	10.10



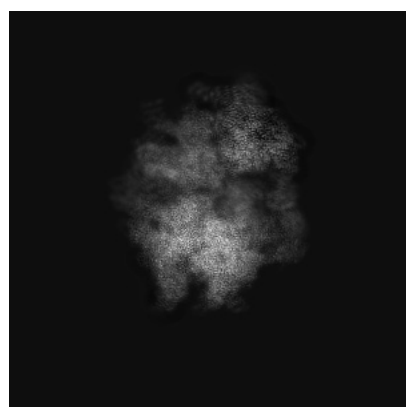
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19460. These allow visual inspection of the internal detail of the map and identification of artifacts.

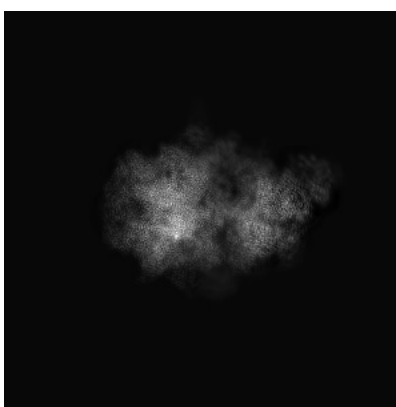
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

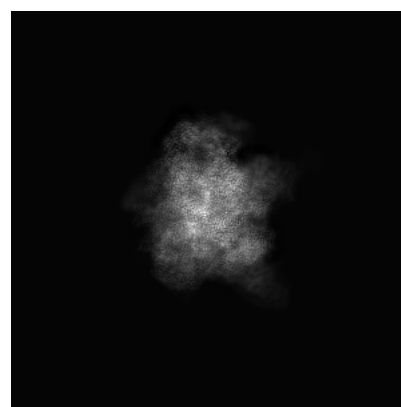
#### 6.1.1 Primary map



X



Y

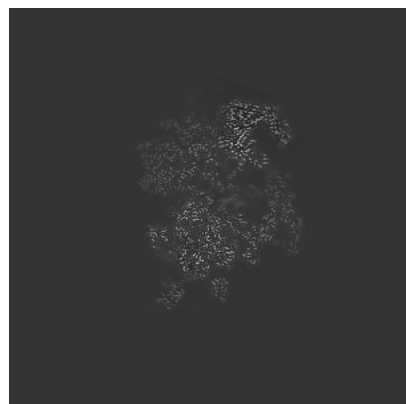


Z

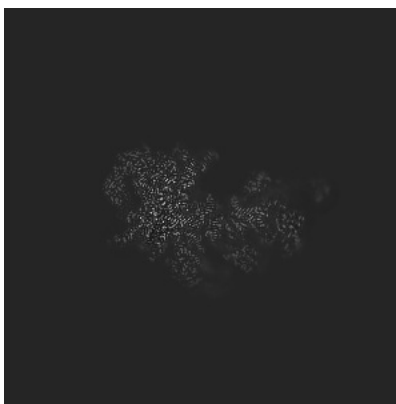
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 256



Y Index: 256

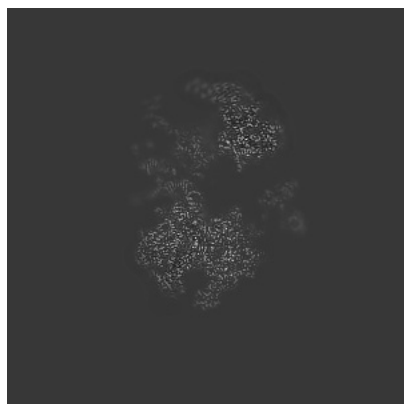


Z Index: 256

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: 276



Y Index: 261

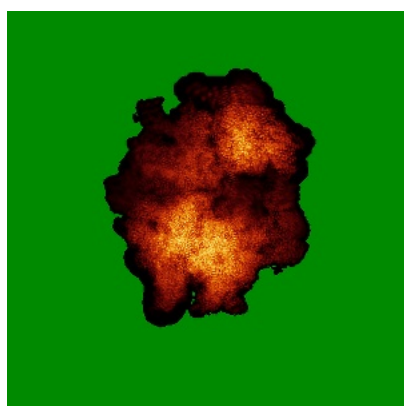


Z Index: 217

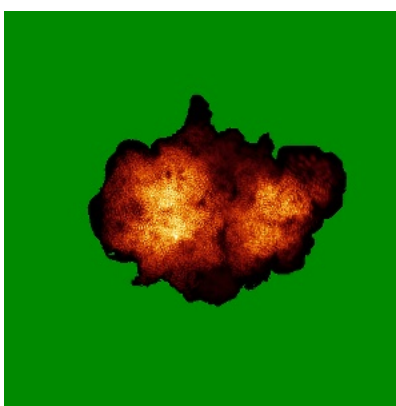
The images above show the largest variance slices of the map in three orthogonal directions.

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

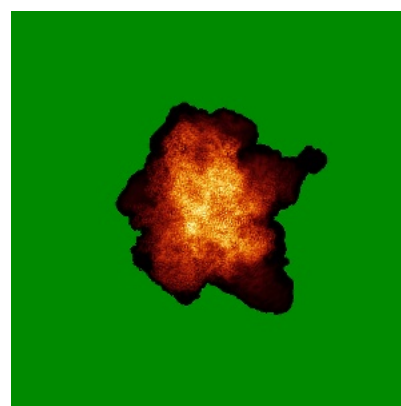
### 6.4.1 Primary map



X



Y

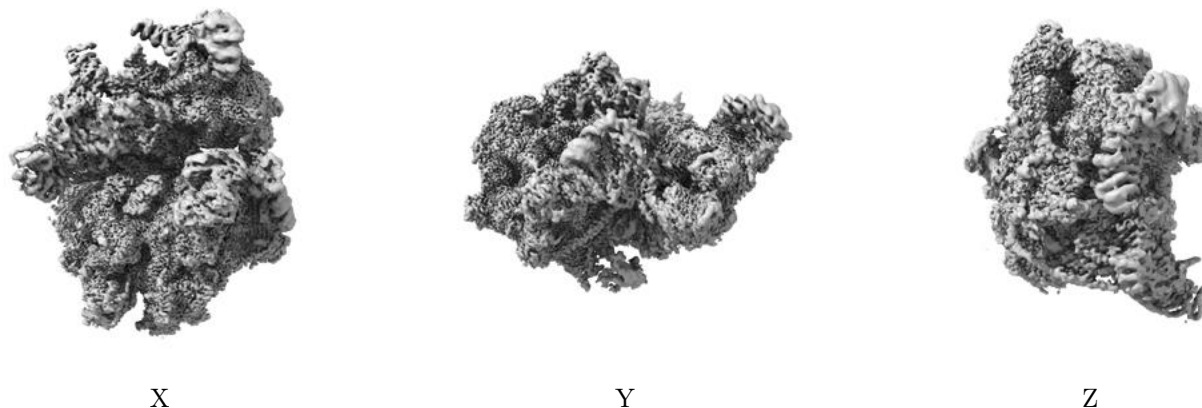


Z

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 1.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

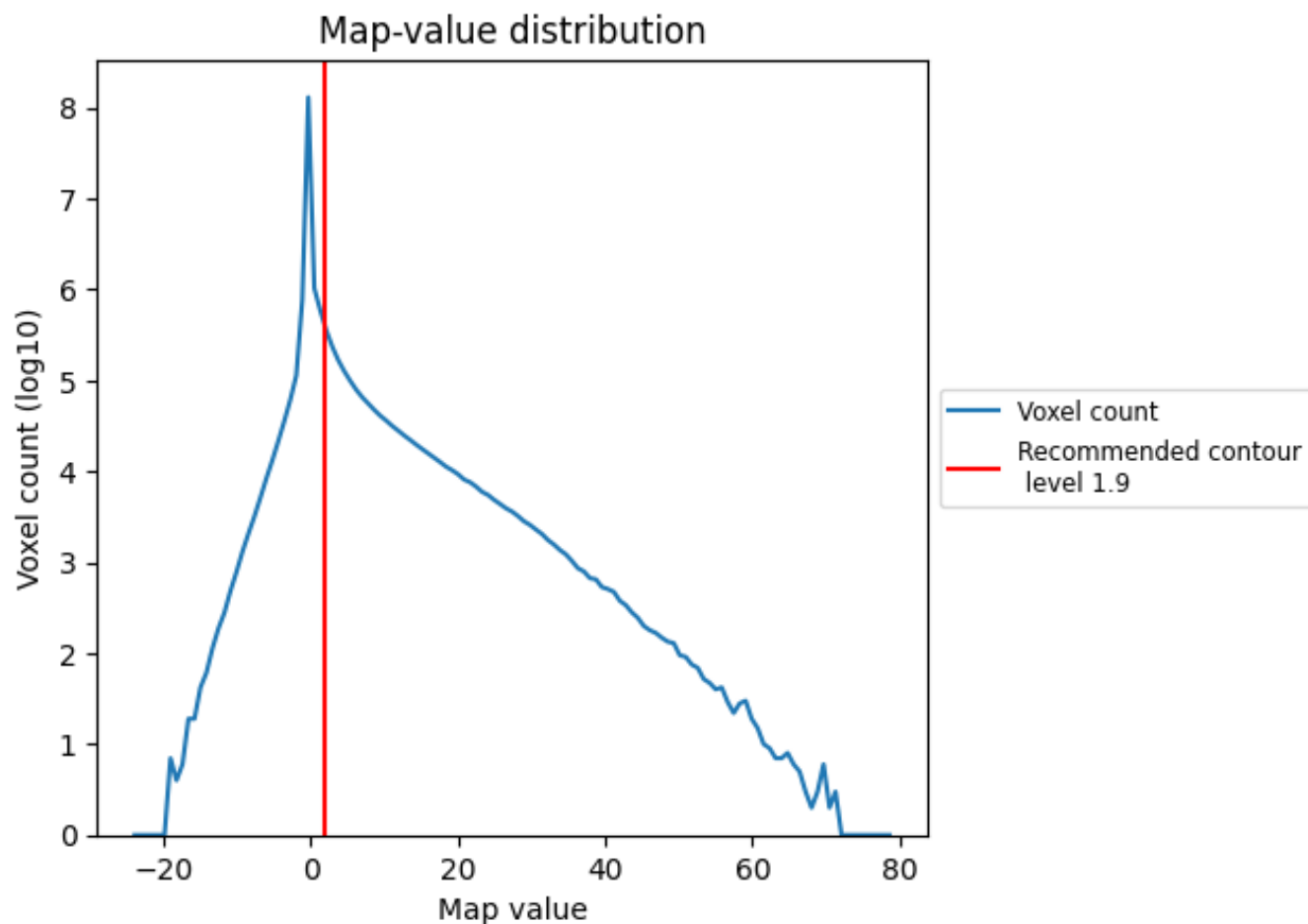
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

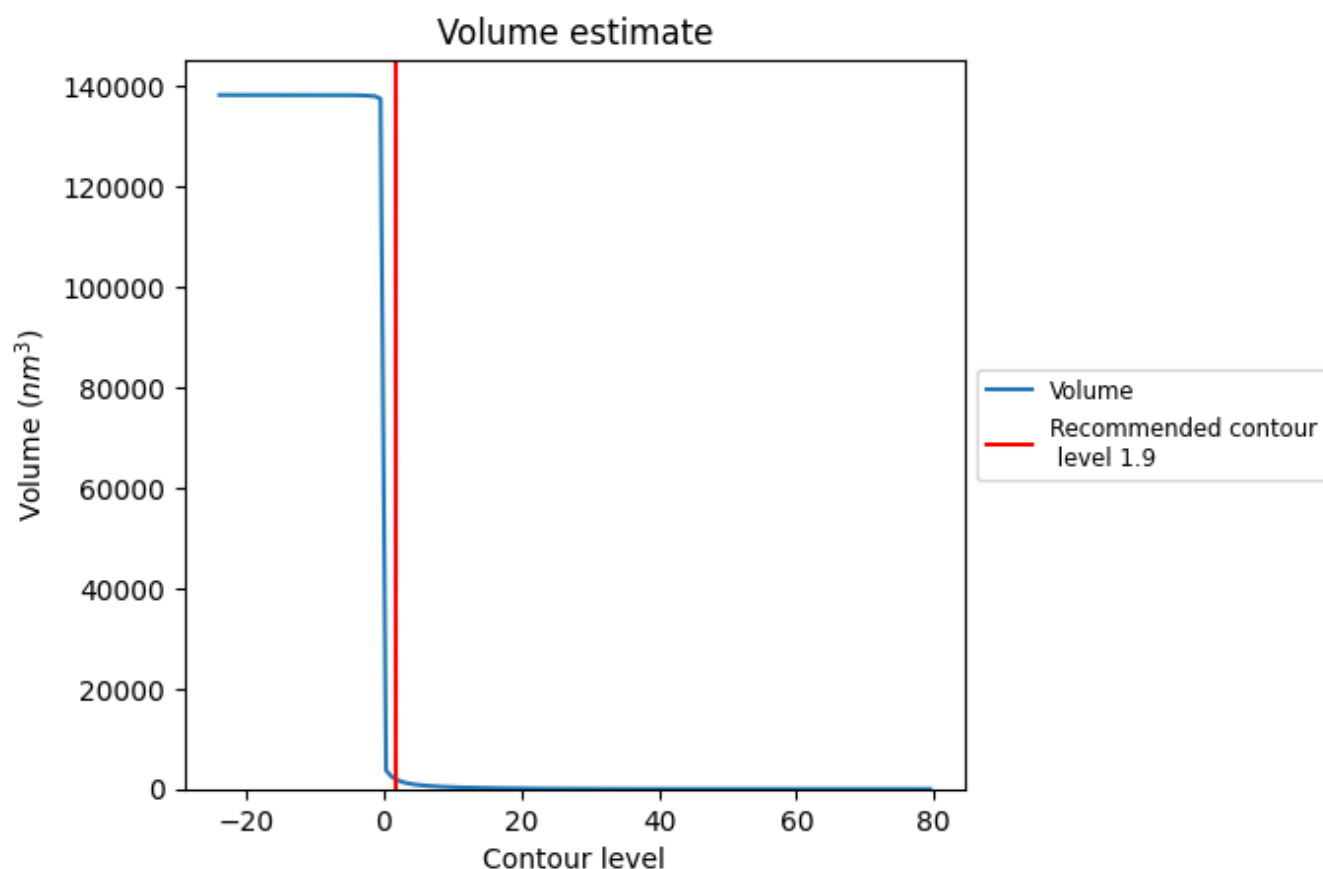
This section contains the results of statistical analysis of the map.

### 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.

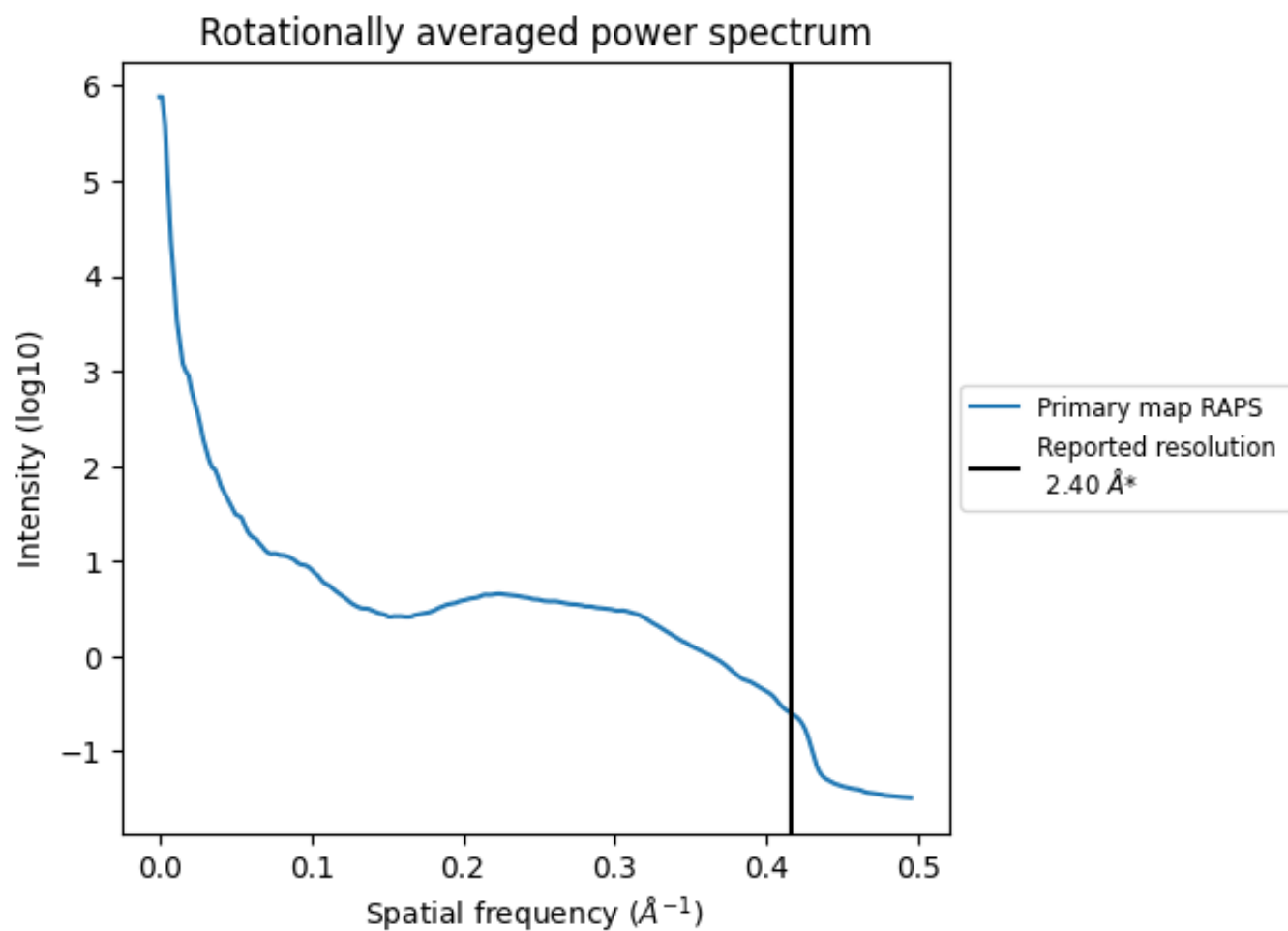
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1834  $\text{nm}^3$ ; this corresponds to an approximate mass of 1657 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 0.417 Å<sup>-1</sup>

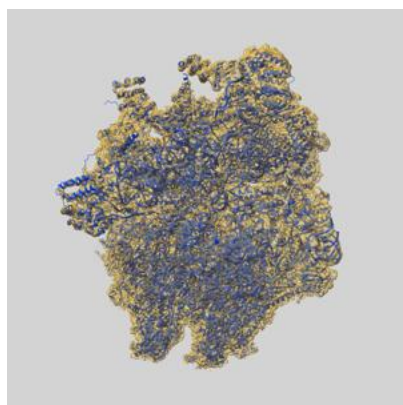
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

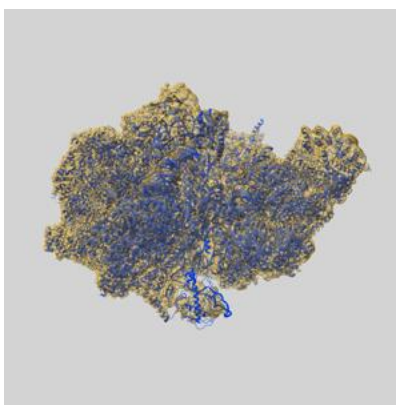
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19460 and PDB model 8RRI. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

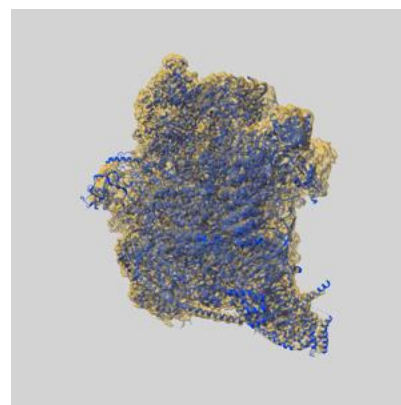
### 9.1 Map-model overlay [i](#)



X



Y

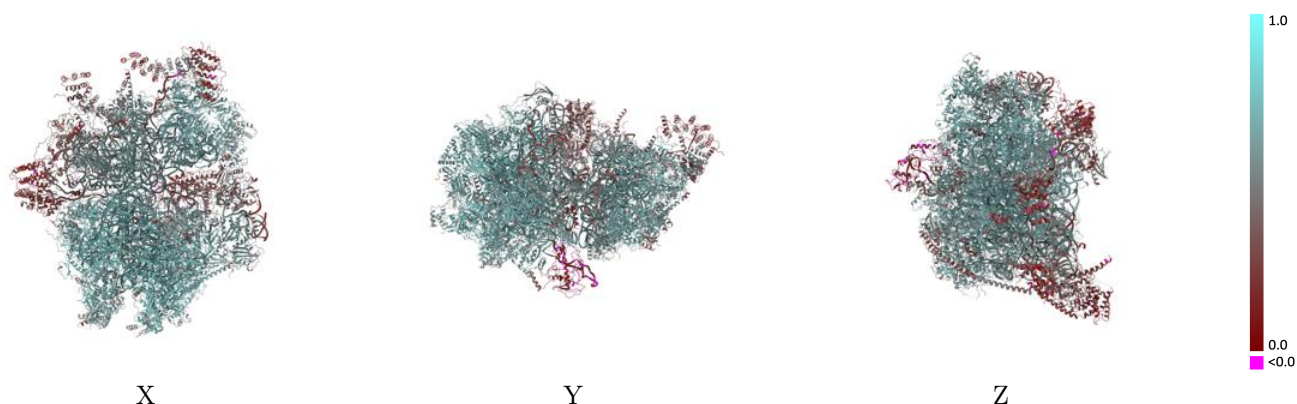


Z

The images above show the 3D surface view of the map at the recommended contour level 1.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

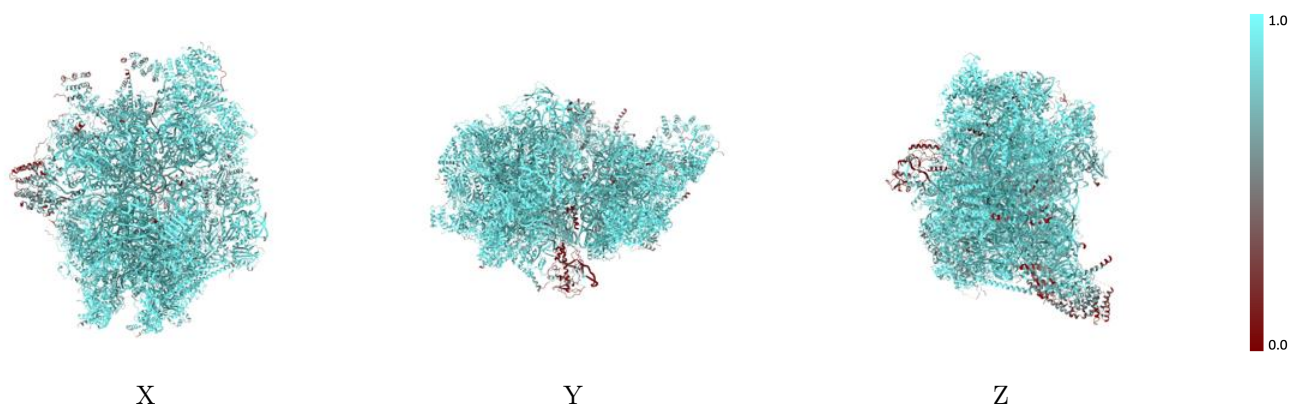


## 9.2 Q-score mapped to coordinate model [i](#)



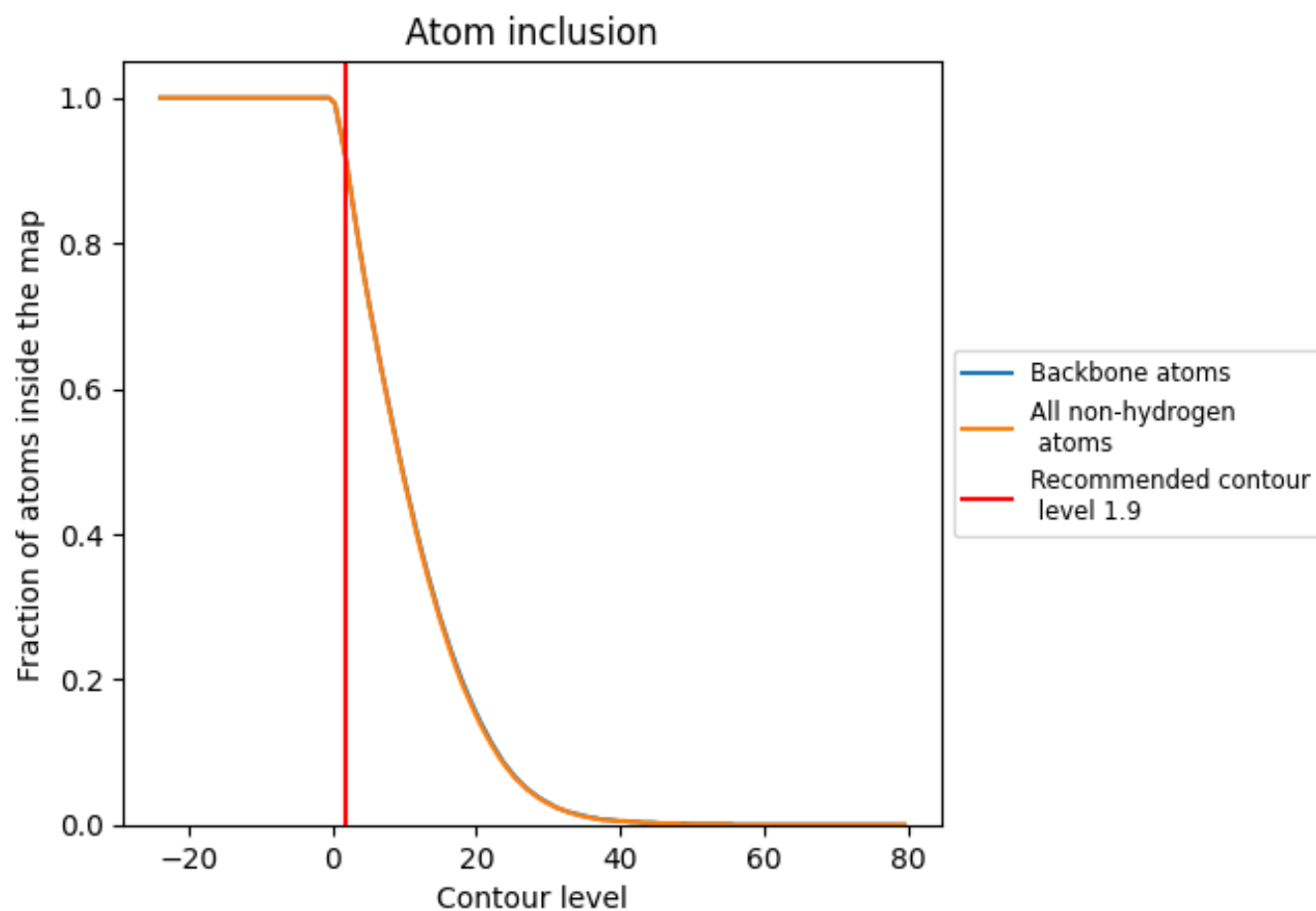
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.9).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 92% 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 (1.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.5820
0	 0.9720	 0.6840
1	 0.9250	 0.6110
2	 0.9890	 0.7470
3	 0.9910	 0.7390
4	 0.9880	 0.6690
5	 0.9650	 0.6340
6	 0.9410	 0.5880
7	 0.9540	 0.6150
8	 0.8120	 0.4130
9	 0.9350	 0.6230
A	 0.9790	 0.6630
A0	 0.7170	 0.3430
A1	 0.9580	 0.5920
A2	 0.9230	 0.5470
A3	 0.9410	 0.5860
A4	 0.8550	 0.3630
AA	 0.9830	 0.6050
AB	 0.9130	 0.5600
AC	 0.9960	 0.6820
AD	 0.9140	 0.5620
AE	 0.9250	 0.5800
AF	 0.9690	 0.6110
AG	 0.9430	 0.5950
AH	 0.9680	 0.6240
AI	 0.9460	 0.5770
AJ	 0.9300	 0.5570
AK	 0.9910	 0.6770
AL	 0.8840	 0.5240
AM	 0.8290	 0.4100
AN	 0.9160	 0.5380
AO	 0.8050	 0.4290
AP	 0.9170	 0.5710
AQ	 0.9720	 0.6000
AR	 0.6930	 0.3510























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Chain	Atom inclusion	Q-score
AS	 0.7970	 0.4530
AT	 0.8750	 0.4910
AU	 0.7940	 0.3920
AV	 0.5410	 0.2340
AW	 0.8720	 0.5240
AX	 0.9830	 0.6200
AY	 0.8550	 0.5110
AZ	 0.9510	 0.6170
Ax	 0.9700	 0.5080
Ay	 0.5830	 0.4360
Az	 0.7820	 0.3050
B	 0.9430	 0.4420
D	 0.9780	 0.6900
E	 0.9770	 0.6980
F	 0.9820	 0.7060
H	 0.5690	 0.3400
J	 0.7420	 0.3080
K	 0.9800	 0.7040
L	 0.9820	 0.6880
M	 0.9780	 0.6940
N	 0.9620	 0.6520
O	 0.9730	 0.6890
P	 0.9730	 0.6490
Q	 0.9010	 0.6310
R	 0.9690	 0.7030
S	 0.9710	 0.6870
T	 0.9850	 0.7100
U	 0.9050	 0.6210
V	 0.9080	 0.5860
W	 0.9880	 0.6990
X	 0.9380	 0.6300
Y	 0.9650	 0.6700
Z	 0.9580	 0.6820
a	 0.9020	 0.6180
b	 0.9750	 0.6900
c	 0.9290	 0.6210
d	 0.9170	 0.5720
e	 0.7890	 0.3670
f	 0.8230	 0.4910
g	 0.9580	 0.6700
h	 0.9230	 0.5870
i	 0.9910	 0.7340

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Chain	Atom inclusion	Q-score
j	 0.9140	 0.6130
k	 0.8690	 0.4520
l	 0.7250	 0.3520
m	 0.7920	 0.4120
o	 0.9880	 0.7100
p	 0.8380	 0.5270
q	 0.7220	 0.4760
r	 0.9620	 0.6280
s	 0.9530	 0.6490
z	 0.2050	 0.0670