



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:10 PM UTC

PDB ID : 6ZM6 / pdb_00006zm6
EMDB ID : EMD-11279
Title : Human mitochondrial ribosome in complex with mRNA, A/A tRNA and P/P tRNA
Authors : Itoh, Y.; Andrell, J.; Amunts, A.
Deposited on : 2020-07-01
Resolution : 2.59 Å (reported)
Based on initial models : 3J9M, 6RW4, 5OOL

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

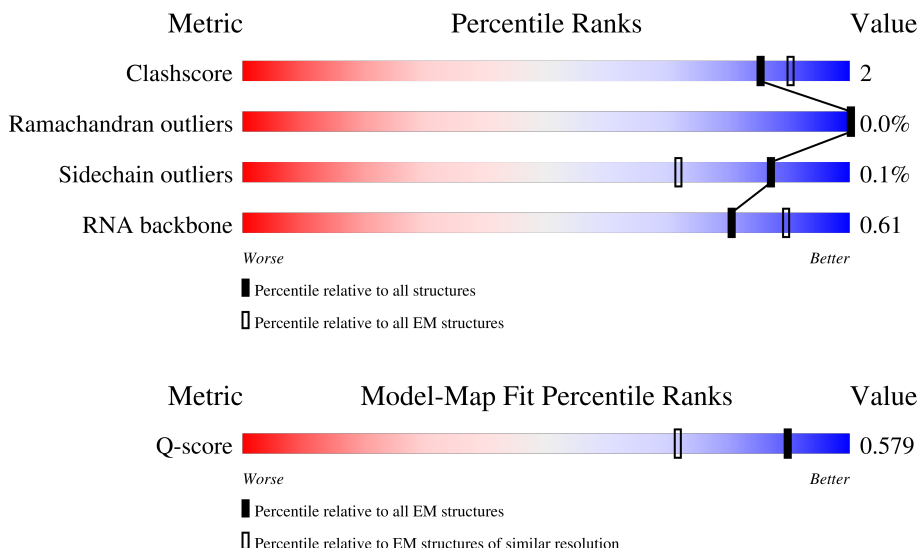
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.59 Å.

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



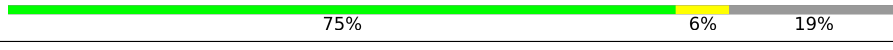
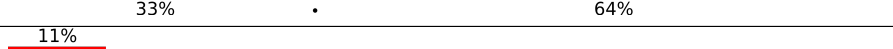
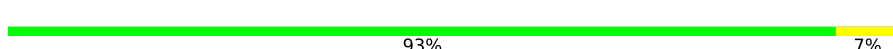
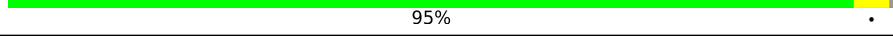
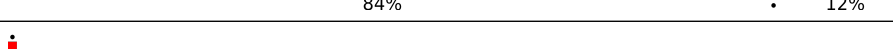
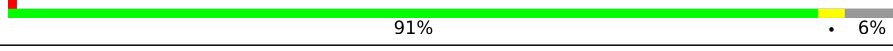
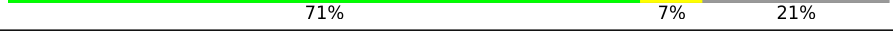
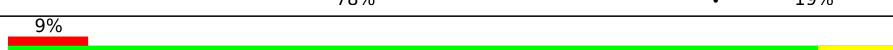
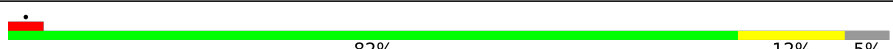
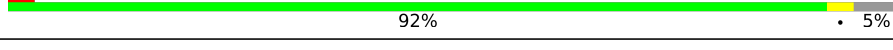
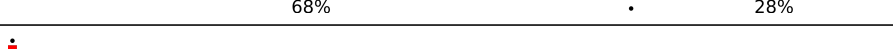
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7741 (2.09 - 3.09)

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

Mol	Chain	Length	Quality of chain
1	A	1561	
2	B	72	
3	D	305	

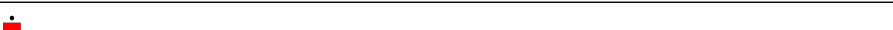
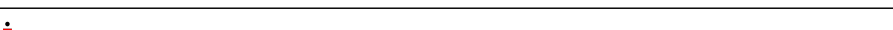
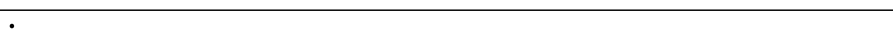
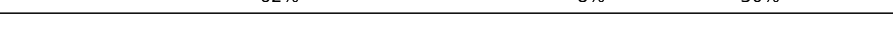
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Mol	Chain	Length	Quality of chain
4	E	348	
5	F	311	
6	H	267	
7	I	261	
8	J	192	
9	K	177	
10	L	145	
11	M	296	
12	N	251	
13	O	175	
14	P	180	
15	Q	292	
16	R	149	
17	S	205	
18	T	206	
19	U	152	
20	V	216	
21	W	148	
22	X	256	
23	Y	250	
24	Z	161	
25	0	188	
26	1	65	
27	2	92	
28	3	188	

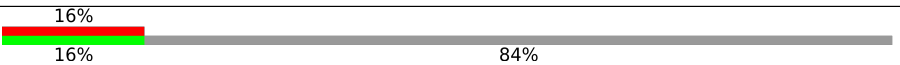
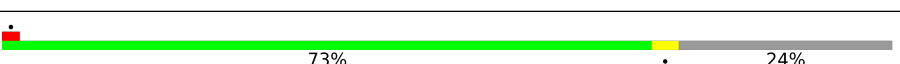
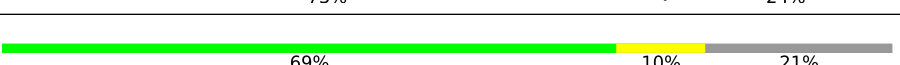
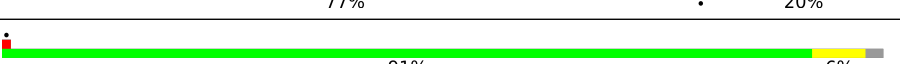
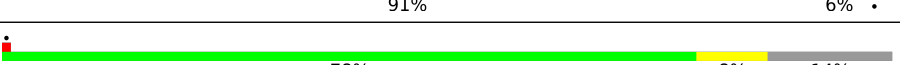
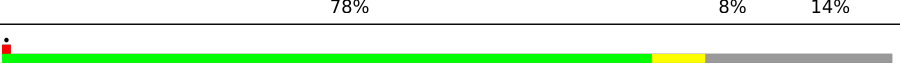
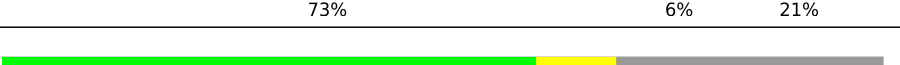
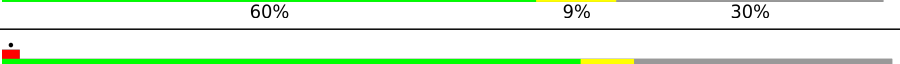
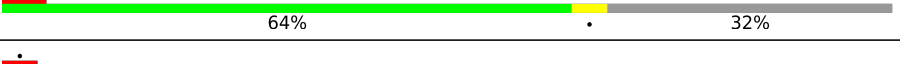
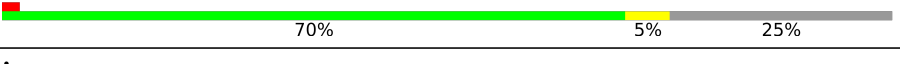
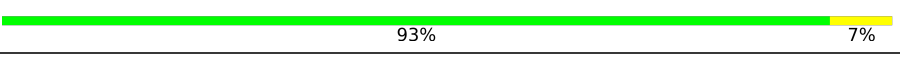
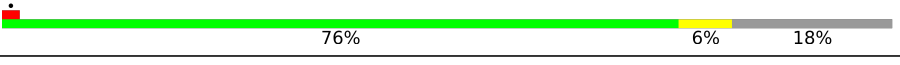
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Mol	Chain	Length	Quality of chain
29	4	103	
30	5	423	
31	6	380	
32	7	338	
33	8	206	
34	9	137	
35	a	142	
36	b	214	
37	c	332	
38	d	306	
39	e	279	
40	f	212	
41	g	166	
42	h	158	
43	i	128	
44	j	123	
45	k	111	
46	l	138	
47	m	128	
48	o	102	
49	p	206	
50	q	222	
51	r	196	
52	s	439	
53	t1	198	

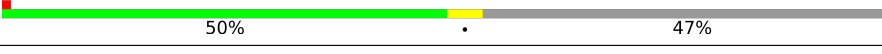
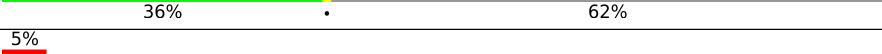
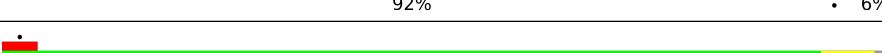
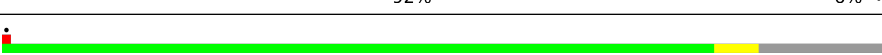
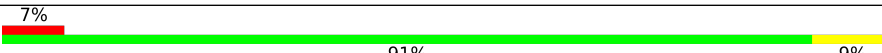
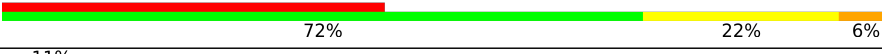
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Mol	Chain	Length	Quality of chain
53	t2	198	
53	t3	198	
53	t4	198	
53	t5	198	
53	t6	198	
54	AA	954	
55	AB	296	
56	AC	167	
57	AD	430	
58	AE	125	
59	AF	242	
60	AG	396	
61	AH	201	
62	AI	194	
63	AJ	138	
64	AK	128	
65	AL	257	
66	AM	137	
67	AN	130	
68	AO	258	
69	AP	142	
70	AQ	86	
71	AR	360	
72	AS	190	
73	AT	173	

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Mol	Chain	Length	Quality of chain
74	AU	205	
75	AV	414	
76	AW	187	
77	AX	398	
78	AY	395	
79	AZ	106	
80	A0	218	
81	A1	323	
82	A2	117	
83	A3	199	
84	A4	689	
85	w	68	
86	x	70	
87	y	19	

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
91	FES	r	201	-	-	X	-

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 326225 atoms, of which 149469 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 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1531	Total	C	H	N	O	P	0	0
			48997	14583	16499	5859	10525	1531		

- Molecule 2 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	72	Total	C	H	N	O	P	0	0
			2298	683	776	269	498	72		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1671	C	G	conflict	GB 1858624630
B	1673	A	U	conflict	GB 1858624630

- Molecule 3 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	238	Total	C	H	N	O	S	0	0
			3780	1157	1921	376	317	9		

- Molecule 4 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	305	Total	C	H	N	O	S	0	0
			4823	1545	2417	418	432	11		

- Molecule 5 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	252	Total	C	H	N	O	S	0	0
			4097	1305	2066	370	350	6		

- Molecule 6 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	97	Total	C	H	N	O	0	0
			1649	508	847	155	139		

- Molecule 7 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	212	Total	C	H	N	O	S	0	0
			3481	1088	1786	304	292	11		

- Molecule 8 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	175	Total	C	H	N	O	S	0	0
			2739	847	1409	237	244	2		

- Molecule 9 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
9	K	177	Total	C	H	N	O	S	0	0
			2909	936	1454	259	253	7		

- Molecule 10 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 11 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	291	Total	C	H	N	O	S	0	0
			4723	1483	2396	430	408	6		

- Molecule 12 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	N	222	Total	C	H	N	O	S	0	0
			3605	1143	1819	326	307	10		

- Molecule 13 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	P	144	Total	C	H	N	O	S	0	0
			2339	733	1166	224	211	5		

- Molecule 15 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Q	238	Total	C	H	N	O	S	0	0
			4002	1268	2023	352	350	9		

- Molecule 16 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	140	Total	C	H	N	O	S	0	0
			2369	732	1215	231	187	4		

- Molecule 17 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	S	161	Total	C	H	N	O	S	0	0
			2659	835	1366	227	227	4		

- Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	166	Total	C	H	N	O	S	0	0
			2780	875	1411	254	233	7		

- Molecule 19 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	U	152	Total	C	H	N	O	S	0	0
			2483	788	1232	234	226	3		

- Molecule 20 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	V	205	Total	C	H	N	O	S	0	0
			3364	1068	1688	298	302	8		

- Molecule 21 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	W	116	Total	C	H	N	O	S	0	0
			1841	577	937	171	153	3		

- Molecule 22 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	X	244	Total	C	H	N	O	S	0	0
			4105	1322	2061	352	365	5		

- Molecule 23 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Y	181	Total	C	H	N	O	S	0	0
			3154	995	1598	298	259	4		

- Molecule 24 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	0	110	Total	C	H	N	O	S	0	0
			1815	554	917	176	162	6		

- Molecule 26 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1	55	Total	C	H	N	O	S	0	0
			954	290	499	87	76	2		

- Molecule 27 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	2	46	Total	C	H	N	O	S	0	0
			784	233	407	83	60	1		

- Molecule 28 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	3	95	Total	C	H	N	O	S	0	0
			1716	539	884	162	128	3		

- Molecule 29 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4	38	Total	C	H	N	O	S	0	0
			704	217	362	72	49	4		

- Molecule 30 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	5	394	Total	C	H	N	O	S	0	0
			6418	2073	3208	560	566	11		

- Molecule 31 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	6	354	Total	C	H	N	O	S	0	0
			5792	1881	2844	525	533	9		

- Molecule 32 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	7	294	Total	C	H	N	O	S	0	0
			4789	1529	2399	405	438	18		

- Molecule 33 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	8	157	Total	C	H	N	O	S	0	0
			2696	844	1369	235	246	2		

- Molecule 34 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	9	124	Total	C	H	N	O	S	0	0
			1985	644	988	170	181	2		

- Molecule 35 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	a	100	Total	C	H	N	O	S	0	0
			1652	529	812	152	154	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
36	b	150	Total	C	H	N	O	S	0	0
			2392	744	1196	231	218	3		

- Molecule 37 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	c	286	Total	C	H	N	O	S	0	0
			4621	1470	2322	397	423	9		

- Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	d	259	Total	C	H	N	O	S	0	0
			4253	1357	2129	369	384	14		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
39	e	228	Total	C	H	N	O	S	0	0
			3699	1174	1851	326	342	6		

- Molecule 40 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	f	157	Total	C	H	N	O	S	0	0
			2523	799	1271	207	242	4		

- Molecule 41 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	h	110	Total	C	H	N	O	S	0	0
			1777	568	882	156	168	3		

- Molecule 43 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	i	97	Total	C	H	N	O	S	0	0
			1687	532	859	165	127	4		

- Molecule 44 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	j	94	Total	C	H	N	O	S	0	0
			1492	463	747	144	136	2		

- Molecule 45 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	k	101	Total	C	H	N	O	S	0	0
			1558	479	784	148	142	5		

- Molecule 46 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	l	82	Total	C	H	N	O	S	0	0
			1363	437	675	120	128	3		

- Molecule 47 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	m	87	Total	C	H	N	O	S	0	0
			1515	466	761	152	134	2		

- Molecule 48 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	o	94	Total	C	H	N	O	S	0	0
			1605	501	807	165	129	3		

- Molecule 49 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	p	147	Total	C	H	N	O	S	0	0
			2431	748	1226	228	225	4		

- Molecule 50 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	q	161	Total	C	H	N	O	S	0	0
			2678	841	1328	260	244	5		

- Molecule 51 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	r	162	Total	C	H	N	O	S	0	0
			2671	839	1349	252	223	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
52	s	386	Total	C	H	N	O	S	0	0
			6298	2023	3143	559	559	14		

- Molecule 53 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t1	46	Total	C	H	N	O	0	0
			732	228	378	56	70		
53	t2	32	Total	C	H	N	O	0	0
			541	168	284	40	49		
53	t3	32	Total	C	H	N	O	0	0
			541	168	284	40	49		
53	t4	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
53	t5	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
53	t6	31	Total	C	H	N	O	0	0
			520	159	275	39	47		

- Molecule 54 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	AA	954	Total	C	H	N	O	P	0	0
			30542	9081	10289	3647	6571	954		

- Molecule 55 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	AB	225	Total	C	H	N	O	S	0	0
			3644	1164	1816	331	323	10		

- Molecule 56 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	AC	132	Total	C	H	N	O	S	0	0
			2172	699	1089	195	185	4		

- Molecule 57 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	AD	343	Total	C	H	N	O	S	0	0
			5536	1713	2805	518	487	13		

- Molecule 58 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	AE	122	Total	C	H	N	O	S	0	0
			1973	614	1001	177	177	4		

- Molecule 59 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	AF	208	Total	C	H	N	O	S	0	0
			3495	1104	1770	312	298	11		

- Molecule 60 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	AG	312	Total	C	H	N	O	S	0	0
			5126	1632	2558	455	467	14		

- Molecule 61 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	AH	140	Total	C	H	N	O	S	0	0
			2336	745	1184	194	210	3		

- Molecule 62 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	AI	137	Total	C	H	N	O	S	0	0
			2076	641	1058	192	181	4		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 63 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	AJ	108	Total	C	H	N	O	S	0	0
			1727	521	888	169	143	6		

- Molecule 64 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	AK	101	Total	C	H	N	O	S	0	0
			1748	537	886	179	141	5		

- Molecule 65 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	AL	174	Total	C	H	N	O	S	0	0
			2994	925	1541	270	251	7		

- Molecule 66 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	AM	119	Total	C	H	N	O	S	0	0
			1908	594	966	185	157	6		

- Molecule 67 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	AN	110	Total	C	H	N	O	S	0	0
			1797	562	929	156	147	3		

- Molecule 68 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 69 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 70 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	AQ	86	Total	C	H	N	O	S	0	0
			1502	460	758	150	126	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	50	ARG	CYS	conflict	UNP P82921

- Molecule 71 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	AR	295	Total	C	H	N	O	S	0	0
			4838	1533	2429	413	455	8		

- Molecule 72 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	AS	135	Total	C	H	N	O	S	0	0
			2227	716	1116	198	196	1		

- Molecule 73 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	AT	168	Total	C	H	N	O	S	0	0
			2765	877	1394	239	244	11		

- Molecule 74 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	AU	176	Total	C	H	N	O	S	0	0
			2988	916	1500	301	267	4		

- Molecule 75 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	AV	362	Total	C	H	N	O	S	0	0
			5933	1904	2964	495	558	12		

- Molecule 76 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	AW	100	Total	C	H	N	O	S	0	0
			1592	498	803	141	146	4		

- Molecule 77 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	AX	352	Total	C	H	N	O	S	0	0
			5694	1822	2845	499	517	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
78	AY	149	Total	C	H	N	O	S	0	0
			2444	801	1198	207	234	4		

- Molecule 79 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	AZ	100	Total	C	H	N	O	S	0	0
			1699	534	860	153	148	4		

- Molecule 80 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	A0	215	Total	C	H	N	O	S	0	0
			3584	1130	1797	339	313	5		

- Molecule 81 is a protein called 28S ribosomal protein S35, mitochondrial.

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

- Molecule 82 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	A2	117	Total	C	H	N	O	S	0	0
			1904	579	969	182	166	8		

- Molecule 83 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	A3	70	Total	C	H	N	O	S	0	0
			1325	401	700	134	89	1		

- Molecule 84 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	A4	588	Total	C	H	N	O	S	0	0
			9536	3053	4768	808	879	28		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
85	w	68	Total	C	H	N	O	P	0	0
			2163	647	725	251	472	68		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
86	x	70	Total	C	H	N	O	P	0	0
			2234	665	751	261	487	70		

- Molecule 87 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	y	19	Total	C	H	N	O	P	0	0
			598	179	199	63	138	19		

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

Mol	Chain	Residues	Atoms		AltConf
88	A	127	Total	Mg	0
			127	127	
88	D	3	Total	Mg	0
			3	3	
88	E	1	Total	Mg	0
			1	1	
88	g	1	Total	Mg	0
			1	1	
88	o	1	Total	Mg	0
			1	1	
88	AA	53	Total	Mg	0
			53	53	
88	AB	1	Total	Mg	0
			1	1	
88	AX	1	Total	Mg	0
			1	1	
88	A3	1	Total	Mg	0
			1	1	

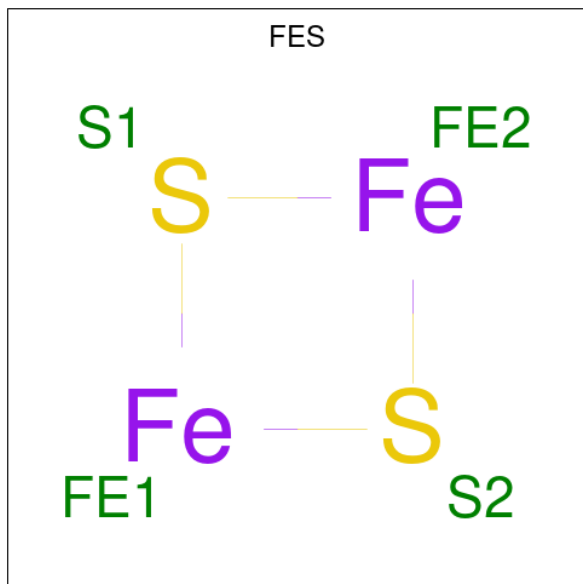
- Molecule 89 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
89	A	31	Total	K	0
			31	31	
89	M	1	Total	K	0
			1	1	
89	P	1	Total	K	0
			1	1	
89	i	1	Total	K	0
			1	1	
89	o	1	Total	K	0
			1	1	
89	AA	9	Total	K	0
			9	9	

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

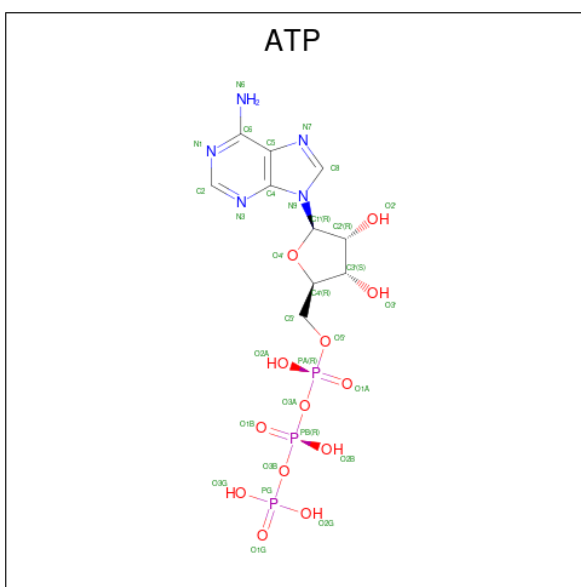
Mol	Chain	Residues	Atoms		AltConf
90	0	1	Total 1	Zn 1	0
90	4	1	Total 1	Zn 1	0
90	AO	1	Total 1	Zn 1	0

- Molecule 91 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



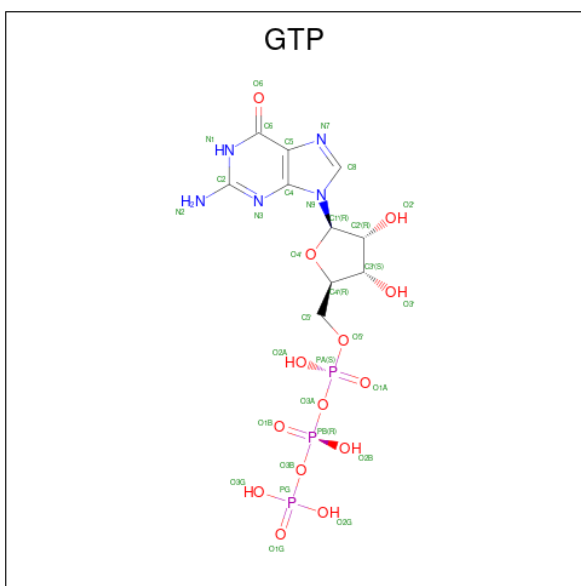
Mol	Chain	Residues	Atoms			AltConf
91	r	1	Total 4	Fe 2	S 2	0
91	AP	1	Total 4	Fe 2	S 2	0
91	AT	1	Total 4	Fe 2	S 2	0

- Molecule 92 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	
92	AX	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 93 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf	
93	AX	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

- Molecule 94 is water.

Mol	Chain	Residues	Atoms		AltConf
94	A	349	Total 349	O 349	0
94	B	1	Total 1	O 1	0
94	D	3	Total 3	O 3	0
94	E	3	Total 3	O 3	0
94	F	4	Total 4	O 4	0
94	K	3	Total 3	O 3	0
94	L	1	Total 1	O 1	0
94	M	5	Total 5	O 5	0
94	N	1	Total 1	O 1	0
94	O	3	Total 3	O 3	0
94	R	1	Total 1	O 1	0
94	S	1	Total 1	O 1	0
94	U	1	Total 1	O 1	0
94	W	1	Total 1	O 1	0
94	6	1	Total 1	O 1	0
94	c	1	Total 1	O 1	0
94	d	1	Total 1	O 1	0
94	f	1	Total 1	O 1	0
94	i	1	Total 1	O 1	0
94	o	2	Total 2	O 2	0
94	r	2	Total 2	O 2	0
94	s	2	Total 2	O 2	0

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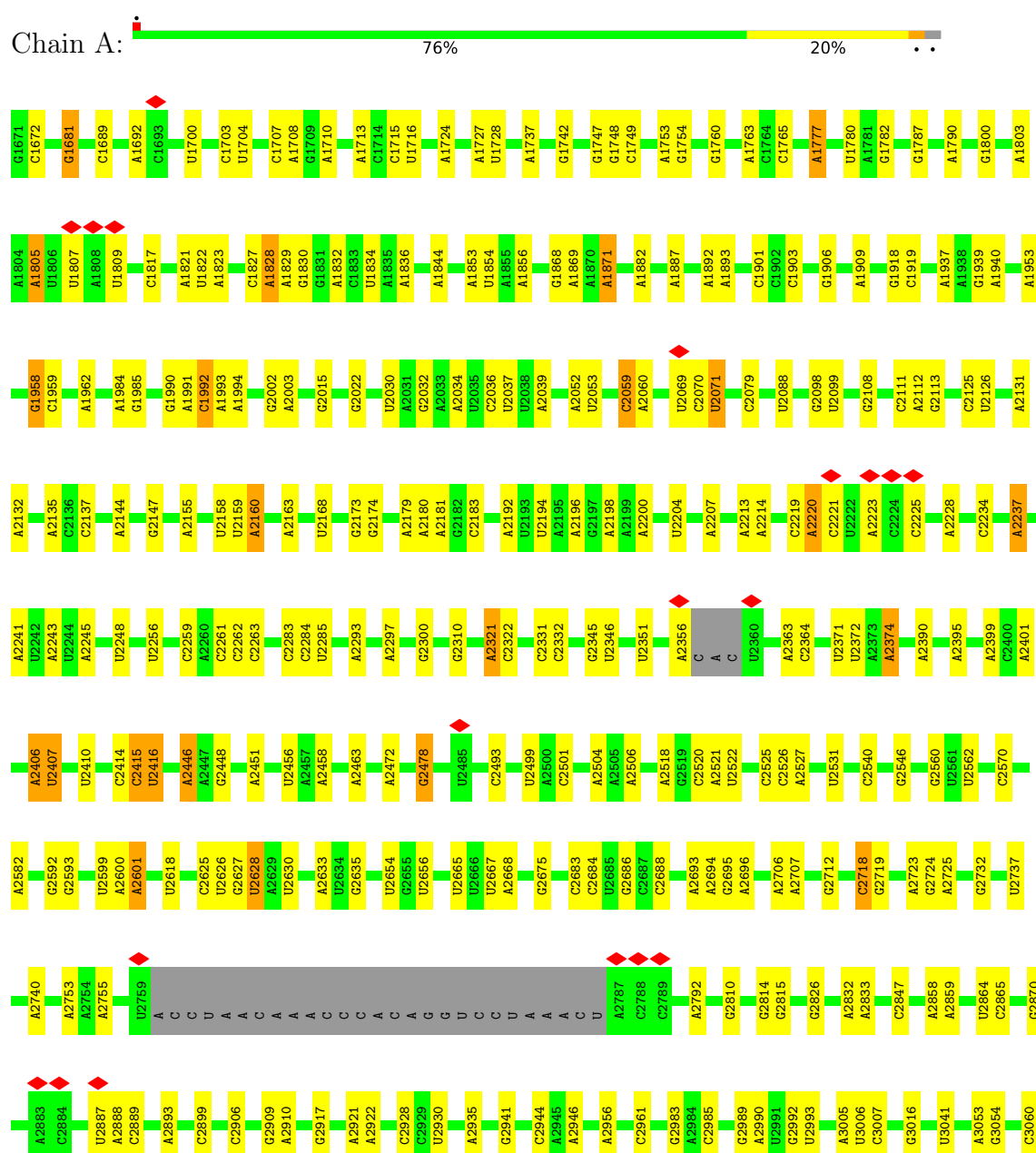
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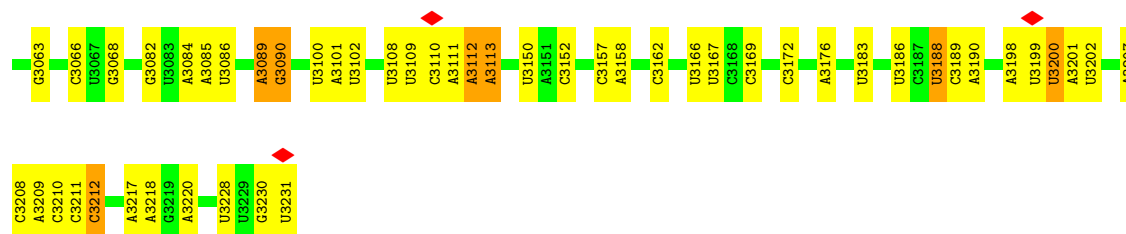
Mol	Chain	Residues	Atoms		AltConf
94	AA	70	Total 70	O 70	0
94	AC	1	Total 1	O 1	0
94	AG	1	Total 1	O 1	0
94	AH	2	Total 2	O 2	0
94	AK	2	Total 2	O 2	0
94	AX	2	Total 2	O 2	0
94	A0	1	Total 1	O 1	0
94	A3	3	Total 3	O 3	0

3 Residue-property plots

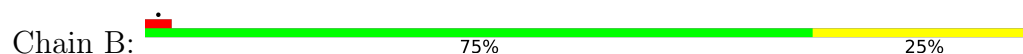
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S mitochondrial rRNA

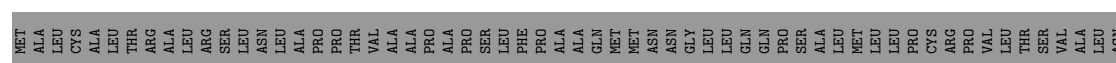




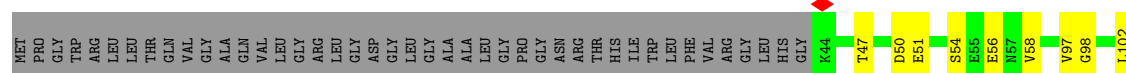
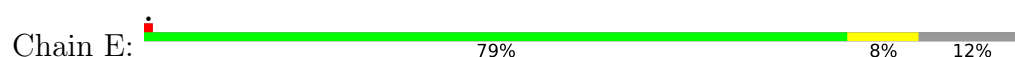
• Molecule 2: mitochondrial tRNAVal



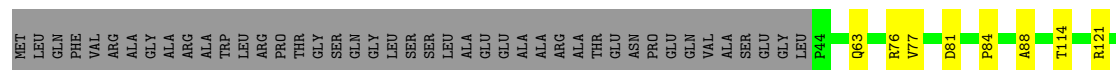
• Molecule 3: 39S ribosomal protein L2, mitochondrial



• Molecule 4: 39S ribosomal protein L3, mitochondrial

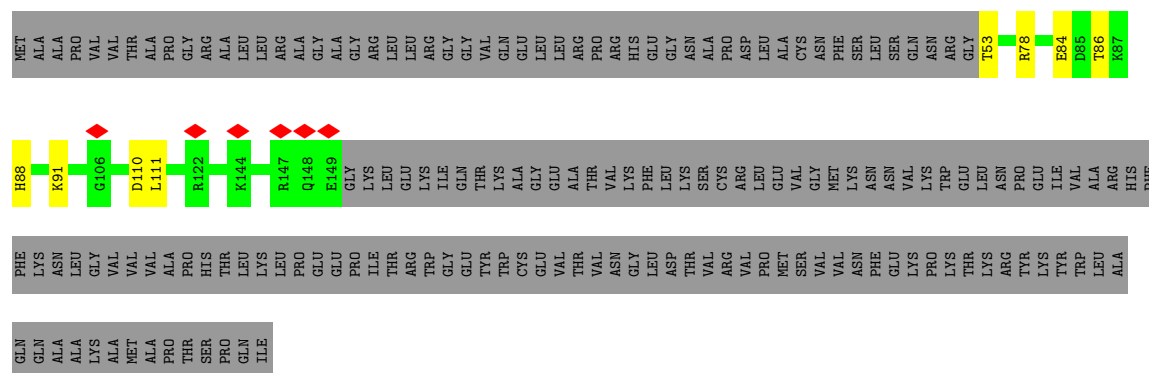


• Molecule 5: 39S ribosomal protein L4, mitochondrial

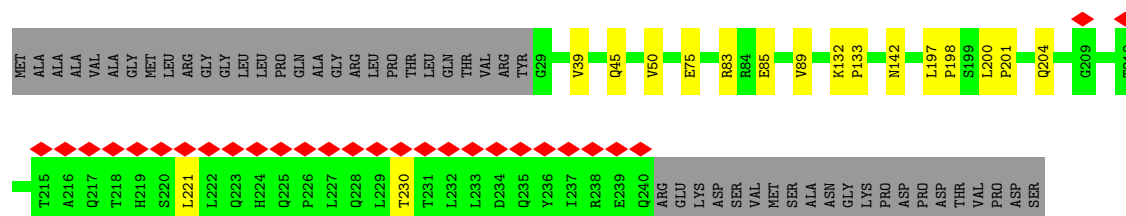


• Molecule 6: 39S ribosomal protein L9, mitochondrial

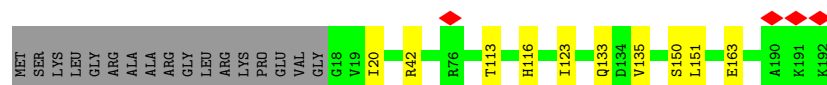
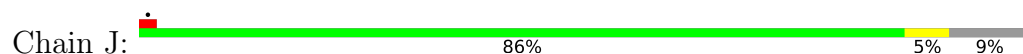




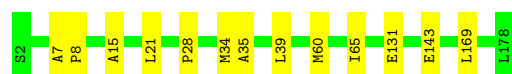
- Molecule 7: 39S ribosomal protein L10, mitochondrial



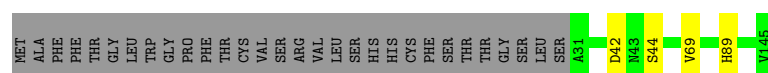
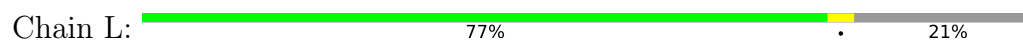
- Molecule 8: 39S ribosomal protein L11, mitochondrial



- Molecule 9: 39S ribosomal protein L13, mitochondrial



- Molecule 10: 39S ribosomal protein L14, mitochondrial



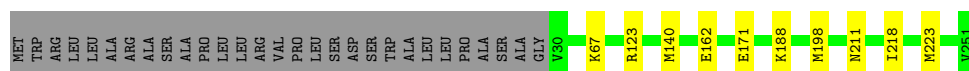
- Molecule 11: 39S ribosomal protein L15, mitochondrial





- Molecule 12: 39S ribosomal protein L16, mitochondrial

Chain N: 84% 12%



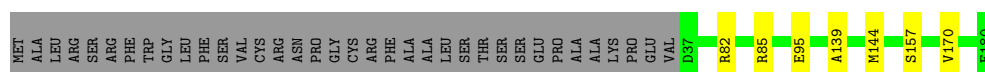
- Molecule 13: 39S ribosomal protein L17, mitochondrial

Chain O: 82% 6% 12%



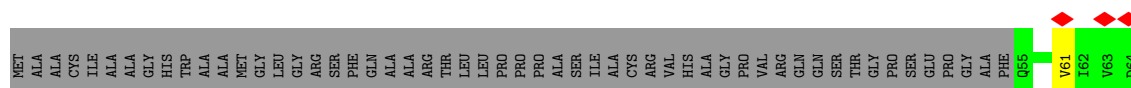
- Molecule 14: 39S ribosomal protein L18, mitochondrial

Chain P: 76% 20%



- Molecule 15: 39S ribosomal protein L19, mitochondrial

Chain Q: 5% 78% 18%



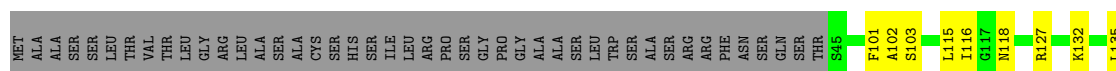
- Molecule 16: 39S ribosomal protein L20, mitochondrial

Chain R: 91% 6%



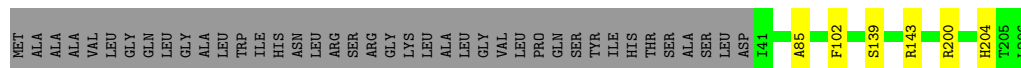
- Molecule 17: 39S ribosomal protein L21, mitochondrial

Chain S: 71% 7% 21%



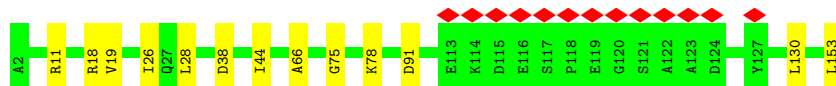
- Molecule 18: 39S ribosomal protein L22, mitochondrial

Chain T: 78% 19%



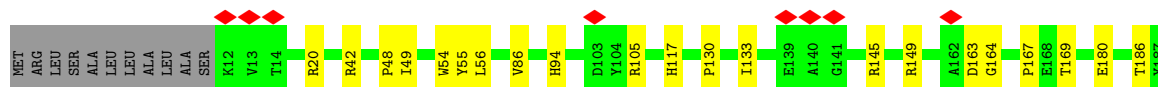
- Molecule 19: 39S ribosomal protein L23, mitochondrial

Chain U: 9% 91% 9%



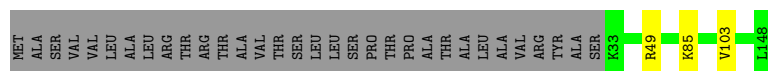
- Molecule 20: 39S ribosomal protein L24, mitochondrial

Chain V: 82% 12% 5%



- Molecule 21: 39S ribosomal protein L27, mitochondrial

Chain W: 76% 22%



- Molecule 22: 39S ribosomal protein L28, mitochondrial

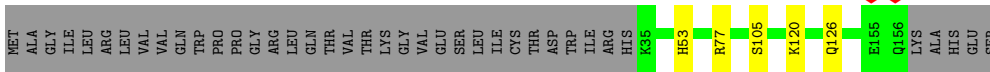
Chain X: 92% 5%



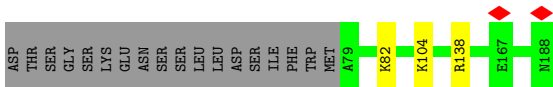
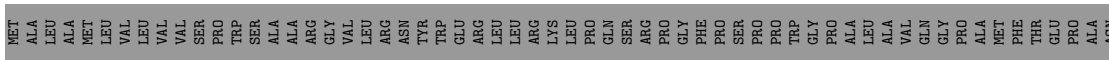
- Molecule 23: 39S ribosomal protein L47, mitochondrial

Chain Y: 68% 28%

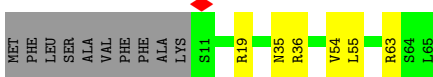
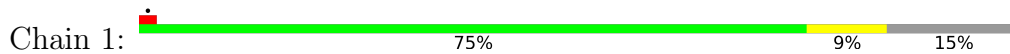
- Molecule 24: 39S ribosomal protein L30, mitochondrial



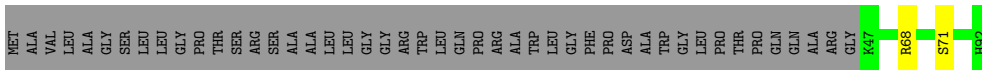
- Molecule 25: 39S ribosomal protein L32, mitochondrial



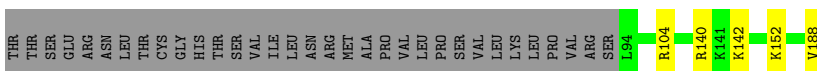
- Molecule 26: 39S ribosomal protein L33, mitochondrial



- Molecule 27: 39S ribosomal protein L34, mitochondrial

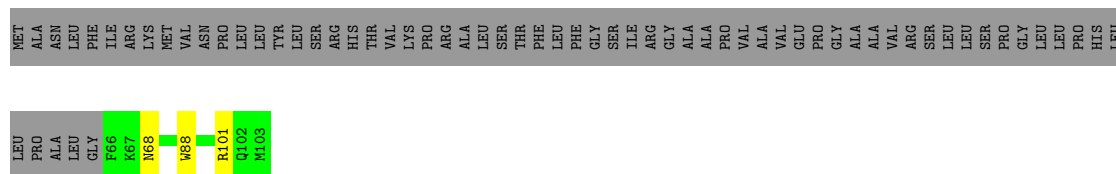


- Molecule 28: 39S ribosomal protein L35, mitochondrial



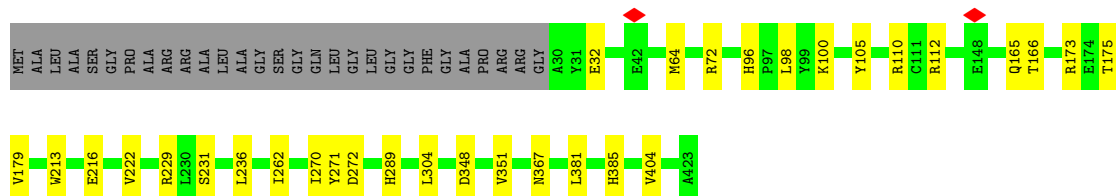
- Molecule 29: 39S ribosomal protein L36, mitochondrial

Chain 4:  34% . 63%

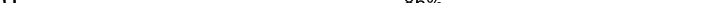


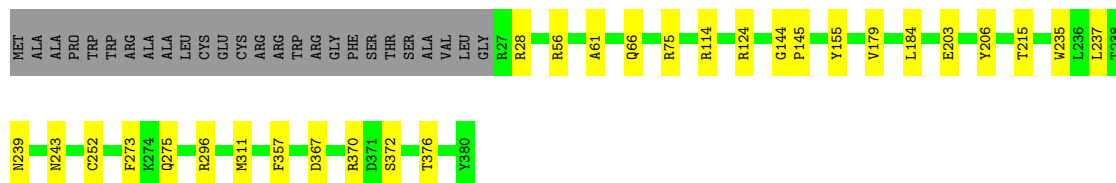
- Molecule 30: 39S ribosomal protein L37, mitochondrial

Chain 5: 86% 8% 7%

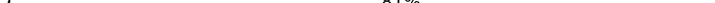


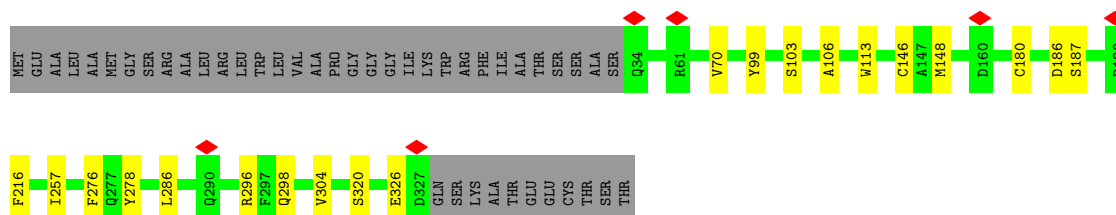
- Molecule 31: 39S ribosomal protein L38, mitochondrial

Chain 6:  86% 8% 7%



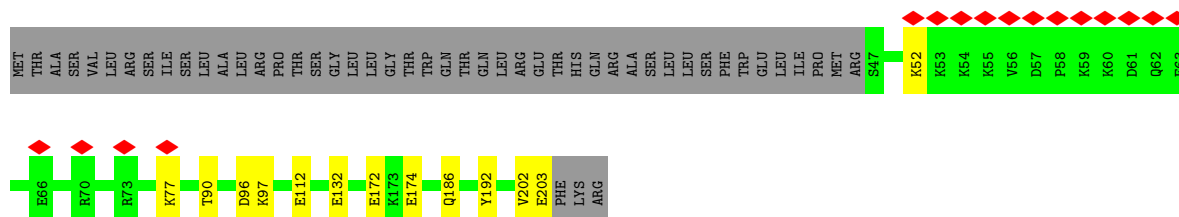
- Molecule 32: 39S ribosomal protein L39, mitochondrial

Chain 7:  81% 6% 13%



- Molecule 33: 39S ribosomal protein L40, mitochondrial

Chain 8:  8% 70% 6% 16%



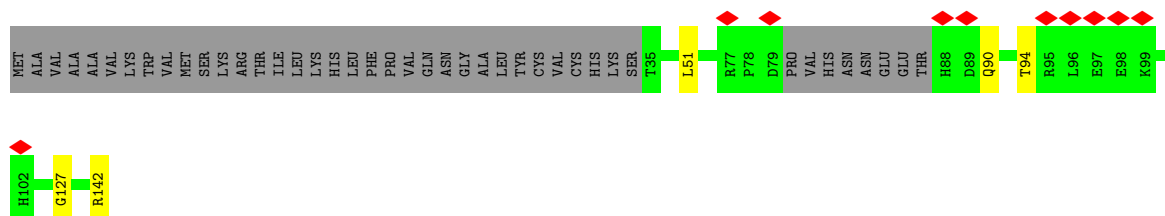
- Molecule 34: 39S ribosomal protein L41, mitochondrial

Chain 9:  86% 9%



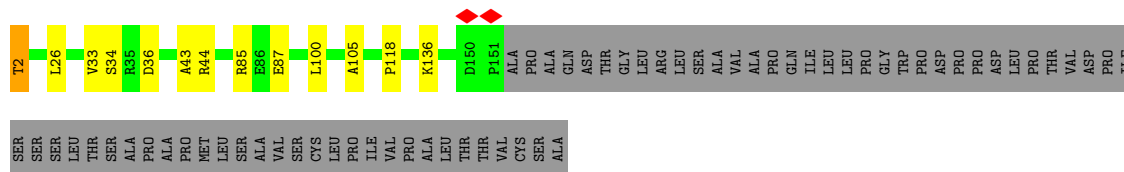
- Molecule 35: 39S ribosomal protein L42, mitochondrial

Chain a:  7% 67% 30%



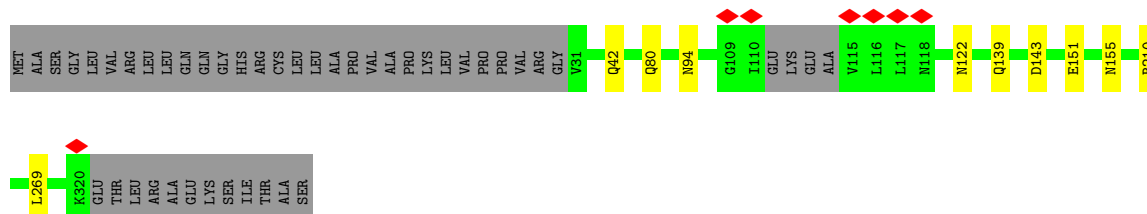
- Molecule 36: 39S ribosomal protein L43, mitochondrial

Chain b:  64% 6% 30%



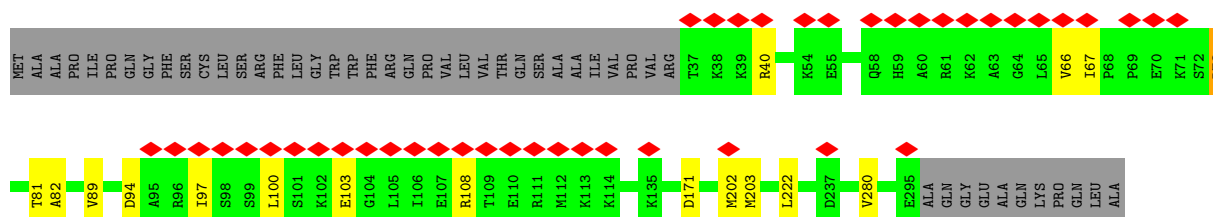
- Molecule 37: 39S ribosomal protein L44, mitochondrial

Chain c:  83% 14%

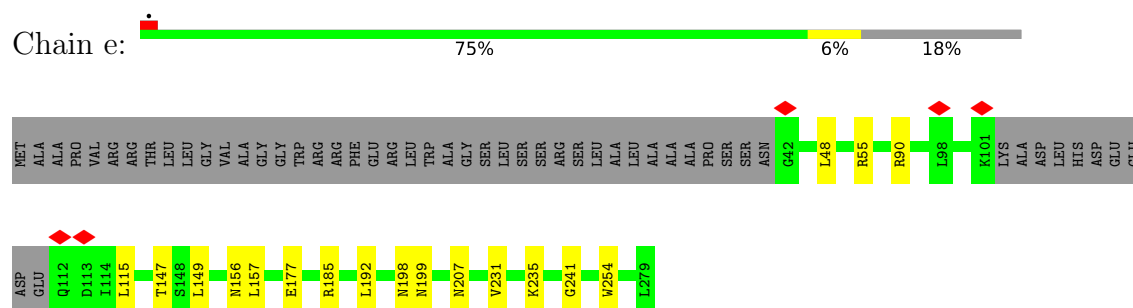


- Molecule 38: 39S ribosomal protein L45, mitochondrial

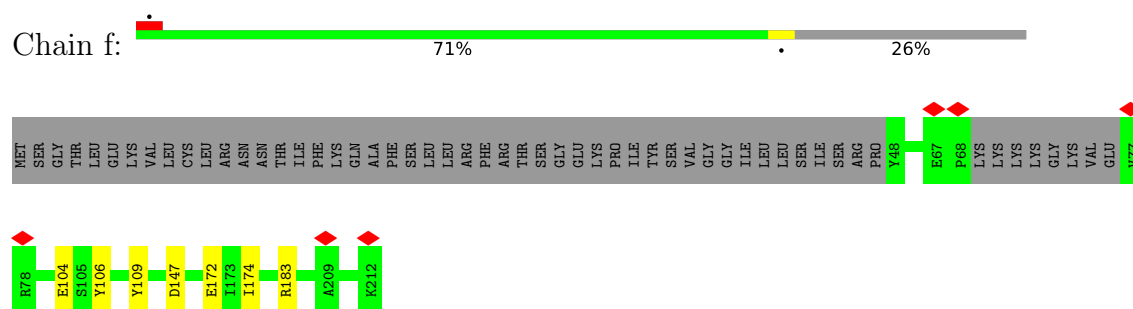
Chain d:  14% 79% 5% 15%



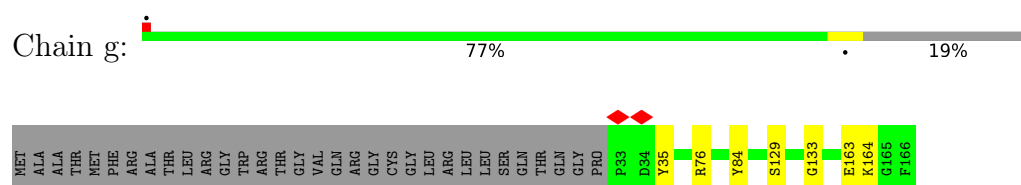
- Molecule 39: 39S ribosomal protein L46, mitochondrial



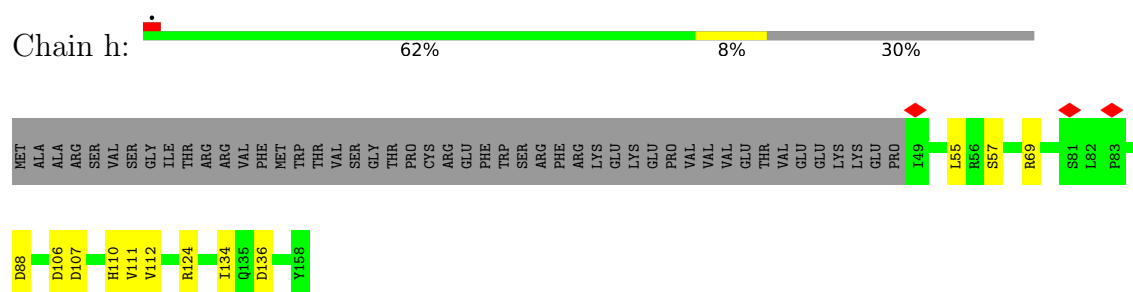
- Molecule 40: 39S ribosomal protein L48, mitochondrial



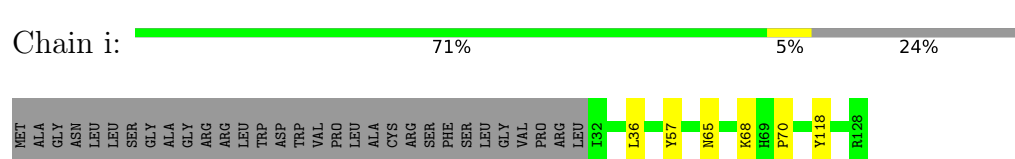
- Molecule 41: 39S ribosomal protein L49, mitochondrial



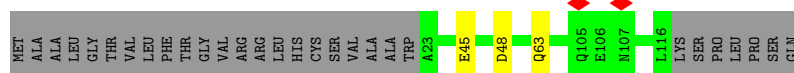
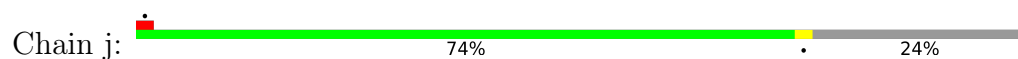
- Molecule 42: 39S ribosomal protein L50, mitochondrial



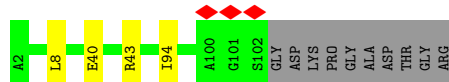
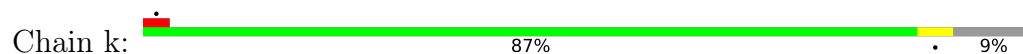
- Molecule 43: 39S ribosomal protein L51, mitochondrial



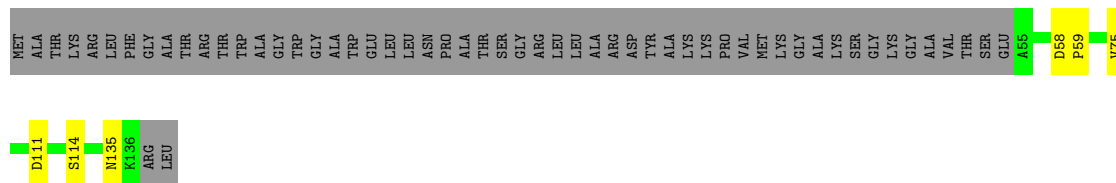
- Molecule 44: 39S ribosomal protein L52, mitochondrial



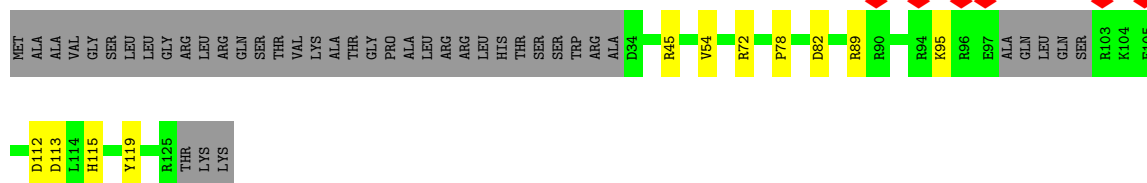
- Molecule 45: 39S ribosomal protein L53, mitochondrial



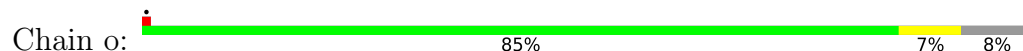
- Molecule 46: 39S ribosomal protein L54, mitochondrial



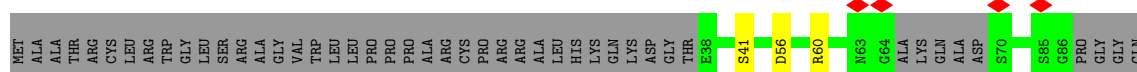
- Molecule 47: 39S ribosomal protein L55, mitochondrial

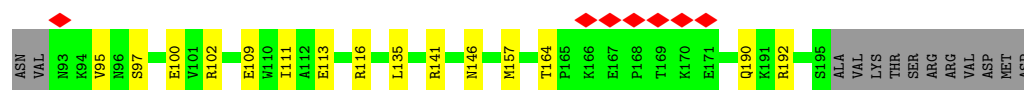


- Molecule 48: Ribosomal protein 63, mitochondrial

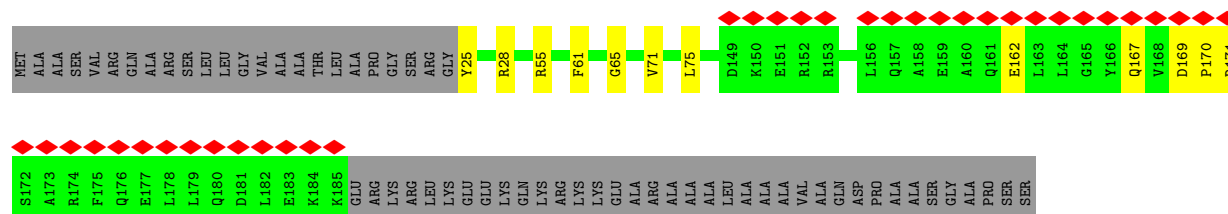


- Molecule 49: Peptidyl-tRNA hydrolase ICT1, mitochondrial

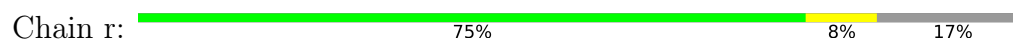




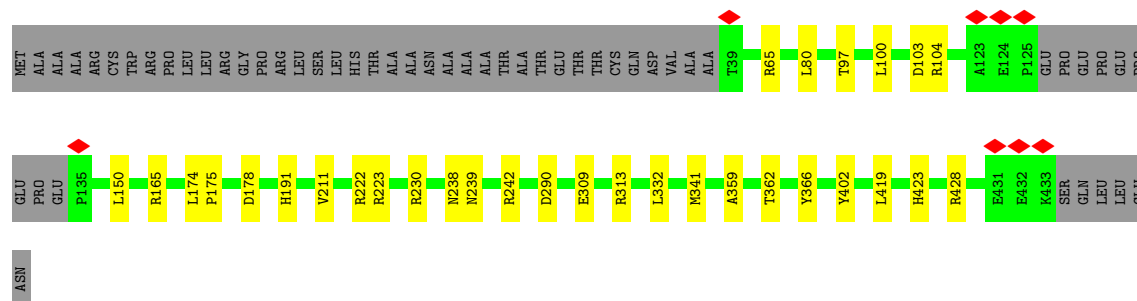
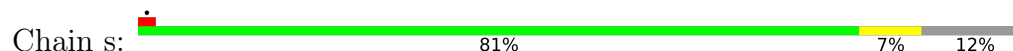
- Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1



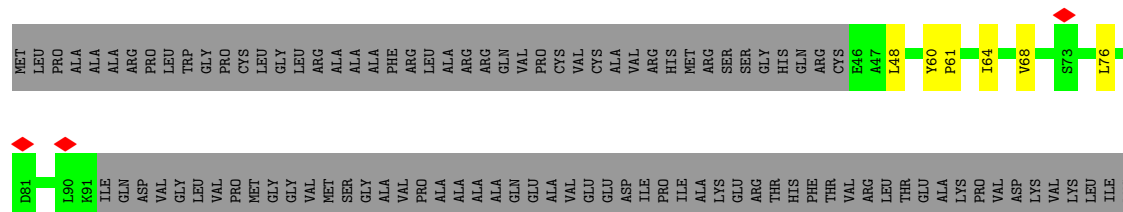
- Molecule 51: 39S ribosomal protein S18a, mitochondrial



- Molecule 52: 39S ribosomal protein S30, mitochondrial

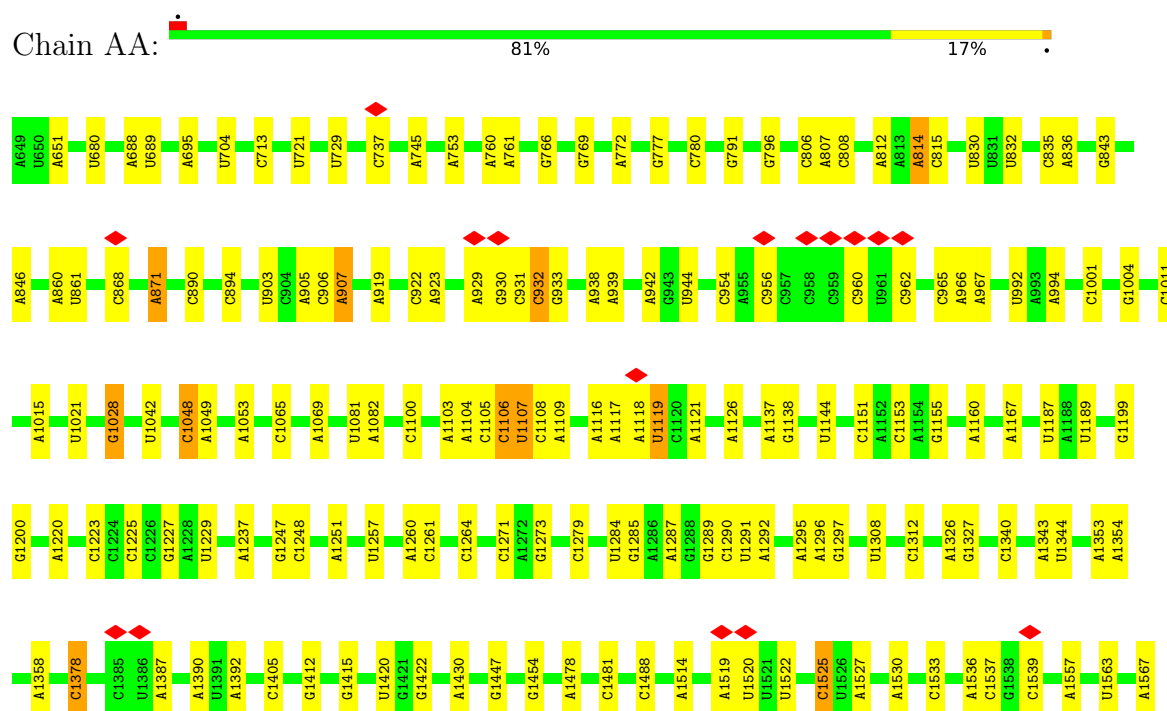


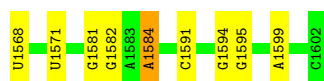
- Molecule 53: 39S ribosomal protein L12, mitochondrial



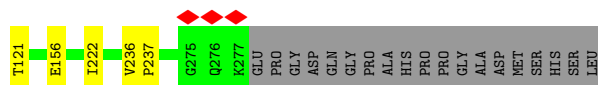
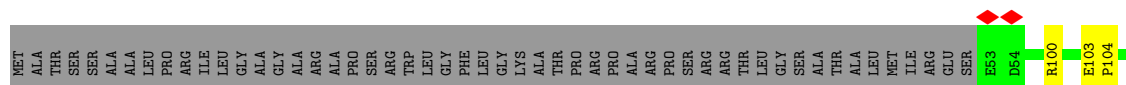
- Molecule 53: 39S ribosomal protein L12, mitochondrial

- Molecule 54: 12S mitochondrial rRNA

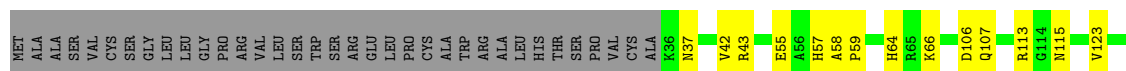




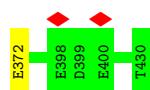
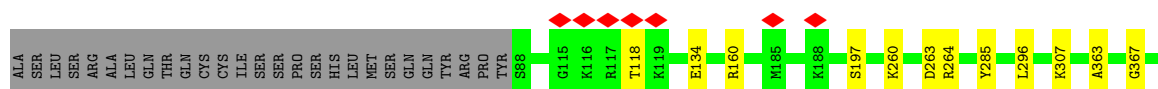
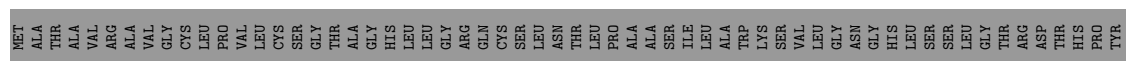
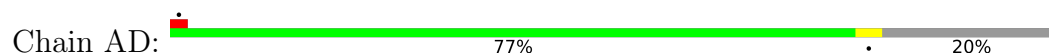
- Molecule 55: 28S ribosomal protein S2, mitochondrial



- Molecule 56: 28S ribosomal protein S24, mitochondrial



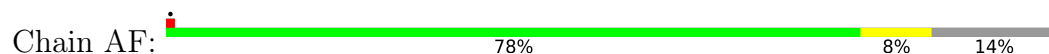
- Molecule 57: 28S ribosomal protein S5, mitochondrial

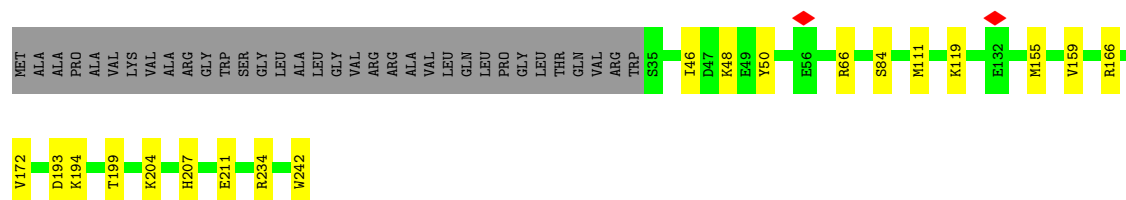


- Molecule 58: 28S ribosomal protein S6, mitochondrial



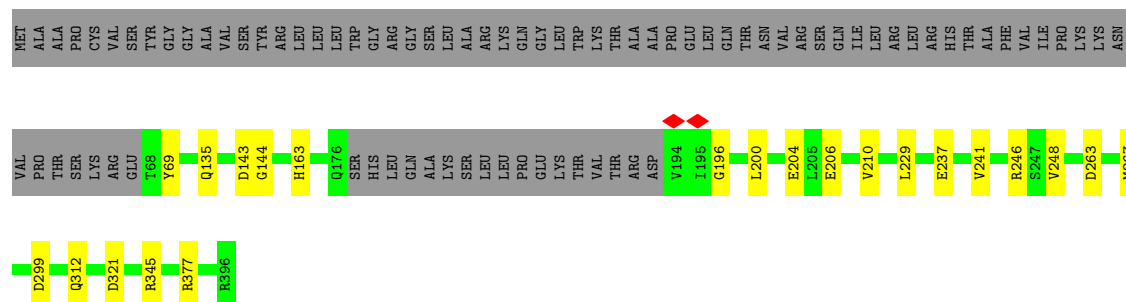
- Molecule 59: 28S ribosomal protein S7, mitochondrial





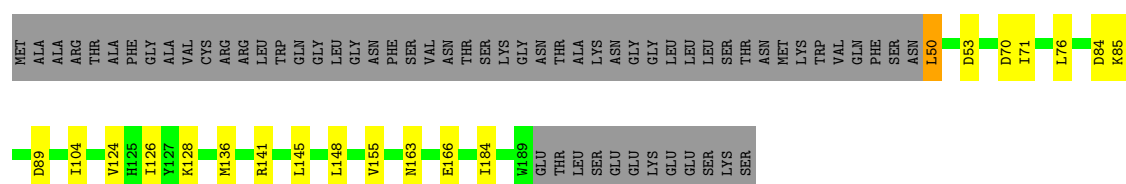
- Molecule 60: 28S ribosomal protein S9, mitochondrial

Chain AG: 73% 6% 21%



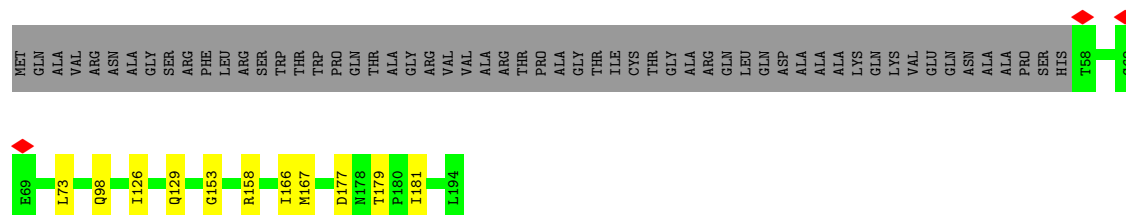
- Molecule 61: 28S ribosomal protein S10, mitochondrial

Chain AH: 60% 9% 30%



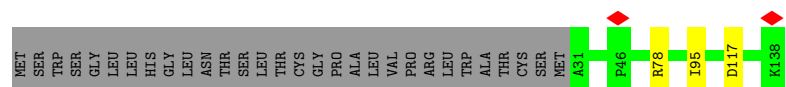
- Molecule 62: 28S ribosomal protein S11, mitochondrial

Chain AI: 65% 6% 29%



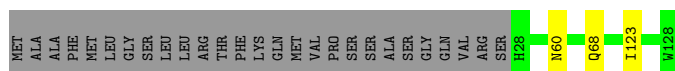
- Molecule 63: 28S ribosomal protein S12, mitochondrial

Chain AJ: 76% 22%



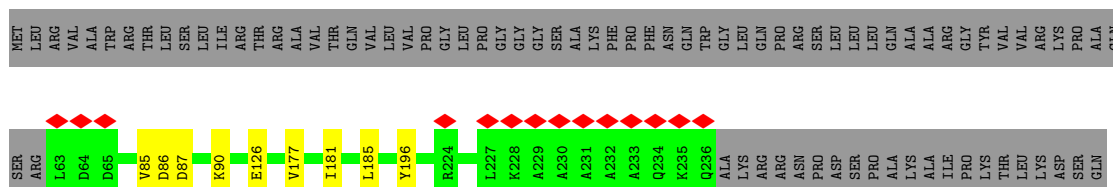
- Molecule 64: 28S ribosomal protein S14, mitochondrial

Chain AK:  77% 21%



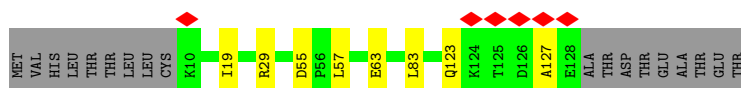
- Molecule 65: 28S ribosomal protein S15, mitochondrial

Chain AL:  5% 64% 32%



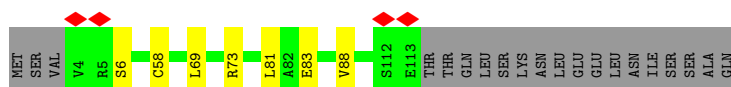
- Molecule 66: 28S ribosomal protein S16, mitochondrial

Chain AM:  81% 6% 13%



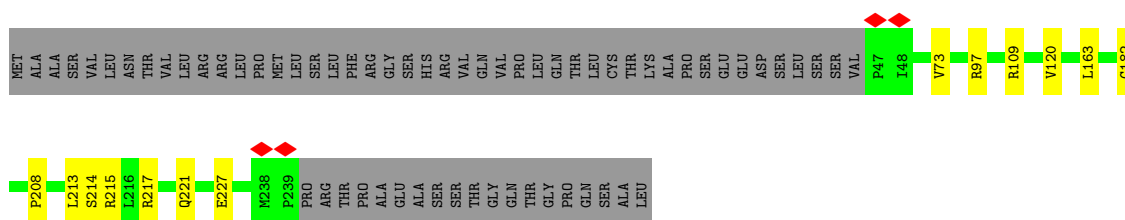
- Molecule 67: 28S ribosomal protein S17, mitochondrial

Chain AN:  79% 5% 15%



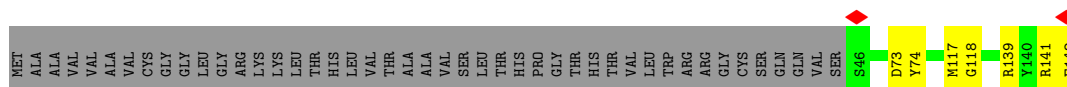
- Molecule 68: 28S ribosomal protein S18b, mitochondrial

Chain AO:  70% 5% 25%

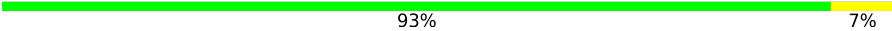


- Molecule 69: 28S ribosomal protein S18c, mitochondrial

Chain AP:  63% 5% 32%



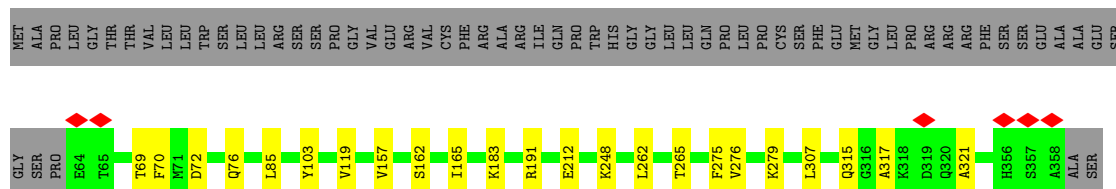
- Molecule 70: 28S ribosomal protein S21, mitochondrial

Chain AQ:  93% 7%



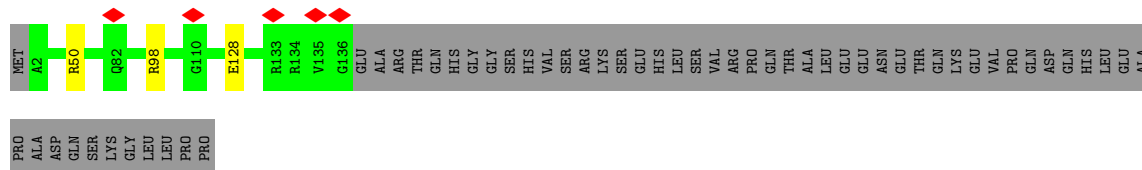
- Molecule 71: 28S ribosomal protein S22, mitochondrial

Chain AR:  76% 6% 18%



- Molecule 72: 28S ribosomal protein S23, mitochondrial

Chain AS:  69% 29%



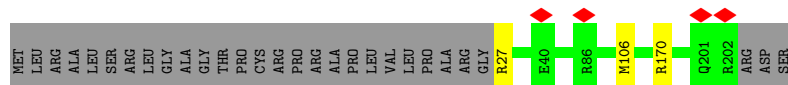
- Molecule 73: 28S ribosomal protein S25, mitochondrial

Chain AT:  92% 5% 3%



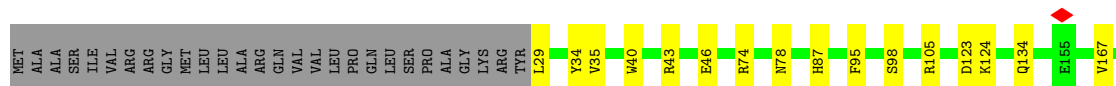
- Molecule 74: 28S ribosomal protein S26, mitochondrial

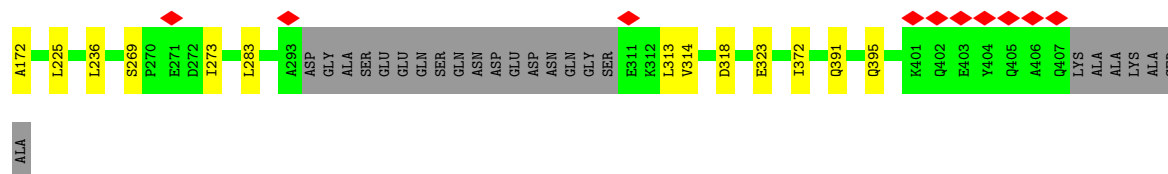
Chain AU:  84% 14%



- Molecule 75: 28S ribosomal protein S27, mitochondrial

Chain AV:  80% 7% 13%

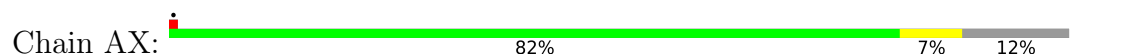




- Molecule 76: 28S ribosomal protein S28, mitochondrial



- Molecule 77: 28S ribosomal protein S29, mitochondrial

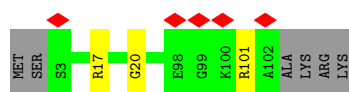


- Molecule 78: 28S ribosomal protein S31, mitochondrial

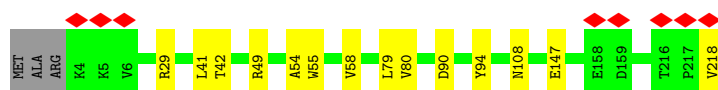


- Molecule 79: 28S ribosomal protein S33, mitochondrial

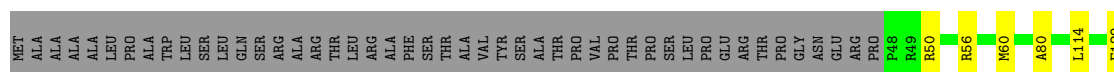
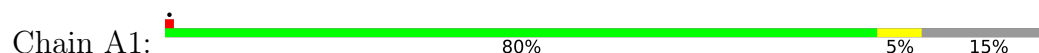




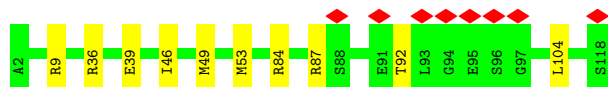
- Molecule 80: 28S ribosomal protein S34, mitochondrial



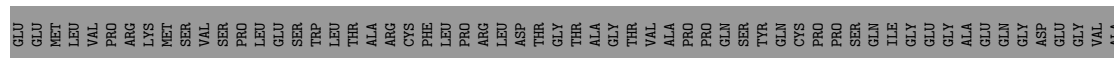
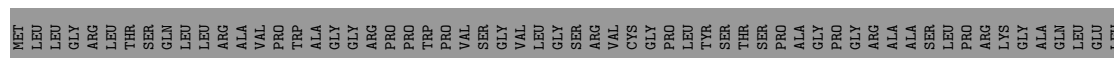
- Molecule 81: 28S ribosomal protein S35, mitochondrial



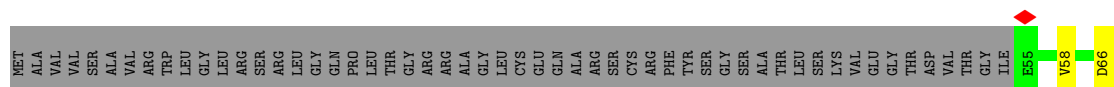
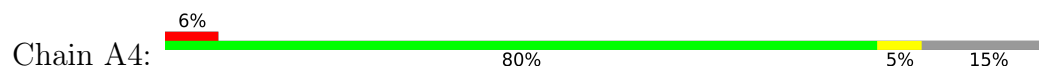
- Molecule 82: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

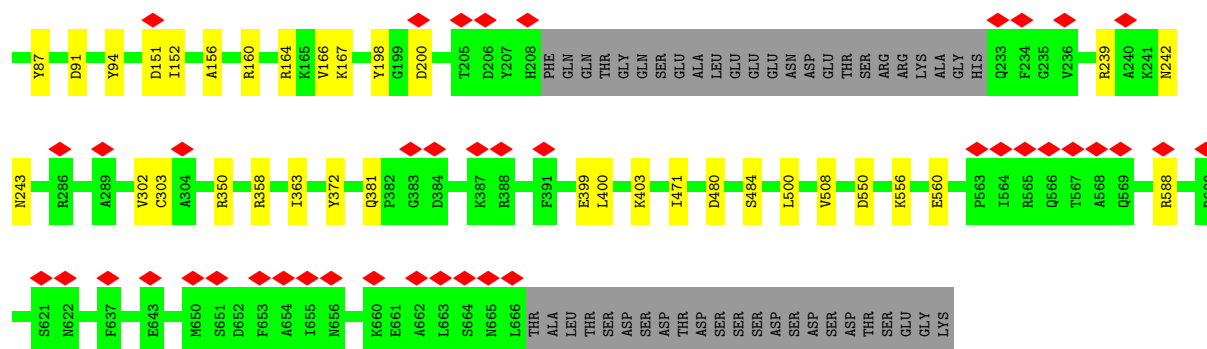


- Molecule 83: Aurora kinase A-interacting protein

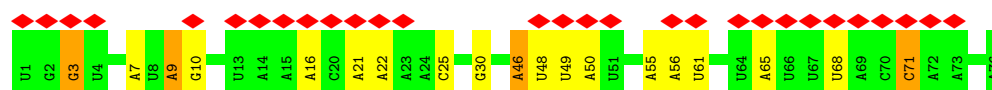
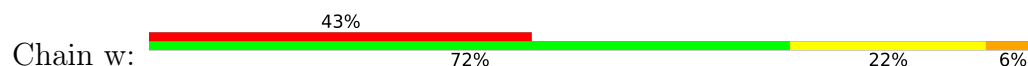


- Molecule 84: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

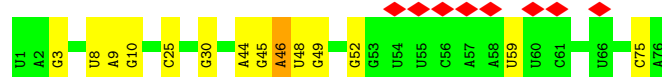
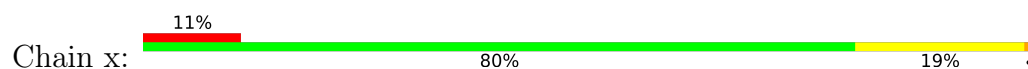




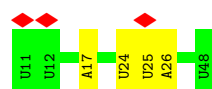
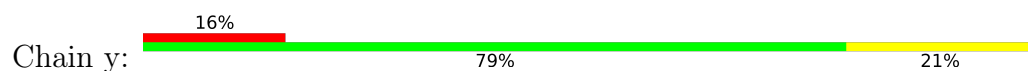
- Molecule 85: A-site tRNA



- Molecule 86: P-site tRNA



- Molecule 87: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93615	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	55.214	Depositor
Minimum map value	-20.948	Depositor
Average map value	0.006	Depositor
Map value standard deviation	1.001	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAC, MG, IAS, FES, AYA, ZN, THC, K, ATP, GTP

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	A	0.13	0/36361	0.21	0/56600
2	B	0.12	0/1700	0.20	0/2641
3	D	0.15	0/1896	0.30	0/2549
4	E	0.14	0/2475	0.25	0/3355
5	F	0.15	0/2090	0.30	0/2842
6	H	0.13	0/816	0.27	0/1097
7	I	0.20	0/1731	0.28	0/2345
8	J	0.17	0/1348	0.27	0/1813
9	K	0.22	0/1490	0.30	0/2021
10	L	0.14	0/905	0.28	0/1218
11	M	0.16	0/2381	0.31	0/3212
12	N	0.19	0/1833	0.29	0/2468
13	O	0.15	0/1283	0.27	0/1727
14	P	0.24	0/1199	0.31	0/1623
15	Q	0.13	0/2027	0.27	0/2734
16	R	0.17	0/1175	0.29	0/1572
17	S	0.16	0/1320	0.31	0/1789
18	T	0.15	0/1403	0.28	0/1886
19	U	0.15	0/1274	0.30	0/1723
20	V	0.12	0/1721	0.28	0/2333
21	W	0.22	0/926	0.30	0/1244
22	X	0.13	0/2099	0.26	0/2837
23	Y	0.15	0/1593	0.28	0/2136
24	Z	0.15	0/1021	0.27	0/1378
25	0	0.14	0/913	0.27	0/1224
26	1	0.16	0/460	0.29	0/610
27	2	0.16	0/383	0.34	0/507
28	3	0.18	0/853	0.32	0/1136
29	4	0.22	0/350	0.31	0/461
30	5	0.13	0/3305	0.26	0/4502
31	6	0.23	0/3043	0.32	0/4140
32	7	0.12	0/2447	0.24	0/3310

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	8	0.17	0/1354	0.27	0/1819
34	9	0.15	0/1025	0.26	0/1379
35	a	0.12	0/866	0.29	0/1174
36	b	0.16	0/1211	0.31	0/1639
37	c	0.14	0/2347	0.26	0/3171
38	d	0.12	0/2181	0.28	0/2949
39	e	0.18	0/1885	0.26	0/2542
40	f	0.20	0/1273	0.27	0/1716
41	g	0.14	0/1151	0.29	0/1569
42	h	0.12	0/918	0.24	0/1249
43	i	0.15	0/850	0.30	0/1135
44	j	0.15	0/760	0.28	0/1023
45	k	0.17	0/777	0.28	0/1048
46	l	0.16	0/707	0.27	0/960
47	m	0.18	0/767	0.31	0/1028
48	o	0.18	0/819	0.32	0/1097
49	p	0.15	0/1223	0.28	0/1641
50	q	0.12	0/1384	0.26	0/1869
51	r	0.24	0/1362	0.31	0/1846
52	s	0.13	0/3239	0.28	0/4400
53	t1	0.08	0/358	0.18	0/486
53	t2	0.08	0/259	0.19	0/350
53	t3	0.05	0/259	0.15	0/350
53	t4	0.06	0/246	0.16	0/331
53	t5	0.05	0/246	0.15	0/331
53	t6	0.06	0/246	0.15	0/331
54	AA	0.10	0/22655	0.17	0/35273
55	AB	0.15	0/1871	0.27	0/2531
56	AC	0.20	0/1113	0.30	0/1505
57	AD	0.15	0/2783	0.27	0/3724
58	AE	0.11	0/989	0.26	0/1335
59	AF	0.11	0/1767	0.25	0/2373
60	AG	0.14	0/2623	0.27	0/3515
61	AH	0.20	0/1178	0.28	0/1598
62	AI	0.12	0/1030	0.26	0/1386
63	AJ	0.14	0/855	0.27	0/1148
64	AK	0.19	0/880	0.32	0/1182
65	AL	0.11	0/1477	0.25	0/1974
66	AM	0.15	0/963	0.29	0/1295
67	AN	0.12	0/886	0.23	0/1199
68	AO	0.13	0/1648	0.27	0/2243
69	AP	0.11	0/798	0.26	0/1070
70	AQ	0.14	0/748	0.31	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
71	AR	0.13	0/2456	0.25	0/3317
72	AS	0.13	0/1138	0.25	0/1533
73	AT	0.12	0/1402	0.26	0/1883
74	AU	0.13	0/1510	0.28	0/2025
75	AV	0.09	0/3030	0.22	0/4093
76	AW	0.13	0/801	0.25	0/1079
77	AX	0.09	0/2921	0.23	0/3954
78	AY	0.14	0/1280	0.23	0/1725
79	AZ	0.15	0/857	0.27	0/1141
80	A0	0.14	0/1834	0.30	0/2484
81	A1	0.16	0/2285	0.26	0/3090
82	A2	0.12	0/941	0.29	0/1257
83	A3	0.16	0/636	0.36	0/839
84	A4	0.12	0/4877	0.24	0/6598
85	w	0.06	0/1608	0.14	0/2497
86	x	0.06	0/1656	0.14	0/2571
87	y	0.09	0/443	0.17	0/684
All	All	0.14	0/185473	0.25	0/263581

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32498	16499	16499	116	0
2	B	1522	776	776	4	0
3	D	1859	1921	1920	14	0
4	E	2406	2417	2415	18	0
5	F	2031	2066	2065	14	0
6	H	802	847	846	6	0
7	I	1695	1786	1785	14	0
8	J	1330	1409	1407	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	1455	1454	1452	8	0
10	L	890	942	941	2	0
11	M	2327	2396	2395	9	0
12	N	1786	1819	1817	7	0
13	O	1259	1295	1294	7	0
14	P	1173	1166	1165	5	0
15	Q	1979	2023	2022	8	0
16	R	1154	1215	1214	4	0
17	S	1293	1366	1365	11	0
18	T	1369	1411	1410	5	0
19	U	1251	1232	1232	12	0
20	V	1676	1688	1687	21	0
21	W	904	937	935	3	0
22	X	2044	2061	2060	5	0
23	Y	1556	1598	1597	9	0
24	Z	996	1045	1044	5	0
25	0	898	917	916	3	0
26	1	455	499	498	4	0
27	2	377	407	406	1	0
28	3	832	884	883	5	0
29	4	342	362	361	2	0
30	5	3210	3208	3206	24	0
31	6	2948	2844	2841	21	0
32	7	2390	2399	2397	12	0
33	8	1327	1369	1368	12	0
34	9	997	988	987	6	0
35	a	840	812	810	4	0
36	b	1196	1196	1190	9	0
37	c	2299	2322	2320	6	0
38	d	2124	2129	2125	12	0
39	e	1848	1851	1849	11	0
40	f	1252	1271	1269	7	0
41	g	1113	1097	1097	4	0
42	h	895	882	881	7	0
43	i	828	859	857	6	0
44	j	745	747	746	2	0
45	k	774	784	784	2	0
46	l	688	675	674	6	0
47	m	754	761	758	11	0
48	o	798	807	804	7	0
49	p	1205	1226	1223	13	0
50	q	1350	1328	1327	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	r	1322	1349	1349	12	0
52	s	3155	3143	3139	20	0
53	t1	354	378	377	11	0
53	t2	257	284	283	10	0
53	t3	257	284	283	0	0
53	t4	245	275	275	4	0
53	t5	245	275	275	1	0
53	t6	245	275	275	0	0
54	AA	20253	10289	10287	52	0
55	AB	1828	1816	1815	5	0
56	AC	1083	1089	1088	11	0
57	AD	2731	2805	2804	9	0
58	AE	972	1001	1000	6	0
59	AF	1725	1770	1769	14	0
60	AG	2568	2558	2554	14	0
61	AH	1152	1184	1183	15	0
62	AI	1018	1058	1056	6	0
63	AJ	839	888	887	3	0
64	AK	862	886	885	3	0
65	AL	1453	1541	1540	5	0
66	AM	942	966	965	6	0
67	AN	868	929	928	5	0
68	AO	1592	1557	1557	10	0
69	AP	781	807	806	5	0
70	AQ	744	758	758	6	0
71	AR	2409	2429	2428	15	0
72	AS	1111	1116	1115	3	0
73	AT	1371	1394	1393	6	0
74	AU	1488	1500	1499	3	0
75	AV	2969	2964	2961	19	0
76	AW	789	803	802	5	0
77	AX	2849	2845	2843	16	0
78	AY	1246	1198	1197	5	0
79	AZ	839	860	858	3	0
80	A0	1787	1797	1796	11	0
81	A1	2238	2269	2269	15	0
82	A2	935	969	973	8	0
83	A3	625	700	699	4	0
84	A4	4768	4768	4766	22	0
85	w	1438	725	726	4	0
86	x	1483	751	753	4	0
87	y	399	199	201	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	A	127	0	0	0	0
88	A3	1	0	0	0	0
88	AA	53	0	0	0	0
88	AB	1	0	0	0	0
88	AX	1	0	0	0	0
88	D	3	0	0	0	0
88	E	1	0	0	0	0
88	g	1	0	0	0	0
88	o	1	0	0	0	0
89	A	31	0	0	0	0
89	AA	9	0	0	0	0
89	M	1	0	0	0	0
89	P	1	0	0	0	0
89	i	1	0	0	0	0
89	o	1	0	0	0	0
90	0	1	0	0	0	0
90	4	1	0	0	0	0
90	AO	1	0	0	0	0
91	AP	4	0	0	0	0
91	AT	4	0	0	0	0
91	r	4	0	0	2	0
92	AX	31	12	12	0	0
93	AX	32	12	12	0	0
94	6	1	0	0	0	0
94	A	349	0	0	6	0
94	A0	1	0	0	0	0
94	A3	3	0	0	0	0
94	AA	70	0	0	5	0
94	AC	1	0	0	0	0
94	AG	1	0	0	0	0
94	AH	2	0	0	0	0
94	AK	2	0	0	0	0
94	AX	2	0	0	0	0
94	B	1	0	0	0	0
94	D	3	0	0	0	0
94	E	3	0	0	0	0
94	F	4	0	0	0	0
94	K	3	0	0	0	0
94	L	1	0	0	0	0
94	M	5	0	0	0	0
94	N	1	0	0	0	0
94	O	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
94	R	1	0	0	0	0
94	S	1	0	0	0	0
94	U	1	0	0	0	0
94	W	1	0	0	0	0
94	c	1	0	0	0	0
94	d	1	0	0	0	0
94	f	1	0	0	0	0
94	i	1	0	0	0	0
94	o	2	0	0	0	0
94	r	2	0	0	0	0
94	s	2	0	0	0	0
All	All	176756	149469	149361	680	0

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

All (680) 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)
54:AA:992:U:O2'	54:AA:994:A:OP2	1.87	0.92
1:A:3063:G:O2'	1:A:3066:C:OP2	1.93	0.86
1:A:3198:A:O2'	1:A:3200:U:O2'	1.93	0.86
31:6:215:THR:OG1	31:6:275:GLN:OE1	1.94	0.85
1:A:1777:A:N6	1:A:1780:U:OP2	2.08	0.85
54:AA:1358:A:O2'	86:x:30:G:OP1	1.97	0.83
1:A:2158:U:OP2	51:r:195:TYR:OH	1.96	0.82
31:6:66:GLN:OE1	31:6:75:ARG:NH2	2.12	0.82
24:Z:105:SER:OG	48:o:59:GLU:OE2	1.98	0.81
51:r:35:PHE:N	51:r:56:THR:HG1	1.79	0.80
49:p:113:GLU:OE1	49:p:116:ARG:NH1	2.14	0.80
6:H:84:GLU:OE1	22:X:44:ARG:NH2	2.15	0.80
56:AC:37:ASN:O	56:AC:43:ARG:NH2	2.14	0.80
84:A4:239:ARG:O	84:A4:242:ASN:ND2	2.15	0.80
5:F:272:LYS:NZ	43:i:65:ASN:OD1	2.15	0.79
52:s:165:ARG:NH2	52:s:309:GLU:OE1	2.15	0.79
47:m:115:HIS:HD1	81:A1:224:TYR:HH	1.22	0.79
1:A:3152:C:OP1	15:Q:141:SER:OG	2.01	0.79
36:b:87:GLU:OE1	36:b:100:LEU:HD11	1.83	0.78
49:p:56:ASP:O	49:p:60:ARG:NE	2.17	0.78
3:D:220:VAL:O	3:D:223:THR:OG1	1.99	0.78
1:A:2416:U:OP1	52:s:313:ARG:NH1	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:AA:729:U:O2	54:AA:745:A:N6	2.17	0.78
82:A2:39:GLU:OE1	82:A2:87:ARG:NE	2.17	0.77
31:6:206:TYR:O	31:6:243:ASN:ND2	2.18	0.76
32:7:180:CYS:SG	32:7:296:ARG:NH1	2.58	0.76
57:AD:285:TYR:OH	57:AD:372:GLU:OE2	2.04	0.75
54:AA:769:G:OP2	67:AN:73:ARG:NH2	2.18	0.75
54:AA:1412:G:OP1	77:AX:279:LYS:NZ	2.19	0.75
54:AA:1591:C:OP1	70:AQ:52:ARG:NH2	2.20	0.75
67:AN:83:GLU:OE2	73:AT:85:GLN:NE2	2.20	0.75
1:A:1760:G:N7	50:q:55:ARG:NH2	2.35	0.74
1:A:2034:A:O2'	11:M:71:GLN:OE1	2.04	0.74
20:V:130:PRO:O	20:V:149:ARG:NH2	2.20	0.74
59:AF:50:TYR:O	59:AF:66:ARG:NH2	2.19	0.74
51:r:166:GLY:O	51:r:171:ARG:NH2	2.20	0.74
77:AX:276:ARG:NH2	77:AX:286:GLU:OE1	2.21	0.73
1:A:2108:G:N7	12:N:67:LYS:NZ	2.35	0.73
31:6:124:ARG:NH1	33:8:112:GLU:OE2	2.20	0.73
68:AO:182:GLY:O	71:AR:183:LYS:NZ	2.20	0.73
3:D:289:LEU:HD12	3:D:290:PRO:HD2	1.71	0.73
1:A:2626:U:O2'	1:A:2628:U:OP2	2.07	0.72
54:AA:906:C:OP1	57:AD:118:THR:HG21	1.89	0.72
86:x:9:A:O2'	86:x:10:G:N7	2.22	0.72
84:A4:550:ASP:OD1	84:A4:588:ARG:NH2	2.23	0.72
69:AP:139:ARG:NH1	69:AP:142:GLU:OE1	2.23	0.72
17:S:127:ARG:NH2	17:S:157:GLU:OE1	2.23	0.72
32:7:146:CYS:O	32:7:278:TYR:OH	2.08	0.71
1:A:3112:A:N6	1:A:3200:U:O2	2.19	0.71
22:X:36:ARG:NH2	22:X:151:GLU:OE2	2.23	0.71
33:8:77:LYS:NZ	86:x:52:G:OP1	2.23	0.71
54:AA:1028:G:OP2	94:AA:1902:HOH:O	2.08	0.71
37:c:94:ASN:OD1	37:c:122:ASN:ND2	2.23	0.71
1:A:2173:G:N3	8:J:150:SER:OG	2.23	0.71
1:A:3198:A:HO2'	1:A:3200:U:HO2'	1.38	0.71
71:AR:212:GLU:OE1	71:AR:248:LYS:NZ	2.18	0.71
39:e:48:LEU:HB2	39:e:231:VAL:HG12	1.71	0.71
1:A:2518:A:OP2	3:D:287:ARG:NH1	2.23	0.71
82:A2:36:ARG:NH1	82:A2:92:THR:OG1	2.24	0.70
54:AA:1021:U:OP2	82:A2:9:ARG:NH2	2.23	0.70
54:AA:1100:C:O2	94:AA:1903:HOH:O	2.09	0.70
12:N:171:GLU:O	46:l:135:ASN:ND2	2.23	0.70
1:A:2740:A:N3	1:A:2921:A:O2'	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2941:G:O6	94:A:3501:HOH:O	2.10	0.69
37:c:42:GLN:NE2	43:i:36:LEU:O	2.25	0.69
43:i:57:TYR:OH	50:q:28:ARG:O	2.07	0.69
1:A:2174:G:H4'	8:J:151:LEU:HD23	1.74	0.69
52:s:178:ASP:OD1	52:s:238:ASN:ND2	2.26	0.69
54:AA:769:G:N2	54:AA:772:A:OP2	2.25	0.69
1:A:3113:A:OP1	1:A:3167:U:O2'	2.11	0.69
47:m:115:HIS:ND1	81:A1:224:TYR:OH	2.14	0.69
30:5:216:GLU:OE2	30:5:367:ASN:ND2	2.26	0.68
84:A4:399:GLU:OE2	84:A4:403:LYS:NZ	2.24	0.68
2:B:1613:U:O2'	2:B:1615:A:OP1	2.11	0.68
1:A:1763:A:OP1	43:i:68:LYS:NZ	2.27	0.67
1:A:2406:A:O2'	1:A:2407:U:O5'	2.13	0.67
56:AC:152:ARG:NH1	84:A4:87:TYR:OH	2.27	0.67
64:AK:60:ASN:OD1	64:AK:68:GLN:NE2	2.27	0.67
15:Q:124:PRO:O	15:Q:129:LYS:NZ	2.16	0.67
59:AF:48:LYS:NZ	60:AG:321:ASP:OD1	2.26	0.67
1:A:1760:G:OP1	11:M:196:ARG:NE	2.27	0.67
1:A:2237:A:OP1	51:r:171:ARG:NH1	2.28	0.67
1:A:2814:G:O2'	1:A:2983:G:OP1	2.13	0.66
41:g:76:ARG:NH2	41:g:163:GLU:O	2.28	0.66
1:A:2930:U:OP2	38:d:40:ARG:NH1	2.28	0.66
54:AA:1287:A:OP2	57:AD:260:LYS:NZ	2.28	0.66
1:A:1953:A:O2'	1:A:2463:A:OP1	2.14	0.66
54:AA:1257:U:O2'	54:AA:1260:A:OP2	2.08	0.66
66:AM:63:GLU:OE2	71:AR:191:ARG:NH1	2.29	0.65
31:6:203:GLU:OE2	49:p:192:ARG:NH1	2.28	0.65
40:f:106:TYR:OH	40:f:174:ILE:O	2.13	0.65
71:AR:262:LEU:O	71:AR:265:THR:OG1	2.13	0.65
75:AV:74:ARG:O	75:AV:78:ASN:ND2	2.30	0.65
82:A2:49:MET:HG2	82:A2:53:MET:HE2	1.79	0.65
45:k:40:GLU:OE2	45:k:43:ARG:NH2	2.30	0.65
75:AV:225:LEU:HD11	75:AV:283:LEU:HD22	1.79	0.65
84:A4:350:ARG:NH2	84:A4:381:GLN:OE1	2.30	0.65
61:AH:104:ILE:HG23	61:AH:148:LEU:HD21	1.79	0.64
84:A4:151:ASP:OD1	84:A4:152:ILE:N	2.30	0.64
1:A:2395:A:OP1	30:5:173:ARG:NH2	2.30	0.64
77:AX:180:GLN:NE2	77:AX:183:GLU:OE1	2.31	0.64
54:AA:1119:U:O4'	72:AS:50:ARG:NH1	2.31	0.64
1:A:2499:U:OP2	1:A:2504:A:N6	2.26	0.64
33:8:192:TYR:OH	47:m:78:PRO:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:c:151:GLU:O	37:c:155:ASN:ND2	2.30	0.64
51:r:70:CYS:SG	91:r:201:FES:FE2	1.89	0.64
36:b:34:SER:OG	36:b:36:ASP:O	2.16	0.64
1:A:2906:C:N3	26:1:19:ARG:NH1	2.47	0.63
54:AA:1415:G:OP2	54:AA:1415:G:N2	2.23	0.63
57:AD:197:SER:O	87:y:26:A:N6	2.31	0.63
7:I:197:LEU:HD12	7:I:198:PRO:HD2	1.81	0.63
54:AA:932:C:O2'	73:AT:2:PRO:O	2.16	0.63
51:r:35:PHE:O	51:r:54:THR:OG1	2.13	0.63
50:q:167:GLN:O	50:q:171:ARG:NE	2.32	0.63
54:AA:1116:A:OP2	55:AB:100:ARG:NH2	2.31	0.63
1:A:2196:A:O2'	1:A:2213:A:N1	2.32	0.62
5:F:76:ARG:NH1	42:h:106:ASP:OD1	2.30	0.62
42:h:88:ASP:OD1	42:h:124:ARG:NH2	2.32	0.62
9:K:21:LEU:HD21	9:K:34:MET:SD	2.39	0.62
61:AH:70:ASP:OD1	61:AH:71:ILE:N	2.31	0.62
84:A4:66:ASP:OD1	84:A4:67:LYS:N	2.33	0.62
54:AA:1107:U:O4	83:A3:128:LYS:NZ	2.32	0.62
1:A:2458:A:O2'	4:E:215:PHE:O	2.18	0.61
54:AA:905:A:O2'	54:AA:907:A:OP1	2.17	0.61
1:A:1753:A:OP1	43:i:118:TYR:OH	2.15	0.61
7:I:221:LEU:HD13	53:t4:86:LEU:HD13	1.82	0.61
31:6:252:CYS:SG	31:6:296:ARG:NH2	2.73	0.61
1:A:1672:C:O2'	18:T:143:ARG:O	2.13	0.61
31:6:367:ASP:OD1	31:6:370:ARG:NH1	2.33	0.61
55:AB:156:GLU:OE1	60:AG:163:HIS:ND1	2.34	0.61
70:AQ:80:ARG:NH1	76:AW:164:GLU:OE1	2.33	0.61
59:AF:155:MET:HE2	59:AF:155:MET:HA	1.82	0.61
54:AA:1454:G:OP2	60:AG:377:ARG:NH2	2.32	0.61
68:AO:221:GLN:NE2	75:AV:314:VAL:O	2.31	0.61
20:V:163:ASP:OD1	20:V:164:GLY:N	2.33	0.61
53:t1:64:ILE:HG23	53:t2:82:LEU:HD13	1.81	0.61
1:A:2069:U:O2'	1:A:2070:C:O4'	2.16	0.61
59:AF:111:MET:HE3	59:AF:111:MET:HA	1.83	0.60
30:5:100:LYS:NZ	30:5:271:TYR:O	2.32	0.60
53:t1:61:PRO:CG	53:t1:64:ILE:HD12	2.31	0.60
19:U:28:LEU:O	23:Y:114:THR:HG23	2.01	0.60
84:A4:363:ILE:HG22	84:A4:363:ILE:O	2.02	0.60
19:U:130:LEU:HD12	38:d:66:VAL:HG13	1.84	0.60
24:Z:53:HIS:ND1	48:o:47:TYR:OH	2.25	0.60
38:d:66:VAL:HG12	38:d:67:ILE:HG13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:AA:1308:U:O2'	56:AC:64:HIS:ND1	2.31	0.60
65:AL:86:ASP:OD1	65:AL:87:ASP:N	2.35	0.60
84:A4:156:ALA:O	84:A4:160:ARG:NH1	2.34	0.60
1:A:2346:U:OP1	52:s:223:ARG:NH2	2.34	0.59
81:A1:50:ARG:NH2	84:A4:94:TYR:O	2.35	0.59
53:t1:61:PRO:HG2	53:t1:64:ILE:HD12	1.82	0.59
1:A:2111:C:O2	1:A:2944:C:O2'	2.17	0.59
4:E:275:ARG:NH2	4:E:331:ASP:OD2	2.35	0.59
59:AF:119:LYS:NZ	77:AX:365:TRP:O	2.24	0.59
8:J:113:THR:OG1	8:J:116:HIS:ND1	2.35	0.59
13:O:57:GLU:OE2	13:O:105:THR:OG1	2.17	0.59
3:D:194:ASN:ND2	3:D:245:GLY:O	2.36	0.59
33:8:132:GLU:OE2	40:f:109:TYR:OH	2.21	0.59
60:AG:69:TYR:O	60:AG:135:GLN:NE2	2.36	0.59
31:6:179:VAL:HG23	31:6:179:VAL:O	2.03	0.59
1:A:2204:U:O2'	1:A:2207:A:N7	2.29	0.58
1:A:3166:U:O2'	4:E:269:TYR:O	2.19	0.58
84:A4:372:TYR:CE2	84:A4:400:LEU:HD21	2.37	0.58
1:A:2562:U:O2'	3:D:284:ARG:O	2.16	0.58
1:A:3068:G:OP2	1:A:3068:G:N2	2.34	0.58
75:AV:46:GLU:OE2	75:AV:74:ARG:NE	2.35	0.58
5:F:63:GLN:NE2	5:F:81:ASP:OD1	2.36	0.58
23:Y:69:ASP:OD1	23:Y:70:ASP:N	2.36	0.58
54:AA:1530:A:OP1	80:A0:29:ARG:NH2	2.36	0.58
1:A:2753:A:O2'	6:H:88:HIS:ND1	2.33	0.58
3:D:111:ARG:NH1	3:D:165:ASN:OD1	2.36	0.58
9:K:7:ALA:HB3	9:K:8:PRO:HD3	1.85	0.58
3:D:113:ARG:O	3:D:147:ARG:NH1	2.34	0.58
32:7:106:ALA:O	32:7:113:TRP:N	2.36	0.58
49:p:100:GLU:OE2	49:p:102:ARG:NH1	2.37	0.58
68:AO:217:ARG:NH2	68:AO:227:GLU:OE2	2.37	0.58
81:A1:60:MET:HE1	81:A1:80:ALA:O	2.04	0.58
84:A4:556:LYS:NZ	84:A4:560:GLU:OE2	2.32	0.57
1:A:2160:A:OP2	29:4:88:TRP:NE1	2.37	0.57
1:A:2456:U:OP1	13:O:16:ARG:NH1	2.35	0.57
41:g:84:TYR:OH	41:g:164:LYS:NZ	2.38	0.57
7:I:75:GLU:OE1	7:I:83:ARG:NH2	2.35	0.57
6:H:78:ARG:NH1	22:X:87:LEU:O	2.38	0.57
33:8:52:LYS:NZ	85:w:25:C:OP1	2.36	0.57
37:c:139:GLN:NE2	37:c:143:ASP:OD2	2.36	0.57
62:AI:166:ILE:HD11	70:AQ:19:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:138:CYS:SG	4:E:144:THR:HG23	2.44	0.56
75:AV:134:GLN:NE2	80:A0:108:ASN:OD1	2.38	0.56
1:A:2712:G:N7	94:A:3520:HOH:O	2.33	0.56
33:8:174:GLU:OE2	40:f:183:ARG:NH2	2.39	0.56
59:AF:193:ASP:OD1	59:AF:194:LYS:N	2.39	0.56
5:F:164:MET:HE1	43:i:70:PRO:HB2	1.86	0.56
37:c:80:GLN:O	37:c:210:ARG:NH2	2.39	0.56
54:AA:1199:G:N1	54:AA:1422:G:OP2	2.37	0.56
56:AC:58:ALA:HB1	56:AC:59:PRO:CD	2.35	0.56
75:AV:391:GLN:O	75:AV:395:GLN:N	2.35	0.56
1:A:2321:A:OP1	25:0:138:ARG:NH2	2.37	0.56
81:A1:235:ASN:ND2	81:A1:237:GLU:OE2	2.39	0.56
77:AX:123:ARG:NH2	77:AX:337:LEU:O	2.39	0.56
1:A:2909:G:OP1	26:1:63:ARG:NH2	2.37	0.56
20:V:20:ARG:NH1	20:V:42:ARG:O	2.39	0.56
57:AD:363:ALA:O	57:AD:367:GLY:N	2.38	0.56
61:AH:50:LEU:HD13	61:AH:53:ASP:O	2.06	0.56
20:V:133:ILE:HD12	20:V:145:ARG:HB2	1.88	0.56
32:7:70:VAL:O	32:7:70:VAL:HG23	2.06	0.55
54:AA:932:C:N3	73:AT:11:ARG:NH1	2.53	0.55
75:AV:40:TRP:O	75:AV:43:ARG:NH1	2.39	0.55
8:J:123:ILE:HD12	46:l:75:VAL:CG1	2.37	0.55
54:AA:713:C:N3	74:AU:27:ARG:N	2.54	0.55
1:A:2259:C:O2'	1:A:2261:C:OP2	2.22	0.55
33:8:186:GLN:OE1	47:m:95:LYS:NZ	2.38	0.55
42:h:57:SER:OG	42:h:136:ASP:OD2	2.24	0.55
61:AH:104:ILE:CG2	61:AH:148:LEU:HD21	2.37	0.55
18:T:85:ALA:O	18:T:139:SER:OG	2.24	0.55
30:5:165:GLN:NE2	30:5:179:VAL:HG21	2.22	0.55
61:AH:76:LEU:HD23	61:AH:145:LEU:HD12	1.88	0.55
73:AT:132:ARG:NH1	73:AT:136:LEU:O	2.39	0.55
4:E:202:GLN:NE2	4:E:301:ASP:OD1	2.40	0.55
32:7:326:GLU:OE2	32:7:326:GLU:N	2.35	0.55
54:AA:871:A:OP2	68:AO:97:ARG:NH2	2.40	0.55
60:AG:229:LEU:HD21	60:AG:241:VAL:HG11	1.86	0.55
62:AI:177:ASP:OD1	62:AI:179:THR:OG1	2.24	0.55
20:V:54:TRP:NE1	20:V:56:LEU:O	2.39	0.54
38:d:89:VAL:HG23	38:d:89:VAL:O	2.07	0.54
54:AA:1053:A:N1	54:AA:1100:C:O2'	2.37	0.54
1:A:2858:A:OP2	28:3:142:LYS:NZ	2.37	0.54
1:A:2826:G:OP1	21:W:49:ARG:NH2	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AD:307:LYS:NZ	71:AR:103:TYR:OH	2.39	0.54
35:a:90:GLN:NE2	35:a:94:THR:OG1	2.38	0.54
52:s:191:HIS:O	52:s:428:ARG:NH2	2.39	0.54
1:A:1871:A:N3	28:3:104:ARG:NH2	2.55	0.54
52:s:103:ASP:OD1	52:s:104:ARG:N	2.39	0.54
4:E:56:GLU:OE2	4:E:56:GLU:N	2.39	0.54
58:AE:31:ASP:OD1	74:AU:170:ARG:NH2	2.41	0.54
1:A:1990:G:OP1	3:D:269:ARG:NH2	2.35	0.54
7:I:221:LEU:CD1	53:t4:86:LEU:HD13	2.37	0.54
4:E:151:THR:HG23	4:E:171:PRO:HB2	1.89	0.54
7:I:39:VAL:HG21	48:o:22:ARG:HD2	1.90	0.54
24:Z:126:GLN:N	24:Z:126:GLN:OE1	2.41	0.54
54:AA:1104:A:OP2	94:AA:1904:HOH:O	2.18	0.54
54:AA:1117:A:OP2	72:AS:50:ARG:NE	2.41	0.54
4:E:47:THR:OG1	4:E:51:GLU:OE2	2.25	0.53
21:W:103:VAL:HG11	31:6:61:ALA:HB1	1.89	0.53
30:5:213:TRP:CZ3	30:5:222:VAL:HG23	2.44	0.53
51:r:117:GLU:HG3	51:r:180:LEU:HD12	1.91	0.53
54:AA:1488:C:O2	54:AA:1584:A:O2'	2.26	0.53
1:A:2256:U:O2'	17:S:118:ASN:ND2	2.42	0.53
20:V:56:LEU:HD13	20:V:86:VAL:HG21	1.91	0.53
1:A:1805:A:OP2	20:V:94:HIS:NE2	2.41	0.53
3:D:204:ALA:O	3:D:208:ARG:NH2	2.40	0.53
61:AH:136:MET:HG2	64:AK:123:ILE:HD13	1.90	0.53
1:A:1747:G:OP2	1:A:1749:C:N4	2.42	0.53
56:AC:106:ASP:OD1	56:AC:107:GLN:N	2.37	0.53
60:AG:263:ASP:OD1	60:AG:267:MET:N	2.39	0.53
1:A:1681:G:OP2	23:Y:230:LYS:NZ	2.29	0.53
18:T:102:PHE:O	25:0:104:LYS:NZ	2.42	0.53
30:5:98:LEU:O	30:5:270:ILE:HG23	2.09	0.53
1:A:2410:U:HO2'	30:5:96:HIS:HD1	1.56	0.53
14:P:139:ALA:O	31:6:155:TYR:OH	2.27	0.52
15:Q:77:SER:OG	15:Q:79:GLU:OE2	2.24	0.52
71:AR:276:VAL:HG11	71:AR:307:LEU:HD12	1.91	0.52
16:R:64:MET:HE1	18:T:204:HIS:CD2	2.43	0.52
62:AI:126:ILE:HD11	82:A2:46:ILE:CG2	2.39	0.52
52:s:150:LEU:HD21	52:s:402:TYR:CD2	2.44	0.52
59:AF:242:TRP:O	82:A2:84:ARG:NH2	2.43	0.52
68:AO:215:ARG:NH1	80:A0:90:ASP:OD1	2.41	0.52
77:AX:253:LEU:HD12	77:AX:255:MET:HE3	1.91	0.52
81:A1:258:SER:O	81:A1:262:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2472:A:O2'	1:A:2478:G:N7	2.26	0.52
66:AM:19:ILE:HB	66:AM:83:LEU:HD23	1.92	0.52
67:AN:58:CYS:SG	67:AN:81:LEU:HD22	2.50	0.52
32:7:186:ASP:OD1	32:7:187:SER:N	2.42	0.52
14:P:82:ARG:NE	14:P:95:GLU:OE2	2.37	0.52
32:7:216:PHE:CE2	32:7:257:ILE:HD11	2.45	0.52
75:AV:95:PHE:O	75:AV:98:SER:OG	2.27	0.52
80:A0:54:ALA:O	80:A0:58:VAL:HG23	2.10	0.52
60:AG:237:GLU:N	60:AG:237:GLU:OE2	2.43	0.52
75:AV:123:ASP:OD1	75:AV:124:LYS:N	2.43	0.51
8:J:163:GLU:OE1	8:J:163:GLU:N	2.38	0.51
52:s:419:LEU:O	52:s:423:HIS:ND1	2.41	0.51
60:AG:196:GLY:O	60:AG:248:VAL:N	2.43	0.51
1:A:2293:A:N6	11:M:37:GLU:OE1	2.42	0.51
3:D:174:VAL:HG22	3:D:186:ALA:O	2.10	0.51
36:b:44:ARG:NH1	48:o:99:LYS:O	2.43	0.51
49:p:135:LEU:HD21	49:p:157:MET:HE1	1.92	0.51
53:t:61:PRO:HD2	53:t:64:ILE:HD12	1.93	0.51
74:AU:106:MET:HE2	74:AU:106:MET:HA	1.92	0.51
31:6:372:SER:HB2	49:p:95:VAL:HG11	1.92	0.51
78:AY:250:ILE:O	84:A4:358:ARG:NE	2.43	0.51
3:D:257:ILE:O	3:D:262:ARG:NH1	2.38	0.51
15:Q:61:VAL:HG12	75:AV:87:HIS:HE1	1.76	0.51
54:AA:812:A:O2'	54:AA:814:A:N1	2.43	0.51
76:AW:87:SER:OG	76:AW:90:THR:OG1	2.28	0.51
30:5:98:LEU:HD13	30:5:272:ASP:HB2	1.92	0.51
66:AM:29:ARG:HD2	66:AM:57:LEU:HD12	1.92	0.51
30:5:105:TYR:CE1	30:5:262:ILE:HD13	2.46	0.51
47:m:119:TYR:OH	81:A1:232:GLU:OE2	2.16	0.50
5:F:220:ASP:OD1	5:F:221:LEU:N	2.42	0.50
30:5:165:GLN:NE2	30:5:175:THR:HG22	2.26	0.50
75:AV:35:VAL:HG22	75:AV:35:VAL:O	2.11	0.50
50:q:61:PHE:O	50:q:65:GLY:N	2.39	0.50
54:AA:1106:C:O2'	54:AA:1108:C:OP2	2.25	0.50
61:AH:136:MET:CG	64:AK:123:ILE:HD13	2.40	0.50
7:I:221:LEU:HD22	53:t4:86:LEU:HB3	1.94	0.50
80:A0:79:LEU:HD22	80:A0:94:TYR:CD1	2.47	0.50
53:t1:64:ILE:CG2	53:t2:82:LEU:HD13	2.42	0.50
1:A:1822:U:O2	1:A:2707:A:O2'	2.29	0.50
52:s:242:ARG:NH2	52:s:290:ASP:OD2	2.44	0.50
69:AP:141:ARG:O	70:AQ:28:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1710:A:N3	30:5:72:ARG:NH2	2.59	0.49
11:M:261:ASP:CG	49:p:41:SER:HG	2.20	0.49
53:t1:60:TYR:CE1	53:t2:85:LEU:HD21	2.47	0.49
63:AJ:78:ARG:NH1	63:AJ:117:ASP:OD2	2.45	0.49
54:AA:1004:G:O2'	62:AI:98:GLN:OE1	2.08	0.49
61:AH:155:VAL:HG21	81:A1:129:PHE:HB2	1.94	0.49
80:A0:41:LEU:HD13	80:A0:55:TRP:CD1	2.47	0.49
1:A:1742:G:O2'	1:A:1754:G:O6	2.27	0.49
69:AP:73:ASP:OD1	69:AP:74:TYR:N	2.46	0.49
80:A0:42:THR:HG22	80:A0:49:ARG:HG2	1.94	0.49
84:A4:471:ILE:HD11	84:A4:500:LEU:HD23	1.94	0.49
1:A:1892:A:N1	31:6:376:THR:OG1	2.39	0.49
1:A:2718:C:OP1	25:0:82:LYS:NZ	2.40	0.49
31:6:273:PHE:HB3	31:6:311:MET:HG2	1.93	0.49
38:d:81:THR:HG22	38:d:82:ALA:N	2.28	0.49
56:AC:113:ARG:NH2	61:AH:166:GLU:OE2	2.38	0.49
47:m:54:VAL:HG12	47:m:72:ARG:O	2.13	0.49
47:m:82:ASP:O	47:m:89:ARG:NH2	2.46	0.49
54:AA:944:U:OP1	94:AA:1905:HOH:O	2.19	0.49
54:AA:994:A:O2'	59:AF:166:ARG:NH1	2.46	0.49
65:AL:85:VAL:HG23	65:AL:90:LYS:HG3	1.93	0.49
1:A:3211:C:HO2'	1:A:3212:C:H5	1.61	0.49
4:E:97:VAL:HG22	4:E:98:GLY:N	2.28	0.49
58:AE:26:ILE:HG23	58:AE:36:VAL:HG21	1.94	0.49
1:A:2531:U:O4	3:D:246:ARG:NH2	2.46	0.49
32:7:286:LEU:HD21	32:7:296:ARG:HE	1.77	0.49
54:AA:1048:C:O2'	65:AL:196:TYR:O	2.30	0.49
15:Q:146:GLY:O	15:Q:148:THR:HG23	2.13	0.49
80:A0:41:LEU:HD13	80:A0:55:TRP:CG	2.48	0.49
54:AA:1525:C:O5'	75:AV:105:ARG:NH1	2.45	0.49
26:1:35:ASN:OD1	26:1:36:ARG:N	2.46	0.48
30:5:229:ARG:NH2	30:5:231:SER:OG	2.47	0.48
52:s:332:LEU:HD21	52:s:359:ALA:HB2	1.96	0.48
53:t1:76:LEU:H	53:t4:68:VAL:HG11	1.77	0.48
76:AW:129:VAL:HG23	76:AW:130:ASP:N	2.28	0.48
77:AX:74:ASP:OD2	77:AX:147:LYS:NZ	2.39	0.48
1:A:1823:A:OP2	35:a:127:GLY:N	2.47	0.48
1:A:2374:A:N1	52:s:97:THR:OG1	2.44	0.48
33:8:172:GLU:OE1	40:f:183:ARG:NH1	2.46	0.48
39:e:156:ASN:OD1	39:e:157:LEU:N	2.46	0.48
39:e:192:LEU:O	39:e:198:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:h:69:ARG:NH1	42:h:107:ASP:OD2	2.43	0.48
20:V:195:GLN:OE1	20:V:195:GLN:N	2.44	0.48
24:Z:120:LYS:NZ	48:o:44:GLU:OE2	2.38	0.48
30:5:236:LEU:HD21	30:5:289:HIS:CD2	2.48	0.48
54:AA:843:G:N2	54:AA:846:A:OP2	2.43	0.48
77:AX:108:LEU:HD23	77:AX:141:VAL:HG21	1.94	0.48
77:AX:272:THR:OG1	77:AX:282:ILE:O	2.26	0.48
1:A:2220:A:OP2	51:r:103:LYS:NZ	2.45	0.48
19:U:153:LEU:HD23	38:d:222:LEU:HB2	1.94	0.48
32:7:276:PHE:HB2	32:7:304:VAL:HG22	1.96	0.48
81:A1:255:ASN:N	81:A1:259:GLU:OE2	2.46	0.48
1:A:1906:G:OP1	94:A:3502:HOH:O	2.19	0.48
1:A:1958:G:O2'	1:A:1959:C:O5'	2.29	0.48
2:B:1643:A:OP1	31:6:114:ARG:NH2	2.47	0.48
20:V:186:THR:HG22	20:V:186:THR:O	2.13	0.48
58:AE:63:TYR:OH	69:AP:118:GLY:O	2.26	0.48
60:AG:143:ASP:OD1	60:AG:144:GLY:N	2.46	0.48
1:A:1787:G:N2	1:A:1790:A:OP2	2.45	0.48
71:AR:317:ALA:O	71:AR:321:ALA:N	2.46	0.48
54:AA:1289:G:O2'	54:AA:1297:G:OP2	2.26	0.48
68:AO:208:PRO:HG2	68:AO:213:LEU:HD21	1.94	0.48
9:K:169:LEU:HD11	51:r:88:LEU:HD13	1.95	0.47
17:S:132:LYS:NZ	44:j:48:ASP:OD1	2.32	0.47
39:e:48:LEU:HD23	39:e:177:GLU:HA	1.95	0.47
59:AF:46:ILE:HG22	59:AF:46:ILE:O	2.14	0.47
66:AM:55:ASP:OD2	73:AT:146:GLN:NE2	2.47	0.47
7:I:200:LEU:HD11	7:I:204:GLN:HE21	1.79	0.47
17:S:101:PHE:HE2	17:S:116:ILE:HD13	1.79	0.47
20:V:48:PRO:HD3	23:Y:234:LEU:HD21	1.95	0.47
75:AV:269:SER:HB2	75:AV:273:ILE:HD12	1.97	0.47
84:A4:480:ASP:O	84:A4:484:SER:OG	2.33	0.47
5:F:220:ASP:O	5:F:245:ALA:N	2.46	0.47
1:A:2059:C:N3	94:A:3523:HOH:O	2.35	0.47
1:A:2364:C:OP2	19:U:78:LYS:NZ	2.47	0.47
6:H:110:ASP:OD1	6:H:111:LEU:N	2.48	0.47
23:Y:194:TYR:OH	30:5:64:MET:O	2.27	0.47
38:d:100:LEU:HD13	38:d:103:GLU:OE1	2.14	0.47
39:e:185:ARG:NH2	39:e:207:ASN:OD1	2.47	0.47
49:p:164:THR:O	49:p:164:THR:HG22	2.14	0.47
56:AC:123:VAL:HG23	56:AC:157:THR:HG22	1.97	0.47
61:AH:89:ASP:OD1	61:AH:141:ARG:NH1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AI:129:GLN:NE2	62:AI:167:MET:SD	2.86	0.47
84:A4:508:VAL:HG12	84:A4:508:VAL:O	2.15	0.47
11:M:156:VAL:O	11:M:176:THR:HA	2.15	0.47
71:AR:162:SER:HB2	71:AR:165:ILE:HD12	1.97	0.47
14:P:144:MET:HE3	14:P:170:VAL:HG11	1.97	0.47
76:AW:162:VAL:HG12	76:AW:162:VAL:O	2.14	0.47
8:J:123:ILE:HD12	46:l:75:VAL:HG13	1.96	0.47
15:Q:61:VAL:O	75:AV:87:HIS:ND1	2.47	0.47
23:Y:83:ALA:N	34:9:74:VAL:O	2.42	0.47
33:8:202:VAL:O	33:8:203:GLU:CB	2.63	0.47
38:d:202:MET:HG2	38:d:203:MET:HG2	1.97	0.47
56:AC:58:ALA:HB1	56:AC:59:PRO:HD2	1.97	0.47
67:AN:88:VAL:HG13	67:AN:88:VAL:O	2.15	0.47
1:A:1906:G:N7	94:A:3522:HOH:O	2.35	0.46
1:A:2135:A:N3	1:A:2135:A:H2'	2.30	0.46
53:t1:64:ILE:HD11	53:t2:78:GLU:CG	2.45	0.46
59:AF:159:VAL:HG23	59:AF:172:VAL:HG21	1.96	0.46
23:Y:154:ARG:O	23:Y:158:THR:OG1	2.24	0.46
53:t1:60:TYR:CZ	53:t2:85:LEU:HD21	2.51	0.46
19:U:66:ALA:HB3	52:s:100:LEU:HD11	1.97	0.46
9:K:60:MET:HE3	9:K:131:GLU:HA	1.97	0.46
12:N:140:MET:HE2	12:N:140:MET:HA	1.97	0.46
7:I:142:ASN:ND2	53:t1:48:LEU:O	2.48	0.46
39:e:90:ARG:NH1	39:e:115:LEU:O	2.47	0.46
66:AM:63:GLU:OE1	71:AR:157:VAL:HG21	2.14	0.46
1:A:2137:C:OP2	24:Z:77:ARG:NH1	2.48	0.46
1:A:2665:U:OP2	13:O:17:ARG:NE	2.44	0.46
1:A:2737:U:O2'	1:A:3084:A:N3	2.48	0.46
4:E:109:LEU:N	4:E:117:HIS:O	2.49	0.46
14:P:144:MET:HE3	14:P:170:VAL:CG1	2.46	0.46
58:AE:94:VAL:HG11	69:AP:117:MET:HE1	1.98	0.46
75:AV:34:TYR:HA	75:AV:372:ILE:HD11	1.97	0.46
81:A1:56:ARG:NH1	84:A4:91:ASP:OD2	2.46	0.46
1:A:1853:A:OP2	17:S:177:ARG:NH2	2.46	0.46
20:V:180:GLU:OE1	20:V:180:GLU:N	2.45	0.46
47:m:112:ASP:OD1	47:m:113:ASP:N	2.49	0.46
73:AT:42:GLU:OE1	73:AT:45:ARG:NH2	2.43	0.46
9:K:15:ALA:CB	37:c:269:LEU:HD22	2.46	0.46
19:U:75:GLY:N	19:U:91:ASP:OD1	2.38	0.46
60:AG:312:GLN:OE1	60:AG:345:ARG:NH2	2.48	0.46
27:2:68:ARG:O	27:2:71:SER:OG	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:5:351:VAL:HG22	30:5:381:LEU:HD23	1.98	0.46
57:AD:263:ASP:OD1	57:AD:264:ARG:N	2.49	0.46
81:A1:278:ILE:HG13	81:A1:278:ILE:O	2.15	0.46
1:A:3201:A:H2'	1:A:3202:U:O4'	2.16	0.46
16:R:141:ILE:HG22	35:a:51:LEU:HD12	1.98	0.46
54:AA:1340:C:O2'	79:AZ:101:ARG:NH2	2.49	0.46
12:N:123:ARG:NH2	12:N:162:GLU:OE1	2.47	0.45
65:AL:126:GLU:HG2	65:AL:177:VAL:HG11	1.98	0.45
1:A:2406:A:O2'	30:5:110:ARG:NH1	2.48	0.45
32:7:298:GLN:NE2	32:7:320:SER:O	2.49	0.45
35:a:142:ARG:O	35:a:142:ARG:HG3	2.16	0.45
34:9:55:GLU:N	34:9:55:GLU:OE1	2.49	0.45
39:e:147:THR:HG22	39:e:147:THR:O	2.16	0.45
55:AB:222:ILE:HD13	55:AB:236:VAL:HB	1.97	0.45
12:N:188:LYS:NZ	12:N:198:MET:HE2	2.30	0.45
4:E:120:THR:OG1	4:E:287:GLY:O	2.28	0.45
7:I:45:GLN:NE2	48:o:25:ARG:O	2.46	0.45
20:V:55:TYR:O	20:V:145:ARG:NH2	2.49	0.45
30:5:385:HIS:O	30:5:404:VAL:N	2.48	0.45
40:f:147:ASP:O	47:m:72:ARG:NH1	2.48	0.45
85:w:46:A:O2'	85:w:48:U:O5'	2.29	0.45
20:V:167:PRO:O	34:9:77:LEU:HD21	2.17	0.45
47:m:115:HIS:NE2	79:AZ:17:ARG:O	2.49	0.45
1:A:1800:G:N1	1:A:1803:A:OP2	2.49	0.45
5:F:114:THR:O	5:F:156:ARG:NH1	2.50	0.45
11:M:250:ASP:OD1	11:M:251:GLU:N	2.49	0.45
38:d:94:ASP:HA	38:d:97:ILE:HD12	1.98	0.45
1:A:3230:G:N7	4:E:156:ARG:NH1	2.62	0.45
19:U:153:LEU:HD23	38:d:222:LEU:CB	2.46	0.45
49:p:109:GLU:OE1	49:p:109:GLU:N	2.50	0.45
54:AA:1279:C:O2'	54:AA:1296:A:N1	2.46	0.45
54:AA:1378:C:O2	77:AX:389:SER:OG	2.30	0.45
59:AF:207:HIS:NE2	59:AF:211:GLU:OE2	2.49	0.45
84:A4:166:VAL:HG23	84:A4:167:LYS:N	2.32	0.45
85:w:3:G:N2	85:w:71:C:O2	2.50	0.45
85:w:9:A:O2'	85:w:10:G:N7	2.42	0.45
53:t1:68:VAL:HG13	53:t2:86:LEU:HD23	1.98	0.45
1:A:3202:U:O2	4:E:303:LYS:NZ	2.50	0.44
20:V:169:THR:HG22	20:V:169:THR:O	2.17	0.44
53:t2:75:THR:O	53:t2:79:ILE:N	2.48	0.44
54:AA:922:C:H2'	54:AA:923:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:AF:84:SER:OG	77:AX:379:GLU:OE1	2.23	0.44
1:A:2248:U:OP1	16:R:99:ARG:NH2	2.44	0.44
30:5:173:ARG:NH1	30:5:348:ASP:O	2.48	0.44
9:K:28:PRO:HG3	9:K:65:ILE:HD12	1.99	0.44
52:s:174:LEU:HB3	52:s:175:PRO:HD3	2.00	0.44
56:AC:115:ASN:ND2	78:AY:309:LYS:O	2.50	0.44
71:AR:69:THR:OG1	71:AR:72:ASP:OD1	2.33	0.44
84:A4:58:VAL:O	84:A4:58:VAL:HG23	2.17	0.44
75:AV:167:VAL:HG13	75:AV:172:ALA:HB3	1.98	0.44
1:A:2144:A:OP1	16:R:57:ARG:NH1	2.50	0.44
12:N:218:ILE:HG23	12:N:223:MET:HB2	2.00	0.44
54:AA:806:C:OP2	54:AA:807:A:N6	2.45	0.44
20:V:49:ILE:HD11	20:V:117:HIS:NE2	2.33	0.44
72:AS:98:ARG:NH2	72:AS:128:GLU:OE1	2.44	0.44
1:A:2416:U:OP2	52:s:165:ARG:NH1	2.51	0.44
1:A:2755:A:OP2	6:H:91:LYS:NZ	2.41	0.44
5:F:84:PRO:O	5:F:88:ALA:N	2.48	0.44
10:L:69:VAL:HG23	10:L:89:HIS:CD2	2.53	0.44
17:S:199:GLU:N	17:S:199:GLU:OE1	2.50	0.44
20:V:188:VAL:O	20:V:188:VAL:HG23	2.17	0.44
1:A:1737:A:H61	1:A:1760:G:H1'	1.82	0.44
54:AA:1264:C:H1'	61:AH:124:VAL:HG13	2.00	0.44
60:AG:200:LEU:HD11	60:AG:204:GLU:HG2	1.99	0.44
32:7:148:MET:HE2	32:7:257:ILE:HG13	2.00	0.43
39:e:55:ARG:NH1	39:e:149:LEU:O	2.51	0.43
41:g:129:SER:O	41:g:133:GLY:N	2.46	0.43
54:AA:1155:G:OP1	83:A3:144:ARG:NH1	2.47	0.43
56:AC:57:HIS:HB2	56:AC:66:LYS:HD2	1.99	0.43
80:A0:218:VAL:HG12	80:A0:218:VAL:O	2.16	0.43
3:D:246:ARG:NH2	3:D:250:VAL:HG13	2.32	0.43
11:M:261:ASP:OD1	11:M:262:PRO:HD2	2.19	0.43
49:p:111:ILE:O	49:p:116:ARG:NH2	2.51	0.43
30:5:351:VAL:HG22	30:5:381:LEU:CD2	2.49	0.43
57:AD:134:GLU:OE2	57:AD:160:ARG:NH1	2.43	0.43
1:A:1828:A:O2'	1:A:2684:C:H5	2.01	0.43
14:P:85:ARG:NH1	14:P:157:SER:OG	2.52	0.43
45:k:8:LEU:HG	45:k:94:ILE:HG21	2.00	0.43
60:AG:206:GLU:O	60:AG:210:VAL:N	2.52	0.43
78:AY:393:GLN:O	78:AY:393:GLN:HG3	2.19	0.43
1:A:2870:G:OP1	28:3:140:ARG:NE	2.49	0.43
11:M:274:VAL:HG11	50:q:75:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:AA:1563:U:O2'	87:y:17:A:OP1	2.27	0.43
68:AO:73:VAL:O	68:AO:109:ARG:NH2	2.50	0.43
71:AR:70:PHE:O	71:AR:76:GLN:NE2	2.52	0.43
75:AV:236:LEU:HD21	75:AV:323:GLU:HB3	2.01	0.43
5:F:234:THR:O	50:q:25:TYR:N	2.52	0.43
7:I:132:LYS:HB2	7:I:133:PRO:HD3	1.99	0.43
33:8:90:THR:O	33:8:90:THR:HG23	2.18	0.43
33:8:202:VAL:O	33:8:203:GLU:HB3	2.18	0.43
36:b:33:VAL:HG12	36:b:43:ALA:HB1	2.00	0.43
54:AA:1581:G:N2	54:AA:1584:A:OP2	2.52	0.43
78:AY:332:ILE:HG23	81:A1:211:ARG:NH1	2.33	0.43
1:A:2415:C:O2'	1:A:2416:U:O4'	2.37	0.43
19:U:38:ASP:OD1	19:U:38:ASP:N	2.51	0.43
20:V:55:TYR:HB2	20:V:133:ILE:HD11	2.00	0.43
38:d:73:ASP:OD1	38:d:73:ASP:N	2.50	0.43
60:AG:200:LEU:HD13	60:AG:246:ARG:CZ	2.48	0.43
1:A:1782:G:O6	5:F:121:ARG:NE	2.48	0.43
1:A:2088:U:O2'	28:3:188:VAL:HG11	2.18	0.43
1:A:2888:A:O2'	21:W:85:LYS:HD2	2.18	0.43
44:j:45:GLU:OE1	44:j:63:GLN:NE2	2.47	0.43
51:r:70:CYS:SG	91:r:201:FES:S1	3.17	0.43
83:A3:170:GLU:HG2	83:A3:191:THR:HG21	2.00	0.43
1:A:1834:U:C4	18:T:200:ARG:HA	2.54	0.42
1:A:2448:G:OP1	52:s:222:ARG:NE	2.50	0.42
39:e:149:LEU:HD21	39:e:254:TRP:CE2	2.54	0.42
55:AB:121:THR:OG1	55:AB:237:PRO:O	2.33	0.42
5:F:211:ARG:HE	42:h:55:LEU:HD11	1.84	0.42
39:e:235:LYS:NZ	40:f:172:GLU:OE2	2.46	0.42
68:AO:214:SER:OG	75:AV:318:ASP:OD1	2.26	0.42
68:AO:221:GLN:OE1	75:AV:313:LEU:HD11	2.19	0.42
84:A4:302:VAL:HG23	84:A4:303:CYS:N	2.35	0.42
1:A:1991:A:H5''	1:A:1992:C:OP1	2.19	0.42
19:U:11:ARG:HE	20:V:211:LYS:HB2	1.84	0.42
19:U:19:VAL:O	19:U:19:VAL:HG13	2.20	0.42
30:5:213:TRP:HZ3	30:5:222:VAL:HG23	1.83	0.42
50:q:162:GLU:O	50:q:162:GLU:HG2	2.19	0.42
56:AC:42:VAL:HG21	56:AC:55:GLU:HG2	2.01	0.42
1:A:2446:A:OP1	52:s:65:ARG:NH2	2.53	0.42
22:X:227:PHE:O	22:X:231:VAL:HG23	2.19	0.42
34:9:16:ASP:OD1	34:9:16:ASP:N	2.51	0.42
1:A:2525:C:OP2	1:A:2526:C:O2'	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:53:THR:N	6:H:86:THR:HG1	2.18	0.42
23:Y:142:LEU:O	23:Y:142:LEU:HD23	2.20	0.42
1:A:2131:A:OP1	48:o:23:ARG:NH1	2.51	0.42
1:A:2546:G:N7	94:A:3527:HOH:O	2.37	0.42
1:A:3082:G:N2	1:A:3085:A:OP2	2.38	0.42
28:3:152:LYS:HD3	31:6:357:PHE:CE2	2.55	0.42
1:A:2310:G:O2'	1:A:2675:G:O6	2.30	0.42
17:S:136:VAL:O	17:S:136:VAL:HG13	2.18	0.42
29:4:68:ASN:OD1	29:4:101:ARG:NH1	2.40	0.42
36:b:85:ARG:NE	36:b:87:GLU:OE2	2.52	0.42
51:r:124:ARG:NH1	51:r:152:THR:O	2.50	0.42
1:A:2522:U:O4	30:5:32:GLU:N	2.45	0.42
4:E:102:LEU:HD21	4:E:294:ASN:HA	2.01	0.42
40:f:104:GLU:OE2	47:m:45:ARG:NH1	2.53	0.42
62:AI:153:GLY:O	62:AI:158:ARG:NH2	2.47	0.42
70:AQ:83:PRO:HA	76:AW:108:VAL:HG21	2.02	0.42
84:A4:164:ARG:NH1	84:A4:198:TYR:OH	2.52	0.42
1:A:2052:A:H2'	1:A:2053:U:O4'	2.20	0.42
23:Y:142:LEU:HD23	23:Y:142:LEU:C	2.45	0.42
63:AJ:95:ILE:HD12	63:AJ:95:ILE:N	2.35	0.42
20:V:105:ARG:NH2	38:d:171:ASP:OD1	2.53	0.42
50:q:169:ASP:N	50:q:170:PRO:HD2	2.34	0.42
61:AH:184:ILE:O	61:AH:184:ILE:HG22	2.19	0.42
77:AX:268:LEU:O	77:AX:294:ARG:NH1	2.41	0.42
86:x:8:U:O2'	86:x:46:A:O2'	2.30	0.42
1:A:2071:U:O2'	31:6:28:ARG:NH1	2.53	0.41
17:S:135:LEU:HD23	17:S:135:LEU:C	2.44	0.41
52:s:178:ASP:HA	52:s:239:ASN:HD21	1.84	0.41
52:s:362:THR:OG1	52:s:366:TYR:O	2.36	0.41
58:AE:3:ARG:NH1	58:AE:67:ASP:OD2	2.45	0.41
2:B:1643:A:H2'	2:B:1644:G:O4'	2.20	0.41
10:L:42:ASP:OD1	10:L:44:SER:OG	2.35	0.41
13:O:55:TYR:OH	15:Q:268:ASP:OD1	2.30	0.41
26:1:54:VAL:HG12	26:1:55:LEU:N	2.35	0.41
70:AQ:72:ILE:HD13	82:A2:104:LEU:HD21	2.02	0.41
5:F:281:ARG:NH2	11:M:128:THR:OG1	2.52	0.41
19:U:18:ARG:NH2	20:V:206:GLU:OE1	2.53	0.41
54:AA:1227:G:OP1	61:AH:128:LYS:NZ	2.53	0.41
55:AB:103:GLU:N	55:AB:104:PRO:CD	2.83	0.41
58:AE:109:VAL:HG23	58:AE:109:VAL:O	2.20	0.41
1:A:2506:A:H1'	1:A:2601:A:N6	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:6:239:ASN:OD1	31:6:275:GLN:NE2	2.44	0.41
1:A:1962:A:OP2	1:A:2501:C:N4	2.52	0.41
4:E:50:ASP:O	13:O:138:ARG:NH2	2.53	0.41
7:I:85:GLU:O	7:I:89:VAL:HG23	2.19	0.41
9:K:35:ALA:O	9:K:39:LEU:HG	2.21	0.41
68:AO:120:VAL:HG13	68:AO:163:LEU:HD13	2.02	0.41
78:AY:319:ALA:O	81:A1:164:ARG:NH1	2.54	0.41
1:A:3089:A:H3'	1:A:3090:G:C5'	2.50	0.41
13:O:64:LYS:NZ	13:O:100:GLN:O	2.54	0.41
13:O:94:ALA:HB3	13:O:95:PRO:HD3	2.01	0.41
20:V:190:CYS:SG	20:V:191:LEU:N	2.89	0.41
22:X:21:CYS:SG	22:X:212:ILE:HD11	2.60	0.41
36:b:26:LEU:HD22	36:b:105:ALA:HA	2.02	0.41
77:AX:62:GLN:OE1	77:AX:62:GLN:N	2.39	0.41
77:AX:203:LYS:O	77:AX:250:GLN:NE2	2.51	0.41
1:A:1749:C:OP2	1:A:2899:C:O2'	2.32	0.41
7:I:230:THR:HG23	53:t5:86:LEU:HD21	2.03	0.41
31:6:235:TRP:CZ2	31:6:237:LEU:HD11	2.56	0.41
57:AD:296:LEU:C	57:AD:296:LEU:HD12	2.45	0.41
77:AX:153:LEU:HD21	77:AX:244:LEU:CD2	2.50	0.41
79:AZ:20:GLY:O	81:A1:211:ARG:NH2	2.46	0.41
1:A:1703:C:OP1	34:9:34:LYS:NZ	2.51	0.41
8:J:133:GLN:HB3	8:J:135:VAL:HG13	2.02	0.41
17:S:164:THR:O	17:S:190:GLN:N	2.50	0.41
19:U:26:ILE:HG22	19:U:44:ILE:HG22	2.03	0.41
31:6:184:LEU:N	49:p:190:GLN:O	2.52	0.41
52:s:211:VAL:HG22	52:s:230:ARG:HG2	2.03	0.41
71:AR:85:LEU:CD2	71:AR:119:VAL:HG13	2.51	0.41
4:E:54:SER:O	4:E:58:VAL:HG23	2.20	0.41
30:5:213:TRP:CH2	30:5:222:VAL:HG23	2.56	0.41
33:8:96:ASP:OD1	33:8:97:LYS:N	2.54	0.41
34:9:16:ASP:OD1	34:9:25:ARG:NH1	2.54	0.41
46:l:58:ASP:OD1	46:l:59:PRO:HD2	2.21	0.41
59:AF:199:THR:HG22	59:AF:204:LYS:HG3	2.03	0.41
61:AH:84:ASP:OD1	61:AH:85:LYS:N	2.54	0.41
65:AL:181:ILE:HG23	65:AL:185:LEU:HD12	2.02	0.41
71:AR:315:GLN:OE1	71:AR:315:GLN:HA	2.21	0.41
84:A4:200:ASP:OD2	84:A4:243:ASN:N	2.54	0.41
1:A:2179:A:N6	1:A:2180:A:H62	2.18	0.41
5:F:77:VAL:O	5:F:77:VAL:HG12	2.20	0.41
7:I:50:VAL:O	12:N:211:ASN:ND2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:5:112:ARG:HG2	30:5:304:LEU:HD21	2.01	0.41
30:5:165:GLN:HG2	30:5:166:THR:HG23	2.03	0.41
32:7:99:TYR:O	32:7:103:SER:OG	2.29	0.41
46:l:111:ASP:O	46:l:114:SER:OG	2.33	0.41
53:t1:68:VAL:HG22	53:t2:82:LEU:HD12	2.02	0.41
54:AA:760:A:N1	54:AA:780:C:O2'	2.40	0.41
66:AM:123:GLN:O	66:AM:127:ALA:N	2.47	0.41
1:A:1830:G:H5''	36:b:2:THC:HG21	2.03	0.40
1:A:3186:U:H2'	1:A:3188:U:OP1	2.21	0.40
5:F:227:PRO:O	5:F:231:VAL:HG23	2.20	0.40
31:6:144:GLY:N	31:6:145:PRO:CD	2.83	0.40
49:p:95:VAL:HG12	49:p:141:ARG:HG2	2.02	0.40
51:r:81:TYR:OH	51:r:111:GLU:OE2	2.30	0.40
59:AF:234:ARG:HB3	82:A2:53:MET:HE1	2.03	0.40
7:I:200:LEU:N	7:I:201:PRO:CD	2.85	0.40
8:J:123:ILE:HD12	46:l:75:VAL:HG12	2.03	0.40
42:h:111:VAL:HG22	42:h:112:VAL:N	2.36	0.40
67:AN:6:SER:OG	67:AN:69:LEU:O	2.29	0.40
71:AR:276:VAL:CG1	71:AR:307:LEU:HD12	2.51	0.40
2:B:1625:A:OP1	31:6:56:ARG:NH2	2.50	0.40
4:E:157:LYS:HB2	4:E:162:LEU:HD21	2.03	0.40
9:K:143:GLU:OE1	36:b:136:LYS:NZ	2.50	0.40
49:p:97:SER:O	49:p:146:ASN:ND2	2.54	0.40
53:t2:60:TYR:N	53:t2:61:PRO:CD	2.84	0.40
54:AA:894:C:N4	63:AJ:117:ASP:OD2	2.55	0.40
80:A0:79:LEU:HD12	80:A0:147:GLU:HG3	2.04	0.40
1:A:2234:C:O2'	1:A:2688:C:O2'	2.35	0.40
1:A:2667:U:H2'	1:A:2668:A:O4'	2.22	0.40
3:D:246:ARG:HH22	3:D:250:VAL:HG13	1.86	0.40
17:S:115:LEU:N	36:b:118:PRO:O	2.44	0.40
39:e:199:ASN:O	39:e:241:GLY:HA3	2.21	0.40
60:AG:299:ASP:OD2	77:AX:385:ASN:ND2	2.54	0.40
71:AR:275:PHE:O	71:AR:279:LYS:N	2.54	0.40
80:A0:80:VAL:O	80:A0:80:VAL:HG23	2.21	0.40
83:A3:177:TRP:CD1	83:A3:177:TRP:C	2.99	0.40
4:E:345:ILE:O	15:Q:172:GLN:NE2	2.54	0.40
8:J:20:ILE:HD11	8:J:42:ARG:HG3	2.04	0.40
17:S:102:ALA:O	17:S:103:SER:OG	2.32	0.40
41:g:35:TYR:CD2	50:q:71:VAL:HG11	2.56	0.40
42:h:110:HIS:CE1	42:h:134:ILE:HD12	2.57	0.40
52:s:80:LEU:HD21	52:s:341:MET:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:AA:1567:A:OP2	94:AA:1906:HOH:O	2.22	0.40
61:AH:163:ASN:HB3	81:A1:114:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	236/305 (77%)	234 (99%)	2 (1%)	0	100	100
4	E	303/348 (87%)	296 (98%)	7 (2%)	0	100	100
5	F	250/311 (80%)	249 (100%)	1 (0%)	0	100	100
6	H	95/267 (36%)	94 (99%)	1 (1%)	0	100	100
7	I	210/261 (80%)	205 (98%)	5 (2%)	0	100	100
8	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
9	K	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
10	L	113/145 (78%)	111 (98%)	2 (2%)	0	100	100
11	M	289/296 (98%)	287 (99%)	2 (1%)	0	100	100
12	N	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
13	O	152/175 (87%)	151 (99%)	1 (1%)	0	100	100
14	P	142/180 (79%)	141 (99%)	1 (1%)	0	100	100
15	Q	236/292 (81%)	235 (100%)	1 (0%)	0	100	100
16	R	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
17	S	159/205 (78%)	159 (100%)	0	0	100	100
18	T	164/206 (80%)	162 (99%)	2 (1%)	0	100	100
19	U	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
20	V	203/216 (94%)	203 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	W	114/148 (77%)	114 (100%)	0	0	100	100
22	X	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
23	Y	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
24	Z	120/161 (74%)	117 (98%)	3 (2%)	0	100	100
25	0	108/188 (57%)	108 (100%)	0	0	100	100
26	1	53/65 (82%)	53 (100%)	0	0	100	100
27	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
28	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
29	4	36/103 (35%)	35 (97%)	1 (3%)	0	100	100
30	5	392/423 (93%)	387 (99%)	5 (1%)	0	100	100
31	6	352/380 (93%)	339 (96%)	13 (4%)	0	100	100
32	7	292/338 (86%)	287 (98%)	5 (2%)	0	100	100
33	8	155/206 (75%)	154 (99%)	1 (1%)	0	100	100
34	9	122/137 (89%)	122 (100%)	0	0	100	100
35	a	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
36	b	148/214 (69%)	144 (97%)	4 (3%)	0	100	100
37	c	282/332 (85%)	276 (98%)	6 (2%)	0	100	100
38	d	257/306 (84%)	252 (98%)	5 (2%)	0	100	100
39	e	224/279 (80%)	220 (98%)	4 (2%)	0	100	100
40	f	153/212 (72%)	151 (99%)	2 (1%)	0	100	100
41	g	132/166 (80%)	129 (98%)	3 (2%)	0	100	100
42	h	108/158 (68%)	105 (97%)	3 (3%)	0	100	100
43	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
44	j	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
45	k	99/111 (89%)	99 (100%)	0	0	100	100
46	l	80/138 (58%)	80 (100%)	0	0	100	100
47	m	83/128 (65%)	81 (98%)	2 (2%)	0	100	100
48	o	92/102 (90%)	92 (100%)	0	0	100	100
49	p	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
50	q	159/222 (72%)	159 (100%)	0	0	100	100
51	r	160/196 (82%)	160 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	s	382/439 (87%)	379 (99%)	3 (1%)	0	100	100
53	t1	44/198 (22%)	43 (98%)	1 (2%)	0	100	100
53	t2	30/198 (15%)	30 (100%)	0	0	100	100
53	t3	30/198 (15%)	30 (100%)	0	0	100	100
53	t4	29/198 (15%)	29 (100%)	0	0	100	100
53	t5	29/198 (15%)	29 (100%)	0	0	100	100
53	t6	29/198 (15%)	29 (100%)	0	0	100	100
55	AB	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
56	AC	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
57	AD	341/430 (79%)	335 (98%)	6 (2%)	0	100	100
58	AE	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
59	AF	206/242 (85%)	206 (100%)	0	0	100	100
60	AG	308/396 (78%)	305 (99%)	3 (1%)	0	100	100
61	AH	138/201 (69%)	135 (98%)	2 (1%)	1 (1%)	18	38
62	AI	133/194 (69%)	131 (98%)	2 (2%)	0	100	100
63	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
64	AK	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
65	AL	172/257 (67%)	171 (99%)	1 (1%)	0	100	100
66	AM	117/137 (85%)	117 (100%)	0	0	100	100
67	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100
68	AO	191/258 (74%)	187 (98%)	4 (2%)	0	100	100
69	AP	95/142 (67%)	95 (100%)	0	0	100	100
70	AQ	84/86 (98%)	84 (100%)	0	0	100	100
71	AR	293/360 (81%)	290 (99%)	3 (1%)	0	100	100
72	AS	133/190 (70%)	133 (100%)	0	0	100	100
73	AT	166/173 (96%)	166 (100%)	0	0	100	100
74	AU	174/205 (85%)	174 (100%)	0	0	100	100
75	AV	358/414 (86%)	357 (100%)	1 (0%)	0	100	100
76	AW	98/187 (52%)	98 (100%)	0	0	100	100
77	AX	350/398 (88%)	346 (99%)	4 (1%)	0	100	100
78	AY	147/395 (37%)	146 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	AZ	98/106 (92%)	98 (100%)	0	0	100	100
80	A0	213/218 (98%)	210 (99%)	3 (1%)	0	100	100
81	A1	274/323 (85%)	268 (98%)	6 (2%)	0	100	100
82	A2	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
83	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
84	A4	584/689 (85%)	575 (98%)	9 (2%)	0	100	100
All	All	14326/19154 (75%)	14162 (99%)	163 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
61	AH	126	ILE

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	
3	D	192/245 (78%)	192 (100%)	0	100	100
4	E	260/290 (90%)	260 (100%)	0	100	100
5	F	219/262 (84%)	219 (100%)	0	100	100
6	H	88/228 (39%)	88 (100%)	0	100	100
7	I	194/232 (84%)	194 (100%)	0	100	100
8	J	138/150 (92%)	138 (100%)	0	100	100
9	K	154/154 (100%)	154 (100%)	0	100	100
10	L	98/124 (79%)	98 (100%)	0	100	100
11	M	246/249 (99%)	246 (100%)	0	100	100
12	N	189/211 (90%)	189 (100%)	0	100	100
13	O	134/150 (89%)	134 (100%)	0	100	100
14	P	126/155 (81%)	126 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	Q	220/256 (86%)	220 (100%)	0	100	100
16	R	118/126 (94%)	118 (100%)	0	100	100
17	S	146/180 (81%)	146 (100%)	0	100	100
18	T	146/176 (83%)	146 (100%)	0	100	100
19	U	134/134 (100%)	134 (100%)	0	100	100
20	V	183/191 (96%)	183 (100%)	0	100	100
21	W	94/119 (79%)	94 (100%)	0	100	100
22	X	220/229 (96%)	220 (100%)	0	100	100
23	Y	163/223 (73%)	163 (100%)	0	100	100
24	Z	113/147 (77%)	113 (100%)	0	100	100
25	0	99/164 (60%)	99 (100%)	0	100	100
26	1	52/60 (87%)	52 (100%)	0	100	100
27	2	40/72 (56%)	40 (100%)	0	100	100
28	3	88/166 (53%)	88 (100%)	0	100	100
29	4	37/89 (42%)	37 (100%)	0	100	100
30	5	353/368 (96%)	353 (100%)	0	100	100
31	6	313/332 (94%)	313 (100%)	0	100	100
32	7	270/303 (89%)	270 (100%)	0	100	100
33	8	146/190 (77%)	146 (100%)	0	100	100
34	9	104/112 (93%)	104 (100%)	0	100	100
35	a	96/133 (72%)	96 (100%)	0	100	100
36	b	131/184 (71%)	131 (100%)	0	100	100
37	c	251/288 (87%)	251 (100%)	0	100	100
38	d	237/274 (86%)	234 (99%)	3 (1%)	61	82
39	e	198/236 (84%)	198 (100%)	0	100	100
40	f	139/188 (74%)	139 (100%)	0	100	100
41	g	124/148 (84%)	124 (100%)	0	100	100
42	h	104/148 (70%)	104 (100%)	0	100	100
43	i	86/110 (78%)	86 (100%)	0	100	100
44	j	74/97 (76%)	74 (100%)	0	100	100
45	k	83/89 (93%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	l	76/116 (66%)	76 (100%)	0	100	100
47	m	81/113 (72%)	81 (100%)	0	100	100
48	o	80/87 (92%)	80 (100%)	0	100	100
49	p	135/181 (75%)	135 (100%)	0	100	100
50	q	138/178 (78%)	138 (100%)	0	100	100
51	r	147/169 (87%)	147 (100%)	0	100	100
52	s	340/381 (89%)	340 (100%)	0	100	100
53	t1	40/158 (25%)	40 (100%)	0	100	100
53	t2	31/158 (20%)	31 (100%)	0	100	100
53	t3	31/158 (20%)	31 (100%)	0	100	100
53	t4	30/158 (19%)	30 (100%)	0	100	100
53	t5	30/158 (19%)	30 (100%)	0	100	100
53	t6	30/158 (19%)	30 (100%)	0	100	100
55	AB	198/249 (80%)	198 (100%)	0	100	100
56	AC	115/143 (80%)	115 (100%)	0	100	100
57	AD	286/357 (80%)	286 (100%)	0	100	100
58	AE	104/107 (97%)	104 (100%)	0	100	100
59	AF	185/209 (88%)	185 (100%)	0	100	100
60	AG	271/342 (79%)	271 (100%)	0	100	100
61	AH	130/180 (72%)	129 (99%)	1 (1%)	73	88
62	AI	104/146 (71%)	102 (98%)	2 (2%)	50	75
63	AJ	93/118 (79%)	93 (100%)	0	100	100
64	AK	91/113 (80%)	91 (100%)	0	100	100
65	AL	158/226 (70%)	158 (100%)	0	100	100
66	AM	97/113 (86%)	97 (100%)	0	100	100
67	AN	96/115 (84%)	96 (100%)	0	100	100
68	AO	174/230 (76%)	174 (100%)	0	100	100
69	AP	88/123 (72%)	88 (100%)	0	100	100
70	AQ	78/78 (100%)	78 (100%)	0	100	100
71	AR	264/318 (83%)	264 (100%)	0	100	100
72	AS	116/164 (71%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	AT	153/157 (98%)	153 (100%)	0	100	100
74	AU	152/174 (87%)	152 (100%)	0	100	100
75	AV	325/364 (89%)	324 (100%)	1 (0%)	86	94
76	AW	87/158 (55%)	87 (100%)	0	100	100
77	AX	311/351 (89%)	310 (100%)	1 (0%)	86	94
78	AY	137/357 (38%)	137 (100%)	0	100	100
79	AZ	90/95 (95%)	90 (100%)	0	100	100
80	A0	188/190 (99%)	188 (100%)	0	100	100
81	A1	254/291 (87%)	254 (100%)	0	100	100
82	A2	100/100 (100%)	100 (100%)	0	100	100
83	A3	65/166 (39%)	65 (100%)	0	100	100
84	A4	526/609 (86%)	526 (100%)	0	100	100
All	All	12825/16498 (78%)	12817 (100%)	8 (0%)	87	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	d	73	ASP
38	d	108	ARG
38	d	280	VAL
61	AH	50	LEU
62	AI	73	LEU
62	AI	181	ILE
75	AV	29	LEU
77	AX	81	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	168	HIS
3	D	276	HIS
5	F	103	GLN
5	F	241	ASN
5	F	251	HIS
7	I	119	HIS
7	I	189	GLN
8	J	178	GLN

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Mol	Chain	Res	Type
9	K	94	GLN
9	K	117	HIS
10	L	89	HIS
11	M	84	ASN
11	M	276	ASN
12	N	237	HIS
14	P	79	HIS
14	P	162	GLN
16	R	12	ASN
16	R	89	ASN
16	R	125	HIS
17	S	118	ASN
18	T	126	HIS
18	T	204	HIS
19	U	77	ASN
21	W	80	HIS
23	Y	179	HIS
24	Z	64	HIS
24	Z	107	ASN
30	5	160	HIS
30	5	165	GLN
30	5	195	HIS
30	5	275	ASN
30	5	353	HIS
30	5	385	HIS
31	6	292	GLN
31	6	295	GLN
31	6	373	HIS
32	7	255	HIS
33	8	158	HIS
35	a	46	ASN
35	a	90	GLN
38	d	77	HIS
38	d	167	HIS
38	d	262	HIS
39	e	75	GLN
39	e	251	HIS
41	g	93	ASN
42	h	110	HIS
42	h	119	GLN
43	i	124	HIS
44	j	31	GLN

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Mol	Chain	Res	Type
45	k	72	HIS
45	k	93	HIS
46	l	82	GLN
48	o	21	HIS
48	o	94	HIS
49	p	194	HIS
50	q	81	GLN
51	r	79	HIS
51	r	96	HIS
51	r	112	HIS
52	s	71	HIS
52	s	107	GLN
52	s	240	GLN
52	s	277	GLN
52	s	387	ASN
57	AD	359	HIS
57	AD	415	GLN
58	AE	58	HIS
59	AF	196	HIS
59	AF	224	HIS
60	AG	87	HIS
60	AG	384	GLN
61	AH	130	HIS
61	AH	163	ASN
61	AH	176	GLN
61	AH	183	HIS
62	AI	87	HIS
62	AI	93	ASN
65	AL	200	HIS
66	AM	16	HIS
66	AM	75	HIS
67	AN	9	HIS
67	AN	52	HIS
68	AO	111	HIS
72	AS	66	HIS
74	AU	102	HIS
74	AU	188	ASN
75	AV	38	HIS
75	AV	215	GLN
75	AV	224	GLN
75	AV	380	GLN
75	AV	391	GLN

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Mol	Chain	Res	Type
76	AW	173	GLN
77	AX	69	ASN
77	AX	159	HIS
77	AX	257	HIS
77	AX	302	HIS
78	AY	257	ASN
78	AY	290	ASN
78	AY	337	HIS
78	AY	378	ASN
79	AZ	56	HIS
80	A0	137	HIS
84	A4	288	HIS
84	A4	577	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1528/1561 (97%)	223 (14%)	1 (0%)
2	B	71/72 (98%)	13 (18%)	0
54	AA	953/954 (99%)	126 (13%)	0
85	w	67/68 (98%)	16 (23%)	0
86	x	68/70 (97%)	9 (13%)	0
87	y	17/19 (89%)	2 (11%)	0
All	All	2704/2744 (98%)	389 (14%)	1 (0%)

All (389) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1681	G
1	A	1689	C
1	A	1692	A
1	A	1700	U
1	A	1704	U
1	A	1707	C
1	A	1708	A
1	A	1713	A
1	A	1715	C
1	A	1716	U
1	A	1724	A
1	A	1727	A
1	A	1728	U

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Mol	Chain	Res	Type
1	A	1748	G
1	A	1765	C
1	A	1777	A
1	A	1805	A
1	A	1807	U
1	A	1809	U
1	A	1817	C
1	A	1821	A
1	A	1827	C
1	A	1828	A
1	A	1829	A
1	A	1832	A
1	A	1836	A
1	A	1844	A
1	A	1854	U
1	A	1856	A
1	A	1868	G
1	A	1869	A
1	A	1871	A
1	A	1882	A
1	A	1887	A
1	A	1893	A
1	A	1901	C
1	A	1903	C
1	A	1909	A
1	A	1918	G
1	A	1919	C
1	A	1937	A
1	A	1939	G
1	A	1940	A
1	A	1958	G
1	A	1984	A
1	A	1985	G
1	A	1992	C
1	A	1993	A
1	A	1994	A
1	A	2002	G
1	A	2003	A
1	A	2015	G
1	A	2022	G
1	A	2030	U
1	A	2032	G

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Mol	Chain	Res	Type
1	A	2036	C
1	A	2037	U
1	A	2039	A
1	A	2059	C
1	A	2060	A
1	A	2071	U
1	A	2079	C
1	A	2098	G
1	A	2099	U
1	A	2113	G
1	A	2125	C
1	A	2126	U
1	A	2132	A
1	A	2147	G
1	A	2155	A
1	A	2159	U
1	A	2160	A
1	A	2163	A
1	A	2168	U
1	A	2181	A
1	A	2183	C
1	A	2192	A
1	A	2194	U
1	A	2198	A
1	A	2200	A
1	A	2214	A
1	A	2219	C
1	A	2220	A
1	A	2221	C
1	A	2223	A
1	A	2225	C
1	A	2228	A
1	A	2237	A
1	A	2241	A
1	A	2243	A
1	A	2245	A
1	A	2262	C
1	A	2263	C
1	A	2283	C
1	A	2284	C
1	A	2285	U
1	A	2297	A

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Mol	Chain	Res	Type
1	A	2300	G
1	A	2321	A
1	A	2322	C
1	A	2331	C
1	A	2332	C
1	A	2345	G
1	A	2351	U
1	A	2356	A
1	A	2363	A
1	A	2371	U
1	A	2372	U
1	A	2374	A
1	A	2390	A
1	A	2399	A
1	A	2401	A
1	A	2406	A
1	A	2407	U
1	A	2414	C
1	A	2415	C
1	A	2416	U
1	A	2446	A
1	A	2451	A
1	A	2478	G
1	A	2493	C
1	A	2520	C
1	A	2521	A
1	A	2527	A
1	A	2540	C
1	A	2560	G
1	A	2570	C
1	A	2582	A
1	A	2592	G
1	A	2593	G
1	A	2599	U
1	A	2600	A
1	A	2601	A
1	A	2618	U
1	A	2625	C
1	A	2627	G
1	A	2628	U
1	A	2630	U
1	A	2633	A

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Mol	Chain	Res	Type
1	A	2635	G
1	A	2654	U
1	A	2656	U
1	A	2683	C
1	A	2686	G
1	A	2693	A
1	A	2694	A
1	A	2695	G
1	A	2696	A
1	A	2706	A
1	A	2718	C
1	A	2719	G
1	A	2723	A
1	A	2724	G
1	A	2725	A
1	A	2732	G
1	A	2792	A
1	A	2810	G
1	A	2815	G
1	A	2832	A
1	A	2833	A
1	A	2847	C
1	A	2859	A
1	A	2864	U
1	A	2865	C
1	A	2887	U
1	A	2889	C
1	A	2893	A
1	A	2910	A
1	A	2917	G
1	A	2922	A
1	A	2928	C
1	A	2935	A
1	A	2946	A
1	A	2956	A
1	A	2961	C
1	A	2985	C
1	A	2989	G
1	A	2990	A
1	A	2992	G
1	A	2993	U
1	A	3005	A

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Mol	Chain	Res	Type
1	A	3006	U
1	A	3007	C
1	A	3016	G
1	A	3041	U
1	A	3053	A
1	A	3054	G
1	A	3060	C
1	A	3086	U
1	A	3089	A
1	A	3090	G
1	A	3100	U
1	A	3101	A
1	A	3102	U
1	A	3108	U
1	A	3109	U
1	A	3110	C
1	A	3111	A
1	A	3112	A
1	A	3113	A
1	A	3150	U
1	A	3157	C
1	A	3158	A
1	A	3162	C
1	A	3169	C
1	A	3172	C
1	A	3176	A
1	A	3183	U
1	A	3188	U
1	A	3189	C
1	A	3190	A
1	A	3199	U
1	A	3200	U
1	A	3207	A
1	A	3208	C
1	A	3209	A
1	A	3210	C
1	A	3212	C
1	A	3217	A
1	A	3218	A
1	A	3220	A
1	A	3228	U
1	A	3231	U

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Mol	Chain	Res	Type
2	B	1603	A
2	B	1605	A
2	B	1609	U
2	B	1611	G
2	B	1617	C
2	B	1621	A
2	B	1646	U
2	B	1650	A
2	B	1652	C
2	B	1653	U
2	B	1654	U
2	B	1661	A
2	B	1664	G
54	AA	651	A
54	AA	680	U
54	AA	688	A
54	AA	689	U
54	AA	695	A
54	AA	704	U
54	AA	721	U
54	AA	737	C
54	AA	753	A
54	AA	761	A
54	AA	766	G
54	AA	777	G
54	AA	791	G
54	AA	796	G
54	AA	808	C
54	AA	814	A
54	AA	815	C
54	AA	830	U
54	AA	832	U
54	AA	835	C
54	AA	836	A
54	AA	860	A
54	AA	861	U
54	AA	868	C
54	AA	871	A
54	AA	890	C
54	AA	903	U
54	AA	907	A
54	AA	919	A

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Mol	Chain	Res	Type
54	AA	929	A
54	AA	930	G
54	AA	931	C
54	AA	932	C
54	AA	933	G
54	AA	938	A
54	AA	939	A
54	AA	942	A
54	AA	954	C
54	AA	956	C
54	AA	960	C
54	AA	962	C
54	AA	965	C
54	AA	966	A
54	AA	967	A
54	AA	1001	C
54	AA	1011	C
54	AA	1015	A
54	AA	1028	G
54	AA	1042	U
54	AA	1048	C
54	AA	1049	A
54	AA	1065	C
54	AA	1069	A
54	AA	1081	U
54	AA	1082	A
54	AA	1103	A
54	AA	1105	C
54	AA	1106	C
54	AA	1107	U
54	AA	1109	A
54	AA	1118	A
54	AA	1119	U
54	AA	1121	A
54	AA	1126	A
54	AA	1137	A
54	AA	1138	G
54	AA	1144	U
54	AA	1151	C
54	AA	1153	C
54	AA	1160	A
54	AA	1167	A

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Mol	Chain	Res	Type
54	AA	1187	U
54	AA	1189	U
54	AA	1200	G
54	AA	1220	A
54	AA	1223	C
54	AA	1225	C
54	AA	1229	U
54	AA	1237	A
54	AA	1247	G
54	AA	1248	C
54	AA	1251	A
54	AA	1261	C
54	AA	1271	C
54	AA	1273	G
54	AA	1284	U
54	AA	1285	G
54	AA	1290	C
54	AA	1291	U
54	AA	1292	A
54	AA	1295	A
54	AA	1312	C
54	AA	1326	A
54	AA	1327	G
54	AA	1343	A
54	AA	1344	U
54	AA	1353	A
54	AA	1354	A
54	AA	1378	C
54	AA	1387	A
54	AA	1390	A
54	AA	1392	A
54	AA	1405	C
54	AA	1420	U
54	AA	1430	A
54	AA	1447	G
54	AA	1478	A
54	AA	1481	C
54	AA	1514	A
54	AA	1519	A
54	AA	1520	U
54	AA	1522	U
54	AA	1525	C

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Mol	Chain	Res	Type
54	AA	1527	A
54	AA	1533	C
54	AA	1536	A
54	AA	1537	C
54	AA	1539	C
54	AA	1557	A
54	AA	1568	U
54	AA	1571	U
54	AA	1582	G
54	AA	1584	A
54	AA	1594	G
54	AA	1595	G
54	AA	1599	A
85	w	3	G
85	w	7	A
85	w	9	A
85	w	16	A
85	w	21	A
85	w	22	A
85	w	30	G
85	w	46	A
85	w	49	U
85	w	50	A
85	w	55	A
85	w	56	A
85	w	61	U
85	w	65	A
85	w	68	U
85	w	71	C
86	x	3	G
86	x	25	C
86	x	44	A
86	x	45	G
86	x	46	A
86	x	48	U
86	x	49	G
86	x	59	U
86	x	75	C
87	y	24	U
87	y	25	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2112	A

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

7 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
36	THC	b	2	36	8,9,10	0.76	0	10,11,13	1.27	2 (20%)
19	AYA	U	2	19	6,7,8	0.81	0	6,8,10	0.55	0
70	AYA	AQ	2	70	6,7,8	0.82	0	6,8,10	0.62	0
82	AYA	A2	2	82	6,7,8	0.82	0	6,8,10	0.61	0
62	IAS	AI	184	62	5,6,8	0.77	0	1,6,10	1.10	0
9	SAC	K	2	9	7,8,9	0.86	0	7,9,11	0.61	0
45	AYA	k	2	45	6,7,8	0.82	0	6,8,10	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	THC	b	2	36	-	0/9/10/12	-
19	AYA	U	2	19	-	2/5/6/8	-
70	AYA	AQ	2	70	-	0/5/6/8	-
82	AYA	A2	2	82	-	0/5/6/8	-
62	IAS	AI	184	62	-	1/3/5/8	-
9	SAC	K	2	9	-	0/7/8/10	-
45	AYA	k	2	45	-	1/5/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	2	THC	C-CA-N1	2.47	113.69	109.80
36	b	2	THC	CB-CA-C	-2.44	107.50	111.55

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	U	2	AYA	O-C-CA-CB
45	k	2	AYA	O-C-CA-CB
62	AI	184	IAS	O-C-CA-CB
19	U	2	AYA	C-CA-N-CT

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	b	2	THC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 241 ligands modelled in this entry, 236 are monoatomic - leaving 5 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	$\# Z > 2$
92	ATP	AX	501	88	32,33,33	1.11	3 (9%)	48,52,52	1.53	7 (14%)
93	GTP	AX	503	-	33,34,34	1.06	2 (6%)	50,54,54	1.56	8 (16%)
91	FES	AP	201	69,58	0,4,4	-	-	-		
91	FES	AT	201	66,73	0,4,4	-	-	-		
91	FES	r	201	51,7	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
92	ATP	AX	501	88	-	1/22/38/38	0/3/3/3
93	GTP	AX	503	-	-	0/22/38/38	0/3/3/3
91	FES	AP	201	69,58	-	-	0/1/1/1
91	FES	AT	201	66,73	-	-	0/1/1/1
91	FES	r	201	51,7	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
93	AX	503	GTP	C6-N1	-2.85	1.33	1.38
92	AX	501	ATP	C5-C6	2.84	1.48	1.41
92	AX	501	ATP	C5-N7	-2.28	1.34	1.39
93	AX	503	GTP	C2-N3	2.22	1.38	1.33
92	AX	501	ATP	C8-N7	2.15	1.35	1.31

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	AX	501	ATP	C5-C4-N3	-5.31	119.41	126.72
93	AX	503	GTP	C5-C4-N3	-4.95	120.51	128.39
93	AX	503	GTP	C2-N1-C6	-4.95	116.14	125.11
92	AX	501	ATP	N3-C4-N9	3.75	133.54	127.17
93	AX	503	GTP	C5-C6-N1	3.40	121.90	113.25
92	AX	501	ATP	N9-C8-N7	-3.29	109.27	113.94
92	AX	501	ATP	C2-N3-C4	3.11	119.42	111.83
93	AX	503	GTP	N9-C4-N3	3.10	132.14	125.95
93	AX	503	GTP	O6-C6-C5	-2.85	119.01	126.53
92	AX	501	ATP	C4-N9-C8	2.63	108.50	105.74
93	AX	503	GTP	N9-C8-N7	-2.57	108.64	113.40
93	AX	503	GTP	C8-N7-C5	2.50	108.72	104.26
92	AX	501	ATP	C5-N7-C8	2.41	107.23	103.45
93	AX	503	GTP	C2-N3-C4	2.34	116.33	112.30
92	AX	501	ATP	C4-C5-N7	-2.30	107.95	110.58

There are no chirality outliers.

All (1) torsion outliers are listed below:

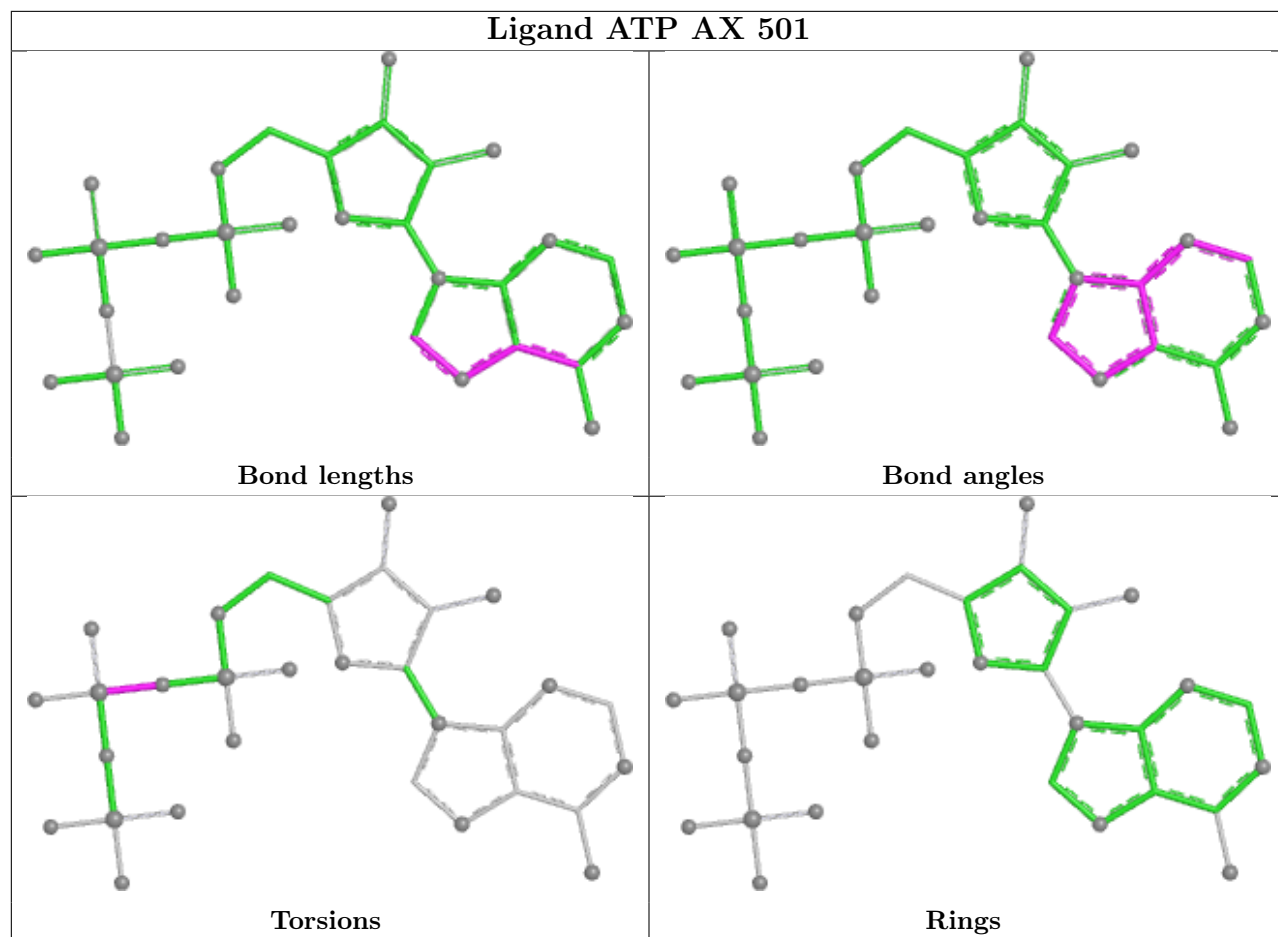
Mol	Chain	Res	Type	Atoms
92	AX	501	ATP	PA-O3A-PB-O2B

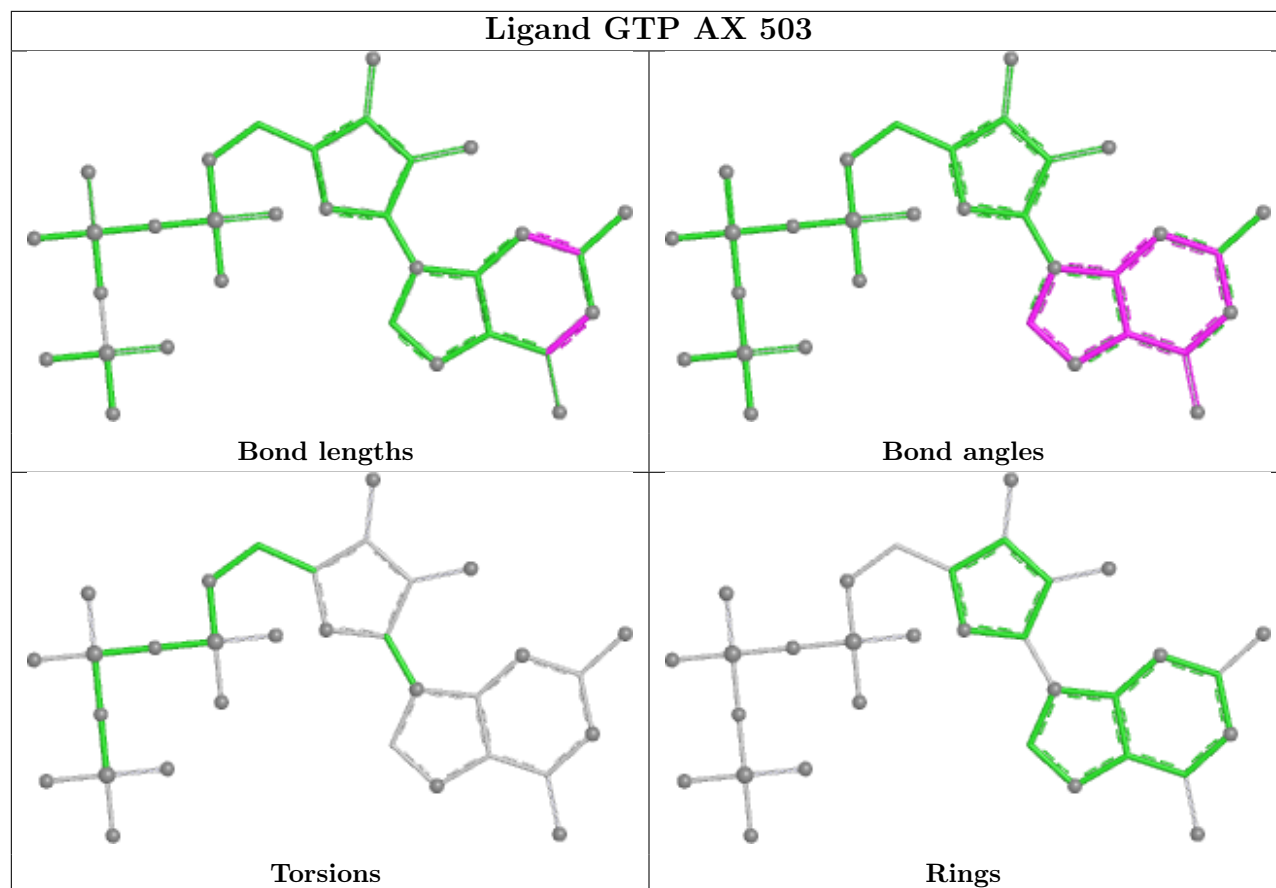
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
91	r	201	FES	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
87	y	1
86	x	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	y	26:A	O3'	46:U	P	66.86
1	x	15:A	O3'	21:A	P	10.04

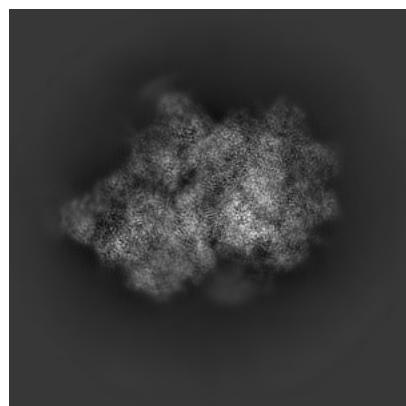
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11279. These allow visual inspection of the internal detail of the map and identification of artifacts.

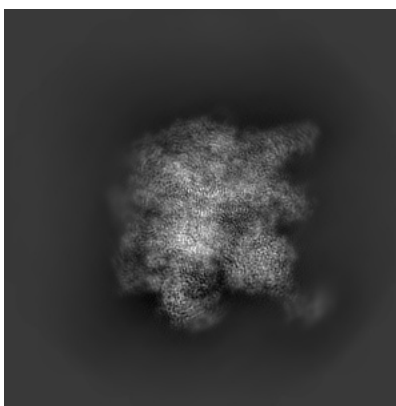
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

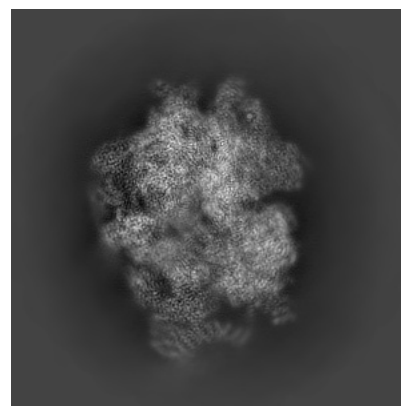
6.1.1 Primary map



X

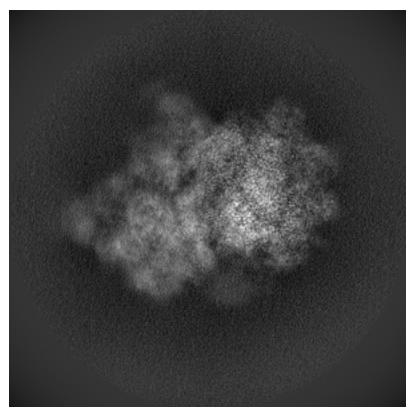


Y

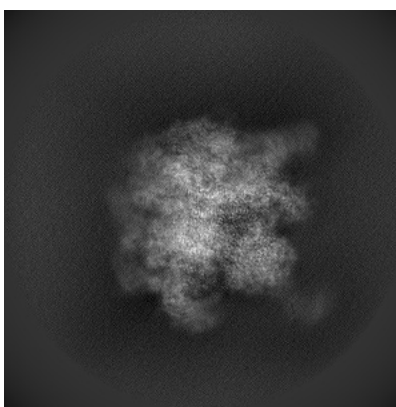


Z

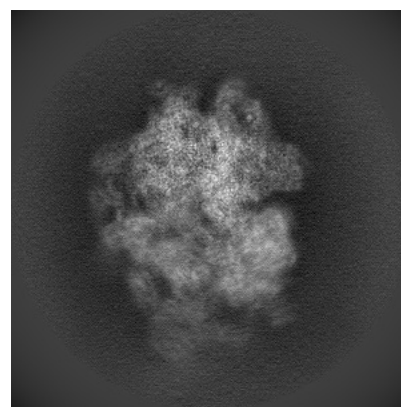
6.1.2 Raw map



X



Y

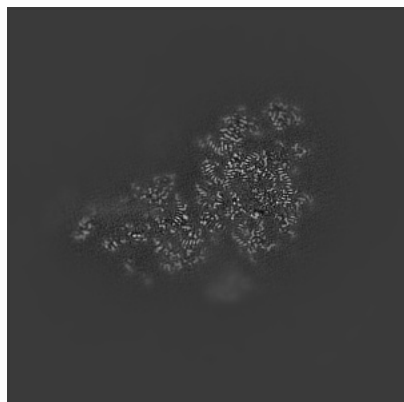


Z

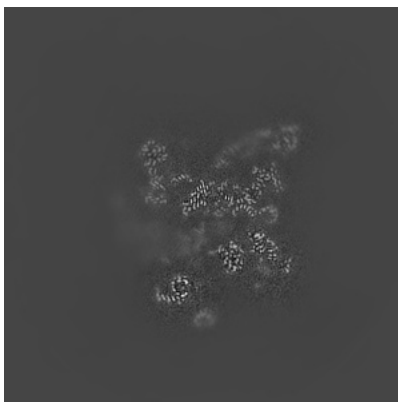
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

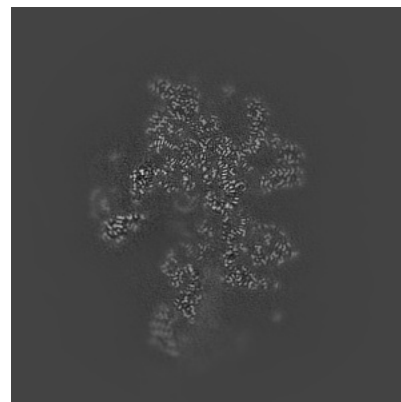
6.2.1 Primary map



X Index: 270

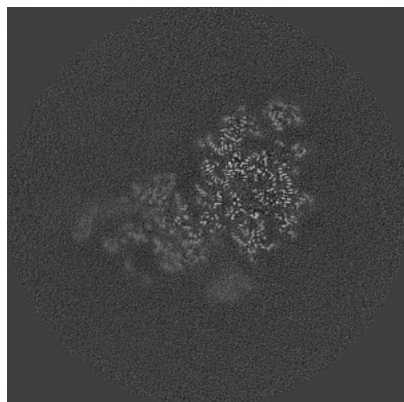


Y Index: 270

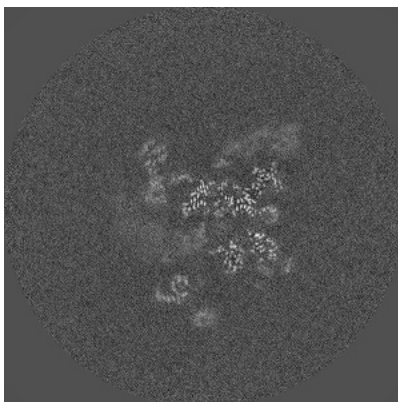


Z Index: 270

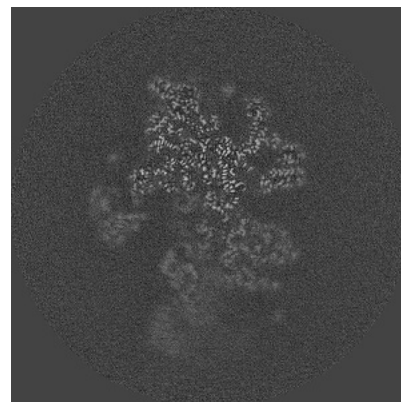
6.2.2 Raw map



X Index: 270



Y Index: 270

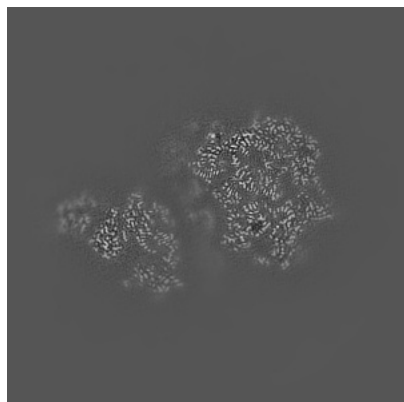


Z Index: 270

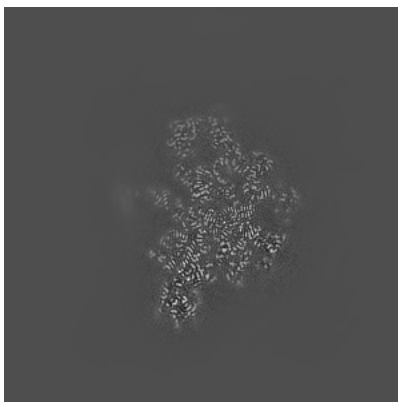
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

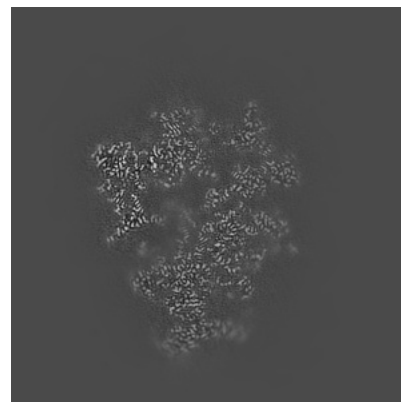
6.3.1 Primary map



X Index: 218

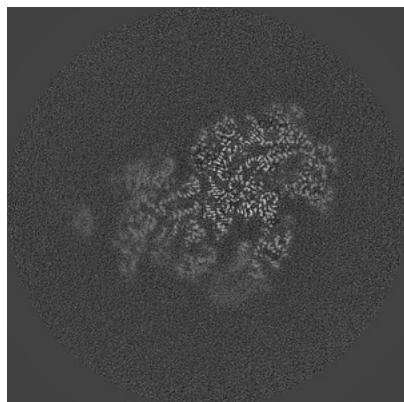


Y Index: 324

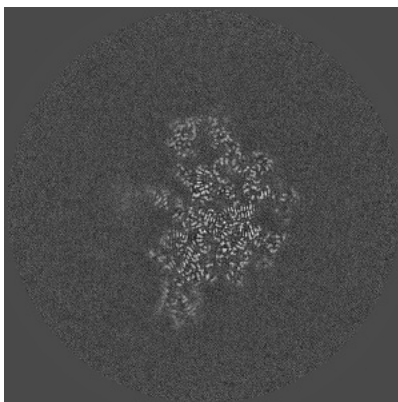


Z Index: 242

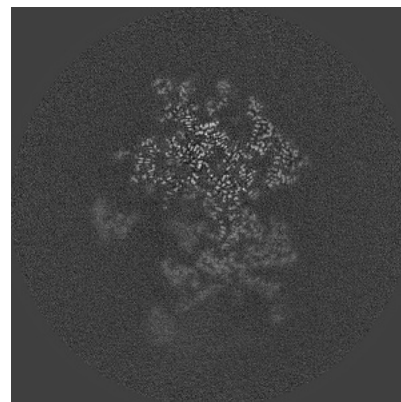
6.3.2 Raw map



X Index: 291



Y Index: 324

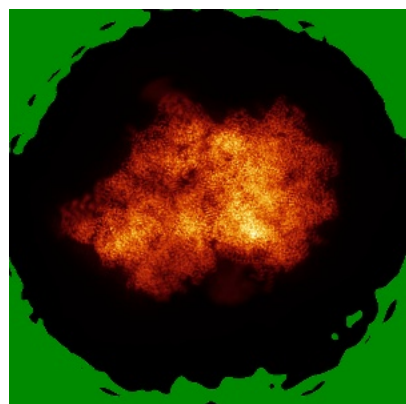


Z Index: 280

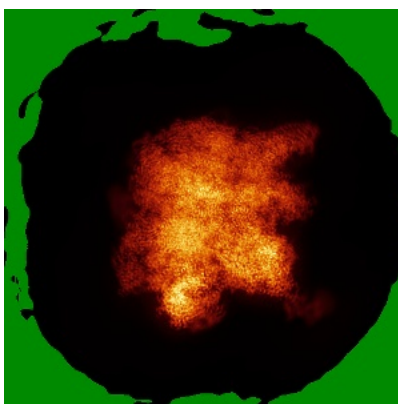
The images above show the largest variance slices of the map in three orthogonal directions.

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

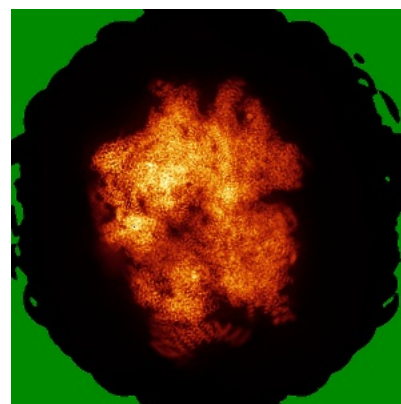
6.4.1 Primary map



X

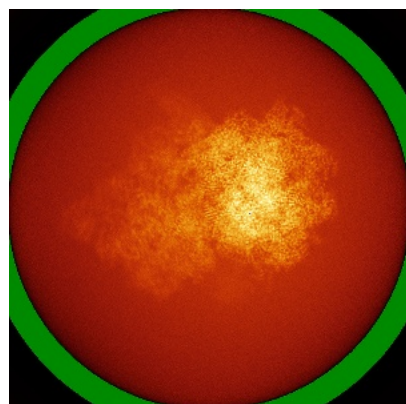


Y

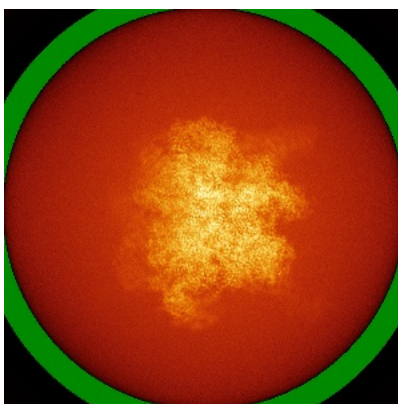


Z

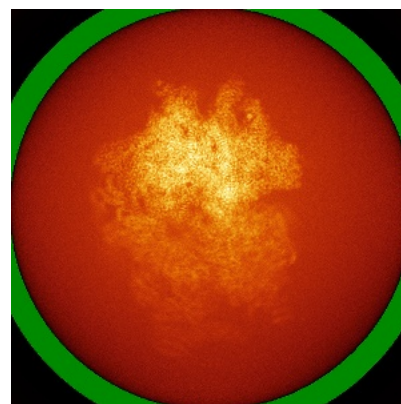
6.4.2 Raw map



X



Y

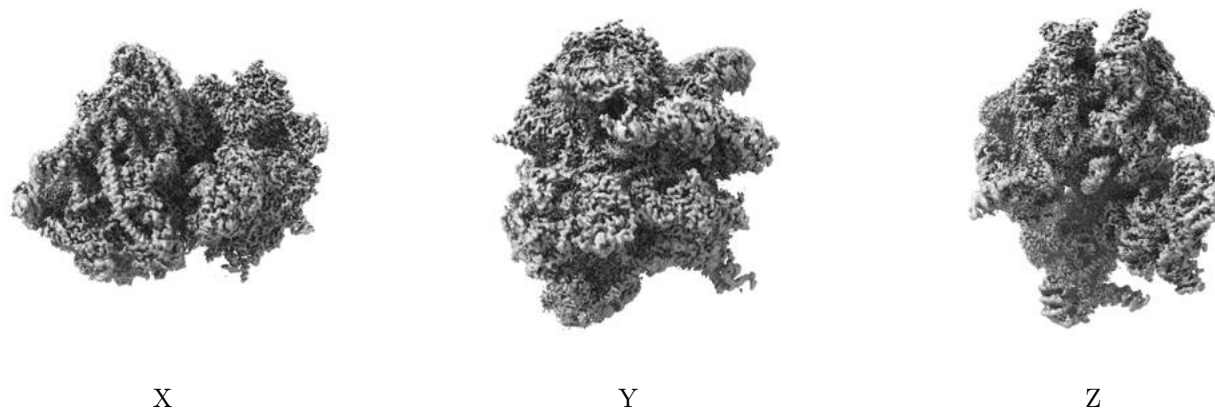


Z

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

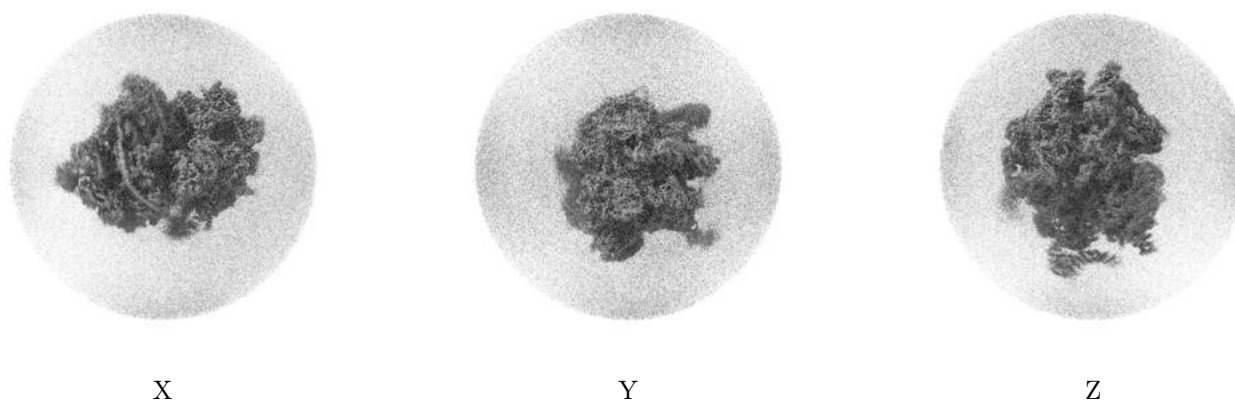
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

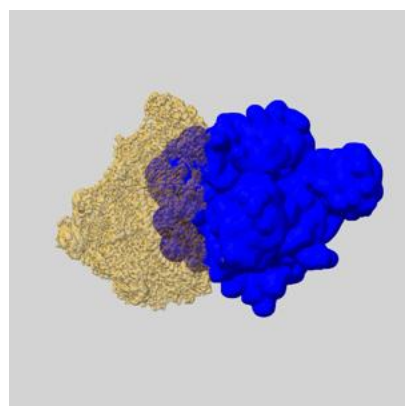
6.6 Mask visualisation [i](#)

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

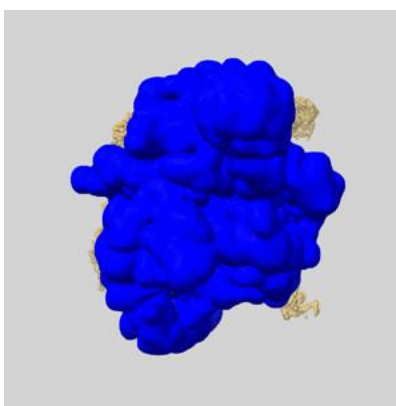
A mask typically either:

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

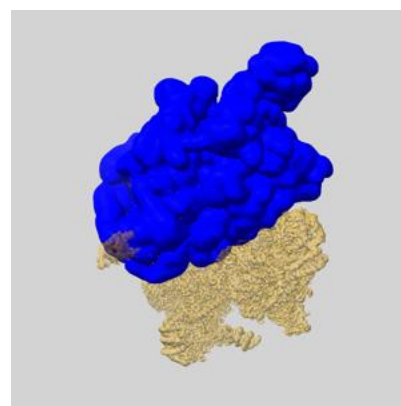
6.6.1 emd_11279_msk_1.map [i](#)



X



Y

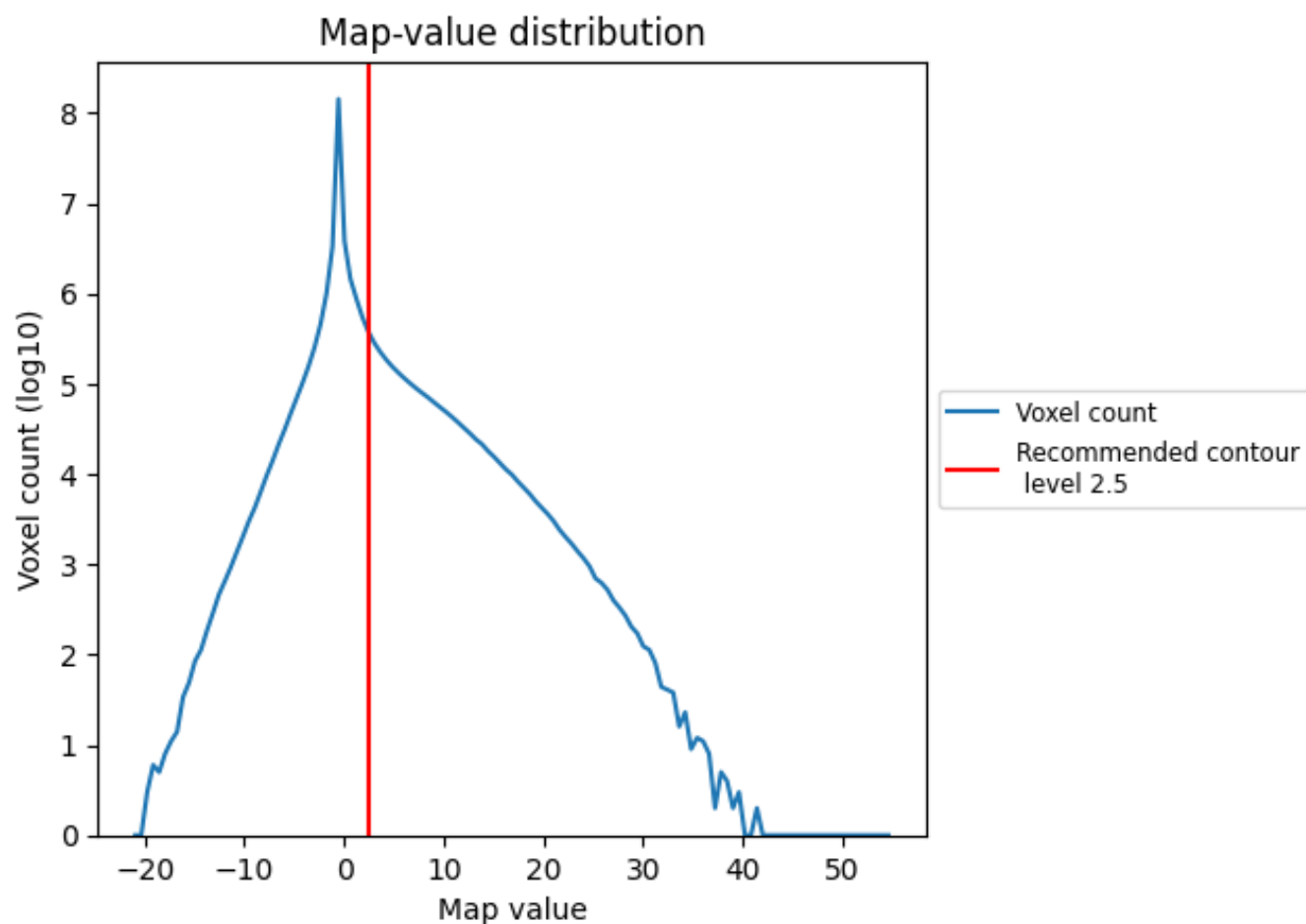


Z

7 Map analysis [i](#)

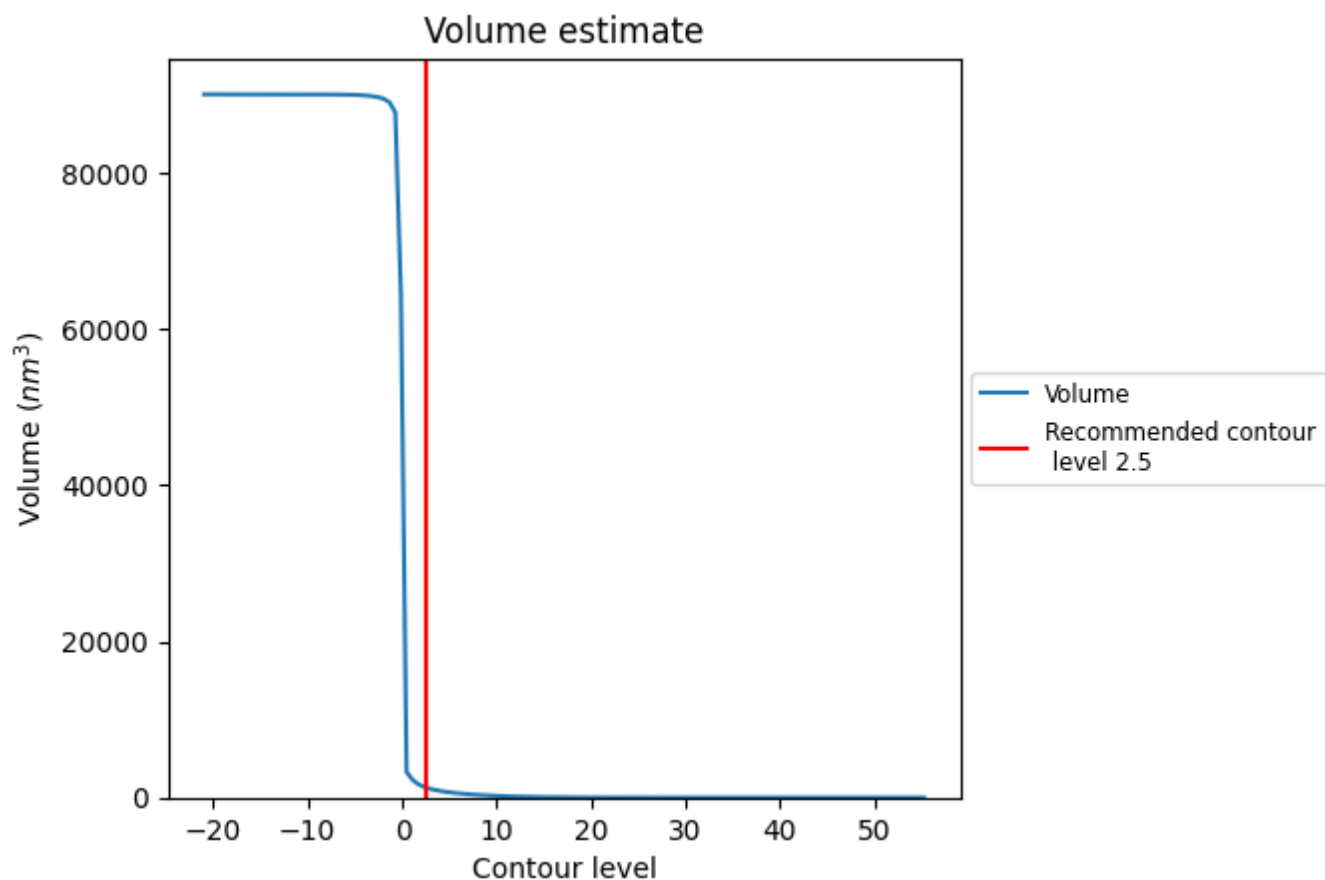
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

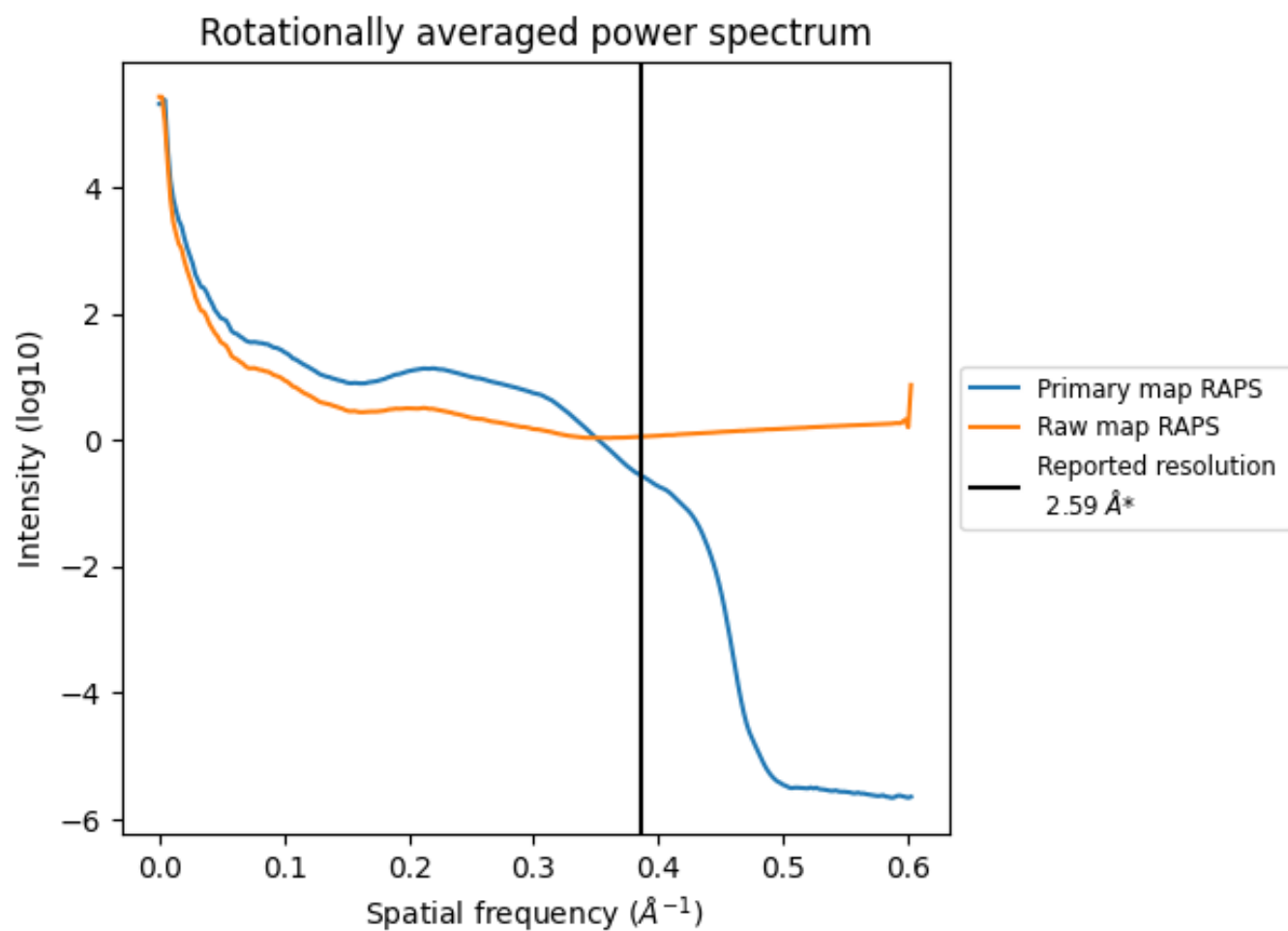
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1293 nm³; this corresponds to an approximate mass of 1168 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 ⓘ

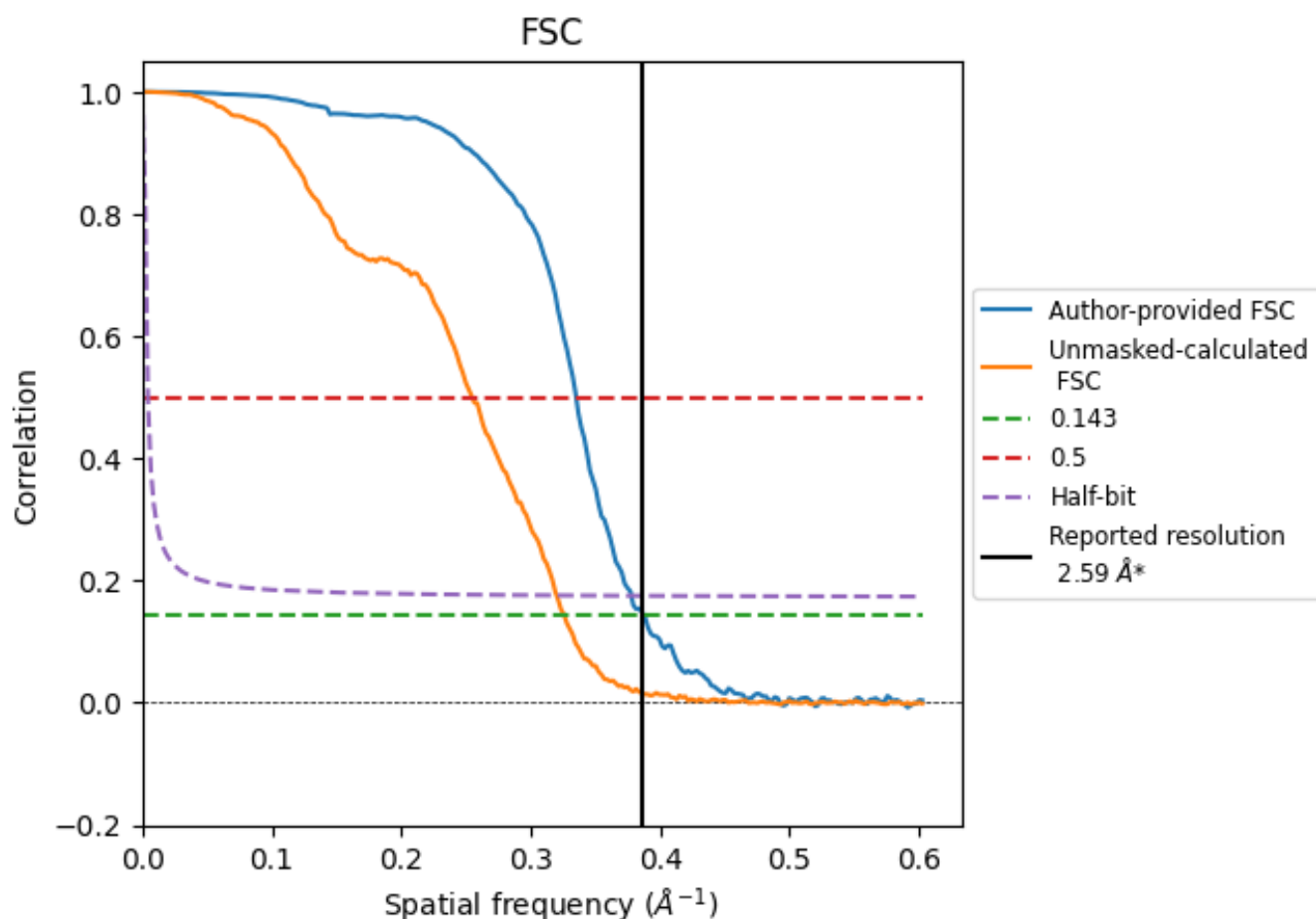


*Reported resolution corresponds to spatial frequency of 0.386 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.386 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

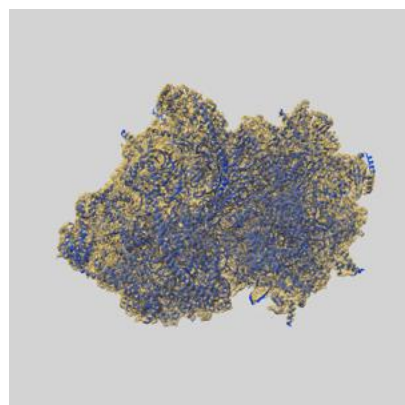
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.58	2.98	2.65
Unmasked-calculated*	3.07	3.92	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.07 differs from the reported value 2.59 by more than 10 %

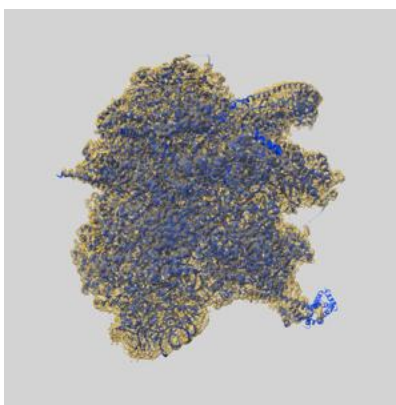
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11279 and PDB model 6ZM6. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

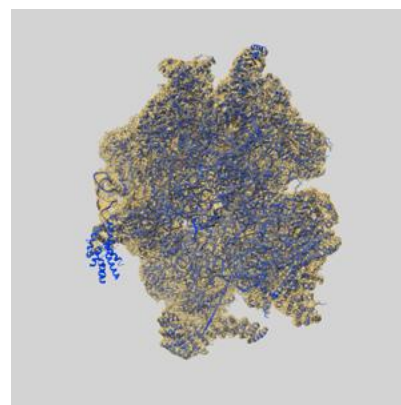
9.1 Map-model overlay [i](#)



X



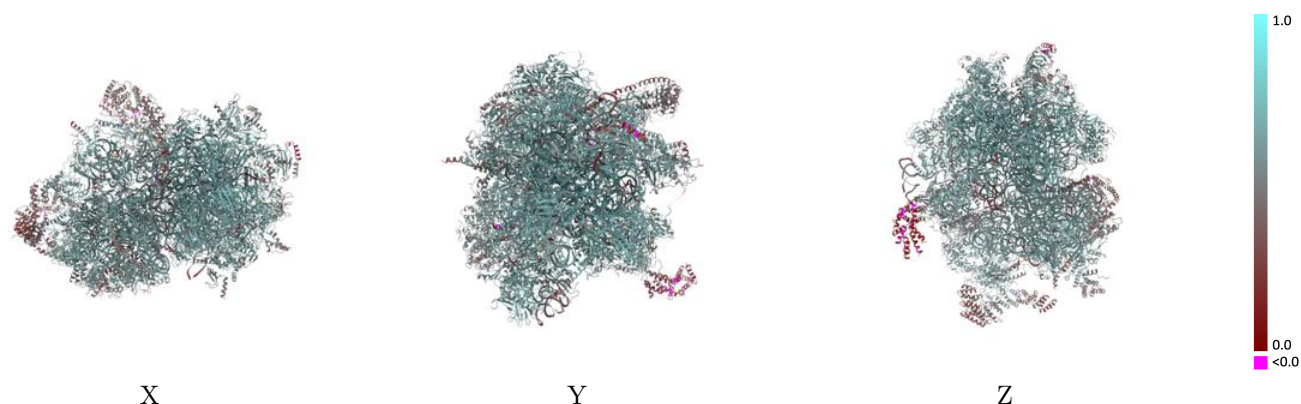
Y



Z

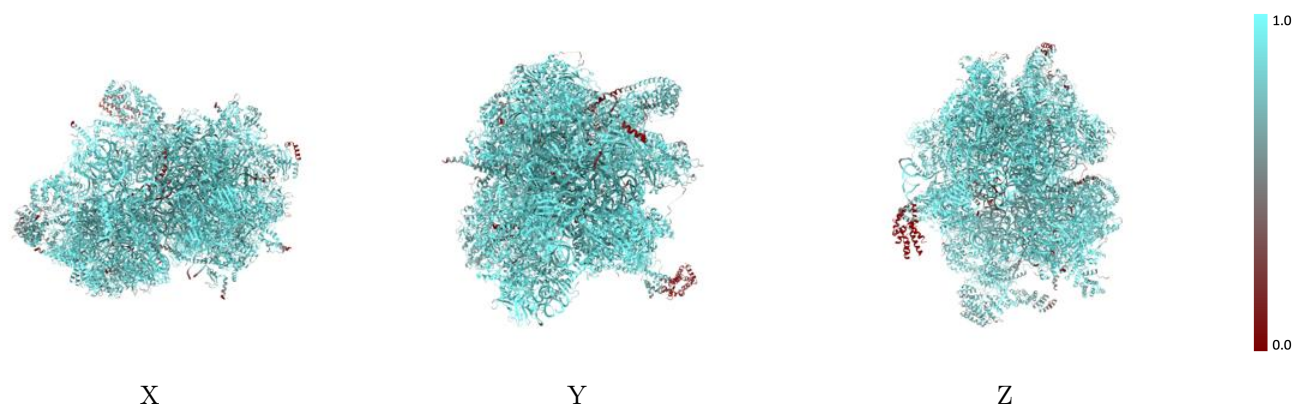
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



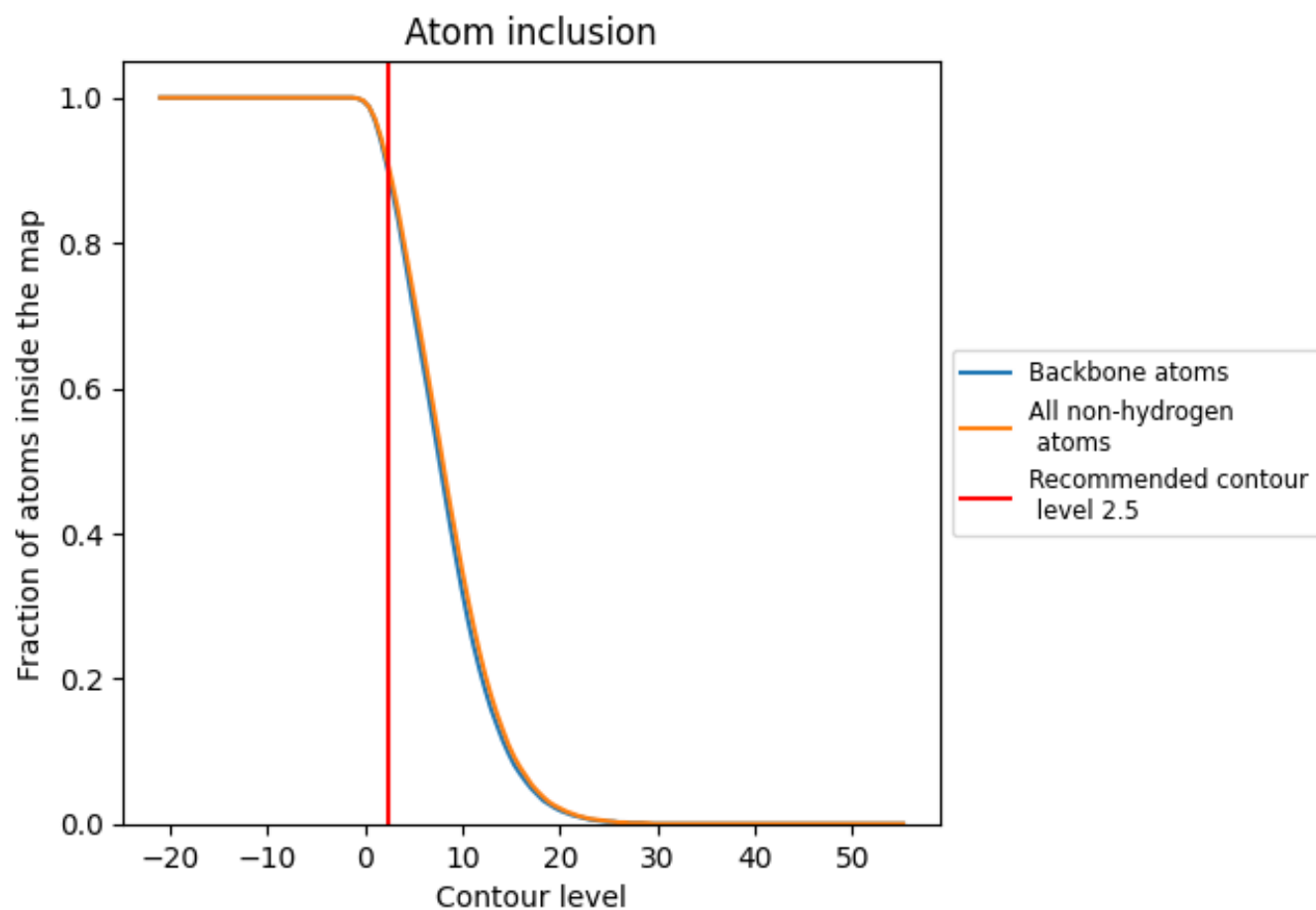
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 90% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9030	 0.5790
0	 0.9080	 0.6210
1	 0.9120	 0.5880
2	 0.9750	 0.6980
3	 0.9780	 0.6710
4	 0.9660	 0.6450
5	 0.9050	 0.5920
6	 0.9520	 0.6100
7	 0.8530	 0.5410
8	 0.8050	 0.4890
9	 0.8820	 0.5840
A	 0.9710	 0.6420
A0	 0.8620	 0.5490
A1	 0.8910	 0.5600
A2	 0.8130	 0.5250
A3	 0.8930	 0.5890
A4	 0.7680	 0.3980
AA	 0.9630	 0.6140
AB	 0.9230	 0.5760
AC	 0.9560	 0.6350
AD	 0.8710	 0.5610
AE	 0.8930	 0.5750
AF	 0.8750	 0.5660
AG	 0.8940	 0.5670
AH	 0.9250	 0.5940
AI	 0.8710	 0.5530
AJ	 0.8310	 0.5590
AK	 0.9710	 0.6420
AL	 0.8120	 0.5220
AM	 0.9100	 0.5920
AN	 0.9120	 0.5900
AO	 0.9070	 0.5700
AP	 0.9010	 0.5710
AQ	 0.9250	 0.5980
AR	 0.8630	 0.5220



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Chain	Atom inclusion	Q-score
AS	 0.8580	 0.5060
AT	 0.8890	 0.5630
AU	 0.8320	 0.5060
AV	 0.7830	 0.4340
AW	 0.9070	 0.5560
AX	 0.8270	 0.5260
AY	 0.8000	 0.5130
AZ	 0.9020	 0.5860
B	 0.9510	 0.5300
D	 0.9510	 0.6310
E	 0.9380	 0.6200
F	 0.9590	 0.6480
H	 0.7940	 0.5310
I	 0.8110	 0.4930
J	 0.8790	 0.4930
K	 0.9620	 0.6450
L	 0.9440	 0.6260
M	 0.9450	 0.6140
N	 0.9490	 0.6200
O	 0.9260	 0.6280
P	 0.9760	 0.6400
Q	 0.8650	 0.5880
R	 0.9680	 0.6610
S	 0.9460	 0.6310
T	 0.9470	 0.6520
U	 0.8670	 0.5910
V	 0.8510	 0.5450
W	 0.9660	 0.6530
X	 0.8840	 0.5850
Y	 0.9180	 0.6220
Z	 0.9370	 0.6160
a	 0.8380	 0.5650
b	 0.9520	 0.6430
c	 0.8920	 0.5850
d	 0.7150	 0.4790
e	 0.9070	 0.5120
f	 0.8720	 0.5450
g	 0.9270	 0.6040
h	 0.8560	 0.5420
i	 0.9650	 0.6820
j	 0.9110	 0.5690
k	 0.9200	 0.5540

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Chain	Atom inclusion	Q-score
l	 0.9100	 0.5190
m	 0.8140	 0.4750
o	 0.9690	 0.6490
p	 0.8390	 0.4940
q	 0.6920	 0.4380
r	 0.9510	 0.6170
s	 0.9170	 0.6100
t1	 0.7000	 0.2820
t2	 0.6950	 0.3040
t3	 0.1290	 0.1420
t4	 0.1060	 0.0540
t5	 0.0000	 0.1240
t6	 0.0000	 0.0560
w	 0.4850	 0.3770
x	 0.7500	 0.4690
y	 0.7690	 0.5000