



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 09:07 AM UTC

PDB ID : 6ZM5 / pdb_00006zm5
EMDB ID : EMD-11278
Title : Human mitochondrial ribosome in complex with OXA1L, mRNA, A/A tRNA, P/P tRNA and nascent polypeptide
Authors : Itoh, Y.; Andrell, J.; Amunts, A.
Deposited on : 2020-07-01
Resolution : 2.89 Å (reported)
Based on initial models : 6RW4, 5OOL, 3J9M

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:

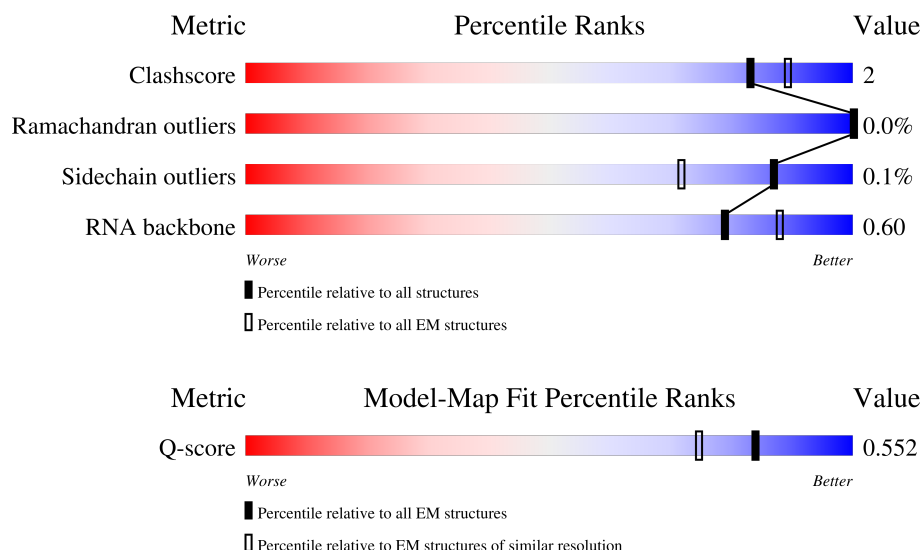
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.89 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.



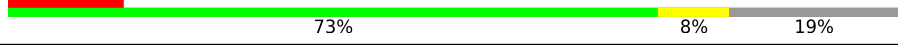
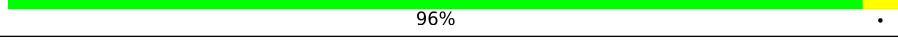
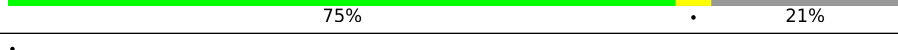
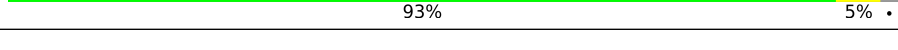
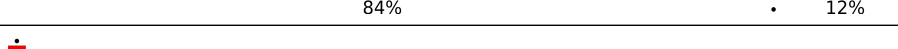
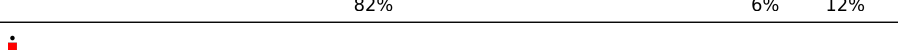
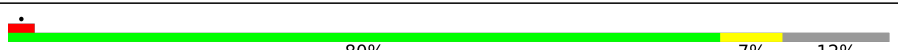
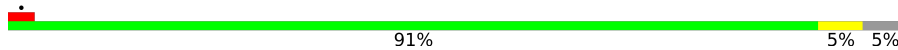
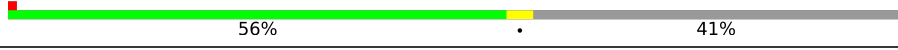
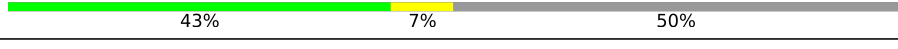
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12148 (2.39 - 3.39)

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	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	

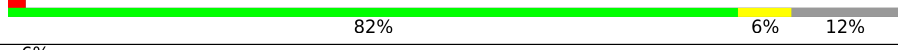
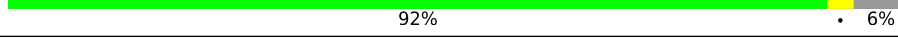
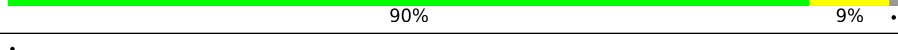
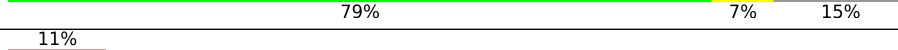
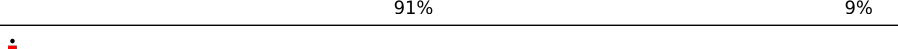
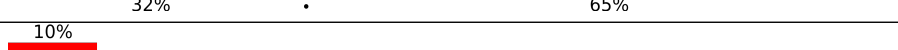
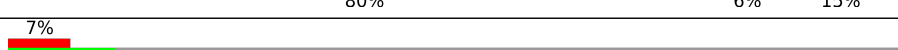
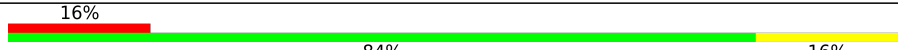
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	t2	198	 5% 12% 5% 84%
53	t3	198	 16% 16% 84%
53	t4	198	 15% 15% 84%
53	t5	198	 16% 15% 84%
53	t6	198	 16% 16% 84%
54	AA	954	 81% 17%
55	AB	296	 73% 24%
56	AC	167	 69% 10% 21%
57	AD	430	 75% 5% 20%
58	AE	125	 91% 6%
59	AF	242	 80% 6% 14%
60	AG	396	 74% 21%
61	AH	201	 62% 7% 30%
62	AI	194	 64% 6% 29%
63	AJ	138	 75% 22%
64	AK	128	 73% 5% 21%
65	AL	257	 5% 65% 32%
66	AM	137	 82% 5% 13%
67	AN	130	 77% 8% 15%
68	AO	258	 71% 25%
69	AP	142	 63% 6% 32%
70	AQ	86	 93% 7%
71	AR	360	 76% 6% 18%
72	AS	190	 68% 29%
73	AT	173	 91% 6%

Continued on next page...

Continued from previous page...

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	u	435	
86	v	32	
87	w	68	
88	x	70	
89	y	19	

2 Entry composition

There are 97 unique types of molecules in this entry. The entry contains 326964 atoms, of which 149830 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	1534	Total	C	H	N	O	P	0	0
			49092	14611	16532	5870	10545	1534		

- 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		

- 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	133	Total	C	H	N	O	S	0	0
			2215	702	1108	214	189	2		

- 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	242	Total	C	H	N	O	S	0	0
			3970	1275	1982	343	358	12		

- 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	variant	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 protein called Mitochondrial inner membrane protein OXA1L.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	u	51	Total	C	H	N	O	S	0	0
			863	265	432	87	77	2		

- Molecule 86 is a protein called Nascent polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	v	32	Total	C	H	N	O		0	0
			320	96	160	32	32			

- Molecule 87 is a RNA chain called A-site tRNA with aminoacylation.

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

- Molecule 88 is a RNA chain called P-site tRNA.

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

- Molecule 89 is a RNA chain called mRNA.

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

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	A	128	Total	Mg	0
			128	128	
90	D	3	Total	Mg	0
			3	3	
90	E	1	Total	Mg	0
			1	1	
90	g	1	Total	Mg	0
			1	1	
90	AA	53	Total	Mg	0
			53	53	
90	AB	1	Total	Mg	0
			1	1	
90	AX	1	Total	Mg	0
			1	1	
90	A3	1	Total	Mg	0
			1	1	

- Molecule 91 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
91	A	30	Total	K	0
			30	30	
91	M	1	Total	K	0
			1	1	
91	N	1	Total	K	0
			1	1	
91	P	1	Total	K	0
			1	1	
91	i	1	Total	K	0
			1	1	

Continued on next page...

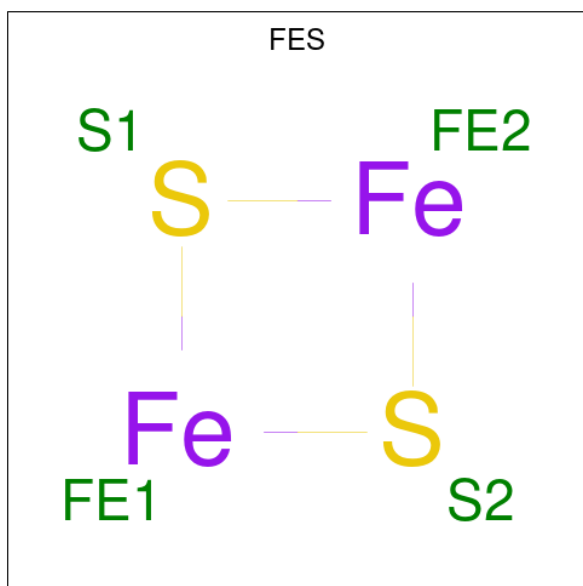
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
91	o	1	Total	K	0
			1	1	
91	AA	9	Total	K	0
			9	9	

- Molecule 92 is ZINC ION (CCD ID: ZN) (formula: Zn).

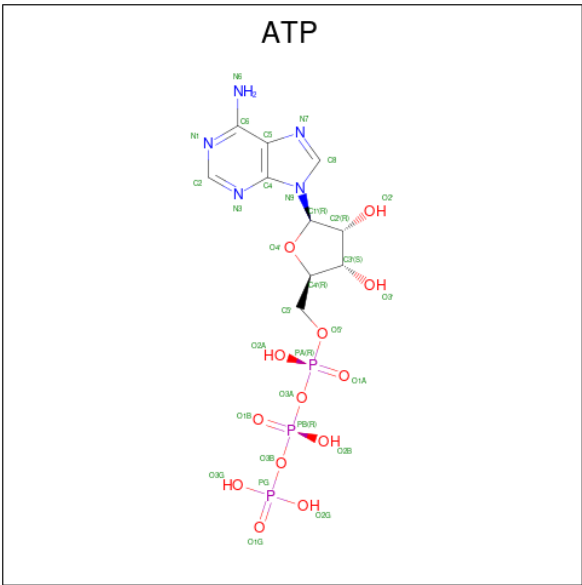
Mol	Chain	Residues	Atoms		AltConf
92	0	1	Total	Zn	0
			1	1	
92	4	1	Total	Zn	0
			1	1	
92	AO	1	Total	Zn	0
			1	1	

- Molecule 93 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



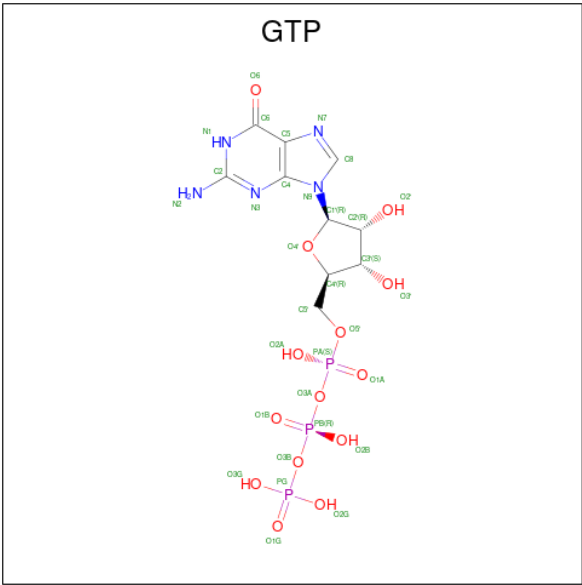
Mol	Chain	Residues	Atoms			AltConf
93	r	1	Total	Fe	S	0
			4	2	2	
93	AP	1	Total	Fe	S	0
			4	2	2	
93	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 94 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



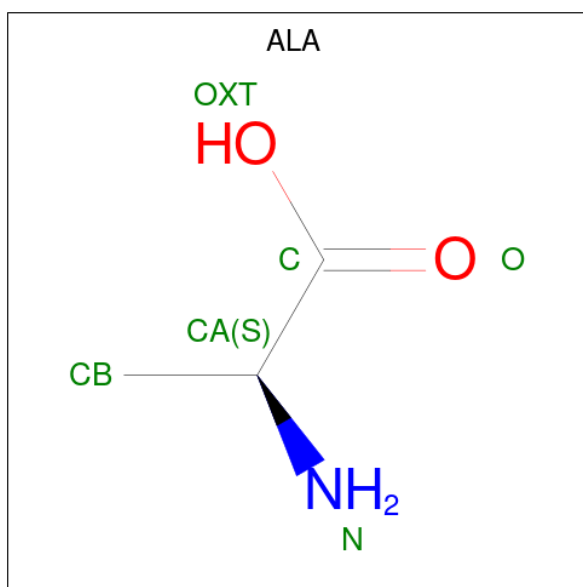
Mol	Chain	Residues	Atoms						AltConf
94	AX	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 95 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 96 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms					AltConf
96	w	1	Total	C	H	N	O	0
			12	3	7	1	1	

- Molecule 97 is water.

Mol	Chain	Residues	Atoms		AltConf
97	A	340	Total	O	0
			340	340	
97	B	1	Total	O	0
			1	1	
97	D	5	Total	O	0
			5	5	
97	E	4	Total	O	0
			4	4	
97	F	6	Total	O	0
			6	6	
97	K	3	Total	O	0
			3	3	
97	L	1	Total	O	0
			1	1	
97	M	7	Total	O	0
			7	7	
97	N	1	Total	O	0
			1	1	
97	O	2	Total	O	0
			2	2	
97	Q	1	Total	O	0
			1	1	

Continued on next page...

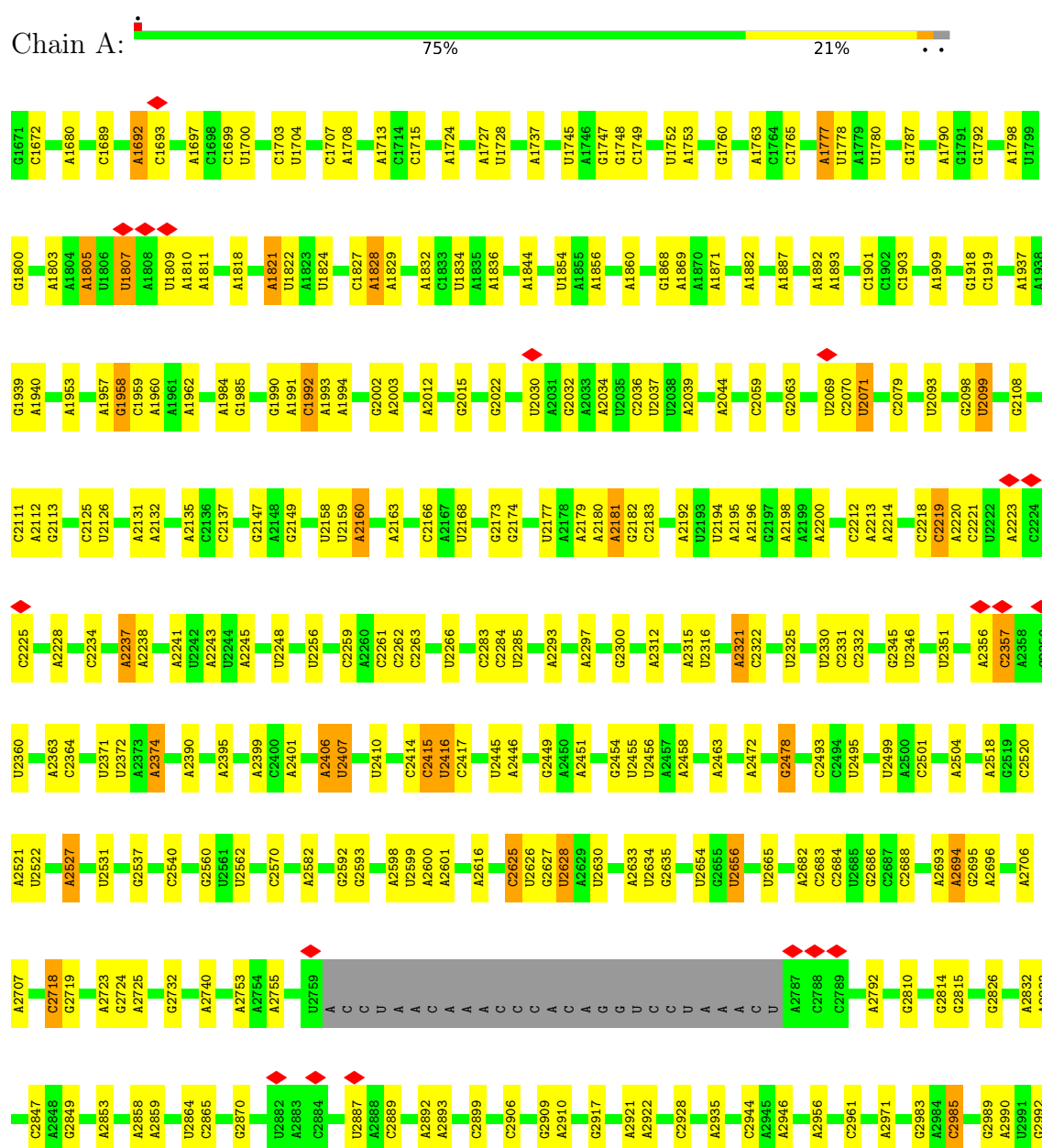
Continued from previous page...

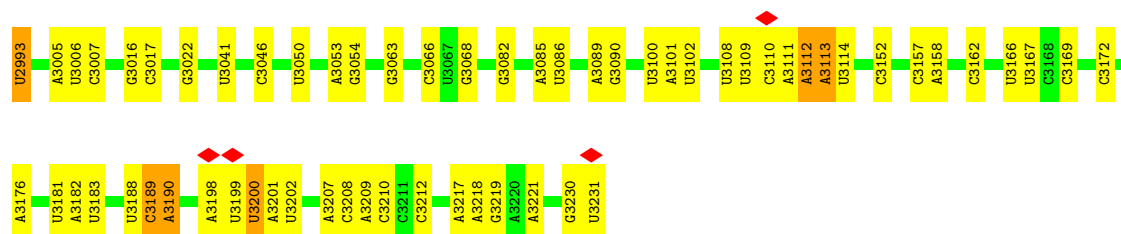
Mol	Chain	Residues	Atoms		AltConf
97	R	3	Total 3	O 3	0
97	S	1	Total 1	O 1	0
97	T	1	Total 1	O 1	0
97	U	1	Total 1	O 1	0
97	W	2	Total 2	O 2	0
97	6	1	Total 1	O 1	0
97	c	1	Total 1	O 1	0
97	f	1	Total 1	O 1	0
97	i	1	Total 1	O 1	0
97	o	2	Total 2	O 2	0
97	r	1	Total 1	O 1	0
97	s	2	Total 2	O 2	0
97	AA	69	Total 69	O 69	0
97	AC	1	Total 1	O 1	0
97	AG	1	Total 1	O 1	0
97	AH	3	Total 3	O 3	0
97	AK	2	Total 2	O 2	0
97	AX	2	Total 2	O 2	0
97	A0	1	Total 1	O 1	0
97	A3	3	Total 3	O 3	0

3 Residue-property plots

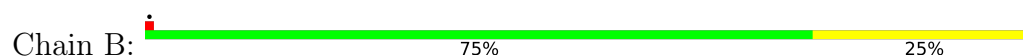
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





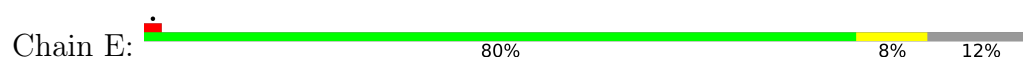
- Molecule 2: mitochondrial tRNA^{Val}



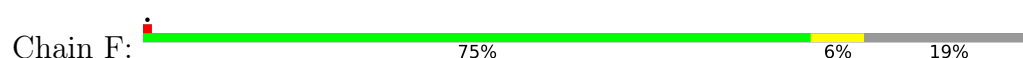
- Molecule 3: 39S ribosomal protein L2, mitochondrial



- Molecule 4: 39S ribosomal protein L3, mitochondrial

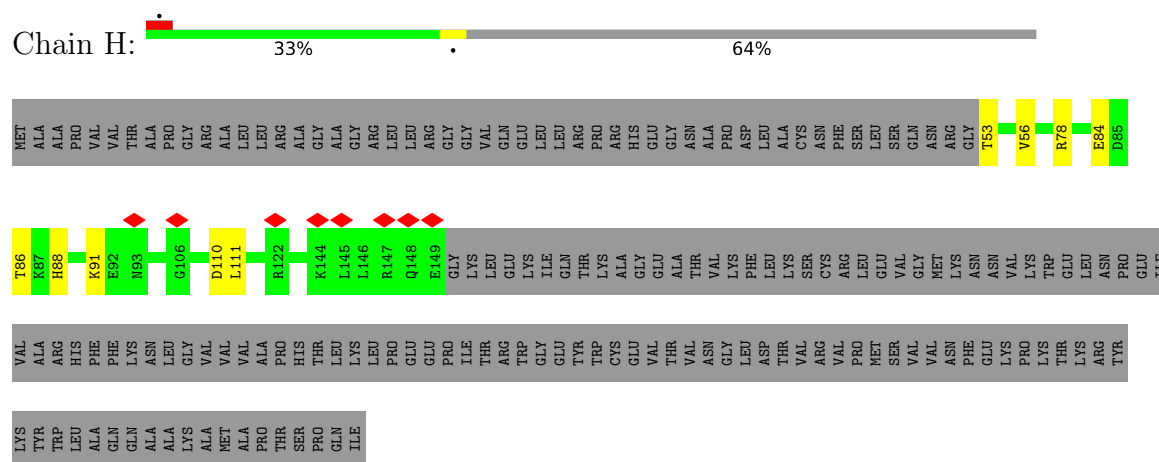


- Molecule 5: 39S ribosomal protein L4, mitochondrial

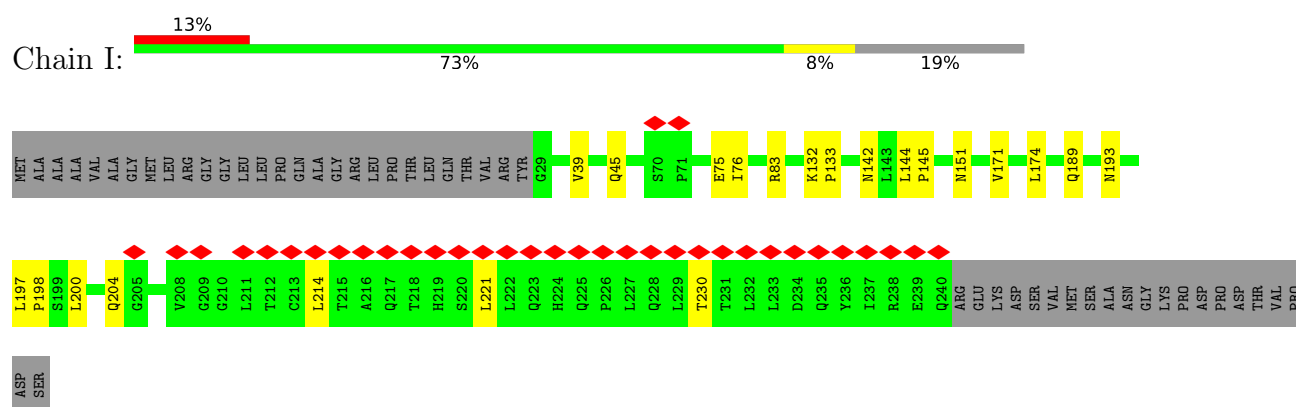


- Molecule 6: 39S ribosomal protein L9, mitochondrial

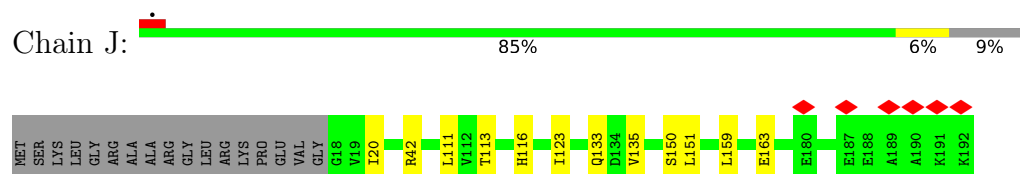




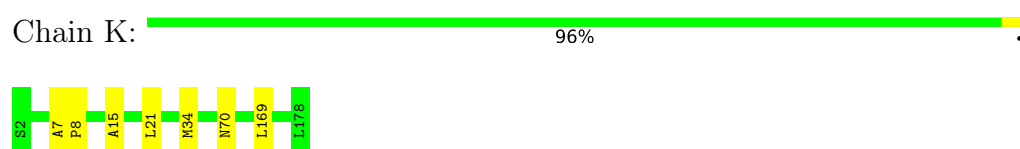
- Molecule 7: 39S ribosomal protein L10, mitochondrial



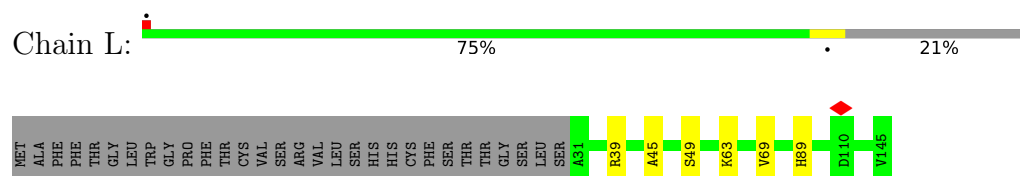
- Molecule 8: 39S ribosomal protein L11, mitochondrial



- Molecule 9: 39S ribosomal protein L13, mitochondrial



- Molecule 10: 39S ribosomal protein L14, mitochondrial



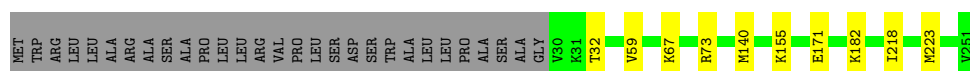
- Molecule 11: 39S ribosomal protein L15, mitochondrial

Chain M:  93% 5%



- Molecule 12: 39S ribosomal protein L16, mitochondrial

Chain N:  84% 12%



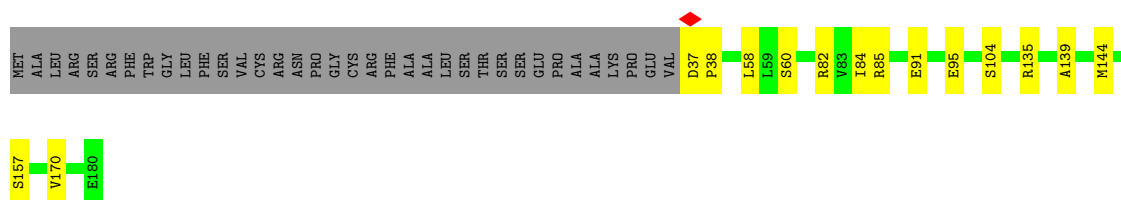
- Molecule 13: 39S ribosomal protein L17, mitochondrial

Chain O:  82% 6% 12%



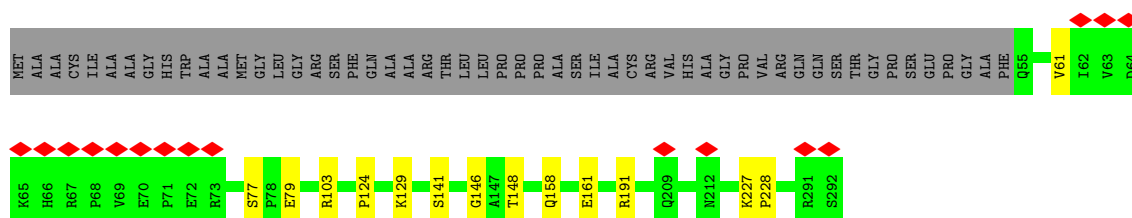
- Molecule 14: 39S ribosomal protein L18, mitochondrial

Chain P:  72% 8% 20%



- Molecule 15: 39S ribosomal protein L19, mitochondrial

Chain Q:  5% 77% 5% 18%

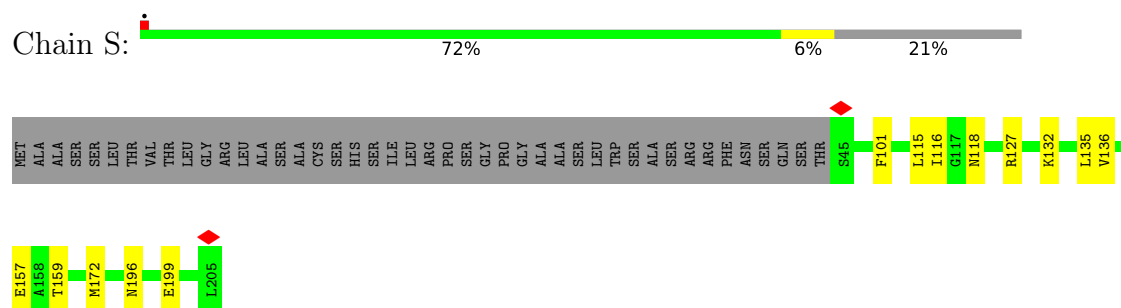


- Molecule 16: 39S ribosomal protein L20, mitochondrial

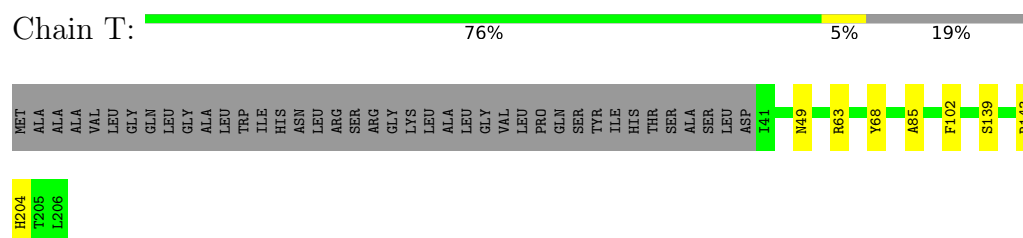
Chain R:  90% 6%



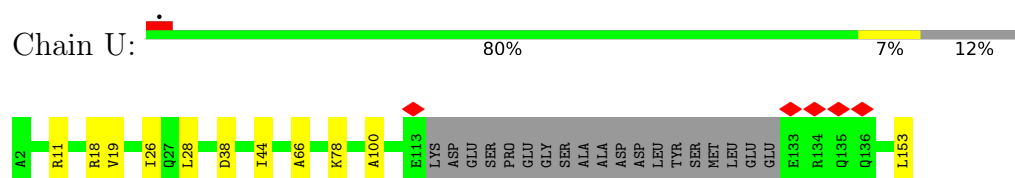
- Molecule 17: 39S ribosomal protein L21, mitochondrial



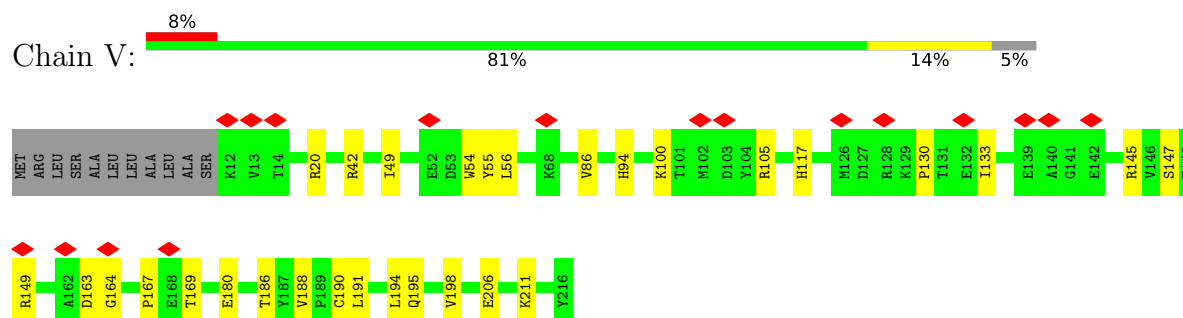
- Molecule 18: 39S ribosomal protein L22, mitochondrial



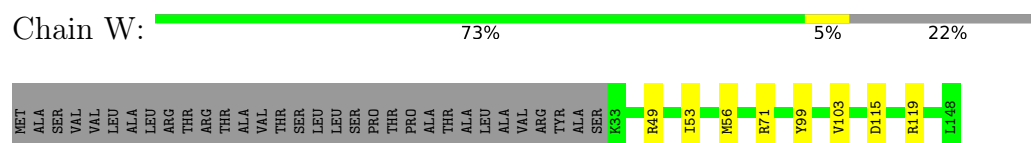
- Molecule 19: 39S ribosomal protein L23, mitochondrial



- Molecule 20: 39S ribosomal protein L24, mitochondrial

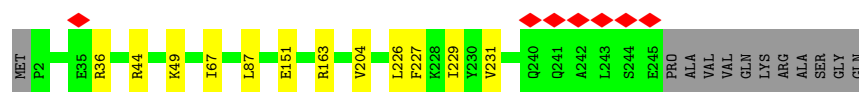


- Molecule 21: 39S ribosomal protein L27, mitochondrial



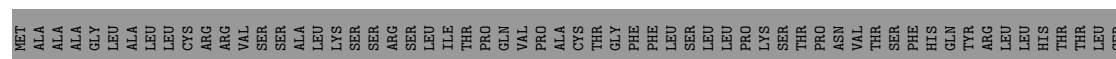
- Molecule 22: 39S ribosomal protein L28, mitochondrial





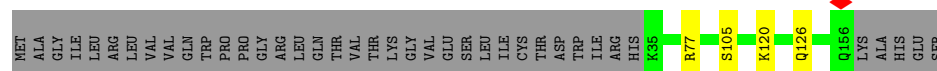
- Molecule 23: 39S ribosomal protein L47, mitochondrial

Chain Y: 68% 28%



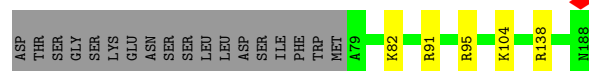
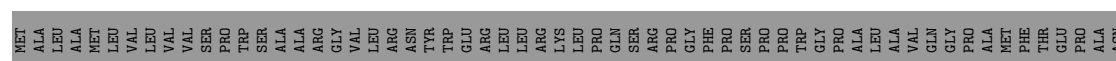
- Molecule 24: 39S ribosomal protein L30, mitochondrial

Chain Z: 73% 24%



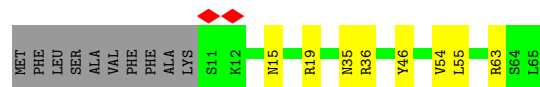
- Molecule 25: 39S ribosomal protein L32, mitochondrial

Chain 0: 56% 41%



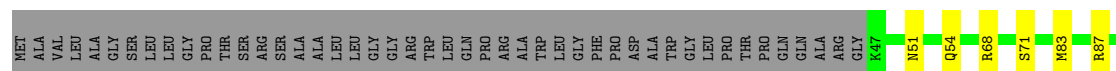
- Molecule 26: 39S ribosomal protein L33, mitochondrial

Chain 1: 72% 12% 15%



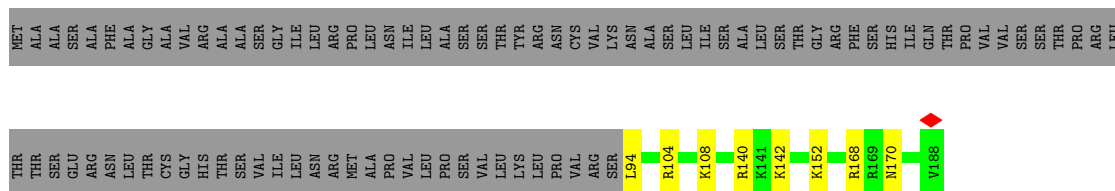
- Molecule 27: 39S ribosomal protein L34, mitochondrial

Chain 2: 43% 7% 50%



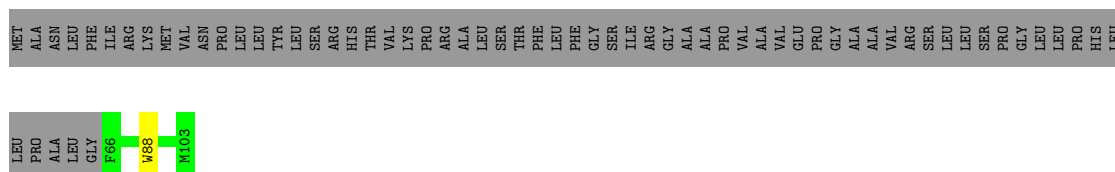
- Molecule 28: 39S ribosomal protein L35, mitochondrial

Chain 3:  46% 49%



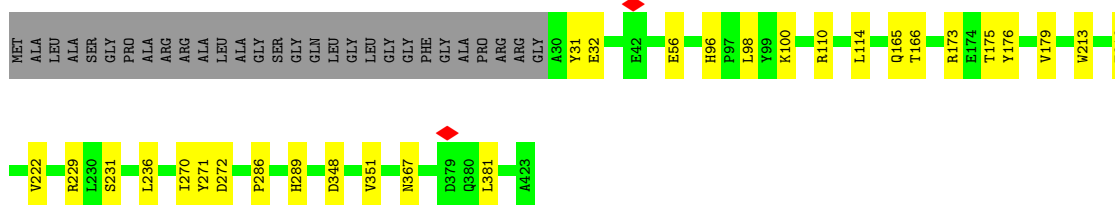
- Molecule 29: 39S ribosomal protein L36, mitochondrial

Chain 4:  36% 63%



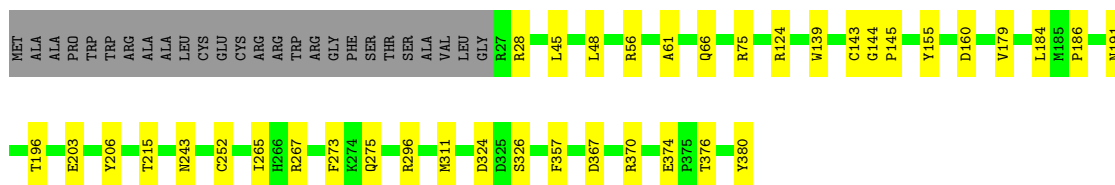
- Molecule 30: 39S ribosomal protein L37, mitochondrial

Chain 5:  86% 7% 7%



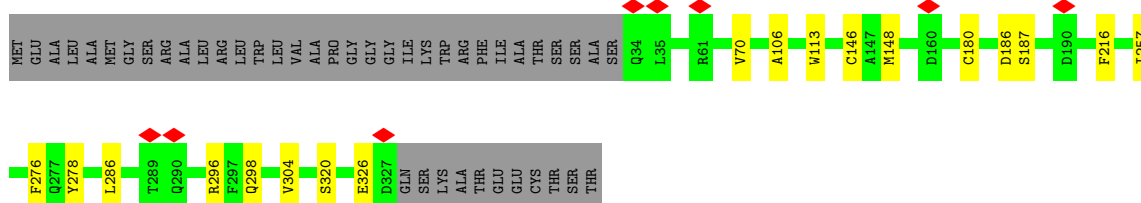
- Molecule 31: 39S ribosomal protein L38, mitochondrial

Chain 6:  83% 10% 7%

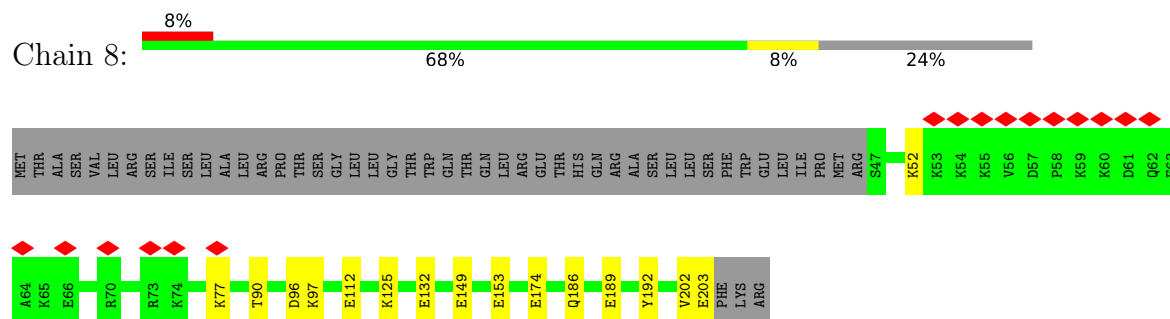


- Molecule 32: 39S ribosomal protein L39, mitochondrial

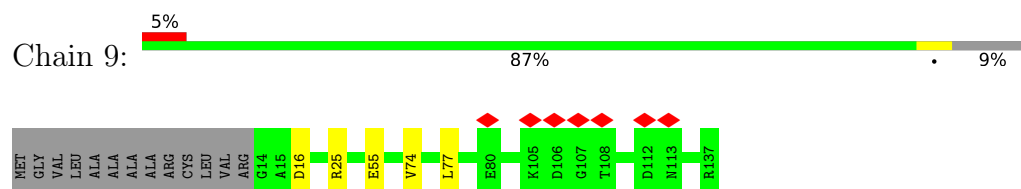
Chain 7:  82% 5% 13%



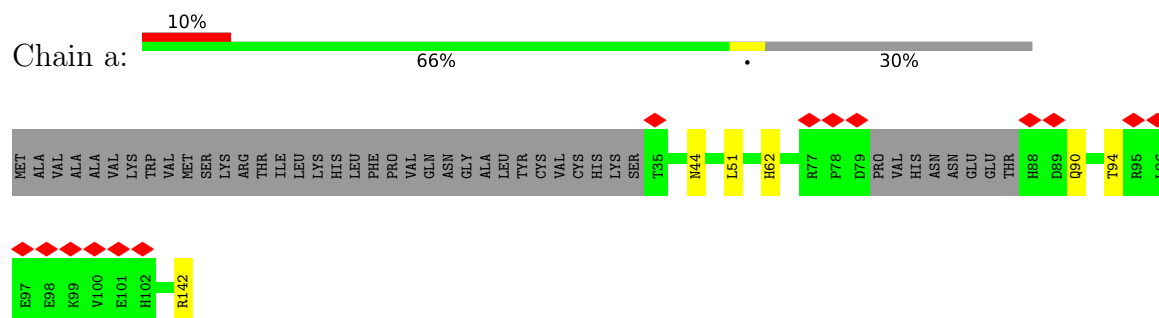
- Molecule 33: 39S ribosomal protein L40, mitochondrial



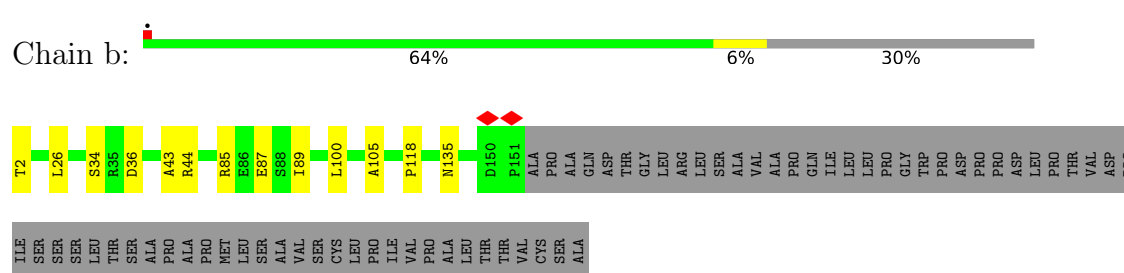
- Molecule 34: 39S ribosomal protein L41, mitochondrial



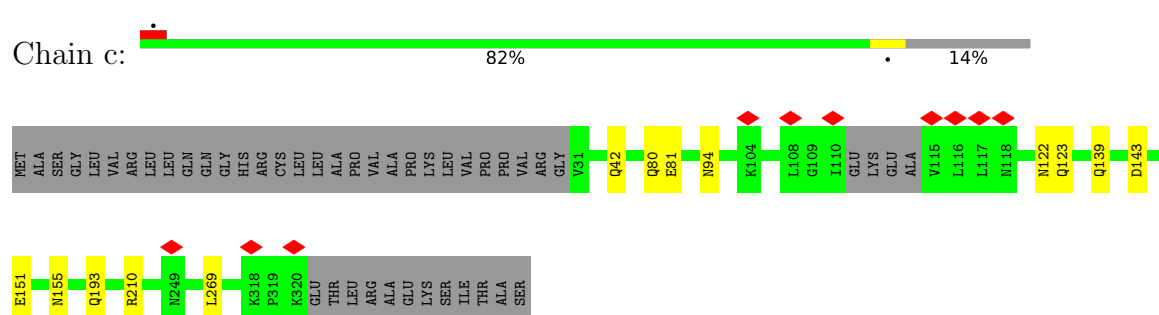
- Molecule 35: 39S ribosomal protein L42, mitochondrial



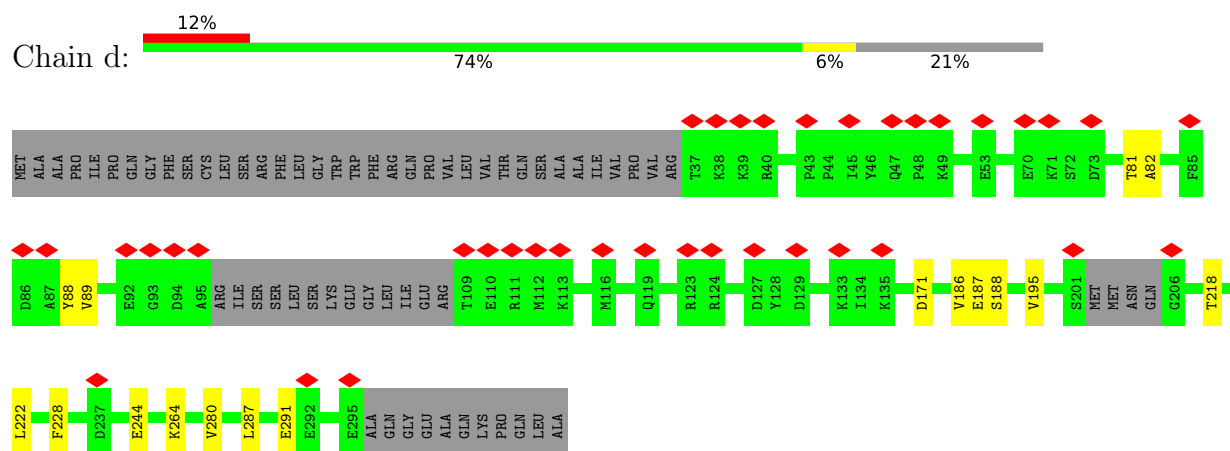
- Molecule 36: 39S ribosomal protein L43, mitochondrial



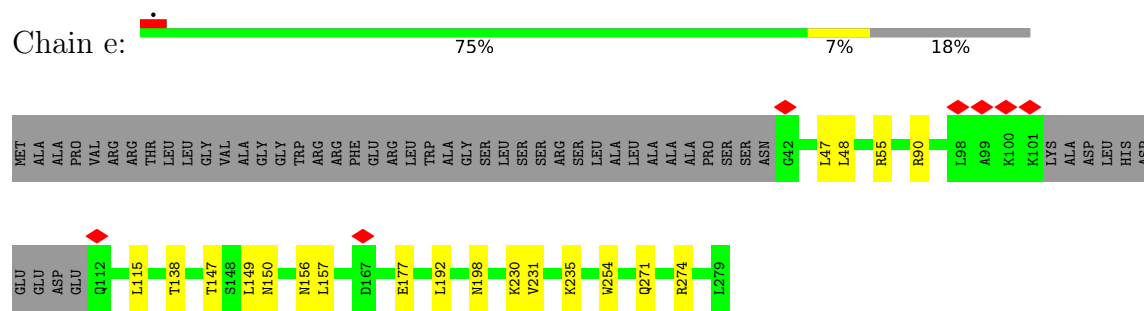
- Molecule 37: 39S ribosomal protein L44, mitochondrial



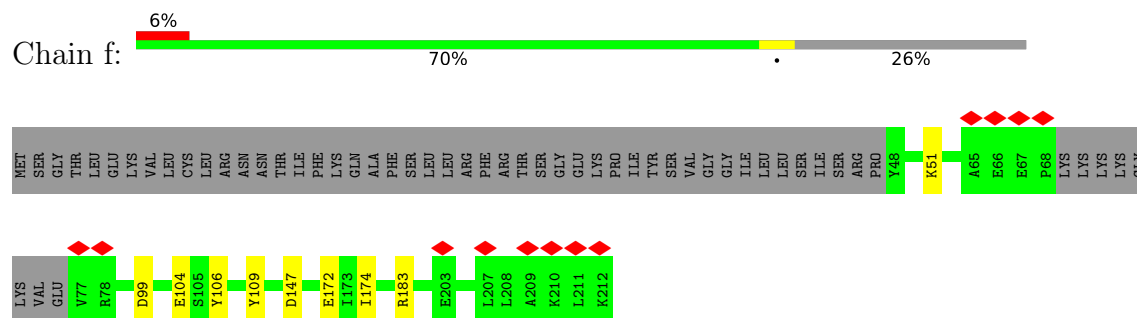
- Molecule 38: 39S ribosomal protein L45, mitochondrial



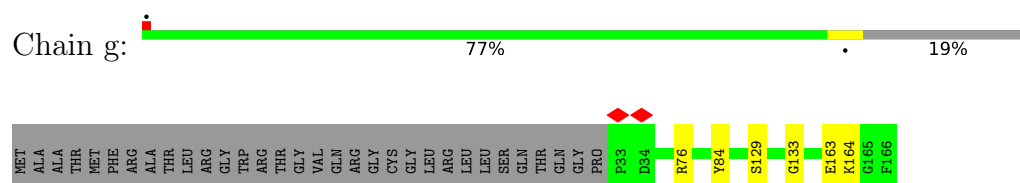
- Molecule 39: 39S ribosomal protein L46, mitochondrial



- Molecule 40: 39S ribosomal protein L48, mitochondrial

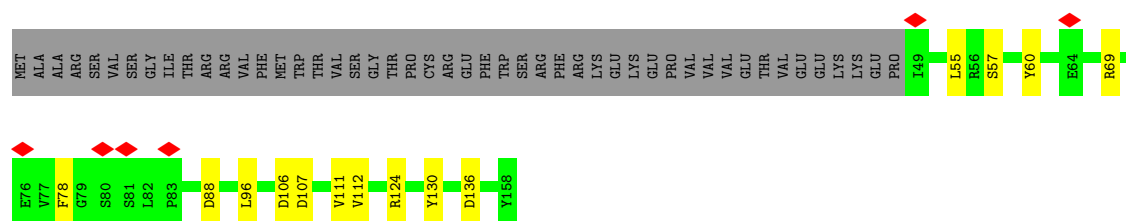


- Molecule 41: 39S ribosomal protein L49, mitochondrial



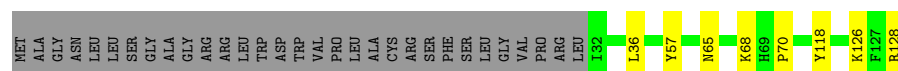
- Molecule 42: 39S ribosomal protein L50, mitochondrial





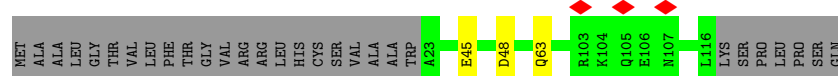
- Molecule 43: 39S ribosomal protein L51, mitochondrial

Chain i: 70% 6% 24%



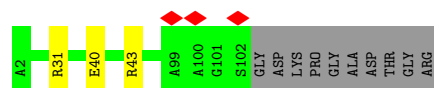
- Molecule 44: 39S ribosomal protein L52, mitochondrial

Chain j: 74% 0% 24%



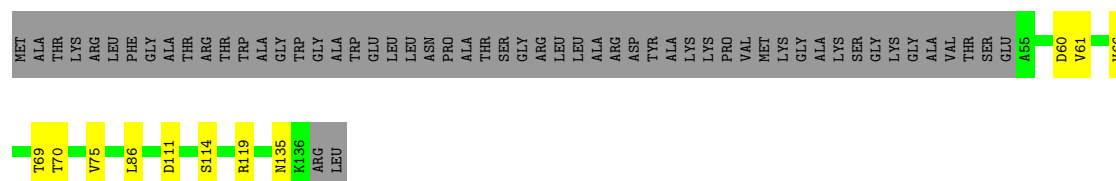
- Molecule 45: 39S ribosomal protein L53, mitochondrial

Chain k: 88% 0% 9%



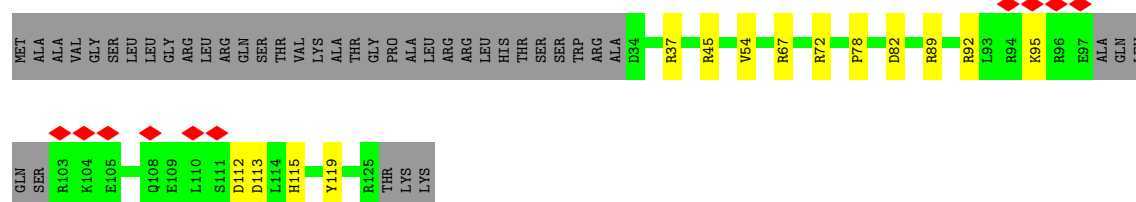
- Molecule 46: 39S ribosomal protein L54, mitochondrial

Chain l: 51% 8% 41%

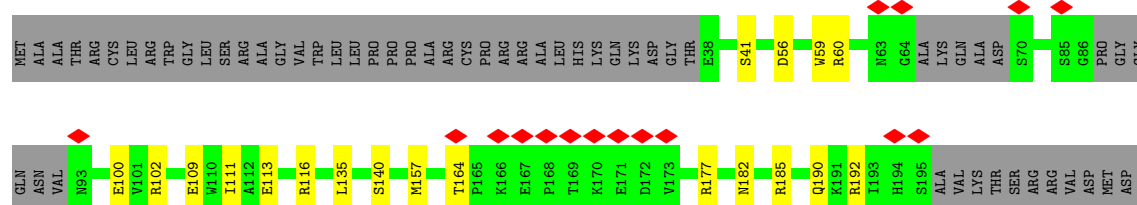


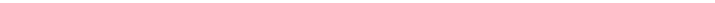
- Molecule 47: 39S ribosomal protein L55, mitochondrial

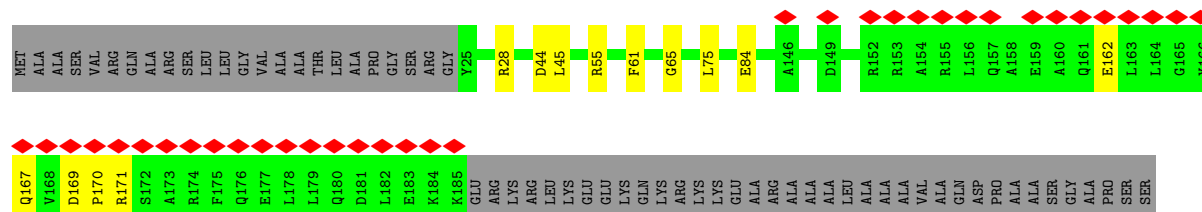
Chain m: 8% 57% 11% 32%

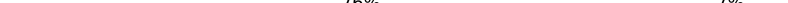


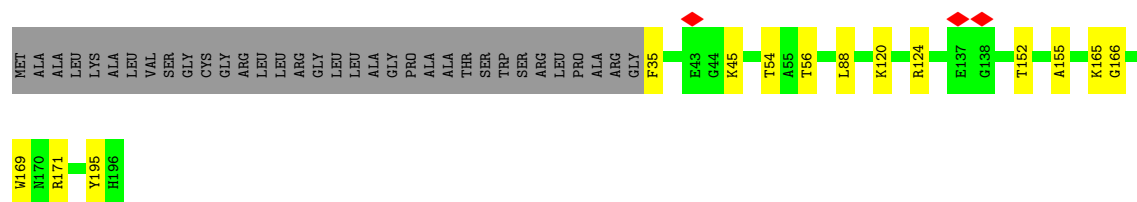
- Chain o: 85% 7% 8%

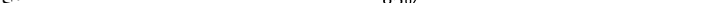


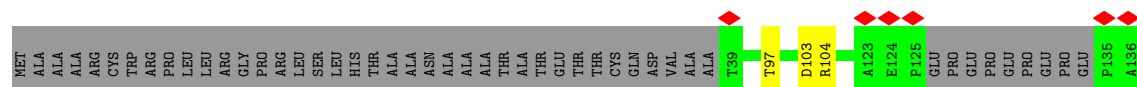
- Chain α :  16% 67% 6% 27%

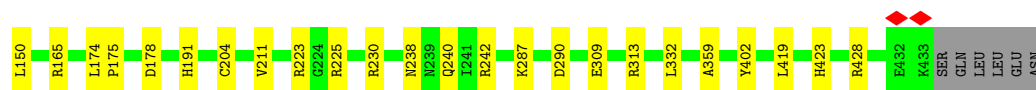


- Chain r: 

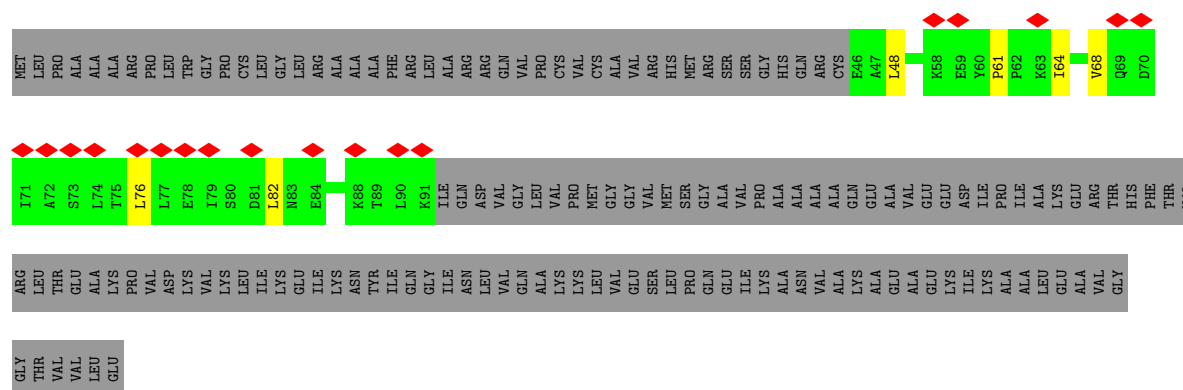


- Chain s:  82% 6% 12%

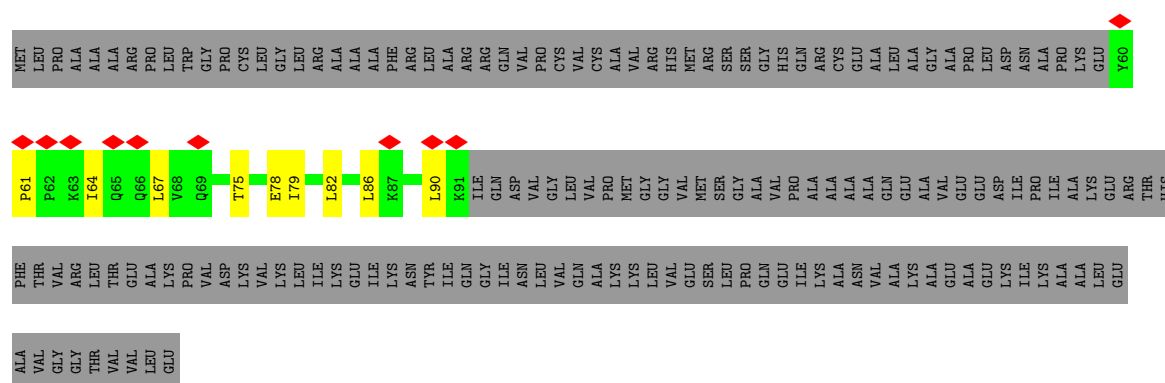




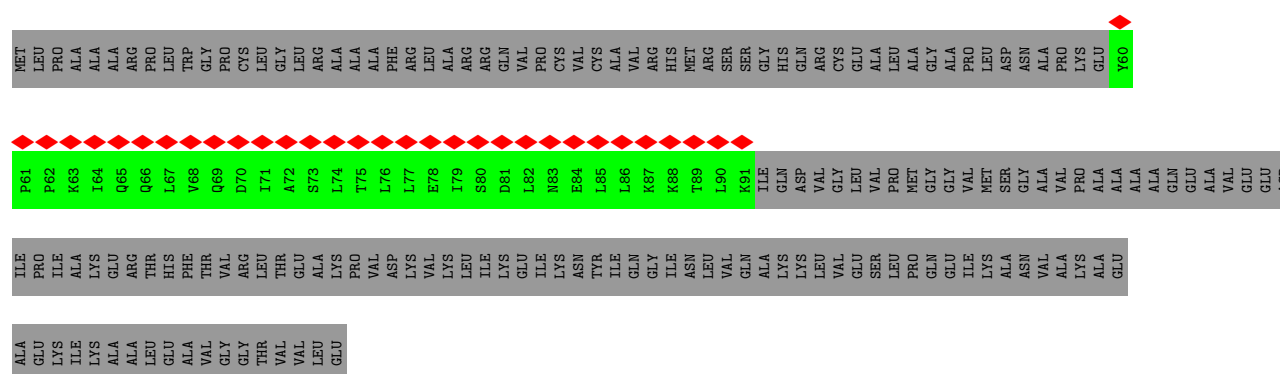
- Molecule 53: 39S ribosomal protein L12, mitochondrial

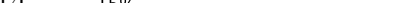


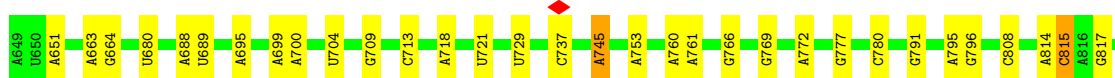
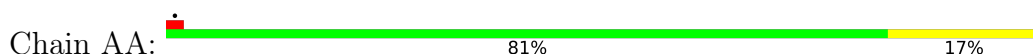
- Molecule 53: 39S ribosomal protein L12, mitochondrial

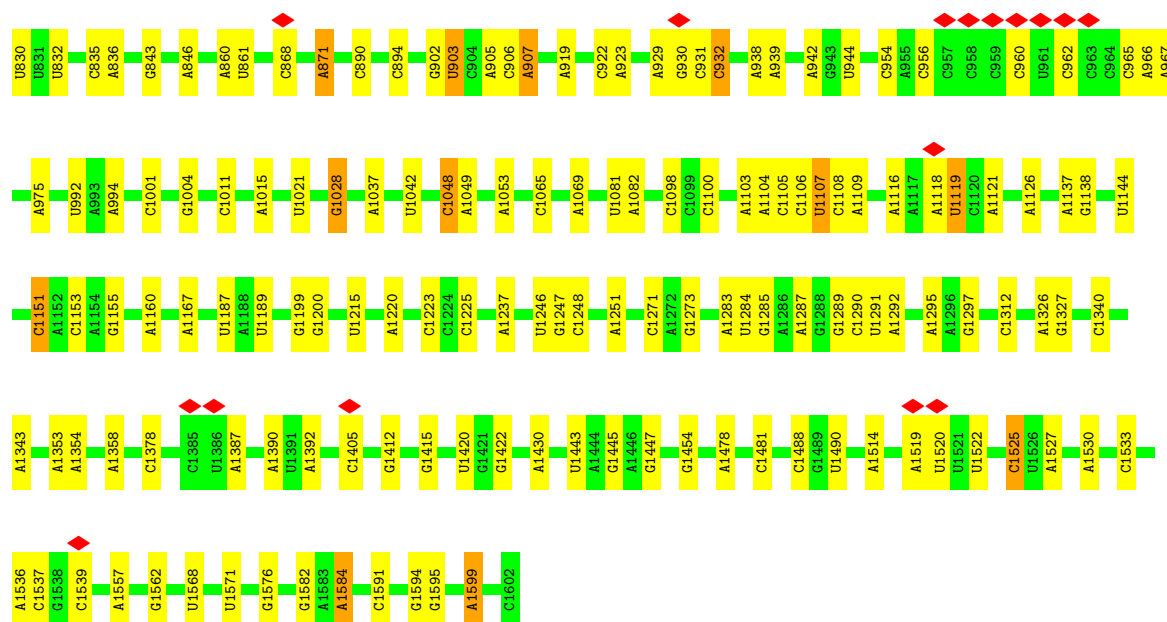


- Molecule 53: 39S ribosomal protein L12, mitochondrial



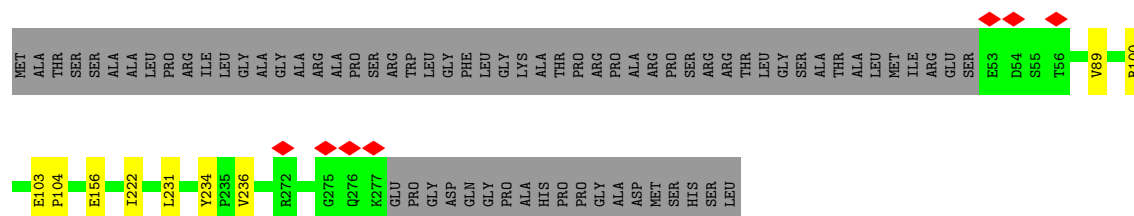
- Chain t4:  15% 15% 84%





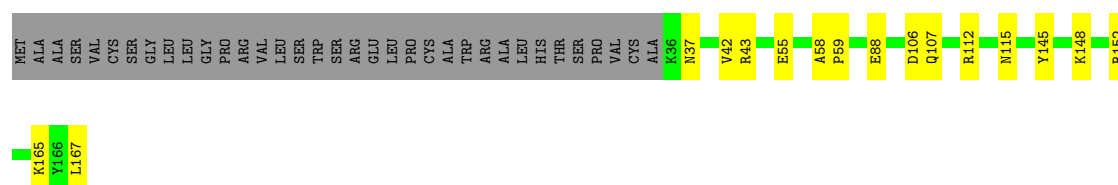
- Molecule 55: 28S ribosomal protein S2, mitochondrial

Chain AB: 73% 24%



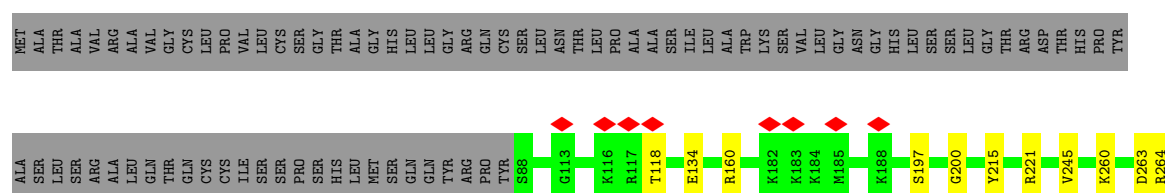
- Molecule 56: 28S ribosomal protein S24, mitochondrial

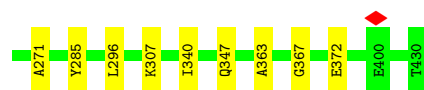
Chain AC: 69% 10% 21%



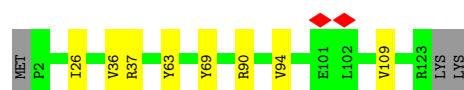
- Molecule 57: 28S ribosomal protein S5, mitochondrial

Chain AD: 75% 5% 20%

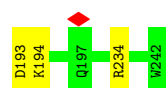
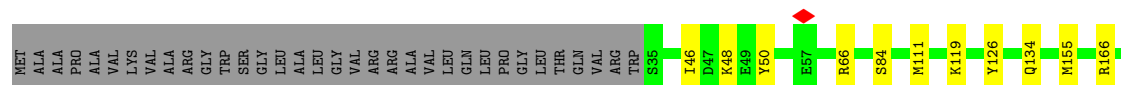
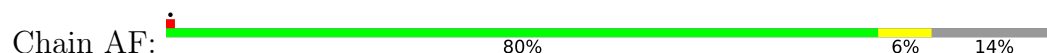




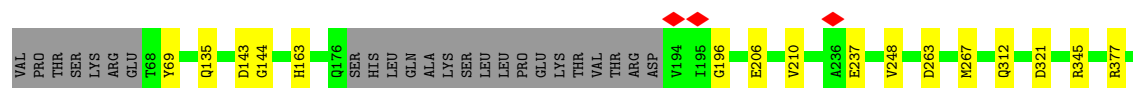
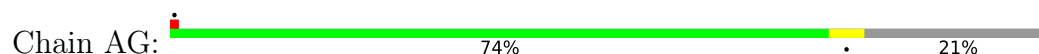
- Molecule 58: 28S ribosomal protein S6, mitochondrial



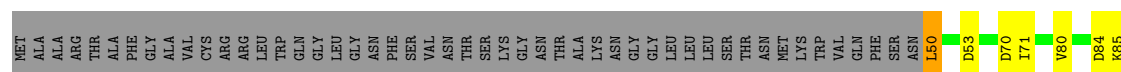
- Molecule 59: 28S ribosomal protein S7, mitochondrial



- Molecule 60: 28S ribosomal protein S9, mitochondrial

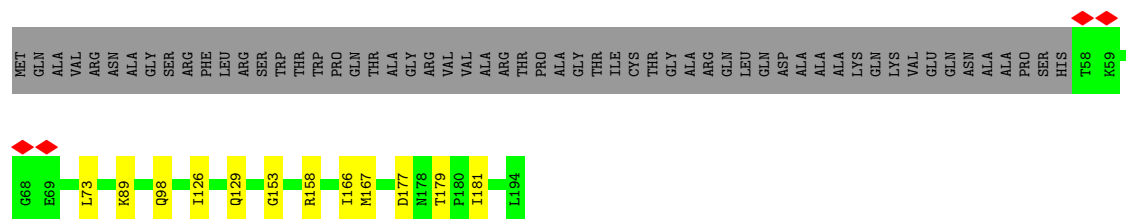


- Molecule 61: 28S ribosomal protein S10, mitochondrial

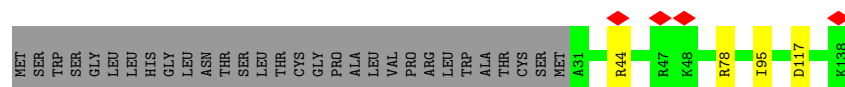
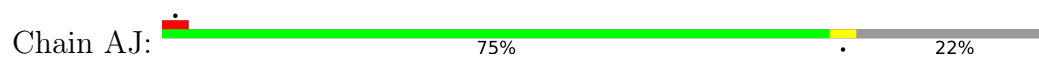


- Molecule 62: 28S ribosomal protein S11, mitochondrial

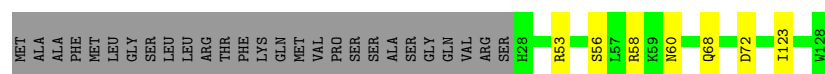
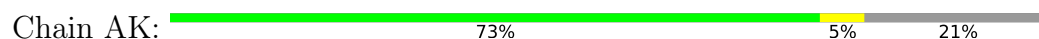




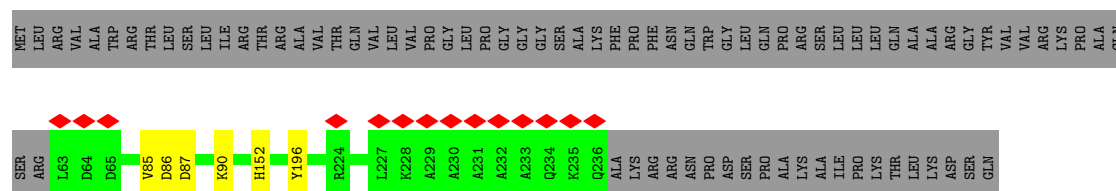
- Molecule 63: 28S ribosomal protein S12, mitochondrial



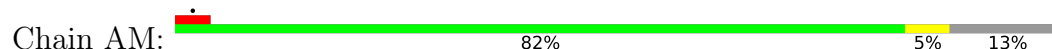
- Molecule 64: 28S ribosomal protein S14, mitochondrial



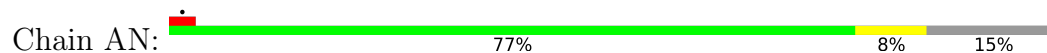
- Molecule 65: 28S ribosomal protein S15, mitochondrial



- Molecule 66: 28S ribosomal protein S16, mitochondrial

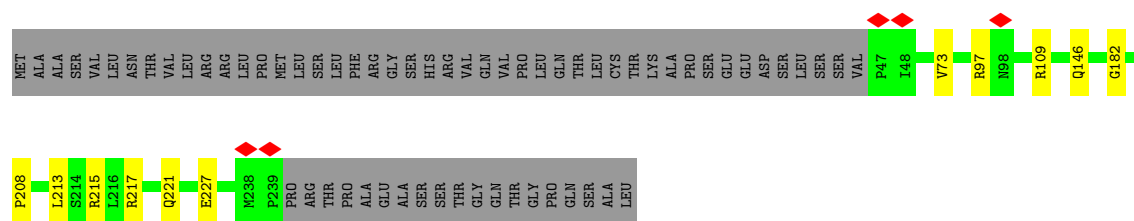


- Molecule 67: 28S ribosomal protein S17, mitochondrial

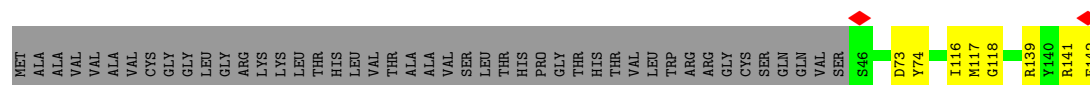


- Molecule 68: 28S ribosomal protein S18b, mitochondrial





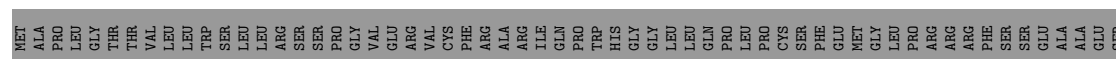
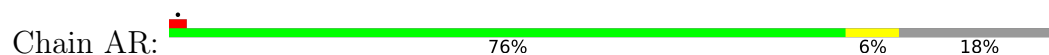
- Molecule 69: 28S ribosomal protein S18c, mitochondrial



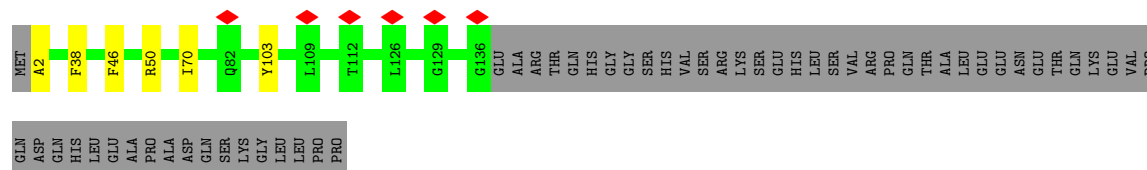
- Molecule 70: 28S ribosomal protein S21, mitochondrial



- Molecule 71: 28S ribosomal protein S22, mitochondrial

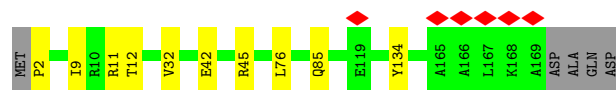


- Molecule 72: 28S ribosomal protein S23, mitochondrial

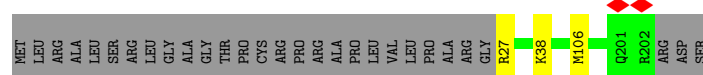
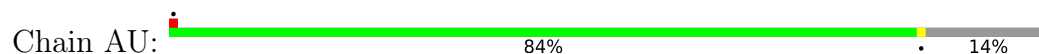


- Molecule 73: 28S ribosomal protein S25, mitochondrial

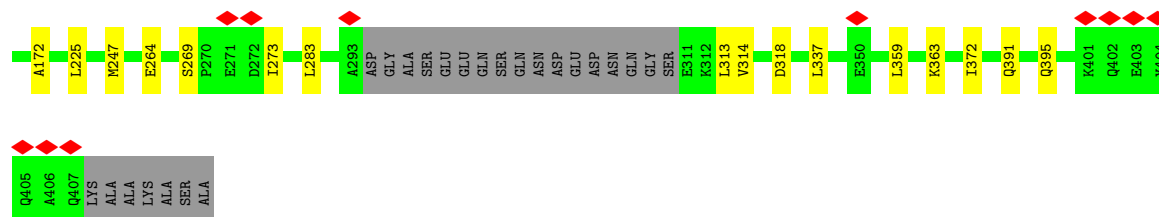
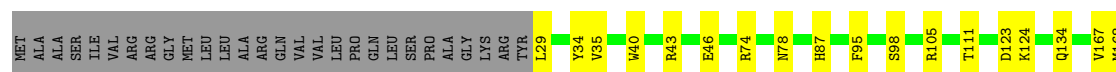
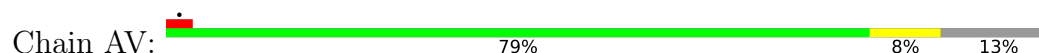




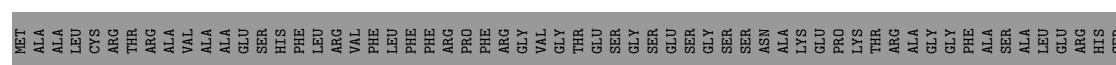
- Molecule 74: 28S ribosomal protein S26, mitochondrial



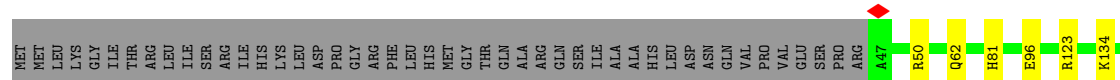
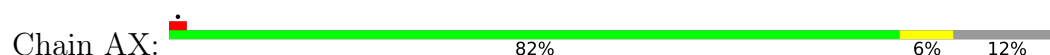
- Molecule 75: 28S ribosomal protein S27, mitochondrial



- Molecule 76: 28S ribosomal protein S28, mitochondrial

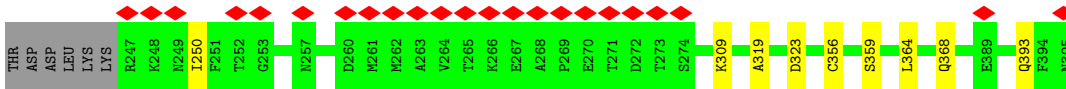


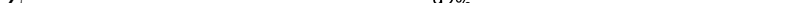
- Molecule 77: 28S ribosomal protein S29, mitochondrial

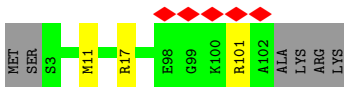


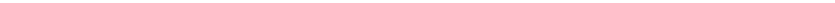
- Molecule 78: 28S ribosomal protein S31, mitochondrial

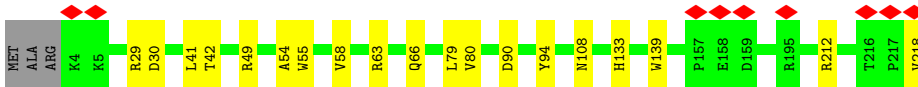




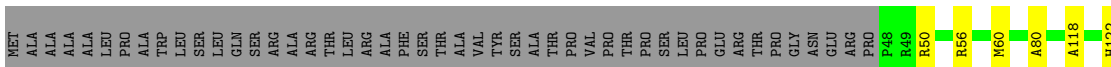
- Chain AZ:  5% 92% 6%

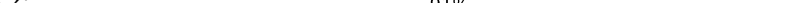


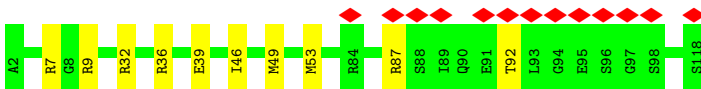
- Chain A0:  90% 9%

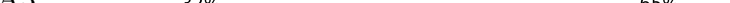


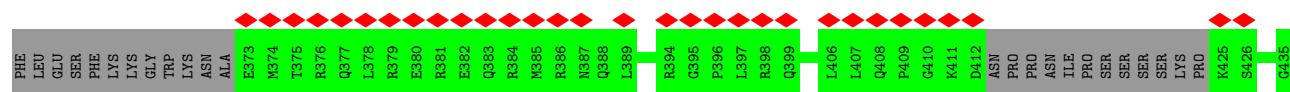
- Chain A1: 79% 7% 15%



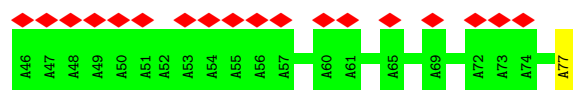
- Chain A2:  11% 91% 9%



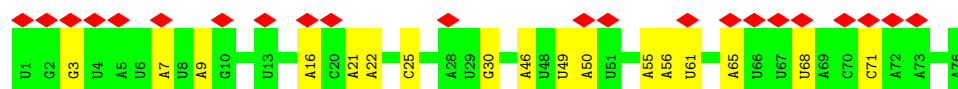
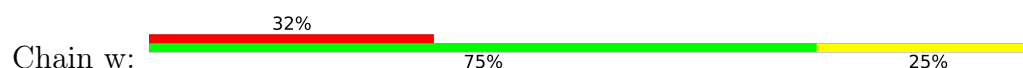
- Chain A3:  32% 3% 65%



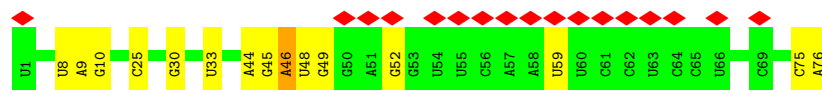
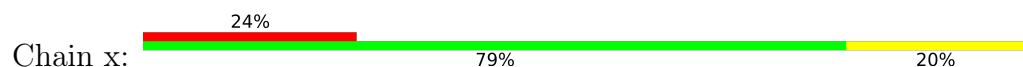
- Molecule 86: Nascent polypeptide



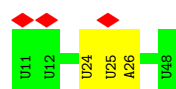
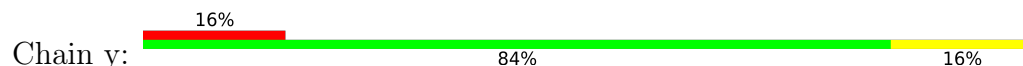
- Molecule 87: A-site tRNA with aminoacylation



- Molecule 88: P-site tRNA



- Molecule 89: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30744	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	42.750	Depositor
Minimum map value	-22.327	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.092	Depositor
Recommended contour level	3	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: FES, SAC, AYA, K, ATP, ZN, THC, MG, GTP, IAS

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	0/36431	0.20	0/56711
2	B	0.11	0/1700	0.19	0/2641
3	D	0.15	0/1896	0.29	0/2549
4	E	0.14	0/2475	0.25	0/3355
5	F	0.16	0/2090	0.29	0/2842
6	H	0.14	0/816	0.27	0/1097
7	I	0.18	0/1731	0.27	0/2345
8	J	0.16	0/1348	0.27	0/1813
9	K	0.19	0/1490	0.28	0/2021
10	L	0.15	0/905	0.28	0/1218
11	M	0.16	0/2381	0.29	0/3212
12	N	0.18	0/1833	0.28	0/2468
13	O	0.16	0/1283	0.27	0/1727
14	P	0.23	0/1199	0.30	0/1623
15	Q	0.13	0/2027	0.26	0/2734
16	R	0.18	0/1175	0.27	0/1572
17	S	0.16	0/1320	0.31	0/1789
18	T	0.16	0/1403	0.28	0/1886
19	U	0.16	0/1127	0.30	0/1523
20	V	0.12	0/1721	0.26	0/2333
21	W	0.23	0/926	0.31	0/1244
22	X	0.13	0/2099	0.25	0/2837
23	Y	0.15	0/1593	0.28	0/2136
24	Z	0.15	0/1021	0.27	0/1378
25	0	0.15	0/913	0.27	0/1224
26	1	0.15	0/460	0.27	0/610
27	2	0.19	0/383	0.33	0/507
28	3	0.19	0/853	0.31	0/1136
29	4	0.21	0/350	0.30	0/461
30	5	0.14	0/3305	0.26	0/4502
31	6	0.21	0/3043	0.31	0/4140
32	7	0.11	0/2447	0.24	0/3310

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	8	0.16	0/1354	0.26	0/1819
34	9	0.15	0/1025	0.25	0/1379
35	a	0.13	0/866	0.30	0/1174
36	b	0.16	0/1211	0.30	0/1639
37	c	0.14	0/2347	0.25	0/3171
38	d	0.10	0/2043	0.23	0/2764
39	e	0.15	0/1885	0.25	0/2542
40	f	0.20	0/1273	0.26	0/1716
41	g	0.15	0/1151	0.29	0/1569
42	h	0.11	0/918	0.23	0/1249
43	i	0.18	0/850	0.30	0/1135
44	j	0.15	0/760	0.27	0/1023
45	k	0.16	0/777	0.27	0/1048
46	l	0.15	0/707	0.27	0/960
47	m	0.17	0/767	0.30	0/1028
48	o	0.18	0/819	0.31	0/1097
49	p	0.13	0/1223	0.27	0/1641
50	q	0.12	0/1384	0.26	0/1869
51	r	0.20	0/1362	0.29	0/1846
52	s	0.15	0/3239	0.28	0/4400
53	t1	0.06	0/358	0.18	0/486
53	t2	0.07	0/259	0.19	0/350
53	t3	0.05	0/259	0.14	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	0.11	0/22655	0.17	0/35273
55	AB	0.15	0/1871	0.26	0/2531
56	AC	0.21	0/1113	0.28	0/1505
57	AD	0.16	0/2783	0.27	0/3724
58	AE	0.12	0/989	0.26	0/1335
59	AF	0.12	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	0.13	0/1030	0.26	0/1386
63	AJ	0.15	0/855	0.27	0/1148
64	AK	0.20	0/880	0.31	0/1182
65	AL	0.12	0/1477	0.25	0/1974
66	AM	0.16	0/963	0.29	0/1295
67	AN	0.14	0/886	0.23	0/1199
68	AO	0.14	0/1648	0.27	0/2243
69	AP	0.13	0/798	0.26	0/1070
70	AQ	0.15	0/748	0.32	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	0.13	0/1402	0.27	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	0.10	0/2921	0.23	0/3954
78	AY	0.14	0/1280	0.22	0/1725
79	AZ	0.16	0/857	0.27	0/1141
80	A0	0.13	0/1834	0.30	0/2484
81	A1	0.16	0/2285	0.25	0/3090
82	A2	0.13	0/941	0.30	0/1257
83	A3	0.17	0/636	0.37	0/839
84	A4	0.11	0/4877	0.24	0/6598
85	u	0.09	0/439	0.25	0/586
86	v	0.06	0/159	0.17	0/221
87	w	0.06	0/1608	0.14	0/2497
88	x	0.06	0/1656	0.15	0/2571
89	y	0.09	0/443	0.17	0/684
All	All	0.14	0/185856	0.24	0/264114

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 [i](#)

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	32560	16532	16529	146	0
2	B	1522	776	776	3	0
3	D	1859	1921	1920	15	0
4	E	2406	2417	2415	17	0
5	F	2031	2066	2065	13	0
6	H	802	847	846	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	1695	1786	1785	17	0
8	J	1330	1409	1407	9	0
9	K	1455	1454	1452	5	0
10	L	890	942	941	4	0
11	M	2327	2396	2395	13	0
12	N	1786	1819	1817	8	0
13	O	1259	1295	1294	8	0
14	P	1173	1166	1165	12	0
15	Q	1979	2023	2022	9	0
16	R	1154	1215	1214	5	0
17	S	1293	1366	1365	11	0
18	T	1369	1411	1410	8	0
19	U	1107	1108	1107	10	0
20	V	1676	1688	1687	24	0
21	W	904	937	935	6	0
22	X	2044	2061	2060	8	0
23	Y	1556	1598	1597	9	0
24	Z	996	1045	1044	4	0
25	0	898	917	916	5	0
26	1	455	499	498	6	0
27	2	377	407	406	4	0
28	3	832	884	883	7	0
29	4	342	362	361	1	0
30	5	3210	3208	3206	21	0
31	6	2948	2844	2841	26	0
32	7	2390	2399	2397	11	0
33	8	1327	1369	1368	15	0
34	9	997	988	987	4	0
35	a	840	812	810	5	0
36	b	1196	1196	1190	8	0
37	c	2299	2322	2320	8	0
38	d	1988	1982	1978	11	0
39	e	1848	1851	1849	13	0
40	f	1252	1271	1269	8	0
41	g	1113	1097	1097	3	0
42	h	895	882	881	8	0
43	i	828	859	857	8	0
44	j	745	747	746	2	0
45	k	774	784	784	2	0
46	l	688	675	674	8	0
47	m	754	761	758	13	0
48	o	798	807	804	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	p	1205	1226	1223	16	0
50	q	1350	1328	1327	9	0
51	r	1322	1349	1349	12	0
52	s	3155	3143	3139	17	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	62	0
55	AB	1828	1816	1815	7	0
56	AC	1083	1089	1088	10	0
57	AD	2731	2805	2804	13	0
58	AE	972	1001	1000	6	0
59	AF	1725	1770	1769	12	0
60	AG	2568	2558	2554	11	0
61	AH	1152	1184	1183	11	0
62	AI	1018	1058	1056	7	0
63	AJ	839	888	887	4	0
64	AK	862	886	885	5	0
65	AL	1453	1541	1540	5	0
66	AM	942	966	965	5	0
67	AN	868	929	928	7	0
68	AO	1592	1557	1557	10	0
69	AP	781	807	806	6	0
70	AQ	744	758	758	6	0
71	AR	2409	2429	2428	15	0
72	AS	1111	1116	1115	6	0
73	AT	1371	1394	1393	8	0
74	AU	1488	1500	1499	3	0
75	AV	2969	2964	2961	21	0
76	AW	789	803	802	5	0
77	AX	2849	2845	2843	15	0
78	AY	1246	1198	1197	8	0
79	AZ	839	860	858	3	0
80	A0	1787	1797	1796	13	0
81	A1	2238	2269	2269	15	0
82	A2	935	969	973	9	0
83	A3	625	700	699	5	0
84	A4	4768	4768	4766	24	0
85	u	431	432	429	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	v	160	160	159	2	0
87	w	1438	725	725	1	0
88	x	1483	751	752	6	0
89	y	399	199	201	1	0
90	A	128	0	0	0	0
90	A3	1	0	0	0	0
90	AA	53	0	0	0	0
90	AB	1	0	0	0	0
90	AX	1	0	0	0	0
90	D	3	0	0	0	0
90	E	1	0	0	0	0
90	g	1	0	0	0	0
91	A	30	0	0	0	0
91	AA	9	0	0	0	0
91	M	1	0	0	0	0
91	N	1	0	0	0	0
91	P	1	0	0	0	0
91	i	1	0	0	0	0
91	o	1	0	0	0	0
92	0	1	0	0	0	0
92	4	1	0	0	0	0
92	AO	1	0	0	0	0
93	AP	4	0	0	0	0
93	AT	4	0	0	0	0
93	r	4	0	0	0	0
94	AX	31	12	12	1	0
95	AX	32	12	12	0	0
96	w	5	7	4	2	0
97	6	1	0	0	0	0
97	A	340	0	0	11	0
97	A0	1	0	0	0	0
97	A3	3	0	0	0	0
97	AA	69	0	0	6	0
97	AC	1	0	0	0	0
97	AG	1	0	0	0	0
97	AH	3	0	0	1	0
97	AK	2	0	0	0	0
97	AX	2	0	0	0	0
97	B	1	0	0	0	0
97	D	5	0	0	0	0
97	E	4	0	0	0	0
97	F	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
97	K	3	0	0	1	0
97	L	1	0	0	0	0
97	M	7	0	0	0	0
97	N	1	0	0	0	0
97	O	2	0	0	0	0
97	Q	1	0	0	0	0
97	R	3	0	0	0	0
97	S	1	0	0	0	0
97	T	1	0	0	0	0
97	U	1	0	0	0	0
97	W	2	0	0	0	0
97	c	1	0	0	0	0
97	f	1	0	0	0	0
97	i	1	0	0	0	0
97	o	2	0	0	0	0
97	r	1	0	0	0	0
97	s	2	0	0	0	0
All	All	177134	149830	149709	755	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 (755) 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)
1:A:1777:A:N6	1:A:1780:U:OP2	2.05	0.90
54:AA:992:U:O2'	54:AA:994:A:OP2	1.91	0.88
1:A:3152:C:OP1	15:Q:141:SER:OG	1.94	0.86
31:6:206:TYR:O	31:6:243:ASN:ND2	2.11	0.84
1:A:3063:G:O2'	1:A:3066:C:OP2	1.96	0.83
12:N:171:GLU:O	46:l:135:ASN:ND2	2.12	0.82
1:A:2416:U:OP1	52:s:313:ARG:NH1	2.12	0.82
51:r:35:PHE:N	51:r:56:THR:HG1	1.79	0.81
1:A:2173:G:N3	8:J:150:SER:OG	2.13	0.81
6:H:84:GLU:OE1	22:X:44:ARG:NH2	2.13	0.81
31:6:215:THR:OG1	31:6:275:GLN:OE1	1.99	0.81
54:AA:1358:A:O2'	88:x:30:G:OP1	1.97	0.81
1:A:2234:C:HO2'	1:A:2688:C:HO2'	1.23	0.80
54:AA:1021:U:OP2	82:A2:9:ARG:NH2	2.16	0.79
84:A4:239:ARG:O	84:A4:242:ASN:ND2	2.16	0.79
20:V:130:PRO:O	20:V:149:ARG:NH2	2.16	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:165:ARG:NH2	52:s:309:GLU:OE1	2.16	0.79
49:p:113:GLU:OE1	49:p:116:ARG:NH1	2.17	0.78
1:A:2158:U:OP2	51:r:195:TYR:OH	2.02	0.78
84:A4:550:ASP:OD1	84:A4:588:ARG:NH2	2.16	0.78
54:AA:729:U:O2	54:AA:745:A:N6	2.16	0.78
69:AP:139:ARG:NH1	69:AP:142:GLU:OE1	2.18	0.77
1:A:2108:G:N7	12:N:67:LYS:NZ	2.32	0.77
1:A:2069:U:O2'	1:A:2070:C:O4'	2.02	0.77
32:7:180:CYS:SG	32:7:296:ARG:NH1	2.58	0.77
51:r:166:GLY:O	51:r:171:ARG:NH2	2.18	0.77
54:AA:769:G:OP2	67:AN:73:ARG:NH2	2.17	0.77
86:v:77:ALA:O	96:w:101:ALA:N	2.18	0.76
24:Z:105:SER:OG	48:o:59:GLU:OE2	2.00	0.76
56:AC:37:ASN:O	56:AC:43:ARG:NH2	2.18	0.76
1:A:2626:U:O2'	1:A:2628:U:OP2	2.03	0.76
59:AF:50:TYR:O	59:AF:66:ARG:NH2	2.19	0.75
31:6:124:ARG:NH1	33:8:112:GLU:OE2	2.19	0.75
54:AA:1028:G:OP2	97:AA:1901:HOH:O	2.03	0.75
1:A:2740:A:N3	1:A:2921:A:O2'	2.20	0.75
49:p:56:ASP:O	49:p:60:ARG:NE	2.20	0.74
54:AA:1119:U:O4'	72:AS:50:ARG:NH1	2.20	0.74
1:A:3113:A:OP1	1:A:3167:U:O2'	2.05	0.74
36:b:87:GLU:OE1	36:b:100:LEU:HD11	1.86	0.74
20:V:105:ARG:NH2	38:d:171:ASP:OD1	2.21	0.74
67:AN:83:GLU:OE2	73:AT:85:GLN:NE2	2.20	0.74
37:c:42:GLN:NE2	43:i:36:LEU:O	2.21	0.74
1:A:2656:U:OP1	97:A:3501:HOH:O	2.06	0.73
54:AA:795:A:OP2	73:AT:134:TYR:OH	2.06	0.73
1:A:1760:G:N7	50:q:55:ARG:NH2	2.36	0.73
59:AF:119:LYS:NZ	77:AX:365:TRP:O	2.20	0.73
84:A4:399:GLU:OE2	84:A4:403:LYS:NZ	2.22	0.73
3:D:289:LEU:HD12	3:D:290:PRO:HD2	1.71	0.72
17:S:127:ARG:NH2	17:S:157:GLU:OE1	2.22	0.72
82:A2:36:ARG:NH1	82:A2:92:THR:OG1	2.22	0.72
88:x:9:A:O2'	88:x:10:G:N7	2.22	0.72
1:A:1892:A:OP2	31:6:380:TYR:OH	2.06	0.72
3:D:220:VAL:O	3:D:223:THR:OG1	2.05	0.72
68:AO:182:GLY:O	71:AR:183:LYS:NZ	2.22	0.72
54:AA:769:G:N2	54:AA:772:A:OP2	2.22	0.71
30:5:216:GLU:OE2	30:5:367:ASN:ND2	2.22	0.71
71:AR:262:LEU:O	71:AR:265:THR:OG1	2.08	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:AF:48:LYS:NZ	60:AG:321:ASP:OD1	2.22	0.71
1:A:2012:A:OP1	97:A:3503:HOH:O	2.08	0.71
54:AA:1454:G:OP2	60:AG:377:ARG:NH2	2.24	0.71
82:A2:49:MET:HG2	82:A2:53:MET:HE2	1.73	0.71
17:S:159:THR:OG1	17:S:196:ASN:OD1	2.09	0.70
75:AV:74:ARG:O	75:AV:78:ASN:ND2	2.25	0.70
5:F:272:LYS:NZ	43:i:65:ASN:OD1	2.25	0.70
1:A:2415:C:O2'	1:A:2416:U:O4'	2.10	0.69
54:AA:1412:G:OP1	77:AX:279:LYS:NZ	2.24	0.69
37:c:94:ASN:OD1	37:c:122:ASN:ND2	2.25	0.69
1:A:2034:A:O2'	11:M:71:GLN:OE1	2.08	0.69
82:A2:39:GLU:OE1	82:A2:87:ARG:NE	2.25	0.69
1:A:2312:A:OP2	97:A:3504:HOH:O	2.09	0.69
1:A:2472:A:O2'	1:A:2478:G:N7	2.24	0.69
1:A:3112:A:N6	1:A:3200:U:O2	2.17	0.69
1:A:1807:U:OP1	20:V:100:LYS:NZ	2.25	0.68
40:f:104:GLU:OE2	47:m:45:ARG:NH1	2.27	0.68
1:A:2458:A:O2'	4:E:215:PHE:O	2.11	0.68
37:c:151:GLU:O	37:c:155:ASN:ND2	2.26	0.68
1:A:1672:C:O2'	18:T:143:ARG:O	2.09	0.68
1:A:2495:U:OP1	97:A:3508:HOH:O	2.12	0.68
47:m:115:HIS:ND1	81:A1:224:TYR:OH	2.12	0.68
57:AD:285:TYR:OH	57:AD:372:GLU:OE2	2.10	0.68
1:A:2149:G:O6	97:A:3505:HOH:O	2.10	0.67
1:A:2718:C:O2	97:A:3506:HOH:O	2.11	0.67
1:A:2454:G:O6	97:A:3507:HOH:O	2.11	0.67
71:AR:212:GLU:OE1	71:AR:248:LYS:NZ	2.20	0.67
32:7:146:CYS:O	32:7:278:TYR:OH	2.13	0.67
68:AO:73:VAL:O	68:AO:109:ARG:NH2	2.27	0.67
41:g:76:ARG:NH2	41:g:163:GLU:O	2.28	0.67
77:AX:276:ARG:NH2	77:AX:286:GLU:OE1	2.28	0.67
37:c:139:GLN:NE2	37:c:143:ASP:OD2	2.28	0.67
33:8:192:TYR:OH	47:m:78:PRO:O	2.11	0.67
1:A:2160:A:OP2	29:4:88:TRP:NE1	2.27	0.66
22:X:36:ARG:NH2	22:X:151:GLU:OE2	2.27	0.66
61:AH:104:ILE:HG23	61:AH:148:LEU:HD21	1.75	0.66
1:A:1753:A:OP1	43:i:118:TYR:OH	2.11	0.66
31:6:66:GLN:OE1	31:6:75:ARG:NH2	2.29	0.66
3:D:113:ARG:O	3:D:147:ARG:NH1	2.27	0.66
81:A1:50:ARG:NH2	84:A4:94:TYR:O	2.28	0.66
1:A:2196:A:O2'	1:A:2213:A:N1	2.27	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2499:U:OP2	1:A:2504:A:N6	2.28	0.66
1:A:2518:A:OP2	3:D:287:ARG:NH1	2.29	0.65
1:A:2892:A:O4'	21:W:71:ARG:NH2	2.28	0.65
84:A4:151:ASP:OD1	84:A4:152:ILE:N	2.29	0.65
54:AA:1591:C:OP1	70:AQ:52:ARG:NH2	2.29	0.65
1:A:2718:C:OP1	25:0:82:LYS:NZ	2.24	0.65
55:AB:156:GLU:OE1	60:AG:163:HIS:ND1	2.30	0.65
1:A:2256:U:O2'	17:S:118:ASN:ND2	2.30	0.65
39:e:235:LYS:NZ	40:f:172:GLU:OE2	2.29	0.65
66:AM:63:GLU:OE2	71:AR:191:ARG:NH1	2.28	0.64
1:A:1778:U:OP2	97:A:3510:HOH:O	2.15	0.64
6:H:78:ARG:NH1	22:X:87:LEU:O	2.29	0.64
15:Q:77:SER:OG	15:Q:79:GLU:OE2	2.14	0.64
15:Q:124:PRO:O	15:Q:129:LYS:NZ	2.22	0.64
33:8:186:GLN:OE1	47:m:95:LYS:NZ	2.30	0.64
54:AA:905:A:O2'	54:AA:907:A:OP1	2.14	0.64
54:AA:906:C:OP1	57:AD:118:THR:HG21	1.98	0.64
52:s:191:HIS:O	52:s:428:ARG:NH2	2.29	0.64
54:AA:1116:A:OP2	55:AB:100:ARG:NH2	2.29	0.64
1:A:3082:G:N2	1:A:3085:A:OP2	2.25	0.64
54:AA:1100:C:O2	97:AA:1902:HOH:O	2.11	0.64
1:A:2174:G:H4'	8:J:151:LEU:HD23	1.79	0.63
20:V:133:ILE:HD12	20:V:145:ARG:HB2	1.81	0.63
40:f:106:TYR:OH	40:f:174:ILE:O	2.15	0.63
42:h:88:ASP:OD1	42:h:124:ARG:NH2	2.31	0.63
84:A4:66:ASP:OD1	84:A4:67:LYS:N	2.32	0.63
1:A:2406:A:O2'	1:A:2407:U:O5'	2.17	0.63
54:AA:1107:U:O4	83:A3:128:LYS:NZ	2.29	0.63
4:E:120:THR:OG1	4:E:287:GLY:O	2.16	0.63
20:V:54:TRP:NE1	20:V:56:LEU:O	2.32	0.63
84:A4:350:ARG:NH2	84:A4:381:GLN:OE1	2.32	0.63
9:K:21:LEU:HD21	9:K:34:MET:SD	2.39	0.62
54:AA:1287:A:OP2	57:AD:260:LYS:NZ	2.31	0.62
1:A:2455:U:O4	97:A:3509:HOH:O	2.13	0.62
53:t1:61:PRO:HG2	53:t1:64:ILE:HD12	1.82	0.62
33:8:77:LYS:NZ	88:x:52:G:OP1	2.32	0.62
1:A:1800:G:N1	1:A:1803:A:OP2	2.31	0.62
1:A:2814:G:O2'	1:A:2983:G:OP1	2.17	0.62
53:t1:64:ILE:HG23	53:t2:82:LEU:HD13	1.80	0.62
75:AV:134:GLN:NE2	80:A0:108:ASN:OD1	2.33	0.62
1:A:2906:C:N3	26:1:19:ARG:NH1	2.48	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:163:ASP:OD1	20:V:164:GLY:N	2.32	0.62
1:A:2357:C:H42	13:O:115:LEU:HD12	1.64	0.62
31:6:203:GLU:OE2	49:p:192:ARG:NH1	2.29	0.62
1:A:1822:U:O2	1:A:2707:A:O2'	2.18	0.61
57:AD:307:LYS:NZ	71:AR:103:TYR:OH	2.32	0.61
60:AG:312:GLN:OE1	60:AG:345:ARG:NH2	2.32	0.61
7:I:75:GLU:OE1	7:I:83:ARG:NH2	2.33	0.61
7:I:221:LEU:HD13	53:t4:86:LEU:HD13	1.82	0.61
56:AC:58:ALA:HB1	56:AC:59:PRO:CD	2.30	0.61
5:F:49:ARG:NH2	5:F:81:ASP:O	2.33	0.61
54:AA:713:C:N3	74:AU:27:ARG:N	2.48	0.61
39:e:48:LEU:HB2	39:e:231:VAL:HG12	1.81	0.61
75:AV:167:VAL:HG13	75:AV:172:ALA:HB3	1.82	0.61
75:AV:40:TRP:O	75:AV:43:ARG:NH1	2.34	0.61
1:A:1747:G:OP2	1:A:1749:C:N4	2.34	0.61
5:F:76:ARG:NH1	42:h:106:ASP:OD1	2.34	0.61
58:AE:63:TYR:OH	69:AP:118:GLY:O	2.11	0.61
61:AH:70:ASP:OD1	61:AH:71:ILE:N	2.32	0.61
84:A4:363:ILE:HG22	84:A4:363:ILE:O	2.01	0.61
54:AA:1525:C:O5'	75:AV:105:ARG:NH1	2.34	0.60
7:I:197:LEU:HD12	7:I:198:PRO:HD2	1.83	0.60
1:A:1760:G:OP1	11:M:196:ARG:NE	2.33	0.60
65:AL:86:ASP:OD1	65:AL:87:ASP:N	2.34	0.60
14:P:144:MET:HE3	14:P:170:VAL:CG1	2.31	0.60
35:a:90:GLN:NE2	35:a:94:THR:OG1	2.34	0.60
68:AO:221:GLN:NE2	75:AV:314:VAL:O	2.35	0.60
1:A:2111:C:O2	1:A:2944:C:O2'	2.17	0.60
57:AD:197:SER:O	89:y:26:A:N6	2.35	0.59
64:AK:60:ASN:OD1	64:AK:68:GLN:NE2	2.35	0.59
1:A:2478:G:O2'	97:A:3502:HOH:O	2.08	0.59
33:8:149:GLU:OE2	39:e:230:LYS:NZ	2.21	0.59
1:A:2293:A:N6	11:M:37:GLU:OE1	2.36	0.59
54:AA:1340:C:O2'	79:AZ:101:ARG:NH2	2.36	0.59
62:AI:166:ILE:HD11	70:AQ:19:VAL:HG21	1.84	0.59
73:AT:42:GLU:OE1	73:AT:45:ARG:NH2	2.34	0.59
1:A:2099:U:OP1	97:A:3511:HOH:O	2.17	0.59
1:A:2315:A:O2'	1:A:2316:U:O2	2.17	0.59
12:N:73:ARG:O	12:N:155:LYS:NZ	2.36	0.59
59:AF:111:MET:HE3	59:AF:111:MET:HA	1.84	0.59
9:K:7:ALA:HB3	9:K:8:PRO:HD3	1.84	0.59
59:AF:155:MET:HE2	59:AF:155:MET:HA	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:q:167:GLN:O	50:q:171:ARG:NE	2.36	0.58
75:AV:46:GLU:OE2	75:AV:74:ARG:NE	2.36	0.58
31:6:160:ASP:OD2	31:6:267:ARG:NH2	2.32	0.58
33:8:132:GLU:OE2	40:f:109:TYR:OH	2.22	0.58
17:S:115:LEU:N	36:b:118:PRO:O	2.33	0.58
1:A:2181:A:O2'	1:A:2182:G:OP1	2.20	0.58
54:AA:1199:G:N1	54:AA:1422:G:OP2	2.36	0.58
2:B:1625:A:OP1	31:6:56:ARG:NH2	2.37	0.58
60:AG:263:ASP:OD1	60:AG:267:MET:N	2.37	0.58
54:AA:1104:A:OP2	97:AA:1904:HOH:O	2.16	0.57
57:AD:363:ALA:O	57:AD:367:GLY:N	2.37	0.57
75:AV:225:LEU:HD11	75:AV:283:LEU:HD22	1.86	0.57
8:J:113:THR:OG1	8:J:116:HIS:ND1	2.35	0.57
31:6:179:VAL:HG23	31:6:179:VAL:O	2.04	0.57
81:A1:56:ARG:NH1	84:A4:91:ASP:OD2	2.36	0.57
23:Y:69:ASP:OD1	23:Y:70:ASP:N	2.37	0.57
30:5:166:THR:O	52:s:287:LYS:NZ	2.25	0.57
80:A0:54:ALA:O	80:A0:58:VAL:HG23	2.04	0.57
1:A:2826:G:OP1	21:W:49:ARG:NH2	2.34	0.57
54:AA:843:G:N2	54:AA:846:A:OP2	2.37	0.57
75:AV:95:PHE:O	75:AV:98:SER:OG	2.22	0.57
1:A:2410:U:HO2'	30:5:96:HIS:HD1	1.52	0.57
1:A:2858:A:OP2	28:3:142:LYS:NZ	2.36	0.57
14:P:82:ARG:NE	14:P:95:GLU:OE2	2.31	0.57
61:AH:104:ILE:CG2	61:AH:148:LEU:HD21	2.34	0.57
67:AN:58:CYS:SG	67:AN:81:LEU:HD22	2.45	0.57
54:AA:815:C:O2'	54:AA:817:G:OP1	2.12	0.57
62:AI:177:ASP:OD1	62:AI:179:THR:OG1	2.21	0.57
1:A:2406:A:O2'	30:5:110:ARG:NH1	2.37	0.56
54:AA:932:C:N3	73:AT:11:ARG:NH1	2.52	0.56
41:g:84:TYR:OH	41:g:164:LYS:NZ	2.39	0.56
77:AX:123:ARG:NH2	77:AX:337:LEU:O	2.38	0.56
1:A:3068:G:OP2	1:A:3068:G:N2	2.37	0.56
18:T:85:ALA:O	18:T:139:SER:OG	2.23	0.56
49:p:182:ASN:OD1	49:p:185:ARG:NH2	2.37	0.56
1:A:1821:A:OP2	25:0:95:ARG:NH1	2.37	0.56
3:D:111:ARG:NH1	3:D:165:ASN:OD1	2.37	0.56
36:b:34:SER:OG	36:b:36:ASP:O	2.21	0.56
54:AA:902:G:O2'	54:AA:903:U:OP1	2.22	0.56
3:D:204:ALA:O	3:D:208:ARG:NH2	2.36	0.56
4:E:202:GLN:NE2	4:E:301:ASP:OD1	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:123:ILE:HD12	46:I:75:VAL:CG1	2.35	0.56
32:7:106:ALA:O	32:7:113:TRP:N	2.38	0.56
45:k:40:GLU:OE2	45:k:43:ARG:NH2	2.38	0.56
1:A:1697:A:N3	1:A:1703:C:O2'	2.39	0.56
1:A:2909:G:OP1	26:1:63:ARG:NH2	2.36	0.56
36:b:44:ARG:NH1	48:o:99:LYS:O	2.38	0.56
52:s:103:ASP:OD1	52:s:104:ARG:N	2.38	0.56
54:AA:1530:A:OP1	80:A0:29:ARG:NH2	2.39	0.56
1:A:1892:A:N1	31:6:376:THR:OG1	2.32	0.55
20:V:20:ARG:NH1	20:V:42:ARG:O	2.38	0.55
21:W:103:VAL:HG11	31:6:61:ALA:HB1	1.87	0.55
32:7:70:VAL:O	32:7:70:VAL:HG23	2.06	0.55
4:E:47:THR:OG1	4:E:51:GLU:OE2	2.21	0.55
43:i:57:TYR:OH	50:q:28:ARG:O	2.15	0.55
7:I:142:ASN:ND2	53:t1:48:LEU:O	2.38	0.55
59:AF:193:ASP:OD1	59:AF:194:LYS:N	2.39	0.55
1:A:3166:U:O2'	4:E:269:TYR:O	2.22	0.55
4:E:151:THR:HG23	4:E:171:PRO:HB2	1.87	0.55
19:U:28:LEU:O	23:Y:114:THR:HG23	2.07	0.55
30:5:100:LYS:NZ	30:5:271:TYR:O	2.38	0.55
53:t1:64:ILE:HD11	53:t2:78:GLU:CG	2.37	0.55
1:A:2137:C:OP2	24:Z:77:ARG:NH1	2.39	0.55
56:AC:106:ASP:OD1	56:AC:107:GLN:N	2.36	0.55
71:AR:276:VAL:HG11	71:AR:307:LEU:HD12	1.89	0.55
81:A1:60:MET:HE1	81:A1:80:ALA:O	2.07	0.55
1:A:1805:A:OP2	20:V:94:HIS:NE2	2.40	0.55
4:E:56:GLU:OE2	4:E:56:GLU:N	2.39	0.54
54:AA:1098:C:O2'	54:AA:1151:C:O2'	2.23	0.54
58:AE:90:ARG:NH2	69:AP:116:ILE:O	2.39	0.54
38:d:287:LEU:HD22	38:d:291:GLU:CD	2.32	0.54
1:A:1871:A:N3	28:3:104:ARG:NH2	2.55	0.54
22:X:49:LYS:NZ	50:q:84:GLU:OE2	2.40	0.54
1:A:1745:U:O4	28:3:108:LYS:NZ	2.40	0.54
2:B:1613:U:O2'	2:B:1615:A:OP1	2.26	0.54
70:AQ:80:ARG:NH1	76:AW:164:GLU:OE1	2.35	0.54
7:I:221:LEU:CD1	53:t4:86:LEU:HD13	2.37	0.54
66:AM:19:ILE:HB	66:AM:83:LEU:HD23	1.90	0.54
14:P:60:SER:HG	49:p:177:ARG:HH21	1.56	0.54
67:AN:6:SER:OG	67:AN:69:LEU:O	2.24	0.54
30:5:229:ARG:NH2	30:5:231:SER:OG	2.41	0.54
39:e:192:LEU:O	39:e:198:ASN:ND2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:178:ASP:OD1	52:s:238:ASN:ND2	2.41	0.54
77:AX:180:GLN:NE2	77:AX:183:GLU:OE1	2.41	0.54
5:F:220:ASP:OD1	5:F:221:LEU:N	2.41	0.54
31:6:374:GLU:OE2	49:p:140:SER:OG	2.20	0.54
33:8:52:LYS:NZ	87:w:25:C:OP1	2.39	0.54
4:E:275:ARG:NH2	4:E:331:ASP:OD2	2.40	0.53
24:Z:120:LYS:NZ	48:o:44:GLU:OE2	2.39	0.53
37:c:80:GLN:O	37:c:210:ARG:NH2	2.41	0.53
3:D:194:ASN:ND2	3:D:245:GLY:O	2.41	0.53
1:A:1953:A:O2'	1:A:2463:A:OP1	2.27	0.53
38:d:81:THR:HG22	38:d:82:ALA:N	2.24	0.53
40:f:99:ASP:OD2	47:m:67:ARG:NH1	2.40	0.53
41:g:129:SER:O	41:g:133:GLY:N	2.39	0.53
53:t1:61:PRO:CG	53:t1:64:ILE:HD12	2.38	0.53
32:7:298:GLN:NE2	32:7:320:SER:O	2.42	0.53
73:AT:9:ILE:O	73:AT:12:THR:OG1	2.24	0.53
61:AH:50:LEU:HD13	61:AH:53:ASP:O	2.09	0.53
84:A4:471:ILE:HD11	84:A4:500:LEU:HD23	1.90	0.53
4:E:138:CYS:SG	4:E:144:THR:HG23	2.48	0.53
32:7:286:LEU:HD21	32:7:296:ARG:HE	1.73	0.53
54:AA:932:C:O2'	73:AT:2:PRO:O	2.27	0.53
49:p:135:LEU:HD21	49:p:157:MET:HE1	1.90	0.53
54:AA:1037:A:HO2'	65:AL:152:HIS:HE2	1.57	0.53
66:AM:29:ARG:HD2	66:AM:57:LEU:HD12	1.91	0.52
7:I:151:ASN:OD1	45:k:31:ARG:NH2	2.42	0.52
15:Q:146:GLY:O	15:Q:148:THR:HG23	2.09	0.52
54:AA:1037:A:O2'	65:AL:152:HIS:NE2	2.39	0.52
59:AF:234:ARG:HB3	82:A2:53:MET:HE1	1.92	0.52
3:D:174:VAL:HG22	3:D:186:ALA:O	2.09	0.52
1:A:2374:A:N1	52:s:97:THR:OG1	2.39	0.52
24:Z:126:GLN:N	24:Z:126:GLN:OE1	2.43	0.52
60:AG:196:GLY:O	60:AG:248:VAL:N	2.42	0.52
5:F:164:MET:HE1	43:i:70:PRO:HB2	1.91	0.52
56:AC:152:ARG:NH1	84:A4:87:TYR:OH	2.43	0.52
60:AG:206:GLU:O	60:AG:210:VAL:N	2.43	0.52
47:m:82:ASP:O	47:m:89:ARG:NH2	2.43	0.52
15:Q:79:GLU:OE1	15:Q:103:ARG:NH2	2.43	0.52
19:U:153:LEU:HD23	38:d:222:LEU:HB2	1.92	0.52
78:AY:250:ILE:O	84:A4:358:ARG:NE	2.43	0.52
1:A:2522:U:O4	30:5:32:GLU:N	2.41	0.52
84:A4:372:TYR:CE2	84:A4:400:LEU:HD21	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3066:C:O2'	4:E:233:GLN:OE1	2.26	0.51
32:7:186:ASP:OD1	32:7:187:SER:N	2.42	0.51
44:j:45:GLU:OE1	44:j:63:GLN:NE2	2.40	0.51
1:A:3189:C:O2'	51:r:155:ALA:N	2.42	0.51
7:I:39:VAL:HG21	48:o:22:ARG:HD2	1.92	0.51
81:A1:255:ASN:N	81:A1:259:GLU:OE2	2.42	0.51
8:J:123:ILE:HD12	46:l:75:VAL:HG13	1.92	0.51
8:J:163:GLU:OE1	8:J:163:GLU:N	2.38	0.51
15:Q:61:VAL:HG12	75:AV:87:HIS:HE1	1.75	0.51
49:p:100:GLU:OE2	49:p:102:ARG:NH1	2.39	0.51
4:E:220:LYS:HG2	4:E:261:MET:HE1	1.93	0.51
7:I:45:GLN:NE2	48:o:25:ARG:O	2.39	0.51
20:V:167:PRO:O	34:9:77:LEU:HD21	2.10	0.51
30:5:98:LEU:HD13	30:5:272:ASP:HB2	1.91	0.51
54:AA:760:A:N1	54:AA:780:C:O2'	2.37	0.51
75:AV:123:ASP:OD1	75:AV:124:LYS:N	2.44	0.51
7:I:189:GLN:NE2	7:I:193:ASN:OD1	2.43	0.51
18:T:63:ARG:NH2	38:d:228:PHE:O	2.43	0.51
1:A:2237:A:OP1	51:r:171:ARG:NH1	2.42	0.51
7:I:200:LEU:HD11	7:I:204:GLN:HE21	1.76	0.51
32:7:216:PHE:CE2	32:7:257:ILE:HD11	2.46	0.51
54:AA:1053:A:N6	54:AA:1100:C:O2'	2.43	0.51
32:7:326:GLU:OE2	32:7:326:GLU:N	2.34	0.51
42:h:69:ARG:NH1	42:h:107:ASP:OD2	2.40	0.51
52:s:211:VAL:HG22	52:s:230:ARG:HG2	1.93	0.51
54:AA:975:A:OP2	70:AQ:3:LYS:NZ	2.42	0.51
81:A1:166:PRO:O	81:A1:169:ARG:NH2	2.44	0.51
14:P:85:ARG:NH1	14:P:157:SER:OG	2.43	0.51
33:8:174:GLU:OE2	40:f:183:ARG:NH2	2.44	0.51
57:AD:200:GLY:O	57:AD:221:ARG:NH1	2.44	0.51
1:A:2753:A:O2'	6:H:88:HIS:ND1	2.43	0.51
5:F:220:ASP:O	5:F:245:ALA:N	2.43	0.51
17:S:132:LYS:NZ	44:j:48:ASP:OD1	2.39	0.51
71:AR:86:ASN:O	71:AR:90:THR:OG1	2.21	0.51
75:AV:168:MET:CE	75:AV:247:MET:HE1	2.41	0.51
54:AA:1490:U:OP1	83:A3:142:LYS:NZ	2.37	0.50
78:AY:250:ILE:HB	84:A4:354:LEU:HD22	1.92	0.50
30:5:98:LEU:O	30:5:270:ILE:HG23	2.11	0.50
52:s:150:LEU:HD21	52:s:402:TYR:CD2	2.46	0.50
9:K:70:ASN:OD1	97:K:201:HOH:O	2.20	0.50
17:S:101:PHE:HE2	17:S:116:ILE:HD13	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:c:123:GLN:OE1	37:c:193:GLN:NE2	2.44	0.50
47:m:119:TYR:OH	81:A1:232:GLU:OE2	2.17	0.50
52:s:419:LEU:O	52:s:423:HIS:ND1	2.44	0.50
65:AL:85:VAL:HG23	65:AL:90:LYS:HG3	1.93	0.50
1:A:2755:A:OP2	6:H:91:LYS:NZ	2.42	0.50
38:d:89:VAL:HG23	38:d:89:VAL:O	2.12	0.50
1:A:2531:U:O4	3:D:246:ARG:NH2	2.45	0.50
9:K:15:ALA:CB	37:c:269:LEU:HD22	2.41	0.50
14:P:58:LEU:HB2	31:6:265:ILE:HD13	1.94	0.50
14:P:139:ALA:O	31:6:155:TYR:OH	2.28	0.50
53:t2:61:PRO:HD2	53:t2:64:ILE:HD12	1.94	0.50
54:AA:1106:C:O2'	54:AA:1108:C:OP2	2.27	0.50
71:AR:317:ALA:O	71:AR:321:ALA:N	2.43	0.50
81:A1:235:ASN:ND2	81:A1:237:GLU:OE2	2.44	0.50
5:F:63:GLN:NE2	5:F:81:ASP:OD1	2.44	0.50
22:X:163:ARG:NH2	22:X:204:VAL:O	2.41	0.50
30:5:165:GLN:NE2	30:5:179:VAL:HG21	2.26	0.50
20:V:56:LEU:HD13	20:V:86:VAL:HG21	1.94	0.50
30:5:173:ARG:NH1	30:5:348:ASP:O	2.42	0.50
74:AU:106:MET:HE2	74:AU:106:MET:HA	1.93	0.50
62:AI:129:GLN:NE2	62:AI:167:MET:SD	2.85	0.50
1:A:1787:G:N2	1:A:1790:A:OP2	2.40	0.49
75:AV:35:VAL:HG22	75:AV:35:VAL:O	2.12	0.49
76:AW:162:VAL:HG12	76:AW:162:VAL:O	2.12	0.49
11:M:261:ASP:OD2	49:p:41:SER:OG	2.31	0.49
20:V:195:GLN:OE1	20:V:195:GLN:N	2.42	0.49
76:AW:129:VAL:HG23	76:AW:130:ASP:N	2.27	0.49
26:1:35:ASN:OD1	26:1:36:ARG:N	2.45	0.49
61:AH:136:MET:HG2	64:AK:123:ILE:HD13	1.94	0.49
1:A:2537:G:O2'	1:A:2634:U:OP2	2.26	0.49
16:R:64:MET:HE1	18:T:204:HIS:CD2	2.48	0.49
56:AC:115:ASN:ND2	78:AY:309:LYS:O	2.46	0.49
38:d:88:TYR:OH	38:d:195:VAL:HG11	2.13	0.49
39:e:55:ARG:NH1	39:e:149:LEU:O	2.45	0.49
50:q:61:PHE:O	50:q:65:GLY:N	2.41	0.49
56:AC:58:ALA:HB1	56:AC:59:PRO:HD2	1.95	0.49
42:h:57:SER:OG	42:h:136:ASP:OD2	2.31	0.49
68:AO:217:ARG:NE	75:AV:318:ASP:OD2	2.45	0.49
20:V:186:THR:HG22	20:V:186:THR:O	2.12	0.49
1:A:2238:A:OP1	51:r:165:LYS:NZ	2.46	0.49
1:A:2870:G:OP1	28:3:140:ARG:NE	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:221:LEU:HD22	53:t4:86:LEU:HB3	1.95	0.49
36:b:26:LEU:HD22	36:b:105:ALA:HA	1.95	0.49
49:p:164:THR:O	49:p:164:THR:HG22	2.12	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:CG	2.48	0.49
54:AA:1415:G:OP2	54:AA:1415:G:N2	2.27	0.48
81:A1:258:SER:O	81:A1:262:ILE:HG22	2.12	0.48
1:A:1990:G:OP1	3:D:269:ARG:NH2	2.39	0.48
39:e:149:LEU:HD21	39:e:254:TRP:CE2	2.48	0.48
55:AB:222:ILE:HD13	55:AB:236:VAL:HB	1.95	0.48
84:A4:200:ASP:OD2	84:A4:243:ASN:N	2.47	0.48
1:A:2456:U:OP1	13:O:16:ARG:NH1	2.46	0.48
1:A:2665:U:OP2	13:O:17:ARG:NE	2.42	0.48
1:A:2527:A:N3	30:5:31:TYR:OH	2.43	0.48
1:A:3181:U:OP2	1:A:3182:A:O2'	2.21	0.48
20:V:55:TYR:O	20:V:145:ARG:NH2	2.45	0.48
63:AJ:78:ARG:NH1	63:AJ:117:ASP:OD2	2.47	0.48
1:A:2562:U:O2'	3:D:284:ARG:O	2.20	0.48
4:E:213:LYS:HD2	4:E:261:MET:HE3	1.95	0.48
1:A:2395:A:OP1	30:5:173:ARG:NH2	2.47	0.48
23:Y:154:ARG:O	23:Y:158:THR:OG1	2.23	0.48
54:AA:1155:G:OP1	83:A3:144:ARG:NH1	2.43	0.48
81:A1:118:ALA:O	81:A1:122:HIS:N	2.43	0.48
82:A2:7:ARG:O	82:A2:9:ARG:NH1	2.47	0.48
1:A:2131:A:OP1	48:o:23:ARG:NH1	2.45	0.48
54:AA:944:U:OP1	97:AA:1905:HOH:O	2.20	0.48
39:e:48:LEU:HD23	39:e:177:GLU:HA	1.95	0.48
13:O:64:LYS:NZ	13:O:100:GLN:O	2.46	0.48
35:a:44:ASN:ND2	36:b:135:ASN:OD1	2.46	0.48
53:t1:64:ILE:CG2	53:t2:82:LEU:HD13	2.44	0.48
54:AA:1104:A:OP1	54:AA:1591:C:O2'	2.26	0.48
68:AO:215:ARG:NH1	80:A0:90:ASP:OD1	2.46	0.48
77:AX:253:LEU:HD12	77:AX:255:MET:HE3	1.95	0.48
39:e:156:ASN:OD1	39:e:157:LEU:N	2.47	0.48
52:s:204:CYS:SG	52:s:240:GLN:NE2	2.87	0.48
11:M:65:LEU:HD13	43:i:128:ARG:OXT	2.14	0.47
30:5:236:LEU:HD21	30:5:289:HIS:CD2	2.49	0.47
34:9:16:ASP:OD1	34:9:25:ARG:NH1	2.47	0.47
54:AA:871:A:OP2	68:AO:97:ARG:NH2	2.45	0.47
59:AF:46:ILE:HG22	59:AF:46:ILE:O	2.14	0.47
71:AR:70:PHE:O	71:AR:76:GLN:NE2	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:102:PHE:O	25:O:104:LYS:NZ	2.45	0.47
20:V:194:LEU:O	20:V:198:VAL:HG23	2.15	0.47
54:AA:1048:C:O2'	65:AL:196:TYR:O	2.32	0.47
4:E:208:ALA:HB2	4:E:297:VAL:HG12	1.96	0.47
54:AA:700:A:N1	54:AA:709:G:O2'	2.46	0.47
60:AG:237:GLU:N	60:AG:237:GLU:OE2	2.43	0.47
61:AH:136:MET:CG	64:AK:123:ILE:HD13	2.43	0.47
62:AI:126:ILE:HD11	82:A2:46:ILE:CG2	2.44	0.47
16:R:141:ILE:HG22	35:a:51:LEU:HD12	1.95	0.47
31:6:45:LEU:HD12	31:6:48:LEU:HD12	1.96	0.47
1:A:2259:C:O2'	1:A:2261:C:OP2	2.28	0.47
59:AF:84:SER:OG	77:AX:379:GLU:OE1	2.21	0.47
80:A0:79:LEU:HD22	80:A0:94:TYR:CD2	2.49	0.47
23:Y:175:ARG:NH2	27:2:83:MET:HE3	2.30	0.47
53:t1:64:ILE:HD11	53:t2:78:GLU:HG3	1.96	0.47
54:AA:1443:U:O2'	54:AA:1445:G:N7	2.40	0.47
60:AG:143:ASP:OD1	60:AG:144:GLY:N	2.47	0.47
4:E:97:VAL:HG22	4:E:98:GLY:N	2.30	0.47
6:H:53:THR:N	6:H:86:THR:HG1	2.13	0.47
18:T:49:ASN:ND2	18:T:68:TYR:O	2.48	0.47
68:AO:221:GLN:OE1	75:AV:313:LEU:HD11	2.15	0.47
69:AP:73:ASP:OD1	69:AP:74:TYR:N	2.48	0.47
75:AV:391:GLN:O	75:AV:395:GLN:N	2.36	0.47
1:A:1818:A:OP2	25:O:91:ARG:NH2	2.42	0.47
36:b:85:ARG:NE	36:b:87:GLU:OE2	2.47	0.47
39:e:147:THR:HG22	39:e:147:THR:O	2.14	0.47
53:t1:76:LEU:H	53:t4:68:VAL:HG11	1.80	0.47
9:K:169:LEU:HD11	51:r:88:LEU:HD13	1.97	0.47
11:M:156:VAL:O	11:M:176:THR:HA	2.15	0.47
75:AV:269:SER:HB2	75:AV:273:ILE:HD12	1.98	0.47
84:A4:556:LYS:NZ	84:A4:560:GLU:OE2	2.44	0.47
1:A:2321:A:OP1	25:O:138:ARG:NH2	2.42	0.46
57:AD:245:VAL:HG22	57:AD:271:ALA:HB1	1.98	0.46
5:F:253:MET:HE3	5:F:259:LEU:HD22	1.97	0.46
17:S:199:GLU:N	17:S:199:GLU:OE1	2.48	0.46
32:7:276:PHE:HB2	32:7:304:VAL:HG22	1.97	0.46
1:A:3198:A:O2'	1:A:3200:U:O2'	2.10	0.46
6:H:110:ASP:OD1	6:H:111:LEU:N	2.49	0.46
58:AE:94:VAL:HG11	69:AP:117:MET:HE1	1.97	0.46
1:A:1798:A:N3	20:V:42:ARG:NH2	2.63	0.46
42:h:60:TYR:OH	42:h:130:TYR:O	2.25	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:332:LEU:HD21	52:s:359:ALA:HB2	1.96	0.46
54:AA:1004:G:OP1	62:AI:89:LYS:NZ	2.47	0.46
54:AA:1576:G:N7	97:AA:1909:HOH:O	2.36	0.46
69:AP:141:ARG:O	70:AQ:28:ARG:NH1	2.48	0.46
81:A1:278:ILE:HG13	81:A1:278:ILE:O	2.15	0.46
1:A:1860:A:O2'	1:A:2682:A:OP1	2.31	0.46
1:A:2449:G:OP2	52:s:225:ARG:NH2	2.40	0.46
1:A:2616:A:HO2'	1:A:3046:C:HO2'	1.61	0.46
4:E:236:THR:HG23	4:E:239:ARG:HD3	1.96	0.46
31:6:252:CYS:SG	31:6:296:ARG:NH2	2.89	0.46
1:A:1749:C:OP2	1:A:2899:C:O2'	2.32	0.46
28:3:168:ARG:NH2	28:3:170:ASN:OD1	2.49	0.46
30:5:229:ARG:NH1	30:5:286:PRO:O	2.47	0.46
14:P:60:SER:OG	49:p:177:ARG:NH2	2.42	0.46
19:U:26:ILE:HG22	19:U:44:ILE:HG22	1.97	0.46
31:6:186:PRO:O	31:6:191:ASN:ND2	2.48	0.46
51:r:124:ARG:NH1	51:r:152:THR:O	2.48	0.46
57:AD:263:ASP:OD1	57:AD:264:ARG:N	2.49	0.46
59:AF:234:ARG:CB	82:A2:53:MET:HE1	2.45	0.46
20:V:169:THR:HG22	20:V:169:THR:O	2.16	0.46
20:V:180:GLU:OE1	20:V:180:GLU:N	2.46	0.46
58:AE:37:ARG:NH1	58:AE:69:TYR:OH	2.48	0.46
1:A:3219:G:O2'	1:A:3221:A:OP2	2.21	0.46
31:6:273:PHE:HB3	31:6:311:MET:HG2	1.97	0.46
84:A4:508:VAL:HG12	84:A4:508:VAL:O	2.16	0.46
1:A:2179:A:N1	1:A:2180:A:N6	2.63	0.45
21:W:53:ILE:HG21	21:W:56:MET:SD	2.56	0.45
66:AM:63:GLU:OE1	71:AR:157:VAL:HG21	2.15	0.45
67:AN:93:ASP:O	67:AN:97:GLY:N	2.44	0.45
71:AR:69:THR:OG1	71:AR:72:ASP:OD1	2.32	0.45
80:A0:218:VAL:HG12	80:A0:218:VAL:O	2.16	0.45
1:A:3190:A:OP2	51:r:120:LYS:NZ	2.50	0.45
14:P:144:MET:HE3	14:P:170:VAL:HG11	1.98	0.45
57:AD:296:LEU:C	57:AD:296:LEU:HD12	2.41	0.45
78:AY:323:ASP:OD2	81:A1:217:GLN:NE2	2.44	0.45
84:A4:156:ALA:O	84:A4:160:ARG:NH1	2.49	0.45
34:9:55:GLU:N	34:9:55:GLU:OE1	2.49	0.45
52:s:242:ARG:NH2	52:s:290:ASP:OD2	2.43	0.45
1:A:2071:U:O2'	31:6:28:ARG:NH1	2.49	0.45
1:A:3201:A:H2'	1:A:3202:U:O4'	2.16	0.45
7:I:171:VAL:HG23	7:I:174:LEU:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:6:324:ASP:OD1	31:6:326:SER:OG	2.34	0.45
54:AA:1053:A:N6	54:AA:1100:C:HO2'	2.14	0.45
84:A4:166:VAL:HG23	84:A4:167:LYS:N	2.32	0.45
8:J:20:ILE:HD11	8:J:42:ARG:HG3	1.97	0.45
33:8:125:LYS:NZ	47:m:37:ARG:O	2.50	0.45
46:l:111:ASP:O	46:l:114:SER:OG	2.29	0.45
49:p:109:GLU:OE1	49:p:109:GLU:N	2.50	0.45
54:AA:1283:A:O2'	57:AD:347:GLN:NE2	2.50	0.45
71:AR:276:VAL:CG1	71:AR:307:LEU:HD12	2.46	0.45
23:Y:142:LEU:C	23:Y:142:LEU:HD23	2.42	0.45
40:f:147:ASP:O	47:m:72:ARG:NH1	2.50	0.45
46:l:66:VAL:O	46:l:70:THR:HG23	2.17	0.45
47:m:112:ASP:OD1	47:m:113:ASP:N	2.50	0.45
54:AA:1004:G:O2'	62:AI:98:GLN:OE1	2.08	0.45
75:AV:34:TYR:HA	75:AV:372:ILE:HD11	1.99	0.45
75:AV:359:LEU:HD11	75:AV:363:LYS:HD2	1.98	0.45
31:6:139:TRP:CD1	31:6:143:CYS:HG	2.35	0.45
33:8:202:VAL:O	33:8:203:GLU:CB	2.64	0.45
47:m:54:VAL:HG12	47:m:72:ARG:O	2.17	0.45
80:A0:133:HIS:O	80:A0:139:TRP:NE1	2.44	0.45
4:E:109:LEU:N	4:E:117:HIS:O	2.50	0.45
12:N:140:MET:HE2	12:N:140:MET:HA	1.99	0.45
17:S:101:PHE:CE2	17:S:116:ILE:HD13	2.52	0.45
58:AE:26:ILE:HG23	58:AE:36:VAL:HG21	1.99	0.45
59:AF:126:TYR:O	59:AF:134:GLN:NE2	2.50	0.45
1:A:2346:U:OP1	52:s:223:ARG:NH2	2.50	0.44
11:M:274:VAL:HG11	50:q:75:LEU:HD13	1.99	0.44
54:AA:922:C:H2'	54:AA:923:A:C8	2.53	0.44
5:F:53:LEU:HD12	5:F:274:LEU:HD12	1.99	0.44
10:L:45:ALA:O	10:L:49:SER:OG	2.26	0.44
15:Q:161:GLU:OE1	15:Q:191:ARG:NH2	2.45	0.44
47:m:115:HIS:NE2	79:AZ:17:ARG:O	2.51	0.44
7:I:76:ILE:HG13	12:N:32:THR:HG22	1.98	0.44
11:M:257:CYS:SG	49:p:59:TRP:NE1	2.90	0.44
11:M:261:ASP:CG	49:p:41:SER:HG	2.25	0.44
30:5:213:TRP:CZ3	30:5:222:VAL:HG23	2.52	0.44
67:AN:88:VAL:HG13	67:AN:88:VAL:O	2.18	0.44
54:AA:1488:C:O2	54:AA:1584:A:O2'	2.35	0.44
1:A:1680:A:OP1	23:Y:230:LYS:NZ	2.49	0.44
1:A:3113:A:O2'	1:A:3114:U:OP2	2.32	0.44
5:F:211:ARG:HE	42:h:55:LEU:HD11	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:A0:42:THR:HG22	80:A0:49:ARG:HG2	1.99	0.44
11:M:250:ASP:OD1	11:M:251:GLU:N	2.50	0.44
12:N:218:ILE:HG23	12:N:223:MET:HB2	1.99	0.44
14:P:104:SER:O	14:P:135:ARG:NH1	2.50	0.44
26:1:54:VAL:HG12	26:1:55:LEU:N	2.33	0.44
60:AG:69:TYR:O	60:AG:135:GLN:NE2	2.45	0.44
73:AT:32:VAL:HG22	73:AT:76:LEU:CD2	2.48	0.44
3:D:246:ARG:NH2	3:D:250:VAL:HG13	2.32	0.44
33:8:90:THR:O	33:8:90:THR:HG23	2.18	0.44
5:F:232:GLU:O	5:F:236:ARG:NH2	2.51	0.44
52:s:174:LEU:HB3	52:s:175:PRO:HD3	2.00	0.44
53:t1:68:VAL:HG13	53:t2:86:LEU:HD23	2.00	0.44
68:AO:217:ARG:NH2	68:AO:227:GLU:OE2	2.51	0.44
88:x:8:U:HO2'	88:x:46:A:HO2'	1.50	0.44
35:a:142:ARG:O	35:a:142:ARG:HG3	2.18	0.43
39:e:138:THR:HG21	39:e:150:ASN:ND2	2.32	0.43
79:AZ:11:MET:SD	81:A1:193:LEU:HD21	2.58	0.43
77:AX:153:LEU:HD21	77:AX:244:LEU:CD2	2.48	0.43
1:A:1763:A:OP1	43:i:68:LYS:NZ	2.46	0.43
1:A:3050:U:O3'	10:L:63:LYS:NZ	2.52	0.43
49:p:111:ILE:O	49:p:116:ARG:NH2	2.51	0.43
77:AX:272:THR:OG1	77:AX:282:ILE:O	2.31	0.43
1:A:2993:U:H1'	96:w:101:ALA:HB1	1.99	0.43
33:8:189:GLU:OE2	47:m:92:ARG:NH1	2.51	0.43
77:AX:153:LEU:HD21	77:AX:244:LEU:HD22	2.00	0.43
1:A:1810:A:H2'	1:A:1811:A:O4'	2.19	0.43
86:v:77:ALA:C	88:x:76:A:O2'	2.62	0.43
1:A:1752:U:OP1	28:3:94:LEU:N	2.51	0.43
1:A:2248:U:OP1	16:R:99:ARG:NH2	2.46	0.43
39:e:90:ARG:NH1	39:e:115:LEU:O	2.50	0.43
77:AX:359:TYR:O	77:AX:363:ASN:ND2	2.52	0.43
80:A0:63:ARG:N	80:A0:66:GLN:OE1	2.41	0.43
30:5:165:GLN:NE2	30:5:175:THR:HG22	2.34	0.43
63:AJ:95:ILE:HD12	63:AJ:95:ILE:N	2.34	0.43
64:AK:58:ARG:NE	64:AK:72:ASP:OD1	2.42	0.43
1:A:2093:U:O2	1:A:2266:U:O2'	2.36	0.43
1:A:3230:G:N7	4:E:156:ARG:NH1	2.59	0.43
3:D:127:ILE:HD13	30:5:114:LEU:HD11	2.01	0.43
54:AA:930:G:N7	63:AJ:44:ARG:NE	2.66	0.43
56:AC:165:LYS:HE3	56:AC:167:LEU:HD21	2.01	0.43
61:AH:80:VAL:HG23	61:AH:88:LEU:HD22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AH:127:TYR:O	97:AH:301:HOH:O	2.21	0.43
68:AO:208:PRO:HG2	68:AO:213:LEU:HD21	2.00	0.43
76:AW:130:ASP:OD2	76:AW:133:LYS:NZ	2.39	0.43
77:AX:62:GLN:OE1	77:AX:62:GLN:N	2.38	0.43
53:t2:75:THR:O	53:t2:79:ILE:N	2.45	0.42
1:A:1958:G:O2'	1:A:1960:A:OP2	2.37	0.42
1:A:1962:A:OP2	1:A:2501:C:N4	2.50	0.42
19:U:38:ASP:OD1	19:U:38:ASP:N	2.51	0.42
20:V:55:TYR:HB2	20:V:133:ILE:HD11	2.01	0.42
50:q:169:ASP:N	50:q:170:PRO:HD2	2.34	0.42
56:AC:42:VAL:HG21	56:AC:55:GLU:HG2	2.01	0.42
78:AY:393:GLN:O	78:AY:393:GLN:HG3	2.19	0.42
84:A4:493:MET:HE2	84:A4:493:MET:HA	2.01	0.42
1:A:1792:G:N7	27:2:87:ARG:NH2	2.61	0.42
1:A:1991:A:H5''	1:A:1992:C:OP1	2.19	0.42
1:A:2598:A:H3'	1:A:2625:C:H42	1.84	0.42
10:L:39:ARG:NH1	15:Q:158:GLN:OE1	2.52	0.42
16:R:22:GLN:OE1	16:R:29:ARG:NH1	2.52	0.42
42:h:78:PHE:CE2	42:h:96:LEU:HD13	2.54	0.42
84:A4:302:VAL:HG23	84:A4:303:CYS:N	2.35	0.42
20:V:190:CYS:SG	20:V:191:LEU:N	2.88	0.42
21:W:115:ASP:O	21:W:119:ARG:NE	2.53	0.42
50:q:162:GLU:O	50:q:162:GLU:HG2	2.19	0.42
56:AC:145:TYR:O	56:AC:148:LYS:NZ	2.47	0.42
1:A:1699:C:N4	23:Y:198:ARG:O	2.51	0.42
1:A:2849:G:OP2	26:1:15:ASN:ND2	2.41	0.42
11:M:261:ASP:OD1	11:M:262:PRO:HD2	2.20	0.42
19:U:153:LEU:HD23	38:d:222:LEU:CB	2.49	0.42
20:V:188:VAL:O	20:V:188:VAL:HG23	2.18	0.42
84:A4:58:VAL:O	84:A4:58:VAL:HG23	2.20	0.42
11:M:203:ARG:NE	11:M:264:GLN:O	2.52	0.42
27:2:68:ARG:O	27:2:71:SER:OG	2.32	0.42
31:6:367:ASP:OD1	31:6:370:ARG:NH1	2.52	0.42
54:AA:1443:U:O2'	97:AA:1906:HOH:O	2.21	0.42
17:S:136:VAL:O	17:S:136:VAL:HG13	2.18	0.42
77:AX:203:LYS:O	77:AX:250:GLN:NE2	2.50	0.42
80:A0:80:VAL:O	80:A0:80:VAL:HG23	2.19	0.42
13:O:38:ARG:NE	13:O:82:GLU:OE1	2.46	0.42
19:U:11:ARG:HE	20:V:211:LYS:HB2	1.84	0.42
33:8:96:ASP:OD1	33:8:97:LYS:N	2.53	0.42
55:AB:103:GLU:N	55:AB:104:PRO:CD	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:AY:364:LEU:HD22	78:AY:368:GLN:OE1	2.20	0.42
7:I:132:LYS:HB2	7:I:133:PRO:HD3	2.01	0.42
23:Y:142:LEU:HD23	23:Y:142:LEU:O	2.20	0.42
51:r:35:PHE:O	51:r:54:THR:OG1	2.35	0.42
53:t1:68:VAL:HG22	53:t2:82:LEU:HD12	2.02	0.42
54:AA:1119:U:OP2	72:AS:50:ARG:NH2	2.49	0.42
60:AG:396:ARG:NH2	88:x:33:U:OP2	2.49	0.42
70:AQ:83:PRO:HA	76:AW:108:VAL:HG21	2.02	0.42
1:A:1737:A:H61	1:A:1760:G:H1'	1.85	0.42
1:A:1749:C:O2'	11:M:80:LYS:NZ	2.44	0.42
10:L:69:VAL:HG23	10:L:89:HIS:CD2	2.55	0.42
20:V:49:ILE:HD11	20:V:117:HIS:NE2	2.34	0.42
30:5:351:VAL:HG22	30:5:381:LEU:HD23	2.02	0.42
1:A:2234:C:O2'	1:A:2688:C:O2'	2.09	0.41
8:J:111:LEU:HG	8:J:159:LEU:HD22	2.02	0.41
32:7:148:MET:HE2	32:7:257:ILE:HG13	2.02	0.41
36:b:43:ALA:HB2	36:b:89:ILE:HD12	2.02	0.41
1:A:2135:A:N3	1:A:2135:A:H2'	2.34	0.41
1:A:2195:A:OP1	46:l:119:ARG:NE	2.53	0.41
8:J:133:GLN:HB3	8:J:135:VAL:HG13	2.02	0.41
14:P:84:ILE:O	14:P:91:GLU:N	2.48	0.41
54:AA:699:A:OP1	74:AU:38:LYS:NZ	2.48	0.41
58:AE:109:VAL:HG23	58:AE:109:VAL:O	2.20	0.41
1:A:2166:C:N4	1:A:2212:C:OP2	2.48	0.41
1:A:2177:U:O2'	1:A:2179:A:N7	2.42	0.41
1:A:3017:C:OP2	1:A:3022:G:N2	2.53	0.41
22:X:227:PHE:O	22:X:231:VAL:HG23	2.20	0.41
42:h:111:VAL:HG22	42:h:112:VAL:N	2.35	0.41
46:l:69:THR:O	46:l:86:LEU:HD12	2.20	0.41
54:AA:994:A:O2'	59:AF:166:ARG:NH1	2.54	0.41
1:A:2330:U:H2'	1:A:2445:U:O4	2.21	0.41
17:S:135:LEU:HD23	17:S:135:LEU:C	2.45	0.41
19:U:18:ARG:NH2	20:V:206:GLU:OE1	2.53	0.41
46:l:60:ASP:OD1	46:l:61:VAL:N	2.54	0.41
54:AA:1599:A:OP2	82:A2:32:ARG:NH1	2.52	0.41
72:AS:70:ILE:HD13	72:AS:103:TYR:CD2	2.56	0.41
80:A0:41:LEU:HD13	80:A0:55:TRP:CD1	2.55	0.41
1:A:2616:A:O2'	1:A:3046:C:O2'	2.34	0.41
5:F:77:VAL:O	5:F:77:VAL:HG12	2.20	0.41
27:2:51:ASN:O	27:2:54:GLN:NE2	2.53	0.41
31:6:144:GLY:N	31:6:145:PRO:CD	2.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:6:184:LEU:N	49:p:190:GLN:O	2.52	0.41
50:q:44:ASP:OD1	50:q:45:LEU:N	2.54	0.41
51:r:45:LYS:O	51:r:45:LYS:HG3	2.20	0.41
54:AA:1289:G:O2'	54:AA:1297:G:OP2	2.35	0.41
1:A:2325:U:O2'	13:O:82:GLU:OE2	2.39	0.41
1:A:2416:U:OP2	52:s:165:ARG:NH1	2.53	0.41
2:B:1643:A:H2'	2:B:1644:G:O4'	2.21	0.41
16:R:47:ILE:HG23	17:S:172:MET:HE2	2.02	0.41
19:U:19:VAL:O	19:U:19:VAL:HG13	2.21	0.41
48:o:12:ILE:HD11	51:r:169:TRP:CZ2	2.55	0.41
71:AR:315:GLN:OE1	71:AR:315:GLN:HA	2.21	0.41
1:A:1958:G:O2'	1:A:1959:C:H3'	2.21	0.41
33:8:202:VAL:O	33:8:203:GLU:HB3	2.20	0.41
35:a:62:HIS:O	35:a:62:HIS:ND1	2.53	0.41
75:AV:40:TRP:HZ2	75:AV:111:THR:HG23	1.85	0.41
84:A4:257:HIS:O	84:A4:261:THR:HG22	2.21	0.41
1:A:2218:C:O2'	1:A:2219:C:OP2	2.35	0.41
56:AC:88:GLU:OE1	56:AC:112:ARG:NH2	2.53	0.41
57:AD:134:GLU:OE2	57:AD:160:ARG:NH1	2.46	0.41
77:AX:134:LYS:NZ	94:AX:501:ATP:O2B	2.50	0.41
78:AY:356:CYS:O	78:AY:359:SER:OG	2.39	0.41
1:A:1828:A:O2'	1:A:2684:C:H5	2.04	0.41
1:A:2971:A:O2'	12:N:182:LYS:O	2.38	0.41
7:I:230:THR:HG23	53:t5:86:LEU:HD21	2.03	0.41
13:O:30:ARG:HD2	13:O:78:PHE:O	2.20	0.41
13:O:77:ASP:O	13:O:83:LYS:NZ	2.54	0.41
19:U:66:ALA:HB2	19:U:100:ALA:HA	2.02	0.41
20:V:133:ILE:HG22	20:V:147:SER:HA	2.03	0.41
22:X:226:LEU:HD23	22:X:229:ILE:HD12	2.03	0.41
23:Y:83:ALA:N	34:9:74:VAL:O	2.48	0.41
38:d:188:SER:HA	38:d:218:THR:HG22	2.02	0.41
57:AD:215:TYR:HE2	72:AS:2:ALA:HB2	1.85	0.41
71:AR:162:SER:HB2	71:AR:165:ILE:HD12	2.02	0.41
80:A0:30:ASP:OD1	80:A0:212:ARG:NH1	2.46	0.41
83:A3:170:GLU:HG2	83:A3:191:THR:HG21	2.02	0.41
1:A:2364:C:OP2	19:U:78:LYS:NZ	2.46	0.41
12:N:59:VAL:O	12:N:59:VAL:HG13	2.21	0.41
14:P:144:MET:HE3	14:P:170:VAL:HG13	2.00	0.41
30:5:56:GLU:HG3	30:5:56:GLU:O	2.21	0.41
54:AA:932:C:OP2	67:AN:38:TYR:OH	2.39	0.41
55:AB:234:TYR:OH	72:AS:38:PHE:O	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AV:264:GLU:CG	75:AV:337:LEU:HD11	2.50	0.41
1:A:2694:A:C6	1:A:2985:C:H1'	2.56	0.40
7:I:144:LEU:N	7:I:145:PRO:HD2	2.36	0.40
21:W:53:ILE:HD12	21:W:99:TYR:OH	2.21	0.40
28:3:152:LYS:HD3	31:6:357:PHE:CE2	2.55	0.40
54:AA:663:A:H2'	54:AA:664:G:C8	2.56	0.40
55:AB:89:VAL:O	55:AB:89:VAL:HG12	2.22	0.40
62:AI:153:GLY:O	62:AI:158:ARG:NH2	2.45	0.40
83:A3:177:TRP:CD1	83:A3:177:TRP:C	2.99	0.40
84:A4:346:HIS:HA	84:A4:378:LEU:HD12	2.03	0.40
1:A:1957:A:OP2	18:T:155:ARG:NE	2.55	0.40
1:A:2063:G:N7	40:f:51:LYS:NZ	2.58	0.40
1:A:2853:A:OP2	26:1:46:TYR:N	2.54	0.40
3:D:246:ARG:HH22	3:D:250:VAL:HG13	1.86	0.40
30:5:176:TYR:CD1	30:5:176:TYR:C	2.99	0.40
31:6:196:THR:OG1	31:6:324:ASP:OD2	2.35	0.40
38:d:186:VAL:HG12	38:d:187:GLU:HG3	2.02	0.40
55:AB:231:LEU:HD21	72:AS:46:PHE:HB2	2.02	0.40
61:AH:84:ASP:OD1	61:AH:85:LYS:N	2.54	0.40
61:AH:184:ILE:O	61:AH:184:ILE:HG22	2.20	0.40
77:AX:50:ARG:NH2	77:AX:96:GLU:OE2	2.49	0.40
78:AY:319:ALA:O	81:A1:164:ARG:NH2	2.54	0.40
5:F:84:PRO:O	5:F:88:ALA:N	2.51	0.40
37:c:81:GLU:OE1	37:c:210:ARG:NE	2.51	0.40
38:d:244:GLU:OE1	38:d:264:LYS:NZ	2.49	0.40
53:t1:82:LEU:HD22	53:t2:67:LEU:HD12	2.03	0.40
54:AA:894:C:N4	63:AJ:117:ASP:OD2	2.54	0.40
66:AM:123:GLN:O	66:AM:127:ALA:N	2.48	0.40
73:AT:32:VAL:HG22	73:AT:76:LEU:HD22	2.03	0.40
1:A:1692:A:H2'	1:A:1693:C:O4'	2.21	0.40
1:A:1834:U:C4	18:T:200:ARG:HA	2.56	0.40
1:A:2634:U:OP1	3:D:278:LYS:NZ	2.44	0.40
6:H:56:VAL:HG23	22:X:67:ILE:CD1	2.52	0.40
7:I:214:LEU:HD21	53:t2:90:LEU:HD13	2.03	0.40
14:P:37:ASP:N	14:P:38:PRO:HD2	2.36	0.40
64:AK:53:ARG:O	64:AK:56:SER:OG	2.38	0.40
71:AR:231:CYS:SG	71:AR:242:TYR:HA	2.62	0.40
1:A:2093:U:H4'	43:i:126:LYS:HE2	2.03	0.40
15:Q:227:LYS:HB3	15:Q:228:PRO:HA	2.04	0.40
33:8:153:GLU:HG2	39:e:47:LEU:HD21	2.02	0.40
39:e:271:GLN:OE1	39:e:274:ARG:NH1	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AO:146:GLN:OE1	68:AO:146:GLN:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	236/305 (77%)	233 (99%)	3 (1%)	0	100	100
4	E	303/348 (87%)	296 (98%)	7 (2%)	0	100	100
5	F	250/311 (80%)	248 (99%)	2 (1%)	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%)	173 (100%)	0	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%)	218 (99%)	2 (1%)	0	100	100
13	O	152/175 (87%)	152 (100%)	0	0	100	100
14	P	142/180 (79%)	141 (99%)	1 (1%)	0	100	100
15	Q	236/292 (81%)	234 (99%)	2 (1%)	0	100	100
16	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
17	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
18	T	164/206 (80%)	164 (100%)	0	0	100	100
19	U	129/152 (85%)	128 (99%)	1 (1%)	0	100	100
20	V	203/216 (94%)	203 (100%)	0	0	100	100
21	W	114/148 (77%)	114 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36 (100%)	0	0	100	100
30	5	392/423 (93%)	388 (99%)	4 (1%)	0	100	100
31	6	352/380 (93%)	338 (96%)	14 (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%)	121 (99%)	1 (1%)	0	100	100
35	a	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
36	b	148/214 (69%)	143 (97%)	5 (3%)	0	100	100
37	c	282/332 (85%)	277 (98%)	5 (2%)	0	100	100
38	d	236/306 (77%)	232 (98%)	4 (2%)	0	100	100
39	e	224/279 (80%)	219 (98%)	5 (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%)	158 (99%)	2 (1%)	0	100	100
52	s	382/439 (87%)	378 (99%)	4 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	128 (98%)	2 (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%)	134 (97%)	3 (2%)	1 (1%)	18	48
62	AI	133/194 (69%)	130 (98%)	3 (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%)	291 (99%)	2 (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%)	172 (99%)	2 (1%)	0	100	100
75	AV	358/414 (86%)	357 (100%)	1 (0%)	0	100	100
76	AW	98/187 (52%)	97 (99%)	1 (1%)	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
79	AZ	98/106 (92%)	98 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	A0	213/218 (98%)	210 (99%)	3 (1%)	0	100	100
81	A1	274/323 (85%)	269 (98%)	5 (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
85	u	47/435 (11%)	47 (100%)	0	0	100	100
86	v	30/32 (94%)	30 (100%)	0	0	100	100
All	All	14361/19621 (73%)	14193 (99%)	167 (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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	P	126/155 (81%)	126 (100%)	0	100	100
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	118/134 (88%)	118 (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	221/274 (81%)	220 (100%)	1 (0%)	81	93
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	k	83/89 (93%)	83 (100%)	0	100	100
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%)	285 (100%)	1 (0%)	86	96
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	90
62	AI	104/146 (71%)	102 (98%)	2 (2%)	50	79
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	AS	116/164 (71%)	116 (100%)	0	100	100
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	96
76	AW	87/158 (55%)	87 (100%)	0	100	100
77	AX	311/351 (89%)	310 (100%)	1 (0%)	86	96
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
85	u	46/373 (12%)	46 (100%)	0	100	100
All	All	12839/16871 (76%)	12832 (100%)	7 (0%)	87	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	d	280	VAL
57	AD	340	ILE
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 (101) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	168	HIS
3	D	276	HIS
4	E	72	GLN
5	F	103	GLN
5	F	241	ASN
5	F	251	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	I	101	ASN
7	I	119	HIS
7	I	189	GLN
7	I	193	ASN
8	J	178	GLN
10	L	89	HIS
10	L	104	ASN
11	M	276	ASN
14	P	79	HIS
15	Q	66	HIS
15	Q	209	GLN
16	R	27	HIS
16	R	89	ASN
16	R	149	HIS
17	S	118	ASN
18	T	56	GLN
21	W	80	HIS
22	X	4	HIS
23	Y	179	HIS
24	Z	64	HIS
24	Z	107	ASN
25	0	144	GLN
30	5	109	HIS
30	5	160	HIS
30	5	165	GLN
30	5	195	HIS
30	5	275	ASN
30	5	385	HIS
31	6	292	GLN
31	6	373	HIS
32	7	255	HIS
33	8	143	GLN
35	a	44	ASN
35	a	46	ASN
35	a	90	GLN
36	b	27	GLN
38	d	59	HIS
38	d	77	HIS
39	e	251	HIS
41	g	93	ASN
41	g	102	HIS
42	h	110	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	i	120	HIS
43	i	124	HIS
44	j	31	GLN
45	k	80	HIS
46	l	82	GLN
48	o	21	HIS
48	o	94	HIS
51	r	79	HIS
51	r	96	HIS
52	s	71	HIS
52	s	107	GLN
52	s	239	ASN
52	s	240	GLN
52	s	277	GLN
52	s	343	GLN
56	AC	60	HIS
57	AD	155	GLN
57	AD	288	HIS
57	AD	415	GLN
60	AG	384	GLN
61	AH	130	HIS
61	AH	147	HIS
61	AH	163	ASN
61	AH	183	HIS
63	AJ	134	HIS
65	AL	218	GLN
66	AM	16	HIS
67	AN	52	HIS
68	AO	111	HIS
71	AR	308	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
77	AX	69	ASN
77	AX	148	GLN
77	AX	159	HIS
77	AX	291	HIS
77	AX	302	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	AY	257	ASN
78	AY	290	ASN
78	AY	337	HIS
79	AZ	56	HIS
80	A0	137	HIS
81	A1	185	HIS
84	A4	243	ASN
84	A4	288	HIS
84	A4	521	HIS
84	A4	540	HIS
84	A4	590	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1532/1561 (98%)	217 (14%)	1 (0%)
2	B	71/72 (98%)	13 (18%)	0
54	AA	953/954 (99%)	125 (13%)	0
87	w	67/68 (98%)	16 (23%)	0
88	x	68/70 (97%)	8 (11%)	0
89	y	17/19 (89%)	2 (11%)	0
All	All	2708/2744 (98%)	381 (14%)	1 (0%)

All (381) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
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	1724	A
1	A	1727	A
1	A	1728	U
1	A	1748	G
1	A	1765	C
1	A	1777	A
1	A	1805	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1807	U
1	A	1809	U
1	A	1821	A
1	A	1824	U
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	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
1	A	2036	C
1	A	2037	U
1	A	2039	A
1	A	2044	A
1	A	2059	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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
1	A	2300	G
1	A	2321	A
1	A	2322	C
1	A	2331	C
1	A	2332	C
1	A	2345	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2351	U
1	A	2356	A
1	A	2357	C
1	A	2360	U
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	2417	C
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	2625	C
1	A	2627	G
1	A	2628	U
1	A	2630	U
1	A	2633	A
1	A	2635	G
1	A	2654	U
1	A	2656	U
1	A	2683	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	A	3006	U
1	A	3007	C
1	A	3016	G
1	A	3041	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3053	A
1	A	3054	G
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	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	3231	U
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	718	A
54	AA	721	U
54	AA	737	C
54	AA	745	A
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
54	AA	929	A
54	AA	931	C
54	AA	932	C
54	AA	938	A
54	AA	939	A
54	AA	942	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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
54	AA	1187	U
54	AA	1189	U
54	AA	1200	G
54	AA	1215	U
54	AA	1220	A
54	AA	1223	C
54	AA	1225	C
54	AA	1237	A
54	AA	1246	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	AA	1247	G
54	AA	1248	C
54	AA	1251	A
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	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
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	1562	G
54	AA	1568	U
54	AA	1571	U
54	AA	1582	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	AA	1584	A
54	AA	1594	G
54	AA	1595	G
54	AA	1599	A
87	w	3	G
87	w	7	A
87	w	9	A
87	w	16	A
87	w	21	A
87	w	22	A
87	w	30	G
87	w	46	A
87	w	49	U
87	w	50	A
87	w	55	A
87	w	56	A
87	w	61	U
87	w	65	A
87	w	68	U
87	w	71	C
88	x	25	C
88	x	44	A
88	x	45	G
88	x	46	A
88	x	48	U
88	x	49	G
88	x	59	U
88	x	75	C
89	y	24	U
89	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 [i](#)

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	$\# Z > 2$
45	AYA	k	2	45	6,7,8	0.82	0	6,8,10	0.68	0
62	IAS	AI	184	62	5,6,8	0.78	0	1,6,10	1.00	0
36	THC	b	2	36	8,9,10	0.80	0	10,11,13	1.16	2 (20%)
70	AYA	AQ	2	70	6,7,8	0.81	0	6,8,10	0.54	0
82	AYA	A2	2	82	6,7,8	0.83	0	6,8,10	0.64	0
9	SAC	K	2	9	7,8,9	0.90	0	7,9,11	0.72	0
19	AYA	U	2	19	6,7,8	0.80	0	6,8,10	0.50	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
45	AYA	k	2	45	-	1/5/6/8	-
62	IAS	AI	184	62	-	1/3/5/8	-
36	THC	b	2	36	-	0/9/10/12	-
70	AYA	AQ	2	70	-	0/5/6/8	-
82	AYA	A2	2	82	-	0/5/6/8	-
9	SAC	K	2	9	-	0/7/8/10	-
19	AYA	U	2	19	-	2/5/6/8	-

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	CB-CA-C	-2.25	107.82	111.55
36	b	2	THC	C-CA-N1	2.13	113.16	109.80

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

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 242 ligands modelled in this entry, 236 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
93	FES	AP	201	58,69	0,4,4	-	-	-		
94	ATP	AX	501	90	32,33,33	1.10	3 (9%)	48,52,52	1.52	7 (14%)
93	FES	r	201	51,7	0,4,4	-	-	-		
95	GTP	AX	503	-	33,34,34	1.04	2 (6%)	50,54,54	1.56	8 (16%)
96	ALA	w	101	87	3,4,5	0.69	0	2,4,6	0.86	0
93	FES	AT	201	73,66	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	FES	AP	201	58,69	-	-	0/1/1/1
94	ATP	AX	501	90	-	1/22/38/38	0/3/3/3
93	FES	r	201	51,7	-	-	0/1/1/1
95	GTP	AX	503	-	-	0/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
96	ALA	w	101	87	-	0/1/2/4	-
93	FES	AT	201	73,66	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
95	AX	503	GTP	C6-N1	-2.86	1.33	1.38
94	AX	501	ATP	C5-C6	2.84	1.48	1.41
94	AX	501	ATP	C5-N7	-2.27	1.34	1.39
95	AX	503	GTP	C2-N3	2.25	1.38	1.33
94	AX	501	ATP	C8-N7	2.08	1.35	1.31

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
94	AX	501	ATP	C5-C4-N3	-5.20	119.56	126.72
95	AX	503	GTP	C2-N1-C6	-4.92	116.19	125.11
95	AX	503	GTP	C5-C4-N3	-4.90	120.58	128.39
94	AX	501	ATP	N3-C4-N9	3.60	133.29	127.17
95	AX	503	GTP	C5-C6-N1	3.41	121.92	113.25
94	AX	501	ATP	N9-C8-N7	-3.24	109.34	113.94
95	AX	503	GTP	N9-C4-N3	3.18	132.32	125.95
94	AX	501	ATP	C2-N3-C4	3.08	119.36	111.83
95	AX	503	GTP	O6-C6-C5	-2.91	118.84	126.53
95	AX	503	GTP	N9-C8-N7	-2.67	108.44	113.40
94	AX	501	ATP	C4-N9-C8	2.56	108.43	105.74
95	AX	503	GTP	C8-N7-C5	2.51	108.74	104.26
94	AX	501	ATP	C5-N7-C8	2.36	107.17	103.45
95	AX	503	GTP	C2-N3-C4	2.33	116.32	112.30
94	AX	501	ATP	C4-C5-N7	-2.33	107.92	110.58

There are no chirality outliers.

All (1) torsion outliers are listed below:

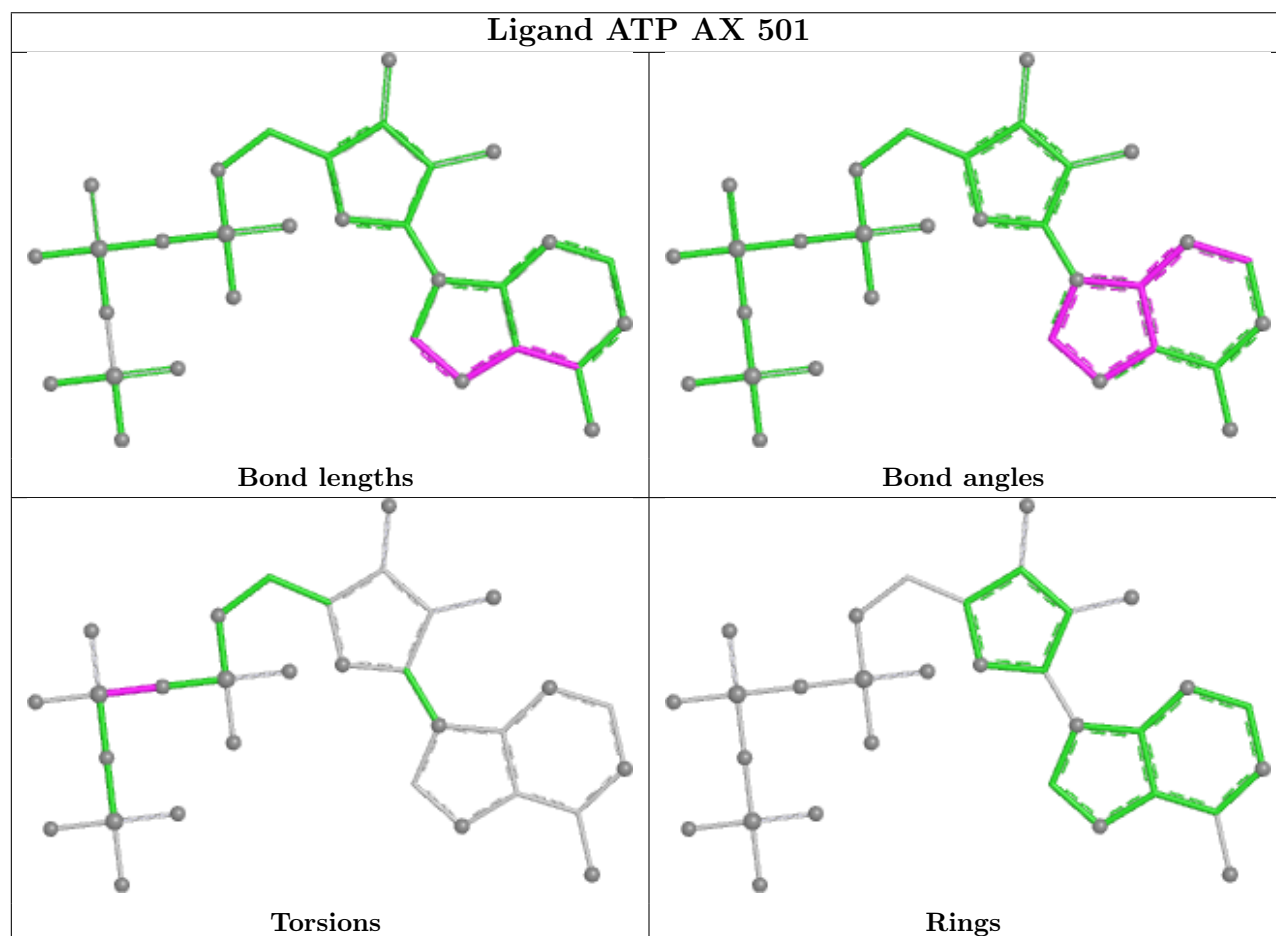
Mol	Chain	Res	Type	Atoms
94	AX	501	ATP	PA-O3A-PB-O2B

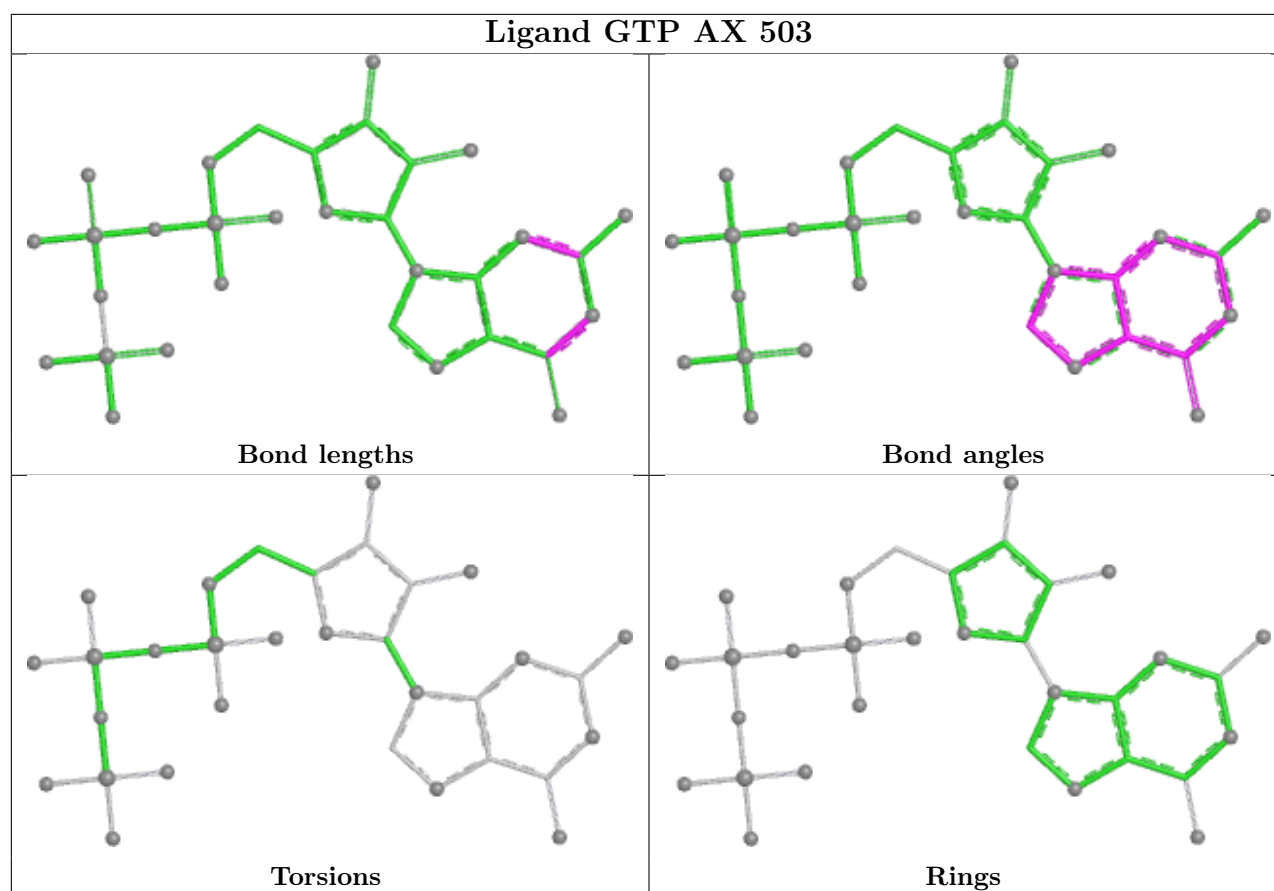
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
94	AX	501	ATP	1	0
96	w	101	ALA	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
89	y	1
88	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	66.64
1	x	15:A	O3'	21:A	P	9.86

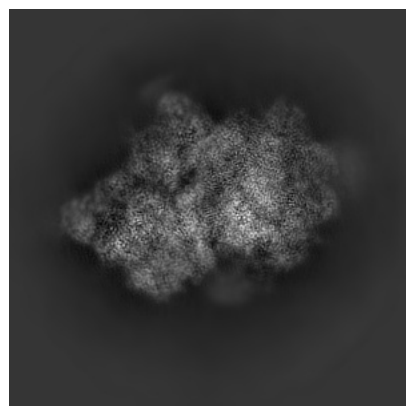
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11278. These allow visual inspection of the internal detail of the map and identification of artifacts.

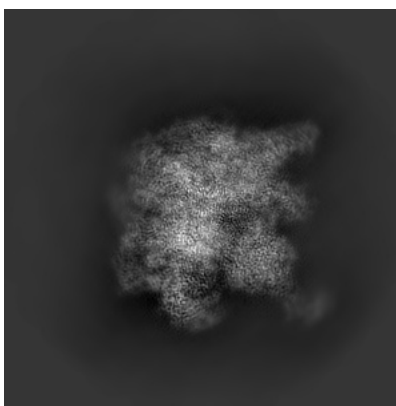
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

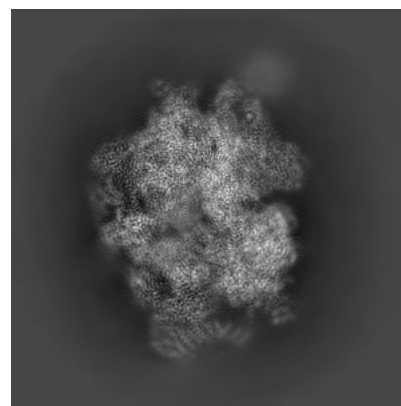
6.1.1 Primary map



X

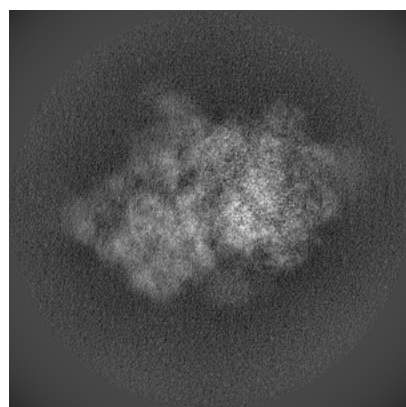


Y

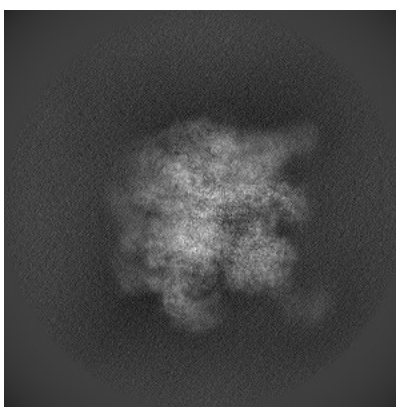


Z

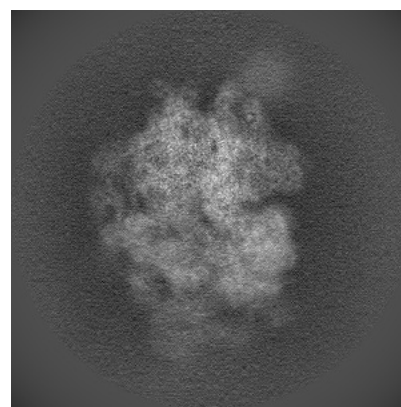
6.1.2 Raw map



X



Y

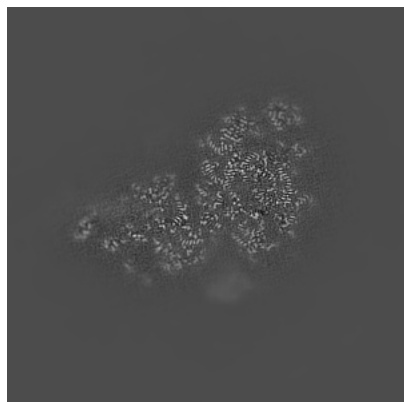


Z

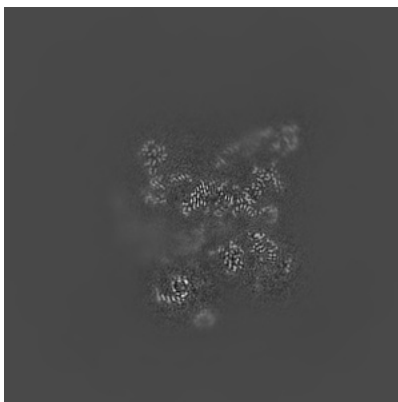
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

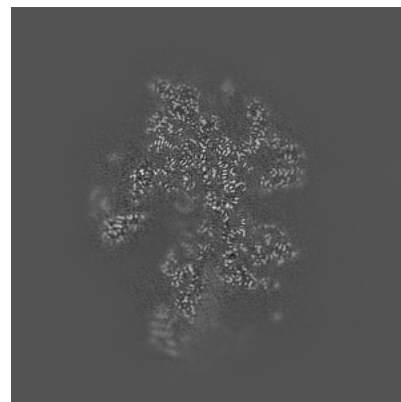
6.2.1 Primary map



X Index: 270

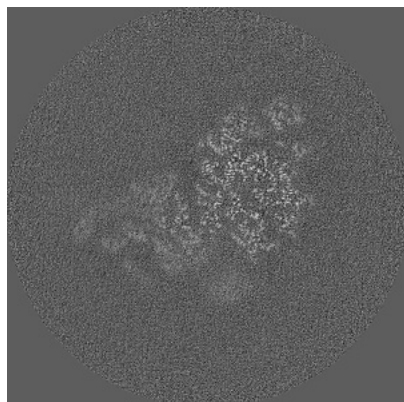


Y Index: 270

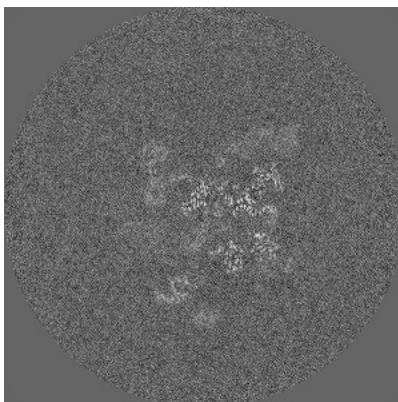


Z Index: 270

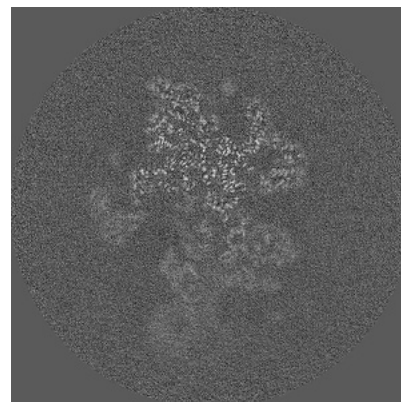
6.2.2 Raw map



X Index: 270



Y Index: 270

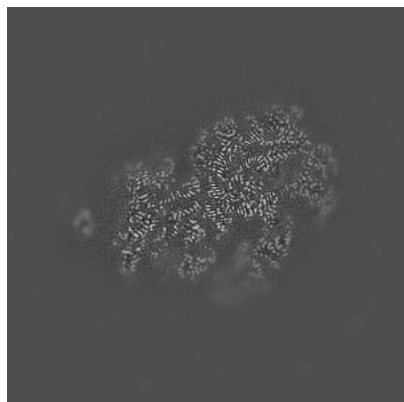


Z Index: 270

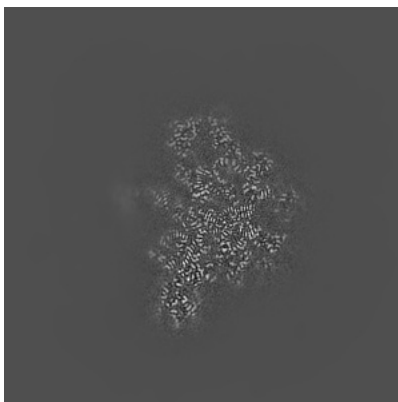
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

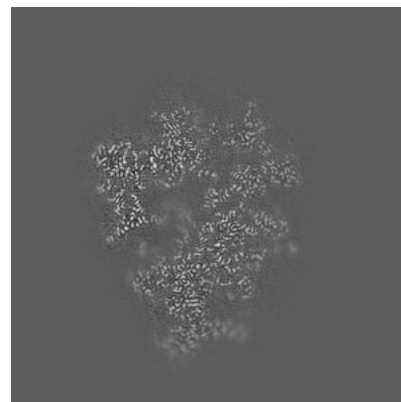
6.3.1 Primary map



X Index: 291

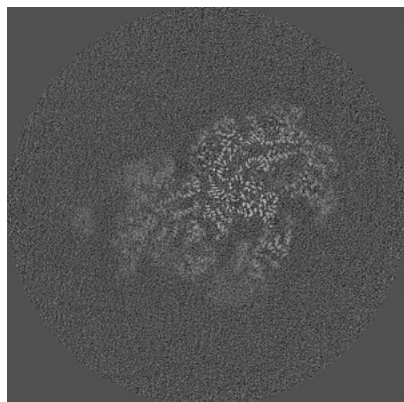


Y Index: 324

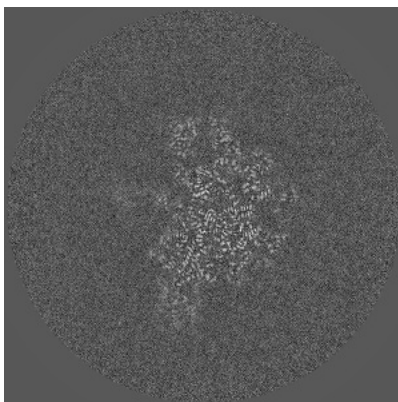


Z Index: 242

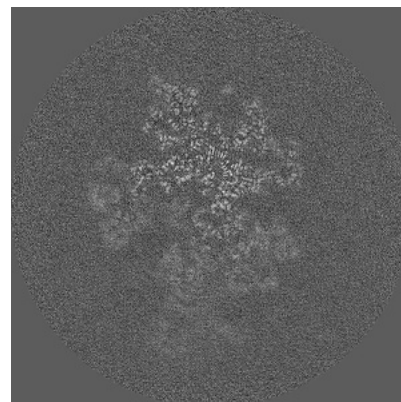
6.3.2 Raw map



X Index: 291



Y Index: 324

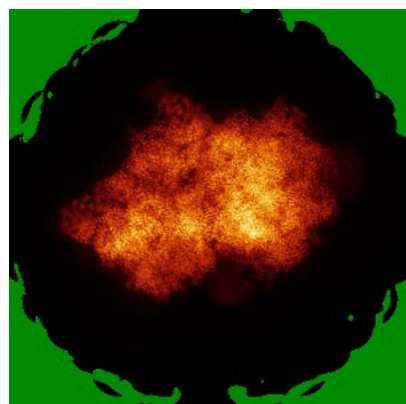


Z Index: 262

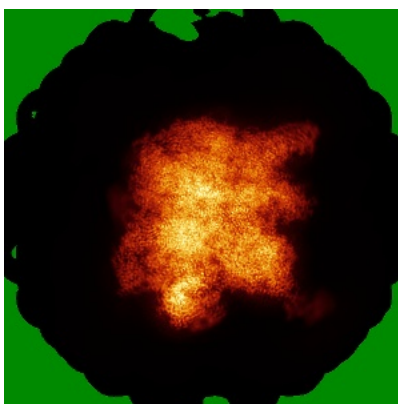
The images above show the largest variance slices of the map in three orthogonal directions.

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

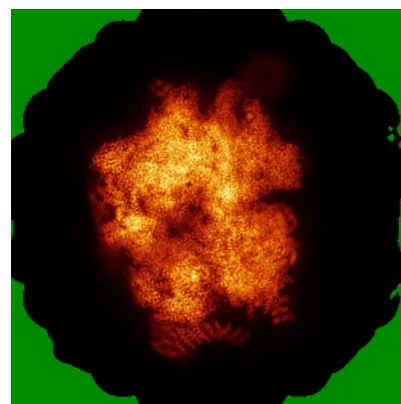
6.4.1 Primary map



X

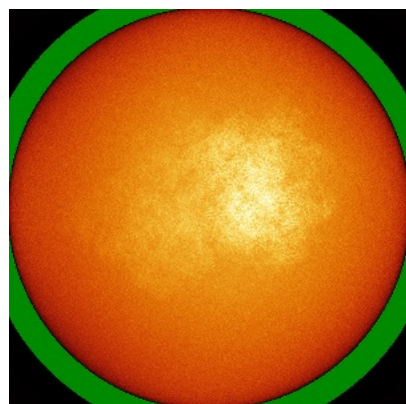


Y

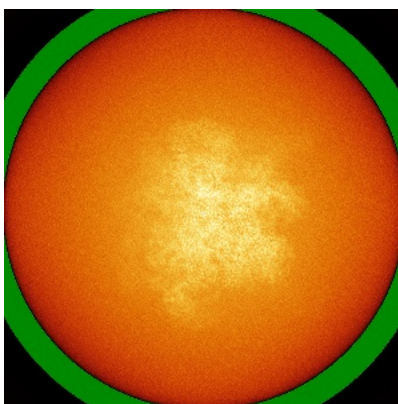


Z

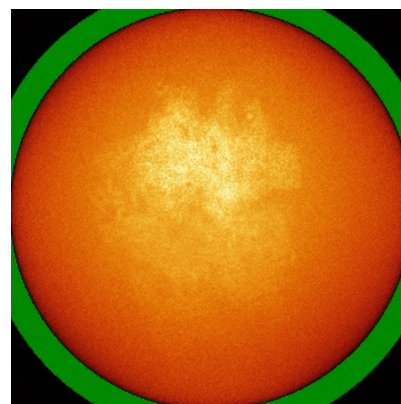
6.4.2 Raw map



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.

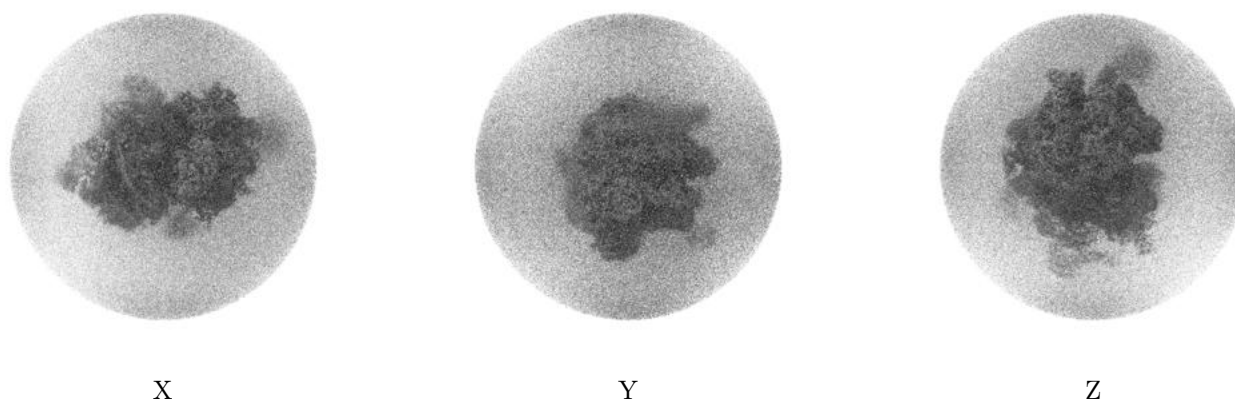
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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.

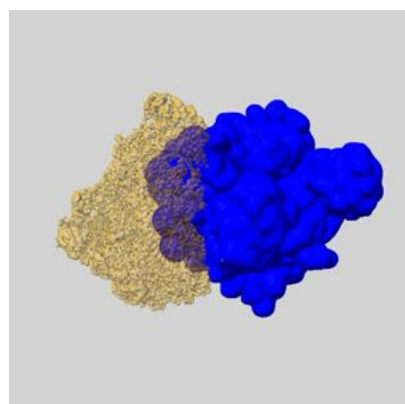
6.6 Mask visualisation [i](#)

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

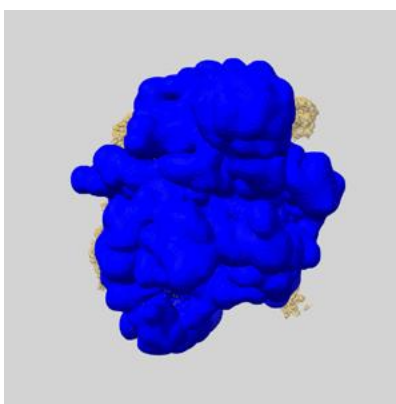
A mask typically either:

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

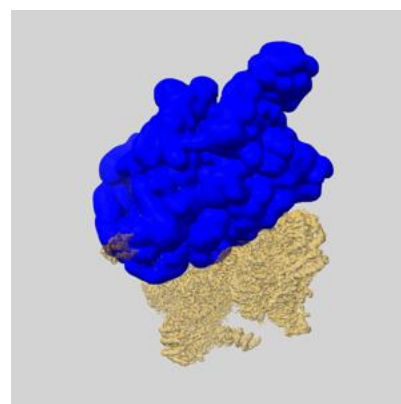
6.6.1 emd_11278_msk_1.map [i](#)



X



Y

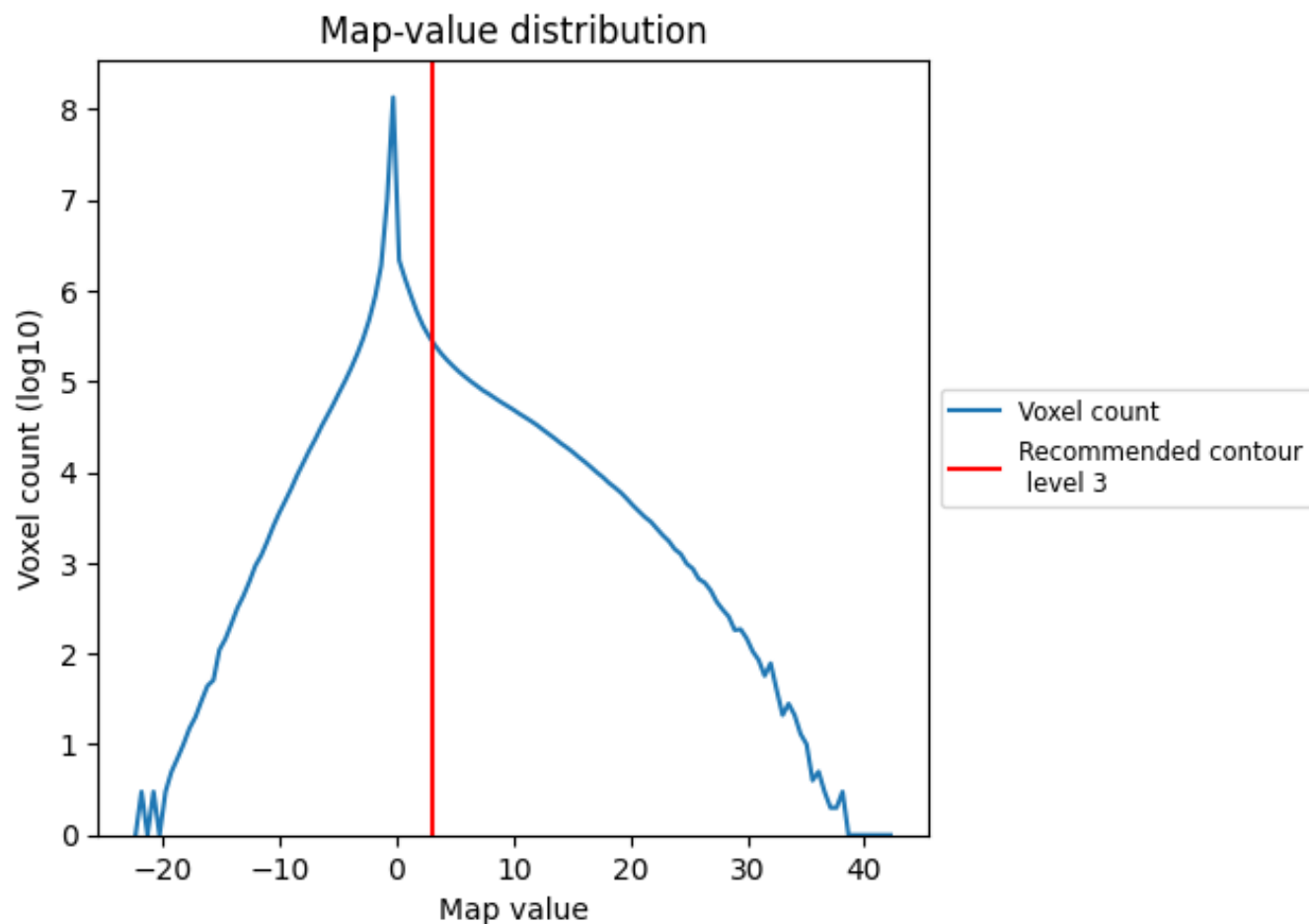


Z

7 Map analysis [i](#)

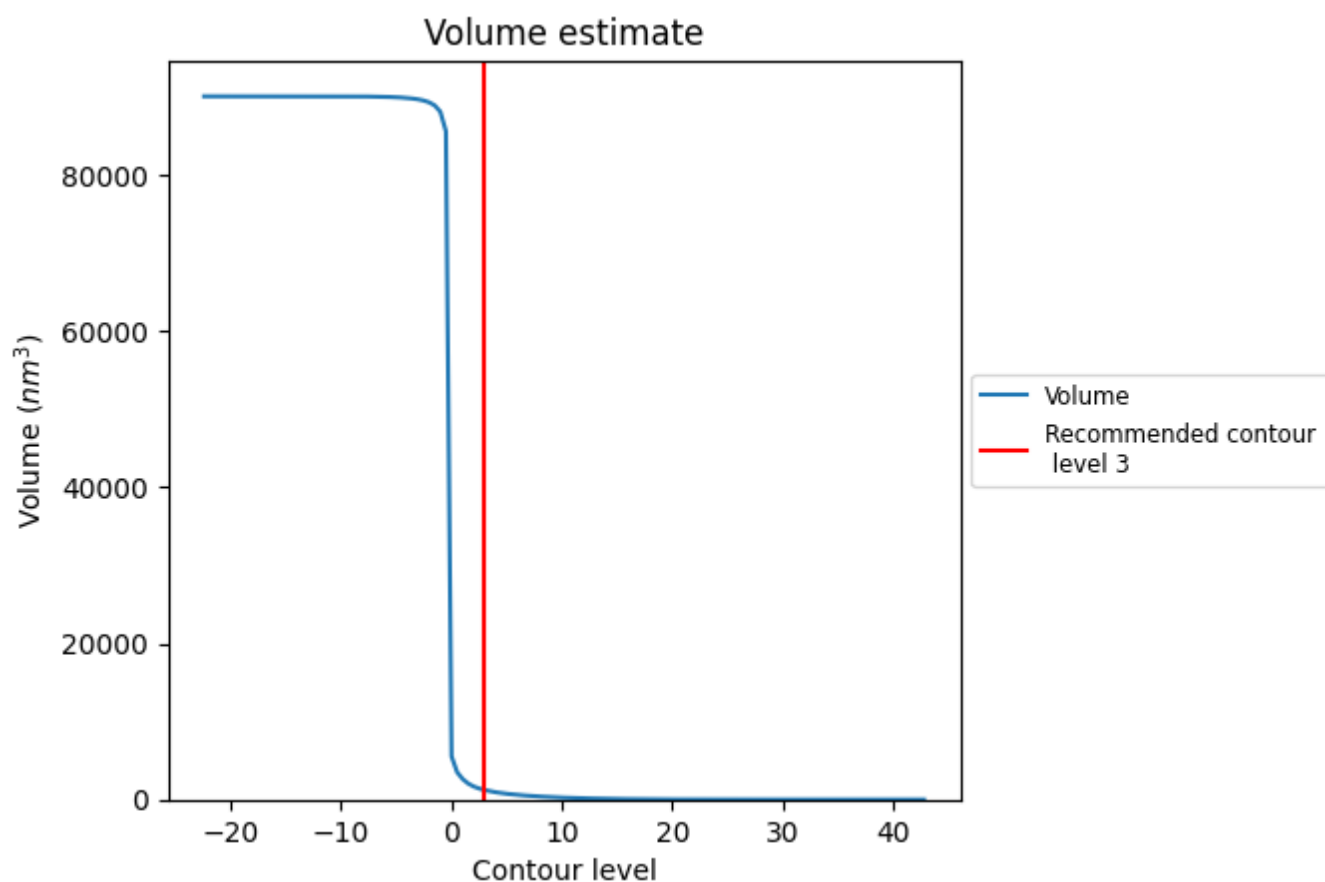
This section contains the results of statistical analysis of the map.

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.

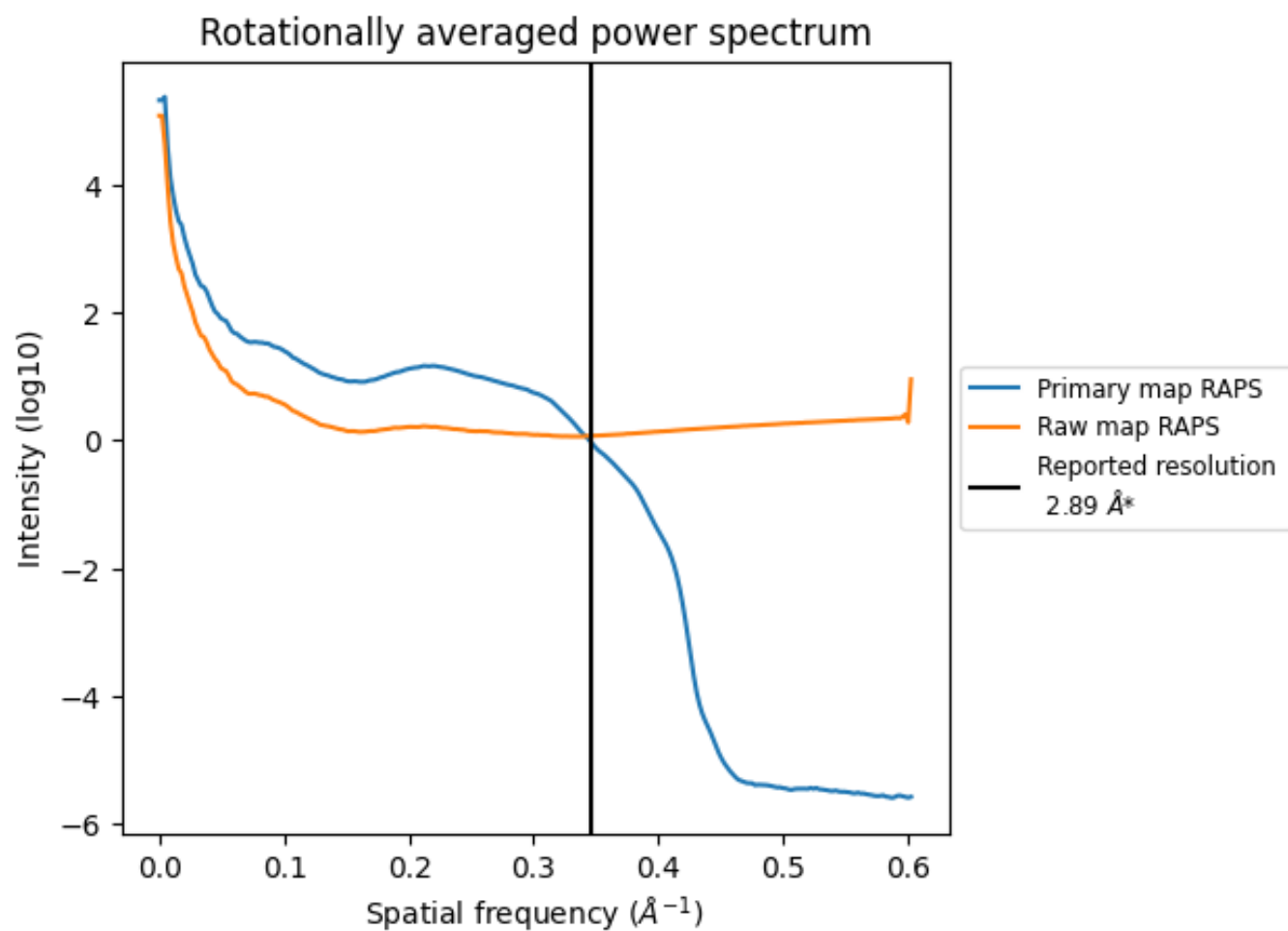
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1233 nm³; this corresponds to an approximate mass of 1114 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 ⓘ

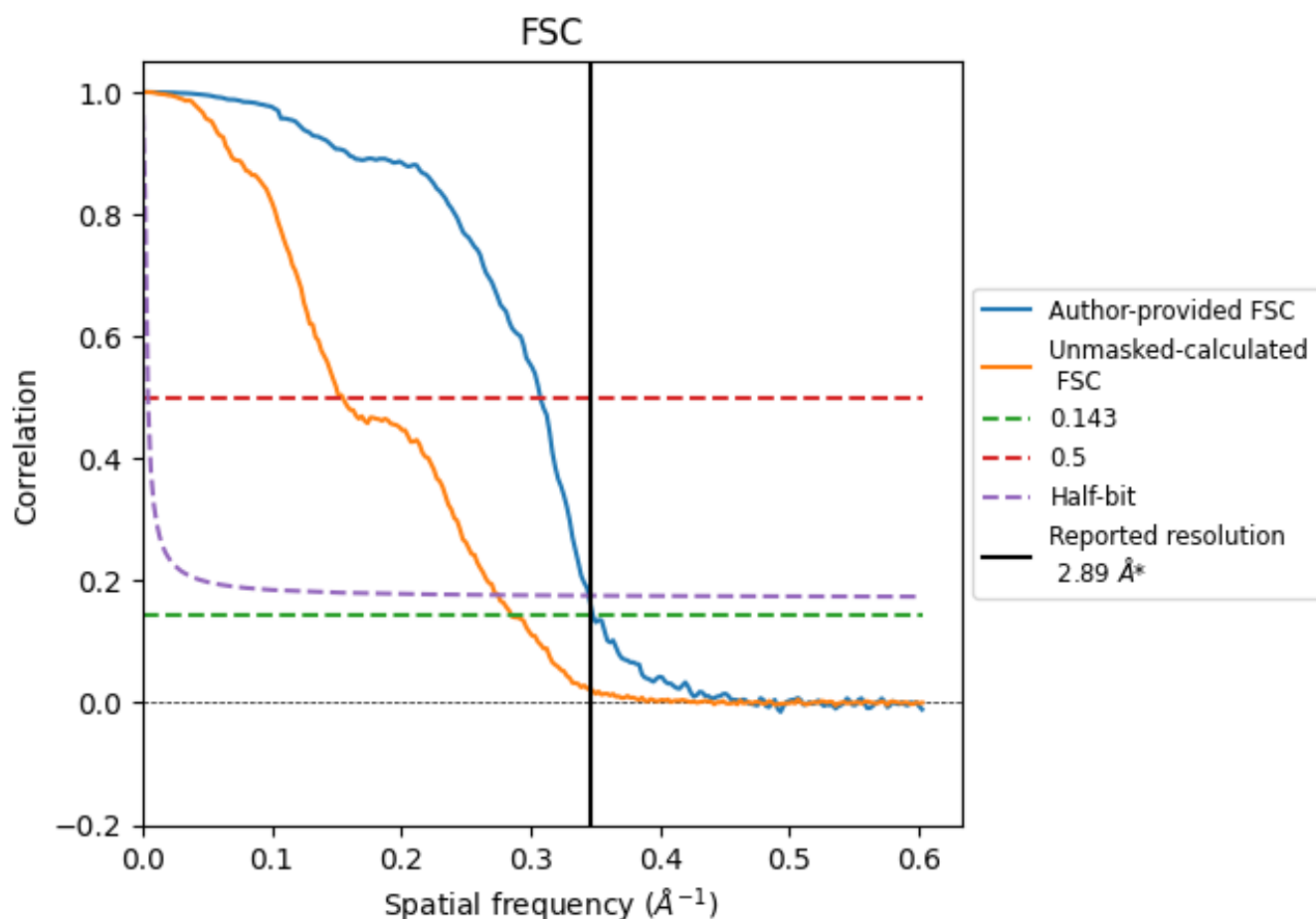


*Reported resolution corresponds to spatial frequency of 0.346 $\text{\AA}^{-1}$

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 0.346 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

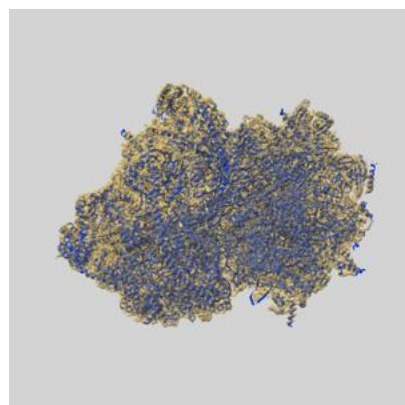
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	2.87	3.25	2.90
Unmasked-calculated*	3.51	6.46	3.64

*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 3.51 differs from the reported value 2.89 by more than 10 %

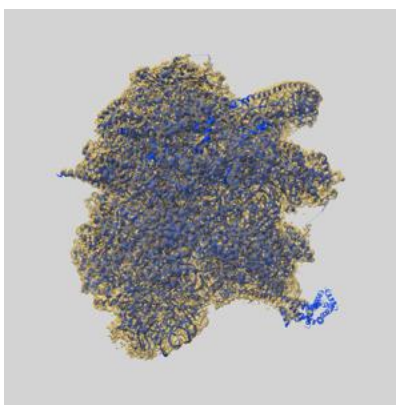
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11278 and PDB model 6ZM5. Per-residue inclusion information can be found in section 3 on page 25.

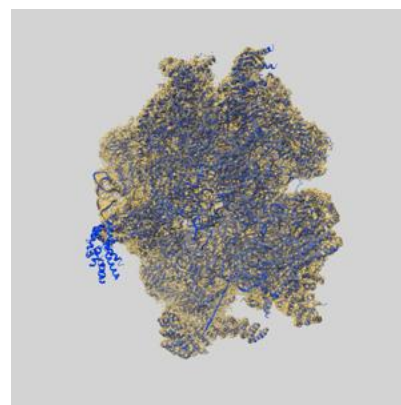
9.1 Map-model overlay [i](#)



X



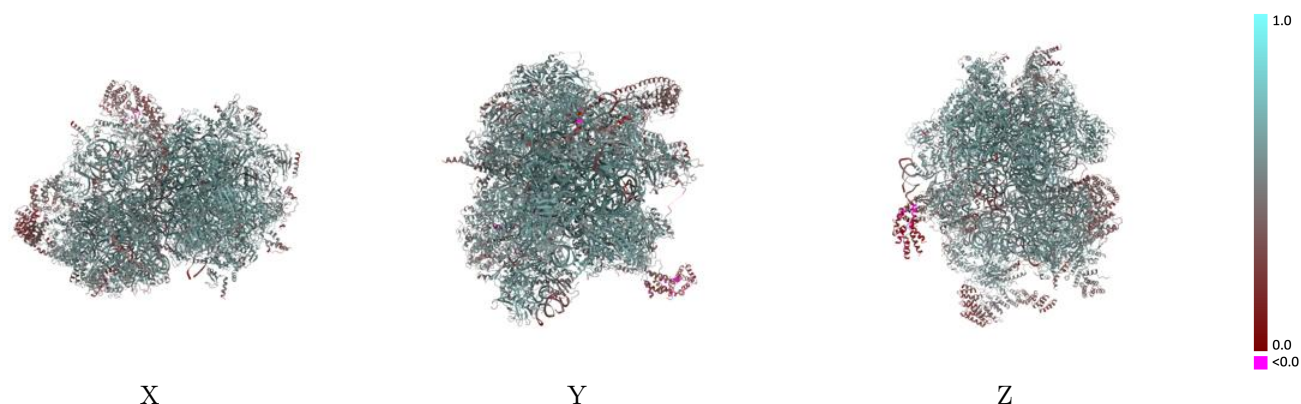
Y



Z

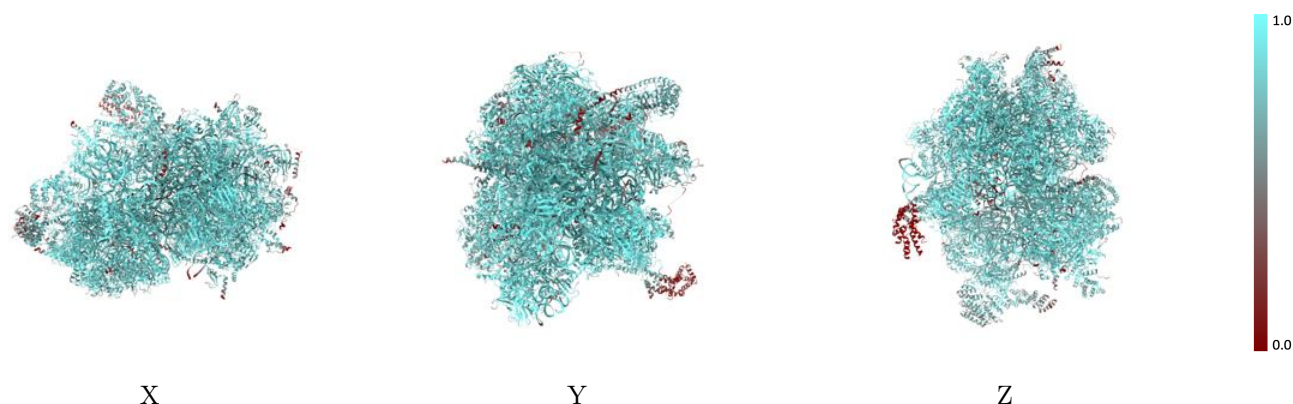
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



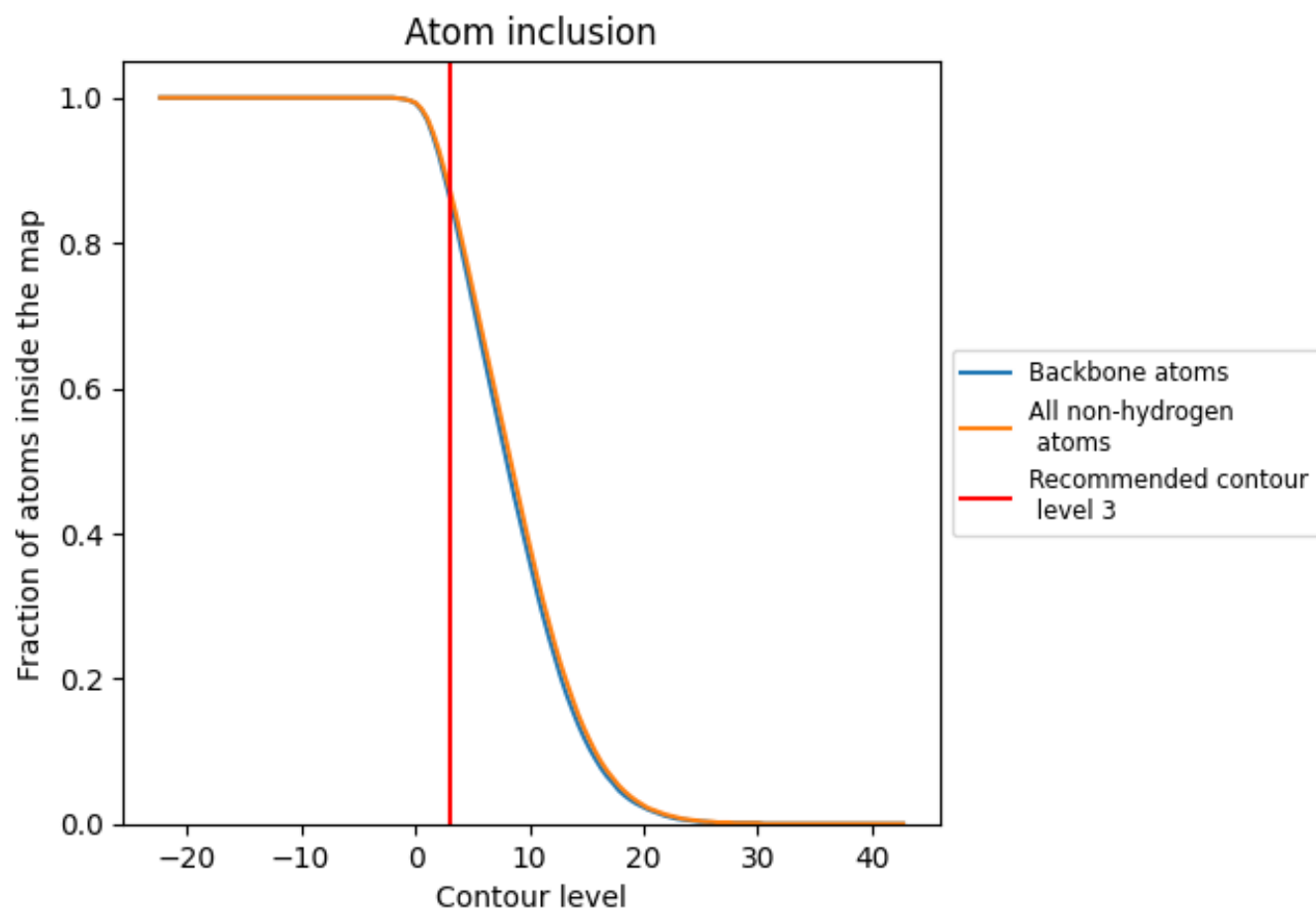
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 88% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.5520
0	 0.8820	 0.5890
1	 0.8480	 0.5640
2	 0.9780	 0.6720
3	 0.9680	 0.6480
4	 0.9540	 0.6260
5	 0.8840	 0.5710
6	 0.9360	 0.5750
7	 0.7890	 0.5120
8	 0.7570	 0.4450
9	 0.8280	 0.5520
A	 0.9610	 0.6190
A0	 0.8280	 0.5040
A1	 0.8660	 0.5250
A2	 0.7960	 0.4880
A3	 0.8730	 0.5660
A4	 0.6960	 0.3580
AA	 0.9560	 0.5930
AB	 0.8990	 0.5480
AC	 0.9520	 0.6120
AD	 0.8670	 0.5370
AE	 0.8540	 0.5520
AF	 0.8410	 0.5300
AG	 0.8720	 0.5320
AH	 0.8960	 0.5580
AI	 0.8540	 0.5320
AJ	 0.8320	 0.5470
AK	 0.9520	 0.6100
AL	 0.7940	 0.5040
AM	 0.8870	 0.5580
AN	 0.9030	 0.5700
AO	 0.8830	 0.5370
AP	 0.8830	 0.5580
AQ	 0.8970	 0.5780
AR	 0.8350	 0.4850



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AS	 0.8260	 0.4760
AT	 0.8730	 0.5430
AU	 0.8010	 0.4630
AV	 0.7220	 0.3790
AW	 0.8720	 0.5280
AX	 0.8310	 0.5180
AY	 0.7560	 0.4600
AZ	 0.8640	 0.5430
B	 0.9130	 0.4760
D	 0.9270	 0.6060
E	 0.9110	 0.5990
F	 0.9290	 0.6170
H	 0.7600	 0.5200
I	 0.7490	 0.4570
J	 0.8090	 0.4410
K	 0.9470	 0.6230
L	 0.9080	 0.5970
M	 0.9140	 0.5970
N	 0.9200	 0.5930
O	 0.9040	 0.6030
P	 0.9480	 0.6050
Q	 0.8320	 0.5490
R	 0.9530	 0.6360
S	 0.9170	 0.6100
T	 0.9220	 0.6210
U	 0.8940	 0.6030
V	 0.7760	 0.5310
W	 0.9400	 0.6220
X	 0.8470	 0.5650
Y	 0.8880	 0.5950
Z	 0.9230	 0.6050
a	 0.7820	 0.5210
b	 0.9370	 0.6190
c	 0.8440	 0.5550
d	 0.6850	 0.4900
e	 0.8640	 0.4610
f	 0.8200	 0.5060
g	 0.9070	 0.5900
h	 0.7800	 0.5210
i	 0.9510	 0.6490
j	 0.8730	 0.5490
k	 0.8500	 0.5150

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
l	 0.8390	 0.4680
m	 0.7720	 0.4420
o	 0.9530	 0.6310
p	 0.7670	 0.4840
q	 0.6420	 0.4280
r	 0.9260	 0.5890
s	 0.8960	 0.5900
t1	 0.5070	 0.2850
t2	 0.4650	 0.2780
t3	 0.0000	 0.1520
t4	 0.0290	 0.0720
t5	 0.0000	 0.1240
t6	 0.0000	 0.0560
u	 0.3830	 0.3490
v	 0.4060	 0.3310
w	 0.5160	 0.3440
x	 0.6590	 0.4180
y	 0.7970	 0.4540