



## Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 05:37 am GMT

PDB ID : 7NQH  
EMDB ID : EMD-12527  
Title : 55S mammalian mitochondrial ribosome with mtRF1a and P-site tRNAMet  
Authors : Kummer, E.; Schubert, K.; Ban, N.  
Deposited on : 2021-03-01  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

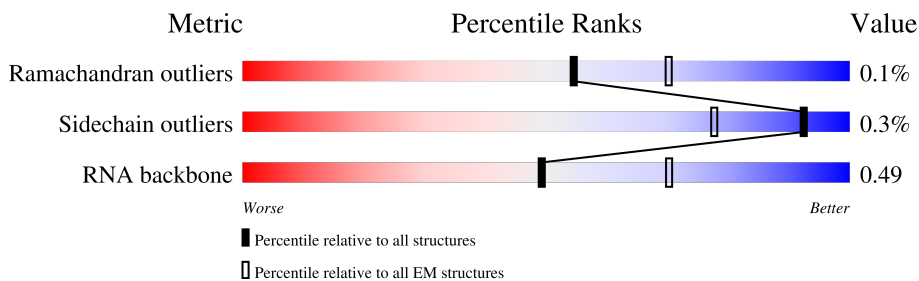
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 3.50 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.



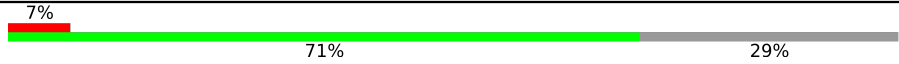
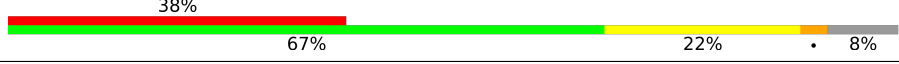
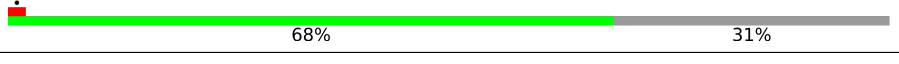


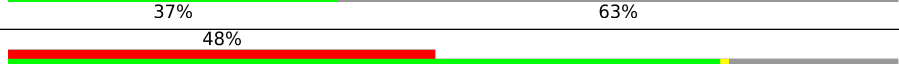

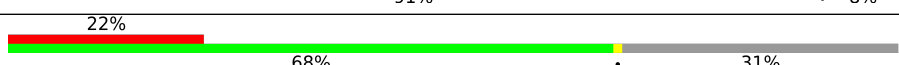
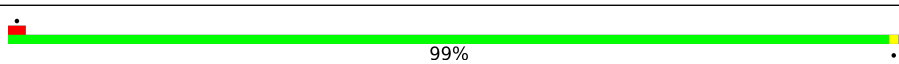

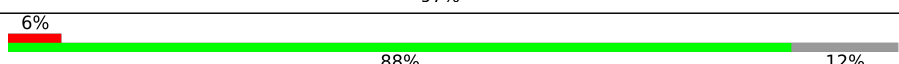
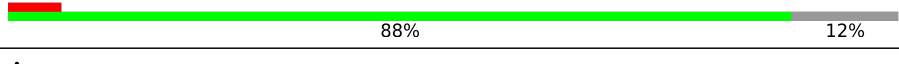
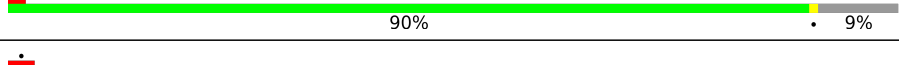

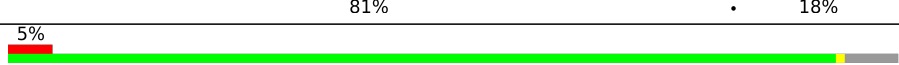
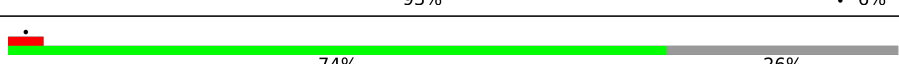

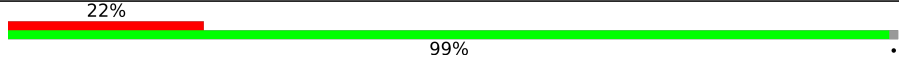
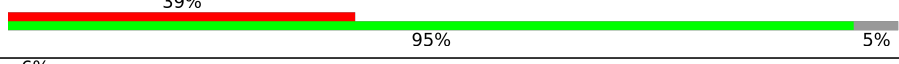
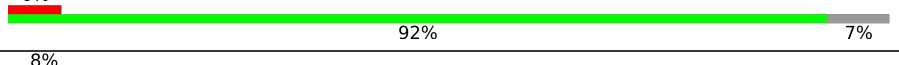
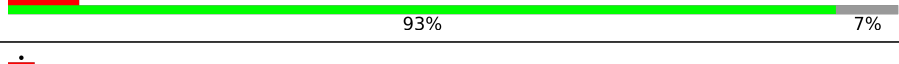

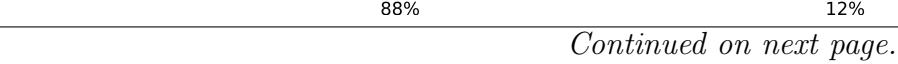


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	CL	198	
1	DL	198	
1	EL	198	
1	FL	198	
1	GL	198	
1	HL	198	
2	B0	148	
3	B1	256	

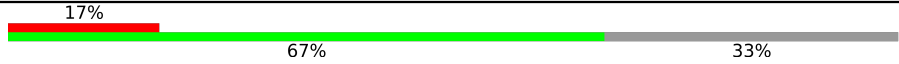
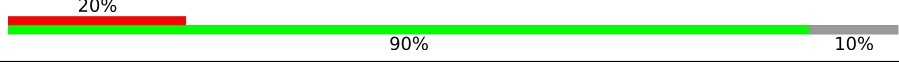
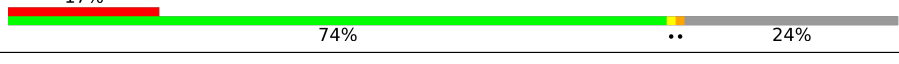
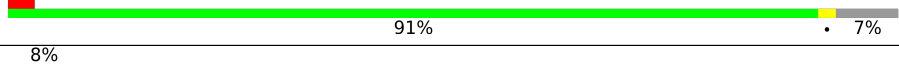

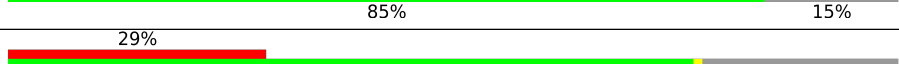
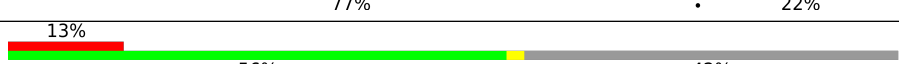
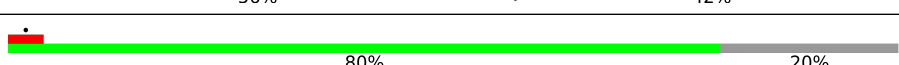
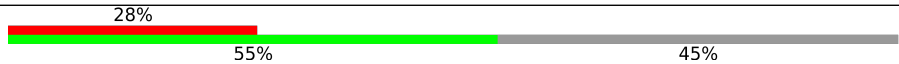



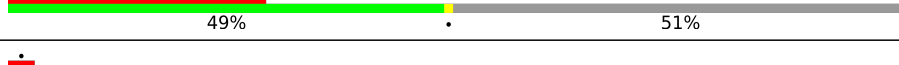
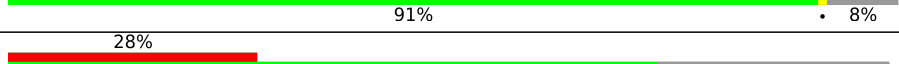
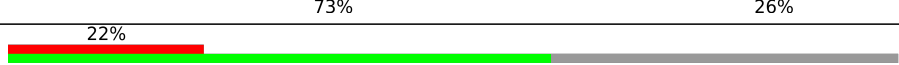










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Mol	Chain	Length	Quality of chain
4	B2	252	
5	BB	73	
6	BD	306	
7	BE	399	
8	BF	294	
9	BI	268	
10	BJ	262	
11	BK	192	
12	BL	362	
13	BN	178	
14	BO	145	
15	BP	296	
16	BQ	251	
17	BR	169	
18	BS	180	
19	BT	292	
20	BU	149	
21	BV	209	
22	BW	210	
23	BX	150	
24	BY	216	
25	Ba	423	
26	Bb	380	
27	B3	161	
28	Bc	334	

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Mol	Chain	Length	Quality of chain
29	Bd	206	
30	Be	135	
31	Bf	142	
32	Bg	159	
33	Bh	332	
34	Bi	306	
35	Bj	279	
36	Bk	269	
37	Bl	166	
38	Bm	198	
39	Bn	128	
40	Bo	124	
41	Bp	112	
42	Bq	138	
43	Bt	102	
44	Bu	205	
45	Bv	222	
46	Bw	433	
47	Bx	196	
48	AA	962	
49	B4	126	
50	B5	188	
51	B6	65	
52	B7	95	
53	AB	289	

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Mol	Chain	Length	Quality of chain
54	AC	167	5% 78% 21%
55	AE	430	17% 79% 20%
56	AF	276	44% 56%
57	AG	240	12% 85% 14%
58	AI	397	18% 83% 17%
59	AJ	200	12% 70% 30%
60	AK	196	70% 30%
61	AL	139	6% 78% 22%
62	AN	128	78% 21%
63	AO	239	13% 73% 27%
64	AP	135	17% 86% 13%
65	AQ	130	7% 85% 14%
66	AR	143	8% 67% 32%
67	AU	87	5% 99%
68	AV	71	17% 48% 51%
69	AX	9	89% 11%
70	AZ	18	56% 100%
71	Aa	382	30% 76% 24%
72	Ab	190	29% 71% 29%
73	Ac	173	13% 95%
74	Ad	205	21% 85% 14%
75	B8	188	51% 49%
76	Ae	455	71% 84% 15%
77	Af	188	8% 52% 47%
78	Ag	410	13% 86% 14%

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Mol	Chain	Length	Quality of chain
79	Ah	387	
80	Ai	106	
81	Aj	218	
82	Ak	325	
83	Am	118	
84	An	199	
85	Ao	699	
86	Ap	258	
87	B9	100	
88	BA	1571	

## 2 Entry composition [i](#)

There are 94 unique types of molecules in this entry. The entry contains 174617 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mitochondrial ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	CL	45	317	203	52	62	0	0
1	DL	27	213	137	33	43	0	0
1	EL	28	222	143	35	44	0	0
1	FL	27	213	137	33	43	0	0
1	GL	27	213	137	33	43	0	0
1	HL	26	205	131	32	42	0	0

- Molecule 2 is a protein called Mitochondrial ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B0	110	857	553	156	145	3	0	0

- Molecule 3 is a protein called Mitochondrial ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B1	244	2036	1315	363	353	5	0	0

- Molecule 4 is a protein called Mitochondrial ribosomal protein L47.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B2	179	1548	992	290	260	6	0	0

- Molecule 5 is a RNA chain called tRNA(Phe) in LSU.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	BB	67	1427	640	261	459	67	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	72	C	-	insertion	GB 76262549
BB	73	A	-	insertion	GB 76262549

- Molecule 6 is a protein called uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	BD	210	1625	1016	323	278	8	0	0

- Molecule 7 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	BE	279	2192	1406	389	388	9	0	0

- Molecule 8 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	BF	223	1792	1155	330	301	6	0	0

- Molecule 9 is a protein called Mitochondrial ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	BI	98	805	509	155	141	0	0

- Molecule 10 is a protein called Mitochondrial ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	BJ	212	1705	1100	306	290	9	0	0

- Molecule 11 is a protein called Mitochondrial ribosomal protein L11.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	BK	176	1303	830	236	235	2	0	0

- Molecule 12 is a protein called Peptide chain release factor 1-like, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	BL	250	2003	1253	362	380	8	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BL	-6	SER	-	expression tag	UNP Q9UGC7
BL	-4	GLY	PRO	conflict	UNP Q9UGC7
BL	-3	SER	ALA	conflict	UNP Q9UGC7
BL	-2	GLY	ARG	conflict	UNP Q9UGC7
BL	-1	SER	ARG	conflict	UNP Q9UGC7
BL	0	GLY	PRO	conflict	UNP Q9UGC7

- Molecule 13 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	BN	177	1444	926	258	253	7	0	0

- Molecule 14 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	BO	115	896	562	176	154	4	0	0

- Molecule 15 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	BP	288	2312	1473	430	403	6	0	0

- Molecule 16 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	BQ	222	1803	1156	331	306	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	237	HIS	TYR	conflict	UNP F1RI89

- Molecule 17 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BR	153	1240	777	236	222	5	0	0

- Molecule 18 is a protein called Mitochondrial ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	BS	143	1168	733	227	204	4	0	0

- Molecule 19 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	BT	240	1954	1253	338	354	9	0	0

- Molecule 20 is a protein called Mitochondrial ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	BU	140	1159	732	239	185	3	0	0

- Molecule 21 is a protein called Mitochondrial ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	BV	155	1231	789	219	219	4	0	0

- Molecule 22 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	BW	166	1374	876	258	234	6	0	0

- Molecule 23 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BX	149	Total	C	N	O	S	0	0
			1181	752	227	200	2		

- Molecule 24 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BY	206	Total	C	N	O	S	0	0
			1678	1056	308	309	5		

- Molecule 25 is a protein called Mitochondrial ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ba	393	Total	C	N	O	S	0	0
			3173	2040	556	565	12		

- Molecule 26 is a protein called Mitochondrial ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Bb	354	Total	C	N	O	S	0	0
			2952	1876	542	525	9		

- Molecule 27 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B3	118	Total	C	N	O	S	0	0
			968	622	178	165	3		

- Molecule 28 is a protein called Mitochondrial ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Bc	295	Total	C	N	O	S	0	0
			2408	1541	410	441	16		

- Molecule 29 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Bd	138	Total	C	N	O	S	0	0
			1158	729	211	217	1		

- Molecule 30 is a protein called Mitochondrial ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Be	122	Total	C	N	O	S	0	0
			972	628	168	173	3		

- Molecule 31 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bf	108	Total	C	N	O	S	0	0
			827	519	154	150	4		

- Molecule 32 is a protein called Mitochondrial ribosomal protein L43.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bg	148	Total	C	N	O	S	0	0
			1167	727	225	212	3		

- Molecule 33 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bh	289	Total	C	N	O	S	0	0
			2319	1486	399	426	8		

- Molecule 34 is a protein called Mitochondrial ribosomal protein L45.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bi	260	Total	C	N	O	S	0	0
			2138	1370	379	379	10		

- Molecule 35 is a protein called Mitochondrial ribosomal protein L46.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bj	217	Total	C	N	O	S	0	0
			1775	1137	311	321	6		

- Molecule 36 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bk	155	Total	C	N	O	S	0	0
			1246	796	214	231	5		

- Molecule 37 is a protein called Mrpl34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	B1	133	1097	709	192	194	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	59	ARG	LYS	conflict	UNP A0A0R4J8D6

- Molecule 38 is a protein called Mitochondrial ribosomal protein L50.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Bm	109	893	568	160	162	3	0	0

- Molecule 39 is a protein called Mitochondrial ribosomal protein L51.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Bn	97	837	539	166	128	4	0	0

- Molecule 40 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Bo	97	772	481	148	141	2	0	0

- Molecule 41 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Bp	97	742	459	143	134	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bp	12	ALA	SER	conflict	UNP A0A341D604
Bp	107	SER	GLY	conflict	UNP A0A341D604

- Molecule 42 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bq	68	Total	C	N	O	S	0	0
			542	344	102	95	1		

- Molecule 43 is a protein called Mitochondrial ribosomal protein L57.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bt	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 44 is a protein called mL62 (ICT1).

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bu	151	Total	C	N	O	S	0	0
			1198	738	233	222	5		

- Molecule 45 is a protein called mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bv	135	Total	C	N	O	S	0	0
			1131	692	223	211	5		

- Molecule 46 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bw	387	Total	C	N	O	S	0	0
			3126	2011	548	555	12		

- Molecule 47 is a protein called Mitochondrial ribosomal protein S18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Bx	162	Total	C	N	O	S	0	0
			1325	845	249	224	7		

- Molecule 48 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AA	960	Total	C	N	O	P	0	0
			20411	9162	3708	6581	960		

- Molecule 49 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B4	63	Total	C	N	O	S	0	0
			479	299	95	82	3		

- Molecule 50 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B5	110	Total	C	N	O	S	0	0
			902	553	181	162	6		

- Molecule 51 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B6	52	Total	C	N	O	S	0	0
			425	274	78	71	2		

- Molecule 52 is a protein called Mitochondrial ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B7	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 53 is a protein called Mitochondrial ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AB	220	Total	C	N	O	S	0	0
			1762	1126	326	304	6		

- Molecule 54 is a protein called Mitochondrial ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AC	132	Total	C	N	O	S	0	0
			1075	695	195	181	4		

- Molecule 55 is a protein called Mitochondrial ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AE	343	Total	C	N	O	S	0	0
			2732	1707	527	487	11		

- Molecule 56 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	AF	122	981	620	178	177	6	0	0

- Molecule 57 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	AG	206	1693	1075	310	297	11	0	0

- Molecule 58 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	AI	328	2650	1678	478	481	13	0	0

- Molecule 59 is a protein called Mitochondrial ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	AJ	140	1155	746	197	208	4	0	0

- Molecule 60 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	AK	137	1007	631	193	180	3	0	0

- Molecule 61 is a protein called Mitochondrial ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	AL	109	840	524	172	138	6	0	0

- Molecule 62 is a protein called Mitochondrial ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	AN	101	858	534	174	144	6	0	0

- Molecule 63 is a protein called uS15m.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	AO	175	1448	919	272	248	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	AP	117	932	588	184	155	5	0	0

- Molecule 65 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	AQ	112	875	568	153	151	3	0	0

- Molecule 66 is a protein called Mitochondrial ribosomal protein S18C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	AR	97	784	507	132	138	7	0	0

- Molecule 67 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	AU	86	734	453	148	125	8	0	0

- Molecule 68 is a RNA chain called tRNAMet.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	69	C	-	insertion	GB 1208989970
AV	70	C	-	insertion	GB 1208989970
AV	71	A	-	insertion	GB 1208989970

- Molecule 69 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
69	AX	9	188	86	35	59	8	0	0

- Molecule 70 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
70	AZ	18	90	54	18	18	0	0

- Molecule 71 is a protein called Mitochondrial ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	Aa	292	2378	1518	409	442	9	0	0

- Molecule 72 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	Ab	135	1101	709	199	192	1	0	0

- Molecule 73 is a protein called Mitochondrial ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	Ac	169	1367	876	236	245	10	0	0

- Molecule 74 is a protein called Mitochondrial ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	Ad	177	1467	904	288	273	2	0	0

- Molecule 75 is a protein called Mitochondrial ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	B8	95	833	539	163	129	2	0	0

- Molecule 76 is a protein called Mitochondrial ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	Ae	388	3109	1971	535	589	14	0	0

- Molecule 77 is a protein called Mitoribosomal protein ms28, mrps28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	Af	99	778	494	134	146	4	0	0

- Molecule 78 is a protein called Death associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	Ag	353	2875	1837	515	513	10	0	0

- Molecule 79 is a protein called Mitochondrial ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	Ah	120	1015	659	168	185	3	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	180	UNK	-	insertion	UNP F1RME2
Ah	181	GLN	-	insertion	UNP F1RME2
Ah	182	LYS	-	insertion	UNP F1RME2
Ah	184	GLY	-	insertion	UNP F1RME2
Ah	185	GLU	LYS	conflict	UNP F1RME2
Ah	187	PRO	LYS	conflict	UNP F1RME2
Ah	189	ILE	LEU	conflict	UNP F1RME2
Ah	190	SER	ILE	conflict	UNP F1RME2
Ah	237	SER	-	insertion	UNP F1RME2
Ah	238	PHE	-	insertion	UNP F1RME2

- Molecule 80 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	Ai	99	824	522	156	143	3	0	0

- Molecule 81 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Aj	213	Total	C	N	O	S	0	0
			1788	1131	338	311	8		

- Molecule 82 is a protein called Mitochondrial ribosomal protein S35.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Ak	275	Total	C	N	O	S	0	0
			2222	1414	380	419	9		

- Molecule 83 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Am	116	Total	C	N	O	S	0	0
			930	577	185	160	8		

- Molecule 84 is a protein called Aurora kinase A interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	An	72	Total	C	N	O	S	0	0
			639	407	139	92	1		

- Molecule 85 is a protein called Pentatricopeptide repeat domain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Ao	572	Total	C	N	O	S	0	0
			4526	2898	770	834	24		

- Molecule 86 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Ap	190	Total	C	N	O	S	0	0
			1564	991	292	273	8		

- Molecule 87 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	B9	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 88 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
88	BA	1544	32844	14750	5972	10578	1544	0	0

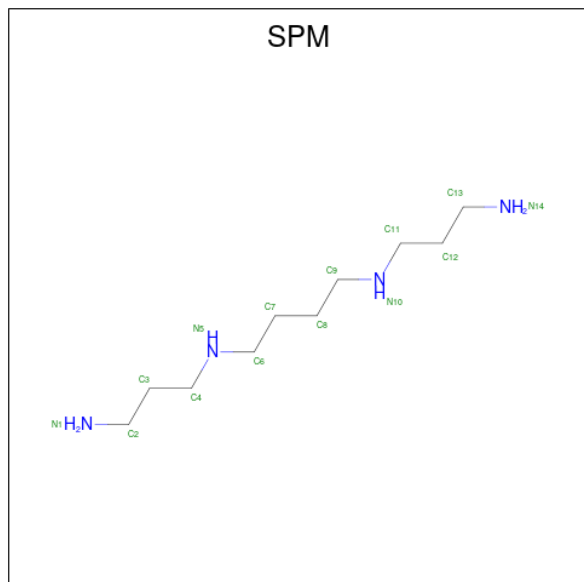
- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	B0	1	Total	Mg	0
			1	1	
89	BB	1	Total	Mg	0
			1	1	
89	BD	3	Total	Mg	0
			3	3	
89	BE	1	Total	Mg	0
			1	1	
89	BP	3	Total	Mg	0
			3	3	
89	BR	1	Total	Mg	0
			1	1	
89	B3	2	Total	Mg	0
			2	2	
89	Be	1	Total	Mg	0
			1	1	
89	Bl	1	Total	Mg	0
			1	1	
89	Bt	2	Total	Mg	0
			2	2	
89	AA	104	Total	Mg	0
			104	104	
89	AB	1	Total	Mg	0
			1	1	
89	AL	2	Total	Mg	0
			2	2	
89	Ag	1	Total	Mg	0
			1	1	
89	Am	1	Total	Mg	0
			1	1	
89	An	1	Total	Mg	0
			1	1	
89	BA	197	Total	Mg	0
			197	197	

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

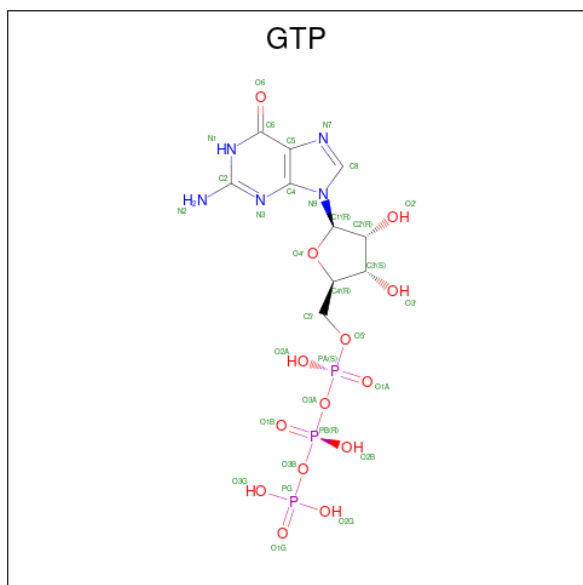
Mol	Chain	Residues	Atoms		AltConf
90	Bx	1	Total	Zn	0
			1	1	
90	B5	1	Total	Zn	0
			1	1	
90	AR	1	Total	Zn	0
			1	1	
90	Ac	1	Total	Zn	0
			1	1	
90	Ap	1	Total	Zn	0
			1	1	
90	B9	1	Total	Zn	0
			1	1	

- Molecule 91 is SPERMINE (three-letter code: SPM) (formula:  $C_{10}H_{26}N_4$ ).



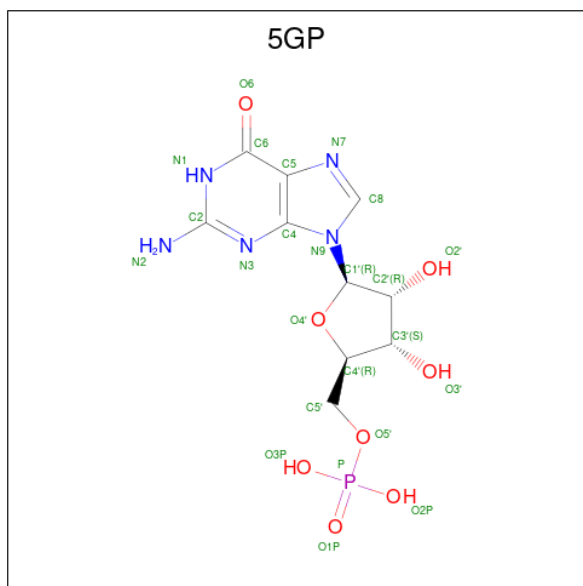
Mol	Chain	Residues	Atoms			AltConf
91	AA	1	Total	C	N	0
			14	10	4	
91	BA	1	Total	C	N	0
			28	20	8	
91	BA	1	Total	C	N	0
			28	20	8	

- Molecule 92 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
92	Ag	1	32	10	5	14	3	0

- Molecule 93 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula:  $C_{10}H_{14}N_5O_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
93	BA	1	48	20	10	16	2	0
93	BA	1	48	20	10	16	2	0

- Molecule 94 is water.

Mol	Chain	Residues	Atoms		AltConf
94	Ag	3	Total 3	O 3	0

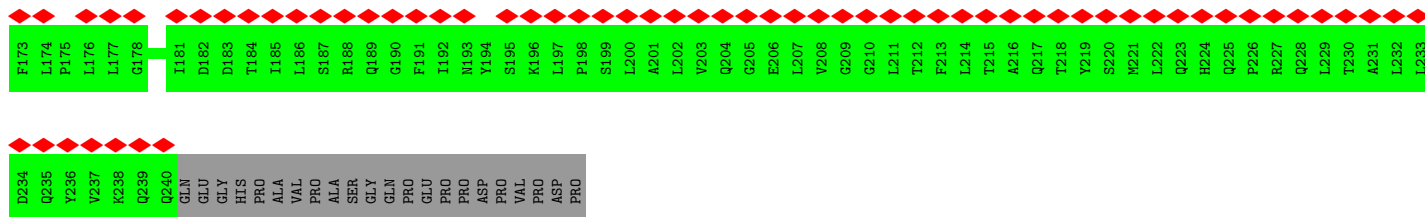




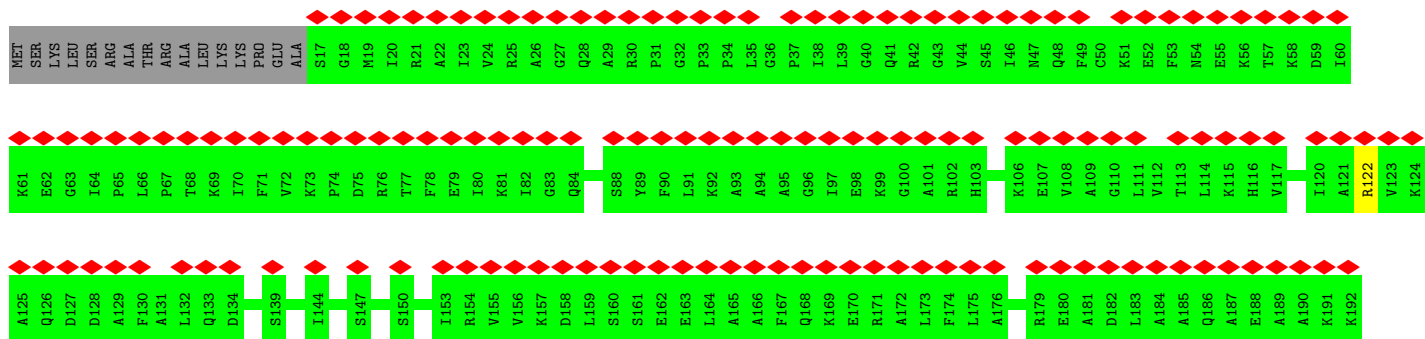
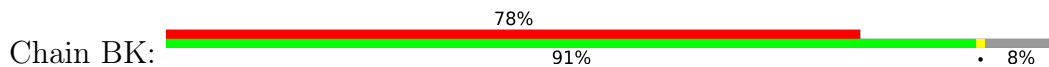




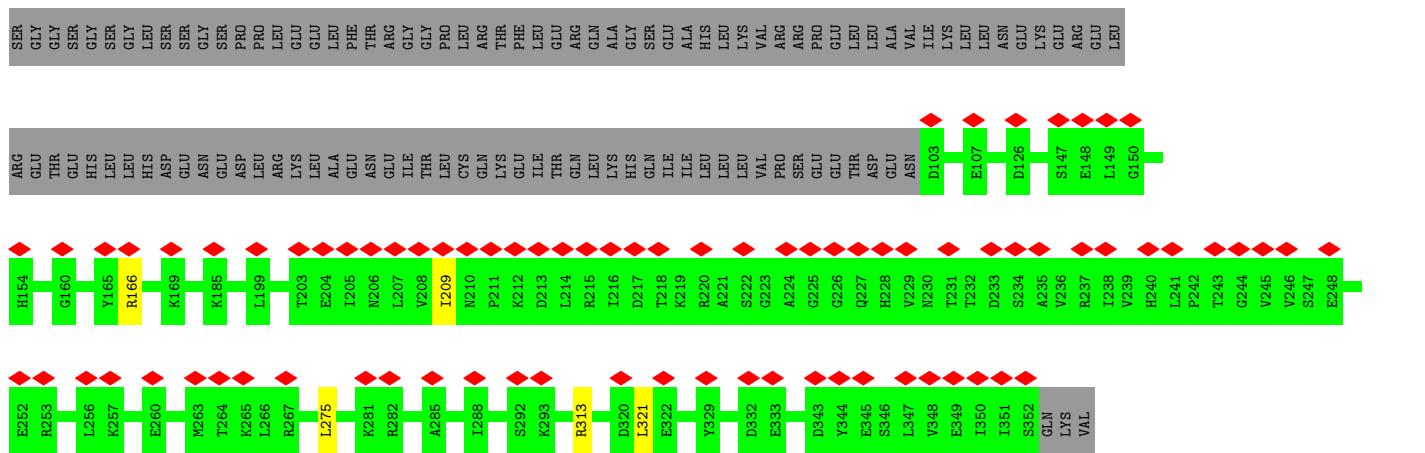




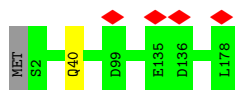
• Molecule 11: Mitochondrial ribosomal protein L11



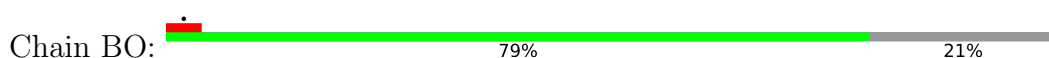
• Molecule 12: Peptide chain release factor 1-like, mitochondrial

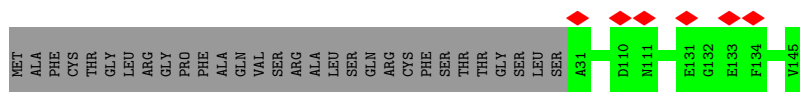


• Molecule 13: uL13m

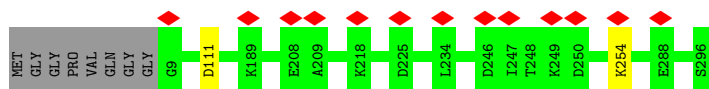


• Molecule 14: uL14m

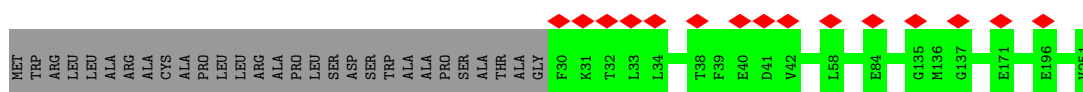
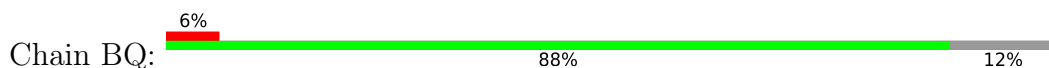




• Molecule 15: uL15m



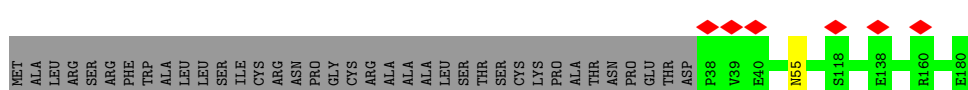
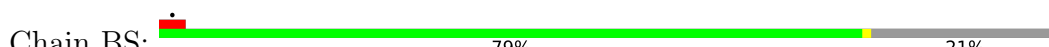
• Molecule 16: uL16m



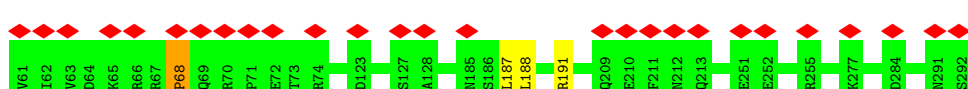
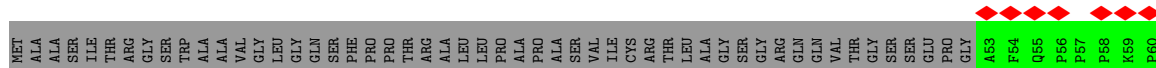
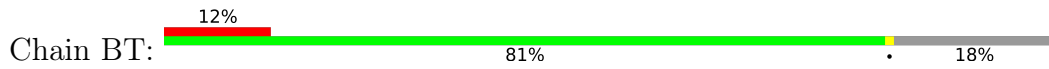
• Molecule 17: bL17m



• Molecule 18: Mitochondrial ribosomal protein L18

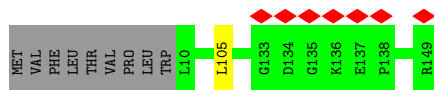


• Molecule 19: Mitochondrial ribosomal protein L19



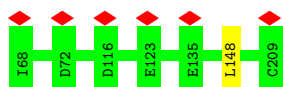
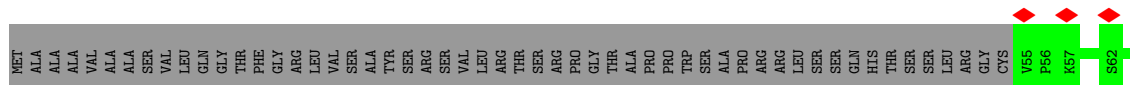
• Molecule 20: Mitochondrial ribosomal protein L20





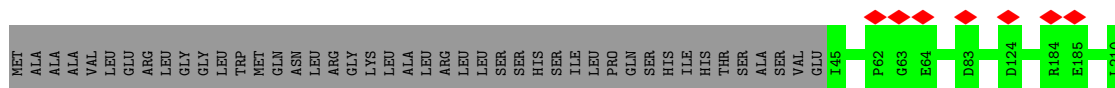
- Molecule 21: Mitochondrial ribosomal protein L21

Chain BV: 74% 26%



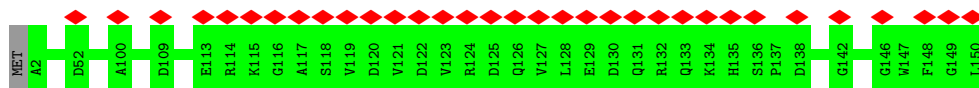
- Molecule 22: uL22m

Chain BW: 79% 21%



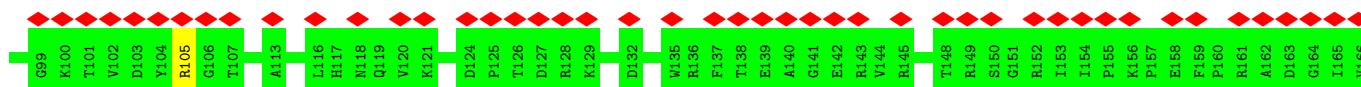
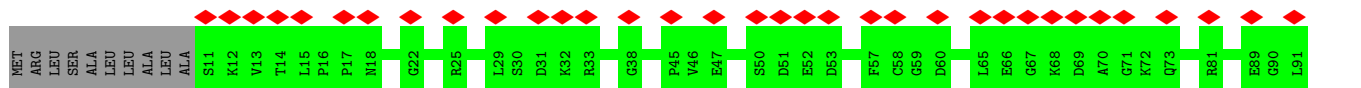
- Molecule 23: uL23m

Chain BX: 22% 99%



- Molecule 24: uL24m

Chain BY: 39% 95% 5%

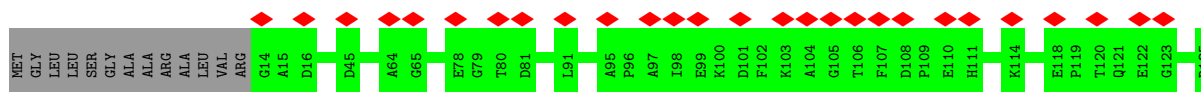


- Molecule 25: Mitochondrial ribosomal protein L37

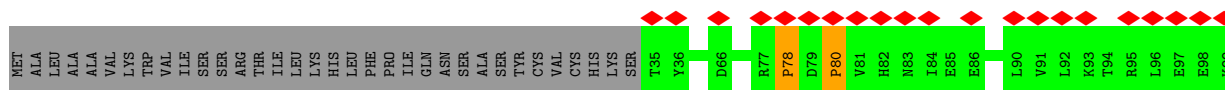
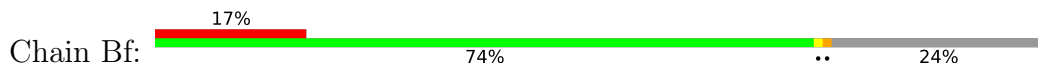
Chain Ba: 6% 92% 7%



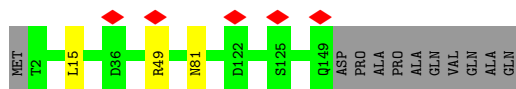




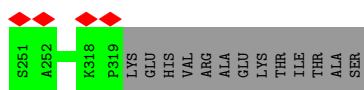
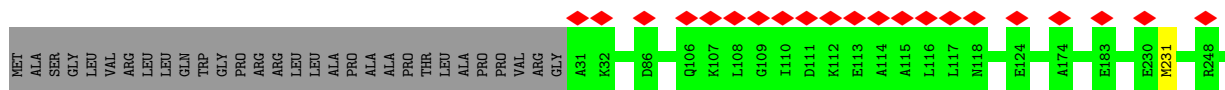
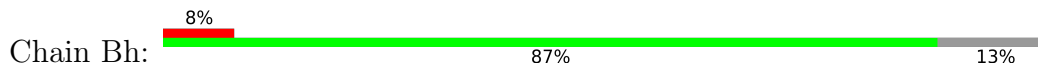
• Molecule 31: mL42



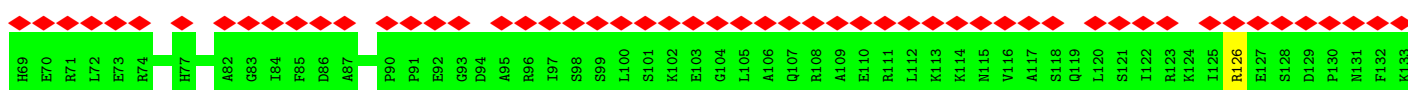
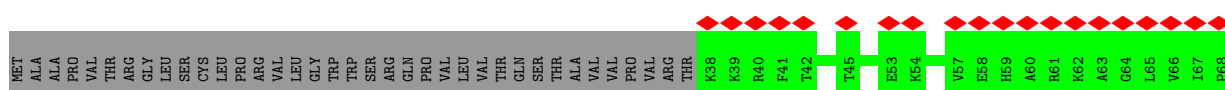
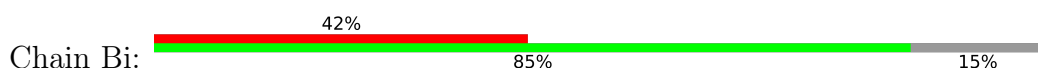
• Molecule 32: Mitochondrial ribosomal protein L43

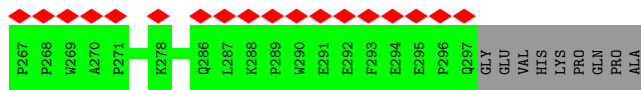


• Molecule 33: mL44

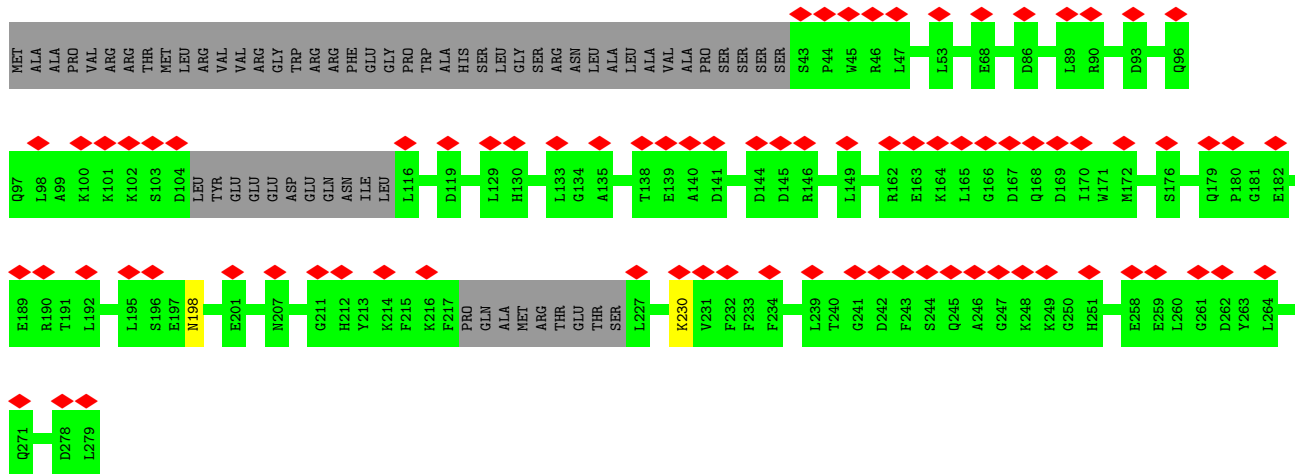
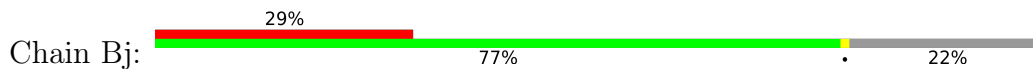


• Molecule 34: Mitochondrial ribosomal protein L45

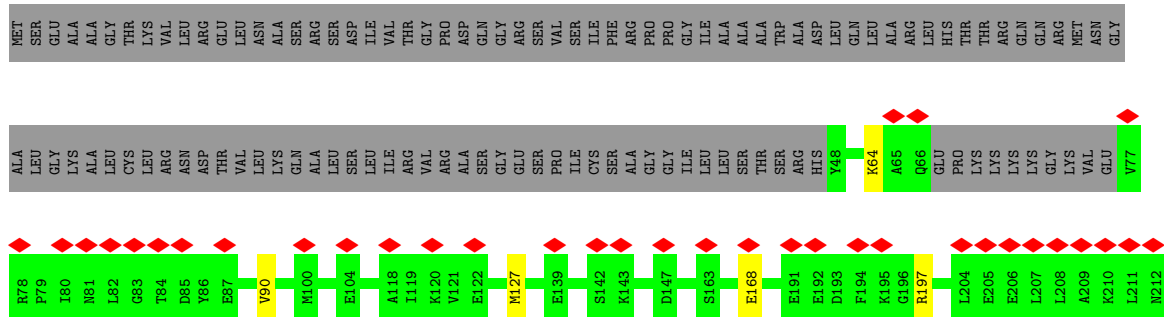




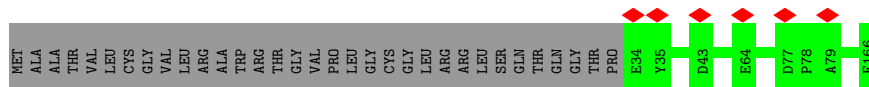
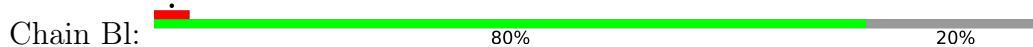
• Molecule 35: Mitochondrial ribosomal protein L46



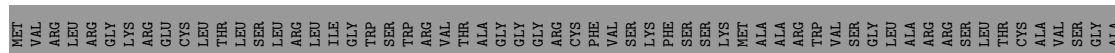
• Molecule 36: 39S ribosomal protein L48, mitochondrial

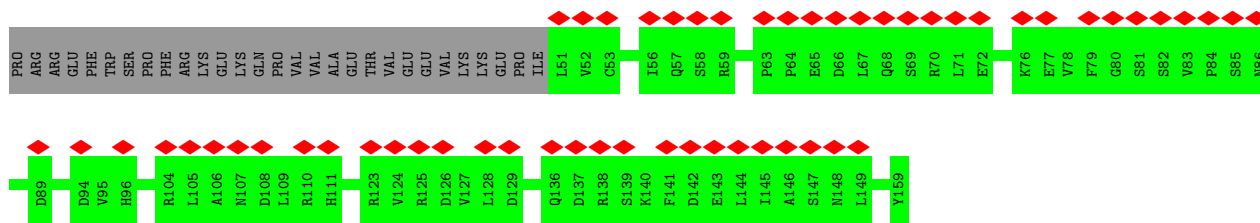


• Molecule 37: Mrpl34

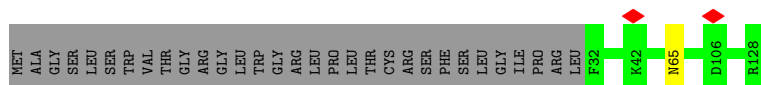
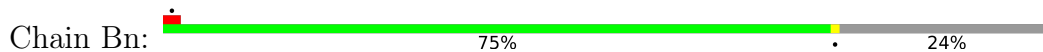


• Molecule 38: Mitochondrial ribosomal protein L50

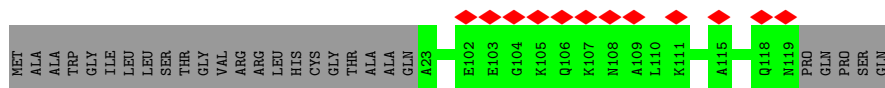
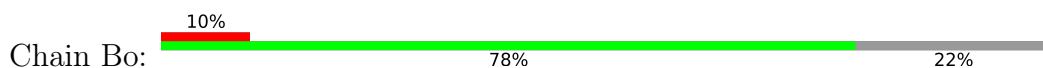




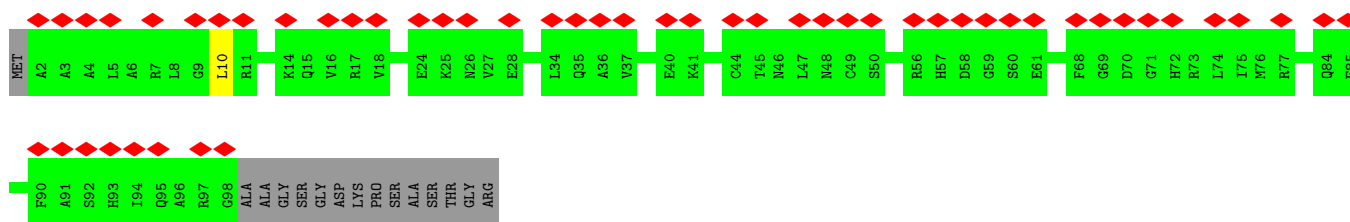
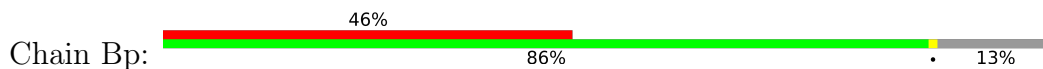
• Molecule 39: Mitochondrial ribosomal protein L51



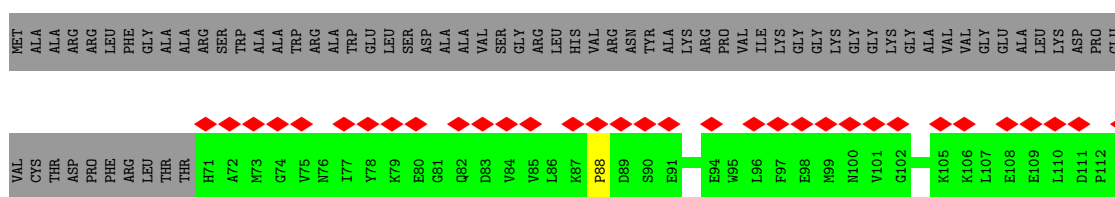
• Molecule 40: mL52



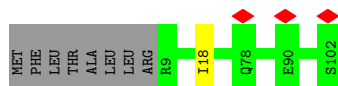
• Molecule 41: mL53



• Molecule 42: mL54

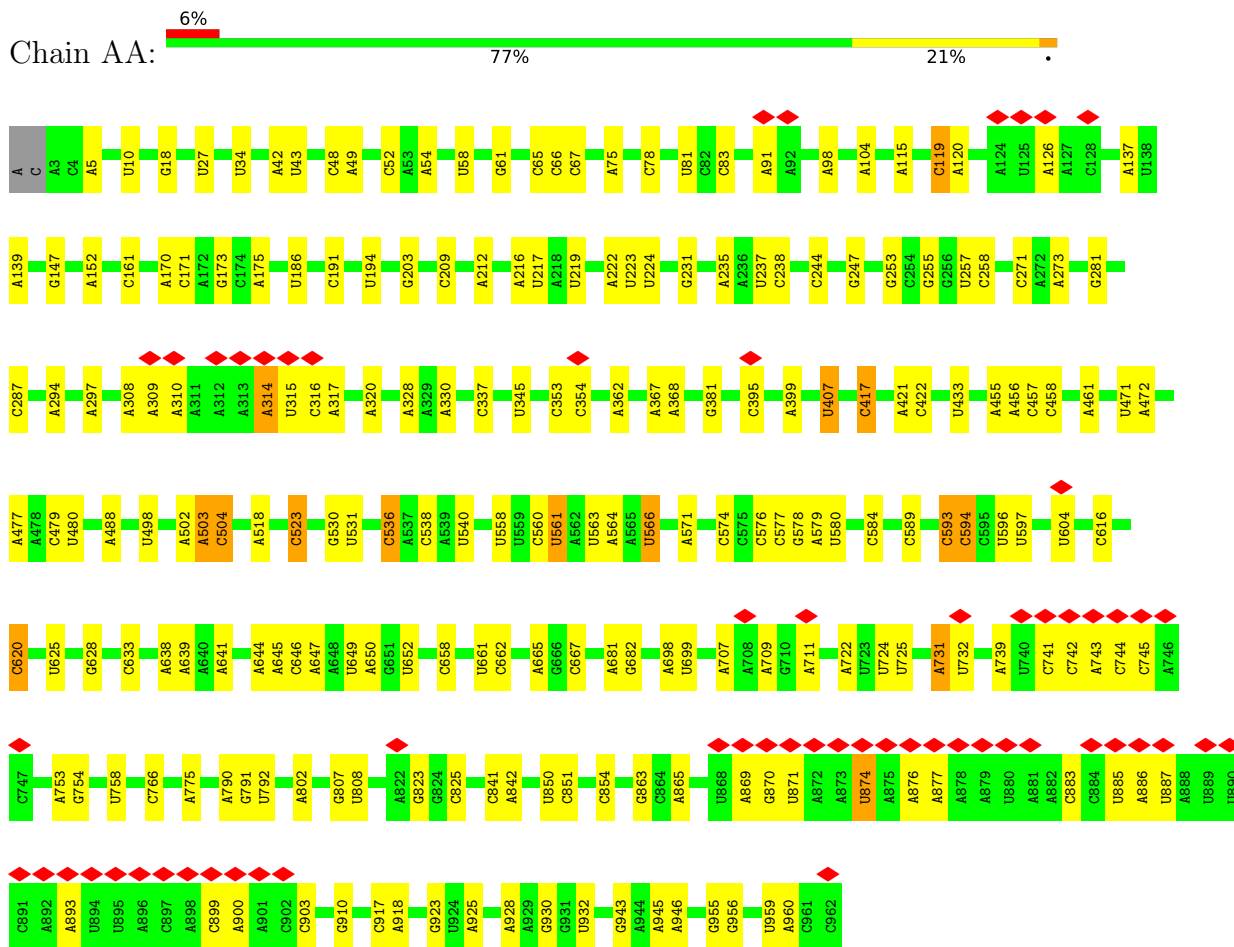


• Molecule 43: Mitochondrial ribosomal protein L57

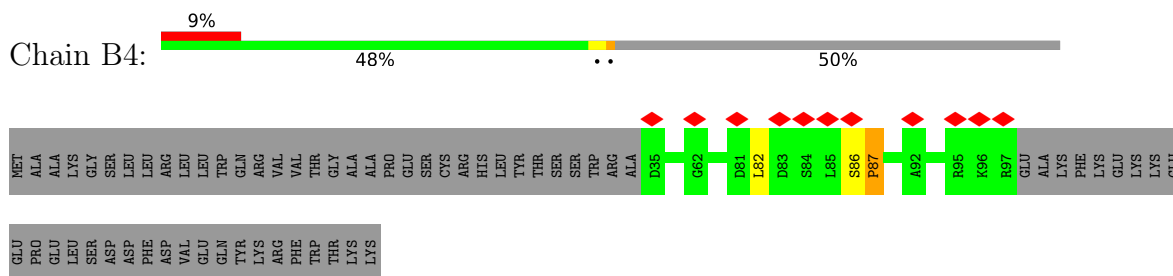




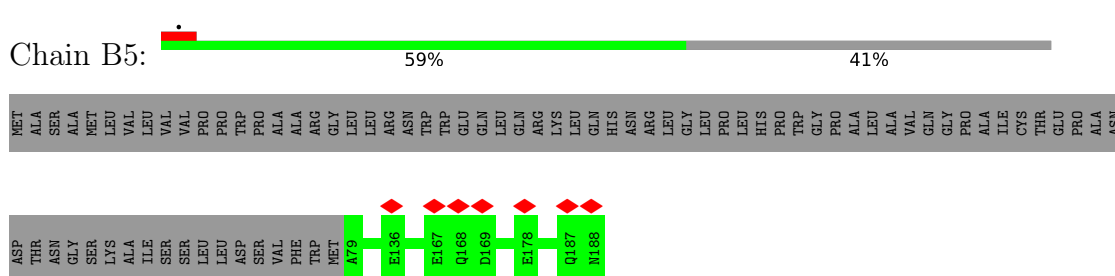
• Molecule 48: 12S rRNA



• Molecule 49: bL31m



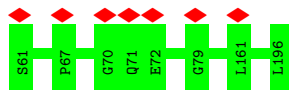
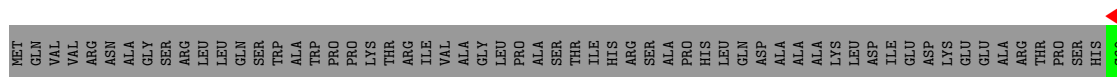
• Molecule 50: bL32m



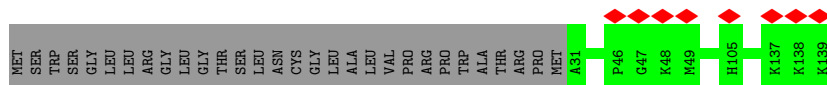
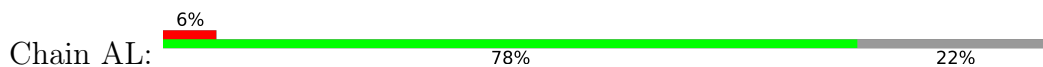
• Molecule 51: bL33m



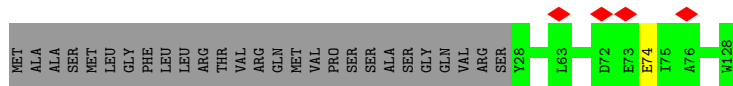
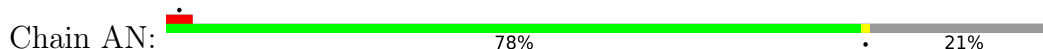




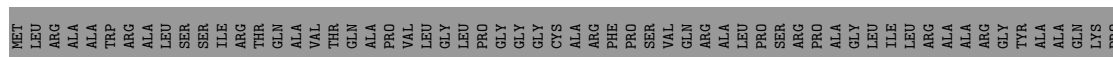
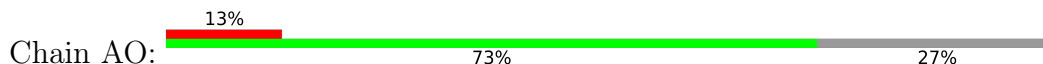
• Molecule 61: Mitochondrial ribosomal protein S12



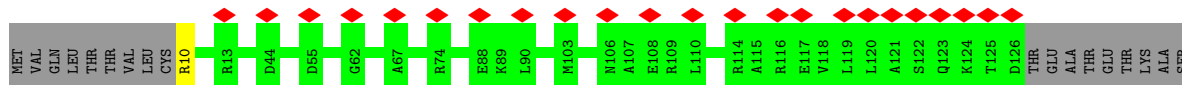
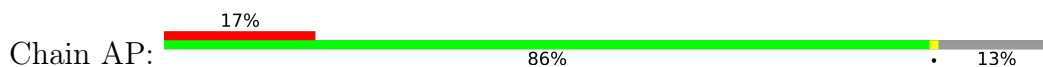
• Molecule 62: Mitochondrial ribosomal protein S14



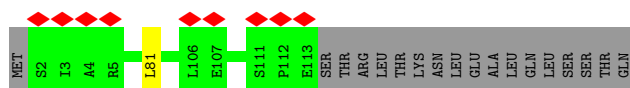
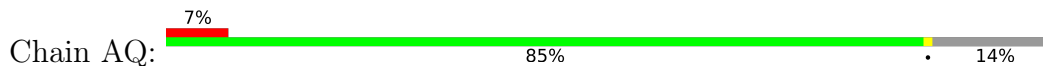
• Molecule 63: uS15m



• Molecule 64: 28S ribosomal protein S16, mitochondrial



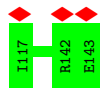
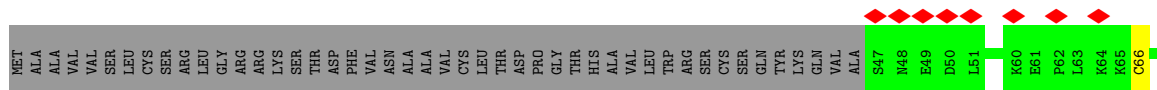
• Molecule 65: uS17m



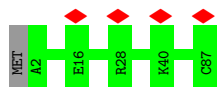
• Molecule 66: Mitochondrial ribosomal protein S18C



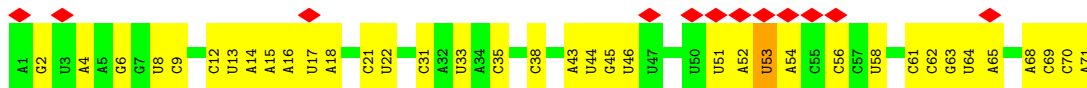




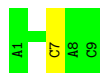
• Molecule 67: bS21m



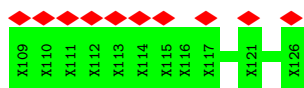
• Molecule 68: tRNAMet



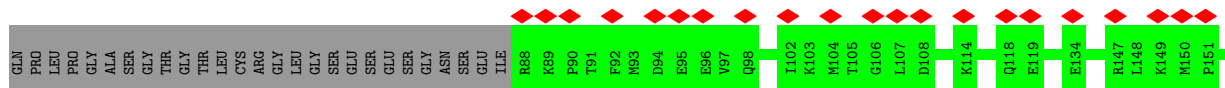
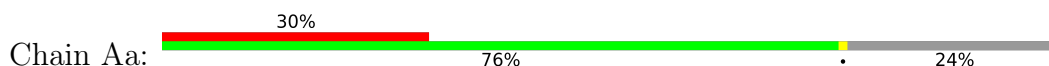
• Molecule 69: mRNA

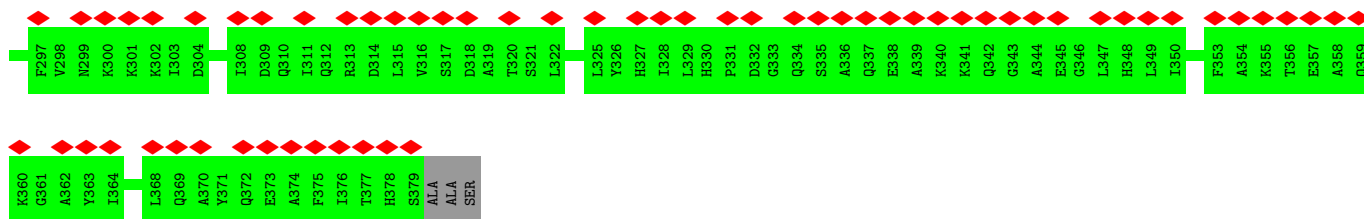


• Molecule 70: unknown

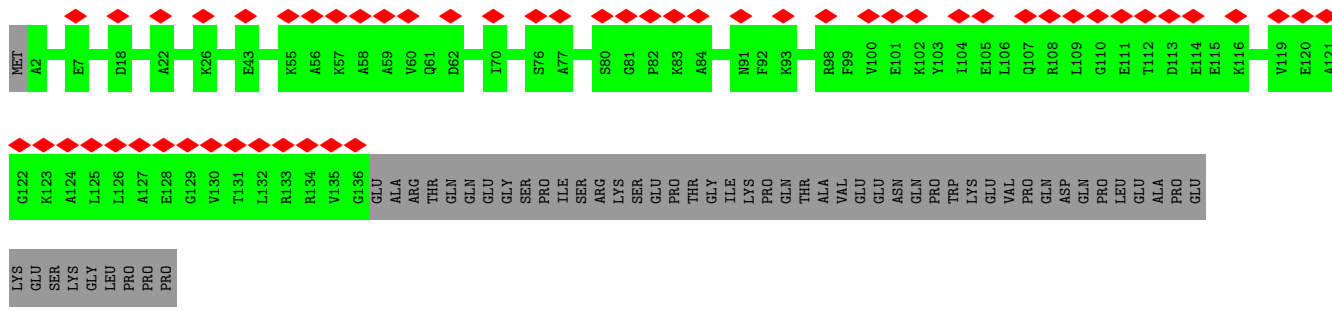
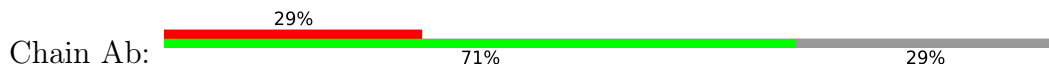


• Molecule 71: Mitochondrial ribosomal protein S22

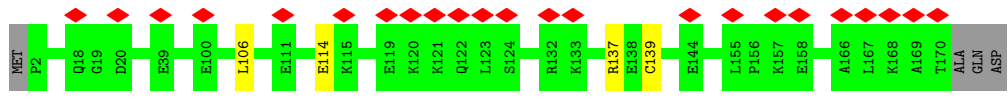




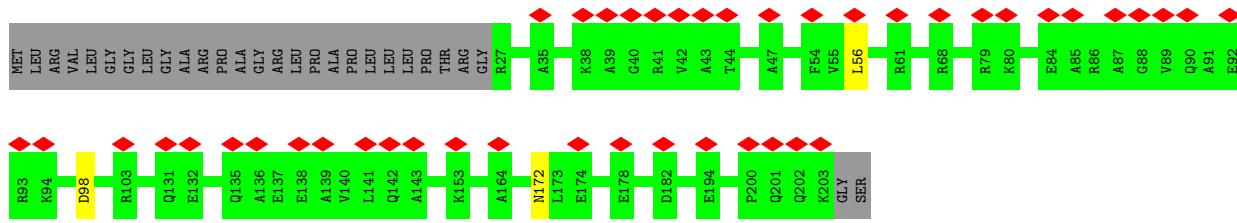
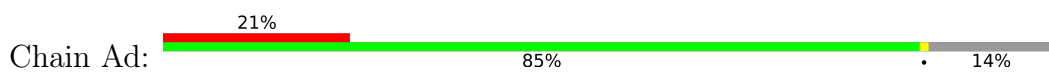
• Molecule 72: mS23



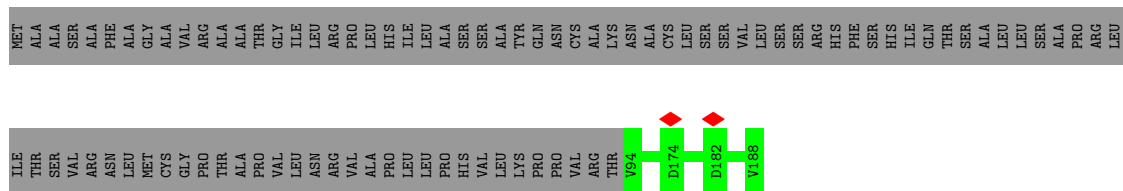
• Molecule 73: Mitochondrial ribosomal protein S25



• Molecule 74: Mitochondrial ribosomal protein S26



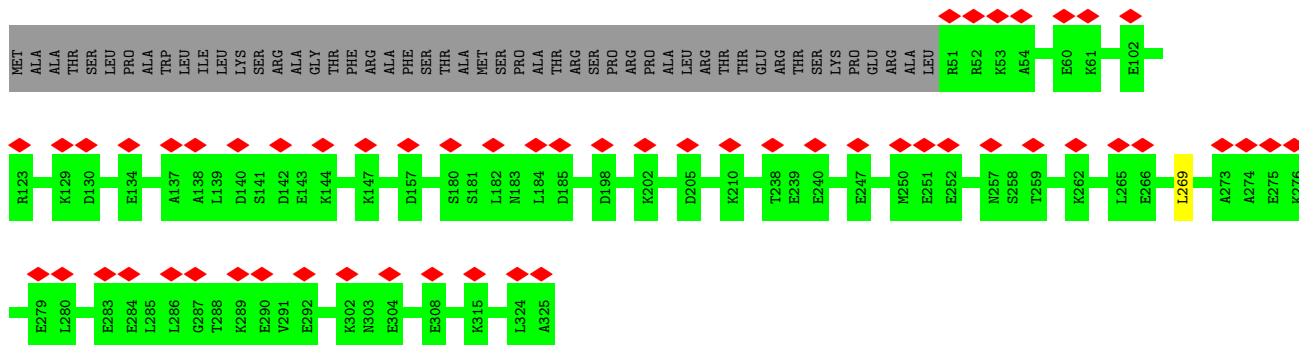
• Molecule 75: Mitochondrial ribosomal protein L35



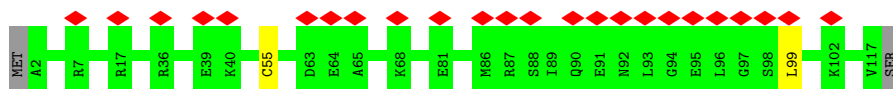
• Molecule 76: Mitochondrial ribosomal protein S27



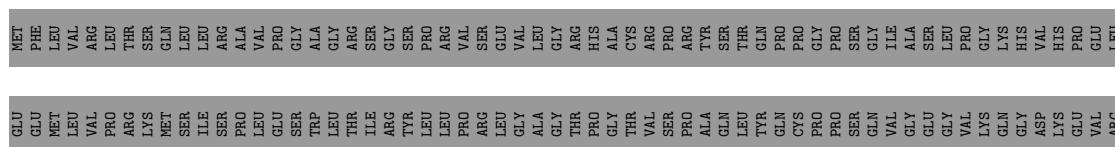




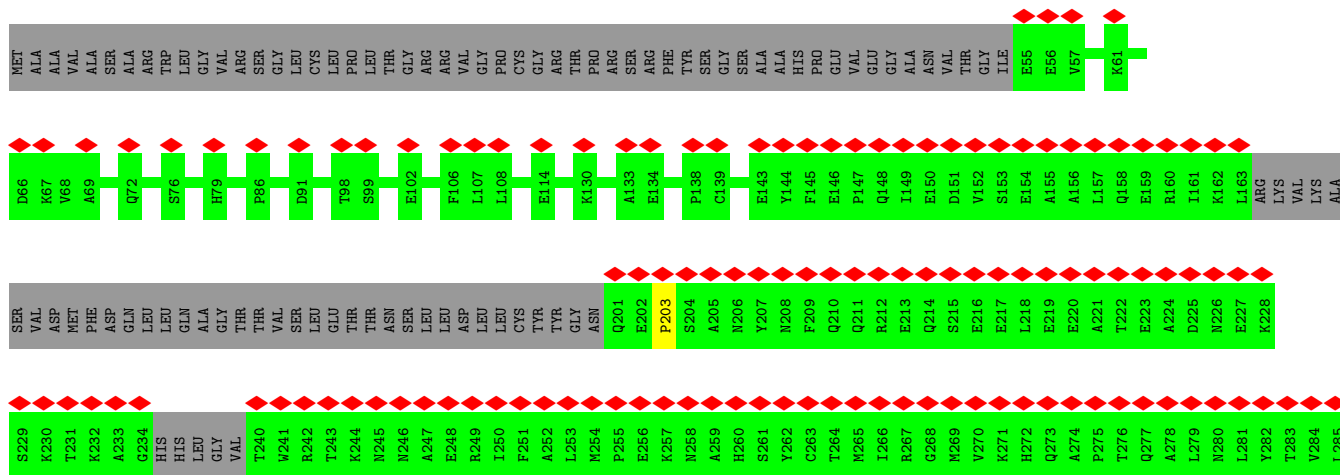
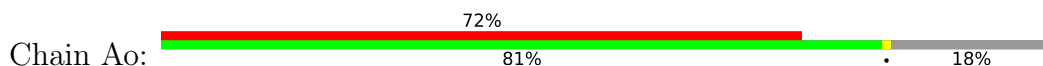
• Molecule 83: mS37

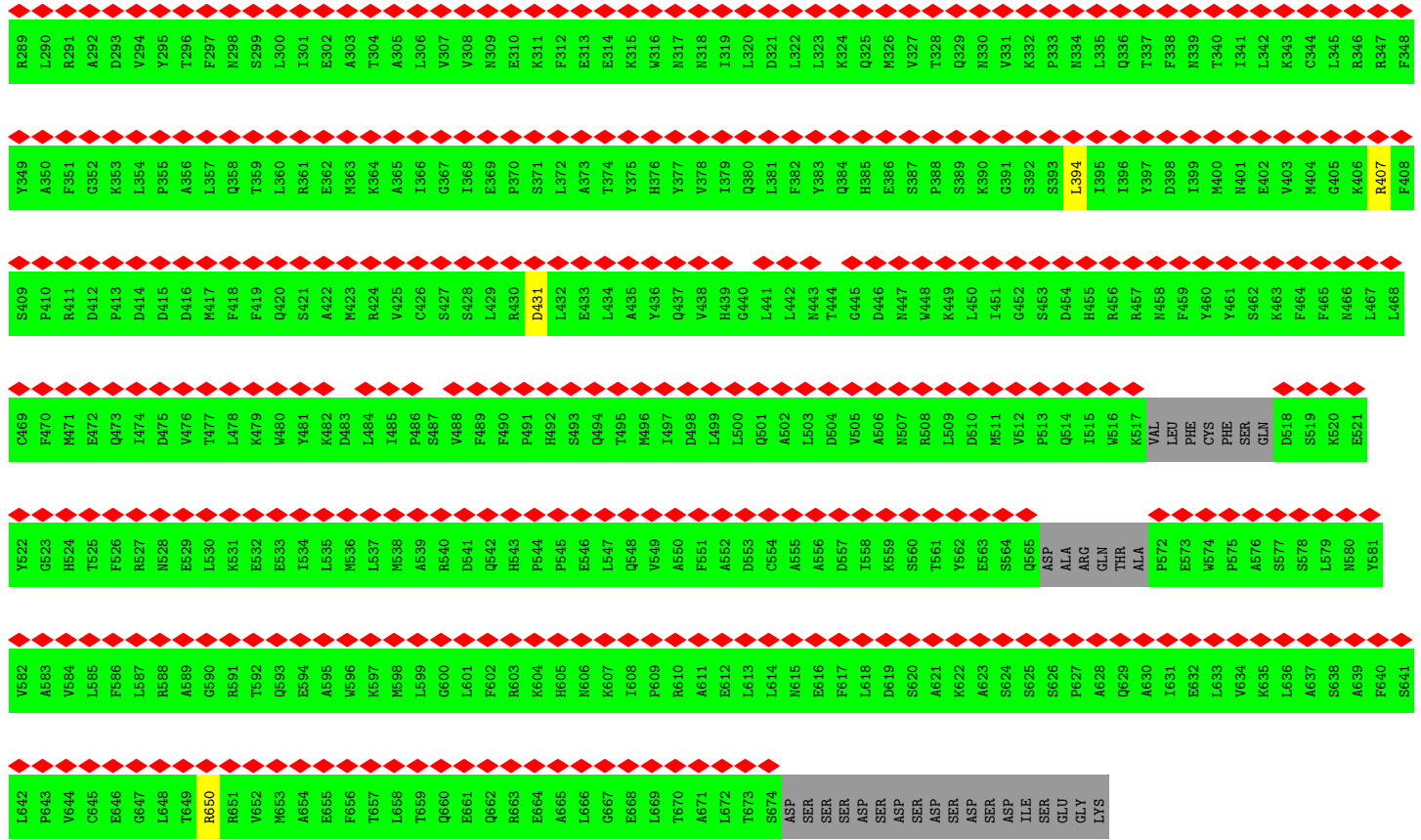


• Molecule 84: Aurora kinase A interacting protein 1

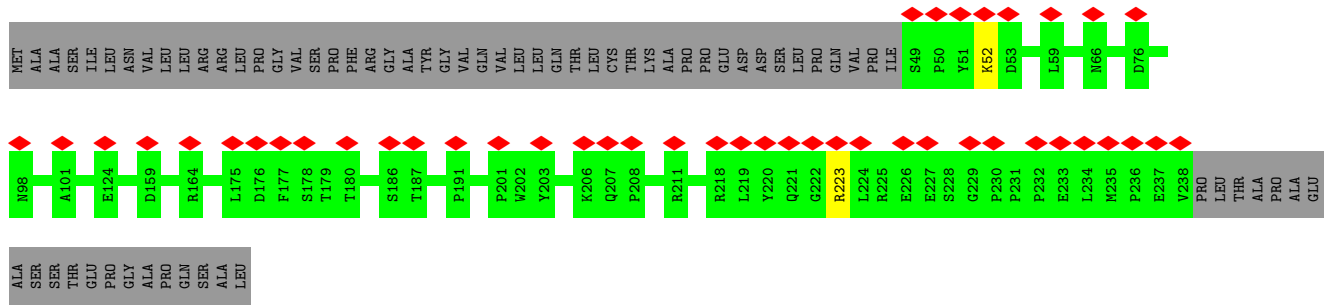
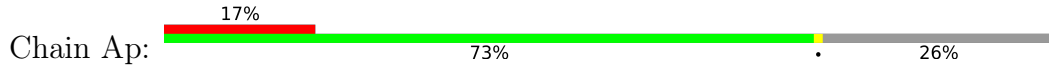


• Molecule 85: Pentatricopeptide repeat domain 3

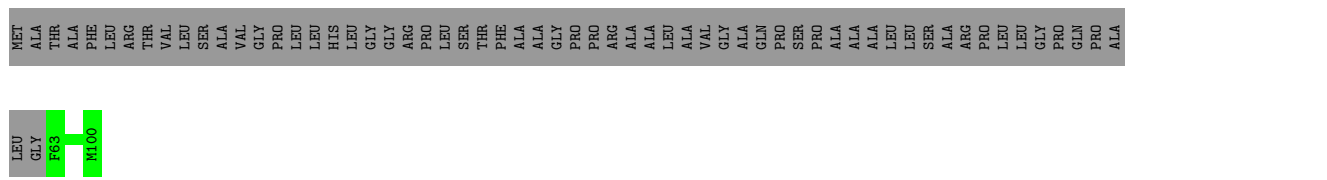




• Molecule 86: 28S ribosomal protein S18b, mitochondrial



• Molecule 87: Ribosomal protein



• Molecule 88: 16S rRNA







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47048	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.933	Depositor
Minimum map value	-0.616	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 5GP, GTP, ZN, SPM, MG

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	CL	0.24	0/319	0.48	0/435
1	DL	0.23	0/212	0.46	0/286
1	EL	0.23	0/221	0.51	0/297
1	FL	0.22	0/212	0.43	0/286
1	GL	0.22	0/212	0.36	0/286
1	HL	0.25	0/204	0.54	0/275
2	B0	0.30	0/880	0.57	0/1189
3	B1	0.26	0/2093	0.57	1/2835 (0.0%)
4	B2	0.31	0/1586	0.62	0/2123
5	BB	0.43	1/1595 (0.1%)	1.14	13/2475 (0.5%)
6	BD	0.27	0/1658	0.61	0/2234
7	BE	0.29	0/2255	0.59	0/3057
8	BF	0.27	0/1843	0.60	1/2505 (0.0%)
9	BI	0.25	0/819	0.63	0/1101
10	BJ	0.32	0/1742	0.70	1/2358 (0.0%)
11	BK	0.27	0/1323	0.59	0/1785
12	BL	0.31	0/2038	0.71	2/2744 (0.1%)
13	BN	0.27	0/1487	0.55	0/2017
14	BO	0.26	0/912	0.61	0/1231
15	BP	0.29	0/2368	0.65	1/3198 (0.0%)
16	BQ	0.28	0/1850	0.60	0/2491
17	BR	0.28	0/1262	0.67	1/1700 (0.1%)
18	BS	0.29	0/1197	0.68	0/1624
19	BT	0.30	0/2002	0.64	3/2708 (0.1%)
20	BU	0.28	0/1179	0.63	1/1578 (0.1%)
21	BV	0.30	0/1256	0.66	1/1706 (0.1%)
22	BW	0.28	0/1407	0.57	0/1891
23	BX	0.28	0/1211	0.61	0/1646
24	BY	0.27	0/1719	0.63	0/2329
25	Ba	0.29	0/3267	0.63	1/4455 (0.0%)
26	Bb	0.29	0/3047	0.63	0/4139
27	B3	0.25	0/993	0.53	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
28	Bc	0.29	0/2464	0.59	1/3330 (0.0%)
29	Bd	0.32	0/1183	0.67	1/1594 (0.1%)
30	Be	0.30	0/1000	0.53	0/1345
31	Bf	0.28	0/851	0.64	2/1159 (0.2%)
32	Bg	0.29	0/1191	0.68	1/1614 (0.1%)
33	Bh	0.29	0/2372	0.60	0/3211
34	Bi	0.27	0/2199	0.58	0/2980
35	Bj	0.32	0/1811	0.65	0/2436
36	Bk	0.35	0/1270	0.75	3/1714 (0.2%)
37	Bl	0.31	0/1135	0.61	0/1549
38	Bm	0.25	0/917	0.54	0/1248
39	Bn	0.29	0/860	0.59	0/1150
40	Bo	0.31	0/787	0.65	0/1056
41	Bp	0.29	0/752	0.67	1/1013 (0.1%)
42	Bq	0.32	0/558	0.66	1/756 (0.1%)
43	Bt	0.29	0/798	0.63	0/1073
44	Bu	0.28	0/1214	0.66	1/1630 (0.1%)
45	Bv	0.27	0/1157	0.59	0/1560
46	Bw	0.29	0/3206	0.58	0/4354
47	Bx	0.30	0/1364	0.63	0/1849
48	AA	0.30	0/22852	1.03	96/35580 (0.3%)
49	B4	0.26	0/486	0.80	2/660 (0.3%)
50	B5	0.30	0/917	0.63	0/1227
51	B6	0.29	0/430	0.68	0/570
52	B7	0.25	0/395	0.62	0/524
53	AB	0.30	0/1804	0.64	0/2445
54	AC	0.32	0/1105	0.69	1/1496 (0.1%)
55	AE	0.28	0/2785	0.66	1/3735 (0.0%)
56	AF	0.29	0/999	0.67	0/1347
57	AG	0.30	0/1731	0.62	0/2322
58	AI	0.29	0/2707	0.61	0/3636
59	AJ	0.31	0/1181	0.66	1/1597 (0.1%)
60	AK	0.27	0/1027	0.59	0/1389
61	AL	0.30	0/858	0.67	0/1152
62	AN	0.29	0/874	0.70	1/1171 (0.1%)
63	AO	0.29	0/1473	0.58	0/1970
64	AP	0.29	0/954	0.65	0/1284
65	AQ	0.27	0/894	0.62	1/1213 (0.1%)
66	AR	0.28	0/802	0.57	1/1079 (0.1%)
67	AU	0.28	0/745	0.60	0/993
68	AV	0.36	0/1673	1.28	22/2602 (0.8%)
69	AX	0.20	0/210	0.79	0/325
71	Aa	0.30	0/2428	0.63	2/3279 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
72	Ab	0.30	0/1126	0.65	0/1514
73	Ac	0.32	0/1399	0.67	3/1881 (0.2%)
74	Ad	0.31	0/1490	0.67	2/2005 (0.1%)
75	B8	0.25	0/853	0.59	0/1136
76	Ae	0.29	0/3171	0.66	2/4292 (0.0%)
77	Af	0.32	0/790	0.76	2/1064 (0.2%)
78	Ag	0.30	0/2945	0.63	2/3984 (0.1%)
79	Ah	0.30	0/1045	0.53	0/1409
80	Ai	0.29	0/841	0.70	1/1121 (0.1%)
81	Aj	0.29	0/1835	0.72	2/2484 (0.1%)
82	Ak	0.28	0/2268	0.60	1/3069 (0.0%)
83	Am	0.29	0/947	0.71	2/1268 (0.2%)
84	An	0.27	0/650	0.66	0/858
85	Ao	0.30	0/4626	0.60	3/6269 (0.0%)
86	Ap	0.29	0/1616	0.61	0/2195
87	B9	0.28	0/342	0.66	0/450
88	BA	0.32	0/36784	1.08	263/57270 (0.5%)
All	All	0.30	1/183516 (0.0%)	0.82	448/260811 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	BE	0	1
10	BJ	0	1
32	Bg	0	1
36	Bk	0	1
39	Bn	0	1
43	Bt	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	BB	1	G	OP3-P	-10.62	1.48	1.61

All (448) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	Af	95	PRO	CA-N-CD	-10.75	96.45	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AA	119	C	C2-N1-C1'	10.40	130.25	118.80
88	BA	1296	U	N1-C2-O2	9.87	129.71	122.80
88	BA	397	C	N1-C2-O2	9.73	124.74	118.90
88	BA	1296	U	N3-C2-O2	-9.72	115.39	122.20
80	Ai	36	LEU	CA-CB-CG	9.66	137.53	115.30
88	BA	890	C	N1-C2-O2	9.57	124.64	118.90
88	BA	848	C	C2-N1-C1'	9.47	129.21	118.80
88	BA	999	C	N1-C2-O2	9.43	124.56	118.90
88	BA	1527	U	C2-N1-C1'	9.39	128.97	117.70
48	AA	745	C	N1-C2-O2	9.35	124.51	118.90
88	BA	1296	U	C2-N1-C1'	9.29	128.85	117.70
48	AA	745	C	C2-N1-C1'	8.89	128.58	118.80
88	BA	890	C	C2-N1-C1'	8.88	128.57	118.80
88	BA	397	C	C2-N1-C1'	8.83	128.51	118.80
48	AA	667	C	N1-C2-O2	8.73	124.14	118.90
88	BA	825	C	N1-C2-O2	8.71	124.13	118.90
88	BA	64	C	C2-N1-C1'	8.70	128.37	118.80
17	BR	77	ASP	CB-CG-OD1	8.69	126.12	118.30
88	BA	1379	C	N1-C2-O2	8.61	124.06	118.90
88	BA	502	U	N3-C2-O2	-8.56	116.21	122.20
88	BA	502	U	N1-C2-O2	8.52	128.77	122.80
88	BA	1288	U	N3-C2-O2	-8.52	116.24	122.20
88	BA	826	C	N3-C2-O2	-8.49	115.95	121.90
88	BA	1428	U	C2-N1-C1'	8.48	127.88	117.70
88	BA	704	U	N3-C2-O2	-8.46	116.28	122.20
88	BA	825	C	C2-N1-C1'	8.40	128.04	118.80
88	BA	394	C	C2-N1-C1'	8.39	128.03	118.80
88	BA	704	U	N1-C2-O2	8.37	128.66	122.80
88	BA	1227	U	N3-C2-O2	-8.35	116.35	122.20
88	BA	1527	U	N1-C2-O2	8.22	128.56	122.80
88	BA	383	C	N1-C2-O2	8.20	123.82	118.90
88	BA	64	C	N1-C2-O2	8.19	123.81	118.90
88	BA	1288	U	N1-C2-O2	8.12	128.49	122.80
88	BA	720	C	N1-C2-O2	8.03	123.72	118.90
88	BA	397	C	N3-C2-O2	-8.01	116.29	121.90
88	BA	549	C	N1-C2-O2	7.98	123.69	118.90
48	AA	67	C	N1-C2-O2	7.97	123.69	118.90
88	BA	890	C	N3-C2-O2	-7.96	116.33	121.90
68	AV	62	C	N1-C2-O2	7.93	123.66	118.90
88	BA	1413	C	C2-N1-C1'	7.93	127.52	118.80
88	BA	1058	C	N1-C2-O2	7.92	123.65	118.90
19	BT	187	LEU	CA-CB-CG	7.88	133.42	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	BA	1227	U	N1-C2-O2	7.85	128.29	122.80
88	BA	704	U	C2-N1-C1'	7.81	127.07	117.70
48	AA	850	U	N1-C2-O2	7.79	128.25	122.80
48	AA	594	C	C2-N1-C1'	7.77	127.34	118.80
48	AA	119	C	N1-C2-O2	7.76	123.56	118.90
88	BA	999	C	N3-C2-O2	-7.75	116.48	121.90
88	BA	848	C	N1-C2-O2	7.72	123.53	118.90
88	BA	826	C	N1-C2-O2	7.70	123.52	118.90
88	BA	999	C	C6-N1-C2	-7.65	117.24	120.30
88	BA	549	C	C2-N1-C1'	7.64	127.21	118.80
88	BA	61	U	N3-C2-O2	-7.61	116.88	122.20
88	BA	60	U	C2-N1-C1'	7.60	126.83	117.70
88	BA	170	U	C2-N1-C1'	7.57	126.79	117.70
5	BB	13	U	C2-N1-C1'	7.55	126.76	117.70
88	BA	170	U	N1-C2-O2	7.55	128.09	122.80
88	BA	170	U	N3-C2-O2	-7.54	116.92	122.20
88	BA	1527	U	N3-C2-O2	-7.52	116.93	122.20
88	BA	1288	U	C2-N1-C1'	7.52	126.72	117.70
88	BA	847	U	C2-N1-C1'	7.51	126.71	117.70
48	AA	745	C	N3-C2-O2	-7.48	116.67	121.90
71	Aa	162	ASP	CB-CG-OD1	7.47	125.03	118.30
41	Bp	10	LEU	CA-CB-CG	7.47	132.48	115.30
5	BB	52	C	N1-C2-O2	7.42	123.35	118.90
88	BA	546	C	C2-N1-C1'	7.38	126.92	118.80
68	AV	62	C	C2-N1-C1'	7.31	126.84	118.80
88	BA	697	C	C2-N1-C1'	7.30	126.83	118.80
48	AA	523	C	C2-N1-C1'	7.27	126.80	118.80
88	BA	60	U	N1-C2-O2	7.26	127.88	122.80
88	BA	259	C	C2-N1-C1'	7.24	126.76	118.80
48	AA	850	U	N3-C2-O2	-7.24	117.14	122.20
32	Bg	15	LEU	CA-CB-CG	7.23	131.93	115.30
88	BA	502	U	C2-N1-C1'	7.20	126.34	117.70
48	AA	119	C	C6-N1-C1'	-7.15	112.22	120.80
42	Bq	88	PRO	CA-N-CD	-7.15	101.49	111.50
5	BB	13	U	N3-C2-O2	-7.14	117.20	122.20
88	BA	720	C	C2-N1-C1'	7.12	126.63	118.80
88	BA	911	C	N1-C2-O2	7.09	123.16	118.90
88	BA	64	C	N3-C2-O2	-7.08	116.94	121.90
68	AV	31	C	C2-N1-C1'	7.08	126.59	118.80
48	AA	744	C	C2-N1-C1'	7.07	126.57	118.80
68	AV	22	U	N3-C2-O2	-7.05	117.26	122.20
88	BA	1227	U	C2-N1-C1'	7.05	126.16	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	BA	1536	U	N1-C2-O2	7.03	127.72	122.80
88	BA	1058	C	C6-N1-C2	-7.02	117.49	120.30
88	BA	1413	C	N1-C2-O2	7.02	123.11	118.90
88	BA	1536	U	C2-N1-C1'	7.00	126.10	117.70
88	BA	104	C	C2-N1-C1'	6.99	126.48	118.80
88	BA	296	C	N1-C2-O2	6.97	123.08	118.90
88	BA	1459	U	N1-C2-O2	6.96	127.67	122.80
5	BB	13	U	N1-C2-O2	6.96	127.67	122.80
48	AA	119	C	C6-N1-C2	-6.96	117.52	120.30
88	BA	825	C	N3-C2-O2	-6.95	117.03	121.90
48	AA	566	U	N3-C2-O2	-6.95	117.33	122.20
88	BA	1379	C	N3-C2-O2	-6.93	117.05	121.90
48	AA	480	U	C2-N1-C1'	6.92	126.00	117.70
88	BA	1058	C	N3-C2-O2	-6.91	117.06	121.90
88	BA	61	U	N1-C2-O2	6.89	127.62	122.80
36	Bk	127	MET	CB-CG-SD	6.87	133.00	112.40
48	AA	593	C	C2-N1-C1'	6.85	126.34	118.80
48	AA	667	C	N3-C2-O2	-6.85	117.10	121.90
88	BA	1297	U	N1-C2-O2	6.85	127.60	122.80
48	AA	480	U	N1-C2-O2	6.85	127.59	122.80
3	B1	24	LEU	CA-CB-CG	6.83	131.01	115.30
5	BB	6	U	N1-C2-O2	6.83	127.58	122.80
44	Bu	167	PRO	N-CA-CB	6.80	111.46	103.30
48	AA	480	U	N3-C2-O2	-6.79	117.45	122.20
48	AA	850	U	C2-N1-C1'	6.78	125.84	117.70
88	BA	890	C	C6-N1-C2	-6.77	117.59	120.30
48	AA	667	C	C2-N1-C1'	6.76	126.24	118.80
88	BA	720	C	N3-C2-O2	-6.76	117.17	121.90
88	BA	383	C	N3-C2-O2	-6.76	117.17	121.90
5	BB	6	U	N3-C2-O2	-6.76	117.47	122.20
81	Aj	138	ASP	CB-CG-OD2	6.75	124.38	118.30
54	AC	114	ALA	C-N-CA	6.72	138.51	121.70
68	AV	22	U	N1-C2-O2	6.72	127.50	122.80
88	BA	821	C	C2-N1-C1'	6.72	126.19	118.80
31	Bf	80	PRO	N-CA-CB	6.72	111.36	103.30
48	AA	662	C	N1-C2-O2	6.71	122.93	118.90
88	BA	1532	U	N3-C2-O2	-6.69	117.52	122.20
10	BJ	144	LEU	CA-CB-CG	6.67	130.65	115.30
88	BA	1297	U	C2-N1-C1'	6.67	125.71	117.70
88	BA	1428	U	N1-C2-O2	6.65	127.46	122.80
88	BA	394	C	C6-N1-C2	-6.65	117.64	120.30
48	AA	48	C	N1-C2-O2	6.65	122.89	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	BA	60	U	N3-C2-O2	-6.62	117.56	122.20
48	AA	725	U	N3-C2-O2	-6.62	117.56	122.20
88	BA	1428	U	N3-C2-O2	-6.61	117.57	122.20
88	BA	848	C	C6-N1-C1'	-6.61	112.87	120.80
5	BB	6	U	C2-N1-C1'	6.61	125.63	117.70
88	BA	285	C	C2-N1-C1'	6.61	126.07	118.80
77	Af	173	LEU	CA-CB-CG	6.59	130.45	115.30
88	BA	1525	C	C6-N1-C2	-6.56	117.67	120.30
55	AE	131	ILE	CG1-CB-CG2	-6.54	97.01	111.40
88	BA	48	U	P-O3'-C3'	6.54	127.55	119.70
78	Ag	337	ASP	CB-CG-OD1	6.54	124.19	118.30
88	BA	1459	U	N3-C2-O2	-6.54	117.62	122.20
88	BA	1543	U	N3-C2-O2	-6.51	117.64	122.20
88	BA	1297	U	N3-C2-O2	-6.51	117.64	122.20
68	AV	35	C	N1-C2-O2	6.50	122.80	118.90
31	Bf	78	PRO	N-CA-CB	6.50	111.10	103.30
88	BA	383	C	C6-N1-C2	-6.47	117.71	120.30
88	BA	1451	U	C2-N1-C1'	6.46	125.45	117.70
88	BA	912	U	C2-N1-C1'	6.46	125.45	117.70
88	BA	999	C	C2-N1-C1'	6.44	125.88	118.80
88	BA	860	G	C4-N9-C1'	6.44	134.87	126.50
48	AA	67	C	N3-C2-O2	-6.43	117.40	121.90
88	BA	383	C	C2-N1-C1'	6.43	125.87	118.80
88	BA	1129	C	N1-C2-O2	6.42	122.75	118.90
88	BA	1379	C	C2-N1-C1'	6.41	125.85	118.80
88	BA	1532	U	N1-C2-O2	6.40	127.28	122.80
48	AA	561	U	C2-N1-C1'	6.40	125.38	117.70
48	AA	498	U	N1-C2-O2	6.39	127.28	122.80
88	BA	704	U	C5-C6-N1	6.38	125.89	122.70
88	BA	1234	U	N1-C2-O2	6.38	127.27	122.80
88	BA	1413	C	C6-N1-C2	-6.38	117.75	120.30
5	BB	52	C	C2-N1-C1'	6.37	125.81	118.80
88	BA	394	C	C5-C6-N1	6.37	124.18	121.00
88	BA	397	C	C6-N1-C2	-6.35	117.76	120.30
88	BA	1570	C	N1-C2-O2	6.35	122.71	118.90
88	BA	1058	C	C2-N1-C1'	6.35	125.78	118.80
76	Ae	342	PRO	N-CA-CB	6.34	110.91	103.30
48	AA	523	C	C6-N1-C2	-6.34	117.76	120.30
88	BA	549	C	N3-C2-O2	-6.33	117.47	121.90
88	BA	1536	U	N3-C2-O2	-6.33	117.77	122.20
88	BA	1296	U	C5-C6-N1	6.33	125.86	122.70
68	AV	62	C	N3-C2-O2	-6.33	117.47	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AA	417	C	N1-C2-O2	6.32	122.69	118.90
88	BA	404	C	N1-C2-O2	6.32	122.69	118.90
88	BA	238	C	C2-N1-C1'	6.32	125.75	118.80
48	AA	745	C	C6-N1-C2	-6.32	117.77	120.30
88	BA	912	U	N3-C2-O2	-6.31	117.78	122.20
48	AA	422	C	N1-C2-O2	6.31	122.68	118.90
88	BA	104	C	N1-C2-O2	6.31	122.69	118.90
48	AA	854	C	N1-C2-O2	6.30	122.68	118.90
15	BP	111	ASP	CB-CG-OD2	6.30	123.97	118.30
88	BA	848	C	C6-N1-C2	-6.27	117.79	120.30
88	BA	64	C	C6-N1-C2	-6.27	117.79	120.30
88	BA	847	U	N1-C2-O2	6.27	127.19	122.80
48	AA	498	U	N3-C2-O2	-6.23	117.84	122.20
48	AA	744	C	N1-C2-O2	6.23	122.64	118.90
88	BA	848	C	C5-C6-N1	6.22	124.11	121.00
88	BA	1527	U	C6-N1-C1'	-6.18	112.55	121.20
83	Am	55	CYS	CA-CB-SG	6.16	125.09	114.00
88	BA	595	C	N1-C2-O2	6.16	122.59	118.90
48	AA	561	U	N1-C2-O2	6.15	127.11	122.80
88	BA	912	U	N1-C2-O2	6.15	127.11	122.80
88	BA	720	C	C6-N1-C2	-6.14	117.84	120.30
88	BA	614	U	N1-C2-O2	6.10	127.07	122.80
88	BA	1297	U	C5-C6-N1	6.09	125.75	122.70
88	BA	1379	C	C6-N1-C2	-6.09	117.86	120.30
48	AA	661	U	N1-C2-O2	6.09	127.06	122.80
88	BA	1235	C	N1-C2-O2	6.07	122.54	118.90
88	BA	826	C	C6-N1-C2	-6.05	117.88	120.30
88	BA	1234	U	N3-C2-O2	-6.05	117.97	122.20
88	BA	1413	C	C5-C6-N1	6.02	124.01	121.00
88	BA	786	U	C2-N1-C1'	6.02	124.92	117.70
48	AA	119	C	N3-C2-O2	-6.02	117.69	121.90
48	AA	594	C	C6-N1-C2	-6.01	117.89	120.30
88	BA	509	C	N1-C2-O2	6.01	122.51	118.90
48	AA	745	C	C6-N1-C1'	-6.01	113.59	120.80
88	BA	846	C	C2-N1-C1'	6.00	125.40	118.80
88	BA	697	C	C6-N1-C2	-6.00	117.90	120.30
88	BA	609	U	C2-N1-C1'	6.00	124.90	117.70
88	BA	786	U	N1-C2-O2	5.98	126.99	122.80
48	AA	662	C	N3-C2-O2	-5.98	117.72	121.90
88	BA	999	C	C5-C6-N1	5.96	123.98	121.00
48	AA	314	A	C2-N3-C4	5.96	113.58	110.60
88	BA	182	C	C2-N1-C1'	5.96	125.36	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	BA	1525	C	N1-C2-O2	5.96	122.48	118.90
88	BA	1525	C	N3-C2-O2	-5.96	117.73	121.90
88	BA	1296	U	C6-N1-C2	-5.96	117.43	121.00
48	AA	661	U	N3-C2-O2	-5.94	118.04	122.20
88	BA	697	C	N1-C2-O2	5.94	122.47	118.90
88	BA	259	C	C6-N1-C2	-5.94	117.92	120.30
88	BA	614	U	N3-C2-O2	-5.93	118.05	122.20
88	BA	821	C	C6-N1-C2	-5.93	117.93	120.30
88	BA	469	C	C2-N1-C1'	5.93	125.32	118.80
48	AA	874	U	N3-C2-O2	-5.92	118.05	122.20
48	AA	584	C	N1-C2-O2	5.92	122.45	118.90
48	AA	561	U	N3-C2-O2	-5.91	118.07	122.20
88	BA	12	C	C6-N1-C2	-5.90	117.94	120.30
88	BA	397	C	C6-N1-C1'	-5.89	113.73	120.80
88	BA	825	C	C6-N1-C1'	-5.89	113.73	120.80
88	BA	1212	U	C2-N1-C1'	5.89	124.76	117.70
68	AV	12	C	C2-N1-C1'	5.88	125.27	118.80
48	AA	871	U	N3-C2-O2	-5.87	118.09	122.20
88	BA	330	A	C2-N3-C4	5.87	113.53	110.60
48	AA	662	C	C6-N1-C2	-5.86	117.96	120.30
88	BA	1429	C	N1-C2-O2	5.84	122.41	118.90
48	AA	584	C	C6-N1-C2	-5.84	117.96	120.30
48	AA	874	U	N1-C2-O2	5.84	126.89	122.80
48	AA	667	C	C6-N1-C2	-5.84	117.97	120.30
88	BA	64	C	C6-N1-C1'	-5.83	113.80	120.80
88	BA	575	C	N1-C2-O2	5.83	122.40	118.90
36	Bk	168	GLU	CA-CB-CG	5.83	126.22	113.40
88	BA	889	C	N1-C2-O2	5.82	122.39	118.90
48	AA	119	C	C5-C6-N1	5.82	123.91	121.00
88	BA	410	U	N1-C2-O2	5.81	126.87	122.80
88	BA	704	U	C6-N1-C2	-5.81	117.51	121.00
88	BA	890	C	C6-N1-C1'	-5.81	113.83	120.80
71	Aa	220	PRO	CA-N-CD	-5.81	103.37	111.50
68	AV	38	C	C2-N1-C1'	5.80	125.18	118.80
88	BA	1212	U	N1-C2-O2	5.80	126.86	122.80
49	B4	87	PRO	N-CA-CB	5.79	110.25	103.30
88	BA	173	C	N1-C2-O2	5.79	122.38	118.90
88	BA	1453	U	C2-N1-C1'	5.79	124.64	117.70
88	BA	410	U	N3-C2-O2	-5.78	118.15	122.20
88	BA	981	U	C2-N1-C1'	5.78	124.64	117.70
48	AA	503	A	C4-N9-C1'	5.77	136.69	126.30
48	AA	504	C	N1-C2-O2	5.77	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	BA	182	C	N1-C2-O2	5.75	122.35	118.90
88	BA	285	C	N1-C2-O2	5.75	122.35	118.90
82	Ak	269	LEU	CA-CB-CG	5.75	128.53	115.30
88	BA	831	U	C2-N1-C1'	5.75	124.60	117.70
48	AA	536	C	C2-N1-C1'	5.75	125.12	118.80
74	Ad	56	LEU	CA-CB-CG	5.74	128.51	115.30
48	AA	48	C	C2-N1-C1'	5.74	125.11	118.80
48	AA	67	C	C2-N1-C1'	5.74	125.11	118.80
48	AA	620	C	C2-N1-C1'	5.74	125.12	118.80
36	Bk	168	GLU	N-CA-CB	5.74	120.93	110.60
48	AA	558	U	C2-N1-C1'	5.74	124.58	117.70
88	BA	238	C	N1-C2-O2	5.73	122.34	118.90
88	BA	614	U	C2-N1-C1'	5.73	124.57	117.70
73	Ac	106	LEU	CA-CB-CG	5.72	128.46	115.30
48	AA	871	U	N1-C2-O2	5.71	126.80	122.80
48	AA	725	U	N1-C2-O2	5.71	126.80	122.80
68	AV	62	C	C6-N1-C2	-5.71	118.02	120.30
48	AA	560	C	N1-C2-O2	5.71	122.32	118.90
88	BA	595	C	C2-N1-C1'	5.70	125.07	118.80
88	BA	1440	U	N3-C2-O2	-5.70	118.21	122.20
88	BA	296	C	N3-C2-O2	-5.70	117.91	121.90
88	BA	860	G	N3-C4-N9	5.70	129.42	126.00
88	BA	404	C	C6-N1-C2	-5.69	118.02	120.30
88	BA	1212	U	N3-C2-O2	-5.69	118.22	122.20
88	BA	12	C	C2-N1-C1'	5.68	125.05	118.80
88	BA	662	C	C2-N1-C1'	5.67	125.04	118.80
88	BA	911	C	N3-C2-O2	-5.65	117.95	121.90
28	Bc	37	LEU	CA-CB-CG	5.63	128.26	115.30
88	BA	423	U	N3-C2-O2	-5.63	118.26	122.20
88	BA	609	U	N1-C2-O2	5.63	126.74	122.80
48	AA	658	C	N1-C2-O2	5.63	122.28	118.90
48	AA	594	C	C5-C6-N1	5.63	123.81	121.00
88	BA	609	U	N3-C2-O2	-5.62	118.27	122.20
88	BA	847	U	C5-C6-N1	5.62	125.51	122.70
85	AO	203	PRO	N-CA-CB	5.60	110.02	103.30
88	BA	697	C	C5-C6-N1	5.60	123.80	121.00
88	BA	509	C	C2-N1-C1'	5.59	124.95	118.80
88	BA	1286	U	N3-C2-O2	-5.59	118.29	122.20
88	BA	405	C	C2-N1-C1'	5.58	124.94	118.80
48	AA	851	C	C6-N1-C2	-5.58	118.07	120.30
88	BA	660	C	C2-N1-C1'	5.58	124.94	118.80
88	BA	1469	C	N1-C2-O2	5.58	122.25	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	Ac	139	CYS	CA-CB-SG	5.57	124.03	114.00
48	AA	67	C	C6-N1-C2	-5.57	118.07	120.30
68	AV	58	U	N1-C2-O2	5.57	126.70	122.80
68	AV	33	U	N3-C2-O2	-5.56	118.31	122.20
5	BB	52	C	N3-C2-O2	-5.55	118.01	121.90
88	BA	1015	C	C2-N1-C1'	5.55	124.90	118.80
68	AV	21	C	C2-N1-C1'	5.55	124.90	118.80
48	AA	503	A	C2-N3-C4	5.54	113.37	110.60
88	BA	860	G	N3-C4-C5	-5.54	125.83	128.60
88	BA	549	C	C6-N1-C2	-5.53	118.09	120.30
78	Ag	337	ASP	CB-CA-C	5.52	121.44	110.40
88	BA	493	A	C2-N3-C4	5.52	113.36	110.60
19	BT	68	PRO	N-CA-CB	5.51	109.91	103.30
88	BA	545	U	N1-C2-O2	5.51	126.66	122.80
88	BA	1145	C	P-O3'-C3'	5.51	126.31	119.70
48	AA	594	C	N1-C2-O2	5.50	122.20	118.90
74	Ad	98	ASP	CB-CG-OD1	5.50	123.25	118.30
88	BA	201	C	C2-N1-C1'	5.50	124.85	118.80
88	BA	394	C	C6-N1-C1'	-5.50	114.19	120.80
88	BA	619	C	N1-C2-O2	5.50	122.20	118.90
48	AA	271	C	C2-N1-C1'	5.50	124.85	118.80
88	BA	1570	C	C2-N1-C1'	5.50	124.85	118.80
88	BA	1453	U	N1-C2-O2	5.48	126.64	122.80
48	AA	792	U	N1-C2-O2	5.48	126.63	122.80
48	AA	52	C	C6-N1-C2	-5.47	118.11	120.30
49	B4	82	LEU	CA-CB-CG	5.47	127.87	115.30
48	AA	52	C	C2-N1-C1'	5.46	124.81	118.80
62	AN	74	GLU	CA-CB-CG	5.46	125.42	113.40
88	BA	847	U	N3-C2-O2	-5.46	118.38	122.20
88	BA	404	C	N3-C2-O2	-5.46	118.08	121.90
21	BV	148	LEU	CA-CB-CG	5.45	127.83	115.30
48	AA	407	U	N1-C2-O2	5.45	126.61	122.80
88	BA	1459	U	C5-C6-N1	5.43	125.41	122.70
5	BB	52	C	C6-N1-C2	-5.42	118.13	120.30
88	BA	1288	U	C5-C6-N1	5.41	125.41	122.70
48	AA	48	C	N3-C2-O2	-5.40	118.12	121.90
48	AA	620	C	C6-N1-C2	-5.39	118.14	120.30
48	AA	560	C	C2-N1-C1'	5.38	124.72	118.80
68	AV	61	C	N1-C2-O2	5.38	122.13	118.90
68	AV	33	U	N1-C2-O2	5.38	126.57	122.80
88	BA	1440	U	N1-C2-O2	5.37	126.56	122.80
88	BA	853	A	C2-N3-C4	5.37	113.29	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AA	498	U	C2-N1-C1'	5.37	124.14	117.70
48	AA	758	U	C2-N1-C1'	5.37	124.14	117.70
88	BA	423	U	N1-C2-O2	5.36	126.55	122.80
88	BA	725	C	N1-C2-O2	5.35	122.11	118.90
88	BA	296	C	C6-N1-C2	-5.35	118.16	120.30
88	BA	545	U	N3-C2-O2	-5.35	118.46	122.20
88	BA	1451	U	C5-C6-N1	5.34	125.37	122.70
88	BA	786	U	N3-C2-O2	-5.34	118.46	122.20
88	BA	1428	U	C6-N1-C1'	-5.34	113.72	121.20
88	BA	1296	U	C6-N1-C1'	-5.34	113.72	121.20
12	BL	275	LEU	CA-CB-CG	5.34	127.57	115.30
48	AA	66	C	N1-C2-O2	5.33	122.10	118.90
48	AA	584	C	N3-C2-O2	-5.33	118.17	121.90
68	AV	70	C	C6-N1-C2	-5.33	118.17	120.30
29	Bd	117	LEU	CA-CB-CG	5.32	127.54	115.30
88	BA	613	U	N3-C2-O2	-5.32	118.48	122.20
88	BA	549	C	C6-N1-C1'	-5.32	114.42	120.80
88	BA	1429	C	C2-N1-C1'	5.32	124.65	118.80
88	BA	860	G	C8-N9-C1'	-5.31	120.09	127.00
83	Am	99	LEU	CA-CB-CG	5.31	127.52	115.30
88	BA	1241	U	P-O3'-C3'	5.30	126.06	119.70
88	BA	77	U	N1-C2-O2	5.30	126.51	122.80
65	AQ	81	LEU	CA-CB-CG	5.30	127.49	115.30
88	BA	825	C	C6-N1-C2	-5.29	118.18	120.30
88	BA	1527	U	C5-C6-N1	5.29	125.35	122.70
48	AA	417	C	N3-C2-O2	-5.29	118.20	121.90
76	Ae	70	LEU	CA-CB-CG	5.29	127.46	115.30
88	BA	468	A	C2-N3-C4	5.28	113.24	110.60
48	AA	503	A	N3-C4-N9	5.28	131.62	127.40
19	BT	188	LEU	CA-CB-CG	5.27	127.43	115.30
25	Ba	363	ASP	CB-CG-OD1	5.27	123.05	118.30
88	BA	562	A	C2-N3-C4	5.27	113.24	110.60
88	BA	61	U	C2-N1-C1'	5.27	124.03	117.70
88	BA	821	C	C5-C6-N1	5.27	123.64	121.00
59	AJ	180	LEU	CA-CB-CG	5.27	127.41	115.30
88	BA	104	C	N3-C2-O2	-5.27	118.21	121.90
88	BA	1532	U	C2-N1-C1'	5.26	124.02	117.70
5	BB	12	U	N3-C2-O2	-5.26	118.52	122.20
88	BA	48	U	OP1-P-O3'	5.26	116.77	105.20
88	BA	79	U	N1-C2-O2	5.25	126.48	122.80
68	AV	53	U	C2-N1-C1'	5.24	123.99	117.70
88	BA	93	U	N1-C2-O2	5.24	126.47	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AA	745	C	C5-C6-N1	5.24	123.62	121.00
88	BA	79	U	C2-N1-C1'	5.23	123.97	117.70
88	BA	259	C	C5-C6-N1	5.22	123.61	121.00
68	AV	35	C	N3-C2-O2	-5.22	118.25	121.90
48	AA	566	U	N1-C2-O2	5.21	126.45	122.80
88	BA	586	C	C2-N1-C1'	5.21	124.53	118.80
88	BA	1288	U	C6-N1-C2	-5.21	117.87	121.00
88	BA	1451	U	N1-C2-O2	5.21	126.44	122.80
20	BU	105	LEU	CA-CB-CG	5.20	127.26	115.30
68	AV	61	C	C2-N1-C1'	5.20	124.52	118.80
88	BA	759	C	C2-N1-C1'	5.20	124.52	118.80
88	BA	546	C	N1-C2-O2	5.20	122.02	118.90
68	AV	58	U	N3-C2-O2	-5.19	118.56	122.20
88	BA	561	C	N1-C2-O2	5.19	122.02	118.90
12	BL	321	LEU	CA-CB-CG	5.19	127.24	115.30
88	BA	1234	U	C2-N1-C1'	5.19	123.93	117.70
88	BA	1558	U	C2-N1-C1'	5.18	123.92	117.70
88	BA	1453	U	N3-C2-O2	-5.17	118.58	122.20
88	BA	405	C	N1-C2-O2	5.17	122.00	118.90
48	AA	422	C	N3-C2-O2	-5.16	118.29	121.90
88	BA	546	C	C6-N1-C1'	-5.16	114.61	120.80
8	BF	289	PRO	CA-N-CD	-5.16	104.28	111.50
48	AA	744	C	N3-C2-O2	-5.16	118.29	121.90
88	BA	190	U	N3-C2-O2	-5.16	118.59	122.20
73	Ac	114	GLU	N-CA-CB	5.15	119.88	110.60
88	BA	468	A	C4-N9-C1'	5.15	135.57	126.30
88	BA	890	C	C5-C6-N1	5.14	123.57	121.00
88	BA	383	C	C5-C6-N1	5.14	123.57	121.00
88	BA	272	A	O4'-C1'-N9	5.14	112.31	108.20
85	Ao	431	ASP	CB-CG-OD2	5.13	122.92	118.30
48	AA	314	A	C4-N9-C1'	5.13	135.54	126.30
88	BA	435	C	C5-C6-N1	5.13	123.56	121.00
88	BA	1129	C	N3-C2-O2	-5.13	118.31	121.90
88	BA	410	U	C2-N1-C1'	5.12	123.85	117.70
88	BA	1413	C	C6-N1-C1'	-5.12	114.66	120.80
68	AV	31	C	C5-C6-N1	5.12	123.56	121.00
48	AA	594	C	C6-N1-C1'	-5.11	114.67	120.80
48	AA	731	A	C2-N3-C4	5.10	113.15	110.60
48	AA	850	U	C5-C6-N1	5.10	125.25	122.70
85	Ao	394	LEU	CA-CB-CG	5.10	127.03	115.30
48	AA	854	C	N3-C2-O2	-5.10	118.33	121.90
5	BB	21	C	N1-C2-O2	5.09	121.96	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	BA	1207	C	C6-N1-C2	-5.08	118.27	120.30
48	AA	417	C	C2-N1-C1'	5.08	124.39	118.80
81	Aj	199	ASP	CB-CG-OD1	5.08	122.87	118.30
88	BA	848	C	N3-C2-O2	-5.06	118.36	121.90
88	BA	1241	U	OP1-P-O3'	5.06	116.33	105.20
88	BA	1058	C	C5-C6-N1	5.06	123.53	121.00
5	BB	12	U	N1-C2-O2	5.06	126.34	122.80
88	BA	79	U	N3-C2-O2	-5.06	118.66	122.20
88	BA	1543	U	N1-C2-O2	5.05	126.34	122.80
88	BA	285	C	C6-N1-C2	-5.05	118.28	120.30
88	BA	397	C	C5-C6-N1	5.05	123.52	121.00
88	BA	1091	U	N3-C2-O2	-5.04	118.67	122.20
88	BA	493	A	C4-N9-C1'	5.04	135.38	126.30
48	AA	407	U	N3-C2-O2	-5.04	118.67	122.20
68	AV	53	U	N1-C2-O2	5.04	126.33	122.80
88	BA	330	A	C4-N9-C1'	5.04	135.37	126.30
88	BA	988	U	N1-C2-O2	5.04	126.33	122.80
66	AR	66	CYS	CA-CB-SG	5.04	123.07	114.00
88	BA	394	C	N1-C2-O2	5.03	121.92	118.90
48	AA	314	A	N3-C4-N9	5.02	131.42	127.40
88	BA	988	U	N3-C2-O2	-5.02	118.69	122.20
48	AA	874	U	C2-N1-C1'	5.01	123.72	117.70
88	BA	595	C	N3-C2-O2	-5.01	118.39	121.90
88	BA	759	C	C6-N1-C2	-5.01	118.30	120.30
88	BA	469	C	C6-N1-C2	-5.01	118.30	120.30
88	BA	708	C	N1-C2-O2	5.01	121.90	118.90
48	AA	633	C	C2-N1-C1'	5.00	124.31	118.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	BE	316	PHE	Peptide
10	BJ	156	SER	Peptide
32	Bg	49	ARG	Peptide
36	Bk	197	ARG	Sidechain
39	Bn	65	ASN	Peptide
43	Bt	18	ILE	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CL	43/198 (22%)	39 (91%)	4 (9%)	0	100	100
1	DL	25/198 (13%)	25 (100%)	0	0	100	100
1	EL	26/198 (13%)	26 (100%)	0	0	100	100
1	FL	25/198 (13%)	24 (96%)	1 (4%)	0	100	100
1	GL	25/198 (13%)	25 (100%)	0	0	100	100
1	HL	24/198 (12%)	24 (100%)	0	0	100	100
2	B0	108/148 (73%)	107 (99%)	1 (1%)	0	100	100
3	B1	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
4	B2	177/252 (70%)	175 (99%)	2 (1%)	0	100	100
6	BD	208/306 (68%)	202 (97%)	5 (2%)	1 (0%)	29	68
7	BE	275/399 (69%)	259 (94%)	15 (6%)	1 (0%)	34	72
8	BF	219/294 (74%)	214 (98%)	5 (2%)	0	100	100
9	BI	96/268 (36%)	92 (96%)	4 (4%)	0	100	100
10	BJ	210/262 (80%)	203 (97%)	7 (3%)	0	100	100
11	BK	174/192 (91%)	171 (98%)	3 (2%)	0	100	100
12	BL	248/362 (68%)	233 (94%)	14 (6%)	1 (0%)	34	72
13	BN	175/178 (98%)	171 (98%)	4 (2%)	0	100	100
14	BO	113/145 (78%)	110 (97%)	3 (3%)	0	100	100
15	BP	286/296 (97%)	277 (97%)	9 (3%)	0	100	100
16	BQ	220/251 (88%)	216 (98%)	4 (2%)	0	100	100
17	BR	151/169 (89%)	147 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	BS	141/180 (78%)	133 (94%)	8 (6%)	0	100	100
19	BT	238/292 (82%)	229 (96%)	8 (3%)	1 (0%)	34	72
20	BU	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
21	BV	153/209 (73%)	148 (97%)	5 (3%)	0	100	100
22	BW	164/210 (78%)	161 (98%)	3 (2%)	0	100	100
23	BX	147/150 (98%)	144 (98%)	3 (2%)	0	100	100
24	BY	204/216 (94%)	198 (97%)	6 (3%)	0	100	100
25	Ba	391/423 (92%)	375 (96%)	16 (4%)	0	100	100
26	Bb	352/380 (93%)	337 (96%)	15 (4%)	0	100	100
27	B3	116/161 (72%)	114 (98%)	2 (2%)	0	100	100
28	Bc	293/334 (88%)	282 (96%)	11 (4%)	0	100	100
29	Bd	136/206 (66%)	132 (97%)	4 (3%)	0	100	100
30	Be	120/135 (89%)	113 (94%)	7 (6%)	0	100	100
31	Bf	106/142 (75%)	102 (96%)	2 (2%)	2 (2%)	8	40
32	Bg	146/159 (92%)	139 (95%)	7 (5%)	0	100	100
33	Bh	287/332 (86%)	277 (96%)	10 (4%)	0	100	100
34	Bi	258/306 (84%)	247 (96%)	11 (4%)	0	100	100
35	Bj	211/279 (76%)	199 (94%)	12 (6%)	0	100	100
36	Bk	151/269 (56%)	142 (94%)	8 (5%)	1 (1%)	22	61
37	Bl	131/166 (79%)	129 (98%)	2 (2%)	0	100	100
38	Bm	107/198 (54%)	103 (96%)	4 (4%)	0	100	100
39	Bn	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
40	Bo	95/124 (77%)	95 (100%)	0	0	100	100
41	Bp	95/112 (85%)	92 (97%)	3 (3%)	0	100	100
42	Bq	66/138 (48%)	62 (94%)	4 (6%)	0	100	100
43	Bt	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
44	Bu	147/205 (72%)	141 (96%)	5 (3%)	1 (1%)	22	61
45	Bv	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
46	Bw	385/433 (89%)	362 (94%)	22 (6%)	1 (0%)	41	75
47	Bx	160/196 (82%)	152 (95%)	8 (5%)	0	100	100
49	B4	61/126 (48%)	51 (84%)	8 (13%)	2 (3%)	4	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	B5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
51	B6	50/65 (77%)	50 (100%)	0	0	100	100
52	B7	44/95 (46%)	43 (98%)	1 (2%)	0	100	100
53	AB	218/289 (75%)	209 (96%)	9 (4%)	0	100	100
54	AC	130/167 (78%)	125 (96%)	5 (4%)	0	100	100
55	AE	341/430 (79%)	324 (95%)	17 (5%)	0	100	100
56	AF	120/276 (44%)	115 (96%)	5 (4%)	0	100	100
57	AG	204/240 (85%)	200 (98%)	4 (2%)	0	100	100
58	AI	326/397 (82%)	318 (98%)	8 (2%)	0	100	100
59	AJ	138/200 (69%)	129 (94%)	9 (6%)	0	100	100
60	AK	135/196 (69%)	125 (93%)	10 (7%)	0	100	100
61	AL	107/139 (77%)	101 (94%)	6 (6%)	0	100	100
62	AN	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
63	AO	173/239 (72%)	166 (96%)	7 (4%)	0	100	100
64	AP	115/135 (85%)	113 (98%)	2 (2%)	0	100	100
65	AQ	110/130 (85%)	108 (98%)	2 (2%)	0	100	100
66	AR	95/143 (66%)	93 (98%)	2 (2%)	0	100	100
67	AU	84/87 (97%)	84 (100%)	0	0	100	100
71	Aa	290/382 (76%)	282 (97%)	8 (3%)	0	100	100
72	Ab	133/190 (70%)	129 (97%)	4 (3%)	0	100	100
73	Ac	167/173 (96%)	163 (98%)	4 (2%)	0	100	100
74	Ad	175/205 (85%)	174 (99%)	1 (1%)	0	100	100
75	B8	93/188 (50%)	88 (95%)	5 (5%)	0	100	100
76	Ae	386/455 (85%)	354 (92%)	30 (8%)	2 (0%)	29	68
77	Af	97/188 (52%)	94 (97%)	3 (3%)	0	100	100
78	Ag	351/410 (86%)	338 (96%)	12 (3%)	1 (0%)	41	75
79	Ah	118/387 (30%)	117 (99%)	1 (1%)	0	100	100
80	Ai	97/106 (92%)	96 (99%)	1 (1%)	0	100	100
81	Aj	211/218 (97%)	206 (98%)	5 (2%)	0	100	100
82	Ak	273/325 (84%)	264 (97%)	9 (3%)	0	100	100
83	Am	114/118 (97%)	112 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	An	70/199 (35%)	67 (96%)	3 (4%)	0	100	100
85	Ao	564/699 (81%)	540 (96%)	24 (4%)	0	100	100
86	Ap	188/258 (73%)	184 (98%)	3 (2%)	1 (0%)	29	68
87	B9	36/100 (36%)	36 (100%)	0	0	100	100
All	All	14349/19793 (72%)	13839 (96%)	495 (3%)	15 (0%)	54	84

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	BT	68	PRO
31	Bf	78	PRO
31	Bf	80	PRO
36	Bk	90	VAL
44	Bu	167	PRO
46	Bw	159	VAL
78	Ag	337	ASP
7	BE	317	PRO
76	Ae	342	PRO
86	Ap	52	LYS
49	B4	87	PRO
76	Ae	75	VAL
49	B4	86	SER
6	BD	208	ILE
12	BL	209	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CL	30/157 (19%)	30 (100%)	0	100	100
1	DL	26/157 (17%)	26 (100%)	0	100	100
1	EL	27/157 (17%)	27 (100%)	0	100	100
1	FL	26/157 (17%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GL	26/157 (17%)	26 (100%)	0	100	100
1	HL	25/157 (16%)	25 (100%)	0	100	100
2	B0	90/115 (78%)	89 (99%)	1 (1%)	73	88
3	B1	219/229 (96%)	219 (100%)	0	100	100
4	B2	164/228 (72%)	164 (100%)	0	100	100
6	BD	167/248 (67%)	167 (100%)	0	100	100
7	BE	237/320 (74%)	237 (100%)	0	100	100
8	BF	194/251 (77%)	193 (100%)	1 (0%)	88	94
9	BI	88/228 (39%)	88 (100%)	0	100	100
10	BJ	192/230 (84%)	191 (100%)	1 (0%)	88	94
11	BK	129/151 (85%)	128 (99%)	1 (1%)	81	91
12	BL	218/318 (69%)	216 (99%)	2 (1%)	78	90
13	BN	156/157 (99%)	155 (99%)	1 (1%)	86	94
14	BO	99/123 (80%)	99 (100%)	0	100	100
15	BP	245/249 (98%)	244 (100%)	1 (0%)	91	96
16	BQ	190/210 (90%)	190 (100%)	0	100	100
17	BR	132/143 (92%)	132 (100%)	0	100	100
18	BS	123/153 (80%)	122 (99%)	1 (1%)	81	91
19	BT	212/258 (82%)	211 (100%)	1 (0%)	88	94
20	BU	118/127 (93%)	118 (100%)	0	100	100
21	BV	136/178 (76%)	136 (100%)	0	100	100
22	BW	144/180 (80%)	144 (100%)	0	100	100
23	BX	116/134 (87%)	116 (100%)	0	100	100
24	BY	185/192 (96%)	184 (100%)	1 (0%)	88	94
25	Ba	348/365 (95%)	347 (100%)	1 (0%)	92	97
26	Bb	310/328 (94%)	309 (100%)	1 (0%)	92	97
27	B3	110/150 (73%)	110 (100%)	0	100	100
28	Bc	271/299 (91%)	271 (100%)	0	100	100
29	Bd	127/181 (70%)	127 (100%)	0	100	100
30	Be	100/108 (93%)	100 (100%)	0	100	100
31	Bf	80/133 (60%)	79 (99%)	1 (1%)	69	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Bg	128/136 (94%)	127 (99%)	1 (1%)	81	91
33	Bh	251/284 (88%)	250 (100%)	1 (0%)	91	96
34	Bi	236/275 (86%)	235 (100%)	1 (0%)	91	96
35	Bj	190/242 (78%)	188 (99%)	2 (1%)	73	88
36	Bk	135/226 (60%)	134 (99%)	1 (1%)	84	93
37	Bl	122/147 (83%)	122 (100%)	0	100	100
38	Bm	103/178 (58%)	103 (100%)	0	100	100
39	Bn	88/113 (78%)	88 (100%)	0	100	100
40	Bo	77/97 (79%)	77 (100%)	0	100	100
41	Bp	79/88 (90%)	79 (100%)	0	100	100
42	Bq	50/114 (44%)	50 (100%)	0	100	100
43	Bt	75/82 (92%)	75 (100%)	0	100	100
44	Bu	126/177 (71%)	125 (99%)	1 (1%)	81	91
45	Bv	115/183 (63%)	115 (100%)	0	100	100
46	Bw	340/373 (91%)	339 (100%)	1 (0%)	92	97
47	Bx	149/173 (86%)	149 (100%)	0	100	100
49	B4	45/114 (40%)	45 (100%)	0	100	100
50	B5	99/163 (61%)	99 (100%)	0	100	100
51	B6	49/60 (82%)	48 (98%)	1 (2%)	55	79
52	B7	41/78 (53%)	41 (100%)	0	100	100
53	AB	187/233 (80%)	186 (100%)	1 (0%)	88	94
54	AC	115/142 (81%)	115 (100%)	0	100	100
55	AE	282/351 (80%)	281 (100%)	1 (0%)	91	96
56	AF	107/210 (51%)	107 (100%)	0	100	100
57	AG	179/203 (88%)	178 (99%)	1 (1%)	86	94
58	AI	273/333 (82%)	273 (100%)	0	100	100
59	AJ	130/180 (72%)	130 (100%)	0	100	100
60	AK	103/151 (68%)	103 (100%)	0	100	100
61	AL	92/116 (79%)	92 (100%)	0	100	100
62	AN	92/114 (81%)	92 (100%)	0	100	100
63	AO	159/205 (78%)	159 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	AP	97/113 (86%)	96 (99%)	1 (1%)	76	88
65	AQ	97/114 (85%)	97 (100%)	0	100	100
66	AR	89/127 (70%)	89 (100%)	0	100	100
67	AU	77/78 (99%)	77 (100%)	0	100	100
71	Aa	258/330 (78%)	258 (100%)	0	100	100
72	Ab	113/162 (70%)	113 (100%)	0	100	100
73	Ac	152/155 (98%)	151 (99%)	1 (1%)	84	93
74	Ad	149/168 (89%)	148 (99%)	1 (1%)	84	93
75	B8	87/162 (54%)	87 (100%)	0	100	100
76	Ae	325/393 (83%)	323 (99%)	2 (1%)	86	94
77	Af	86/160 (54%)	86 (100%)	0	100	100
78	Ag	312/361 (86%)	312 (100%)	0	100	100
79	Ah	109/346 (32%)	109 (100%)	0	100	100
80	Ai	86/93 (92%)	86 (100%)	0	100	100
81	Aj	188/190 (99%)	186 (99%)	2 (1%)	73	88
82	Ak	249/289 (86%)	249 (100%)	0	100	100
83	Am	100/102 (98%)	100 (100%)	0	100	100
84	An	66/174 (38%)	65 (98%)	1 (2%)	65	84
85	Ao	478/611 (78%)	476 (100%)	2 (0%)	91	96
86	Ap	170/225 (76%)	169 (99%)	1 (1%)	86	94
87	B9	36/77 (47%)	36 (100%)	0	100	100
All	All	12601/16899 (75%)	12564 (100%)	37 (0%)	92	97

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B0	86	ASN
8	BF	60	ARG
10	BJ	63	ARG
11	BK	122	ARG
12	BL	166	ARG
12	BL	313	ARG
13	BN	40	GLN
15	BP	254	LYS
18	BS	55	ASN

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Mol	Chain	Res	Type
19	BT	191	ARG
24	BY	105	ARG
25	Ba	310	ARG
26	Bb	52	ARG
31	Bf	131	ARG
32	Bg	81	ASN
33	Bh	231	MET
34	Bi	126	ARG
35	Bj	198	ASN
35	Bj	230	LYS
36	Bk	64	LYS
44	Bu	159	GLU
46	Bw	347	ARG
51	B6	34	ARG
53	AB	263	ARG
55	AE	92	LYS
57	AG	139	ARG
64	AP	10	ARG
73	Ac	137	ARG
74	Ad	172	ASN
76	Ae	399	GLN
76	Ae	424	HIS
81	Aj	17	ARG
81	Aj	83	LYS
84	An	197	LYS
85	Ao	407	ARG
85	Ao	650	ARG
86	Ap	223	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B0	86	ASN
10	BJ	128	ASN
10	BJ	235	GLN
12	BL	319	HIS
15	BP	120	GLN
18	BS	41	ASN
18	BS	55	ASN
18	BS	115	HIS
23	BX	98	GLN
27	B3	102	ASN

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Mol	Chain	Res	Type
32	Bg	24	GLN
32	Bg	58	ASN
35	Bj	175	GLN
36	Bk	189	HIS
55	AE	155	GLN
55	AE	344	ASN
58	AI	87	HIS
62	AN	68	GLN
73	Ac	118	GLN
87	B9	97	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
48	AA	959/962 (99%)	192 (20%)	1 (0%)
5	BB	64/73 (87%)	14 (21%)	0
68	AV	70/71 (98%)	26 (37%)	0
69	AX	8/9 (88%)	1 (12%)	0
88	BA	1542/1571 (98%)	418 (27%)	5 (0%)
All	All	2643/2686 (98%)	651 (24%)	6 (0%)

All (651) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	BB	3	U
5	BB	5	A
5	BB	7	G
5	BB	8	U
5	BB	13	U
5	BB	21	C
5	BB	34	U
5	BB	43	C
5	BB	44	U
5	BB	46	G
5	BB	47	A
5	BB	48	U
5	BB	69	C
5	BB	70	A
48	AA	5	A
48	AA	10	U
48	AA	18	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	AA	27	U
48	AA	34	U
48	AA	42	A
48	AA	43	U
48	AA	49	A
48	AA	54	A
48	AA	58	U
48	AA	61	G
48	AA	65	C
48	AA	75	A
48	AA	78	C
48	AA	81	U
48	AA	83	C
48	AA	91	A
48	AA	98	A
48	AA	104	A
48	AA	115	A
48	AA	119	C
48	AA	120	A
48	AA	126	A
48	AA	137	A
48	AA	139	A
48	AA	147	G
48	AA	152	A
48	AA	161	C
48	AA	170	A
48	AA	171	C
48	AA	173	G
48	AA	175	A
48	AA	186	U
48	AA	191	C
48	AA	194	U
48	AA	203	G
48	AA	209	C
48	AA	212	A
48	AA	216	A
48	AA	217	U
48	AA	219	U
48	AA	222	A
48	AA	223	U
48	AA	224	U
48	AA	231	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	AA	235	A
48	AA	237	U
48	AA	238	C
48	AA	244	C
48	AA	247	G
48	AA	253	G
48	AA	255	G
48	AA	257	U
48	AA	258	C
48	AA	273	A
48	AA	281	G
48	AA	287	C
48	AA	294	A
48	AA	297	A
48	AA	308	A
48	AA	309	A
48	AA	310	A
48	AA	314	A
48	AA	315	U
48	AA	316	C
48	AA	317	A
48	AA	320	A
48	AA	328	A
48	AA	330	A
48	AA	337	C
48	AA	345	U
48	AA	353	C
48	AA	354	C
48	AA	362	A
48	AA	367	A
48	AA	368	A
48	AA	381	G
48	AA	395	C
48	AA	399	A
48	AA	407	U
48	AA	417	C
48	AA	421	A
48	AA	433	U
48	AA	455	A
48	AA	456	A
48	AA	457	C
48	AA	458	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	AA	461	A
48	AA	471	U
48	AA	472	A
48	AA	477	A
48	AA	479	C
48	AA	488	A
48	AA	502	A
48	AA	503	A
48	AA	504	C
48	AA	518	A
48	AA	523	C
48	AA	530	G
48	AA	531	U
48	AA	536	C
48	AA	538	C
48	AA	540	U
48	AA	561	U
48	AA	563	U
48	AA	564	A
48	AA	566	U
48	AA	571	A
48	AA	574	C
48	AA	576	C
48	AA	577	C
48	AA	578	G
48	AA	579	A
48	AA	580	U
48	AA	589	C
48	AA	593	C
48	AA	594	C
48	AA	596	U
48	AA	597	U
48	AA	604	U
48	AA	616	C
48	AA	620	C
48	AA	625	U
48	AA	628	G
48	AA	638	A
48	AA	639	A
48	AA	641	A
48	AA	644	A
48	AA	645	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	AA	646	C
48	AA	647	A
48	AA	649	U
48	AA	650	A
48	AA	652	U
48	AA	665	A
48	AA	681	A
48	AA	682	G
48	AA	698	A
48	AA	699	U
48	AA	707	A
48	AA	709	A
48	AA	711	A
48	AA	722	A
48	AA	724	U
48	AA	731	A
48	AA	732	U
48	AA	739	A
48	AA	741	C
48	AA	742	C
48	AA	743	A
48	AA	753	A
48	AA	754	G
48	AA	766	C
48	AA	775	A
48	AA	790	A
48	AA	791	G
48	AA	802	A
48	AA	807	G
48	AA	808	U
48	AA	823	G
48	AA	825	C
48	AA	841	C
48	AA	842	A
48	AA	863	G
48	AA	865	A
48	AA	869	A
48	AA	870	G
48	AA	874	U
48	AA	876	A
48	AA	877	A
48	AA	883	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	AA	885	U
48	AA	886	A
48	AA	887	U
48	AA	893	A
48	AA	899	C
48	AA	900	A
48	AA	903	C
48	AA	910	G
48	AA	918	A
48	AA	923	G
48	AA	925	A
48	AA	928	A
48	AA	930	G
48	AA	932	U
48	AA	943	G
48	AA	945	A
48	AA	946	A
48	AA	955	G
48	AA	956	G
48	AA	959	U
48	AA	960	A
68	AV	2	G
68	AV	4	A
68	AV	6	G
68	AV	8	U
68	AV	9	C
68	AV	13	U
68	AV	14	A
68	AV	15	A
68	AV	16	A
68	AV	17	U
68	AV	18	A
68	AV	43	A
68	AV	44	U
68	AV	45	G
68	AV	46	U
68	AV	51	U
68	AV	52	A
68	AV	53	U
68	AV	54	A
68	AV	56	C
68	AV	63	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
68	AV	64	U
68	AV	65	A
68	AV	68	A
68	AV	69	C
68	AV	71	A
69	AX	7	C
88	BA	4	A
88	BA	7	G
88	BA	11	G
88	BA	19	U
88	BA	20	A
88	BA	21	C
88	BA	22	U
88	BA	27	A
88	BA	31	A
88	BA	32	C
88	BA	33	A
88	BA	36	A
88	BA	40	C
88	BA	41	A
88	BA	42	C
88	BA	45	A
88	BA	46	A
88	BA	49	A
88	BA	56	A
88	BA	57	A
88	BA	59	A
88	BA	60	U
88	BA	63	A
88	BA	66	U
88	BA	67	A
88	BA	68	A
88	BA	75	A
88	BA	82	G
88	BA	83	A
88	BA	96	U
88	BA	97	A
88	BA	104	C
88	BA	105	G
88	BA	109	U
88	BA	115	U
88	BA	118	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
88	BA	122	G
88	BA	126	G
88	BA	129	A
88	BA	132	G
88	BA	135	G
88	BA	139	G
88	BA	140	A
88	BA	141	A
88	BA	142	U
88	BA	143	A
88	BA	147	U
88	BA	149	A
88	BA	153	U
88	BA	163	C
88	BA	164	A
88	BA	168	A
88	BA	172	C
88	BA	178	C
88	BA	179	U
88	BA	180	A
88	BA	186	U
88	BA	190	U
88	BA	192	A
88	BA	205	A
88	BA	218	A
88	BA	219	A
88	BA	223	A
88	BA	224	A
88	BA	225	C
88	BA	228	U
88	BA	229	A
88	BA	231	C
88	BA	237	A
88	BA	238	C
88	BA	239	C
88	BA	243	A
88	BA	245	A
88	BA	254	G
88	BA	263	G
88	BA	271	U
88	BA	272	A
88	BA	273	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
88	BA	275	A
88	BA	277	A
88	BA	295	G
88	BA	309	A
88	BA	311	A
88	BA	312	C
88	BA	322	G
88	BA	323	A
88	BA	324	G
88	BA	329	A
88	BA	330	A
88	BA	331	A
88	BA	336	A
88	BA	337	A
88	BA	338	C
88	BA	339	G
88	BA	340	A
88	BA	352	G
88	BA	359	G
88	BA	366	A
88	BA	368	A
88	BA	369	G
88	BA	371	A
88	BA	372	U
88	BA	373	U
88	BA	374	U
88	BA	376	A
88	BA	390	A
88	BA	393	A
88	BA	394	C
88	BA	398	A
88	BA	403	C
88	BA	404	C
88	BA	409	A
88	BA	414	A
88	BA	417	G
88	BA	427	G
88	BA	428	A
88	BA	429	G
88	BA	440	A
88	BA	445	A
88	BA	446	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
88	BA	448	G
88	BA	459	A
88	BA	460	C
88	BA	467	A
88	BA	468	A
88	BA	473	G
88	BA	474	A
88	BA	479	A
88	BA	480	G
88	BA	488	U
88	BA	490	U
88	BA	491	U
88	BA	492	A
88	BA	493	A
88	BA	494	U
88	BA	497	U
88	BA	500	C
88	BA	501	A
88	BA	503	A
88	BA	505	U
88	BA	506	A
88	BA	507	G
88	BA	514	A
88	BA	515	A
88	BA	516	G
88	BA	517	C
88	BA	518	A
88	BA	526	A
88	BA	527	U
88	BA	530	A
88	BA	532	A
88	BA	533	A
88	BA	541	A
88	BA	545	U
88	BA	547	A
88	BA	548	A
88	BA	549	C
88	BA	552	A
88	BA	553	U
88	BA	554	U
88	BA	557	C
88	BA	560	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
88	BA	561	C
88	BA	562	A
88	BA	563	U
88	BA	570	A
88	BA	574	A
88	BA	576	U
88	BA	578	A
88	BA	579	U
88	BA	584	A
88	BA	586	C
88	BA	592	G
88	BA	595	C
88	BA	596	A
88	BA	617	A
88	BA	618	A
88	BA	625	A
88	BA	631	A
88	BA	634	G
88	BA	640	A
88	BA	648	C
88	BA	649	A
88	BA	650	A
88	BA	660	C
88	BA	665	C
88	BA	673	C
88	BA	683	U
88	BA	684	A
88	BA	689	A
88	BA	691	A
88	BA	693	U
88	BA	694	A
88	BA	695	U
88	BA	697	C
88	BA	704	U
88	BA	707	A
88	BA	713	A
88	BA	714	A
88	BA	718	A
88	BA	719	C
88	BA	720	C
88	BA	722	A
88	BA	723	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
88	BA	724	A
88	BA	725	C
88	BA	727	A
88	BA	728	C
88	BA	737	G
88	BA	743	U
88	BA	744	A
88	BA	745	A
88	BA	746	U
88	BA	747	U
88	BA	748	A
88	BA	753	G
88	BA	761	A
88	BA	763	C
88	BA	764	A
88	BA	773	C
88	BA	775	C
88	BA	777	A
88	BA	778	A
88	BA	780	G
88	BA	782	A
88	BA	825	C
88	BA	828	G
88	BA	834	C
88	BA	847	U
88	BA	848	C
88	BA	849	U
88	BA	851	G
88	BA	852	C
88	BA	853	A
88	BA	854	U
88	BA	855	U
88	BA	856	A
88	BA	859	A
88	BA	864	U
88	BA	868	G
88	BA	872	A
88	BA	883	G
88	BA	889	C
88	BA	892	G
88	BA	896	A
88	BA	897	A

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
88	BA	899	G
88	BA	902	C
88	BA	908	A
88	BA	909	U
88	BA	911	C
88	BA	922	A
88	BA	923	A
88	BA	924	G
88	BA	925	G
88	BA	933	A
88	BA	935	C
88	BA	938	U
88	BA	939	U
88	BA	948	A
88	BA	950	U
88	BA	958	U
88	BA	959	G
88	BA	960	U
88	BA	961	A
88	BA	962	U
88	BA	964	A
88	BA	965	A
88	BA	967	G
88	BA	970	C
88	BA	977	G
88	BA	981	U
88	BA	983	U
88	BA	986	U
88	BA	987	G
88	BA	992	U
88	BA	1015	C
88	BA	1016	C
88	BA	1018	U
88	BA	1026	A
88	BA	1027	G
88	BA	1028	A
88	BA	1034	G
88	BA	1038	A
88	BA	1041	A
88	BA	1045	U
88	BA	1050	C
88	BA	1055	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
88	BA	1056	G
88	BA	1057	A
88	BA	1063	U
88	BA	1064	G
88	BA	1071	U
88	BA	1072	A
88	BA	1074	U
88	BA	1081	U
88	BA	1089	G
88	BA	1092	A
88	BA	1093	A
88	BA	1127	A
88	BA	1137	A
88	BA	1138	G
88	BA	1140	A
88	BA	1146	G
88	BA	1167	C
88	BA	1168	A
88	BA	1169	A
88	BA	1180	G
88	BA	1183	U
88	BA	1188	U
88	BA	1194	U
88	BA	1195	A
88	BA	1201	A
88	BA	1204	A
88	BA	1206	U
88	BA	1207	C
88	BA	1215	C
88	BA	1217	A
88	BA	1218	U
88	BA	1219	A
88	BA	1220	A
88	BA	1221	C
88	BA	1222	A
88	BA	1226	C
88	BA	1233	A
88	BA	1238	A
88	BA	1239	A
88	BA	1240	A
88	BA	1241	U
88	BA	1242	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
88	BA	1246	A
88	BA	1247	U
88	BA	1248	C
88	BA	1249	A
88	BA	1252	G
88	BA	1253	G
88	BA	1254	A
88	BA	1258	A
88	BA	1264	C
88	BA	1268	G
88	BA	1271	A
88	BA	1287	G
88	BA	1288	U
88	BA	1291	U
88	BA	1292	A
88	BA	1294	A
88	BA	1296	U
88	BA	1298	C
88	BA	1299	C
88	BA	1303	C
88	BA	1314	U
88	BA	1325	G
88	BA	1326	A
88	BA	1328	G
88	BA	1332	G
88	BA	1336	A
88	BA	1341	A
88	BA	1342	C
88	BA	1352	G
88	BA	1353	C
88	BA	1358	G
88	BA	1385	U
88	BA	1387	A
88	BA	1388	A
88	BA	1389	A
88	BA	1390	G
88	BA	1395	A
88	BA	1396	C
88	BA	1405	A
88	BA	1413	C
88	BA	1420	A
88	BA	1425	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
88	BA	1426	G
88	BA	1428	U
88	BA	1432	U
88	BA	1433	U
88	BA	1436	U
88	BA	1438	U
88	BA	1445	U
88	BA	1448	A
88	BA	1457	A
88	BA	1458	G
88	BA	1459	U
88	BA	1466	G
88	BA	1468	A
88	BA	1474	G
88	BA	1475	A
88	BA	1476	A
88	BA	1482	A
88	BA	1485	A
88	BA	1492	C
88	BA	1493	A
88	BA	1494	A
88	BA	1498	C
88	BA	1504	A
88	BA	1505	G
88	BA	1509	U
88	BA	1514	A
88	BA	1521	U
88	BA	1522	A
88	BA	1525	C
88	BA	1526	U
88	BA	1527	U
88	BA	1528	A
88	BA	1531	C
88	BA	1532	U
88	BA	1533	A
88	BA	1536	U
88	BA	1538	A
88	BA	1548	A
88	BA	1549	A
88	BA	1551	C
88	BA	1552	C
88	BA	1553	A

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Mol	Chain	Res	Type
88	BA	1558	U
88	BA	1559	A
88	BA	1570	C
88	BA	1571	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	AA	917	C
88	BA	48	U
88	BA	1145	C
88	BA	1219	A
88	BA	1220	A
88	BA	1241	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 335 ligands modelled in this entry, 329 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	$\# Z  > 2$
91	SPM	AA	3001	-	13,13,13	0.33	0	12,12,12	0.77	0
92	GTP	Ag	500	89	26,34,34	1.16	2 (7%)	32,54,54	1.56	7 (21%)
93	5GP	BA	1792	89	22,26,26	1.25	2 (9%)	26,40,40	1.25	4 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
93	5GP	BA	1791	-	22,26,26	1.22	2 (9%)	26,40,40	1.27	4 (15%)
91	SPM	BA	1793	-	13,13,13	0.32	0	12,12,12	0.79	0
91	SPM	BA	1794	-	13,13,13	0.34	0	12,12,12	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	SPM	AA	3001	-	-	3/11/11/11	-
92	GTP	Ag	500	89	-	2/18/38/38	0/3/3/3
93	5GP	BA	1792	89	-	0/6/26/26	0/3/3/3
93	5GP	BA	1791	-	-	2/6/26/26	0/3/3/3
91	SPM	BA	1793	-	-	3/11/11/11	-
91	SPM	BA	1794	-	-	3/11/11/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	Ag	500	GTP	C5-C6	-4.22	1.38	1.47
93	BA	1792	5GP	C5-C6	-4.14	1.39	1.47
93	BA	1791	5GP	C5-C6	-3.96	1.39	1.47
93	BA	1791	5GP	C6-N1	-2.55	1.34	1.37
93	BA	1792	5GP	C6-N1	-2.52	1.34	1.37
92	Ag	500	GTP	C2-N3	2.20	1.38	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	Ag	500	GTP	PA-O3A-PB	-3.44	121.03	132.83
92	Ag	500	GTP	PB-O3B-PG	-3.21	121.82	132.83
92	Ag	500	GTP	C5-C6-N1	3.20	119.60	113.95
93	BA	1791	5GP	C5-C6-N1	3.20	119.60	113.95
93	BA	1792	5GP	C5-C6-N1	3.17	119.55	113.95
92	Ag	500	GTP	C2-N1-C6	-2.94	119.68	125.10
92	Ag	500	GTP	C3'-C2'-C1'	2.91	105.36	100.98
92	Ag	500	GTP	C8-N7-C5	2.83	108.37	102.99
92	Ag	500	GTP	O6-C6-C5	-2.44	119.61	124.37
93	BA	1791	5GP	C8-N7-C5	2.40	107.57	102.99
93	BA	1791	5GP	C2-N1-C6	-2.38	120.72	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
93	BA	1792	5GP	C8-N7-C5	2.33	107.44	102.99
93	BA	1792	5GP	C2-N1-C6	-2.31	120.85	125.10
93	BA	1792	5GP	O6-C6-C5	-2.17	120.13	124.37
93	BA	1791	5GP	O6-C6-C5	-2.02	120.42	124.37

There are no chirality outliers.

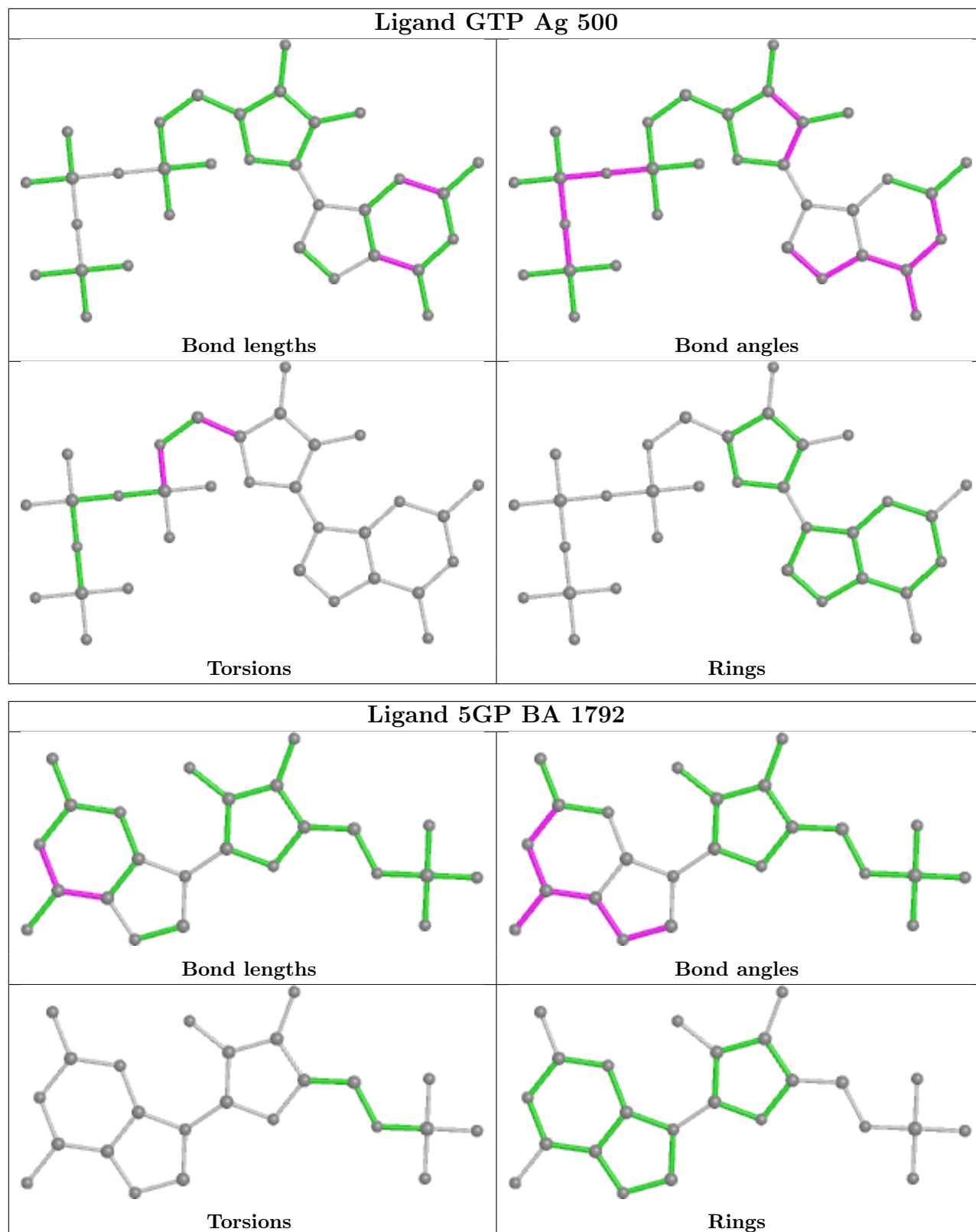
All (13) torsion outliers are listed below:

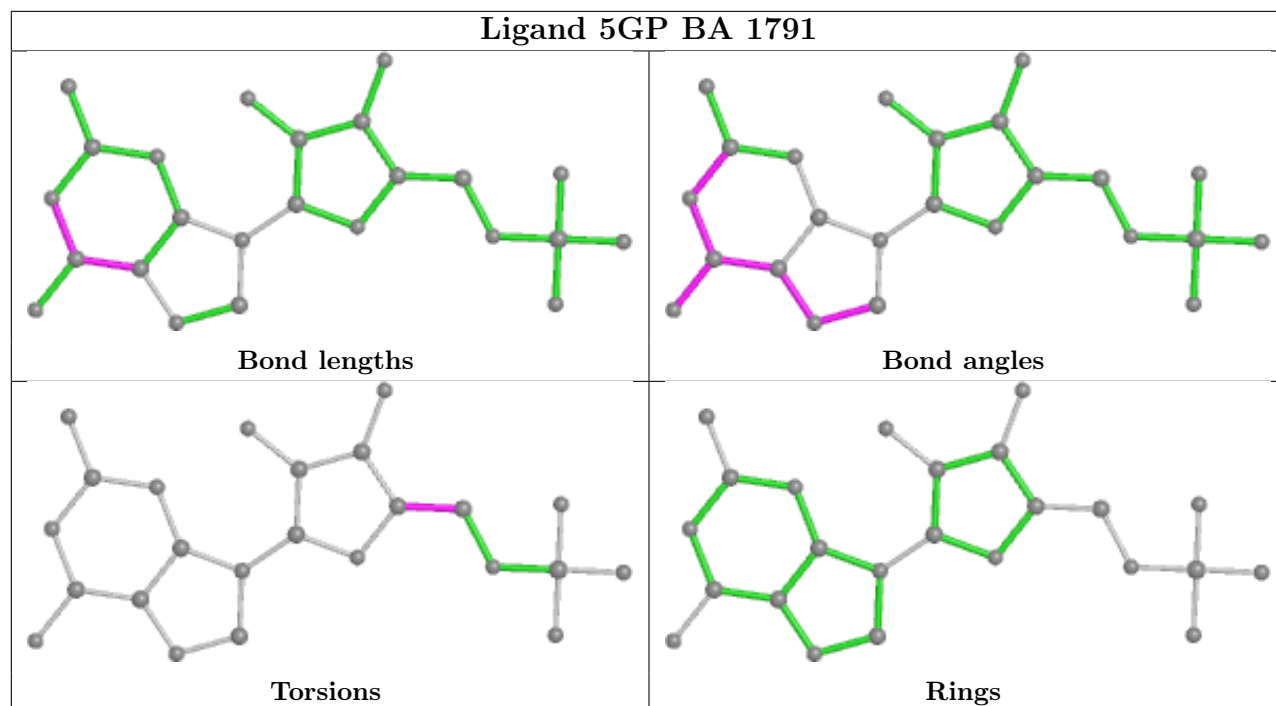
Mol	Chain	Res	Type	Atoms
93	BA	1791	5GP	O4'-C4'-C5'-O5'
91	BA	1794	SPM	C12-C11-N10-C9
91	AA	3001	SPM	C7-C8-C9-N10
91	BA	1794	SPM	C6-C7-C8-C9
93	BA	1791	5GP	C3'-C4'-C5'-O5'
91	AA	3001	SPM	C6-C7-C8-C9
92	Ag	500	GTP	O4'-C4'-C5'-O5'
91	BA	1793	SPM	C7-C8-C9-N10
91	BA	1793	SPM	N5-C6-C7-C8
91	BA	1793	SPM	C7-C6-N5-C4
91	AA	3001	SPM	C7-C6-N5-C4
92	Ag	500	GTP	C5'-O5'-PA-O1A
91	BA	1794	SPM	C8-C9-N10-C11

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

There are no chain breaks in this entry.

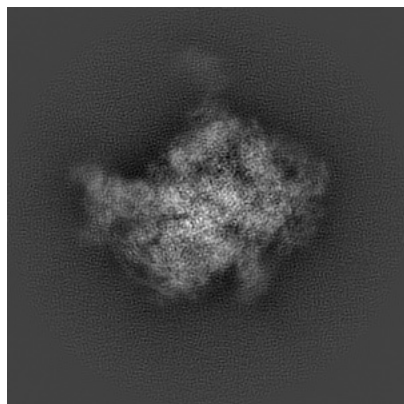
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12527. These allow visual inspection of the internal detail of the map and identification of artifacts.

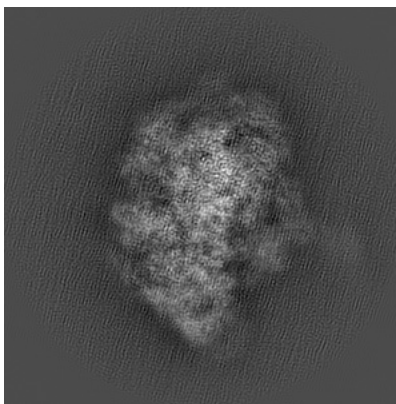
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

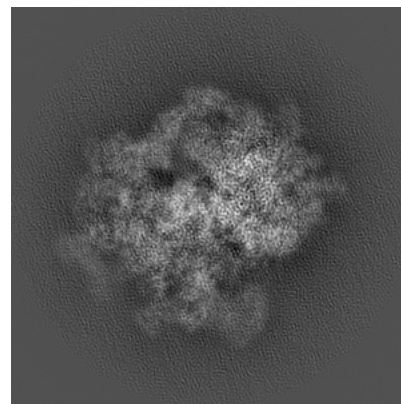
#### 6.1.1 Primary map



X

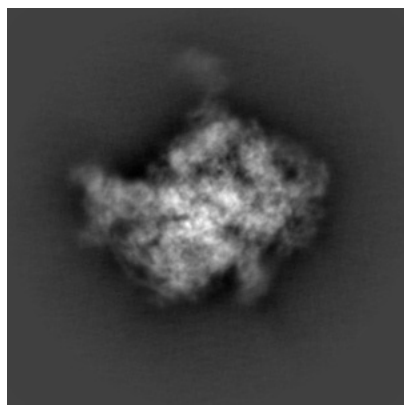


Y

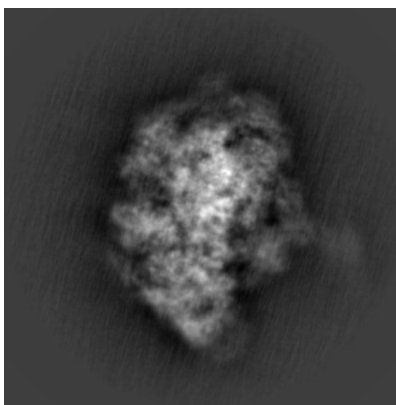


Z

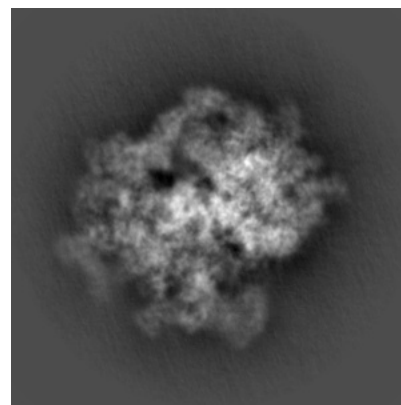
#### 6.1.2 Raw map



X



Y

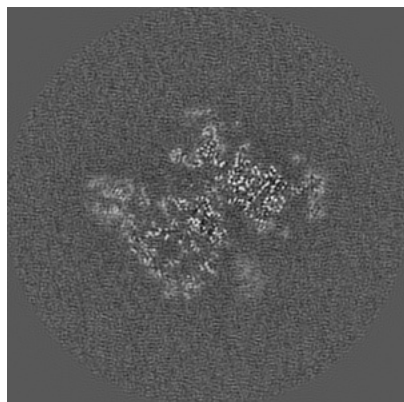


Z

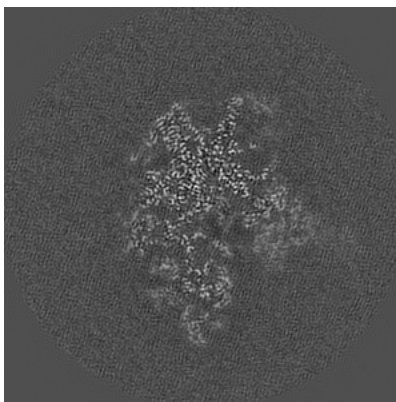
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

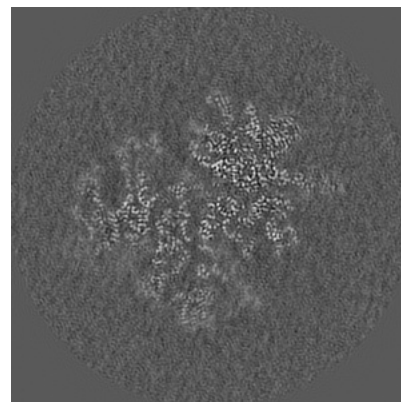
### 6.2.1 Primary map



X Index: 160

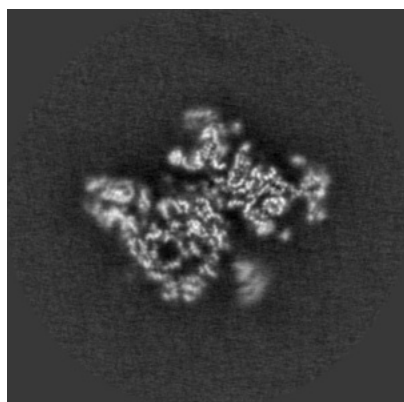


Y Index: 160

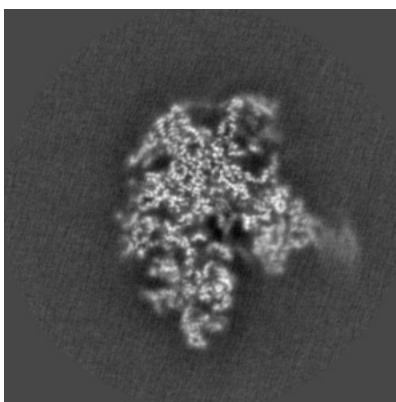


Z Index: 160

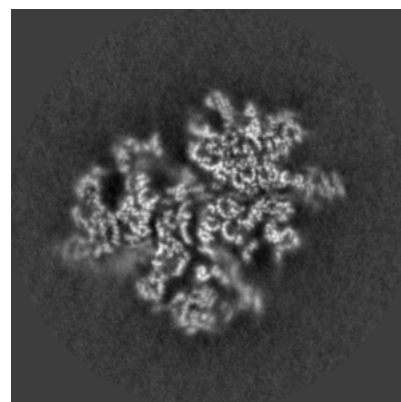
### 6.2.2 Raw map



X Index: 160



Y Index: 160

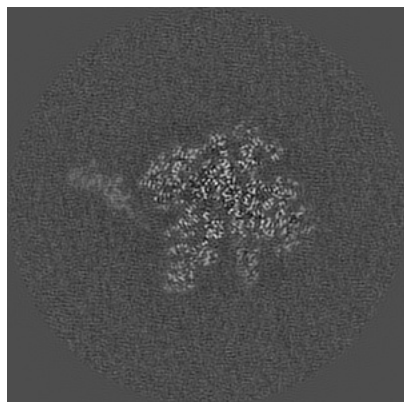


Z Index: 160

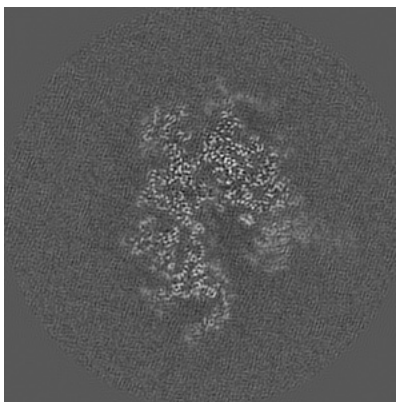
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

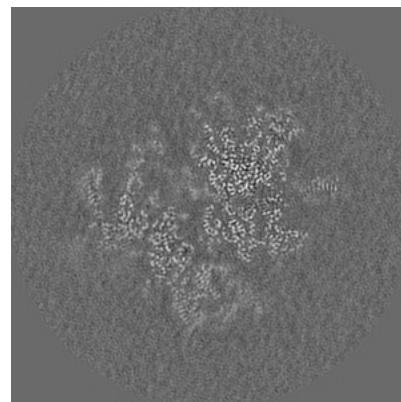
### 6.3.1 Primary map



X Index: 187

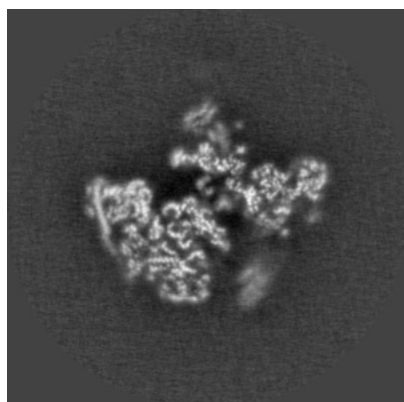


Y Index: 165

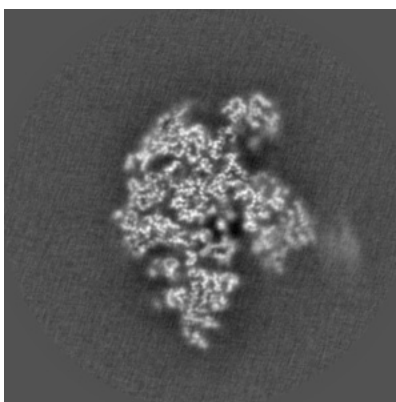


Z Index: 165

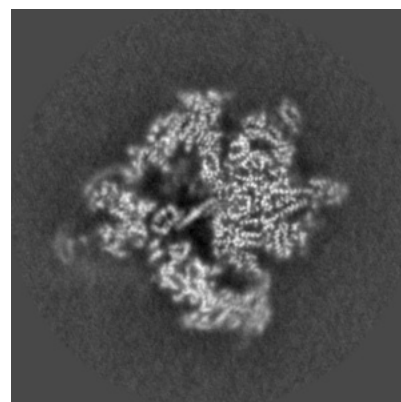
### 6.3.2 Raw map



X Index: 154



Y Index: 156

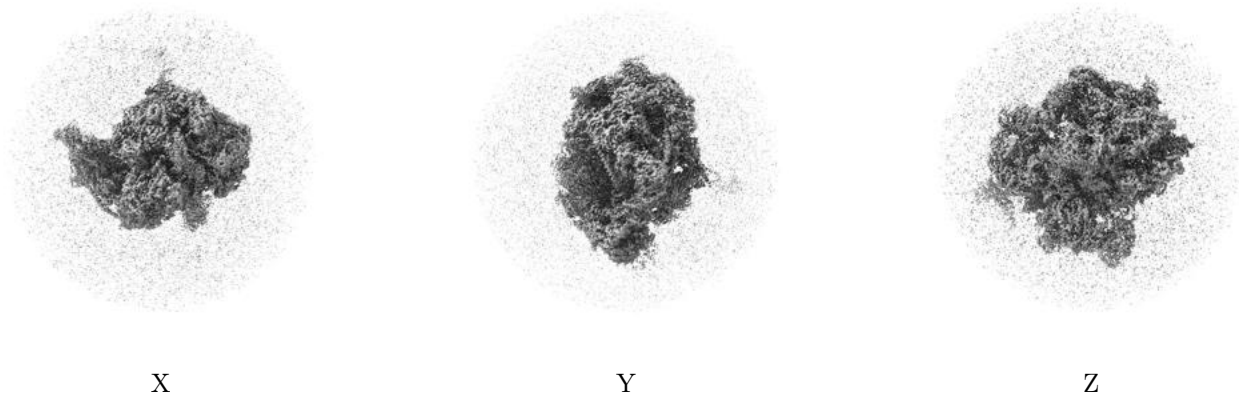


Z Index: 174

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.



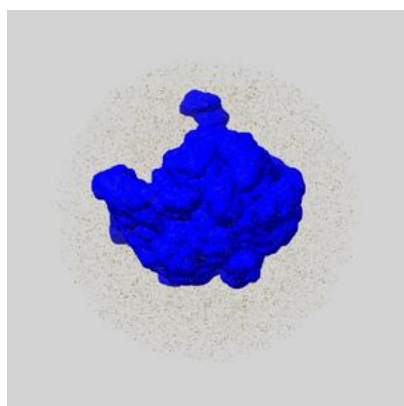
## 6.5 Mask visualisation [i](#)

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

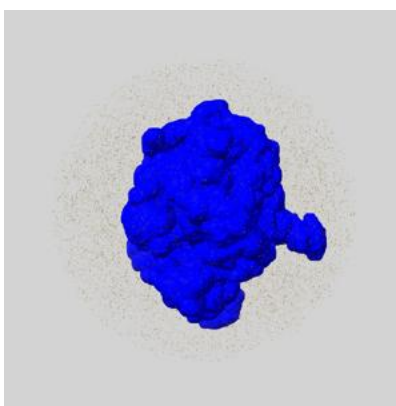
A mask typically either:

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

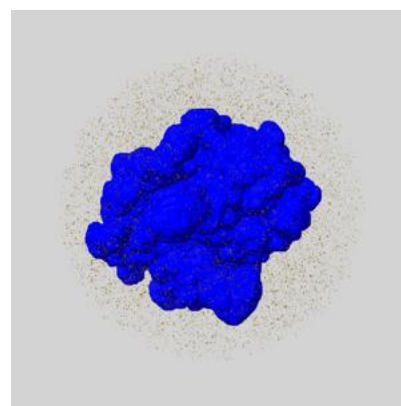
### 6.5.1 emd\_12527\_msk\_1.map [i](#)



X



Y

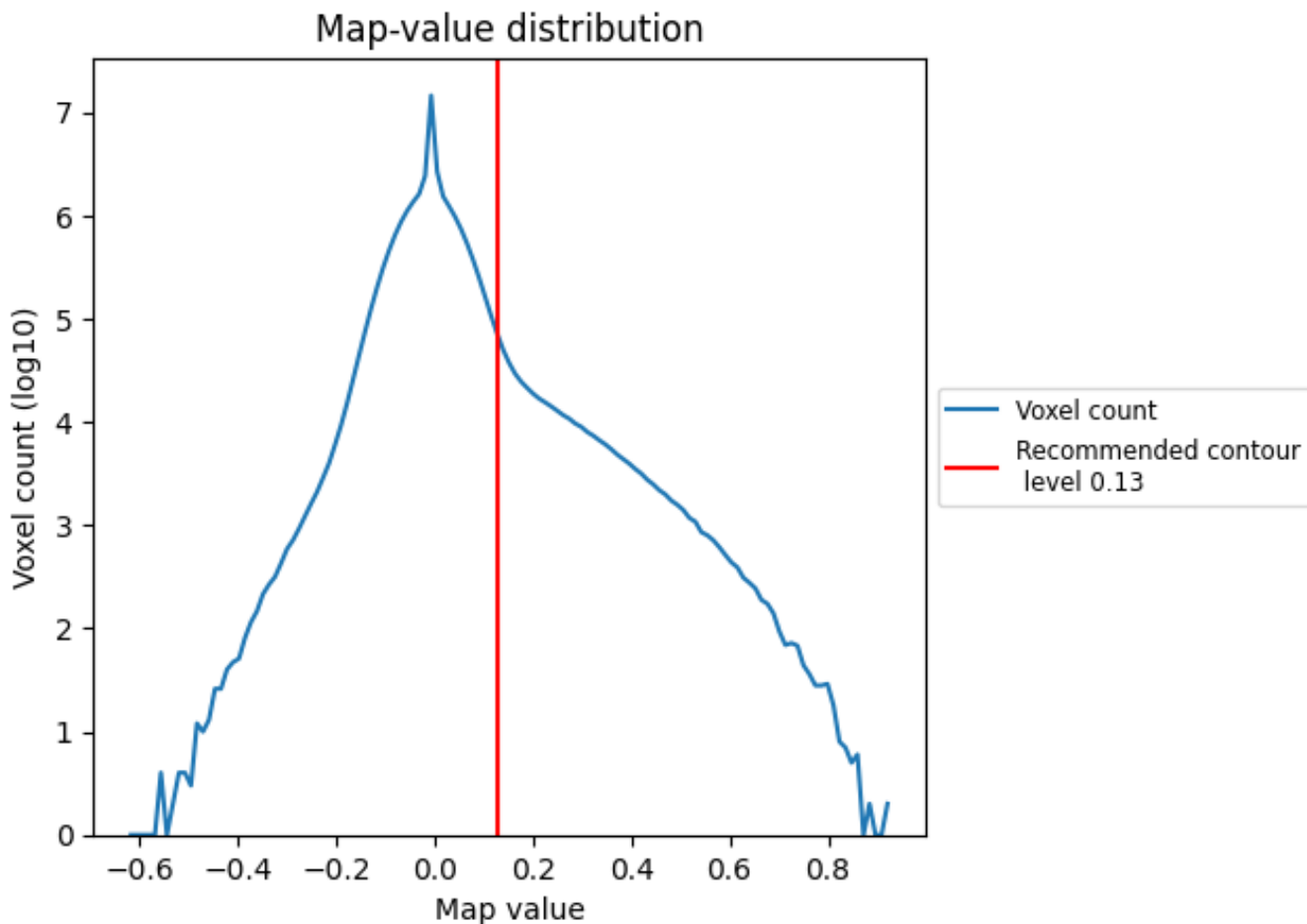


Z

## 7 Map analysis [i](#)

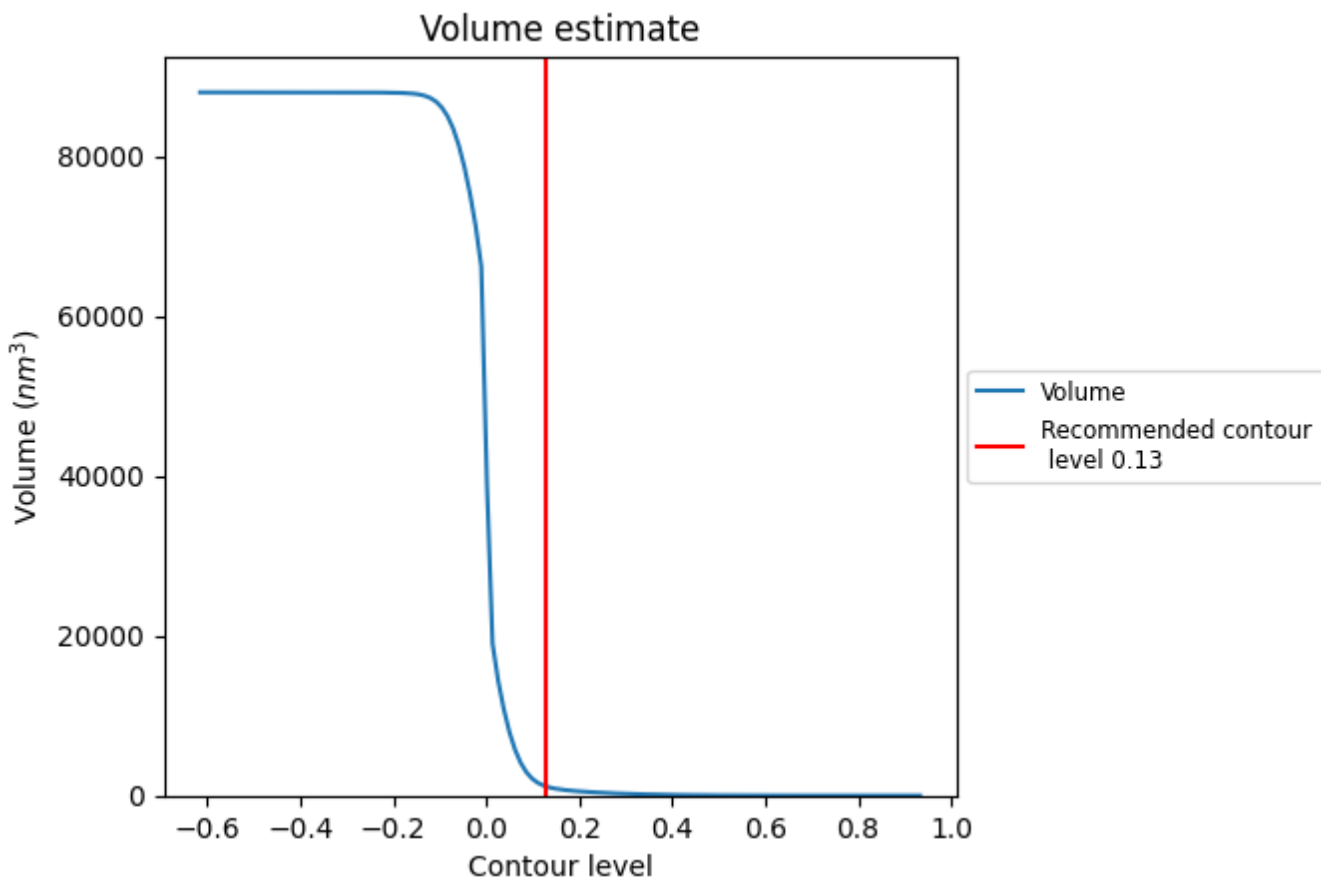
This section contains the results of statistical analysis of the map.

### 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.

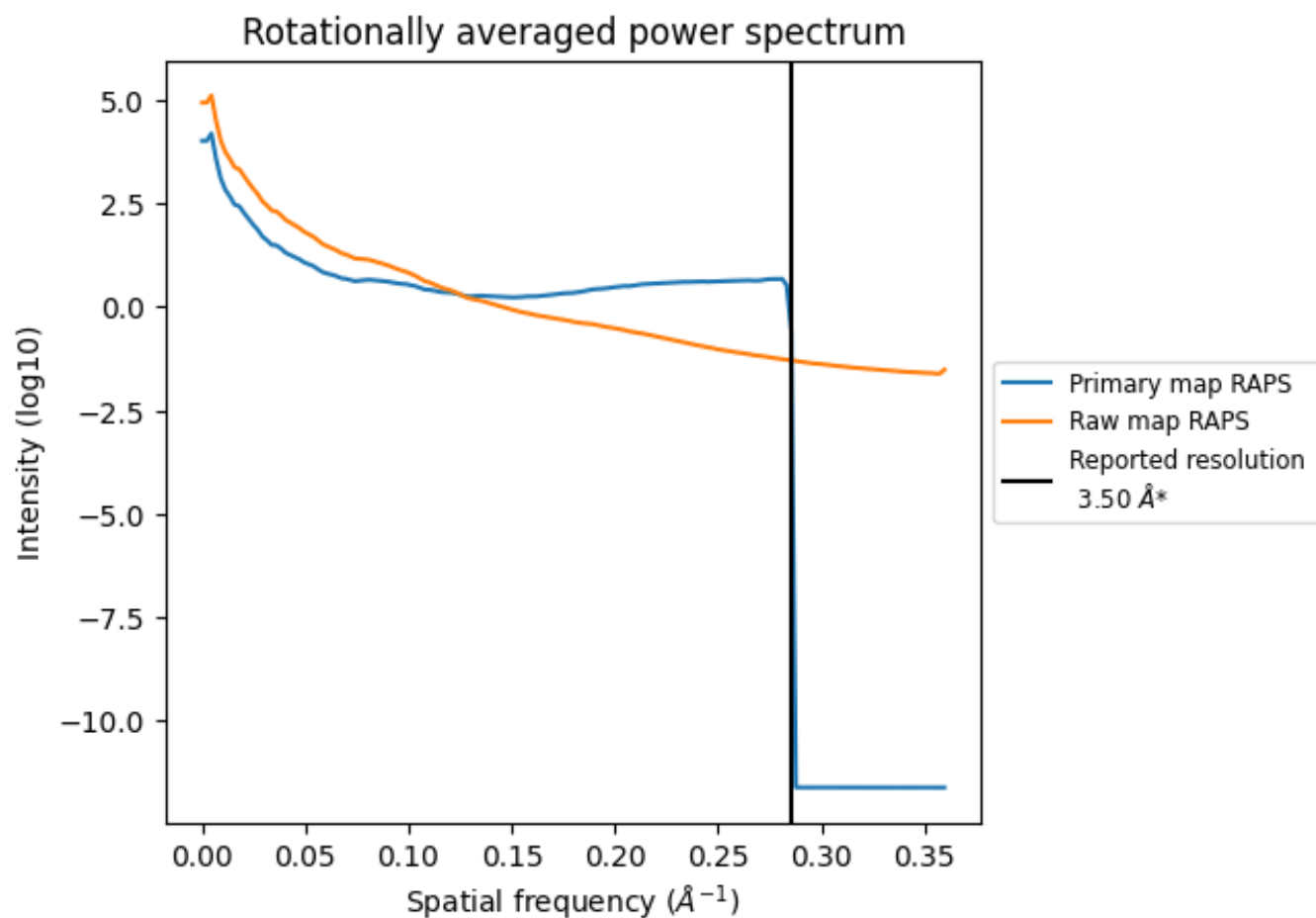
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $1125 \text{ nm}^3$ ; this corresponds to an approximate mass of 1016 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 [i](#)

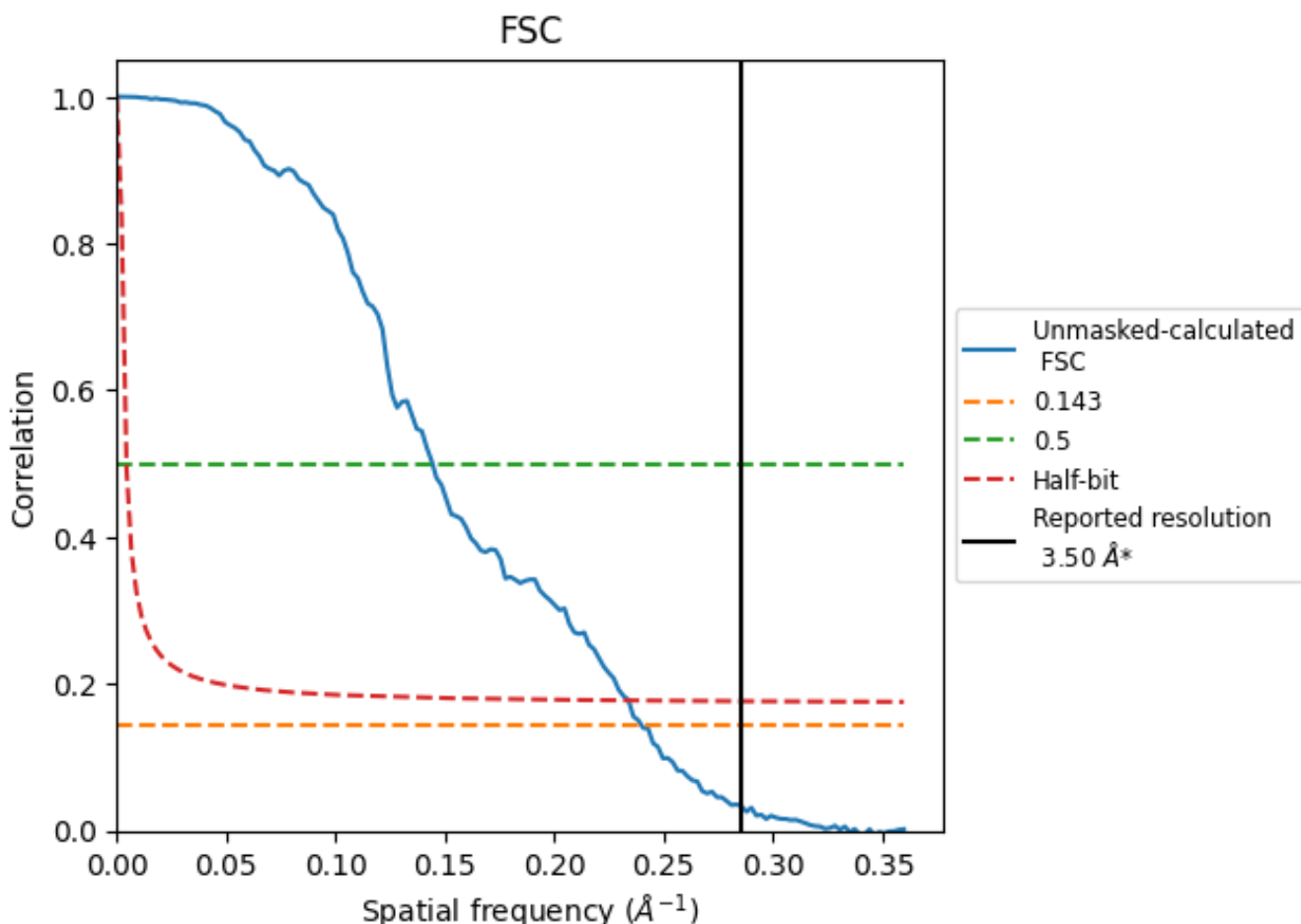


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 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 0.286 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

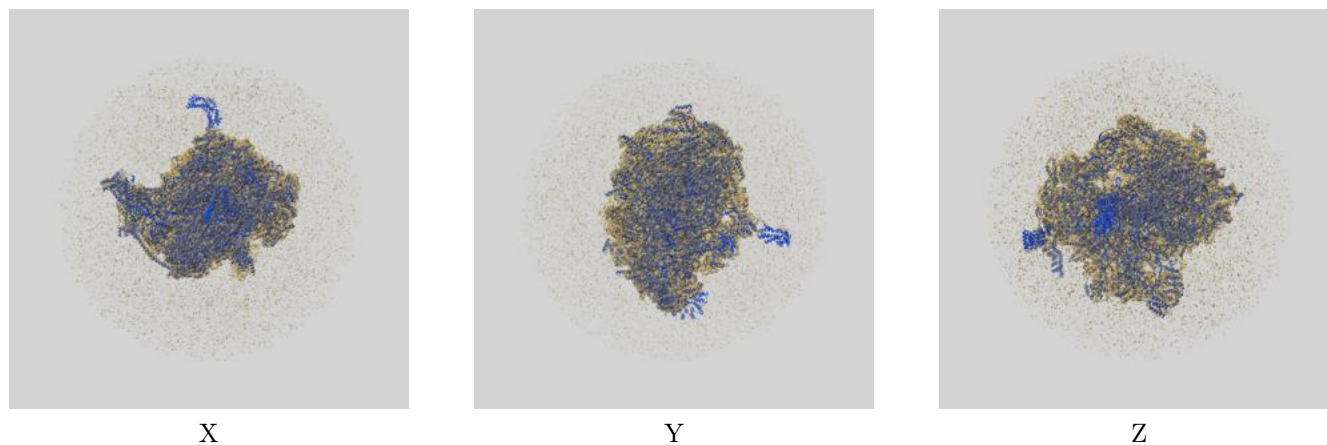
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.17	6.93	4.28

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.5 by more than 10 %

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

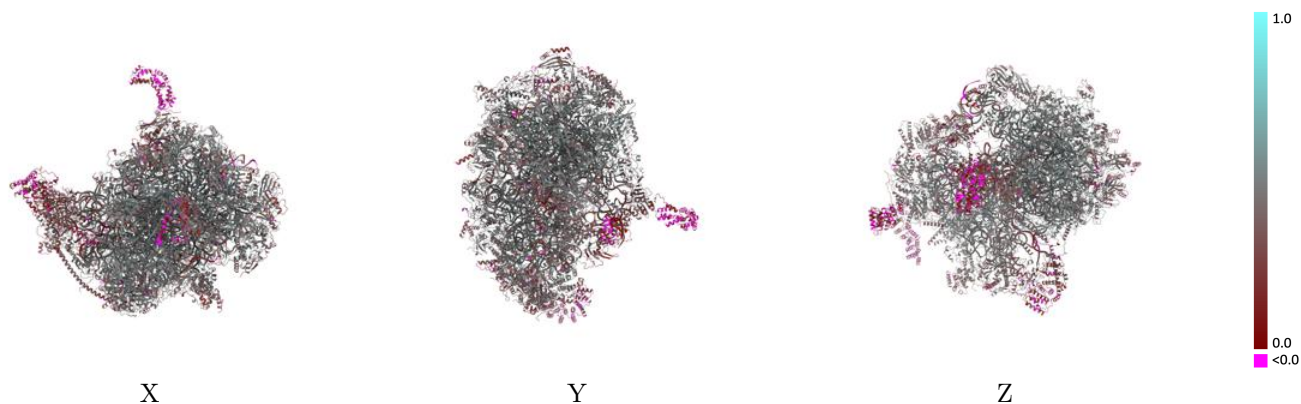
This section contains information regarding the fit between EMDB map EMD-12527 and PDB model 7NQH. Per-residue inclusion information can be found in section [3](#) on page [25](#).

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



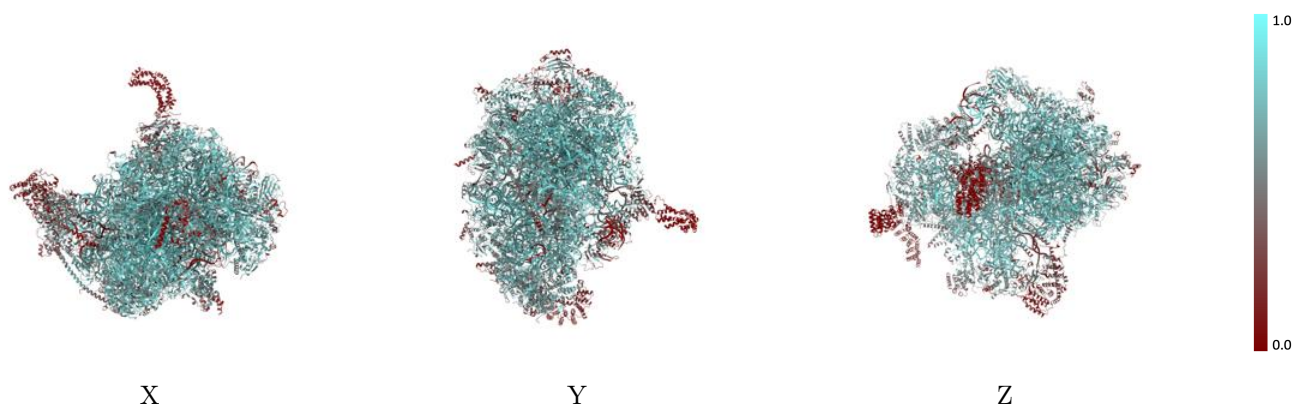
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

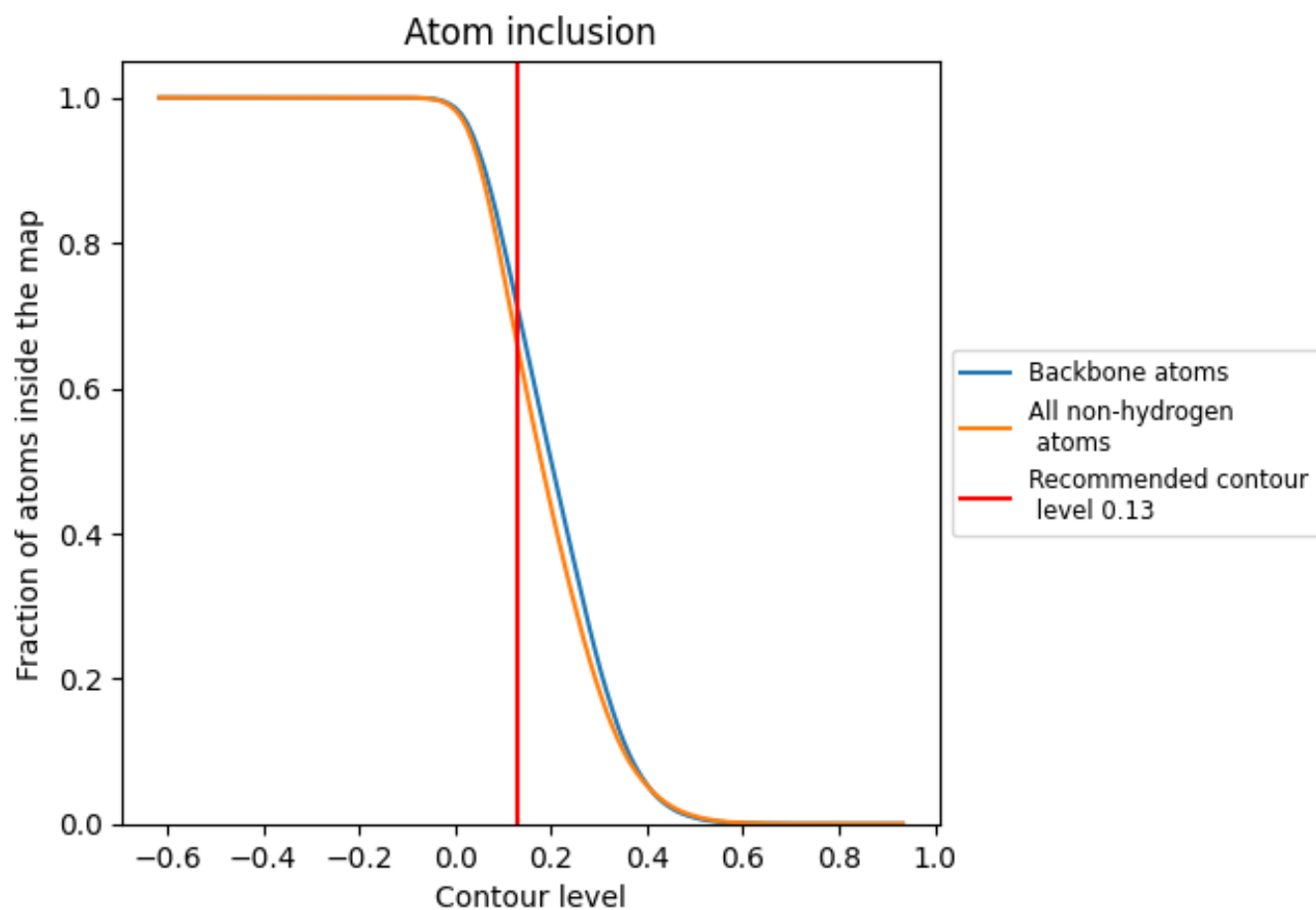
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6583	 0.4210
AA	 0.8039	 0.4400
AB	 0.6814	 0.4490
AC	 0.6635	 0.4700
AE	 0.6060	 0.4490
AF	 0.6656	 0.4600
AG	 0.6420	 0.4280
AI	 0.6023	 0.4120
AJ	 0.6048	 0.4060
AK	 0.6802	 0.4510
AL	 0.7174	 0.4850
AN	 0.7276	 0.4830
AO	 0.5939	 0.4180
AP	 0.5851	 0.4010
AQ	 0.6465	 0.4440
AR	 0.6727	 0.4640
AU	 0.7221	 0.4760
AV	 0.6402	 0.3540
AX	 0.8032	 0.4770
AZ	 0.4889	 0.2550
Aa	 0.4687	 0.3540
Ab	 0.5094	 0.3780
Ac	 0.6379	 0.4300
Ad	 0.5413	 0.3620
Ae	 0.2311	 0.1960
Af	 0.6021	 0.4340
Ag	 0.6045	 0.3830
Ah	 0.5420	 0.3590
Ai	 0.6285	 0.4340
Aj	 0.4024	 0.3200
Ak	 0.5698	 0.3960
Am	 0.5987	 0.4200
An	 0.6787	 0.4730
Ao	 0.1210	 0.1730
Ap	 0.5865	 0.4050





































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Chain	Atom inclusion	Q-score
B0	 0.7779	 0.5170
B1	 0.5976	 0.4480
B2	 0.6954	 0.4680
B3	 0.7571	 0.5040
B4	 0.6196	 0.3890
B5	 0.7164	 0.4780
B6	 0.4423	 0.4050
B7	 0.8211	 0.5380
B8	 0.7892	 0.5150
B9	 0.8224	 0.5150
BA	 0.8227	 0.4640
BB	 0.5378	 0.2700
BD	 0.7462	 0.4970
BE	 0.7434	 0.4830
BF	 0.7563	 0.4890
BI	 0.5353	 0.4050
BJ	 0.3539	 0.3030
BK	 0.1986	 0.2230
BL	 0.5048	 0.3960
BN	 0.7711	 0.5030
BO	 0.7241	 0.4860
BP	 0.7289	 0.4800
BQ	 0.7246	 0.4780
BR	 0.7502	 0.4890
BS	 0.7442	 0.4790
BT	 0.6616	 0.4460
BU	 0.7579	 0.4980
BV	 0.7347	 0.4920
BW	 0.7494	 0.5070
BX	 0.6596	 0.4470
BY	 0.4732	 0.3890
Ba	 0.7032	 0.4580
Bb	 0.6972	 0.4330
Bc	 0.6257	 0.4140
Bd	 0.5540	 0.3790
Be	 0.5922	 0.4160
Bf	 0.6754	 0.4500
Bg	 0.7467	 0.4940
Bh	 0.6811	 0.4430
Bi	 0.4041	 0.3380
Bj	 0.4730	 0.3060
Bk	 0.5670	 0.3950

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Chain	Atom inclusion	Q-score
Bl	 0.7343	 0.4650
Bm	 0.3945	 0.3760
Bn	 0.7717	 0.4990
Bo	 0.6911	 0.4400
Bp	 0.4019	 0.3190
Bq	 0.4057	 0.3030
Bt	 0.7668	 0.4970
Bu	 0.4991	 0.3670
Bv	 0.4968	 0.3860
Bw	 0.7003	 0.4570
Bx	 0.6900	 0.4400
CL	 0.0158	 0.0630
DL	 0.0000	 -0.0080
EL	 0.0090	 0.0110
FL	 0.0047	 0.0280
GL	 0.0094	 0.0460
HL	 0.0000	 0.0150