Full wwPDB EM Validation Report ⓘ

Nov 6, 2023 – 07:01 am GMT

PDB ID	:	8OIQ
EMDB ID	:	EMD-16896
Title	:	39S mammalian mitochondrial large ribosomal subunit with mtRF1 and P-site tRNA
Authors	:	Saurer, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.; Ban, N.
Deposited on	:	2023-03-23
Resolution	:	3.50 Å(reported)
Based on initial models	:	7QI4, 7NQH, .

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

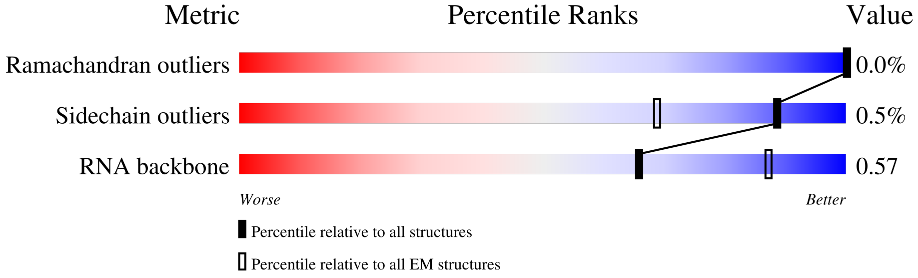
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

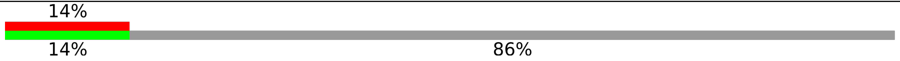
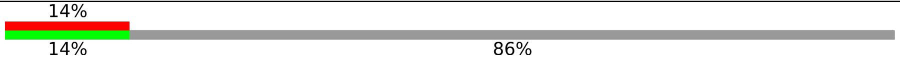
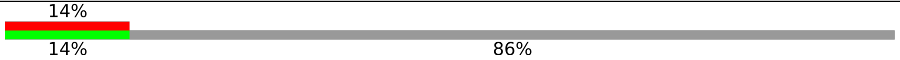
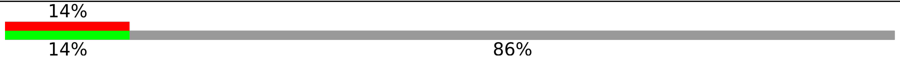
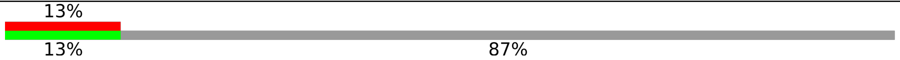
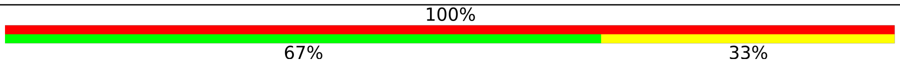
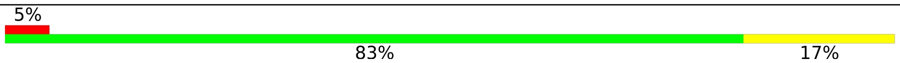
The reported resolution of this entry is 3.50 Å.

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 >=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 <=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	B1	198	
1	B2	198	
1	B3	198	
1	B4	198	
1	B5	198	
1	B6	198	
2	B7	3	
3	B8	1571	

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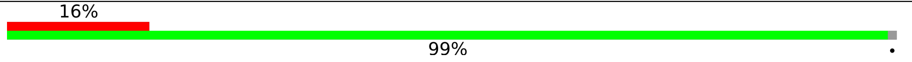
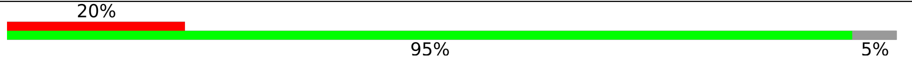
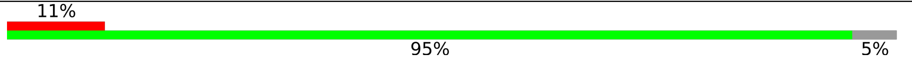
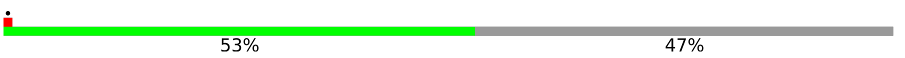
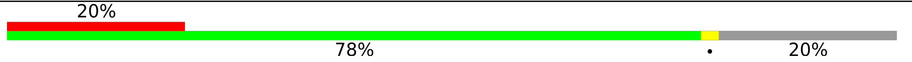
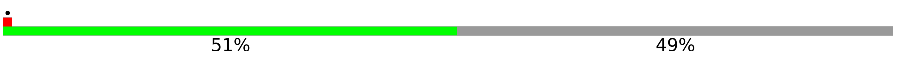
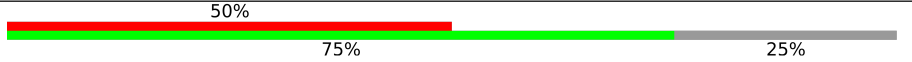
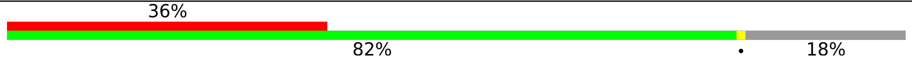
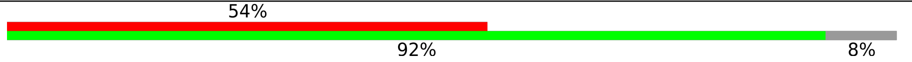
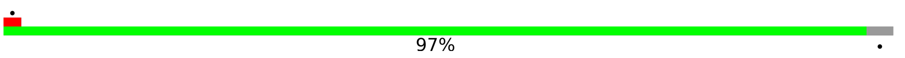
Mol	Chain	Length	Quality of chain
4	B9	73	
5	BA	210	
6	BB	150	
7	BC	216	
8	BD	148	
9	BE	256	
10	BF	250	
11	BG	161	
12	BH	207	
13	BI	65	
14	BJ	95	
15	BK	188	
16	BL	306	
17	BM	399	
18	BN	294	
19	BO	268	
20	BP	257	
21	BQ	192	
22	BR	197	
23	BS	325	
24	BT	296	
25	BU	251	
26	BV	169	
27	BW	188	
28	BX	303	

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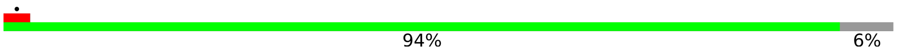
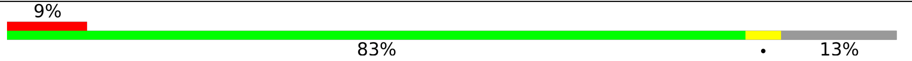
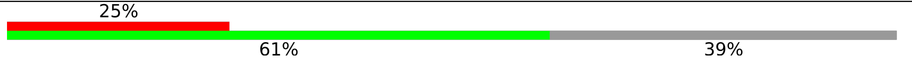
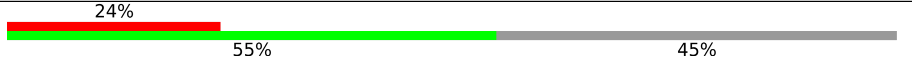
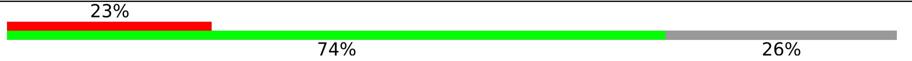
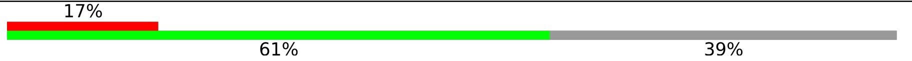
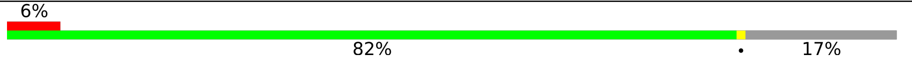
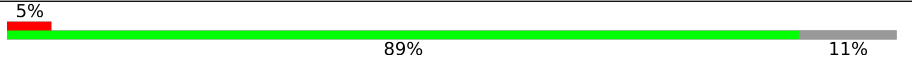
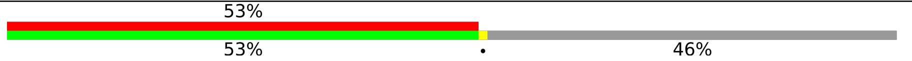
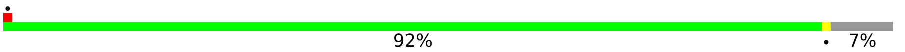
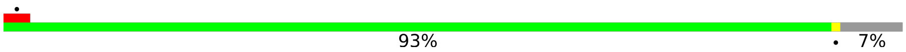
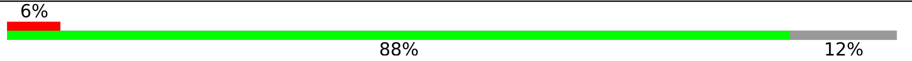
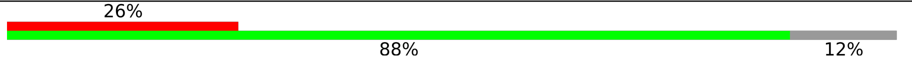
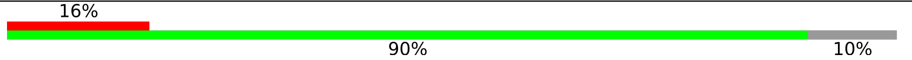
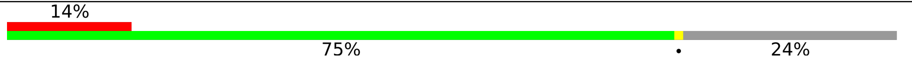
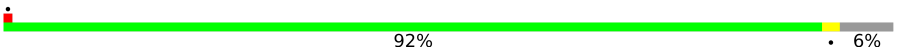
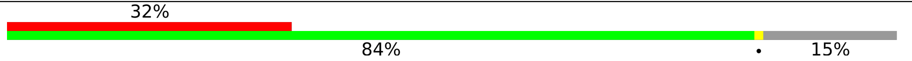
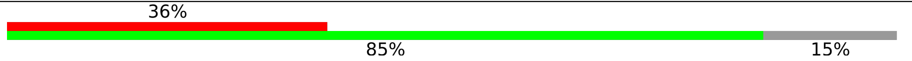
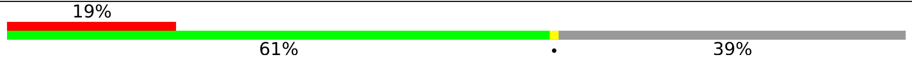
Mol	Chain	Length	Quality of chain
29	BY	149	
30	BZ	209	
31	Ba	160	
32	Bb	112	
33	Bc	138	
34	Bd	126	
35	Be	102	
36	Bf	205	
37	Bg	222	
38	Bh	196	
39	Bi	433	
40	Bj	304	
41	Bl	100	
42	Bm	423	
43	Bn	380	
44	Bo	334	
45	Bp	162	
46	Bq	135	
47	Br	142	
48	Bs	159	
49	Bt	332	
50	Bu	306	
51	Bv	279	
52	Bw	269	
53	Bx	166	

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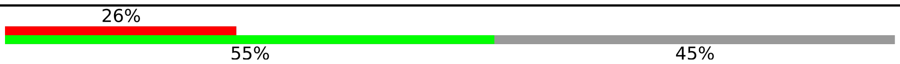
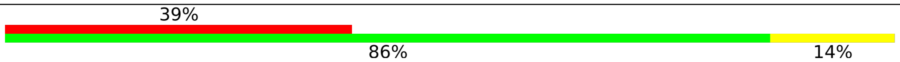
Mol	Chain	Length	Quality of chain
54	By	198	
55	Bz	128	
56	AG	71	
57	Aa	474	

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 112981 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
1	B1	45	Total C N O 317 203 52 62	0	0
1	B2	27	Total C N O 213 137 33 43	0	0
1	B3	28	Total C N O 222 143 35 44	0	0
1	B4	27	Total C N O 213 137 33 43	0	0
1	B5	27	Total C N O 213 137 33 43	0	0
1	B6	26	Total C N O 205 131 32 42	0	0

- Molecule 2 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	B7	3	Total C N O P 62 28 11 20 3	0	0

- Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	B8	1571	Total C N O P 33427 15015 6087 10754 1571	0	0

- Molecule 4 is a RNA chain called CP Phe-tRNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	B9	73	Total C N O P S 1560 703 283 500 73 1	0	0

- Molecule 5 is a protein called uL22m.

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

- Molecule 6 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	BB	149	1184	754	227	201	2	0	0

- Molecule 7 is a protein called uL24m.

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

- Molecule 8 is a protein called Mitochondrial ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	BD	112	867	558	158	148	3	0	0

- Molecule 9 is a protein called Mitochondrial ribosomal protein L28.

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

- Molecule 10 is a protein called Mitochondrial ribosomal protein L47.

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

- Molecule 11 is a protein called uL30m.

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

- Molecule 12 is a protein called Mitochondrial ribosomal protein L32.

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

- Molecule 13 is a protein called bL33m.

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

- Molecule 14 is a protein called Mitochondrial ribosomal protein L34.

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

- Molecule 15 is a protein called 39S ribosomal protein L35, mitochondrial.

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

- Molecule 16 is a protein called Mitochondrial ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	BL	240	1860	1160	371	319	10	0	0

- Molecule 17 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BM	307	2420	1554	426	430	10	0	0

- Molecule 18 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	BN	250	2019	1299	370	344	6	1	0

- Molecule 19 is a protein called Mitochondrial ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BO	202	Total	C	N	O	S	0	0
			1660	1059	311	286	4		

- Molecule 20 is a protein called Mitochondrial ribosomal protein L10.

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

- Molecule 21 is a protein called Mitochondrial ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BQ	176	Total	C	N	O	S	0	0
			1339	851	243	243	2		

- Molecule 22 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BR	177	Total	C	N	O	S	0	0
			1447	928	258	254	7		

- Molecule 23 is a protein called Mitochondrial ribosomal protein L14.

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

- Molecule 24 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 25 is a protein called uL16m.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 26 is a protein called bL17m.

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

- Molecule 27 is a protein called Mitochondrial ribosomal protein L18.

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

- Molecule 28 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BX	225	Total 1855	C 1187	N 321	O 338	S 9	0	0

- Molecule 29 is a protein called Mitochondrial ribosomal protein L20.

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

- Molecule 30 is a protein called Mitochondrial ribosomal protein L21.

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

- Molecule 31 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 32 is a protein called Mitochondrial ribosomal protein L53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Bb	97	745	461	143	135	6	0	0

- Molecule 33 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Bc	84	716	458	128	127	3	0	0

- Molecule 34 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Bd	69	571	353	117	98	3	0	0

- Molecule 35 is a protein called Mitochondrial ribosomal protein L57.

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

- Molecule 36 is a protein called mL62 (ICT1).

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

- Molecule 37 is a protein called mL64.

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

- Molecule 38 is a protein called Mitochondrial ribosomal protein S18A.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Bj	164	1325	853	217	251	4	0	0

- Molecule 41 is a protein called Ribosomal protein.

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

- Molecule 42 is a protein called Mitochondrial ribosomal protein L37.

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

- Molecule 43 is a protein called Mitochondrial ribosomal protein L38.

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

- Molecule 44 is a protein called Mitochondrial ribosomal protein L39.

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

- Molecule 45 is a protein called Mitochondrial ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Bp	143	1202	757	217	227	1	0	0

- Molecule 46 is a protein called Mitochondrial ribosomal protein L41.

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

- Molecule 47 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Br	108	906	570	167	165	4	0	0

- Molecule 48 is a protein called 39S ribosomal protein L43, mitochondrial isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Bs	150	1185	738	227	217	3	0	0

- Molecule 49 is a protein called mL44.

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

- Molecule 50 is a protein called Mitochondrial ribosomal protein L45.

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

- Molecule 51 is a protein called Mitochondrial ribosomal protein L46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Bv	238	1948	1240	338	363	7	0	0

- Molecule 52 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Bw	165	1295	825	224	241	5	0	0

- Molecule 53 is a protein called 39S ribosomal protein L49, mitochondrial.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bx	59	ARG	LYS	conflict	UNP A0A287A0K2

- Molecule 54 is a protein called Mitochondrial ribosomal protein L50.

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

- Molecule 55 is a protein called Mitochondrial ribosomal protein L51.

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

- Molecule 56 is a RNA chain called P-site Met-tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	AG	71	1502	673	264	494	71	0	0

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 57 is a protein called Peptide chain release factor 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	Aa	381	3120	1943	572	592	13	1	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	446	GLY	-	expression tag	UNP O75570
Aa	447	GLY	-	expression tag	UNP O75570
Aa	448	SER	-	expression tag	UNP O75570
Aa	449	GLY	-	expression tag	UNP O75570
Aa	450	GLY	-	expression tag	UNP O75570
Aa	451	SER	-	expression tag	UNP O75570
Aa	452	GLY	-	expression tag	UNP O75570
Aa	453	ASP	-	expression tag	UNP O75570
Aa	454	TYR	-	expression tag	UNP O75570
Aa	455	LYS	-	expression tag	UNP O75570
Aa	456	ASP	-	expression tag	UNP O75570
Aa	457	HIS	-	expression tag	UNP O75570
Aa	458	ASP	-	expression tag	UNP O75570
Aa	459	GLY	-	expression tag	UNP O75570
Aa	460	ASP	-	expression tag	UNP O75570
Aa	461	TYR	-	expression tag	UNP O75570
Aa	462	LYS	-	expression tag	UNP O75570
Aa	463	ASP	-	expression tag	UNP O75570
Aa	464	HIS	-	expression tag	UNP O75570
Aa	465	ASP	-	expression tag	UNP O75570
Aa	466	ILE	-	expression tag	UNP O75570
Aa	467	ASP	-	expression tag	UNP O75570
Aa	468	TYR	-	expression tag	UNP O75570
Aa	469	LYS	-	expression tag	UNP O75570
Aa	470	ASP	-	expression tag	UNP O75570
Aa	471	ASP	-	expression tag	UNP O75570
Aa	472	ASP	-	expression tag	UNP O75570
Aa	473	ASP	-	expression tag	UNP O75570
Aa	474	LYS	-	expression tag	UNP O75570

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
58	B8	193	Total Mg 193 193	0
58	B9	1	Total Mg 1 1	0
58	BL	2	Total Mg 2 2	0
58	BM	2	Total Mg 2 2	0
58	BT	1	Total Mg 1 1	0

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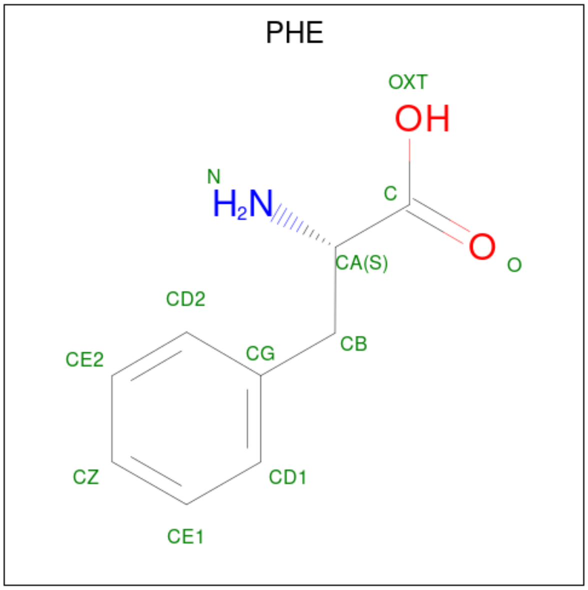
Mol	Chain	Residues	Atoms	AltConf
58	BV	3	Total Mg 3 3	0
58	Be	1	Total Mg 1 1	0
58	Bq	1	Total Mg 1 1	0
58	Bx	1	Total Mg 1 1	0

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
59	B8	26	Total K 26 26	0
59	BL	1	Total K 1 1	0
59	BU	1	Total K 1 1	0
59	BW	1	Total K 1 1	0
59	Be	1	Total K 1 1	0

- Molecule 60 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).

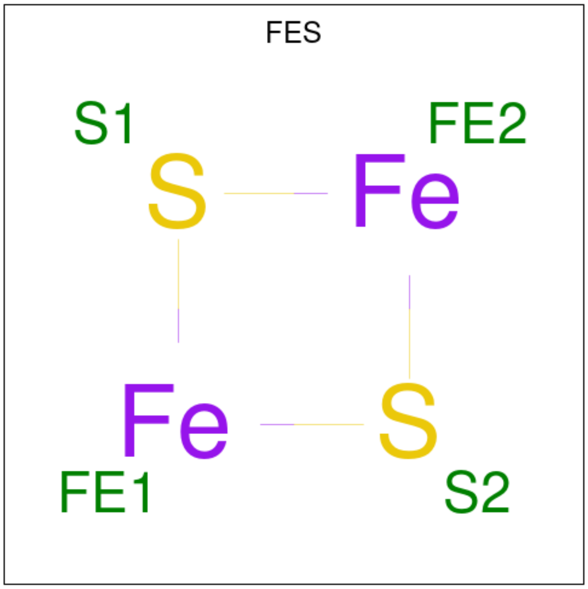


Mol	Chain	Residues	Atoms	AltConf
60	B9	1	Total C N O 11 9 1 1	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

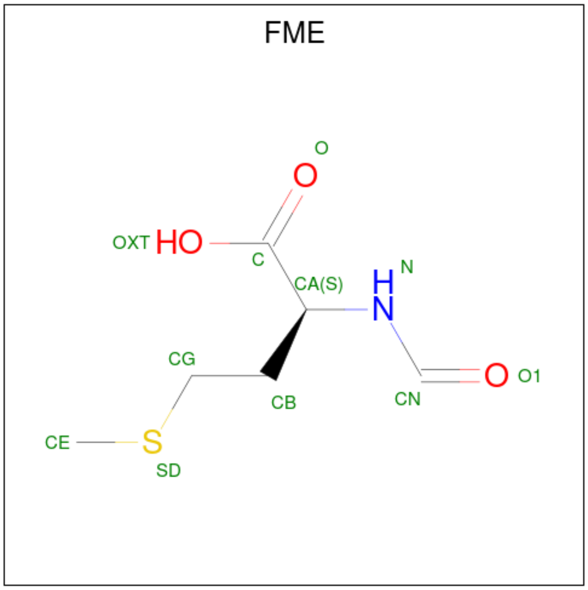
Mol	Chain	Residues	Atoms	AltConf
61	BH	1	Total Zn 1 1	0
61	Bl	1	Total Zn 1 1	0

- Molecule 62 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
62	Bh	1	Total Fe S 4 2 2	0

- Molecule 63 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



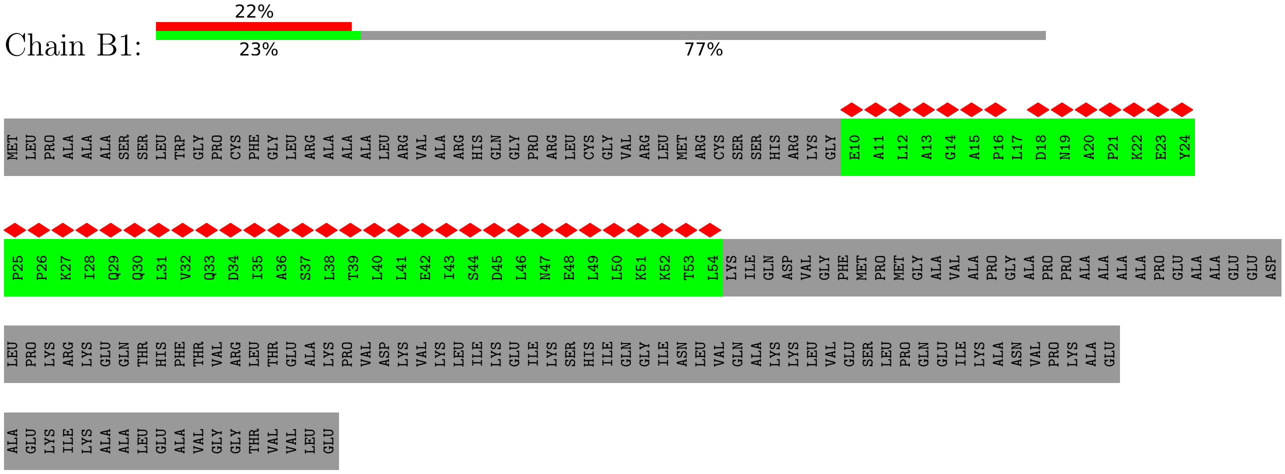
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
63	AG	1	10	6	1	2	1	0

3 Residue-property plots ⓘ

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

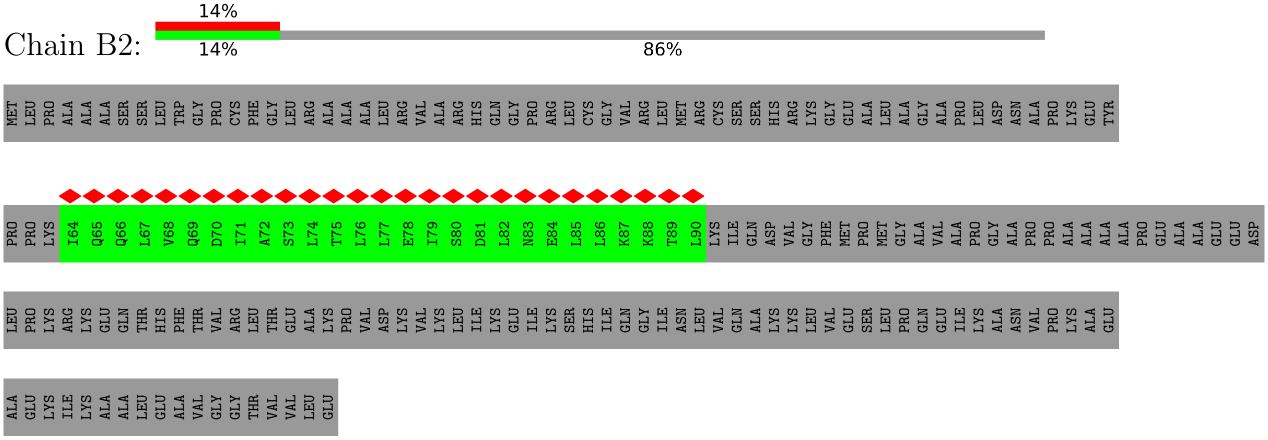
- Molecule 1: Mitochondrial ribosomal protein L12

Chain B1:



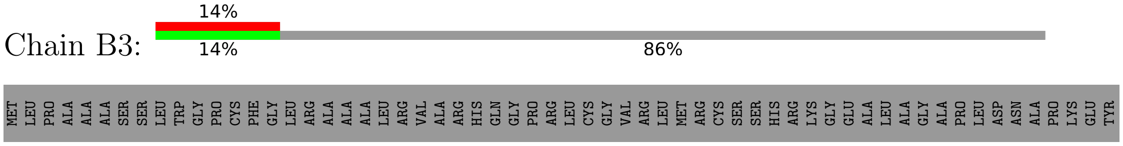
- Molecule 1: Mitochondrial ribosomal protein L12

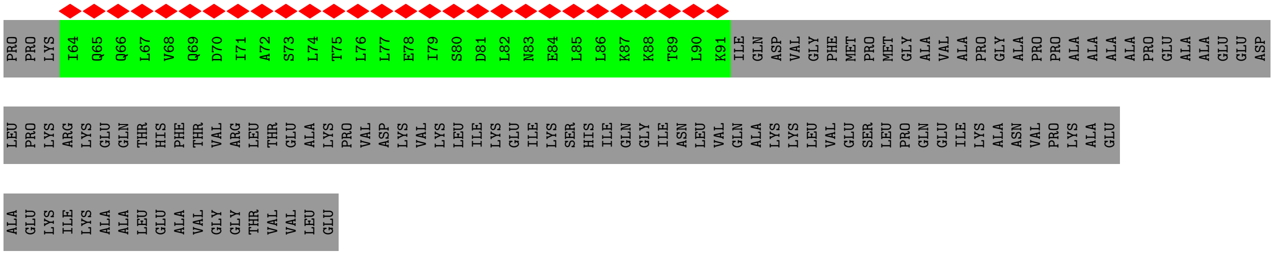
Chain B2:



- Molecule 1: Mitochondrial ribosomal protein L12

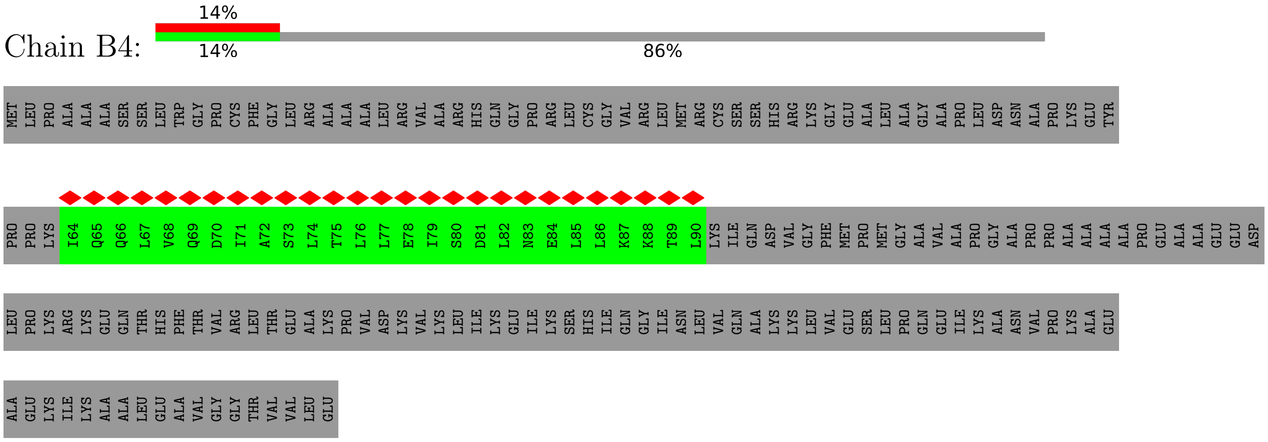
Chain B3:





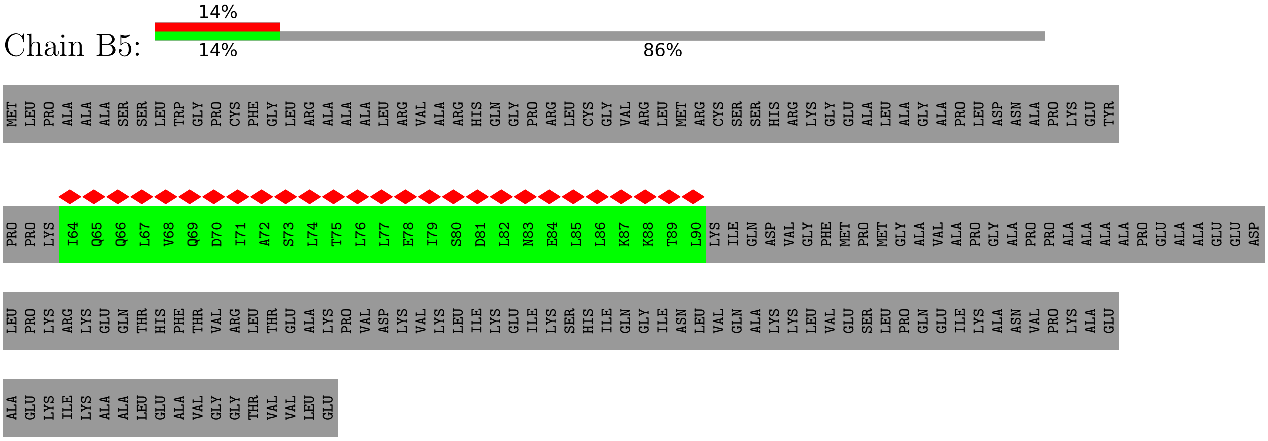
- Molecule 1: Mitochondrial ribosomal protein L12

Chain B4:



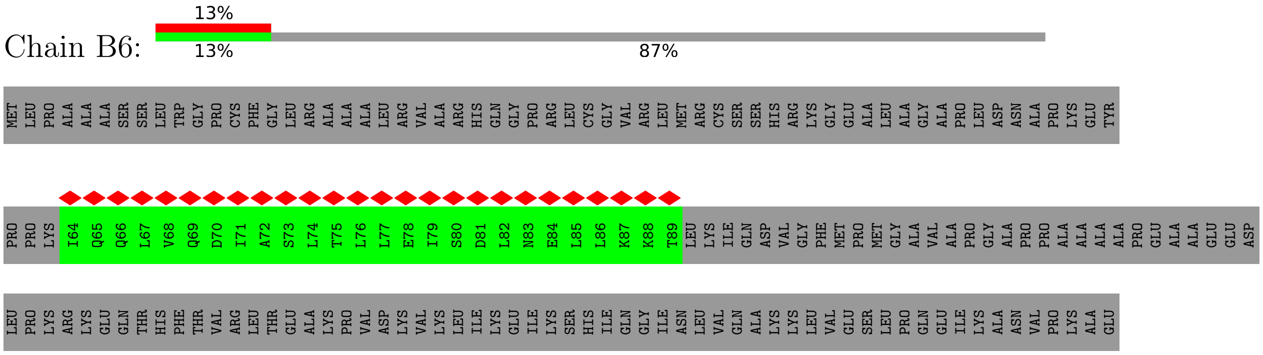
- Molecule 1: Mitochondrial ribosomal protein L12

Chain B5:



- Molecule 1: Mitochondrial ribosomal protein L12

Chain B6:

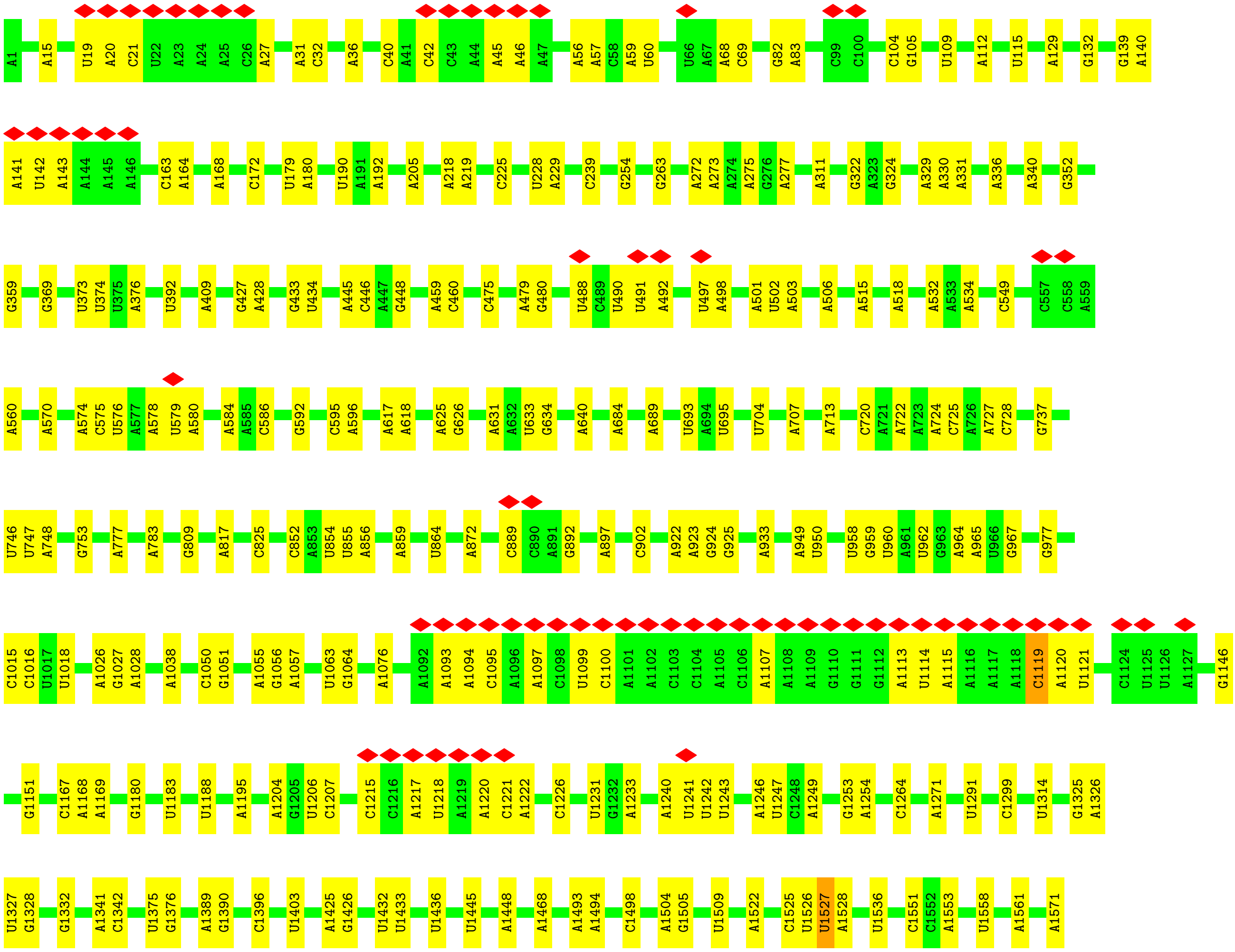


- Molecule 2: E-site tRNA

Chain B7:

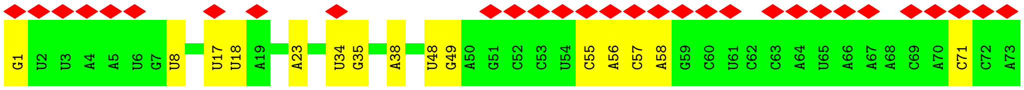
- Molecule 3: 16S rRNA

Chain B8:

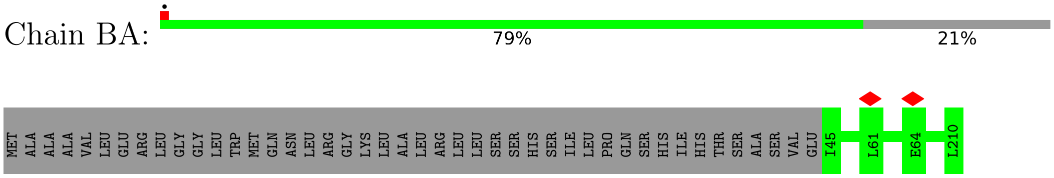


- Molecule 4: CP Phe-tRNA

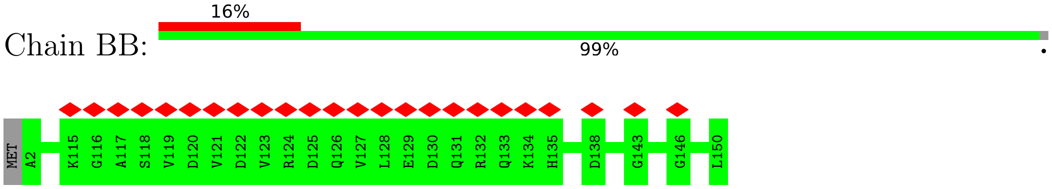
Chain B9:



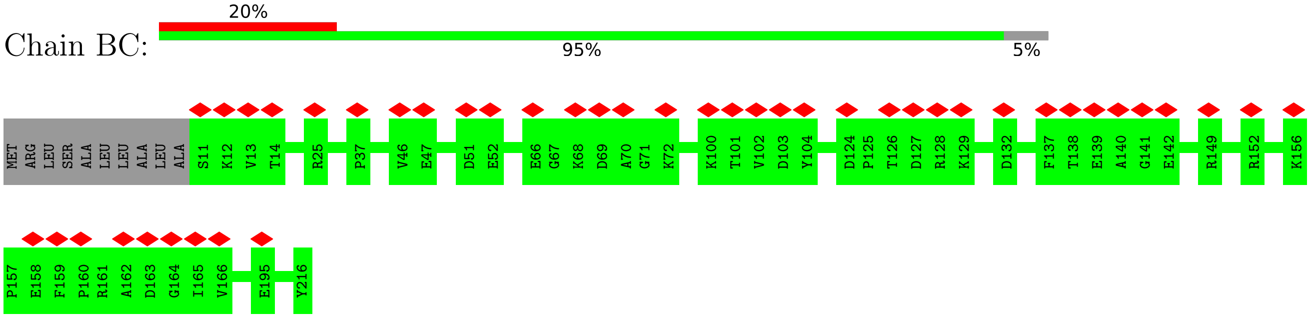
- Molecule 5: uL22m



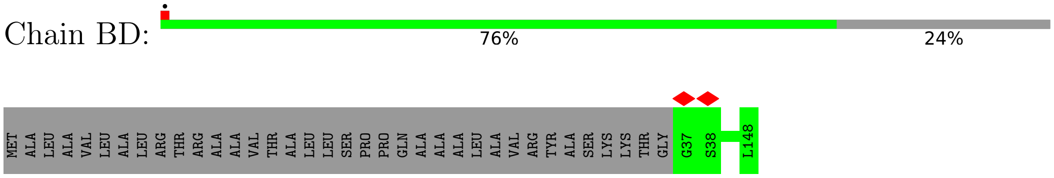
- Molecule 6: 39S ribosomal protein L23, mitochondrial



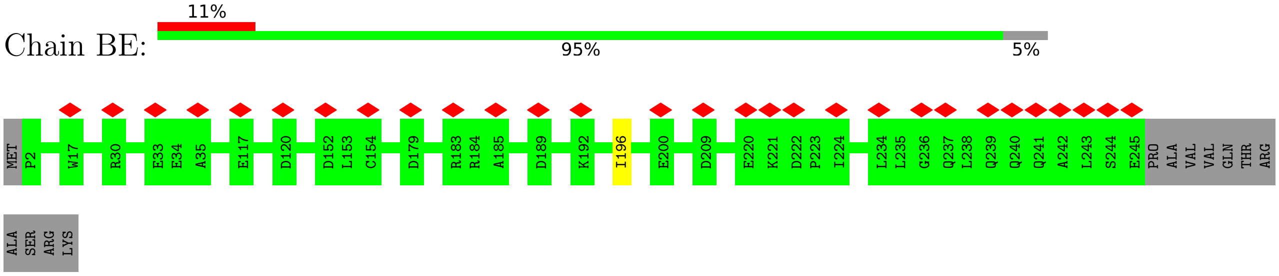
- Molecule 7: uL24m



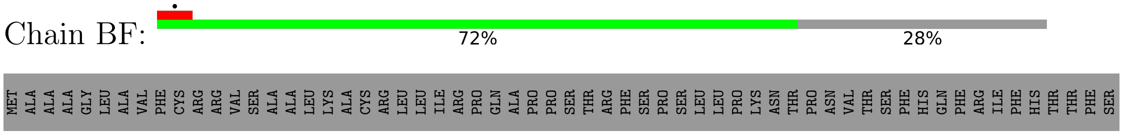
- Molecule 8: Mitochondrial ribosomal protein L27

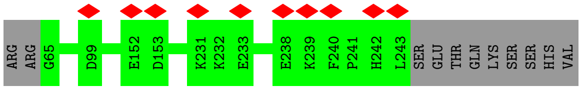


- Molecule 9: Mitochondrial ribosomal protein L28

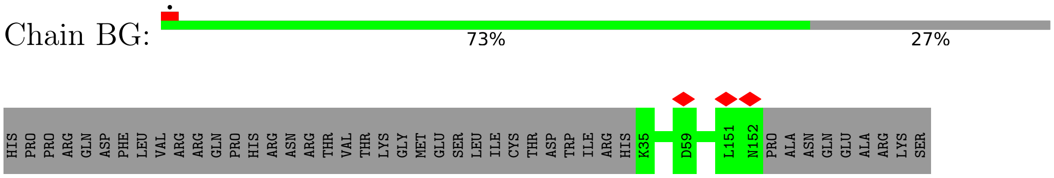


- Molecule 10: Mitochondrial ribosomal protein L47

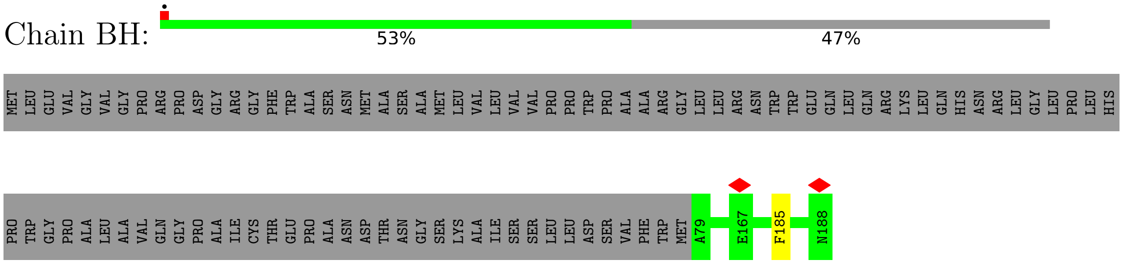




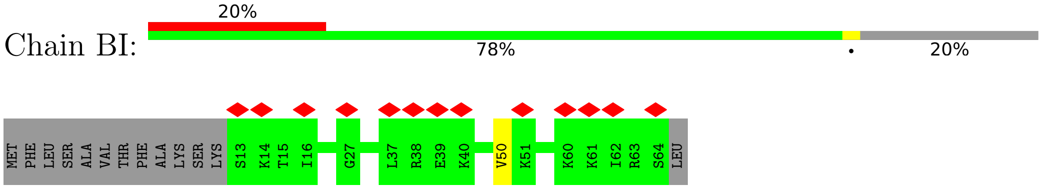
- Molecule 11: uL30m



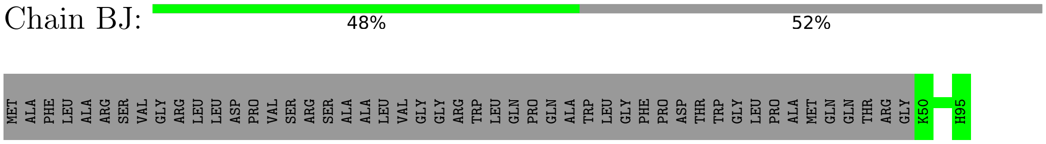
- Molecule 12: Mitochondrial ribosomal protein L32



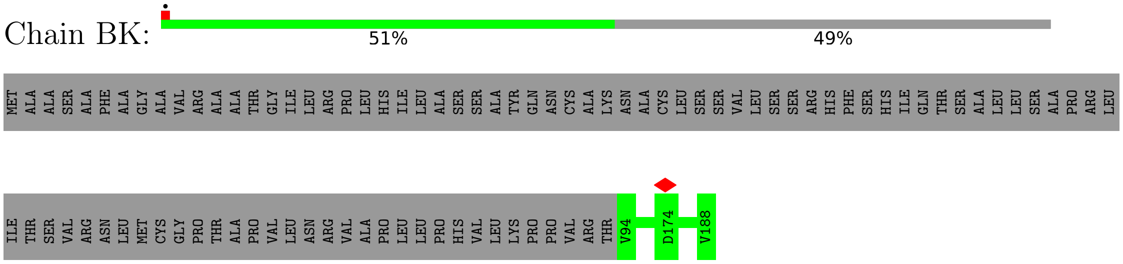
- Molecule 13: bL33m



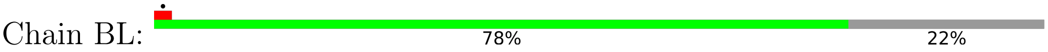
- Molecule 14: Mitochondrial ribosomal protein L34

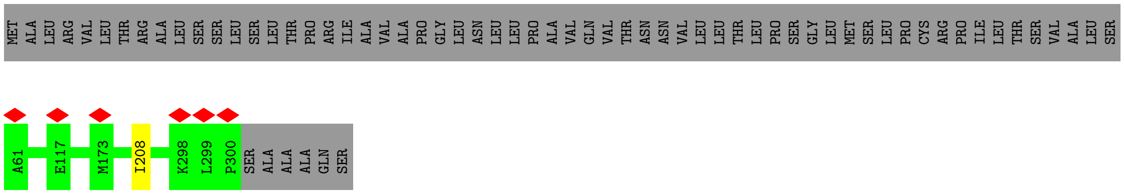


- Molecule 15: 39S ribosomal protein L35, mitochondrial



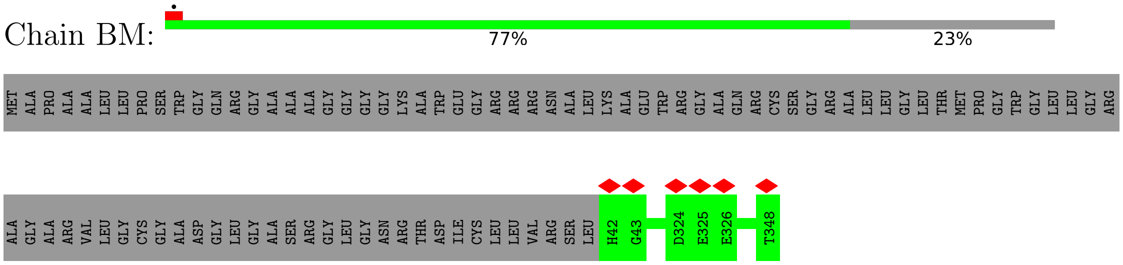
- Molecule 16: Mitochondrial ribosomal protein L2





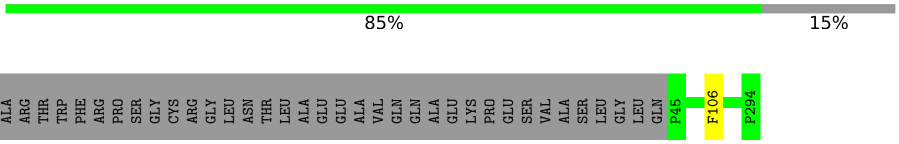
- Molecule 17: ICT1

Chain BM:



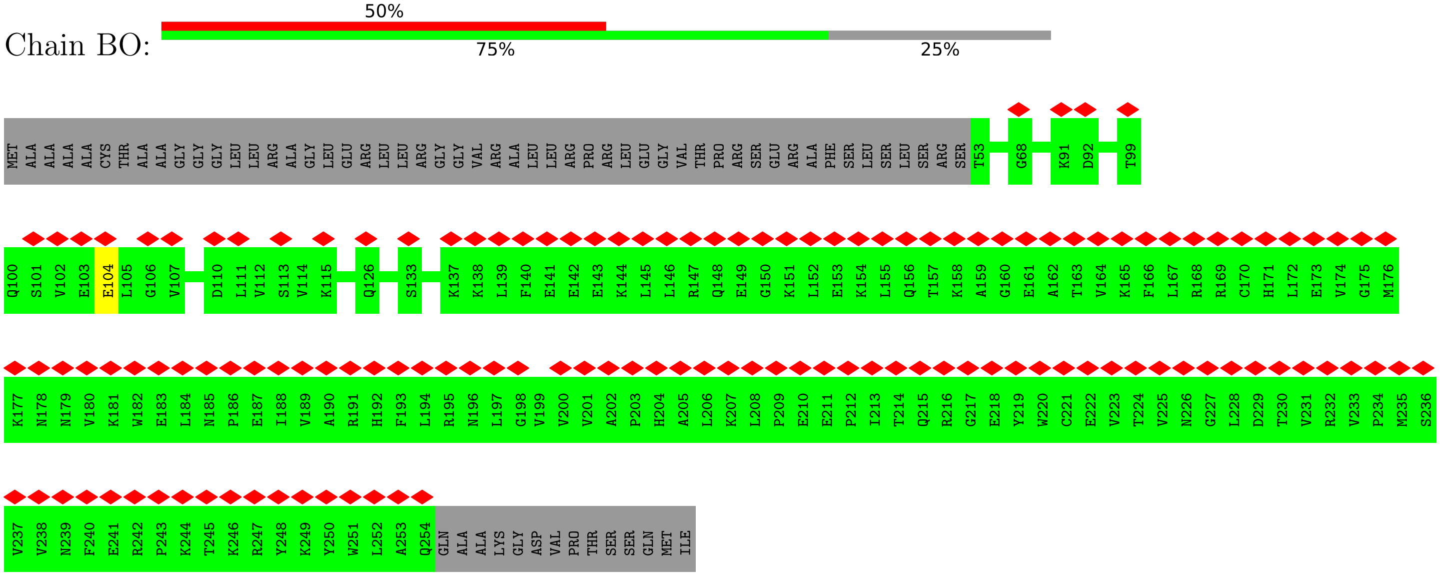
- Molecule 18: Mitochondrial ribosomal protein L4

Chain BN:



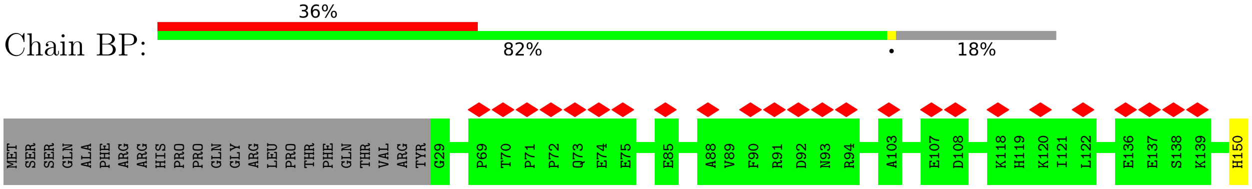
- Molecule 19: Mitochondrial ribosomal protein L9

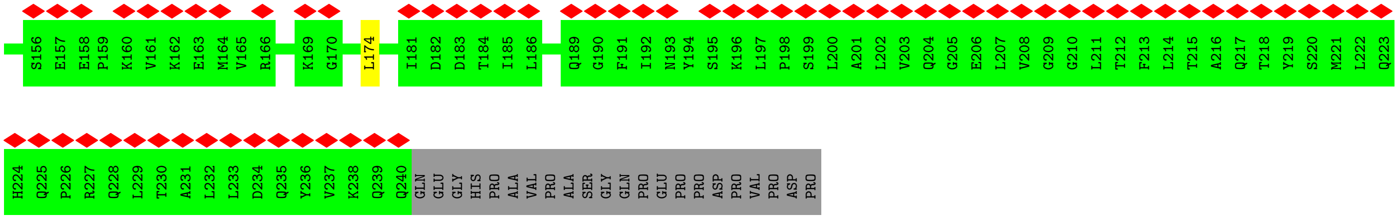
Chain BO:



- Molecule 20: Mitochondrial ribosomal protein L10

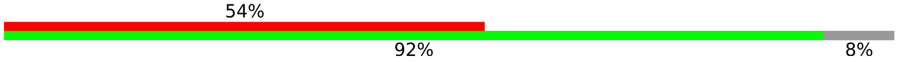
Chain BP:

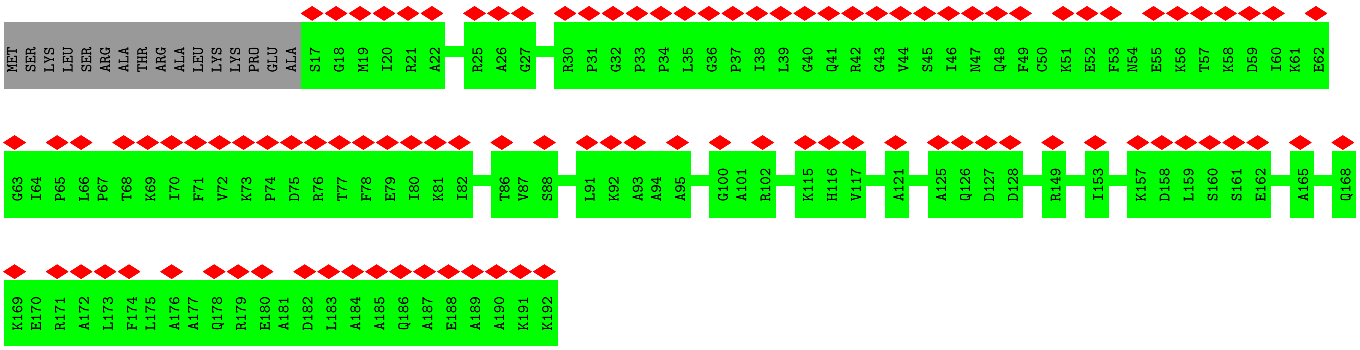




- Molecule 21: Mitochondrial ribosomal protein L11

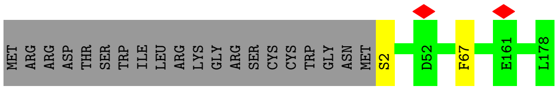
Chain BQ:





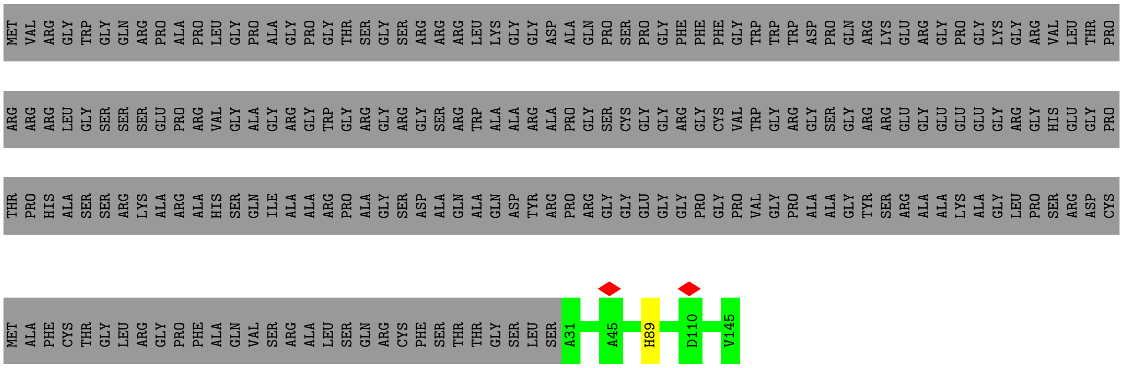
- Molecule 22: 39S ribosomal protein L13, mitochondrial

Chain BR:



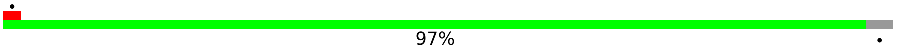
- Molecule 23: Mitochondrial ribosomal protein L14

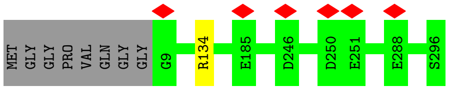
Chain BS:



- Molecule 24: 39S ribosomal protein L15, mitochondrial

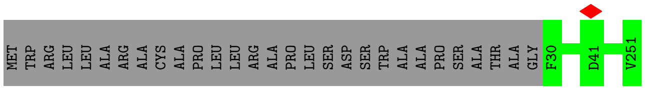
Chain BT:





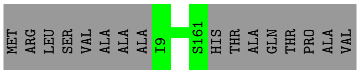
- Molecule 25: uL16m

Chain BU:



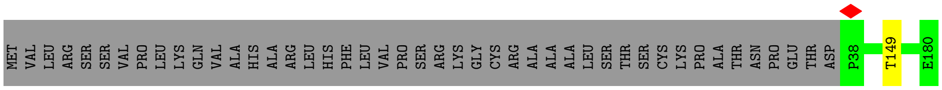
- Molecule 26: bL17m

Chain BV:



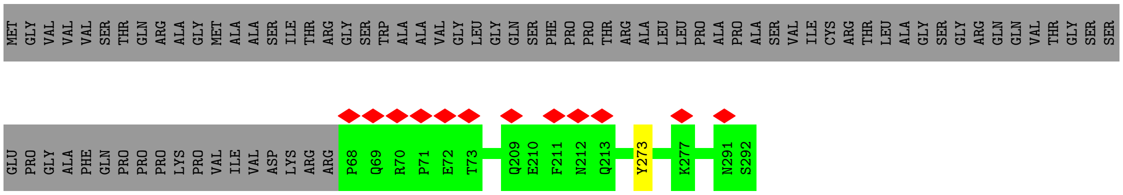
- Molecule 27: Mitochondrial ribosomal protein L18

Chain BW:



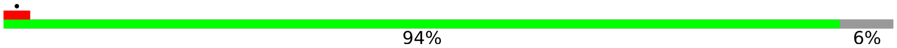
- Molecule 28: 39S ribosomal protein L19, mitochondrial

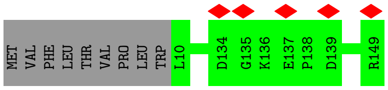
Chain BX:



- Molecule 29: Mitochondrial ribosomal protein L20

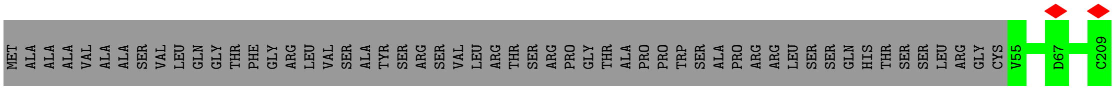
Chain BY:



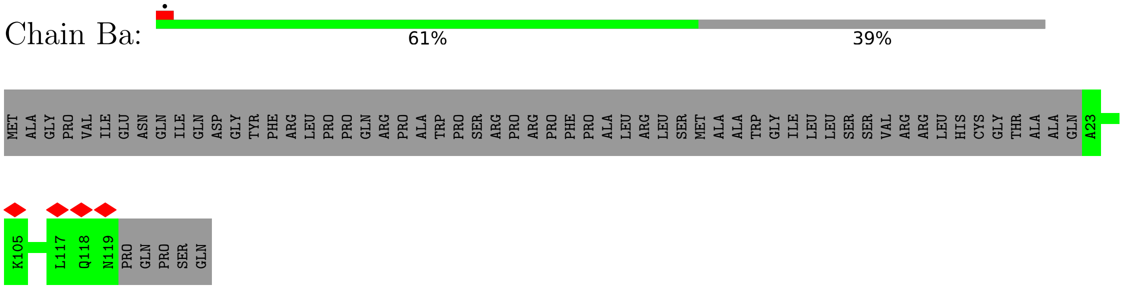


- Molecule 30: Mitochondrial ribosomal protein L21

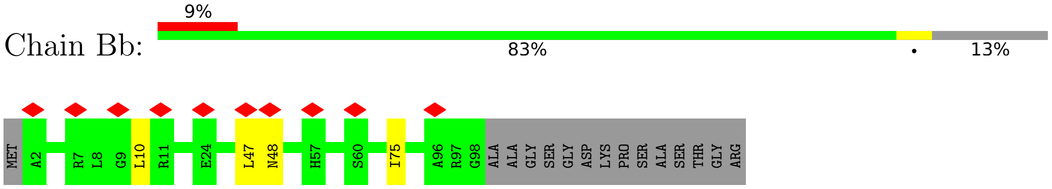
Chain BZ:



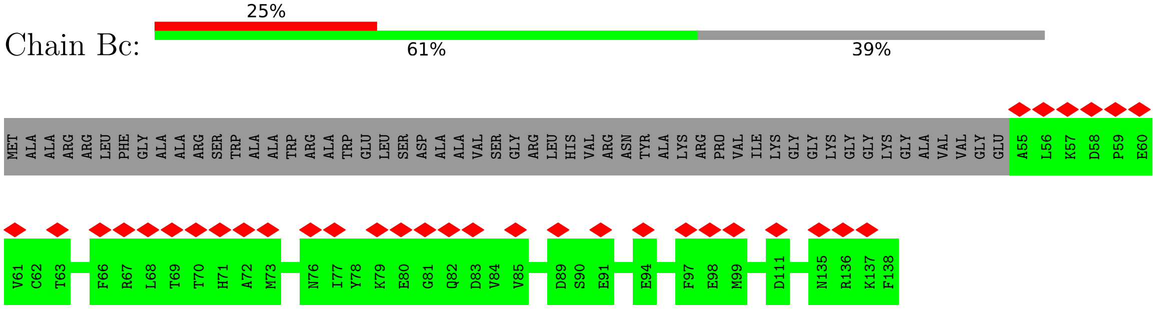
- Molecule 31: 39S ribosomal protein L52, mitochondrial



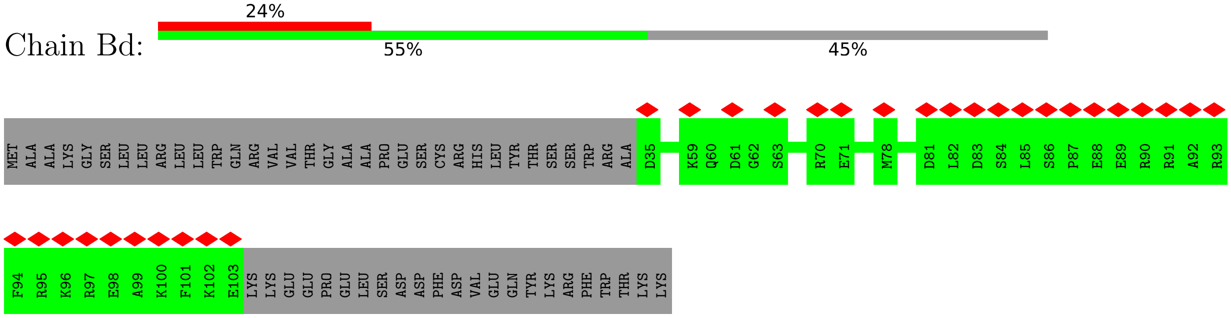
- Molecule 32: Mitochondrial ribosomal protein L53



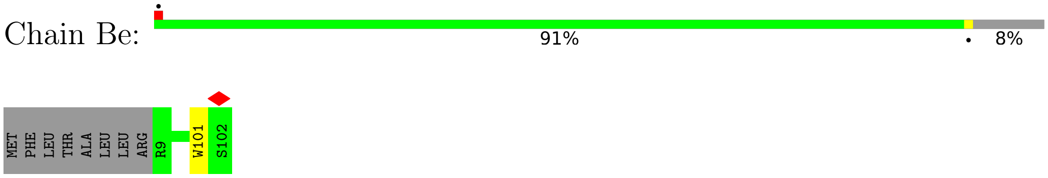
- Molecule 33: mL54



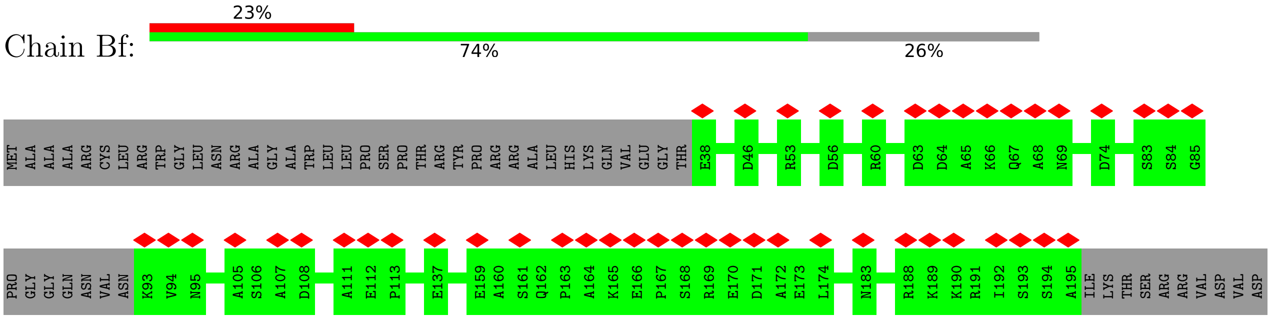
- Molecule 34: bL31m



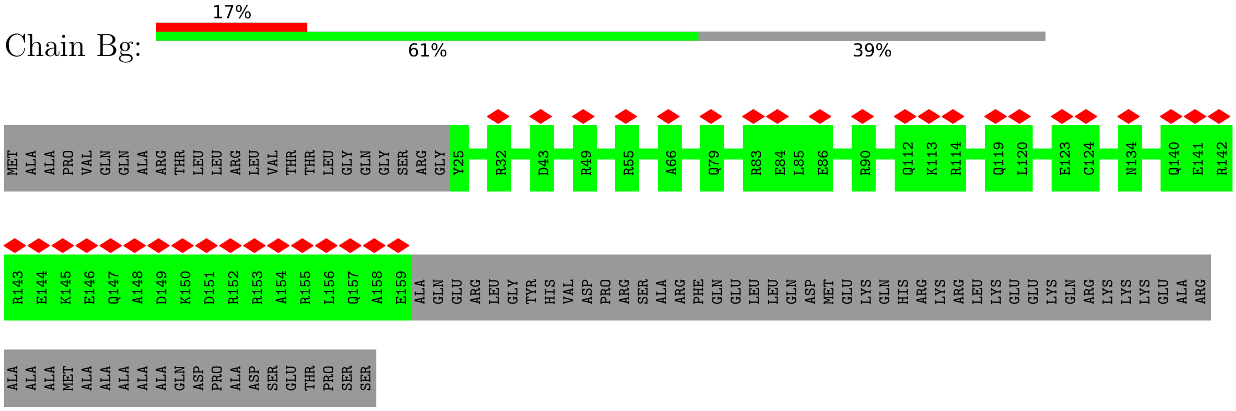
- Molecule 35: Mitochondrial ribosomal protein L57



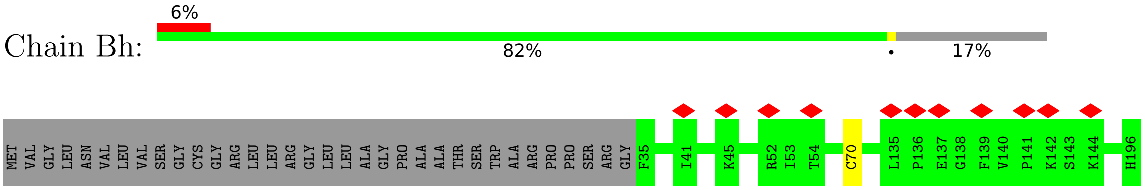
- Molecule 36: mL62 (ICT1)



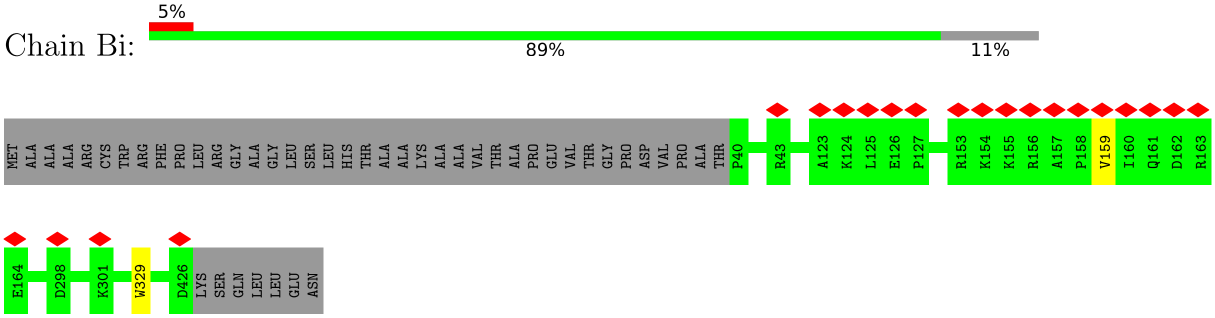
- Molecule 37: mL64



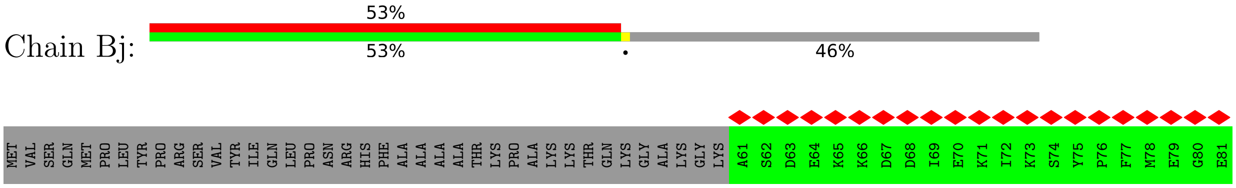
- Molecule 38: Mitochondrial ribosomal protein S18A

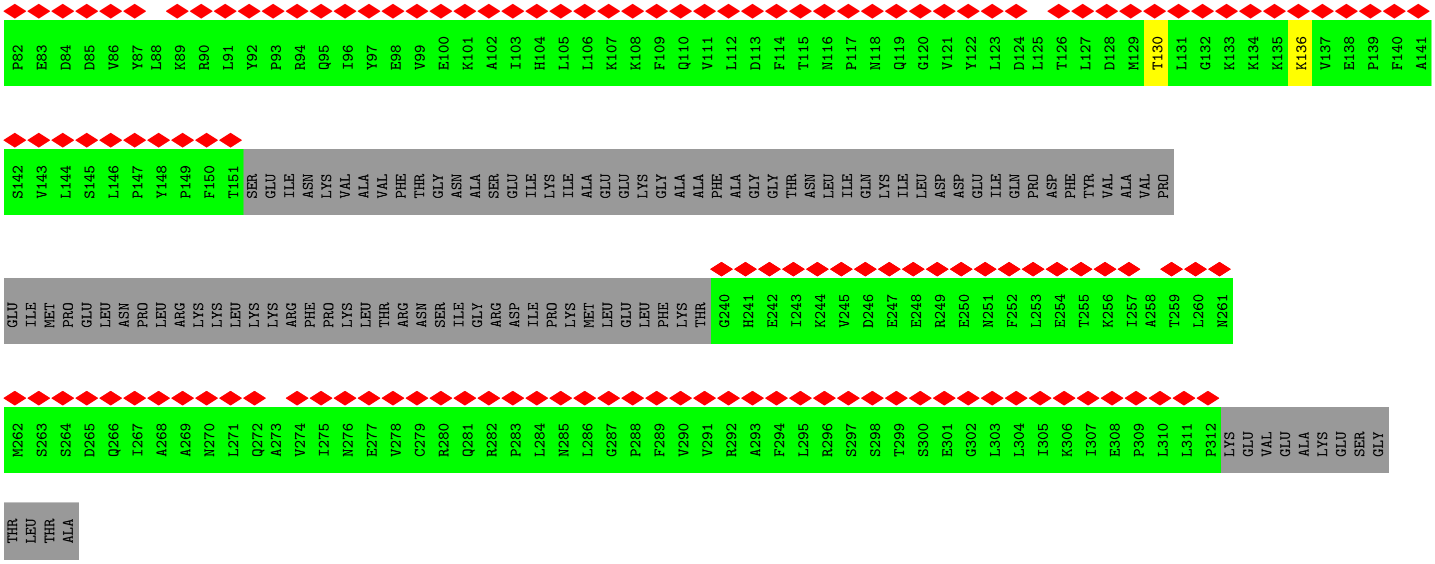


- Molecule 39: 39S ribosomal protein S30, mitochondrial



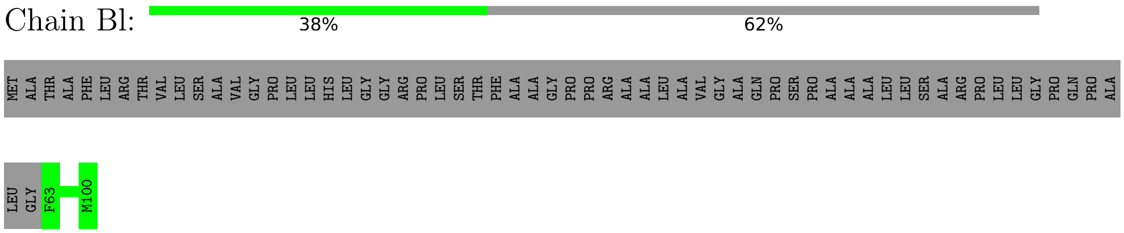
- Molecule 40: 39S ribosomal protein L1, mitochondrial





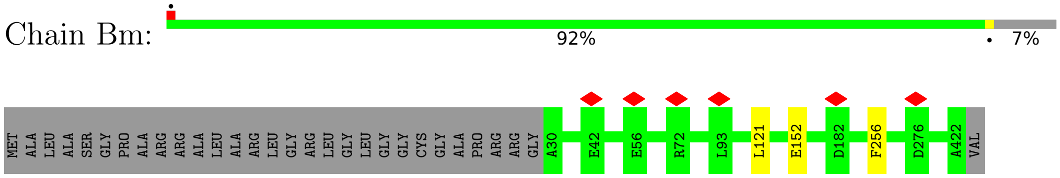
- Molecule 41: Ribosomal protein

Chain Bl:



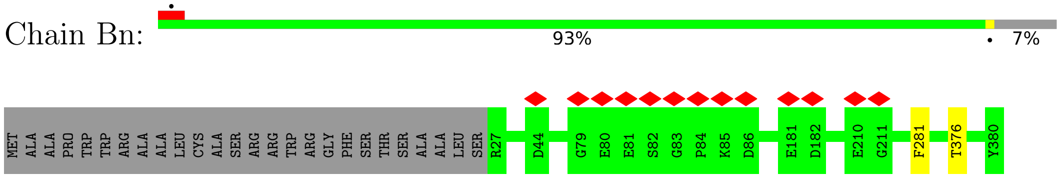
- Molecule 42: Mitochondrial ribosomal protein L37

Chain Bm:



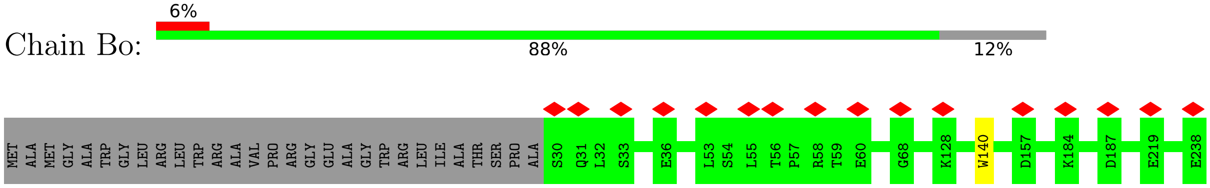
- Molecule 43: Mitochondrial ribosomal protein L38

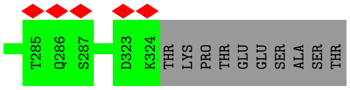
Chain Bn:



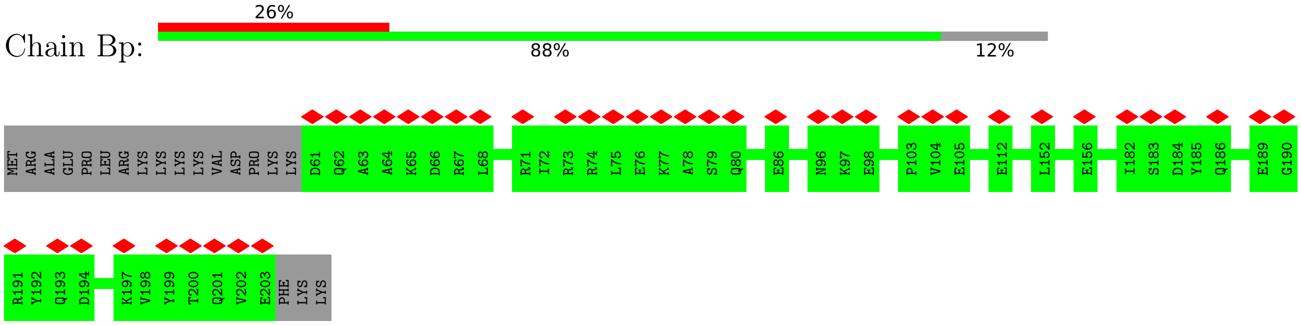
- Molecule 44: Mitochondrial ribosomal protein L39

Chain Bo:

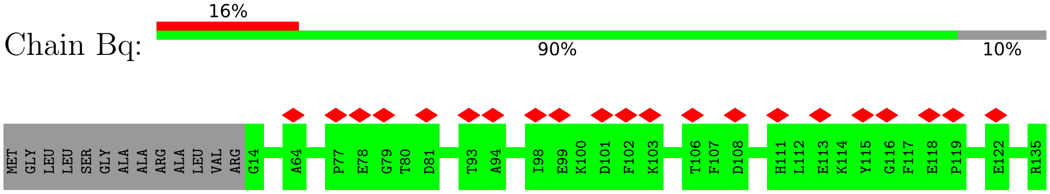




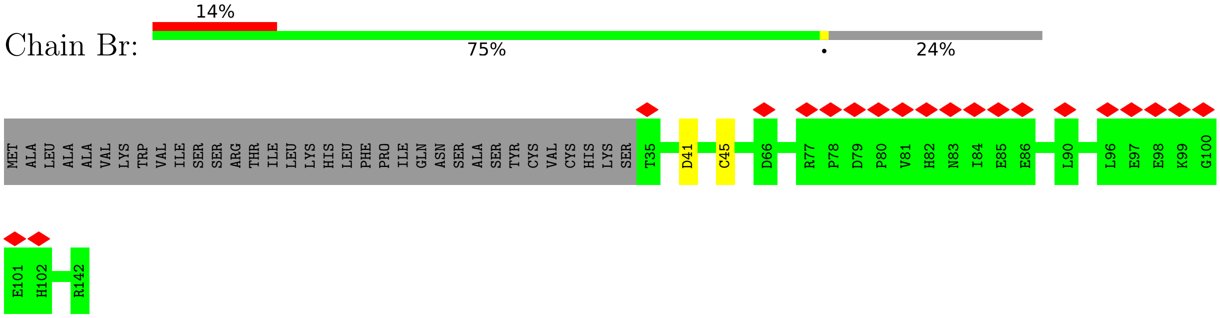
- Molecule 45: Mitochondrial ribosomal protein L40



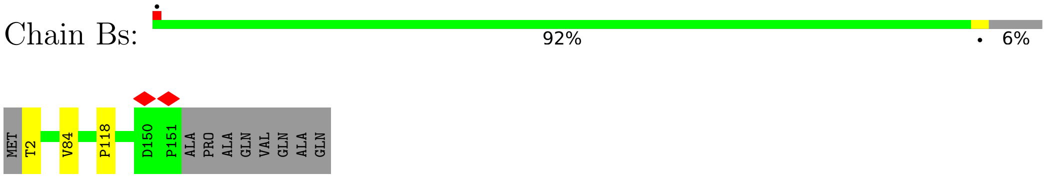
- Molecule 46: Mitochondrial ribosomal protein L41



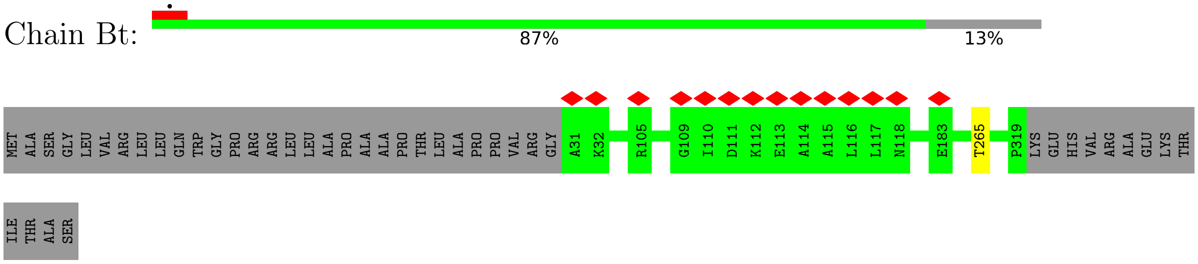
- Molecule 47: mL42



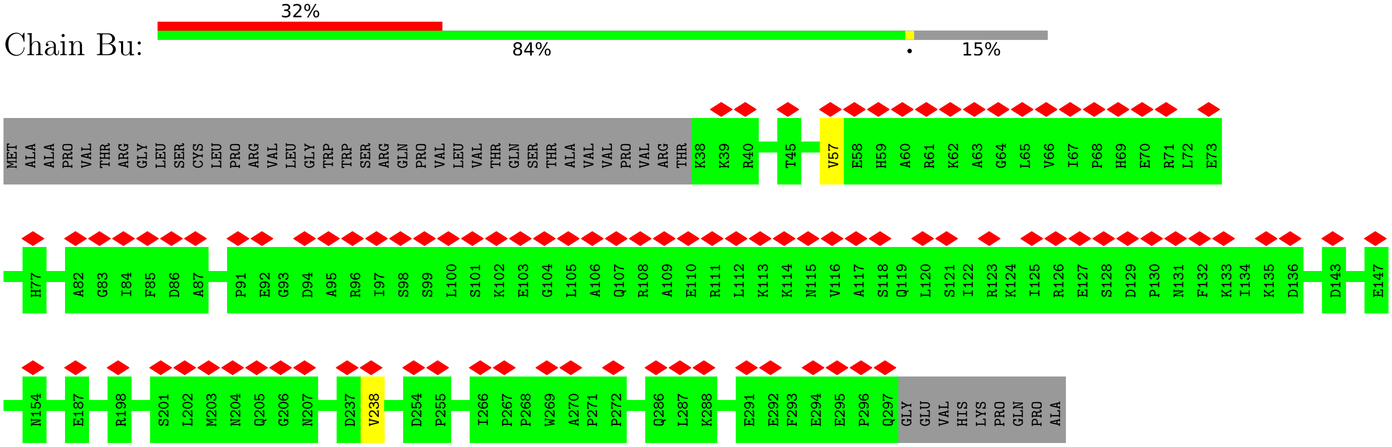
- Molecule 48: 39S ribosomal protein L43, mitochondrial isoform X2



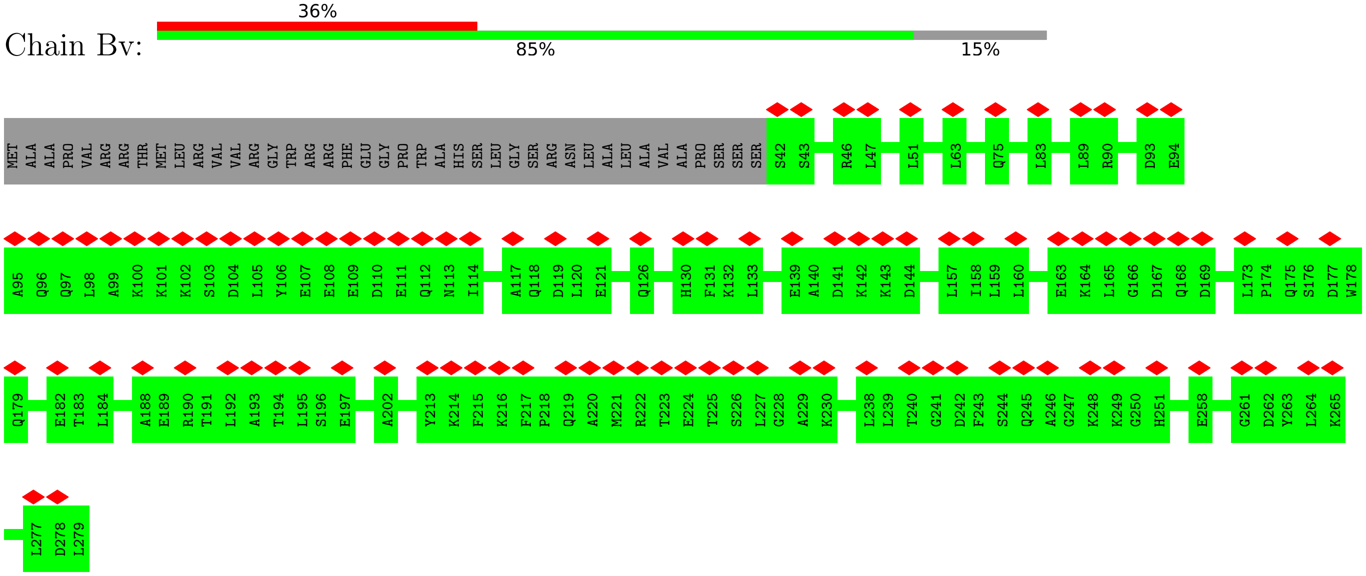
- Molecule 49: mL44



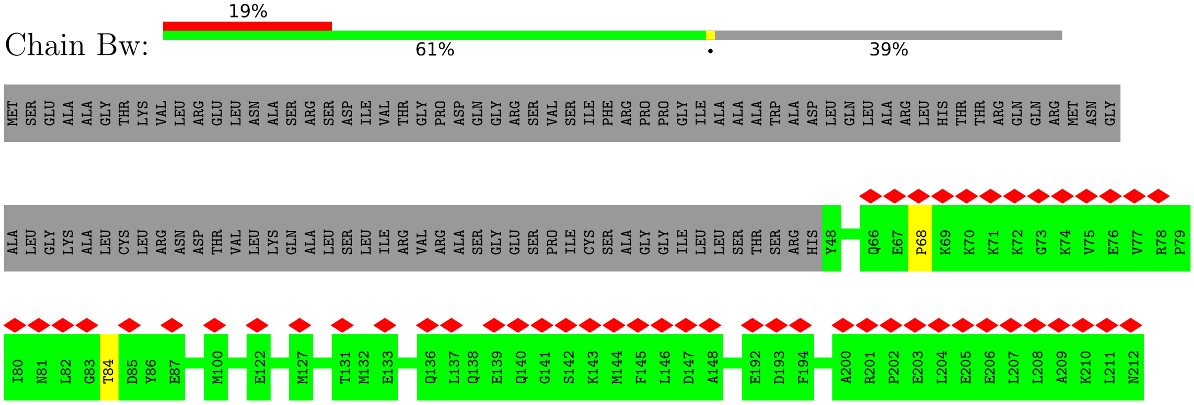
• Molecule 50: Mitochondrial ribosomal protein L45



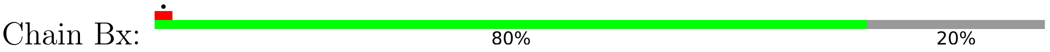
• Molecule 51: Mitochondrial ribosomal protein L46

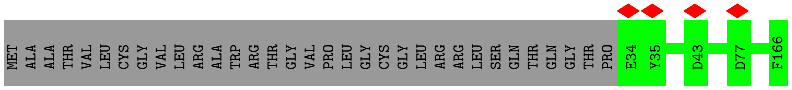


• Molecule 52: 39S ribosomal protein L48, mitochondrial



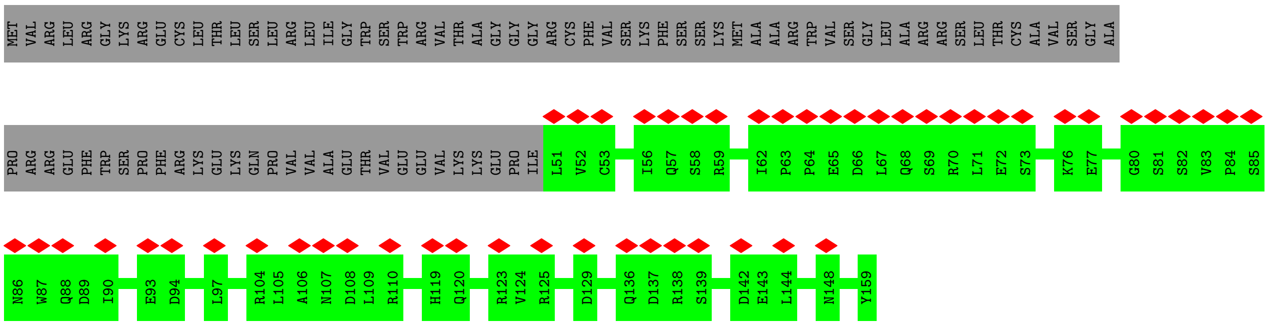
• Molecule 53: 39S ribosomal protein L49, mitochondrial





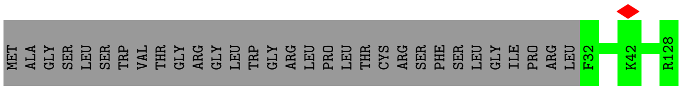
• Molecule 54: Mitochondrial ribosomal protein L50

Chain By:



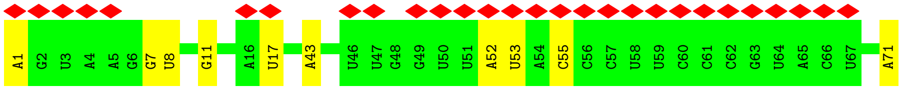
• Molecule 55: Mitochondrial ribosomal protein L51

Chain Bz:



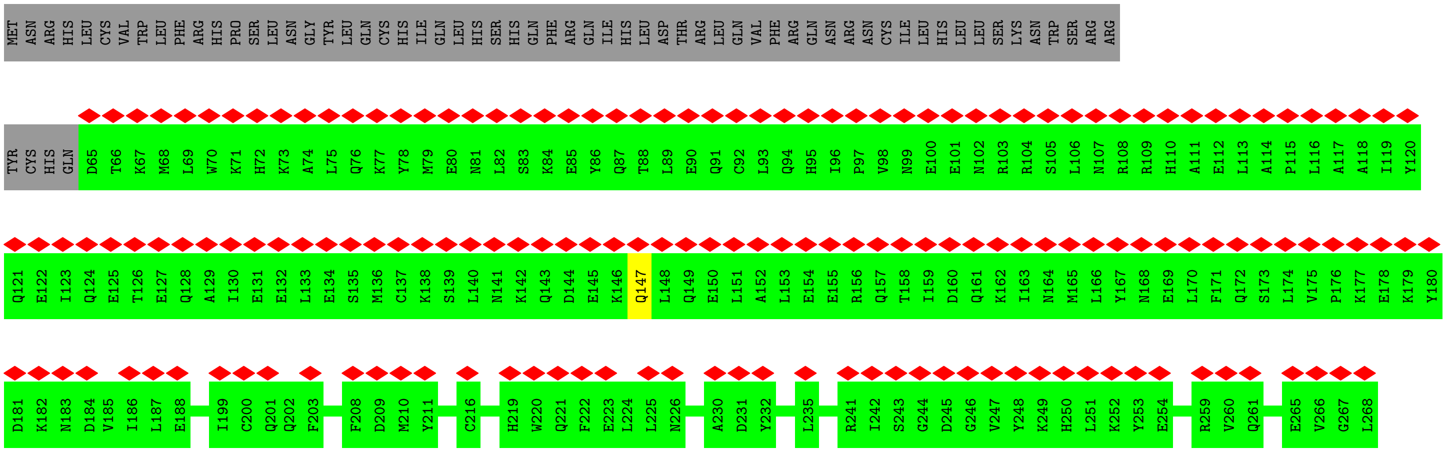
• Molecule 56: P-site Met-tRNA(fMet)

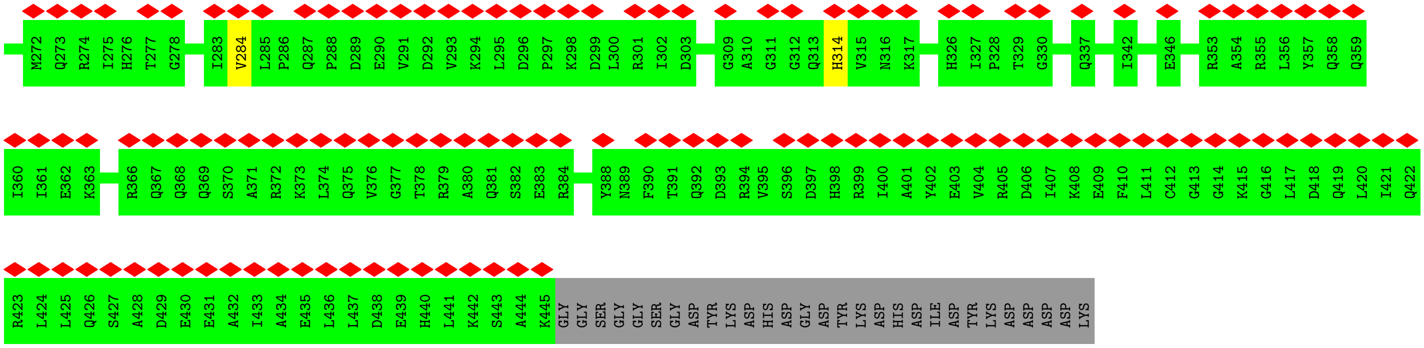
Chain AG:



• Molecule 57: Peptide chain release factor 1, mitochondrial

Chain Aa:




M272
Q273
R274
I275
H276
T277
G278
I283
V284
L285
P286
Q287
P288
D289
E290
V291
D292
V293
K294
L295
D296
P297
K298
D299
L300
R301
I302
D303
G309
A310
G311
G312
Q313
H314
V315
N316
K317
H326
I327
P328
T329
G330
Q337
I342
E346
R353
A354
R355
L356
Y357
Q358
Q359
I360
I361
E362
K363
R366
Q367
Q368
Q369
S370
A371
R372
K373
L374
Q375
V376
G377
T378
R379
A380
Q381
S382
E383
R384
Y388
N389
F390
T391
Q392
D393
R394
V395
S396
D397
H398
R399
I400
A401
Y402
E403
V404
R405
D406
I407
K408
E409
F410
L411
C412
G413
G414
K415
G416
L417
D418
Q419
L420
I421
Q422
R423
L424
L425
Q426
S427
A428
D429
E430
E431
A432
I433
A434
E435
L436
L437
D438
E439
H440
L441
K442
S443
A444
K445
GLY
GLY
SER
GLY
GLY
SER
GLY
ASP
TYR
LYS
ASP
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GLY
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TYR
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ASP
HIS
ASP
ILE
ASP
TYR
LYS
ASP
ASP
ASP
ASP
LYS

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50622	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 ($e^-/\text{Å}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.800	Depositor
Minimum map value	-2.487	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.130	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	532.5, 532.5, 532.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FME, PSU, AYA, MIA, 1MA, MG, OMG, K, FES, ZN, THC, OMU, SAC

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	B1	0.23	0/319	0.37	0/435
1	B2	0.21	0/212	0.36	0/286
1	B3	0.22	0/221	0.36	0/297
1	B4	0.22	0/212	0.33	0/286
1	B5	0.22	0/212	0.32	0/286
1	B6	0.22	0/204	0.37	0/275
2	B7	0.13	0/68	0.66	0/103
3	B8	0.21	0/37315	0.69	5/58099 (0.0%)
4	B9	0.30	1/1712 (0.1%)	0.69	0/2659
5	BA	0.25	0/1407	0.48	0/1891
6	BB	0.25	0/1206	0.52	0/1639
7	BC	0.24	0/1719	0.51	0/2329
8	BD	0.26	0/890	0.46	0/1202
9	BE	0.23	0/2093	0.46	0/2835
10	BF	0.23	0/1586	0.47	0/2123
11	BG	0.24	0/993	0.46	0/1341
12	BH	0.24	0/917	0.51	0/1227
13	BI	0.23	0/430	0.48	0/570
14	BJ	0.23	0/395	0.55	0/524
15	BK	0.25	0/853	0.52	0/1136
16	BL	0.24	0/1898	0.52	0/2555
17	BM	0.25	0/2493	0.44	0/3387
18	BN	0.24	0/2080	0.49	0/2830
19	BO	0.23	0/1695	0.50	0/2288
20	BP	0.24	0/1742	0.46	0/2358
21	BQ	0.25	0/1359	0.46	0/1828
22	BR	0.28	0/1481	0.44	0/2009
23	BS	0.25	0/912	0.52	0/1231
24	BT	0.25	0/2368	0.51	0/3198
25	BU	0.25	0/1850	0.50	0/2491
26	BV	0.24	0/1262	0.51	0/1700
27	BW	0.23	0/1197	0.51	0/1624

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
28	BX	0.24	0/1898	0.48	0/2562
29	BY	0.24	0/1179	0.52	0/1578
30	BZ	0.24	0/1256	0.49	0/1706
31	Ba	0.24	0/787	0.46	0/1056
32	Bb	0.24	0/747	0.52	0/1006
33	Bc	0.23	0/737	0.46	0/997
34	Bd	0.23	0/580	0.58	0/780
35	Be	0.24	0/798	0.54	0/1073
36	Bf	0.23	0/1214	0.51	0/1630
37	Bg	0.23	0/1157	0.48	0/1560
38	Bh	0.24	0/1364	0.49	0/1849
39	Bi	0.25	0/3206	0.47	0/4354
40	Bj	0.24	0/1350	0.44	0/1823
41	Bl	0.24	0/342	0.53	0/450
42	Bm	0.25	0/3267	0.47	0/4455
43	Bn	0.25	0/3047	0.50	0/4139
44	Bo	0.24	0/2464	0.43	0/3330
45	Bp	0.24	0/1228	0.48	0/1656
46	Bq	0.26	0/1000	0.46	0/1345
47	Br	0.25	0/934	0.51	0/1267
48	Bs	0.25	0/1200	0.53	0/1627
49	Bt	0.24	0/2372	0.46	0/3211
50	Bu	0.24	0/2199	0.46	0/2980
51	Bv	0.23	0/1988	0.44	0/2678
52	Bw	0.25	0/1320	0.47	1/1785 (0.1%)
53	Bx	0.25	0/1135	0.47	0/1549
54	By	0.23	0/917	0.45	0/1248
55	Bz	0.24	0/860	0.48	0/1150
56	AG	0.29	1/1677 (0.1%)	0.68	0/2606
57	Aa	0.23	0/3171	0.45	0/4263
All	All	0.23	2/118695 (0.0%)	0.57	6/168755 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	AG	1	A	OP3-P	-10.67	1.48	1.61
4	B9	1	G	OP3-P	-10.54	1.48	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B8	1119	C	N1-C2-O2	6.16	122.59	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B8	1527	U	C2-N1-C1’	6.05	124.96	117.70
52	Bw	68	PRO	N-CA-CB	5.89	110.37	103.30
3	B8	1119	C	N3-C2-O2	-5.22	118.25	121.90
3	B8	1527	U	N1-C2-O2	5.17	126.42	122.80
3	B8	1119	C	C2-N1-C1’	5.13	124.44	118.80

There are no chirality outliers.

There are no planarity outliers.

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	B1	43/198 (22%)	40 (93%)	3 (7%)	0	100	100
1	B2	25/198 (13%)	25 (100%)	0	0	100	100
1	B3	26/198 (13%)	26 (100%)	0	0	100	100
1	B4	25/198 (13%)	25 (100%)	0	0	100	100
1	B5	25/198 (13%)	25 (100%)	0	0	100	100
1	B6	24/198 (12%)	24 (100%)	0	0	100	100
5	BA	164/210 (78%)	158 (96%)	6 (4%)	0	100	100
6	BB	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
7	BC	204/216 (94%)	196 (96%)	8 (4%)	0	100	100
8	BD	110/148 (74%)	109 (99%)	1 (1%)	0	100	100
9	BE	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
10	BF	177/250 (71%)	175 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	BG	116/161 (72%)	114 (98%)	2 (2%)	0	100	100
12	BH	108/207 (52%)	108 (100%)	0	0	100	100
13	BI	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
14	BJ	44/95 (46%)	44 (100%)	0	0	100	100
15	BK	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
16	BL	238/306 (78%)	230 (97%)	7 (3%)	1 (0%)	34	72
17	BM	305/399 (76%)	295 (97%)	10 (3%)	0	100	100
18	BN	249/294 (85%)	246 (99%)	3 (1%)	0	100	100
19	BO	200/268 (75%)	192 (96%)	8 (4%)	0	100	100
20	BP	210/257 (82%)	208 (99%)	2 (1%)	0	100	100
21	BQ	174/192 (91%)	170 (98%)	4 (2%)	0	100	100
22	BR	175/197 (89%)	170 (97%)	5 (3%)	0	100	100
23	BS	113/325 (35%)	111 (98%)	2 (2%)	0	100	100
24	BT	286/296 (97%)	274 (96%)	12 (4%)	0	100	100
25	BU	220/251 (88%)	216 (98%)	4 (2%)	0	100	100
26	BV	151/169 (89%)	147 (97%)	4 (3%)	0	100	100
27	BW	141/188 (75%)	134 (95%)	7 (5%)	0	100	100
28	BX	223/303 (74%)	221 (99%)	2 (1%)	0	100	100
29	BY	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
30	BZ	153/209 (73%)	149 (97%)	4 (3%)	0	100	100
31	Ba	95/160 (59%)	94 (99%)	1 (1%)	0	100	100
32	Bb	95/112 (85%)	90 (95%)	5 (5%)	0	100	100
33	Bc	82/138 (59%)	82 (100%)	0	0	100	100
34	Bd	67/126 (53%)	64 (96%)	3 (4%)	0	100	100
35	Be	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
36	Bf	147/205 (72%)	143 (97%)	4 (3%)	0	100	100
37	Bg	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
38	Bh	160/196 (82%)	154 (96%)	6 (4%)	0	100	100
39	Bi	385/433 (89%)	370 (96%)	14 (4%)	1 (0%)	41	75
40	Bj	160/304 (53%)	155 (97%)	5 (3%)	0	100	100
41	Bl	36/100 (36%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	Bm	391/423 (92%)	380 (97%)	11 (3%)	0	100	100
43	Bn	352/380 (93%)	336 (96%)	16 (4%)	0	100	100
44	Bo	293/334 (88%)	282 (96%)	11 (4%)	0	100	100
45	Bp	141/162 (87%)	135 (96%)	6 (4%)	0	100	100
46	Bq	120/135 (89%)	114 (95%)	6 (5%)	0	100	100
47	Br	106/142 (75%)	101 (95%)	5 (5%)	0	100	100
48	Bs	148/159 (93%)	144 (97%)	4 (3%)	0	100	100
49	Bt	287/332 (86%)	282 (98%)	5 (2%)	0	100	100
50	Bu	258/306 (84%)	251 (97%)	7 (3%)	0	100	100
51	Bv	236/279 (85%)	232 (98%)	4 (2%)	0	100	100
52	Bw	163/269 (61%)	151 (93%)	12 (7%)	0	100	100
53	Bx	131/166 (79%)	128 (98%)	3 (2%)	0	100	100
54	By	107/198 (54%)	105 (98%)	2 (2%)	0	100	100
55	Bz	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
57	Aa	380/474 (80%)	372 (98%)	8 (2%)	0	100	100
All	All	9259/12922 (72%)	9009 (97%)	248 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	Bi	159	VAL
16	BL	208	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B1	30/157 (19%)	30 (100%)	0	100	100
1	B2	26/157 (17%)	26 (100%)	0	100	100
1	B3	27/157 (17%)	27 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B4	26/157 (17%)	26 (100%)	0	100	100
1	B5	26/157 (17%)	26 (100%)	0	100	100
1	B6	25/157 (16%)	25 (100%)	0	100	100
5	BA	144/180 (80%)	144 (100%)	0	100	100
6	BB	116/134 (87%)	116 (100%)	0	100	100
7	BC	185/192 (96%)	185 (100%)	0	100	100
8	BD	91/115 (79%)	91 (100%)	0	100	100
9	BE	219/229 (96%)	218 (100%)	1 (0%)	88	94
10	BF	164/226 (73%)	164 (100%)	0	100	100
11	BG	110/150 (73%)	110 (100%)	0	100	100
12	BH	99/177 (56%)	98 (99%)	1 (1%)	76	88
13	BI	49/60 (82%)	48 (98%)	1 (2%)	55	79
14	BJ	41/78 (53%)	41 (100%)	0	100	100
15	BK	87/162 (54%)	87 (100%)	0	100	100
16	BL	193/248 (78%)	193 (100%)	0	100	100
17	BM	263/320 (82%)	263 (100%)	0	100	100
18	BN	218/251 (87%)	217 (100%)	1 (0%)	88	94
19	BO	181/228 (79%)	180 (99%)	1 (1%)	86	94
20	BP	192/231 (83%)	190 (99%)	2 (1%)	76	88
21	BQ	138/151 (91%)	138 (100%)	0	100	100
22	BR	155/173 (90%)	154 (99%)	1 (1%)	86	94
23	BS	99/243 (41%)	98 (99%)	1 (1%)	76	88
24	BT	245/249 (98%)	244 (100%)	1 (0%)	91	96
25	BU	190/210 (90%)	190 (100%)	0	100	100
26	BV	132/143 (92%)	132 (100%)	0	100	100
27	BW	123/161 (76%)	122 (99%)	1 (1%)	81	91
28	BX	204/266 (77%)	203 (100%)	1 (0%)	88	94
29	BY	118/127 (93%)	118 (100%)	0	100	100
30	BZ	136/178 (76%)	136 (100%)	0	100	100
31	Ba	77/129 (60%)	77 (100%)	0	100	100
32	Bb	79/88 (90%)	75 (95%)	4 (5%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	Bc	79/114 (69%)	79 (100%)	0	100	100
34	Bd	60/114 (53%)	60 (100%)	0	100	100
35	Be	75/82 (92%)	74 (99%)	1 (1%)	69	86
36	Bf	126/177 (71%)	126 (100%)	0	100	100
37	Bg	115/183 (63%)	115 (100%)	0	100	100
38	Bh	149/173 (86%)	148 (99%)	1 (1%)	84	93
39	Bi	340/373 (91%)	339 (100%)	1 (0%)	92	97
40	Bj	150/267 (56%)	148 (99%)	2 (1%)	69	86
41	Bl	36/77 (47%)	36 (100%)	0	100	100
42	Bm	348/365 (95%)	345 (99%)	3 (1%)	78	90
43	Bn	310/328 (94%)	308 (99%)	2 (1%)	86	94
44	Bo	271/299 (91%)	270 (100%)	1 (0%)	91	96
45	Bp	132/150 (88%)	132 (100%)	0	100	100
46	Bq	100/108 (93%)	100 (100%)	0	100	100
47	Br	103/133 (77%)	101 (98%)	2 (2%)	57	80
48	Bs	129/135 (96%)	127 (98%)	2 (2%)	62	83
49	Bt	251/284 (88%)	250 (100%)	1 (0%)	91	96
50	Bu	236/275 (86%)	234 (99%)	2 (1%)	81	91
51	Bv	210/242 (87%)	210 (100%)	0	100	100
52	Bw	135/226 (60%)	134 (99%)	1 (1%)	84	93
53	Bx	122/147 (83%)	122 (100%)	0	100	100
54	By	103/178 (58%)	103 (100%)	0	100	100
55	Bz	88/113 (78%)	88 (100%)	0	100	100
57	Aa	339/424 (80%)	336 (99%)	3 (1%)	78	90
All	All	8215/11008 (75%)	8177 (100%)	38 (0%)	89	94

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	BE	196	ILE
12	BH	185	PHE
13	BI	50	VAL
18	BN	106	PHE
19	BO	104	GLU

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Mol	Chain	Res	Type
20	BP	150	HIS
20	BP	174	LEU
22	BR	67	PHE
23	BS	89	HIS
24	BT	134	ARG
27	BW	149	THR
28	BX	273	TYR
32	Bb	10	LEU
32	Bb	47	LEU
32	Bb	48	ASN
32	Bb	75	ILE
35	Be	101	TRP
38	Bh	70	CYS
39	Bi	329	TRP
40	Bj	130	THR
40	Bj	136	LYS
42	Bm	121	LEU
42	Bm	152	GLU
42	Bm	256	PHE
43	Bn	281	PHE
43	Bn	376	THR
44	Bo	140	TRP
47	Br	41	ASP
47	Br	45	CYS
48	Bs	84	VAL
48	Bs	118	PRO
49	Bt	265	THR
50	Bu	57	VAL
50	Bu	238	VAL
52	Bw	84	THR
57	Aa	147	GLN
57	Aa	284	VAL
57	Aa	314	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
5	BA	60	GLN
5	BA	99	GLN
5	BA	113	GLN
5	BA	171	HIS
5	BA	199	GLN

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Mol	Chain	Res	Type
8	BD	107	ASN
10	BF	112	ASN
12	BH	96	ASN
12	BH	118	GLN
12	BH	144	GLN
14	BJ	57	GLN
15	BK	118	HIS
15	BK	154	GLN
16	BL	183	HIS
17	BM	117	HIS
17	BM	277	ASN
18	BN	97	HIS
18	BN	241	ASN
18	BN	276	HIS
18	BN	277	ASN
19	BO	178	ASN
19	BO	239	ASN
20	BP	61	ASN
20	BP	73	GLN
20	BP	115	GLN
20	BP	224	HIS
21	BQ	84	GLN
21	BQ	133	GLN
22	BR	160	GLN
23	BS	33	GLN
23	BS	59	HIS
23	BS	142	GLN
24	BT	87	HIS
24	BT	94	GLN
24	BT	170	ASN
25	BU	138	GLN
26	BV	98	GLN
26	BV	116	GLN
27	BW	52	ASN
27	BW	79	HIS
27	BW	96	HIS
28	BX	253	GLN
29	BY	94	GLN
29	BY	147	GLN
30	BZ	183	ASN
32	Bb	84	GLN
33	Bc	82	GLN

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Mol	Chain	Res	Type
34	Bd	60	GLN
35	Be	30	GLN
35	Be	45	ASN
37	Bg	106	GLN
37	Bg	119	GLN
37	Bg	130	GLN
38	Bh	164	ASN
39	Bi	173	GLN
39	Bi	201	HIS
39	Bi	228	ASN
39	Bi	379	GLN
39	Bi	414	GLN
40	Bj	266	GLN
42	Bm	119	GLN
42	Bm	149	ASN
42	Bm	186	GLN
42	Bm	266	GLN
42	Bm	280	GLN
42	Bm	343	GLN
42	Bm	358	GLN
43	Bn	307	HIS
44	Bo	197	HIS
44	Bo	305	HIS
45	Bp	186	GLN
45	Bp	193	GLN
47	Br	71	HIS
48	Bs	24	GLN
48	Bs	58	ASN
48	Bs	129	GLN
49	Bt	42	GLN
49	Bt	69	HIS
49	Bt	193	GLN
50	Bu	69	HIS
50	Bu	167	ASN
50	Bu	196	GLN
50	Bu	217	HIS
51	Bv	113	ASN
51	Bv	251	HIS
52	Bw	54	HIS
52	Bw	136	GLN
53	Bx	93	ASN
53	Bx	155	GLN

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Mol	Chain	Res	Type
54	By	88	GLN
54	By	96	HIS
55	Bz	69	HIS
57	Aa	107	ASN
57	Aa	124	GLN
57	Aa	183	ASN
57	Aa	341	GLN
57	Aa	381	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B7	2/3 (66%)	1 (50%)	0
3	B8	1570/1571 (99%)	262 (16%)	0
4	B9	71/73 (97%)	13 (18%)	0
56	AG	70/71 (98%)	9 (12%)	0
All	All	1713/1718 (99%)	285 (16%)	0

All (285) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B7	76	A
3	B8	15	A
3	B8	19	U
3	B8	20	A
3	B8	21	C
3	B8	27	A
3	B8	31	A
3	B8	32	C
3	B8	36	A
3	B8	40	C
3	B8	42	C
3	B8	45	A
3	B8	46	A
3	B8	56	A
3	B8	57	A
3	B8	59	A
3	B8	60	U
3	B8	68	A
3	B8	69	C
3	B8	82	G

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Mol	Chain	Res	Type
3	B8	83	A
3	B8	104	C
3	B8	105	G
3	B8	109	U
3	B8	112	A
3	B8	115	U
3	B8	129	A
3	B8	132	G
3	B8	139	G
3	B8	140	A
3	B8	141	A
3	B8	142	U
3	B8	143	A
3	B8	163	C
3	B8	164	A
3	B8	168	A
3	B8	172	C
3	B8	179	U
3	B8	180	A
3	B8	190	U
3	B8	192	A
3	B8	205	A
3	B8	218	A
3	B8	219	A
3	B8	225	C
3	B8	228	U
3	B8	229	A
3	B8	239	C
3	B8	254	G
3	B8	263	G
3	B8	272	A
3	B8	273	A
3	B8	275	A
3	B8	277	A
3	B8	311	A
3	B8	322	G
3	B8	324	G
3	B8	329	A
3	B8	330	A
3	B8	331	A
3	B8	336	A
3	B8	340	A

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Mol	Chain	Res	Type
3	B8	352	G
3	B8	359	G
3	B8	369	G
3	B8	373	U
3	B8	374	U
3	B8	376	A
3	B8	392	U
3	B8	409	A
3	B8	427	G
3	B8	428	A
3	B8	433	G
3	B8	434	U
3	B8	445	A
3	B8	446	C
3	B8	448	G
3	B8	459	A
3	B8	460	C
3	B8	475	C
3	B8	479	A
3	B8	480	G
3	B8	488	U
3	B8	490	U
3	B8	491	U
3	B8	492	A
3	B8	497	U
3	B8	498	A
3	B8	501	A
3	B8	502	U
3	B8	503	A
3	B8	506	A
3	B8	515	A
3	B8	518	A
3	B8	532	A
3	B8	534	A
3	B8	549	C
3	B8	560	A
3	B8	570	A
3	B8	574	A
3	B8	575	C
3	B8	576	U
3	B8	578	A
3	B8	579	U

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Mol	Chain	Res	Type
3	B8	580	A
3	B8	584	A
3	B8	586	C
3	B8	592	G
3	B8	595	C
3	B8	596	A
3	B8	617	A
3	B8	618	A
3	B8	625	A
3	B8	626	G
3	B8	631	A
3	B8	633	U
3	B8	634	G
3	B8	640	A
3	B8	684	A
3	B8	689	A
3	B8	693	U
3	B8	695	U
3	B8	704	U
3	B8	707	A
3	B8	713	A
3	B8	720	C
3	B8	722	A
3	B8	724	A
3	B8	725	C
3	B8	727	A
3	B8	728	C
3	B8	737	G
3	B8	746	U
3	B8	747	U
3	B8	748	A
3	B8	753	G
3	B8	777	A
3	B8	783	A
3	B8	809	G
3	B8	817	A
3	B8	825	C
3	B8	852	C
3	B8	854	U
3	B8	855	U
3	B8	856	A
3	B8	859	A

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Mol	Chain	Res	Type
3	B8	864	U
3	B8	872	A
3	B8	889	C
3	B8	892	G
3	B8	897	A
3	B8	902	C
3	B8	922	A
3	B8	923	A
3	B8	924	G
3	B8	925	G
3	B8	933	A
3	B8	950	U
3	B8	958	U
3	B8	959	G
3	B8	960	U
3	B8	962	U
3	B8	964	A
3	B8	965	A
3	B8	967	G
3	B8	977	G
3	B8	1015	C
3	B8	1016	C
3	B8	1018	U
3	B8	1026	A
3	B8	1027	G
3	B8	1028	A
3	B8	1038	A
3	B8	1050	C
3	B8	1051	G
3	B8	1055	A
3	B8	1056	G
3	B8	1057	A
3	B8	1063	U
3	B8	1064	G
3	B8	1076	A
3	B8	1093	A
3	B8	1094	A
3	B8	1095	C
3	B8	1097	A
3	B8	1099	U
3	B8	1100	C
3	B8	1107	A

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Mol	Chain	Res	Type
3	B8	1113	A
3	B8	1114	U
3	B8	1115	A
3	B8	1119	C
3	B8	1120	A
3	B8	1121	U
3	B8	1146	G
3	B8	1167	C
3	B8	1168	A
3	B8	1169	A
3	B8	1180	G
3	B8	1183	U
3	B8	1188	U
3	B8	1195	A
3	B8	1204	A
3	B8	1206	U
3	B8	1207	C
3	B8	1215	C
3	B8	1217	A
3	B8	1218	U
3	B8	1220	A
3	B8	1221	C
3	B8	1222	A
3	B8	1226	C
3	B8	1231	U
3	B8	1233	A
3	B8	1240	A
3	B8	1241	U
3	B8	1242	U
3	B8	1243	U
3	B8	1246	A
3	B8	1247	U
3	B8	1249	A
3	B8	1253	G
3	B8	1254	A
3	B8	1264	C
3	B8	1271	A
3	B8	1291	U
3	B8	1299	C
3	B8	1314	U
3	B8	1325	G
3	B8	1326	A

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Mol	Chain	Res	Type
3	B8	1327	U
3	B8	1328	G
3	B8	1332	G
3	B8	1341	A
3	B8	1342	C
3	B8	1389	A
3	B8	1390	G
3	B8	1396	C
3	B8	1425	A
3	B8	1426	G
3	B8	1432	U
3	B8	1433	U
3	B8	1436	U
3	B8	1445	U
3	B8	1448	A
3	B8	1468	A
3	B8	1493	A
3	B8	1494	A
3	B8	1498	C
3	B8	1504	A
3	B8	1505	G
3	B8	1509	U
3	B8	1522	A
3	B8	1525	C
3	B8	1526	U
3	B8	1527	U
3	B8	1528	A
3	B8	1536	U
3	B8	1551	C
3	B8	1553	A
3	B8	1558	U
3	B8	1561	A
3	B8	1571	A
4	B9	8	U
4	B9	17	U
4	B9	18	U
4	B9	23	A
4	B9	34	U
4	B9	35	G
4	B9	48	U
4	B9	49	G
4	B9	55	C

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Mol	Chain	Res	Type
4	B9	56	A
4	B9	57	C
4	B9	58	A
4	B9	71	C
56	AG	7	G
56	AG	8	U
56	AG	11	G
56	AG	17	U
56	AG	43	A
56	AG	52	A
56	AG	53	U
56	AG	55	C
56	AG	71	A

There are no RNA pucker outliers to report.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OMU	B8	1375	59,3	19,22,23	1.18	2 (10%)	26,31,34	1.67	5 (19%)
3	1MA	B8	949	3	16,25,26	0.89	2 (12%)	18,37,40	1.05	2 (11%)
3	PSU	B8	1403	3	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)
48	THC	Bs	2	48	8,9,10	0.56	0	9,11,13	0.91	1 (11%)
3	OMG	B8	1151	56,59,3	18,26,27	0.91	1 (5%)	19,38,41	1.01	2 (10%)
22	SAC	BR	2	22	7,8,9	0.53	0	8,9,11	0.94	1 (12%)
4	MIA	B9	38	4	24,31,32	0.87	1 (4%)	26,44,47	4.87	2 (7%)
6	AYA	BB	2	6	6,7,8	0.77	0	5,8,10	0.23	0
32	AYA	Bb	2	32	6,7,8	0.71	0	5,8,10	0.39	0
3	OMG	B8	1376	3	18,26,27	0.92	1 (5%)	19,38,41	0.96	2 (10%)

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
3	OMU	B8	1375	59,3	-	0/9/27/28	0/2/2/2
3	1MA	B8	949	3	-	0/3/25/26	0/3/3/3
3	PSU	B8	1403	3	-	0/7/25/26	0/2/2/2
48	THC	Bs	2	48	-	1/8/10/12	-
3	OMG	B8	1151	56,59,3	-	0/5/27/28	0/3/3/3
22	SAC	BR	2	22	-	4/7/8/10	-
4	MIA	B9	38	4	-	0/11/33/34	0/3/3/3
6	AYA	BB	2	6	-	0/4/6/8	-
32	AYA	Bb	2	32	-	3/4/6/8	-
3	OMG	B8	1376	3	-	0/5/27/28	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B8	1403	PSU	C6-C5	3.14	1.39	1.35
3	B8	1403	PSU	C4-N3	-2.72	1.33	1.38
3	B8	1376	OMG	C6-N1	-2.61	1.34	1.37
3	B8	1151	OMG	C6-N1	-2.58	1.34	1.37
3	B8	1375	OMU	C4-N3	-2.41	1.34	1.38
3	B8	949	1MA	C8-N7	-2.37	1.31	1.35
4	B9	38	MIA	C2-S10	2.30	1.77	1.75
3	B8	1375	OMU	C2-N3	-2.12	1.34	1.38
3	B8	949	1MA	C5-C4	-2.08	1.37	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B9	38	MIA	C11-S10-C2	24.47	120.54	102.27
3	B8	1403	PSU	N1-C2-N3	5.79	121.69	115.13
3	B8	1375	OMU	C4-N3-C2	-4.44	120.73	126.58
3	B8	1375	OMU	N3-C2-N1	4.07	120.29	114.89
3	B8	1403	PSU	C4-N3-C2	-3.77	120.90	126.34
3	B8	1375	OMU	C5-C4-N3	3.50	120.07	114.84
3	B8	1403	PSU	O2-C2-N1	-3.29	119.17	122.79
4	B9	38	MIA	C5-C6-N1	-3.27	118.09	120.81
3	B8	1375	OMU	O4-C4-C5	-3.03	119.84	125.16
22	BR	2	SAC	O-C-CA	-2.54	118.13	124.78
48	Bs	2	THC	O-C-CA	-2.36	118.25	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B8	1375	OMU	O2-C2-N1	-2.31	119.72	122.79
3	B8	949	1MA	C5-C6-N1	-2.14	110.71	113.90
3	B8	1376	OMG	C8-N7-C5	2.10	106.98	102.99
3	B8	949	1MA	N1-C6-N6	2.06	125.02	119.77
3	B8	1151	OMG	C5-C6-N1	2.06	117.58	113.95
3	B8	1151	OMG	C8-N7-C5	2.03	106.85	102.99
3	B8	1376	OMG	C5-C6-N1	2.01	117.50	113.95

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	BR	2	SAC	C2A-C1A-N-CA
22	BR	2	SAC	OAC-C1A-N-CA
22	BR	2	SAC	C-CA-CB-OG
32	Bb	2	AYA	CM-CT-N-CA
32	Bb	2	AYA	OT-CT-N-CA
22	BR	2	SAC	N-CA-CB-OG
32	Bb	2	AYA	C-CA-N-CT
48	Bs	2	THC	CB-CA-N1-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 240 ligands modelled in this entry, 237 are monoatomic - leaving 3 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	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
60	PHE	B9	101	4	10,11,12	0.38	0	10,13,15	0.29	0
62	FES	Bh	201	20,38	0,4,4	-	-	-		
63	FME	AG	101	56	8,9,10	0.54	0	7,9,11	0.96	1 (14%)

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
60	PHE	B9	101	4	-	1/5/6/8	0/1/1/1
62	FES	Bh	201	20,38	-	-	0/1/1/1
63	FME	AG	101	56	-	2/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	AG	101	FME	O-C-CA	-2.51	118.21	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	B9	101	PHE	O-C-CA-CB
63	AG	101	FME	O1-CN-N-CA
63	AG	101	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

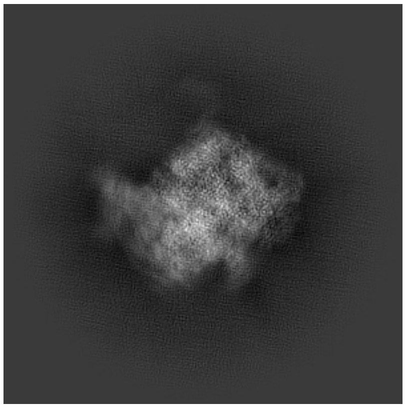
6 Map visualisation

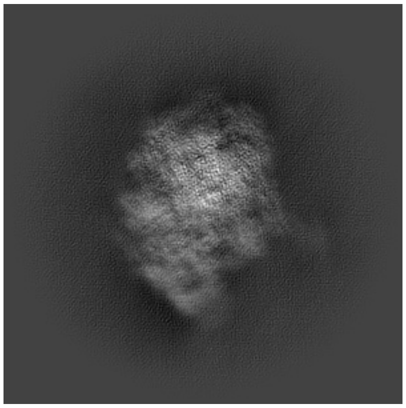
This section contains visualisations of the EMDB entry EMD-16896. These allow visual inspection of the internal detail of the map and identification of artifacts.

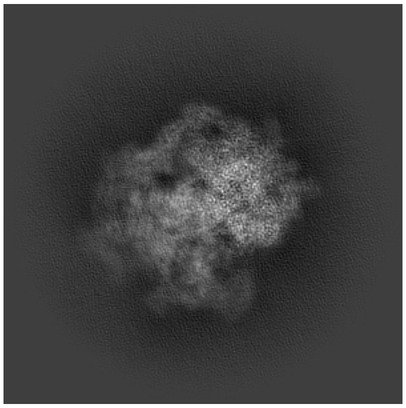
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

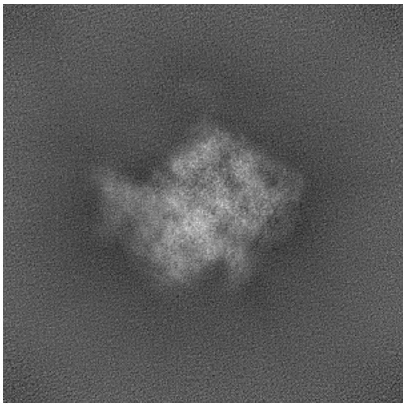
6.1.1 Primary map

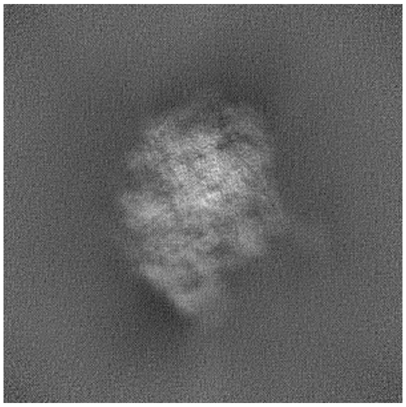

X

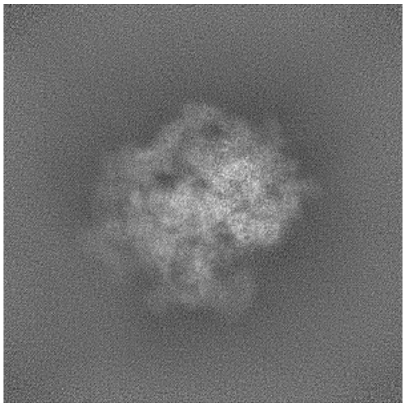

Y


Z

6.1.2 Raw map


X

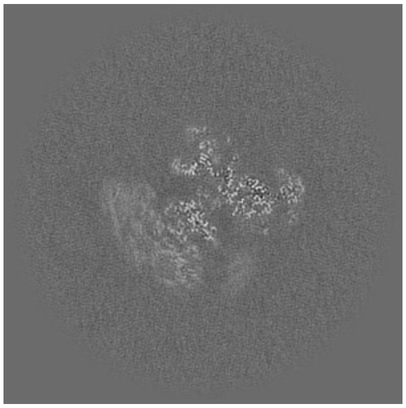

Y


Z

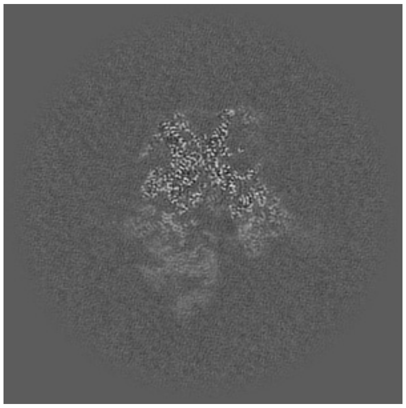
The images above show the map projected in three orthogonal directions.

6.2 Central slices

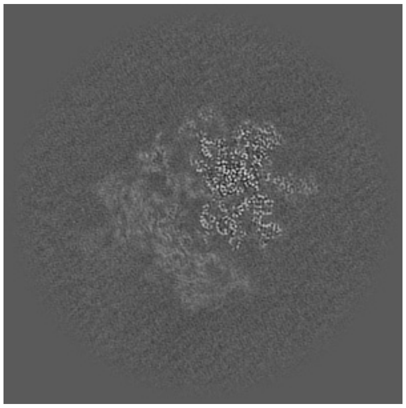
6.2.1 Primary map



X Index: 250

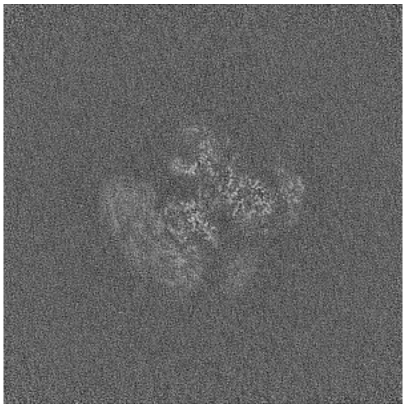


Y Index: 250

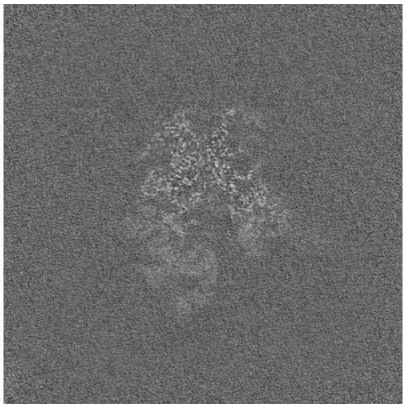


Z Index: 250

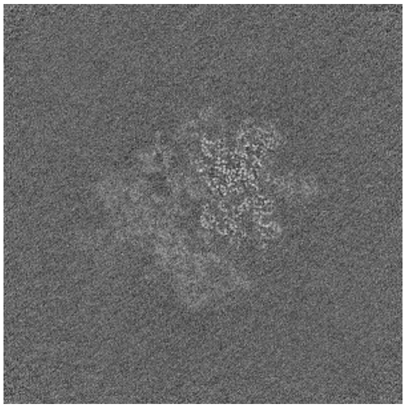
6.2.2 Raw map



X Index: 250



Y Index: 250

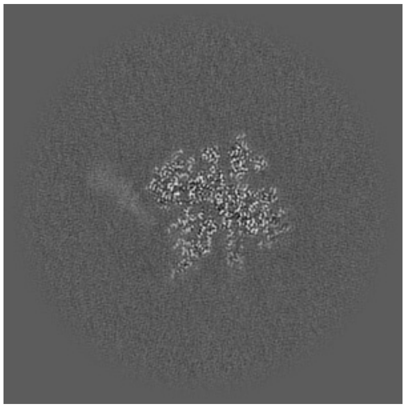


Z Index: 250

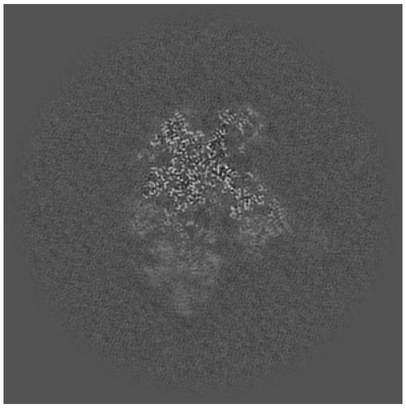
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

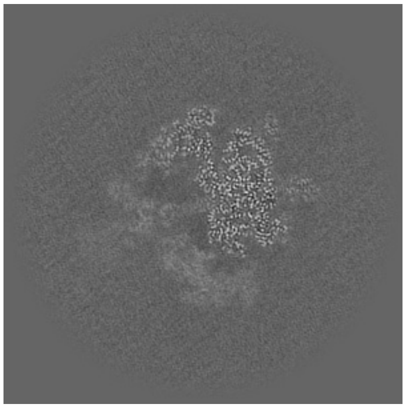
6.3.1 Primary map



X Index: 291

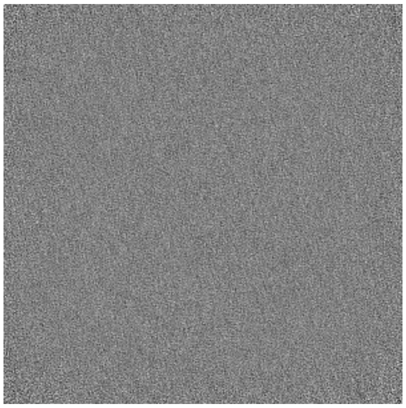


Y Index: 247

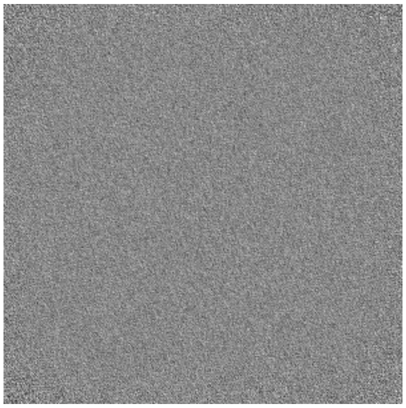


Z Index: 263

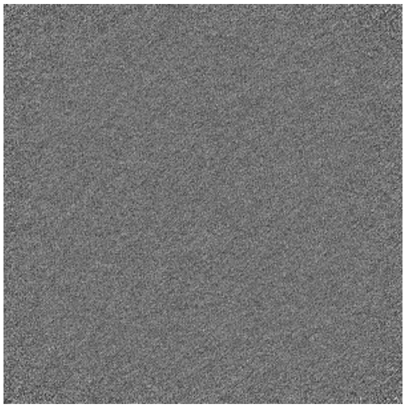
6.3.2 Raw map



X Index: 0



Y Index: 0

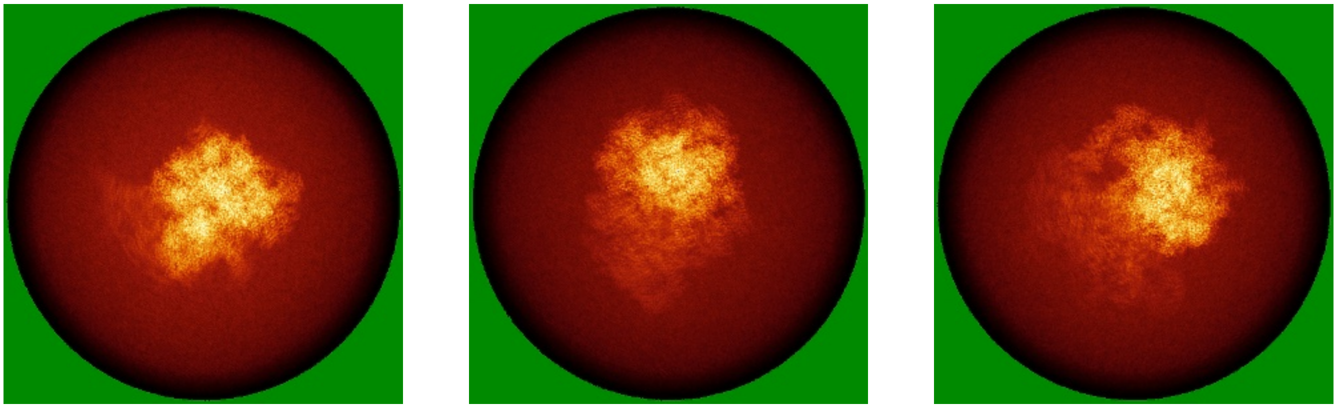


Z Index: 0

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

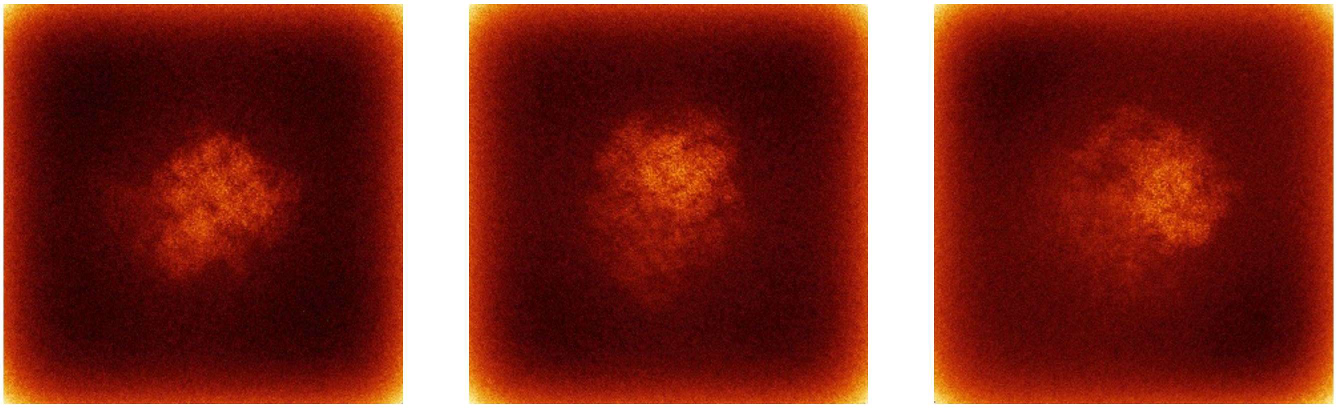
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

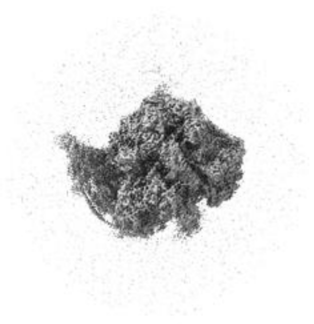


X Y Z

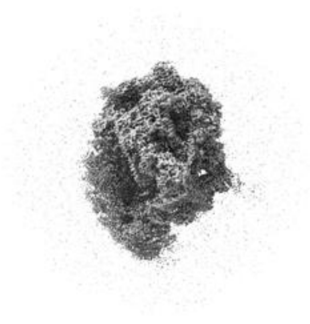
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

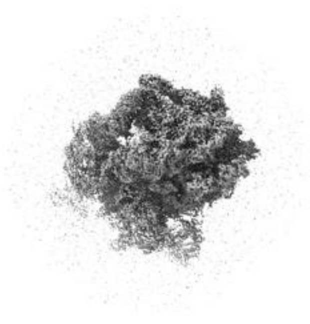
6.5.1 Primary map



X



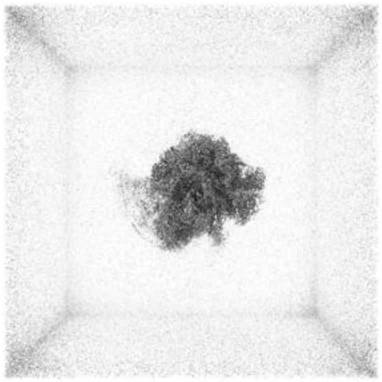
Y



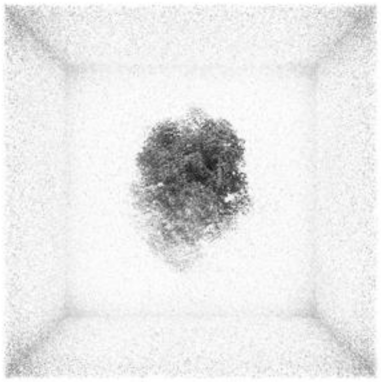
Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y

Z

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

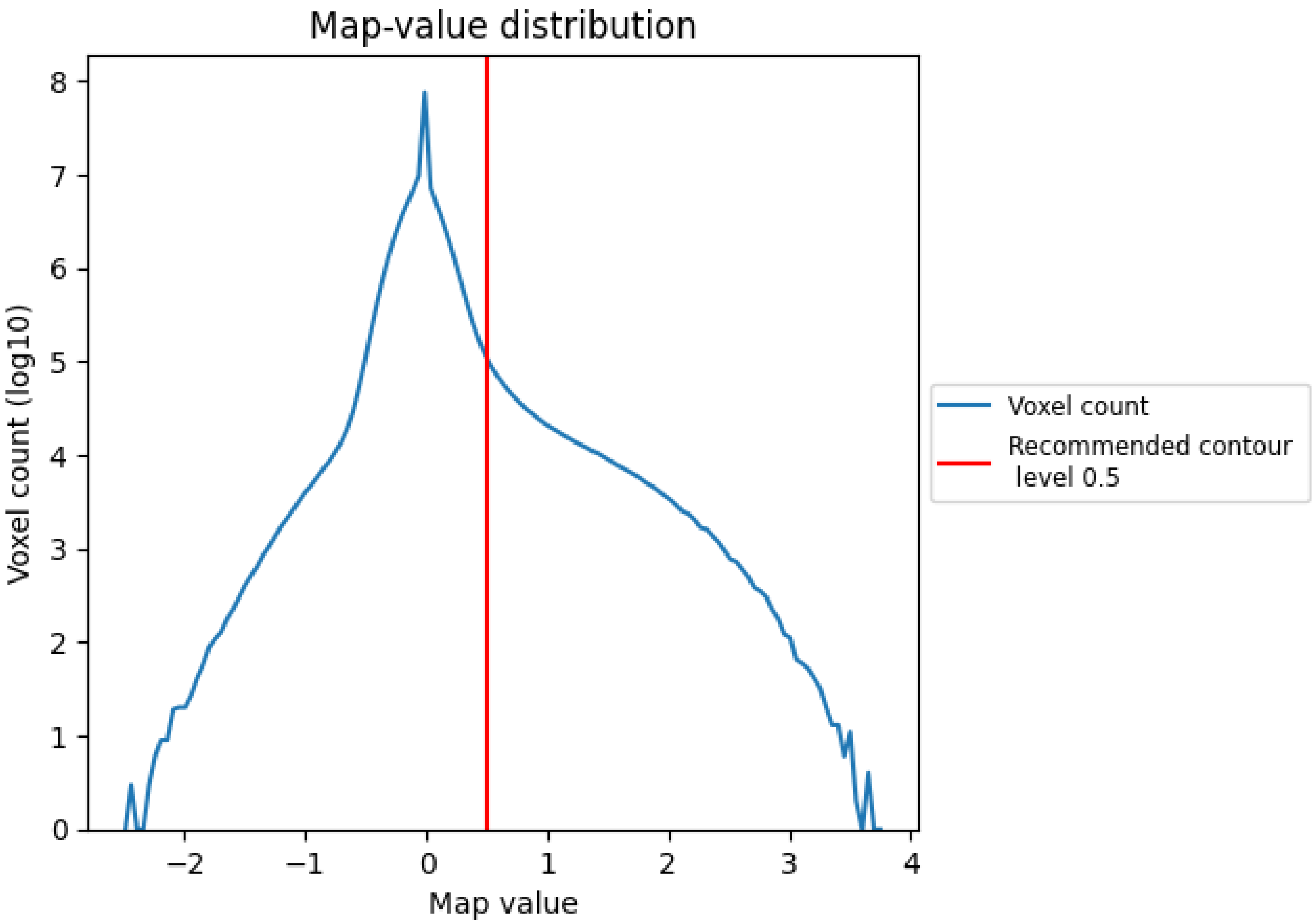
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

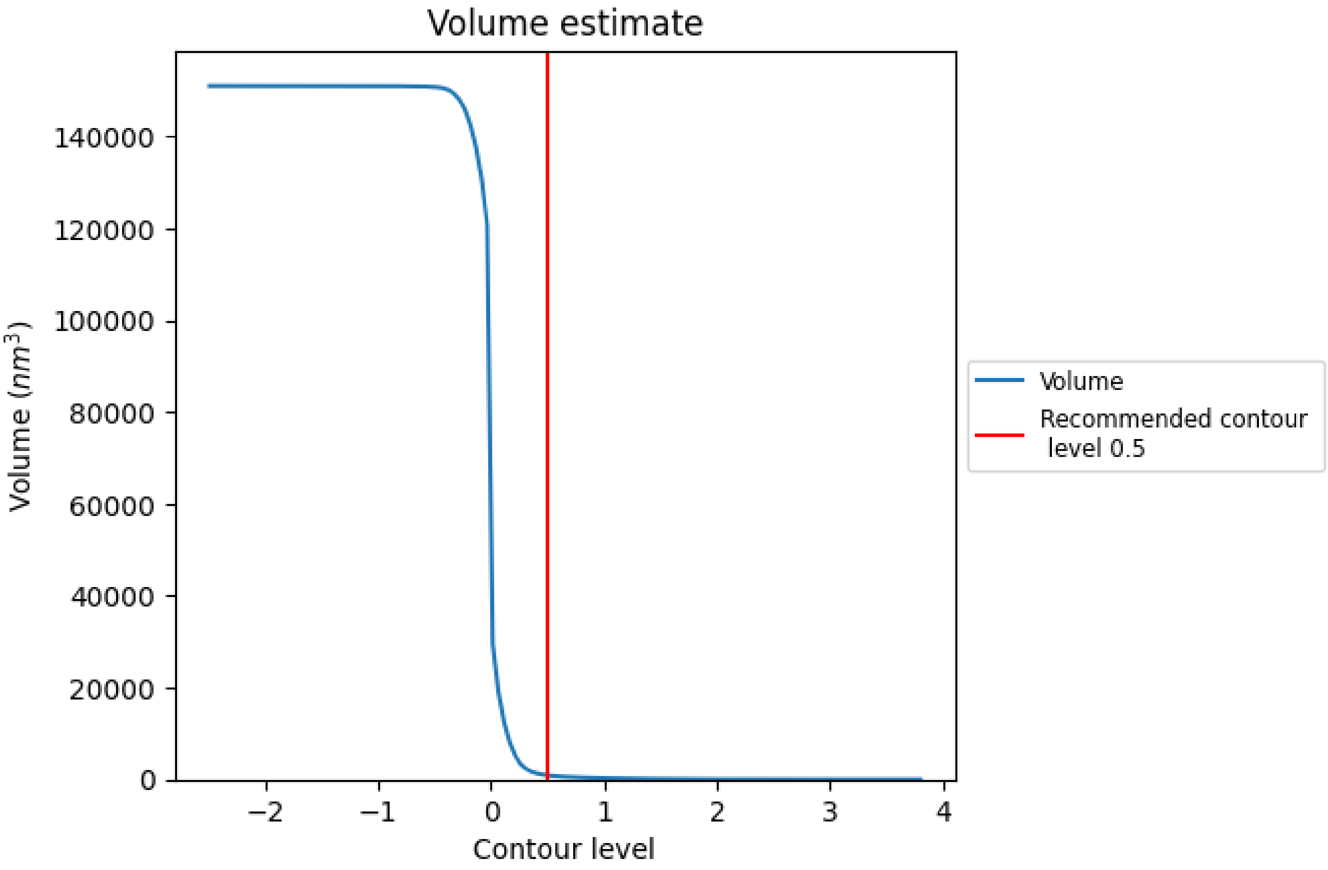
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

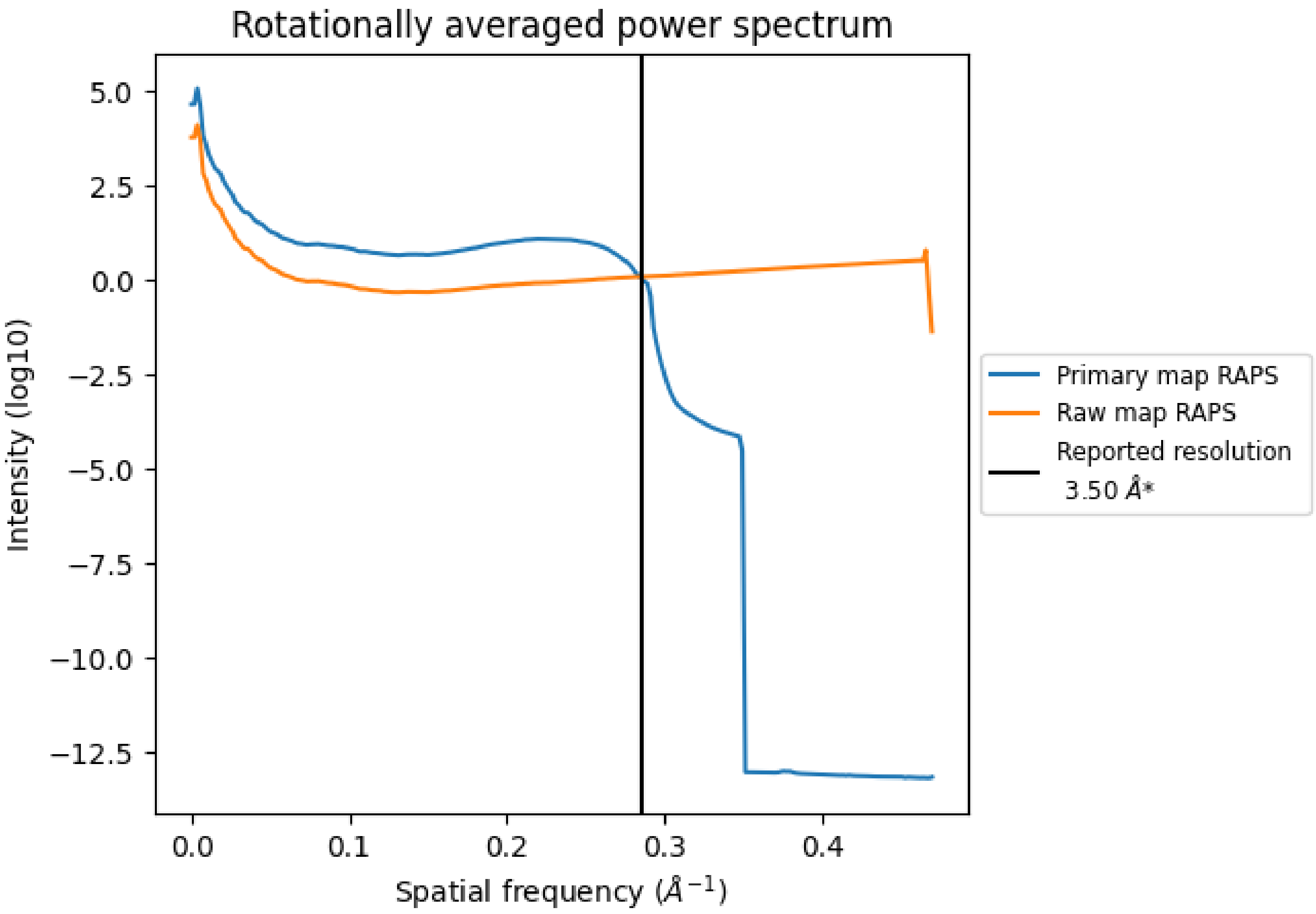
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 905 nm^3; this corresponds to an approximate mass of 817 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

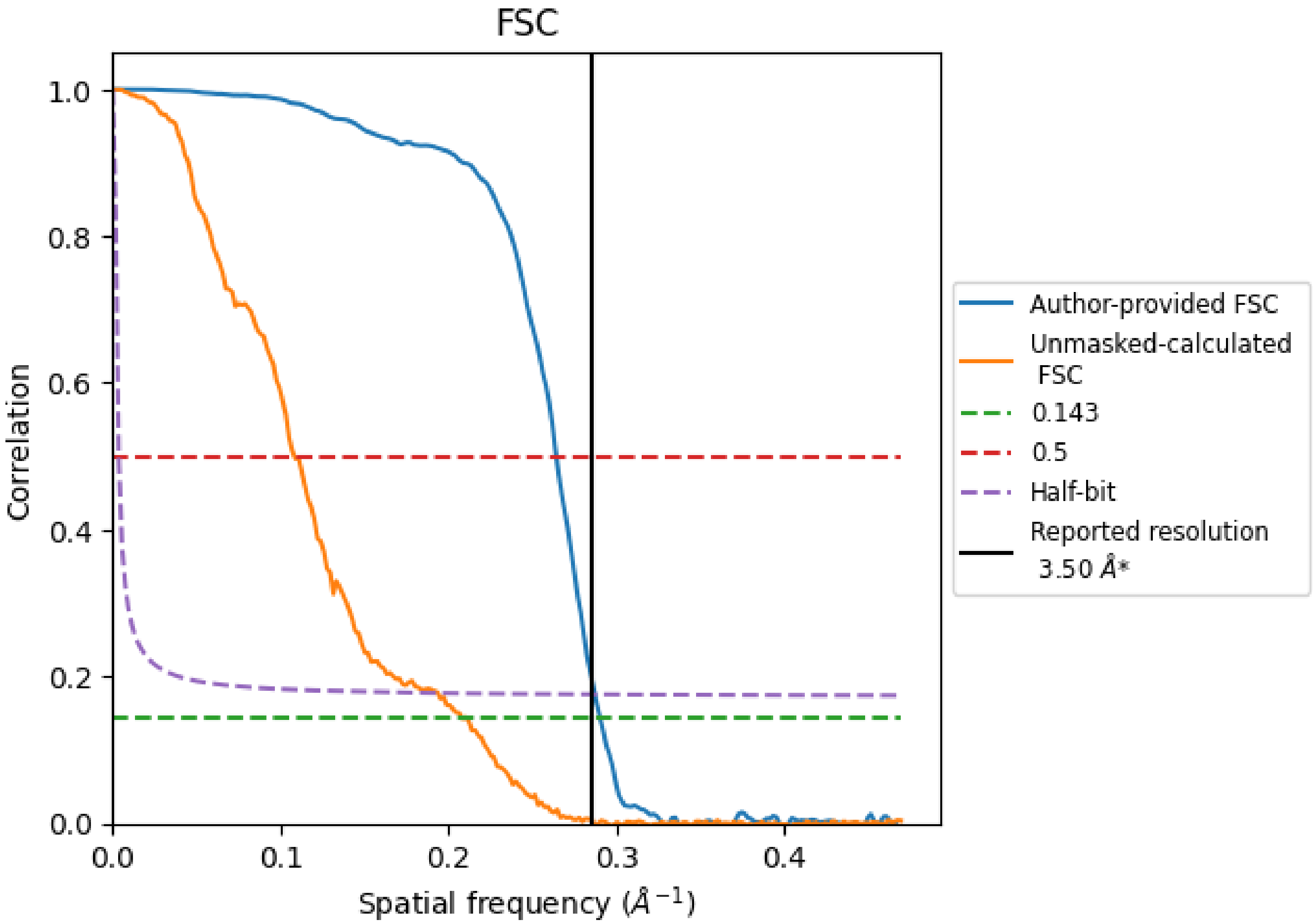


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates ⓘ

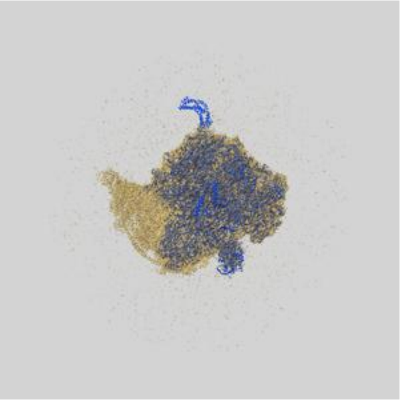
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.44	3.78	3.48
Unmasked-calculated*	4.80	9.23	5.16

*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 4.80 differs from the reported value 3.5 by more than 10 %

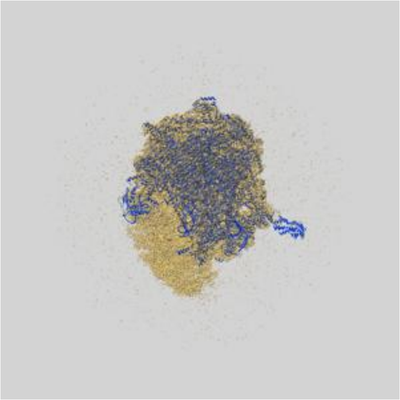
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-16896 and PDB model 8OIQ. Per-residue inclusion information can be found in section 3 on page 19.

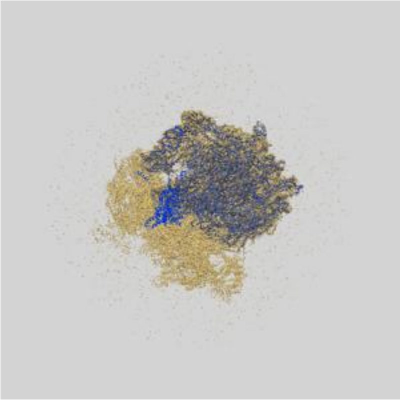
9.1 Map-model overlay ⓘ



X



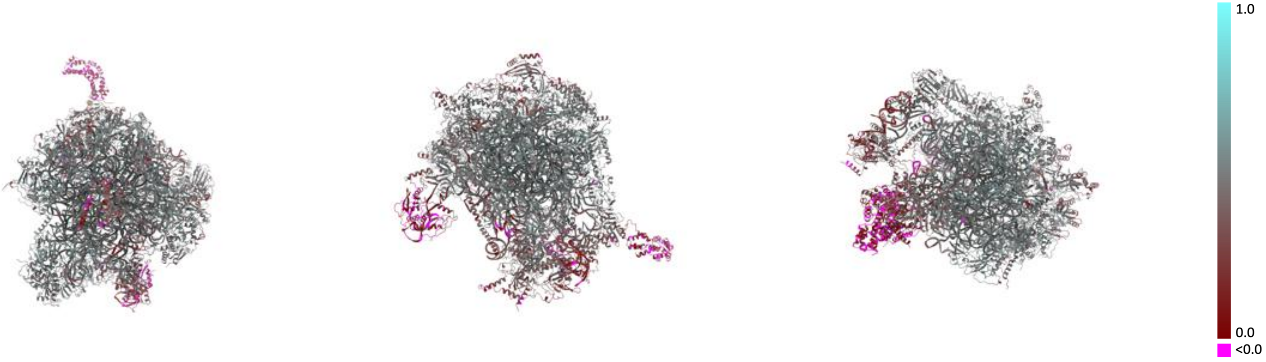
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

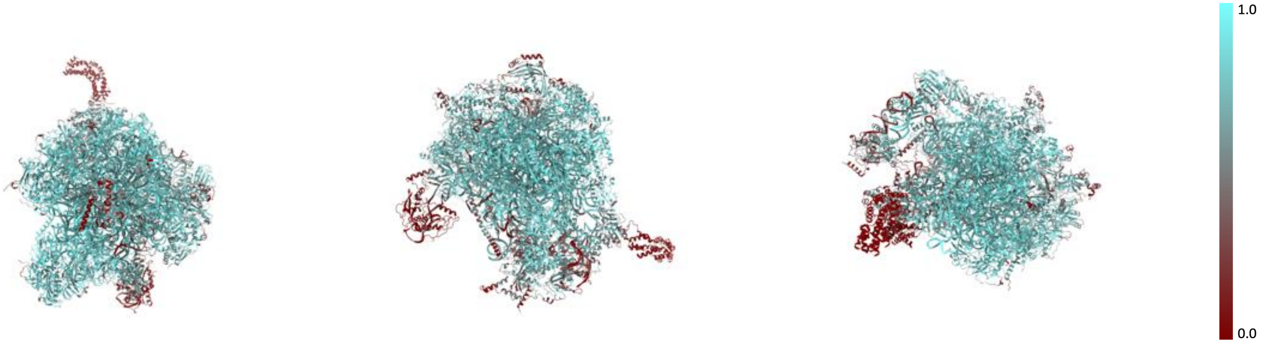
9.2 Q-score mapped to coordinate model



X Y Z

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.

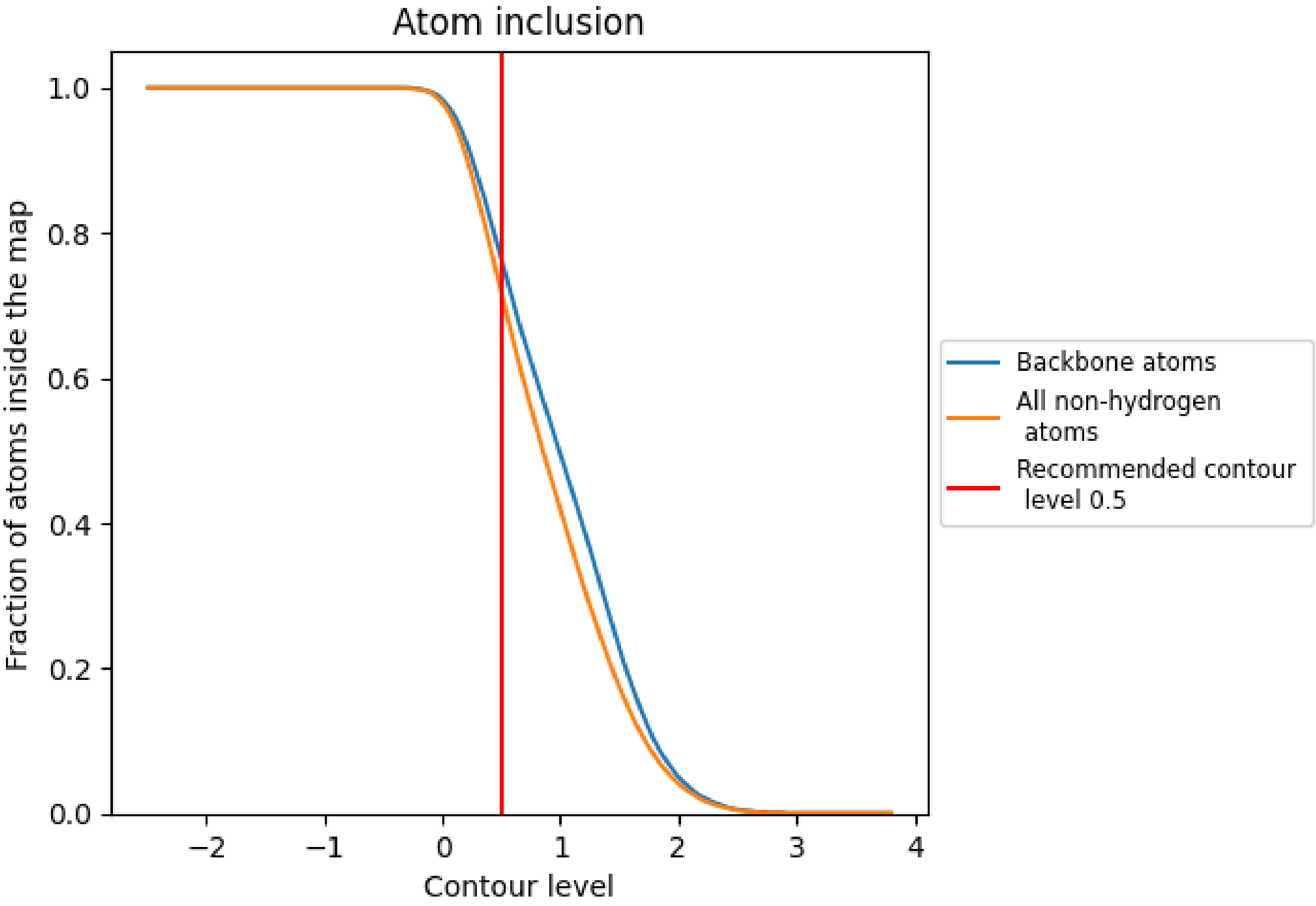
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7180	0.4400
AG	0.4970	0.2890
Aa	0.2050	0.2120
B1	0.0350	0.1140
B2	0.0190	0.0840
B3	0.0040	0.0300
B4	0.0000	0.0580
B5	0.0000	0.0230
B6	0.0000	0.1040
B7	0.0650	0.1160
B8	0.8600	0.4750
B9	0.5470	0.3000
BA	0.7980	0.5140
BB	0.7380	0.4670
BC	0.5800	0.4200
BD	0.8270	0.5200
BE	0.6880	0.4490
BF	0.7760	0.4820
BG	0.8290	0.5030
BH	0.7880	0.5010
BI	0.5940	0.4180
BJ	0.8700	0.5320
BK	0.8490	0.5340
BL	0.8170	0.5020
BM	0.8200	0.5020
BN	0.8170	0.5120
BO	0.2900	0.2460
BP	0.4590	0.3120
BQ	0.3480	0.2810
BR	0.8470	0.5160
BS	0.7840	0.5100
BT	0.7930	0.4960
BU	0.8260	0.5090
BV	0.8190	0.5210
BW	0.7730	0.4910

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Chain	Atom inclusion	Q-score
BX	0.7600	0.4910
BY	0.8330	0.5210
BZ	0.8220	0.5090
Ba	0.7680	0.4810
Bb	0.6300	0.4050
Bc	0.4880	0.3300
Bd	0.4560	0.3370
Be	0.8630	0.5220
Bf	0.5440	0.4040
Bg	0.5520	0.3990
Bh	0.7960	0.4820
Bi	0.7890	0.4830
Bj	0.0580	0.0750
Bl	0.8660	0.5290
Bm	0.7800	0.4760
Bn	0.7690	0.4650
Bo	0.7190	0.4560
Bp	0.5200	0.3680
Bq	0.6630	0.4440
Br	0.6750	0.4630
Bs	0.8200	0.5130
Bt	0.7760	0.4760
Bu	0.5020	0.3710
Bv	0.4480	0.2810
Bw	0.5440	0.4000
Bx	0.7990	0.4980
By	0.4460	0.4140
Bz	0.8420	0.5210