Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:32 am GMT

PDB ID	:	6GB2
EMDB ID	:	EMD-4370
Title	:	Unique features of mammalian mitochondrial translation initiation revealed by cryo-EM. This file contains the 39S ribosomal subunit.
Authors	:	Kummer, E.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on	:	2018-04-13
Resolution	:	3.20 Å(reported)

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

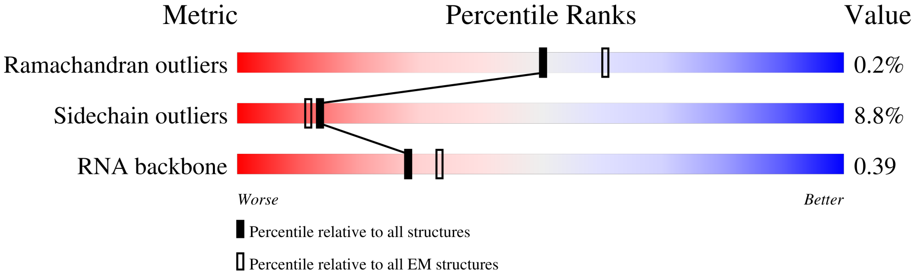
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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

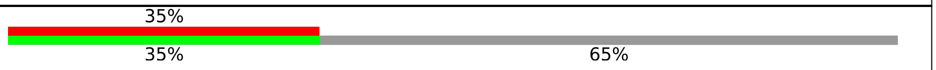
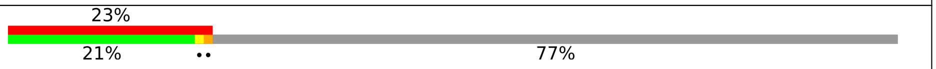
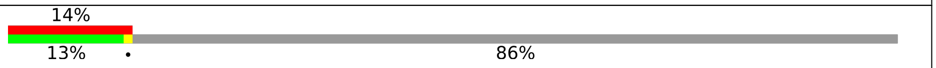
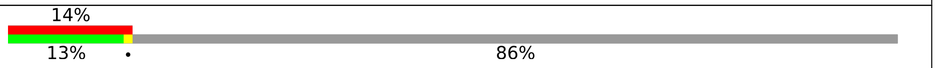
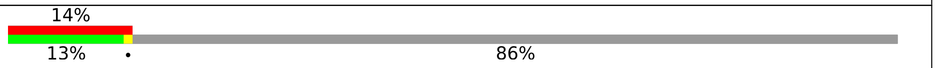
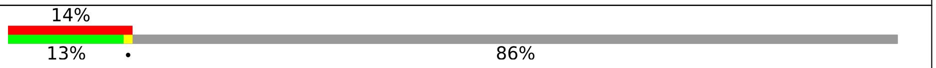
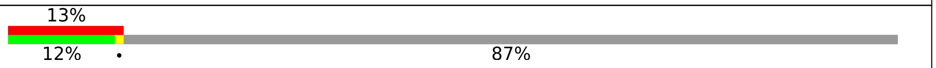
The reported resolution of this entry is 3.20 Å.

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	BL	198	
1	CL	198	
1	DL	198	
1	EL	198	
1	FL	198	
1	GL	198	
1	HL	198	
2	B0	148	

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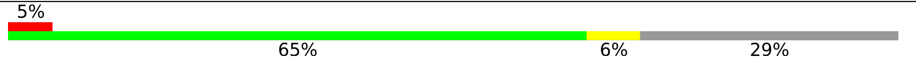
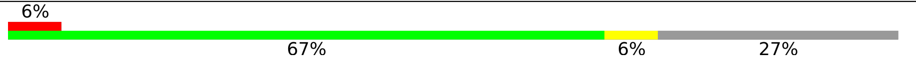
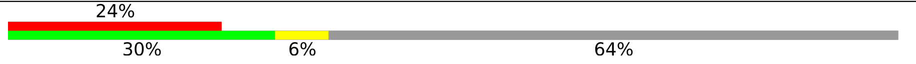
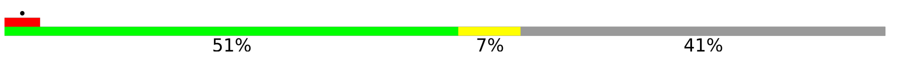
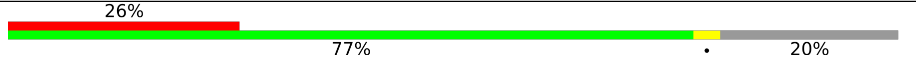
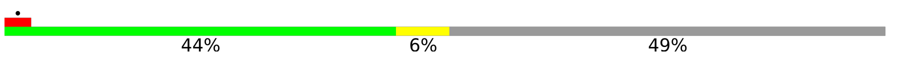
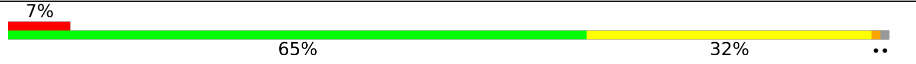
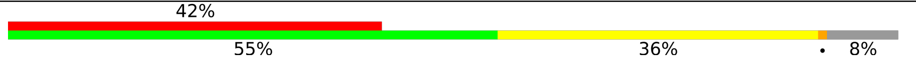
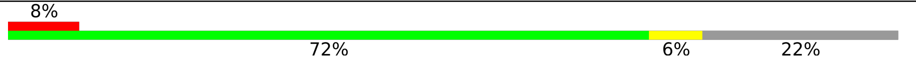
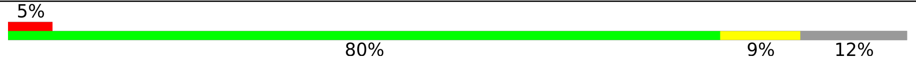
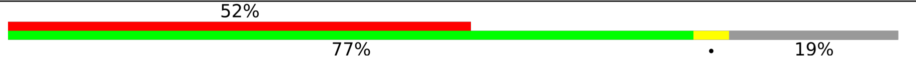
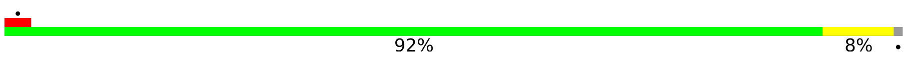
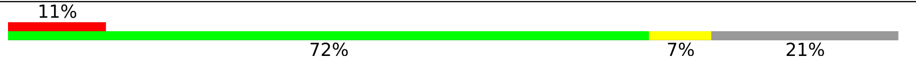
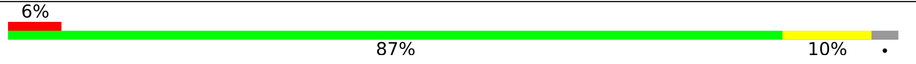
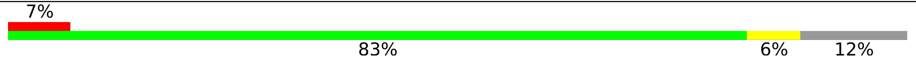
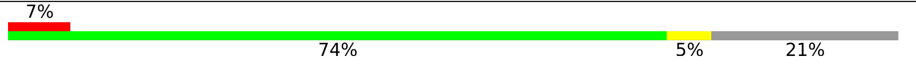
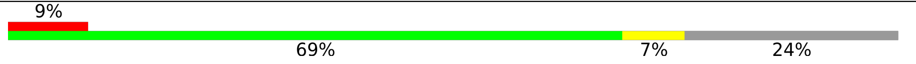
Mol	Chain	Length	Quality of chain
3	B1	256	
4	B2	252	
5	B3	161	
6	B4	126	
7	B5	188	
8	B6	65	
9	B7	95	
10	B8	188	
11	B9	100	
12	BA	1571	
13	BB	73	
14	BC	657	
15	BD	306	
16	BE	348	
17	BF	294	
18	BI	268	
19	BJ	262	
20	BK	192	
21	BN	178	
22	BO	145	
23	BP	296	
24	BQ	251	
25	BR	169	
26	BS	180	
27	BT	292	

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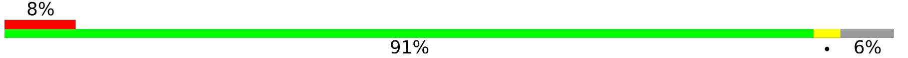
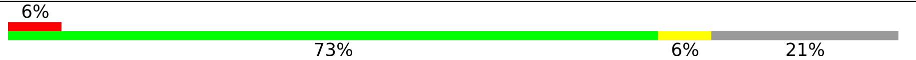
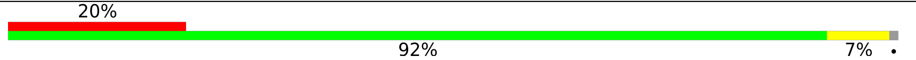
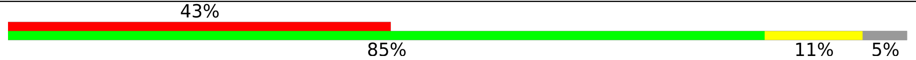
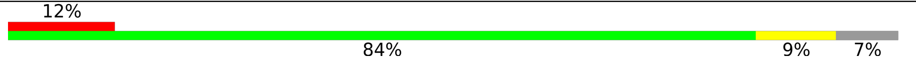
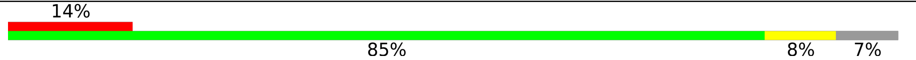
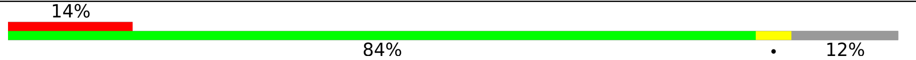
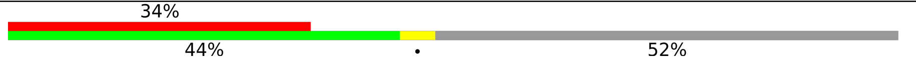
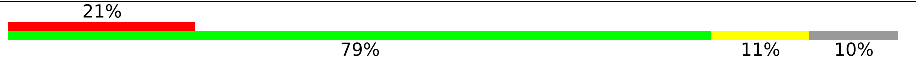
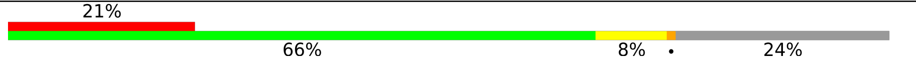
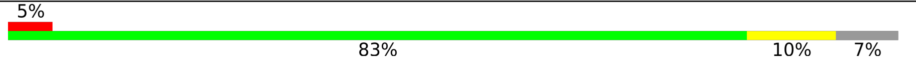
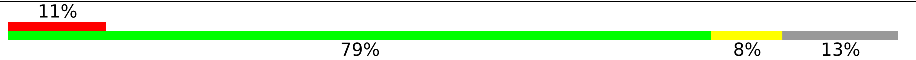
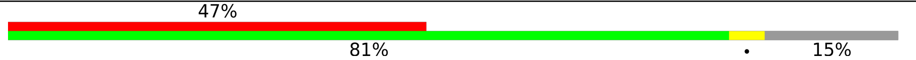
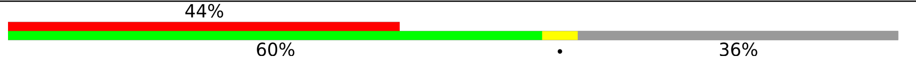
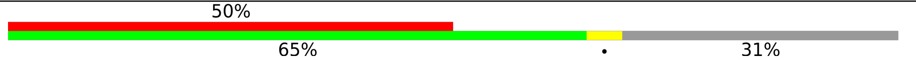
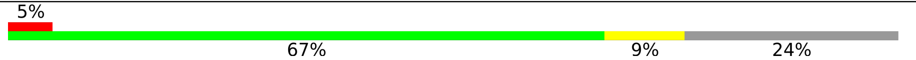
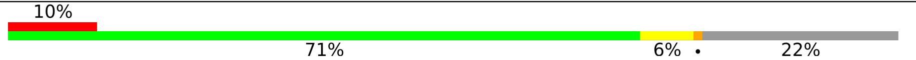
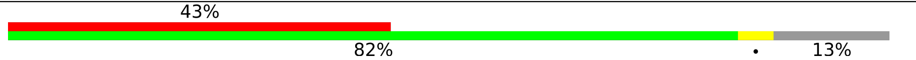
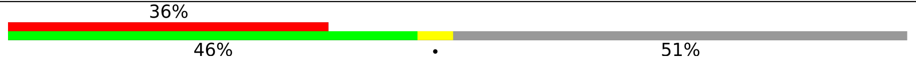
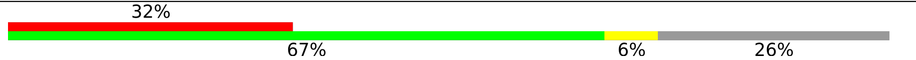
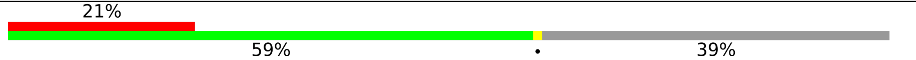
Mol	Chain	Length	Quality of chain
28	BU	149	
29	BV	209	
30	BW	210	
31	BX	150	
32	BY	216	
33	Ba	423	
34	Bb	380	
35	Bc	334	
36	Bd	206	
37	Be	135	
38	Bf	142	
39	Bg	159	
40	Bh	332	
41	Bi	306	
42	Bj	279	
43	Bk	212	
44	Bl	166	
45	Bm	159	
46	Bn	128	
47	Bo	124	
48	Bp	112	
49	Bq	138	
50	Bt	102	
51	Bu	205	
52	Bv	222	

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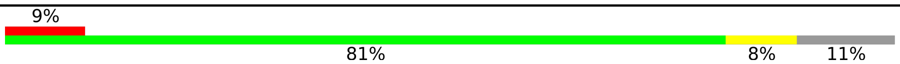
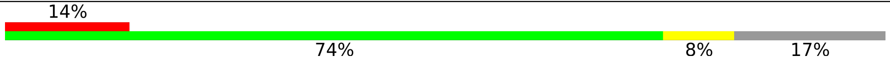
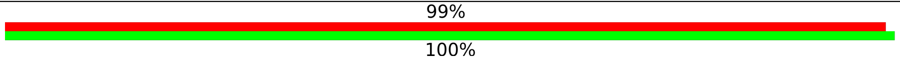
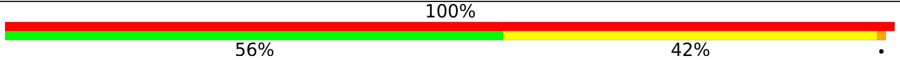
Mol	Chain	Length	Quality of chain
53	Bw	433	
54	Bx	196	
55	Bz	82	
56	AV	71	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 111109 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
1	BL	70	537	346	93	98	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 protein called 'Mitochondrial ribosomal protein L30.

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

- Molecule 6 is a protein called 'Mitochondrial ribosomal protein L55.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B4	45	381	239	77	62	3	0	0

- Molecule 7 is a protein called Mitochondrial ribosomal protein L32.

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

- Molecule 8 is a protein called Mitochondrial ribosomal protein L33.

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

- Molecule 9 is a protein called Mitochondrial ribosomal protein L34.

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

- Molecule 10 is a protein called Mitochondrial ribosomal protein L35.

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

- Molecule 11 is a protein called Ribosomal protein.

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

- Molecule 12 is a RNA chain called 16S ribosomal RNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	BA	1549	32950	14798	5993	10610	1549	0	0

- Molecule 13 is a RNA chain called CP tRNAPhe, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	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 14 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	BC	571	4364	2743	765	839	17	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	71	SER	-	expression tag	UNP P46199
BC	72	GLY	-	expression tag	UNP P46199
BC	73	GLY	-	expression tag	UNP P46199
BC	74	SER	-	expression tag	UNP P46199
BC	75	GLY	-	expression tag	UNP P46199
BC	76	SER	-	expression tag	UNP P46199
BC	77	GLY	-	expression tag	UNP P46199

- Molecule 15 is a protein called Mitochondrial ribosomal protein L2.

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

- Molecule 16 is a protein called ICT1.

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

- Molecule 17 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BF	250	2011	1294	367	344	6	0	0

- Molecule 18 is a protein called Mitochondrial ribosomal protein L9.

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

- Molecule 19 is a protein called Mitochondrial ribosomal protein L10.

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

- Molecule 20 is a protein called Mitochondrial ribosomal protein L11.

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

- Molecule 21 is a protein called Mitochondrial ribosomal protein L13.

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

- Molecule 22 is a protein called Mitochondrial ribosomal protein L14.

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

- Molecule 23 is a protein called Mitochondrial ribosomal protein L15.

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

- Molecule 24 is a protein called Mitochondrial ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	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 25 is a protein called Mitochondrial ribosomal protein L17.

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

- Molecule 26 is a protein called Mitochondrial ribosomal protein L18.

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

- Molecule 27 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	BT	223	1845	1181	319	336	9	0	0

- Molecule 28 is a protein called Mitochondrial ribosomal protein L20.

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

- Molecule 29 is a protein called Mitochondrial ribosomal protein L21.

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

- Molecule 30 is a protein called Mitochondrial ribosomal protein L22.

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

- Molecule 31 is a protein called Mitochondrial ribosomal protein L23.

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

- Molecule 32 is a protein called Mitochondrial ribosomal protein L24.

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

- Molecule 33 is a protein called Mitochondrial ribosomal protein L37.

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

- Molecule 34 is a protein called Mitochondrial ribosomal protein L38.

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

- Molecule 35 is a protein called Mitochondrial ribosomal protein L39.

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

- Molecule 36 is a protein called Mitochondrial ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bd	99	Total 832	C 528	N 148	O 155	S 1	0	0

- Molecule 37 is a protein called Mitochondrial ribosomal protein L41.

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

- Molecule 38 is a protein called Mitochondrial ribosomal protein L42.

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

- Molecule 39 is a protein called Mitochondrial ribosomal protein L43.

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

- Molecule 40 is a protein called Mitochondrial ribosomal protein L44.

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

- Molecule 41 is a protein called Mitochondrial ribosomal protein L45.

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

- Molecule 42 is a protein called Mitochondrial ribosomal protein L46.

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

- Molecule 43 is a protein called Mitochondrial ribosomal protein L48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Bk	136	1087	692	185	205	5	0	0

- Molecule 44 is a protein called Mrpl34.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 45 is a protein called Mitochondrial ribosomal protein L50.

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

- Molecule 46 is a protein called Mitochondrial ribosomal protein L51.

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

- Molecule 47 is a protein called Mitochondrial ribosomal protein L52.

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

- Molecule 48 is a protein called mL53, MRPL53.

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

- Molecule 49 is a protein called Uncharacterized protein.

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

- Molecule 50 is a protein called Mitochondrial ribosomal protein L57.

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

- Molecule 51 is a protein called Mitochondrial ribosomal protein L58.

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

- Molecule 52 is a protein called 'Mitochondrial ribosomal protein L59.

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

- Molecule 53 is a protein called mL65, MRPS30.

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

- Molecule 54 is a protein called Mitochondrial ribosomal protein S18A.

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

- Molecule 55 is a protein called unassigned secondary structure elements.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	Bz	82	Total 410	C 246	N 82	O 82	0	0

- Molecule 56 is a RNA chain called P-site fMet-tRNAMet, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	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

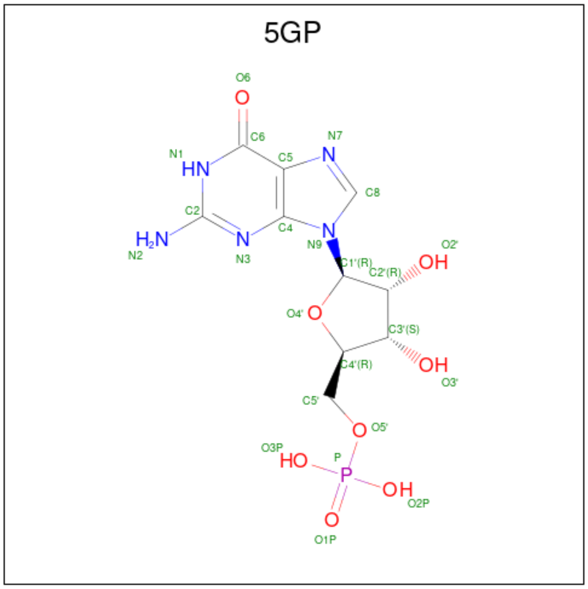
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	B3	1	1	1	0
57	BA	203	203	203	0
57	BB	1	1	1	0
57	BC	1	1	1	0
57	BD	3	3	3	0
57	BP	2	2	2	0
57	BQ	1	1	1	0
57	Be	2	2	2	0
57	Bl	1	1	1	0
57	Bt	1	1	1	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

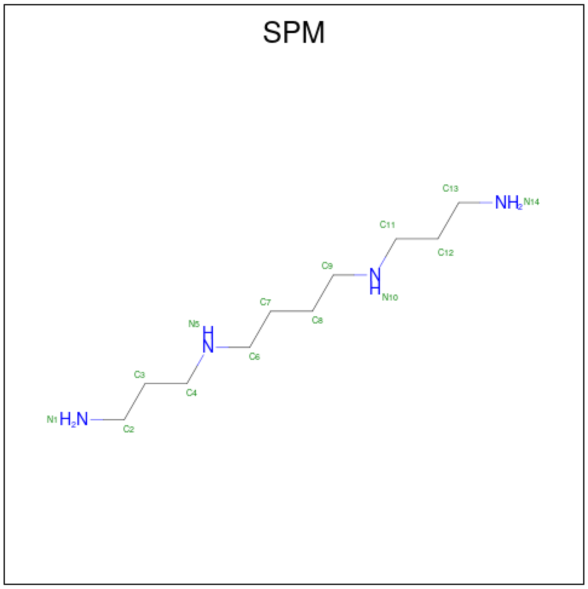
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
58	B5	1	1	1	0
58	B9	1	1	1	0
58	BJ	1	1	1	0

- Molecule 59 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



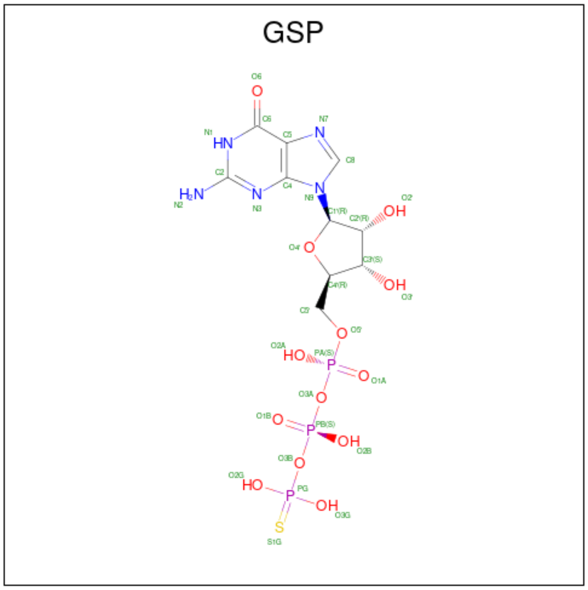
Mol	Chain	Residues	Atoms					AltConf
59	BA	1	Total 48	C 20	N 10	O 16	P 2	0
59	BA	1	Total 48	C 20	N 10	O 16	P 2	0

- Molecule 60 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	AltConf
60	BA	1	Total C N 14 10 4	0
60	BR	1	Total C N 14 10 4	0

- Molecule 61 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$) (labeled as "Ligand of Interest" by depositor).

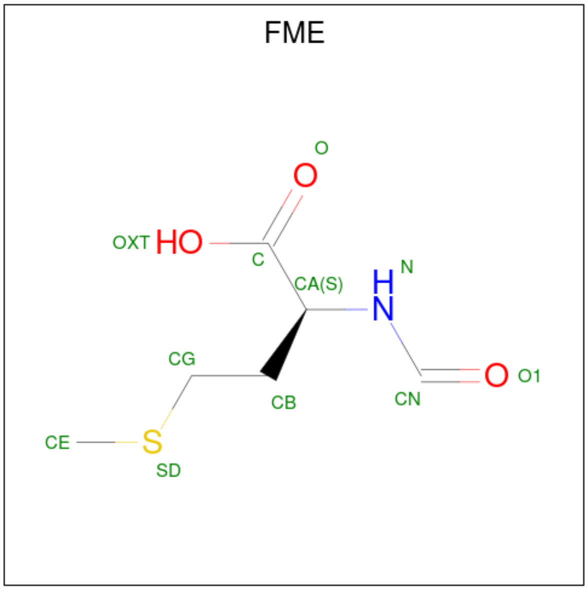


Mol	Chain	Residues	Atoms	AltConf
61	BC	1	Total C N O P S 32 10 5 13 3 1	0

- Molecule 62 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
62	BC	1	Total Na 1 1	0

- Molecule 63 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$) (labeled as "Ligand of Interest" by depositor).



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

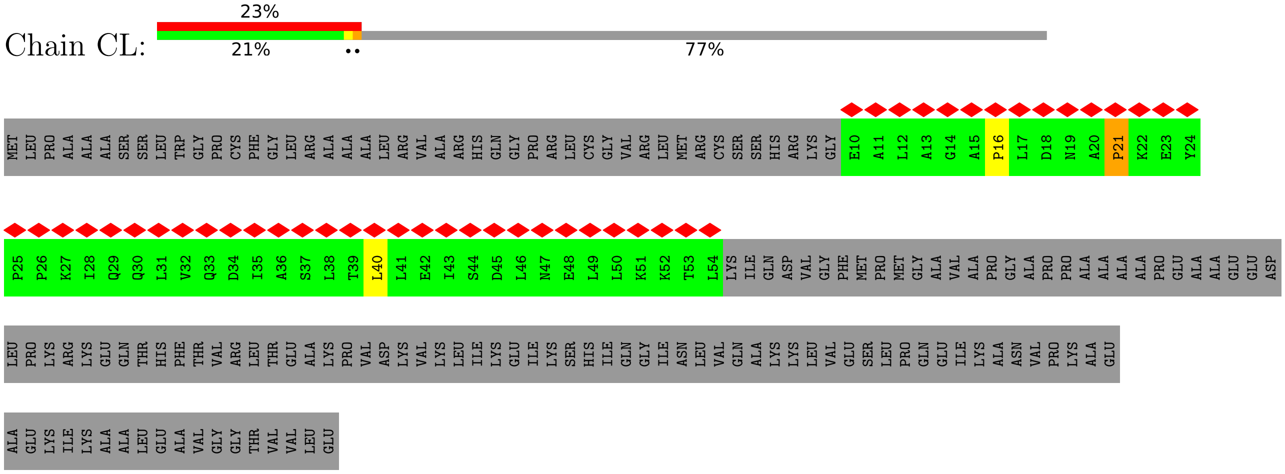
- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
64	BC	2	2	2	0

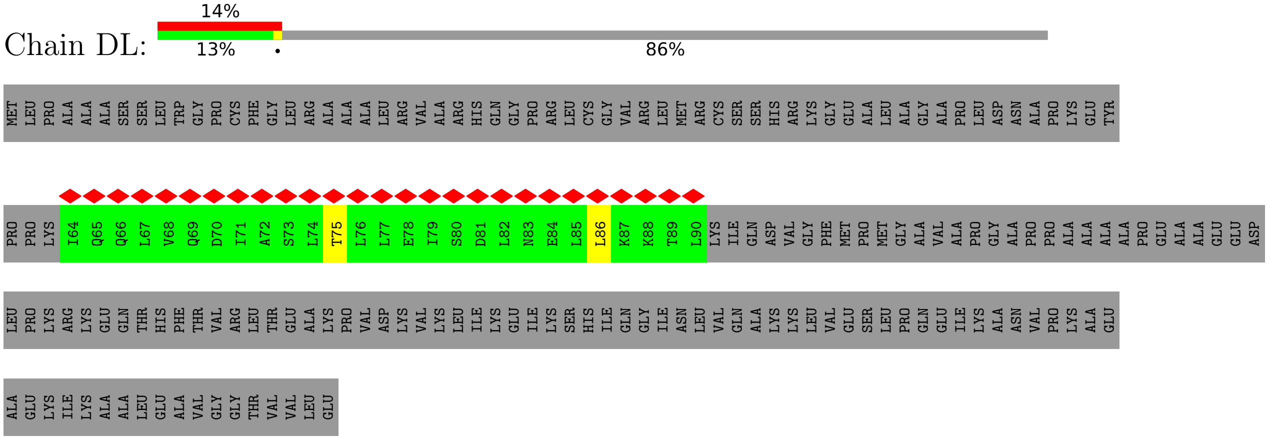
3 Residue-property plots ⓘ

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.

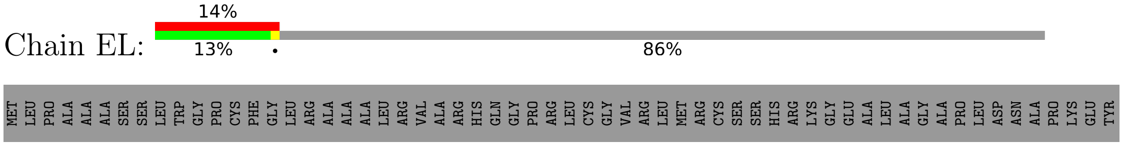
- Molecule 1: Mitochondrial ribosomal protein L12

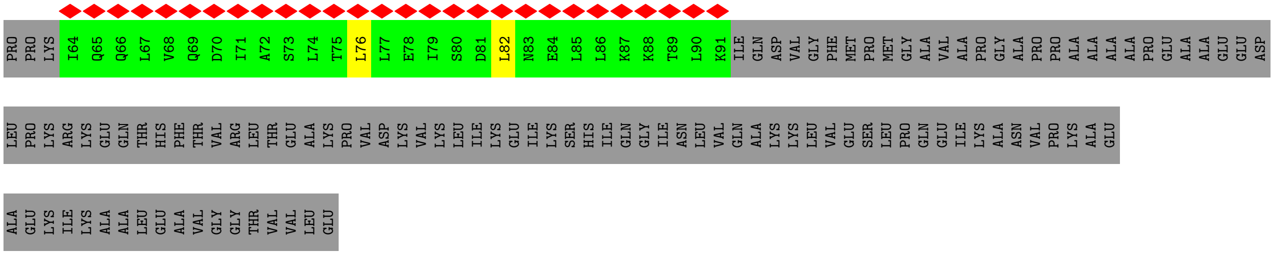


- Molecule 1: Mitochondrial ribosomal protein L12



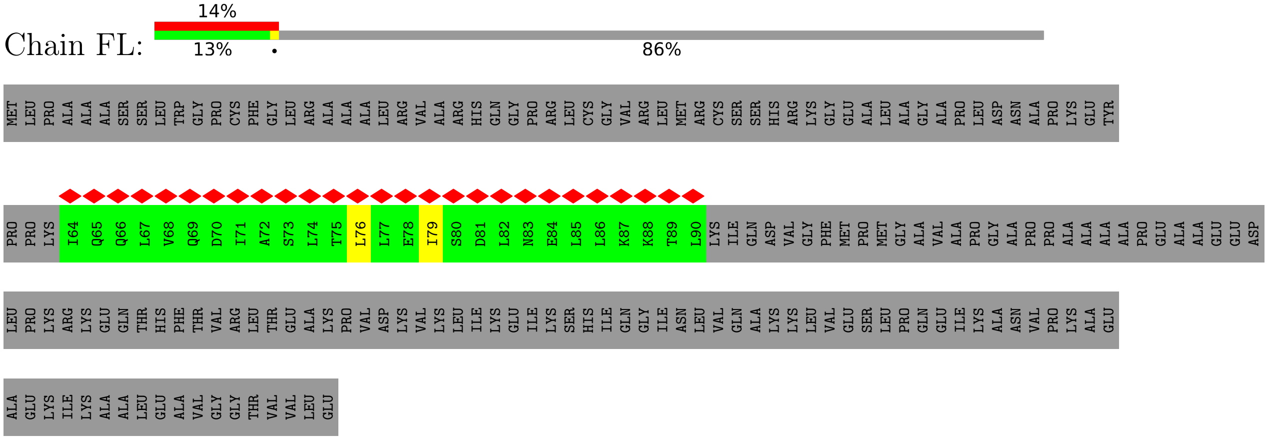
- Molecule 1: Mitochondrial ribosomal protein L12





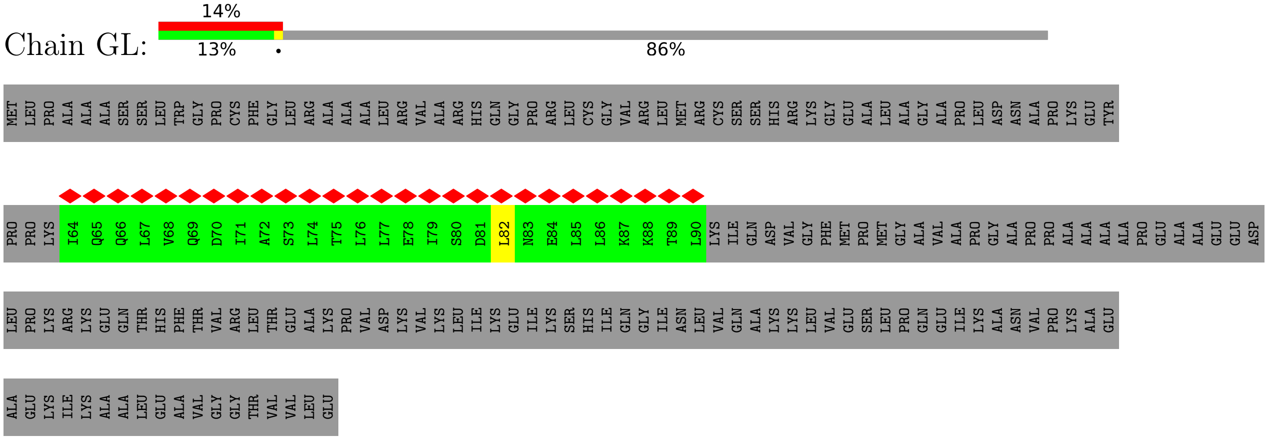
- Molecule 1: Mitochondrial ribosomal protein L12

Chain FL:



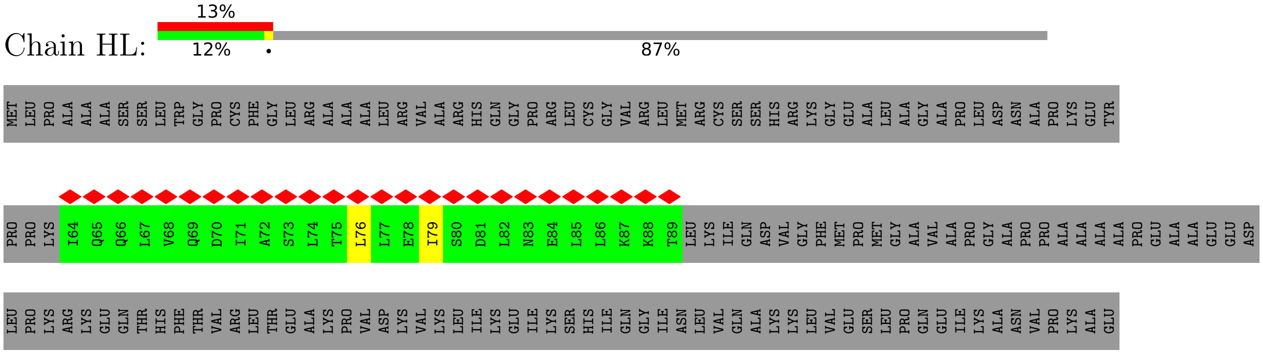
- Molecule 1: Mitochondrial ribosomal protein L12

Chain GL:

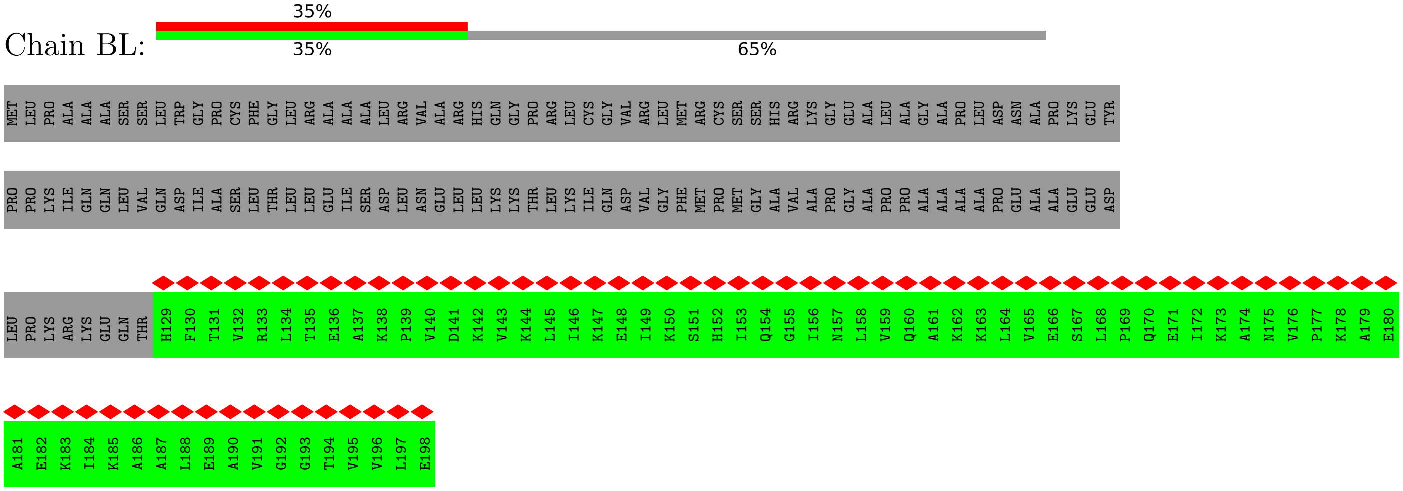


- Molecule 1: Mitochondrial ribosomal protein L12

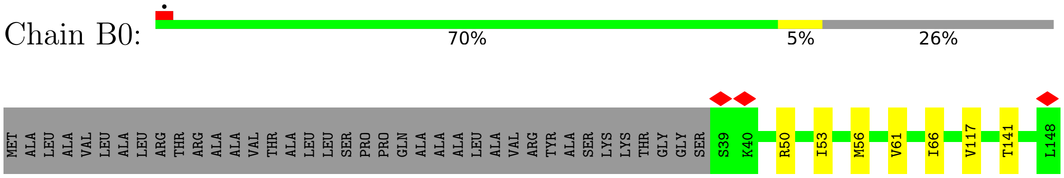
Chain HL:



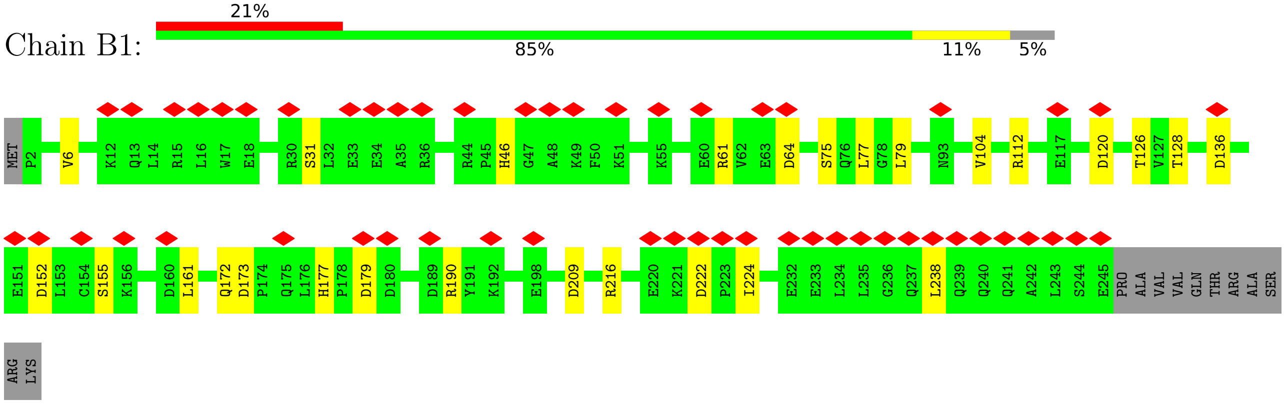
- Molecule 1: Mitochondrial ribosomal protein L12



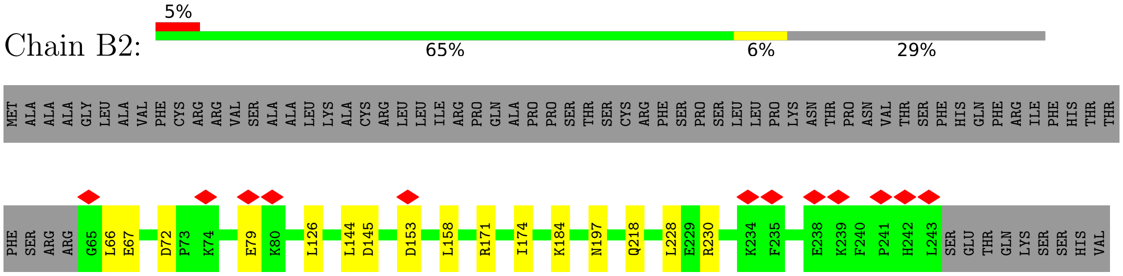
- Molecule 2: Mitochondrial ribosomal protein L27



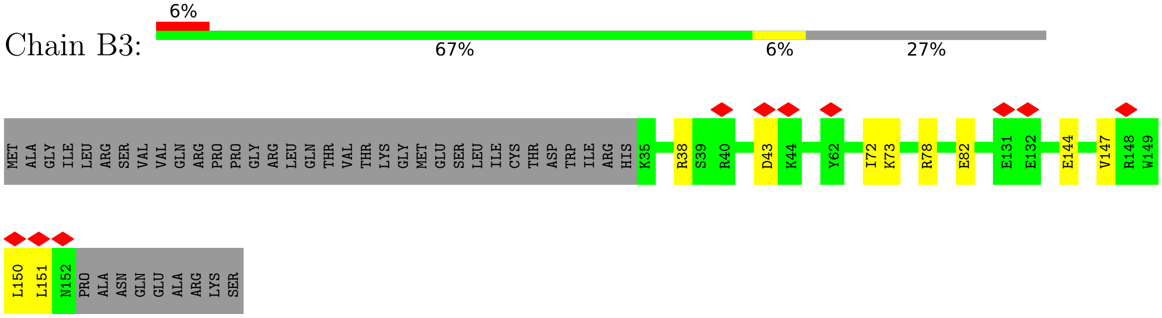
- Molecule 3: Mitochondrial ribosomal protein L28



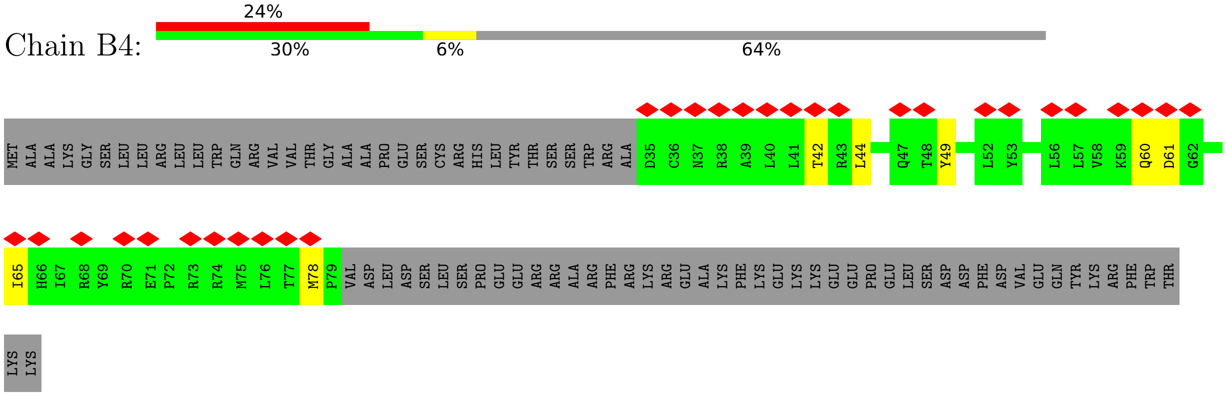
- Molecule 4: Mitochondrial ribosomal protein L47



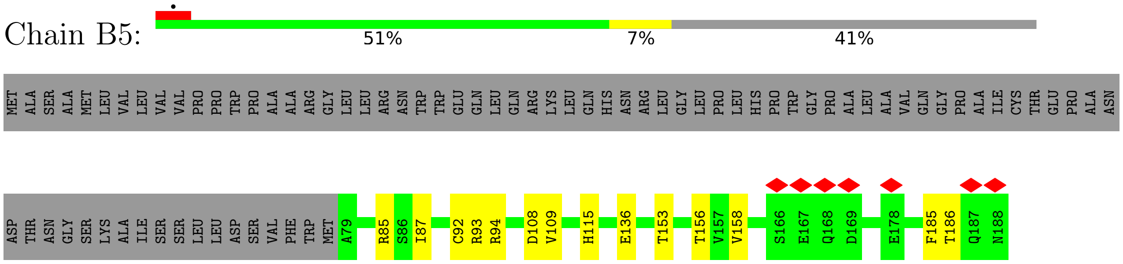
- Molecule 5: 'Mitochondrial ribosomal protein L30



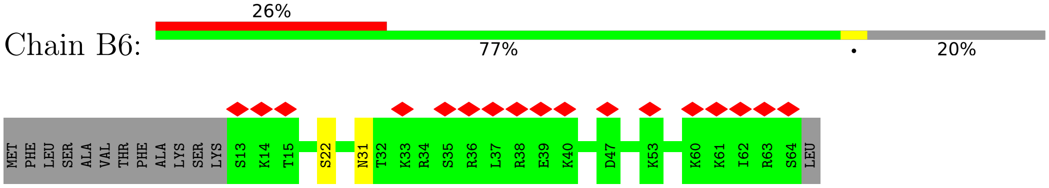
- Molecule 6: 'Mitochondrial ribosomal protein L55



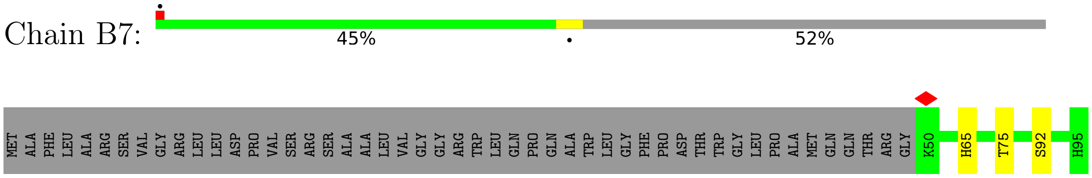
- Molecule 7: Mitochondrial ribosomal protein L32



- Molecule 8: Mitochondrial ribosomal protein L33

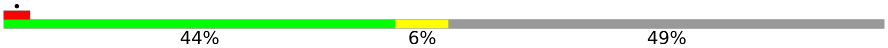


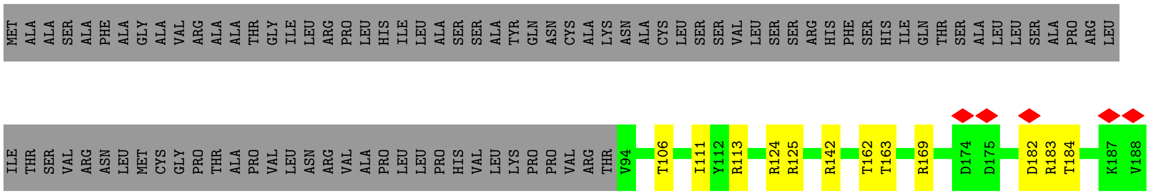
- Molecule 9: Mitochondrial ribosomal protein L34



- Molecule 10: Mitochondrial ribosomal protein L35

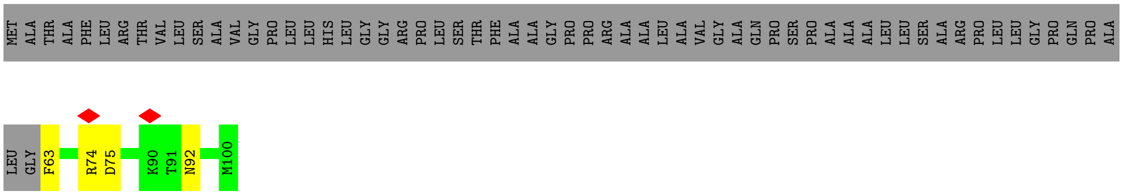
Chain B8:





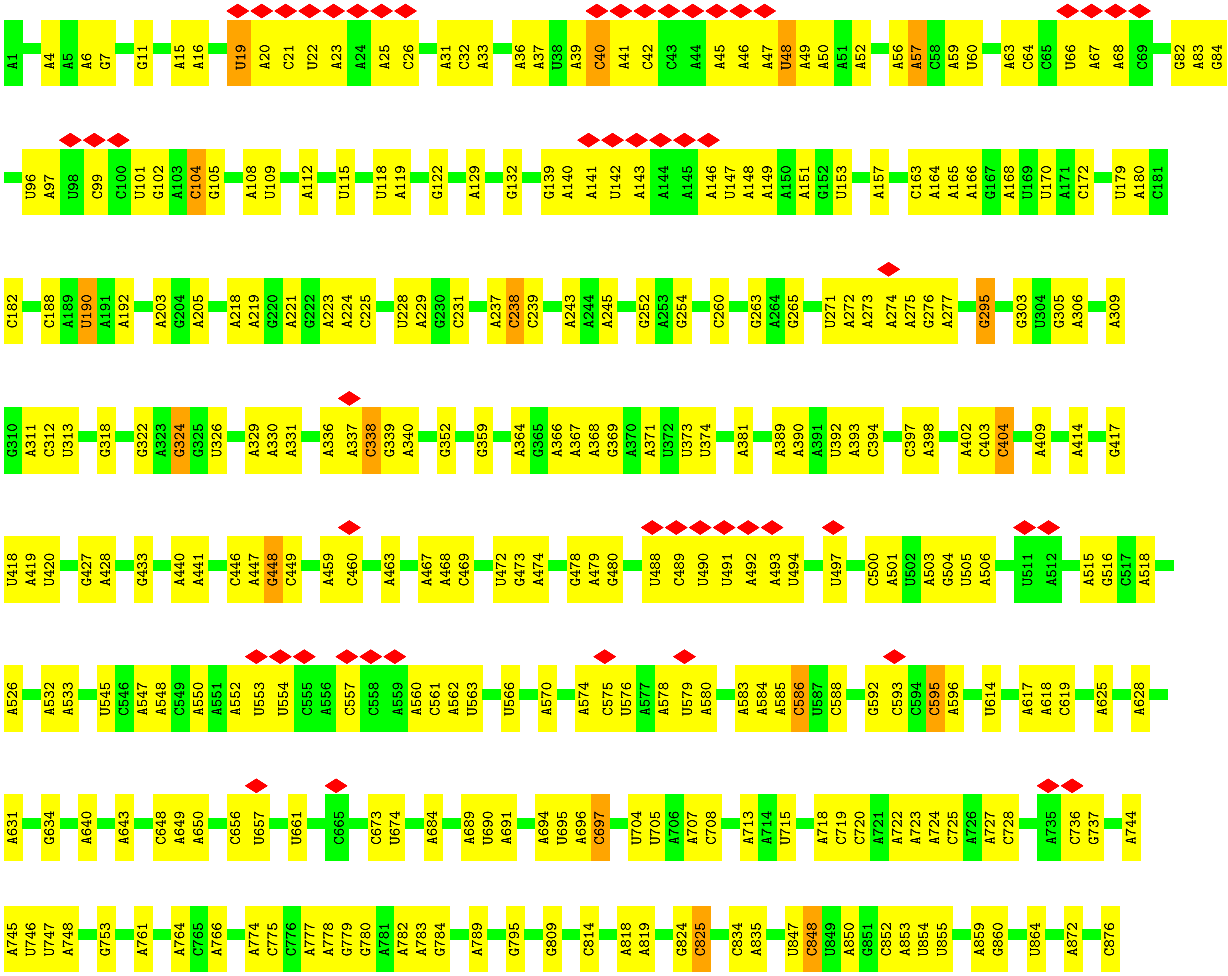
- Molecule 11: Ribosomal protein

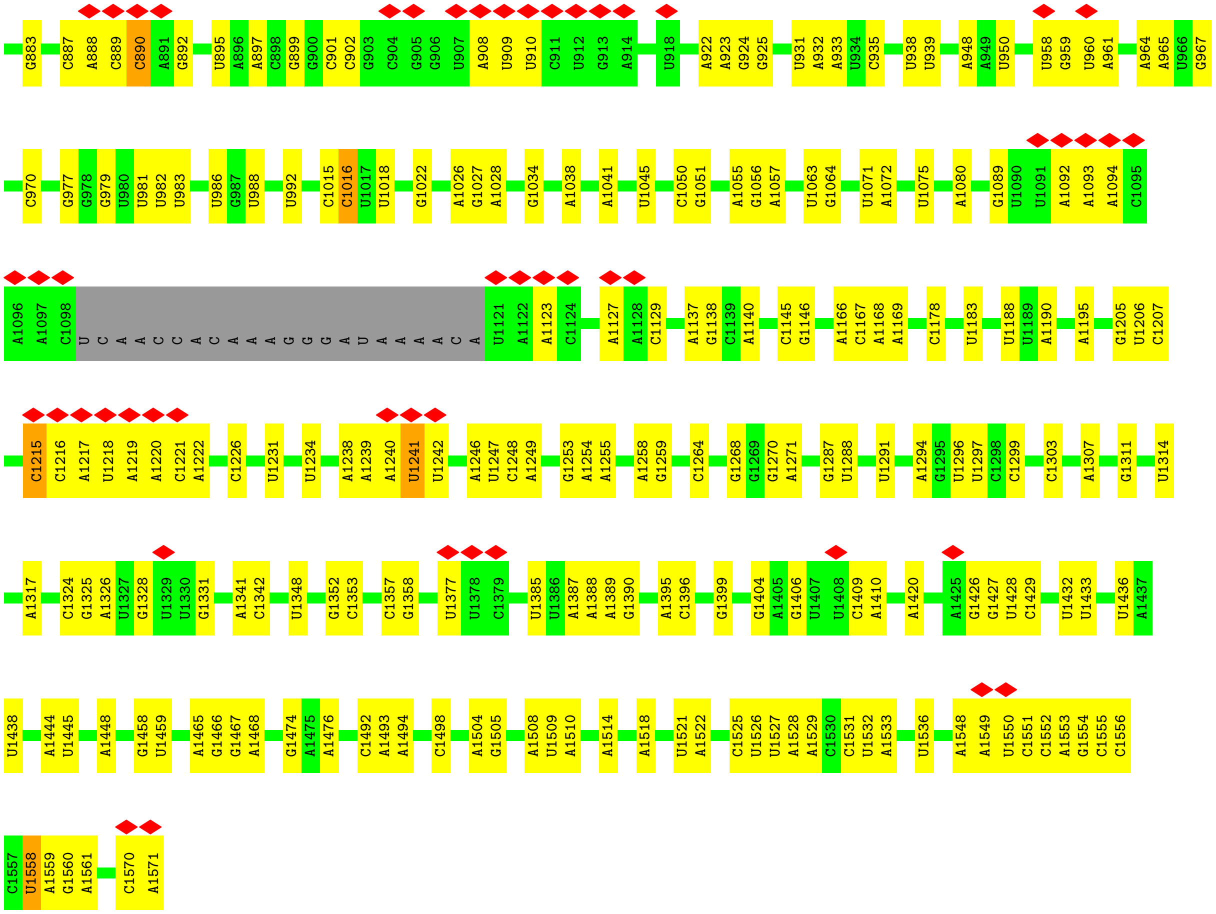
Chain B9:



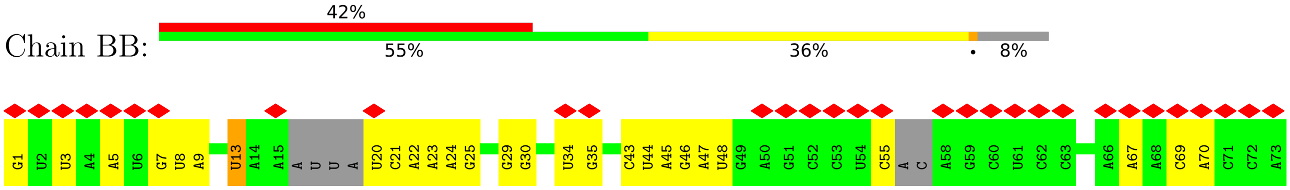
- Molecule 12: 16S ribosomal RNA, mitochondrial

Chain BA:

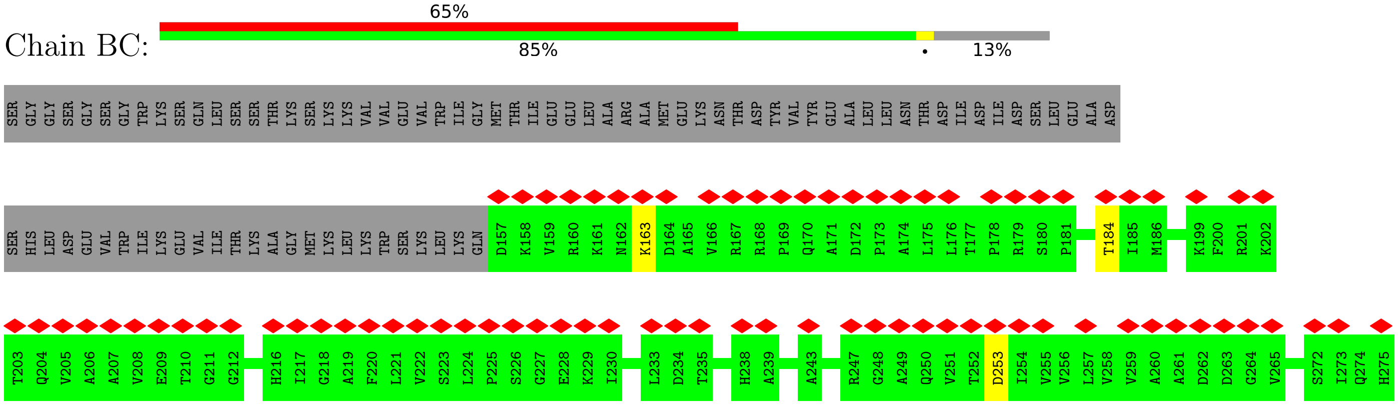


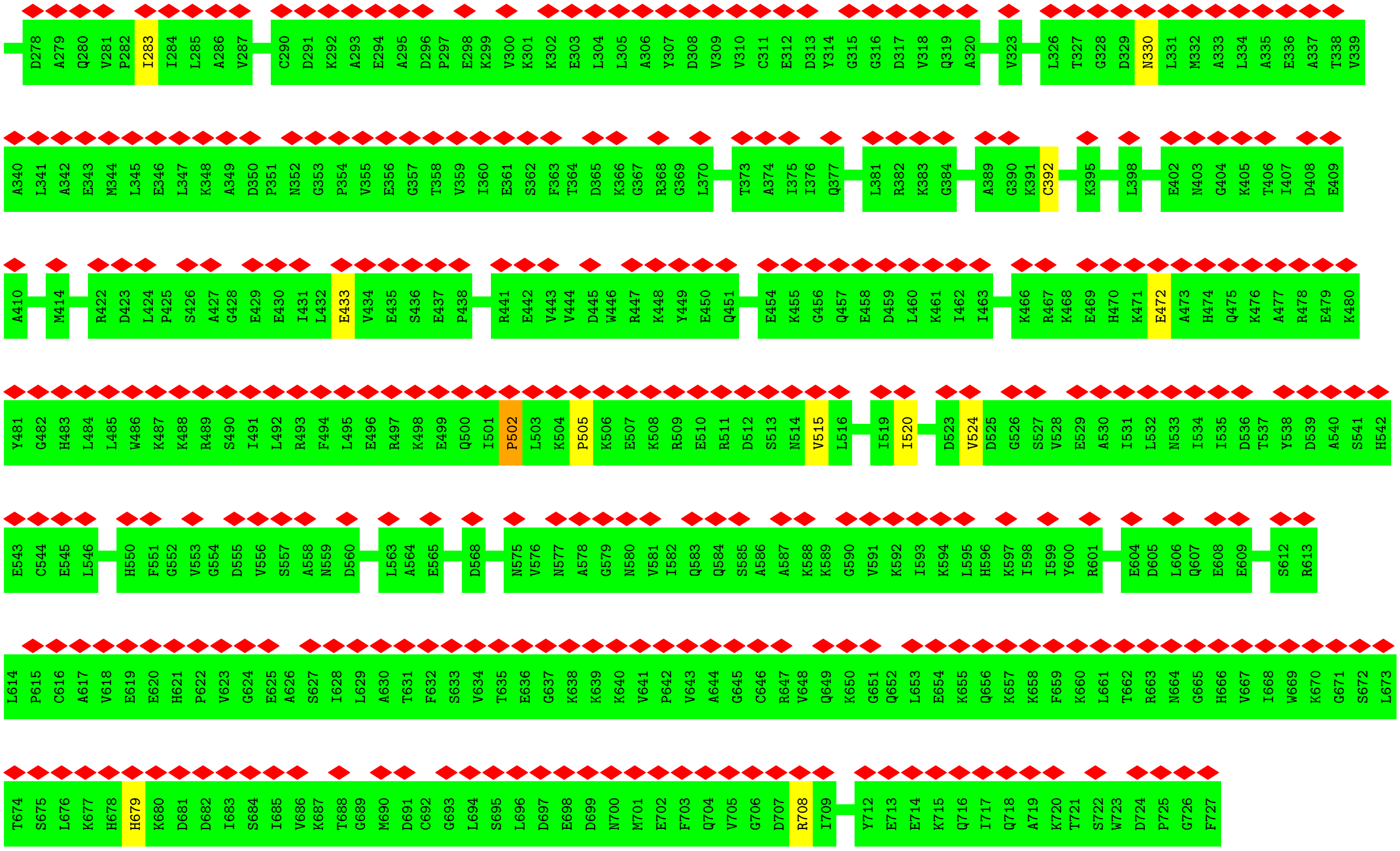


- Molecule 13: CP tRNAPhe, mitochondrial



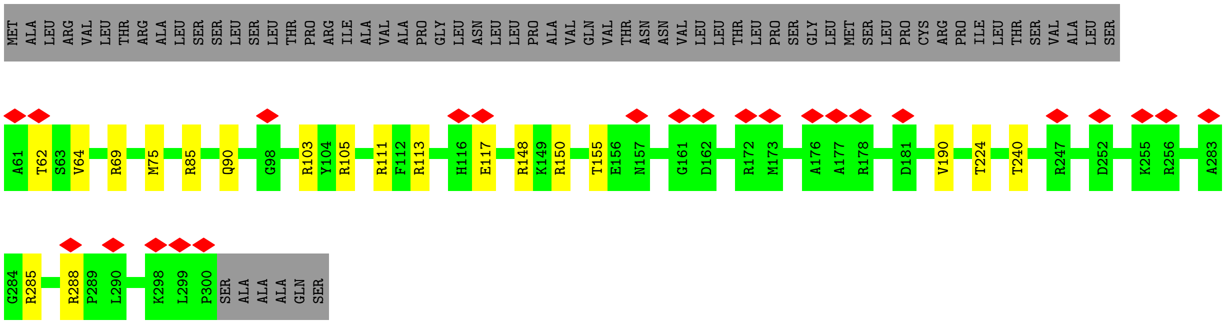
- Molecule 14: Translation initiation factor IF-2, mitochondrial





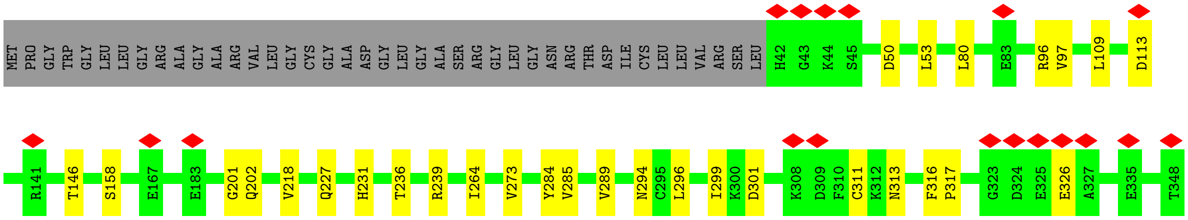
- Molecule 15: Mitochondrial ribosomal protein L2

Chain BD:

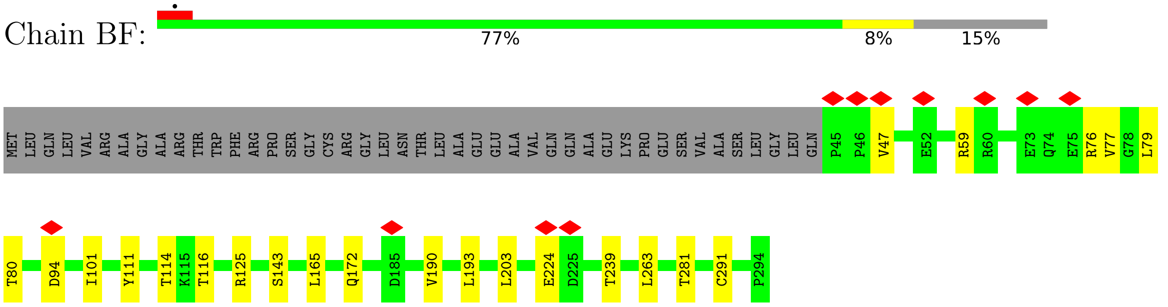


- Molecule 16: ICT1

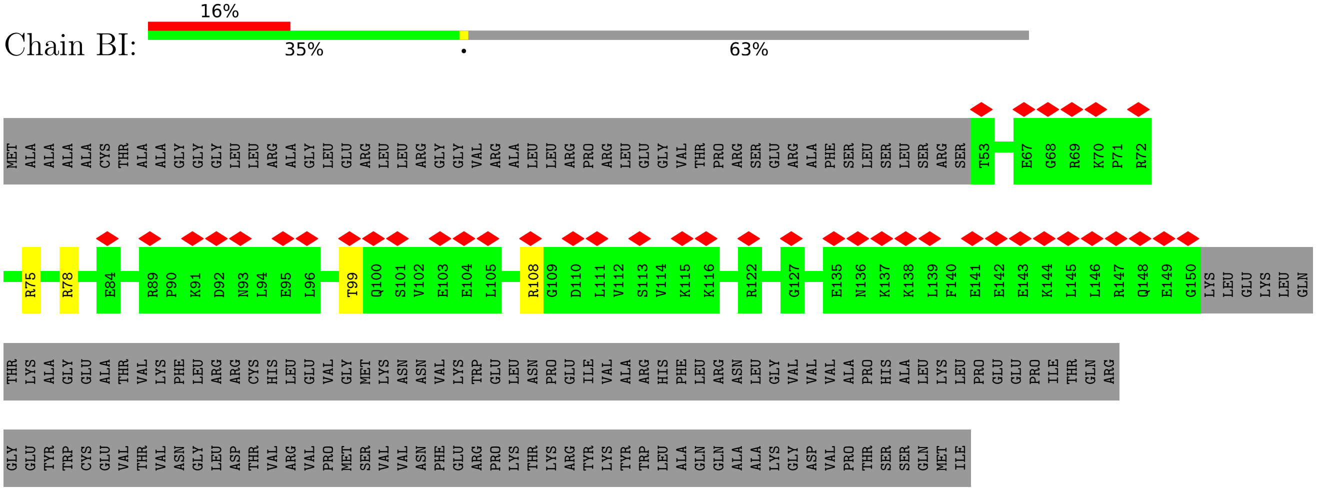
Chain BE:



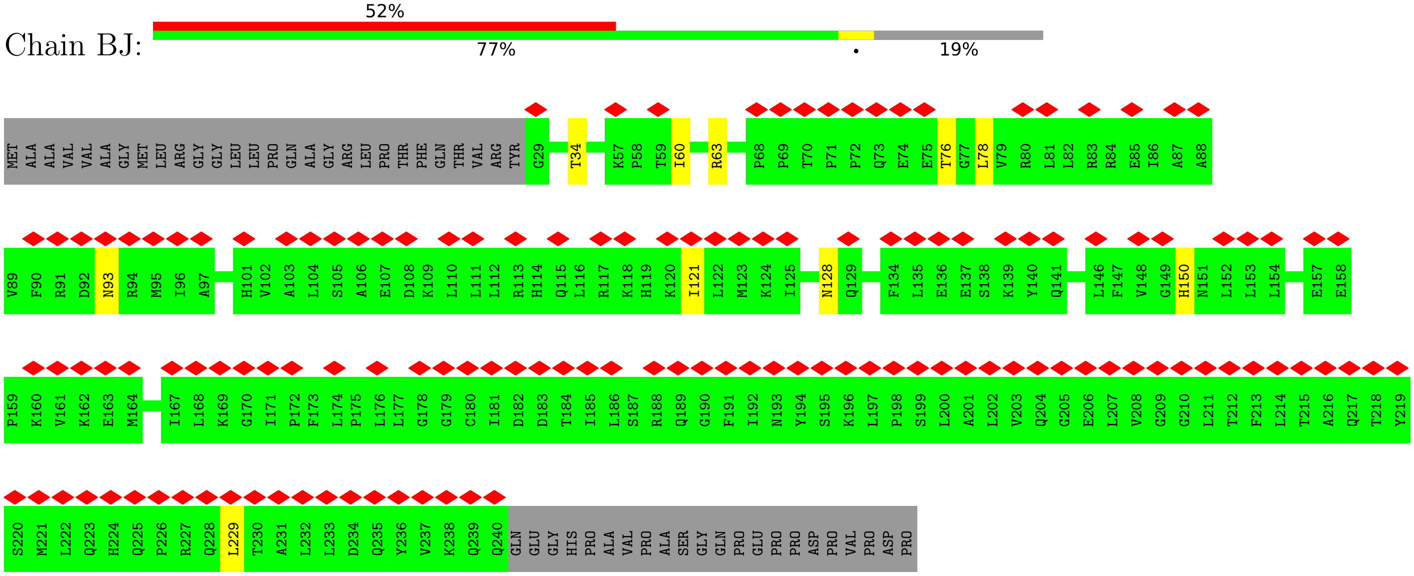
- Molecule 17: Mitochondrial ribosomal protein L4



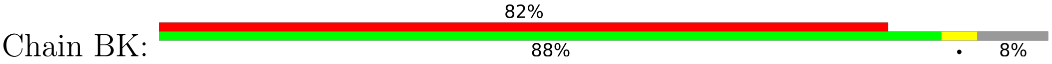
- Molecule 18: Mitochondrial ribosomal protein L9

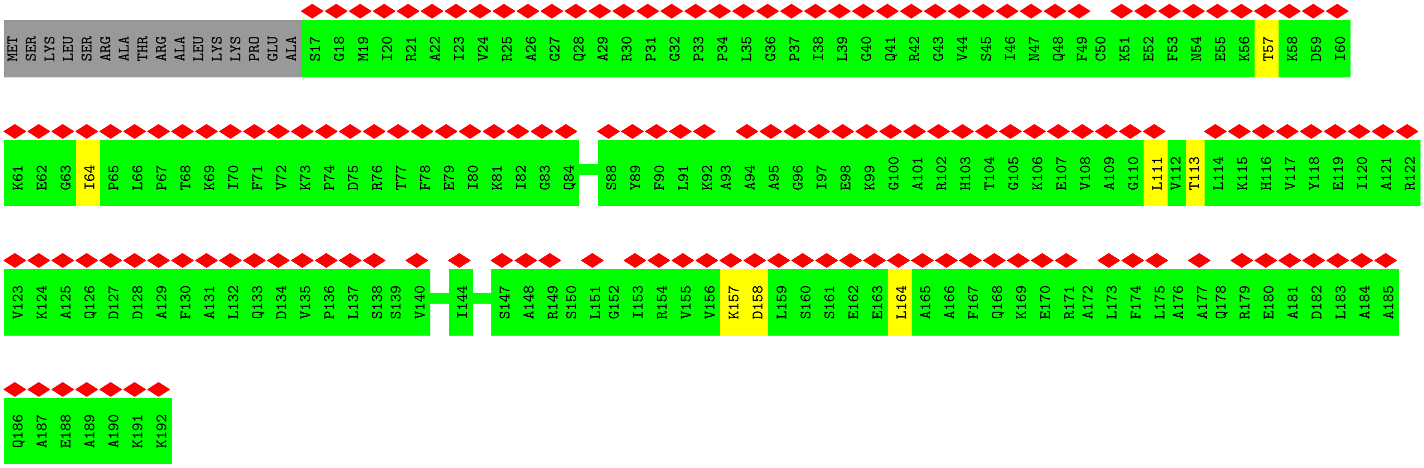


- Molecule 19: Mitochondrial ribosomal protein L10



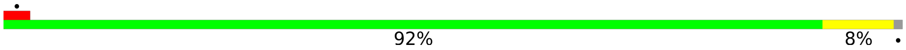
- Molecule 20: Mitochondrial ribosomal protein L11

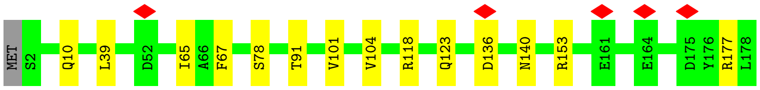




- Molecule 21: Mitochondrial ribosomal protein L13

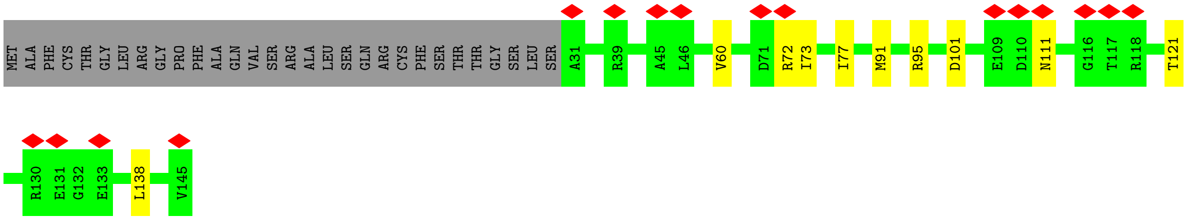
Chain BN:





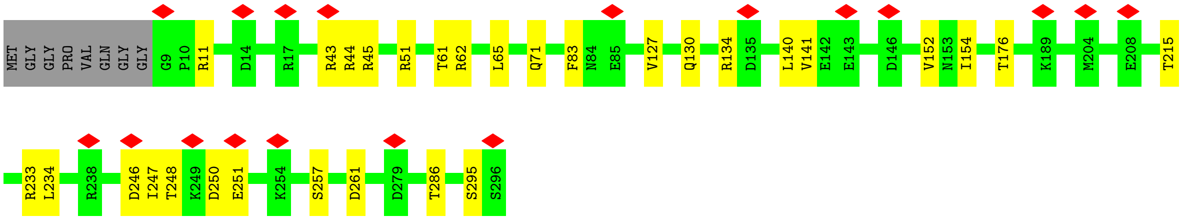
- Molecule 22: Mitochondrial ribosomal protein L14

Chain BO:



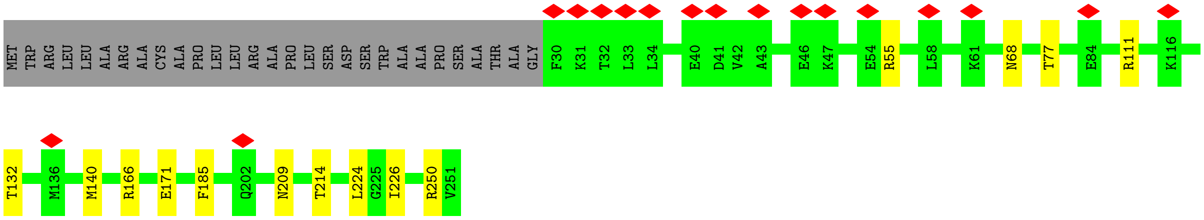
- Molecule 23: Mitochondrial ribosomal protein L15

Chain BP:



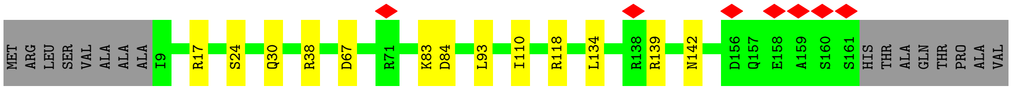
- Molecule 24: Mitochondrial ribosomal protein L16

Chain BQ:



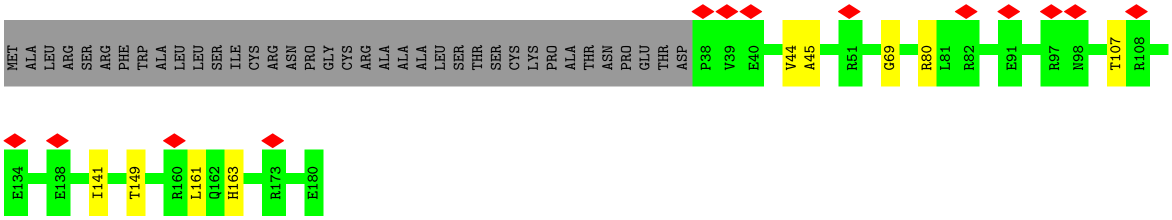
- Molecule 25: Mitochondrial ribosomal protein L17

Chain BR:



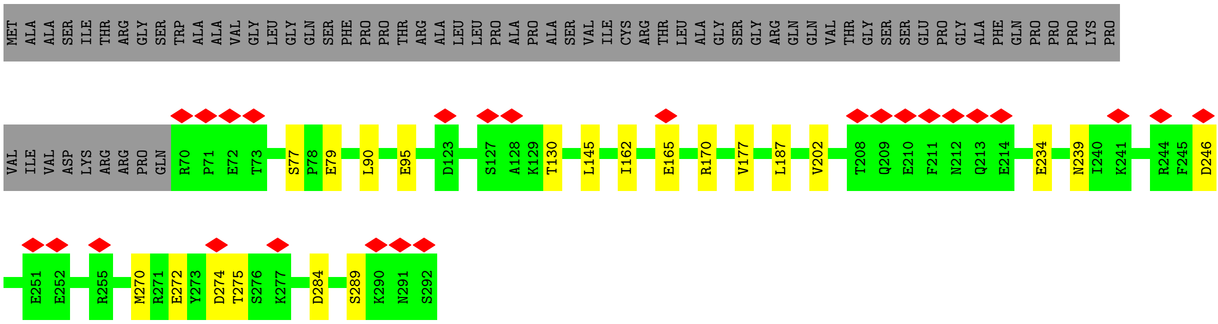
- Molecule 26: Mitochondrial ribosomal protein L18

Chain BS:



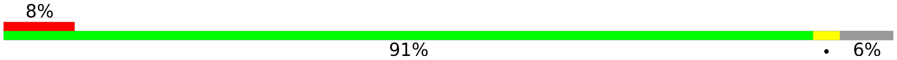
- Molecule 27: Mitochondrial ribosomal protein L19

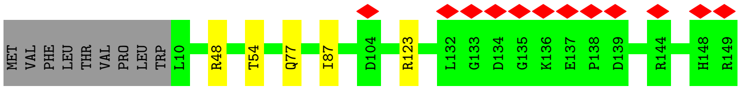
Chain BT:



- Molecule 28: Mitochondrial ribosomal protein L20

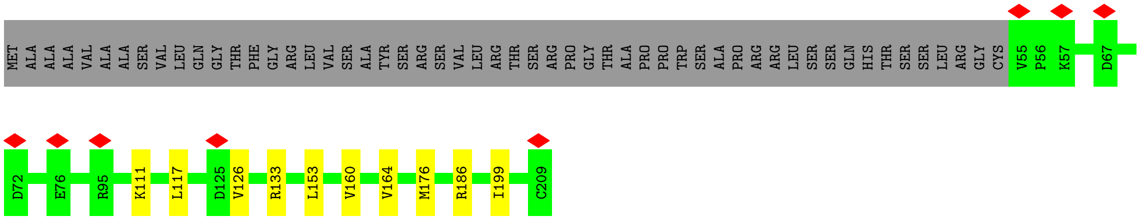
Chain BU:



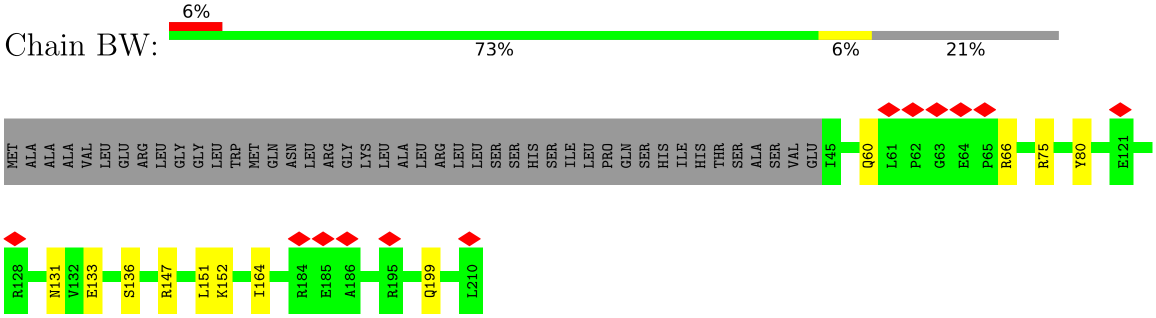


- Molecule 29: Mitochondrial ribosomal protein L21

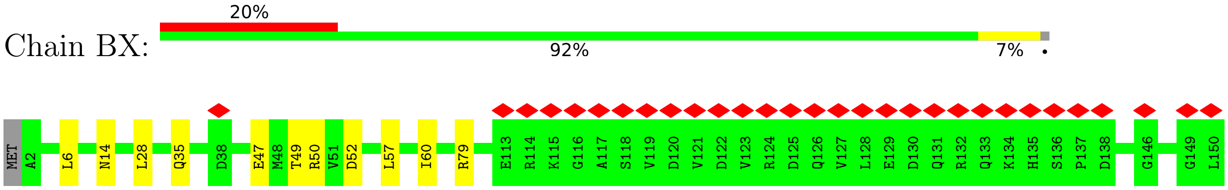
Chain BV:



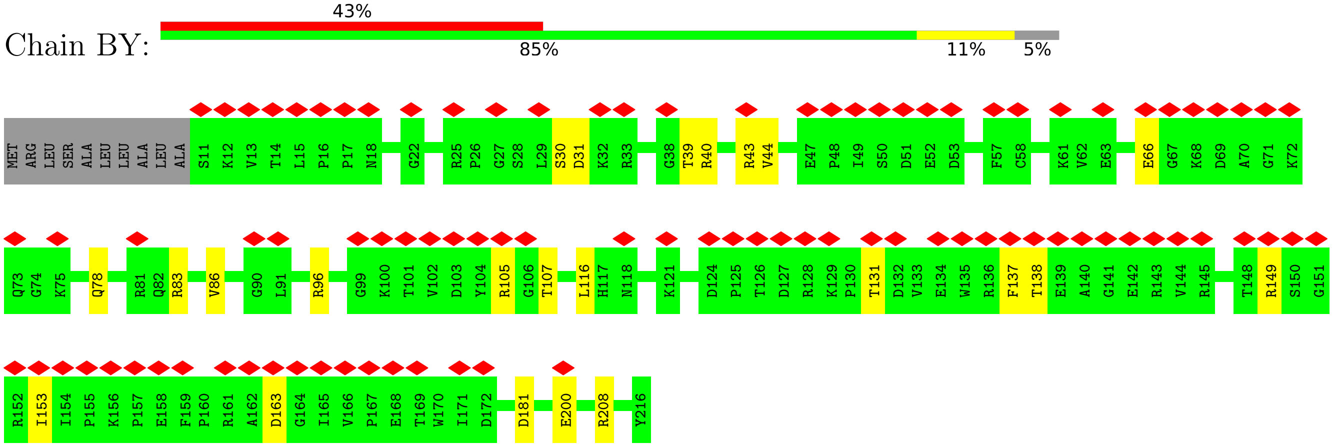
- Molecule 30: Mitochondrial ribosomal protein L22



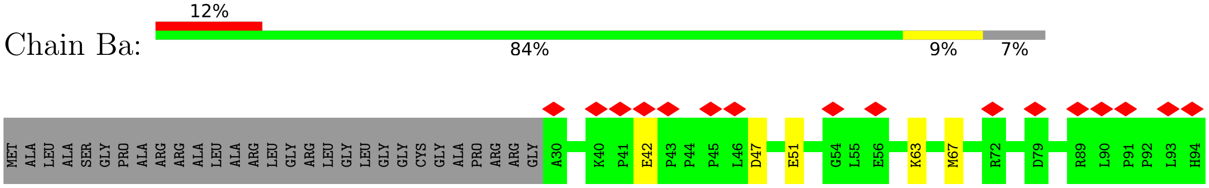
- Molecule 31: Mitochondrial ribosomal protein L23

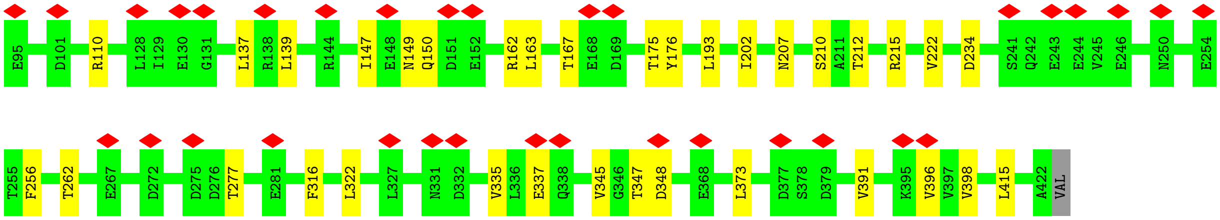


- Molecule 32: Mitochondrial ribosomal protein L24



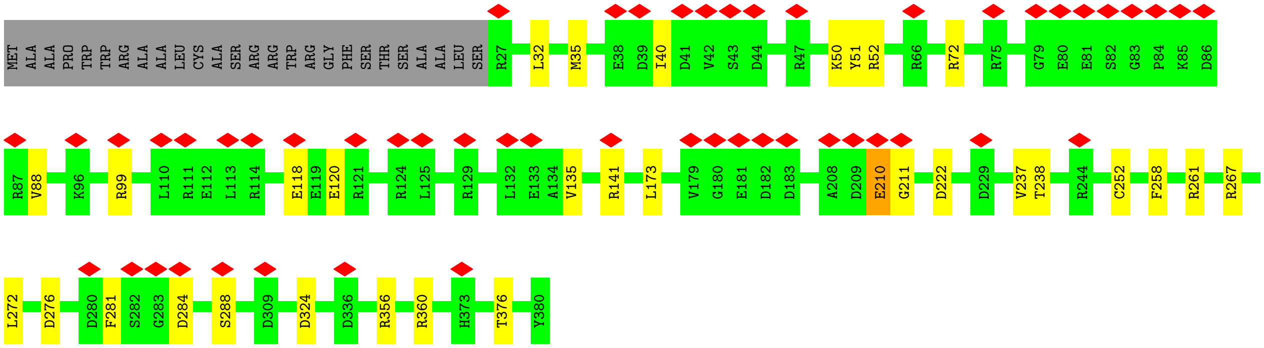
- Molecule 33: Mitochondrial ribosomal protein L37





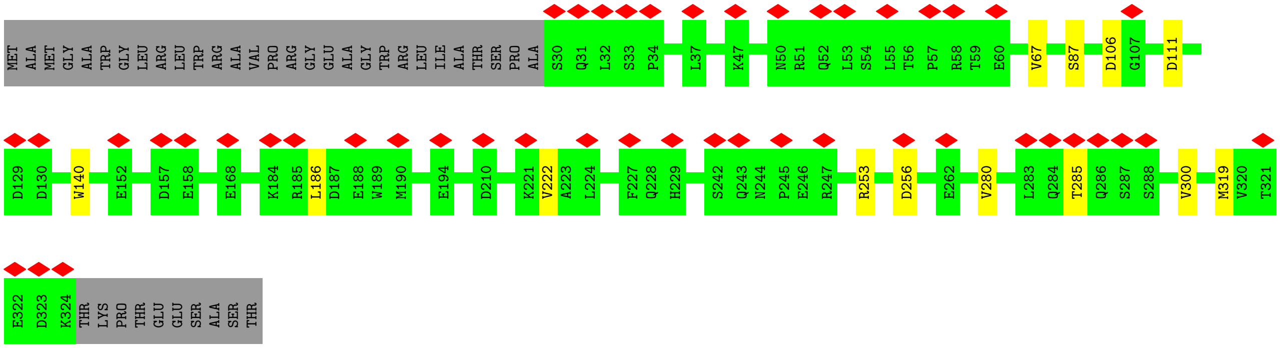
- Molecule 34: Mitochondrial ribosomal protein L38

Chain Bb:



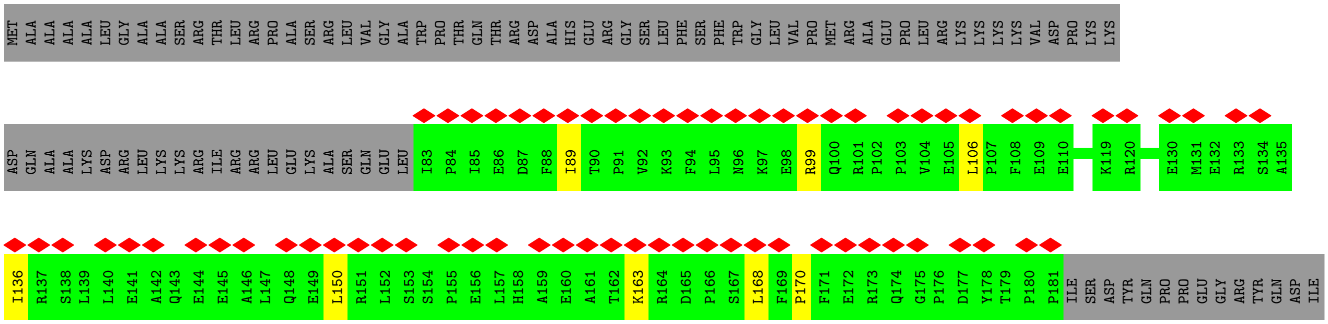
- Molecule 35: Mitochondrial ribosomal protein L39

Chain Bc:



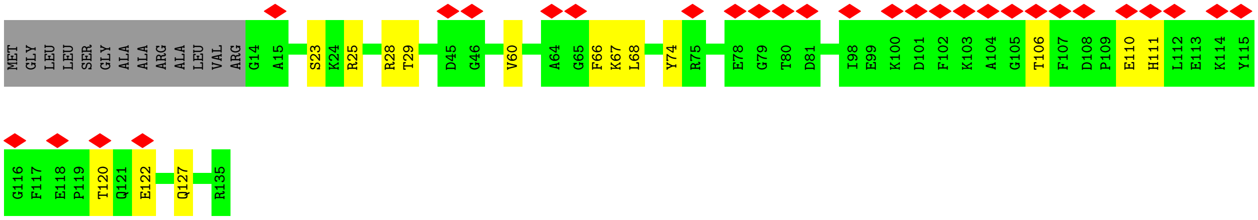
- Molecule 36: Mitochondrial ribosomal protein L40

Chain Bd:



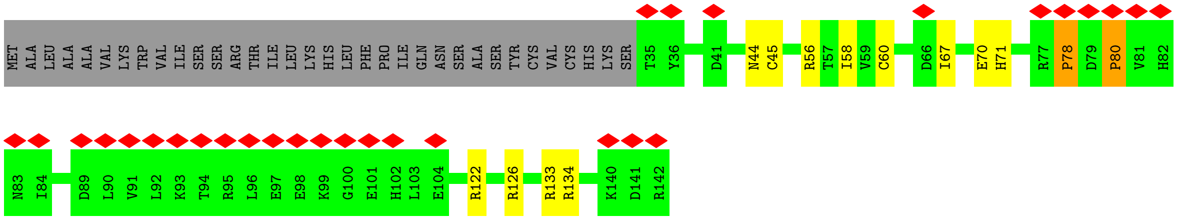
- Molecule 37: Mitochondrial ribosomal protein L41

Chain Be:



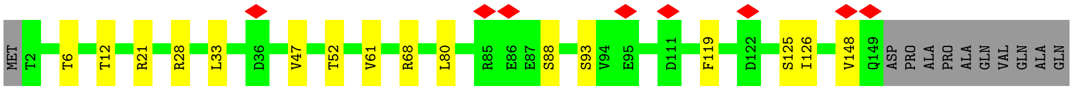
- Molecule 38: Mitochondrial ribosomal protein L42

Chain Bf:



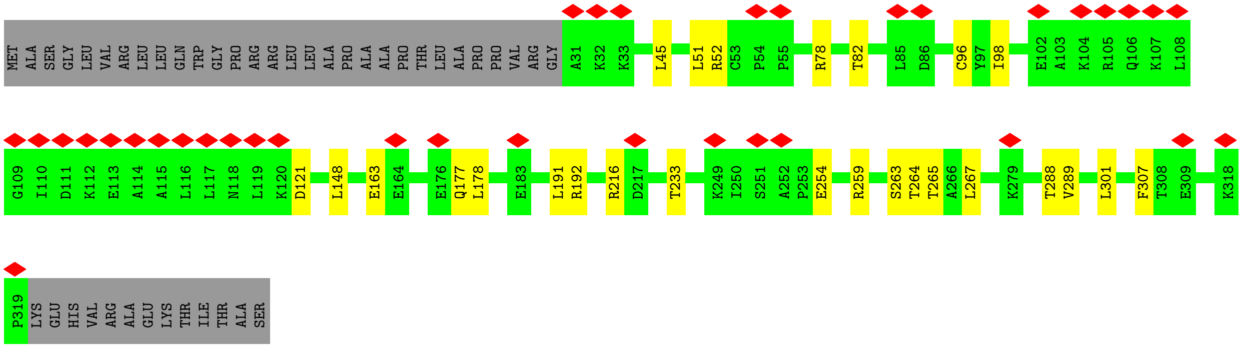
- Molecule 39: Mitochondrial ribosomal protein L43

Chain Bg:

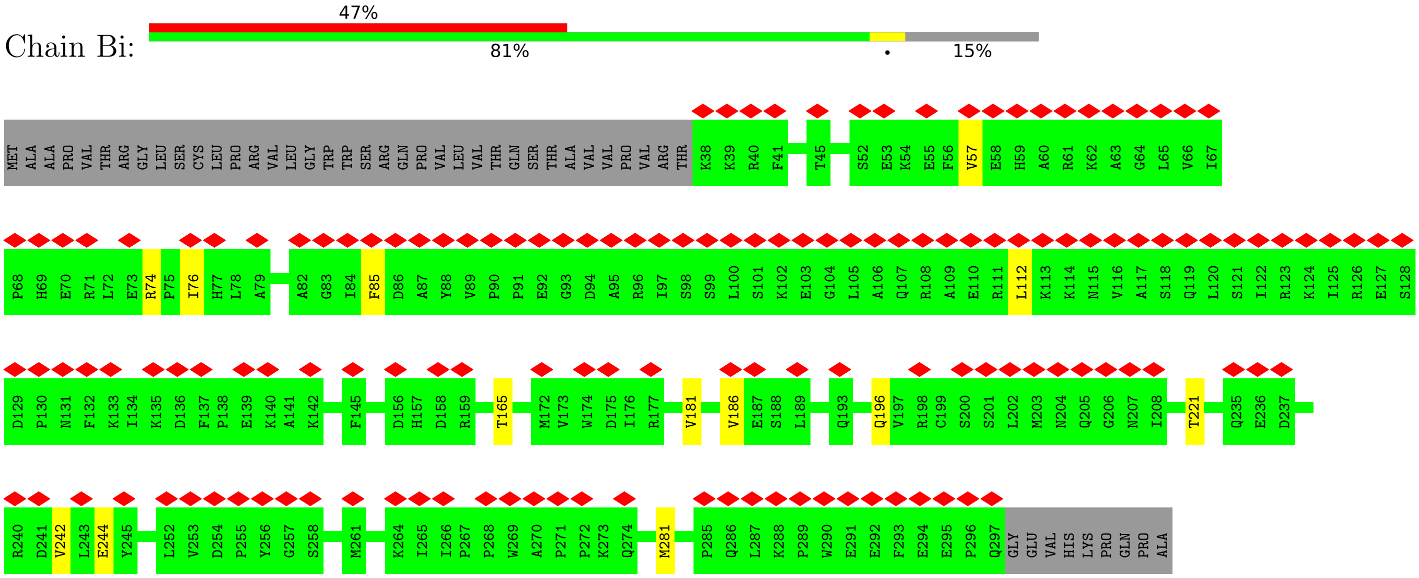


- Molecule 40: Mitochondrial ribosomal protein L44

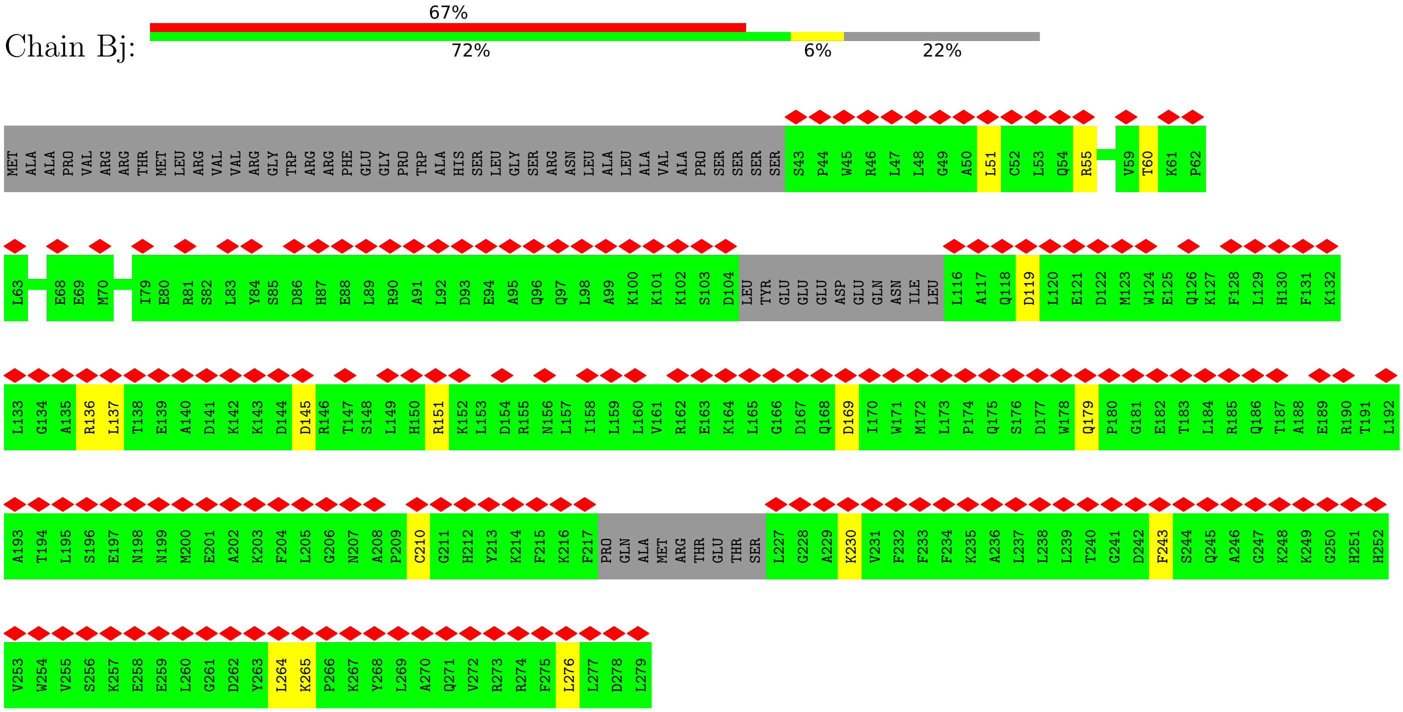
Chain Bh:



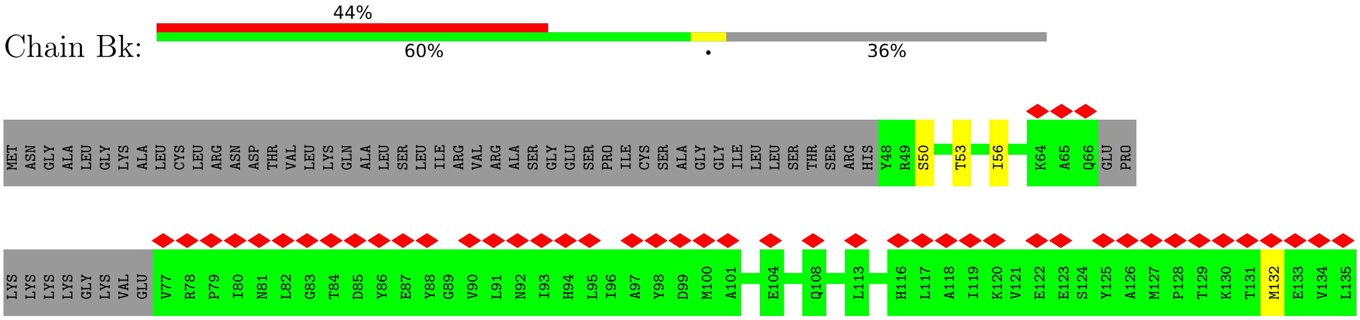
- Molecule 41: Mitochondrial ribosomal protein L45

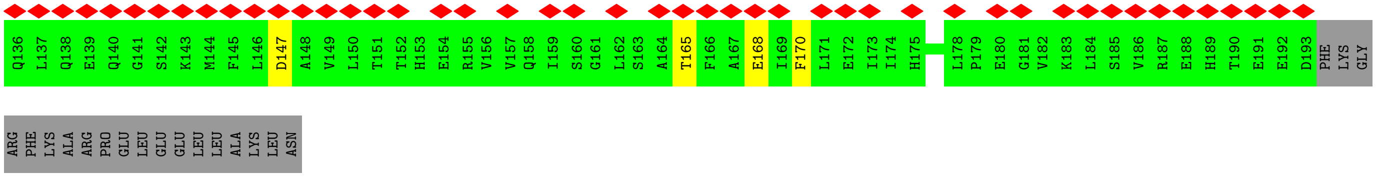


- Molecule 42: Mitochondrial ribosomal protein L46



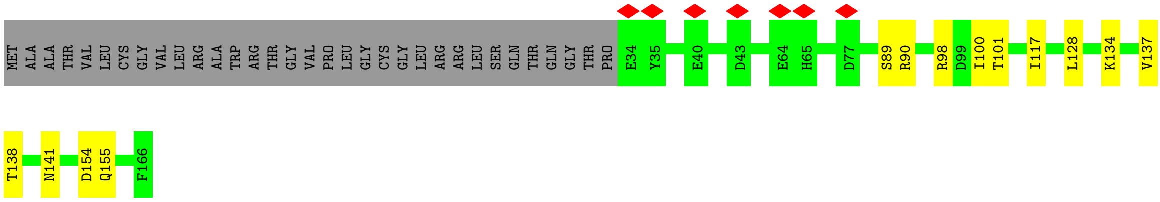
- Molecule 43: Mitochondrial ribosomal protein L48





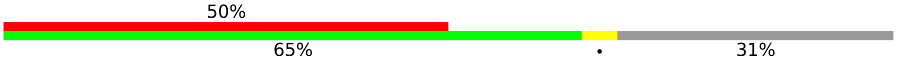
- Molecule 44: Mrpl34

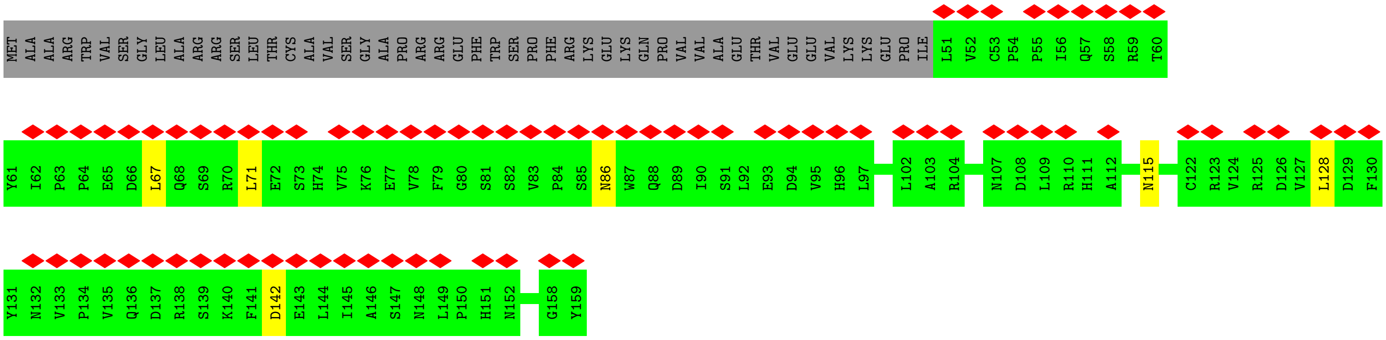
Chain Bl:



- Molecule 45: Mitochondrial ribosomal protein L50

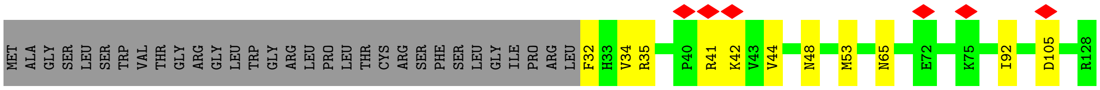
Chain Bm:





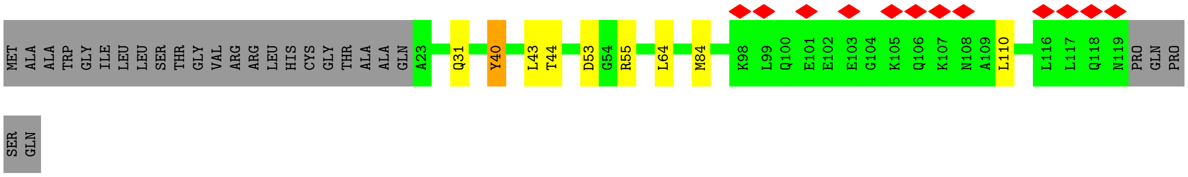
- Molecule 46: Mitochondrial ribosomal protein L51

Chain Bn:



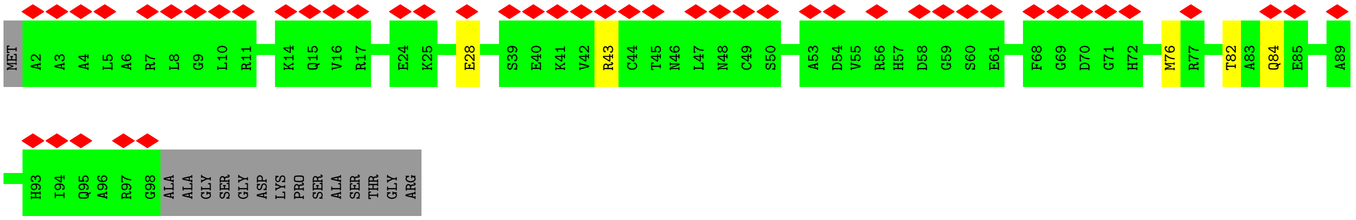
- Molecule 47: Mitochondrial ribosomal protein L52

Chain Bo:



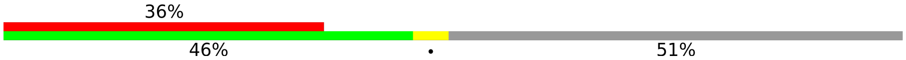
- Molecule 48: mL53, MRPL53

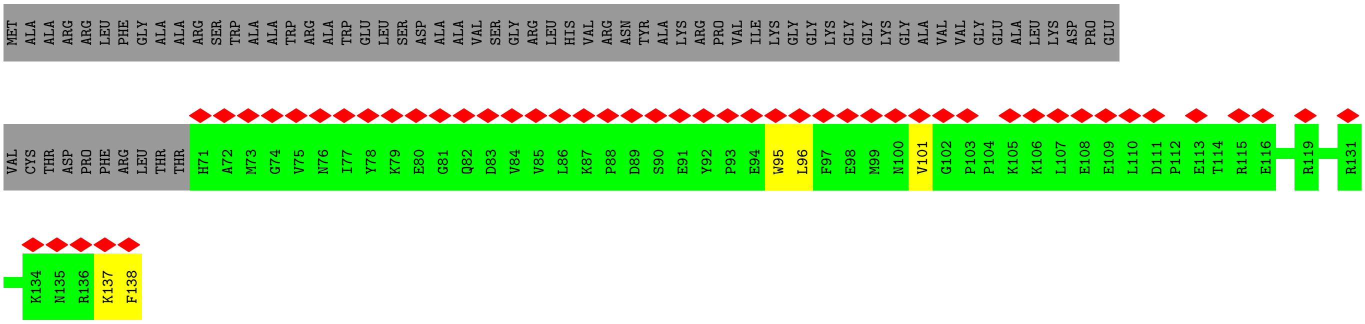
Chain Bp:



- Molecule 49: Uncharacterized protein

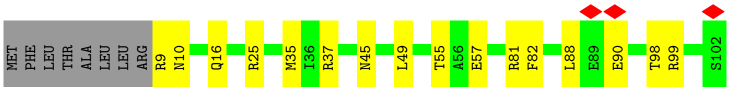
Chain Bq:





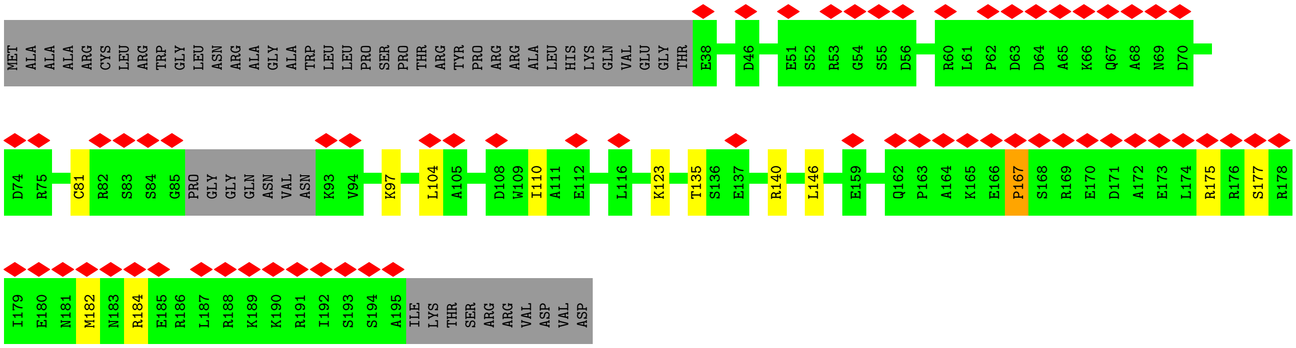
- Molecule 50: Mitochondrial ribosomal protein L57

Chain Bt:



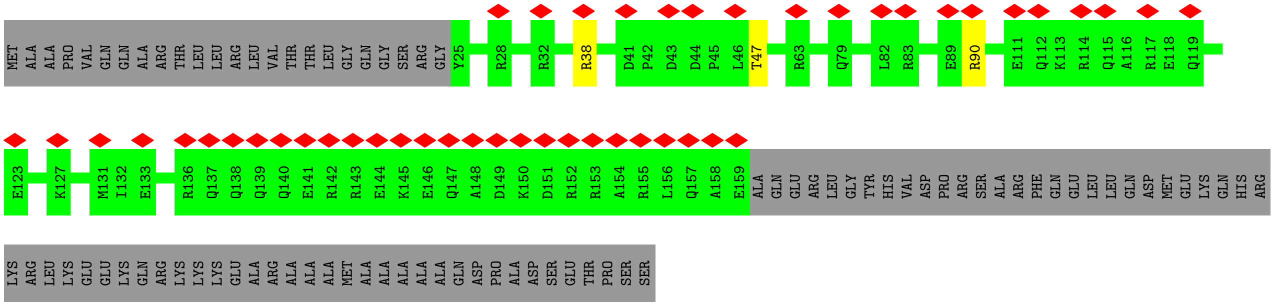
- Molecule 51: Mitochondrial ribosomal protein L58

Chain Bu:



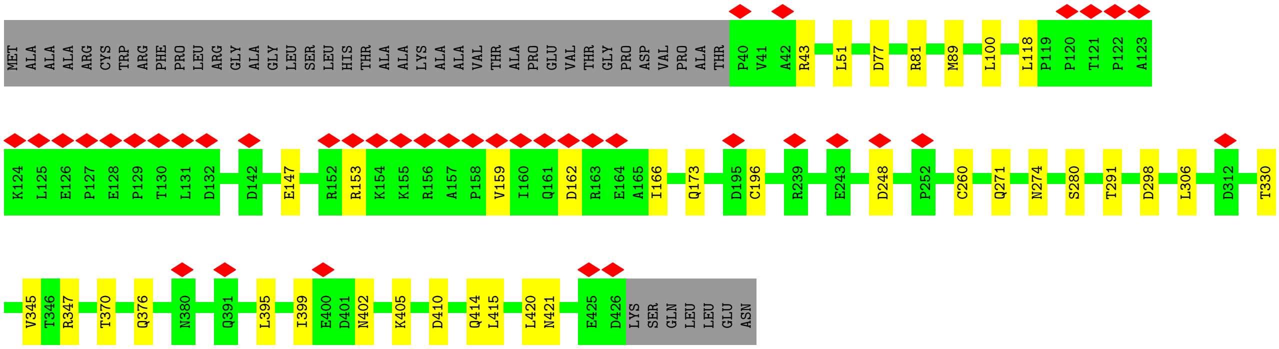
- Molecule 52: ’Mitochondrial ribosomal protein L59

Chain Bv:



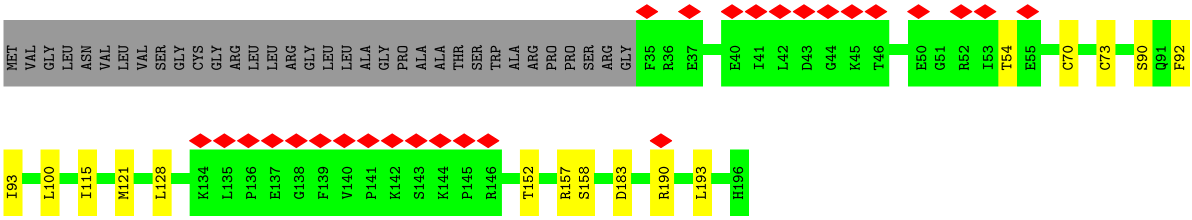
- Molecule 53: mL65, MRPS30

Chain Bw:



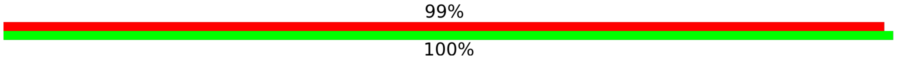
- Molecule 54: Mitochondrial ribosomal protein S18A

Chain Bx:



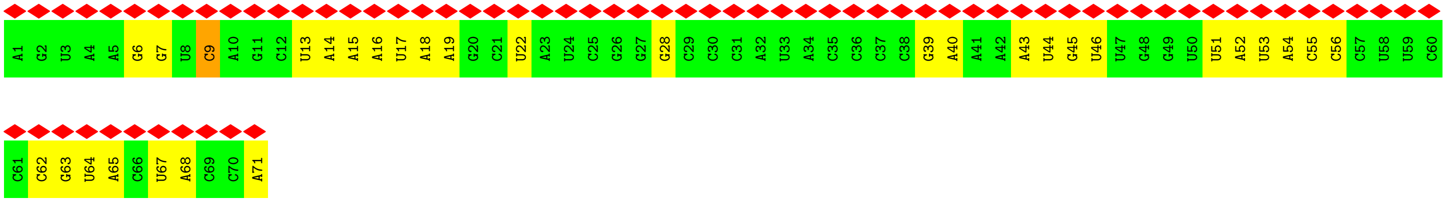
- Molecule 55: unassigned secondary structure elements

Chain Bz:



- Molecule 56: P-site fMet-tRNAMet, mitochondrial

Chain AV:


A1
G2
U3
A4
A5
G6
G7
U8
C9
A10
G11
C12
U13
A14
A15
A16
U17
A18
A19
G20
C21
U22
A23
U24
C25
G26
G27
G28
C29
C30
C31
A32
U33
A34
C35
C36
C37
C38
G39
A40
A41
A42
A43
U44
G45
U46
U47
G48
G49
U50
U51
A52
U53
A54
C55
C56
C57
U58
U59
C60
C61
C62
G63
U64
A65
C66
U67
A68
C69
C70
A71

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75666	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 ($e^-/\text{Å}^2$)	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	0.658	Depositor
Minimum map value	-0.328	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	390.59, 390.59, 390.59	wwPDB
Map dimensions	281, 281, 281	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	BL	0.35	0/542	0.50	0/729
1	CL	0.44	0/319	0.71	2/435 (0.5%)
1	DL	0.37	0/212	0.48	0/286
1	EL	0.43	0/221	0.53	0/297
1	FL	0.40	0/212	0.53	0/286
1	GL	0.40	0/212	0.49	0/286
1	HL	0.46	0/204	0.55	0/275
2	B0	0.45	0/880	0.53	0/1189
3	B1	0.33	0/2093	0.50	0/2835
4	B2	0.37	0/1586	0.53	0/2123
5	B3	0.38	0/993	0.57	0/1341
6	B4	0.27	0/388	0.51	0/523
7	B5	0.37	0/917	0.54	0/1227
8	B6	0.38	0/430	0.54	0/570
9	B7	0.44	0/395	0.56	0/524
10	B8	0.43	0/853	0.58	0/1136
11	B9	0.42	0/342	0.54	0/450
12	BA	0.60	0/36903	1.01	45/57455 (0.1%)
13	BB	0.50	1/1595 (0.1%)	0.92	1/2475 (0.0%)
14	BC	0.33	0/4432	0.52	2/5989 (0.0%)
15	BD	0.35	0/1898	0.57	0/2555
16	BE	0.39	0/2493	0.62	1/3387 (0.0%)
17	BF	0.41	0/2069	0.57	0/2816
18	BI	0.35	0/819	0.54	0/1101
19	BJ	0.34	0/1742	0.50	0/2358
20	BK	0.32	0/1323	0.51	0/1785
21	BN	0.39	0/1487	0.55	0/2017
22	BO	0.34	0/912	0.56	0/1231
23	BP	0.38	0/2368	0.54	0/3198
24	BQ	0.37	0/1850	0.54	0/2491
25	BR	0.39	0/1262	0.57	0/1700
26	BS	0.37	0/1197	0.56	0/1624

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	BT	0.37	0/1888	0.55	0/2548
28	BU	0.47	0/1179	0.59	0/1578
29	BV	0.43	0/1256	0.60	0/1706
30	BW	0.42	0/1407	0.58	0/1891
31	BX	0.38	0/1211	0.56	0/1646
32	BY	0.30	0/1719	0.51	0/2329
33	Ba	0.33	0/3267	0.54	0/4455
34	Bb	0.34	0/3047	0.54	1/4139 (0.0%)
35	Bc	0.33	0/2464	0.50	0/3330
36	Bd	0.32	0/853	0.52	0/1153
37	Be	0.36	0/1000	0.58	0/1345
38	Bf	0.36	0/851	0.57	2/1159 (0.2%)
39	Bg	0.39	0/1191	0.56	0/1614
40	Bh	0.37	0/2372	0.55	0/3211
41	Bi	0.33	0/2199	0.51	0/2980
42	Bj	0.30	0/1811	0.49	0/2436
43	Bk	0.31	0/1108	0.50	0/1499
44	Bl	0.37	0/1135	0.51	0/1549
45	Bm	0.28	0/917	0.46	0/1248
46	Bn	0.41	0/860	0.63	0/1150
47	Bo	0.36	0/787	0.53	1/1056 (0.1%)
48	Bp	0.31	0/752	0.52	0/1013
49	Bq	0.35	0/558	0.49	0/756
50	Bt	0.38	0/798	0.56	0/1073
51	Bu	0.29	0/1214	0.48	1/1630 (0.1%)
52	Bv	0.28	0/1157	0.40	0/1560
53	Bw	0.38	0/3206	0.55	0/4354
54	Bx	0.40	0/1364	0.60	1/1849 (0.1%)
55	Bz	0.35	0/404	0.30	0/556
56	AV	0.45	0/1673	0.97	5/2602 (0.2%)
All	All	0.45	1/116797 (0.0%)	0.75	62/166109 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	B4	0	1
16	BE	0	1
26	BS	0	1
34	Bb	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
46	Bn	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	BB	1	G	OP3-P	-10.38	1.48	1.61

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	BA	448	G	O5’-P-OP2	-8.78	97.80	105.70
12	BA	52	A	O4’-C1’-N9	7.63	114.30	108.20
56	AV	9	C	C2-N1-C1’	7.62	127.18	118.80
12	BA	697	C	C2-N1-C1’	7.51	127.06	118.80
56	AV	9	C	N1-C2-O2	7.33	123.30	118.90
12	BA	170	U	N3-C2-O2	-7.02	117.29	122.20
12	BA	104	C	C6-N1-C2	-6.82	117.57	120.30
12	BA	19	U	C5-C6-N1	6.81	126.11	122.70
1	CL	21	PRO	N-CA-CB	6.45	111.04	103.30
12	BA	825	C	C2-N1-C1’	6.34	125.78	118.80
1	CL	16	PRO	N-CA-CB	6.29	110.85	103.30
16	BE	201	GLY	N-CA-C	-6.29	97.38	113.10
12	BA	697	C	C6-N1-C2	-6.28	117.79	120.30
12	BA	586	C	C2-N1-C1’	6.26	125.68	118.80
12	BA	595	C	C6-N1-C2	-6.15	117.84	120.30
14	BC	502	PRO	N-CA-CB	6.14	110.67	103.30
56	AV	9	C	N3-C2-O2	-6.04	117.67	121.90
12	BA	57	A	O5’-P-OP1	-5.99	100.31	105.70
12	BA	1016	C	C5-C6-N1	-5.87	118.07	121.00
12	BA	190	U	N3-C2-O2	-5.84	118.11	122.20
38	Bf	80	PRO	N-CA-CB	5.82	110.28	103.30
12	BA	448	G	C8-N9-C4	5.79	108.72	106.40
51	Bu	167	PRO	N-CA-CB	5.78	110.24	103.30
12	BA	697	C	C5-C6-N1	5.74	123.87	121.00
12	BA	48	U	P-O3’-C3’	5.74	126.58	119.70
12	BA	112	A	O4’-C1’-N9	5.73	112.78	108.20
56	AV	9	C	C6-N1-C2	-5.71	118.02	120.30
12	BA	469	C	C2-N1-C1’	5.70	125.07	118.80
12	BA	588	C	C6-N1-C2	-5.70	118.02	120.30
12	BA	324	G	N3-C4-C5	-5.69	125.75	128.60
12	BA	151	A	N1-C6-N6	5.66	122.00	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	BC	505	PRO	N-CA-CB	5.61	110.03	103.30
12	BA	104	C	N3-C2-O2	-5.59	117.99	121.90
12	BA	1215	C	C2-N1-C1'	5.59	124.95	118.80
12	BA	433	G	C8-N9-C4	5.58	108.63	106.40
12	BA	64	C	N3-C2-O2	-5.57	118.00	121.90
38	Bf	78	PRO	N-CA-CB	5.54	109.95	103.30
12	BA	1016	C	C4-C5-C6	5.54	120.17	117.40
12	BA	238	C	O4'-C1'-N1	5.46	112.57	108.20
12	BA	463	A	C8-N9-C4	5.40	107.96	105.80
12	BA	848	C	N1-C2-O2	5.39	122.14	118.90
12	BA	848	C	C2-N1-C1'	5.39	124.73	118.80
12	BA	404	C	N1-C2-O2	5.37	122.12	118.90
13	BB	13	U	C2-N1-C1'	5.34	124.11	117.70
12	BA	1241	U	P-O3'-C3'	5.34	126.10	119.70
12	BA	1395	A	C8-N9-C4	5.32	107.93	105.80
12	BA	890	C	N1-C2-O2	5.28	122.07	118.90
12	BA	338	C	C6-N1-C2	5.26	122.40	120.30
12	BA	104	C	C2-N1-C1'	5.25	124.58	118.80
34	Bb	211	GLY	N-CA-C	-5.24	100.00	113.10
12	BA	40	C	O5'-P-OP1	-5.23	100.99	105.70
12	BA	326	U	C5-C6-N1	-5.21	120.09	122.70
54	Bx	73	CYS	CA-CB-SG	-5.18	104.68	114.00
12	BA	1558	U	N1-C2-O2	5.12	126.39	122.80
12	BA	595	C	C2-N1-C1'	5.12	124.43	118.80
12	BA	166	A	C8-N9-C4	5.11	107.84	105.80
47	Bo	40	TYR	CA-CB-CG	5.10	123.09	113.40
12	BA	1215	C	C5-C6-N1	5.08	123.54	121.00
12	BA	433	G	N7-C8-N9	-5.05	110.58	113.10
56	AV	9	C	C6-N1-C1'	-5.05	114.74	120.80
12	BA	151	A	N9-C4-C5	-5.04	103.78	105.80
12	BA	295	G	C5-C6-N1	5.01	114.01	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B4	61	ASP	Peptide
16	BE	316	PHE	Peptide
26	BS	69	GLY	Peptide
34	Bb	210	GLU	Peptide
46	Bn	65	ASN	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BL	68/198 (34%)	65 (96%)	3 (4%)	0	100	100
1	CL	43/198 (22%)	41 (95%)	1 (2%)	1 (2%)	6	34
1	DL	25/198 (13%)	25 (100%)	0	0	100	100
1	EL	26/198 (13%)	25 (96%)	1 (4%)	0	100	100
1	FL	25/198 (13%)	25 (100%)	0	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%)	105 (97%)	3 (3%)	0	100	100
3	B1	242/256 (94%)	238 (98%)	4 (2%)	0	100	100
4	B2	177/252 (70%)	171 (97%)	6 (3%)	0	100	100
5	B3	116/161 (72%)	114 (98%)	2 (2%)	0	100	100
6	B4	43/126 (34%)	40 (93%)	3 (7%)	0	100	100
7	B5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
8	B6	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
9	B7	44/95 (46%)	43 (98%)	1 (2%)	0	100	100
10	B8	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
11	B9	36/100 (36%)	36 (100%)	0	0	100	100
14	BC	569/657 (87%)	545 (96%)	23 (4%)	1 (0%)	47	79
15	BD	238/306 (78%)	225 (94%)	13 (6%)	0	100	100
16	BE	305/348 (88%)	282 (92%)	20 (7%)	3 (1%)	15	54
17	BF	248/294 (84%)	237 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	BI	96/268 (36%)	91 (95%)	5 (5%)	0	100	100
19	BJ	210/262 (80%)	203 (97%)	7 (3%)	0	100	100
20	BK	174/192 (91%)	164 (94%)	9 (5%)	1 (1%)	25	64
21	BN	175/178 (98%)	172 (98%)	3 (2%)	0	100	100
22	BO	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
23	BP	286/296 (97%)	276 (96%)	10 (4%)	0	100	100
24	BQ	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
25	BR	151/169 (89%)	146 (97%)	5 (3%)	0	100	100
26	BS	141/180 (78%)	128 (91%)	12 (8%)	1 (1%)	22	61
27	BT	221/292 (76%)	214 (97%)	7 (3%)	0	100	100
28	BU	138/149 (93%)	134 (97%)	4 (3%)	0	100	100
29	BV	153/209 (73%)	147 (96%)	6 (4%)	0	100	100
30	BW	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
31	BX	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
32	BY	204/216 (94%)	192 (94%)	12 (6%)	0	100	100
33	Ba	391/423 (92%)	375 (96%)	16 (4%)	0	100	100
34	Bb	352/380 (93%)	330 (94%)	22 (6%)	0	100	100
35	Bc	293/334 (88%)	279 (95%)	14 (5%)	0	100	100
36	Bd	97/206 (47%)	89 (92%)	7 (7%)	1 (1%)	15	54
37	Be	120/135 (89%)	114 (95%)	6 (5%)	0	100	100
38	Bf	106/142 (75%)	102 (96%)	2 (2%)	2 (2%)	8	39
39	Bg	146/159 (92%)	137 (94%)	9 (6%)	0	100	100
40	Bh	287/332 (86%)	274 (96%)	13 (4%)	0	100	100
41	Bi	258/306 (84%)	250 (97%)	8 (3%)	0	100	100
42	Bj	211/279 (76%)	200 (95%)	10 (5%)	1 (0%)	29	67
43	Bk	132/212 (62%)	126 (96%)	6 (4%)	0	100	100
44	Bl	131/166 (79%)	127 (97%)	4 (3%)	0	100	100
45	Bm	107/159 (67%)	103 (96%)	4 (4%)	0	100	100
46	Bn	95/128 (74%)	89 (94%)	6 (6%)	0	100	100
47	Bo	95/124 (77%)	91 (96%)	4 (4%)	0	100	100
48	Bp	95/112 (85%)	89 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	Bq	66/138 (48%)	64 (97%)	1 (2%)	1 (2%)	10	44
50	Bt	92/102 (90%)	86 (94%)	6 (6%)	0	100	100
51	Bu	147/205 (72%)	137 (93%)	9 (6%)	1 (1%)	22	61
52	Bv	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
53	Bw	385/433 (89%)	364 (94%)	20 (5%)	1 (0%)	41	74
54	Bx	160/196 (82%)	156 (98%)	3 (2%)	1 (1%)	25	64
55	Bz	70/82 (85%)	70 (100%)	0	0	100	100
All	All	9175/12712 (72%)	8795 (96%)	365 (4%)	15 (0%)	50	79

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CL	21	PRO
38	Bf	78	PRO
38	Bf	80	PRO
51	Bu	167	PRO
16	BE	202	GLN
53	Bw	159	VAL
54	Bx	93	ILE
14	BC	502	PRO
16	BE	317	PRO
20	BK	157	LYS
49	Bq	101	VAL
42	Bj	151	ARG
16	BE	264	ILE
36	Bd	170	PRO
26	BS	45	ALA

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	BL	59/157 (38%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CL	30/157 (19%)	29 (97%)	1 (3%)	38	71
1	DL	26/157 (17%)	24 (92%)	2 (8%)	13	44
1	EL	27/157 (17%)	25 (93%)	2 (7%)	13	46
1	FL	26/157 (17%)	24 (92%)	2 (8%)	13	44
1	GL	26/157 (17%)	25 (96%)	1 (4%)	33	67
1	HL	25/157 (16%)	23 (92%)	2 (8%)	12	42
2	B0	90/115 (78%)	83 (92%)	7 (8%)	12	43
3	B1	219/229 (96%)	192 (88%)	27 (12%)	4	21
4	B2	164/228 (72%)	148 (90%)	16 (10%)	8	31
5	B3	110/147 (75%)	100 (91%)	10 (9%)	9	34
6	B4	42/114 (37%)	36 (86%)	6 (14%)	3	15
7	B5	99/163 (61%)	85 (86%)	14 (14%)	3	16
8	B6	49/60 (82%)	47 (96%)	2 (4%)	30	66
9	B7	41/78 (53%)	38 (93%)	3 (7%)	14	46
10	B8	87/162 (54%)	75 (86%)	12 (14%)	3	16
11	B9	36/77 (47%)	32 (89%)	4 (11%)	6	25
14	BC	464/556 (84%)	451 (97%)	13 (3%)	43	74
15	BD	193/248 (78%)	174 (90%)	19 (10%)	8	31
16	BE	263/290 (91%)	238 (90%)	25 (10%)	8	32
17	BF	217/251 (86%)	194 (89%)	23 (11%)	6	27
18	BI	88/228 (39%)	84 (96%)	4 (4%)	27	63
19	BJ	192/230 (84%)	182 (95%)	10 (5%)	23	59
20	BK	129/151 (85%)	123 (95%)	6 (5%)	26	62
21	BN	156/157 (99%)	142 (91%)	14 (9%)	9	34
22	BO	99/123 (80%)	89 (90%)	10 (10%)	7	29
23	BP	245/249 (98%)	215 (88%)	30 (12%)	5	22
24	BQ	190/210 (90%)	176 (93%)	14 (7%)	13	46
25	BR	132/143 (92%)	119 (90%)	13 (10%)	8	31
26	BS	123/153 (80%)	116 (94%)	7 (6%)	20	56
27	BT	204/258 (79%)	183 (90%)	21 (10%)	7	29
28	BU	118/127 (93%)	113 (96%)	5 (4%)	30	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BV	136/178 (76%)	126 (93%)	10 (7%)	13	46
30	BW	144/180 (80%)	132 (92%)	12 (8%)	11	40
31	BX	116/134 (87%)	105 (90%)	11 (10%)	8	32
32	BY	185/192 (96%)	162 (88%)	23 (12%)	4	21
33	Ba	348/365 (95%)	309 (89%)	39 (11%)	6	25
34	Bb	310/328 (94%)	279 (90%)	31 (10%)	7	30
35	Bc	271/299 (91%)	258 (95%)	13 (5%)	25	61
36	Bd	92/181 (51%)	85 (92%)	7 (8%)	13	45
37	Be	100/108 (93%)	85 (85%)	15 (15%)	3	14
38	Bf	80/133 (60%)	68 (85%)	12 (15%)	3	14
39	Bg	128/136 (94%)	112 (88%)	16 (12%)	4	21
40	Bh	251/284 (88%)	225 (90%)	26 (10%)	7	28
41	Bi	236/275 (86%)	223 (94%)	13 (6%)	21	57
42	Bj	190/242 (78%)	175 (92%)	15 (8%)	12	43
43	Bk	119/181 (66%)	111 (93%)	8 (7%)	16	50
44	Bl	122/147 (83%)	109 (89%)	13 (11%)	6	27
45	Bm	103/145 (71%)	97 (94%)	6 (6%)	20	55
46	Bn	88/113 (78%)	78 (89%)	10 (11%)	5	24
47	Bo	77/97 (79%)	68 (88%)	9 (12%)	5	23
48	Bp	79/88 (90%)	74 (94%)	5 (6%)	18	52
49	Bq	50/114 (44%)	46 (92%)	4 (8%)	12	42
50	Bt	75/82 (92%)	59 (79%)	16 (21%)	1	5
51	Bu	126/177 (71%)	114 (90%)	12 (10%)	8	32
52	Bv	115/183 (63%)	112 (97%)	3 (3%)	46	76
53	Bw	340/373 (91%)	305 (90%)	35 (10%)	7	29
54	Bx	149/173 (86%)	135 (91%)	14 (9%)	8	33
All	All	7999/10754 (74%)	7296 (91%)	703 (9%)	13	36

All (703) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CL	40	LEU
1	DL	75	THR

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Mol	Chain	Res	Type
1	DL	86	LEU
1	EL	76	LEU
1	EL	82	LEU
1	FL	76	LEU
1	FL	79	ILE
1	GL	82	LEU
1	HL	76	LEU
1	HL	79	ILE
2	B0	50	ARG
2	B0	53	ILE
2	B0	56	MET
2	B0	61	VAL
2	B0	66	ILE
2	B0	117	VAL
2	B0	141	THR
3	B1	6	VAL
3	B1	31	SER
3	B1	46	HIS
3	B1	61	ARG
3	B1	64	ASP
3	B1	75	SER
3	B1	77	LEU
3	B1	79	LEU
3	B1	104	VAL
3	B1	112	ARG
3	B1	120	ASP
3	B1	126	THR
3	B1	128	THR
3	B1	136	ASP
3	B1	152	ASP
3	B1	155	SER
3	B1	161	LEU
3	B1	172	GLN
3	B1	173	ASP
3	B1	177	HIS
3	B1	179	ASP
3	B1	190	ARG
3	B1	209	ASP
3	B1	216	ARG
3	B1	222	ASP
3	B1	224	ILE
3	B1	238	LEU

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Mol	Chain	Res	Type
4	B2	66	LEU
4	B2	67	GLU
4	B2	72	ASP
4	B2	79	GLU
4	B2	126	LEU
4	B2	144	LEU
4	B2	145	ASP
4	B2	153	ASP
4	B2	158	LEU
4	B2	171	ARG
4	B2	174	ILE
4	B2	184	LYS
4	B2	197	ASN
4	B2	218	GLN
4	B2	228	LEU
4	B2	230	ARG
5	B3	38	ARG
5	B3	43	ASP
5	B3	72	ILE
5	B3	73	LYS
5	B3	78	ARG
5	B3	82	GLU
5	B3	144	GLU
5	B3	147	VAL
5	B3	150	LEU
5	B3	151	LEU
6	B4	42	THR
6	B4	44	LEU
6	B4	49	TYR
6	B4	60	GLN
6	B4	65	ILE
6	B4	78	MET
7	B5	85	ARG
7	B5	87	ILE
7	B5	92	CYS
7	B5	93	ARG
7	B5	94	ARG
7	B5	108	ASP
7	B5	109	VAL
7	B5	115	HIS
7	B5	136	GLU
7	B5	153	THR

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Mol	Chain	Res	Type
7	B5	156	THR
7	B5	158	VAL
7	B5	185	PHE
7	B5	186	THR
8	B6	22	SER
8	B6	31	ASN
9	B7	65	HIS
9	B7	75	THR
9	B7	92	SER
10	B8	106	THR
10	B8	111	ILE
10	B8	113	ARG
10	B8	124	ARG
10	B8	125	ARG
10	B8	142	ARG
10	B8	162	THR
10	B8	163	THR
10	B8	169	ARG
10	B8	182	ASP
10	B8	183	ARG
10	B8	184	THR
11	B9	63	PHE
11	B9	74	ARG
11	B9	75	ASP
11	B9	92	ASN
14	BC	163	LYS
14	BC	184	THR
14	BC	253	ASP
14	BC	283	ILE
14	BC	330	ASN
14	BC	392	CYS
14	BC	433	GLU
14	BC	472	GLU
14	BC	515	VAL
14	BC	520	ILE
14	BC	524	VAL
14	BC	679	HIS
14	BC	708	ARG
15	BD	62	THR
15	BD	64	VAL
15	BD	69	ARG
15	BD	75	MET

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Mol	Chain	Res	Type
15	BD	85	ARG
15	BD	90	GLN
15	BD	103	ARG
15	BD	105	ARG
15	BD	111	ARG
15	BD	113	ARG
15	BD	117	GLU
15	BD	148	ARG
15	BD	150	ARG
15	BD	155	THR
15	BD	190	VAL
15	BD	224	THR
15	BD	240	THR
15	BD	285	ARG
15	BD	288	ARG
16	BE	50	ASP
16	BE	53	LEU
16	BE	80	LEU
16	BE	96	ARG
16	BE	97	VAL
16	BE	109	LEU
16	BE	113	ASP
16	BE	146	THR
16	BE	158	SER
16	BE	218	VAL
16	BE	227	GLN
16	BE	231	HIS
16	BE	236	THR
16	BE	239	ARG
16	BE	273	VAL
16	BE	284	TYR
16	BE	285	VAL
16	BE	289	VAL
16	BE	294	ASN
16	BE	296	LEU
16	BE	299	ILE
16	BE	301	ASP
16	BE	311	CYS
16	BE	313	ASN
16	BE	326	GLU
17	BF	47	VAL
17	BF	59	ARG

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Mol	Chain	Res	Type
17	BF	76	ARG
17	BF	77	VAL
17	BF	79	LEU
17	BF	80	THR
17	BF	94	ASP
17	BF	101	ILE
17	BF	111	TYR
17	BF	114	THR
17	BF	116	THR
17	BF	125	ARG
17	BF	143	SER
17	BF	165	LEU
17	BF	172	GLN
17	BF	190	VAL
17	BF	193	LEU
17	BF	203	LEU
17	BF	224	GLU
17	BF	239	THR
17	BF	263	LEU
17	BF	281	THR
17	BF	291	CYS
18	BI	75	ARG
18	BI	78	ARG
18	BI	99	THR
18	BI	108	ARG
19	BJ	34	THR
19	BJ	60	ILE
19	BJ	63	ARG
19	BJ	76	THR
19	BJ	78	LEU
19	BJ	93	ASN
19	BJ	121	ILE
19	BJ	128	ASN
19	BJ	150	HIS
19	BJ	229	LEU
20	BK	57	THR
20	BK	64	ILE
20	BK	111	LEU
20	BK	113	THR
20	BK	158	ASP
20	BK	164	LEU
21	BN	10	GLN

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Mol	Chain	Res	Type
21	BN	39	LEU
21	BN	65	ILE
21	BN	67	PHE
21	BN	78	SER
21	BN	91	THR
21	BN	101	VAL
21	BN	104	VAL
21	BN	118	ARG
21	BN	123	GLN
21	BN	136	ASP
21	BN	140	ASN
21	BN	153	ARG
21	BN	177	ARG
22	BO	60	VAL
22	BO	72	ARG
22	BO	73	ILE
22	BO	77	ILE
22	BO	91	MET
22	BO	95	ARG
22	BO	101	ASP
22	BO	111	ASN
22	BO	121	THR
22	BO	138	LEU
23	BP	11	ARG
23	BP	43	ARG
23	BP	44	ARG
23	BP	45	ARG
23	BP	51	ARG
23	BP	61	THR
23	BP	62	ARG
23	BP	65	LEU
23	BP	71	GLN
23	BP	83	PHE
23	BP	127	VAL
23	BP	130	GLN
23	BP	134	ARG
23	BP	140	LEU
23	BP	141	VAL
23	BP	152	VAL
23	BP	154	ILE
23	BP	176	THR
23	BP	215	THR

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Mol	Chain	Res	Type
23	BP	233	ARG
23	BP	234	LEU
23	BP	246	ASP
23	BP	247	ILE
23	BP	248	THR
23	BP	250	ASP
23	BP	251	GLU
23	BP	257	SER
23	BP	261	ASP
23	BP	286	THR
23	BP	295	SER
24	BQ	55	ARG
24	BQ	68	ASN
24	BQ	77	THR
24	BQ	111	ARG
24	BQ	132	THR
24	BQ	140	MET
24	BQ	166	ARG
24	BQ	171	GLU
24	BQ	185	PHE
24	BQ	209	ASN
24	BQ	214	THR
24	BQ	224	LEU
24	BQ	226	ILE
24	BQ	250	ARG
25	BR	17	ARG
25	BR	24	SER
25	BR	30	GLN
25	BR	38	ARG
25	BR	67	ASP
25	BR	83	LYS
25	BR	84	ASP
25	BR	93	LEU
25	BR	110	ILE
25	BR	118	ARG
25	BR	134	LEU
25	BR	139	ARG
25	BR	142	ASN
26	BS	44	VAL
26	BS	80	ARG
26	BS	107	THR
26	BS	141	ILE

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Mol	Chain	Res	Type
26	BS	149	THR
26	BS	161	LEU
26	BS	163	HIS
27	BT	77	SER
27	BT	79	GLU
27	BT	90	LEU
27	BT	95	GLU
27	BT	130	THR
27	BT	145	LEU
27	BT	162	ILE
27	BT	165	GLU
27	BT	170	ARG
27	BT	177	VAL
27	BT	187	LEU
27	BT	202	VAL
27	BT	234	GLU
27	BT	239	ASN
27	BT	246	ASP
27	BT	270	MET
27	BT	272	GLU
27	BT	274	ASP
27	BT	275	THR
27	BT	284	ASP
27	BT	289	SER
28	BU	48	ARG
28	BU	54	THR
28	BU	77	GLN
28	BU	87	ILE
28	BU	123	ARG
29	BV	111	LYS
29	BV	117	LEU
29	BV	126	VAL
29	BV	133	ARG
29	BV	153	LEU
29	BV	160	VAL
29	BV	164	VAL
29	BV	176	MET
29	BV	186	ARG
29	BV	199	ILE
30	BW	60	GLN
30	BW	66	ARG
30	BW	75	ARG

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Mol	Chain	Res	Type
30	BW	80	TYR
30	BW	131	ASN
30	BW	133	GLU
30	BW	136	SER
30	BW	147	ARG
30	BW	151	LEU
30	BW	152	LYS
30	BW	164	ILE
30	BW	199	GLN
31	BX	6	LEU
31	BX	14	ASN
31	BX	28	LEU
31	BX	35	GLN
31	BX	47	GLU
31	BX	49	THR
31	BX	50	ARG
31	BX	52	ASP
31	BX	57	LEU
31	BX	60	ILE
31	BX	79	ARG
32	BY	30	SER
32	BY	31	ASP
32	BY	39	THR
32	BY	40	ARG
32	BY	43	ARG
32	BY	44	VAL
32	BY	66	GLU
32	BY	78	GLN
32	BY	83	ARG
32	BY	86	VAL
32	BY	96	ARG
32	BY	105	ARG
32	BY	107	THR
32	BY	116	LEU
32	BY	131	THR
32	BY	137	PHE
32	BY	138	THR
32	BY	149	ARG
32	BY	153	ILE
32	BY	163	ASP
32	BY	181	ASP
32	BY	200	GLU

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Mol	Chain	Res	Type
32	BY	208	ARG
33	Ba	42	GLU
33	Ba	47	ASP
33	Ba	51	GLU
33	Ba	63	LYS
33	Ba	67	MET
33	Ba	110	ARG
33	Ba	137	LEU
33	Ba	139	LEU
33	Ba	147	ILE
33	Ba	149	ASN
33	Ba	150	GLN
33	Ba	162	ARG
33	Ba	163	LEU
33	Ba	167	THR
33	Ba	175	THR
33	Ba	176	TYR
33	Ba	193	LEU
33	Ba	202	ILE
33	Ba	207	ASN
33	Ba	210	SER
33	Ba	212	THR
33	Ba	215	ARG
33	Ba	222	VAL
33	Ba	234	ASP
33	Ba	256	PHE
33	Ba	262	THR
33	Ba	277	THR
33	Ba	316	PHE
33	Ba	322	LEU
33	Ba	335	VAL
33	Ba	337	GLU
33	Ba	345	VAL
33	Ba	347	THR
33	Ba	348	ASP
33	Ba	373	LEU
33	Ba	391	VAL
33	Ba	396	VAL
33	Ba	398	VAL
33	Ba	415	LEU
34	Bb	32	LEU
34	Bb	35	MET

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Mol	Chain	Res	Type
34	Bb	40	ILE
34	Bb	50	LYS
34	Bb	51	TYR
34	Bb	52	ARG
34	Bb	72	ARG
34	Bb	88	VAL
34	Bb	99	ARG
34	Bb	118	GLU
34	Bb	120	GLU
34	Bb	135	VAL
34	Bb	141	ARG
34	Bb	173	LEU
34	Bb	210	GLU
34	Bb	222	ASP
34	Bb	237	VAL
34	Bb	238	THR
34	Bb	252	CYS
34	Bb	258	PHE
34	Bb	261	ARG
34	Bb	267	ARG
34	Bb	272	LEU
34	Bb	276	ASP
34	Bb	281	PHE
34	Bb	284	ASP
34	Bb	288	SER
34	Bb	324	ASP
34	Bb	356	ARG
34	Bb	360	ARG
34	Bb	376	THR
35	Bc	67	VAL
35	Bc	87	SER
35	Bc	106	ASP
35	Bc	111	ASP
35	Bc	140	TRP
35	Bc	186	LEU
35	Bc	222	VAL
35	Bc	253	ARG
35	Bc	256	ASP
35	Bc	280	VAL
35	Bc	285	THR
35	Bc	300	VAL
35	Bc	319	MET

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Mol	Chain	Res	Type
36	Bd	89	ILE
36	Bd	99	ARG
36	Bd	106	LEU
36	Bd	136	ILE
36	Bd	150	LEU
36	Bd	163	LYS
36	Bd	168	LEU
37	Be	23	SER
37	Be	25	ARG
37	Be	28	ARG
37	Be	29	THR
37	Be	60	VAL
37	Be	66	PHE
37	Be	67	LYS
37	Be	68	LEU
37	Be	74	TYR
37	Be	106	THR
37	Be	110	GLU
37	Be	111	HIS
37	Be	120	THR
37	Be	122	GLU
37	Be	127	GLN
38	Bf	44	ASN
38	Bf	45	CYS
38	Bf	56	ARG
38	Bf	58	ILE
38	Bf	60	CYS
38	Bf	67	ILE
38	Bf	70	GLU
38	Bf	71	HIS
38	Bf	122	ARG
38	Bf	126	ARG
38	Bf	133	ARG
38	Bf	134	ARG
39	Bg	6	THR
39	Bg	12	THR
39	Bg	21	ARG
39	Bg	28	ARG
39	Bg	33	LEU
39	Bg	47	VAL
39	Bg	52	THR
39	Bg	61	VAL

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Mol	Chain	Res	Type
39	Bg	68	ARG
39	Bg	80	LEU
39	Bg	88	SER
39	Bg	93	SER
39	Bg	119	PHE
39	Bg	125	SER
39	Bg	126	ILE
39	Bg	148	VAL
40	Bh	45	LEU
40	Bh	51	LEU
40	Bh	52	ARG
40	Bh	78	ARG
40	Bh	82	THR
40	Bh	96	CYS
40	Bh	98	ILE
40	Bh	121	ASP
40	Bh	148	LEU
40	Bh	163	GLU
40	Bh	177	GLN
40	Bh	178	LEU
40	Bh	191	LEU
40	Bh	192	ARG
40	Bh	216	ARG
40	Bh	233	THR
40	Bh	254	GLU
40	Bh	259	ARG
40	Bh	263	SER
40	Bh	264	THR
40	Bh	265	THR
40	Bh	267	LEU
40	Bh	288	THR
40	Bh	289	VAL
40	Bh	301	LEU
40	Bh	307	PHE
41	Bi	57	VAL
41	Bi	74	ARG
41	Bi	76	ILE
41	Bi	85	PHE
41	Bi	112	LEU
41	Bi	165	THR
41	Bi	181	VAL
41	Bi	186	VAL

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Mol	Chain	Res	Type
41	Bi	196	GLN
41	Bi	221	THR
41	Bi	242	VAL
41	Bi	244	GLU
41	Bi	281	MET
42	Bj	51	LEU
42	Bj	55	ARG
42	Bj	60	THR
42	Bj	119	ASP
42	Bj	136	ARG
42	Bj	137	LEU
42	Bj	145	ASP
42	Bj	169	ASP
42	Bj	179	GLN
42	Bj	210	CYS
42	Bj	230	LYS
42	Bj	243	PHE
42	Bj	264	LEU
42	Bj	265	LYS
42	Bj	276	LEU
43	Bk	50	SER
43	Bk	53	THR
43	Bk	56	ILE
43	Bk	132	MET
43	Bk	147	ASP
43	Bk	165	THR
43	Bk	168	GLU
43	Bk	170	PHE
44	Bl	89	SER
44	Bl	90	ARG
44	Bl	98	ARG
44	Bl	100	ILE
44	Bl	101	THR
44	Bl	117	ILE
44	Bl	128	LEU
44	Bl	134	LYS
44	Bl	137	VAL
44	Bl	138	THR
44	Bl	141	ASN
44	Bl	154	ASP
44	Bl	155	GLN
45	Bm	67	LEU

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Mol	Chain	Res	Type
45	Bm	71	LEU
45	Bm	86	ASN
45	Bm	115	ASN
45	Bm	128	LEU
45	Bm	142	ASP
46	Bn	32	PHE
46	Bn	34	VAL
46	Bn	35	ARG
46	Bn	41	ARG
46	Bn	42	LYS
46	Bn	44	VAL
46	Bn	48	ASN
46	Bn	53	MET
46	Bn	92	ILE
46	Bn	105	ASP
47	Bo	31	GLN
47	Bo	40	TYR
47	Bo	43	LEU
47	Bo	44	THR
47	Bo	53	ASP
47	Bo	55	ARG
47	Bo	64	LEU
47	Bo	84	MET
47	Bo	110	LEU
48	Bp	28	GLU
48	Bp	43	ARG
48	Bp	76	MET
48	Bp	82	THR
48	Bp	84	GLN
49	Bq	95	TRP
49	Bq	96	LEU
49	Bq	137	LYS
49	Bq	138	PHE
50	Bt	9	ARG
50	Bt	10	ASN
50	Bt	16	GLN
50	Bt	25	ARG
50	Bt	35	MET
50	Bt	37	ARG
50	Bt	45	ASN
50	Bt	49	LEU
50	Bt	55	THR

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Mol	Chain	Res	Type
50	Bt	57	GLU
50	Bt	81	ARG
50	Bt	82	PHE
50	Bt	88	LEU
50	Bt	90	GLU
50	Bt	98	THR
50	Bt	99	ARG
51	Bu	81	CYS
51	Bu	97	LYS
51	Bu	104	LEU
51	Bu	110	ILE
51	Bu	123	LYS
51	Bu	135	THR
51	Bu	140	ARG
51	Bu	146	LEU
51	Bu	175	ARG
51	Bu	177	SER
51	Bu	182	MET
51	Bu	184	ARG
52	Bv	38	ARG
52	Bv	47	THR
52	Bv	90	ARG
53	Bw	43	ARG
53	Bw	51	LEU
53	Bw	77	ASP
53	Bw	81	ARG
53	Bw	89	MET
53	Bw	100	LEU
53	Bw	118	LEU
53	Bw	147	GLU
53	Bw	153	ARG
53	Bw	162	ASP
53	Bw	166	ILE
53	Bw	173	GLN
53	Bw	196	CYS
53	Bw	248	ASP
53	Bw	260	CYS
53	Bw	271	GLN
53	Bw	274	ASN
53	Bw	280	SER
53	Bw	291	THR
53	Bw	298	ASP

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Mol	Chain	Res	Type
53	Bw	306	LEU
53	Bw	330	THR
53	Bw	345	VAL
53	Bw	347	ARG
53	Bw	370	THR
53	Bw	376	GLN
53	Bw	395	LEU
53	Bw	399	ILE
53	Bw	402	ASN
53	Bw	405	LYS
53	Bw	410	ASP
53	Bw	414	GLN
53	Bw	415	LEU
53	Bw	420	LEU
53	Bw	421	ASN
54	Bx	54	THR
54	Bx	70	CYS
54	Bx	90	SER
54	Bx	92	PHE
54	Bx	100	LEU
54	Bx	115	ILE
54	Bx	121	MET
54	Bx	128	LEU
54	Bx	152	THR
54	Bx	157	ARG
54	Bx	158	SER
54	Bx	183	ASP
54	Bx	190	ARG
54	Bx	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (158) such sidechains are listed below:

Mol	Chain	Res	Type
2	B0	41	ASN
2	B0	59	HIS
2	B0	65	ASN
2	B0	76	HIS
3	B1	27	HIS
3	B1	42	HIS
3	B1	172	GLN
4	B2	75	ASN
4	B2	90	GLN

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Mol	Chain	Res	Type
5	B3	67	HIS
6	B4	37	ASN
6	B4	47	GLN
7	B5	83	ASN
7	B5	118	GLN
7	B5	144	GLN
7	B5	170	GLN
10	B8	118	HIS
14	BC	215	GLN
14	BC	268	GLN
14	BC	319	GLN
14	BC	330	ASN
14	BC	475	GLN
14	BC	596	HIS
16	BE	231	HIS
16	BE	281	ASN
16	BE	292	HIS
16	BE	313	ASN
17	BF	74	GLN
17	BF	83	HIS
17	BF	97	HIS
17	BF	103	GLN
17	BF	105	ASN
17	BF	249	ASN
18	BI	88	HIS
18	BI	93	ASN
19	BJ	41	HIS
19	BJ	93	ASN
19	BJ	217	GLN
20	BK	84	GLN
20	BK	103	HIS
1	BL	152	HIS
21	BN	40	GLN
21	BN	74	GLN
21	BN	80	HIS
21	BN	94	GLN
22	BO	89	HIS
22	BO	103	ASN
23	BP	84	ASN
23	BP	87	HIS
23	BP	170	ASN
23	BP	219	ASN

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Mol	Chain	Res	Type
24	BQ	68	ASN
24	BQ	98	HIS
24	BQ	110	ASN
24	BQ	209	ASN
25	BR	27	HIS
25	BR	91	GLN
25	BR	112	ASN
25	BR	116	GLN
25	BR	147	ASN
26	BS	52	ASN
26	BS	79	HIS
26	BS	115	HIS
27	BT	239	ASN
28	BU	77	GLN
29	BV	88	ASN
29	BV	109	GLN
29	BV	122	ASN
29	BV	144	ASN
30	BW	73	HIS
30	BW	157	HIS
30	BW	171	HIS
30	BW	199	GLN
30	BW	203	ASN
31	BX	14	ASN
31	BX	77	ASN
32	BY	35	ASN
32	BY	78	GLN
32	BY	84	ASN
32	BY	210	HIS
33	Ba	65	HIS
33	Ba	108	HIS
33	Ba	119	GLN
33	Ba	156	ASN
33	Ba	195	HIS
33	Ba	207	ASN
33	Ba	223	HIS
33	Ba	266	GLN
33	Ba	358	GLN
33	Ba	360	ASN
34	Bb	220	ASN
34	Bb	224	HIS
34	Bb	266	HIS

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Mol	Chain	Res	Type
34	Bb	275	GLN
34	Bb	308	GLN
34	Bb	354	GLN
35	Bc	243	GLN
35	Bc	252	HIS
35	Bc	274	GLN
35	Bc	294	GLN
35	Bc	301	HIS
35	Bc	305	HIS
35	Bc	310	ASN
36	Bd	143	GLN
38	Bf	44	ASN
38	Bf	62	HIS
38	Bf	121	HIS
39	Bg	17	ASN
39	Bg	127	GLN
39	Bg	129	GLN
39	Bg	131	HIS
39	Bg	135	ASN
40	Bh	118	ASN
40	Bh	172	ASN
40	Bh	177	GLN
41	Bi	115	ASN
41	Bi	161	HIS
41	Bi	167	ASN
41	Bi	196	GLN
42	Bj	87	HIS
42	Bj	150	HIS
42	Bj	175	GLN
42	Bj	251	HIS
43	Bk	111	HIS
43	Bk	175	HIS
43	Bk	177	ASN
44	Bl	141	ASN
45	Bm	111	HIS
45	Bm	115	ASN
46	Bn	48	ASN
46	Bn	59	ASN
46	Bn	69	HIS
46	Bn	122	ASN
47	Bo	63	GLN
48	Bp	15	GLN

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Mol	Chain	Res	Type
48	Bp	84	GLN
48	Bp	93	HIS
49	Bq	129	HIS
50	Bt	30	GLN
50	Bt	34	ASN
50	Bt	45	ASN
50	Bt	85	HIS
51	Bu	103	HIS
51	Bu	145	ASN
52	Bv	107	GLN
53	Bw	96	GLN
53	Bw	146	GLN
53	Bw	173	GLN
53	Bw	201	HIS
53	Bw	234	GLN
53	Bw	271	GLN
53	Bw	381	ASN
53	Bw	385	ASN
53	Bw	421	ASN
54	Bx	112	HIS
54	Bx	164	ASN
54	Bx	184	ASN
54	Bx	196	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	BA	1547/1571 (98%)	509 (32%)	10 (0%)
13	BB	65/73 (89%)	25 (38%)	1 (1%)
56	AV	70/71 (98%)	31 (44%)	0
All	All	1682/1715 (98%)	565 (33%)	11 (0%)

All (565) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	BA	4	A
12	BA	6	A
12	BA	7	G
12	BA	11	G
12	BA	15	A
12	BA	16	A

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Mol	Chain	Res	Type
12	BA	19	U
12	BA	20	A
12	BA	21	C
12	BA	22	U
12	BA	23	A
12	BA	25	A
12	BA	26	C
12	BA	31	A
12	BA	32	C
12	BA	33	A
12	BA	36	A
12	BA	37	A
12	BA	39	A
12	BA	40	C
12	BA	41	A
12	BA	42	C
12	BA	45	A
12	BA	46	A
12	BA	47	A
12	BA	48	U
12	BA	49	A
12	BA	50	A
12	BA	56	A
12	BA	57	A
12	BA	59	A
12	BA	60	U
12	BA	63	A
12	BA	66	U
12	BA	67	A
12	BA	68	A
12	BA	82	G
12	BA	83	A
12	BA	84	G
12	BA	96	U
12	BA	97	A
12	BA	99	C
12	BA	101	U
12	BA	102	G
12	BA	104	C
12	BA	105	G
12	BA	108	A
12	BA	109	U

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Mol	Chain	Res	Type
12	BA	115	U
12	BA	118	U
12	BA	119	A
12	BA	122	G
12	BA	129	A
12	BA	132	G
12	BA	139	G
12	BA	140	A
12	BA	141	A
12	BA	142	U
12	BA	143	A
12	BA	146	A
12	BA	147	U
12	BA	148	A
12	BA	149	A
12	BA	153	U
12	BA	157	A
12	BA	163	C
12	BA	164	A
12	BA	165	A
12	BA	168	A
12	BA	172	C
12	BA	179	U
12	BA	180	A
12	BA	182	C
12	BA	188	C
12	BA	190	U
12	BA	192	A
12	BA	203	A
12	BA	205	A
12	BA	218	A
12	BA	219	A
12	BA	221	A
12	BA	223	A
12	BA	224	A
12	BA	225	C
12	BA	228	U
12	BA	229	A
12	BA	231	C
12	BA	237	A
12	BA	238	C
12	BA	239	C

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Mol	Chain	Res	Type
12	BA	243	A
12	BA	245	A
12	BA	252	G
12	BA	254	G
12	BA	260	C
12	BA	263	G
12	BA	265	G
12	BA	271	U
12	BA	272	A
12	BA	273	A
12	BA	274	A
12	BA	275	A
12	BA	276	G
12	BA	277	A
12	BA	295	G
12	BA	303	G
12	BA	305	G
12	BA	306	A
12	BA	309	A
12	BA	311	A
12	BA	312	C
12	BA	313	U
12	BA	318	G
12	BA	322	G
12	BA	324	G
12	BA	329	A
12	BA	330	A
12	BA	331	A
12	BA	336	A
12	BA	337	A
12	BA	338	C
12	BA	339	G
12	BA	340	A
12	BA	352	G
12	BA	359	G
12	BA	364	A
12	BA	366	A
12	BA	367	A
12	BA	368	A
12	BA	369	G
12	BA	371	A
12	BA	373	U

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Mol	Chain	Res	Type
12	BA	374	U
12	BA	381	A
12	BA	389	A
12	BA	390	A
12	BA	392	U
12	BA	393	A
12	BA	394	C
12	BA	397	C
12	BA	398	A
12	BA	402	A
12	BA	403	C
12	BA	404	C
12	BA	409	A
12	BA	414	A
12	BA	417	G
12	BA	418	U
12	BA	419	A
12	BA	420	U
12	BA	427	G
12	BA	428	A
12	BA	440	A
12	BA	441	A
12	BA	446	C
12	BA	447	A
12	BA	448	G
12	BA	449	C
12	BA	459	A
12	BA	460	C
12	BA	467	A
12	BA	468	A
12	BA	472	U
12	BA	473	G
12	BA	474	A
12	BA	478	G
12	BA	479	A
12	BA	480	G
12	BA	488	U
12	BA	489	C
12	BA	490	U
12	BA	491	U
12	BA	492	A
12	BA	493	A

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Mol	Chain	Res	Type
12	BA	494	U
12	BA	497	U
12	BA	500	C
12	BA	501	A
12	BA	503	A
12	BA	504	G
12	BA	505	U
12	BA	506	A
12	BA	515	A
12	BA	516	G
12	BA	518	A
12	BA	526	A
12	BA	532	A
12	BA	533	A
12	BA	545	U
12	BA	547	A
12	BA	548	A
12	BA	550	A
12	BA	552	A
12	BA	553	U
12	BA	554	U
12	BA	557	C
12	BA	560	A
12	BA	561	C
12	BA	562	A
12	BA	563	U
12	BA	566	U
12	BA	570	A
12	BA	574	A
12	BA	575	C
12	BA	576	U
12	BA	578	A
12	BA	579	U
12	BA	580	A
12	BA	583	A
12	BA	584	A
12	BA	585	A
12	BA	586	C
12	BA	592	G
12	BA	593	C
12	BA	595	C
12	BA	596	A

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Mol	Chain	Res	Type
12	BA	614	U
12	BA	617	A
12	BA	618	A
12	BA	619	C
12	BA	625	A
12	BA	628	A
12	BA	631	A
12	BA	634	G
12	BA	640	A
12	BA	643	A
12	BA	648	C
12	BA	649	A
12	BA	650	A
12	BA	656	C
12	BA	657	U
12	BA	661	U
12	BA	673	C
12	BA	674	U
12	BA	684	A
12	BA	689	A
12	BA	690	U
12	BA	691	A
12	BA	694	A
12	BA	695	U
12	BA	696	A
12	BA	697	C
12	BA	704	U
12	BA	705	U
12	BA	707	A
12	BA	708	C
12	BA	713	A
12	BA	715	U
12	BA	718	A
12	BA	719	C
12	BA	720	C
12	BA	722	A
12	BA	723	A
12	BA	724	A
12	BA	725	C
12	BA	727	A
12	BA	728	C
12	BA	736	C

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Mol	Chain	Res	Type
12	BA	737	G
12	BA	744	A
12	BA	745	A
12	BA	746	U
12	BA	747	U
12	BA	748	A
12	BA	753	G
12	BA	761	A
12	BA	764	A
12	BA	766	A
12	BA	774	A
12	BA	775	C
12	BA	777	A
12	BA	778	A
12	BA	779	G
12	BA	780	G
12	BA	782	A
12	BA	783	A
12	BA	784	G
12	BA	789	A
12	BA	795	G
12	BA	809	G
12	BA	814	C
12	BA	818	A
12	BA	819	A
12	BA	824	G
12	BA	825	C
12	BA	834	C
12	BA	835	A
12	BA	847	U
12	BA	848	C
12	BA	850	A
12	BA	852	C
12	BA	853	A
12	BA	854	U
12	BA	855	U
12	BA	859	A
12	BA	860	G
12	BA	864	U
12	BA	872	A
12	BA	876	C
12	BA	883	G

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Mol	Chain	Res	Type
12	BA	887	C
12	BA	888	A
12	BA	889	C
12	BA	890	C
12	BA	892	G
12	BA	895	U
12	BA	897	A
12	BA	899	G
12	BA	901	C
12	BA	902	C
12	BA	908	A
12	BA	909	U
12	BA	910	U
12	BA	922	A
12	BA	923	A
12	BA	924	G
12	BA	925	G
12	BA	931	U
12	BA	932	A
12	BA	933	A
12	BA	935	C
12	BA	938	U
12	BA	939	U
12	BA	948	A
12	BA	950	U
12	BA	958	U
12	BA	959	G
12	BA	960	U
12	BA	961	A
12	BA	964	A
12	BA	965	A
12	BA	967	G
12	BA	970	C
12	BA	977	G
12	BA	979	G
12	BA	981	U
12	BA	982	U
12	BA	983	U
12	BA	986	U
12	BA	988	U
12	BA	992	U
12	BA	1015	C

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Mol	Chain	Res	Type
12	BA	1016	C
12	BA	1018	U
12	BA	1022	G
12	BA	1026	A
12	BA	1027	G
12	BA	1028	A
12	BA	1034	G
12	BA	1038	A
12	BA	1041	A
12	BA	1045	U
12	BA	1050	C
12	BA	1051	G
12	BA	1055	A
12	BA	1056	G
12	BA	1057	A
12	BA	1063	U
12	BA	1064	G
12	BA	1071	U
12	BA	1072	A
12	BA	1075	U
12	BA	1080	A
12	BA	1089	G
12	BA	1092	A
12	BA	1093	A
12	BA	1094	A
12	BA	1123	A
12	BA	1127	A
12	BA	1129	C
12	BA	1137	A
12	BA	1138	G
12	BA	1140	A
12	BA	1145	C
12	BA	1146	G
12	BA	1166	A
12	BA	1167	C
12	BA	1168	A
12	BA	1169	A
12	BA	1178	C
12	BA	1183	U
12	BA	1188	U
12	BA	1190	A
12	BA	1195	A

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Mol	Chain	Res	Type
12	BA	1205	G
12	BA	1206	U
12	BA	1207	C
12	BA	1215	C
12	BA	1216	C
12	BA	1217	A
12	BA	1218	U
12	BA	1219	A
12	BA	1220	A
12	BA	1221	C
12	BA	1222	A
12	BA	1226	C
12	BA	1231	U
12	BA	1234	U
12	BA	1238	A
12	BA	1239	A
12	BA	1240	A
12	BA	1241	U
12	BA	1242	U
12	BA	1246	A
12	BA	1247	U
12	BA	1248	C
12	BA	1249	A
12	BA	1253	G
12	BA	1254	A
12	BA	1255	A
12	BA	1258	A
12	BA	1259	G
12	BA	1264	C
12	BA	1268	G
12	BA	1270	G
12	BA	1271	A
12	BA	1287	G
12	BA	1288	U
12	BA	1291	U
12	BA	1294	A
12	BA	1296	U
12	BA	1297	U
12	BA	1299	C
12	BA	1303	C
12	BA	1307	A
12	BA	1311	G

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Mol	Chain	Res	Type
12	BA	1314	U
12	BA	1317	A
12	BA	1324	C
12	BA	1325	G
12	BA	1326	A
12	BA	1328	G
12	BA	1331	G
12	BA	1341	A
12	BA	1342	C
12	BA	1348	U
12	BA	1352	G
12	BA	1353	C
12	BA	1357	C
12	BA	1358	G
12	BA	1377	U
12	BA	1385	U
12	BA	1387	A
12	BA	1388	A
12	BA	1389	A
12	BA	1390	G
12	BA	1396	C
12	BA	1399	G
12	BA	1404	G
12	BA	1406	G
12	BA	1409	C
12	BA	1410	A
12	BA	1420	A
12	BA	1426	G
12	BA	1427	G
12	BA	1428	U
12	BA	1429	C
12	BA	1432	U
12	BA	1433	U
12	BA	1436	U
12	BA	1438	U
12	BA	1444	A
12	BA	1445	U
12	BA	1448	A
12	BA	1458	G
12	BA	1459	U
12	BA	1465	A
12	BA	1466	G

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Mol	Chain	Res	Type
12	BA	1467	G
12	BA	1468	A
12	BA	1474	G
12	BA	1476	A
12	BA	1492	C
12	BA	1493	A
12	BA	1494	A
12	BA	1498	C
12	BA	1504	A
12	BA	1505	G
12	BA	1508	A
12	BA	1509	U
12	BA	1510	A
12	BA	1514	A
12	BA	1518	A
12	BA	1521	U
12	BA	1522	A
12	BA	1525	C
12	BA	1526	U
12	BA	1527	U
12	BA	1528	A
12	BA	1529	A
12	BA	1531	C
12	BA	1532	U
12	BA	1533	A
12	BA	1536	U
12	BA	1548	A
12	BA	1549	A
12	BA	1550	U
12	BA	1551	C
12	BA	1552	C
12	BA	1553	A
12	BA	1554	G
12	BA	1555	C
12	BA	1556	C
12	BA	1558	U
12	BA	1559	A
12	BA	1560	G
12	BA	1561	A
12	BA	1570	C
12	BA	1571	A
13	BB	3	U

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Mol	Chain	Res	Type
13	BB	5	A
13	BB	7	G
13	BB	8	U
13	BB	9	A
13	BB	13	U
13	BB	21	C
13	BB	22	A
13	BB	23	A
13	BB	24	A
13	BB	25	G
13	BB	29	G
13	BB	30	G
13	BB	34	U
13	BB	35	G
13	BB	43	C
13	BB	44	U
13	BB	45	A
13	BB	46	G
13	BB	47	A
13	BB	48	U
13	BB	55	C
13	BB	67	A
13	BB	69	C
13	BB	70	A
56	AV	6	G
56	AV	7	G
56	AV	9	C
56	AV	13	U
56	AV	14	A
56	AV	15	A
56	AV	16	A
56	AV	17	U
56	AV	18	A
56	AV	19	A
56	AV	22	U
56	AV	28	G
56	AV	39	G
56	AV	40	A
56	AV	43	A
56	AV	44	U
56	AV	45	G
56	AV	46	U

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Mol	Chain	Res	Type
56	AV	51	U
56	AV	52	A
56	AV	53	U
56	AV	54	A
56	AV	55	C
56	AV	56	C
56	AV	62	C
56	AV	63	G
56	AV	64	U
56	AV	65	A
56	AV	67	U
56	AV	68	A
56	AV	71	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	BA	39	A
12	BA	48	U
12	BA	101	U
12	BA	553	U
12	BA	1093	A
12	BA	1145	C
12	BA	1219	A
12	BA	1220	A
12	BA	1240	A
12	BA	1241	U
13	BB	20	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 226 ligands modelled in this entry, 220 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	$\#\|Z\| > 2$
61	GSP	BC	901	62,57	26,34,34	2.17	3 (11%)	27,54,54	1.51	6 (22%)
59	5GP	BA	3204	-	22,26,26	1.07	1 (4%)	26,40,40	1.29	3 (11%)
59	5GP	BA	3203	-	22,26,26	1.07	2 (9%)	26,40,40	1.46	4 (15%)
63	FME	AV	101	56	8,9,10	0.96	0	7,9,11	0.67	0
60	SPM	BA	3205	-	13,13,13	0.37	0	12,12,12	0.81	0
60	SPM	BR	201	-	13,13,13	0.48	0	12,12,12	0.77	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**
61	GSP	BC	901	62,57	-	0/17/38/38	0/3/3/3
59	5GP	BA	3204	-	-	5/6/26/26	0/3/3/3
59	5GP	BA	3203	-	-	5/6/26/26	0/3/3/3
63	FME	AV	101	56	-	4/7/9/11	-
60	SPM	BA	3205	-	-	6/11/11/11	-
60	SPM	BR	201	-	-	7/11/11/11	-

All (6) bond length outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(Å)**	**Ideal(Å)**
61	BC	901	GSP	PG-S1G	-9.35	1.70	1.90
61	BC	901	GSP	C5-C6	-3.70	1.39	1.47
59	BA	3204	5GP	C5-C6	-3.24	1.40	1.47
59	BA	3203	5GP	C6-N1	-2.73	1.33	1.37
59	BA	3203	5GP	C5-C6	-2.45	1.42	1.47
61	BC	901	GSP	C2-N3	2.37	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	3203	5GP	C5-C6-N1	3.66	120.42	113.95
59	BA	3203	5GP	O6-C6-N1	-3.21	116.86	120.65
59	BA	3203	5GP	C8-N7-C5	3.18	109.06	102.99
61	BC	901	GSP	C5-C6-N1	3.12	119.46	113.95
61	BC	901	GSP	C8-N7-C5	3.05	108.80	102.99
59	BA	3204	5GP	C5-C6-N1	3.00	119.25	113.95
61	BC	901	GSP	PA-O3A-PB	-2.84	123.07	132.83
59	BA	3203	5GP	C2-N1-C6	-2.79	119.96	125.10
61	BC	901	GSP	C2-N1-C6	-2.74	120.06	125.10
59	BA	3204	5GP	C8-N7-C5	2.62	107.98	102.99
59	BA	3204	5GP	C2-N1-C6	-2.51	120.47	125.10
61	BC	901	GSP	C3'-C2'-C1'	2.25	104.37	100.98
61	BC	901	GSP	O6-C6-C5	-2.04	120.40	124.37

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	BA	3203	5GP	C5'-O5'-P-O1P
59	BA	3203	5GP	C5'-O5'-P-O2P
59	BA	3203	5GP	C5'-O5'-P-O3P
59	BA	3204	5GP	C5'-O5'-P-O1P
59	BA	3204	5GP	C5'-O5'-P-O2P
59	BA	3204	5GP	C5'-O5'-P-O3P
59	BA	3204	5GP	O4'-C4'-C5'-O5'
59	BA	3204	5GP	C3'-C4'-C5'-O5'
63	AV	101	FME	C-CA-CB-CG
63	AV	101	FME	CA-CB-CG-SD
60	BR	201	SPM	N5-C6-C7-C8
60	BA	3205	SPM	C7-C8-C9-N10
60	BA	3205	SPM	C2-C3-C4-N5
60	BR	201	SPM	C2-C3-C4-N5
63	AV	101	FME	N-CA-CB-CG
60	BR	201	SPM	C8-C9-N10-C11
63	AV	101	FME	CB-CG-SD-CE
60	BR	201	SPM	N1-C2-C3-C4
60	BA	3205	SPM	C6-C7-C8-C9
60	BR	201	SPM	C6-C7-C8-C9
59	BA	3203	5GP	C4'-C5'-O5'-P
60	BA	3205	SPM	N1-C2-C3-C4
60	BA	3205	SPM	C7-C6-N5-C4
60	BR	201	SPM	N10-C11-C12-C13
60	BR	201	SPM	C12-C11-N10-C9

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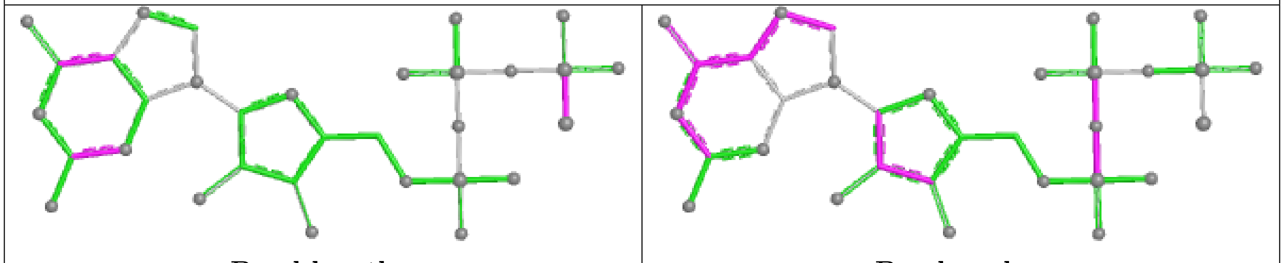
Mol	Chain	Res	Type	Atoms
60	BA	3205	SPM	N5-C6-C7-C8
59	BA	3203	5GP	O4'-C4'-C5'-O5'

There are no ring outliers.

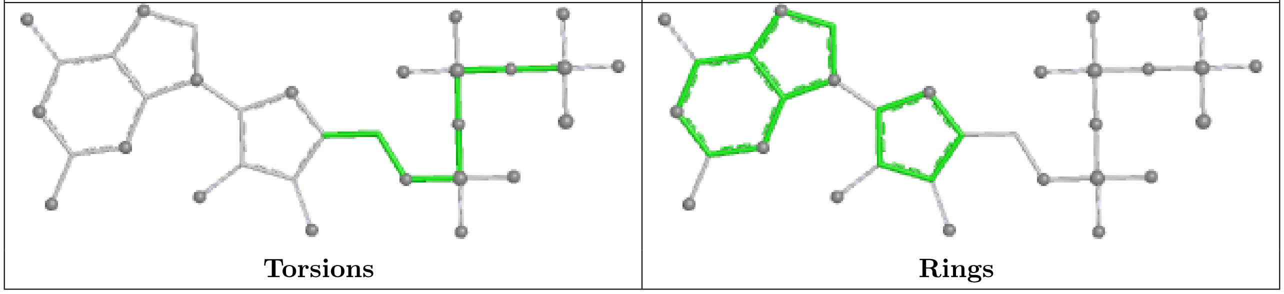
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GSP BC 901

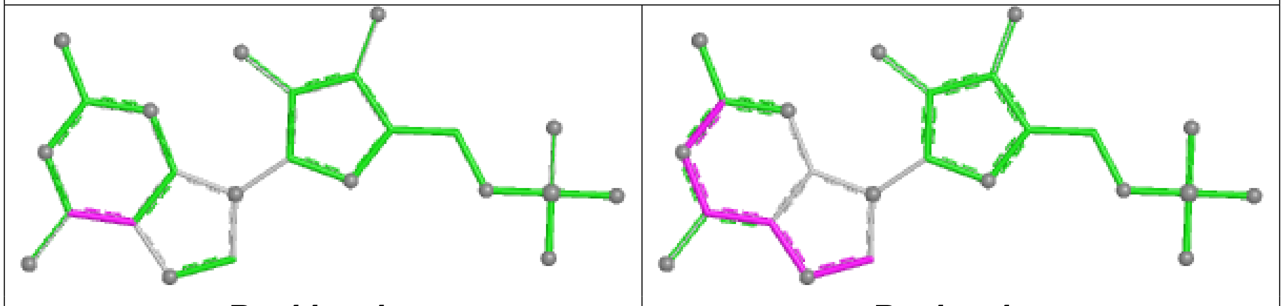


Bond lengths **Bond angles**



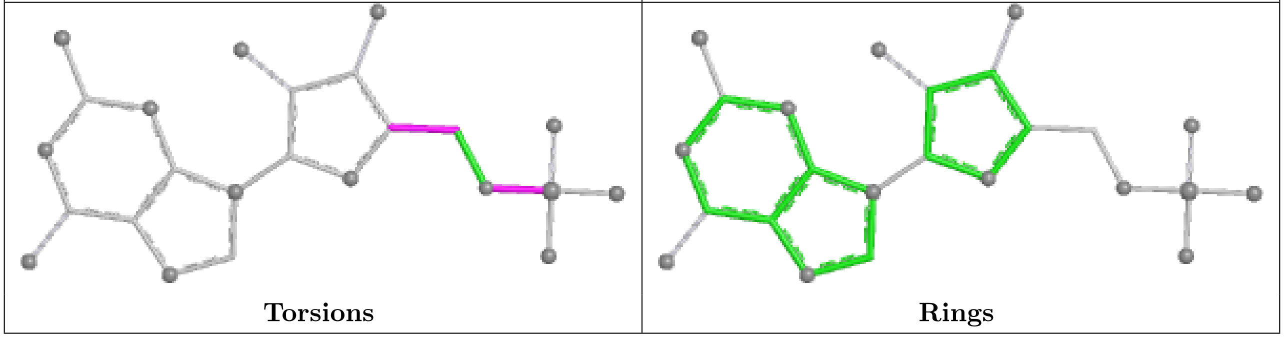
Torsions **Rings**

Ligand 5GP BA 3204



Bond lengths

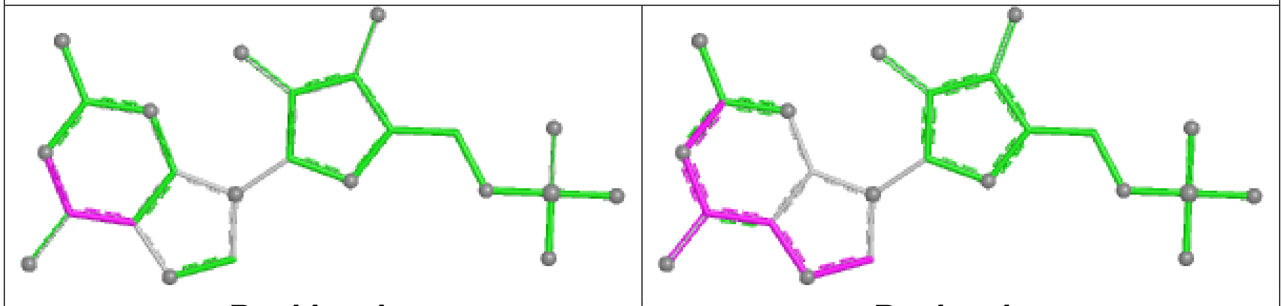
Bond angles



Torsions

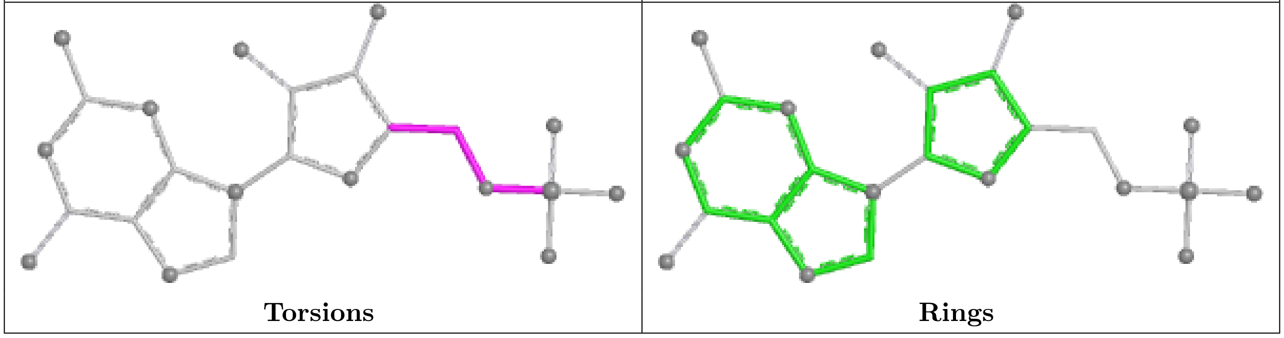
Rings

Ligand 5GP BA 3203



Bond lengths

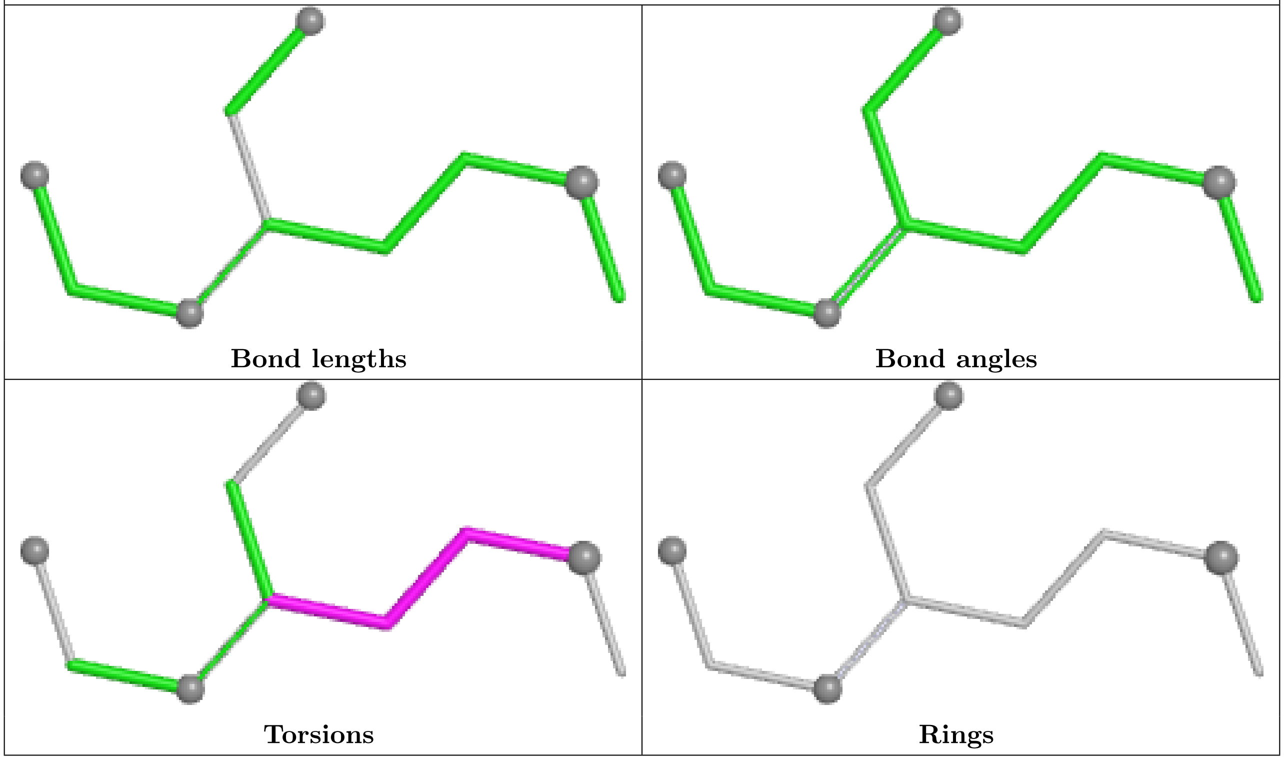
Bond angles



Torsions

Rings

Ligand FME AV 101



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	Bz	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bz	710:ALA	C	1001:ALA	N	60.04
1	Bz	415:ALA	C	601:ALA	N	51.34
1	Bz	106:ALA	C	301:ALA	N	30.40
1	Bz	615:ALA	C	700:ALA	N	17.65
1	Bz	315:ALA	C	399:ALA	N	16.53

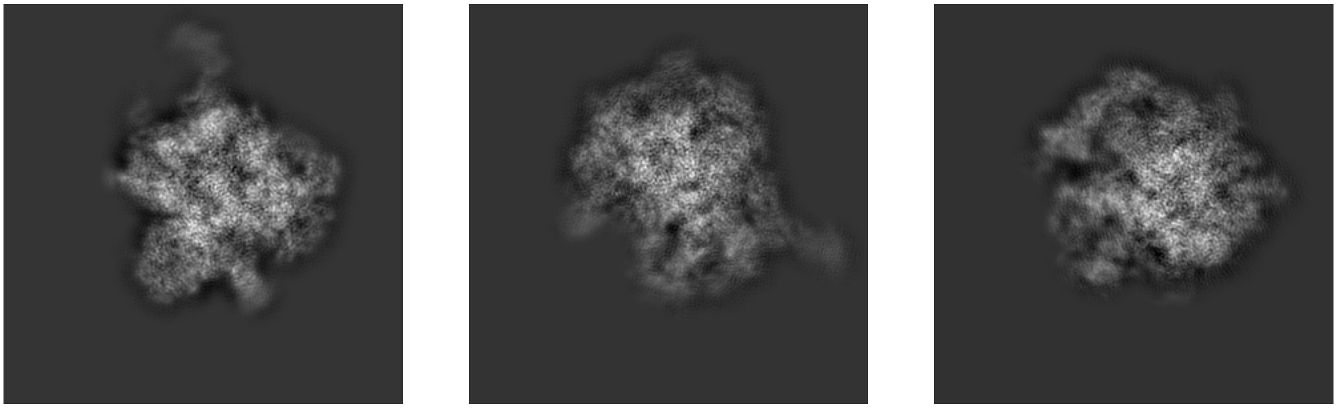
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-4370. 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.

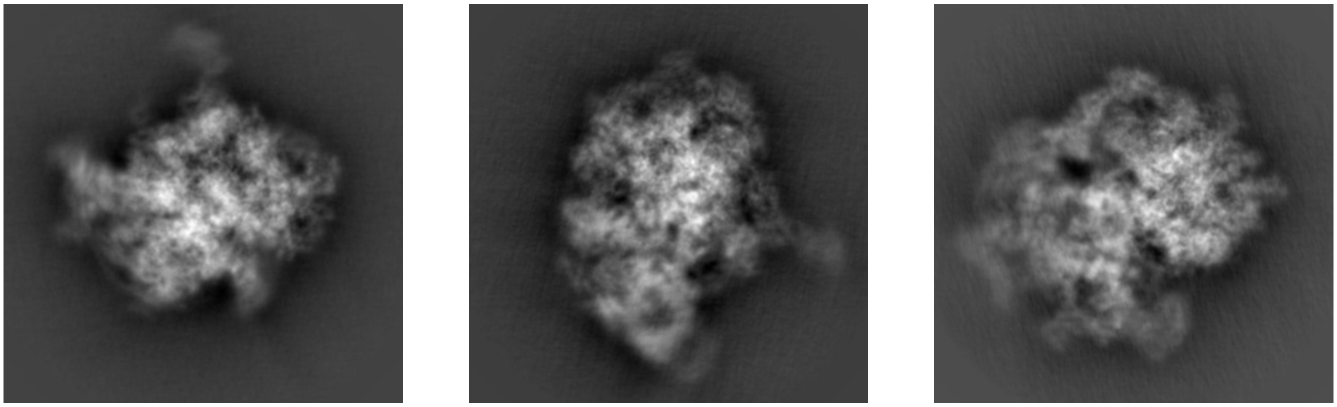
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

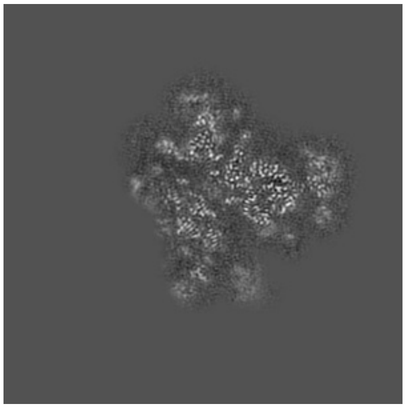


X Y Z

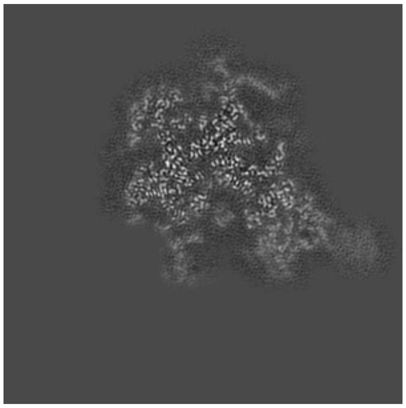
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

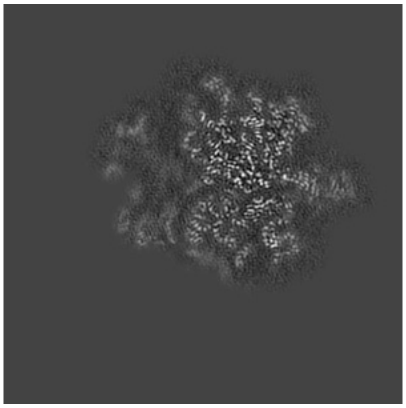
6.2.1 Primary map



X Index: 140

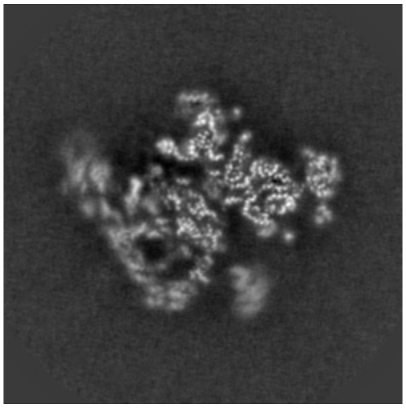


Y Index: 140

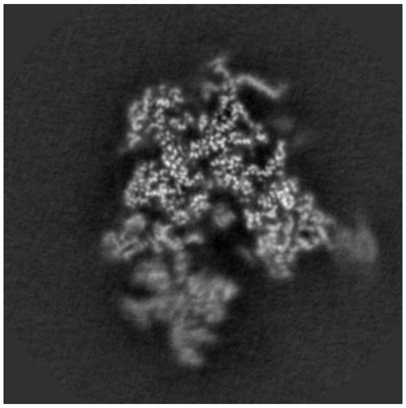


Z Index: 140

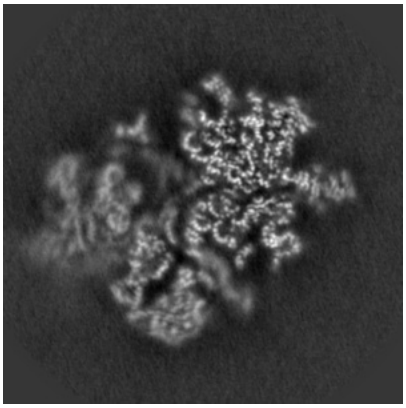
6.2.2 Raw map



X Index: 140



Y Index: 140

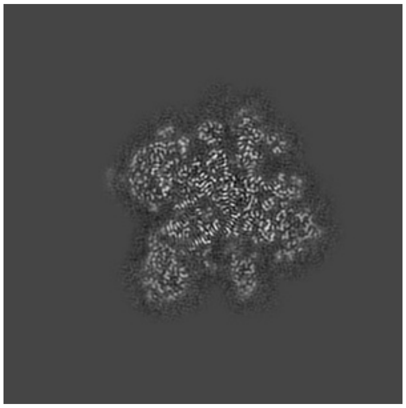


Z Index: 140

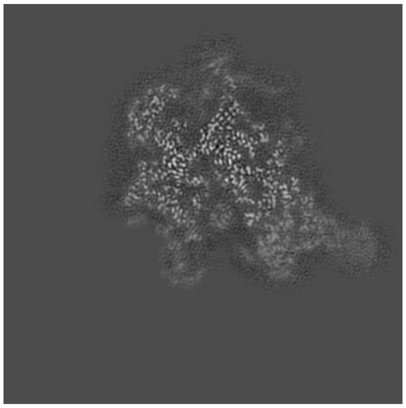
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

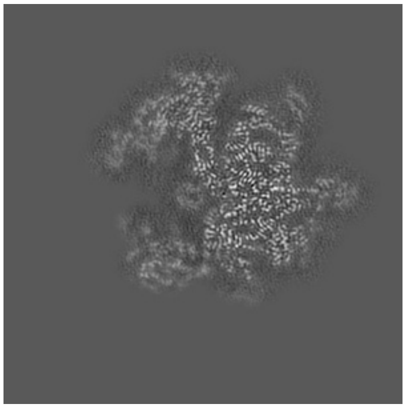
6.3.1 Primary map



X Index: 169

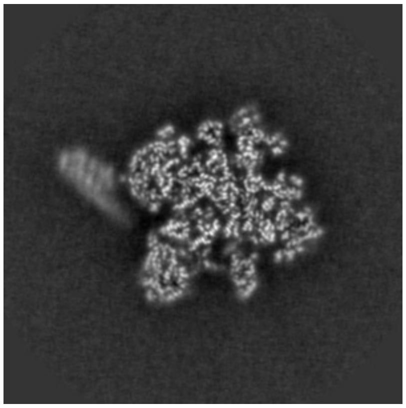


Y Index: 142

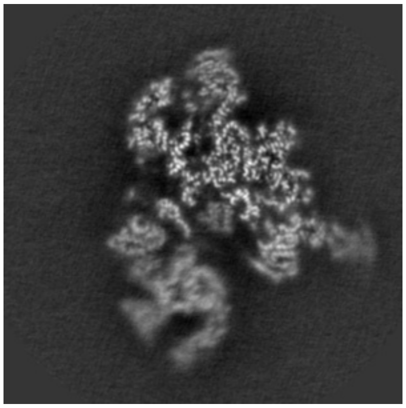


Z Index: 153

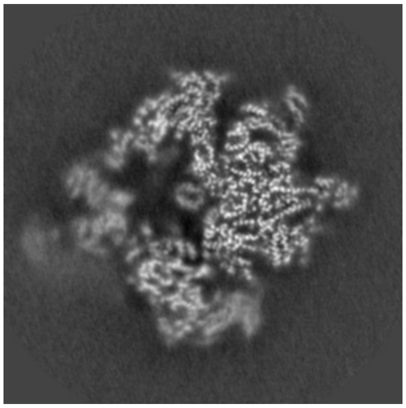
6.3.2 Raw map



X Index: 169



Y Index: 148



Z Index: 153

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. 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

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.

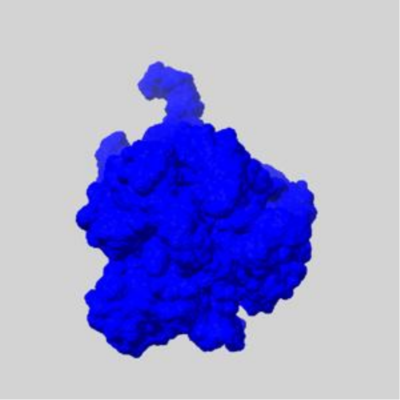
6.5 Mask visualisation ⓘ

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

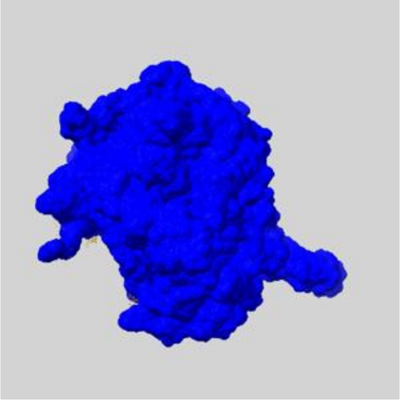
A mask typically either:

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

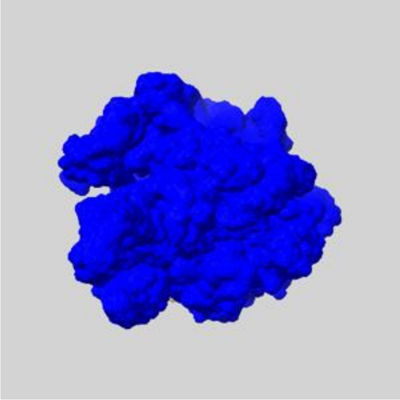
6.5.1 emd_4370_msk_1.map ⓘ



X



Y

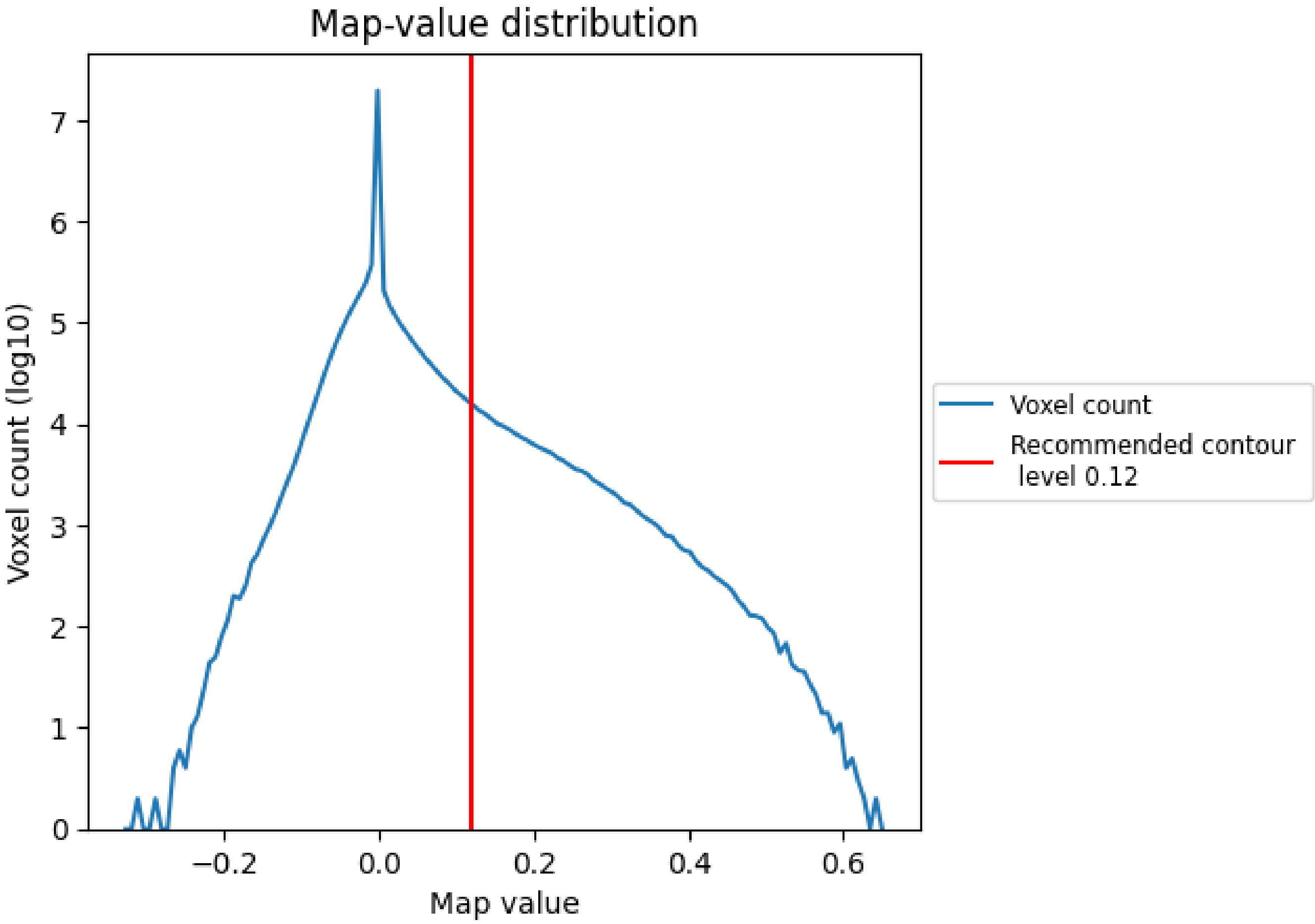


Z

7 Map analysis ⓘ

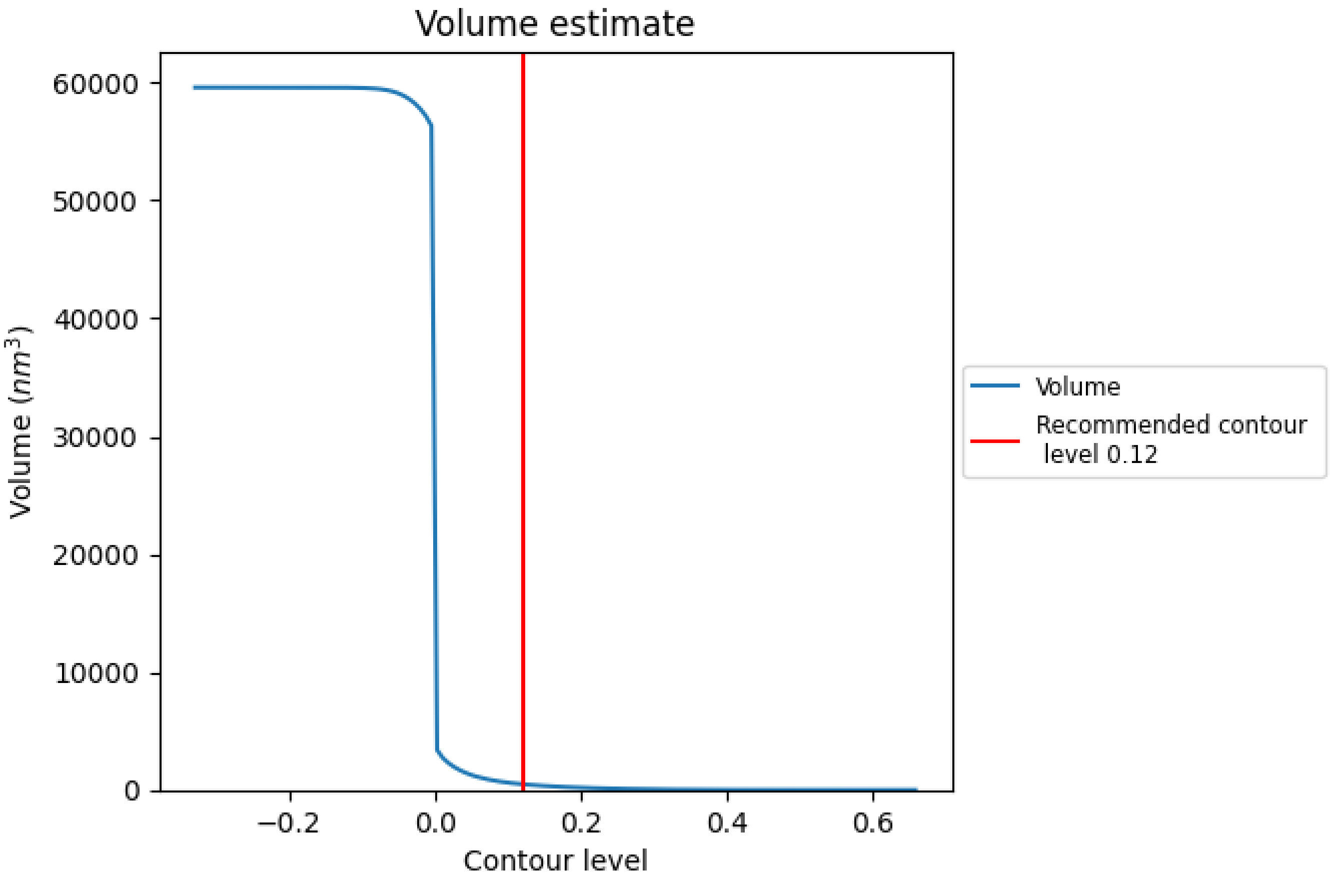
This section contains the results of statistical analysis of the map.

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.

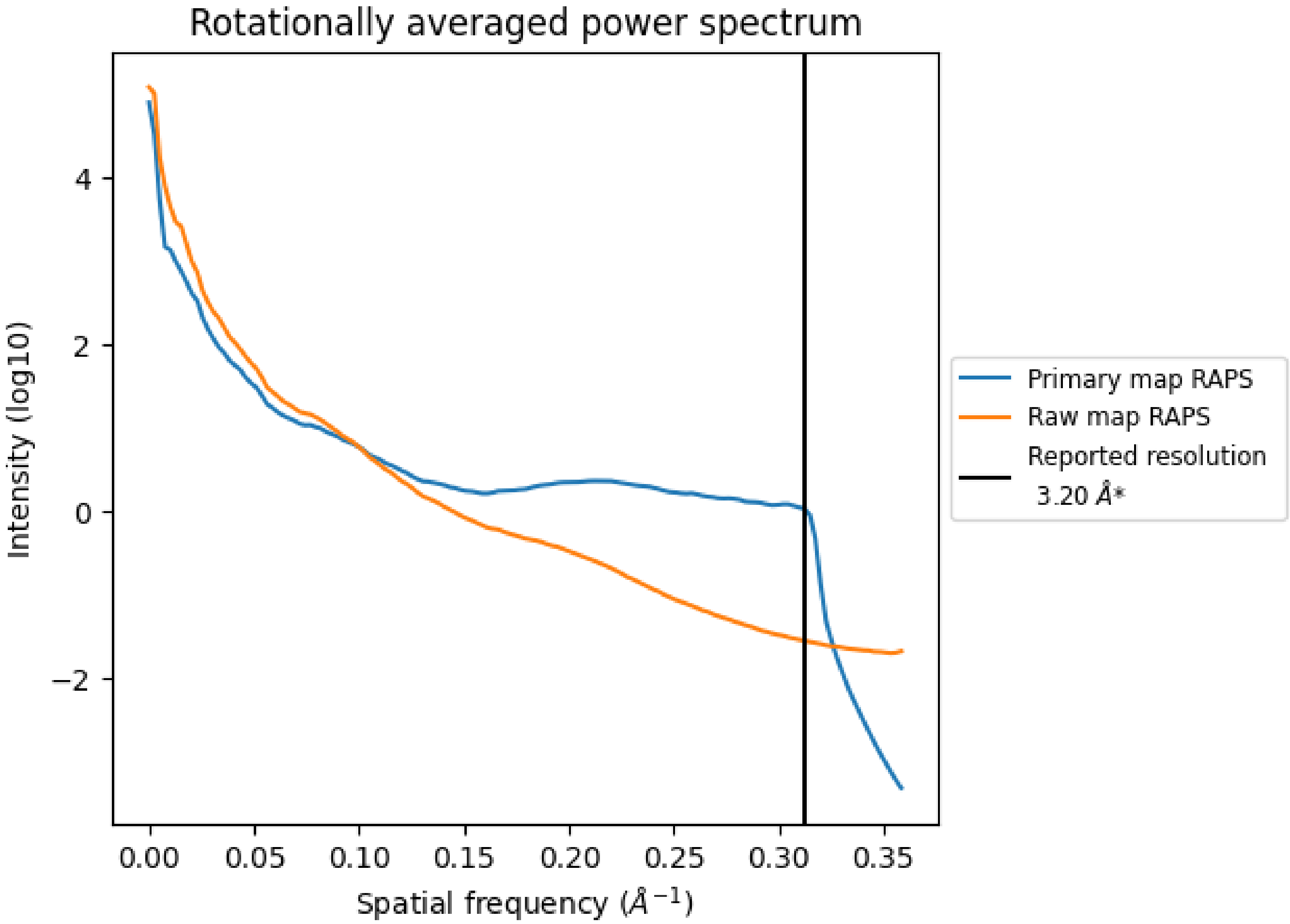
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 485 nm^3; this corresponds to an approximate mass of 438 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 ⓘ

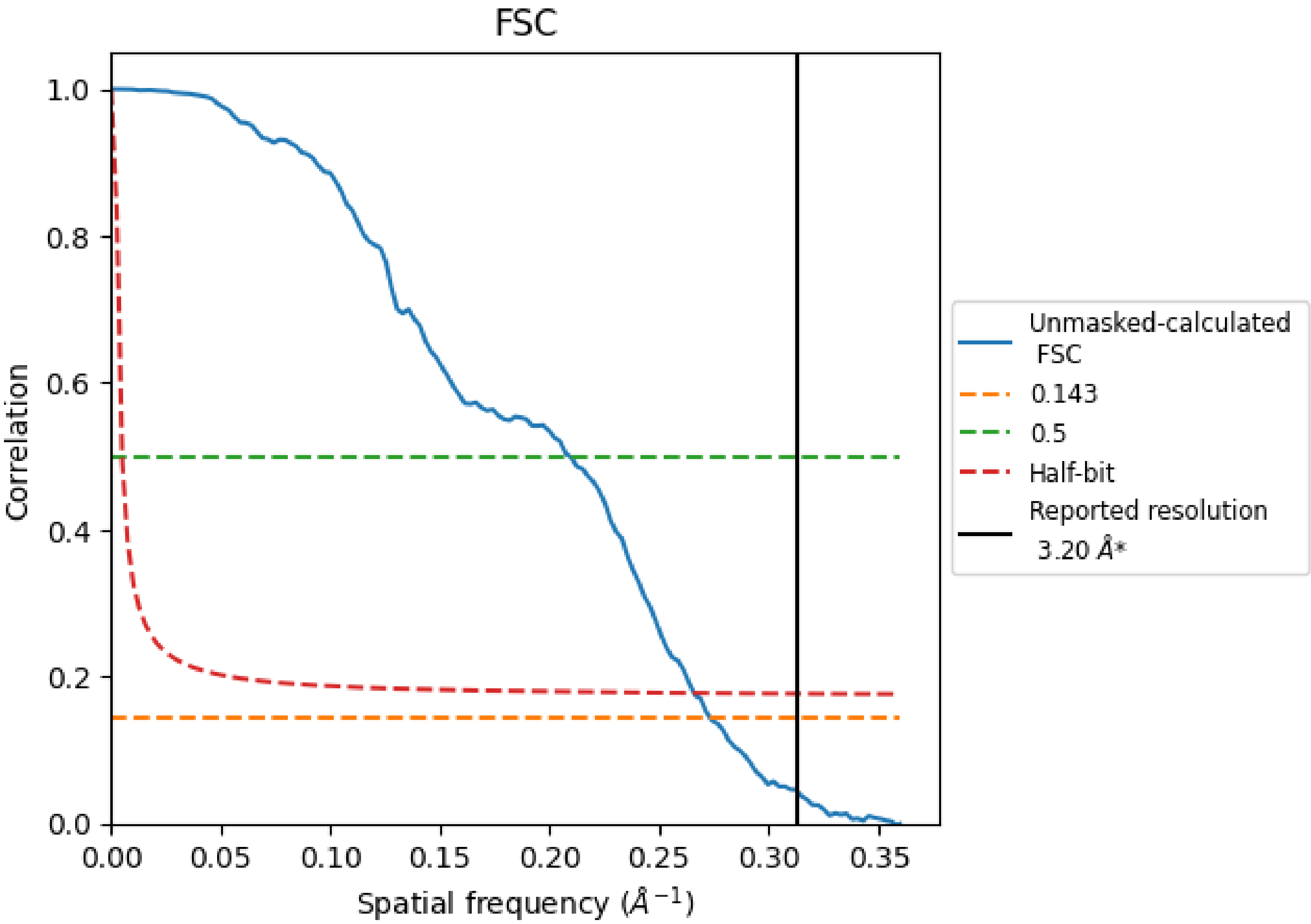


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

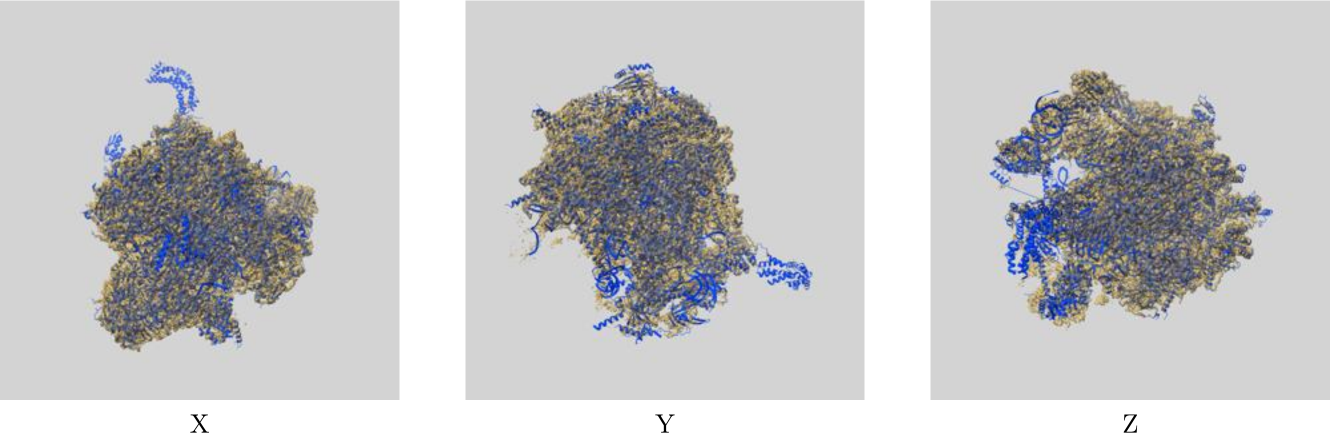
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.78	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 3.2 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-4370 and PDB model 6GB2. Per-residue inclusion information can be found in section 3 on page 19.

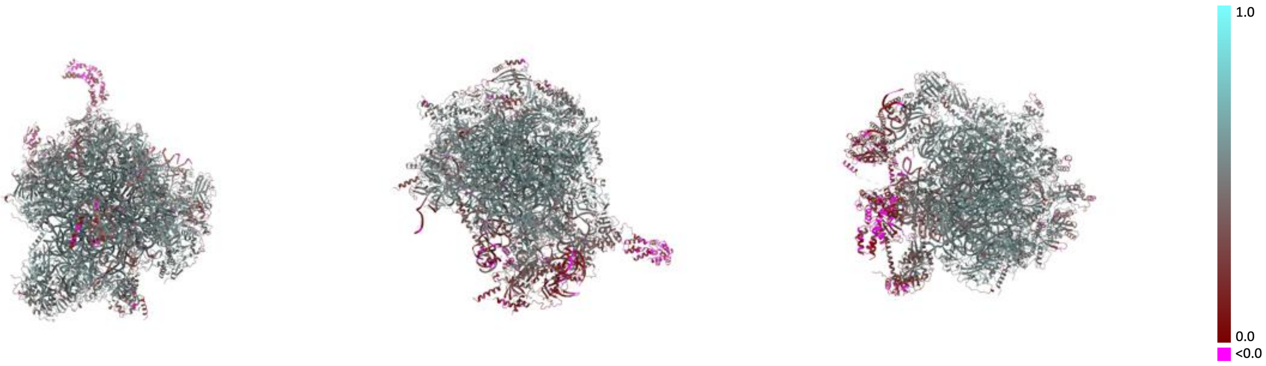
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

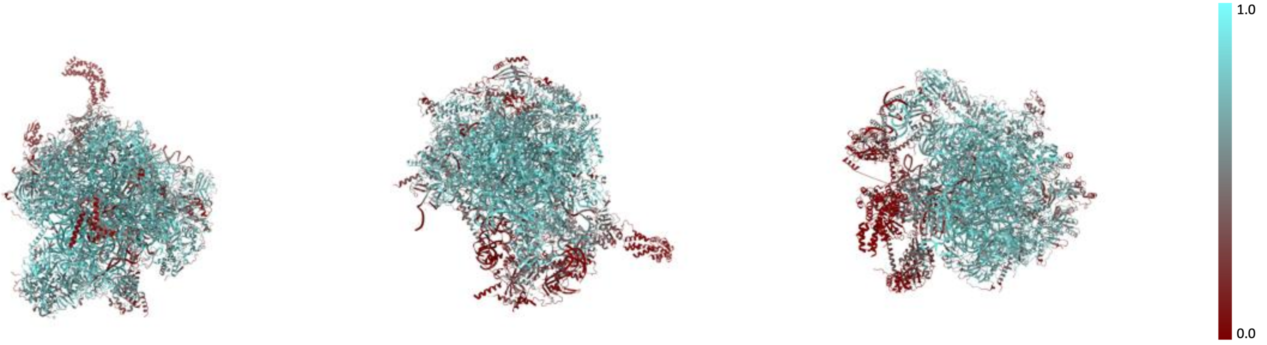
9.2 Q-score mapped to coordinate model ⓘ



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.

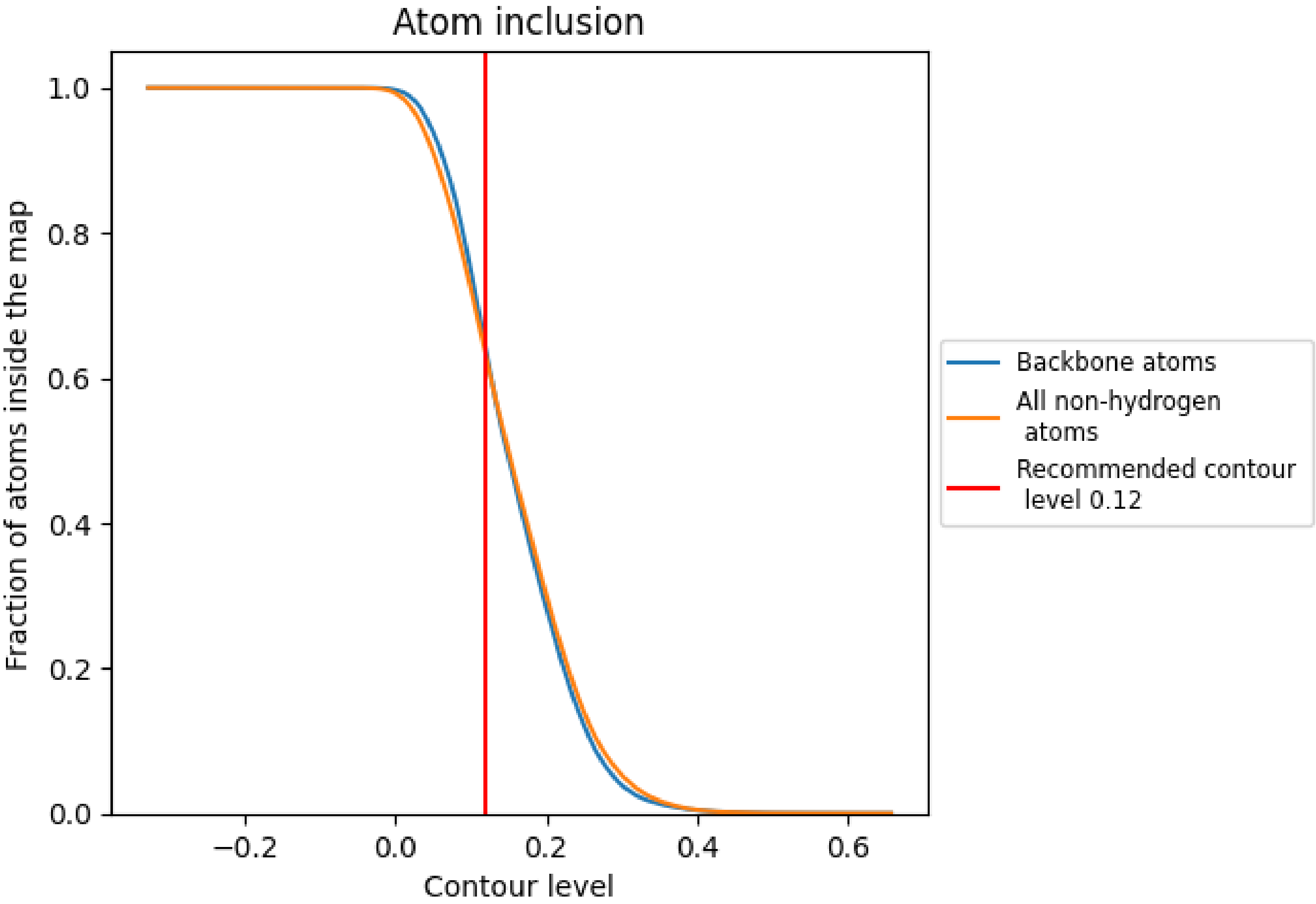
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 64% of all backbone atoms, 63% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6311	0.4810
AV	0.0438	0.1900
B0	0.7586	0.5630
B1	0.6001	0.4850
B2	0.7181	0.5260
B3	0.7274	0.5410
B4	0.3343	0.2940
B5	0.6980	0.5220
B6	0.4808	0.4760
B7	0.8022	0.5900
B8	0.7716	0.5710
B9	0.7819	0.5530
BA	0.8424	0.5520
BB	0.4944	0.2870
BC	0.2591	0.3620
BD	0.6689	0.5360
BE	0.7181	0.5320
BF	0.7373	0.5480
BI	0.4801	0.4340
BJ	0.3393	0.3300
BK	0.1665	0.2330
BL	0.0037	0.1550
BN	0.7753	0.5590
BO	0.6184	0.5250
BP	0.7332	0.5470
BQ	0.6825	0.5310
BR	0.7364	0.5470
BS	0.6812	0.5090
BT	0.6411	0.5130
BU	0.7543	0.5500
BV	0.7222	0.5330
BW	0.7246	0.5520
BX	0.6799	0.5080
BY	0.4295	0.4340
Ba	0.6584	0.4990

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Chain	Atom inclusion	Q-score
Bb	0.6589	0.4740
Bc	0.6016	0.4650
Bd	0.2788	0.2660
Be	0.5853	0.4820
Bf	0.6393	0.4810
Bg	0.7219	0.5470
Bh	0.6648	0.4940
Bi	0.3581	0.3980
Bj	0.1741	0.1960
Bk	0.3152	0.3150
Bl	0.7222	0.5250
Bm	0.2810	0.3950
Bn	0.7643	0.5620
Bo	0.6578	0.5030
Bp	0.3785	0.3700
Bq	0.3295	0.3570
Bt	0.7463	0.5540
Bu	0.4533	0.3870
Bv	0.4931	0.4090
Bw	0.6908	0.5090
Bx	0.6750	0.5040
Bz	0.0146	0.0900
CL	0.0095	0.1490
DL	0.0047	0.1210
EL	0.0000	0.0300
FL	0.0047	0.0730
GL	0.0000	0.0360
HL	0.0000	0.0780