



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 04:14 PM UTC

PDB ID : 7A5H / pdb_00007a5h
EMDB ID : EMD-11643
Title : Structure of the split human mitoribosomal large subunit with rescue factors mtRF-R and MTRES1
Authors : Desai, N.; Yang, H.; Chandrasekaran, V.; Kazi, R.; Minczuk, M.; Ramakrishnan, V.
Deposited on : 2020-08-21
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

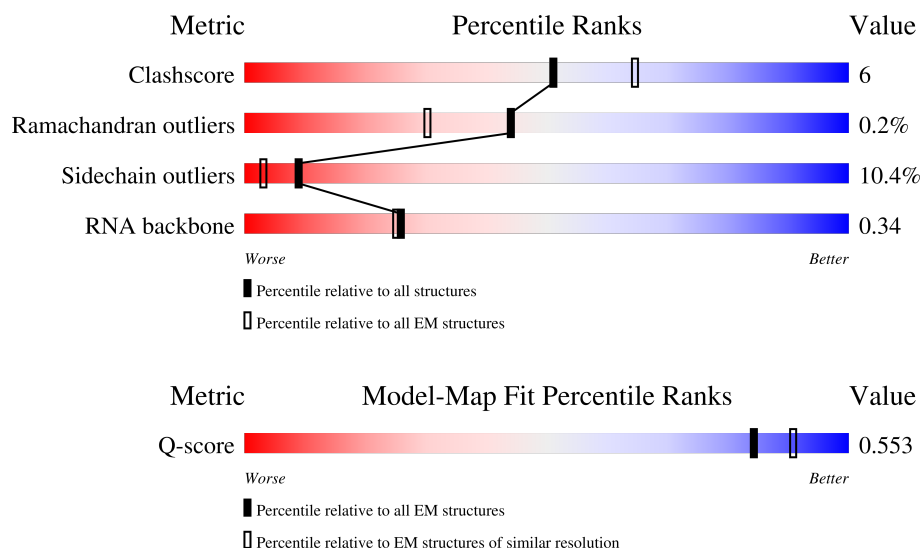
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	D	305	
2	E	348	
3	F	311	

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Mol	Chain	Length	Quality of chain
4	H	267	
5	I	261	
6	J	192	
7	K	178	
8	L	145	
9	M	296	
10	N	251	
11	O	175	
12	P	179	
13	Q	292	
14	R	149	
15	S	205	
16	T	212	
17	U	153	
18	V	216	
19	W	148	
20	X	256	
21	Y	250	
22	Z	161	
23	0	188	
24	1	65	
25	2	92	
26	3	188	
27	5	423	
28	6	380	

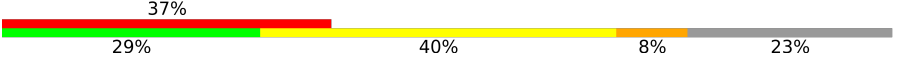
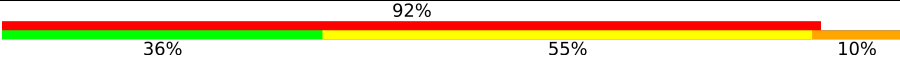
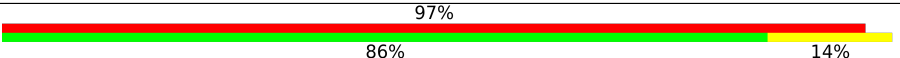
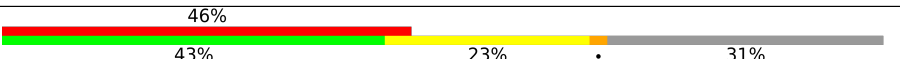
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Mol	Chain	Length	Quality of chain
29	7	338	
30	8	206	
31	9	137	
32	a	142	
33	b	155	
34	c	332	
35	d	306	
36	e	279	
37	f	194	
38	g	166	
39	h	158	
40	i	128	
41	j	123	
42	k	112	
43	l	138	
44	m	128	
45	o	102	
46	p	206	
47	q	222	
48	r	196	
49	s	439	
50	t	28	
51	u	234	
52	v	70	
53	w	156	

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Mol	Chain	Length	Quality of chain
54	A	1559	
55	B	73	
56	24	73	
57	Y2	29	
58	C	166	
59	G	240	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 102610 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 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	236	Total	C	N	O	S	0	0
			1842	1145	373	315	9		

- Molecule 2 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	304	Total	C	N	O	S	0	0
			2396	1539	416	430	11		

- Molecule 3 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 4 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	95	Total	C	N	O	S	0	0
			784	498	152	134			

- Molecule 5 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 6 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 7 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 8 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 9 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 10 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 11 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 12 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	141	Total	C	N	O	S	0	0
			1148	719	221	203	5		

- Molecule 13 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	217	Total	C	N	O	S	0	0
			1805	1159	317	320	9		

- Molecule 14 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 15 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 16 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 17 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	152	Total	C	N	O	S	0	0
			1218	772	233	210	3		

- Molecule 18 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	202	Total	C	N	O	S	0	0
			1624	1032	291	293	8		

- Molecule 19 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	109	Total	C	N	O	S	0	0
			859	552	162	142	3		

- Molecule 20 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	243	Total	C	N	O	S	0	0
			2035	1317	351	362	5		

- Molecule 21 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 22 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 23 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 24 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 25 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	45	Total	C	N	O	S	0	0
			367	227	81	58	1		

- Molecule 26 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 27 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	387	Total	C	N	O	S	0	0
			3156	2039	548	558	11		

- Molecule 28 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 29 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 30 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	110	Total	C	N	O	S	0	0
			890	567	155	166	2		

- Molecule 31 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 32 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	82	Total	C	N	O	S	0	0
			686	434	124	123	5		

- Molecule 33 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 34 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 35 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	211	Total	C	N	O	S	0	0
			1741	1123	299	309	10		

- Molecule 36 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 37 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	116	Total	C	N	O	S	0	0
			915	585	152	175	3		

- Molecule 38 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 40 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 41 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 42 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	80	Total	C	N	O	S	0	0
			627	392	116	114	5		

- Molecule 43 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	l	23	Total	C	N	O	0	0
			221	137	52	32		

- Molecule 44 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 45 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	91	Total	C	N	O	S	0	0
			771	487	156	125	3		

- Molecule 46 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 47 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 48 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 49 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 50 is a protein called Unknown protein/protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	t	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 51 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	111	Total	C	N	O	S	0	0
			927	595	155	167	10		

- Molecule 52 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	v	69	Total	C	N	O	0	0
			588	372	116	100		

- Molecule 53 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	79	Total	C	N	O	S	0	0
			638	410	95	128	5		

- Molecule 54 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	A	1457	Total	C	N	O	P	0	0
			30945	13883	5590	10015	1457		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3107	U	UNK	conflict	GB 1025814679

- Molecule 55 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 56 is a RNA chain called mt-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	24	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		

- Molecule 57 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	Y2	29	Total	C	N	O	0	0
			157	96	32	29		

- Molecule 58 is a protein called Probable peptide chain release factor C12orf65, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	C	114	Total	C	N	O	S	1	0
			928	578	177	171	2		

- Molecule 59 is a protein called Mitochondrial transcription rescue factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	G	96	Total	C	N	O	S	0	0
			809	523	142	143	1		

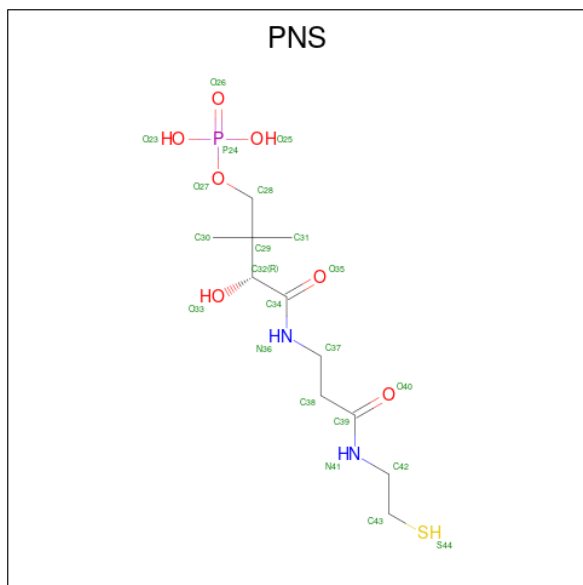
- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	D	1	Total	Mg	0
			1	1	
60	W	1	Total	Mg	0
			1	1	
60	g	1	Total	Mg	0
			1	1	
60	A	89	Total	Mg	0
			89	89	

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	0	1	Total	Zn	0
			1	1	
61	r	1	Total	Zn	0
			1	1	

- Molecule 62 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).

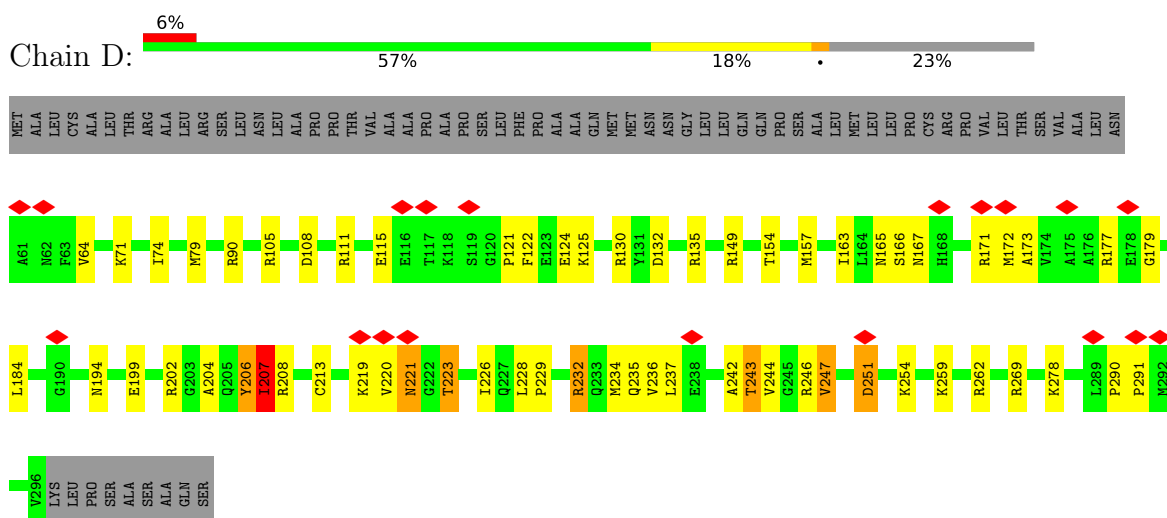


Mol	Chain	Residues	Atoms						AltConf
62	v	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

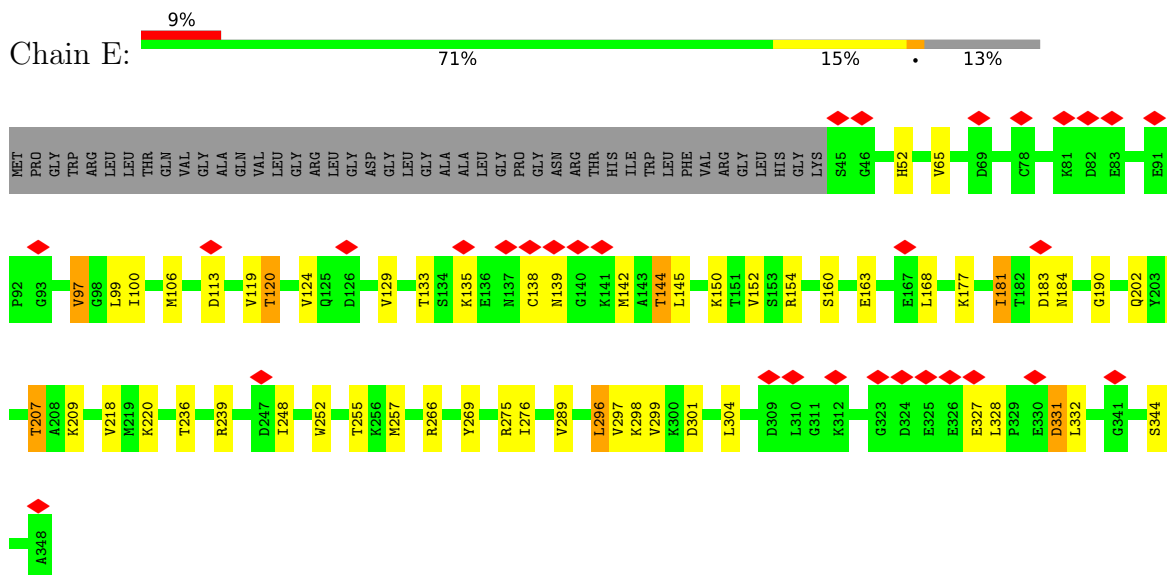
3 Residue-property plots

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.

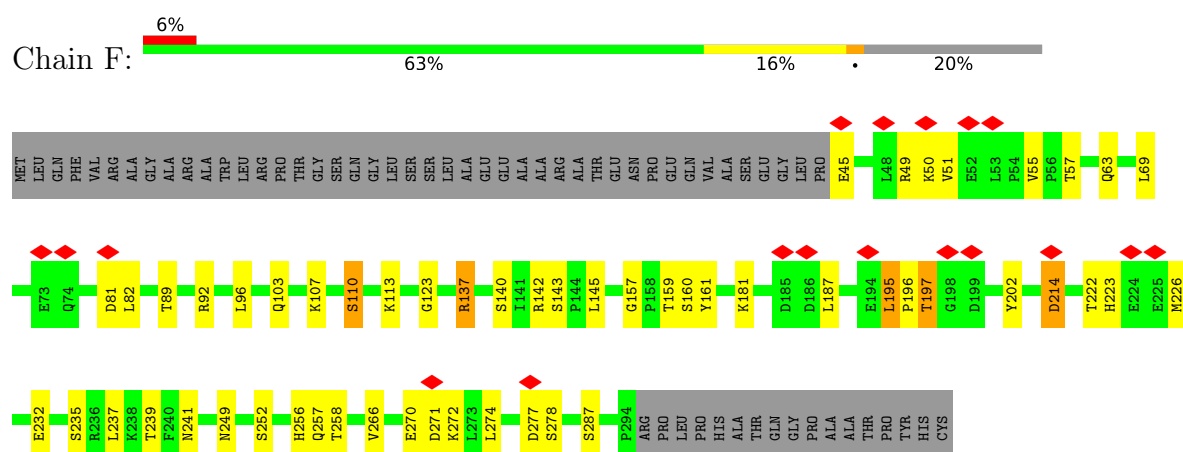
- Molecule 1: 39S ribosomal protein L2, mitochondrial



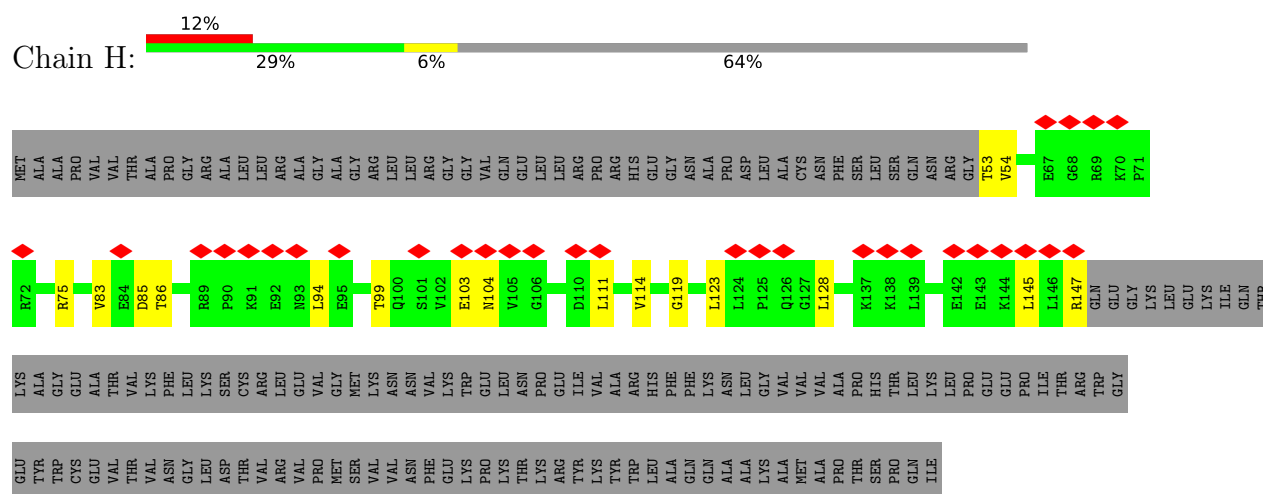
- Molecule 2: 39S ribosomal protein L3, mitochondrial



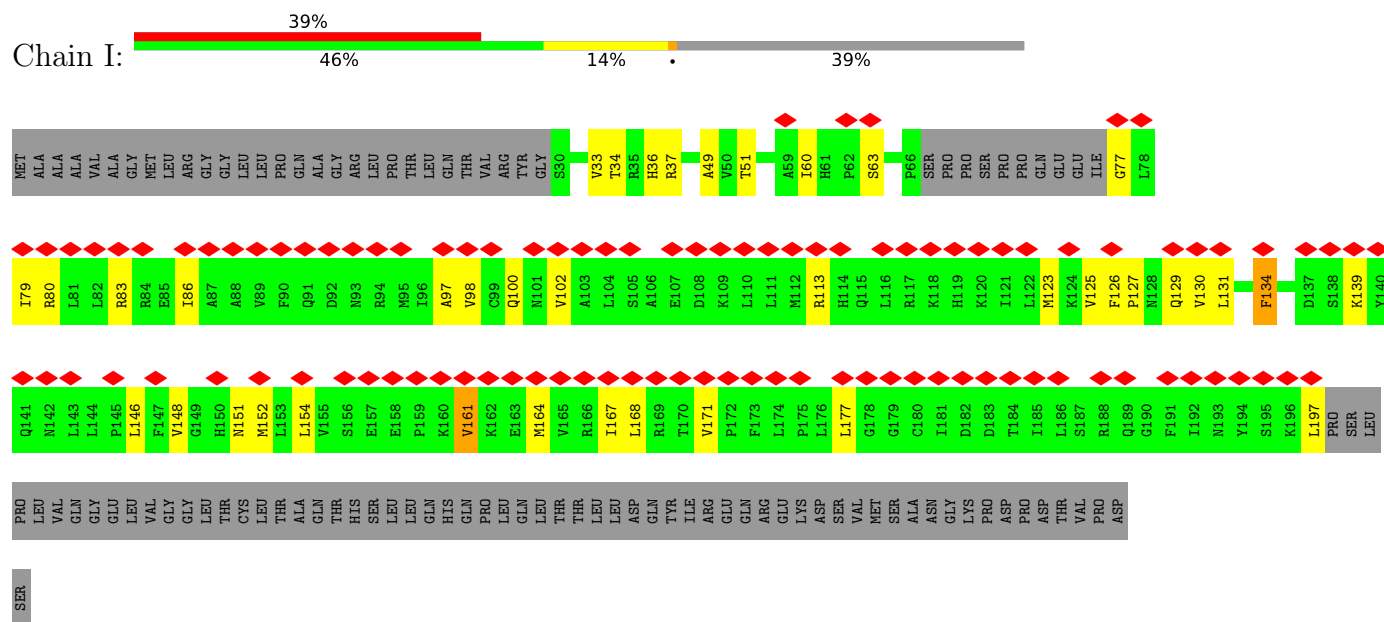
- Molecule 3: 39S ribosomal protein L4, mitochondrial



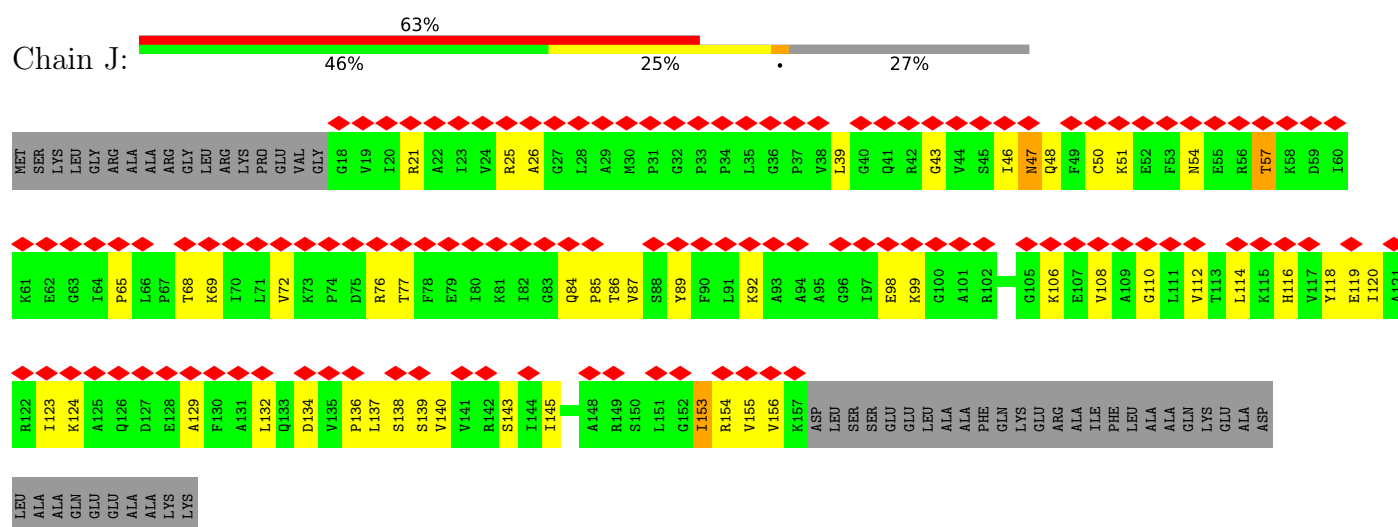
- Molecule 4: 39S ribosomal protein L9, mitochondrial



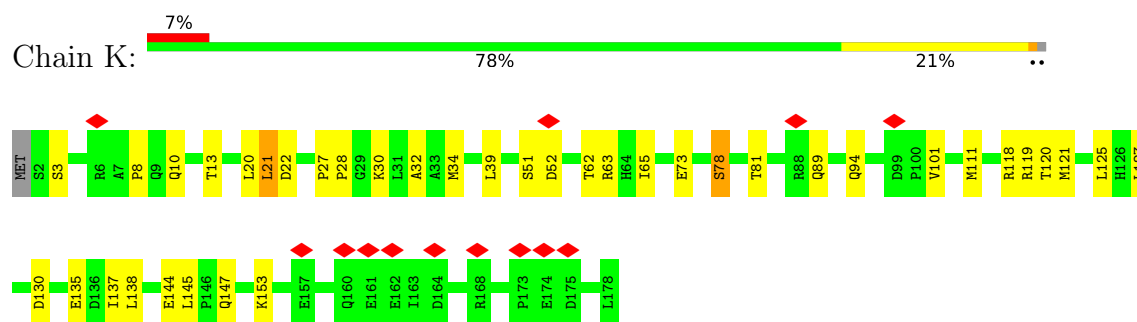
- Molecule 5: 39S ribosomal protein L10, mitochondrial



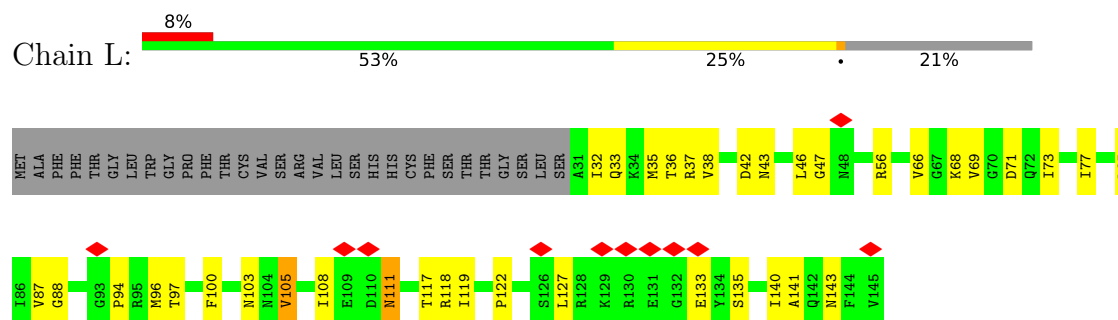
- Molecule 6: 39S ribosomal protein L11, mitochondrial



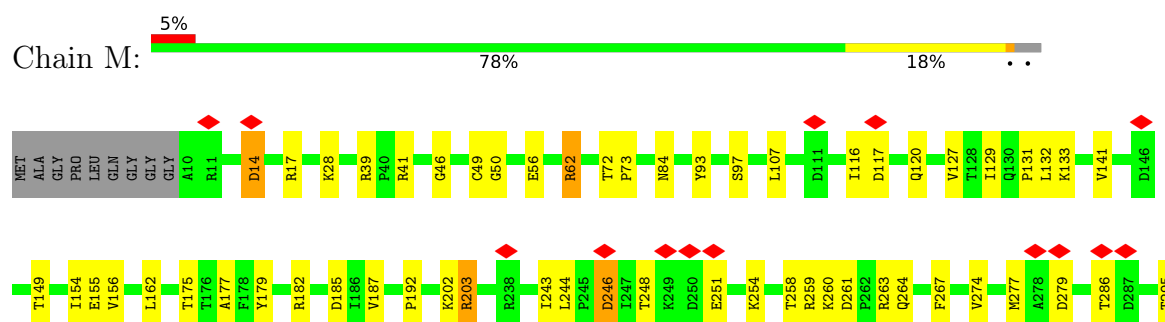
- Molecule 7: 39S ribosomal protein L13, mitochondrial



- Molecule 8: 39S ribosomal protein L14, mitochondrial



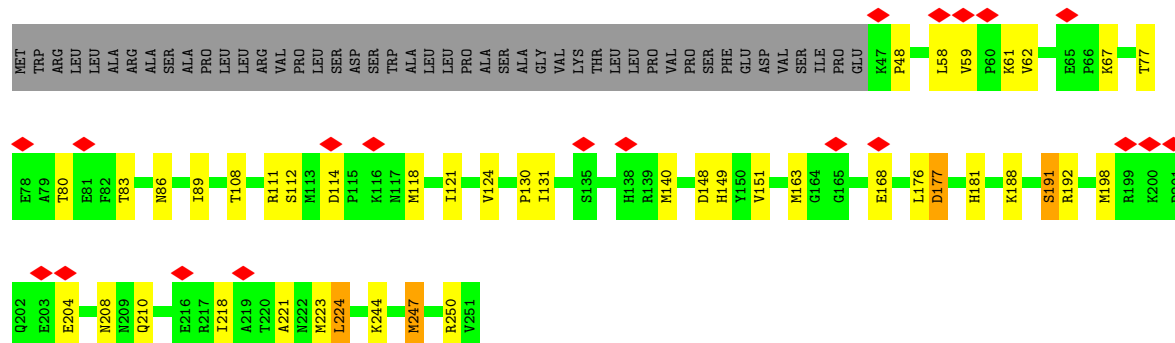
- Molecule 9: 39S ribosomal protein L15, mitochondrial





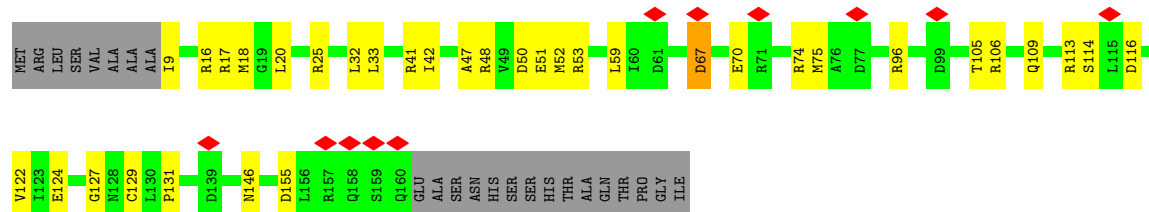
- Molecule 10: 39S ribosomal protein L16, mitochondrial

Chain N: 8% 65% 16% 18%



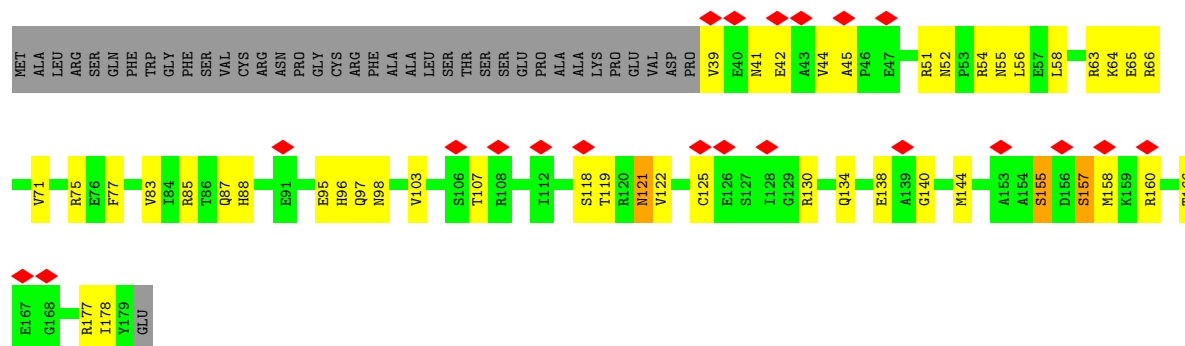
- Molecule 11: 39S ribosomal protein L17, mitochondrial

Chain O: 6% 67% 19% 13%



- Molecule 12: Mitochondrial ribosomal protein L18, isoform CRA_b

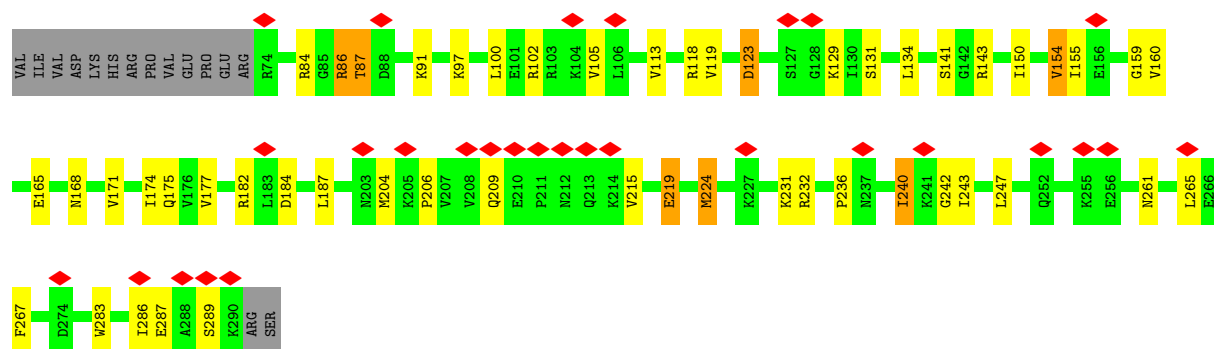
Chain P: 12% 54% 23% 21%



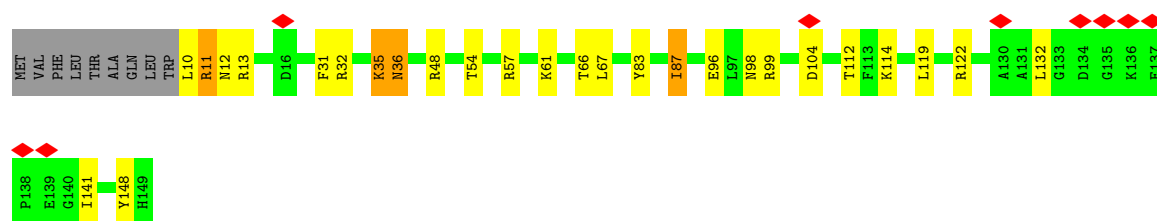
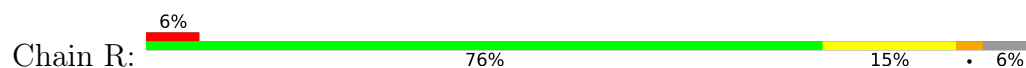
- Molecule 13: 39S ribosomal protein L19, mitochondrial

Chain Q: 10% 57% 15% 26%

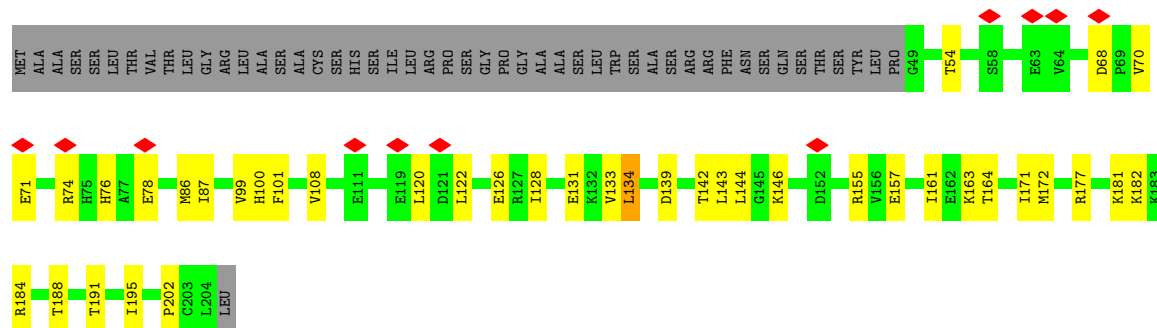




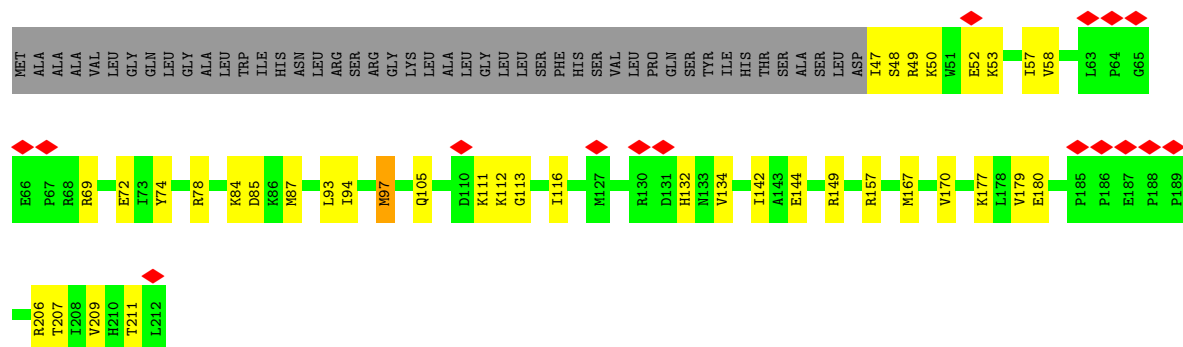
- Molecule 14: 39S ribosomal protein L20, mitochondrial



- Molecule 15: 39S ribosomal protein L21, mitochondrial

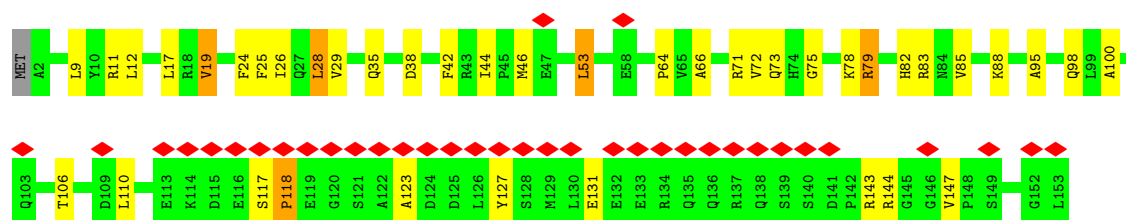


- Molecule 16: 39S ribosomal protein L22, mitochondrial



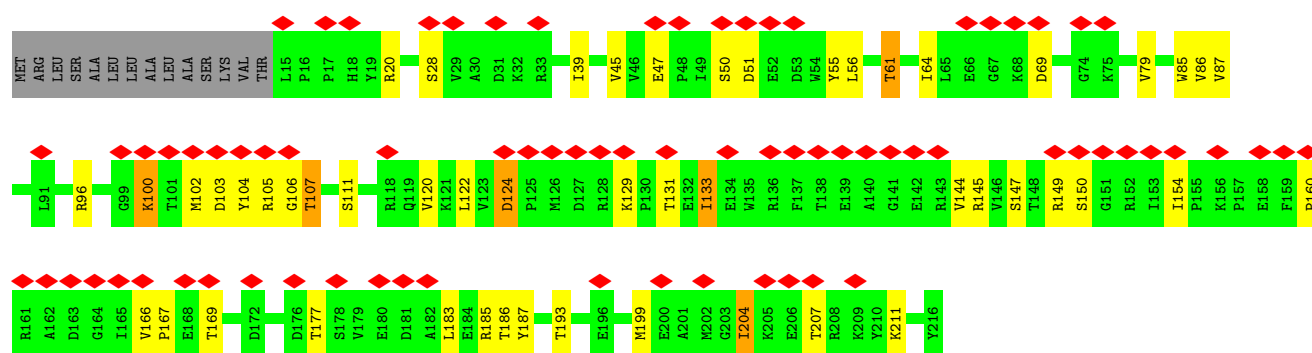
- Molecule 17: 39S ribosomal protein L23, mitochondrial

Chain U: 



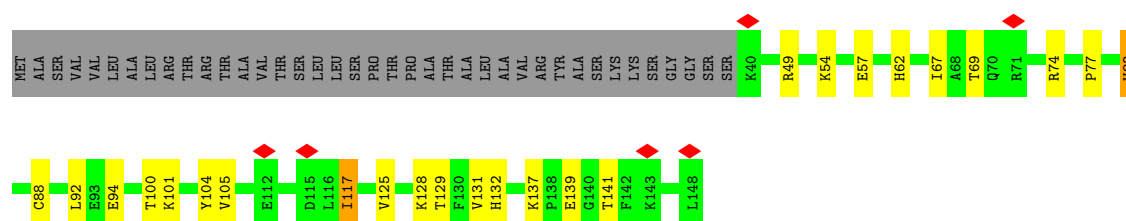
- Molecule 18: 39S ribosomal protein L24, mitochondrial

Chain V: 



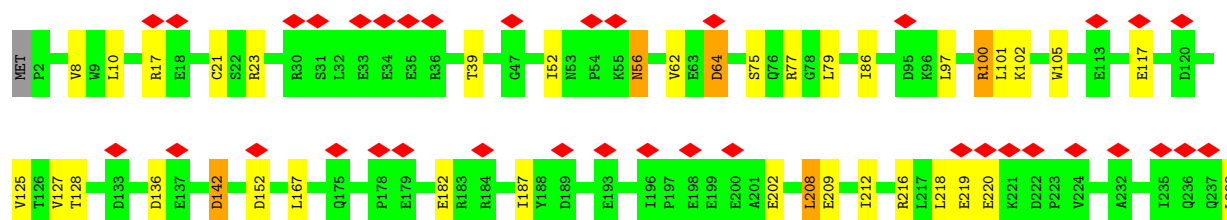
- Molecule 19: 39S ribosomal protein L27, mitochondrial

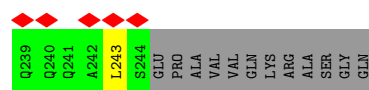
Chain W: 



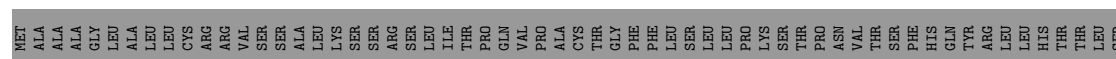
- Molecule 20: 39S ribosomal protein L28, mitochondrial

Chain X: 

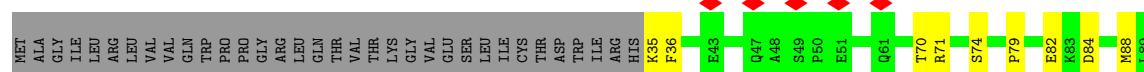




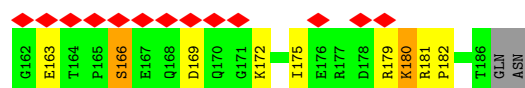
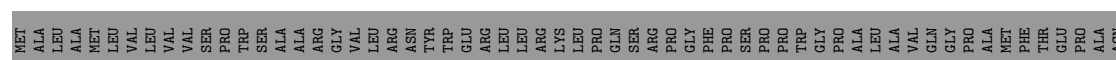
- Molecule 21: 39S ribosomal protein L47, mitochondrial



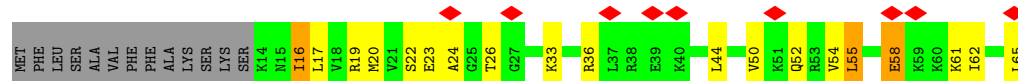
- Molecule 22: 39S ribosomal protein L30, mitochondrial

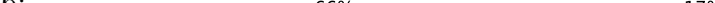


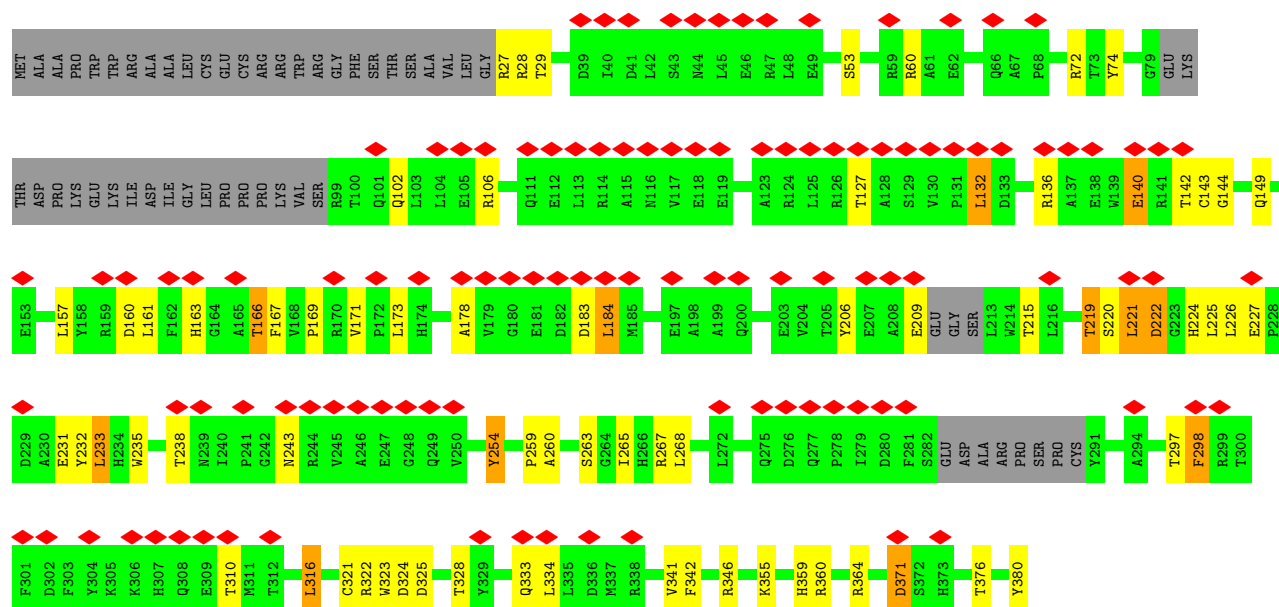
- Molecule 23: 39S ribosomal protein L32, mitochondrial



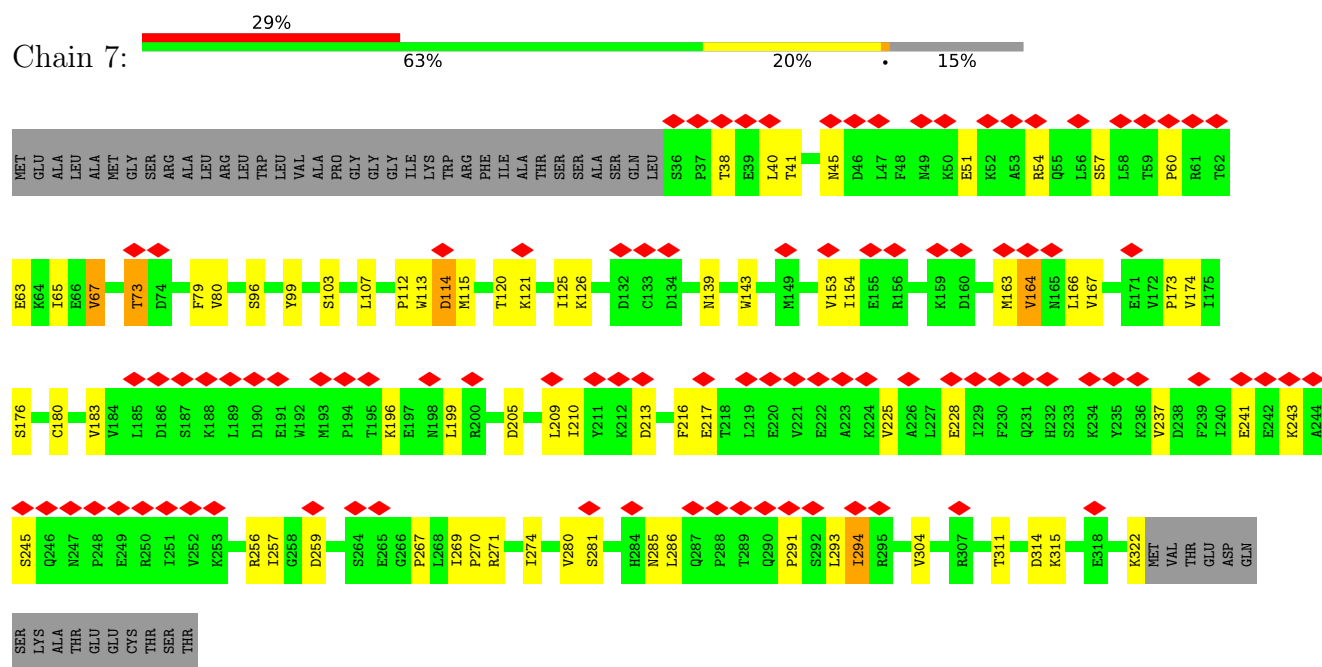
- Molecule 24: 39S ribosomal protein L33, mitochondrial



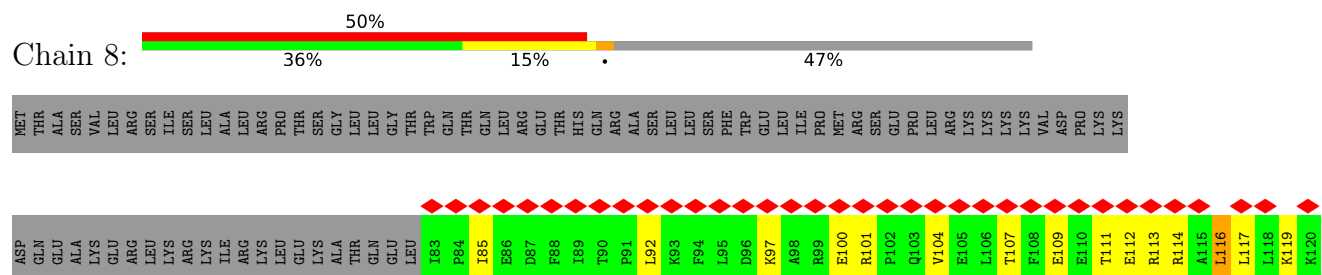
- Chain 6: 



• Molecule 29: 39S ribosomal protein L39, mitochondrial

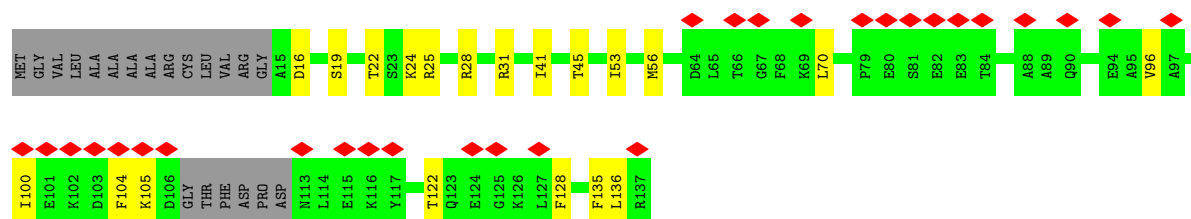


• Molecule 30: 39S ribosomal protein L40, mitochondrial

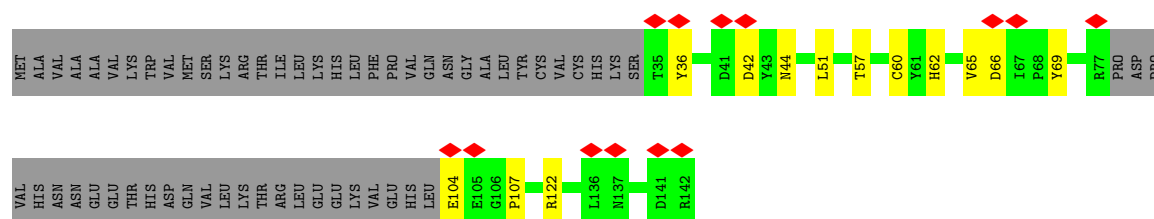




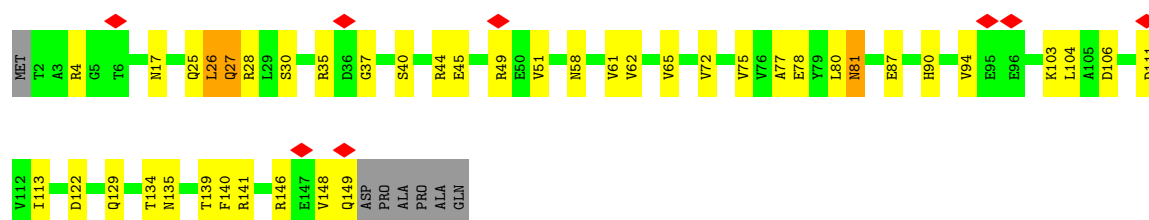
• Molecule 31: 39S ribosomal protein L41, mitochondrial



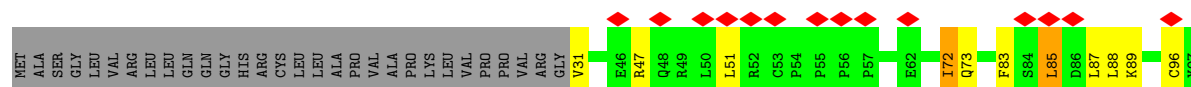
• Molecule 32: 39S ribosomal protein L42, mitochondrial

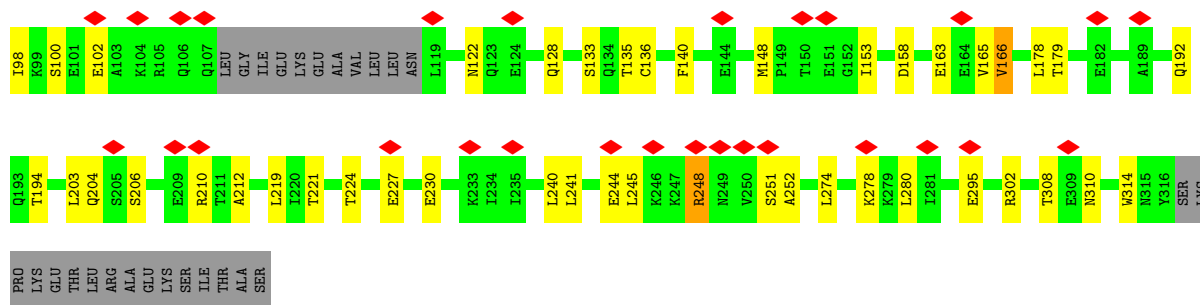


• Molecule 33: 39S ribosomal protein L43, mitochondrial

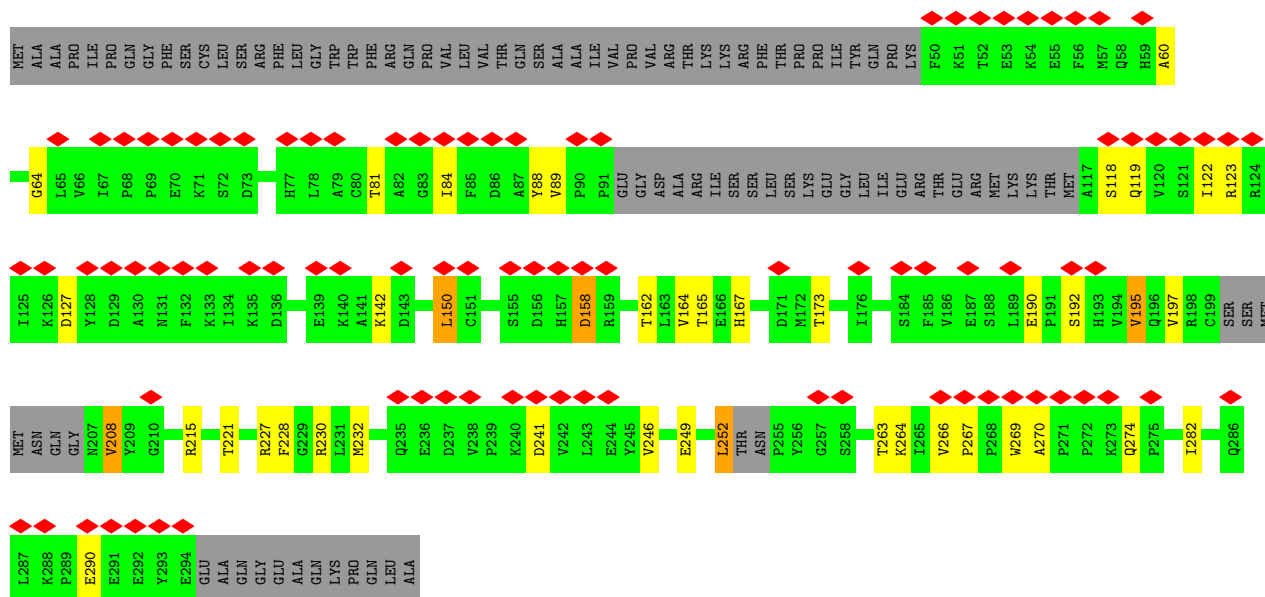


• Molecule 34: 39S ribosomal protein L44, mitochondrial

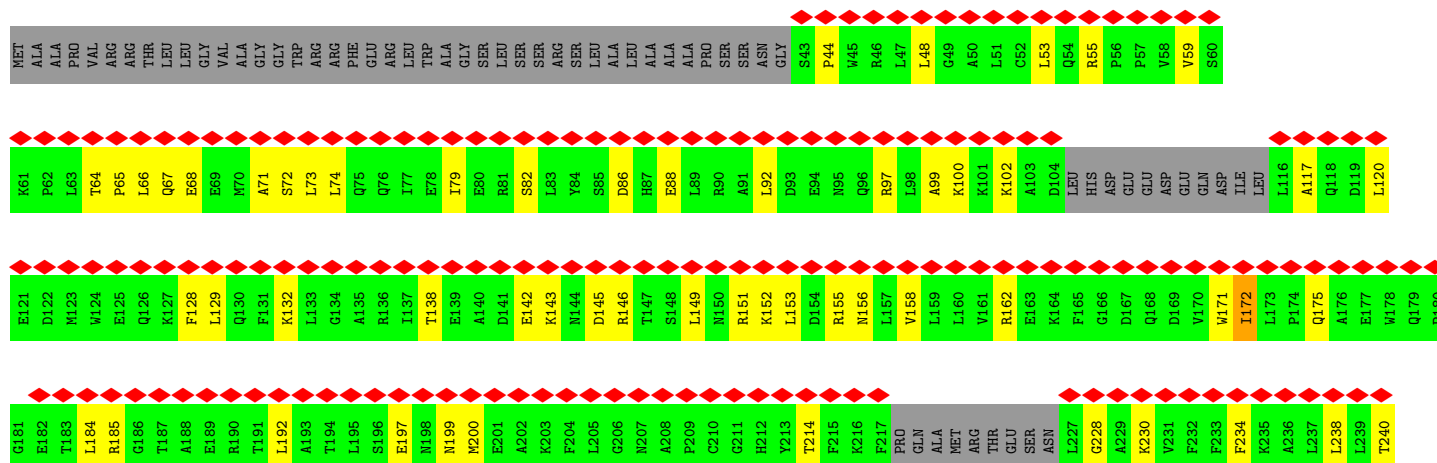
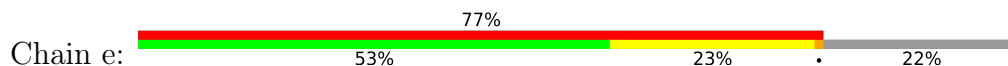




• Molecule 35: 39S ribosomal protein L45, mitochondrial



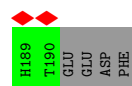
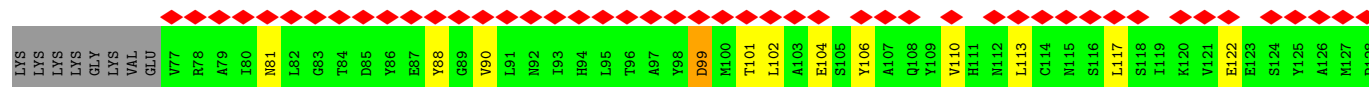
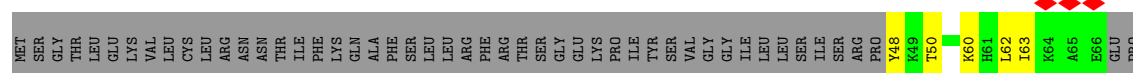
• Molecule 36: 39S ribosomal protein L46, mitochondrial





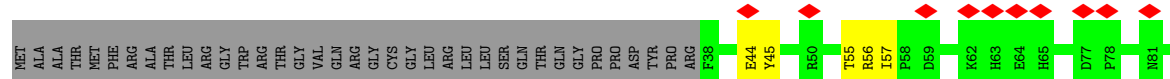
- Molecule 37: 39S ribosomal protein L48, mitochondrial

Chain f:



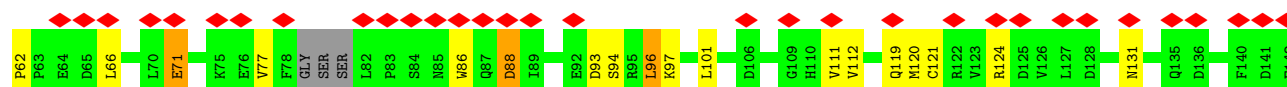
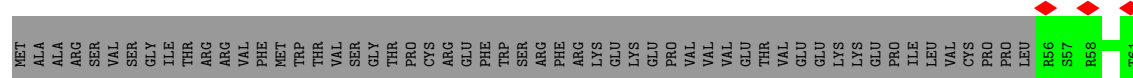
- Molecule 38: 39S ribosomal protein L49, mitochondrial

Chain g:



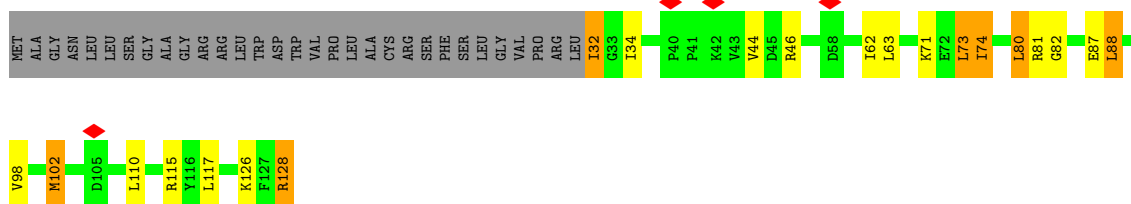
- Molecule 39: 39S ribosomal protein L50, mitochondrial

Chain h:



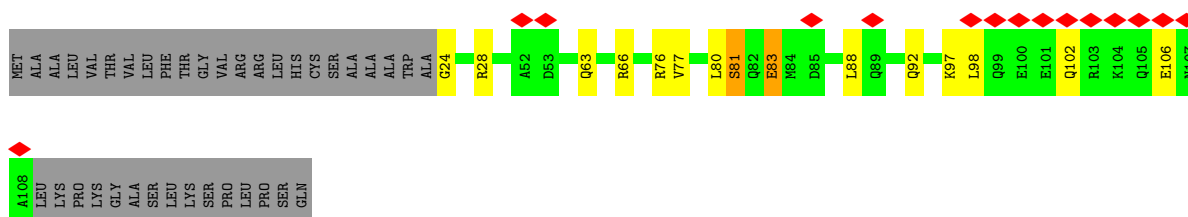
- Molecule 40: 39S ribosomal protein L51, mitochondrial

Chain i: 



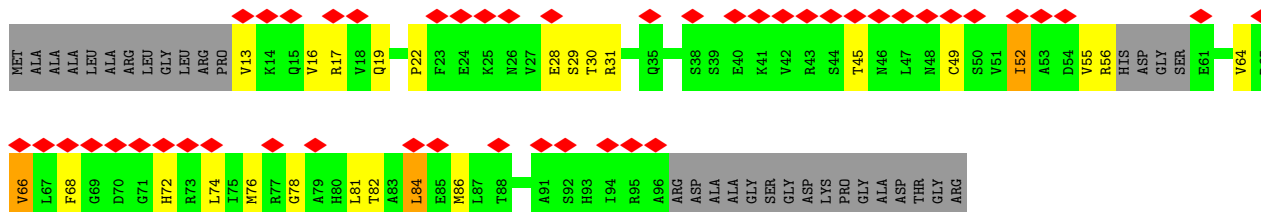
- Molecule 41: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA

Chain j: 



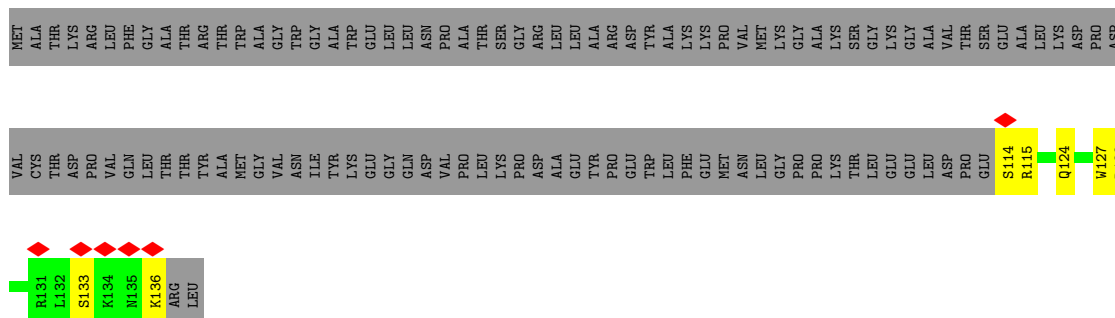
- Molecule 42: 39S ribosomal protein L53, mitochondrial

Chain k: 



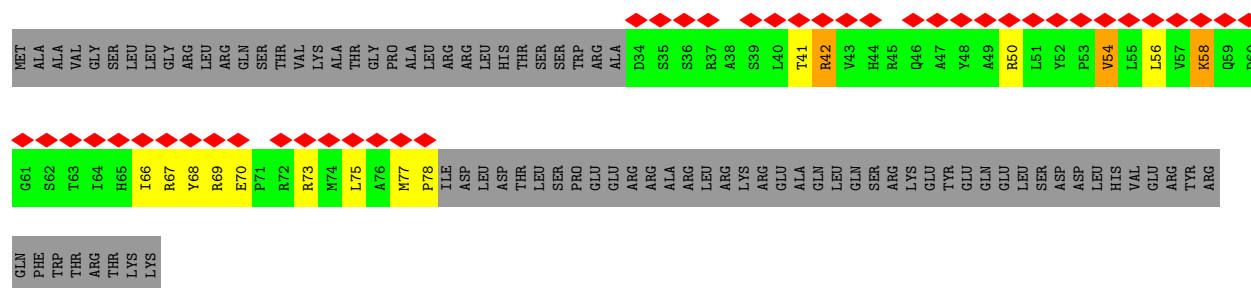
- Molecule 43: 39S ribosomal protein L54, mitochondrial

Chain l: 

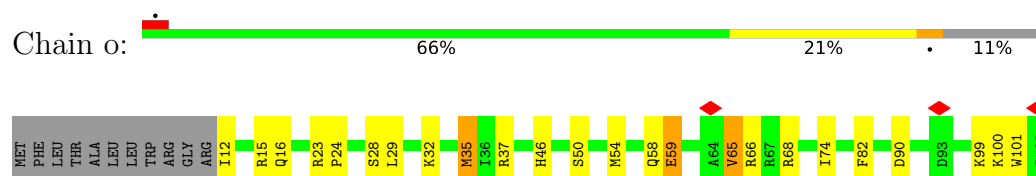


- Molecule 44: 39S ribosomal protein L55, mitochondrial

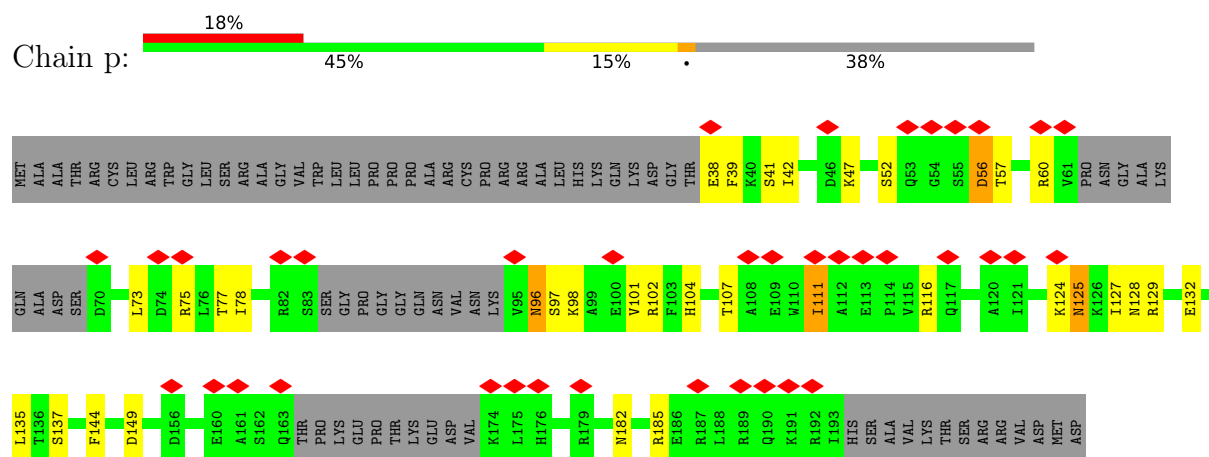
Chain m: 



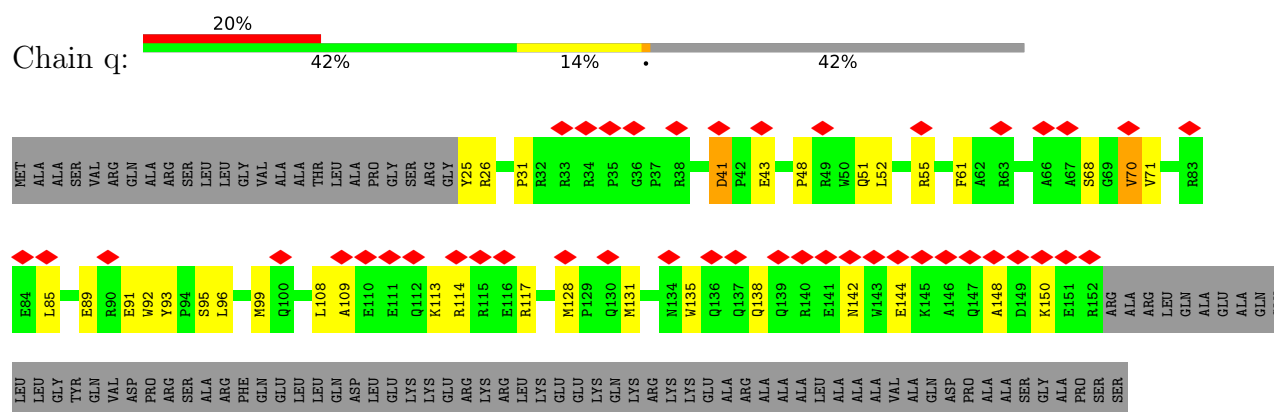
- Molecule 45: Ribosomal protein 63, mitochondrial



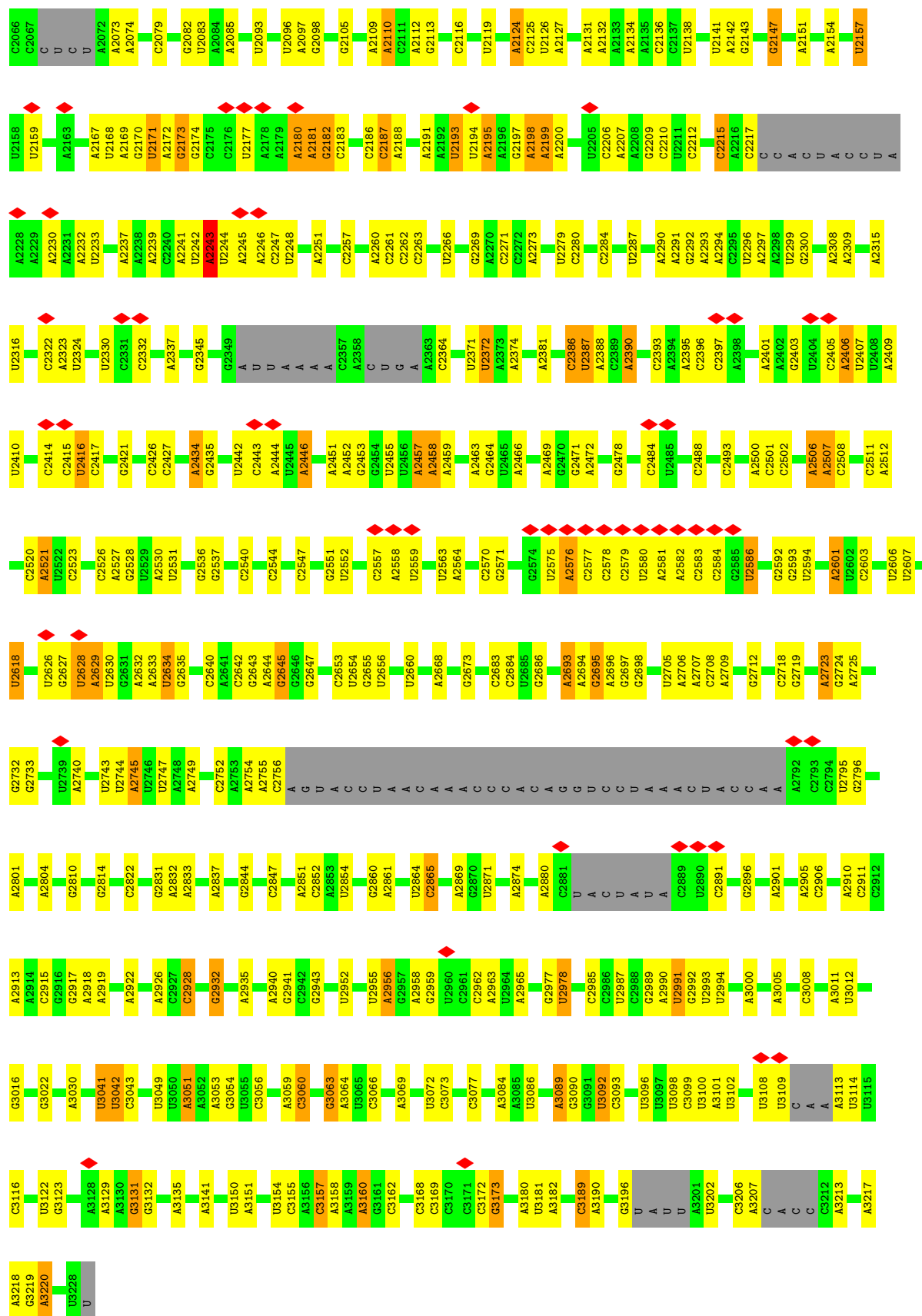
- Molecule 46: Peptidyl-tRNA hydrolase ICT1, mitochondrial



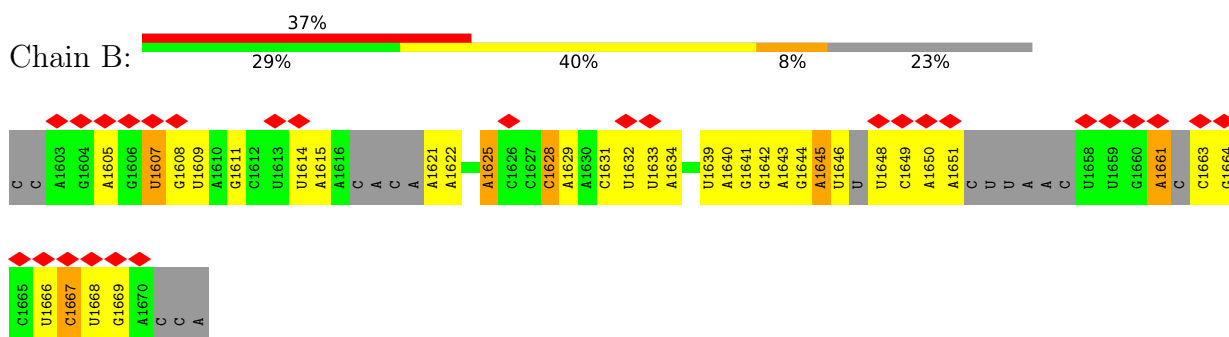
- Molecule 47: Growth arrest and DNA damage-inducible proteins-interacting protein 1



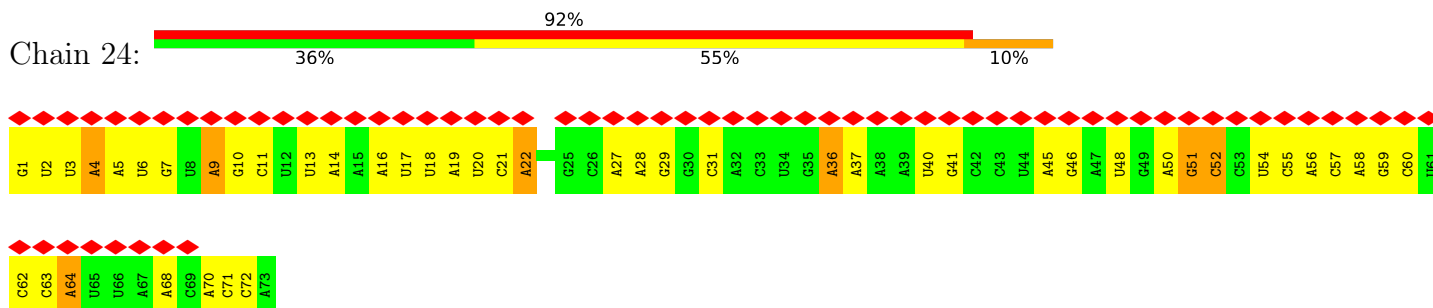
- Molecule 48: 39S ribosomal protein S18a, mitochondrial



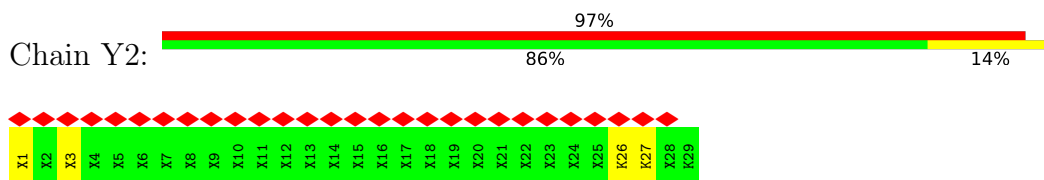
- Molecule 55: mt-tRNAVal



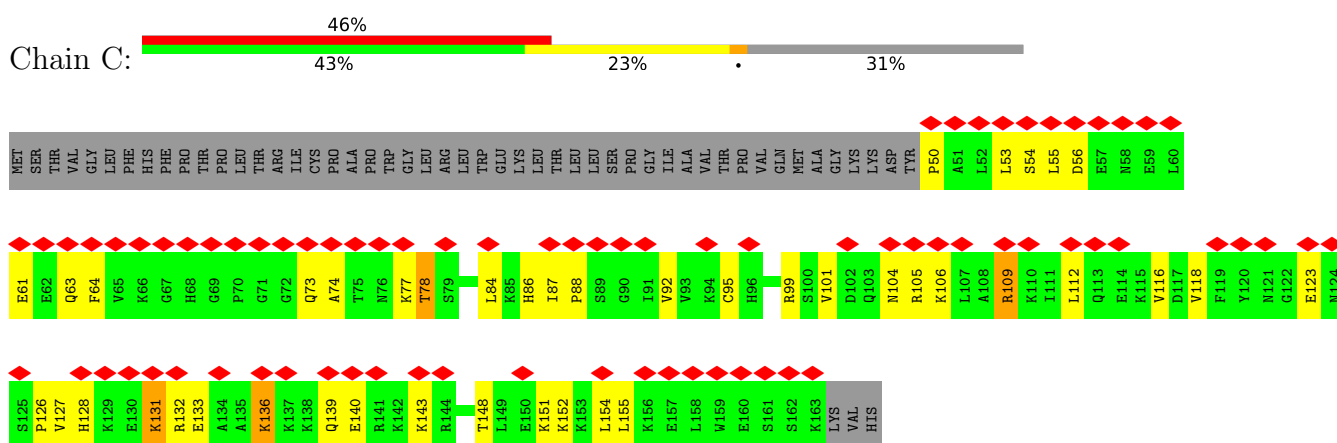
- Molecule 56: mt-tRNA



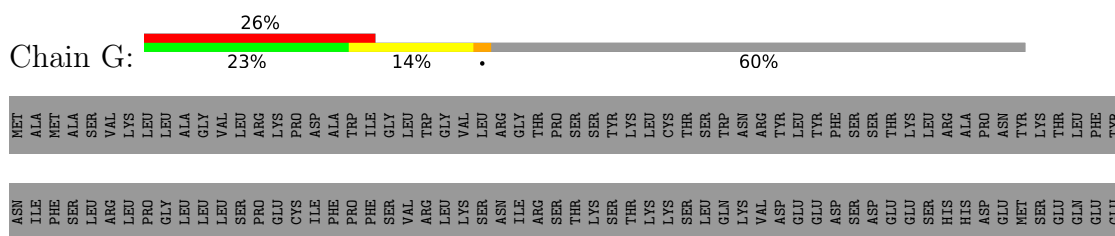
- Molecule 57: nascent chain

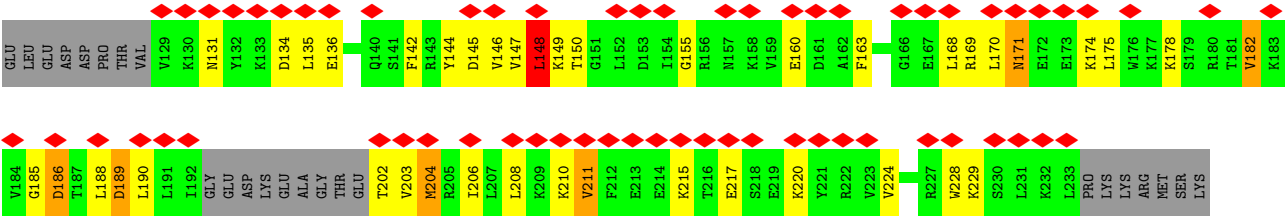


- Molecule 58: Probable peptide chain release factor C12orf65, mitochondrial



- Molecule 59: Mitochondrial transcription rescue factor 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48245	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	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	0.675	Depositor
Minimum map value	-0.378	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.11	Depositor
Map size ($\text{\AA}$)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PNS, ZN, MG, MEQ

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	D	0.66	0/1879	0.78	1/2527 (0.0%)
2	E	0.67	0/2465	0.71	0/3344
3	F	0.70	0/2071	0.68	0/2817
4	H	0.53	0/798	0.73	0/1073
5	I	0.44	0/1308	0.78	1/1761 (0.1%)
6	J	0.37	0/1077	0.81	2/1452 (0.1%)
7	K	0.70	0/1495	0.68	1/2029 (0.0%)
8	L	0.64	0/904	0.80	0/1218
9	M	0.68	0/2359	0.72	0/3185
10	N	0.63	0/1697	0.70	0/2281
11	O	0.66	0/1269	0.71	0/1708
12	P	0.55	0/1173	0.68	0/1588
13	Q	0.59	0/1846	0.73	2/2487 (0.1%)
14	R	0.73	0/1174	0.65	0/1572
15	S	0.70	0/1276	0.73	0/1729
16	T	0.68	1/1402 (0.1%)	0.69	0/1886
17	U	0.62	0/1247	0.84	1/1689 (0.1%)
18	V	0.50	0/1666	0.72	4/2260 (0.2%)
19	W	0.70	0/881	0.62	0/1188
20	X	0.57	0/2090	0.68	0/2825
21	Y	0.66	1/1552 (0.1%)	0.66	0/2079
22	Z	0.64	0/1003	0.69	0/1354
23	0	0.62	0/895	0.73	0/1201
24	1	0.61	0/438	0.71	0/583
25	2	0.82	0/373	0.76	0/496
26	3	0.76	0/852	0.71	0/1136
27	5	0.56	0/3250	0.71	0/4429
28	6	0.55	1/2726 (0.0%)	0.71	2/3715 (0.1%)
29	7	0.51	0/2391	0.70	0/3234
30	8	0.38	0/909	0.96	9/1227 (0.7%)
31	9	0.59	0/972	0.72	0/1306
32	a	0.55	0/709	0.65	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.65	0/1202	0.73	0/1626
34	c	0.55	0/2264	0.67	0/3059
35	d	0.45	0/1790	0.67	0/2423
36	e	0.37	0/1797	0.71	0/2422
37	f	0.43	0/931	0.68	0/1259
38	g	0.66	0/1102	0.75	0/1503
39	h	0.44	0/847	0.68	0/1150
40	i	0.77	0/849	0.73	0/1135
41	j	0.54	0/698	0.63	0/940
42	k	0.43	0/635	0.68	0/855
43	l	0.48	0/226	0.56	0/299
44	m	0.37	0/379	0.88	0/510
45	o	0.68	0/792	0.74	0/1064
46	p	0.44	0/1071	0.64	0/1433
47	q	0.45	0/1107	0.60	0/1498
48	r	0.63	0/1238	0.66	0/1676
49	s	0.62	0/3114	0.68	0/4225
51	u	0.48	0/949	0.69	0/1281
52	v	0.42	0/597	0.74	0/796
53	w	0.29	0/647	0.70	0/871
54	A	0.77	0/34613	0.60	6/53854 (0.0%)
55	B	0.36	0/1328	0.53	0/2056
56	24	0.33	0/1731	0.56	0/2693
57	Y2	0.51	0/25	0.83	0/27
58	C	0.45	0/929	0.90	1/1235 (0.1%)
59	G	0.50	0/818	1.18	4/1090 (0.4%)
All	All	0.64	3/107826 (0.0%)	0.68	34/153322 (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
1	D	0	1
15	S	0	1
18	V	0	1
27	5	0	2
30	8	0	3
48	r	0	2
49	s	0	1
57	Y2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
59	G	0	2
All	All	0	14

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	6	28	ARG	C-N	-11.02	1.18	1.33
16	T	58	VAL	C-N	-6.08	1.15	1.33
21	Y	195	ASN	CA-C	-5.75	1.44	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	102	VAL	N-CA-C	-9.60	103.98	113.20
59	G	145	ASP	N-CA-C	-8.59	104.83	114.62
59	G	189	ASP	CA-C-N	8.28	137.36	121.54
59	G	189	ASP	C-N-CA	8.28	137.36	121.54
17	U	118	PRO	N-CA-CB	8.10	111.75	103.25

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	5	216	GLU	Peptide
27	5	217	SER	Peptide
1	D	206	TYR	Peptide
15	S	101	PHE	Peptide
18	V	100	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1842	0	1896	34	0
2	E	2396	0	2402	28	0
3	F	2013	0	2044	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	784	0	832	5	0
5	I	1283	0	1369	26	0
6	J	1061	0	1141	24	0
7	K	1451	0	1448	20	0
8	L	889	0	941	19	0
9	M	2305	0	2378	30	0
10	N	1654	0	1681	22	0
11	O	1245	0	1283	19	0
12	P	1148	0	1148	30	0
13	Q	1805	0	1841	25	0
14	R	1153	0	1214	19	0
15	S	1251	0	1322	19	0
16	T	1368	0	1409	23	0
17	U	1218	0	1186	24	0
18	V	1624	0	1606	20	0
19	W	859	0	888	11	0
20	X	2035	0	2054	21	0
21	Y	1517	0	1561	16	0
22	Z	978	0	1030	16	0
23	0	880	0	902	16	0
24	1	433	0	475	12	0
25	2	367	0	393	3	0
26	3	831	0	883	16	0
27	5	3156	0	3138	45	0
28	6	2640	0	2464	41	0
29	7	2334	0	2343	26	0
30	8	890	0	864	18	0
31	9	947	0	949	11	0
32	a	686	0	658	7	0
33	b	1178	0	1180	21	0
34	c	2217	0	2220	25	0
35	d	1741	0	1727	23	0
36	e	1762	0	1767	36	0
37	f	915	0	917	13	0
38	g	1067	0	1056	12	0
39	h	827	0	806	11	0
40	i	827	0	857	14	0
41	j	684	0	673	10	0
42	k	627	0	636	14	0
43	l	221	0	227	4	0
44	m	372	0	387	10	0
45	o	771	0	775	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	p	1058	0	1083	16	0
47	q	1076	0	1049	16	0
48	r	1203	0	1220	17	0
49	s	3036	0	3022	43	0
50	t	140	0	30	0	0
51	u	927	0	921	21	0
52	v	588	0	604	19	0
53	w	638	0	636	13	0
54	A	30945	0	15722	152	0
55	B	1191	0	607	13	0
56	24	1547	0	787	11	0
57	Y2	157	0	80	2	0
58	C	928	0	974	23	0
59	G	809	0	869	17	0
60	A	89	0	0	0	0
60	D	1	0	0	0	0
60	W	1	0	0	0	0
60	g	1	0	0	0	0
61	0	1	0	0	0	0
61	r	1	0	0	0	0
62	v	21	0	21	4	0
All	All	102610	0	86596	1018	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1018 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:39:VAL:HG12	12:P:41:ASN:H	1.51	0.74
42:k:64:VAL:HB	42:k:76:MET:HB2	1.72	0.70
9:M:246:ASP:OD1	9:M:246:ASP:N	2.26	0.69
12:P:118:SER:OG	12:P:121:ASN:ND2	2.27	0.68
6:J:89:TYR:HA	6:J:92:LYS:HE2	1.76	0.67

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	234/305 (77%)	219 (94%)	14 (6%)	1 (0%)	30	60
2	E	302/348 (87%)	284 (94%)	18 (6%)	0	100	100
3	F	248/311 (80%)	240 (97%)	8 (3%)	0	100	100
4	H	93/267 (35%)	86 (92%)	7 (8%)	0	100	100
5	I	154/261 (59%)	135 (88%)	19 (12%)	0	100	100
6	J	138/192 (72%)	127 (92%)	11 (8%)	0	100	100
7	K	175/178 (98%)	165 (94%)	10 (6%)	0	100	100
8	L	113/145 (78%)	102 (90%)	11 (10%)	0	100	100
9	M	285/296 (96%)	267 (94%)	18 (6%)	0	100	100
10	N	203/251 (81%)	193 (95%)	9 (4%)	1 (0%)	24	55
11	O	150/175 (86%)	144 (96%)	6 (4%)	0	100	100
12	P	139/179 (78%)	129 (93%)	10 (7%)	0	100	100
13	Q	215/292 (74%)	202 (94%)	13 (6%)	0	100	100
14	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
15	S	154/205 (75%)	148 (96%)	6 (4%)	0	100	100
16	T	164/212 (77%)	156 (95%)	8 (5%)	0	100	100
17	U	148/153 (97%)	132 (89%)	14 (10%)	2 (1%)	9	33
18	V	200/216 (93%)	187 (94%)	13 (6%)	0	100	100
19	W	107/148 (72%)	104 (97%)	3 (3%)	0	100	100
20	X	241/256 (94%)	231 (96%)	10 (4%)	0	100	100
21	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
22	Z	118/161 (73%)	113 (96%)	5 (4%)	0	100	100
23	0	106/188 (56%)	104 (98%)	2 (2%)	0	100	100
24	1	50/65 (77%)	48 (96%)	2 (4%)	0	100	100
25	2	43/92 (47%)	42 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	3	93/188 (50%)	88 (95%)	5 (5%)	0	100	100
27	5	383/423 (90%)	361 (94%)	22 (6%)	0	100	100
28	6	316/380 (83%)	293 (93%)	23 (7%)	0	100	100
29	7	285/338 (84%)	267 (94%)	17 (6%)	1 (0%)	30	60
30	8	108/206 (52%)	86 (80%)	19 (18%)	3 (3%)	4	21
31	9	113/137 (82%)	106 (94%)	7 (6%)	0	100	100
32	a	78/142 (55%)	74 (95%)	4 (5%)	0	100	100
33	b	146/155 (94%)	133 (91%)	13 (9%)	0	100	100
34	c	271/332 (82%)	263 (97%)	8 (3%)	0	100	100
35	d	203/306 (66%)	189 (93%)	14 (7%)	0	100	100
36	e	211/279 (76%)	189 (90%)	22 (10%)	0	100	100
37	f	110/194 (57%)	95 (86%)	15 (14%)	0	100	100
38	g	127/166 (76%)	119 (94%)	8 (6%)	0	100	100
39	h	96/158 (61%)	92 (96%)	4 (4%)	0	100	100
40	i	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
41	j	83/123 (68%)	79 (95%)	4 (5%)	0	100	100
42	k	76/112 (68%)	68 (90%)	8 (10%)	0	100	100
43	l	21/138 (15%)	19 (90%)	2 (10%)	0	100	100
44	m	43/128 (34%)	34 (79%)	9 (21%)	0	100	100
45	o	89/102 (87%)	86 (97%)	3 (3%)	0	100	100
46	p	119/206 (58%)	115 (97%)	4 (3%)	0	100	100
47	q	126/222 (57%)	121 (96%)	5 (4%)	0	100	100
48	r	140/196 (71%)	133 (95%)	7 (5%)	0	100	100
49	s	366/439 (83%)	347 (95%)	19 (5%)	0	100	100
51	u	109/234 (47%)	99 (91%)	10 (9%)	0	100	100
52	v	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
53	w	77/156 (49%)	66 (86%)	11 (14%)	0	100	100
57	Y2	2/29 (7%)	0	2 (100%)	0	100	100
58	C	112/166 (68%)	96 (86%)	15 (13%)	1 (1%)	14	43
59	G	92/240 (38%)	60 (65%)	28 (30%)	4 (4%)	2	14
All	All	8249/11388 (72%)	7695 (93%)	541 (7%)	13 (0%)	44	71

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	207	ILE
17	U	118	PRO
30	8	186	GLN
30	8	187	PRO
30	8	188	PRO

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	D	190/245 (78%)	172 (90%)	18 (10%)	8	29
2	E	259/290 (89%)	235 (91%)	24 (9%)	8	30
3	F	217/262 (83%)	193 (89%)	24 (11%)	6	22
4	H	86/228 (38%)	77 (90%)	9 (10%)	6	25
5	I	145/232 (62%)	135 (93%)	10 (7%)	14	41
6	J	113/150 (75%)	98 (87%)	15 (13%)	4	17
7	K	155/156 (99%)	145 (94%)	10 (6%)	15	43
8	L	98/124 (79%)	86 (88%)	12 (12%)	5	19
9	M	245/249 (98%)	223 (91%)	22 (9%)	9	31
10	N	172/211 (82%)	156 (91%)	16 (9%)	8	30
11	O	133/150 (89%)	123 (92%)	10 (8%)	12	38
12	P	123/154 (80%)	110 (89%)	13 (11%)	6	24
13	Q	199/256 (78%)	177 (89%)	22 (11%)	6	22
14	R	118/126 (94%)	108 (92%)	10 (8%)	10	33
15	S	141/180 (78%)	124 (88%)	17 (12%)	5	20
16	T	146/182 (80%)	138 (94%)	8 (6%)	19	48
17	U	124/135 (92%)	114 (92%)	10 (8%)	11	36
18	V	172/191 (90%)	144 (84%)	28 (16%)	2	11
19	W	89/119 (75%)	78 (88%)	11 (12%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	X	219/229 (96%)	199 (91%)	20 (9%)	9	31
21	Y	159/223 (71%)	145 (91%)	14 (9%)	9	32
22	Z	111/147 (76%)	103 (93%)	8 (7%)	13	40
23	0	97/164 (59%)	85 (88%)	12 (12%)	4	19
24	1	49/60 (82%)	43 (88%)	6 (12%)	5	19
25	2	39/72 (54%)	36 (92%)	3 (8%)	12	37
26	3	88/166 (53%)	78 (89%)	10 (11%)	5	21
27	5	348/368 (95%)	308 (88%)	40 (12%)	5	21
28	6	265/332 (80%)	231 (87%)	34 (13%)	4	18
29	7	263/303 (87%)	231 (88%)	32 (12%)	5	19
30	8	91/190 (48%)	81 (89%)	10 (11%)	6	23
31	9	99/112 (88%)	94 (95%)	5 (5%)	21	50
32	a	78/133 (59%)	72 (92%)	6 (8%)	12	37
33	b	130/135 (96%)	113 (87%)	17 (13%)	4	17
34	c	241/288 (84%)	220 (91%)	21 (9%)	9	32
35	d	193/274 (70%)	175 (91%)	18 (9%)	8	30
36	e	188/236 (80%)	174 (93%)	14 (7%)	13	38
37	f	101/173 (58%)	88 (87%)	13 (13%)	4	17
38	g	119/148 (80%)	109 (92%)	10 (8%)	10	34
39	h	95/148 (64%)	83 (87%)	12 (13%)	4	18
40	i	86/110 (78%)	73 (85%)	13 (15%)	3	13
41	j	68/97 (70%)	64 (94%)	4 (6%)	18	46
42	k	71/90 (79%)	63 (89%)	8 (11%)	5	21
43	l	23/116 (20%)	22 (96%)	1 (4%)	26	54
44	m	40/113 (35%)	36 (90%)	4 (10%)	7	27
45	o	78/87 (90%)	68 (87%)	10 (13%)	4	18
46	p	117/181 (65%)	105 (90%)	12 (10%)	7	25
47	q	110/178 (62%)	97 (88%)	13 (12%)	5	20
48	r	133/169 (79%)	120 (90%)	13 (10%)	7	28
49	s	326/381 (86%)	291 (89%)	35 (11%)	6	24
51	u	105/200 (52%)	92 (88%)	13 (12%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	v	59/60 (98%)	51 (86%)	8 (14%)	3	16
53	w	73/136 (54%)	63 (86%)	10 (14%)	3	16
57	Y2	3/3 (100%)	2 (67%)	1 (33%)	0	1
58	C	102/146 (70%)	90 (88%)	12 (12%)	5	20
59	G	90/221 (41%)	76 (84%)	14 (16%)	2	12
All	All	7382/9829 (75%)	6617 (90%)	765 (10%)	9	25

5 of 765 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	7	281	SER
38	g	55	THR
30	8	137	ARG
29	7	280	VAL
34	c	206	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 136 such sidechains are listed below:

Mol	Chain	Res	Type
48	r	62	ASN
49	s	107	GLN
58	C	97	GLN
19	W	51	GLN
18	V	92	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	A	1443/1559 (92%)	421 (29%)	22 (1%)
55	B	51/73 (69%)	23 (45%)	1 (1%)
56	24	73/73 (100%)	37 (50%)	1 (1%)
All	All	1567/1705 (91%)	481 (30%)	24 (1%)

5 of 481 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
54	A	1674	A
54	A	1676	A

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Mol	Chain	Res	Type
54	A	1677	C
54	A	1678	C
54	A	1679	U

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	A	2606	U
54	A	2910	A
54	A	2905	A
54	A	2989	G
54	A	2125	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	MEQ	C	73	58	8,9,10	0.98	1 (12%)	5,10,12	0.72	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
58	MEQ	C	73	58	-	4/8/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	C	73	MEQ	CE-NE2	-2.03	1.42	1.45

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	C	73	MEQ	C-CA-CB-CG
58	C	73	MEQ	CG-CD-NE2-CE
58	C	73	MEQ	OE1-CD-NE2-CE
58	C	73	MEQ	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 95 ligands modelled in this entry, 94 are monoatomic - leaving 1 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
62	PNS	v	101	53	14,20,21	2.22	4 (28%)	18,26,29	1.87	5 (27%)

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
62	PNS	v	101	53	-	9/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	v	101	PNS	C39-N41	5.17	1.45	1.33
62	v	101	PNS	C34-N36	5.00	1.45	1.33
62	v	101	PNS	O40-C39	-2.86	1.17	1.23
62	v	101	PNS	O35-C34	-2.24	1.19	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	v	101	PNS	C37-N36-C34	-4.01	115.34	122.55
62	v	101	PNS	C31-C29-C32	3.34	114.47	108.77
62	v	101	PNS	C38-C39-N41	3.34	122.42	116.34
62	v	101	PNS	C32-C34-N36	2.47	121.16	116.48
62	v	101	PNS	O40-C39-C38	-2.10	118.21	122.02

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

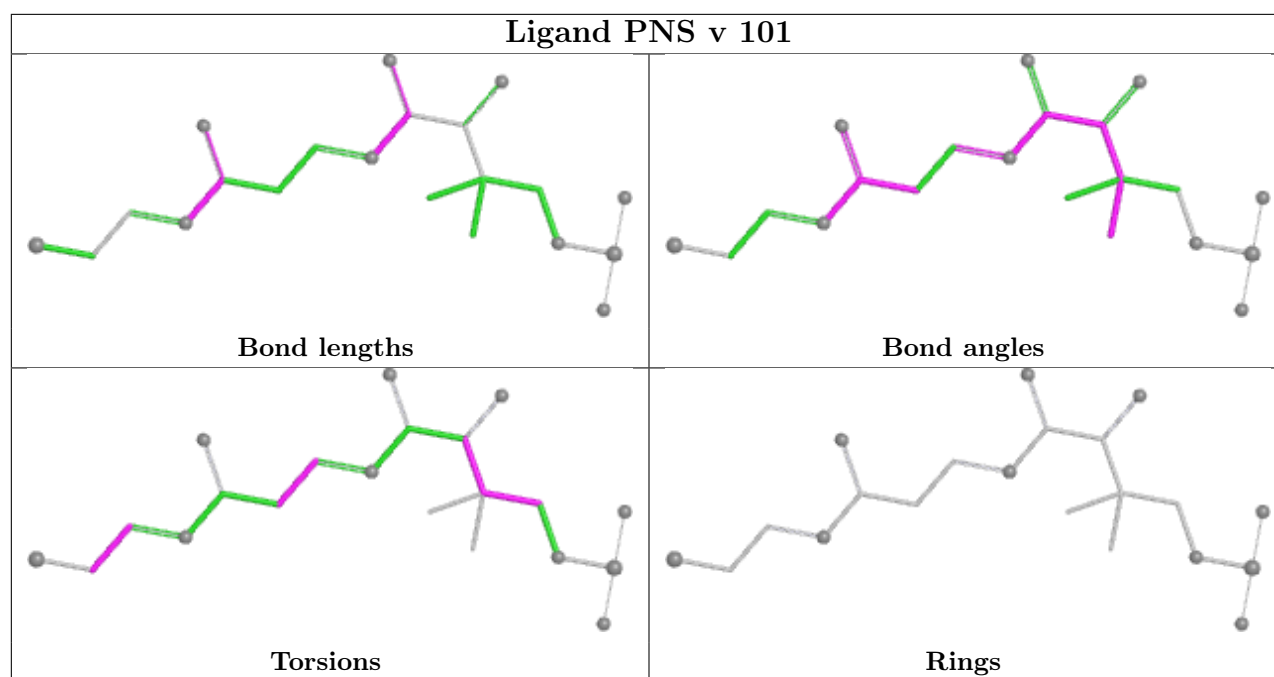
Mol	Chain	Res	Type	Atoms
62	v	101	PNS	C28-C29-C32-O33
62	v	101	PNS	C28-C29-C32-C34
62	v	101	PNS	C30-C29-C32-O33
62	v	101	PNS	C30-C29-C32-C34
62	v	101	PNS	C31-C29-C32-O33

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	v	101	PNS	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	U	1
28	6	1
16	T	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	124:ASP	C	125:ASP	N	3.71
1	6	28:ARG	C	29:THR	N	1.18
1	T	58:VAL	C	59:TYR	N	1.14

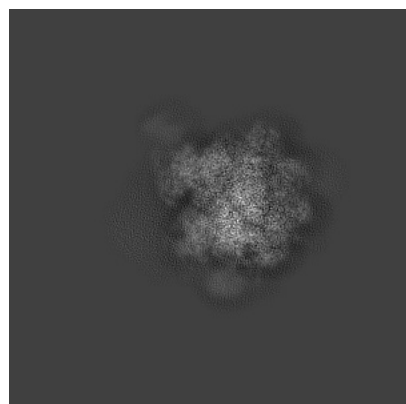
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11643. These allow visual inspection of the internal detail of the map and identification of artifacts.

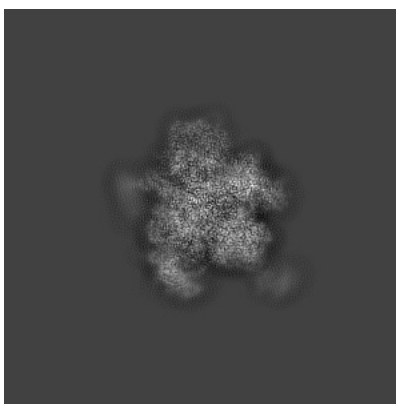
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

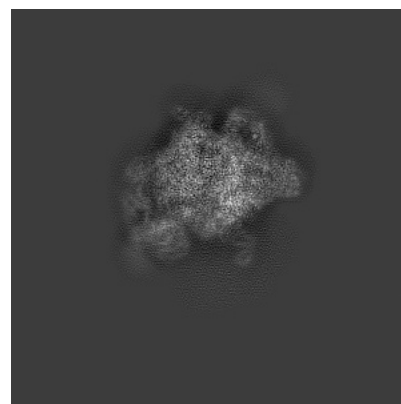
6.1.1 Primary map



X

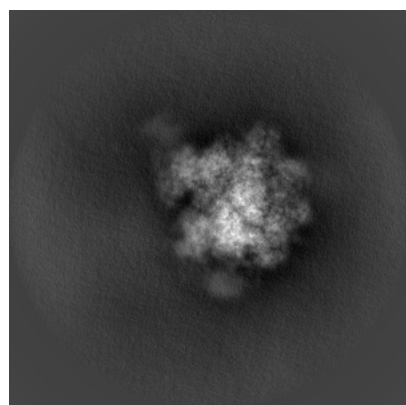


Y

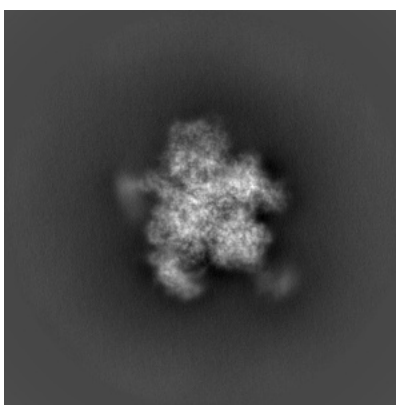


Z

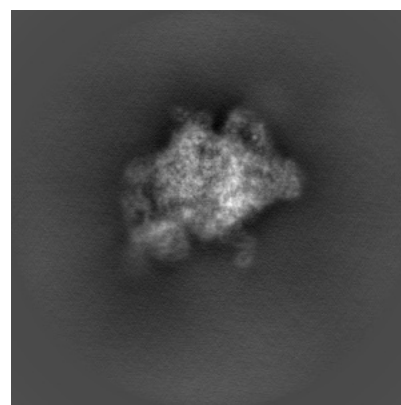
6.1.2 Raw map



X



Y

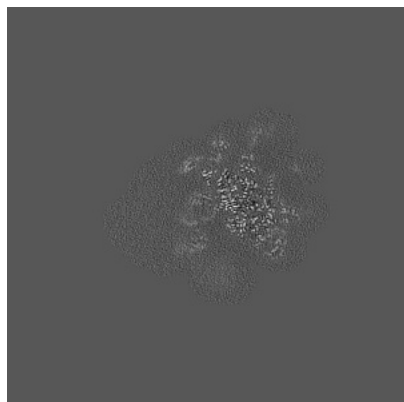


Z

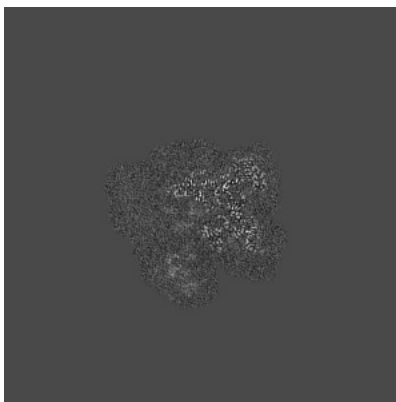
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

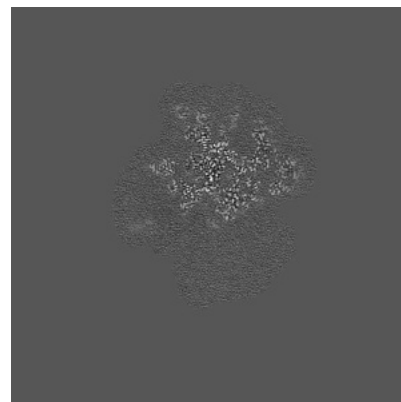
6.2.1 Primary map



X Index: 256

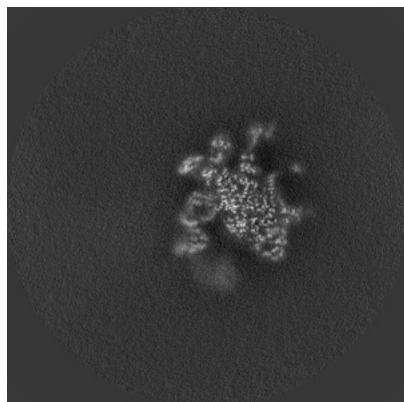


Y Index: 256

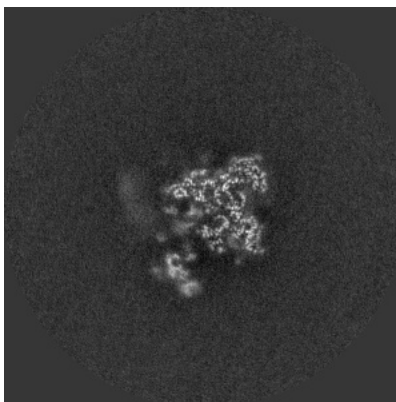


Z Index: 256

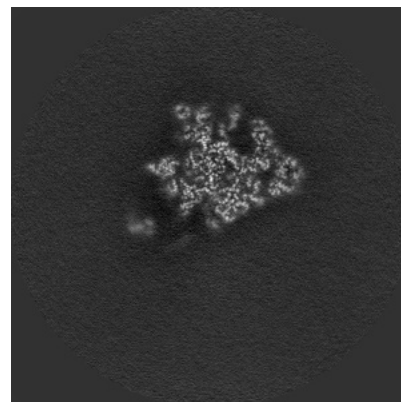
6.2.2 Raw map



X Index: 256



Y Index: 256

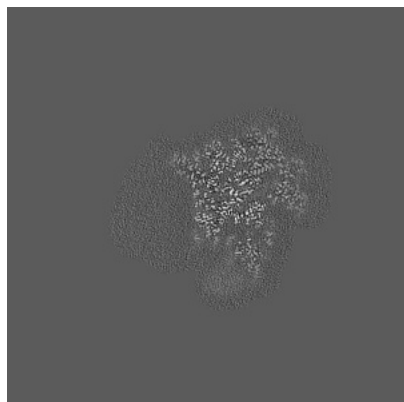


Z Index: 256

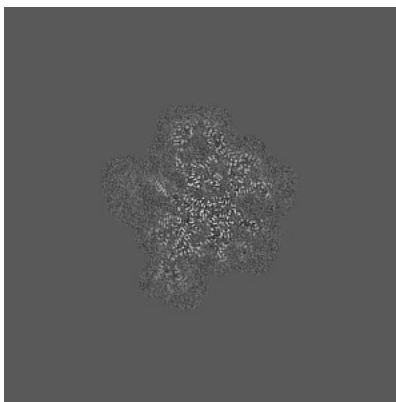
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

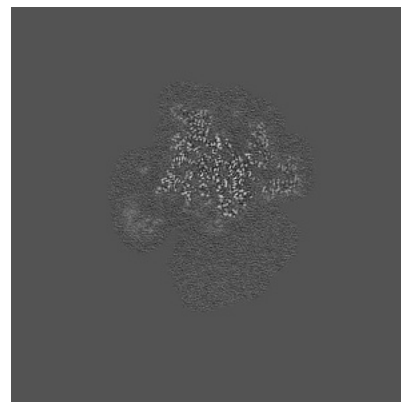
6.3.1 Primary map



X Index: 284

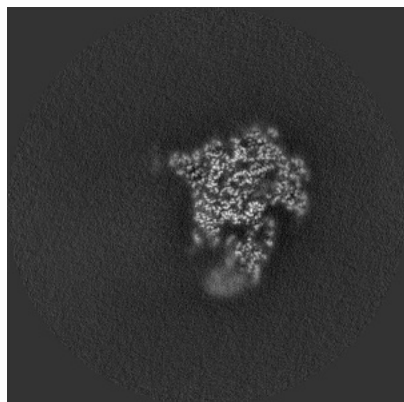


Y Index: 293

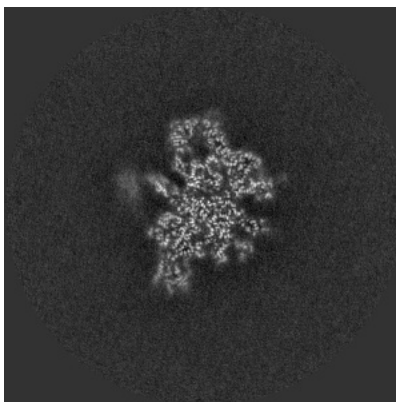


Z Index: 246

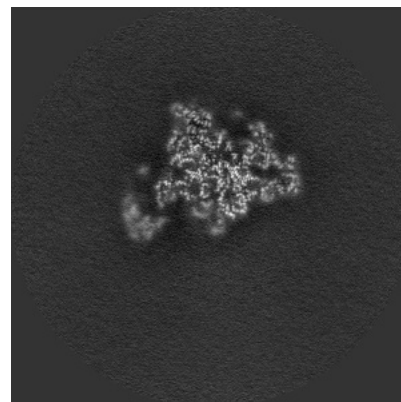
6.3.2 Raw map



X Index: 285



Y Index: 293

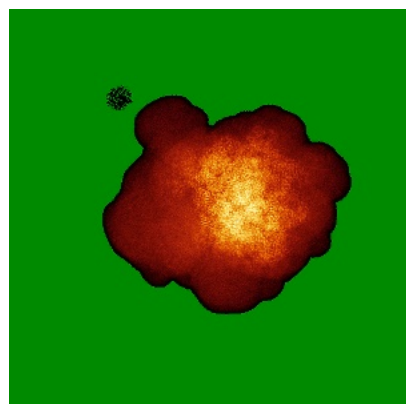


Z Index: 243

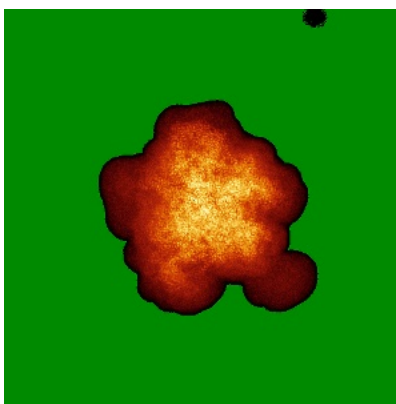
The images above show the largest variance slices of the map in three orthogonal directions.

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

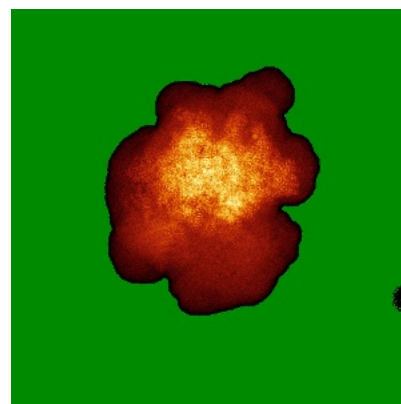
6.4.1 Primary map



X

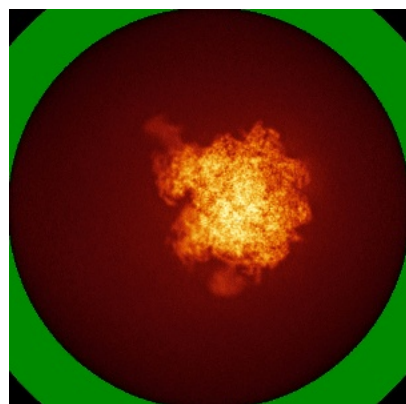


Y

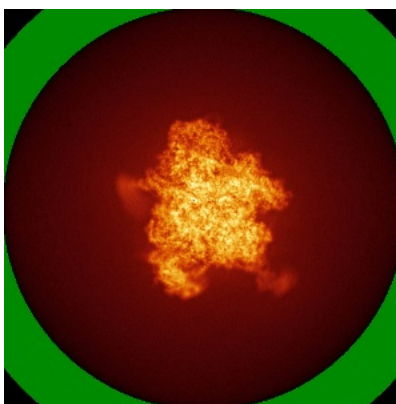


Z

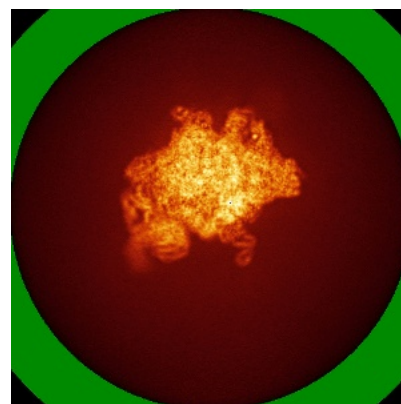
6.4.2 Raw map



X



Y

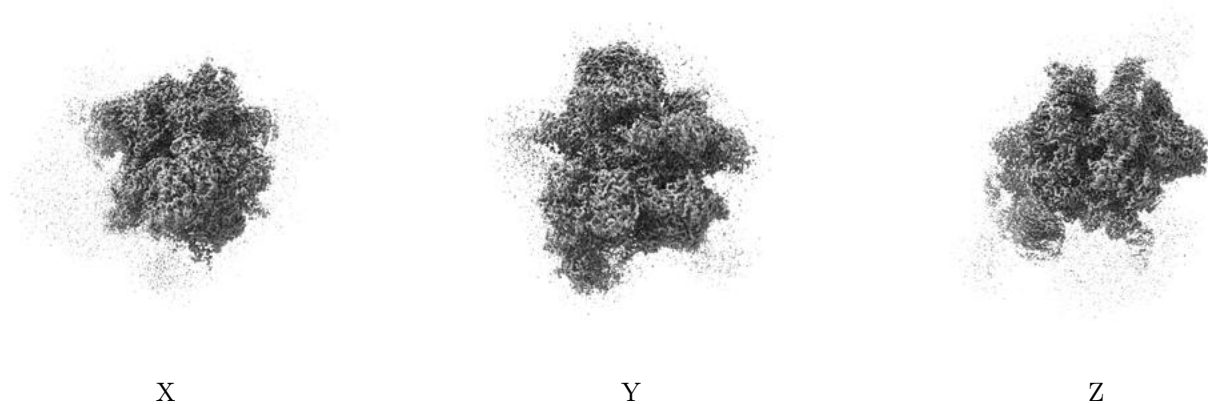


Z

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

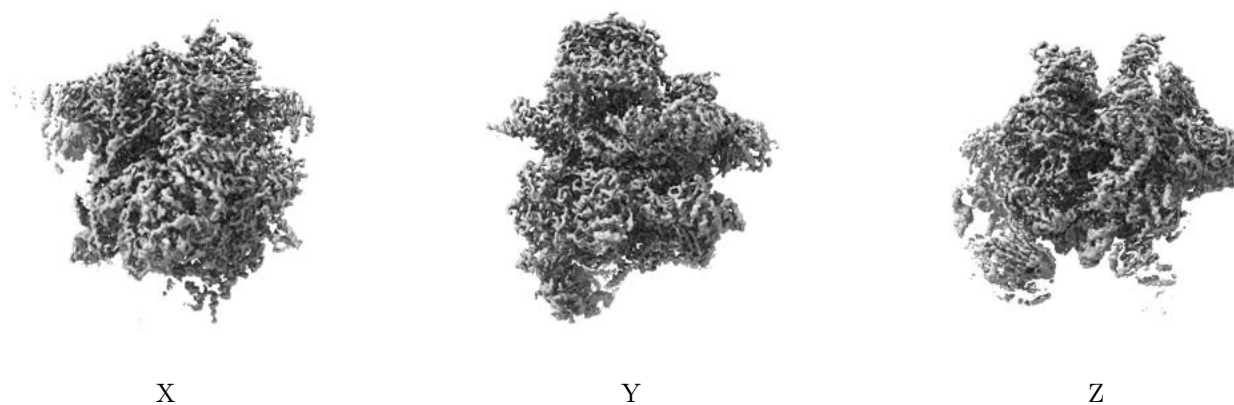
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

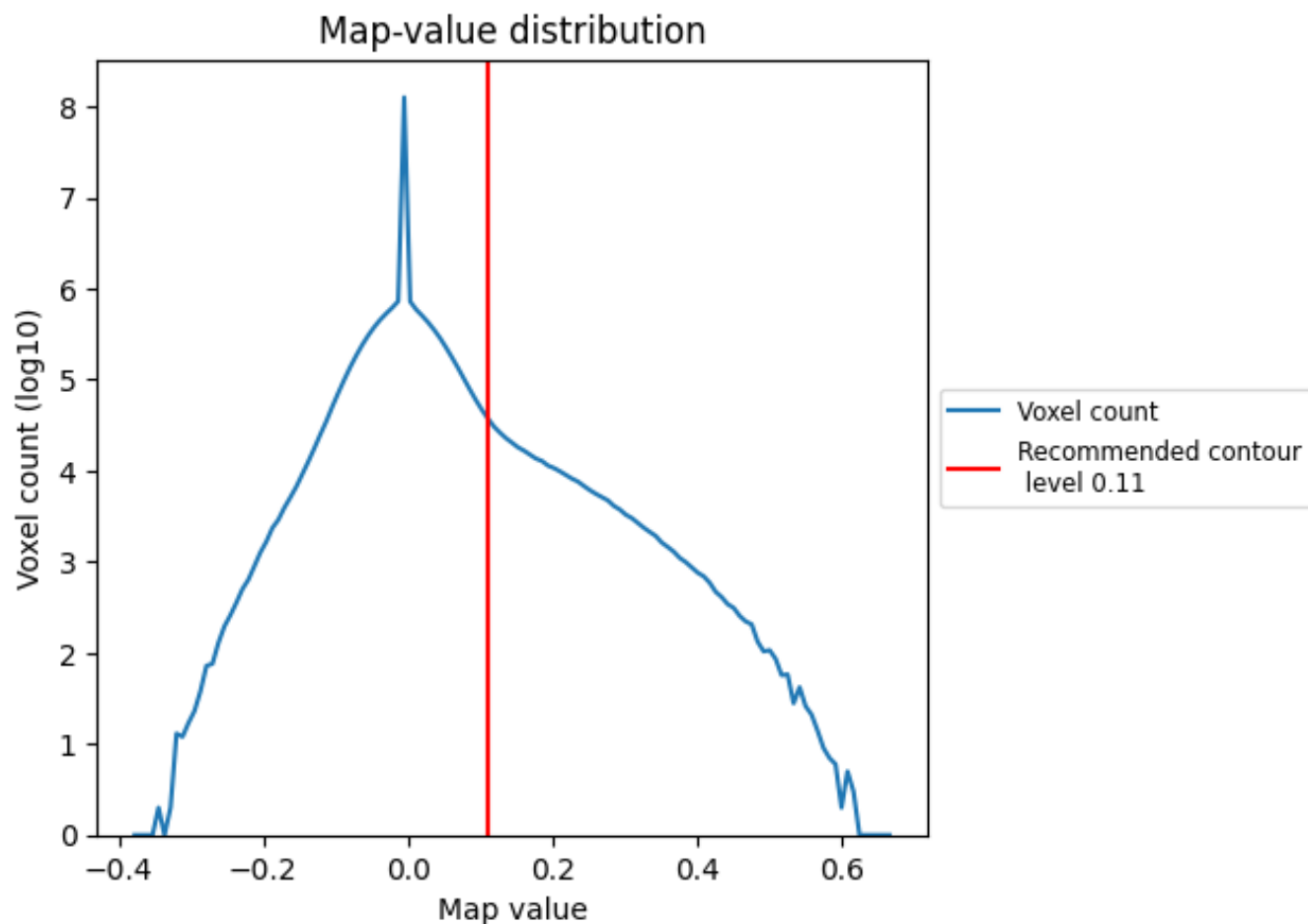
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

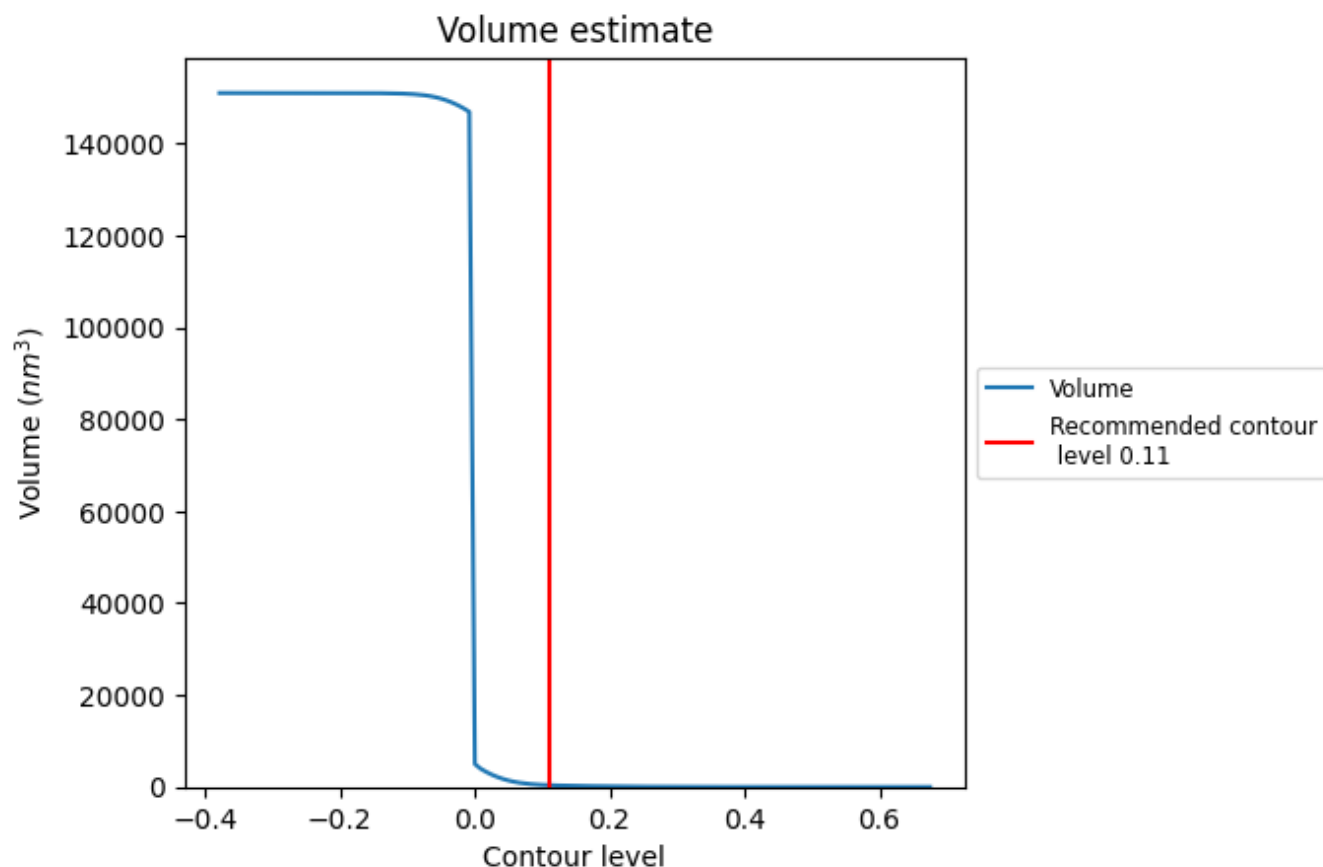
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

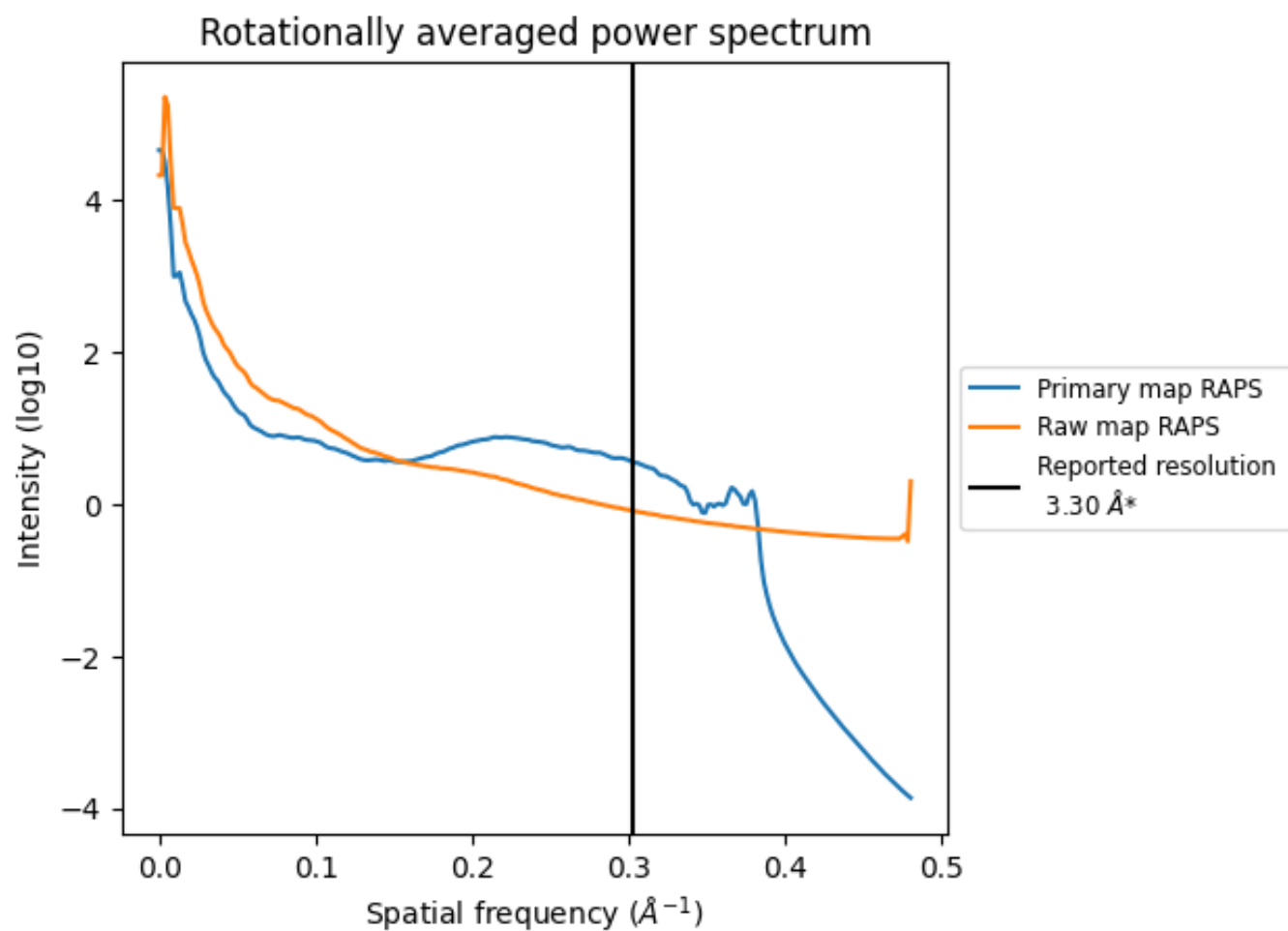
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 383 nm³; this corresponds to an approximate mass of 346 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 ⓘ

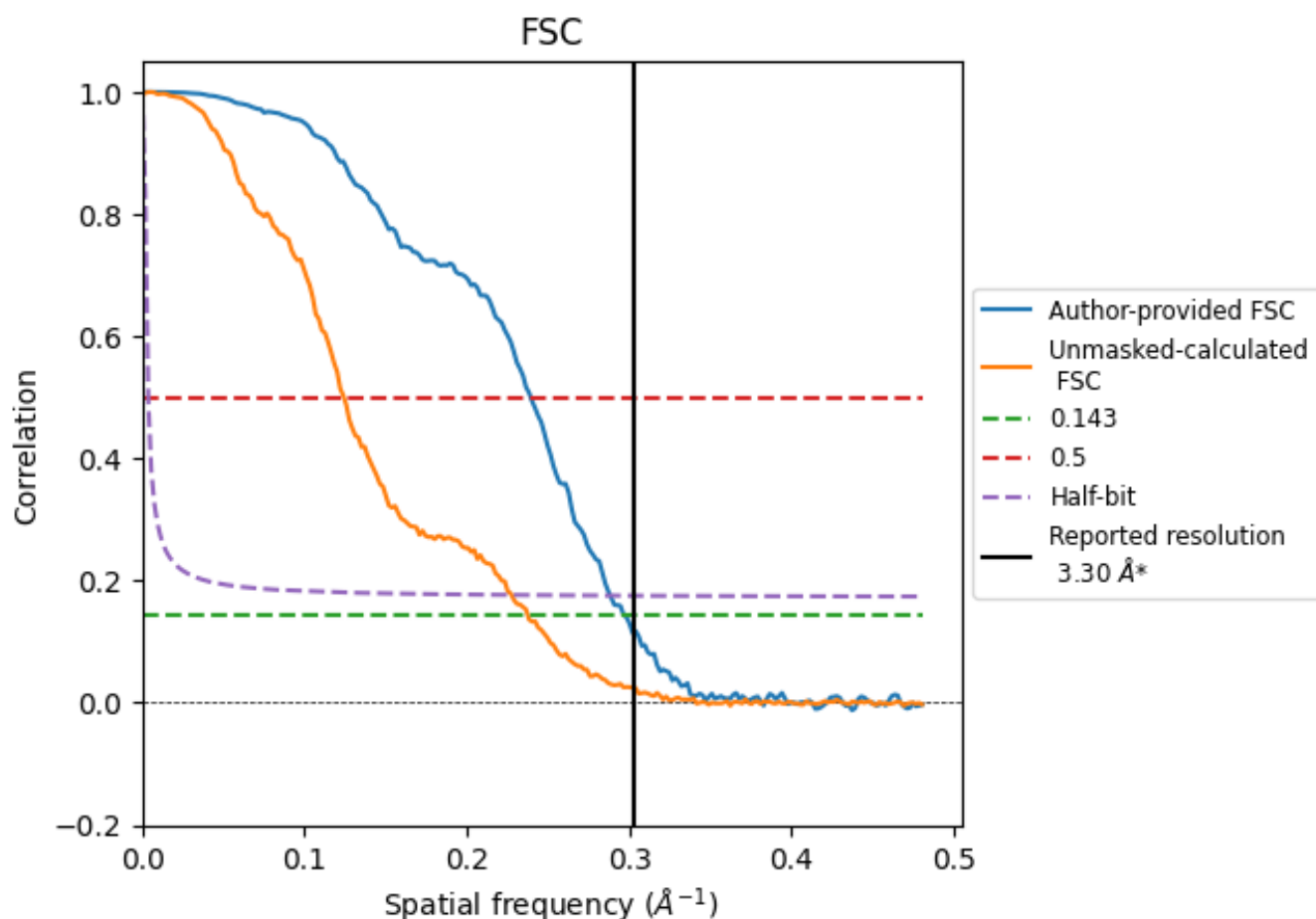


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.36	4.18	3.47
Unmasked-calculated*	4.21	8.05	4.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 3.3 by more than 10 %

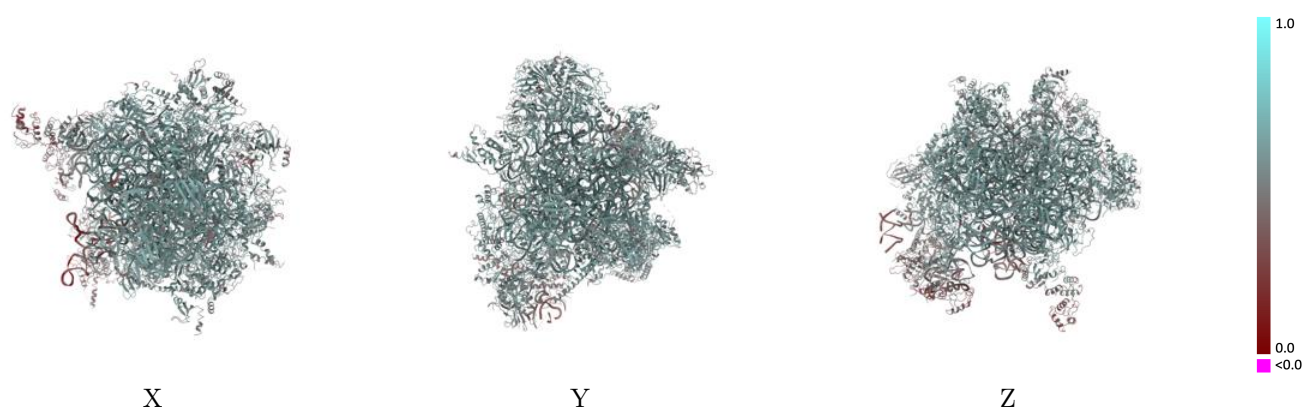
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11643 and PDB model 7A5H. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)

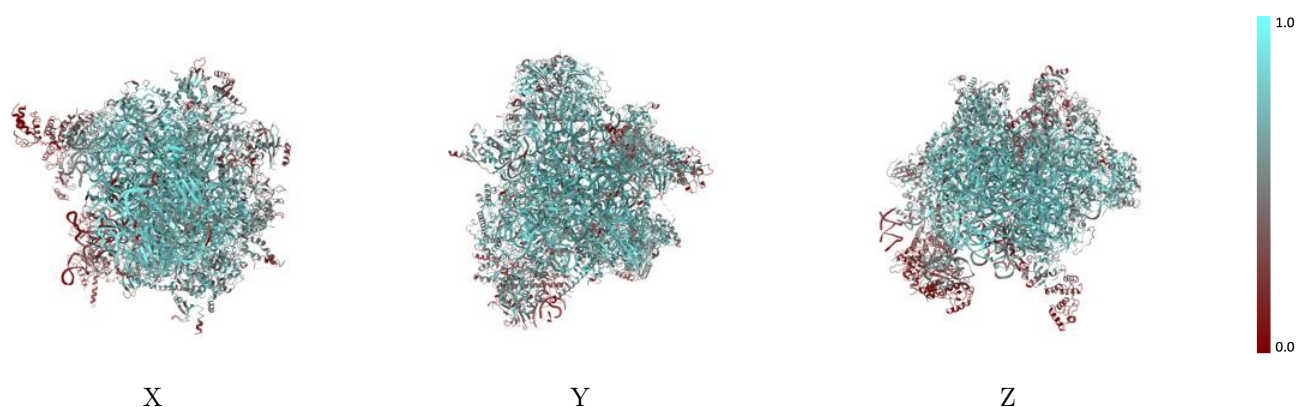
This section was not generated.

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



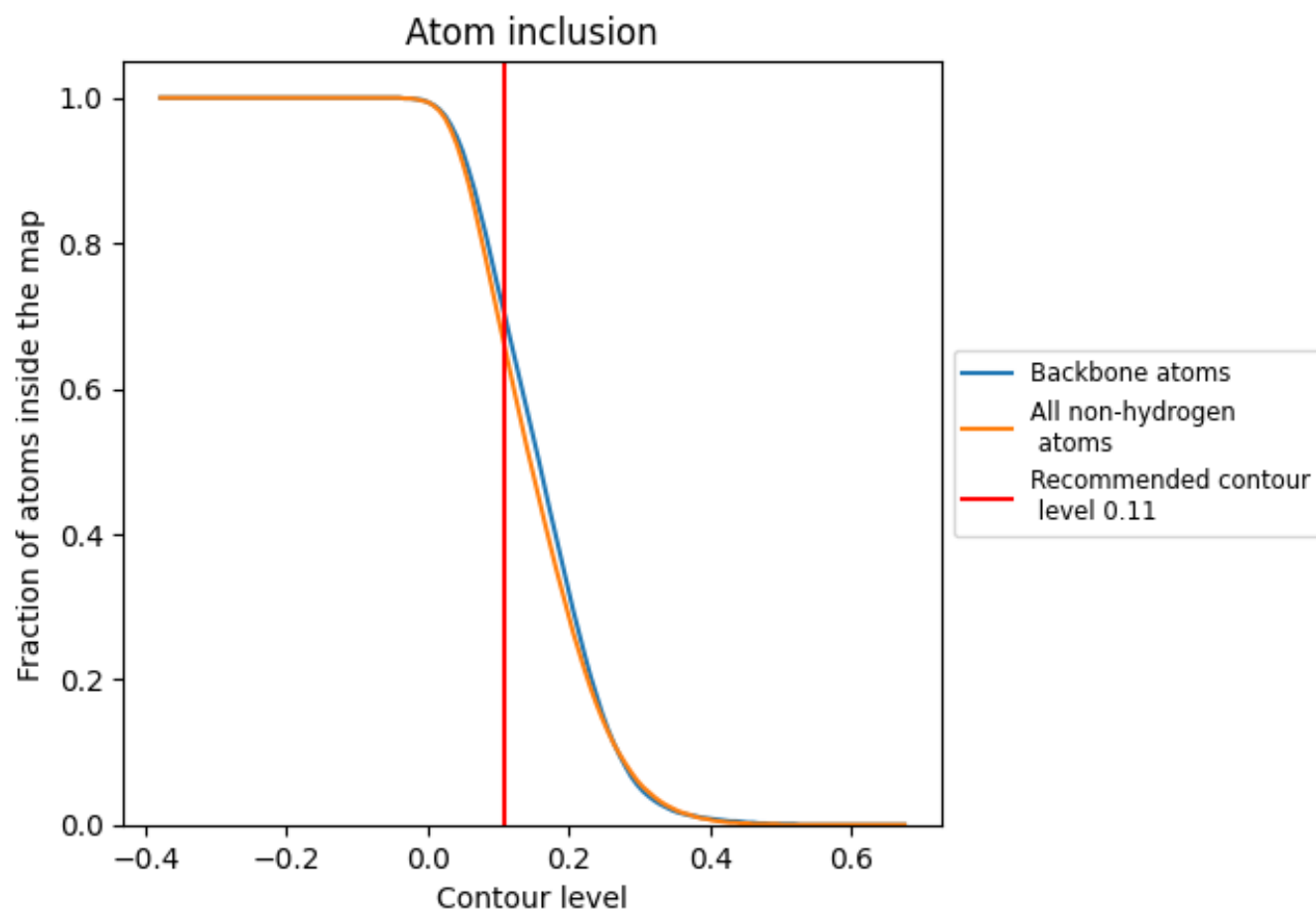
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 65% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6530	 0.5530
0	 0.6350	 0.5740
1	 0.6480	 0.5620
2	 0.8260	 0.6210
24	 0.1940	 0.2980
3	 0.7890	 0.6150
5	 0.6450	 0.5580
6	 0.5390	 0.5260
7	 0.5050	 0.5290
8	 0.1420	 0.3890
9	 0.6120	 0.5630
A	 0.8360	 0.5920
B	 0.3870	 0.3880
C	 0.3120	 0.5120
D	 0.7190	 0.5840
E	 0.7120	 0.5830
F	 0.7100	 0.5860
G	 0.3440	 0.4660
H	 0.5320	 0.5450
I	 0.3490	 0.4630
J	 0.1800	 0.3930
K	 0.7510	 0.5950
L	 0.6890	 0.5770
M	 0.7260	 0.5850
N	 0.6970	 0.5850
O	 0.7350	 0.5850
P	 0.6260	 0.5610
Q	 0.6390	 0.5660
R	 0.7600	 0.6050
S	 0.7230	 0.5880
T	 0.7110	 0.5900
U	 0.6160	 0.5460
V	 0.4920	 0.5220
W	 0.7480	 0.6040
X	 0.6310	 0.5630



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Chain	Atom inclusion	Q-score
Y	 0.6850	 0.5840
Y2	 0.1080	 0.3260
Z	 0.7380	 0.5940
a	 0.6840	 0.5760
b	 0.7270	 0.5900
c	 0.6200	 0.5600
d	 0.4410	 0.5170
e	 0.0630	 0.3440
f	 0.2610	 0.4430
g	 0.6850	 0.5700
h	 0.4980	 0.5120
i	 0.7690	 0.6050
j	 0.6470	 0.5720
k	 0.3740	 0.4680
l	 0.5100	 0.5350
m	 0.1330	 0.3850
o	 0.7610	 0.6000
p	 0.5090	 0.5370
q	 0.4950	 0.5090
r	 0.7200	 0.5850
s	 0.6890	 0.5740
t	 0.1430	 0.3980
u	 0.4300	 0.5050
v	 0.2290	 0.4320
w	 0.0470	 0.3360