wwPDB EM Validation Summary Report

Oct 19, 2022 – 02:16 am BST

PDB ID	:	8APH
EMDB ID	:	EMD-15571
Title	:	rotational state 2c of the Trypanosoma brucei mitochondrial ATP synthase dimer
Authors	:	Muehleip, A.; Gahura, O.; Zikova, A.; Amunts, A.
Deposited on	:	2022-08-09
Resolution	:	3.80 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:

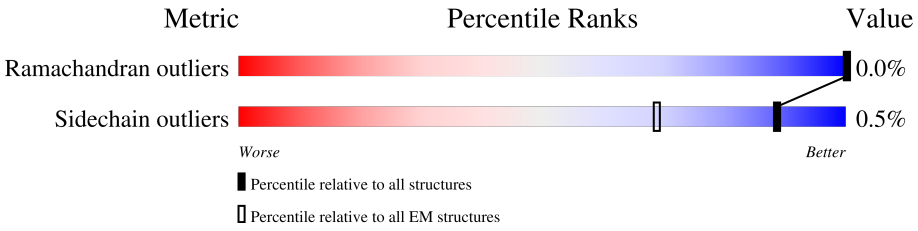
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	FAILED
MolProbity	:	4.02b-467
buster-report	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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

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	L	92	16% 71% 29%
1	l	92	25% 71% 29%
2	M	144	29% 90% 10%
2	m	144	22% 90% 10%
3	a	231	99%
4	c	114	11% 75% 25%
5	d	370	28% 89% 10%
6	e	396	96%
7	f	145	92% 7%

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Mol	Chain	Length	Quality of chain
8	g	269	86% 100%
9	h	157	71% 87% 13%
10	i	104	99%
11	j	169	99%
12	k	124	9% 85% 15%
13	n	156	89% 11%
14	o	101	94% 5%
15	p	105	76% 24%
16	q	98	87% 13%
17	r	62	100%
18	H1	182	49% 87% 12%
19	I1	75	64% 85% 13%
20	J1	188	63% 88% 12%
20	K1	188	50% 88% 12%
20	L1	188	57% 88% 12%
21	M1	255	43% 92% 8%
22	O1	118	42% 65% 34%
22	P1	118	49% 65% 34%
22	Q1	118	49% 65% 34%
22	R1	118	52% 65% 34%
22	S1	118	47% 64% 34%
22	T1	118	44% 64% 34%
22	U1	118	45% 65% 34%
22	V1	118	46% 65% 34%
22	W1	118	50% 65% 34%

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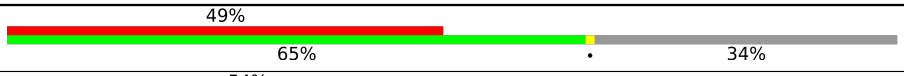
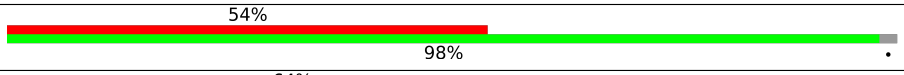
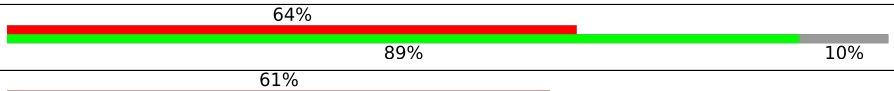
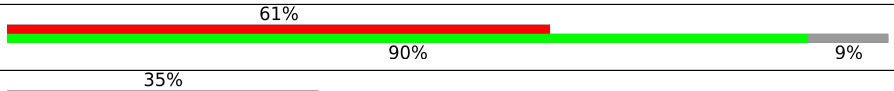
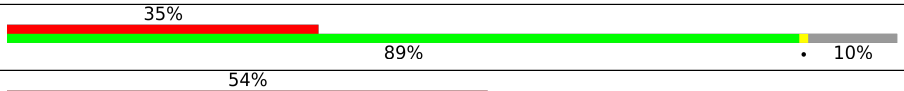
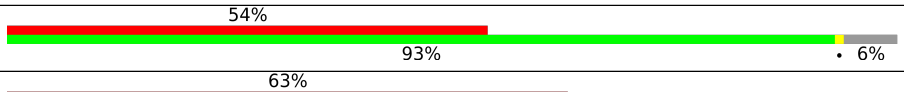
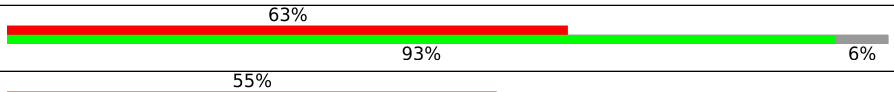
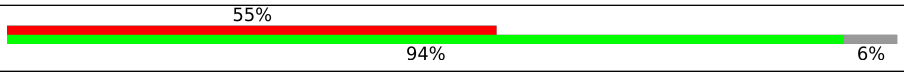
Mol	Chain	Length	Quality of chain
22	X1	118	
23	G1	305	
24	A1	584	
24	B1	584	
24	C1	584	
25	D1	519	
25	E1	519	
25	F1	519	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	Q7G	e	407	X	-	-	-
29	Q7G	n	201	X	-	-	-

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 129563 atoms, of which 65460 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 subunit-e.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	L	65	Total	C	H	N	O	S	0	0
			1082	340	545	104	92	1		
1	l	65	Total	C	H	N	O	S	0	0
			1082	340	545	104	92	1		

- Molecule 2 is a protein called subunit-g.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	M	129	Total	C	H	N	O	S	0	0
			2069	662	1042	177	186	2		
2	m	129	Total	C	H	N	O	S	0	0
			2069	662	1042	177	186	2		

- Molecule 3 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	a	231	Total	C	H	N	O	S	0	0
			4076	1459	2044	261	284	28		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	23	TRP	-	insertion	UNP P24499
a	180	TRP	-	insertion	UNP P24499

- Molecule 4 is a protein called subunit-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	c	86	Total	C	H	N	O	S	0	0
			1460	494	715	116	130	5		

- Molecule 5 is a protein called subunit-d.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	d	332	Total	C	H	N	O	S	0	0
			5499	1710	2762	505	514	8		

- Molecule 6 is a protein called ATPTB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	e	383	Total	C	H	N	O	S	0	0
			6270	2060	3050	558	585	17		

- Molecule 7 is a protein called subunit-f.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	f	135	Total	C	H	N	O	S	0	0
			2256	744	1111	201	195	5		

- Molecule 8 is a protein called ATPTB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	g	268	Total	C	H	N	O	S	0	0
			3953	1211	2020	343	378	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	176	ALA	VAL	conflict	UNP A0A3L6KRX7

- Molecule 9 is a protein called ATPTB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	h	137	Total	C	H	N	O	S	0	0
			2158	680	1088	184	203	3		

- Molecule 10 is a protein called subunit-i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	i	103	Total	C	H	N	O	S	0	0
			1740	574	857	152	151	6		

- Molecule 11 is a protein called ATPTB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	j	168	Total	C	H	N	O	S	0	0
			2835	919	1411	249	249	7		

- Molecule 12 is a protein called subunit-k.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	k	105	Total	C	H	N	O	S	0	0
			1749	577	876	149	141	6		

- Molecule 13 is a protein called ATPTB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	n	139	Total	C	H	N	O	S	0	0
			2210	730	1082	183	208	7		

- Molecule 14 is a protein called ATPTB12.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	o	96	Total	C	H	N	O	S	0	0
			1556	506	767	140	140	3		

- Molecule 15 is a protein called subunit-b.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	80	Total	C	H	N	O	S	0	0
			1335	448	651	108	125	3		

- Molecule 16 is a protein called ATPEG3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	85	Total	C	H	N	O	0	0
			1486	499	720	142	125		

- Molecule 17 is a protein called ATPEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	r	62	Total	C	H	N	O	S	0	0
			1040	358	498	94	85	5		

- Molecule 18 is a protein called ATP synthase, epsilon chain, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	H1	161	Total	C	H	N	O	S	0	0
			2483	788	1232	211	248	4		

- Molecule 19 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	I1	65	Total	C	H	N	O	S	0	0
			1046	332	513	97	102	2		

- Molecule 20 is a protein called ATP synthase subunit p18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	J1	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		
20	K1	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		
20	L1	165	Total	C	H	N	O	S	0	0
			2581	819	1271	220	257	14		

- Molecule 21 is a protein called OSCP.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	M1	234	Total	C	H	N	O	S	0	0
			3750	1212	1873	302	360	3		

- Molecule 22 is a protein called ATPase subunit 9, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	O1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
22	P1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
22	Q1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
22	R1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
22	S1	78	Total	C	H	N	O	S	0	0
			1166	376	601	89	96	4		
22	T1	78	Total	C	H	N	O	S	0	0
			1166	376	601	89	96	4		
22	U1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
22	V1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
22	W1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
22	X1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		

- Molecule 23 is a protein called ATP synthase gamma subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	G1	300	Total	C	H	N	O	S	0	0
			4774	1507	2387	423	448	9		

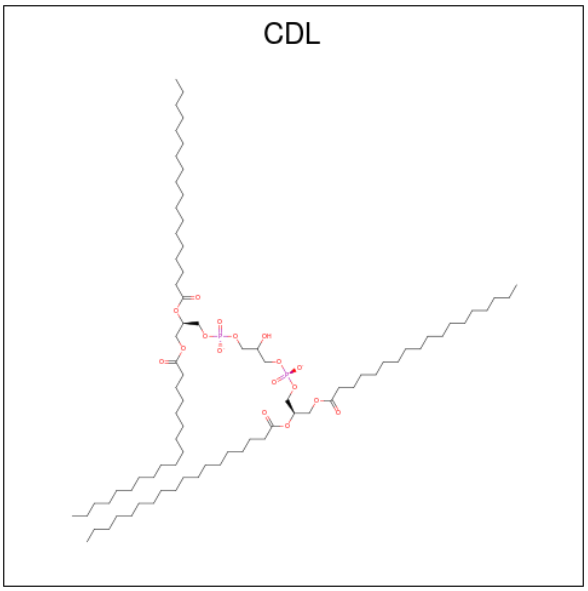
- Molecule 24 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A1	523	Total	C	H	N	O	S	0	0
			8193	2587	4154	701	731	20		
24	B1	529	Total	C	H	N	O	S	0	0
			8260	2603	4187	709	741	20		
24	C1	524	Total	C	H	N	O	S	0	0
			8219	2594	4170	703	732	20		

- Molecule 25 is a protein called ATP synthase subunit beta, mitochondrial.

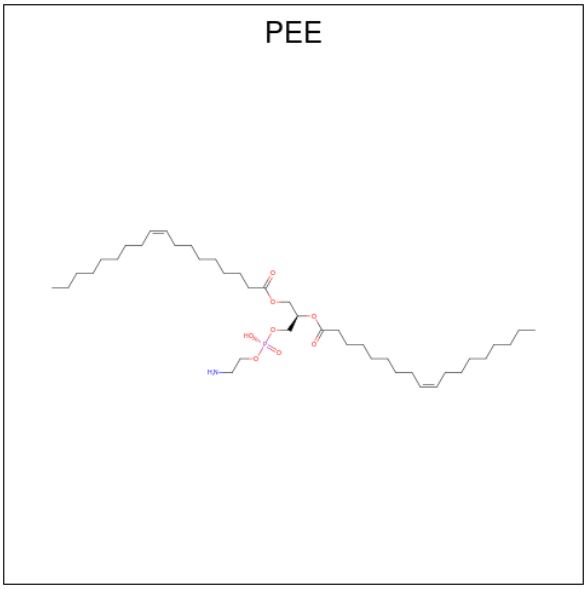
Mol	Chain	Residues	Atoms						AltConf	Trace
25	D1	488	Total	C	H	N	O	S	0	0
			7446	2334	3750	632	711	19		
25	E1	486	Total	C	H	N	O	S	0	0
			7414	2324	3732	630	709	19		
25	F1	488	Total	C	H	N	O	S	0	0
			7446	2334	3750	632	711	19		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



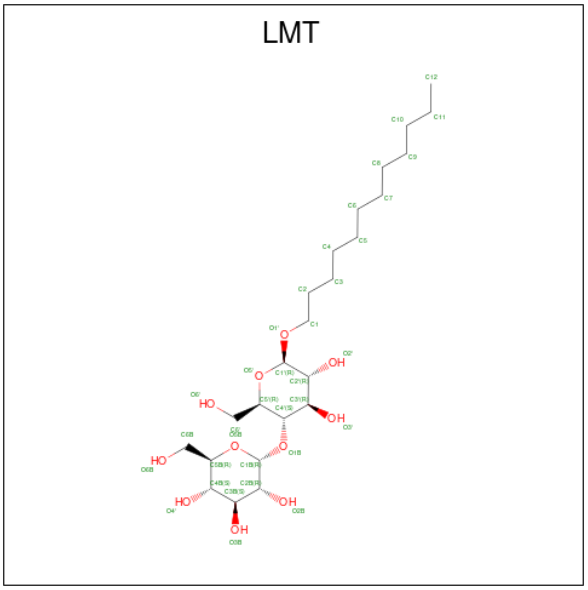
Mol	Chain	Residues	Atoms					AltConf
26	L	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	M	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
26	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
26	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
26	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
26	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
26	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	j	1	Total	C	H	O	P	0
			512	162	312	34	4	
26	j	1	Total	C	H	O	P	0
			512	162	312	34	4	
26	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	m	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	q	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 27 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



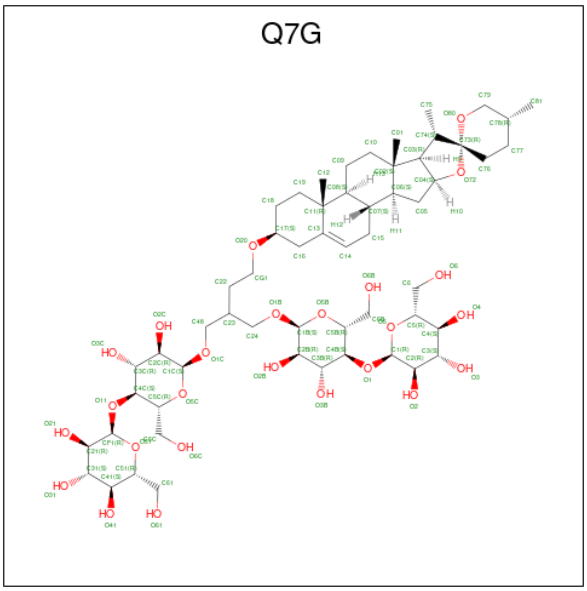
Mol	Chain	Residues	Atoms						AltConf
27	M	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
27	f	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
27	m	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



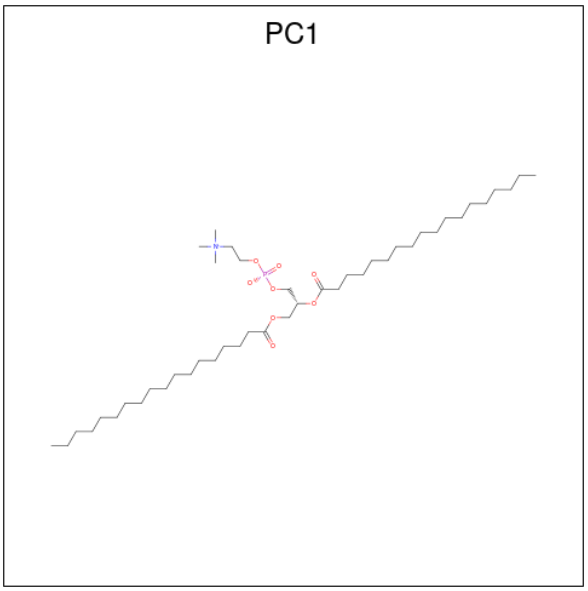
Mol	Chain	Residues	Atoms				AltConf
28	e	1	Total	C	H	O	0
			74	24	39	11	
28	j	1	Total	C	H	O	0
			74	24	39	11	

- Molecule 29 is 2-{[(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl}-4-{[(3beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy}butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (three-letter code: Q7G) (formula: $C_{56}H_{92}O_{25}$).



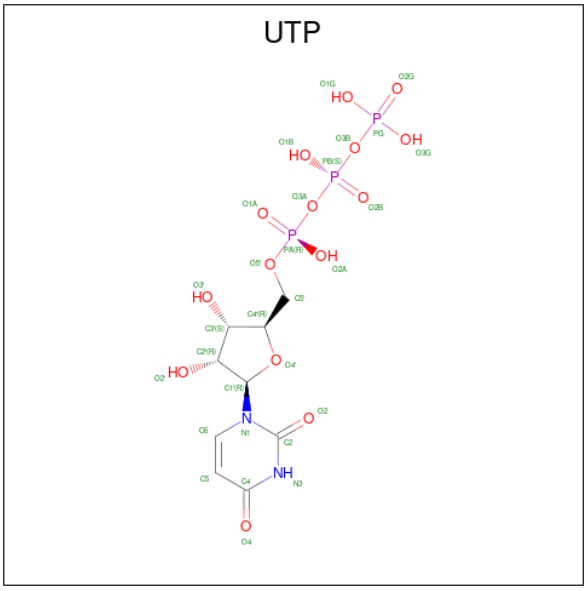
Mol	Chain	Residues	Atoms				AltConf
29	e	1	Total	C	H	O	0
			108	38	60	10	
29	n	1	Total	C	H	O	0
			129	44	70	15	

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



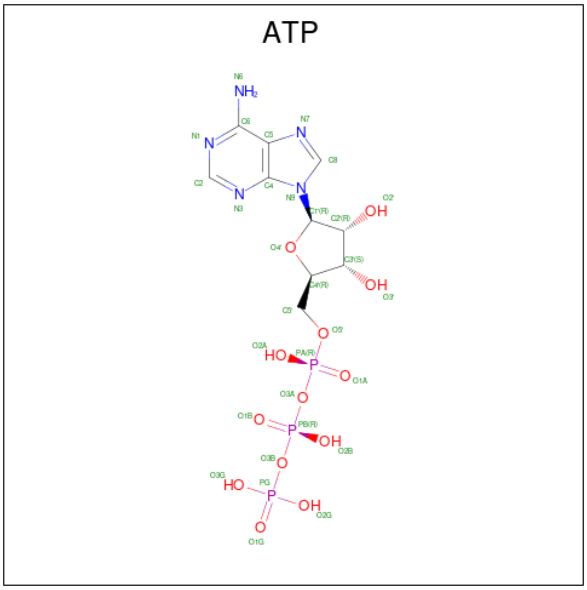
Mol	Chain	Residues	Atoms						AltConf
30	f	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	i	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	j	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	p	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 31 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
31	H1	1	Total	C	H	N	O	P	0
			40	9	11	2	15	3	

- Molecule 32 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
32	A1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
32	B1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
32	C1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
32	D1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
33	A1	1	Total	Mg	0
			1	1	
33	B1	1	Total	Mg	0
			1	1	
33	C1	1	Total	Mg	0
			1	1	
33	D1	1	Total	Mg	0
			1	1	

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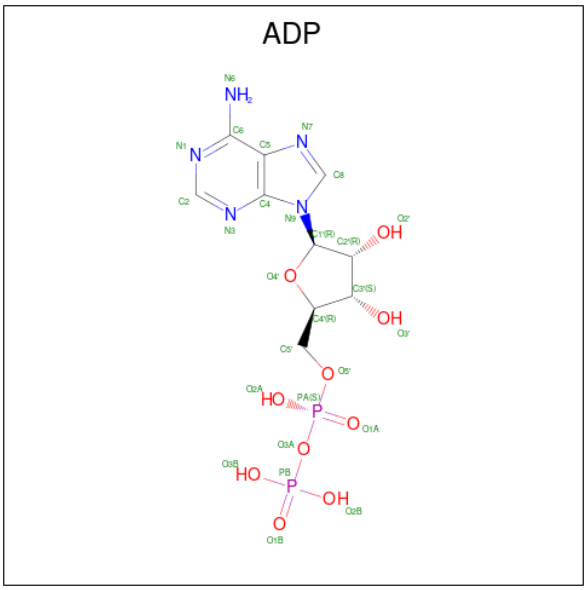
Mol	Chain	Residues	Atoms	AltConf
33	E1	1	Total Mg 1 1	0

- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



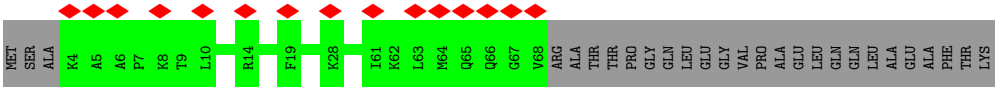
Mol	Chain	Residues	Atoms	AltConf
34	E1	1	Total C H N O P 39 10 12 5 10 2	0

3 Residue-property plots (i)

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.

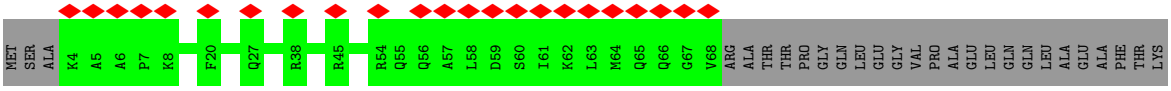
• Molecule 1: subunit-e

Chain L:



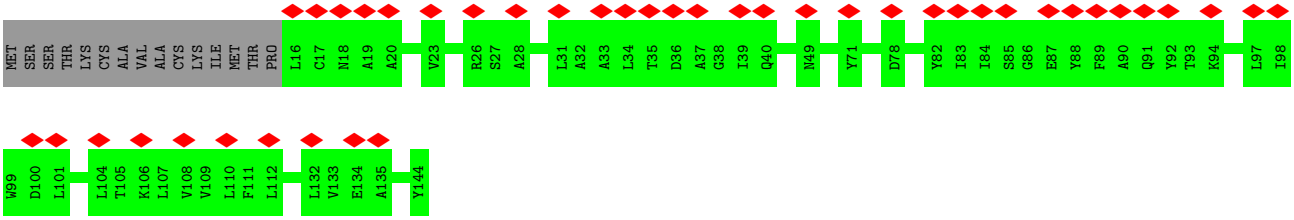
• Molecule 1: subunit-e

Chain l:



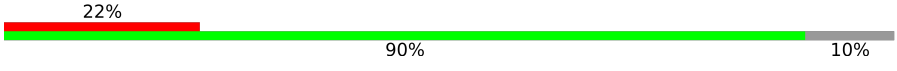
• Molecule 2: subunit-g

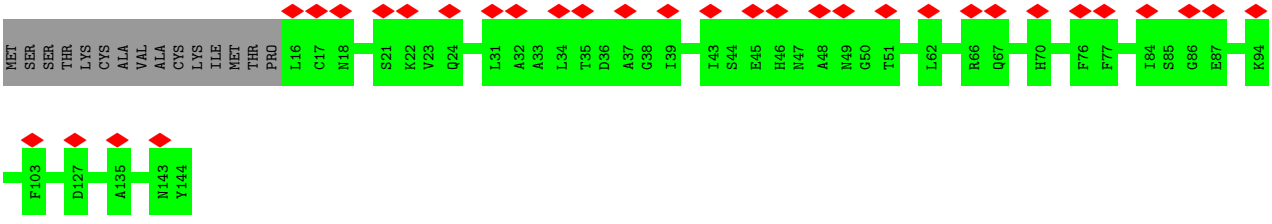
Chain M:



• Molecule 2: subunit-g

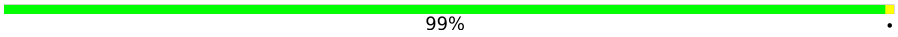
Chain m:

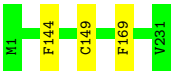




• Molecule 3: ATP synthase subunit a

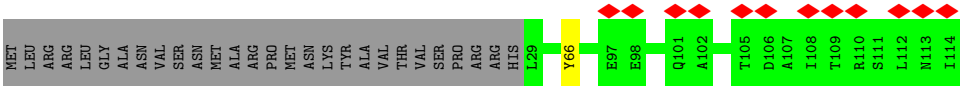
Chain a:





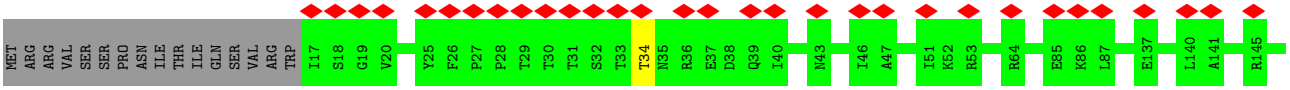
• Molecule 4: subunit-8

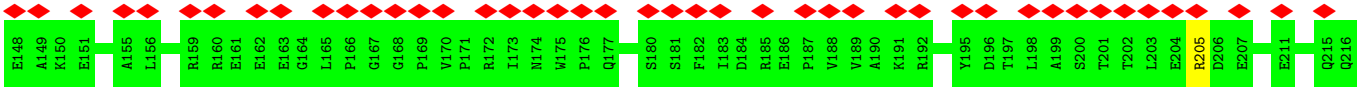
Chain c:

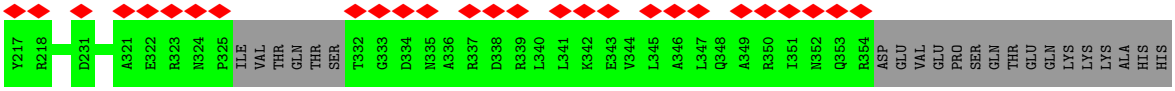


• Molecule 5: subunit-d

Chain d:

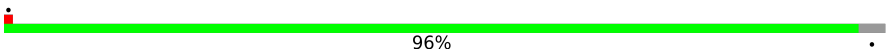


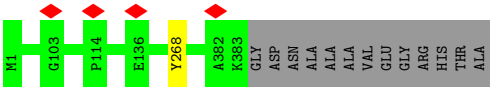




• Molecule 6: ATPTB1

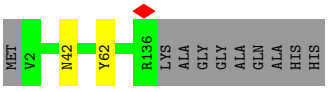
Chain e:





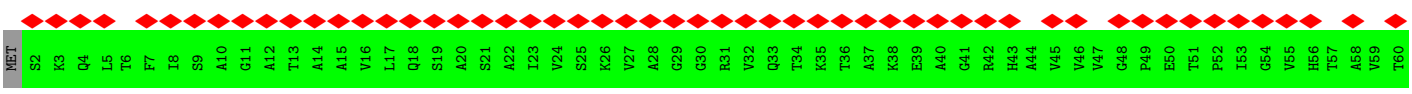
• Molecule 7: subunit-f

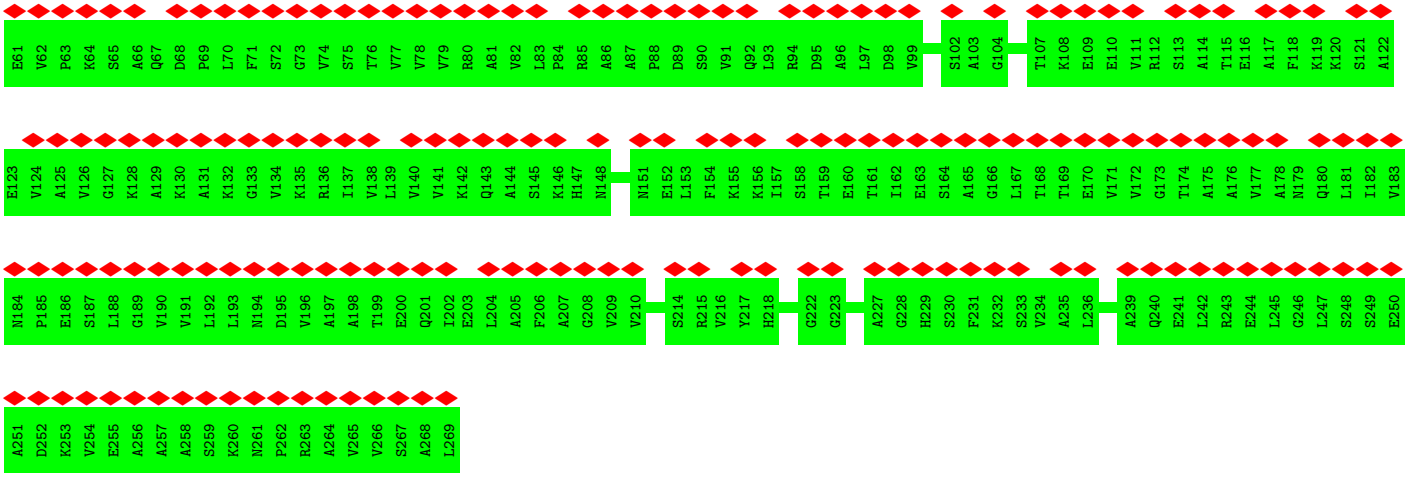
Chain f:



• Molecule 8: ATPTB3

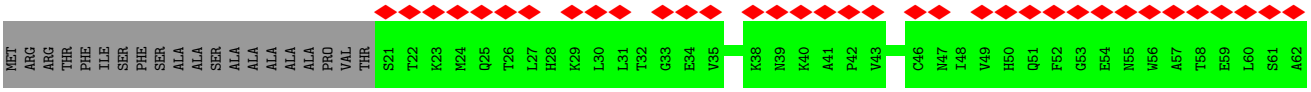
Chain g:

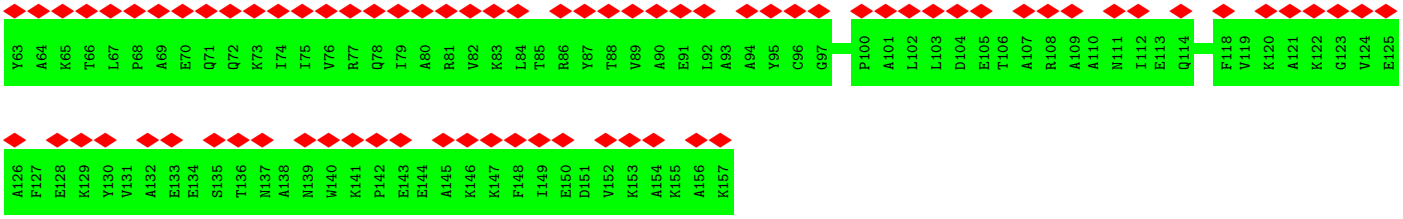




- Molecule 9: ATPTB4

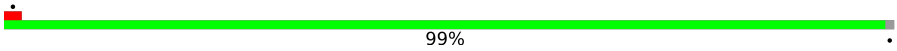
Chain h:

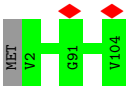




- Molecule 10: subunit-i/j

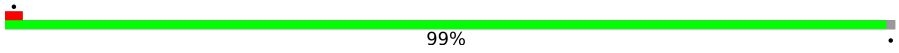
Chain i:

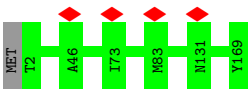




- Molecule 11: ATPTB6

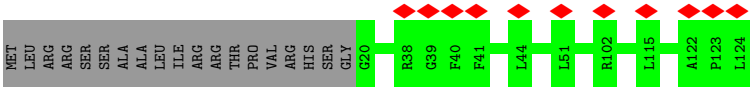
Chain j:





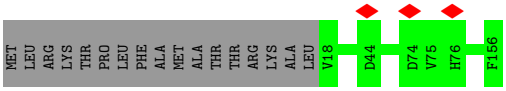
- Molecule 12: subunit-k

Chain k:



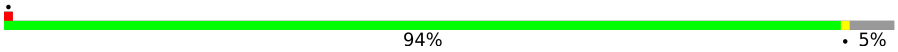
• Molecule 13: ATPTB11

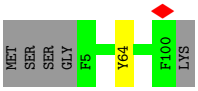
Chain n:



• Molecule 14: ATPTB12

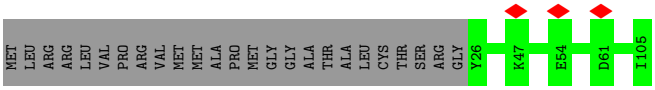
Chain o:





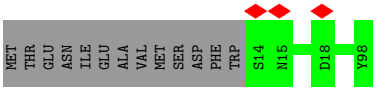
• Molecule 15: subunit-b

Chain p:



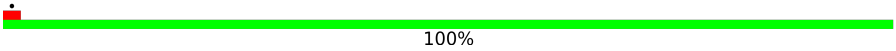
• Molecule 16: ATPEG3

Chain q:



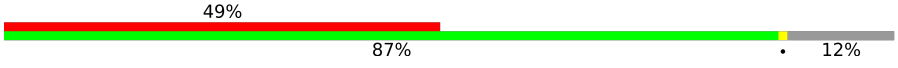
• Molecule 17: ATPEG4

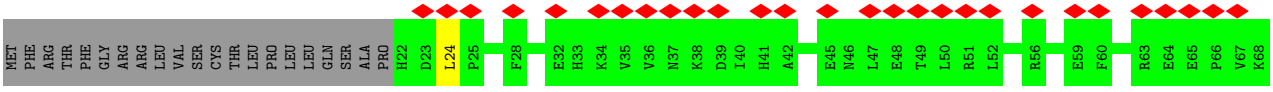
Chain r:

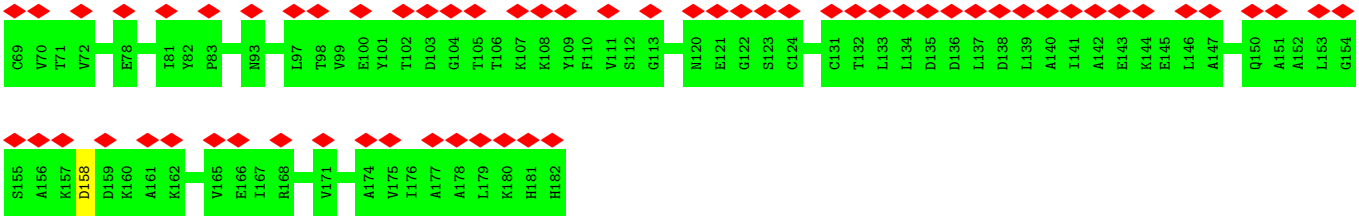


• Molecule 18: ATP synthase, epsilon chain, putative

Chain H1:

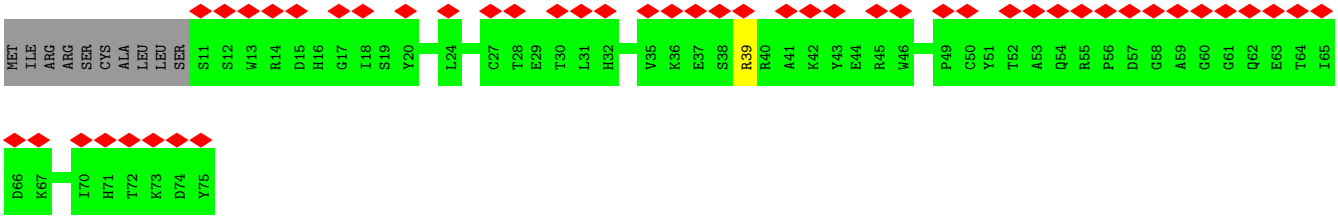






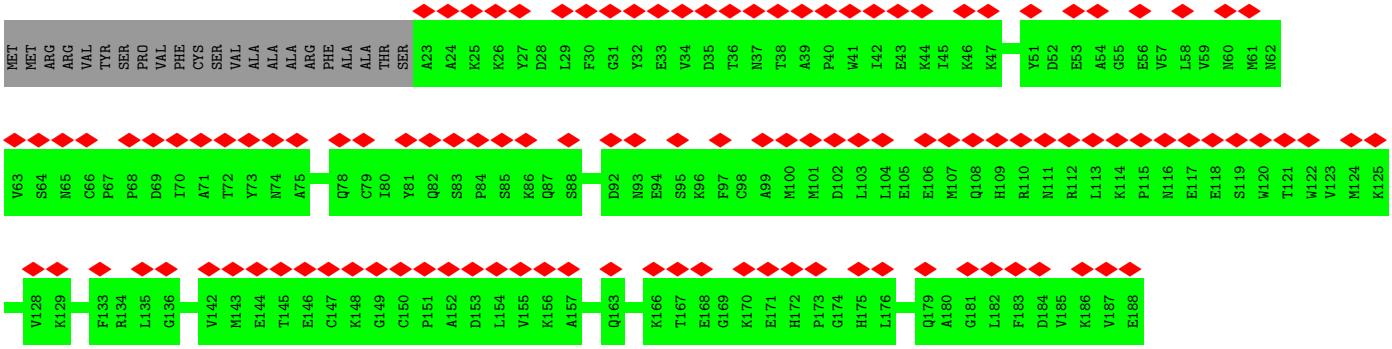
• Molecule 19: ATP synthase subunit epsilon, mitochondrial

Chain I1:



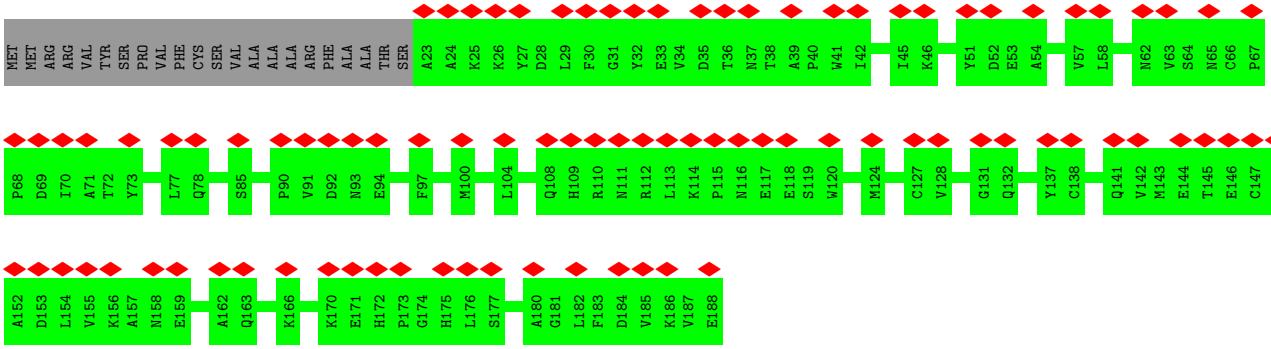
• Molecule 20: ATP synthase subunit p18, mitochondrial

Chain J1:



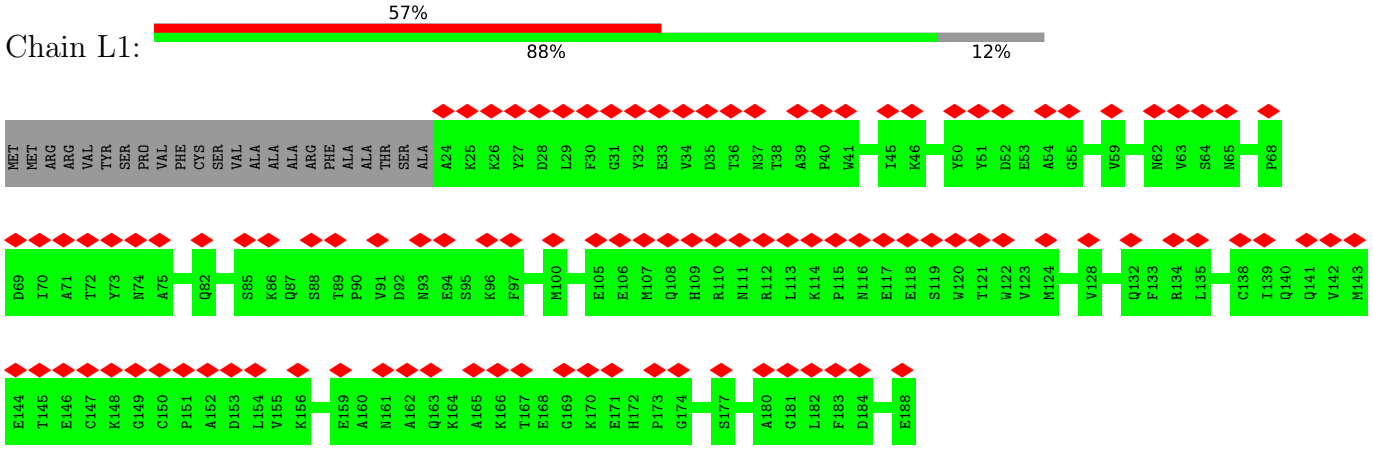
• Molecule 20: ATP synthase subunit p18, mitochondrial

Chain K1:



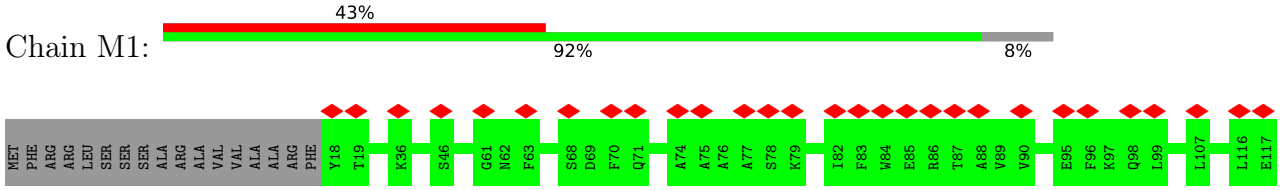
• Molecule 20: ATP synthase subunit p18, mitochondrial

Chain L1:



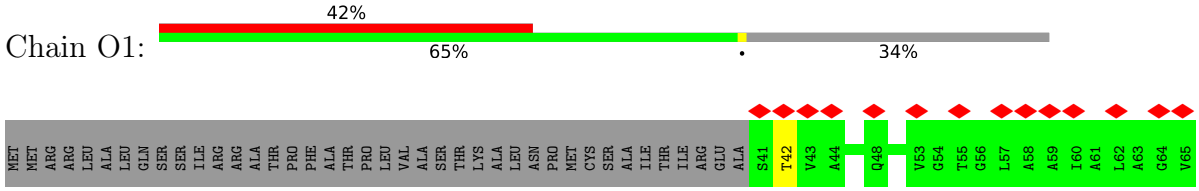
• Molecule 21: OSCP

Chain M1:



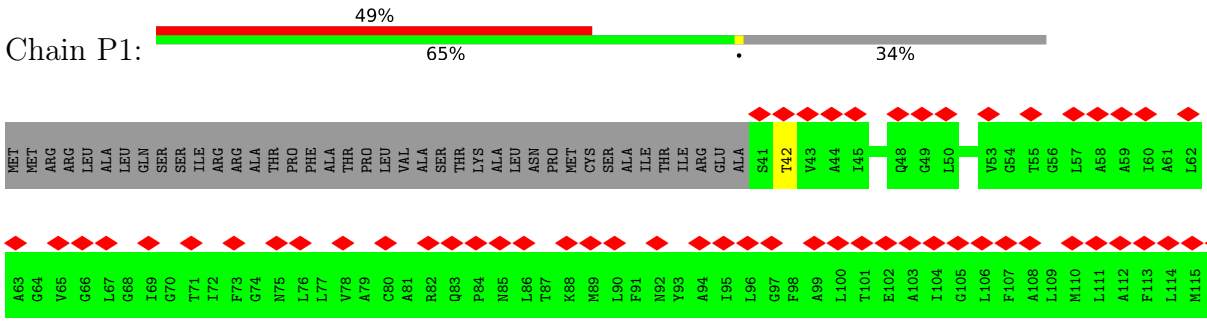
• Molecule 22: ATPase subunit 9, putative

Chain O1:



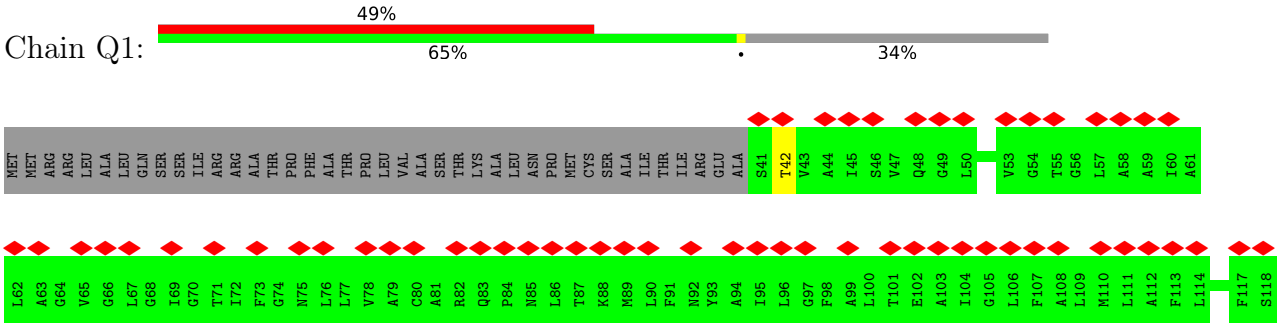
• Molecule 22: ATPase subunit 9, putative

Chain P1:



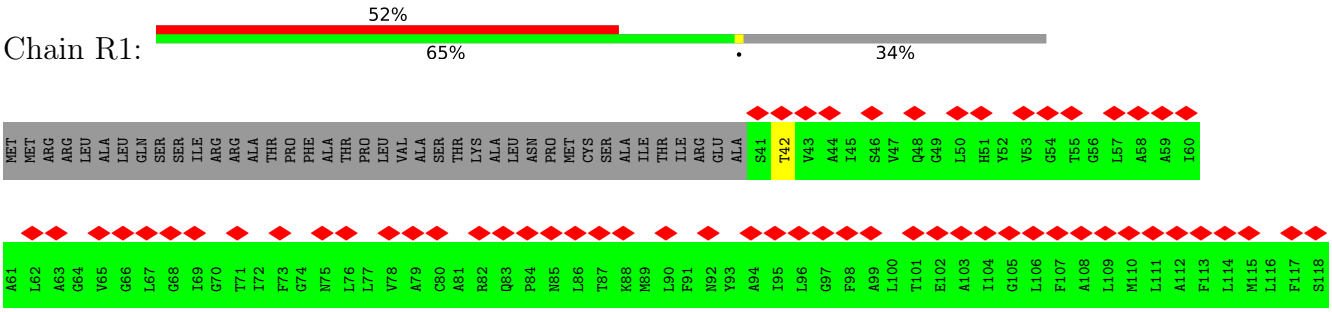
• Molecule 22: ATPase subunit 9, putative

Chain Q1:



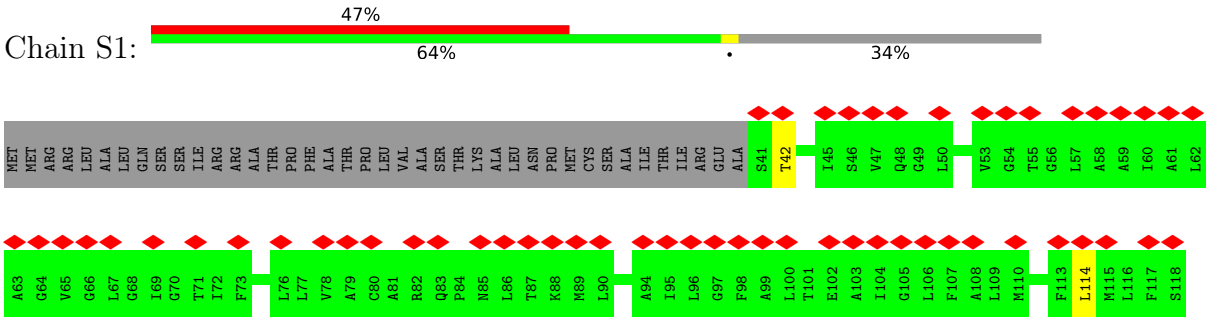
• Molecule 22: ATPase subunit 9, putative

Chain R1:



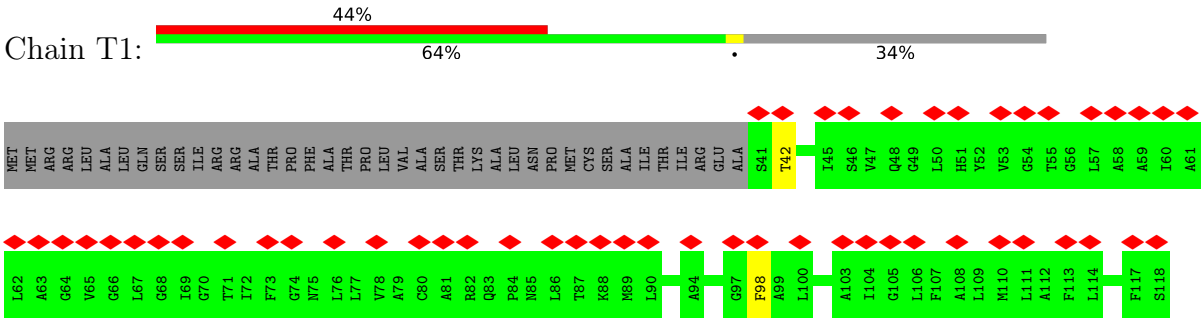
• Molecule 22: ATPase subunit 9, putative

Chain S1:



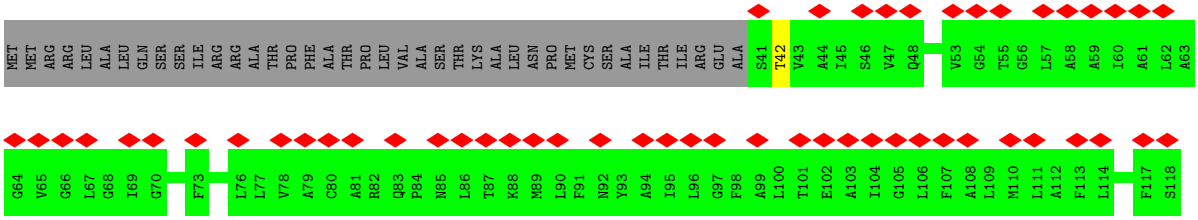
• Molecule 22: ATPase subunit 9, putative

Chain T1:

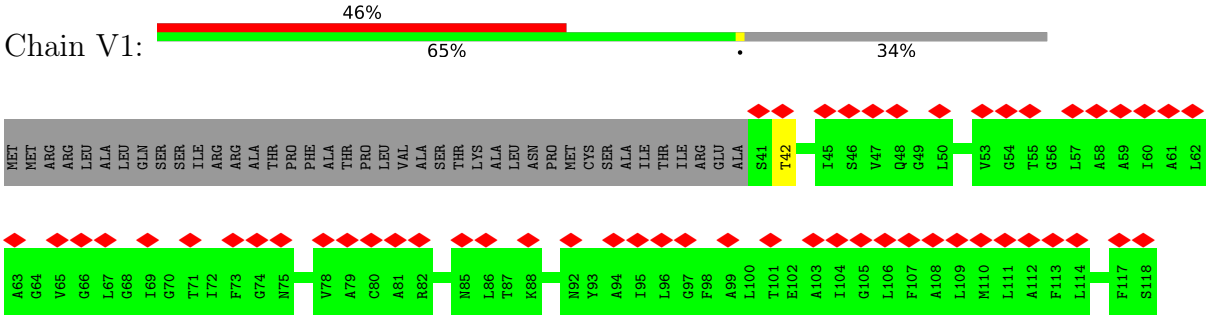


• Molecule 22: ATPase subunit 9, putative

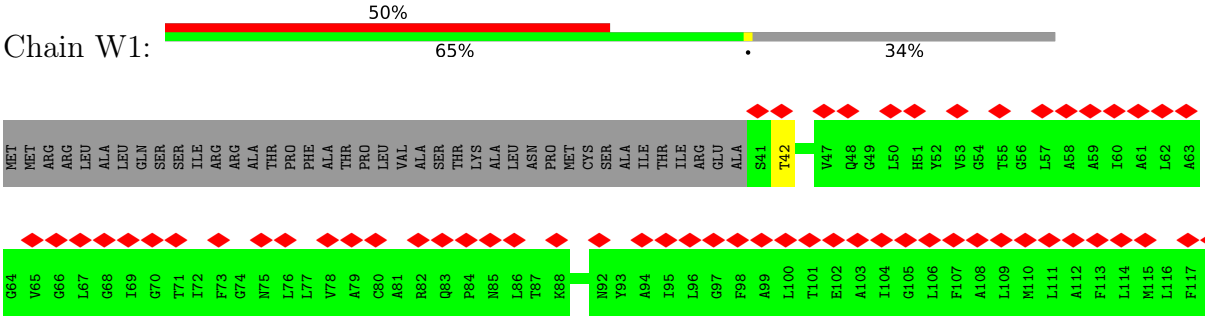
Chain U1:



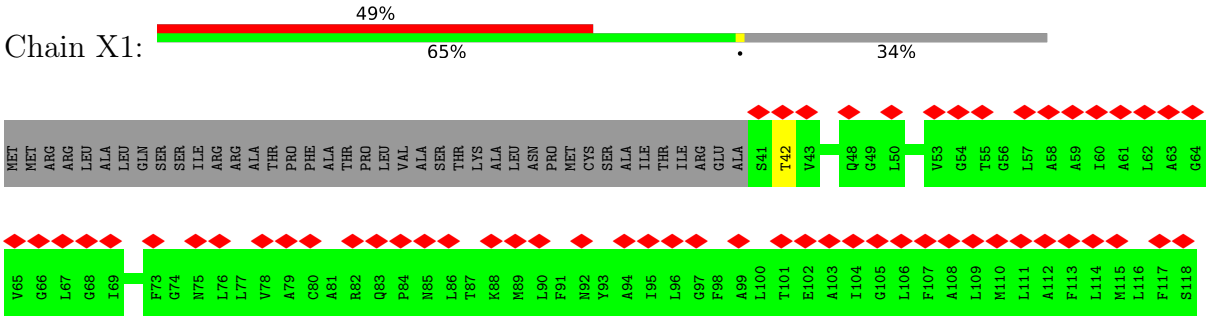
• Molecule 22: ATPase subunit 9, putative



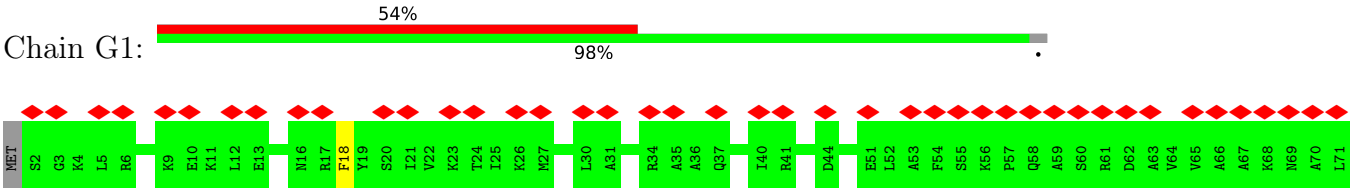
• Molecule 22: ATPase subunit 9, putative

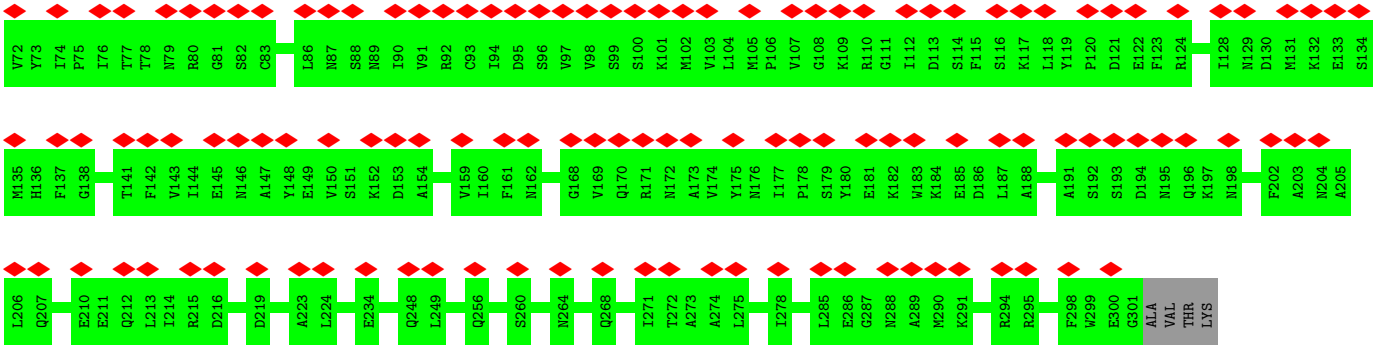


• Molecule 22: ATPase subunit 9, putative



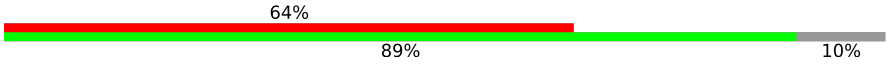
• Molecule 23: ATP synthase gamma subunit

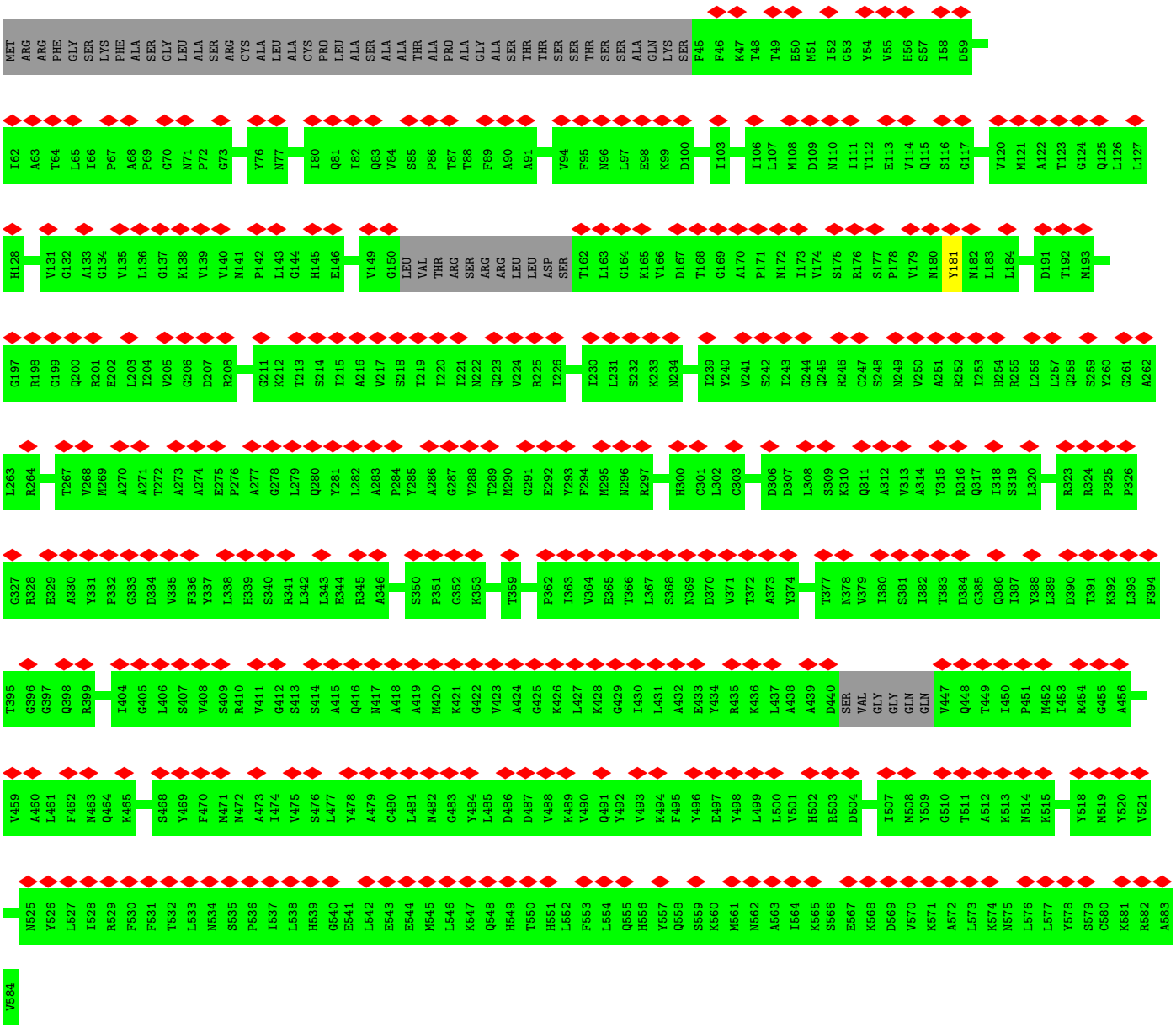




• Molecule 24: ATP synthase subunit alpha, mitochondrial

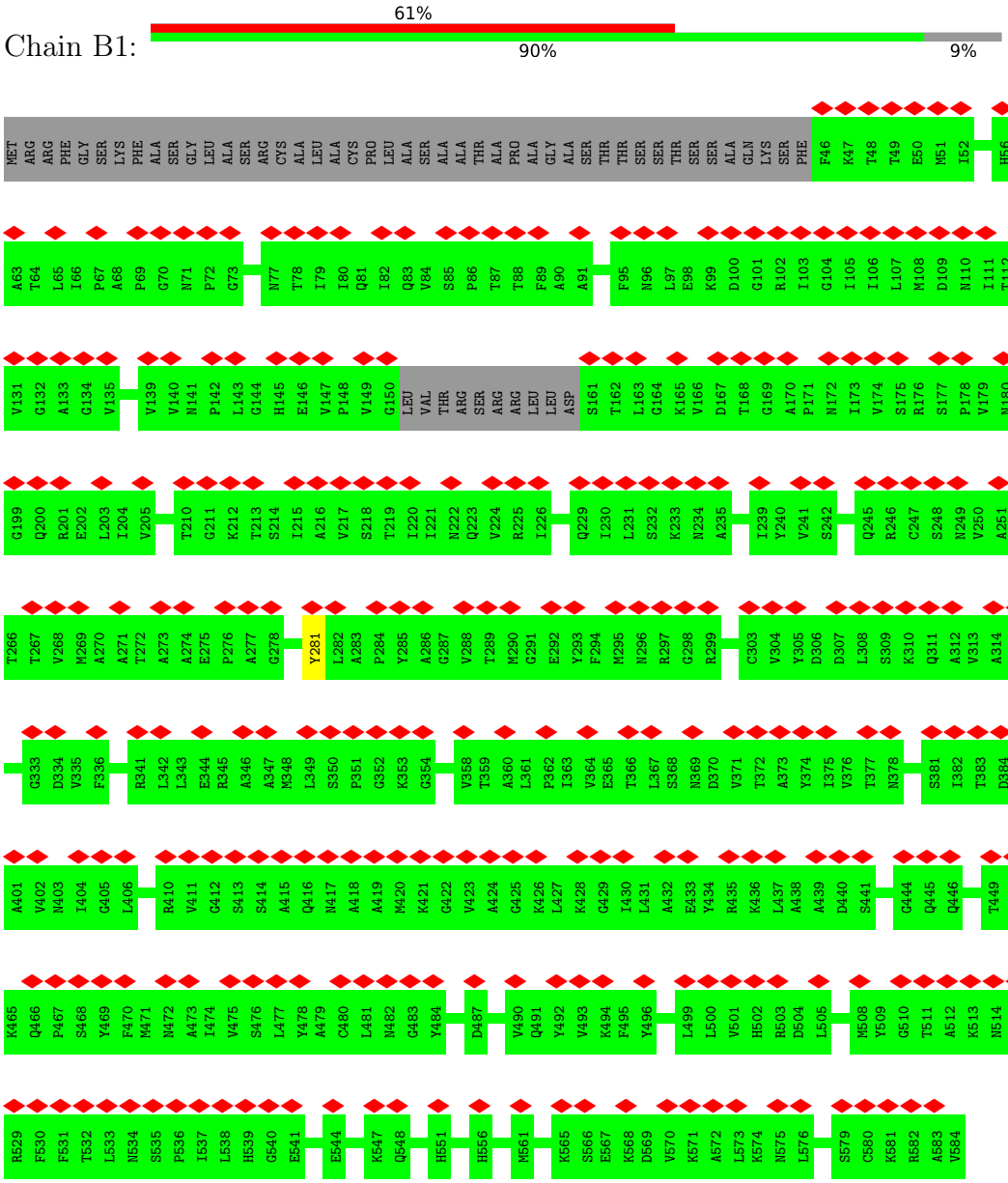
Chain A1:





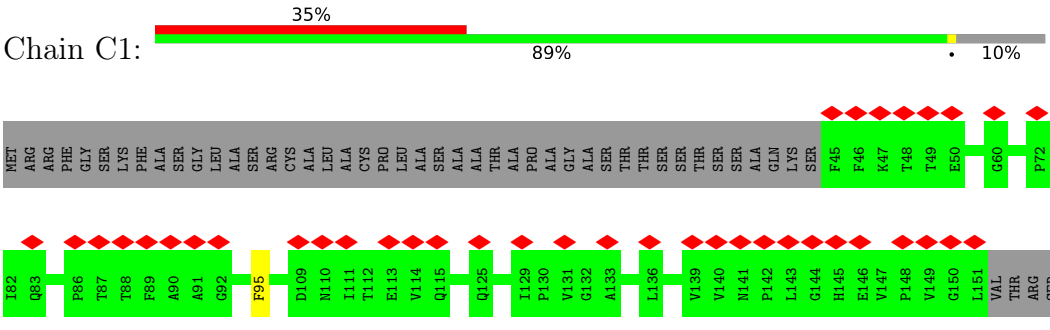
• Molecule 24: ATP synthase subunit alpha, mitochondrial

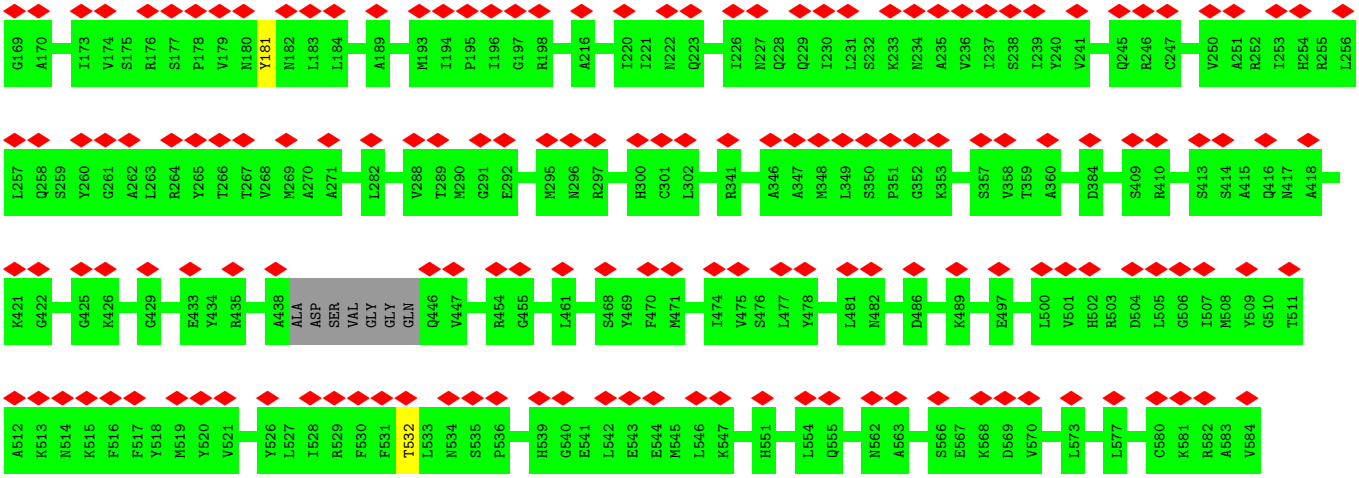
Chain B1:



• Molecule 24: ATP synthase subunit alpha, mitochondrial

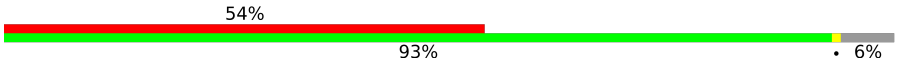
Chain C1:

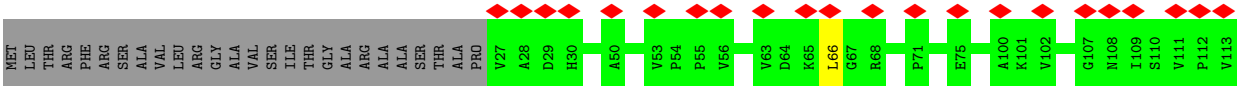


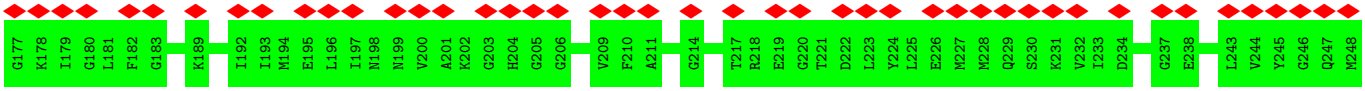


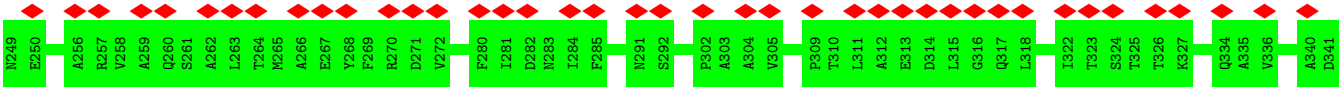
• Molecule 25: ATP synthase subunit beta, mitochondrial

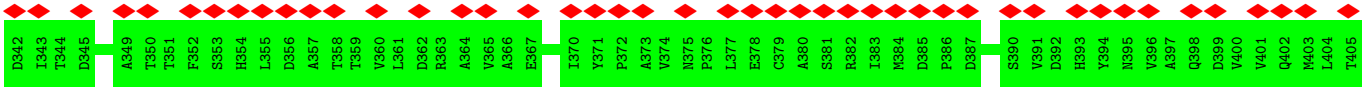
Chain D1:

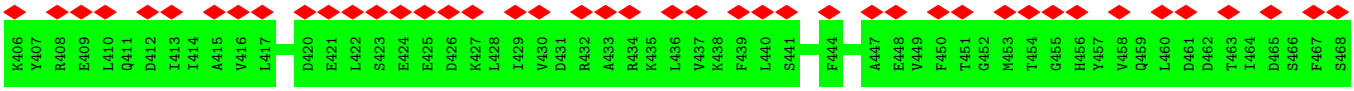


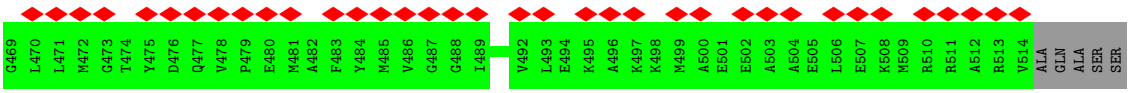






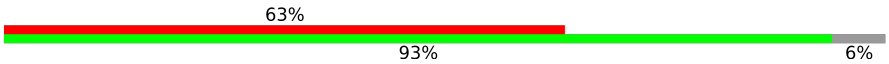


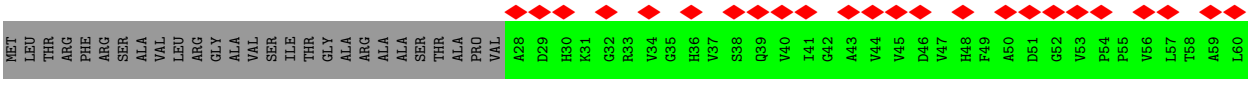


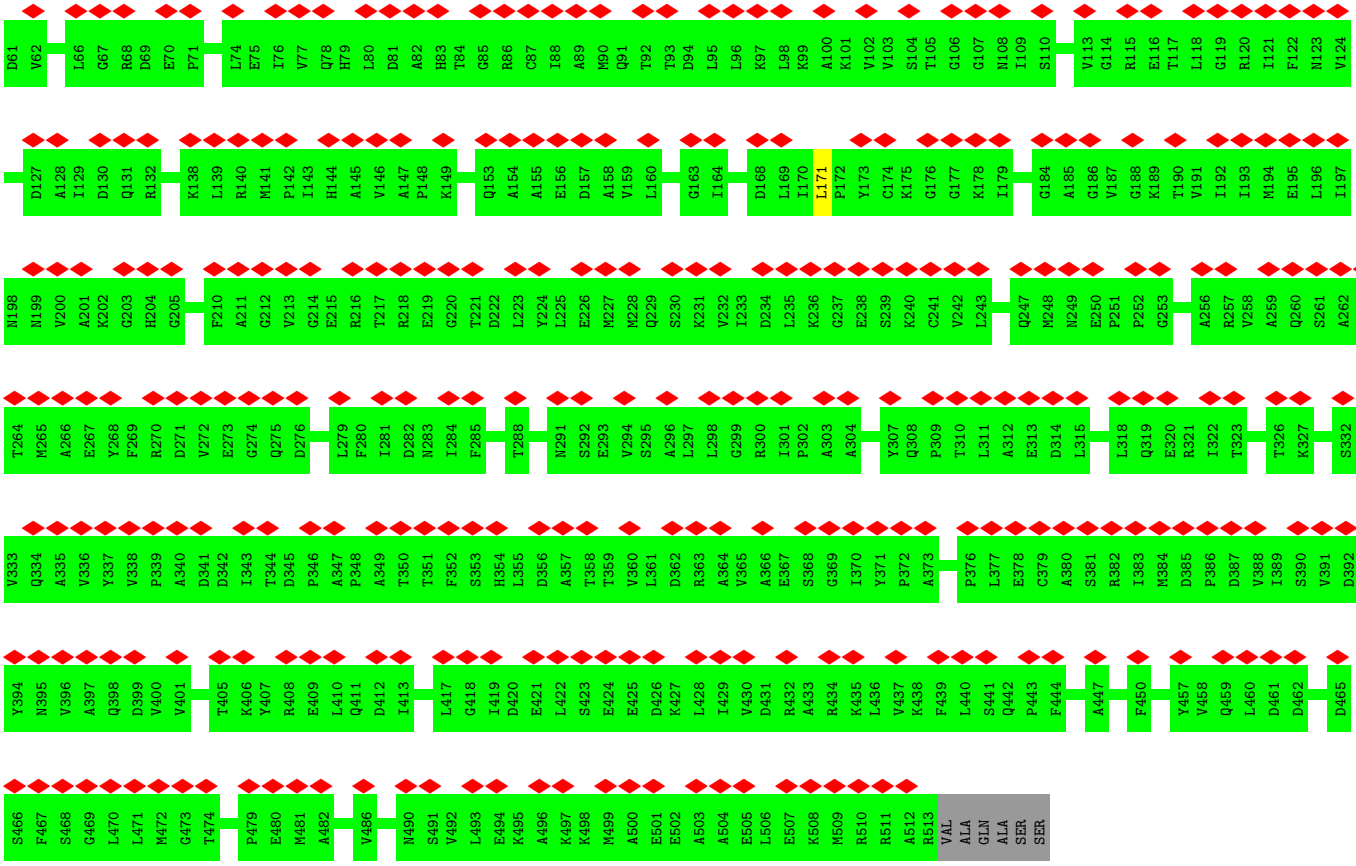


• Molecule 25: ATP synthase subunit beta, mitochondrial

Chain E1:

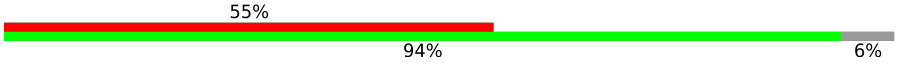


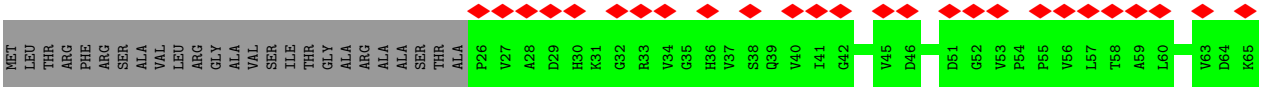


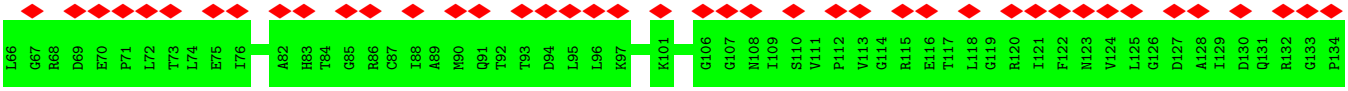


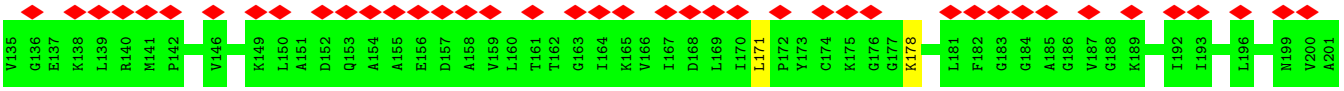
• Molecule 25: ATP synthase subunit beta, mitochondrial

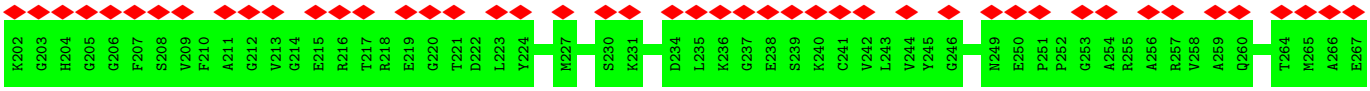
Chain F1:

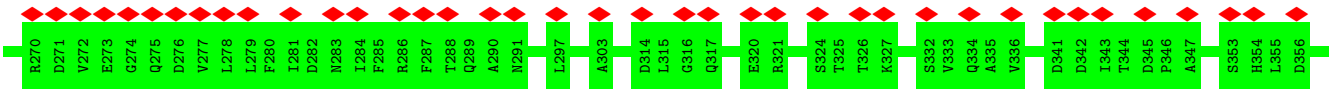


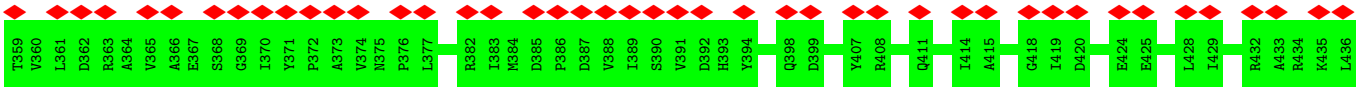













L440 S441 Q442 P443 F444 Q445 V446 A447 E448 V449 F450 T451 G452 M453 T454 G455 H456 Y457 V458 Q459 L460 D461
I464 D465 S466 F467 S468 G469 L470 L471 M472 G473 T474
Q477 V478 P479 E480 M481 A482 F483
G487 G488 I489 N490
L493 E494 K495 A496 K497 K498 M499 A500 E501 E502 A503
A504 E505 L506 E507 K508 M509 R510 R511 A512 R513 VAL ALA GLN ALA SER SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11035	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 ($e^-/Å^2$)	33	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.081	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CDL, UTP, LMT, PC1, PEE, AME, Q7G, ATP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	L	0.24	0/547	0.44	0/735
1	l	0.24	0/547	0.44	0/735
2	M	0.25	0/1049	0.42	0/1423
2	m	0.25	0/1049	0.42	0/1423
3	a	0.36	0/2111	0.41	0/2861
4	c	0.33	0/772	0.46	0/1054
5	d	0.25	0/2786	0.50	0/3760
6	e	0.28	0/3305	0.45	0/4482
7	f	0.31	0/1183	0.49	0/1601
8	g	0.24	0/1953	0.44	0/2650
9	h	0.24	0/1088	0.39	0/1466
10	i	0.31	0/913	0.47	0/1240
11	j	0.27	0/1462	0.48	0/1973
12	k	0.28	0/904	0.49	0/1228
13	n	0.32	0/1166	0.45	0/1581
14	o	0.27	0/814	0.39	0/1100
15	p	0.29	0/707	0.44	0/957
16	q	0.30	0/799	0.49	0/1091
17	r	0.30	0/567	0.45	0/767
18	H1	0.29	0/1274	0.46	0/1728
19	I1	0.24	0/547	0.50	0/738
20	J1	0.24	0/1342	0.39	0/1810
20	K1	0.24	0/1342	0.39	0/1810
20	L1	0.24	0/1337	0.39	0/1803
21	M1	0.24	0/1916	0.41	0/2591
22	O1	0.25	0/574	0.41	0/777
22	P1	0.25	0/574	0.39	0/777
22	Q1	0.25	0/574	0.39	0/777
22	R1	0.25	0/574	0.40	0/777
22	S1	0.26	0/574	0.42	0/777
22	T1	0.26	0/574	0.41	0/777
22	U1	0.25	0/574	0.42	0/777

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
22	V1	0.25	0/574	0.39	0/777
22	W1	0.25	0/574	0.40	0/777
22	X1	0.25	0/574	0.39	0/777
23	G1	0.26	0/2427	0.49	0/3268
24	A1	0.28	0/4113	0.47	0/5569
24	B1	0.27	0/4147	0.48	0/5616
24	C1	0.27	0/4123	0.47	0/5582
25	D1	0.27	0/3752	0.47	0/5087
25	E1	0.27	0/3738	0.47	0/5067
25	F1	0.26	0/3753	0.47	0/5088
All	All	0.27	0/63273	0.45	0/85654

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	L	63/92 (68%)	63 (100%)	0	0	100	100
1	l	63/92 (68%)	63 (100%)	0	0	100	100
2	M	127/144 (88%)	127 (100%)	0	0	100	100
2	m	127/144 (88%)	127 (100%)	0	0	100	100
3	a	229/231 (99%)	227 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	c	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
5	d	328/370 (89%)	317 (97%)	10 (3%)	1 (0%)	41	74
6	e	381/396 (96%)	376 (99%)	5 (1%)	0	100	100
7	f	133/145 (92%)	130 (98%)	3 (2%)	0	100	100
8	g	266/269 (99%)	264 (99%)	2 (1%)	0	100	100
9	h	135/157 (86%)	134 (99%)	1 (1%)	0	100	100
10	i	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
11	j	166/169 (98%)	163 (98%)	3 (2%)	0	100	100
12	k	103/124 (83%)	100 (97%)	3 (3%)	0	100	100
13	n	137/156 (88%)	129 (94%)	8 (6%)	0	100	100
14	o	94/101 (93%)	93 (99%)	1 (1%)	0	100	100
15	p	78/105 (74%)	76 (97%)	2 (3%)	0	100	100
16	q	83/98 (85%)	82 (99%)	1 (1%)	0	100	100
17	r	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
18	H1	159/182 (87%)	155 (98%)	3 (2%)	1 (1%)	25	62
19	I1	63/75 (84%)	59 (94%)	4 (6%)	0	100	100
20	J1	164/188 (87%)	160 (98%)	4 (2%)	0	100	100
20	K1	164/188 (87%)	163 (99%)	1 (1%)	0	100	100
20	L1	163/188 (87%)	163 (100%)	0	0	100	100
21	M1	230/255 (90%)	221 (96%)	9 (4%)	0	100	100
22	O1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
22	P1	76/118 (64%)	76 (100%)	0	0	100	100
22	Q1	76/118 (64%)	76 (100%)	0	0	100	100
22	R1	76/118 (64%)	76 (100%)	0	0	100	100
22	S1	76/118 (64%)	76 (100%)	0	0	100	100
22	T1	76/118 (64%)	76 (100%)	0	0	100	100
22	U1	76/118 (64%)	76 (100%)	0	0	100	100
22	V1	76/118 (64%)	76 (100%)	0	0	100	100
22	W1	76/118 (64%)	76 (100%)	0	0	100	100
22	X1	76/118 (64%)	76 (100%)	0	0	100	100
23	G1	298/305 (98%)	290 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	A1	517/584 (88%)	513 (99%)	4 (1%)	0	100	100
24	B1	525/584 (90%)	515 (98%)	10 (2%)	0	100	100
24	C1	518/584 (89%)	511 (99%)	6 (1%)	1 (0%)	47	79
25	D1	486/519 (94%)	478 (98%)	8 (2%)	0	100	100
25	E1	484/519 (93%)	471 (97%)	13 (3%)	0	100	100
25	F1	486/519 (94%)	473 (97%)	13 (3%)	0	100	100
All	All	7775/8943 (87%)	7644 (98%)	128 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	H1	158	ASP
5	d	34	THR
24	C1	532	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	55/75 (73%)	55 (100%)	0	100	100
1	l	55/75 (73%)	55 (100%)	0	100	100
2	M	111/124 (90%)	111 (100%)	0	100	100
2	m	111/124 (90%)	111 (100%)	0	100	100
3	a	225/225 (100%)	222 (99%)	3 (1%)	69	82
4	c	80/104 (77%)	79 (99%)	1 (1%)	69	82
5	d	297/334 (89%)	296 (100%)	1 (0%)	92	96
6	e	334/341 (98%)	333 (100%)	1 (0%)	92	96
7	f	119/124 (96%)	117 (98%)	2 (2%)	60	78
8	g	205/206 (100%)	205 (100%)	0	100	100
9	h	110/123 (89%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	i	95/96 (99%)	95 (100%)	0	100	100
11	j	149/150 (99%)	149 (100%)	0	100	100
12	k	91/107 (85%)	91 (100%)	0	100	100
13	n	123/137 (90%)	123 (100%)	0	100	100
14	o	82/86 (95%)	81 (99%)	1 (1%)	71	84
15	p	75/94 (80%)	75 (100%)	0	100	100
16	q	80/92 (87%)	80 (100%)	0	100	100
17	r	56/56 (100%)	56 (100%)	0	100	100
18	H1	137/156 (88%)	136 (99%)	1 (1%)	84	91
19	I1	58/67 (87%)	57 (98%)	1 (2%)	60	78
20	J1	145/162 (90%)	145 (100%)	0	100	100
20	K1	145/162 (90%)	145 (100%)	0	100	100
20	L1	145/162 (90%)	145 (100%)	0	100	100
21	M1	200/215 (93%)	200 (100%)	0	100	100
22	O1	56/89 (63%)	55 (98%)	1 (2%)	59	77
22	P1	56/89 (63%)	55 (98%)	1 (2%)	59	77
22	Q1	56/89 (63%)	55 (98%)	1 (2%)	59	77
22	R1	56/89 (63%)	55 (98%)	1 (2%)	59	77
22	S1	56/89 (63%)	54 (96%)	2 (4%)	35	63
22	T1	56/89 (63%)	54 (96%)	2 (4%)	35	63
22	U1	56/89 (63%)	55 (98%)	1 (2%)	59	77
22	V1	56/89 (63%)	55 (98%)	1 (2%)	59	77
22	W1	56/89 (63%)	55 (98%)	1 (2%)	59	77
22	X1	56/89 (63%)	55 (98%)	1 (2%)	59	77
23	G1	253/257 (98%)	252 (100%)	1 (0%)	91	95
24	A1	434/479 (91%)	433 (100%)	1 (0%)	93	97
24	B1	438/479 (91%)	436 (100%)	2 (0%)	88	94
24	C1	436/479 (91%)	433 (99%)	3 (1%)	84	91
25	D1	399/420 (95%)	396 (99%)	3 (1%)	81	89
25	E1	397/420 (94%)	396 (100%)	1 (0%)	92	96
25	F1	399/420 (95%)	397 (100%)	2 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6599/7441 (89%)	6563 (100%)	36 (0%)	89 94

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	C1	95	PHE
25	F1	178	LYS
24	C1	181	TYR
25	D1	171	LEU
22	P1	42	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
24	B1	115	GLN
24	B1	514	ASN
24	B1	463	ASN
25	E1	78	GLN
20	J1	175	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

Mogul failed to run properly - this section is therefore empty.

5.5 Carbohydrates (i)

Mogul failed to run properly - this section is therefore empty.

5.6 Ligand geometry (i)

Mogul failed to run properly - this section is therefore empty.

5.7 Other polymers (i)

Mogul failed to run properly - this section is therefore empty.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

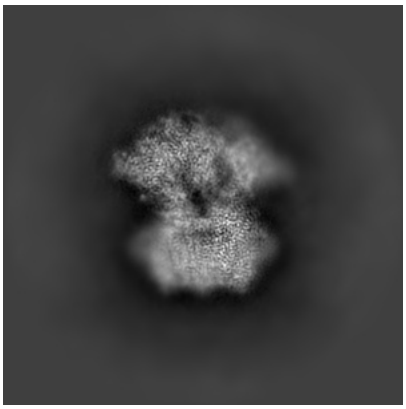
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15571. These allow visual inspection of the internal detail of the map and identification of artifacts.

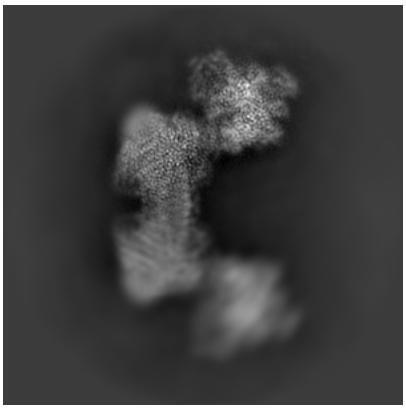
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

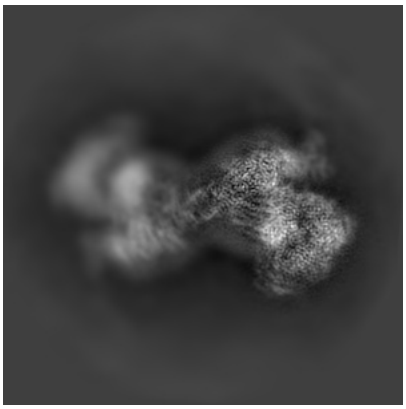
6.1.1 Primary map



X

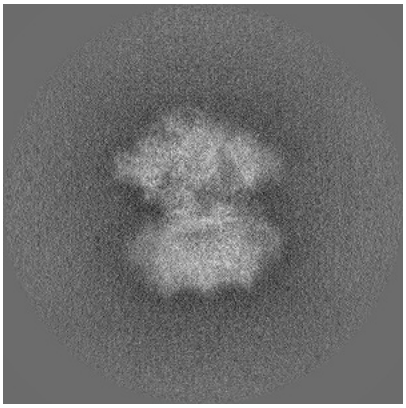


Y

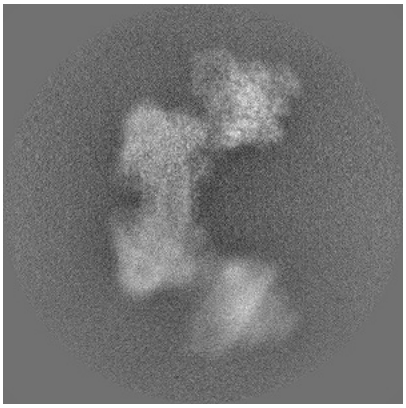


Z

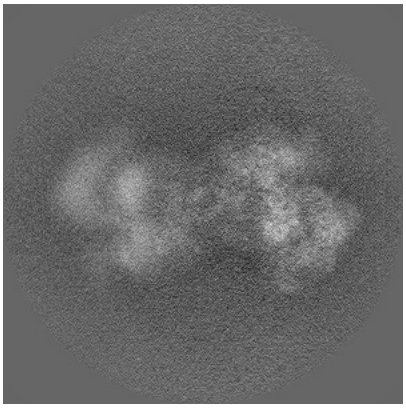
6.1.2 Raw map



X



Y

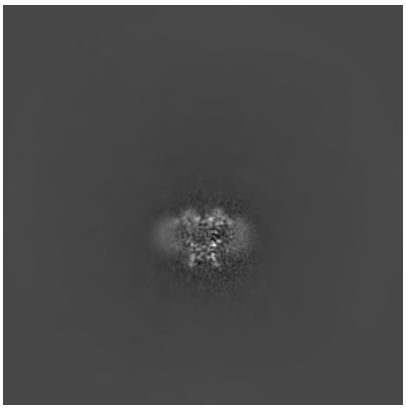


Z

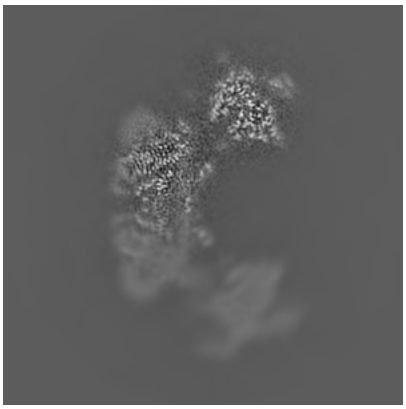
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

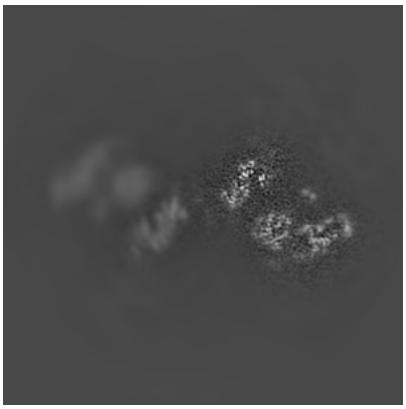
6.2.1 Primary map



X Index: 280

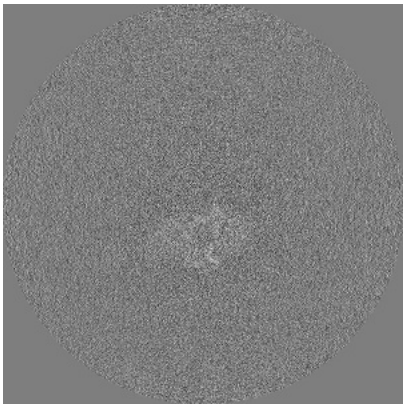


Y Index: 280

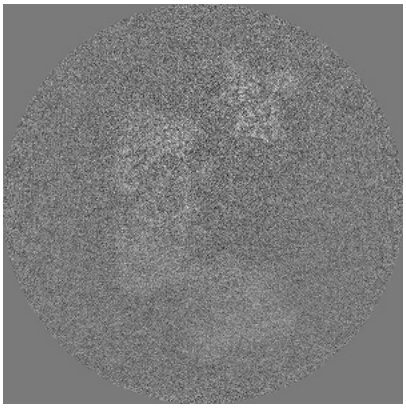


Z Index: 280

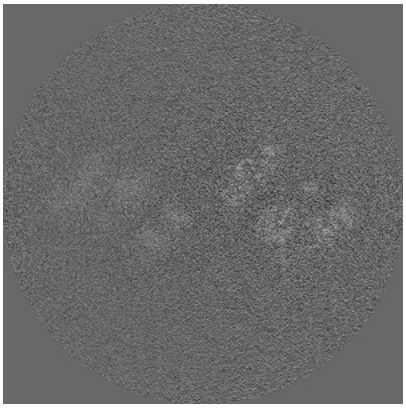
6.2.2 Raw map



X Index: 280



Y Index: 280

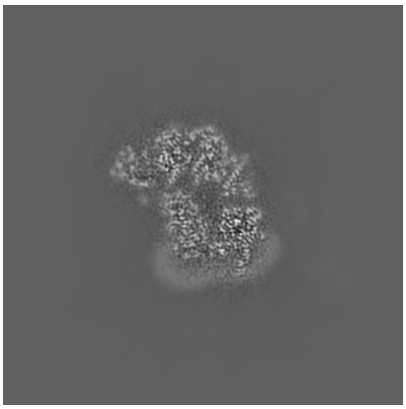


Z Index: 280

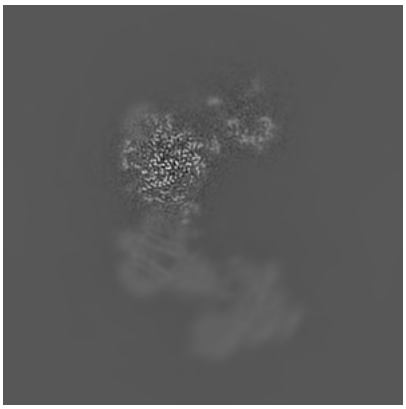
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

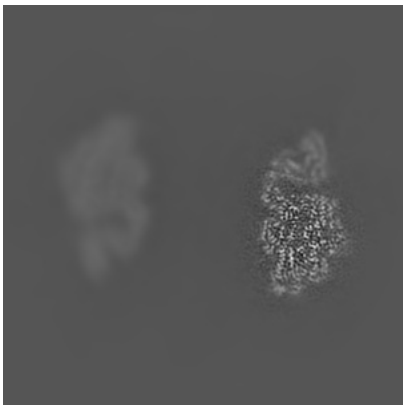
6.3.1 Primary map



X Index: 377

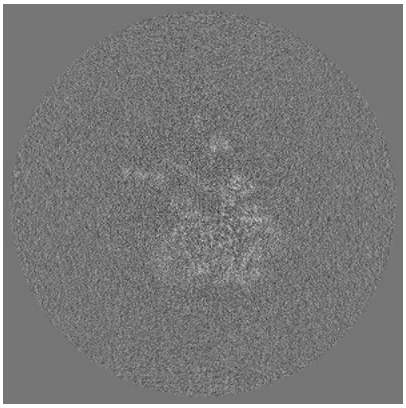


Y Index: 305

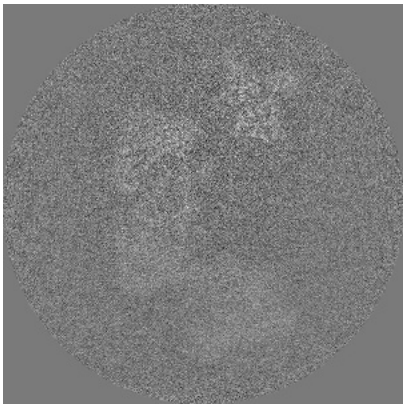


Z Index: 343

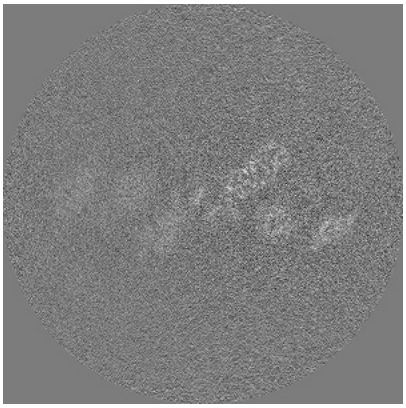
6.3.2 Raw map



X Index: 360



Y Index: 280



Z Index: 271

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

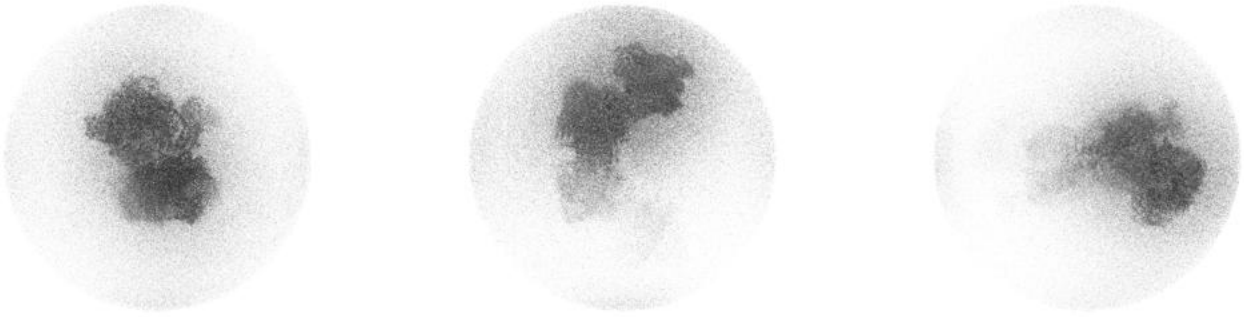
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

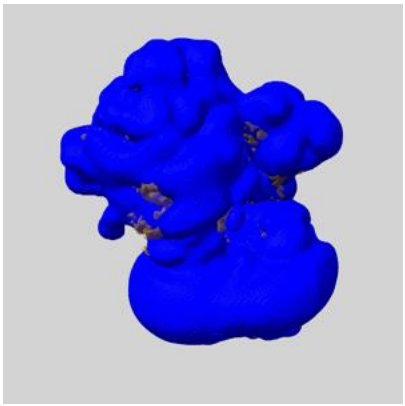
6.5 Mask visualisation (i)

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

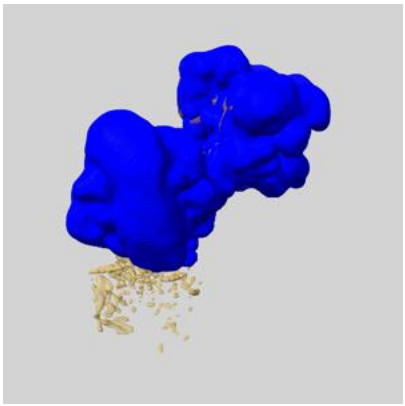
A mask typically either:

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

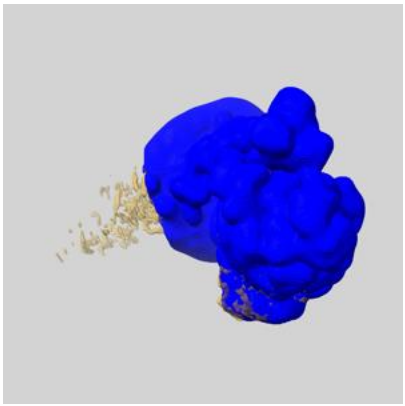
6.5.1 emd_15571_msk_1.map (i)



X



Y

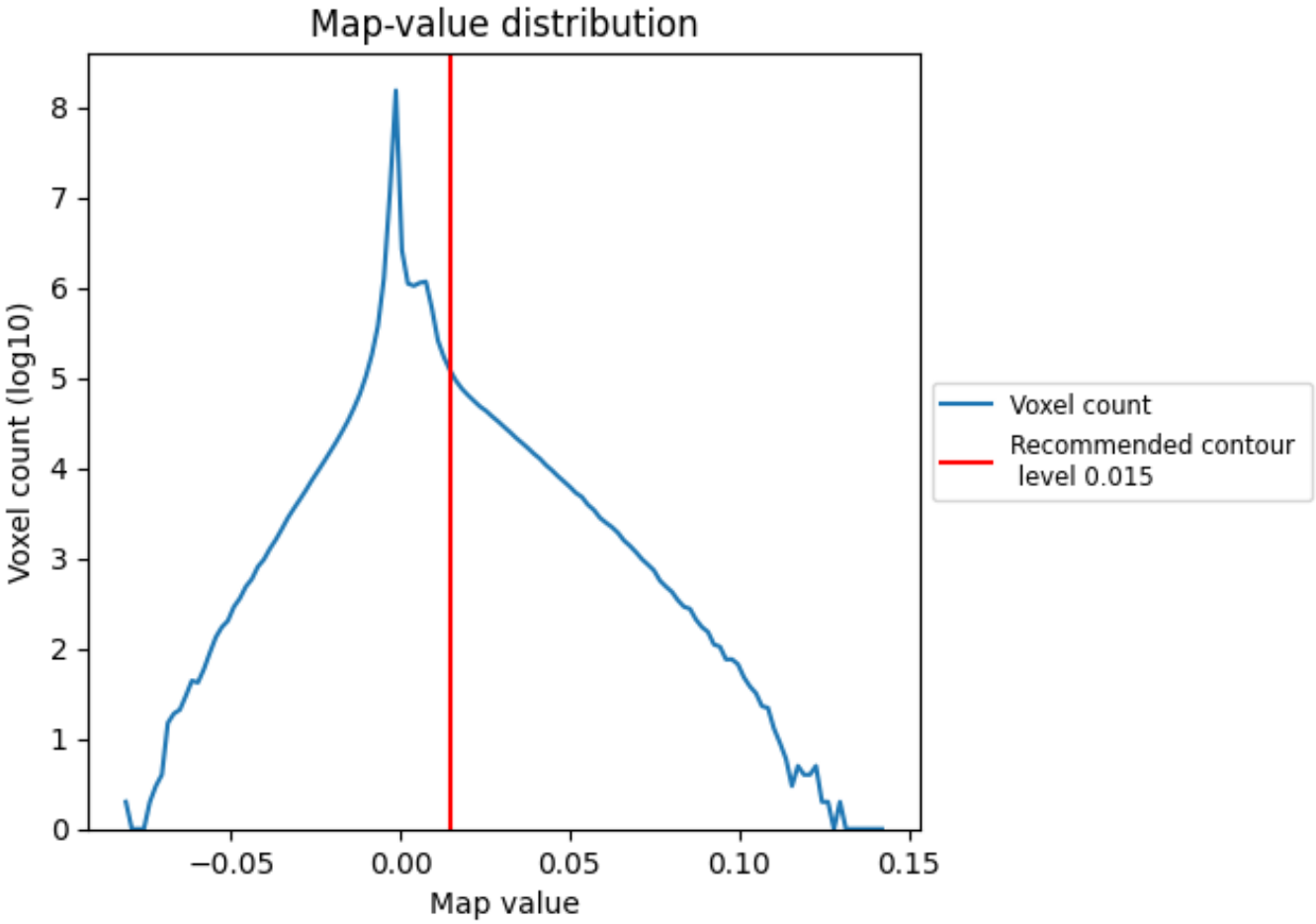


Z

7 Map analysis

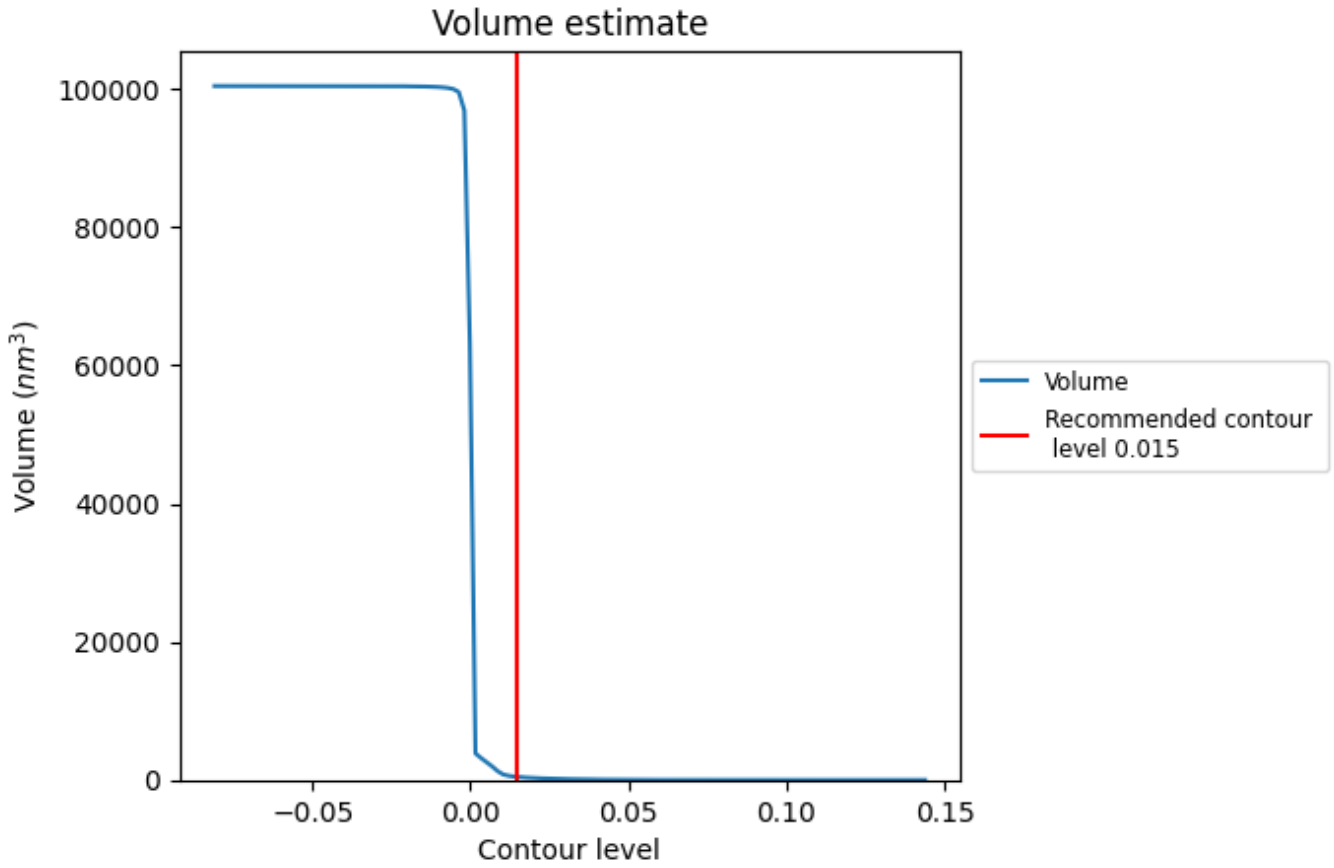
This section contains the results of statistical analysis of the map.

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.

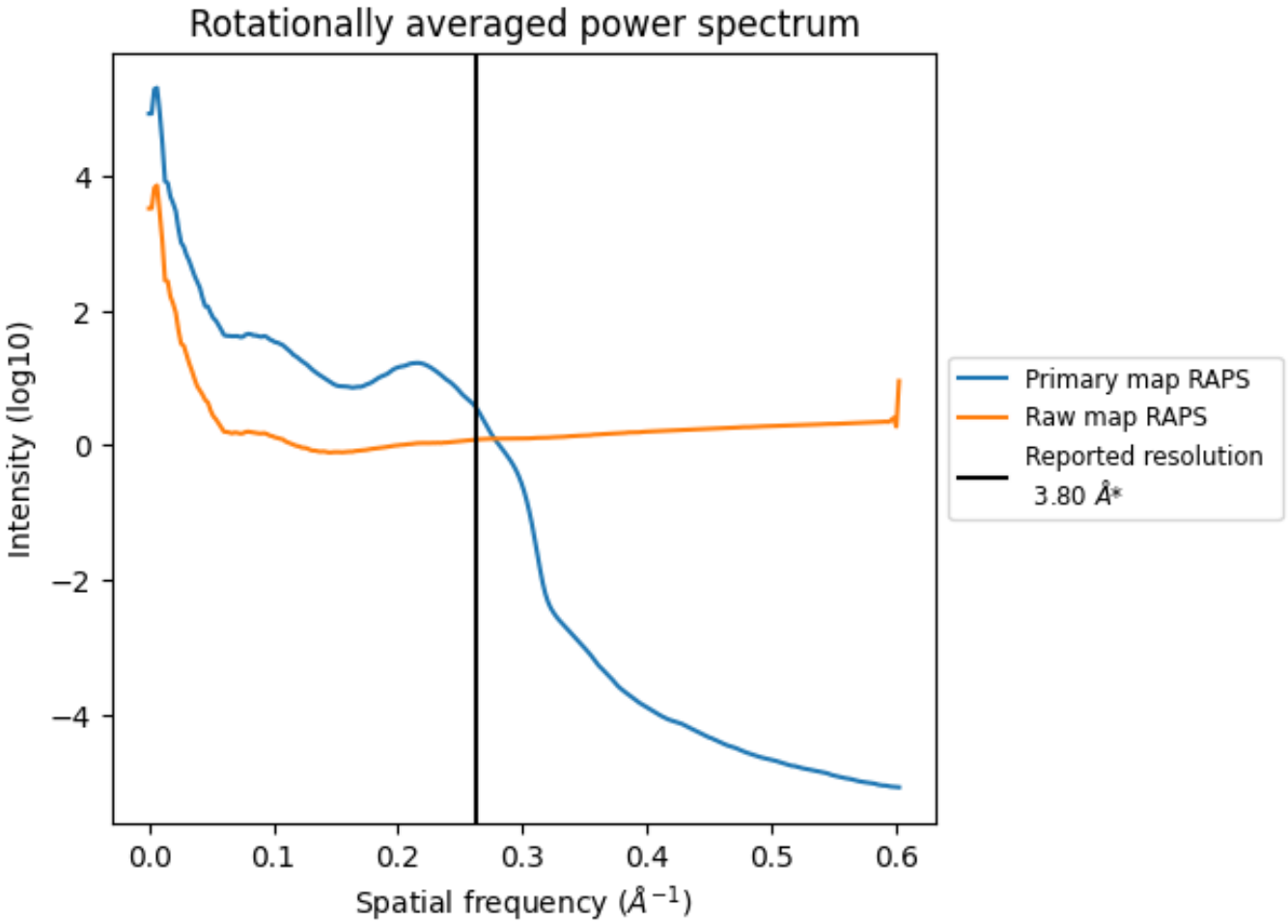
7.2 Volume estimate (i)



The volume at the recommended contour level is 440 nm^3; this corresponds to an approximate mass of 398 kDa.

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

7.3 Rotationally averaged power spectrum (i)

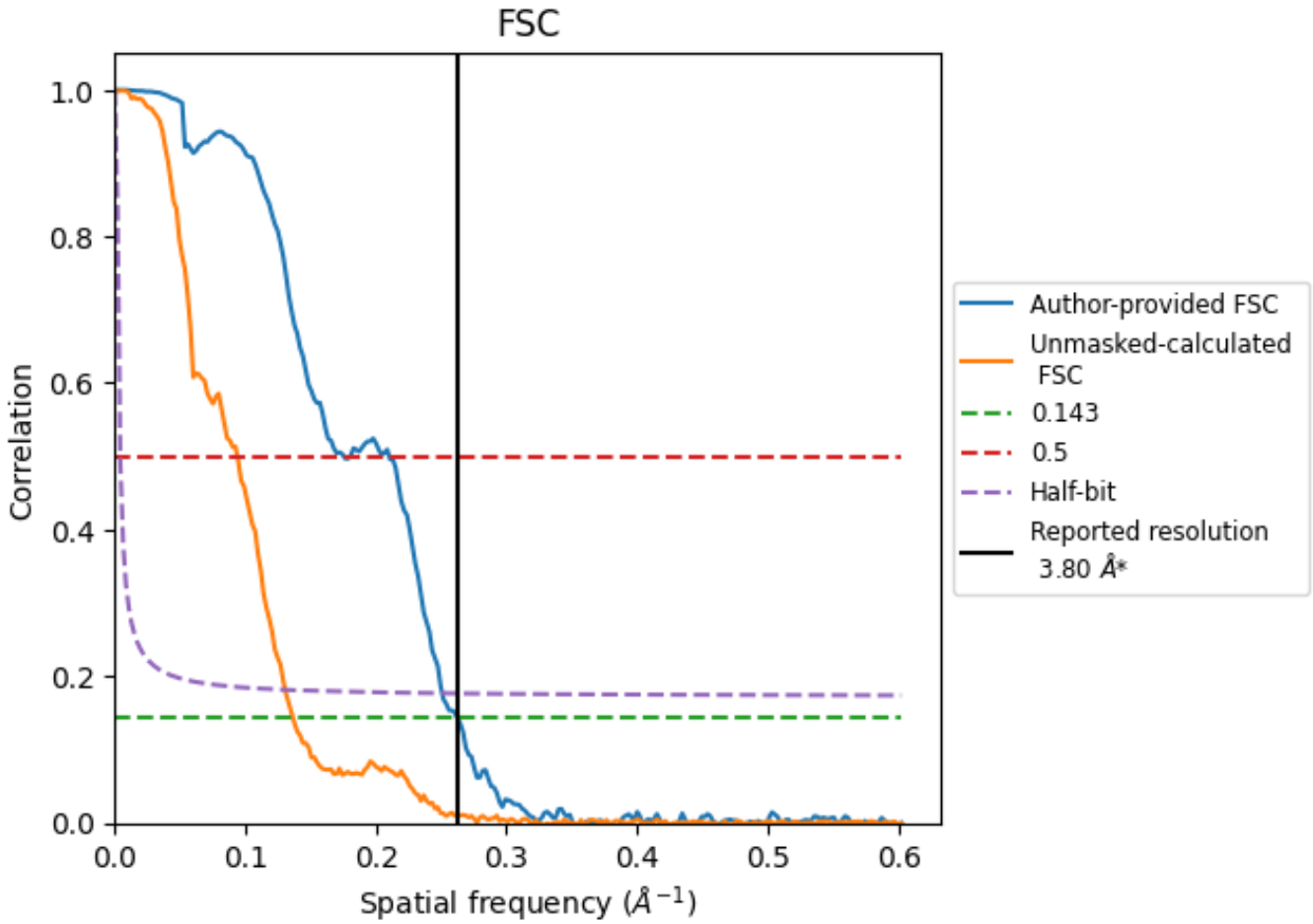


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

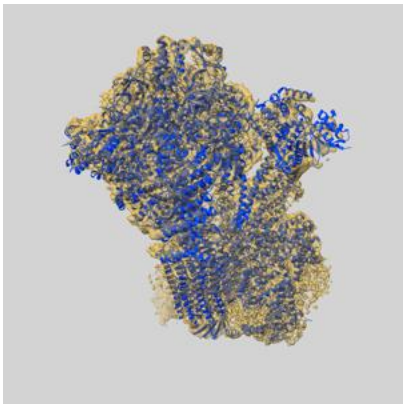
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	5.70	3.99
Unmasked-calculated*	7.33	10.65	7.66

*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 7.33 differs from the reported value 3.8 by more than 10 %

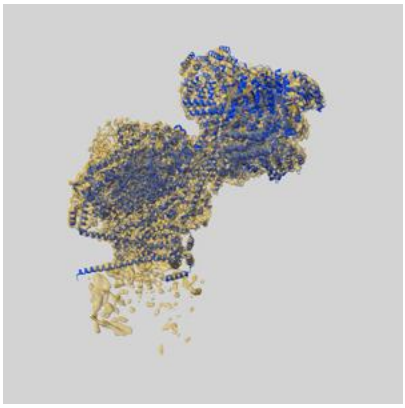
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15571 and PDB model 8APH. Per-residue inclusion information can be found in section 3 on page 16.

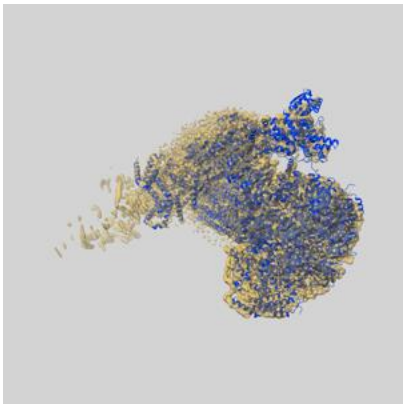
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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

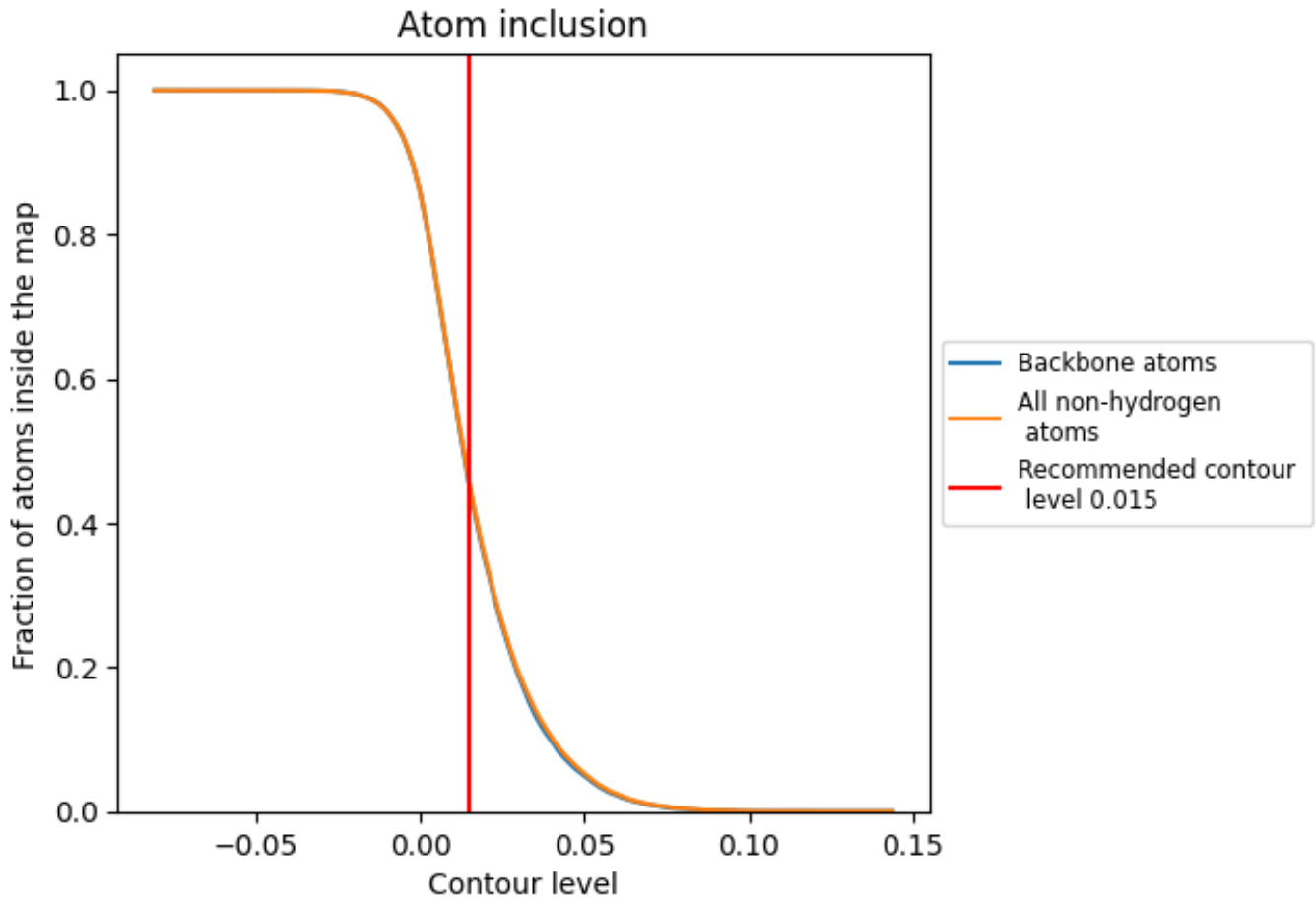
This section was not generated.

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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 45% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.4549
A1	0.2766
B1	0.3093
C1	0.4851
D1	0.3708
E1	0.3056
F1	0.3653
G1	0.3887
H1	0.3631
I1	0.2674
J1	0.2764
K1	0.3672
L	0.4655
L1	0.3076
M	0.4564
M1	0.4252
O1	0.2977
P1	0.2638
Q1	0.2620
R1	0.2460
S1	0.2995
T1	0.3440
U1	0.3422
V1	0.3066
W1	0.2406
X1	0.2389
a	0.8218
c	0.7228
d	0.5754
e	0.7663
f	0.7796
g	0.1491
h	0.1866
i	0.8240
j	0.7228

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Chain	Atom inclusion
k	0.7199
l	0.4366
m	0.5264
n	0.8575
o	0.7636
p	0.7295
q	0.8043
r	0.8229