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

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 43
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)	${f EM} {f structures} \ (\#{f Entries})$
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%	29%						
1	1	92	25%	29%						
2	М	144	90%	10%						
2	m	144	90%	10%						
3	a	231	99%	•						
4	с	114	75%	• 25%						
5	d	370	28%	• 10%						
6	е	396	• 96%	·						
7	f	145	92%	• 7%						



Conti	nued fron	<i>i</i> previous	page									
Mol	Chain	Length	Quality of chain									
			86%									
8	g	269	100%									
			71%									
9	h	157	87% 13%									
			_									
10	i	104	99%									
1.1		1.00	÷									
11	J	169	99%	•								
10	1.	194	9%									
12	К	124	85%	15%								
13	n	156	9 00/	110/								
10	11	100										
14	0	101	94%	• 5%								
	-		•									
15	р	105	76%	24%								
	-											
16	q	98	87%	13%								
			_									
17	r	62	100%									
10	114	100	49%									
18	HI	182	87%	• 12%								
10	T1	75	64%									
19	11	61										
20	T1	188	000/	1.20/								
	01	100	50%	12 %								
20	K1	188	88%	12%								
			57%									
20	L1	188	88%	12%								
			43%									
21	M1	255	92%	8%								
			42%									
22	01	118	65% •	34%								
	D1	110	49%									
22	PI	118	65% ·	34%								
22	01	119	4970	240/								
		110	52% •	34%								
22	R1	118	65%	34%								
	101	110	47%									
22	S1	118	64% ·	34%								
			44%									
22	T1	118	64%	34%								
			45%									
22	U1	118	65% .	34%								
	T.T	4.4.0	46%									
22	V1	118	65%	34%								
0.0	1171	110	50%									
22	VV 1	118	•	34%								



Mol	Chain	Length	Quality of chain	Quality of chain						
			49%							
22	X1	118	65% •	34%						
	<i></i>		54%							
23	G1	305	98%	•						
			64%							
24	A1	584	89%	10%						
0.1	D1	504	61%							
24	BI	584	90%	9%						
0.1	C1	594	35%							
24	UI	384	<u> </u>	• 10%						
25	D1	510	J+ /0	60/						
20		519	63%	• 6%						
25	E1	519	029/	60/						
	1.71	515	55%	0%						
25	F1	519	94%	6%						

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	е	407	Х			-
29	Q7G	n	201	Х	-	-	-



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.

Mol	Chain	Residues	Atoms						AltConf	Trace
1 L	65	Total	С	Η	Ν	Ο	S	0	0	
	Г	05	1082	340	545	104	92	1	0	0
1 1	1	65	Total	С	Н	Ν	Ο	S	0	0
	1	00	1082	340	545	104	92	1	0	0

• Molecule 1 is a protein called subunit-e.

• Molecule 2 is a protein called subunit-g.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2 M	120	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
	111	129	2069	662	1042	177	186	2	0	0
2 m	120	Total	С	Η	Ν	0	S	0	0	
	111	129	2069	662	1042	177	186	2	0	0

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

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

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	С	86	Total 1460	C 494	Н 715	N 116	O 130	${ m S}{ m 5}$	0	0

• Molecule 5 is a protein called subunit-d.



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

• Molecule 6 is a protein called ATPTB1.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
6	е	383	Total 6270	C 2060	Н 3050	N 558	O 585	${ m S}$ 17	0	0

• Molecule 7 is a protein called subunit-f.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
7	f	135	Total 2256	С 744	H 1111	N 201	O 195	${ m S}{ m 5}$	0	0

• Molecule 8 is a protein called ATPTB3.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
8	g	268	Total	C 1911	H 2020	N 242	$\begin{array}{c} 0 \\ 278 \end{array}$	S 1	0	0
			3905	1211	2020	343	310	T		

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			Atom	.S			AltConf	Trace
9	h	137	Total 2158	C 680	Н 1088	N 184	O 203	${ m S} { m 3}$	0	0

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

Mol	Chain	Residues			Aton	ns			AltConf	Trace
10	i	103	Total 1740	C 574	Н 857	N 152	0 151	S 6	0	0

• Molecule 11 is a protein called ATPTB6.



Mol	Chain	Residues			Atom	IS			AltConf	Trace
11	j	168	Total 2835	C 919	H 1411	N 249	O 249	${ m S} 7$	0	0

• Molecule 12 is a protein called subunit-k.

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

• Molecule 13 is a protein called ATPTB11.

Mol	Chain	Residues			Atom	S			AltConf	Trace
13	n	139	Total 2210	C 730	Н 1082	N 183	O 208	${f S}{7}$	0	0

• Molecule 14 is a protein called ATPTB12.

Mol	Chain	Residues			Aton	ıs			AltConf	Trace
14	О	96	Total 1556	C 506	Н 767	N 140	O 140	${ m S} { m 3}$	0	0

• Molecule 15 is a protein called subunit-b.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
15	р	80	Total 1335	C 448	Н 651	N 108	0 125	${ m S} { m 3}$	0	0

• Molecule 16 is a protein called ATPEG3.

Mol	Chain	Residues		Α	toms			AltConf	Trace
16	q	85	Total 1486	C 499	Н 720	N 142	O 125	0	0

• Molecule 17 is a protein called ATPEG4.

Mol	Chain	Residues		ŀ	Atom	s			AltConf	Trace
17	r	62	Total 1040	C 358	Н 498	N 94	O 85	${f S}{5}$	0	0

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



Mol	Chain	Residues			Atom	S			AltConf	Trace
19	Π1	161	Total	С	Η	Ν	0	\mathbf{S}	0	0
10	111	101	2483	788	1232	211	248	4	0	0

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

Mol	Chain	Residues			Atom	.S			AltConf	Trace
19	I1	65	Total 1046	C 332	Н 513	N 97	0 102	${ m S} { m 2}$	0	0

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

Mol	Chain	Residues			Aton	ns			AltConf	Trace
20	T1	166	Total	С	Η	Ν	0	\mathbf{S}	0	0
20	91	100	2591	822	1276	221	258	14	0	0
20	K1	166	Total	С	Η	Ν	0	\mathbf{S}	0	0
20	171	100	2591	822	1276	221	258	14	0	0
20	T 1	165	Total	С	Η	Ν	0	S	0	0
20		105	2581	819	1271	220	257	14	0	0

• Molecule 21 is a protein called OSCP.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
21	M1	234	Total 3750	C 1212	Н 1873	N 302	O 360	${ m S} { m 3}$	0	0

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

$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	Frace	AltConf			s	Atoms	A		Residues	Chain	Mol
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	0	0	S	0	Ν	Η	С	Total	79	01	- 22
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	0	0	4	96	89	600	376	1165	10	01	
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	0	0	S	Ο	Ν	Η	С	Total	70	D1	- 22
22 Q1 78 Total C H N O S 0 1165 376 600 89 96 4 0	0	0	4	96	89	600	376	1165	10	ГІ	
22 01 78 1165 376 600 89 96 4 0 1165 376 600 89 96 4 0 1165 376 600 89 96 4 0 10	0	0	S	Ο	Ν	Η	С	Total	70	01	- 22
	0	0	4	96	89	600	376	1165	10	QI	
22 P1 79 Total C H N O S 0	0	0	S	Ο	Ν	Η	С	Total	70	D1	- 22
$\begin{bmatrix} 22 & R1 & 78 & 1165 & 376 & 600 & 89 & 96 & 4 \\ \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$	0	0	4	96	89	600	376	1165	10	n1	
22 S1 78 Total C H N O S 0	0	0	S	0	Ν	Н	С	Total	79	C 1	- 22
$\begin{bmatrix} 22 & 51 & 78 \\ 1166 & 376 & 601 & 89 & 96 & 4 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	0	0	4	96	89	601	376	1166	10	51	
22 T1 78 Total C H N O S 0	0	0	S	0	Ν	Н	С	Total	79	TT1	- 22
$\begin{bmatrix} 22 & 11 & 78 \\ 1166 & 376 & 601 & 89 & 96 & 4 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	0	0	4	96	89	601	376	1166	10	11	
22 III 78 Total C H N O S 0	0	0	S	Ο	Ν	Η	С	Total	78	TT1	22
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	0	0	4	96	89	600	376	1165	10		



Mol	Chain	Residues		A	Atoms	S			AltConf	Trace
าา	$\mathbf{V}1$	78	Total	С	Η	Ν	Ο	S	0	0
	V I	10	1165	376	600	89	96	4	0	0
าา	W/1	79	Total	С	Н	Ν	Ο	S	0	0
	VV 1	10	1165	376	600	89	96	4	0	0
าา	V1	79	Total	С	Н	Ν	Ο	S	0	0
		10	1165	376	600	89	96	4	0	0

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

Mol	Chain	Residues			Atom	S			AltConf	Trace
23	G1	300	Total 4774	C 1507	Н 2387	N 423	0 448	S 9	0	0

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

Mol	Chain	Residues			Atom	.S			AltConf	Trace
94	Δ.1	502	Total	С	Η	Ν	0	S	0	0
24	AI	525	8193	2587	4154	701	731	20	0	0
94	D1	520	Total	С	Η	Ν	0	S	0	0
24	DI	529	8260	2603	4187	709	741	20	0	0
94	C1	594	Total	С	Η	Ν	0	S	0	0
24	01	524	8219	2594	4170	703	732	20	0	0

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

Mol	Chain	Residues			Atom	.s			AltConf	Trace
25	D1	199	Total	С	Η	Ν	0	\mathbf{S}	0	0
20		400	7446	2334	3750	632	711	19	0	0
25	F 1	486	Total	С	Η	Ν	0	S	0	0
20	171	400	7414	2324	3732	630	709	19	0	0
25	F 1	199	Total	С	Η	Ν	0	S	0	0
20	L L	400	7446	2334	3750	632	711	19	0	0

• 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
200	т	1	Total C H	O P	0
26	L	1	256 81 156	17 2	0
90	М	1	Total C H	O P	0
20	IVI	1	256 81 156	17 2	0
00	_	1	Total C H	O P	0
20	С	1	256 81 156	17 2	0
26		1	Total C H	O P	0
20	е	1	1280 405 780	85 10	0
26	0	1	Total C H	O P	0
20	е	1	1280 405 780	85 10	0
26	0	1	Total C H	O P	0
20	е	1	1280 405 780	85 10	0
26	0	1	Total C H	O P	0
20	е	1	1280 405 780	85 10	0
26	0	1	Total C H	0 P	0
20	е	1	1280 405 780	85 10	0
26	f	1	Total C H	O P	0
20	1	I	256 81 156	17 2	0
26	;	1	Total C H	O P	0
20	J	1	512 162 312	34 4	0
26	;	1	Total C H	O P	0
20	J	1	512 162 312	34 4	0
26	1	1	Total C H	O P	0
	1	1	256 81 156	17 2	U
26	m	1	Total C H	0 P	0
20	111	1	256 81 156	17 2	U
26	0	1	Total C H	0 P	0
20	Ч		256 81 156	17 2	U



• Molecule 27 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Atoms					AltConf
27 M	М	1	Total	С	Н	Ν	0	Р	0
	1	133	41	82	1	8	1	0	
27	97 f	1	Total	С	Η	Ν	0	Р	0
	1	133	41	82	1	8	1	0	
27	m	m 1	Total	С	Η	Ν	0	Р	0
			133	41	82	1	8	1	0

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





Mol	Chain	Residues	Atoms	AltConf
20	0	1	Total C H O	0
28	е	1	74 24 39 11	0
20	;	1	Total C H O	0
28	J	1	74 24 39 11	U

• Molecule 29 is 2-{[(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl}-4-{[(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy}butyl 4-O-alpha-D-glucopyranosyl-alp ha-D-glucopyranoside (three-letter code: Q7G) (formula: C₅₆H₉₂O₂₅).



Mol	Chain	Residues	Ato	AltConf		
29	е	1	Total C 108 38	Н 60	O 10	0
29	n	1	Total C 129 44	Н 70	0 15	0

• 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
20	f	1	Total	С	Η	Ν	Ο	Р	0
30	30 1	I	142	44	88	1	8	1	0
20	;	1	Total	С	Η	Ν	Ο	Р	0
30	1	1	142	44	88	1	8	1	0
20	;	1	Total	С	Η	Ν	Ο	Р	0
30	J	1	142	44	88	1	8	1	0
20	30 p	1	Total	С	Η	Ν	Ο	Р	0
- 50			142	44	88	1	8	1	U

• 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	
91	U1	1	Total	С	Η	Ν	Ο	Р	0
51	пі	1	40	9	11	2	15	3	0

• 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	Λ1	1	Total	С	Η	Ν	Ο	Р	0	
	1	43	10	12	5	13	3	0		
20	D1	D1	1	Total	С	Η	Ν	Ο	Р	0
32 D1	DI	T	43	10	12	5	13	3	0	
20	32 C1	1	Total	С	Η	Ν	0	Р	0	
32			43	10	12	5	13	3	0	
32	D1	D1 1	Total	С	Η	Ν	0	Р	0	
			43	10	12	5	13	3	0	

• 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 1 1	0
33	B1	1	Total Mg 1 1	0
33	C1	1	Total Mg 1 1	0
33	D1	1	Total Mg 1 1	0

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	
24	F 1	1	Total	С	Η	Ν	Ο	Р	0
- 54	171	I	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 a:	99%				
M1 F144 C149 F169 V231					
• Molecule 4: subunit-8					
Chain c:	75%	·	25%		
MET LEU LEU ARG ARG CLY CLY ASN ASN ASN ASN ASN ASN ASN ASN ASN ATA TYR TYR TYR	VAL PRO ARG ARG HIS HIS E97 E97 E97	q101 4102 1105 1105 1108 1108 R110	L112		
• Molecule 5: subunit-d					
Chain d:	89%		• 10%		
MET ARG ARG VAL SER SER PRO ASC ASC ASC ASC ASC ASC ASC ASC ASC ASC	Y25 F26 P27 P28 T30 T31 S32 S32 S32 S32 S32 N35	Ra6 E37 D38 039 140 M3 M3 146	A47 151 K52 R53 R64	E85 K86 L87 E137	R145
El 48 A1 49 K150 E151 A155 A155 A155 A155 A156 E161 E161 E161 E162 E163 E164 C164 C165 C165 C165 C165 C165 C165 C165 C165	P169 V170 P171 P171 R172 N172 N175 P176 P176 Q177 S180 S180	5101 5182 1183 0194 8185 7185 7185 7185 7188 7188	K191 R192 Y195 D196 T197	A199 8200 7201 7202 1203 8204	2005 E207
Y217 R218 R218 A321 A321 A321 A321 C122 R323 N324 P326 R323 R324 CLN THR CLN THR CLN THR CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	N3355 A3355 B3355 B3355 B3355 C355 C35	L345 L347 Q348 A349 R350 I351 N352 Q353 R354	ASP CLU VAL GLU PRO SER CLN GLU GLU	GLN LYS LYS LYS ALA HIS HIS	
• Molecule 6: ATPTB1					
Chain e:	96%		·		
M1 G103 G103 P114 P114 C103 C1	ARG HIS THR ALA				
• Molecule 7: subunit-f					
Chain f:	92%		• 7%		
MET V2 N42 N42 SUY C2 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1					
• Molecule 8: ATPTB3	0.0%				
Chain g:	100%				
MET S2 K3 P4 P4 P5 F7 F7 F7 F7 F7 F1 S9 A10 C11 F1 A12 C11 S1 C11 F1	Q18 q 319 4 219 4 221 4 723 4 123 4 724 4 726 4 726 4 728 4 729 729 729 729 729 729 729 729 729 729	629 630 131 132 133 6 133 134 136 136 136	K38 E39 A40 G41 F42 H43	V45 V46 V47 G48 P49 E50 T51	F52 153 G54 V55 H56 T57 A58 V59 V59

• Molecule 3: ATP synthase subunit a







MET LEU LEU ARG SER SER ALA ALA ALA ALA ARG THE PRO PRO PRO	Stern G20 G20 R33 R41 F41 L44 F41 F41 L44 F41 F41 F41 F41 F41 F41 F41 F41 F41 F	◆ 	
• Molecule 13: ATPTB	11	-	
Chain n:	89%	11%	
MET LEU LEU LYS LYS PRO THR ALA MET ALA ALA ALA ARG ALA ALSU ALEU	P14 D74 H75 F156		
• Molecule 14: ATPTB	12		
Chain o:	94%	• 5%	
MET SER SER SER FIL FIL FIL FIL FIL FIL FIL FIL FIL FIL			
• Molecule 15: subunit-	b		
Chain p:	76%	24%	
MET LEU ARG ARG ARG LEU VAL PRO PRO ARA MET ARA ALA ALA ALA	ALIAR ALIA LLEU CYS SER SER ARG GLY K47 K47 C F25 B61 D61 D61 D61		
• Molecule 16: ATPEG	3		
Chain q:	87%	13%	
MET THR GLU ASN ASN ASN ASN ASN MET SER THP S14 MI S14 MI S14 MI S14 MI S14 MI S14 MI S14 MI S14 MI S14 MI S14 MI S14 MI S14 MI S14 MI S11 MI S11 MI S11 MI S11 MI S11 MI S11 MI S11 MI S11 MI S11 MI S11 MI S11 MI S11 MI S12 MI S11 MI S12 MI MI MI MI MI MI MI MI MI MI MI MI MI			
• Molecule 17: ATPEG	4		
Chain r:	100%		
HR 22			
• Molecule 18: ATP syr	nthase, epsilon chain, putative		
Chain H1:	49% 87%	• 12%	
MET PHE ARG CLFR CLEU CLEU CLEU CVA CVA CVA CVA CVA CVA CVA CVA CVA CVA	SER ALA ALA HZ2 HZ2 D23 F28 F28 H33 H33 V35 V35 V35 V35 V35 V35 D39	140 441 441 442 645 848 149 149 149 149 149 149 851 851 850 859	F664 F665 V67





• Molecule 19: ATP synthase subunit epsilon, mitochondrial





• Molecule 20: ATP synthase subunit p18, mitochondrial



• Molecule 20: ATP synthase subunit p18, mitochondrial

































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	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	33	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM $(4k \ge 4k)$	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).

Mal	Chain	Bond lengths		Bond	angles
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	L	0.24	0/547	0.44	0/735
1	1	0.24	0/547	0.44	0/735
2	М	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	с	0.33	0/772	0.46	0/1054
5	d	0.25	0/2786	0.50	0/3760
6	е	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	0	0.27	0/814	0.39	0/1100
15	р	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	01	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



Mal	Chain	Bond	lengths	Bond	angles
	Unam	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 (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
1	L	63/92~(68%)	63~(100%)	0	0	100	100
1	1	63/92~(68%)	63~(100%)	0	0	100	100
2	М	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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Bercenti	
4	с	84/114~(74%)	83~(99%)	1 (1%)	0	100	100
5	d	328/370~(89%)	317~(97%)	10 (3%)	1 (0%)	41	74
6	е	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	О	94/101~(93%)	93 (99%)	1 (1%)	0	100	100
15	р	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	01	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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
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 side chain 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	Perce	ntiles
1	L	55/75~(73%)	55~(100%)	0	100	100
1	1	55/75~(73%)	55~(100%)	0	100	100
2	М	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	с	80/104~(77%)	79~(99%)	1 (1%)	69	82
5	d	297/334~(89%)	296 (100%)	1 (0%)	92	96
6	е	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



Mol	Chain	Analysed	Rotameric Outliers		Perce	ntiles
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	О	82/86~(95%)	81 (99%)	1 (1%)	71	84
15	р	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%)	145 (100%) 0 10		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%) 8		84	91
25	D1	399/420~(95%)	396 (99%)	(99%) 3 (1%) 81 89		89
25	E1	397/420~(94%)	396 (100%)	1 (0%)	92	96
25	F1	399/420~(95%)	397 (100%) 2 (0%)		88	94



Continued from previous page...

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

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	a	144	PHE
3	a	149	CYS
3	a	169	PHE
4	с	66	TYR
5	d	205	ARG
6	е	268	TYR
7	f	42	ASN
7	f	62	TYR
14	0	64	TYR
18	H1	24	LEU
19	I1	39	ARG
22	01	42	THR
22	P1	42	THR
22	Q1	42	THR
22	R1	42	THR
22	S1	42	THR
22	S1	114	LEU
22	T1	42	THR
22	T1	98	PHE
22	U1	42	THR
22	V1	42	THR
22	W1	42	THR
22	X1	42	THR
23	G1	18	PHE
24	A1	181	TYR
$2\overline{4}$	B1	181	TYR
24	B1	281	TYR
24	C1	77	ASN
24	C1	95	PHE
24	C1	181	TYR
$\overline{25}$	D1	66	LEU
25	D1	116	GLU
$\overline{25}$	D1	171	LEU
25	E1	171	LEU
25	F1	171	LEU
25	F1	178	LYS



Mol	Chain	Res	Type
3	a	155	HIS
6	е	41	GLN
15	р	95	GLN
20	J1	82	GLN
20	J1	93	ASN
20	J1	108	GLN
20	J1	175	HIS
20	K1	74	ASN
22	V1	75	ASN
22	V1	85	ASN
23	G1	129	ASN
24	A1	502	HIS
24	A1	522	GLN
24	B1	81	GLN
24	B1	115	GLN
24	B1	398	GLN
24	B1	463	ASN
24	B1	514	ASN
25	E1	78	GLN
25	E1	144	HIS
25	F1	30	HIS
25	F1	411	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

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 (i)

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 (i)

6.1.1 Primary map



6.1.2 Raw map



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



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



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



6.4 Orthogonal surface views (i)

6.4.1 Primary map



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



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.



Mask visualisation (i) 6.5

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

$emd_{15571}msk_{1.map}$ (i) 6.5.1



Υ



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 440 $\rm nm^3;$ 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 ${\rm \AA^{-1}}$



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 0.263 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estim	Estimation criterion (FSC cut-off)			
resolution estimate (A)	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 (i)

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 (i)



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 (i)

This section was not generated.

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 (0.015).



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
М	0.4564
M1	0.4252
01	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
с	0.7228
d	0.5754
е	0.7663
f	0.7796
g	0.1491
h	0.1866
i	0.8240
j	0.7228





Chain	Atom inclusion
k	0.7199
1	0.4366
m	0.5264
n	0.8575
0	0.7636
р	0.7295
q	0.8043
r	0.8229

