

wwPDB EM Validation Summary Report (i)

Nov 30, 2022 – 05:12 pm GMT

DDB ID		8 A D 6
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EMDB ID	:	EMD-15559
Title	:	Trypanosoma brucei mitochondrial F1Fo ATP synthase dimer
Authors	:	Muehleip, A.; Gahura, O.; Zikova, A.; Amunts, A.
Deposited on	:	2022-08-09
Resolution	:	3.20 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 (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.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.20 Å.

Ramachandran outliers

Sidechain outliers

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		Percentile Ranks	Value
Ramachandran outliers			0.0%
Sidechain outliers			0.4%
	Worse		Better
	Percentile relativ	ve to all structures	
	Percentile relativ	ve to all EM structures	
[
Metric		Whole archive	EM structures
		(# Entries)	$(\# {\rm Entries})$

154571

154315

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.

4023

3826

Mol	Chain	Length	Quality of chain	
1	А	231	99%	·
1	a	231	99%	•
2	A1	584	9%91%	9%
2	A2	584	9%91%	9%
2	B1	584	8%	10%
2	B2	584	8%	10%
2	C1	584	5% 89%	10%
2	C2	584	5%	10%
3	С	114	• 74% •	25%



Mol	Chain	Length	Quality of chain	
3	с	114	• 74% •	25%
4	D	370	• 89%	10%
4	d	370	• 89%	10%
5	D1	519	10%	6%
5	D2	519	10%	6%
5	$\mathrm{E1}$	519	9%	6%
5	E2	519	9%	6%
5	F1	519	<u>8%</u> 94%	6%
5	F2	519	<u>8%</u> 94%	6%
6	Ε	396	96%	•••
6	е	396	96%	•••
7	F	145	92%	• 7%
7	f	145	92%	• 7%
8	G	269	10%	
8	g	269	10%	
9	G1	305	15%	•••
9	G2	305	98%	•••
10	Н	157	6% 87%	13%
10	h	157	<u>6%</u> 87%	13%
11	H1	182	8%	• 12%
11	H2	182	8%	• 12%
12	Ι	104	99%	•
12	i	104	99%	•
13	I1	75	87%	13%
13	I2	75	15% 87%	13%

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 Mol
 Chain
 Length



Chain Length Quality of chain Mol J 1416999% 14j 16999% 32% 15J1 188 88% 12% 32% J21518888% 12% 11% 15K118888% 12% 11% K21518888% 12% 21% 15L118888% 12% 21% L21518812% 88% Κ 124 1685% 15% i 16k 12485% 15% i 17L 92 71% 29% 92 1 1771% 29% 18 М 14489% • 10% 18 \mathbf{m} 14489% • 10% 12% 19M12558% 91% 11% 19M225591% 8% 20Ν 15688% 11% • 20156n 11% 88% Ο 21101• 5% 94% 21101• 5% 0 94% 22O111834% 66% 22O211866% 34% i 22P111866% 34% i P22211866% 34% 22Q111866% 34%



Mol	Chain	Length	Quality of chain	
22	Q2	118	• 66%	34%
22	R1	118	66%	34%
22	R2	118	6 6%	34%
22	S1	118	66%	34%
22	S2	118	66%	34%
22	T1	118	● 66%	34%
22	T2	118	6 6%	34%
22	U1	118	66%	34%
22	U2	118	66%	34%
22	V1	118	66%	34%
22	V2	118	6 6%	34%
22	W1	118	6 6%	34%
22	W2	118	6 6%	34%
22	X1	118	6 4% •	34%
22	X2	118	6 4% •	34%
23	Р	105	76%	24%
23	р	105	76%	24%
24	Q	98	87%	13%
24	q	98	87%	13%
25	R	62	100%	
25	r	62	100%	

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
31	Q7G	Ε	402	Х	-	-	-
31	Q7G	Ν	201	Х	-	-	-



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	Q7G	е	407	Х	-	-	-
31	Q7G	n	201	Х	-	-	-



2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 251552 atoms, of which 126980 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 ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1 A	921	Total	С	Η	Ν	0	\mathbf{S}	0	0
	Π	231	4076	1459	2044	261	284	28	0
1 a	991	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
	a	231	4076	1459	2044	261	284	28	0

There are 4 discrepancies between the modelled and reference sequences:

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

• Molecule 2 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues			Atom	s			AltConf	Trace
9	Δ.1	520	Total	С	Η	Ν	0	S	0	0
2	AI	550	8280	2612	4196	710	742	20	0	0
9	٨٥	520	Total	С	Н	Ν	0	S	0	0
2	ΛL	000	8280	2612	4196	710	742	20	0	0
9	R1	523	Total	С	Η	Ν	0	S	0	0
2			8198	2585	4161	702	730	20		0
9	Bo	523	Total	С	Н	Ν	0	S	0	0
2	D_{2}		8198	2585	4161	702	730	20		0
9	C1	523	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
2 01	525	8193	2587	4154	701	731	20	0	0	
2	C2	523	Total	С	Η	Ν	0	S	0	0
	$2 \qquad C2$	525	8193	2587	4154	701	731	20		0

• Molecule 3 is a protein called subunit-8.



Mol	Chain	Residues			Aton	ns			AltConf	Trace
2	C	86	Total	С	Η	Ν	0	S	0	0
3	C	80	1460	494	715	116	130	5	0	0
2		86	Total	С	Η	Ν	0	S	0	0
3	C		1460	494	715	116	130	5		U

• Molecule 4 is a protein called subunit-d.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
4	Л	220	Total	С	Η	Ν	0	S	0	0
4	D	552	5499	1710	2762	505	514	8	0	0
4	d	220	Total	С	Η	Ν	0	S	0	0
4	u	552	5499	1710	2762	505	514	8	0	0

• Molecule 5 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
5	D1	487	Total	С	Η	Ν	0	S	0	0
5		407	7430	2329	3741	631	710	19	0	0
5	DЭ	497	Total	С	Η	Ν	0	S	0	0
5	D^2	407	7430	2329	3741	631	710	19	0	0
E	L 1	196	Total	С	Η	Ν	0	S	0	0
0	EI	400	7415	2324	3733	630	709	19	0	0
E	ГO	196	Total	С	Η	Ν	0	S	0	0
0	$\mathbf{E}\mathbf{Z}$	400	7415	2324	3733	630	709	19	0	0
5	L ¹	480	Total	С	Η	Ν	0	S	0	0
5	I I	409	7461	2339	3758	633	712	19	0	0
5	Го	480	Total	С	Н	Ν	0	S	0	0
0	$\Gamma \Delta$	409	7461	2339	3758	633	712	19		U

• Molecule 6 is a protein called ATPTB1.

Mol	Chain	Residues			Atom	S			AltConf	Trace
6	F	383	Total	С	Η	Ν	0	\mathbf{S}	0	0
0	Ľ	000	6281	2060	3061	558	585	17	0	0
6	0	202	Total	С	Η	Ν	0	S	0	0
0	е	000	6281	2060	3061	558	585	17	0	0

• Molecule 7 is a protein called subunit-f.

Mol	Chain	Residues			Atom	S			AltConf	Trace
7	F	135	Total 2256	С 744	H 1111	N 201	0 195	${S \atop 5}$	0	0



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Mol	Chain	Residues			Atom	.S			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	С	268	Total	С	Η	Ν	0	S	0	0
0	G	200	3953	1211	2020	343	378	1	0	0
0	۵.	268	Total	С	Η	Ν	0	S	0	0
0	g	208	3953	1211	2020	343	378	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

• Molecule 9 is a protein called ATP synthase gamma subunit.

Mol	Chain	Residues			Atom	5			AltConf	Trace
0	C1	200	Total	С	Η	Ν	0	S	0	0
9	GI	300	4774	1507	2387	423	448	9	0	0
0	Co	200	Total	С	Η	Ν	0	S	0	0
9	62	300	4774	1507	2387	423	448	9	0	U

• Molecule 10 is a protein called ATPTB4.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
10	п	127	Total	С	Η	Ν	Ο	S	0	0
10	11	137	2158	680	1088	184	203	3	0	0
10	h	127	Total	С	Η	Ν	0	S	0	0
10	11	137	2158	680	1088	184	203	3	0	0

• Molecule 11 is a protein called ATP synthase, epsilon chain, putative.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
11	Ц1	161	Total	С	Η	Ν	0	\mathbf{S}	0	0
11	111	101	2483	788	1232	211	248	4	0	0
11	ЦЭ	161	Total	С	Η	Ν	0	\mathbf{S}	0	0
	112	101	2483	788	1232	211	248	4	0	0

• Molecule 12 is a protein called subunit-i/j.



Mol	Chain	Residues			Aton	ns			AltConf	Trace
19	т	103	Total	С	Η	Ν	0	\mathbf{S}	0	0
12	1	105	1740	574	857	152	151	6	0	0
19	i	103	Total	С	Η	Ν	0	S	0	0
	1	103	1740	574	857	152	151	6		0

• Molecule 13 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues		-	Atom	s			AltConf	Trace
12	T1	65	Total	С	Η	Ν	0	S	0	0
10	11	05	1046	332	513	97	102	2	0	0
12	10	65	Total	С	Н	Ν	0	S	0	0
10	12	00	1046	332	513	97	102	2	0	U

• Molecule 14 is a protein called ATPTB6.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
14	T	168	Total	С	Η	Ν	Ο	S	Ο	0
14	0	100	2835	919	1411	249	249	7	0	0
14	i	168	Total	С	Η	Ν	Ο	S	0	0
14	J	108	2835	919	1411	249	249	7	0	0

• Molecule 15 is a protein called ATP synthase subunit p18, mitochondrial.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
15	T1	166	Total	С	Η	Ν	0	\mathbf{S}	0	0
10	JI	100	2590	822	1276	221	257	14	0	0
15	10	166	Total	С	Н	Ν	0	S	0	0
10	52	100	2590	822	1276	221	257	14	0	0
15	K1	166	Total	С	Η	Ν	0	S	0	0
10	171	100	2591	822	1276	221	258	14	0	0
15	K9	166	Total	С	Н	Ν	0	S	0	0
10	112	100	2591	822	1276	221	258	14	0	0
15	T 1	165	Total	С	Η	Ν	0	S	0	0
10		105	2581	819	1271	220	257	14	0	0
15	1.0	165	Total	С	Н	Ν	0	S	0	0
10		105	2581	819	1271	220	257	14		

• Molecule 16 is a protein called subunit-k.

Mol	Chain	Residues			Atom	ns			AltConf	Trace
16	К	105	Total 1749	C 577	Н 876	N 149	0 141	S 6	0	0



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

• Molecule 17 is a protein called subunit-e.

Mol	Chain	Residues		-	Atom	S			AltConf	Trace
17	т	65	Total	С	Η	Ν	Ο	S	0	0
11		05	1082	340	545	104	92	1	0	0
17	1	65	Total	С	Η	Ν	Ο	S	0	0
11	1	05	1082	340	545	104	92	1	0	0

• Molecule 18 is a protein called subunit-g.

Mol	Chain	Residues			Atom	S			AltConf	Trace
19	М	120	Total	С	Η	Ν	Ο	S	0	0
10	111	129	2069	662	1042	177	186	2	0	0
19	m	120	Total	С	Η	Ν	0	S	0	0
10	111	129	2069	662	1042	177	186	2	U	

• Molecule 19 is a protein called oligomycin sensitivity conferring protein.

Mol	Chain	Residues			Atom	5			AltConf	Trace
10	M1	234	Total	С	Η	Ν	0	S	0	0
19	1/11	234	3750	1212	1873	302	360	3	0	0
10	Mo	224	Total	С	Η	Ν	Ο	S	0	0
19	IVI Z	204	3750	1212	1873	302	360	3	0	0

• Molecule 20 is a protein called ATPTB11.

Mol	Chain	Residues			Atom	S			AltConf	Trace
20	N	130	Total	С	Η	Ν	0	S	0	0
20	11	159	2210	730	1082	183	208	7	0	0
20	n	120	Total	С	Η	Ν	0	S	0	0
20	11	159	2210	730	1082	183	208	7	0	0

• Molecule 21 is a protein called ATPTB12.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
91	0	06	Total	С	Η	Ν	0	S	0	0
21	0	90	1556	506	767	140	140	3	0	0
91	0	06	Total	С	Η	Ν	0	\mathbf{S}	0	0
	0	90	1556	506	767	140	140	3	0	U



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

22 O1 78 Total C H N O S 0 0 22 O2 78 Total C H N O S 0 0 22 O2 78 Total C H N O S 0 0 22 P1 78 Total C H N O S 0 0 22 P2 78 Total C H N O S 0 0 22 Q1 78 Total C H N O S 0 0 22 Q2 78 Total C H N O S 0 0 0 22 R1 78 Total C H N O S 0 0 0 22 R1 78 Total C H<	Mol	Chain	Residues		A	Atom	s			AltConf	Trace
22 O1 78 1165 376 600 89 96 4 0 0 22 O2 78 Total C H N O S 0 0 22 P1 78 Total C H N O S 0 0 22 P1 78 Total C H N O S 0 0 22 P2 78 Total C H N O S 0 0 22 Q1 78 Total C H N O S 0 0 22 Q2 78 Total C H N O S 0 0 22 R1 78 Total C H N O S 0 0 22 S1 78 Total C H N <	00	01	70	Total	С	Η	Ν	0	S	0	0
22 O2 78 Total C H N O S 0 0 22 P1 78 Total C H N O S 0 0 22 P1 78 Total C H N O S 0 0 22 P2 78 Total C H N O S 0 0 22 Q1 78 Total C H N O S 0 0 22 Q2 78 Total C H N O S 0 0 22 R1 78 Total C H N O S 0 0 0 22 R1 78 Total C H N O S 0 0 0 22 S1 78 Total C H<	22	01	18	1165	376	600	89	96	4	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		02	70	Total	С	Н	Ν	0	S	0	0
22 P1 78 Total C H N O S 0 0 22 P2 78 Total C H N O S 0 0 22 P2 78 Total C H N O S 0 0 22 Q1 78 Total C H N O S 0 0 22 Q2 78 Total C H N O S 0 0 22 R1 78 Total C H N O S 0 0 22 R1 78 Total C H N O S 0 0 0 22 R1 78 Total C H N O S 0 0 0 22 S1 78 Total C H<		02	10	1165	376	600	89	96	4	0	0
22 P1 78 1165 376 600 89 96 4 0 0 22 P2 78 Total C H N O S 0 0 22 Q1 78 Total C H N O S 0 0 22 Q2 78 Total C H N O S 0 0 22 Q2 78 Total C H N O S 0 0 22 R1 78 Total C H N O S 0 0 22 R2 78 Total C H N O S 0 0 22 S1 78 Total C H N O S 0 0 22 S2 78 Total C H N <	22	D1	70	Total	С	Η	Ν	Ο	S	0	0
22 P2 78 Total C H N O S 0 0 22 Q1 78 Total C H N O S 0 0 22 Q2 78 Total C H N O S 0 0 22 Q2 78 Total C H N O S 0 0 22 Q2 78 Total C H N O S 0 0 22 R1 78 Total C H N O S 0 0 22 R2 78 Total C H N O S 0 0 22 S1 78 Total C H N O S 0 0 22 S1 78 Total C H N O<		ГІ	10	1165	376	600	89	96	4	0	0
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$\begin{array}{c c c c c c c c c c c c c c c c c c c $	22	01	78	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		QI	10	1165	376	600	89	96	4	0	0
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		101	10	1165	376	600	89	96	4	0	0
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		51	10	1166	376	601	89	96	4	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	22	ຽງ	78	Total	С	Η	Ν	0	\mathbf{S}	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		52	10	1166	376	601	89	96	4	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	- 22	TT1	79	Total	С	Η	Ν	Ο	S	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		11	10	1166	376	601	89	96	4	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	- 22	ТЭ	70	Total	С	Η	Ν	0	S	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		12	10	1166	376	601	89	96	4	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	22	TT1	70	Total	С	Η	Ν	Ο	S	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		UI	10	1165	376	600	89	96	4	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	- 22	119	70	Total	С	Η	Ν	Ο	S	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		02	10	1165	376	600	89	96	4	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	222	V1	70	Total	С	Н	Ν	Ο	S	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		V I	10	1165	376	600	89	96	4	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		Vo	70	Total	С	Н	Ν	Ο	S	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		V Z	18	1165	376	600	89	96	4	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	00	W 71	70	Total	С	Н	Ν	0	S	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	22	VV 1	(8	1165	376	600	89	96	4	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		WO	70	Total	С	Н	Ν	0	S	0	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	22	W2	(8	1165	376	600	89	96	4	U	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	00	V1	70	Total	С	Н	Ν	Ο	S	0	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	22		(8	1165	376	600	89	96	4	0	0
$\begin{vmatrix} 22 \\ -22 \end{vmatrix}$ X2 $\begin{vmatrix} 78 \\ -78 \end{vmatrix}$ 1165 376 600 89 96 4 $\begin{vmatrix} 0 \\ -0 \end{vmatrix}$ 0	00	Vo	70	Total	С	Н	Ν	Ο	S	0	0
	22	X2	18	1165	376	600	89	96	4	0	0

• Molecule 23 is a protein called subunit-b.



Mol	Chain	Residues			Aton	ıs			AltConf	Trace
23	р	80	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
20	1	80	1335	448	651	108	125	3	0	0
93	n	80	Total	С	Н	Ν	0	S	0	0
20	Р	80	1335	448	651	108	125	3	0	0

• Molecule 24 is a protein called ATPEG3.

Mol	Chain	Residues		A	toms			AltConf	Trace
24	0	85	Total	С	Η	Ν	Ο	0	0
24	Q	85	1486	499	720	142	125	0	0
24	a	85	Total	С	Н	Ν	Ο	0	0
24	q	00	1486	499	720	142	125	0	0

• Molecule 25 is a protein called ATPEG4.

Mol	Chain	Residues		ŀ	Atom	5			AltConf	Trace
25	В	62	Total	С	Η	Ν	Ο	S	0	0
20	п	02	1040	358	498	94	85	5	0	0
25	r	62	Total	С	Н	Ν	Ο	S	0	0
20	1	02	1040	358	498	94	85	5	0	0

• Molecule 26 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
26	Λ 1	1	Total	С	Η	Ν	0	Р	0
20	AI	1	43	10	12	5	13	3	0



Mol	Chain	Residues		A	Atom	ıs			AltConf
26	10	1	Total	С	Η	Ν	Ο	Р	0
20	A2	1	43	10	12	5	13	3	0
26	P1	1	Total	С	Η	Ν	Ο	Р	0
20	DI	1	43	10	12	5	13	3	0
26	Рŋ	1	Total	С	Η	Ν	Ο	Р	0
20	DZ	1	43	10	12	5	13	3	0
26	C1	1	Total	С	Η	Ν	Ο	Р	0
20	01	1	43	10	12	5	13	3	0
26	CD	1	Total	С	Η	Ν	Ο	Р	0
20	02	1	43	10	12	5	13	3	0
26	F 1	1	Total	С	Η	Ν	Ο	Р	0
20	I, I	1	43	10	12	5	13	3	0
26	FЭ	1	Total	С	Η	Ν	Ο	Р	0
20	ΓZ	1	43	10	12	5	13	3	0

• Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
27	A1	1	Total Mg 1 1	0
27	A2	1	Total Mg 1 1	0
27	B1	1	Total Mg 1 1	0
27	B2	1	Total Mg 1 1	0
27	C1	1	Total Mg 1 1	0
27	C2	1	Total Mg 1 1	0
27	D1	1	Total Mg 1 1	0
27	D2	1	Total Mg 1 1	0
27	F1	1	Total Mg 1 1	0
27	F2	1	Total Mg 1 1	0

• Molecule 28 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
	C	1	Total C H O P	0
28	C	1	256 81 156 17 2	0
00	Б	1	Total C H O P	0
28	E	1	1280 405 780 85 10	0
00	Б	1	Total C H O P	0
28	Ľ	1	1280 405 780 85 10	0
	F	1	Total C H O P	0
28	E	1	1280 405 780 85 10	0
20	F	1	Total C H O P	0
28	E	1	1280 405 780 85 10	0
20	F	1	Total C H O P	0
28	E	1	1280 405 780 85 10	0
20	F	1	Total C H O P	0
28	F	1	256 81 156 17 2	0
20	т	1	Total C H O P	0
28	J	1	512 162 312 34 4	0
20	т	1	Total C H O P	0
28	J	1	512 162 312 34 4	0
20	т	1	Total C H O P	0
28	L	1	256 81 156 17 2	0
	М	1	Total C H O P	0
28	M	1	256 81 156 17 2	0
	0	1	Total C H O P	0
28	Q		256 81 156 17 2	U
90	6	1	Total C H O P	0
28	С		256 81 156 17 2	U
20		1	Total C H O P	0
20	е		1280 405 780 85 10	U



Mol	Chain	Residues	-	Atoms			AltConf
28	0	1	Total (C H	Ο	Р	0
20	е	1	1280 40	05 780	85	10	0
28	0	1	Total (C H	Ο	Р	0
20	е	1	1280 40	05 780	85	10	0
28	0	1	Total (C H	Ο	Р	0
20	е	1	1280 40	05 780	85	10	0
28	0	1	Total (C H	Ο	Р	0
20	е	I	1280 40	05 780	85	10	0
28	f	1	Total (С Н	Ο	Р	0
20	L	1	256 8	31 156	17	2	0
28	i	1	Total (C H	Ο	Р	0
20	J	1	512 1	62 312	34	4	0
28	i	1	Total (C H	Ο	Р	0
20	J	1	512 1	62 312	34	4	0
28	1	1	Total (С Н	Ο	Р	0
20	1	1	256 8	81 156	17	2	0
28	m	1	Total (С Н	Ο	Р	0
	111	1	256 8	31 156	17	2	U
28	a	1	Total	СН	Ο	Р	0
20	Ч	L	256 8	81 156	17	2	U

• Molecule 29 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
20	D1	1	Total	С	Η	Ν	Ο	Р	0
29	DI	1	39	10	12	5	10	2	0



Mol	Chain	Residues		Atoms					
20	DЭ	1	Total	С	Η	Ν	0	Р	0
29	D_2	1	39	10	12	5	10	2	0

• Molecule 30 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $\rm C_{24}H_{46}O_{11}).$



Mol	Chain	Residues	Atoms	AltConf
20	F	1	Total C H O	0
30	Ľ	1	74 24 39 11	0
20	т	1	Total C H O	0
30	J	1	74 24 39 11	0
30	0	1	Total C H O	0
50	е	1	74 24 39 11	0
30	i	1	Total C H O	0
30	J	1	74 24 39 11	0

• Molecule 31 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	Atoms	AltConf
21	F	1	Total C H O	0
51	Ľ	1	108 38 60 10	0
91	N	1	Total C H O	0
51	IN	1	129 44 70 15	0
91	0	1	Total C H O	0
51	е	1	108 38 60 10	0
91		1	Total C H O	0
51	11	1	129 44 70 15	0

• Molecule 32 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		A	tom	IS			AltConf
20	Б	1	Total	С	Η	Ν	Ο	Р	0
32	Г	1	133	41	82	1	8	1	0
20	D	1	Total	С	Η	Ν	Ο	Р	0
32	n	1	133	41	82	1	8	1	0
20	t	1	Total	С	Η	Ν	Ο	Р	0
32	1	1	133	41	82	1	8	1	0
20	r	1	Total	С	Η	Ν	Ο	Р	0
52	1	1	133	41	82	1	8	1	U

• Molecule 33 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	5	AltConf
22	Б	1	Total C H	N O P	0
55	Г	1	284 88 176	2 16 2	0
22	Б	1	Total C H	N O P	0
55	Г	1	284 88 176	2 16 2	0
22	т	1	Total C H	N O P	0
55	1	1	142 44 88	1 8 1	0
22	Т	1	Total C H	N O P	0
55	J	1	142 44 88	1 8 1	0
22	f	1	Total C H	N O P	0
55	1	1	284 88 176	2 16 2	0
22	f	1	Total C H	N O P	0
55	1	1	284 88 176	2 16 2	0
22	;	1	Total C H	N O P	0
55	1	1	142 44 88	1 8 1	



Mol	Chain	Residues	Atoms					AltConf	
22	;	1	Total	С	Η	Ν	Ο	Р	0
00	J	1	142	44	88	1	8	1	0

• Molecule 34 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		
24	Π1	1	Total	С	Η	Ν	Ο	Р	0
34	пі	1	40	9	11	2	15	3	0
24	Цэ	1	Total	С	Η	Ν	Ο	Р	0
04	112		40	9	11	2	15	3	



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: ATP synthase subunit a







• Molecule 2: ATP synthase subunit alpha, mitochondrial

Chain B1:	89%	10%
MET ARG ARG PHE GLY SER LTY ALA ALA SER SER SER SER	ARG CYS CYS CYS CYS CYS CYS ALA ALA ALA ALA ALA CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	F46 G60 F69 G70 F71 F85 F95 F95 F95
A133 G134 G134 H145 E146 V147 P148 L151 VAL THR ARG	SER ARG ARG LEU LEU LEU V166 P167 P185 M193 P281 T185 M193 P368 M193 B368 M373 A373	6425 K426 K426 K428 K428 K435 K436 K436 K436 A43 A43 A43 A43 A43 A43 A43 A44 A44 A44
Y509 6510 ← A512 ← K513 ← K513 ← K513 ← N534 ←	× 1 × 1 × 1 × 1 × 1 × 1 × 1 × 1 × 1 × 1	
• Molecule 2: ATF	' synthase subunit alpha, mitochondrial	
Chain B2:	89%	10%
MET ARG ARG PHE PHE CLYS CLYS PHE SER SER CLY CLEU CLEU SER SER SER	ARG CYS ALA ALA ALA ALA CYS CYS CYS CYS FLO FLO ALA ALA ALA ALA ALA ALA ALA ALA ALA A	F46 660 660 660 761 761 769 770 871 870 870 890 795
D100	THR THR SER ARG SER ARG LLEU LLEU LLEU LLEU LLEU LLEU LLEU LLE	8414 8414 6425 6425 6426 6426 6426 8435 8435 8436 8436 A1A A38 A38 A438 A38 A438 A38 A38 A438 A38 A438 A38 A446 CUY CUY
V447 0448 10468 1000000000000000000000000000000000000	N562	
• Molecule 2: ATF	' synthase subunit alpha, mitochondrial	
Chain C1:	89%	10%
MET ARG ARG CLY GLY CLYS PHE PLY ALA CLEU CLEU SER SER SER	ALA ARC CYS CYS ALLA ALLA ALLA ALLA ALLA ALLA ALLA AL	F45 F46 K47 D59 D59 G60 T61 V74 M108 G150 V1LL V1LL THR

• Molecule 2: ATP synthase subunit alpha, mitochondrial



Chain C2:	89%	10%
MET ARG ARG ARG CLY CLY CLEU CLEU ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	SER ALA ALA ALA ALA ALA ALA ALA ALA SER SER SER SER SER SER SER SER SER SER	EVS E46 F45 F45 F45 F45 F45 F45 F45 F47 F11 F11 F11 F12 F45 F45 F45 F45 F45 F45 F45 F45 F45 F45
ARG SER ARG ARG ARG LEU LEU LEU ASP SER T162 LI63 Y181 Y181 Y181 T165 M193 M193	R225	N440 SRR VAL GLY GLN V447 V447 T552 T553 A553 T564 W553 V584
• Molecule 3: subunit-8		
Chain C:	74%	• 25%
MET LEU LEU ARG ARG CLY CLEU ARG ASN MET ASN MET ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	VAL SER PRO ARG ARG HIS L29 193 T93 T193 T193 T114	
• Molecule 3: subunit-8		
Chain c:	74%	• 25%
MET LEU ARG ARG CLFU CLEU CLFU ARG ASN MET ASN MET ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	SER PRG ARG ARG L29 L29 T93 T93 T114 T114	
• Molecule 4: subunit-d		
Chain D:	89%	10%
MET ARG VARG SER SER SER ASD ASD ASD ARG CLN CLN TTRP SER TTRP TTRP TTRP TTRP TTRP SER TTS1	133 P325 P325 TLE VAL THR THR THR THR THR THR THR THR THR THR	VAL PRO SER CLU CLN THR CLN CLN CLN CLN CLN CLN STH ALA HIS HIS
• Molecule 4: subunit-d		
Chain d:	89%	10%
MET ARG ARG ARG SER SER SER SER ASN ASN ASN ASN CLN CLN CLN THR CLN THR CLN THR TTR TTR TTR TTR TTR CLN TTR CON TTR TTR TTR TTR TTR TTR TTR TTR TTR TT	R145 P325 P325 T112 T112 T112 T1132 C333 C333 C333 C333 C333 C333 C333	VAL CLU CLU CLU CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN
• Molecule 5: ATP synthase su	ıbunit beta, mitochondrial	
Chain D1:	94%	6%
MET LIEU ARG ARG ARG SER ALA ALA ALA ARG ALA ARG ALA ARG ARA ARG ARA ARA ARA	THR ALA PRO V27 A28 A28 A28 A28 A28 A28 A28 A28 A28 A28	A127 A128 D130 Q131 C133 Q131 R132 G133 G133 G133 G136 G136 G136 G136 A147 A147 A155 C138 D157
L171 G180 A201 H204 G205 G205 G205 G205 G205 C205 C205 C205 C205 C205 C205 C205 C	S332 × V333 ↓ V3333 ↓ L361 ↓ L361 ↓ L361 ↓ L377 ↓ L377 ↓ L377 ↓ A380 ↑ A380 ↓ A380 ↓ D387 ↓ D387	D420 R434 R434 Q477 Q477 M499 R510 R511 A512 A512 A512 A513 A512 A513 A513 A513 A513 A513 A513 A513 A513



• Molecule 5: ATP sy	vnthase subunit beta, mitochondrial	
Chain D2:	94%	6%
MET LEU THR ARG ARG ARG ALA ALA ALA ALA ALA ALA ALA SER TLE SER	THR ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	1129 1129 (131 (132) (133 (133 (135 (135 (135 (135 (135 (135
G180 V200 A201 K202 G203 G205 C233 C2337 C2337 C238	L297 • L297 • V305 • V305 • S332 • S332 • S336 E367 • S368 • S368 • S368 • S368 • S368 • S368 • S376 • C379 • A380 • A380 • D3877 • D3	T451 4477 4477 4499 8510 8510 8511 8513 8513 8513 8513 8513 8513 8513
• Molecule 5: ATP sy	vnthase subunit beta, mitochondrial	
Chain E1:	93%	6%
MET LEU THR THR ARG PHE ARG ARG CARG CLY ALA ALA ALA ALA ALA TLE SER	THR GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	v.187 C.188 K.202 K.202 A.340 A.340 A.340 A.340 B.342 D.342 D.342 D.342 D.342 B.343 C.236 C.266
D387 L410 L417 6418 6418 1419 2420 1420 1449	4452 4453 7454 6477 6477 6477 6477 6477 6477 6494 6503 6504 6503 6504 6503 6504 6505 6505 6505 6505 6505 8506 8506 8501 8510 8511 8510 8511 8511 8511 8511	VAL VAL ALA ALA ALA ALA SER SER SER
• Molecule 5: ATP sy	vnthase subunit beta, mitochondrial	
Chain E2:	93%	6%
MET LEU THR ARG ARG ARG ALA ARG ALA ARG ALA ARG CLY VAL SER TLE	THR ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	V187 C188 K202 K202 K236 K236 K236 K236 K236 K236 K236 K23
G369 D387 L410 G417 G418 G418 1419 E420 E424	V449 G452 M453 Q477 Q477 Q477 Q477 C454 E501 E501 E501 E501 E503 A504 A503 A504 A503 A503 A503 A503 A503 A503 A503 A503	A512 A512 VAL ALA GLN GLN SER SER SER
• Molecule 5: ATP sy	vnthase subunit beta, mitochondrial	
Chain F1:	94%	6%
MET LEU THR THR ARG ARG ALA ARG GLY VAL ALA ALA TLE SER TLE	THR ALA ALA ALA ALA ALA ALA P26 A23 A23 A33 A33 C57 C67 C67 C67 C133 C133	P134 P135 C136 E137 K138 L139 E166 D157 K175 K175 C203 C203 C203 C203 C203 C203 C203 C203
K236 (237 (237 (237 (2337 (2337)) (2337) (2361) (2361) (2361) (2362) (2362) (2362) (2362) (2362) (2362) (2362) (2362) (2372) (2372) (2372) (2372) (2372) (2377) (23	S368 E378 E378 E378 C452 C452 C452 C452 C452 K451 K511 K512 K512 K512 K513 K513 K513 K513 K513 K513 K513 K513	
• Molecule 5: ATP sy	vnthase subunit beta, mitochondrial	
Chain F2:	94%	6%



MET LEU THE ARG ARG ARG ARG ARG ALA VAL ALA ALA ALA ALA ALA ALA ALA ALA	A156 K175 K202 K203 K203 K203 K204
 Molecule 6: ATPTB1 	
Chain E: 96%	
M1 7266 K383 ALA ALA ALA ALA ALA ALA ALA ALA ALA	
• Molecule 6: ATPTB1	
Chain e: 96%	
M1 7268 7268 ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 7: subunit-f	
Chain F: 92% ·	7%
MET V2 LV3 GLY GLY HIS HIS	
• Molecule 7: subunit-f	
Chain f: 92%	7%
MET V2 M136 ALA ALA ALA HIS HIS HIS	
• Molecule 8: ATPTB3	
Chain G: 100%	_
MET S2 K3 K3 K3 K3 K3 K3 K3 K3 K3 K3	
• Molecule 8: ATPTB3	
Chain g: 10%	_
MET S2 K3 A14 A14 A14 C29 C29 C29 C30 A13 A37 A37 A37 A37 A37 A37 A37 A37 A37 A3	





MET PHE PHE CLY ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG
• Molecule 12: subunit-i/j
Chain I: 99%
MET V2 V104
• Molecule 12: subunit-i/j
Chain i: 99%
• Molecule 13: ATP synthase subunit epsilon, mitochondrial
Chain I1: 87% 13%
MET ILLE ARG CYS ARA ARA ARA ALA ILLU SER B115 B115 B115 B115 B115 B115 B115 B11
• Molecule 13: ATP synthase subunit epsilon, mitochondrial
15% Chain I2: 87% 13%
MET ILLE ARG ARG ARG SER ALA LLEU SER B11 G17 G60 G60 G60 G60 G60 C60 C75 C75 C75 C75 C75 C75 C75 C75 C75 C75
• Molecule 14: ATPTB6
Chain J: 99%
12 12 16 16
• Molecule 14: ATPTB6
• Molecule 14: ATPTB6 Chain j: 99%
• Molecule 14: ATPTB6 Chain j: 99% .
 Molecule 14: ATPTB6 Chain j: 99% . 99% . Molecule 15: ATP synthase subunit p18, mitochondrial
 Molecule 14: ATPTB6 Chain j: 99% . Molecule 15: ATP synthase subunit p18, mitochondrial 32% Chain J1: 88% 12%



	** * *	••	******	* *	* *	****	•••• •
MET MET ARG ARG ARG ARG ARG ARG SER PRO PRO PRO SER VAL PHE ALA ALA ALA ALA ALA ALA ALA ALA	SER ALA A24 K25 K25 C48 C48 K49	Q82 S83 P84	S88 T89 P90 V91 D92 N93 E94	K114 K148	A152 D153	q163 K164 A165 K166 T167	E168 G169 K170 E171 H172 P173
6174 H175 L176 3177 0178 0178 0178 0181 1182 F183 F183 F183 F183 F183 F183 F183 F183							
• Molecule 16: subunit-k							
Chain K:	85%				15%	-	
MET LEU LEU ARG ARG SER SER ALA ALA ALA ALA ALA ARG THR THR THR THR THR THR CO CO	L124						
• Molecule 16: subunit-k							
Chain k:	85%				15%	-	
MET LEU ARG ARG SER ARG ARA ALA ALA ALA ALA ALA ALA ALA ALA ALA	L124						
• Molecule 17: subunit-e							
Chain L:	71%			29%	_	-	
MET SER ALLA V68 V68 CLV PRO CLV PRO CLV VAL CLU PRO CLV VAL CLU CLU	GLN GLN LEU ALA GLU GLU PHE THR THR						
• Molecule 17: subunit-e							
Chain 1:	71%			29%	_	-	
MET SER ALLA V68 V68 V68 ALA ALA PTHR THR THR THR THR THR THR THR THR THR	GLN GLN LEU ALA GLU GLU PHE THR THR						
• Molecule 18: subunit-g							
Chain M:	89%				• 10%	%	
MET SER SER THR THR LYS CYS ALA ALA ALA MET THR MET THR THR THR THR THR THR THR THR THR TH							
• Molecule 18: subunit-g							
Chain m:	89%				• 109	%	
MET SER SER SER SER LYS VAL VAL CYS CYS CYS CYS THR THR THR THR V109 V109 V109 V109 V109							
		W O R L PROTEIN					

• Molecule 19: oligomycin sensitiviy conferring protein 12% Chain M1: 91% 8% MET PHE ARG ARG SER SER SER SER ALA ALA ALA ALA ALA ALA ALA ALA ALA LYS GLN ALA GLY • Molecule 19: oligomycin sensitiviy conferring protein 11% Chain M2: 91% 8% MET PHE ARG ARG ARG SER SER SER ALA ARG ALA ARG ALA ALA ALA ARG ALA ARG LYS GLN ALA GLY • Molecule 20: ATPTB11 Chain N: 88% 11% MET LEU LYS LYS PRO PRO PRO LEU ALA ALA ALA ALA ALA ALA ALA ALA ALA • Molecule 20: ATPTB11 Chain n: 88% 11% • MET LEU ARG LYS THR PRO LEU ALA ALA ALA ALA ALA ALA CYS LYS LEU • Molecule 21: ATPTB12 Chain O: 94% • 5% • Molecule 21: ATPTB12 Chain o: 94% • 5%



• Molecule 22: ATPase subun	it 9, putative	
Chain O1:	66%	34%
MET MET MET ARG ARG LEU ALU CLEU ALA ALA ALA ARG PHE PHE PHE ALA ALA ALA ALA ALA ALA VAL	ALA THR ILYS SER ILYS ALA ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	
• Molecule 22: ATPase subun	it 9, putative	
Chain O2:	66%	34%
MET MET ARG ARG ARG LEU ALG CLU CLU CLU CLU ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG	ALA THR LYS LYS LYS LZS ALA ALA ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	
• Molecule 22: ATPase subun	it 9, putative	
Chain P1:	66%	34%
MET MET MET ARG ARG ARG CLEU ALLA ALLA ALLA ALLA ALLA ALLA ALLA A	ALA ALA THR LIVS LIVS LIVS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 22: ATPase subun	it 9, putative	
Chain P2:	66%	34%
MET MET MET ARG ARG LEU LEU LEU SER SER ARG ARG ARG ARG ARG ARG ARG ARG ARG AR	ALA ALA TTHR LLYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 22: ATPase subun	it 9, putative	
Chain Q1:	66%	34%
MET MET ARG ARG LEU LEU LEU LEU SER SER ARG GLN SER ARG PRO PRO PRO PRO PRO PRO PRO VAL	ALA ALA THR LYS SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 22: ATPase subun	it 9, putative	
Chain Q2:	66%	34%
MET MET ARG ARG ARG ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	ALA ALA CYSS CYSS CYSS ASN ASN ASN ASN ASN ASN ASN CYSS CYS CYS CYS CYS CYS CYS CYS CYS CY	
• Molecule 22: ATPase subun	it 9, putative	
Chain R1:	66%	34%



MET MET ARG ARG ARG ARG ARG CLN CLEU ALA ARG ARG ARG ARA ARG ARA ARA ARA ARA AR	
• Molecule 22: ATPase subunit 9, putative	
Chain R2: 66%	34%
MET MET ARG ALEU ALLA LLEU LLEU CLEU ALA ARG ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 22: ATPase subunit 9, putative	
Chain S1: 66%	34%
MET MET ARG ARG ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 22: ATPase subunit 9, putative	
Chain S2: 66%	34%
MET MET MET ARIG LLEU LLEU LLEU LLEU LLEU ALIA ALIA ALIA ALIA ALIA ALIA ALIA ALI	
• Molecule 22: ATPase subunit 9, putative	
Chain T1: 66%	34%
MET MET ARG ARG ARG ALLA ALLA CLEU CLEU CLEU ALLA ALA ALA ALA ALA ALA ALA ALA ALA A	
• Molecule 22: ATPase subunit 9, putative	
Chain T2: 66%	34%
MET MET ARG ARG CLEU ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 22: ATPase subunit 9, putative	
Chain U1: 66%	34%
MET MET ARIG ARIG ARIG ARIG ALLA LLEU ALIA ALIA ALIA ALIA ALIA ALIA ALIA ALI	

• Molecule 22: ATPase subunit 9, putative



Chain U2:	66%	34%
	•	•
MET MET MET ARG ARG ALA ALA CLN SER SER SER	ARG ARG ARG ARG ARG ARG ARA ARA ARA ARA	A108
• Molecule 22:	ATPase subunit 9, putative	
Chain V1:	66%	34%
MET MET ARG ARG LEU LEU CLEU GLN SER SER	ARG ARG ARG ARG ARG ARG ARA ARA ALA ALA ALA ALA ALA ARG CONS SER ARA ARG CONS SER ARA ARA ARA ARA ARA ARA ARA ARA ARA A	A108
• Molecule 22:	ATPase subunit 9, putative	
Chain V2:	66%	34%
MET MET ARG ARG ARG LEU CLU CLU CLN SER SER SER	ARG ARG ARG ARG ALA ARG ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	A108
• Molecule 22:	ATPase subunit 9, putative	
Chain W1:	66%	34%
MET MET ARG ARG LEU LEU LEU GLN SER SER	ALC ARC ARC ARC ARC ARC ARC ARC ARLA ARLA	<mark></mark>
• Molecule 22:	ATPase subunit 9, putative	
Chain W2:	66%	34%
MET MET ARG ARG LEU LEU LEU CER SER SER	ALLA ARG ARG ALLA ALLA ALLA ALLA ALLA AL	111 111 111
• Molecule 22:	ATPase subunit 9, putative	
Chain X1:	64% ·	34%
MET MET MET ARG ARG ARG LEU LEU CLN SER SER	ALLA ARG ARG ARG ARG ARA ARA ARA ARA ARA AR	1104 8118
• Molecule 22:	ATPase subunit 9, putative	
Chain X2:	64% ·	34%
MET MET ARG ARG LEU LEU LEU CLN SER SER	ARG ARG ARG ARG ARG ARG ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	F104 F107 S118
	WORLDWIDE PROTEIN DATA BANK	

• Molecule 23: subunit-b

Chain P:	76%	24%
MET LEU ARG ARG ARG VAL PRO PRO MET ALA ALA MET PRO PRO	GLY ALA THR ALA LEU CLEU CLEU CLEU CLEU CLEU CLEU CLEU	
• Molecule 23: subur	ait-b	
Chain p:	76%	24%
MET LEU LEU ARG ARG ARG PRO PRO MET MET MET MET MET MET	dLY ALA ALA ALA ILEU CYS SER ARG CLY TOS ILOS	
• Molecule 24: ATPI	EG3	
Chain Q:	87%	13%
MET THR GLU GLU ASN ASP ALA VAL ALA SER SER SER TRP SER TRP TRP TRP		
• Molecule 24: ATPI	EG3	
Chain q:	87%	13%
MET THR GLU GLU ASN ASP ASP ASP ASP ASP TRP ASP TRP N15		
• Molecule 25: ATPI	EG4	
Chain R:	100%	
There are no outlier	residues recorded for this chain.	
• Molecule 25: ATPI	EG4	
Chain r:	100%	

There are no outlier residues recorded for this chain.



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36925	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 x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	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: ATP, CDL, ADP, MG, UTP, Q7G, PC1, AME, PEE, LMT

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	ond lengths Bond angles		l angles
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.34	0/2111	0.41	0/2861
1	a	0.34	0/2111	0.41	0/2861
2	A1	0.24	0/4159	0.47	0/5632
2	A2	0.24	0/4159	0.47	0/5632
2	B1	0.24	0/4110	0.46	0/5566
2	B2	0.24	0/4110	0.46	0/5566
2	C1	0.24	0/4113	0.47	0/5569
2	C2	0.24	0/4113	0.47	0/5569
3	С	0.30	0/772	0.44	0/1054
3	с	0.30	0/772	0.45	0/1054
4	D	0.25	0/2786	0.50	0/3760
4	d	0.25	0/2786	0.50	0/3760
5	D1	0.24	0/3745	0.46	0/5077
5	D2	0.24	0/3745	0.47	0/5077
5	E1	0.24	0/3738	0.46	0/5067
5	E2	0.24	0/3738	0.46	0/5067
5	F1	0.24	0/3760	0.47	0/5098
5	F2	0.24	0/3760	0.47	0/5098
6	Е	0.28	0/3305	0.45	0/4482
6	е	0.28	0/3305	0.45	0/4482
7	F	0.31	0/1183	0.50	0/1601
7	f	0.31	0/1183	0.50	0/1601
8	G	0.24	0/1953	0.45	0/2650
8	g	0.24	0/1953	0.45	0/2650
9	G1	0.24	0/2427	0.47	0/3268
9	G2	0.24	0/2427	0.47	0/3268
10	Н	0.24	0/1088	0.39	0/1466
10	h	0.24	0/1088	0.39	0/1466
11	H1	0.25	0/1274	0.45	0/1728
11	H2	0.25	0/1274	0.45	0/1728
12	Ι	0.30	0/913	0.47	0/1240
12	i	0.30	0/913	0.47	0/1240


	Chain	Bond	lengths	Bond angles		
IVI01	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
13	I1	0.23	0/547	0.48	0/738	
13	I2	0.23	0/547	0.48	0/738	
14	J	0.27	0/1462	0.48	0/1973	
14	j	0.27	0/1462	0.48	0/1973	
15	J1	0.23	0/1341	0.39	0/1810	
15	J2	0.23	0/1341	0.39	0/1810	
15	K1	0.23	0/1342	0.38	0/1810	
15	K2	0.23	0/1342	0.38	0/1810	
15	L1	0.23	0/1337	0.39	0/1803	
15	L2	0.23	0/1337	0.38	0/1803	
16	Κ	0.27	0/904	0.49	0/1228	
16	k	0.27	0/904	0.49	0/1228	
17	L	0.27	0/547	0.44	0/735	
17	1	0.27	0/547	0.44	0/735	
18	М	0.29	0/1049	0.44	0/1423	
18	m	0.29	0/1049	0.44	0/1423	
19	M1	0.24	0/1916	0.41	0/2591	
19	M2	0.24	0/1916	0.41	0/2591	
20	Ν	0.30	0/1166	0.45	0/1581	
20	n	0.30	0/1166	0.45	0/1581	
21	0	0.27	0/814	0.39	0/1100	
21	0	0.27	0/814	0.39	0/1100	
22	01	0.25	0/574	0.40	0/777	
22	O2	0.25	0/574	0.41	0/777	
22	P1	0.26	0/574	0.41	0/777	
22	P2	0.26	0/574	0.41	0/777	
22	Q1	0.25	0/574	0.40	0/777	
22	Q2	0.25	0/574	0.40	0/777	
22	R1	0.25	0/574	0.40	0/777	
22	R2	0.25	0/574	0.40	0/777	
22	S1	0.25	0/574	0.39	0/777	
22	S2	0.24	0/574	0.39	0/777	
22	T1	0.25	0/574	0.39	0/777	
22	T2	0.25	0/574	0.39	0/777	
22	U1	0.24	0/574	0.38	0/777	
22	U2	0.24	0/574	0.38	0/777	
22	V1	0.24	0/574	0.38	0/777	
22	V2	0.24	0/574	0.38	0/777	
22	W1	0.25	0/574	0.39	0/777	
22	W2	0.25	0/574	0.39	0/777	
22	X1	0.25	0/574	0.38	0/777	
22	X2	0.25	0/574	0.38	0/777	
23	Р	0.30	0/707	0.44	0/957	



Mal	Chain	Bond	Bond lengths		l angles
	Unam	RMSZ # Z > 5		RMSZ	# Z > 5
23	р	0.30	0/707	0.44	0/957
24	Q	0.29	0/799	0.50	0/1091
24	q	0.29	0/799	0.50	0/1091
25	R	0.32	0/567	0.45	0/767
25	r	0.32	0/567	0.45	0/767
All	All	0.26	0/123350	0.45	0/166992

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	ntiles
1	А	229/231~(99%)	227~(99%)	2 (1%)	0	100	100
1	a	229/231~(99%)	227~(99%)	2 (1%)	0	100	100
2	A1	526/584~(90%)	523~(99%)	3 (1%)	0	100	100
2	A2	526/584~(90%)	523~(99%)	3 (1%)	0	100	100
2	B1	517/584~(88%)	510 (99%)	7 (1%)	0	100	100
2	B2	517/584~(88%)	510 (99%)	7 (1%)	0	100	100
2	C1	517/584~(88%)	512 (99%)	4 (1%)	1 (0%)	47	79
2	C2	517/584~(88%)	512 (99%)	4 (1%)	1 (0%)	47	79
3	С	84/114~(74%)	83 (99%)	1 (1%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
3	с	84/114~(74%)	84 (100%)	0	0	100	100
4	D	328/370~(89%)	321 (98%)	7 (2%)	0	100	100
4	d	328/370~(89%)	321 (98%)	7 (2%)	0	100	100
5	D1	485/519~(93%)	478 (99%)	7 (1%)	0	100	100
5	D2	485/519~(93%)	478 (99%)	7 (1%)	0	100	100
5	E1	484/519~(93%)	471 (97%)	13 (3%)	0	100	100
5	E2	484/519~(93%)	471 (97%)	13 (3%)	0	100	100
5	F1	487/519~(94%)	479 (98%)	8 (2%)	0	100	100
5	F2	487/519~(94%)	479 (98%)	8 (2%)	0	100	100
6	Е	381/396~(96%)	375~(98%)	6 (2%)	0	100	100
6	е	381/396~(96%)	376 (99%)	5 (1%)	0	100	100
7	F	133/145~(92%)	131 (98%)	2 (2%)	0	100	100
7	f	133/145~(92%)	131 (98%)	2 (2%)	0	100	100
8	G	266/269~(99%)	263 (99%)	3 (1%)	0	100	100
8	g	266/269~(99%)	263~(99%)	3 (1%)	0	100	100
9	G1	298/305~(98%)	296 (99%)	2 (1%)	0	100	100
9	G2	298/305~(98%)	296 (99%)	2 (1%)	0	100	100
10	Н	135/157~(86%)	133~(98%)	2 (2%)	0	100	100
10	h	135/157~(86%)	133~(98%)	2 (2%)	0	100	100
11	H1	159/182~(87%)	158 (99%)	1 (1%)	0	100	100
11	H2	159/182~(87%)	158 (99%)	1 (1%)	0	100	100
12	Ι	101/104~(97%)	100 (99%)	1 (1%)	0	100	100
12	i	101/104~(97%)	100 (99%)	1 (1%)	0	100	100
13	I1	63/75~(84%)	63 (100%)	0	0	100	100
13	I2	63/75~(84%)	63 (100%)	0	0	100	100
14	J	166/169~(98%)	163 (98%)	3 (2%)	0	100	100
14	j	166/169~(98%)	163 (98%)	3 (2%)	0	100	100
15	J1	$\overline{164/188} \ (87\%)$	161 (98%)	3 (2%)	0	100	100
15	J2	164/188~(87%)	161 (98%)	3 (2%)	0	100	100
15	K1	164/188~(87%)	159 (97%)	5 (3%)	0	100	100
15	K2	164/188~(87%)	159 (97%)	5 (3%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
15	L1	163/188~(87%)	163 (100%)	0	0	100	100
15	L2	163/188~(87%)	162 (99%)	1 (1%)	0	100	100
16	Κ	103/124~(83%)	99~(96%)	4 (4%)	0	100	100
16	k	103/124~(83%)	99 (96%)	4 (4%)	0	100	100
17	L	63/92~(68%)	63 (100%)	0	0	100	100
17	1	63/92~(68%)	63 (100%)	0	0	100	100
18	М	127/144~(88%)	127 (100%)	0	0	100	100
18	m	127/144~(88%)	127 (100%)	0	0	100	100
19	M1	230/255~(90%)	226 (98%)	4 (2%)	0	100	100
19	M2	230/255~(90%)	226 (98%)	4 (2%)	0	100	100
20	Ν	137/156~(88%)	131 (96%)	6 (4%)	0	100	100
20	n	137/156~(88%)	131 (96%)	6 (4%)	0	100	100
21	Ο	94/101~(93%)	94 (100%)	0	0	100	100
21	О	94/101~(93%)	94 (100%)	0	0	100	100
22	01	76/118~(64%)	71 (93%)	5 (7%)	0	100	100
22	O2	76/118~(64%)	71 (93%)	5 (7%)	0	100	100
22	P1	76/118~(64%)	73 (96%)	3 (4%)	0	100	100
22	P2	76/118~(64%)	73 (96%)	3 (4%)	0	100	100
22	Q1	76/118~(64%)	76 (100%)	0	0	100	100
22	Q2	76/118~(64%)	76 (100%)	0	0	100	100
22	R1	76/118~(64%)	76 (100%)	0	0	100	100
22	R2	76/118~(64%)	76 (100%)	0	0	100	100
22	S1	76/118~(64%)	74 (97%)	2(3%)	0	100	100
22	S2	76/118~(64%)	74 (97%)	2 (3%)	0	100	100
22	T1	76/118~(64%)	75 (99%)	1 (1%)	0	100	100
22	T2	76/118~(64%)	75~(99%)	1 (1%)	0	100	100
22	U1	76/118 (64%)	72 (95%)	4 (5%)	0	100	100
22	U2	$76/\overline{118}\ (64\%)$	72 (95%)	4(5%)	0	100	100
22	V1	76/118 (64%)	74 (97%)	2 (3%)	0	100	100
22	V2	76/118~(64%)	74 (97%)	2 (3%)	0	100	100
22	W1	76/118 (64%)	74 (97%)	2(3%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
22	W2	76/118~(64%)	74 (97%)	2(3%)	0	100	100
22	X1	76/118~(64%)	75~(99%)	1 (1%)	0	100	100
22	X2	76/118~(64%)	75~(99%)	1 (1%)	0	100	100
23	Р	78/105~(74%)	77~(99%)	1 (1%)	0	100	100
23	р	78/105~(74%)	77~(99%)	1 (1%)	0	100	100
24	Q	83/98~(85%)	80~(96%)	3(4%)	0	100	100
24	q	83/98~(85%)	80~(96%)	3~(4%)	0	100	100
25	R	60/62~(97%)	59~(98%)	1 (2%)	0	100	100
25	r	60/62 $(97%)$	59~(98%)	1 (2%)	0	100	100
All	All	15170/17414~(87%)	14931 (98%)	237 (2%)	2(0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C2	532	THR
2	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	Percentiles
1	А	225/225~(100%)	223~(99%)	2(1%)	78 91
1	a	225/225~(100%)	223~(99%)	2 (1%)	78 91
2	A1	439/479~(92%)	438 (100%)	1 (0%)	93 98
2	A2	439/479~(92%)	438 (100%)	1 (0%)	93 98
2	B1	435/479~(91%)	433 (100%)	2 (0%)	88 95
2	B2	435/479~(91%)	433 (100%)	2 (0%)	88 95
2	C1	434/479~(91%)	433 (100%)	1 (0%)	93 98
2	C2	434/479~(91%)	433 (100%)	1 (0%)	93 98
3	С	80/104~(77%)	78 (98%)	2 (2%)	47 77



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
3	с	80/104~(77%)	78~(98%)	2(2%)	47	77
4	D	297/334~(89%)	296 (100%)	1 (0%)	92	96
4	d	297/334~(89%)	296 (100%)	1 (0%)	92	96
5	D1	398/420~(95%)	397 (100%)	1 (0%)	92	96
5	D2	398/420~(95%)	397~(100%)	1 (0%)	92	96
5	E1	397/420~(94%)	396 (100%)	1 (0%)	92	96
5	E2	397/420~(94%)	396 (100%)	1 (0%)	92	96
5	F1	400/420~(95%)	399 (100%)	1 (0%)	92	96
5	F2	400/420~(95%)	399 (100%)	1 (0%)	92	96
6	Е	334/341~(98%)	332 (99%)	2 (1%)	86	94
6	е	334/341~(98%)	332 (99%)	2 (1%)	86	94
7	F	119/124~(96%)	118 (99%)	1 (1%)	81	93
7	f	119/124~(96%)	118 (99%)	1 (1%)	81	93
8	G	205/206~(100%)	205 (100%)	0	100	100
8	g	205/206~(100%)	205 (100%)	0	100	100
9	G1	253/257~(98%)	251 (99%)	2 (1%)	81	93
9	G2	253/257~(98%)	251 (99%)	2 (1%)	81	93
10	Н	110/123~(89%)	110 (100%)	0	100	100
10	h	110/123~(89%)	110 (100%)	0	100	100
11	H1	137/156~(88%)	136 (99%)	1 (1%)	84	94
11	H2	137/156~(88%)	136 (99%)	1 (1%)	84	94
12	Ι	95/96~(99%)	95 (100%)	0	100	100
12	i	95/96~(99%)	95 (100%)	0	100	100
13	I1	58/67~(87%)	58 (100%)	0	100	100
13	I2	58/67~(87%)	58 (100%)	0	100	100
14	J	149/150~(99%)	149 (100%)	0	100	100
14	j	149/150~(99%)	149 (100%)	0	100	100
15	J1	145/162~(90%)	145 (100%)	0	100	100
15	J2	145/162~(90%)	145 (100%)	0	100	100
15	K1	145/162~(90%)	145 (100%)	0	100	100
15	K2	145/162~(90%)	145 (100%)	0	100	100



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Mol	Chain	Analysed	Rotameric	Outliers	I	Perce	ntiles
15	L1	145/162~(90%)	145 (100%)	0		100	100
15	L2	145/162~(90%)	145 (100%)	0		100	100
16	Κ	91/107~(85%)	91~(100%)	0		100	100
16	k	91/107~(85%)	91 (100%)	0		100	100
17	L	55/75~(73%)	55 (100%)	0		100	100
17	1	55/75~(73%)	55 (100%)	0		100	100
18	М	111/124 (90%)	110 (99%)	1 (1%)		78	91
18	m	111/124 (90%)	110 (99%)	1 (1%)		78	91
19	M1	200/215~(93%)	199 (100%)	1 (0%)		88	95
19	M2	200/215~(93%)	199 (100%)	1 (0%)		88	95
20	Ν	123/137~(90%)	122 (99%)	1 (1%)		81	93
20	n	123/137~(90%)	122 (99%)	1 (1%)		81	93
21	О	82/86~(95%)	81 (99%)	1 (1%)		71	88
21	О	82/86~(95%)	81 (99%)	1 (1%)		71	88
22	01	56/89~(63%)	56 (100%)	0		100	100
22	O2	56/89~(63%)	56 (100%)	0		100	100
22	P1	56/89~(63%)	56 (100%)	0		100	100
22	P2	56/89~(63%)	56 (100%)	0		100	100
22	Q1	56/89~(63%)	56 (100%)	0		100	100
22	Q2	56/89~(63%)	56 (100%)	0		100	100
22	R1	56/89~(63%)	56 (100%)	0		100	100
22	R2	56/89~(63%)	56 (100%)	0		100	100
22	S1	56/89~(63%)	56~(100%)	0		100	100
22	S2	56/89~(63%)	56 (100%)	0		100	100
22	T1	56/89~(63%)	56 (100%)	0		100	100
22	T2	56/89~(63%)	56 (100%)	0		100	100
22	U1	56/89~(63%)	56 (100%)	0		100	100
22	U2	56/89~(63%)	56 (100%)	0		100	100
22	V1	56/89~(63%)	56 (100%)	0		100	100
22	V2	56/89~(63%)	56 (100%)	0		100	100
22	W1	56/89~(63%)	56 (100%)	0		100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
22	W2	56/89~(63%)	56~(100%)	0	100	100
22	X1	56/89~(63%)	54 (96%)	2(4%)	35	69
22	X2	56/89~(63%)	54~(96%)	2(4%)	35	69
23	Р	75/94~(80%)	75 (100%)	0	100	100
23	р	75/94~(80%)	75~(100%)	0	100	100
24	Q	80/92~(87%)	80 (100%)	0	100	100
24	q	80/92~(87%)	80 (100%)	0	100	100
25	R	56/56~(100%)	56~(100%)	0	100	100
25	r	56/56~(100%)	56 (100%)	0	100	100
All	All	12866/14484~(89%)	12818 (100%)	48 (0%)	91	95

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	М	109	VAL
22	X2	104	ILE
19	M1	247	ASP
21	0	64	TYR
1	a	144	PHE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such side chains are listed below:

Mol	Chain	Res	Type
9	G2	233	ASN
15	J1	93	ASN
1	a	150	ASN
22	V1	75	ASN
22	V2	75	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



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

Mal	Tuno	Chain	Dog	Dec	Dec	Dec	Tink	B	ond leng	gths	B	ond ang	gles
IVIOI	туре	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2			
6	AME	E	1	6	9,10,11	0.24	0	9,11,13	0.49	0			
6	AME	e	1	6	9,10,11	0.25	0	9,11,13	0.48	0			

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AME	Е	1	6	-	2/9/10/12	-
6	AME	е	1	6	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Ε	1	AME	N-CA-CB-CG
6	е	1	AME	N-CA-CB-CG
6	Е	1	AME	C-CA-CB-CG
6	е	1	AME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

Of 66 ligands modelled in this entry, 10 are monoatomic - leaving 56 for Mogul analysis.

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

Mal	Type	Chain	Dog	Link	Bo	ond leng	$_{\rm sths}$	Boi	nd angle	es
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CDL	j	202	-	$99,\!99,\!99$	0.29	0	105,111,111	0.26	0
28	CDL	Е	406	-	99,99,99	0.29	0	105,111,111	0.25	0
26	ATP	A1	601	27	$26,\!33,\!33$	0.60	0	$31,\!52,\!52$	0.60	1 (3%)
26	ATP	B2	601	27	$26,\!33,\!33$	0.61	0	$31,\!52,\!52$	0.61	1 (3%)
28	CDL	Q	101	-	99,99,99	0.29	0	105,111,111	0.29	0
31	Q7G	Е	402	-	$54,\!54,\!90$	0.13	0	82,84,138	0.32	0
33	PC1	J	204	-	$53,\!53,\!53$	0.28	0	$59,\!61,\!61$	0.27	0
32	PEE	r	101	-	50, 50, 50	0.74	2 (4%)	$53,\!55,\!55$	0.51	0
26	ATP	F2	601	27	26,33,33	0.62	0	31,52,52	0.60	1 (3%)
34	UTP	H2	201	-	22,30,30	0.91	1 (4%)	27,47,47	0.85	1 (3%)
26	ATP	F1	601	27	26,33,33	0.62	0	31,52,52	0.60	1 (3%)
28	CDL	J	203	-	99,99,99	0.29	0	105,111,111	0.26	0
31	Q7G	е	407	-	54,54,90	0.13	0	82,84,138	0.31	0
33	PC1	j	203	-	$53,\!53,\!53$	0.29	0	59,61,61	0.27	0
30	LMT	j	204	-	$36,\!36,\!36$	0.17	0	$47,\!47,\!47$	0.54	0
29	ADP	D1	601	27	$24,\!29,\!29$	0.70	0	$29,\!45,\!45$	0.79	1 (3%)
33	PC1	Ι	201	-	$53,\!53,\!53$	0.28	0	$59,\!61,\!61$	0.27	0
33	PC1	f	204	-	$53,\!53,\!53$	0.27	0	$59,\!61,\!61$	0.27	0
28	CDL	q	101	-	$99,\!99,\!99$	0.29	0	105,111,111	0.29	0
26	ATP	A2	601	27	$26,\!33,\!33$	0.61	0	$31,\!52,\!52$	0.61	1 (3%)
30	LMT	Е	401	-	36,36,36	0.15	0	47,47,47	0.46	1 (2%)
26	ATP	C1	601	27	26,33,33	0.61	0	$31,\!52,\!52$	0.61	1 (3%)
34	UTP	H1	201	-	22,30,30	0.91	1 (4%)	$27,\!47,\!47$	0.85	1 (3%)
28	CDL	е	401	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	m	201	-	99,99,99	0.30	0	105,111,111	0.28	0
29	ADP	D2	601	27	24,29,29	0.69	0	29,45,45	0.79	1 (3%)
30	LMT	e	406	-	36,36,36	0.15	0	47,47,47	0.47	1 (2%)
28	CDL	е	402	-	99,99,99	0.30	0	105,111,111	0.28	0
28	CDL	е	404	-	$99,\!99,\!99$	0.29	0	105,111,111	0.25	0



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	ths	Bond angles		
INIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
33	PC1	i	201	-	53,53,53	0.29	0	59,61,61	0.27	0
28	CDL	е	405	-	99,99,99	0.29	0	105,111,111	0.26	0
31	Q7G	N	201	-	66,66,90	0.13	0	100,102,138	0.31	0
28	CDL	Е	403	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	j	201	-	99,99,99	0.29	0	105,111,111	0.25	0
28	CDL	С	201	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	с	201	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	J	202	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	F	201	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	Е	404	-	99,99,99	0.30	0	105,111,111	0.28	0
26	ATP	B1	601	27	26,33,33	0.61	0	$31,\!52,\!52$	0.61	1 (3%)
28	CDL	М	201	-	99,99,99	0.30	0	105,111,111	0.28	0
26	ATP	C2	601	27	26,33,33	0.61	0	31,52,52	0.61	1 (3%)
28	CDL	1	101	-	99,99,99	0.30	0	105,111,111	0.26	0
32	PEE	f	202	-	50,50,50	0.76	2 (4%)	$53,\!55,\!55$	0.45	0
33	PC1	F	203	-	53,53,53	0.28	0	59,61,61	0.27	0
33	PC1	f	203	-	53,53,53	0.28	0	59,61,61	0.28	0
32	PEE	F	202	-	50,50,50	0.76	2 (4%)	$53,\!55,\!55$	0.45	0
28	CDL	е	403	-	99,99,99	0.29	0	105,111,111	0.26	0
32	PEE	R	101	-	50,50,50	0.73	2 (4%)	$53,\!55,\!55$	0.51	0
28	CDL	L	101	-	99,99,99	0.29	0	105,111,111	0.25	0
33	PC1	F	204	-	53,53,53	0.27	0	59,61,61	0.27	0
28	CDL	f	201	-	99,99,99	0.29	0	105,111,111	0.26	0
30	LMT	J	201	-	36,36,36	0.16	0	47,47,47	0.54	0
31	Q7G	n	201	-	66,66,90	0.14	0	100,102,138	0.31	0
28	CDL	Е	407	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	Е	405	-	99,99,99	0.29	0	105,111,111	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CDL	j	202	-	-	29/110/110/110	-
28	CDL	Е	406	-	-	19/110/110/110	-
26	ATP	A1	601	27	-	5/18/38/38	0/3/3/3
31	Q7G	Е	402	-	1/1/19/34	5/15/123/200	0/7/7/10
26	ATP	B2	601	27	-	4/18/38/38	0/3/3/3
28	CDL	Q	101	-	-	28/110/110/110	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PC1	J	204	-	-	14/57/57/57	-
32	PEE	r	101	-	-	29/54/54/54	-
26	ATP	F2	601	27	-	4/18/38/38	0/3/3/3
34	UTP	H2	201	-	-	5/20/38/38	0/2/2/2
26	ATP	F1	601	27	-	4/18/38/38	0/3/3/3
28	CDL	J	203	-	-	29/110/110/110	_
31	Q7G	е	407	-	1/1/19/34	5/15/123/200	0/7/7/10
33	PC1	j	203	-	-	14/57/57/57	-
30	LMT	j	204	-	_	5/21/61/61	0/2/2/2
29	ADP	D1	601	27	-	1/12/32/32	0/3/3/3
33	PC1	Ι	201	-	-	10/57/57/57	-
33	PC1	f	204	-	-	10/57/57/57	-
28	CDL	q	101	-	_	28/110/110/110	_
26	ATP	A2	601	27	-	5/18/38/38	0/3/3/3
30	LMT	Е	401	-	-	1/21/61/61	0/2/2/2
26	ATP	C1	601	27	-	6/18/38/38	0/3/3/3
34	UTP	H1	201	-	-	4/20/38/38	0/2/2/2
28	CDL	е	401	-	-	23/110/110/110	-
28	CDL	m	201	-	-	41/110/110/110	-
29	ADP	D2	601	27	-	1/12/32/32	0/3/3/3
30	LMT	е	406	-	-	1/21/61/61	0/2/2/2
28	CDL	е	402	-	-	30/110/110/110	-
28	CDL	е	404	-	-	19/110/110/110	-
33	PC1	i	201	-	-	10/57/57/57	-
31	Q7G	Ν	201	-	2/2/24/34	6/20/148/200	0/8/8/10
28	CDL	е	405	-	-	34/110/110/110	-
28	CDL	Е	403	-	-	23/110/110/110	-
28	CDL	j	201	-	-	25/110/110/110	-
28	CDL	С	201	-	-	24/110/110/110	-
28	CDL	С	201	-	-	24/110/110/110	-
28	CDL	J	202	-	-	25/110/110/110	-
28	CDL	F	201	-	-	22/110/110/110	-
28	CDL	Е	404	-	-	30/110/110/110	-
26	ATP	B1	601	27	-	4/18/38/38	0/3/3/3
28	CDL	М	201	-	-	42/110/110/110	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	ATP	C2	601	27	-	6/18/38/38	0/3/3/3
28	CDL	1	101	-	-	23/110/110/110	-
32	PEE	f	202	-	-	17/54/54/54	-
33	PC1	F	203	-	-	10/57/57/57	-
33	PC1	f	203	-	-	10/57/57/57	-
32	PEE	F	202	-	-	17/54/54/54	-
28	CDL	е	403	-	-	30/110/110/110	-
32	PEE	R	101	-	-	29/54/54/54	-
28	CDL	L	101	-	-	23/110/110/110	-
33	PC1	F	204	-	-	10/57/57/57	-
28	CDL	f	201	-	-	22/110/110/110	-
30	LMT	J	201	-	-	5/21/61/61	0/2/2/2
31	Q7G	n	201	-	2/2/24/34	6/20/148/200	0/8/8/10
28	CDL	Е	407	-	-	35/110/110/110	-
28	CDL	Е	405	-	-	30/110/110/110	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
32	f	202	PEE	C39-C38	3.57	1.52	1.31
32	F	202	PEE	C39-C38	3.56	1.52	1.31
32	f	202	PEE	C18-C19	3.51	1.52	1.31
32	F	202	PEE	C18-C19	3.51	1.52	1.31
32	r	101	PEE	C18-C19	3.46	1.51	1.31

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
34	H2	201	UTP	C5-C4-N3	-3.87	114.79	123.31
34	H1	201	UTP	C5-C4-N3	-3.86	114.82	123.31
26	C2	601	ATP	C5-C6-N6	2.35	123.92	120.35
26	B2	601	ATP	C5-C6-N6	2.35	123.92	120.35
29	D1	601	ADP	C5-C6-N6	2.34	123.90	120.35

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	Е	402	Q7G	C1B
Continued on next nage				



Mol	Chain	Res	Type	Atom
31	Ν	201	Q7G	C1B
31	Ν	201	Q7G	C1C
31	е	407	Q7G	C1B
31	n	201	Q7G	C1B

5 of 921 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A1	601	ATP	PB-O3B-PG-O2G
26	A2	601	ATP	PB-O3B-PG-O2G
26	B1	601	ATP	PB-O3B-PG-O3G
26	B2	601	ATP	PB-O3B-PG-O3G
26	C1	601	ATP	PB-O3B-PG-O2G

There are no ring outliers.

No monomer is involved in short contacts.

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








































































































5.7 Other polymers (i)

There are no such residues in this entry.

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-15559. 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





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: 195



Y Index: 256



Z Index: 254

6.3.2 Raw map



X Index: 322

Y Index: 304



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 0.008. 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

$emd_{15559}msk_{1.map}$ (i) 6.5.1





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 1696 $\rm nm^3;$ this corresponds to an approximate mass of 1532 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 0.312 ${\rm \AA^{-1}}$



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 0.312 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

B osolution ostimato $(\hat{\lambda})$	Estimation criterion (FSC cut-off)		
resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.14	3.70	3.19
Unmasked-calculated*	3.89	7.22	4.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.2 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15559 and PDB model 8AP6. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.008 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 (0.008).



9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.8126
А	0.9541
A1	0.7552
A2	0.7545
B1	0.8002
B2	0.7972
С	0.9153
C1	0.7772
C2	0.7742
D	0.8587
D1	0.7226
D2	0.7188
E	0.9366
E1	0.7712
E2	0.7688
F	0.9257
F1	0.7609
F2	0.7582
G	0.8080
G1	0.7240
G2	0.7257
Н	0.8267
H1	0.7545
H2	0.7569
Ι	0.9604
I1	0.7171
I2	0.7190
J	0.9176
J1	0.5971
J2	0.5948
K	0.9350
K1	0.7159
K2	0.7105
L	0.8636
L1	0.6484



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Chain	Atom inclusion
L2	0.6491
М	0.9177
M1	0.7596
M2	0.7574
N	0.9751
0	0.9483
01	0.8164
O2	0.8164
Р	0.9357
P1	0.8414
P2	0.8360
Q	0.9292
Q1	0.7950
Q2	0.7932
R	0.9444
R1	0.8360
R2	0.8342
S1	0.8592
S2	0.8538
T1	0.8360
T2	0.8378
U1	0.8414
U2	0.8467
V1	0.7897
V2	0.7950
W1	0.8039
W2	0.8057
X1	0.8235
X2	0.8271
a	0.9556
с	0.9092
d	0.8572
е	0.9355
f	0.9242
g	0.8085
h	0.8277
i	0.9604
j	0.9140
k	0.9338
1	0.8555
m	0.9150
n	0.9734

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Chain	Atom inclusion
0	0.9470
р	0.9297
q	0.9316
r	0.9479

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