



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Dec 9, 2019 – 03:02 AM EST

PDB ID : 6RDF
EMDB ID: : EMD-4816
Title : CryoEM structure of Polytomella F-ATP synthase, Primary rotary state 3, monomer-masked refinement
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on : 2019-04-12
Resolution : 3.20 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

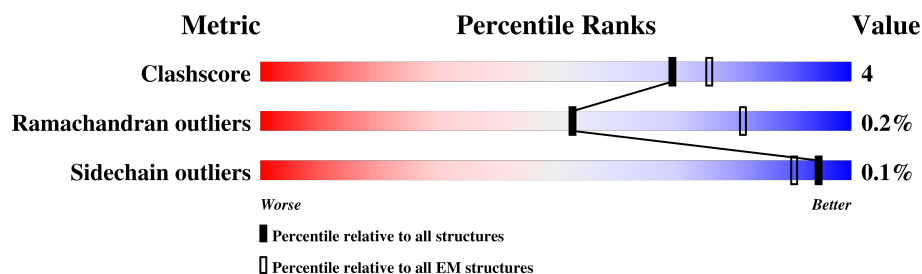
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	82	91% 7% .
2	1	618	87% 9% .
3	2	441	85% 15%
4	3	325	66% 9% 25%
5	4	294	90% 9% .
6	5	123	88% 12%
7	6	151	76% 6% 18%
8	7	190	79% 13% 7%
9	8	89	90% 9% .

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Mol	Chain	Length	Quality of chain
10	9	97	<div><div></div><div>94%</div><div>6%</div></div>
11	M	327	<div><div></div><div>61%</div><div>6%</div><div>34%</div></div>
12	P	229	<div><div></div><div>31%</div><div>•</div><div>65%</div></div>
13	T	562	<div><div></div><div>5%</div><div>•</div><div>93%</div></div>

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 19855 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ASA-10: Polytomella F-ATP synthase associated subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	81	Total	C	N	O	S	0	0
			607	388	107	110	2		

- Molecule 2 is a protein called ATP synthase associated protein ASA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	595	Total	C	N	O	S	0	0
			4661	2958	798	900	5		

- Molecule 3 is a protein called ASA-2: Polytomella F-ATP synthase associated subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	2	441	Total	C	N	O	0	0
			3163	2020	532	611		

- Molecule 4 is a protein called Mitochondrial F1F0 ATP synthase associated 32 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	245	Total	C	N	O	S	0	0
			1874	1204	299	370	1		

- Molecule 5 is a protein called Mitochondrial ATP synthase associated protein ASA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	290	Total	C	N	O	S	0	0
			2177	1385	356	434	2		

- Molecule 6 is a protein called Mitochondrial F1F0 ATP synthase associated 14 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	123	Total	C	N	O	S	0	0
			986	640	172	170	4		

- Molecule 7 is a protein called Mitochondrial ATP synthase subunit ASA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	124	Total	C	N	O	S	0	0
			926	599	154	172	1		

- Molecule 8 is a protein called Mitochondrial ATP synthase associated protein ASA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	176	Total	C	N	O	S	0	0
			1347	860	227	259	1		

- Molecule 9 is a protein called Mitochondrial ATP synthase subunit ASA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	88	Total	C	N	O	0	0
			692	456	115	121		

- Molecule 10 is a protein called ASA-9: Polytomella F-ATP synthase associated subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	97	Total	C	N	O	S	0	0
			776	514	124	132	6		

- Molecule 11 is a protein called Mitochondrial ATP synthase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	217	Total	C	N	O	S	0	0
			1640	1077	267	288	8		

- Molecule 12 is a protein called Mitochondrial ATP synthase subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	80	Total	C	N	O	S	0	0
			646	418	105	120	3		

- Molecule 13 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	T	40	Total	C	N	O	0	0
			330	215	56	59		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	266	ARG	LYS	conflict	UNP A0ZW40

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	M	1	Total 1	Zn 1	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	1	2	Total 2	O 2	0
15	5	3	Total 3	O 3	0
15	6	2	Total 2	O 2	0
15	M	22	Total 22	O 22	0

3 Residue-property plots


These plots are drawn for all protein, RNA and DNA 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. 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. 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.

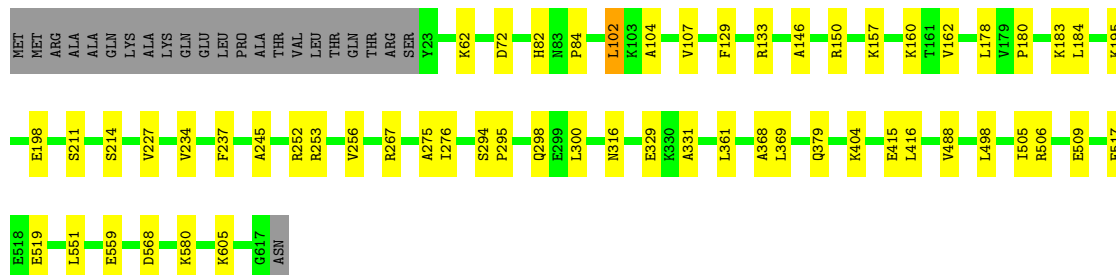
- Molecule 1: ASA-10: *Polytomella* F-ATP synthase associated subunit 10

Chain 0: 




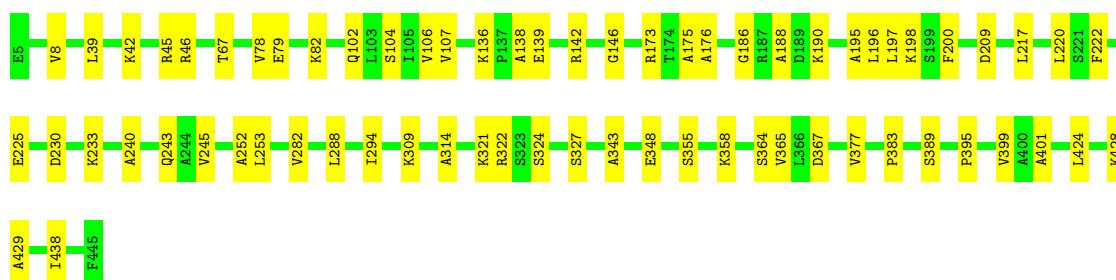
- Molecule 2: ATP synthase associated protein ASA1

Chain 1: 



- Molecule 3: ASA-2: *Polytomella* F-ATP synthase associated subunit 2

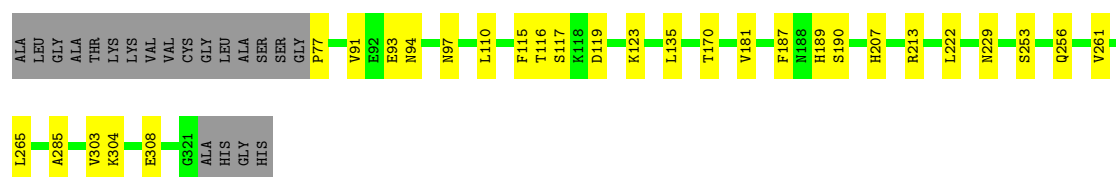
Chain 2: 



- Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein

Chain 3: 





- Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4: 90% 9%



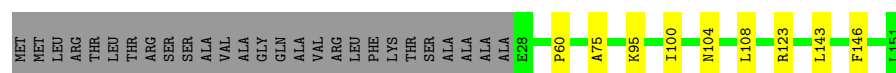
- Molecule 6: Mitochondrial F1F0 ATP synthase associated 14 kDa protein

Chain 5: 88% 12%



- Molecule 7: Mitochondrial ATP synthase subunit ASA6

Chain 6: 76% 6% 18%



- Molecule 8: Mitochondrial ATP synthase associated protein ASA7

Chain 7: 79% 13% 7%



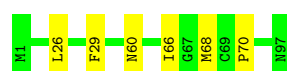
- Molecule 9: Mitochondrial ATP synthase subunit ASA8

Chain 8: 90% 9%



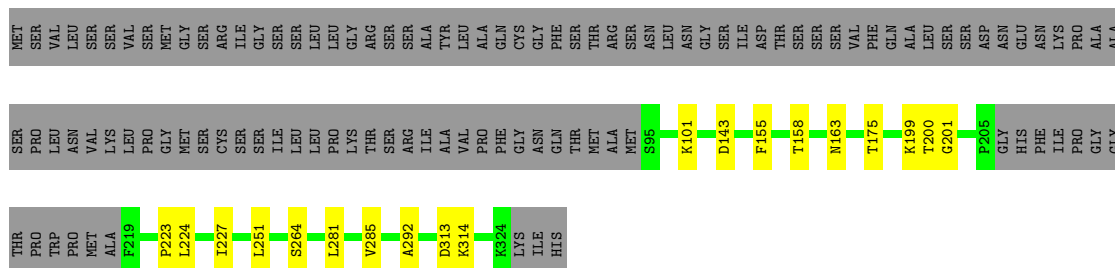
- Molecule 10: ASA-9: Polytomella F-ATP synthase associated subunit 9

Chain 9: 94% 6%

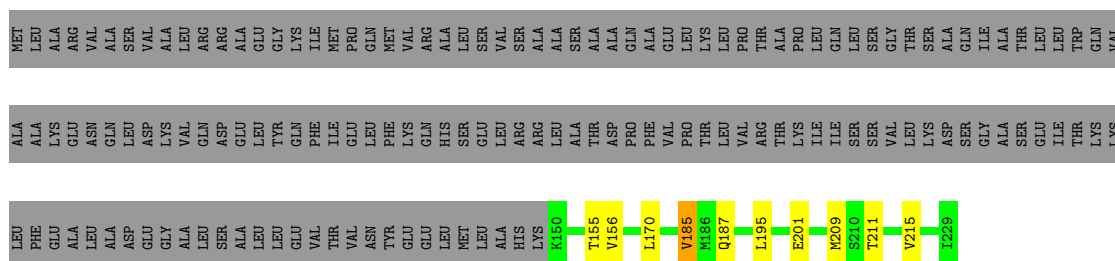


- Molecule 11: Mitochondrial ATP synthase subunit 6

Chain M: 61% 6% 34%



- Molecule 12: Mitochondrial ATP synthase subunit OSCP



- Molecule 13: ATP synthase subunit alpha



ALA

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	163259	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	0	0.39	0/628	0.55	1/856 (0.1%)
10	9	0.34	0/802	0.49	0/1084
11	M	0.45	0/1683	0.57	0/2295
12	P	0.34	0/653	0.60	0/872
13	T	0.38	0/338	0.55	0/454
2	1	0.38	0/4750	0.49	0/6434
3	2	0.34	0/3212	0.52	0/4371
4	3	0.36	0/1911	0.50	1/2601 (0.0%)
5	4	0.38	0/2216	0.49	0/3000
6	5	0.46	0/1011	0.62	2/1376 (0.1%)
7	6	0.39	0/946	0.51	0/1287
8	7	0.44	0/1374	0.52	0/1865
9	8	0.42	0/715	0.54	0/974
All	All	0.39	0/20239	0.52	4/27469 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	P	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	106	LEU	CA-CB-CG	6.05	129.21	115.30
4	3	77	PRO	N-CA-CB	5.87	110.34	103.30
1	0	31	CYS	CA-CB-SG	5.72	124.30	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	106	LEU	CB-CG-CD2	-5.01	102.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	P	185	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	607	0	584	4	0
2	1	4661	0	4695	36	0
3	2	3163	0	3262	41	0
4	3	1874	0	1826	17	0
5	4	2177	0	2169	19	0
6	5	986	0	1021	13	0
7	6	926	0	941	9	0
8	7	1347	0	1345	24	0
9	8	692	0	694	6	0
10	9	776	0	757	4	0
11	M	1640	0	1665	18	0
12	P	646	0	681	6	0
13	T	330	0	342	5	0
14	M	1	0	0	0	0
15	1	2	0	0	0	0
15	5	3	0	0	0	0
15	6	2	0	0	0	0
15	M	22	0	0	6	0
All	All	19855	0	19982	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 161 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:224:LEU:HG	15:M:709:HOH:O	1.66	0.93
11:M:224:LEU:CD2	15:M:709:HOH:O	2.21	0.87
11:M:224:LEU:CG	15:M:709:HOH:O	2.22	0.86
11:M:199:LYS:HE3	11:M:313:ASP:OD2	1.78	0.84
11:M:224:LEU:HD23	15:M:709:HOH:O	1.77	0.81

There are no symmetry-related clashes.

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	Percentiles	
1	0	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
2	1	593/618 (96%)	574 (97%)	19 (3%)	0	100	100
3	2	439/441 (100%)	417 (95%)	21 (5%)	1 (0%)	49	83
4	3	243/325 (75%)	234 (96%)	9 (4%)	0	100	100
5	4	288/294 (98%)	277 (96%)	11 (4%)	0	100	100
6	5	121/123 (98%)	114 (94%)	6 (5%)	1 (1%)	21	62
7	6	122/151 (81%)	111 (91%)	11 (9%)	0	100	100
8	7	174/190 (92%)	171 (98%)	3 (2%)	0	100	100
9	8	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
10	9	95/97 (98%)	84 (88%)	11 (12%)	0	100	100
11	M	213/327 (65%)	206 (97%)	7 (3%)	0	100	100
12	P	78/229 (34%)	71 (91%)	6 (8%)	1 (1%)	13	52
13	T	38/562 (7%)	31 (82%)	6 (16%)	1 (3%)	6	35
All	All	2569/3528 (73%)	2445 (95%)	120 (5%)	4 (0%)	53	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	383	PRO
13	T	56	LYS
6	5	120	PRO
12	P	185	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	63/64 (98%)	63 (100%)	0	100	100
2	1	493/512 (96%)	491 (100%)	2 (0%)	92	96
3	2	312/312 (100%)	311 (100%)	1 (0%)	93	97
4	3	195/258 (76%)	195 (100%)	0	100	100
5	4	220/223 (99%)	220 (100%)	0	100	100
6	5	107/107 (100%)	107 (100%)	0	100	100
7	6	96/115 (84%)	96 (100%)	0	100	100
8	7	140/150 (93%)	140 (100%)	0	100	100
9	8	71/72 (99%)	71 (100%)	0	100	100
10	9	79/79 (100%)	79 (100%)	0	100	100
11	M	178/272 (65%)	178 (100%)	0	100	100
12	P	73/196 (37%)	73 (100%)	0	100	100
13	T	36/448 (8%)	36 (100%)	0	100	100
All	All	2063/2808 (74%)	2060 (100%)	3 (0%)	94	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	102	LEU
2	1	605	LYS
3	2	428	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
4	3	206	ASN
6	5	29	GLN
12	P	220	ASN
4	3	229	ASN
4	3	256	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.