



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 9, 2019 – 02:46 AM EST

PDB ID : 6RD6
EMDB ID: : EMD-4807
Title : CryoEM structure of Polytomella F-ATP synthase, focussed refinement of upper peripheral stalk
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on : 2019-04-12
Resolution : 2.75 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation 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

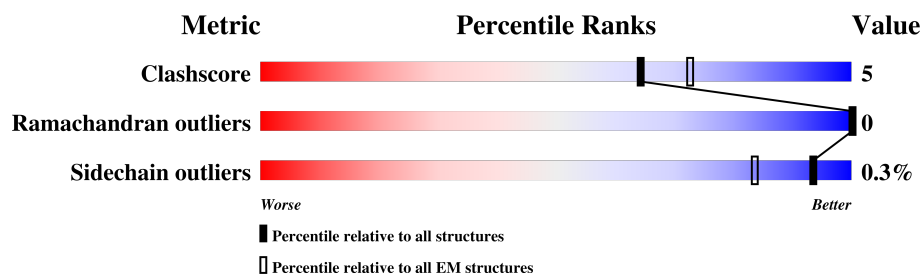
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.75 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	2	441	88% 12%
2	4	294	90% 8% .
3	7	190	82% 11% 7%
4	P	229	32% . 64%
5	T	562	7% . 92%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7758 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-2: Polytomella F-ATP synthase associated subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2	441	Total	C	N	O	0	0
			3163	2020	532	611		

- Molecule 2 is a protein called Mitochondrial ATP synthase associated protein ASA4.

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

- Molecule 3 is a protein called Mitochondrial ATP synthase associated protein ASA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	176	Total	C	N	O	S	0	0
			1347	860	227	259	1		

- Molecule 4 is a protein called Mitochondrial ATP synthase subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	82	Total	C	N	O	S	0	0
			665	430	110	122	3		

- Molecule 5 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	T	46	Total	C	N	O	0	0
			374	245	64	65		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	2	6	Total 6	O 6	0
6	4	8	Total 8	O 8	0
6	7	13	Total 13	O 13	0
6	P	1	Total 1	O 1	0
6	T	4	Total 4	O 4	0

[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	777340	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 [i](#)

5.1 Standard geometry [i](#)

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	2	0.31	0/3212	0.47	0/4371
2	4	0.35	0/2216	0.48	0/3000
3	7	0.34	0/1374	0.48	0/1865
4	P	0.27	0/673	0.50	0/898
5	T	0.32	0/384	0.48	0/518
All	All	0.32	0/7859	0.48	0/10652

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](#)

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	2	3163	0	3262	37	0
2	4	2177	0	2169	24	0
3	7	1347	0	1345	17	0
4	P	665	0	701	8	0
5	T	374	0	390	8	0
6	2	6	0	0	0	0
6	4	8	0	0	0	0
6	7	13	0	0	0	0
6	P	1	0	0	0	0
6	T	4	0	0	0	0
All	All	7758	0	7867	71	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 5.

All (71) 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)
2:4:48:LEU:HD11	4:P:215:VAL:HG12	1.04	1.02
2:4:48:LEU:HD11	4:P:215:VAL:CG1	1.98	0.91
2:4:48:LEU:CD1	4:P:215:VAL:HG12	1.99	0.87
2:4:49:ILE:CD1	5:T:70:VAL:HG13	2.15	0.77
3:7:170:HIS:HD2	3:7:172:ALA:H	1.42	0.65
2:4:49:ILE:HD11	5:T:70:VAL:HG13	1.78	0.65
2:4:49:ILE:HD13	5:T:70:VAL:HG13	1.79	0.63
1:2:240:ALA:H	1:2:243:GLN:HE21	1.49	0.59
4:P:209:MET:HG2	5:T:79:PRO:HG2	1.85	0.58
3:7:165:ARG:NH2	3:7:171:PRO:O	2.38	0.56
1:2:282:VAL:HG21	2:4:14:LEU:HD22	1.88	0.55
1:2:84:VAL:HA	1:2:87:LEU:HD12	1.88	0.54
4:P:150:LYS:HB3	4:P:182:PHE:HA	1.88	0.54
1:2:108:GLU:HB2	1:2:142:ARG:HB3	1.89	0.53
4:P:156:VAL:HG21	4:P:170:LEU:HD21	1.90	0.53
1:2:322:ARG:NH2	1:2:367:ASP:OD2	2.35	0.53
1:2:321:LYS:NZ	2:4:94:GLN:O	2.42	0.52
1:2:42:LYS:NZ	3:7:69:LEU:O	2.40	0.52
1:2:278:ASP:HB2	2:4:26:LYS:HG2	1.92	0.52
1:2:288:LEU:HD23	1:2:307:VAL:HG11	1.92	0.52
1:2:95:LEU:HD12	1:2:98:LEU:HD12	1.92	0.52
1:2:245:VAL:HG23	1:2:269:VAL:HG21	1.91	0.52
2:4:270:ASP:HB3	5:T:52:LYS:HB3	1.92	0.52
3:7:39:VAL:HG12	3:7:48:VAL:HG12	1.94	0.50
3:7:123:HIS:HD2	3:7:125:GLU:H	1.58	0.50
3:7:170:HIS:CD2	3:7:172:ALA:H	2.26	0.50
2:4:49:ILE:HD12	5:T:71:LYS:HG3	1.94	0.49
4:P:162:LEU:HD21	4:P:170:LEU:HD23	1.94	0.49
1:2:70:LEU:HD12	1:2:106:VAL:HG22	1.94	0.49
1:2:366:LEU:HD22	1:2:378:LEU:HD11	1.94	0.48
1:2:42:LYS:HA	3:7:74:ILE:HD11	1.96	0.47
2:4:7:LYS:NZ	2:4:41:THR:OG1	2.48	0.47
1:2:143:VAL:HG12	1:2:157:LEU:HD21	1.96	0.47
1:2:290:VAL:HG22	1:2:405:VAL:HG21	1.96	0.46
2:4:84:TYR:OH	3:7:161:TYR:OH	2.32	0.46
1:2:128:VAL:HG21	1:2:143:VAL:HG11	1.96	0.46
1:2:137:PRO:HA	1:2:140:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:147:VAL:HG21	1:2:157:LEU:HD23	1.97	0.46
1:2:215:PHE:HA	1:2:250:GLY:HA3	1.96	0.46
1:2:104:SER:OG	1:2:142:ARG:NH1	2.44	0.46
2:4:45:ALA:HB1	2:4:49:ILE:HG22	1.98	0.46
3:7:23:LEU:HG	3:7:66:LEU:HD12	1.98	0.46
1:2:126:ALA:O	1:2:130:SER:HB3	2.17	0.45
2:4:5:VAL:HG21	2:4:10:VAL:HB	1.99	0.44
1:2:412:ALA:HB1	1:2:441:VAL:HG12	1.98	0.44
2:4:71:LEU:HD13	2:4:221:ILE:HG21	1.99	0.44
1:2:45:ARG:NH1	3:7:75:SER:O	2.46	0.44
1:2:364:SER:OG	1:2:406:ARG:NH2	2.48	0.43
2:4:7:LYS:HA	2:4:10:VAL:HG12	1.99	0.43
1:2:282:VAL:HG22	2:4:29:LEU:HD11	2.00	0.43
2:4:100:PRO:HG3	3:7:170:HIS:CD2	2.53	0.43
4:P:206:ARG:N	5:T:82:ILE:O	2.49	0.43
1:2:382:VAL:HB	1:2:417:PRO:HA	1.99	0.43
3:7:117:ASP:OD2	3:7:117:ASP:N	2.51	0.43
2:4:168:ALA:HA	2:4:171:VAL:HG12	2.01	0.43
2:4:73:LEU:HD23	2:4:218:VAL:HG13	2.00	0.42
1:2:80:HIS:HB2	3:7:76:LEU:HB2	2.01	0.42
3:7:180:GLY:O	3:7:183:THR:OG1	2.31	0.42
5:T:50:LYS:HE2	5:T:50:LYS:HB3	1.83	0.42
1:2:419:ASN:N	1:2:419:ASN:OD1	2.53	0.42
1:2:19:VAL:HG11	1:2:51:VAL:HG22	2.01	0.42
1:2:111:GLY:HA3	1:2:146:GLY:HA2	2.01	0.42
1:2:139:GLU:N	1:2:139:GLU:OE1	2.53	0.41
1:2:70:LEU:HA	1:2:70:LEU:HD23	1.90	0.41
2:4:232:HIS:CG	3:7:153:LEU:HD11	2.56	0.41
1:2:98:LEU:HD22	1:2:102:GLN:HB3	2.03	0.41
1:2:266:PHE:HA	1:2:269:VAL:HG12	2.02	0.40
1:2:67:THR:HG21	1:2:102:GLN:HG2	2.02	0.40
1:2:36:LEU:HD11	1:2:47:LEU:HG	2.03	0.40
2:4:217:GLU:OE2	3:7:165:ARG:NH1	2.55	0.40
2:4:182:ILE:HG22	3:7:184:ASN:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	439/441 (100%)	430 (98%)	9 (2%)	0	100	100
2	4	288/294 (98%)	282 (98%)	6 (2%)	0	100	100
3	7	174/190 (92%)	169 (97%)	5 (3%)	0	100	100
4	P	80/229 (35%)	77 (96%)	3 (4%)	0	100	100
5	T	44/562 (8%)	41 (93%)	3 (7%)	0	100	100
All	All	1025/1716 (60%)	999 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	2	312/312 (100%)	312 (100%)	0	100	100
2	4	220/223 (99%)	218 (99%)	2 (1%)	81	89
3	7	140/150 (93%)	140 (100%)	0	100	100
4	P	75/196 (38%)	75 (100%)	0	100	100
5	T	41/448 (9%)	41 (100%)	0	100	100
All	All	788/1329 (59%)	786 (100%)	2 (0%)	93	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	4	46	SER
2	4	49	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	68	ASN
1	2	122	ASN
1	2	243	GLN
1	2	427	GLN
2	4	239	GLN
3	7	123	HIS
3	7	170	HIS
3	7	184	ASN
4	P	220	ASN
4	P	223	ASN
5	T	64	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.