



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 11, 2019 – 03:11 AM EST

PDB ID : 6N2D
EMDB ID: : EMD-9327
Title : Bacillus PS3 ATP synthase membrane region
Authors : Guo, H.; Rubinstein, J.L.
Deposited on : 2018-11-12
Resolution : 3.30 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

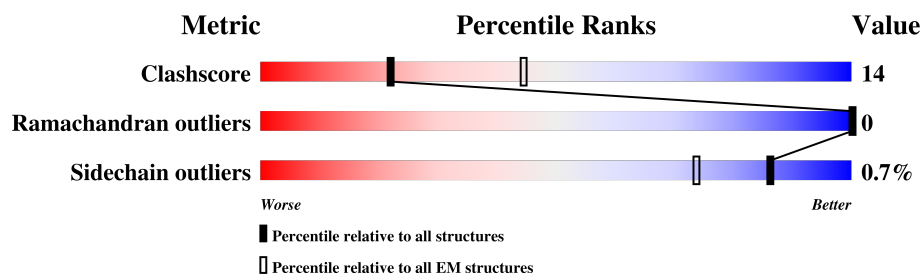
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	b1	167	26% 74%
1	b2	167	22% 78%
2	a	237	85% 14%
3	c0	72	99% .
3	c1	72	97% ..
3	c2	72	99% .
3	c3	72	99% .
3	c4	72	97% ..
3	c5	72	99% .

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Mol	Chain	Length	Quality of chain
3	c6	72	<div><div></div><div>97%</div><div>..</div></div>
3	c7	72	<div><div></div><div>97%</div><div>..</div></div>
3	c8	72	<div><div></div><div>99%</div><div>.</div></div>
3	c9	72	<div><div></div><div>97%</div><div>..</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7162 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 ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	b2	37	Total	C	N	O	S	0	0
			286	192	50	42	2		
1	b1	43	Total	C	N	O	S	0	0
			320	215	53	51	1		

- Molecule 2 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	203	Total	C	N	O	S	0	0
			1486	990	238	250	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c0	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
3	c1	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
3	c2	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
3	c3	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
3	c4	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
3	c5	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
3	c6	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
3	c7	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
3	c8	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
3	c9	71	Total	C	N	O	S	0	0
			507	333	86	87	1		

3 Residue-property plots [i](#)

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: ATP synthase subunit b

Chain b2:  22% 78%

GLU
ALA
ALA
HIS
GLY
ILE
S7
H43
ILE
ALA
ASN
GLU
ILE
ASP
GLN
ALA
GLU
LYS
ARG
GLN
GLU
LEU
GLU
GLN
ARG
GLU
MET
LYS
GLN
SER
GLN
ALA
ALA
LEU
GLU
GLN
ASN
ALA
ARG
LYS
ALA
GLU
GLN
LYS
ILE

VAL
ALA
SER
ILE
LYS
ARG
ALA
GLU
GLN
VAL
GLU
ARG
GLN
LYS
THR
ALA
LYS
GLY
ILE
GLU
ARG
GLU
GLN
GLY
MET
ALA
LEU
ARG
GLU
GLN
SER
LEU
SER
VAL
ILE
TLE
SER
LYS
VAL
ILE
GLY
LYS
THR
GLU
ASP
GLN
GLN
ARG
LYS
LEU
GLU
ILE

ALA
TYR
ILE
LYS
ASP
VAL
GLN
GLU
VAL
GLY
ALA
ARG

- Molecule 1: ATP synthase subunit b


Chain b1:  26% 74%

GLU
ALA
ALA
HIS
GLY
ILE
S7
D49
ALA
GLU
LYS
ARG
ARG
GLN
GLU
ALA
GLU
LYS
GLY
LYS
GLN
ALA
LEU
GLU
MET
LYS
GLN
SER
SER
ARG
GLU
VAL
GLN
GLY
ALA
ALA
LEU
SER
LEU
SER
VAL
ILE
TLE
GLU
ASN
ALA
ARG
LYS
LEU
GLU
ALA
GLY
ASP
GLU
GLN
LYS
GLU
TLE
ILE
GLN
VAL
SER
ALA
ALA

GLU
ALA
GLU
ARG
VAL
LYS
GLU
THR
ALA
LYS
LYS
TLE
GLU
GLU
ARG
GLY
LYS
GLN
ALA
MET
GLU
ALA
VAL
VAL
ALA
SER
LEU
SER
VAL
TLE
ILE
LYS
GLU
LYS
GLU
THR
GLN
ASP
GLU
ARG
LYS
LEU
TLE
ILE
GLN
TYR
TLE
LYS
ASP
VAL

GLN
GLU
VAL
GLY
GLY
ALA
ALA
ARG

- Molecule 2: ATP synthase subunit a

Chain a:  85% 14%

MET
GLU
HIS
LYS
ALA
P6
N16
G131
VAL
LYS
MET
LYS
GLY
ALA
SER
ASP
TYR
LEU
ARG
ASP
VAL
ALA
TRP
LEU
F152
Y191
GLY
VAL
LEU
GLY
ALA
VAL
G198
S234
HIS
ASP
HIS

- Molecule 3: ATP synthase subunit c

Chain c0:  99%

MET
S2
R72

- Molecule 3: ATP synthase subunit c

Chain c1:  97% ..



- Molecule 3: ATP synthase subunit c

Chain c2:  99% .



- Molecule 3: ATP synthase subunit c

Chain c3:  99% .



- Molecule 3: ATP synthase subunit c

Chain c4:  97% ..



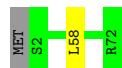
- Molecule 3: ATP synthase subunit c

Chain c5:  99% .



- Molecule 3: ATP synthase subunit c

Chain c6:  97% ..



- Molecule 3: ATP synthase subunit c

Chain c7:  97% ..



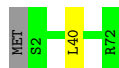
- Molecule 3: ATP synthase subunit c

Chain c8:  99% .



- Molecule 3: ATP synthase subunit c

Chain c9:  97% ..



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	895574	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 ($e^-/\text{\AA}^2$)	0.71	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	132075	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	b1	0.30	0/326	0.65	0/444
1	b2	0.31	0/292	0.59	0/395
2	a	0.32	0/1520	0.61	0/2079
3	c0	0.37	0/513	0.67	0/697
3	c1	0.37	0/513	0.66	0/697
3	c2	0.34	0/513	0.64	0/697
3	c3	0.35	0/513	0.64	0/697
3	c4	0.32	0/513	0.66	1/697 (0.1%)
3	c5	0.34	0/513	0.64	0/697
3	c6	0.36	0/513	0.70	0/697
3	c7	0.34	0/513	0.73	0/697
3	c8	0.36	0/513	0.69	0/697
3	c9	0.35	0/513	0.71	0/697
All	All	0.34	0/7268	0.66	1/9888 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	c4	54	LEU	CA-CB-CG	5.40	127.72	115.30

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	b1	320	0	316	0	0
1	b2	286	0	287	0	0
2	a	1486	0	1455	0	0
3	c0	507	0	552	0	0
3	c1	507	0	552	0	0
3	c2	507	0	552	0	0
3	c3	507	0	552	0	0
3	c4	507	0	552	0	0
3	c5	507	0	552	0	0
3	c6	507	0	552	0	0
3	c7	507	0	552	0	0
3	c8	507	0	552	0	0
3	c9	507	0	552	0	0
All	All	7162	0	7578	0	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 14.

There are no clashes within the asymmetric unit.

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	b1	41/167 (25%)	40 (98%)	1 (2%)	0	100	100
1	b2	35/167 (21%)	34 (97%)	1 (3%)	0	100	100
2	a	197/237 (83%)	186 (94%)	11 (6%)	0	100	100
3	c0	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
3	c1	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
3	c2	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
3	c3	69/72 (96%)	68 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c4	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
3	c5	69/72 (96%)	69 (100%)	0	0	100	100
3	c6	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
3	c7	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
3	c8	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
3	c9	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
All	All	963/1291 (75%)	938 (97%)	25 (3%)	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	b1	29/139 (21%)	29 (100%)	0	100	100
1	b2	26/139 (19%)	26 (100%)	0	100	100
2	a	143/198 (72%)	142 (99%)	1 (1%)	85	91
3	c0	51/52 (98%)	51 (100%)	0	100	100
3	c1	51/52 (98%)	50 (98%)	1 (2%)	58	80
3	c2	51/52 (98%)	51 (100%)	0	100	100
3	c3	51/52 (98%)	51 (100%)	0	100	100
3	c4	51/52 (98%)	51 (100%)	0	100	100
3	c5	51/52 (98%)	51 (100%)	0	100	100
3	c6	51/52 (98%)	50 (98%)	1 (2%)	58	80
3	c7	51/52 (98%)	50 (98%)	1 (2%)	58	80
3	c8	51/52 (98%)	51 (100%)	0	100	100
3	c9	51/52 (98%)	50 (98%)	1 (2%)	58	80
All	All	708/996 (71%)	703 (99%)	5 (1%)	86	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	a	16	ASN
3	c1	41	ARG
3	c6	58	LEU
3	c7	10	ILE
3	c9	40	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	a	231	HIS
3	c7	37	GLN
3	c5	23	ASN
2	a	173	ASN
3	c1	37	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.