



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 17, 2019 – 10:32 AM EDT

PDB ID : 6PWF
EMDB ID: : EMD-20507
Title : Cryo-EM structure of the ATPase domain of chromatin remodeling factor ISWI
bound to the nucleosome
Authors : Chittori, S.; Subramaniam, S.
Deposited on : 2019-07-22
Resolution : 4.07 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

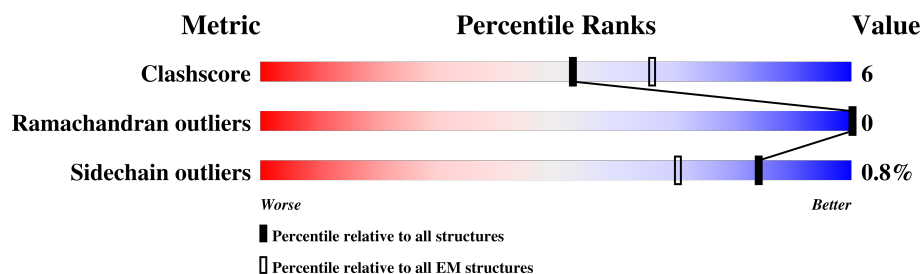
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.07 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	A	136	63% 7% 29%
1	E	136	63% 7% 29%
2	B	103	78% 8% 15%
2	F	103	66% 11% 23%
3	C	124	74% 10% 16%
3	G	124	80% 5% 15%
4	D	123	63% 12% 25%
4	H	123	65% 11% 24%
5	I	147	73% 26% .

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Mol	Chain	Length	Quality of chain
6	J	147	 78% 19% ..
7	K	640	 56% 15% 29%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15197 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	96	Total	C	N	O	S	0	0
			790	499	151	137	3		
1	E	96	Total	C	N	O	S	0	0
			790	499	151	137	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	88	Total	C	N	O	S	0	0
			671	422	130	118	1		
2	F	79	Total	C	N	O	S	0	0
			626	395	121	109	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	104	Total	C	N	O	S	0	0
			798	503	155	139	1		
3	G	105	Total	C	N	O	S	0	0
			807	509	157	140	1		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	92	Total	C	N	O	S	0	0
			723	456	129	136	2		
4	H	94	Total	C	N	O	S	0	0
			743	468	135	138	2		

- Molecule 5 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

- Molecule 6 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 7 is a protein called chromatin remodeling factor ISWI.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	454	Total	C	N	O	S	0	0
			3263	2085	579	586	13		

There are 26 discrepancies between the modelled and reference sequences:

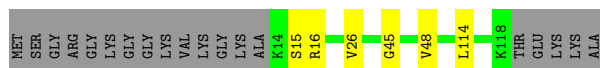
Chain	Residue	Modelled	Actual	Comment	Reference
K	83	MET	-	expression tag	UNP G0S9L5
K	84	ALA	-	expression tag	UNP G0S9L5
K	85	HIS	-	expression tag	UNP G0S9L5
K	86	HIS	-	expression tag	UNP G0S9L5
K	87	HIS	-	expression tag	UNP G0S9L5
K	88	HIS	-	expression tag	UNP G0S9L5
K	89	HIS	-	expression tag	UNP G0S9L5
K	90	HIS	-	expression tag	UNP G0S9L5
K	91	GLY	-	expression tag	UNP G0S9L5
K	92	HIS	-	expression tag	UNP G0S9L5
K	93	HIS	-	expression tag	UNP G0S9L5
K	94	HIS	-	expression tag	UNP G0S9L5
K	95	GLU	-	expression tag	UNP G0S9L5
K	96	ASN	-	expression tag	UNP G0S9L5
K	97	LEU	-	expression tag	UNP G0S9L5
K	98	TYR	-	expression tag	UNP G0S9L5
K	99	PHE	-	expression tag	UNP G0S9L5
K	100	GLN	-	expression tag	UNP G0S9L5
K	101	GLY	-	expression tag	UNP G0S9L5
K	102	SER	-	expression tag	UNP G0S9L5
K	103	SER	-	expression tag	UNP G0S9L5
K	104	SER	-	expression tag	UNP G0S9L5
K	163	GLY	-	linker	UNP G0S9L5
K	164	SER	-	linker	UNP G0S9L5
K	165	SER	-	linker	UNP G0S9L5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	166	GLY	-	linker	UNP G0S9L5

Chain G:



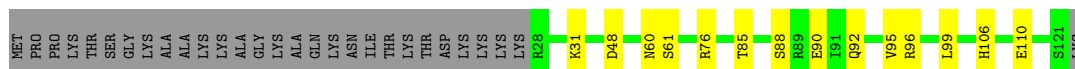
- Molecule 4: Histone H2B

Chain D:



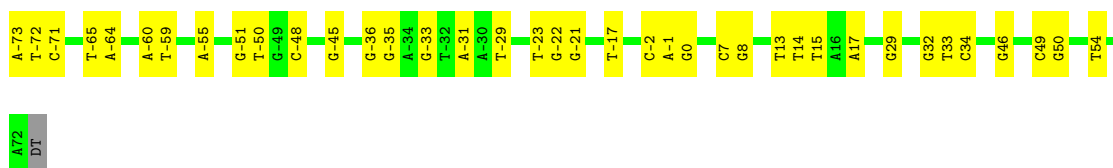
- Molecule 4: Histone H2B

Chain H:



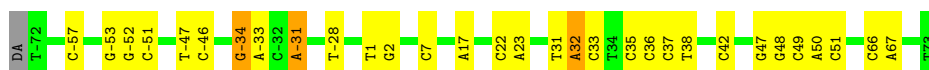
- Molecule 5: DNA (147-MER)

Chain I:



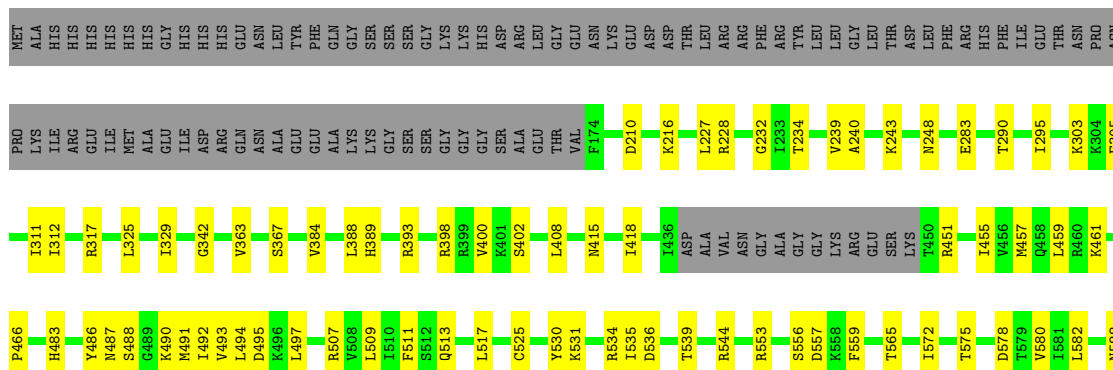
- Molecule 6: DNA (147-MER)

Chain J:



- Molecule 7: chromatin remodeling factor ISWI

Chain K:



THR	LYS	GLY	ALA	PHE	GLY	LEU	MET	ALA	GLU	LYS	GLY	ALA	ASN	LEU	ASP	ASP	ASP	ILE	ASP	ALA	ILE	LEU	LYS	ALA	GLY	GLU	GLU	ARG	THR	ARG	GLU	LEU	ASN	GLN	ILE	ALA	LYS	TYR	GLU	LYS	ALA	LEU	GLY	ILE	ASN	LYS	ASP	GLU	LEU	GLN	LYS	PHE	THR	SER	ILE	GLN	HIS	GLY	ALA	GLU	LYS	VAL	PHE	GLN
PE89	Q590	A591	D592	L593	Q594	A595	H600	R601	Q604	Y610	F611	R612	F613	V614	T615	A618	F619	E620	E621	L624	E625	L636	Q640	GLY	ARG	ALA	GLN	ILE	ALA	THR	LYS	ALA	ALA	ASN	LYS	ASP	GLU	LEU	GLN	LYS	PHE	THR	SER	MET	THR	ILE	GLN	HIS	GLY	ALA	GLU	LYS	VAL	PHE	GLN									

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32529	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 ($e^-/\text{\AA}^2$)	39	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	A	0.42	0/802	0.59	0/1076
1	E	0.42	0/802	0.59	0/1076
2	B	0.50	0/678	0.68	0/911
2	F	0.52	0/633	0.64	0/848
3	C	0.44	0/808	0.63	0/1090
3	G	0.45	0/817	0.60	0/1101
4	D	0.45	0/734	0.65	0/988
4	H	0.51	0/754	0.65	0/1013
5	I	0.90	0/3381	0.98	0/5221
6	J	0.89	0/3333	0.99	3/5137 (0.1%)
7	K	0.38	0/3324	0.66	1/4535 (0.0%)
All	All	0.67	0/16066	0.81	4/22996 (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
4	H	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	J	-31	DA	O4'-C4'-C3'	-7.30	101.58	104.50
7	K	517	LEU	CB-CG-CD1	-5.61	101.46	111.00
6	J	-34	DG	P-O3'-C3'	5.42	126.21	119.70
6	J	32	DA	P-O3'-C3'	5.24	125.99	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	31	LYS	Peptide

5.2 Too-close contacts ⓘ

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	A	790	0	826	7	0
1	E	790	0	826	9	0
2	B	671	0	684	7	0
2	F	626	0	663	10	0
3	C	798	0	848	10	0
3	G	807	0	861	4	0
4	D	723	0	746	11	0
4	H	743	0	772	9	0
5	I	3011	0	1639	37	0
6	J	2975	0	1639	29	0
7	K	3263	0	2967	58	0
All	All	15197	0	12471	150	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 6.

The worst 5 of 150 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)
6:J:23:DA:OP1	7:K:588:ASN:ND2	2.07	0.88
5:I:-73:DA:H2'	5:I:-72:DT:H72	1.57	0.85
5:I:-73:DA:H2'	5:I:-72:DT:C7	2.21	0.69
2:F:68:ASP:OD2	2:F:92:ARG:NH2	2.30	0.65
5:I:-21:DG:N2	6:J:22:DC:O2	2.29	0.65

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	A	94/136 (69%)	89 (95%)	5 (5%)	0	100	100
1	E	94/136 (69%)	89 (95%)	5 (5%)	0	100	100
2	B	86/103 (84%)	77 (90%)	9 (10%)	0	100	100
2	F	77/103 (75%)	72 (94%)	5 (6%)	0	100	100
3	C	102/124 (82%)	99 (97%)	3 (3%)	0	100	100
3	G	103/124 (83%)	96 (93%)	7 (7%)	0	100	100
4	D	90/123 (73%)	86 (96%)	4 (4%)	0	100	100
4	H	92/123 (75%)	76 (83%)	16 (17%)	0	100	100
7	K	450/640 (70%)	388 (86%)	62 (14%)	0	100	100
All	All	1188/1612 (74%)	1072 (90%)	116 (10%)	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	A	84/111 (76%)	83 (99%)	1 (1%)	74	87
1	E	84/111 (76%)	83 (99%)	1 (1%)	74	87
2	B	64/79 (81%)	64 (100%)	0	100	100
2	F	64/79 (81%)	64 (100%)	0	100	100
3	C	81/94 (86%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	82/94 (87%)	82 (100%)	0	100	100
4	D	79/104 (76%)	77 (98%)	2 (2%)	50	75
4	H	81/104 (78%)	80 (99%)	1 (1%)	74	87
7	K	289/555 (52%)	287 (99%)	2 (1%)	85	93
All	All	908/1331 (68%)	901 (99%)	7 (1%)	84	91

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	116	ARG
7	K	534	ARG
4	H	60	ASN
4	D	30	ARG
7	K	248	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	25	ASN
7	K	513	GLN
7	K	248	ASN
4	D	81	ASN
7	K	389	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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 [i](#)

There are no chain breaks in this entry.