



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 1, 2023 – 12:34 PM JST

PDB ID : 5HEK
Title : crystal structure of M1.HpyAVI
Authors : Ma, B.; Zhang, H.; Liu, W.
Deposited on : 2016-01-06
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

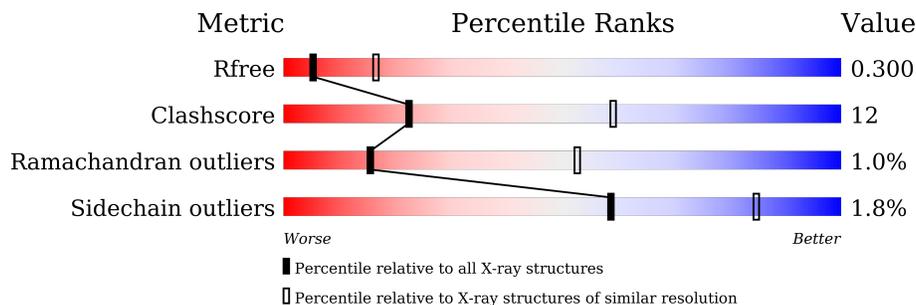
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	240	62% (green), 18% (yellow), 18% (grey)
1	B	240	54% (green), 22% (yellow), 23% (grey)
1	C	240	57% (green), 19% (yellow), 23% (grey)
1	D	240	54% (green), 18% (yellow), 26% (grey)

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 6166 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Adenine specific DNA methyltransferase (DpnA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	197	Total 1638	C 1074	N 274	O 282	S 8	0	0	0
1	B	185	Total 1532	C 1004	N 254	O 266	S 8	0	0	0
1	C	185	Total 1533	C 1004	N 257	O 265	S 7	0	0	0
1	D	177	Total 1463	C 962	N 243	O 251	S 7	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	LEU	-	expression tag	UNP O24891
A	234	GLU	-	expression tag	UNP O24891
A	235	HIS	-	expression tag	UNP O24891
A	236	HIS	-	expression tag	UNP O24891
A	237	HIS	-	expression tag	UNP O24891
A	238	HIS	-	expression tag	UNP O24891
A	239	HIS	-	expression tag	UNP O24891
A	240	HIS	-	expression tag	UNP O24891
B	233	LEU	-	expression tag	UNP O24891
B	234	GLU	-	expression tag	UNP O24891
B	235	HIS	-	expression tag	UNP O24891
B	236	HIS	-	expression tag	UNP O24891
B	237	HIS	-	expression tag	UNP O24891
B	238	HIS	-	expression tag	UNP O24891
B	239	HIS	-	expression tag	UNP O24891
B	240	HIS	-	expression tag	UNP O24891
C	233	LEU	-	expression tag	UNP O24891
C	234	GLU	-	expression tag	UNP O24891
C	235	HIS	-	expression tag	UNP O24891
C	236	HIS	-	expression tag	UNP O24891
C	237	HIS	-	expression tag	UNP O24891

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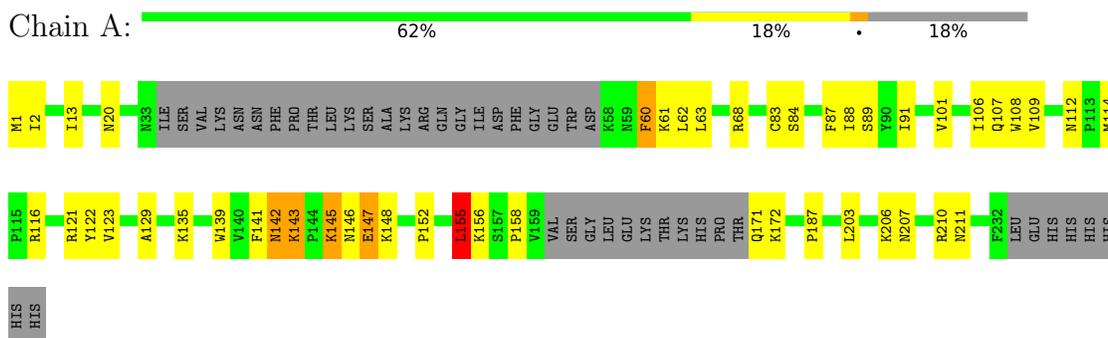
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Chain	Residue	Modelled	Actual	Comment	Reference
C	238	HIS	-	expression tag	UNP O24891
C	239	HIS	-	expression tag	UNP O24891
C	240	HIS	-	expression tag	UNP O24891
D	233	LEU	-	expression tag	UNP O24891
D	234	GLU	-	expression tag	UNP O24891
D	235	HIS	-	expression tag	UNP O24891
D	236	HIS	-	expression tag	UNP O24891
D	237	HIS	-	expression tag	UNP O24891
D	238	HIS	-	expression tag	UNP O24891
D	239	HIS	-	expression tag	UNP O24891
D	240	HIS	-	expression tag	UNP O24891

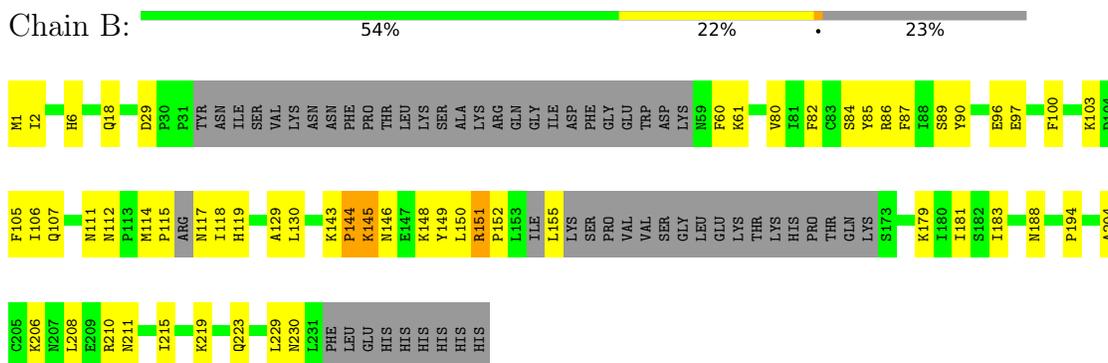
3 Residue-property plots [i](#)

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. 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.

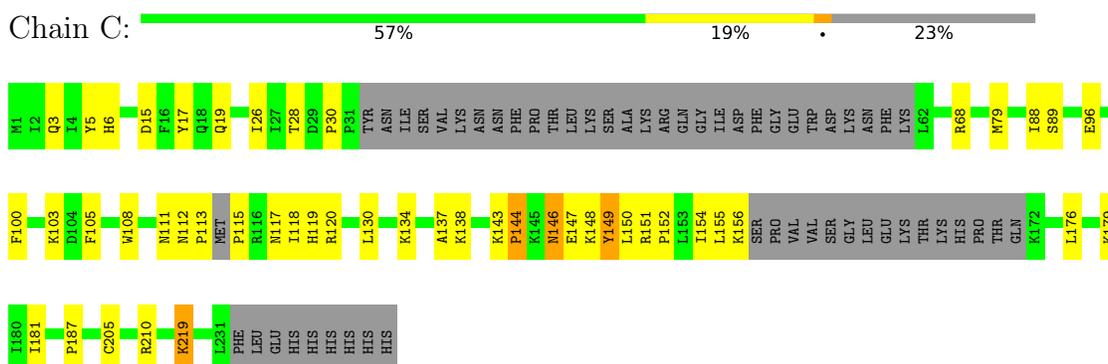
- Molecule 1: Adenine specific DNA methyltransferase (DpnA)



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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.72Å 69.72Å 532.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 3.00 48.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.09-3.00) 99.0 (48.16-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.251 , 0.308 0.248 , 0.300	Depositor DCC
R_{free} test set	1275 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtrriage
Anisotropy	0.489	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	6166	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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 >5	RMSZ	# Z >5
1	A	0.41	0/1680	0.72	2/2268 (0.1%)
1	B	0.40	0/1569	0.62	0/2117
1	C	0.39	0/1570	0.67	0/2118
1	D	0.40	0/1495	0.64	0/2012
All	All	0.40	0/6314	0.66	2/8515 (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
1	A	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	MET	C-N-CD	-6.75	105.76	120.60
1	A	155	LEU	CA-CB-CG	6.61	130.49	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ASN	Peptide
1	A	145	LYS	Peptide
1	A	147	GLU	Peptide
1	A	60	PHE	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	A	1638	0	1662	43	0
1	B	1532	0	1544	45	0
1	C	1533	0	1559	44	0
1	D	1463	0	1496	34	0
All	All	6166	0	6261	144	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 12.

The worst 5 of 144 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)
1:B:229:LEU:O	1:B:230:ASN:ND2	2.14	0.81
1:C:146:ASN:OD1	1:C:147:GLU:N	2.14	0.79
1:B:29:ASP:HB2	1:B:82:PHE:HD2	1.46	0.79
1:B:119:HIS:HA	1:D:143:LYS:HE3	1.66	0.76
1:C:6:HIS:CE1	1:C:219:LYS:HD2	2.21	0.76

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 X-ray entries followed by that with respect to entries of similar resolution.

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	191/240 (80%)	169 (88%)	20 (10%)	2 (1%)	15 53
1	B	176/240 (73%)	155 (88%)	20 (11%)	1 (1%)	25 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	177/240 (74%)	159 (90%)	15 (8%)	3 (2%)	9	39
1	D	166/240 (69%)	152 (92%)	13 (8%)	1 (1%)	25	64
All	All	710/960 (74%)	635 (89%)	68 (10%)	7 (1%)	15	53

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	149	TYR
1	A	155	LEU
1	C	144	PRO
1	D	144	PRO
1	B	144	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	179/218 (82%)	178 (99%)	1 (1%)	86	95
1	B	167/218 (77%)	164 (98%)	3 (2%)	59	85
1	C	167/218 (77%)	165 (99%)	2 (1%)	71	90
1	D	159/218 (73%)	153 (96%)	6 (4%)	33	69
All	All	672/872 (77%)	660 (98%)	12 (2%)	59	85

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	103	LYS
1	D	125	ASP
1	D	219	LYS
1	D	142	ASN
1	B	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	6	HIS
1	C	112	ASN
1	C	142	ASN
1	C	186	ASN
1	D	142	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](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.