



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Nov 11, 2019 – 05:09 PM EST

PDB ID : 6PPR
EMDB ID: : EMD-20446
Title : Cryo-EM structure of AdnA(D934A)-AdnB(D1014A) in complex with
AMPPNP and DNA
Authors : Jia, N.; Unciuleac, M.; Shuman, S.; Patel, D.J.
Deposited on : 2019-07-08
Resolution : 3.50 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
Mogul : 1.8.0 (224370), CSD as540be (2019)
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

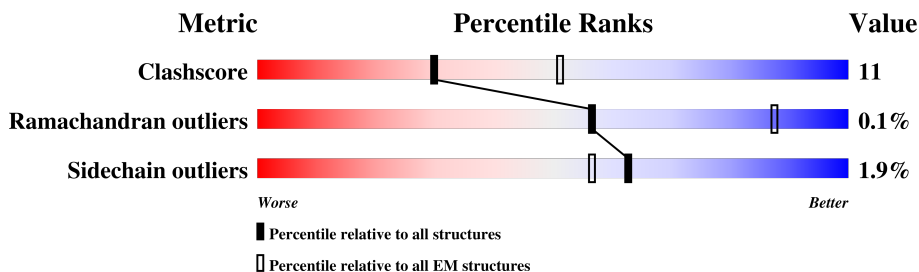
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	B	1095	
2	A	1045	
3	X	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ANP	A	1101	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11995 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 UvrD/REP helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	760	Total	C	N	O	S	0	0
			5558	3523	1029	990	16		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	537	THR	SER	variant	UNP A0A0D6HIW1
B	540	VAL	LEU	variant	UNP A0A0D6HIW1
B	559	GLU	GLN	variant	UNP A0A0D6HIW1
B	599	ALA	VAL	variant	UNP A0A0D6HIW1
B	627	GLY	SER	variant	UNP A0A0D6HIW1
B	1014	ALA	ASP	engineered mutation	UNP A0A0D6HIW1

- Molecule 2 is a protein called ATP-dependent DNA helicase (UvrD/REP).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	834	Total	C	N	O	S	0	0
			5746	3634	1074	1018	20		

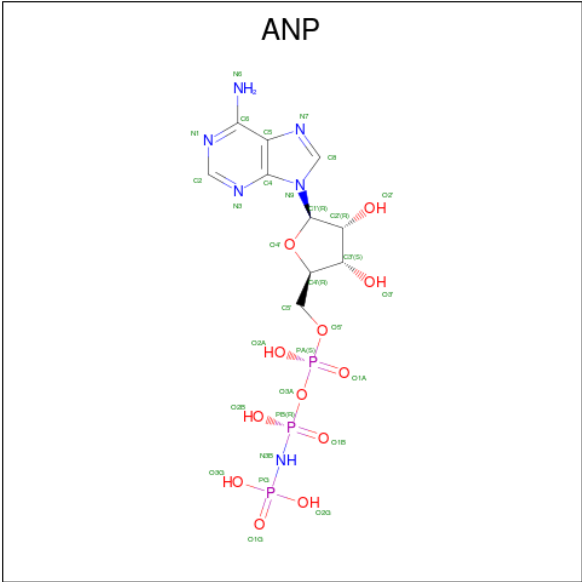
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	934	ALA	ASP	engineered mutation	UNP A0A0D6HKQ2

- Molecule 3 is a DNA chain called DNA (70-MER).

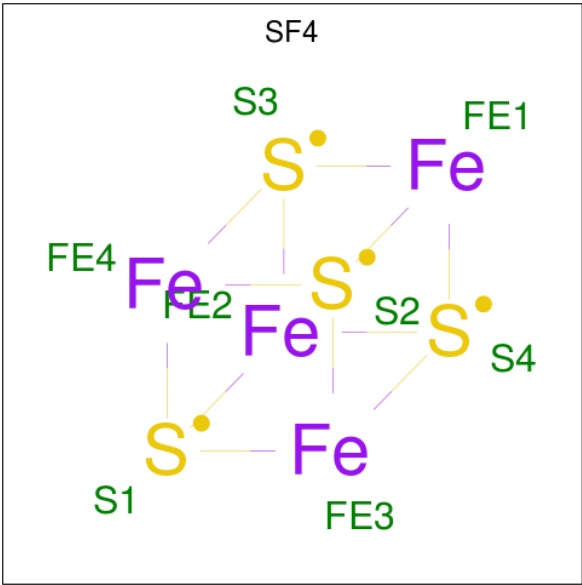
Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	32	Total	C	N	O	P	0	0
			652	316	101	203	32		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



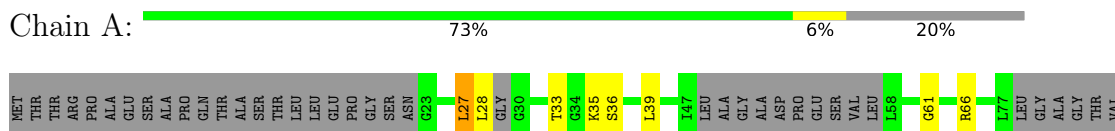
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

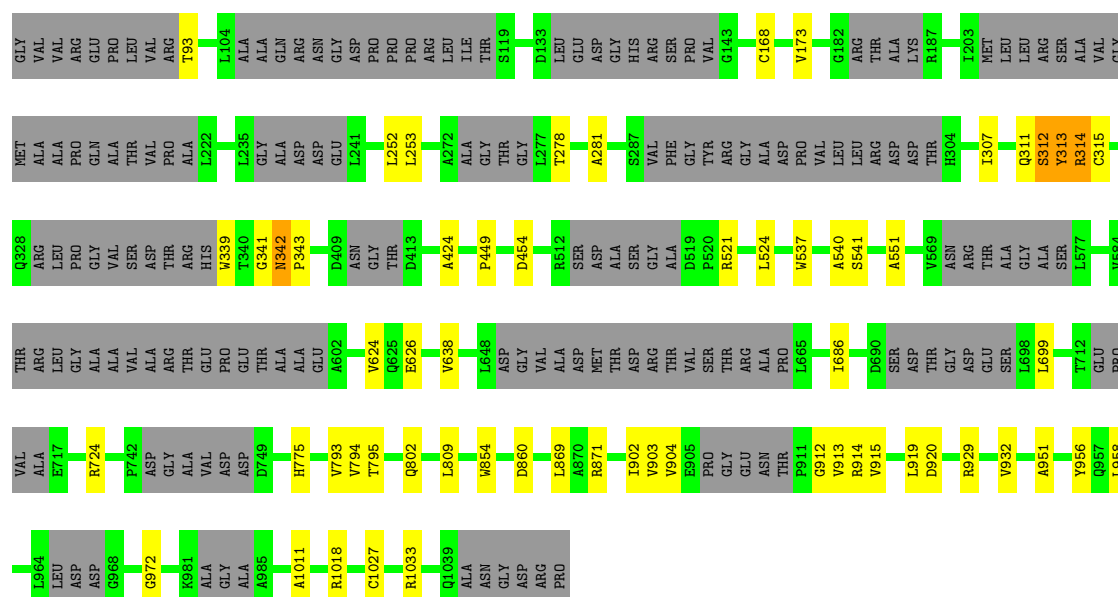
- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



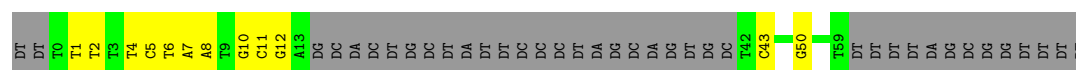
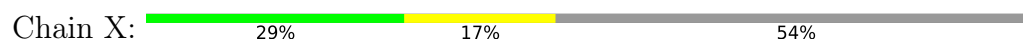
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Fe	S	0
			8	4	4	

- Molecule 1: UvrD/REP helicase





- Molecule 3: DNA (70-MER)



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	61579	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 ($e^-/\text{\AA}^2$)	2.16	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ANP

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	B	0.44	0/5662	0.66	2/7732 (0.0%)
2	A	0.36	0/5836	0.60	0/7988
3	X	0.66	0/725	1.03	0/1115
All	All	0.42	0/12223	0.67	2/16835 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	PRO	N-CA-CB	6.69	111.33	103.30
1	B	211	PRO	N-CA-CB	5.87	110.34	103.30

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	B	5558	0	5441	144	0
2	A	5746	0	5463	97	0
3	X	652	0	371	24	0
4	A	31	0	13	10	0
5	A	8	0	0	0	0
All	All	11995	0	11288	253	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 11.

The worst 5 of 253 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:143:LEU:CD2	1:B:251:VAL:HB	1.43	1.44
2:A:27:LEU:HD11	2:A:281:ALA:CB	1.60	1.32
1:B:614:ARG:NH1	1:B:648:ALA:HB1	1.44	1.29
2:A:27:LEU:CD1	2:A:281:ALA:HA	1.60	1.29
1:B:143:LEU:HD21	1:B:251:VAL:CB	1.62	1.28

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	B	730/1095 (67%)	647 (89%)	82 (11%)	1 (0%)	53	86
2	A	788/1045 (75%)	716 (91%)	72 (9%)	0	100	100
All	All	1518/2140 (71%)	1363 (90%)	154 (10%)	1 (0%)	56	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208	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 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	B	521/851 (61%)	511 (98%)	10 (2%)	60	82
2	A	495/796 (62%)	486 (98%)	9 (2%)	62	83
All	All	1016/1647 (62%)	997 (98%)	19 (2%)	63	82

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	780	ARG
2	A	27	LEU
2	A	314	ARG
1	B	709	ARG
2	A	342	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	770	HIS
2	A	342	ASN
2	A	643	HIS

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ANP	A	1101	-	28,33,33	1.44	5 (17%)	29,52,52	1.14	2 (6%)
5	SF4	A	1102	-	0,12,12	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	1101	-	-	5/13/38/38	0/3/3/3
5	SF4	A	1102	-	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	ANP	PG-O1G	4.41	1.51	1.46
4	A	1101	ANP	PB-O1B	4.12	1.50	1.46
4	A	1101	ANP	PB-O2B	-2.16	1.50	1.56
4	A	1101	ANP	PG-O2G	-2.03	1.51	1.56
4	A	1101	ANP	PG-O3G	-2.00	1.51	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1101	ANP	O2B-PB-O1B	4.17	118.47	109.87
4	A	1101	ANP	C5'-C6-N6	2.20	123.83	120.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	ANP	PA-O3A-PB-O2B
4	A	1101	ANP	C5'-O5'-PA-O3A

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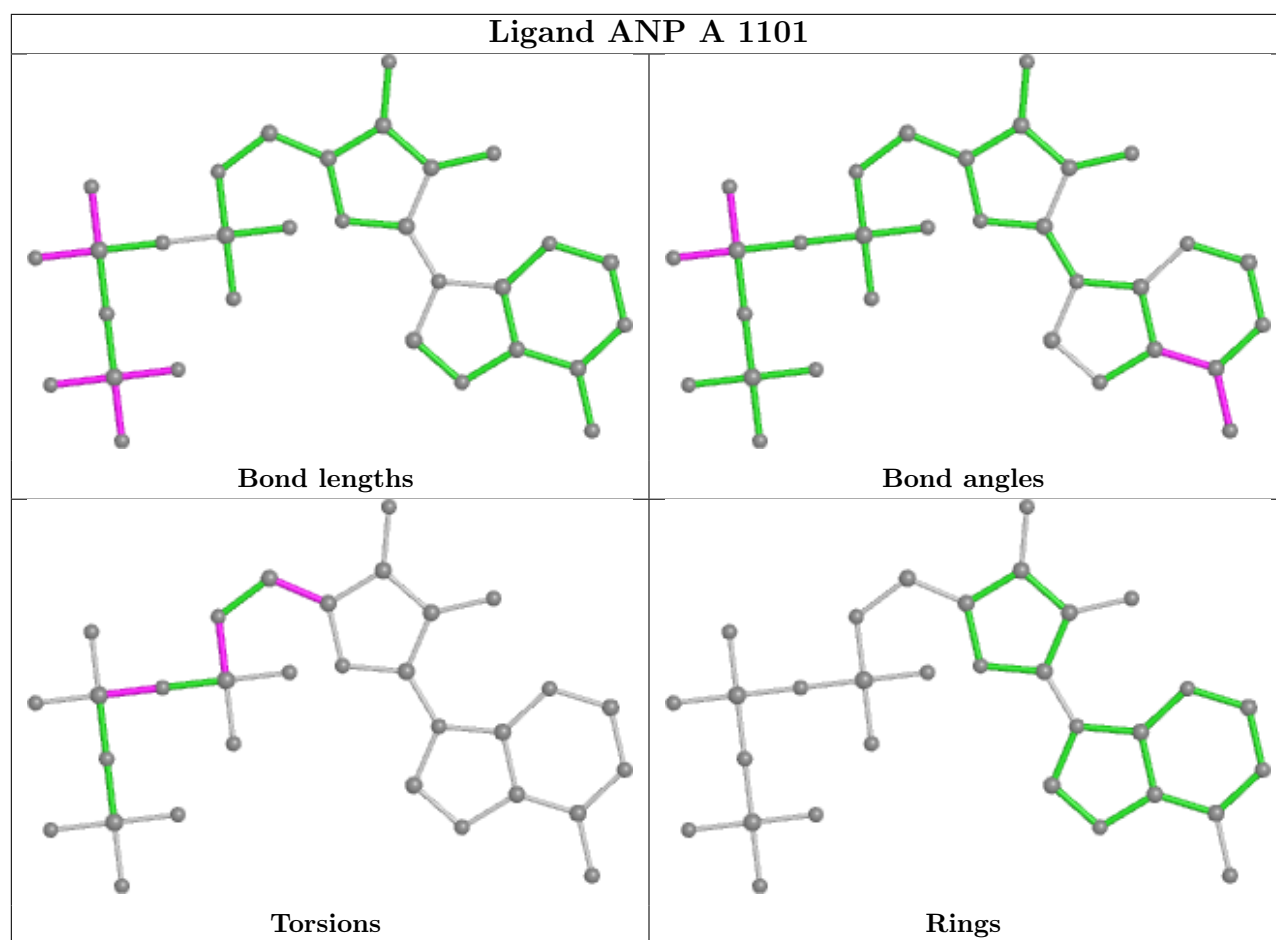
Mol	Chain	Res	Type	Atoms
4	A	1101	ANP	O4'-C4'-C5'-O5'
4	A	1101	ANP	C3'-C4'-C5'-O5'
4	A	1101	ANP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	ANP	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.