



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2025 – 04:47 PM EDT

PDB ID : 9OND / pdb_00009ond
Title : Crystal structure of E. coli ApaH in complex with ppAGG
Authors : Nuthanakanti, A.; Serganov, A.
Deposited on : 2025-05-15
Resolution : 2.16 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

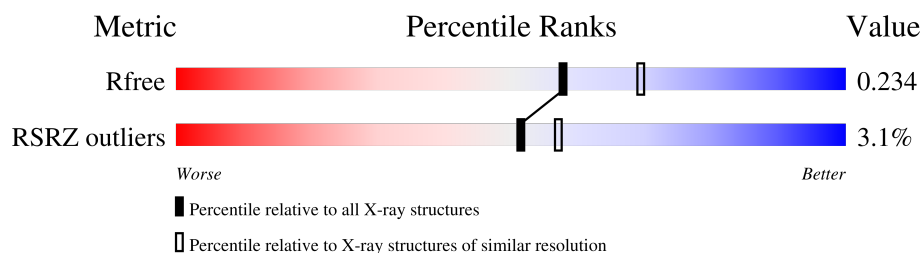
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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}	164625	1881 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4595 atoms, of which 39 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 Bis(5'-nucleosyl)-tetraphosphatase [symmetrical].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2096	1349	351	385	11			
1	B	269	Total	C	N	O	S	0	1	0
			2114	1355	360	388	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	HIS	-	expression tag	UNP P05637
A	282	HIS	-	expression tag	UNP P05637
A	283	HIS	-	expression tag	UNP P05637
A	284	HIS	-	expression tag	UNP P05637
A	285	HIS	-	expression tag	UNP P05637
A	286	HIS	-	expression tag	UNP P05637
B	281	HIS	-	expression tag	UNP P05637
B	282	HIS	-	expression tag	UNP P05637
B	283	HIS	-	expression tag	UNP P05637
B	284	HIS	-	expression tag	UNP P05637
B	285	HIS	-	expression tag	UNP P05637
B	286	HIS	-	expression tag	UNP P05637

- Molecule 2 is a RNA chain called RNA ppAGG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	2	Total	C	H	N	O	P	0	0	0
			44	12	11	5	13	3			
2	E	2	Total	C	H	N	O	P	0	0	0
			42	10	11	5	13	3			

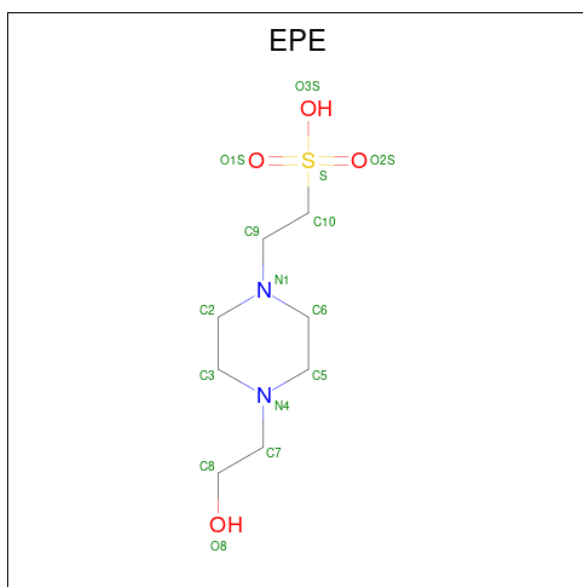
- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	1
			2	2		
3	B	2	Total	Mn	0	1
			2	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	1
			1	1		
4	B	1	Total	Mg	0	1
			1	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	126	Total	O	0	0
			126	126		
6	D	2	Total	O	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	129	Total 129	O 129	0	0
6	E	4	Total 4	O 4	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.33Å 54.82Å 119.17Å 90.00° 129.28° 90.00°	Depositor
Resolution (Å)	82.88 – 2.16 82.88 – 2.16	Depositor EDS
% Data completeness (in resolution range)	96.8 (82.88-2.16) 96.8 (82.88-2.16)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.196 , 0.235 0.195 , 0.234	Depositor DCC
R_{free} test set	2181 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4595	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	EPE	B	301	-	15,15,15	0.82	1 (6%)	19,20,20	2.06	5 (26%)

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
5	EPE	B	301	-	-	1/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	EPE	C10-S	2.77	1.81	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	EPE	C5-N4-C3	5.93	121.61	108.84
5	B	301	EPE	C7-N4-C3	3.42	120.35	111.24
5	B	301	EPE	O2S-S-C10	3.40	111.86	106.73
5	B	301	EPE	C6-C5-N4	2.80	116.31	110.65
5	B	301	EPE	C7-N4-C5	2.17	117.01	111.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	EPE	C8-C7-N4-C3

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	269/286 (94%)	0.30	10 (3%) 45 51	28, 38, 58, 73	0
1	B	269/286 (94%)	0.23	6 (2%) 62 67	21, 38, 52, 66	1 (0%)
2	D	1/3 (33%)	3.18	1 (100%) 0 0	61, 61, 61, 61	1 (100%)
2	E	1/3 (33%)	1.86	0 100 100	61, 61, 61, 61	1 (100%)
All	All	540/578 (93%)	0.27	17 (3%) 51 57	21, 38, 55, 73	3 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ARG	4.9
1	B	155	MET	4.1
1	A	195	TYR	3.6
1	B	150	PHE	3.4
1	B	151	PHE	3.4
1	A	155	MET	3.3
1	A	203	ALA	3.3
1	B	156	TYR	3.2
2	D	2	G	3.2
1	A	249	TRP	2.6
1	A	173	LEU	2.6
1	A	150	PHE	2.5
1	B	249	TRP	2.3
1	A	159	MET	2.2
1	A	166	GLU	2.1
1	A	151	PHE	2.0
1	B	83	LYS	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EPE	B	301	15/15	0.80	0.22	56,69,78,82	28
4	MG	B	303[B]	1/1	0.98	0.05	38,38,38,38	1
3	MN	B	302[A]	1/1	0.98	0.06	38,38,38,38	1
4	MG	A	302[B]	1/1	0.99	0.03	37,37,37,37	1
3	MN	A	301[A]	1/1	0.99	0.04	38,38,38,38	1
3	MN	B	304	1/1	0.99	0.07	35,35,35,35	0
3	MN	A	303	1/1	1.00	0.05	42,42,42,42	0

5.5 Other polymers [i](#)

There are no such residues in this entry.