



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2024 – 12:53 AM EDT

PDB ID : 4DE4
Title : Crystal structure of aminoglycoside phosphotransferase APH(2'')-Id/APH(2'')-IVa in complex with HEPES
Authors : Stogios, P.J.; Minasov, G.; Tan, K.; Nocek, B.; Evdokimova, E.; Egorova, O.; Di Leo, R.; Li, H.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2012-01-19
Resolution : 2.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

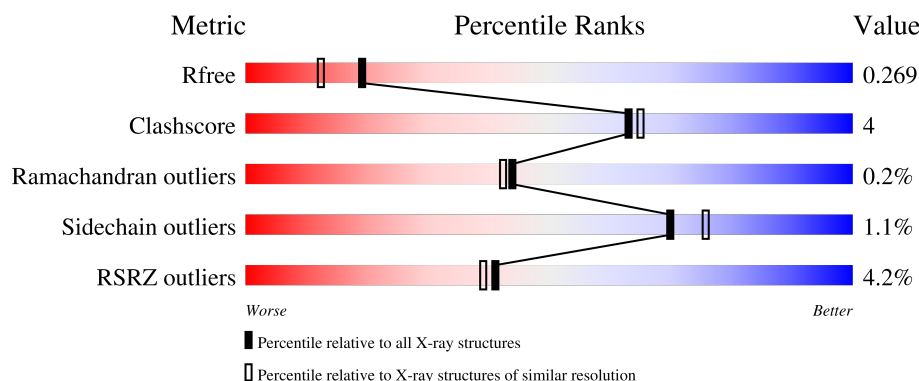
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	322	 4% 82% 10% 8%
1	B	322	 3% 82% 11% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5238 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 APH(2")-Id.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	Se	0	2	0
			2463	1589	397	465	3	9			
1	B	298	Total	C	N	O	S	Se	0	1	0
			2474	1596	399	467	3	9			

There are 42 discrepancies between the modelled and reference sequences:

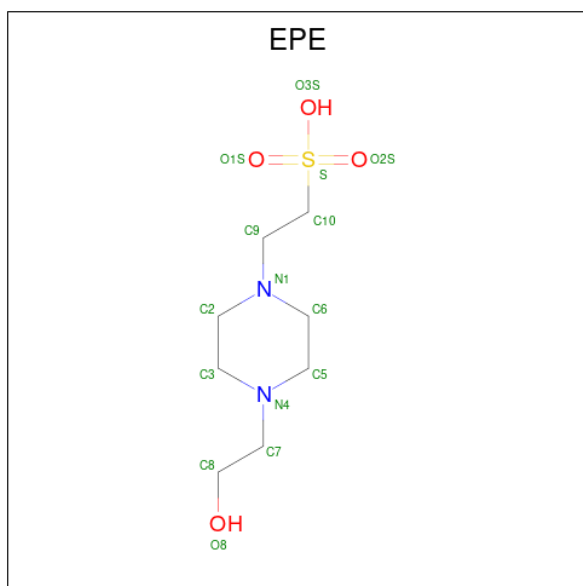
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MSE	-	expression tag	UNP O68183
A	-19	GLY	-	expression tag	UNP O68183
A	-18	SER	-	expression tag	UNP O68183
A	-17	SER	-	expression tag	UNP O68183
A	-16	HIS	-	expression tag	UNP O68183
A	-15	HIS	-	expression tag	UNP O68183
A	-14	HIS	-	expression tag	UNP O68183
A	-13	HIS	-	expression tag	UNP O68183
A	-12	HIS	-	expression tag	UNP O68183
A	-11	HIS	-	expression tag	UNP O68183
A	-10	SER	-	expression tag	UNP O68183
A	-9	SER	-	expression tag	UNP O68183
A	-8	GLY	-	expression tag	UNP O68183
A	-7	ARG	-	expression tag	UNP O68183
A	-6	GLU	-	expression tag	UNP O68183
A	-5	ASN	-	expression tag	UNP O68183
A	-4	LEU	-	expression tag	UNP O68183
A	-3	TYR	-	expression tag	UNP O68183
A	-2	PHE	-	expression tag	UNP O68183
A	-1	GLN	-	expression tag	UNP O68183
A	0	GLY	-	expression tag	UNP O68183
B	-20	MSE	-	expression tag	UNP O68183
B	-19	GLY	-	expression tag	UNP O68183
B	-18	SER	-	expression tag	UNP O68183
B	-17	SER	-	expression tag	UNP O68183

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP O68183
B	-15	HIS	-	expression tag	UNP O68183
B	-14	HIS	-	expression tag	UNP O68183
B	-13	HIS	-	expression tag	UNP O68183
B	-12	HIS	-	expression tag	UNP O68183
B	-11	HIS	-	expression tag	UNP O68183
B	-10	SER	-	expression tag	UNP O68183
B	-9	SER	-	expression tag	UNP O68183
B	-8	GLY	-	expression tag	UNP O68183
B	-7	ARG	-	expression tag	UNP O68183
B	-6	GLU	-	expression tag	UNP O68183
B	-5	ASN	-	expression tag	UNP O68183
B	-4	LEU	-	expression tag	UNP O68183
B	-3	TYR	-	expression tag	UNP O68183
B	-2	PHE	-	expression tag	UNP O68183
B	-1	GLN	-	expression tag	UNP O68183
B	0	GLY	-	expression tag	UNP O68183

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).

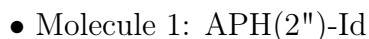


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total 115	O 115	0	1
3	B	156	Total 156	O 156	0	0

- Molecule 1: APH(2'')-Id



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.54Å 101.21Å 71.17Å 90.00° 97.51° 90.00°	Depositor
Resolution (Å)	28.99 – 2.00 28.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (28.99-2.00) 95.8 (28.99-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.222 , 0.272 0.217 , 0.269	Depositor DCC
R_{free} test set	2000 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5238	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% 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

5.1 Standard geometry

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

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	0.22	0/2521	0.37	0/3386
1	B	0.22	0/2529	0.37	0/3397
All	All	0.22	0/5050	0.37	0/6783

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2463	0	2427	17	0
1	B	2474	0	2438	22	0
2	A	15	0	17	1	0
2	B	15	0	17	2	0
3	A	115	0	0	0	0
3	B	156	0	0	1	0
All	All	5238	0	4899	38	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 4.

All (38) 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:161:LEU:HD11	1:B:276:ILE:HD13	1.76	0.66
1:B:177:TYR:HA	1:B:180:ILE:HD12	1.80	0.63
1:B:66:ARG:NH1	3:B:618:HOH:O	2.32	0.62
1:A:177:TYR:HA	1:A:180:ILE:HD12	1.84	0.60
1:B:10:GLU:HG3	1:B:22:ILE:HD12	1.84	0.59
1:B:143:VAL:HA	1:B:223:ILE:HB	1.86	0.58
1:B:61:VAL:HG21	1:B:90:MSE:HE3	1.86	0.58
1:B:71:LEU:HD12	1:B:75:ILE:HD13	1.86	0.57
1:A:152:GLU:HG2	1:A:156:LYS:HE3	1.87	0.56
1:A:83[B]:MSE:HE2	1:A:84:PRO:HD2	1.88	0.55
1:B:16:LEU:HD21	1:B:83[B]:MSE:SE	2.58	0.54
1:A:159:LYS:HD3	1:B:83[A]:MSE:HE3	1.91	0.53
1:B:234:MSE:HE2	1:B:245:VAL:HG11	1.90	0.53
1:A:68:HIS:HA	1:A:75:ILE:HD11	1.92	0.51
1:A:16:LEU:HD21	1:A:83[A]:MSE:SE	2.61	0.51
1:A:10:GLU:HG3	1:A:22:ILE:HD12	1.96	0.48
1:B:2:ARG:N	1:B:49:LYS:O	2.38	0.48
1:A:83[B]:MSE:HE3	1:B:159:LYS:HD3	1.96	0.47
1:A:161:LEU:HD11	1:A:276:ILE:HD13	1.98	0.46
1:A:234:MSE:HE2	1:A:245:VAL:HG11	1.97	0.45
1:A:147:ARG:NH2	1:A:181:LEU:O	2.48	0.45
1:B:27:ILE:HD12	1:B:35:ILE:HD11	1.99	0.45
1:B:16:LEU:HD11	1:B:83[B]:MSE:HG3	1.98	0.44
1:B:172:LYS:HD3	1:B:298:ILE:HD12	2.01	0.43
1:B:280:LYS:HE3	1:B:280:LYS:HB3	1.91	0.43
2:B:401:EPE:H61	2:B:401:EPE:H102	1.31	0.43
1:B:264:TYR:O	1:B:268:GLU:HG2	2.19	0.42
1:A:87:THR:HA	1:B:51:SER:HB3	2.00	0.42
1:A:30:GLU:HG3	1:A:35:ILE:HD13	2.02	0.42
2:A:401:EPE:H52	2:A:401:EPE:H82	1.77	0.42
1:A:16:LEU:HD11	1:A:83[A]:MSE:HG3	2.01	0.42
1:B:138:PHE:CZ	1:B:193:LEU:HD22	2.55	0.42
1:A:225:ASP:HA	1:A:226:PRO:HD2	1.91	0.41
1:B:225:ASP:HA	1:B:226:PRO:HD2	1.89	0.41
1:A:143:VAL:HA	1:A:223:ILE:HB	2.03	0.41
1:B:271:TRP:CZ2	2:B:401:EPE:H62	2.56	0.41
1:A:22:ILE:HG23	1:A:39:ILE:HG23	2.03	0.40
1:B:243:GLU:CD	1:B:243:GLU:H	2.24	0.40

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 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	296/322 (92%)	285 (96%)	10 (3%)	1 (0%)	37	35
1	B	297/322 (92%)	284 (96%)	13 (4%)	0	100	100
All	All	593/644 (92%)	569 (96%)	23 (4%)	1 (0%)	44	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ILE

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 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	276/288 (96%)	272 (99%)	4 (1%)	62	68
1	B	277/288 (96%)	275 (99%)	2 (1%)	81	86
All	All	553/576 (96%)	547 (99%)	6 (1%)	70	76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	MSE
1	A	266	MSE
1	A	284	TYR
1	A	285	MSE
1	B	2	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	231	ILE

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

Mol	Chain	Res	Type
1	A	56	ASN
1	B	68	HIS
1	B	89	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 oligosaccharides 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	$\# Z > 2$
2	EPE	B	401	-	15,15,15	0.89	1 (6%)	19,20,20	1.94	5 (26%)
2	EPE	A	401	-	15,15,15	0.80	1 (6%)	19,20,20	1.80	3 (15%)

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
2	EPE	B	401	-	-	6/9/19/19	0/1/1/1
2	EPE	A	401	-	-	8/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	EPE	C10-S	2.93	1.81	1.77
2	A	401	EPE	C10-S	2.76	1.81	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	EPE	C5-N4-C3	5.03	119.67	108.84
2	B	401	EPE	C5-N4-C3	4.58	118.70	108.84
2	B	401	EPE	C7-N4-C3	3.61	120.86	111.24
2	B	401	EPE	C7-N4-C5	3.45	120.44	111.24
2	A	401	EPE	C7-N4-C5	3.09	119.47	111.24
2	B	401	EPE	O1S-S-C10	3.04	111.32	106.73
2	B	401	EPE	C6-N1-C2	2.49	114.20	108.84
2	A	401	EPE	C7-N4-C3	2.36	117.52	111.24

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	EPE	C10-C9-N1-C2
2	A	401	EPE	C10-C9-N1-C6
2	A	401	EPE	S-C10-C9-N1
2	A	401	EPE	C9-C10-S-O2S
2	B	401	EPE	C10-C9-N1-C6
2	A	401	EPE	C8-C7-N4-C5
2	A	401	EPE	C9-C10-S-O3S
2	B	401	EPE	C9-C10-S-O3S
2	B	401	EPE	S-C10-C9-N1
2	B	401	EPE	C10-C9-N1-C2
2	A	401	EPE	C9-C10-S-O1S
2	B	401	EPE	C9-C10-S-O1S
2	B	401	EPE	C9-C10-S-O2S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	401	EPE	N4-C7-C8-O8

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	EPE	2	0
2	A	401	EPE	1	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	288/322 (89%)	0.41	13 (4%) 39 37	19, 49, 85, 106	1 (0%)
1	B	290/322 (90%)	0.23	11 (3%) 44 42	23, 41, 73, 100	0
All	All	578/644 (89%)	0.32	24 (4%) 41 39	19, 44, 83, 106	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	THR	4.0
1	B	279	GLY	3.7
1	A	283	GLY	3.5
1	A	288	TYR	3.1
1	B	241	GLY	3.0
1	A	279	GLY	2.9
1	B	141	ASN	2.8
1	B	298	ILE	2.7
1	B	68	HIS	2.7
1	A	140	SER	2.6
1	B	138	PHE	2.5
1	A	284	TYR	2.4
1	B	140	SER	2.4
1	B	235	GLU	2.4
1	A	287	TRP	2.4
1	A	25	ILE	2.4
1	A	18	PRO	2.3
1	A	278	TYR	2.3
1	B	137	GLY	2.3
1	B	69	ASN	2.3
1	A	293	ASN	2.2
1	B	278	TYR	2.2
1	A	286	ASP	2.2
1	A	136	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 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
2	EPE	B	401	15/15	0.69	0.15	68,70,147,147	0
2	EPE	A	401	15/15	0.75	0.15	87,88,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.