W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2024 – 10:49 AM EDT

PDB ID	:	4GA4
Title	:	Crystal structure of AMP phosphorylase N-terminal deletion mutant
Authors	:	Nishitani, Y.; Aono, R.; Nakamura, A.; Sato, T.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on	:	2012-07-25
Resolution	:	3.51 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:

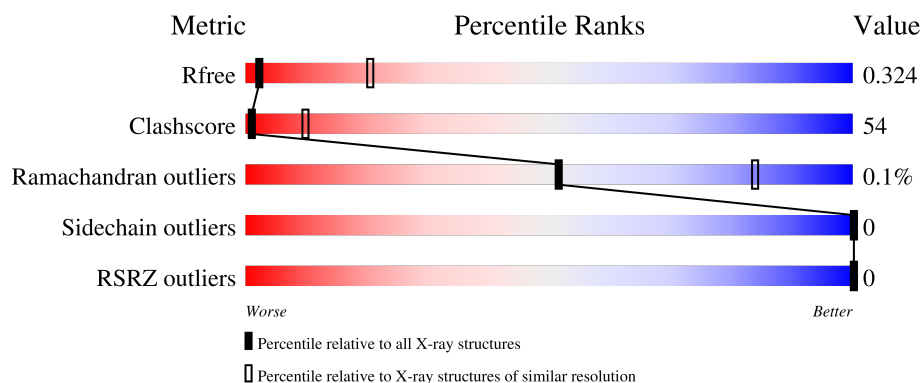|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
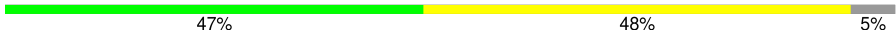*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.51 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	Percentile Ranks	Value
Rfree		0.324
Clashscore		54
Ramachandran outliers		0.1%
Sidechain outliers		0
RSRZ outliers		0

Worse ────────────────── *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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 <=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	440	55% 40% 5%
1	B	440	47% 48% 5%

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
2	PO4	B	601	-	-	X	-

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 5680 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 Putative thymidine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			2835	1771	484	566	14			
1	B	418	Total	C	N	O	S	0	0	0
			2835	1771	484	566	14			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	MET	-	expression tag	UNP Q5JCX3
A	504	GLY	-	expression tag	UNP Q5JCX3
A	505	ASN	-	expression tag	UNP Q5JCX3
A	506	SER	-	expression tag	UNP Q5JCX3
A	507	SER	-	expression tag	UNP Q5JCX3
A	508	SER	-	expression tag	UNP Q5JCX3
A	509	VAL	-	expression tag	UNP Q5JCX3
A	510	ASP	-	expression tag	UNP Q5JCX3
A	511	LYS	-	expression tag	UNP Q5JCX3
A	512	LEU	-	expression tag	UNP Q5JCX3
A	513	ALA	-	expression tag	UNP Q5JCX3
A	514	ALA	-	expression tag	UNP Q5JCX3
A	515	ALA	-	expression tag	UNP Q5JCX3
A	516	LEU	-	expression tag	UNP Q5JCX3
A	517	GLU	-	expression tag	UNP Q5JCX3
A	518	HIS	-	expression tag	UNP Q5JCX3
A	519	HIS	-	expression tag	UNP Q5JCX3
A	520	HIS	-	expression tag	UNP Q5JCX3
A	521	HIS	-	expression tag	UNP Q5JCX3
A	522	HIS	-	expression tag	UNP Q5JCX3
A	523	HIS	-	expression tag	UNP Q5JCX3
B	84	MET	-	expression tag	UNP Q5JCX3
B	504	GLY	-	expression tag	UNP Q5JCX3
B	505	ASN	-	expression tag	UNP Q5JCX3
B	506	SER	-	expression tag	UNP Q5JCX3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	507	SER	-	expression tag	UNP Q5JCX3
B	508	SER	-	expression tag	UNP Q5JCX3
B	509	VAL	-	expression tag	UNP Q5JCX3
B	510	ASP	-	expression tag	UNP Q5JCX3
B	511	LYS	-	expression tag	UNP Q5JCX3
B	512	LEU	-	expression tag	UNP Q5JCX3
B	513	ALA	-	expression tag	UNP Q5JCX3
B	514	ALA	-	expression tag	UNP Q5JCX3
B	515	ALA	-	expression tag	UNP Q5JCX3
B	516	LEU	-	expression tag	UNP Q5JCX3
B	517	GLU	-	expression tag	UNP Q5JCX3
B	518	HIS	-	expression tag	UNP Q5JCX3
B	519	HIS	-	expression tag	UNP Q5JCX3
B	520	HIS	-	expression tag	UNP Q5JCX3
B	521	HIS	-	expression tag	UNP Q5JCX3
B	522	HIS	-	expression tag	UNP Q5JCX3
B	523	HIS	-	expression tag	UNP Q5JCX3

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
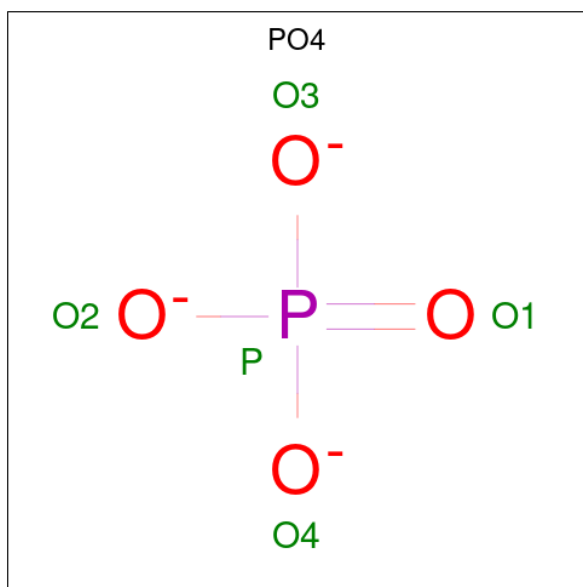
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0

3 Residue-property plots ⓘ

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Putative thymidine phosphorylase

Chain A:

- Molecule 1: Putative thymidine phosphorylase

Chain B:
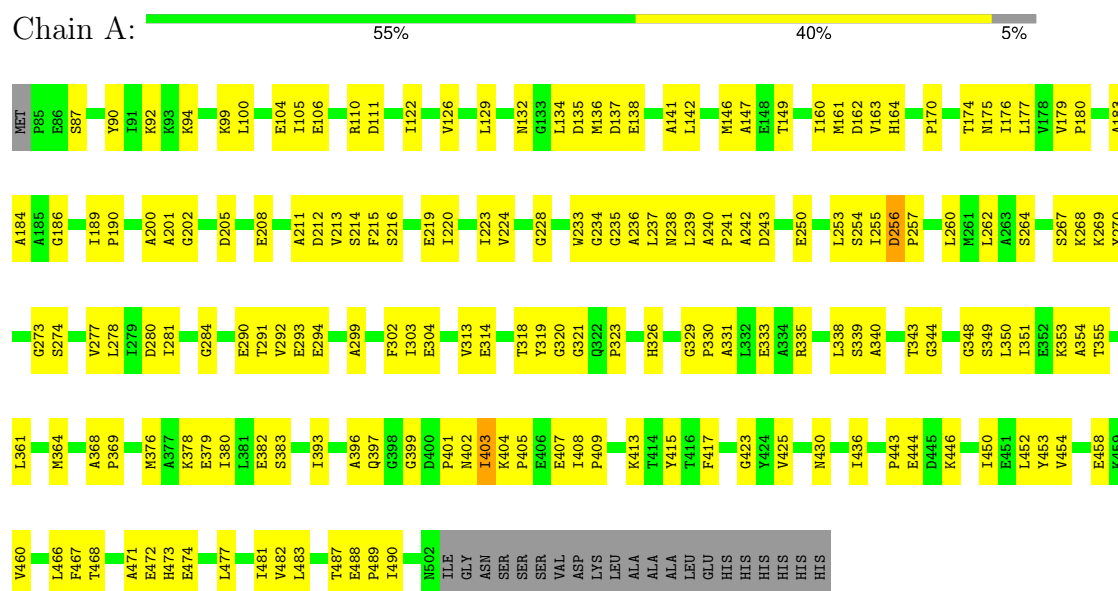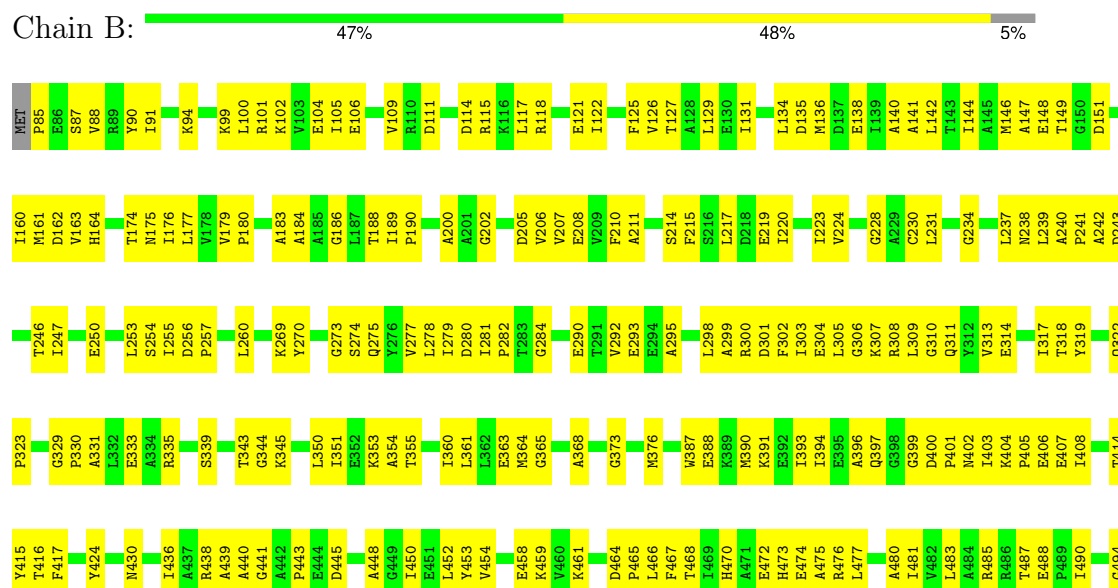
M495 V496 L497 G501 N502 ILE GLY ASN SER SER VAL ASP LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	166.12Å 166.12Å 93.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.51 42.66 – 3.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.51) 99.9 (42.66-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.272 , 0.322 0.277 , 0.324	Depositor DCC
R_{free} test set	943 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	91.5	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 69.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5680	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4

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	0.64	0/2874	0.72	1/3920 (0.0%)
1	B	0.59	1/2874 (0.0%)	0.72	1/3920 (0.0%)
All	All	0.62	1/5748 (0.0%)	0.72	2/7840 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	323	PRO	N-CD	5.93	1.56	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	256	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	256	ASP	CB-CG-OD2	5.16	122.94	118.30

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	2835	0	2565	246	0
1	B	2835	0	2565	345	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	3	0
All	All	5680	0	5130	585	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 54.

The worst 5 of 585 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:A:368:ALA:HB2	1:A:376:MET:CE	1.29	1.59
1:B:368:ALA:HB2	1:B:376:MET:CE	1.40	1.44
1:B:416:THR:HG23	1:B:467:PHE:O	1.28	1.31
1:B:136:MET:CE	1:B:304:GLU:HG3	1.61	1.29
1:B:180:PRO:HG3	1:B:390:MET:CE	1.64	1.26

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	416/440 (94%)	412 (99%)	3 (1%)	1 (0%)	47	80
1	B	416/440 (94%)	411 (99%)	5 (1%)	0	100	100
All	All	832/880 (94%)	823 (99%)	8 (1%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	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	240/344 (70%)	240 (100%)	0	100	100
1	B	240/344 (70%)	240 (100%)	0	100	100
All	All	480/688 (70%)	480 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	HIS
1	B	430	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	PO4	B	601	-	4,4,4	0.96	0	6,6,6	0.46	0
2	PO4	A	601	-	4,4,4	0.95	0	6,6,6	0.46	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	PO4	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	418/440 (95%)	-0.65	0	100	100	26, 65, 102, 146	0
1	B	418/440 (95%)	-0.45	0	100	100	37, 89, 138, 199	0
All	All	836/880 (95%)	-0.55	0	100	100	26, 75, 126, 199	0

There are no RSRZ outliers to report.

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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(Å^2)	Q<0.9
2	PO4	B	601	5/5	0.88	0.26	78,78,78,78	0
2	PO4	A	601	5/5	0.90	0.44	78,78,78,78	0

6.5   Other polymers ⓘ

There are no such residues in this entry.

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