

Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 09:14 PM EST

PDB ID : 4D98

Title : Crystal structure of the hexameric purine nucleoside phosphorylase from Bacil-

lus subtilis in space group H32 at pH 7.5

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Deposited on : 2012-01-11

Resolution : 1.70 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 (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

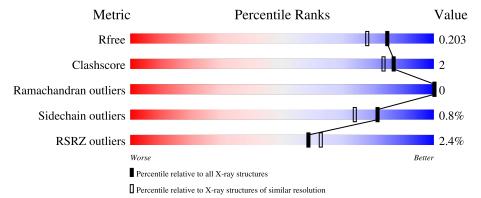
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	253	89%		9%			
1	В	253	86%	6%	9%			



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3954 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 Purine nucleoside phosphorylase deoD-type.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	231	Total 1818	C 1151	N 298	O 359	S 10	0	12	0
1	В	231		C 1128		O 353	S 9	0	6	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O34925
A	-18	GLY	-	- expression tag	
A	-17	SER	-	expression tag	UNP O34925
A	-16	SER	-	expression tag	UNP O34925
A	-15	HIS	-	expression tag	UNP O34925
A	-14	HIS	-	expression tag	UNP O34925
A	-13	HIS	-	expression tag	UNP O34925
A	-12	HIS	-	expression tag	UNP O34925
A	-11	HIS	-	expression tag	UNP O34925
A	-10	HIS	-	expression tag	UNP O34925
A	-9	SER	-	expression tag	UNP O34925
A	-8	SER	-	expression tag	UNP O34925
A	-7	GLY	-	expression tag	UNP O34925
A	-6	LEU	-	expression tag	UNP O34925
A	-5	VAL	-	expression tag	UNP O34925
A	-4	PRO	-	expression tag	UNP O34925
A	-3	ARG	-	expression tag	UNP O34925
A	-2	GLY	-	expression tag	UNP O34925
A	-1	SER	-	expression tag	UNP O34925
A	0	HIS	-	expression tag	UNP O34925
A	225	ASP	GLU	SEE REMARK 999	UNP O34925
В	-19	MET	-	expression tag	UNP O34925
В	-18	GLY	-	expression tag	UNP O34925
В	-17	SER	-	expression tag	UNP O34925
В	-16	SER	-	expression tag	UNP O34925

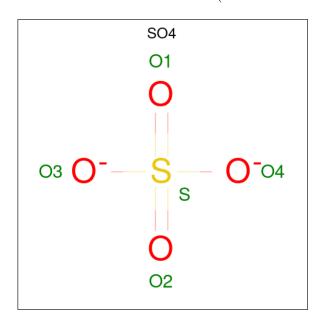
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Chain	Residue	Modelled	Actual	Comment	Reference
В	-15	HIS	- expression tag		UNP O34925
В	-14	HIS	-	expression tag	UNP O34925
В	-13	HIS	-	expression tag	UNP O34925
В	-12	HIS	-	expression tag	UNP O34925
В	-11	HIS	-	expression tag	UNP O34925
В	-10	HIS	-	expression tag	UNP O34925
В	-9	SER	-	expression tag	UNP O34925
В	-8	SER	-	expression tag	UNP O34925
В	-7	GLY	-	expression tag	UNP O34925
В	-6	LEU	-	expression tag	UNP O34925
В	-5	VAL	-	expression tag	UNP O34925
В	-4	PRO	-	expression tag	UNP O34925
В	-3	ARG	-	expression tag	UNP O34925
В	-2	GLY	-	expression tag	UNP O34925
В	-1	SER	-	expression tag	UNP O34925
В	0	HIS	-	expression tag	UNP O34925
В	225	ASP	GLU	SEE REMARK 999	UNP O34925

 \bullet Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



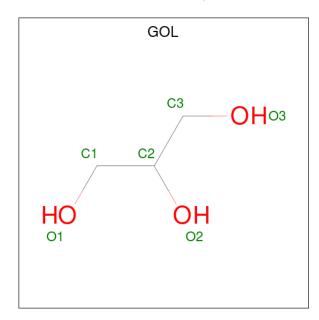
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	В	1	Total O S 5 4 1	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	В	1	Total Cl 1 1	0	0

 \bullet Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total C O 6 3 3	0	0

• Molecule 5 is water.

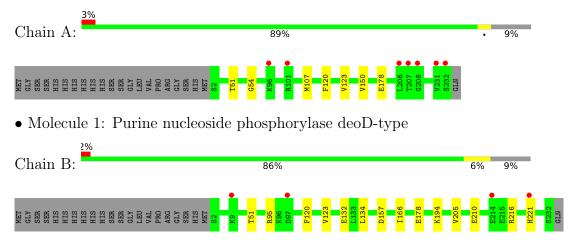
M	[ol	Chain	Residues	Atoms	ZeroOcc	AltConf
ļ	5	A	171	Total O 171 171	0	0
ţ	5	В	163	Total O 163 163	0	0



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 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: Purine nucleoside phosphorylase deoD-type





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	H 3 2	Depositor	
Cell constants	158.26Å 158.26Å 93.87Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	1	
Resolution (Å)	29.81 - 1.70	Depositor	
, ,	29.81 - 1.70	EDS	
% Data completeness	95.1 (29.81-1.70)	Depositor	
(in resolution range)	95.1 (29.81-1.70)	EDS	
R_{merge}	0.09	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	4.39 (at 1.70Å)	Xtriage	
Refinement program	REFMAC	Depositor	
D D	0.168 , 0.206	Depositor	
R, R_{free}	0.166 , 0.203	DCC	
R_{free} test set	2375 reflections (5.06%)	wwPDB-VP	
Wilson B-factor (Å ²)	23.0	Xtriage	
Anisotropy	0.063	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37, 41.9	EDS	
L-test for twinning ²	$< L > = 0.51, < L^2> = 0.34$	Xtriage	
	0.015 for -2/3 *h- 1/3 *k- 4/3 *l,- 1/3 *h- 2/3 *k+		
	4/3*l,-1/3*h+1/3*k+1/3*l		
Estimated twinning fraction	0.007 for -h, 1/3 *h-1/3 *k-4/3 *l, -1/3 *h-2/3 *k	Xtriage	
	+1/3*1	120210080	
	0.001 for $-1/3*h+1/3*k+4/3*l,-k,2/3*h+1/$		
E E completion	3*k+1/3*l	EDC	
F_o, F_c correlation	0.97	EDS	
Total number of atoms	3954	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	24.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 15.99% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: SO4, CL, GOL

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	Bo	nd angles
IVIOI	Chain	RMSZ # Z > 5		RMSZ	# Z > 5
1	A	0.75	0/1881	0.76	0/2546
1	В	0.75	0/1829	0.79	1/2477 (0.0%)
All	All	0.75	0/3710	0.77	1/5023 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
1	В	157	ASP	CB-CG-OD1	5.90	123.61	118.30

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	A	1818	0	1842	6	0
1	В	1784	0	1795	9	0
2	A	5	0	0	0	0
2	В	5	0	0	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
4	В	6	0	8	2	0
5	A	171	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	В	163	0	0	2	0
All	All	3954	0	3645	15	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 2.

All (15) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	$ ext{overlap }(\mathring{\mathbf{A}})$
1:B:95:ARG:HH22	4:B:303:GOL:H12	1.49	0.76
1:A:51[A]:THR:HG22	5:A:455:HOH:O	1.86	0.75
1:B:120:PHE:HB3	1:B:123:VAL:HB	1.72	0.70
1:A:120:PHE:HB3	1:A:123:VAL:HB	1.80	0.63
1:B:51[A]:THR:HG22	5:B:472:HOH:O	2.12	0.49
1:B:95:ARG:NH2	4:B:303:GOL:H12	2.23	0.47
1:A:51[A]:THR:HG23	1:A:54:GLY:C	2.36	0.46
1:A:107[A]:MET:HG3	1:A:150:VAL:HG12	1.98	0.45
1:B:210:GLU:HG3	1:B:216:ARG:NH2	2.34	0.43
1:A:51[A]:THR:CG2	1:A:54:GLY:H	2.33	0.42
1:B:51[A]:THR:CG2	5:B:472:HOH:O	2.67	0.41
1:B:132:GLU:OE1	1:B:194:LYS:NZ	2.52	0.41
1:A:51[A]:THR:CG2	1:A:54:GLY:CA	2.99	0.41
1:B:166:ILE:HD13	1:B:205:VAL:HG11	2.02	0.40

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	Perce	ntiles
1	A	241/253 (95%)	240 (100%)	1 (0%)	0	100	100
1	В	235/253 (93%)	232 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	476/506 (94%)	472 (99%)	4 (1%)	0	100 100

There are no Ramachandran outliers to report.

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	204/211 (97%)	203 (100%)	1 (0%)	88 83		
1	В	198/211 (94%)	196 (99%)	2 (1%)	76 67		
All	All	402/422 (95%)	399 (99%)	3 (1%)	81 77		

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	В	178	GLU
1	В	221	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	B	ond leng	gths	В	ond ang	gles
MIOI	туре	Chain	Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.18	0
2	SO4	В	301	-	4,4,4	0.06	0	6,6,6	0.51	0
4	GOL	В	303	-	5,5,5	0.49	0	5,5,5	0.35	0

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	GOL	В	303	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	303	GOL	O1-C1-C2-O2
4	В	303	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	303	GOL	2	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 (i)

6.1 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, 95^{th} 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	231/253 (91%)	-0.00	7 (3%) 50 54	15, 21, 36, 45	0
1	В	231/253 (91%)	-0.10	4 (1%) 70 74	15, 21, 33, 39	0
All	All	462/506 (91%)	-0.05	11 (2%) 59 63	15, 21, 34, 45	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	A	232	SER	6.7	
1	A	231	VAL	4.5	
1	В	9	LYS	2.8	
1	В	214	GLU	2.7	
1	A	208	GLY	2.7	
1	A	206	LEU	2.5	
1	В	97	ASP	2.5	
1	В	221	HIS	2.4	
1	A	207[A]	THR	2.4	
1	A	101	ARG	2.3	
1	A	96	LYS	2.2	

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	GOL	В	303	6/6	0.81	0.23	53,53,56,59	0
3	CL	В	302	1/1	0.98	0.06	30,30,30,30	0
3	CL	A	302	1/1	0.98	0.07	30,30,30,30	0
2	SO4	A	301	5/5	0.99	0.04	23,24,26,27	0
2	SO4	В	301	5/5	1.00	0.06	18,19,20,21	0

6.5 Other polymers (i)

There are no such residues in this entry.

