Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 06:15 am GMT

PDB ID	:	1ODK
Title	:	PURINE NUCLEOSIDE PHOSPHORYLASE FROM THERMUS THERMOPHILUS
Authors	:	Tahirov, T.H.; Inagaki, E.; Miyano, M.
Deposited on	:	2003-02-19
Resolution	:	1.90 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 (i)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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

PERCENTILES INFOmissingINFO

1 Entry composition (i)

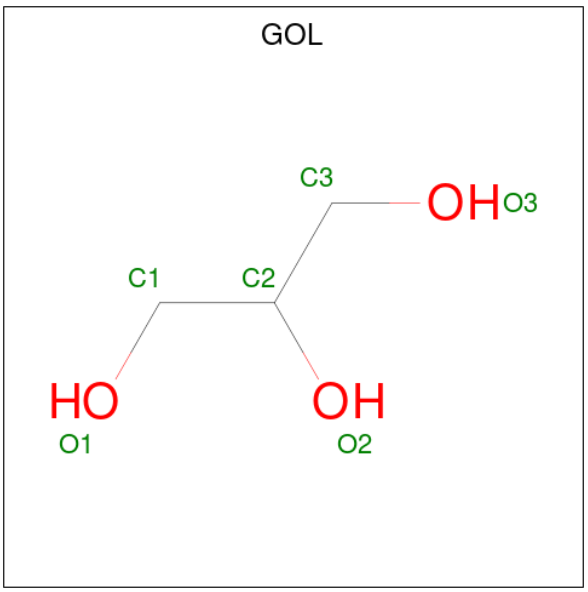
There are 3 unique types of molecules in this entry. The entry contains 11369 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	228	1745	1108	319	314	4	0	0	0
1	B	234	1782	1131	325	322	4	0	0	0
1	C	228	1745	1108	319	314	4	0	0	0
1	D	234	1786	1133	325	324	4	0	0	0
1	E	226	1727	1096	317	310	4	0	0	0
1	F	234	1782	1131	325	322	4	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	B	1	6	3	3	0	0
			Total	C	O		
2	C	1	6	3	3	0	0
			Total	C	O		
2	D	1	6	3	3	0	0
			Total	C	O		
2	E	1	6	3	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	158	158	158	0	0
			Total	O		
3	B	149	149	149	0	0
			Total	O		
3	C	113	113	113	0	0
			Total	O		
3	D	106	106	106	0	0
			Total	O		
3	E	112	112	112	0	0
			Total	O		
3	F	128	128	128	0	0

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	131.92Å 131.92Å 169.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 1.90 19.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.98-1.90) 98.8 (19.98-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.09 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.208 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 62.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11369	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

3 Model quality (i)

3.1 Standard geometry (i)

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

3.2 Too-close contacts (i)

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

3.3 Torsion angles (i)

3.3.1 Protein backbone (i)

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

3.3.2 Protein sidechains (i)

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

3.3.3 RNA (i)

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

3.4 Non-standard residues in protein, DNA, RNA chains (i)

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

3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

3.6 Ligand geometry (i)

6 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	GOL	D	1236	-	5,5,5	0.29	0	5,5,5	0.17	0
2	GOL	B	1236	-	5,5,5	0.29	0	5,5,5	0.28	0
2	GOL	A	1236	-	5,5,5	0.26	0	5,5,5	0.16	0
2	GOL	A	1237	-	5,5,5	0.21	0	5,5,5	0.12	0
2	GOL	C	1236	-	5,5,5	0.30	0	5,5,5	0.13	0
2	GOL	E	1236	-	5,5,5	0.30	0	5,5,5	0.22	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
2	GOL	D	1236	-	-	2/4/4/4	-
2	GOL	B	1236	-	-	2/4/4/4	-
2	GOL	A	1236	-	-	0/4/4/4	-
2	GOL	A	1237	-	-	1/4/4/4	-
2	GOL	C	1236	-	-	0/4/4/4	-
2	GOL	E	1236	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1236	GOL	O1-C1-C2-C3
2	D	1236	GOL	C1-C2-C3-O3
2	B	1236	GOL	O1-C1-C2-O2
2	D	1236	GOL	O2-C2-C3-O3
2	A	1237	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Fit of model and data (i)

4.1 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	228/235 (97%)	-0.24	6 (2%)	56	58	7, 15, 34, 60	0
1	B	234/235 (99%)	-0.17	11 (4%)	31	34	8, 15, 37, 49	0
1	C	228/235 (97%)	-0.03	12 (5%)	26	29	10, 20, 41, 60	0
1	D	234/235 (99%)	0.31	21 (8%)	9	10	9, 24, 53, 65	0
1	E	226/235 (96%)	-0.12	7 (3%)	49	51	8, 18, 42, 55	0
1	F	234/235 (99%)	0.04	15 (6%)	19	22	8, 17, 51, 77	0
All	All	1384/1410 (98%)	-0.03	72 (5%)	27	30	7, 18, 44, 77	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	211	LEU	9.0
1	F	209	PRO	8.5
1	A	214	PRO	7.4
1	F	210	GLU	7.2
1	F	207	GLY	5.8
1	D	209	PRO	5.7
1	F	9	HIS	5.4
1	F	208	ASP	5.4
1	F	10	PRO	5.3
1	C	215	GLU	5.2
1	E	205	ARG	5.2
1	B	10	PRO	4.9
1	D	2	SER	4.8
1	D	210	GLU	4.6
1	A	213	PRO	4.6
1	A	215	GLU	4.4
1	F	96	SER	4.4
1	E	215	GLU	4.3
1	F	216	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	97	ASP	4.1
1	D	215	GLU	4.0
1	F	213	PRO	3.9
1	C	205	ARG	3.9
1	D	216	VAL	3.8
1	D	207	GLY	3.7
1	D	213	PRO	3.7
1	A	216	VAL	3.7
1	C	2	SER	3.6
1	D	211	LEU	3.6
1	D	36	ASN	3.4
1	C	96	SER	3.3
1	B	9	HIS	3.3
1	D	205	ARG	3.3
1	B	2	SER	3.2
1	E	147	PRO	3.2
1	D	212	ALA	3.2
1	F	2	SER	3.2
1	D	35	GLN	3.0
1	B	95	SER	2.9
1	B	96	SER	2.9
1	C	95	SER	2.9
1	C	9	HIS	2.9
1	D	95	SER	2.9
1	E	145	GLY	2.9
1	B	214	PRO	2.8
1	F	97	ASP	2.7
1	F	212	ALA	2.7
1	F	95	SER	2.7
1	F	215	GLU	2.7
1	B	207	GLY	2.7
1	A	205	ARG	2.6
1	C	216	VAL	2.6
1	B	38	ARG	2.5
1	D	96	SER	2.5
1	B	209	PRO	2.5
1	E	100	PRO	2.5
1	C	97	ASP	2.5
1	D	214	PRO	2.4
1	C	212	PRO	2.4
1	E	146	TYR	2.3
1	A	2	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	206	ILE	2.3
1	D	31	LYS	2.3
1	D	208	ASP	2.3
1	C	100	PRO	2.2
1	C	31	LYS	2.2
1	B	215	GLU	2.2
1	E	2	SER	2.2
1	C	36	ASN	2.1
1	D	235	VAL	2.1
1	D	56	VAL	2.1
1	D	99	ALA	2.0

4.2 Non-standard residues in protein, DNA, RNA chains (i)

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

4.3 Carbohydrates (i)

There are no monosaccharides in this entry.

4.4 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(Å^2)	Q<0.9
2	GOL	E	1236	6/6	0.63	0.22	47,51,53,55	0
2	GOL	C	1236	6/6	0.64	0.23	52,54,55,59	0
2	GOL	D	1236	6/6	0.69	0.22	42,44,45,53	0
2	GOL	A	1236	6/6	0.73	0.25	43,44,47,53	0
2	GOL	B	1236	6/6	0.77	0.21	45,46,46,51	0
2	GOL	A	1237	6/6	0.78	0.17	43,45,46,48	0

4.5 Other polymers (i)

There are no such residues in this entry.