wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2024 – 08:30 AM EST

PDB ID	:	1PYP
Title	:	X-RAY DIFFRACTION STUDY OF INORGANIC PYROPHOSPHATASE FROM BAKER,S YEAST AT THE 3 ANGSTROMS RESOLUTION (RUSSIAN)
Authors	:	Harutyunyan, E.H.; Terzyan, S.S.; Vainshtein, B.K.
Deposited on	:	1983-02-03
Resolution	:	3.00 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 (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:

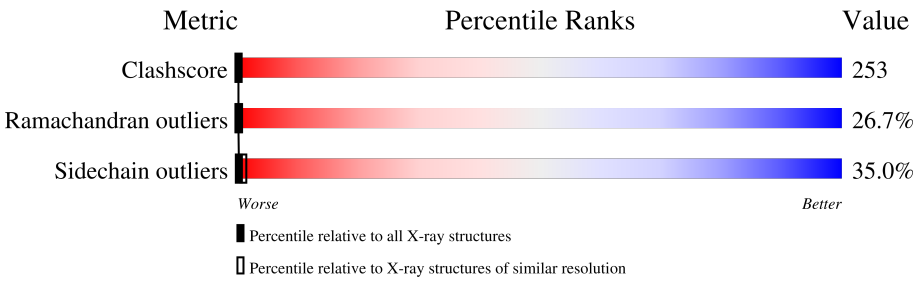
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	285	6% 38% 39% 16% .
1	B	285	6% 38% 39% 16% .

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4472 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 INORGANIC PYROPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	281	2236	1435	369	429	3	0	0	1
1	B	281	2236	1435	369	429	3	0	0	1

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ASP	ASN	conflict	UNP P00817
A	71	ASN	ASP	conflict	UNP P00817
A	?	-	LYS	deletion	UNP P00817
A	116	ASN	ASP	conflict	UNP P00817
A	122	GLN	GLU	conflict	UNP P00817
A	135	GLU	GLN	conflict	UNP P00817
A	185	ASP	ASN	conflict	UNP P00817
A	223	ASN	ASP	conflict	UNP P00817
A	265	PRO	LEU	conflict	UNP P00817
B	40	ASP	ASN	conflict	UNP P00817
B	71	ASN	ASP	conflict	UNP P00817
B	?	-	LYS	deletion	UNP P00817
B	116	ASN	ASP	conflict	UNP P00817
B	122	GLN	GLU	conflict	UNP P00817
B	135	GLU	GLN	conflict	UNP P00817
B	185	ASP	ASN	conflict	UNP P00817
B	223	ASN	ASP	conflict	UNP P00817
B	265	PRO	LEU	conflict	UNP P00817

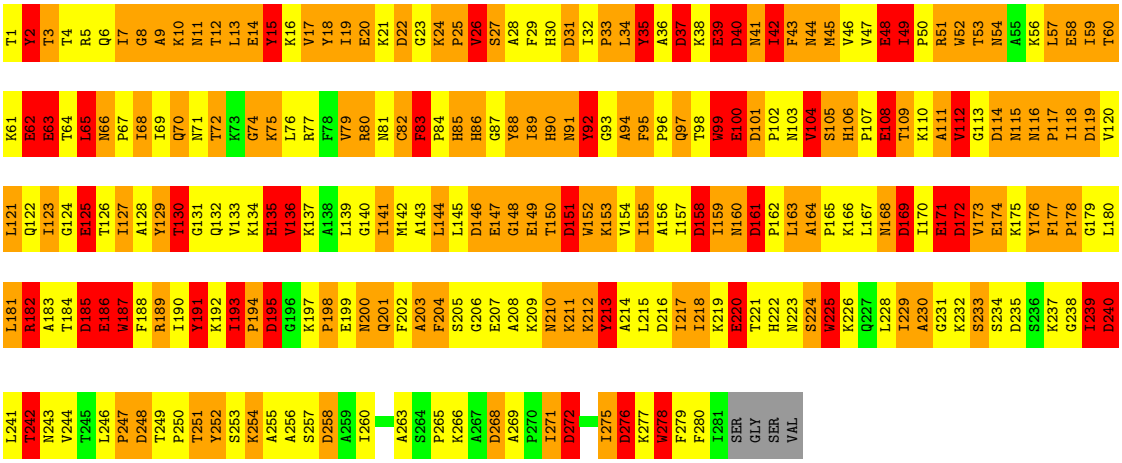
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

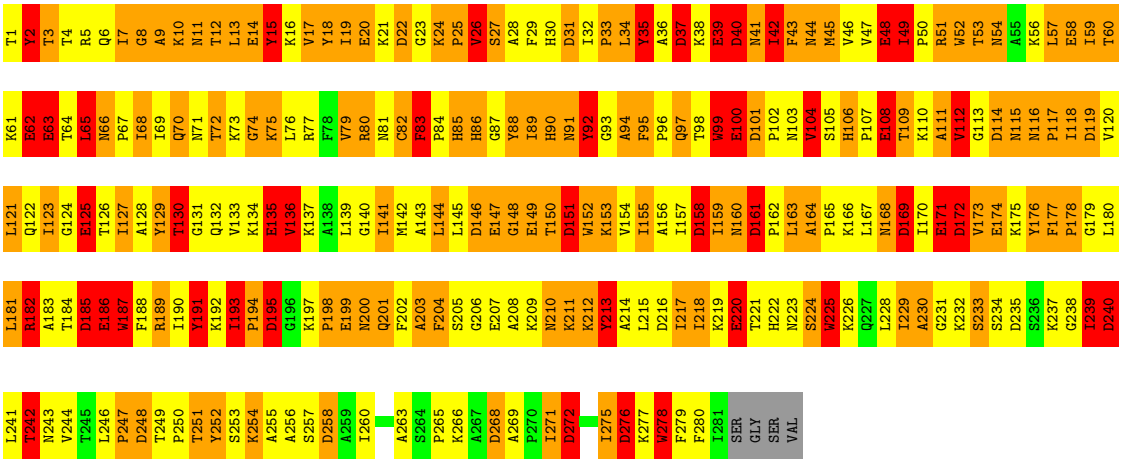
• Molecule 1: INORGANIC PYROPHOSPHATASE

Chain A: 6% 38% 39% 16%



• Molecule 1: INORGANIC PYROPHOSPHATASE

Chain B: 6% 38% 39% 16%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 1 21	Depositor
Cell constants a, b, c, α, β, γ	52.23Å 70.29Å 95.47Å 90.00° 90.00° 99.59°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4472	wwPDB-VP
Average B, all atoms (Å^2)	0.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	1.18	25/2295 (1.1%)	1.40	72/3123 (2.3%)
1	B	1.18	25/2295 (1.1%)	1.40	72/3123 (2.3%)
All	All	1.18	50/4590 (1.1%)	1.40	144/6246 (2.3%)

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	TRP	NE1-CE2	-7.35	1.28	1.37
1	A	278	TRP	NE1-CE2	-7.34	1.28	1.37
1	B	278	TRP	NE1-CE2	-7.34	1.28	1.37
1	A	99	TRP	NE1-CE2	-7.34	1.28	1.37
1	B	99	TRP	NE1-CE2	-7.33	1.28	1.37

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	172	ASP	CB-CG-OD1	7.35	124.92	118.30
1	A	172	ASP	CB-CG-OD1	7.35	124.91	118.30
1	B	169	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	158	ASP	CB-CG-OD1	7.33	124.90	118.30
1	B	22	ASP	CB-CG-OD1	7.32	124.89	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	2236	0	2198	1132	10
1	B	2236	0	2198	1138	13
All	All	4472	0	4396	2241	13

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 253.

The worst 5 of 2241 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:1:THR:HG21	1:B:19:ILE:CD1	1.22	1.68
1:B:19:ILE:CD1	1:B:26:VAL:HG11	1.27	1.64
1:A:1:THR:HG21	1:A:19:ILE:CD1	1.22	1.62
1:B:9:ALA:CB	1:B:15:TYR:HB2	1.19	1.61
1:B:42:ILE:HD12	1:B:159:ILE:CD1	1.29	1.60

The worst 5 of 13 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:CG	1:B:108:GLU:OE2[1_445]	1.56	0.64
1:A:115:ASN:ND2	1:B:75:LYS:NZ[1_455]	1.71	0.49
1:A:174:GLU:OE1	1:B:248:ASP:CG[2_775]	1.72	0.48
1:B:2:TYR:OH	1:B:199:GLU:OE2[2_774]	1.82	0.38
1:A:247:PRO:CG	1:B:108:GLU:CG[1_445]	1.84	0.36

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	Percentiles
1	A	279/285 (98%)	151 (54%)	53 (19%)	75 (27%)	0 0
1	B	279/285 (98%)	152 (54%)	53 (19%)	74 (26%)	0 0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	558/570 (98%)	303 (54%)	106 (19%)	149 (27%)	0 0

5 of 149 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	TYR
1	A	8	GLY
1	A	9	ALA
1	A	12	THR
1	A	13	LEU

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	243/247 (98%)	158 (65%)	85 (35%)	0 1
1	B	243/247 (98%)	158 (65%)	85 (35%)	0 1
All	All	486/494 (98%)	316 (65%)	170 (35%)	0 1

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	99	TRP
1	B	177	PHE
1	B	109	THR
1	B	141	ILE
1	B	210	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	ASN
1	B	122	GLN
1	B	200	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	160	ASN
1	A	160	ASN

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)

There are no ligands in this entry.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.