wwPDB Geometry-Only Validation Summary Report

May 27, 2024 – 06:35 PM EDT

PDB ID	:	5TY5
Title	:	Neutron structure from microgravity-grown crystals of Inorganic Pyrophosphatase from Thermococcus theoreducens
Authors	:	Inoguchi, N.; Coates, L.; Morris, M.L.; Singhal, A.; Monaco, D.A.; Garcia-Ruiz, J.M.; Pusey, M.L.; Ng, J.D.
Deposited on	:	2016-11-18
Resolution	:	2.30 Å(reported)

This is a wwPDB Geometry-Only 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	:	FAILED
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)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
NEUTRON DIFFRACTION

The reported resolution of this entry is 2.30 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19178 atoms, of which 8119 are hydrogens and 2034 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
1	A	174	Total	C	D	H	N	O	S	0	152	0
			3000	941	225	1337	226	266	5			
1	B	175	Total	C	D	H	N	O	S	0	155	0
			3047	946	233	1368	227	267	6			
1	C	174	Total	C	D	H	N	O	S	0	155	0
			3038	944	234	1362	226	266	6			
1	D	174	Total	C	D	H	N	O	S	0	151	0
			3017	941	228	1351	226	266	5			
1	E	174	Total	C	D	H	N	O	S	0	151	0
			3034	944	231	1361	226	266	6			
1	F	173	Total	C	D	H	N	O	S	0	153	0
			3009	939	235	1340	225	265	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	67	Total	D	O	0	0
			171	104	67		
2	B	73	Total	D	O	0	0
			187	114	73		
2	C	71	Total	D	O	0	0
			201	130	71		
2	D	52	Total	D	O	0	0
			148	96	52		
2	E	58	Total	D	O	0	0
			152	94	58		
2	F	64	Total	D	O	0	0
			174	110	64		

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.

3 Model quality

3.1 Standard geometry

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

3.2 Too-close contacts

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

3.3 Torsion angles

3.3.1 Protein backbone

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

3.3.2 Protein sidechains

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

3.3.3 RNA

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

3.4 Non-standard residues in protein, DNA, RNA chains

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

3.5 Carbohydrates

There are no monosaccharides in this entry.

3.6 Ligand geometry

There are no ligands in this entry.

3.7 Other polymers

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.