Full wwPDB Geometry-Only Validation Report (i)

Sep 24, 2023 – 11:51 AM 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 Full wwPDB Geometry-Only 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:

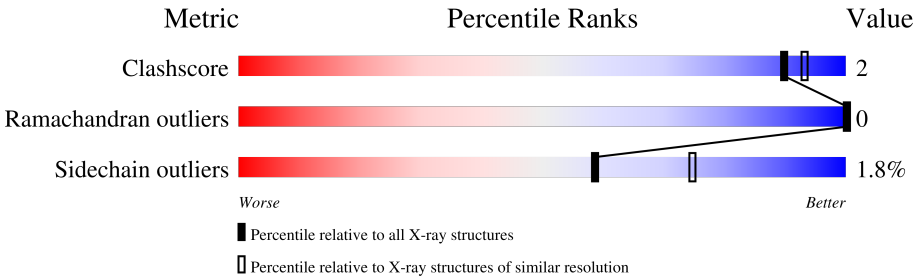
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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.

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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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	178	96%
1	B	178	96%
1	C	178	95%
1	D	178	95%
1	E	178	93%
1	F	178	97%

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		

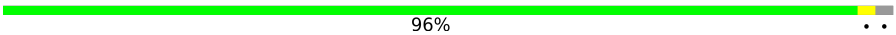
3 Residue-property plots (i)

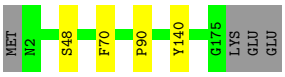
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

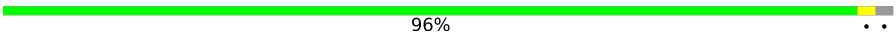
Chain A:

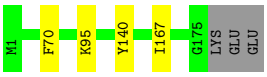




• Molecule 1: Inorganic pyrophosphatase

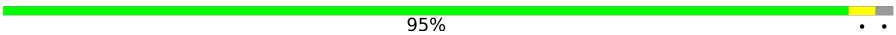
Chain B:

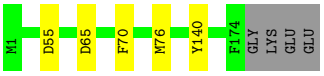




• Molecule 1: Inorganic pyrophosphatase

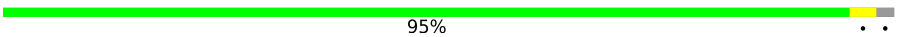
Chain C:

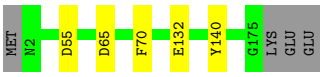




• Molecule 1: Inorganic pyrophosphatase

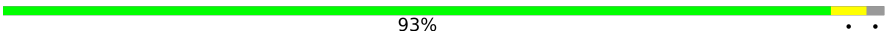
Chain D:





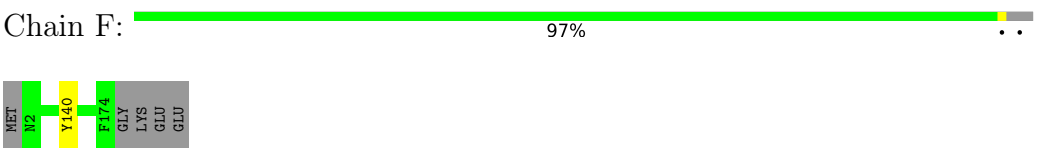
• Molecule 1: Inorganic pyrophosphatase

Chain E:



• Molecule 1: Inorganic pyrophosphatase

Chain F:



4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOD

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	0.39	2/2393 (0.1%)	0.44	0/3237
1	B	0.26	0/2478	0.43	0/3351
1	C	0.26	0/2453	0.41	0/3321
1	D	0.27	0/2455	0.45	0/3320
1	E	0.27	0/2528	0.42	0/3424
1	F	0.25	0/2460	0.45	0/3333
All	All	0.29	2/14767 (0.0%)	0.43	0/19986

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48[A]	SER	C-N	9.24	1.51	1.34
1	A	48[B]	SER	C-N	9.24	1.51	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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4.2 Torsion angles

4.2.1 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	275/178 (154%)	264 (96%)	11 (4%)	0	100	100
1	B	286/178 (161%)	278 (97%)	8 (3%)	0	100	100
1	C	280/178 (157%)	273 (98%)	7 (2%)	0	100	100
1	D	283/178 (159%)	272 (96%)	11 (4%)	0	100	100
1	E	286/178 (161%)	277 (97%)	9 (3%)	0	100	100
1	F	281/178 (158%)	276 (98%)	5 (2%)	0	100	100
All	All	1691/1068 (158%)	1640 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

4.2.2 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	250/159 (157%)	246 (98%)	4 (2%)	62	78
1	B	257/159 (162%)	254 (99%)	3 (1%)	71	84
1	C	255/159 (160%)	248 (97%)	7 (3%)	44	61
1	D	256/159 (161%)	249 (97%)	7 (3%)	44	61
1	E	264/159 (166%)	256 (97%)	8 (3%)	41	57
1	F	255/159 (160%)	253 (99%)	2 (1%)	81	91
All	All	1537/954 (161%)	1506 (98%)	31 (2%)	59	72

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70[A]	PHE
1	A	70[B]	PHE
1	A	140[B]	TYR
1	A	140[A]	TYR
1	B	70[A]	PHE
1	B	140[B]	TYR
1	B	140[A]	TYR

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Mol	Chain	Res	Type
1	C	55[B]	ASP
1	C	65[A]	ASP
1	C	65[B]	ASP
1	C	70[A]	PHE
1	C	70[B]	PHE
1	C	140[A]	TYR
1	C	140[B]	TYR
1	D	55[B]	ASP
1	D	65[A]	ASP
1	D	65[B]	ASP
1	D	70[A]	PHE
1	D	70[B]	PHE
1	D	140[A]	TYR
1	D	140[B]	TYR
1	E	1[A]	MET
1	E	1[B]	MET
1	E	70[A]	PHE
1	E	70[B]	PHE
1	E	140[A]	TYR
1	E	140[B]	TYR
1	E	172[A]	GLU
1	E	172[B]	GLU
1	F	140[A]	TYR
1	F	140[B]	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

4.2.3 RNA

There are no RNA molecules in this entry.

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

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

4.4 Carbohydrates

There are no monosaccharides in this entry.

4.5 Ligand geometry (i)

There are no ligands in this entry.

4.6 Other polymers (i)

There are no such residues in this entry.

4.7 Polymer linkage issues (i)

There are no chain breaks in this entry.