Full wwPDB Geometry-Only Validation Report (i)

Sep 2, 2023 – 11:12 AM EDT

PDB ID	:	3Q3L
Title	:	The neutron crystallographic structure of inorganic pyrophosphatase from Thermococcus thioreducens
Authors	:	Hughes, R.C.; Coates, L.; Blakeley, M.P.; Tomanicek, S.J.; Meehan, E.J.; Garcia-Ruiz, J.M.; Ng, J.D.
Deposited on	:	2010-12-22
Resolution	:	2.50 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:

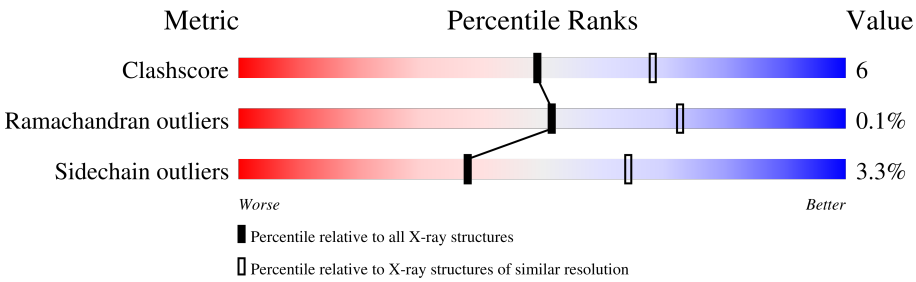
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	91% 6% • •
1	B	178	94% • • •
1	C	178	96% • •
1	D	178	93% 5% •
1	E	178	96% • •
1	F	178	93% 6% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18607 atoms, of which 8043 are hydrogens and 1726 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 Tt-IPPase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S			
1	A	175	3099	949	258	1389	227	269	7	95	155	0
1	B	175	2961	936	254	1276	224	265	6	69	147	0
1	C	175	3074	940	266	1370	225	267	6	82	154	0
1	D	175	3040	933	264	1350	223	265	5	87	156	0
1	E	174	3011	928	257	1336	221	264	5	90	153	0
1	F	175	3002	933	251	1322	222	268	6	87	152	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	D	O		
3	A	40	88	48	40	0	1
			Total	D	O		
3	B	54	78	24	54	0	1
			Total	D	O		
3	C	34	58	24	34	0	0
			Total	D	O		
3	D	37	55	18	37	0	0
			Total	D	O		
3	E	36	80	44	36	0	0
			Total	D	O		
3	F	37	55	18	37	0	0

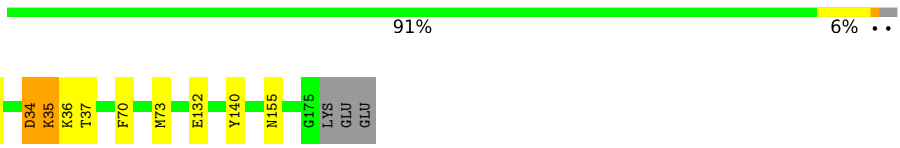
3 Residue-property plots (i)

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. 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.

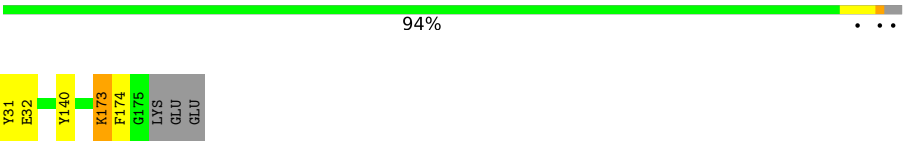
• Molecule 1: Tt-IPPase

Chain A:



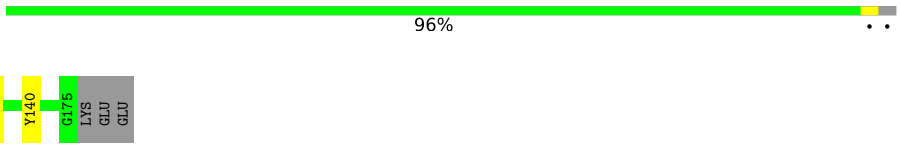
• Molecule 1: Tt-IPPase

Chain B:



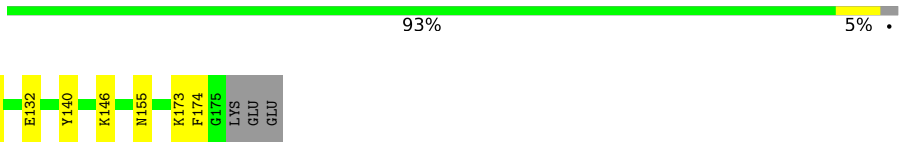
• Molecule 1: Tt-IPPase

Chain C:



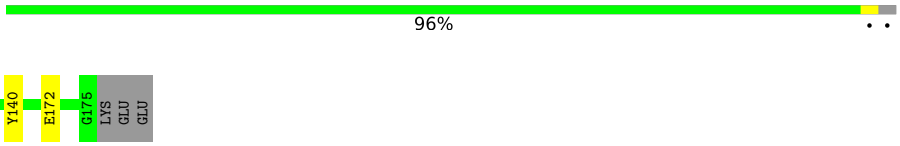
• Molecule 1: Tt-IPPase

Chain D:



• Molecule 1: Tt-IPPase

Chain E:



• Molecule 1: Tt-IPPase

Chain F:

M1
L33
F70
P82
E132
Y140
E151
K173
F174
G175
LYS
GLU
GLU

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.36	0/2817	0.51	2/3824 (0.1%)
1	B	0.35	0/2718	0.51	0/3693
1	C	0.35	0/2797	0.52	0/3797
1	D	0.35	0/2789	0.50	0/3793
1	E	0.34	0/2763	0.51	0/3759
1	F	0.35	0/2750	0.51	0/3745
All	All	0.35	0/16634	0.51	2/22611 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35[A]	LYS	CD-CE-NZ	5.02	123.24	111.70
1	A	35[B]	LYS	CD-CE-NZ	5.02	123.24	111.70

There are no chirality outliers.

There are no planarity outliers.

4.2 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	1710	1389	180	25	0
1	B	1685	1276	216	8	0
1	C	1704	1370	141	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1690	1350	132	1	0
1	E	1675	1336	136	0	0
1	F	1680	1322	165	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	88	0	0	3	0
3	B	78	0	0	3	0
3	C	58	0	0	1	0
3	D	55	0	0	7	0
3	E	80	0	0	9	0
3	F	55	0	0	6	0
All	All	10564	8043	970	65	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 6.

All (65) 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:173:LYS:HG2	1:B:174:PHE:CE2	2.17	0.73
1:A:35[A]:LYS:NZ	3:A:428:DOD:O	2.16	0.66
1:F:174:PHE:O	1:F:175:GLY:C	2.39	0.61
1:B:22:GLU:O	1:B:31:TYR:HB2	2.02	0.55
1:B:173:LYS:HG2	1:B:174:PHE:CD2	2.36	0.55
1:A:35[B]:LYS:HE2	3:A:428:DOD:O	2.03	0.53
1:A:34:ASP:C	1:A:36[B]:LYS:H	2.07	0.52
1:A:34:ASP:C	1:A:36[A]:LYS:H	2.08	0.52
1:F:82:PRO:O	3:F:337:HOH:O	2.22	0.51
1:D:173:LYS:HD3	1:D:174:PHE:CE2	2.48	0.44
1:F:173:LYS:HG3	1:F:174:PHE:CD1	2.47	0.44

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	329/178 (185%)	317 (96%)	11 (3%)	1 (0%)	41	61
1	B	319/178 (179%)	313 (98%)	6 (2%)	0	100	100
1	C	326/178 (183%)	320 (98%)	6 (2%)	0	100	100
1	D	328/178 (184%)	321 (98%)	7 (2%)	0	100	100
1	E	324/178 (182%)	317 (98%)	7 (2%)	0	100	100
1	F	325/178 (183%)	318 (98%)	7 (2%)	0	100	100
All	All	1951/1068 (183%)	1906 (98%)	44 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ASP

4.3.2 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	290/159 (182%)	274 (94%)	16 (6%)	21	41
1	B	278/159 (175%)	273 (98%)	5 (2%)	59	81
1	C	290/159 (182%)	282 (97%)	8 (3%)	43	70
1	D	283/159 (178%)	269 (95%)	14 (5%)	25	47
1	E	281/159 (177%)	273 (97%)	8 (3%)	43	70
1	F	279/159 (176%)	271 (97%)	8 (3%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1701/954 (178%)	1642 (96%)	59 (4%)	38 62

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6[A]	GLU
1	A	6[B]	GLU
1	A	7[A]	LEU
1	A	7[B]	LEU
1	A	8[A]	GLU
1	A	8[B]	GLU
1	A	37[A]	THR
1	A	37[B]	THR
1	A	70[A]	PHE
1	A	70[B]	PHE
1	A	132[A]	GLU
1	A	132[B]	GLU
1	A	140[A]	TYR
1	A	140[B]	TYR
1	A	155[A]	ASN
1	A	155[B]	ASN
1	B	8[A]	GLU
1	B	8[B]	GLU
1	B	140[A]	TYR
1	B	140[B]	TYR
1	B	173	LYS
1	C	6[A]	GLU
1	C	6[B]	GLU
1	C	33[A]	LEU
1	C	33[B]	LEU
1	C	132[A]	GLU
1	C	132[B]	GLU
1	C	140[A]	TYR
1	C	140[B]	TYR
1	D	6[A]	GLU
1	D	6[B]	GLU
1	D	33[A]	LEU
1	D	33[B]	LEU
1	D	70[A]	PHE
1	D	70[B]	PHE
1	D	132[A]	GLU
1	D	132[B]	GLU

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Mol	Chain	Res	Type
1	D	140[A]	TYR
1	D	140[B]	TYR
1	D	146[A]	LYS
1	D	146[B]	LYS
1	D	155[A]	ASN
1	D	155[B]	ASN
1	E	65[A]	ASP
1	E	65[B]	ASP
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	33[A]	LEU
1	F	33[B]	LEU
1	F	70[A]	PHE
1	F	70[B]	PHE
1	F	132[A]	GLU
1	F	132[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.

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.