Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:04 PM GMT

PDB ID	:	1IME
Title	:	STRUCTURAL STUDIES OF METAL BINDING BY INOSITOL MONOPHOSPHATASE: EVIDENCE FOR TWO-METAL ION CATALYSIS
Authors	:	Bone, R.
Deposited on	:	1994-02-08
Resolution	:	2.25 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

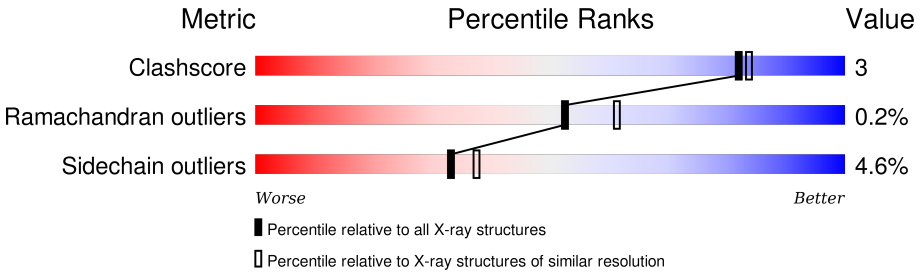
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.25 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	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	277	87% 10%
1	B	277	82% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4331 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 INOSITOL MONOPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	55	0	1
			2073	1307	352	396	18			
1	B	273	Total	C	N	O	S	62	0	1
			2073	1307	352	396	18			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total	O	0	0
			92	92		
3	B	91	Total	O	0	0
			91	91		

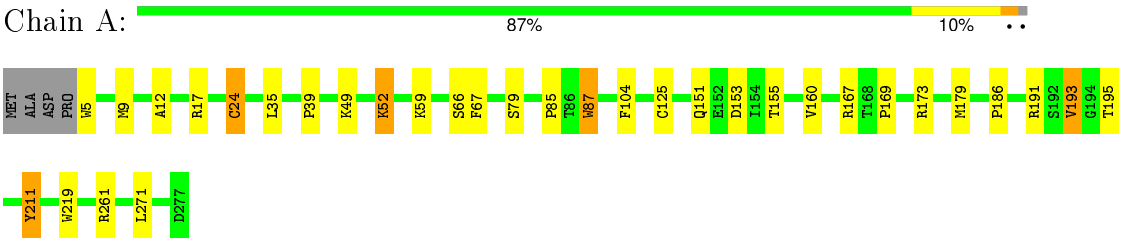
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

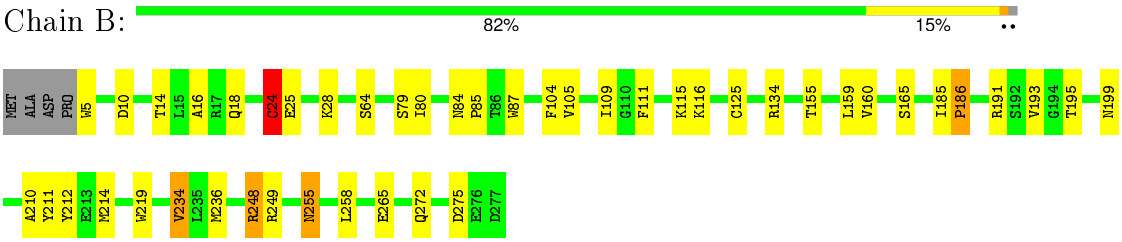
- Molecule 1: INOSITOL MONOPHOSPHATASE

Chain A:



- Molecule 1: INOSITOL MONOPHOSPHATASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.00Å 86.00Å 154.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4331	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.79	0/2106	1.41	23/2849 (0.8%)
1	B	0.81	0/2106	1.47	20/2849 (0.7%)
All	All	0.80	0/4212	1.44	43/5698 (0.8%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	105	VAL	CG1-CB-CG2	-9.88	95.10	110.90
1	B	236	MET	CG-SD-CE	-9.29	85.34	100.20
1	B	219	TRP	CD1-CG-CD2	9.04	113.54	106.30
1	A	191	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	A	5	TRP	CD1-CG-CD2	8.77	113.31	106.30
1	A	219	TRP	CD1-CG-CD2	8.67	113.23	106.30
1	B	87	TRP	CD1-CG-CD2	8.43	113.04	106.30
1	A	5	TRP	CE2-CD2-CG	-7.87	101.01	107.30
1	B	5	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	B	87	TRP	CE2-CD2-CG	-7.53	101.28	107.30
1	B	5	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	A	219	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	A	191	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	87	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	B	219	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	B	24	CYS	CA-CB-SG	-6.98	101.43	114.00
1	B	212	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	A	87	TRP	CD1-CG-CD2	6.85	111.78	106.30
1	B	134	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	B	5	TRP	CG-CD2-CE3	6.26	139.53	133.90
1	A	211	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	A	5	TRP	CB-CG-CD1	-5.96	119.25	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	5	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	B	219	TRP	CG-CD1-NE1	-5.79	104.31	110.10
1	A	17	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	219	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	A	87	TRP	CG-CD2-CE3	5.71	139.04	133.90
1	A	261	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	191	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	134	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	179	MET	CG-SD-CE	-5.62	91.21	100.20
1	B	248	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	167	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	5	TRP	CG-CD1-NE1	-5.44	104.66	110.10
1	A	219	TRP	CG-CD2-CE3	5.41	138.76	133.90
1	A	24	CYS	CA-CB-SG	-5.36	104.35	114.00
1	A	87	TRP	CB-CG-CD1	-5.35	120.04	127.00
1	A	5	TRP	CG-CD2-CE3	5.28	138.65	133.90
1	B	234	VAL	N-CA-CB	-5.20	100.05	111.50
1	B	248	ARG	CA-CB-CG	-5.09	102.21	113.40
1	A	193	VAL	N-CA-CB	-5.08	100.33	111.50
1	B	5	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	A	9	MET	CG-SD-CE	-5.01	92.19	100.20

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	2073	0	2090	11	0
1	B	2073	0	2090	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	92	0	0	0	0
3	B	91	0	0	0	0
All	All	4331	0	4180	26	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 3.

All (26) 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:A:151:GLN:HE21	1:A:153:ASP:H	1.28	0.79
1:A:49:LYS:HA	1:A:52:LYS:HD2	1.63	0.79
1:B:214:MET:HG2	1:B:249:ARG:HG2	1.79	0.65
1:B:80:ILE:HD12	1:B:275:ASP:HB2	1.79	0.64
1:B:185:ILE:HD11	1:B:265:GLU:HG3	1.82	0.62
1:B:25:GLU:O	1:B:28:LYS:HG2	2.03	0.58
1:B:160:VAL:HG23	1:B:211:TYR:HB2	1.86	0.57
1:A:155:THR:HA	1:A:186:PRO:O	2.08	0.54
1:B:24:CYS:SG	1:B:125:CYS:HB3	2.46	0.54
1:A:24:CYS:SG	1:A:125:CYS:HB3	2.49	0.53
1:B:159:LEU:HD22	1:B:210:ALA:HB3	1.92	0.52
1:B:85:PRO:HB3	1:B:111:PHE:CZ	2.45	0.52
1:A:151:GLN:NE2	1:A:153:ASP:HB3	2.28	0.49
1:A:160:VAL:HG23	1:A:211:TYR:HB2	1.94	0.49
1:B:193:VAL:HG22	1:B:199:ASN:ND2	2.27	0.48
1:B:248:ARG:HD3	1:B:272:GLN:O	2.14	0.47
1:A:59:LYS:HE2	1:A:67:PHE:CE1	2.50	0.46
1:B:16:ALA:HB2	1:B:109:ILE:HD12	1.97	0.46
1:A:35:LEU:HD13	1:A:39:PRO:HA	1.96	0.46
1:A:151:GLN:HE21	1:A:153:ASP:N	2.05	0.45
1:B:155:THR:HA	1:B:186:PRO:O	2.19	0.42
1:B:84:ASN:OD1	1:B:85:PRO:HD2	2.19	0.42
1:A:12:ALA:HB2	1:A:87:TRP:HZ3	1.84	0.42
1:A:104:PHE:CZ	1:B:104:PHE:HZ	2.37	0.42
1:B:255:ASN:ND2	1:B:258:LEU:H	2.18	0.41
1:B:248:ARG:HD3	1:B:248:ARG:HH11	1.70	0.40

There are no symmetry-related clashes.

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	271/277 (98%)	263 (97%)	7 (3%)	1 (0%)	39 43
1	B	271/277 (98%)	260 (96%)	11 (4%)	0	100 100
All	All	542/554 (98%)	523 (96%)	18 (3%)	1 (0%)	52 61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	PRO

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	227/231 (98%)	219 (96%)	8 (4%)	43 53
1	B	227/231 (98%)	214 (94%)	13 (6%)	25 26
All	All	454/462 (98%)	433 (95%)	21 (5%)	33 37

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	66	SER
1	A	79	SER
1	A	169	PRO
1	A	173	ARG
1	A	193	VAL
1	A	195	THR
1	A	271	LEU
1	B	10	ASP
1	B	14	THR
1	B	18	GLN
1	B	24	CYS

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Mol	Chain	Res	Type
1	B	64	SER
1	B	79	SER
1	B	115	LYS
1	B	116	LYS
1	B	165	SER
1	B	186	PRO
1	B	195	THR
1	B	234	VAL
1	B	255	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	151	GLN
1	B	48	GLN
1	B	151	GLN
1	B	199	ASN
1	B	255	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.