



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:04 PM UTC

PDB ID : 1IMF / pdb_00001imf
Title : STRUCTURAL STUDIES OF METAL BINDING BY INOSITOL MONOPHOSPHATASE: EVIDENCE FOR TWO-METAL ION CATALYSIS
Authors : Bone, R.
Deposited on : 1994-02-08
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

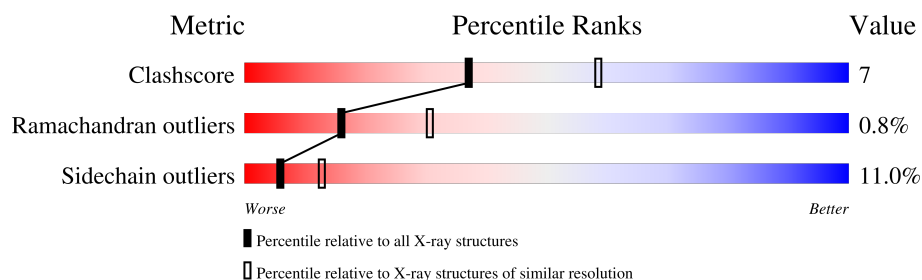
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	277	 60% 27% 7% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2043 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	264	Total	C	N	O	S	36	0	2
			1998	1260	341	381	16			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total	O	0	0
			45	45		

Note EDS was not executed.

Chain A:

60% 27% 7% 5%

MET ALA ASP PRO Q6 Q6 M9 D10 R17 E21 V22 V23 C24 I27 K28 N29 E30 MET ASN VAL MET LEU LYS SER SER PRO V40 D41 Q48 K49 K52 H53 S56 E60 K61 Y62 F63 S64 H65 S66 F67 E77 K78 S79 L80 L81

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.83Å 100.83Å 62.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2043	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.20	7/2029 (0.3%)	1.98	54/2745 (2.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	ILE	CA-CB	8.24	1.58	1.54
1	A	100	HIS	CD2-NE2	-7.27	1.29	1.37
1	A	29	ASN	C-N	-7.00	1.23	1.33
1	A	217	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	65	HIS	CD2-NE2	-5.39	1.31	1.37
1	A	270	PRO	CA-CB	-5.14	1.47	1.53
1	A	188	HIS	CD2-NE2	-5.03	1.32	1.37

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ASN	OD1-CG-ND2	-9.07	113.53	122.60
1	A	119	PHE	CA-CB-CG	8.96	122.76	113.80
1	A	269	ILE	N-CA-C	-8.84	98.14	107.60
1	A	48	GLN	OE1-CD-NE2	-7.31	115.29	122.60
1	A	95	THR	CA-CB-OG1	-7.24	98.74	109.60
1	A	193	VAL	N-CA-CB	-7.17	101.18	112.07
1	A	165	SER	N-CA-C	-7.16	103.64	112.88
1	A	168	THR	CA-C-N	7.10	127.09	119.28
1	A	168	THR	C-N-CA	7.10	127.09	119.28
1	A	199	ASN	OD1-CG-ND2	-7.07	115.53	122.60
1	A	185	ILE	CB-CA-C	-6.92	107.13	113.70
1	A	99	VAL	N-CA-CB	-6.68	102.73	110.55
1	A	77	GLU	CB-CG-CD	6.41	123.50	112.60
1	A	114	ASN	CB-CG-ND2	6.33	125.89	116.40
1	A	52	LYS	N-CA-C	-6.25	104.38	111.07
1	A	90	ASP	CA-CB-CG	6.22	118.83	112.60
1	A	153	ASP	CA-CB-CG	6.22	118.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	HIS	CB-CG-CD2	-6.19	123.16	131.20
1	A	142	ASN	OD1-CG-ND2	-6.09	116.50	122.60
1	A	89	ILE	O-C-N	-6.06	116.50	122.93
1	A	100	HIS	CA-CB-CG	-6.05	107.75	113.80
1	A	267	GLN	CA-CB-CG	-6.04	102.02	114.10
1	A	95	THR	N-CA-C	6.03	117.54	110.97
1	A	95	THR	N-CA-CB	-5.90	101.30	109.91
1	A	274	ASP	CA-C-N	5.81	128.06	120.28
1	A	274	ASP	C-N-CA	5.81	128.06	120.28
1	A	275	ASP	N-CA-C	5.76	117.56	111.28
1	A	141	CYS	N-CA-C	-5.75	99.15	108.52
1	A	21	GLU	N-CA-C	5.71	117.50	111.28
1	A	64	SER	N-CA-CB	-5.70	101.44	110.28
1	A	261	ARG	CD-NE-CZ	-5.65	116.49	124.40
1	A	111	PHE	CA-CB-CG	5.62	119.42	113.80
1	A	89	ILE	N-CA-CB	-5.60	101.90	110.86
1	A	9	MET	CA-CB-CG	-5.54	103.01	114.10
1	A	80	ILE	N-CA-C	-5.51	99.56	107.78
1	A	268	VAL	CG1-CB-CG2	-5.48	98.74	110.80
1	A	150	GLN	CA-CB-CG	-5.46	103.17	114.10
1	A	265	GLU	CA-CB-CG	-5.46	103.19	114.10
1	A	103	PRO	N-CA-C	5.44	123.68	112.47
1	A	240	GLY	N-CA-C	-5.38	107.49	113.79
1	A	79	SER	CA-CB-OG	-5.35	100.40	111.10
1	A	64	SER	CA-CB-OG	5.26	121.62	111.10
1	A	272	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	A	84	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	A	49	LYS	CA-CB-CG	-5.21	103.67	114.10
1	A	95	THR	CA-CB-CG2	5.16	119.28	110.50
1	A	206	GLY	N-CA-C	-5.11	108.28	114.92
1	A	140	PHE	O-C-N	-5.09	117.17	123.33
1	A	81	LEU	N-CA-CB	-5.09	101.77	110.16
1	A	83	ASP	N-CA-C	5.08	119.33	113.18
1	A	56	SER	N-CA-C	-5.07	105.94	111.82
1	A	254	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	A	28	LYS	CA-C-N	5.02	130.73	121.70
1	A	28	LYS	C-N-CA	5.02	130.73	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1998	0	2009	28	0
2	A	45	0	0	2	0
All	All	2043	0	2009	28	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 7.

All (28) 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:22:VAL:HG21	1:A:53:MET:HE1	1.56	0.86
1:A:226:ILE:O	1:A:226:ILE:HG13	2.04	0.57
1:A:254:ASN:OD1	1:A:258:LEU:HD22	2.05	0.56
1:A:23:VAL:O	1:A:27:ILE:HG13	2.06	0.55
1:A:61:LYS:HE3	1:A:62:TYR:CZ	2.42	0.54
1:A:155:THR:HA	1:A:186:PRO:O	2.08	0.53
1:A:106:ALA:HA	1:A:123:TYR:O	2.10	0.51
1:A:214:MET:HG2	1:A:249:ARG:HB3	1.94	0.49
1:A:261:ARG:NH1	1:A:265:GLU:OE1	2.46	0.49
1:A:61:LYS:HE3	1:A:62:TYR:CE2	2.48	0.48
1:A:6:GLN:HG3	1:A:10:ASP:OD1	2.13	0.48
1:A:17:ARG:O	1:A:21:GLU:HG3	2.14	0.47
1:A:96:THR:O	1:A:100:HIS:HD2	1.97	0.47
1:A:104:PHE:CD2	1:A:198:VAL:HG11	2.48	0.47
1:A:130:MET:H	1:A:142:ASN:ND2	2.13	0.47
1:A:174:MET:HE1	2:A:308:HOH:O	2.15	0.45
1:A:236:MET:HE1	1:A:260:GLU:HG3	1.97	0.45
1:A:65:HIS:CG	1:A:85:PRO:HB2	2.52	0.44
1:A:90:ASP:HB3	1:A:108:SER:HB3	2.00	0.44
1:A:238:VAL:HG22	1:A:266:ILE:HD11	2.01	0.43
1:A:181:LYS:HD2	2:A:294:HOH:O	2.19	0.43
1:A:168:THR:O	1:A:172:VAL:HG23	2.20	0.41
1:A:200:MET:HE3	1:A:252:ALA:HB2	2.01	0.41
1:A:273:ARG:HE	1:A:275:ASP:HB2	1.86	0.41
1:A:160:VAL:HG12	1:A:191:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HE3	1:A:62:TYR:OH	2.22	0.40
1:A:130:MET:HB3	1:A:142:ASN:ND2	2.36	0.40
1:A:157:SER:O	1:A:188:HIS:HB2	2.22	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	260/277 (94%)	248 (95%)	10 (4%)	2 (1%)	16	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	103	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	210/231 (91%)	187 (89%)	23 (11%)	6	13

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	CYS
1	A	40	VAL
1	A	41	ASP
1	A	60	GLU
1	A	61	LYS
1	A	67	PHE
1	A	80	ILE
1	A	89	ILE
1	A	95	THR
1	A	134	ARG
1	A	166	SER
1	A	173	ARG
1	A	179	MET
1	A	193	VAL
1	A	195	THR
1	A	226	ILE
1	A	238	VAL
1	A	256	ARG
1	A	258	LEU
1	A	261	ARG
1	A	265	GLU
1	A	267	GLN
1	A	271	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	142	ASN
1	A	199	ASN
1	A	267	GLN

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 [i](#)

There are no oligosaccharides 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.