



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:22 pm BST

PDB ID : 2BJI
Title : High Resolution Structure of myo-Inositol Monophosphatase, The Target of Lithium Therapy
Authors : Gill, R.; Mohammed, F.; Badyal, R.; Coates, L.; Erskine, P.; Thompson, D.; Cooper, J.; Gore, M.; Wood, S.
Deposited on : 2005-02-03
Resolution : 1.24 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

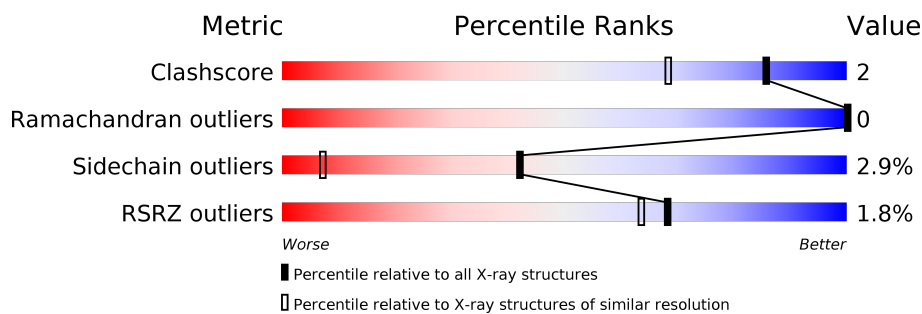
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.24 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	1007 (1.26-1.22)
Ramachandran outliers	138981	2053 (1.28-1.20)
Sidechain outliers	138945	2051 (1.28-1.20)
RSRZ outliers	127900	1987 (1.28-1.20)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	277	<div> <div>2%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	B	277	<div> <div>%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4706 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-1(OR 4)-MONOPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	27	3	1
			2090	1321	351	402	16			
1	B	275	Total	C	N	O	S	29	5	1
			2092	1319	354	404	15			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Mg	0	0
			3	3		
2	A	3	Total	Mg	0	0
			3	3		

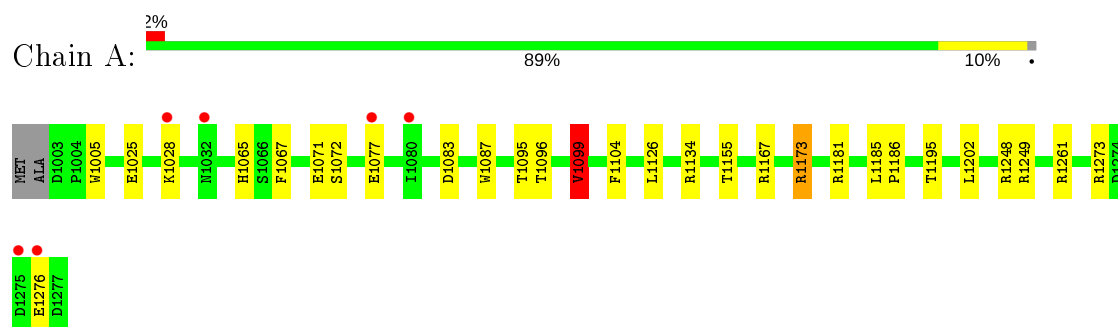
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	266	Total	O	0	0
			266	266		
3	B	252	Total	O	0	0
			252	252		

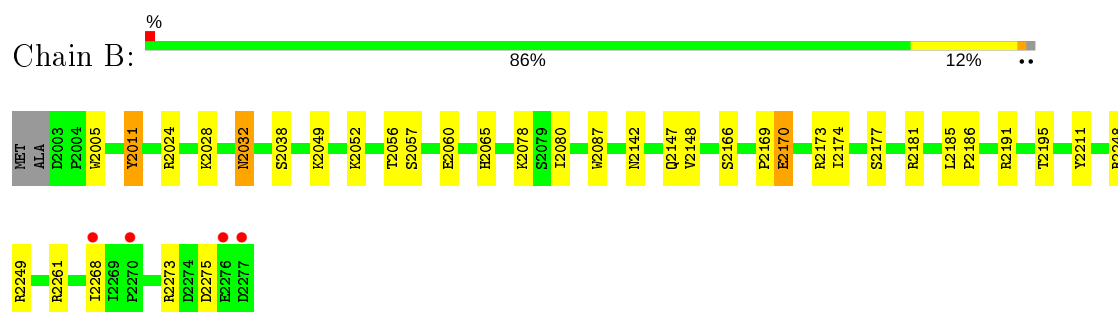
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

• Molecule 1: INOSITOL-1(OR 4)-MONOPHOSPHATASE



• Molecule 1: INOSITOL-1(OR 4)-MONOPHOSPHATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.23Å 55.15Å 60.88Å 67.22° 69.65° 85.14°	Depositor
Resolution (Å)	10.00 – 1.24 9.99 – 1.30	Depositor EDS
% Data completeness (in resolution range)	84.7 (10.00-1.24) 68.4 (9.99-1.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.30Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.153 , 0.191 0.149 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4706	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.55	0/2138	1.28	23/2895 (0.8%)
1	B	0.55	0/2156	1.31	23/2917 (0.8%)
All	All	0.55	0/4294	1.29	46/5812 (0.8%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2249	ARG	NE-CZ-NH1	12.09	126.35	120.30
1	A	1249	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	B	2249	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	B	2087	TRP	CD1-NE1-CE2	10.38	118.34	109.00
1	B	2181	ARG	NE-CZ-NH2	10.35	125.47	120.30
1	A	1249	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	B	2065	HIS	CG-ND1-CE1	9.87	122.01	108.20
1	A	1181	ARG	NE-CZ-NH1	9.85	125.23	120.30
1	A	1273	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	B	2191	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	1065	HIS	CG-ND1-CE1	8.56	120.18	108.20
1	A	1087	TRP	CD1-NE1-CE2	8.53	116.67	109.00
1	A	1173	ARG	CD-NE-CZ	8.35	135.30	123.60
1	A	1261	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	B	2011	TYR	CB-CG-CD1	-7.28	116.64	121.00
1	B	2087	TRP	CG-CD1-NE1	-7.09	103.00	110.10
1	B	2261[A]	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	B	2261[B]	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	A	1273	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	1261	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	2273	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	1248	ARG	CD-NE-CZ	6.36	132.51	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2060	GLU	OE1-CD-OE2	6.32	130.89	123.30
1	A	1087	TRP	CG-CD1-NE1	-6.24	103.86	110.10
1	B	2024	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	2191	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	2065	HIS	ND1-CG-CD2	-5.90	97.74	106.00
1	A	1083	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	B	2024	ARG	CD-NE-CZ	5.75	131.65	123.60
1	B	2087	TRP	NE1-CE2-CD2	-5.58	101.72	107.30
1	B	2211	TYR	CB-CG-CD2	5.55	124.33	121.00
1	A	1005	TRP	CG-CD2-CE3	5.46	138.82	133.90
1	A	1099[A]	VAL	CA-CB-CG1	5.44	119.06	110.90
1	A	1099[B]	VAL	CA-CB-CG1	5.44	119.06	110.90
1	A	1134	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	1067	PHE	CB-CG-CD2	5.30	124.51	120.80
1	B	2261[A]	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	2261[B]	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	1167	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	A	1104	PHE	CB-CG-CD1	-5.22	117.15	120.80
1	B	2275	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	2011	TYR	CB-CG-CD2	5.14	124.09	121.00
1	B	2248	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	1071	GLU	OE1-CD-OE2	-5.13	117.14	123.30
1	A	1173	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	1087	TRP	NE1-CE2-CD2	-5.07	102.23	107.30

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	2090	0	2113	8	2
1	B	2092	0	2100	10	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	266	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	252	0	0	4	0
All	All	4706	0	4213	18	3

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 2.

All (18) 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:2166:SER:HB3	3:B:3194:HOH:O	1.87	0.74
1:B:2052:LYS:O	1:B:2056:THR:HG23	1.94	0.67
1:B:2169:PRO:O	1:B:2173:ARG:HG3	1.97	0.64
1:A:1095:THR:O	1:A:1099[A]:VAL:HG12	2.07	0.54
1:A:1202:LEU:HG	3:A:2170:HOH:O	2.07	0.54
1:B:2049:LYS:HE2	3:B:3004:HOH:O	2.08	0.52
1:B:2011:TYR:OH	1:B:2057[B]:SER:OG	2.29	0.51
1:A:1096:THR:O	1:A:1099[A]:VAL:HG13	2.11	0.51
1:A:1155:THR:HA	1:A:1186:PRO:O	2.12	0.49
1:A:1185:LEU:N	1:A:1186:PRO:HA	2.29	0.48
1:A:1096:THR:HA	1:A:1099[A]:VAL:CG1	2.46	0.46
1:B:2185:LEU:N	1:B:2186:PRO:HA	2.32	0.44
1:B:2147[A]:GLN:HG3	1:B:2148:VAL:O	2.18	0.44
1:B:2169:PRO:HG2	3:B:3197:HOH:O	2.18	0.43
1:B:2032:ASN:ND2	3:B:3070:HOH:O	2.51	0.42
1:B:2174:ILE:HA	1:B:2177[A]:SER:OG	2.19	0.42
1:A:1276:GLU:HB3	3:A:2224:HOH:O	2.20	0.41
1:A:1072:SER:O	1:A:1077:GLU:HB2	2.20	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:GLU:OE2	1:A:1173:ARG:NH1[1_655]	1.14	1.06
1:A:1025:GLU:OE2	1:A:1173:ARG:CZ[1_655]	1.73	0.47
1:B:2142:ASN:O	1:B:2170:GLU:OE2[1_655]	2.18	0.02

5.3 Torsion angles

5.3.1 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	276/277 (100%)	269 (98%)	7 (2%)	0	100	100
1	B	278/277 (100%)	271 (98%)	7 (2%)	0	100	100
All	All	554/554 (100%)	540 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	230/229 (100%)	225 (98%)	5 (2%)	52	14
1	B	232/229 (101%)	223 (96%)	9 (4%)	32	4
All	All	462/458 (101%)	448 (97%)	14 (3%)	42	6

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1028	LYS
1	A	1099[A]	VAL
1	A	1099[B]	VAL
1	A	1126	LEU
1	A	1195	THR
1	B	2005	TRP
1	B	2028	LYS
1	B	2032	ASN

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Mol	Chain	Res	Type
1	B	2038	SER
1	B	2078	LYS
1	B	2080	ILE
1	B	2170	GLU
1	B	2195	THR
1	B	2268	ILE

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	1018	GLN
1	A	1114	ASN
1	A	1267	GLN
1	B	2032	ASN
1	B	2048	GLN
1	B	2114	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 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.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	274/277 (98%)	-0.21	6 (2%) 62 56	9, 14, 29, 50	8 (2%)
1	B	275/277 (99%)	-0.14	4 (1%) 73 69	9, 14, 30, 76	8 (2%)
All	All	549/554 (99%)	-0.18	10 (1%) 68 63	9, 14, 30, 76	16 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2277	ASP	4.9
1	A	1276	GLU	4.2
1	B	2270	PRO	3.0
1	B	2276	GLU	2.5
1	A	1032	ASN	2.3
1	A	1080	ILE	2.2
1	B	2268	ILE	2.2
1	A	1275	ASP	2.2
1	A	1077	GLU	2.1
1	A	1028	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	A	2278	1/1	0.99	0.06	15,15,15,15	0
2	MG	A	2279	1/1	0.99	0.19	22,22,22,22	0
2	MG	B	3277	1/1	1.00	0.03	10,10,10,10	0
2	MG	A	2277	1/1	1.00	0.04	10,10,10,10	0
2	MG	B	3278	1/1	1.00	0.05	11,11,11,11	0
2	MG	B	3279	1/1	1.00	0.08	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.