



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:22 AM UTC

PDB ID : 1MJZ / pdb_00001mjz
Title : STRUCTURE OF INORGANIC PYROPHOSPHATASE MUTANT D97N
Authors : Oganessian, V.; Harutyunyan, E.H.; Avaeva, S.M.; Huber, R.
Deposited on : 1997-02-08
Resolution : 2.20 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

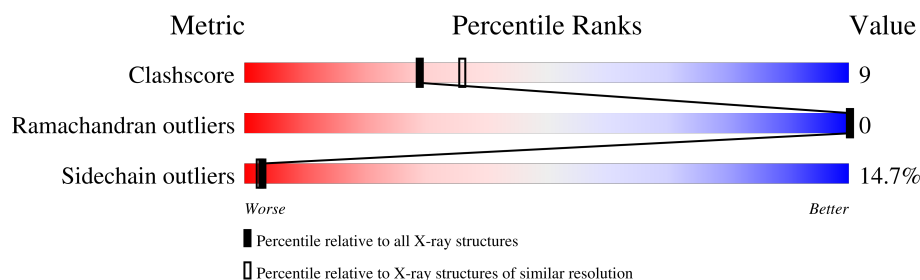
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 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	175	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1441 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 INORGANIC PYROPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1381	889	225	262	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASN	ASP	engineered mutation	UNP P0A7A9

- Molecule 2 is water.

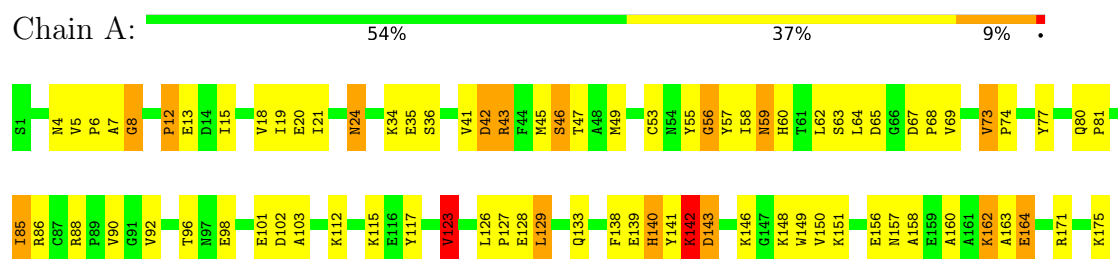
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	60	Total	O	0	0
			60	60		

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



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	110.64Å 110.64Å 77.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1441	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.13	2/1416 (0.1%)	2.16	63/1923 (3.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	ILE	C-O	-5.69	1.17	1.24
1	A	20	GLU	N-CA	-5.64	1.39	1.46

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASN	OD1-CG-ND2	10.88	133.48	122.60
1	A	53	CYS	CA-C-O	-9.31	111.08	121.51
1	A	69	VAL	CA-C-N	9.05	133.56	120.71
1	A	69	VAL	C-N-CA	9.05	133.56	120.71
1	A	102	ASP	CA-CB-CG	8.91	121.51	112.60
1	A	123	VAL	CB-CA-C	-8.69	98.69	112.16
1	A	43	ARG	CD-NE-CZ	8.25	135.95	124.40
1	A	90	VAL	CA-C-O	-7.97	110.81	120.78
1	A	88	ARG	NE-CZ-NH1	-7.97	113.53	121.50
1	A	138	PHE	CA-CB-CG	-7.26	106.54	113.80
1	A	162	LYS	CA-C-O	-6.88	112.50	120.20
1	A	43	ARG	O-C-N	6.86	130.15	123.29
1	A	164	GLU	N-CA-C	6.85	119.62	111.33
1	A	86	ARG	CA-C-O	-6.84	112.56	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ARG	NE-CZ-NH2	6.68	125.21	119.20
1	A	163	ALA	N-CA-C	-6.62	103.54	111.69
1	A	36	SER	CA-C-O	6.60	126.99	119.27
1	A	57	TYR	CA-C-O	6.50	128.35	121.33
1	A	123	VAL	O-C-N	6.30	128.23	121.87
1	A	171	ARG	CD-NE-CZ	6.29	133.21	124.40
1	A	35	GLU	CA-C-O	-6.18	114.51	121.00
1	A	73	VAL	CA-CB-CG2	6.12	120.80	110.40
1	A	90	VAL	N-CA-CB	6.10	121.29	111.23
1	A	133	GLN	CA-C-N	6.03	128.16	120.56
1	A	133	GLN	C-N-CA	6.03	128.16	120.56
1	A	77	TYR	O-C-N	6.03	127.63	121.72
1	A	55	TYR	N-CA-CB	5.99	120.17	110.77
1	A	69	VAL	O-C-N	-5.98	115.09	122.57
1	A	24	ASN	CA-CB-CG	-5.89	106.71	112.60
1	A	43	ARG	CA-C-N	-5.89	114.67	122.85
1	A	43	ARG	C-N-CA	-5.89	114.67	122.85
1	A	8	GLY	CA-C-O	-5.81	115.92	121.62
1	A	126	LEU	O-C-N	5.80	127.93	121.43
1	A	150	VAL	CA-C-O	-5.80	114.44	120.64
1	A	127	PRO	CA-C-N	5.58	128.08	120.54
1	A	127	PRO	C-N-CA	5.58	128.08	120.54
1	A	77	TYR	CB-CG-CD1	-5.56	112.47	120.80
1	A	117	TYR	N-CA-C	-5.55	106.56	113.38
1	A	77	TYR	CA-C-O	-5.52	113.55	120.23
1	A	74	PRO	CA-C-O	-5.48	114.91	121.48
1	A	56	GLY	O-C-N	5.46	129.80	122.70
1	A	24	ASN	CB-CA-C	-5.46	102.88	111.51
1	A	58	ILE	CB-CA-C	-5.43	103.46	110.84
1	A	41	VAL	N-CA-CB	5.40	116.82	110.82
1	A	90	VAL	CA-C-N	-5.40	112.56	121.04
1	A	90	VAL	C-N-CA	-5.40	112.56	121.04
1	A	142	LYS	CA-CB-CG	-5.39	103.32	114.10
1	A	143	ASP	CB-CG-OD2	5.38	130.78	118.40
1	A	63	SER	N-CA-C	-5.38	102.56	110.52
1	A	160	ALA	CA-C-N	5.35	127.71	120.65
1	A	160	ALA	C-N-CA	5.35	127.71	120.65
1	A	140	HIS	CA-CB-CG	-5.30	108.50	113.80
1	A	158	ALA	N-CA-CB	-5.27	102.38	110.12
1	A	4	ASN	CB-CA-C	-5.22	102.32	110.94
1	A	21	ILE	CB-CG1-CD1	5.17	124.67	113.80
1	A	13	GLU	N-CA-CB	5.14	118.54	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ARG	CB-CA-C	5.14	117.02	110.13
1	A	19	ILE	N-CA-CB	5.09	116.07	110.53
1	A	36	SER	O-C-N	-5.06	115.53	122.46
1	A	43	ARG	NE-CZ-NH1	5.03	126.53	121.50
1	A	77	TYR	CA-CB-CG	-5.02	104.86	113.90
1	A	58	ILE	CA-C-O	-5.02	115.20	120.57
1	A	24	ASN	CA-C-O	-5.01	114.60	120.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	ASN	Mainchain

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	1381	0	1371	24	0
2	A	60	0	0	3	0
All	All	1441	0	1371	24	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 9.

All (24) 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:98:GLU:HG3	1:A:149:TRP:HE1	1.40	0.84
1:A:67:ASP:HB2	1:A:68:PRO:CD	2.12	0.80
1:A:73:VAL:HG11	1:A:85:ILE:HD13	1.84	0.59
1:A:67:ASP:HB2	1:A:68:PRO:HD2	1.85	0.58
1:A:8:GLY:HA3	1:A:15:ILE:HA	1.86	0.57
1:A:123:VAL:HG22	1:A:157:ASN:HA	1.88	0.56
1:A:98:GLU:HG3	1:A:149:TRP:NE1	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:PRO:HG2	1:A:162:LYS:HG2	1.92	0.52
1:A:46:SER:HB2	2:A:177:HOH:O	2.10	0.51
1:A:65:ASP:OD2	1:A:67:ASP:OD1	2.30	0.49
1:A:140:HIS:ND1	1:A:143:ASP:OD2	2.39	0.49
1:A:45:MET:HE1	1:A:142:LYS:HG3	1.94	0.48
1:A:42:ASP:O	1:A:43:ARG:HB3	2.14	0.47
1:A:7:ALA:HB3	2:A:218:HOH:O	2.16	0.45
1:A:129:LEU:O	1:A:129:LEU:HD12	2.19	0.43
1:A:5:VAL:HA	1:A:6:PRO:HD2	1.87	0.43
1:A:115:LYS:HG3	2:A:185:HOH:O	2.19	0.43
1:A:47:THR:HB	1:A:49:MET:HG3	2.01	0.42
1:A:103:ALA:HB3	1:A:164:GLU:OE2	2.19	0.42
1:A:67:ASP:HB2	1:A:68:PRO:HD3	1.97	0.42
1:A:80:GLN:HA	1:A:81:PRO:HD3	1.80	0.42
1:A:18:VAL:O	1:A:56:GLY:HA3	2.20	0.41
1:A:59:ASN:O	1:A:60:HIS:HB2	2.21	0.41
1:A:8:GLY:CA	1:A:15:ILE:HA	2.51	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	173/175 (99%)	158 (91%)	15 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	150/150 (100%)	128 (85%)	22 (15%)	3 2

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	34	LYS
1	A	42	ASP
1	A	46	SER
1	A	62	LEU
1	A	64	LEU
1	A	85	ILE
1	A	92	VAL
1	A	96	THR
1	A	101	GLU
1	A	112	LYS
1	A	123	VAL
1	A	128	GLU
1	A	129	LEU
1	A	139	GLU
1	A	141	TYR
1	A	142	LYS
1	A	146	LYS
1	A	148	LYS
1	A	151	LYS
1	A	156	GLU
1	A	175	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	133	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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.