

wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 09:03 AM EDT

PDB ID : 1MJX

Title : STRUCTURE OF INORGANIC PYROPHOSPHATASE MUTANT D65N

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Deposited on : 1997-02-08

Resolution : 2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (i)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

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)

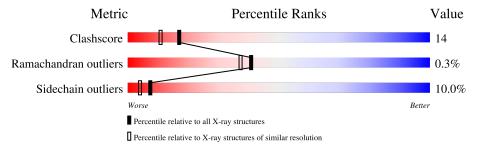
Validation Pipeline (wwPDB-VP) : 2.23.2

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 2.15 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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	175	68%	24%	6% •
1	В	175	74%	21%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2943 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.

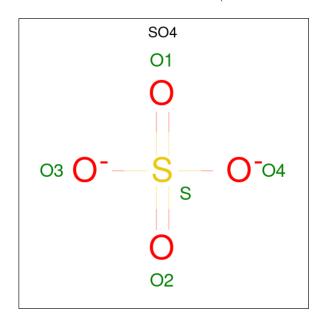
• Molecule 1 is a protein called INORGANIC PYROPHOSPHATASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	175	Total 1381			O 262	S 5	0	0	0
1	D	175	Total			O	$\frac{s}{S}$	0	0	0
1	1 B	175	1381	889	225	262	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	ASN	ASP	engineered mutation	UNP P0A7A9
В	65	ASN	ASP	engineered mutation	UNP P0A7A9

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total O 5 4	S 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total O S 5 4 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	84	Total O 84 84	0	0
3	В	87	Total O 87 87	0	0

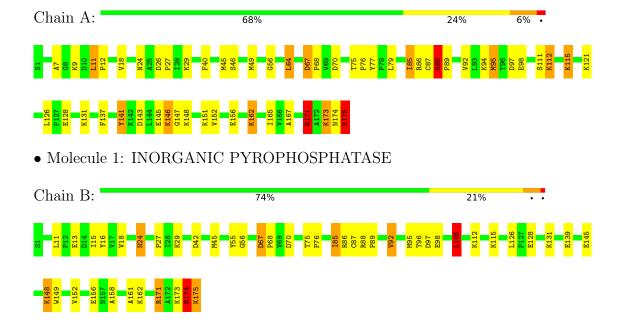


3 Residue-property plots (i)

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: INORGANIC PYROPHOSPHATASE





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	H 3 2	Depositor	
Cell constants	110.20Å 110.20Å 155.20Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	15.00 - 2.15	Depositor	
% Data completeness	(Not available) (15.00-2.15)	Depositor	
(in resolution range)	(1100 available) (15.00 2.15)		
R_{merge}	0.12	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	REFMAC	Depositor	
R, R_{free}	0.190 , 0.263	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2943	wwPDB-VP	
Average B, all atoms (Å ²)	34.0	wwPDB-VP	



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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		nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	1.87	1/1416 (0.1%)	1.48	$13/1923 \ (0.7\%)$	
1	В	1.20	2/1416 (0.1%)	1.43	13/1923 (0.7%)	
All	All	1.57	3/2832 (0.1%)	1.45	$26/3846 \ (0.7\%)$	

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 maintain group or atoms of a sidechain that are expected to be planar.

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\mathbf{Ideal}(exttt{\AA})$
1	A	175	LYS	C-OXT	63.73	2.44	1.23
1	В	175	LYS	C-OXT	34.88	1.89	1.23
1	В	174	ASN	C-N	-9.36	1.12	1.34

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
1	В	174	ASN	O-C-N	-12.36	102.92	122.70
1	A	174	ASN	O-C-N	-8.57	108.99	122.70
1	В	88	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	A	70	ASP	CB-CG-OD2	7.79	125.31	118.30
1	В	174	ASN	C-N-CA	7.44	140.30	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	В	174	ASN	Mainchain

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	1381	0	1371	51	0
1	В	1381	0	1370	26	0
2	A	5	0	0	0	0
2	В	5	0	0	0	0
3	A	84	0	0	0	0
3	В	87	0	0	0	0
All	All	2943	0	2741	77	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 14.

The worst 5 of 77 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$	
1:B:175:LYS:C	1:B:175:LYS:OXT	1.89	1.11	
1:A:86:ARG:HH11	1:A:112:LYS:HD3	1.34	0.91	
1:B:86:ARG:NH1	1:B:112:LYS:HD2	1.86	0.90	
1:A:111:SER:HB3	1:A:115:LYS:HZ1	1.37	0.89	
1:A:151:LYS:NZ	1:A:152:VAL:H	1.71	0.88	

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	n Analysed Favoured Allowed C		Outliers	Perce	entiles	
1	A	173/175~(99%)	167 (96%)	6 (4%)	0	100	100
1	В	173/175~(99%)	166 (96%)	6 (4%)	1 (1%)	25	18
All	All	346/350~(99%)	333 (96%)	12 (4%)	1 (0%)	41	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	174	ASN

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%)	134 (89%)	16 (11%)	6 3		
1	В	150/150~(100%)	136 (91%)	14 (9%)	9 5		
All	All	300/300 (100%)	270 (90%)	30 (10%)	7 4		

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	LYS
1	В	128	GLU
1	В	24	ASN
1	В	173	LYS
1	В	96	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	174	ASN



5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type Chain Re		Res Link	Bond lengths			Bond angles			
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	SO4	A	176	-	4,4,4	0.59	0	6,6,6	0.23	0
2	SO4	В	176	-	4,4,4	0.65	0	6,6,6	0.27	0

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 (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	В	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	В	174:ASN	С	175:LYS	N	1.12



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

