

# Full wwPDB X-ray Structure Validation Report (i)

#### Mar 4, 2024 – 06:43 PM EST

PDB ID	:	2CXN
Title	:	Crystal structure of mouse AMF $/$ phosphate complex
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Deposited on	:	2005-06-30
Resolution	:	1.40  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 (i) 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 (i)) were used in the production of this report:

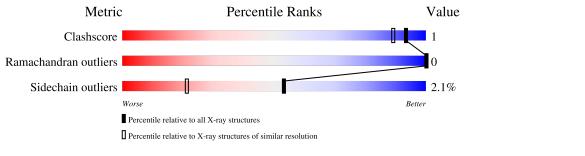
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.40 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	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)

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	А	557	94%	6%
1	В	557	94%	6%



#### $2\mathrm{CXN}$

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10053 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.

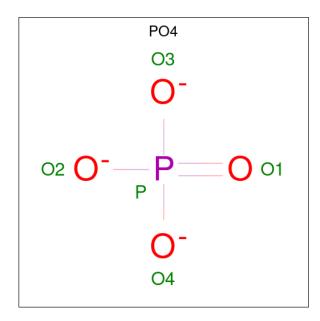
• Molecule 1 is a protein called Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	557	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	I A	557	4416	2826	764	807	19	0		
1	Р	557	Total	С	Ν	0	S	0	0	0
	I B	557	4416	2826	764	807	19	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P06745
А	61	SER	ASN	conflict	UNP P06745
В	1	MET	-	initiating methionine	UNP P06745
В	61	SER	ASN	conflict	UNP P06745

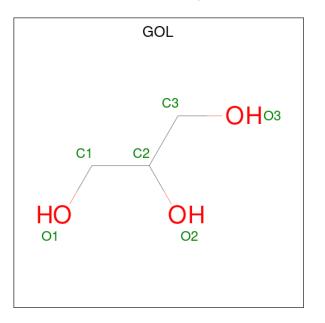
• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	А	1	Total 5	0 4	Р 1	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	601	Total O 601 601	0	0
4	В	591	Total O 591 591	0	0

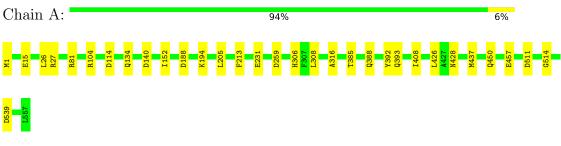


# 3 Residue-property plots (i)

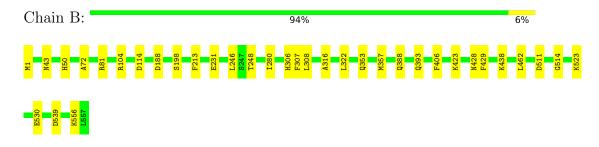
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Glucose-6-phosphate isomerase



• Molecule 1: Glucose-6-phosphate isomerase





## 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	69.95Å 116.03Å 73.21Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $101.67^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	40.00 - 1.40	Depositor	
% Data completeness	96.0 (40.00-1.40)	Depositor	
(in resolution range)	30.0 (40.00-1.40)	Depositor	
$R_{merge}$	(Not available)	Depositor	
R <sub>sym</sub>	(Not available)	Depositor	
Refinement program	REFMAC 5.1.24	Depositor	
$R, R_{free}$	0.171 , $0.188$	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	10053	wwPDB-VP	
Average B, all atoms $(Å^2)$	14.0	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: PO4, GOL

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	А	0.31	0/4525	0.61	6/6124~(0.1%)	
1	В	0.31	0/4525	0.60	4/6124~(0.1%)	
All	All	0.31	0/9050	0.61	10/12248~(0.1%)	

There are no bond length outliers.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	188	ASP	CB-CG-OD2	5.98	123.68	118.30
1	В	511	ASP	CB-CG-OD2	5.82	123.54	118.30
1	А	140	ASP	CB-CG-OD2	5.77	123.50	118.30
1	В	188	ASP	CB-CG-OD2	5.65	123.39	118.30
1	А	511	ASP	CB-CG-OD2	5.63	123.36	118.30
1	А	114	ASP	CB-CG-OD2	5.26	123.03	118.30
1	В	114	ASP	CB-CG-OD2	5.21	122.99	118.30
1	А	539	ASP	CB-CG-OD2	5.20	122.98	118.30
1	А	259	ASP	CB-CG-OD2	5.14	122.93	118.30
1	В	539	ASP	CB-CG-OD2	5.12	122.91	118.30

All (10) bond angle outliers are listed below:

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	А	4416	0	4398	13	0
1	В	4416	0	4398	16	0
2	А	5	0	0	0	0
3	А	12	0	16	0	0
3	В	12	0	16	0	0
4	А	601	0	0	0	0
4	В	591	0	0	1	0
All	All	10053	0	8828	25	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 1.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A / 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:306:HIS:HE1	1:A:316:ALA:H	1.16	0.94
1:B:306:HIS:HE1	1:B:316:ALA:H	1.16	0.93
1:A:514:GLY:H	1:B:393:GLN:HE22	1.20	0.88
1:A:393:GLN:HE22	1:B:514:GLY:H	1.27	0.81
1:A:306:HIS:CE1	1:A:316:ALA:H	2.08	0.58
1:B:248:THR:HG23	4:B:2257:HOH:O	2.05	0.56
1:A:152:ILE:HD12	1:A:205:LEU:HD23	1.89	0.55
1:B:306:HIS:CE1	1:B:316:ALA:H	2.09	0.54
1:B:388:GLN:HE22	1:B:428:ASN:HB3	1.71	0.54
1:B:246:LEU:HD13	1:B:280:ILE:HA	1.93	0.51
1:B:81:ARG:HD2	1:B:308:LEU:HA	1.95	0.49
1:A:388:GLN:HE22	1:A:428:ASN:HB3	1.78	0.48
1:B:43:ASN:OD1	1:B:50:HIS:HD2	1.98	0.46
1:A:388:GLN:HA	1:A:392:TYR:CD1	2.51	0.46
1:A:81:ARG:HD2	1:A:308:LEU:HA	1.99	0.45
1:A:514:GLY:N	1:B:393:GLN:HE22	2.00	0.45
1:A:514:GLY:H	1:B:393:GLN:NE2	2.02	0.42
1:B:523:LYS:HD2	1:B:523:LYS:HA	1.88	0.42
1:B:353:GLN:O	1:B:357:MET:HB2	2.18	0.42
1:A:385:THR:O	1:A:388:GLN:HB3	2.19	0.42
1:A:26:LEU:HB3	1:A:437:MET:HG2	2.02	0.42
1:B:406:PHE:HB3	1:B:429:PHE:CE1	2.55	0.42
1:B:72:ALA:HB2	1:B:322:LEU:HD21	2.00	0.41
1:A:408:ILE:HD13	1:A:426:LEU:HD23	2.02	0.41
1:B:81:ARG:HG3	1:B:307:PHE:CE2	2.56	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	Perce	entiles
1	А	555/557~(100%)	544~(98%)	11 (2%)	0	100	100
1	В	555/557~(100%)	541 (98%)	14 (2%)	0	100	100
All	All	1110/1114 (100%)	1085~(98%)	25~(2%)	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	Analysed Rotameric Outliers		Percentiles		
1	А	475/475~(100%)	465~(98%)	10 (2%)	53 21		
1	В	475/475 (100%)	465~(98%)	10 (2%)	53 21		
All	All	950/950~(100%)	930~(98%)	20~(2%)	53 21		

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1	MET
1	А	15	GLU
1	А	27	ARG
1	А	104	ARG
1	А	134	GLN
1	А	194	LYS
1	А	213	PHE
1	А	231	GLU

Continued on next page...



Mol	Chain	Res	Type
1	А	450	GLN
1	А	457	GLU
1	В	1	MET
1	В	104	ARG
1	В	198	SER
1	В	213	PHE
1	В	231	GLU
1	В	423	LYS
1	В	438	LYS
1	В	462	LEU
1	В	530	GLU
1	В	556	LYS

Continued from previous page...

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	47	ASN
1	А	58	ASN
1	А	134	GLN
1	А	306	HIS
1	А	388	GLN
1	А	393	GLN
1	А	397	GLN
1	А	475	ASN
1	В	23	ASN
1	В	50	HIS
1	В	58	ASN
1	В	261	GLN
1	В	306	HIS
1	В	388	GLN
1	В	393	GLN
1	В	397	GLN
1	В	475	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)

5 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	Turne	Chain	Res	Res Link Bond lengths			Bond angles			
10101	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	GOL	В	1703	-	$5,\!5,\!5$	0.34	0	$5,\!5,\!5$	0.34	0
3	GOL	А	1704	-	$5,\!5,\!5$	0.35	0	$5,\!5,\!5$	0.34	0
3	GOL	А	1701	-	$5,\!5,\!5$	0.33	0	$5,\!5,\!5$	0.33	0
2	PO4	А	1601	-	$4,\!4,\!4$	0.84	0	$6,\!6,\!6$	0.49	0
3	GOL	В	1702	-	$5,\!5,\!5$	0.35	0	$5,\!5,\!5$	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	А	1701	-	-	0/4/4/4	-
3	GOL	В	1703	-	-	0/4/4/4	-
3	GOL	А	1704	-	-	2/4/4/4	-
3	GOL	В	1702	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
3	А	1704	GOL	O1-C1-C2-C3
3	В	1702	GOL	O1-C1-C2-C3
3	В	1702	GOL	O1-C1-C2-O2
3	А	1704	GOL	O1-C1-C2-O2

All (4) torsion outliers are listed below:

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)

There are no chain breaks in this entry.



## 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.

