

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

#### Jan 30, 2021 - 08:05 PM EST

PDB ID	:	3M7V
Title	:	Crystal structure of phosphopentomutase from streptococcus mutans
Authors	:	Fedorov, A.A.; Bonanno, J.; Fedorov, E.V.; Burley, S.K.; Almo, S.C.; New
		York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-03-17
Resolution	:	2.00  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 following versions of software and data (see references (1)) were used in the production of this report:

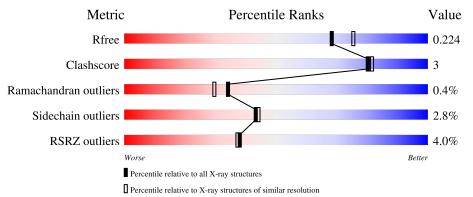
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

## 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 2.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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% 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	А	413	88%	8%	•
1	В	413	90%	7%	·



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6466 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 Phosphopentomutase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	401	Total	С	Ν	0	$\mathbf{S}$	0	1	0
		401	3072	1947	524	591	10	0	1	0
1	В	401	Total	С	Ν	0	S	0	1	0
1	D	401	3069	1947	523	589	10	0		0

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	MET	-	expression tag	UNP Q8DTU0
А	0	SER	-	expression tag	UNP Q8DTU0
А	1	LEU	-	expression tag	UNP Q8DTU0
А	404	GLU	-	expression tag	UNP Q8DTU0
A	405	GLY	-	expression tag	UNP Q8DTU0
A	406	HIS	-	expression tag	UNP Q8DTU0
А	407	HIS	-	expression tag	UNP Q8DTU0
А	408	HIS	-	expression tag	UNP Q8DTU0
A	409	HIS	-	expression tag	UNP Q8DTU0
A	410	HIS	-	expression tag	UNP Q8DTU0
A	411	HIS	-	expression tag	UNP Q8DTU0
В	-1	MET	-	expression tag	UNP Q8DTU0
В	0	SER	-	expression tag	UNP Q8DTU0
В	1	LEU	-	expression tag	UNP Q8DTU0
В	404	GLU	-	expression tag	UNP Q8DTU0
В	405	GLY	-	expression tag	UNP Q8DTU0
В	406	HIS	-	expression tag	UNP Q8DTU0
В	407	HIS	-	expression tag	UNP Q8DTU0
В	408	HIS	-	expression tag	UNP Q8DTU0
В	409	HIS	-	expression tag	UNP Q8DTU0
В	410	HIS	-	expression tag	UNP Q8DTU0
В	411	HIS	-	expression tag	UNP Q8DTU0

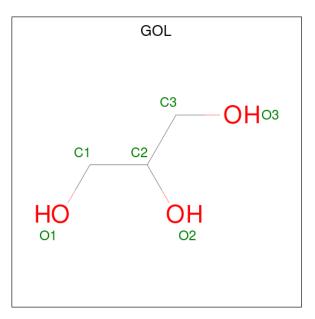
There are 22 discrepancies between the modelled and reference sequences:

• Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	2	Total Mn 2 2	0	0
2	А	2	Total Mn 2 2	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

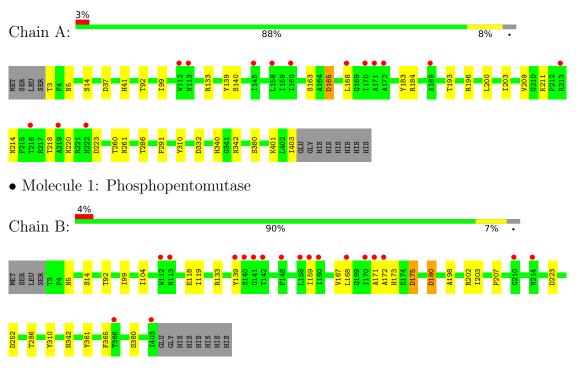
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	166	Total O 166 166	0	0
4	В	149	Total O 149 149	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 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: Phosphopentomutase



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	69.79Å 63.69Å 104.77Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $98.85^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	20.00 - 2.00	Depositor
Resolution (A)	19.93 - 2.00	EDS
% Data completeness	97.5 (20.00-2.00)	Depositor
(in resolution range)	96.9(19.93-2.00)	EDS
R <sub>merge</sub>	0.07	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.07 (at 2.01 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
D D.	0.181 , 0.211	Depositor
$R, R_{free}$	0.192 , $0.224$	DCC
$R_{free}$ test set	3011 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	26.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38 , $44.2$	EDS
L-test for twinning <sup>2</sup>	$ L  > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6466	wwPDB-VP
Average B, all atoms $(Å^2)$	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: GOL, MN

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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.66	0/3147	0.70	1/4284~(0.0%)	
1	В	0.66	0/3146	0.70	0/4287	
All	All	0.66	0/6293	0.70	1/8571~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	332	ASP	CB-CG-OD2	5.04	122.84	118.30

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	3072	0	2991	17	0
1	В	3069	0	2973	15	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
3	А	6	0	8	2	0
4	А	166	0	0	4	0
4	В	149	0	0	1	0
All	All	6466	0	5972	33	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 3.

All (33) 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:193:THR:HG21	1:A:200:LEU:HD12	1.71	0.71
1:B:5:ASN:ND2	1:B:286:THR:O	2.23	0.70
1:B:173:HIS:CE1	1:B:175:ASP:HB2	2.35	0.61
1:B:180:ASP:OD1	1:B:180:ASP:N	2.33	0.57
1:A:209:VAL:HG13	1:A:218:THR:HG21	1.88	0.56
1:B:92:THR:HG22	4:B:425:HOH:O	2.06	0.55
1:A:92:THR:HG22	4:A:459:HOH:O	2.07	0.53
1:B:119:ILE:HD11	1:B:198:ALA:CB	2.40	0.52
1:B:99:ILE:O	1:B:380:SER:HB3	2.12	0.50
1:A:209:VAL:HG13	1:A:218:THR:CG2	2.41	0.50
1:A:193:THR:CG2	1:A:200:LEU:HD12	2.42	0.50
1:A:165:ASP:OD2	1:A:165:ASP:N	2.44	0.50
1:B:104:ILE:N	1:B:104:ILE:HD12	2.27	0.49
1:A:3:THR:CB	1:A:403:ILE:CD1	2.93	0.46
1:A:183:TYR:OH	1:A:220:ASN:O	2.26	0.46
1:B:202:ARG:NH2	1:B:252:ASP:O	2.49	0.46
1:B:14:SER:HB2	1:B:342:ASN:HB2	1.98	0.46
1:B:167:VAL:HG23	1:B:202:ARG:HG3	1.97	0.46
1:A:260:THR:OG1	1:A:261:ASN:ND2	2.48	0.45
1:A:14:SER:HB2	1:A:342:ASN:HB2	1.97	0.45
1:B:172:ALA:O	1:B:207:PRO:HA	2.17	0.44
1:A:3:THR:CB	1:A:403:ILE:HD13	2.48	0.44
1:B:119:ILE:HD11	1:B:198:ALA:HB1	2.01	0.43
1:A:401:LYS:NZ	4:A:494:HOH:O	2.52	0.43
1:B:361:TYR:HA	1:B:365:PHE:CE1	2.53	0.43
1:B:159:ILE:HB	1:B:171:ALA:HB3	2.01	0.43
1:A:196:ARG:HD2	4:A:493:HOH:O	2.18	0.42
1:B:168:LEU:HB3	1:B:203:ILE:HD12	2.01	0.42
3:A:414:GOL:H11	4:A:487:HOH:O	2.19	0.42
1:A:41:HIS:NE2	3:A:414:GOL:O2	2.49	0.41
1:A:99:ILE:O	1:A:380:SER:HB3	2.20	0.41
1:A:168:LEU:HD23	1:A:168:LEU:C	2.42	0.41
1:A:5:ASN:ND2	1:A:286:THR:O	2.54	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	Percentile	es
1	А	400/413~(97%)	383~(96%)	14 (4%)	3 (1%)	19 13	
1	В	400/413~(97%)	382~(96%)	18 (4%)	0	100 100	)
All	All	800/826~(97%)	765 (96%)	32~(4%)	3~(0%)	34 30	

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	214	ASN
1	А	37	ASP
1	А	340	HIS

#### 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	А	328/343~(96%)	317~(97%)	11 (3%)	37 36		
1	В	326/343~(95%)	319~(98%)	7 (2%)	53 57		
All	All	654/686~(95%)	636~(97%)	18 (3%)	43 44		

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	133	ARG
1	А	139	TYR
1	А	140	SER

Continued on next page...



Mol	Chain	Res	Type
1	А	163	SER
1	А	165	ASP
1	А	184	ARG
1	А	203	ILE
1	А	211	LYS
1	А	223	ASP
1	А	291	PHE
1	А	310	TYR
1	В	118	GLU
1	В	133	ARG
1	В	139	TYR
1	В	175	ASP
1	В	180	ASP
1	В	223	ASP
1	В	310	TYR

Continued from previous page...

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	74	ASN
1	А	261	ASN
1	В	173	HIS
1	В	255	ASN
1	В	261	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)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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).

ſ	Mol	Type	Chain	Res	Link	B	ond leng	gths	B	ond ang	gles
	WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
	3	GOL	А	414	-	$5,\!5,\!5$	1.06	0	$5,\!5,\!5$	1.15	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	414	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms
3	А	414	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	414	GOL	2	0

### 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)

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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	А	401/413~(97%)	0.01	14 (3%) 44 43	25, 38, 74, 95	0
1	В	401/413~(97%)	0.08	18 (4%) 33 32	25, 39, 75, 97	0
All	All	802/826~(97%)	0.05	32 (3%) 38 37	25, 39, 75, 97	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	В	159	ILE	5.5	
1	В	112[A]	TRP	5.1	
1	В	141	GLY	4.2	
1	В	160	ILE	3.9	
1	В	214	ASN	3.8	
1	А	170	ILE	3.7	
1	В	172	ALA	3.7	
1	В	170	ILE	3.7	
1	В	158	LEU	3.6	
1	А	171	ALA	3.4	
1	А	145	ILE	3.4	
1	В	171	ALA	3.3	
1	А	213	ARG	3.1	
1	В	139	TYR	3.1	
1	В	366	THR	3.0	
1	А	158	LEU	3.0	
1	А	222	HIS	2.9	
1	В	403	ILE	2.8	
1	В	210	GLY	2.7	
1	В	148	PHE	2.6	
1	А	216	THR	2.6	
1	А	189	ALA	2.6	
1	А	219	ALA	2.5	
1	В	142	THR	2.5	

Continued on next page...



Mol	Chain	Res	Type	RSRZ	
1	А	112	TRP	2.5	
1	В	140	SER	2.5	
1	В	168	LEU	2.4	
1	А	160	ILE	2.4	
1	В	113	ASN	2.2	
1	А	113	ASN	2.2	
1	А	172	ALA	2.1	
1	А	168	LEU	2.1	

Continued from previous page...

#### 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 monosaccharides 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,  $95^{th}$  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	$B-factors(Å^2)$	Q < 0.9
3	GOL	А	414	6/6	0.89	0.15	34,37,39,45	0
2	MN	В	413	1/1	0.98	0.04	34,34,34,34	0
2	MN	В	412	1/1	0.99	0.05	27,27,27,27	0
2	MN	А	412	1/1	0.99	0.04	30,30,30,30	0
2	MN	А	413	1/1	0.99	0.08	34,34,34,34	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

