



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 11:13 AM GMT

PDB ID : 1YJX  
Title : Crystal structure of human B type phosphoglycerate mutase  
Authors : Wang, Y.; Wei, Z.; Liu, L.; Gong, W.  
Deposited on : 2005-01-16  
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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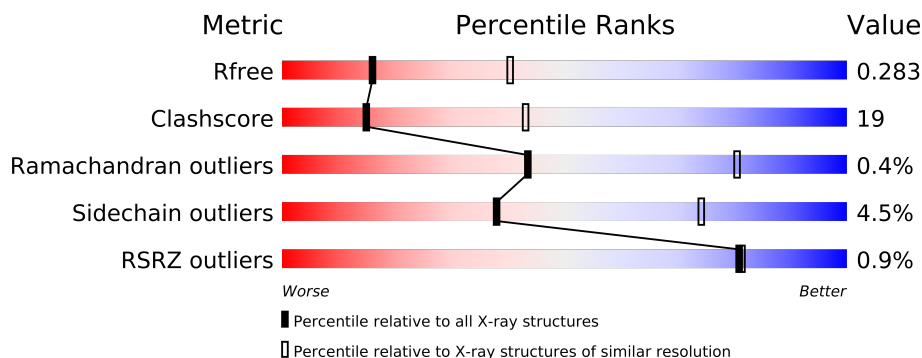
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	262	
1	B	262	
1	C	262	
1	D	262	
1	E	262	
1	F	262	
1	G	262	
1	H	262	
1	I	262	
1	J	262	
1	K	262	
1	L	262	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CIT	A	601	-	X
3	CIT	B	602	-	X
3	CIT	F	606	-	X
3	CIT	H	608	-	X
3	CIT	I	609	-	X
3	CIT	K	611	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23286 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Phosphoglycerate mutase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1913	1218	337	351	7			
1	B	242	Total	C	N	O	S	0	0	0
			1903	1211	335	350	7			
1	C	243	Total	C	N	O	S	0	0	0
			1898	1209	332	351	6			
1	D	245	Total	C	N	O	S	0	0	0
			1914	1218	336	353	7			
1	E	243	Total	C	N	O	S	0	0	0
			1897	1208	332	351	6			
1	F	242	Total	C	N	O	S	0	0	0
			1890	1204	332	347	7			
1	G	245	Total	C	N	O	S	0	0	0
			1887	1200	329	351	7			
1	H	241	Total	C	N	O	S	0	0	0
			1875	1196	328	345	6			
1	I	242	Total	C	N	O	S	0	0	0
			1904	1213	332	352	7			
1	J	244	Total	C	N	O	S	0	0	0
			1918	1220	339	352	7			
1	K	239	Total	C	N	O	S	0	0	0
			1870	1193	332	340	5			
1	L	245	Total	C	N	O	S	0	0	0
			1921	1222	342	350	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	LEU	-	EXPRESSION TAG	UNP P18669
A	256	GLU	-	EXPRESSION TAG	UNP P18669
A	257	HIS	-	EXPRESSION TAG	UNP P18669
A	258	HIS	-	EXPRESSION TAG	UNP P18669
A	259	HIS	-	EXPRESSION TAG	UNP P18669

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Chain	Residue	Modelled	Actual	Comment	Reference
A	260	HIS	-	EXPRESSION TAG	UNP P18669
A	261	HIS	-	EXPRESSION TAG	UNP P18669
A	262	HIS	-	EXPRESSION TAG	UNP P18669
B	255	LEU	-	EXPRESSION TAG	UNP P18669
B	256	GLU	-	EXPRESSION TAG	UNP P18669
B	257	HIS	-	EXPRESSION TAG	UNP P18669
B	258	HIS	-	EXPRESSION TAG	UNP P18669
B	259	HIS	-	EXPRESSION TAG	UNP P18669
B	260	HIS	-	EXPRESSION TAG	UNP P18669
B	261	HIS	-	EXPRESSION TAG	UNP P18669
B	262	HIS	-	EXPRESSION TAG	UNP P18669
C	255	LEU	-	EXPRESSION TAG	UNP P18669
C	256	GLU	-	EXPRESSION TAG	UNP P18669
C	257	HIS	-	EXPRESSION TAG	UNP P18669
C	258	HIS	-	EXPRESSION TAG	UNP P18669
C	259	HIS	-	EXPRESSION TAG	UNP P18669
C	260	HIS	-	EXPRESSION TAG	UNP P18669
C	261	HIS	-	EXPRESSION TAG	UNP P18669
C	262	HIS	-	EXPRESSION TAG	UNP P18669
D	255	LEU	-	EXPRESSION TAG	UNP P18669
D	256	GLU	-	EXPRESSION TAG	UNP P18669
D	257	HIS	-	EXPRESSION TAG	UNP P18669
D	258	HIS	-	EXPRESSION TAG	UNP P18669
D	259	HIS	-	EXPRESSION TAG	UNP P18669
D	260	HIS	-	EXPRESSION TAG	UNP P18669
D	261	HIS	-	EXPRESSION TAG	UNP P18669
D	262	HIS	-	EXPRESSION TAG	UNP P18669
E	255	LEU	-	EXPRESSION TAG	UNP P18669
E	256	GLU	-	EXPRESSION TAG	UNP P18669
E	257	HIS	-	EXPRESSION TAG	UNP P18669
E	258	HIS	-	EXPRESSION TAG	UNP P18669
E	259	HIS	-	EXPRESSION TAG	UNP P18669
E	260	HIS	-	EXPRESSION TAG	UNP P18669
E	261	HIS	-	EXPRESSION TAG	UNP P18669
E	262	HIS	-	EXPRESSION TAG	UNP P18669
F	255	LEU	-	EXPRESSION TAG	UNP P18669
F	256	GLU	-	EXPRESSION TAG	UNP P18669
F	257	HIS	-	EXPRESSION TAG	UNP P18669
F	258	HIS	-	EXPRESSION TAG	UNP P18669
F	259	HIS	-	EXPRESSION TAG	UNP P18669
F	260	HIS	-	EXPRESSION TAG	UNP P18669
F	261	HIS	-	EXPRESSION TAG	UNP P18669

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Chain	Residue	Modelled	Actual	Comment	Reference
F	262	HIS	-	EXPRESSION TAG	UNP P18669
G	255	LEU	-	EXPRESSION TAG	UNP P18669
G	256	GLU	-	EXPRESSION TAG	UNP P18669
G	257	HIS	-	EXPRESSION TAG	UNP P18669
G	258	HIS	-	EXPRESSION TAG	UNP P18669
G	259	HIS	-	EXPRESSION TAG	UNP P18669
G	260	HIS	-	EXPRESSION TAG	UNP P18669
G	261	HIS	-	EXPRESSION TAG	UNP P18669
G	262	HIS	-	EXPRESSION TAG	UNP P18669
H	255	LEU	-	EXPRESSION TAG	UNP P18669
H	256	GLU	-	EXPRESSION TAG	UNP P18669
H	257	HIS	-	EXPRESSION TAG	UNP P18669
H	258	HIS	-	EXPRESSION TAG	UNP P18669
H	259	HIS	-	EXPRESSION TAG	UNP P18669
H	260	HIS	-	EXPRESSION TAG	UNP P18669
H	261	HIS	-	EXPRESSION TAG	UNP P18669
H	262	HIS	-	EXPRESSION TAG	UNP P18669
I	255	LEU	-	EXPRESSION TAG	UNP P18669
I	256	GLU	-	EXPRESSION TAG	UNP P18669
I	257	HIS	-	EXPRESSION TAG	UNP P18669
I	258	HIS	-	EXPRESSION TAG	UNP P18669
I	259	HIS	-	EXPRESSION TAG	UNP P18669
I	260	HIS	-	EXPRESSION TAG	UNP P18669
I	261	HIS	-	EXPRESSION TAG	UNP P18669
I	262	HIS	-	EXPRESSION TAG	UNP P18669
J	255	LEU	-	EXPRESSION TAG	UNP P18669
J	256	GLU	-	EXPRESSION TAG	UNP P18669
J	257	HIS	-	EXPRESSION TAG	UNP P18669
J	258	HIS	-	EXPRESSION TAG	UNP P18669
J	259	HIS	-	EXPRESSION TAG	UNP P18669
J	260	HIS	-	EXPRESSION TAG	UNP P18669
J	261	HIS	-	EXPRESSION TAG	UNP P18669
J	262	HIS	-	EXPRESSION TAG	UNP P18669
K	255	LEU	-	EXPRESSION TAG	UNP P18669
K	256	GLU	-	EXPRESSION TAG	UNP P18669
K	257	HIS	-	EXPRESSION TAG	UNP P18669
K	258	HIS	-	EXPRESSION TAG	UNP P18669
K	259	HIS	-	EXPRESSION TAG	UNP P18669
K	260	HIS	-	EXPRESSION TAG	UNP P18669
K	261	HIS	-	EXPRESSION TAG	UNP P18669
K	262	HIS	-	EXPRESSION TAG	UNP P18669
L	255	LEU	-	EXPRESSION TAG	UNP P18669

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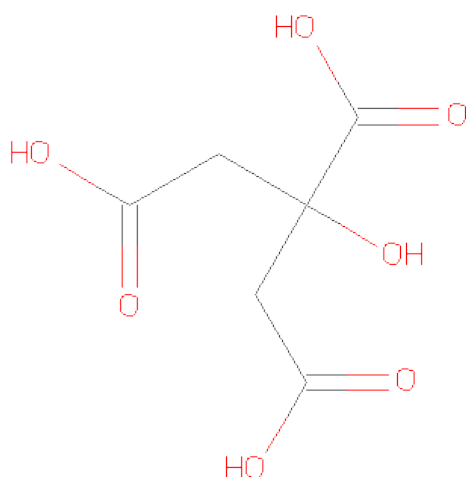
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Chain	Residue	Modelled	Actual	Comment	Reference
L	256	GLU	-	EXPRESSION TAG	UNP P18669
L	257	HIS	-	EXPRESSION TAG	UNP P18669
L	258	HIS	-	EXPRESSION TAG	UNP P18669
L	259	HIS	-	EXPRESSION TAG	UNP P18669
L	260	HIS	-	EXPRESSION TAG	UNP P18669
L	261	HIS	-	EXPRESSION TAG	UNP P18669
L	262	HIS	-	EXPRESSION TAG	UNP P18669

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total Cl 1 1	0	0
2	K	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	0	0
3	E	1	Total C O 13 6 7	0	0
3	F	1	Total C O 13 6 7	0	0
3	G	1	Total C O 13 6 7	0	0
3	H	1	Total C O 13 6 7	0	0
3	I	1	Total C O 13 6 7	0	0
3	J	1	Total C O 13 6 7	0	0
3	K	1	Total C O 13 6 7	0	0
3	L	1	Total C O 13 6 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	43	Total O 43 43	0	0
4	B	45	Total O 45 45	0	0
4	C	21	Total O 21 21	0	0
4	D	33	Total O 33 33	0	0
4	E	17	Total O 17 17	0	0
4	F	27	Total O 27 27	0	0
4	G	12	Total O 12 12	0	0
4	H	18	Total O 18 18	0	0

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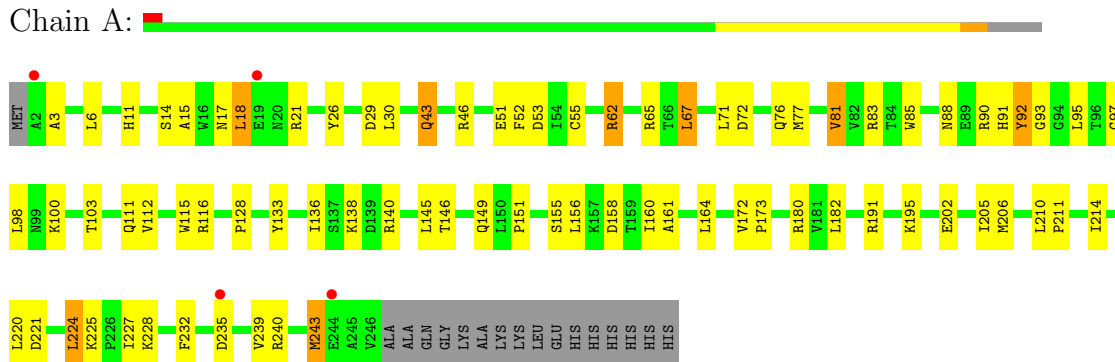
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	19	Total 19	O 19	0	0
4	J	15	Total 15	O 15	0	0
4	K	35	Total 35	O 35	0	0
4	L	49	Total 49	O 49	0	0

### 3 Residue-property plots

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

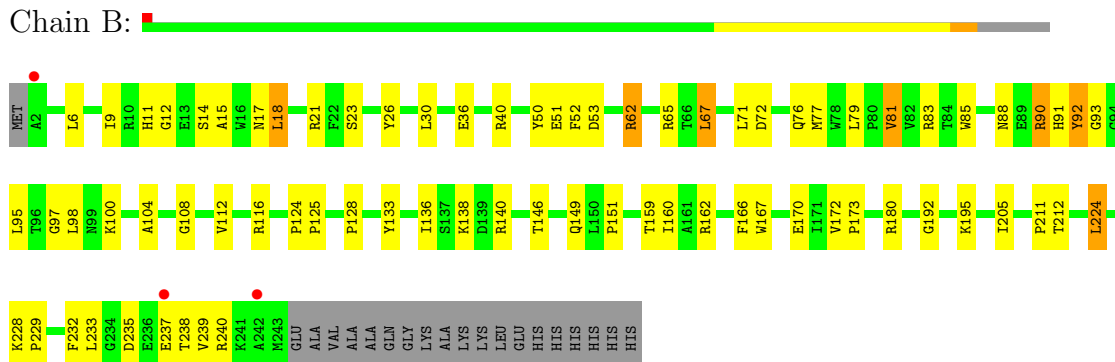
#### • Molecule 1: Phosphoglycerate mutase 1

Chain A:



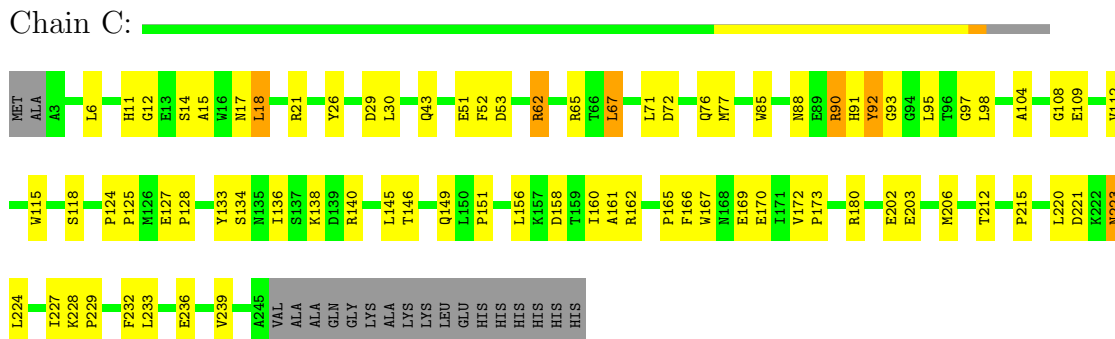
#### • Molecule 1: Phosphoglycerate mutase 1

Chain B:



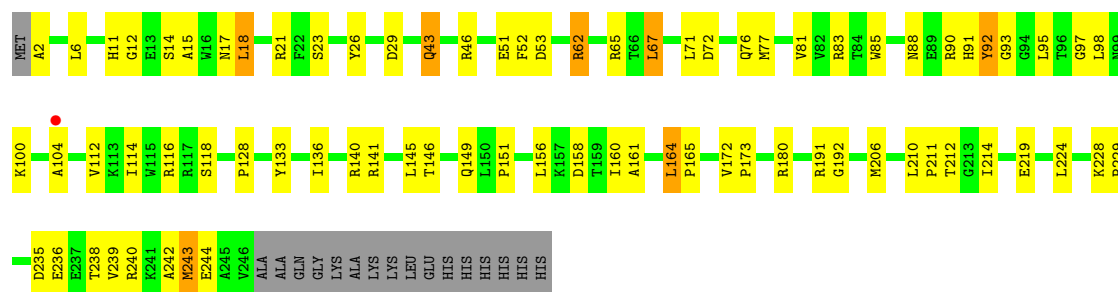
#### • Molecule 1: Phosphoglycerate mutase 1

Chain C:



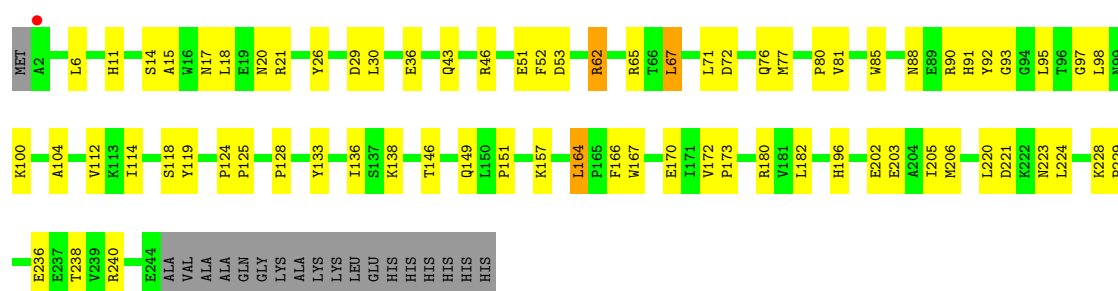
#### • Molecule 1: Phosphoglycerate mutase 1

## Chain D:



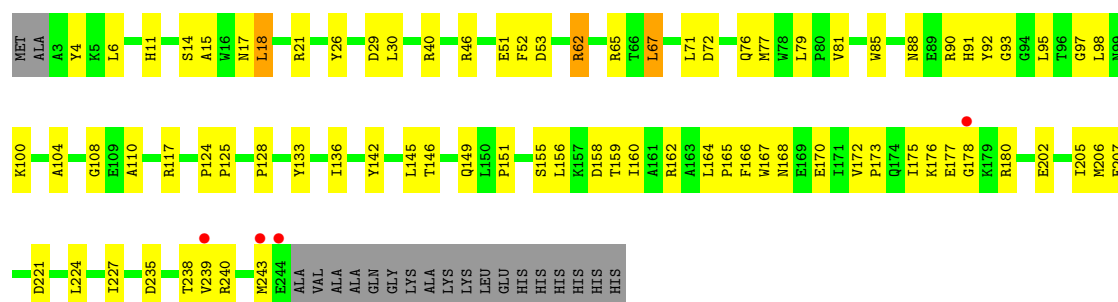
- Molecule 1: Phosphoglycerate mutase 1

## Chain E:



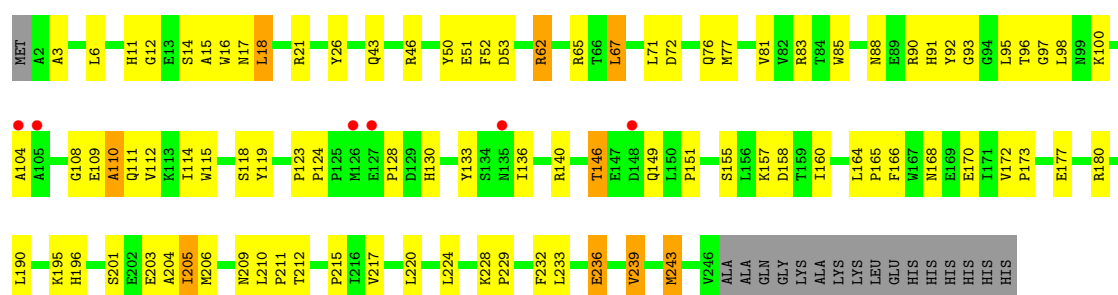
- Molecule 1: Phosphoglycerate mutase 1

## Chain F:



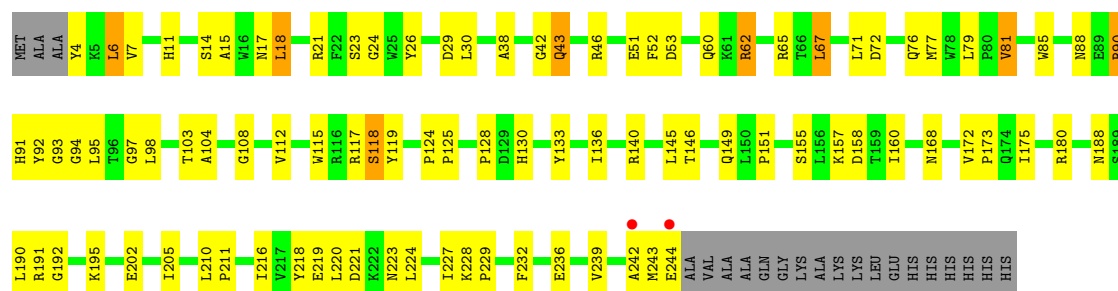
- Molecule 1: Phosphoglycerate mutase 1

## Chain G:



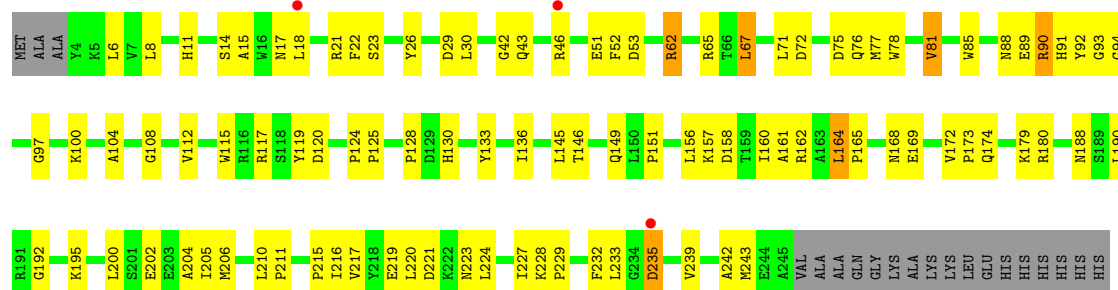
- Molecule 1: Phosphoglycerate mutase 1

## Chain H:



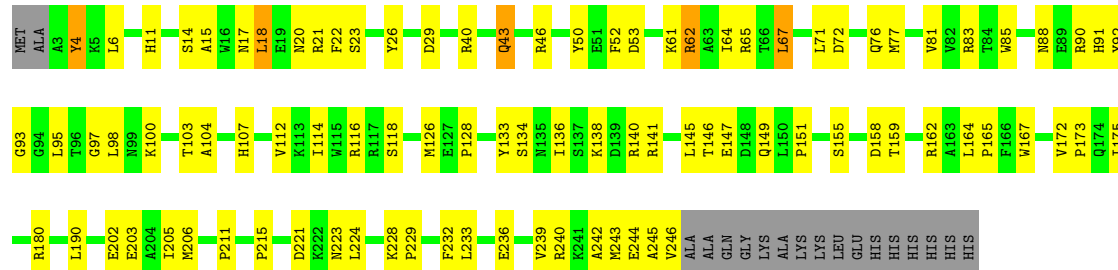
• Molecule 1: Phosphoglycerate mutase 1

Chain I:



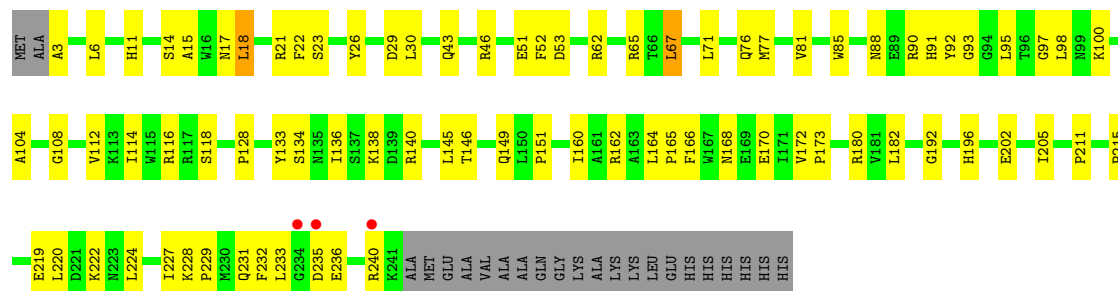
• Molecule 1: Phosphoglycerate mutase 1

Chain J:



• Molecule 1: Phosphoglycerate mutase 1

Chain K:



• Molecule 1: Phosphoglycerate mutase 1

Chain L:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.53Å 75.93Å 186.98Å 90.00° 94.42° 90.00°	Depositor
Resolution (Å)	29.91 – 2.80 29.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.91-2.80) 93.9 (29.91-2.80)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.233 , 0.272 0.249 , 0.283	Depositor DCC
$R_{free}$ test set	8542 reflections (10.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 8.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 84989 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23286	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.38	0/1962	0.60	0/2671
1	B	0.38	0/1952	0.62	0/2655
1	C	0.36	0/1947	0.61	0/2652
1	D	0.37	0/1963	0.61	0/2673
1	E	0.37	0/1946	0.60	0/2650
1	F	0.36	0/1939	0.61	0/2641
1	G	0.36	0/1936	0.60	0/2641
1	H	0.37	0/1924	0.61	0/2621
1	I	0.37	0/1953	0.61	0/2657
1	J	0.37	0/1967	0.62	0/2676
1	K	0.37	0/1919	0.61	0/2612
1	L	0.38	0/1970	0.62	0/2679
All	All	0.37	0/23378	0.61	0/31828

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1913	0	1848	68	0
1	B	1903	0	1845	64	0
1	C	1898	0	1827	63	0
1	D	1914	0	1843	66	0
1	E	1897	0	1822	62	0
1	F	1890	0	1819	77	0
1	G	1887	0	1786	83	0
1	H	1875	0	1800	84	0
1	I	1904	0	1844	96	0
1	J	1918	0	1858	83	0
1	K	1870	0	1806	72	0
1	L	1921	0	1865	73	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
3	A	13	0	5	1	0
3	B	13	0	5	2	0
3	C	13	0	5	1	0
3	D	13	0	5	2	0
3	E	13	0	5	0	0
3	F	13	0	5	1	0
3	G	13	0	5	1	0
3	H	13	0	5	2	0
3	I	13	0	5	1	0
3	J	13	0	5	2	0
3	K	13	0	5	3	0
3	L	13	0	5	3	0
4	A	43	0	0	2	0
4	B	45	0	0	1	0
4	C	21	0	0	1	0
4	D	33	0	0	3	0
4	E	17	0	0	3	0
4	F	27	0	0	5	0
4	G	12	0	0	1	0
4	H	18	0	0	2	0
4	I	19	0	0	2	0
4	J	15	0	0	1	0
4	K	35	0	0	8	0
4	L	49	0	0	3	0
All	All	23286	0	22023	861	0



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

The worst 5 of 861 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:195:LYS:HB2	1:A:205:ILE:HD12	1.22	1.11
1:H:195:LYS:HB2	1:H:205:ILE:HD12	1.34	1.09
1:A:91:HIS:HD2	1:A:93:GLY:H	1.12	0.98
1:F:206:MET:HE2	1:F:206:MET:HA	1.45	0.96
1:I:43:GLN:HE21	1:I:46:ARG:HH22	1.10	0.96

There are no symmetry-related clashes.

## 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	243/262 (93%)	223 (92%)	19 (8%)	1 (0%)	43	80
1	B	240/262 (92%)	220 (92%)	20 (8%)	0	100	100
1	C	241/262 (92%)	221 (92%)	20 (8%)	0	100	100
1	D	243/262 (93%)	226 (93%)	15 (6%)	2 (1%)	27	65
1	E	241/262 (92%)	224 (93%)	17 (7%)	0	100	100
1	F	240/262 (92%)	221 (92%)	19 (8%)	0	100	100
1	G	243/262 (93%)	221 (91%)	18 (7%)	4 (2%)	14	44
1	H	239/262 (91%)	221 (92%)	16 (7%)	2 (1%)	27	65
1	I	240/262 (92%)	222 (92%)	17 (7%)	1 (0%)	43	80
1	J	242/262 (92%)	227 (94%)	15 (6%)	0	100	100
1	K	237/262 (90%)	225 (95%)	10 (4%)	2 (1%)	27	65
1	L	243/262 (93%)	224 (92%)	18 (7%)	1 (0%)	43	80
All	All	2892/3144 (92%)	2675 (92%)	204 (7%)	13 (0%)	43	80

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	235	ASP
1	D	243	MET
1	G	110	ALA
1	G	146	THR
1	K	235	ASP

### 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	194/220 (88%)	185 (95%)	9 (5%)	37	73
1	B	195/220 (89%)	187 (96%)	8 (4%)	41	77
1	C	193/220 (88%)	184 (95%)	9 (5%)	36	73
1	D	194/220 (88%)	185 (95%)	9 (5%)	37	73
1	E	192/220 (87%)	185 (96%)	7 (4%)	47	82
1	F	192/220 (87%)	183 (95%)	9 (5%)	36	73
1	G	188/220 (86%)	178 (95%)	10 (5%)	32	67
1	H	190/220 (86%)	181 (95%)	9 (5%)	36	73
1	I	196/220 (89%)	188 (96%)	8 (4%)	41	77
1	J	196/220 (89%)	186 (95%)	10 (5%)	33	69
1	K	189/220 (86%)	183 (97%)	6 (3%)	51	85
1	L	195/220 (89%)	186 (95%)	9 (5%)	37	73
All	All	2314/2640 (88%)	2211 (96%)	103 (4%)	38	74

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	81	VAL
1	G	92	TYR
1	L	18	LEU
1	F	90	ARG
1	G	18	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	188	ASN
1	H	17	ASN
1	L	17	ASN
1	G	17	ASN
1	G	43	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	CIT	A	601	-	12,12,12	2.26	3 (25%)	17,17,17	3.20	5 (29%)
3	CIT	B	602	-	12,12,12	1.98	3 (25%)	17,17,17	3.28	10 (58%)
3	CIT	C	603	-	12,12,12	2.00	4 (33%)	17,17,17	3.36	9 (52%)
3	CIT	D	604	-	12,12,12	2.32	4 (33%)	17,17,17	2.70	8 (47%)
3	CIT	E	605	-	12,12,12	2.36	4 (33%)	17,17,17	3.03	7 (41%)
3	CIT	F	606	-	12,12,12	1.87	3 (25%)	17,17,17	3.26	7 (41%)
3	CIT	G	607	-	12,12,12	2.45	4 (33%)	17,17,17	3.10	6 (35%)
3	CIT	H	608	-	12,12,12	2.13	3 (25%)	17,17,17	3.11	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CIT	I	609	-	12,12,12	2.01	2 (16%)	17,17,17	3.28	8 (47%)
3	CIT	J	610	-	12,12,12	2.33	3 (25%)	17,17,17	2.83	6 (35%)
3	CIT	K	611	-	12,12,12	2.02	3 (25%)	17,17,17	3.26	9 (52%)
3	CIT	L	612	-	12,12,12	2.37	3 (25%)	17,17,17	3.07	6 (35%)

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	CIT	A	601	-	-	0/16/16/16	0/0/0/0
3	CIT	B	602	-	-	0/16/16/16	0/0/0/0
3	CIT	C	603	-	-	0/16/16/16	0/0/0/0
3	CIT	D	604	-	-	0/16/16/16	0/0/0/0
3	CIT	E	605	-	-	0/16/16/16	0/0/0/0
3	CIT	F	606	-	-	0/16/16/16	0/0/0/0
3	CIT	G	607	-	-	0/16/16/16	0/0/0/0
3	CIT	H	608	-	-	0/16/16/16	0/0/0/0
3	CIT	I	609	-	-	0/16/16/16	0/0/0/0
3	CIT	J	610	-	-	0/16/16/16	0/0/0/0
3	CIT	K	611	-	-	0/16/16/16	0/0/0/0
3	CIT	L	612	-	-	0/16/16/16	0/0/0/0

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	612	CIT	C3-C6	5.94	1.59	1.53
3	G	607	CIT	C3-C6	5.77	1.59	1.53
3	H	608	CIT	C3-C6	5.59	1.59	1.53
3	J	610	CIT	C3-C6	5.53	1.59	1.53
3	D	604	CIT	C3-C6	5.48	1.59	1.53

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	CIT	O7-C3-C6	-7.05	98.79	108.95
3	K	611	CIT	O6-C6-C3	-6.84	102.95	112.89
3	F	606	CIT	O6-C6-C3	-6.83	102.96	112.89
3	C	603	CIT	O6-C6-C3	-6.82	102.98	112.89
3	I	609	CIT	O6-C6-C3	-6.71	103.14	112.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	245/262 (93%)	-0.32	4 (1%) 68 69	19, 33, 55, 81	0
1	B	242/262 (92%)	-0.27	3 (1%) 75 76	18, 33, 49, 78	0
1	C	243/262 (92%)	-0.21	0 100 100	18, 34, 51, 84	0
1	D	245/262 (93%)	-0.24	1 (0%) 90 91	18, 36, 54, 74	0
1	E	243/262 (92%)	-0.10	1 (0%) 90 91	21, 36, 56, 88	0
1	F	242/262 (92%)	-0.19	4 (1%) 67 68	20, 36, 56, 95	0
1	G	245/262 (93%)	-0.07	6 (2%) 56 57	21, 38, 61, 85	0
1	H	241/262 (91%)	-0.15	2 (0%) 83 83	21, 37, 53, 90	0
1	I	242/262 (92%)	-0.06	3 (1%) 75 76	20, 37, 60, 91	0
1	J	244/262 (93%)	-0.18	0 100 100	20, 38, 58, 91	0
1	K	239/262 (91%)	-0.21	3 (1%) 74 75	19, 35, 49, 102	0
1	L	245/262 (93%)	-0.15	0 100 100	18, 32, 52, 82	0
All	All	2916/3144 (92%)	-0.18	27 (0%) 81 81	18, 35, 57, 102	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	234	GLY	4.9
1	K	235	ASP	4.2
1	G	104	ALA	3.7
1	E	2	ALA	3.1
1	B	2	ALA	3.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CIT	F	606	13/13	0.35	5.03	73,76,81,82	0
3	CIT	H	608	13/13	0.37	4.65	72,74,81,81	0
3	CIT	B	602	13/13	0.31	2.71	69,70,73,74	0
3	CIT	K	611	13/13	0.34	2.33	61,62,63,64	0
3	CIT	I	609	13/13	0.26	2.19	55,56,58,58	0
3	CIT	A	601	13/13	0.25	2.02	48,50,55,58	0
3	CIT	E	605	13/13	0.28	1.70	69,71,72,72	0
3	CIT	D	604	13/13	0.27	1.68	65,67,70,71	0
3	CIT	G	607	13/13	0.30	1.31	72,74,77,77	0
3	CIT	C	603	13/13	0.24	1.30	55,57,59,59	0
3	CIT	J	610	13/13	0.27	1.12	64,65,69,71	0
3	CIT	L	612	13/13	0.22	0.11	49,52,55,56	0
2	CL	K	263	1/1	0.12	-1.20	21,21,21,21	0
2	CL	C	263	1/1	0.15	-1.27	23,23,23,23	0
2	CL	F	263	1/1	0.13	-2.07	31,31,31,31	0
2	CL	J	263	1/1	0.07	-2.57	32,32,32,32	0
2	CL	H	263	1/1	0.09	-2.98	25,25,25,25	0
2	CL	A	263	1/1	0.08	-4.83	22,22,22,22	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.