



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 04:49 am GMT

PDB ID : 2G9V  
Title : The crystal structure of glycogen phosphorylase in complex with (3R,4R,5R)-5-hydroxymethylpiperidine-3,4-diol and phosphate  
Authors : Oikonomakos, N.G.; Tiraidis, C.; Leonidas, D.D.; Zographos, S.E.  
Deposited on : 2006-03-07  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

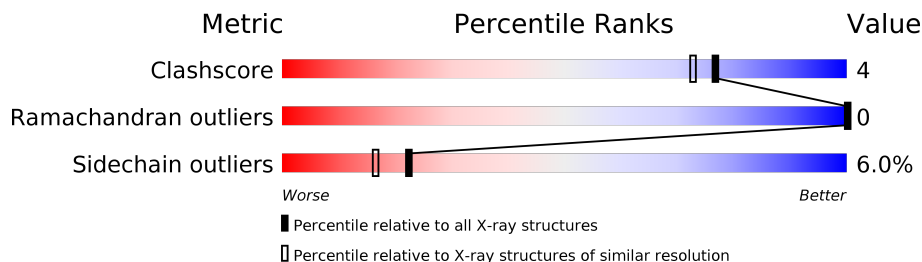
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6823 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 Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	807	Total	C	N	O	P	S	0	0	0
			6579	4196	1156	1197	1	29			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	680	LLP	LYS	MODIFIED RESIDUE	UNP P00489

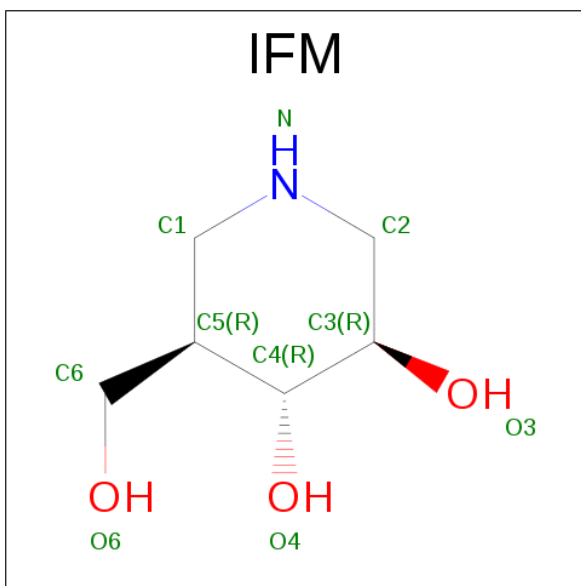
- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (three-letter code:

IFM) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	224	Total	O	0	0
			224	224		



Note EDS was not executed.

- Chain A:  85% 10%

Row	Block 1	Block 2	Block 3	Block 4	Block 5	Block 6	Block 7	Block 8	Block 9	Block 10	Block 11	Block 12	Block 13	Block 14	Block 15
1	SER	ARG	PRO	LEU	LEU	ASP	ASP	GLN	GLY	ARG	LYS	LYS	GLN	THR	THR
2	L254	LYS	ASP	PHE	ASN	ASN	VAL	GLY	GLY	L271	N282	ASP	ASN	F285	R292
3	L444	S449	H450	V455	H459	K478	V493	I512	L522	F545	A546	L549	I557	N558	P569
4	E716	L721	Y726	E730	Y731	Y732	D733	R734	R739	E743	L765	F774	L790	R803	R831
5	L562	L566	K568	R569	K574	R575	N579	L586	K596	R601	Y613	L622	L645	V656	L662
6	R833	A836	PRO	ASP	GLU	LYS	ILE	PRO	D327	A328	F329	P330	D355	K363	V367
7	R334	L334	LYS	PHE	GLY	CYS	ARG	ASP	PRO	VAL	ARG	T324	N325	F326	D327
8	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155	K191	L198
9	T398	T398	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155
10	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155	K191	L198
11	T398	T398	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155
12	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155	K191	L198
13	T398	T398	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155
14	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155	K191	L198
15	T398	T398	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155
16	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155	K191	L198
17	T398	T398	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155
18	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155	K191	L198
19	T398	T398	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155
20	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155	K191	L198
21	T398	T398	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155
22	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155	K191	L198
23	T398	T398	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155
24	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155	K191	L198
25	T398	T398	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y155
26	R43	D61	R81	L85	Y90	R93	L104	A111	L115	L122	E126	R138	Y15		

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.64Å 128.64Å 116.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.91 – 2.15	Depositor
% Data completeness (in resolution range)	95.8 (90.91-2.15)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.193 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IFM, PO4, LLP

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	0.40	0/6700	0.56	0/9065

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	6579	0	6520	46	0
2	A	10	0	0	1	0
3	A	10	0	13	0	0
4	A	224	0	0	4	0
All	All	6823	0	6533	46	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 4.

The worst 5 of 46 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:93:ARG:NH2	1:A:126:GLU:O	2.18	0.77
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.68	0.75
1:A:367:VAL:O	1:A:371:THR:HG23	1.87	0.75
1:A:138:ARG:HD3	1:A:138:ARG:O	1.92	0.70
1:A:455:VAL:H	1:A:459:HIS:HD2	1.39	0.68

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	798/842 (95%)	771 (97%)	27 (3%)	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	697/730 (96%)	655 (94%)	42 (6%)	22	16

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	THR
1	A	522	LEU

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Mol	Chain	Res	Type
1	A	765	LEU
1	A	384	LEU
1	A	400	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	481	ASN
1	A	484	ASN
1	A	727	ASN
1	A	459	HIS
1	A	678	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	LLP	A	680	1	24,24,25	1.67	4 (16%)	28,32,34	1.30	3 (10%)

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
1	LLP	A	680	1	-	0/15/17/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	O3-C3	-5.46	1.24	1.37
1	A	680	LLP	C4'-NZ	2.27	1.34	1.27
1	A	680	LLP	CA-C	2.56	1.53	1.50
1	A	680	LLP	C4-C4'	2.91	1.51	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	CE-NZ-C4'	-3.21	109.72	119.03
1	A	680	LLP	C5-C6-N1	-2.52	119.61	123.87
1	A	680	LLP	C4-C4'-NZ	-2.33	113.34	124.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	680	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PO4	A	996	-	4,4,4	0.69	0	6,6,6	0.52	0
2	PO4	A	997	-	4,4,4	1.02	0	6,6,6	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	IFM	A	998	-	9,10,10	1.65	2 (22%)	9,13,13	0.67	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
2	PO4	A	996	-	-	0/0/0/0	0/0/0/0
2	PO4	A	997	-	-	0/0/0/0	0/0/0/0
3	IFM	A	998	-	-	0/2/16/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	998	IFM	C1-N	2.10	1.50	1.46
3	A	998	IFM	C2-C3	3.06	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	997	PO4	1	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](#)

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.