



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:12 pm GMT

PDB ID : 1A3X  
Title : PYRUVATE KINASE FROM SACCHAROMYCES CEREVISIAE COM-  
PLEXED WITH PG, MN<sup>2+</sup> AND K<sup>+</sup>  
Authors : Jurica, M.S.; Mesecar, A.; Heath, P.J.; Shi, W.; Nowak, T.; Stoddard, B.L.  
Deposited on : 1998-01-26  
Resolution : 3.00 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

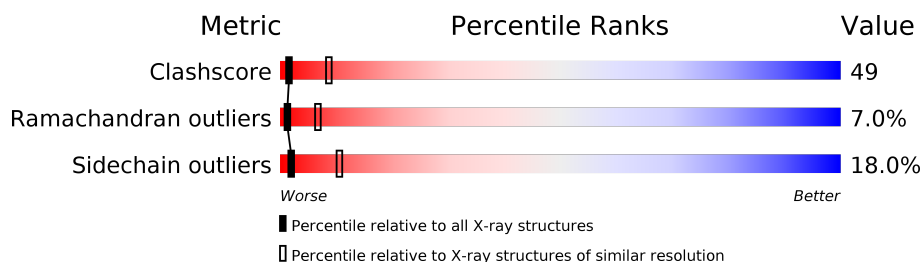
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)

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 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	500	
1	B	500	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGA	A	1005	-	-	X	-

## 2 Entry composition [i](#)

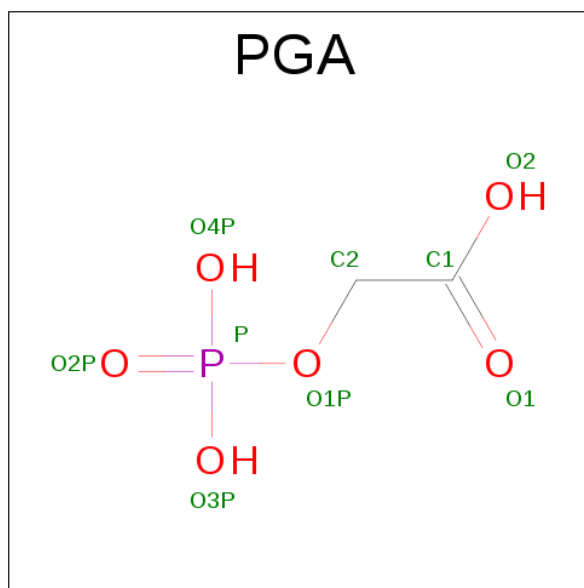
There are 4 unique types of molecules in this entry. The entry contains 7472 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PYRUVATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3725	2347	642	718	18			
1	B	487	Total	C	N	O	S	0	0	0
			3725	2347	642	718	18			

- Molecule 2 is SUGAR (2-PHOSPHOGLYCOLIC ACID) (three-letter code: PGA) (formula:  $C_2H_5O_6P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	2	6	1		
2	B	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mn 1	0	0
3	A	1	Total 1	Mn 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	K 1	0	0
4	A	1	Total 1	K 1	0	0



PHE	L422	M348	L273	E197	V136
LYS	V423	A349	P272	D198	I137
ALA	T425	E350	P273	L199	S138
GLY	R425	Q357	P274	R200	A139
ALA	C426	A358	E275	F201	G140
GLY	P427	I359			R141
HIS	R428	A360	V279	H208	I142
SER	A429	Y361	Q280	M209	I143
N493	A430	K281	K282	V210	Y144
T494	R431	L362	L283	F211	V145
L495	F432	P363	L284	A212	D146
Q496	S433	D366	L289	S213	D147
H434	H434			F214	G148
V497	L435			I215	V149
S498	T436	R369	K292	R216	L150
T499	R437	N370	P293	S151	S151
V500	G438	T372	V294	D220	F152
	V439	C371	P294	V221	I153
	F440	P373	L295	L222	V154
	P441	K374	C296	T223	L155
		P375	A297	I224	E156
	F444	T376	T298	E226	V157
	E445	S377	Q299	R225	V158
	K446	T378	N300	V227	D159
	E447		L301	L228	D160
PRO		V382	E302		K161
VAL		S303	S303	Q231	T162
SER		A386	K304	G232	L163
ASP		V387	T305		K164
TRP		A388		V235	V165
T453	T453	A389	P308		K166
D454	D454	V390	R309	V239	A167
V456	V456	F391	P310	K240	L168
E457	E457		T311	I241	N169
A458	A458	A395	E314	E242	A170
R459	R459	K396	V315	N243	G171
I460	I460	I398	S316	Q244	K172
R461	R461	I399	D317	Q245	I173
F462	F462	V400	V318	G246	C174
G463	G463	L401	L323	V247	S175
I464	I464	S402	D324	N248	H176
E465	E465	T403		N249	K177
K466	K466	S404			G178
A467	A467		D327	L254	V179
F468	F468	T407	C328	K255	N180
E469	E469	P408	V329	V256	L181
		R409	R409	T257	P182
		L410	L330	D258	G183
L473	L473	V411	L331	G259	T184
K474	K474	S412	A336	V260	D185
K475	K475	R413	K337	M261	V186
G476	G476	Y414	G338	V262	D187
D477	D477	R415		A263	L188
T478	T478	P416	I342	R264	P189
V479	V479	N417	N343	G265	A190
V480	V480	C418	K344	D266	L191
S481	S481	P419	V345	L267	
T482	T482	I420	T346	G268	K194
Q483	Q483	I421	T347	I269	D195
G484	G484			E270	K196

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.30Å 106.40Å 105.50Å 90.00° 110.80° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00	Depositor
% Data completeness (in resolution range)	85.0 (100.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.227 , 0.341	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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: K, MN, PGA

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	0.59	2/3781 (0.1%)	0.88	4/5124 (0.1%)
1	B	0.41	0/3781	1.03	7/5124 (0.1%)
All	All	0.51	2/7562 (0.0%)	0.96	11/10248 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	LYS	C-N	-26.09	0.84	1.34
1	A	375	PRO	C-N	5.31	1.46	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	375	PRO	O-C-N	-31.91	71.64	122.70
1	B	375	PRO	CA-C-N	-31.09	48.81	117.20
1	A	375	PRO	O-C-N	-25.38	82.10	122.70
1	A	375	PRO	CA-C-N	-24.09	64.20	117.20
1	B	374	LYS	O-C-N	-21.78	79.71	121.10

There are no chirality outliers.



All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	LYS	Peptide
1	A	375	PRO	Mainchain
1	B	374	LYS	Mainchain,Peptide

## 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	3725	0	3804	369	1
1	B	3725	0	3804	375	1
2	A	9	0	2	5	0
2	B	9	0	2	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	7472	0	7612	744	1

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 49.

The worst 5 of 744 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:374:LYS:HG2	1:A:375:PRO:HD3	1.25	1.11
1:B:186:VAL:HG23	1:B:216:ARG:HE	1.19	1.06
1:A:272:PRO:HB2	1:A:275:GLU:HG3	1.28	1.06
1:B:272:PRO:HB2	1:B:275:GLU:HG3	1.37	1.05
1:A:390:VAL:HB	1:A:395:ALA:HB3	1.37	1.02

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:NH2	1:B:268:GLY:O[1_545]	2.06	0.14

## 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	481/500 (96%)	382 (79%)	65 (14%)	34 (7%)	1	6
1	B	481/500 (96%)	377 (78%)	71 (15%)	33 (7%)	1	7
All	All	962/1000 (96%)	759 (79%)	136 (14%)	67 (7%)	1	7

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	12	VAL
1	A	96	THR
1	A	99	VAL
1	A	106	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	412/423 (97%)	337 (82%)	75 (18%)	2	10
1	B	412/423 (97%)	339 (82%)	73 (18%)	2	11
All	All	824/846 (97%)	676 (82%)	148 (18%)	2	10

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	417	ASN
1	B	33	ASN
1	B	410	LEU
1	A	432	PHE
1	B	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	493	ASN
1	B	66	ASN
1	B	483	GLN
1	B	33	ASN
1	B	106	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
2	PGA	A	1005	1,3,4	5,8,8	2.35	2 (40%)	6,11,11	3.19	2 (33%)
2	PGA	B	1006	3,4	5,8,8	2.17	2 (40%)	6,11,11	3.23	2 (33%)

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	PGA	A	1005	1,3,4	-	0/4/6/6	0/0/0/0
2	PGA	B	1006	3,4	-	0/4/6/6	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	PGA	O1P-C2	-2.08	1.36	1.44
2	B	1006	PGA	P-O2P	2.06	1.57	1.50
2	B	1006	PGA	P-O3P	3.73	1.70	1.54
2	A	1005	PGA	P-O3P	3.84	1.70	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1006	PGA	O3P-P-O1P	2.35	112.97	106.73
2	A	1005	PGA	O3P-P-O1P	2.88	114.39	106.73
2	A	1005	PGA	O1P-P-O2P	6.63	125.08	106.47
2	B	1006	PGA	O1P-P-O2P	6.95	125.98	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1005	PGA	5	0
2	B	1006	PGA	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.