



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 03:49 pm BST

PDB ID : 1A3X
Title : PYRUVATE KINASE FROM SACCHAROMYCES CEREVISIAE COM-
PLEXED WITH PG, MN²⁺ AND K⁺
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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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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) : 2.11

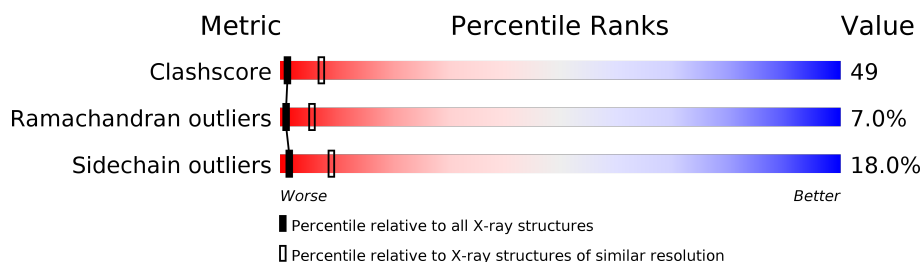
1 Overall quality at a glance

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 ≥ 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 $\leq 5\%$.

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](#)

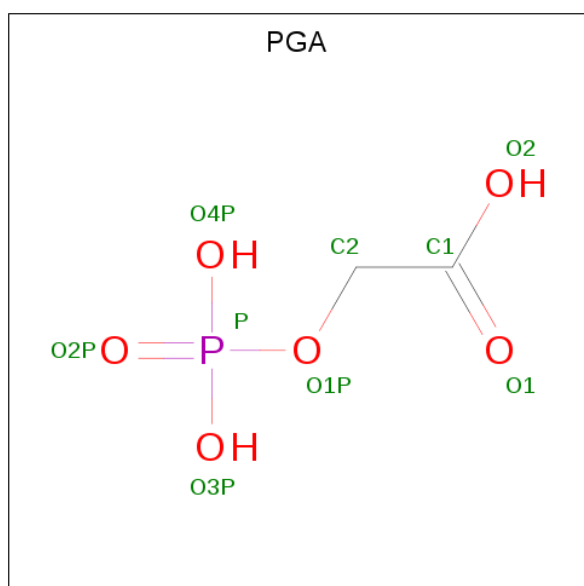
There are 4 unique types of molecules in this entry. The entry contains 7472 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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).

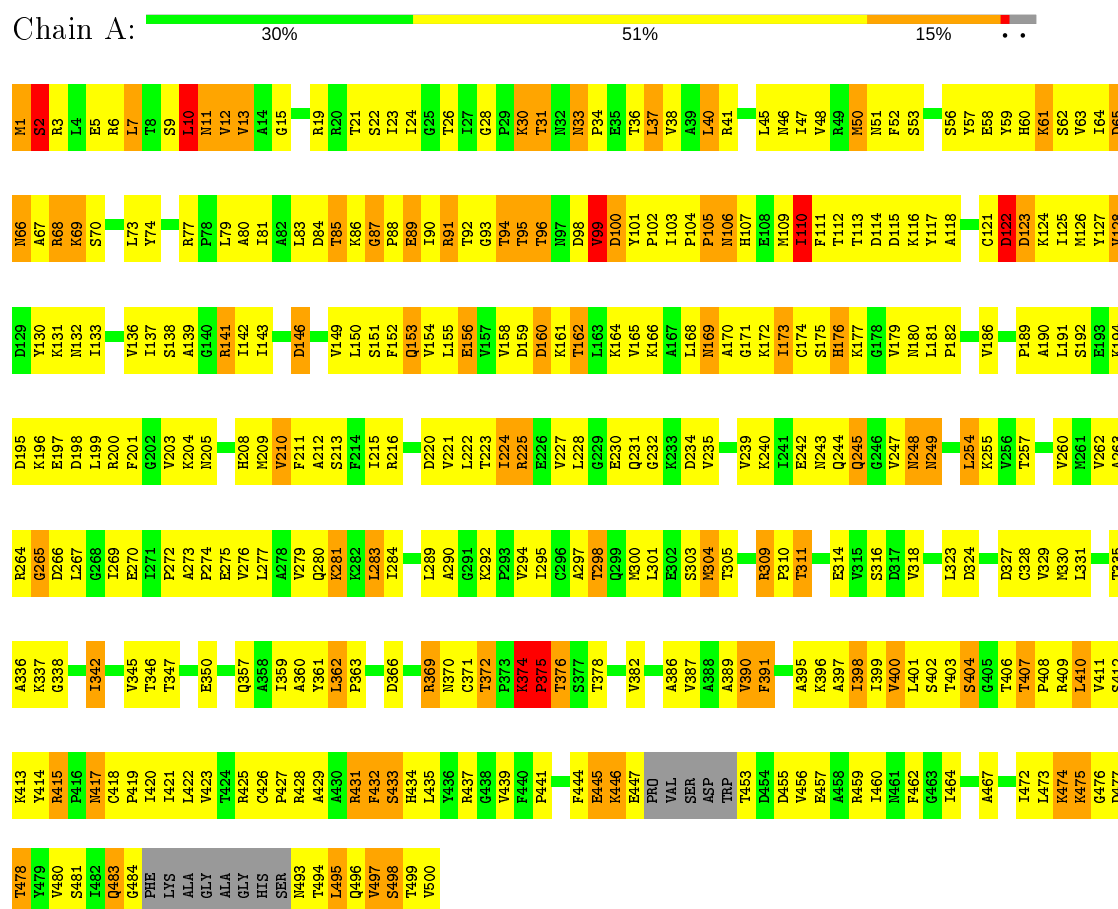
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	K 1	0	0
4	A	1	Total 1	K 1	0	0

3 Residue-property plots

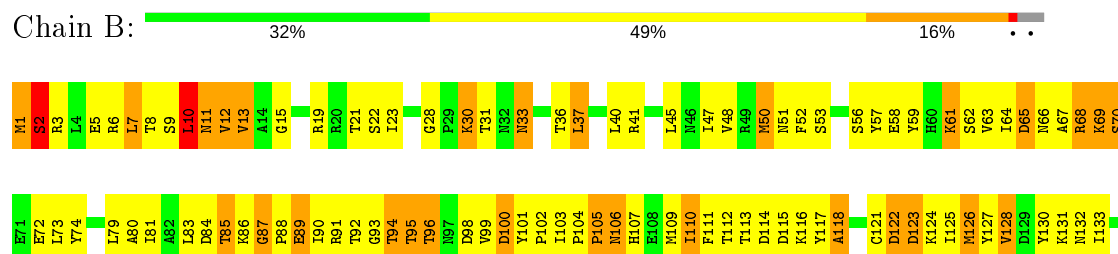
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



• Molecule 1: PYRUVATE KINASE



PHE	L422	M348	I271	E197	V136
LYS	V423	A349	P272	D198	I137
ALA	T424	E350	A273	L199	S138
GLY	R425	Q357	P274	R200	A139
ALA	C426	A358	E275	F201	G140
GLY	P427	I359	V279	H208	R141
HIS	R428	A360	Q280	M209	I142
SER	A429	Y361	R281	V210	I143
M493	A430	L362	K282	F211	Y144
T494	R431	P363	L283	A212	V145
L495	L432	P363	L283	S213	D146
Q496	S433	D366	I284	P214	D147
V497	H434	R369	L289	G148	G148
S498	L435	N370	L289	V149	V149
V500	Y436	N370	K292	L150	L150
	R437	T372	P293	S151	S151
	G438	C371	V294	D220	F152
	V439	T372	P294	V221	Q153
	P440	P373	L295	L222	V154
	P441	K374	C296	T223	L155
	F444	P375	A297	I224	E156
	E445	T376	T298	R225	V157
	K446	S377	Q299	E226	V158
	E447	T378	M300	V227	D159
	PRO	V382	L301	L228	D160
	VAL	A386	E302	K161	K161
	SER	A387	S303	Q231	T162
	ASP	V387	M304	G232	L163
	TRP	A388	T305	V235	K164
	T453	A389	P308	V235	V165
	D454	V390	R309	V239	K166
	D455	F391	F310	K240	A167
	V456	A395	T311	E241	L168
	E457	K396	E314	E242	M169
	A458	A397	V315	N243	G171
	R459	I398	S316	Q244	K172
	I460	I399	S316	Q245	I173
	M461	V400	D317	G246	C174
	G463	L401	V318	V247	S175
	I464	S402	L323	N248	H176
	E465	T403	D324	N249	K177
	K466	S404	D327	L254	G178
	A467	T407	C328	K255	V179
	E469	P408	V329	V256	M180
	L473	R409	M330	T257	L181
	K474	L410	L331	D258	P182
	K475	V411	A336	G259	G183
	G476	S412	K337	V260	T184
	D477	K413	G338	M261	D185
	T478	Y414	A337	V262	V186
	T478	R415	K337	A263	D187
	Y479	P416	G338	R264	L188
	V480	M417	I342	G265	P189
	S481	M417	N343	D266	A190
	I482	C418	I343	L267	L191
	Q483	P419	V345	G268	K194
	G484	I420	T346	I269	D195
		I421	T347	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, α , β , γ	108.30 Å 106.40 Å 105.50 Å 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 ²)	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	5
1	B	481/500 (96%)	377 (78%)	71 (15%)	33 (7%)	1	6
All	All	962/1000 (96%)	759 (79%)	136 (14%)	67 (7%)	1	6

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%)	1	9
1	B	412/423 (97%)	339 (82%)	73 (18%)	2	9
All	All	824/846 (97%)	676 (82%)	148 (18%)	1	9

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 ⓘ

There are no RNA molecules 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 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	B	1006	3,4	5,8,8	2.31	2 (40%)	6,11,11	3.24	2 (33%)
2	PGA	A	1005	1,3,4	5,8,8	2.49	3 (60%)	6,11,11	3.21	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	B	1006	3,4	-	2/4/6/6	-
2	PGA	A	1005	1,3,4	-	0/4/6/6	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	PGA	P-O3P	4.09	1.70	1.54
2	B	1006	PGA	P-O3P	3.97	1.70	1.54
2	B	1006	PGA	P-O2P	2.24	1.57	1.50
2	A	1005	PGA	O1P-C2	-2.20	1.36	1.45
2	A	1005	PGA	P-O2P	2.08	1.57	1.50

All (4) bond angle outliers are listed below:

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

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1006	PGA	C2-O1P-P-O3P
2	B	1006	PGA	C2-O1P-P-O4P

There are no ring outliers.

2 monomers are involved in 7 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	374:LYS	C	375:PRO	N	0.84

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.