



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:11 AM UTC

PDB ID : 1A3X / pdb_00001a3x
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

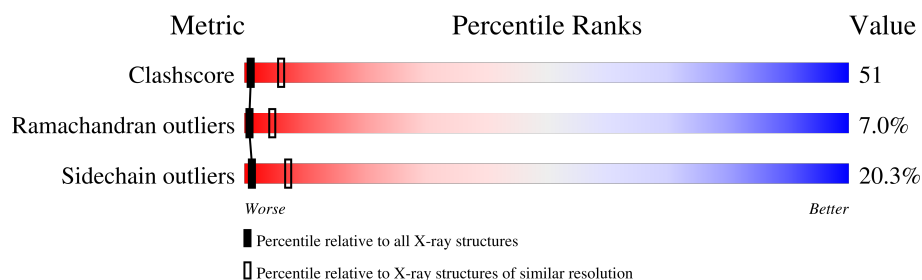
1 Overall quality at a glance

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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 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 $\leq 5\%$.

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	PGA	B	1006	-	X	-	-

2 Entry composition [i](#)

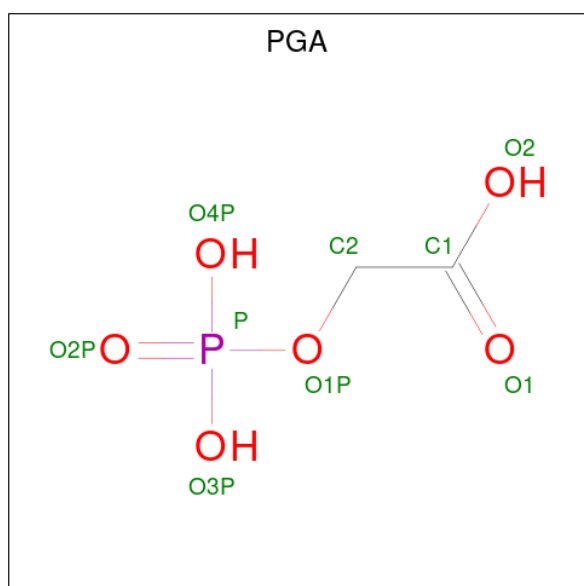
There are 4 unique types of molecules in this entry. The entry contains 7472 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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 (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

D477	T478	V411	S412	K342	L267	I133
T479	V479	K413	K343	K344	G268	V136
V480	V480	V414	A344	E270	D198	I137
S481	V481	R415	V345	I271	L199	S138
I482	V482	P416	T346	P272	R200	A139
Q483	V483	M417	T347	A273	G140	F201
G484	V484	C418	M348	P274	R201	R141
PHE	PHE	P419	A349	E275	H208	I142
LYS	LYS	L420	E350	V276	M209	I143
ALA	ALA	L421	Q357	L277	V210	I144
GLY	GLY	L422	A358	A278	F211	V145
ALA	ALA	V423	I359	Q280	A212	D146
GLY	GLY	T424	A360	K281	S213	D147
HIS	HIS	R425	A361	V294	F214	G148
SER	SER	C426	Y361	K282	I215	G149
N493	N493	P427	L362	L283	R216	L150
T494	T494	R428	P363	I284	S151	L151
L495	L495	A429	D366	N288	D220	F152
Q496	Q496	A430	D367	L289	V221	Q153
V497	V497	R431	M368	K292	L222	V154
S498	S498	F432	R369	P293	T223	L155
T499	T499	S433	N370	R225	I224	E156
V500	V500	H434	C371	V294	E226	V157
		L435	T372	I295	V227	L158
		V436	F373	C296	L228	D159
		R437	K374	A297	Q229	D160
		G438	P375	T298	E230	K161
		V439	T376	Q299	Q231	T162
		F440	S377	M300	G232	L163
		P441	T378	L301	V165	K164
				E302	K166	V165
		F444	V382	S303	V235	K167
		E445		K304	K236	L168
		K446	A386	T305	V239	M169
		E447	V387	P308	K240	A170
		PRO	A388	R309	I241	G171
		VAL	A389	E242	K172	
		SER	V390	P310	N243	
		ASP	F391	T311	Q244	I173
		TRP	E392		Q245	C174
		T453	Q393	E314	G246	H176
		D454	K394	V315	V247	K177
		D455	A395	S316	N248	G178
		V456	K396	D317	N249	V179
		E457	A397	V318		
		A458	I398	L323		
		R459	I399	D324	L254	L181
		L460	V400		K255	P182
		K461	L401		V256	G183
		F462	S402	D327	T257	T184
		G463	T403	C328	D258	D185
		I464	S404	V329	G259	V186
			G405	M330	V260	D187
				L331	M261	L188
		A467	T406		V262	P189
					A263	A190
		L473	P408		R264	L191
		K474	R409	A336	G265	
		K475	L410	K337	D266	
		G476		G338	K194	

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	108.30Å 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 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: PGA, K, 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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	2/3781 (0.1%)	1.24	38/5124 (0.7%)
1	B	0.51	2/3781 (0.1%)	1.31	37/5124 (0.7%)
All	All	0.57	4/7562 (0.1%)	1.27	75/10248 (0.7%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	LYS	C-N	-21.01	0.84	1.33
1	A	375	PRO	C-N	8.96	1.46	1.33
1	B	375	PRO	C-N	-6.05	1.25	1.33
1	B	188	LEU	CA-C	-5.23	1.47	1.53

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	LYS	O-C-N	-36.18	79.71	121.32
1	A	375	PRO	O-C-N	-30.03	82.10	122.64
1	B	375	PRO	O-C-N	-26.03	71.64	121.10
1	A	374	LYS	CA-C-N	-22.84	91.29	119.84
1	A	374	LYS	C-N-CA	-22.84	91.29	119.84

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	Peptide,Mainchain

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	382	1
1	B	3725	0	3804	393	1
2	A	9	0	2	6	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	775	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 51.

The worst 5 of 775 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	4
1	B	481/500 (96%)	377 (78%)	71 (15%)	33 (7%)	1	5
All	All	962/1000 (96%)	759 (79%)	136 (14%)	67 (7%)	1	4

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%)	328 (80%)	84 (20%)	1	7
1	B	412/423 (97%)	329 (80%)	83 (20%)	1	7
All	All	824/846 (97%)	657 (80%)	167 (20%)	1	7

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	128	VAL
1	B	324	ASP
1	B	153	GLN
1	B	230	GLU
1	B	390	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	243	ASN
1	B	417	ASN
1	B	244	GLN
1	B	343	ASN
1	B	461	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 oligosaccharides 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	4,3	8,8,8	2.31	3 (37%)	10,11,11	2.98	4 (40%)
2	PGA	A	1005	4,3	8,8,8	3.04	3 (37%)	10,11,11	2.95	4 (40%)

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	4,3	-	4/6/6/6	-
2	PGA	A	1005	4,3	-	2/6/6/6	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	PGA	O1P-C2	-6.62	1.36	1.43
2	A	1005	PGA	P-O3P	4.25	1.70	1.54
2	B	1006	PGA	P-O3P	4.12	1.70	1.54
2	B	1006	PGA	O1P-C2	-3.62	1.39	1.43
2	B	1006	PGA	P-O2P	2.34	1.57	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1006	PGA	O1P-P-O2P	7.23	125.98	106.44
2	A	1005	PGA	O1P-P-O2P	6.90	125.08	106.44
2	B	1006	PGA	O1P-C2-C1	3.78	116.24	110.54
2	A	1005	PGA	O1P-C2-C1	3.66	116.06	110.54
2	A	1005	PGA	O3P-P-O1P	2.96	114.39	106.67

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1006	PGA	C2-O1P-P-O3P
2	A	1005	PGA	O2-C1-C2-O1P
2	A	1005	PGA	O1-C1-C2-O1P
2	B	1006	PGA	O2-C1-C2-O1P
2	B	1006	PGA	O1-C1-C2-O1P

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1006	PGA	2	0
2	A	1005	PGA	6	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.