



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2018 – 07:45 am GMT

PDB ID : 1A3W
Title : PYRUVATE KINASE FROM SACCHAROMYCES CEREVISIAE COM-
PLEXED WITH FBP, 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

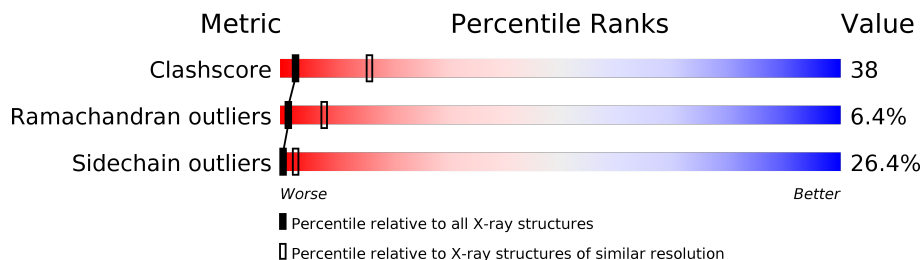
1 Overall quality at a glance

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	122078	2167 (3.00-3.00)
Ramachandran outliers	120005	2101 (3.00-3.00)
Sidechain outliers	119972	2104 (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. 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	

2 Entry composition [i](#)

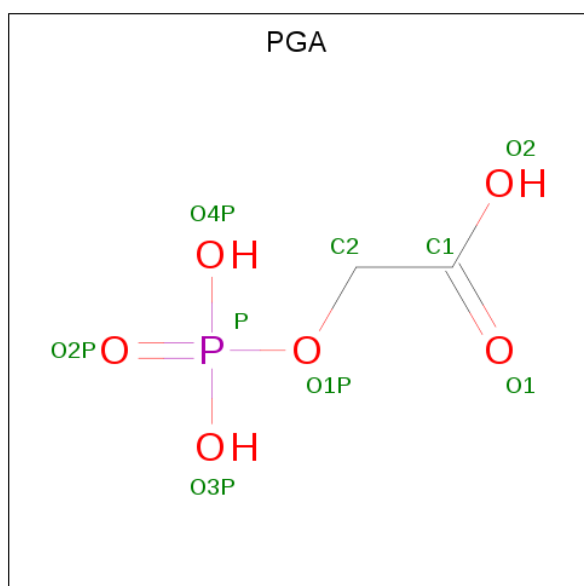
There are 5 unique types of molecules in this entry. The entry contains 7581 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

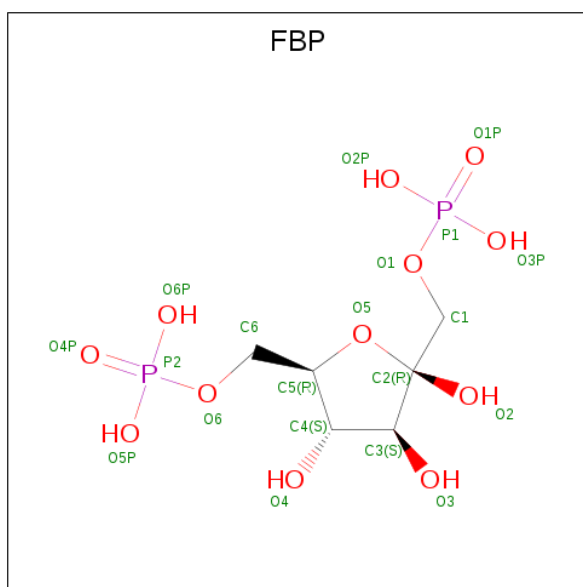
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3773	2380	650	726	17			
1	B	489	Total	C	N	O	S	0	0	0
			3746	2362	647	720	17			

- 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 BETA-FRUCTOSE-1,6-DIPHOSPHATE (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			20	6	12	2		
3	B	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

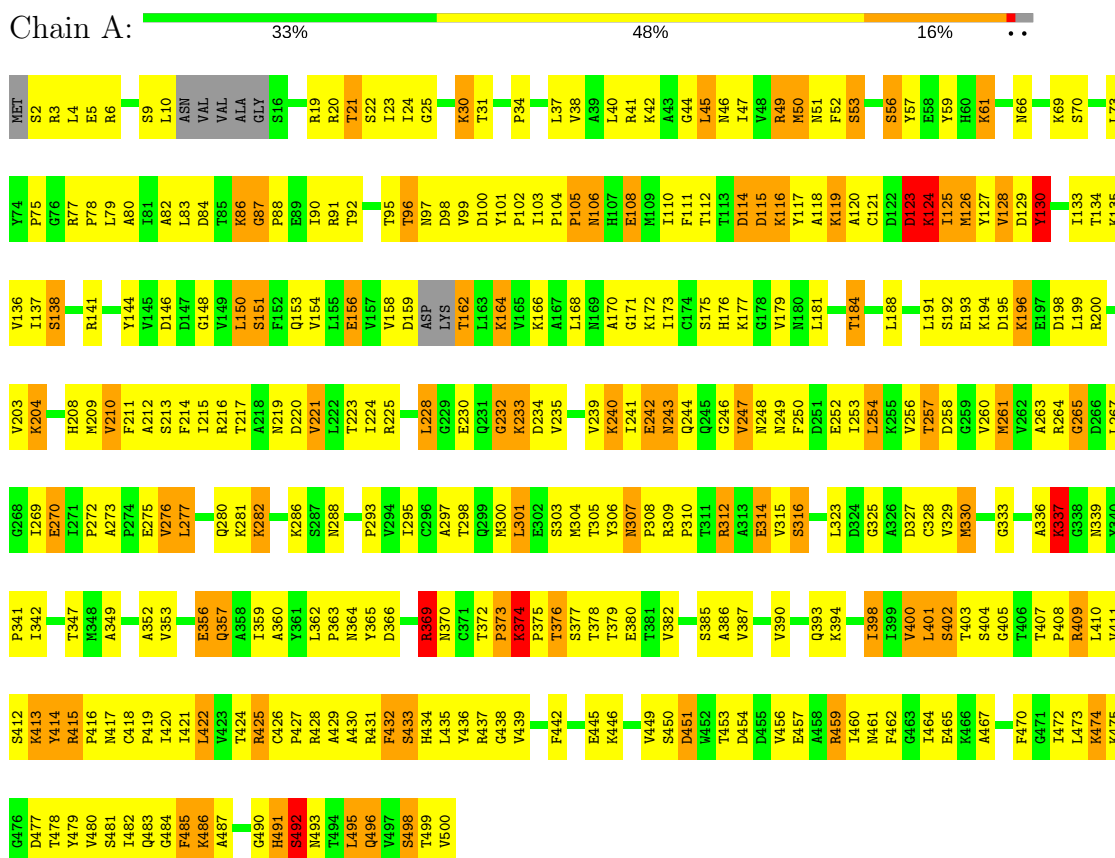
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	K	0	0
			1	1		
5	A	1	Total	K	0	0
			1	1		

3 Residue-property plots

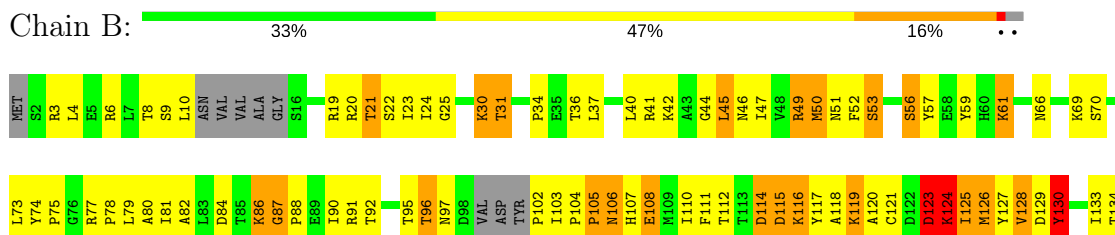
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

• Molecule 1: PYRUVATE KINASE



• Molecule 1: PYRUVATE KINASE



S481	M417	T347	I269	K204	K135
I482	C418	M348	E270		V136
Q483	P419	A349	T271	H208	I137
G484	T420		P272	M209	S138
F485	T421	A352	A273	V210	
K486	L422	V353	P274	F211	R141
A487	V423		E275	A212	
	T424	E386	V276	S213	Y144
G490	R425	Q357	L277	F214	Y145
H491		A358		I215	D146
S492	R428	I359	Q280	R216	D147
N493	A429	A360	K281	T217	G148
T494	A430	Y361	K282	A218	V149
L495	R431	L362		N219	L150
Q496	F432	P363	N288	D220	S151
S498	S433	N364		V221	F152
T499	H434	Y365	P293	L222	Q153
V500	L435	D366	V294	T223	V154
	Y436		T295	I224	L155
	R437	K369	C296	R225	E156
	G438	N370	A297		V157
	V439	C371	T298	L228	V158
		T372	Q299	G229	D159
	F442	P373	N300	E230	ASP
		K374	L301	Q231	LYS
E445	E445	P375	E302	G232	T162
K446	K446	T376	S303	K233	L163
		S377	N304	D234	K164
V449	S450	T378	T305	V235	V165
D451	D451	T379	Y306		K166
V452	V452	E380	N307	V239	A167
T453	T453	T381	P308	K240	L168
D454	D454	V382	R309	I241	N169
V456	V456		P310	E242	A170
E457	E457	S385	T311	N243	G171
A458	A458	A386	R312	Q244	K172
		V387	A313	G245	I173
			E314	G246	G174
		Q393	S315	V247	S175
		K394	S316	N248	H176
				N249	K177
		T398	L323	F250	G178
		I399	D324	D251	V179
		V400	G325	E252	N180
		L401	A326	I253	L181
		S402	D327	K255	
		T403	C328	V256	T184
		S404	V329	T257	
		G405	N330	D258	L191
		T406		G259	S192
		T407	G333	V260	E193
		P408		M261	K194
		R409	A336	D195	D196
		L410	K337	V262	K196
		V411	G338	A263	E197
		S412	N339	R264	D198
		K413	V340	G265	L199
		Y414	P341	D266	R200
		R415	I342	L267	
		P416		G268	V203

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	109.40Å 102.70Å 110.90Å 90.00° 112.30° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00	Depositor
% Data completeness (in resolution range)	75.9 (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}	0.218 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7581	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, FBP, PGA, 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	0.29	0/3834	0.63	7/5196 (0.1%)
1	B	0.31	0/3805	0.65	8/5153 (0.2%)
All	All	0.30	0/7639	0.64	15/10349 (0.1%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	ARG	NE-CZ-NH2	-12.25	114.17	120.30
1	B	369	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	A	369	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	A	369	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	B	409	ARG	NE-CZ-NH2	-10.42	115.09	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3773	0	3844	296	0
1	B	3746	0	3822	298	0
2	A	9	0	2	1	0
2	B	9	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	20	0	10	3	0
3	B	20	0	10	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	7581	0	7690	579	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 38.

The worst 5 of 579 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:B:374:LYS:H	1:B:375:PRO:HA	1.16	1.11
1:A:374:LYS:H	1:A:375:PRO:HA	1.19	1.05
1:B:398:ILE:HD11	1:B:482:ILE:HD11	1.43	1.01
1:A:242:GLU:HG3	1:A:263:ALA:CB	1.95	0.96
1:B:242:GLU:HG3	1:B:263:ALA:CB	1.97	0.95

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	486/500 (97%)	398 (82%)	56 (12%)	32 (7%)	1	7
1	B	481/500 (96%)	394 (82%)	57 (12%)	30 (6%)	1	9
All	All	967/1000 (97%)	792 (82%)	113 (12%)	62 (6%)	1	8

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	99	VAL
1	A	106	ASN
1	A	170	ALA
1	A	337	LYS

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	417/423 (99%)	307 (74%)	110 (26%)	0	3
1	B	414/423 (98%)	305 (74%)	109 (26%)	0	3
All	All	831/846 (98%)	612 (74%)	219 (26%)	0	3

5 of 219 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	ASP
1	B	50	MET
1	B	422	LEU
1	A	461	ASN
1	B	4	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	HIS
1	B	106	ASN
1	B	434	HIS
1	A	483	GLN
1	B	46	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	5,4	5,8,8	2.39	2 (40%)	6,11,11	3.72	3 (50%)
3	FBP	A	1007	-	18,20,20	1.01	0	23,32,32	0.68	0
2	PGA	B	1006	5,4	5,8,8	2.33	2 (40%)	6,11,11	3.55	3 (50%)
3	FBP	B	1008	-	18,20,20	1.06	1 (5%)	23,32,32	0.82	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	PGA	A	1005	5,4	-	0/4/6/6	0/0/0/0
3	FBP	A	1007	-	-	0/13/32/32	0/1/1/1
2	PGA	B	1006	5,4	-	0/4/6/6	0/0/0/0
3	FBP	B	1008	-	-	0/13/32/32	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	PGA	P-O2P	2.34	1.58	1.50
3	B	1008	FBP	O5-C2	2.40	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1006	PGA	P-O2P	2.43	1.58	1.50
2	A	1005	PGA	P-O3P	3.87	1.70	1.54
2	B	1006	PGA	P-O3P	3.98	1.70	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1005	PGA	O4P-P-O1P	-2.41	100.32	106.73
2	B	1006	PGA	O4P-P-O1P	-2.11	101.13	106.73
2	A	1005	PGA	O3P-P-O1P	2.97	114.64	106.73
2	B	1006	PGA	O3P-P-O1P	3.09	114.94	106.73
2	B	1006	PGA	O1P-P-O2P	7.30	126.95	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1005	PGA	1	0
3	A	1007	FBP	3	0
3	B	1008	FBP	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.