



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:26 PM GMT

PDB ID : 1OZF  
Title : The crystal structure of Klebsiella pneumoniae acetolactate synthase with enzyme-bound cofactors  
Authors : Pang, S.S.; Duggleby, R.G.; Schowen, R.L.; Guddat, L.W.  
Deposited on : 2003-04-09  
Resolution : 2.30 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

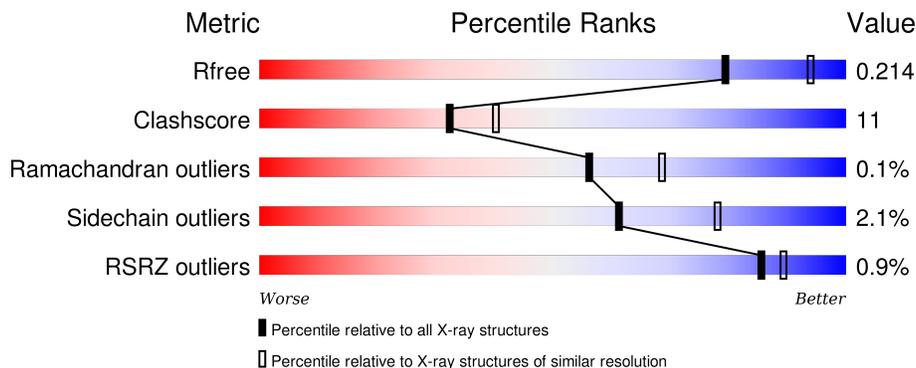
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	566	 75% 20% . .
1	B	566	 72% 23% . .

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
5	PEG	A	693	-	-	-	X
5	PEG	A	696	-	-	-	X
5	PEG	B	701	-	-	-	X
5	PEG	B	702	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8858 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.

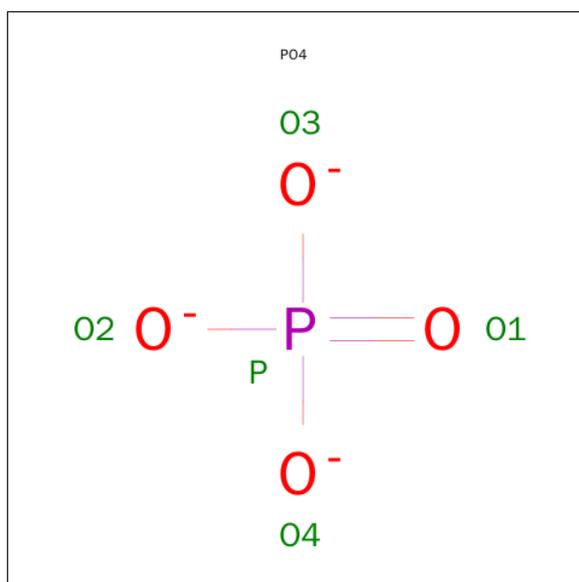
- Molecule 1 is a protein called Acetolactate synthase, catabolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	545	4125	2603	731	773	18	0	0	0
1	B	542	4079	2583	711	767	18	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	GLU	-	EXPRESSION TAG	UNP P27696
A	561	HIS	-	EXPRESSION TAG	UNP P27696
A	562	HIS	-	EXPRESSION TAG	UNP P27696
A	563	HIS	-	EXPRESSION TAG	UNP P27696
A	564	HIS	-	EXPRESSION TAG	UNP P27696
A	565	HIS	-	EXPRESSION TAG	UNP P27696
A	566	HIS	-	EXPRESSION TAG	UNP P27696
B	560	GLU	-	EXPRESSION TAG	UNP P27696
B	561	HIS	-	EXPRESSION TAG	UNP P27696
B	562	HIS	-	EXPRESSION TAG	UNP P27696
B	563	HIS	-	EXPRESSION TAG	UNP P27696
B	564	HIS	-	EXPRESSION TAG	UNP P27696
B	565	HIS	-	EXPRESSION TAG	UNP P27696
B	566	HIS	-	EXPRESSION TAG	UNP P27696

- 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 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	280	Total O 280 280	0	0
6	B	247	Total O 247 247	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.82Å 160.57Å 129.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30 76.29 – 2.29	Depositor EDS
% Data completeness (in resolution range)	88.5 (100.00-2.30) 88.0 (76.29-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.93 (at 2.29Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.165 , 0.214 0.165 , 0.214	Depositor DCC
$R_{free}$ test set	4848 reflections (10.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtrriage
Anisotropy	0.451	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 62.4	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Outliers	1 of 48069 reflections (0.002%)	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8858	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: PO4, PEG, MG, TPP

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	0.31	0/4204	0.57	0/5717
1	B	0.30	0/4157	0.57	0/5655
All	All	0.31	0/8361	0.57	0/11372

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 [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	4125	0	4114	88	0
1	B	4079	0	4056	85	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	26	0	16	3	0
4	B	26	0	16	3	0
5	A	49	0	70	6	0
5	B	14	0	20	1	0
6	A	280	0	0	11	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	247	0	0	9	0
All	All	8858	0	8292	175	2

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 11.

The worst 5 of 175 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:353:GLN:HE21	5:A:692:PEG:H11	1.40	0.86
1:A:371:LEU:HD21	1:A:518:ALA:HA	1.58	0.86
1:A:352:ARG:HA	1:A:355:GLN:HE21	1.41	0.84
1:A:360:ASP:HB3	6:A:892:HOH:O	1.87	0.75
1:B:478:ASN:HD21	1:B:546:ASN:HD22	1.34	0.73

All (2) 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)
6:A:701:HOH:O	6:A:701:HOH:O 4_556	1.56	0.64
6:A:708:HOH:O	6:A:708:HOH:O 4_556	2.15	0.05

## 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	541/566 (96%)	525 (97%)	16 (3%)	0	<b>100</b> <b>100</b>
1	B	534/566 (94%)	512 (96%)	21 (4%)	1 (0%)	52 64
All	All	1075/1132 (95%)	1037 (96%)	37 (3%)	1 (0%)	56 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	310	GLU

### 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	430/452 (95%)	421 (98%)	9 (2%)	61	78
1	B	424/452 (94%)	415 (98%)	9 (2%)	61	78
All	All	854/904 (94%)	836 (98%)	18 (2%)	61	78

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	455	MET
1	B	180	VAL
1	B	311	GLU
1	A	411	ARG
1	A	447	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	554	HIS
1	B	87	ASN
1	B	385	ASN
1	B	12	HIS
1	B	56	HIS

### 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 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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
5	PEG	A	690	-	6,6,6	0.60	0	5,5,5	1.53	1 (20%)
5	PEG	A	691	-	6,6,6	0.65	0	5,5,5	1.52	1 (20%)
5	PEG	A	692	-	6,6,6	0.65	0	5,5,5	1.59	1 (20%)
5	PEG	A	693	-	6,6,6	0.67	0	5,5,5	1.54	1 (20%)
5	PEG	A	694	-	6,6,6	0.64	0	5,5,5	1.53	1 (20%)
5	PEG	A	695	-	6,6,6	0.73	0	5,5,5	1.58	1 (20%)
5	PEG	A	696	-	6,6,6	0.71	0	5,5,5	1.51	1 (20%)
2	PO4	A	697	-	4,4,4	1.03	0	6,6,6	0.27	0
4	TPP	A	700	3	20,27,27	2.22	8 (40%)	31,40,40	2.43	12 (38%)
5	PEG	B	701	-	6,6,6	0.72	0	5,5,5	1.55	1 (20%)
5	PEG	B	702	-	6,6,6	0.66	0	5,5,5	1.53	1 (20%)
2	PO4	B	703	-	4,4,4	1.14	0	6,6,6	0.27	0
4	TPP	B	705	3	20,27,27	2.37	10 (50%)	31,40,40	2.41	12 (38%)

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
5	PEG	A	690	-	-	0/4/4/4	0/0/0/0
5	PEG	A	691	-	-	0/4/4/4	0/0/0/0
5	PEG	A	692	-	-	0/4/4/4	0/0/0/0
5	PEG	A	693	-	-	0/4/4/4	0/0/0/0
5	PEG	A	694	-	-	0/4/4/4	0/0/0/0
5	PEG	A	695	-	-	0/4/4/4	0/0/0/0
5	PEG	A	696	-	-	0/4/4/4	0/0/0/0
2	PO4	A	697	-	-	0/0/0/0	0/0/0/0
4	TPP	A	700	3	-	0/16/17/17	0/2/2/2
5	PEG	B	701	-	-	0/4/4/4	0/0/0/0
5	PEG	B	702	-	-	0/4/4/4	0/0/0/0
2	PO4	B	703	-	-	0/0/0/0	0/0/0/0
4	TPP	B	705	3	-	0/16/17/17	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	TPP	CM4-C4	-4.34	1.40	1.49
4	B	705	TPP	CM4-C4	-4.28	1.40	1.49
4	B	705	TPP	PB-O1B	-2.27	1.43	1.51
4	A	700	TPP	PB-O1B	-2.26	1.43	1.51
4	B	705	TPP	PA-O2A	-2.22	1.45	1.54

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	TPP	C6-C5-C4	-6.21	122.00	127.56
4	B	705	TPP	C6-C5-C4	-5.94	122.24	127.56
4	A	700	TPP	N1'-C2'-N3'	-3.83	118.51	125.60
4	B	705	TPP	N1'-C2'-N3'	-3.78	118.61	125.60
4	B	705	TPP	CM4-C4-C5	-2.63	122.99	128.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	692	PEG	2	0
5	A	694	PEG	1	0
5	A	695	PEG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	TPP	3	0
5	B	701	PEG	1	0
4	B	705	TPP	3	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](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	545/566 (96%)	-0.23	3 (0%) 90 93	9, 20, 41, 63	0
1	B	542/566 (95%)	-0.20	7 (1%) 79 84	11, 24, 49, 68	0
All	All	1087/1132 (96%)	-0.21	10 (0%) 85 89	9, 22, 46, 68	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	TYR	4.0
1	B	364	ALA	3.3
1	B	337	HIS	3.3
1	B	309	TYR	2.8
1	A	363	GLY	2.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PEG	B	701	7/7	0.87	0.20	7.40	47,48,52,53	0
5	PEG	A	693	7/7	0.92	0.16	4.42	37,39,41,41	0
5	PEG	A	696	7/7	0.80	0.20	3.37	41,45,47,47	0
5	PEG	B	702	7/7	0.93	0.14	2.43	48,49,51,53	0
5	PEG	A	692	7/7	0.81	0.24	1.42	44,44,46,46	0
5	PEG	A	690	7/7	0.93	0.22	0.90	49,50,53,53	0
4	TPP	B	705	26/26	0.98	0.11	0.80	14,25,29,29	0
5	PEG	A	691	7/7	0.93	0.14	0.65	34,37,41,42	0
5	PEG	A	694	7/7	0.90	0.18	0.55	41,43,44,45	0
5	PEG	A	695	7/7	0.92	0.17	0.40	38,40,41,44	0
4	TPP	A	700	26/26	0.98	0.11	-0.54	7,21,26,29	0
3	MG	A	699	1/1	0.97	0.10	-0.86	12,12,12,12	0
2	PO4	B	703	5/5	0.99	0.10	-1.38	16,17,20,20	0
2	PO4	A	697	5/5	0.99	0.08	-2.12	12,12,14,17	0
3	MG	B	704	1/1	0.98	0.06	-3.62	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.