



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:24 PM GMT

PDB ID : 1K49
Title : Crystal Structure of 3,4-dihydroxy-2-butanone 4-phosphate synthase (cation free form)
Authors : Liao, D.-I.; Zheng, Y.-J.; Viitanen, P.V.; Jordan, D.B.
Deposited on : 2001-10-06
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at 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.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

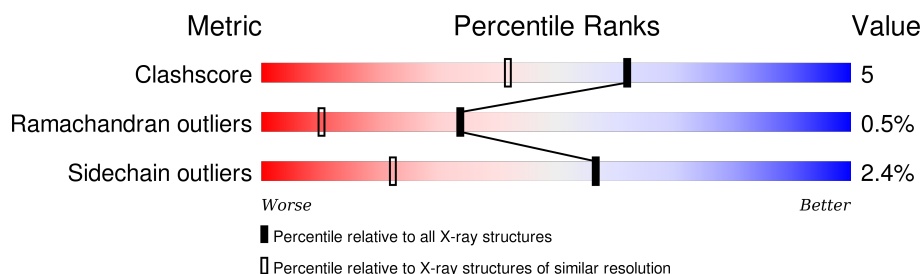
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)

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	233	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1810 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 3,4-Dihydroxy-2-Butanone 4-Phosphate Synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1566	969	289	297	11			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



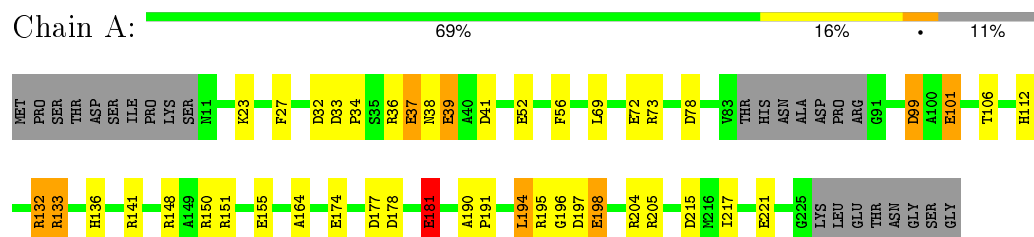
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	224	Total 224	O 224	0	0

Note EDS was not executed.

- Molecule 1: 3,4-Dihydroxy-2-Butanone 4-Phosphate Synthase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	53.70 Å 87.83 Å 43.96 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.50)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.201 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1810	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: SO4

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	1.02	9/1593 (0.6%)	1.52	35/2161 (1.6%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	GLU	CD-OE2	8.23	1.34	1.25
1	A	155	GLU	CD-OE2	6.77	1.33	1.25
1	A	198	GLU	CD-OE2	6.63	1.32	1.25
1	A	72	GLU	CD-OE2	6.61	1.32	1.25
1	A	52	GLU	CD-OE2	5.78	1.32	1.25
1	A	39	GLU	CD-OE2	5.50	1.31	1.25
1	A	37	GLU	CD-OE2	5.39	1.31	1.25
1	A	101	GLU	CD-OE2	5.14	1.31	1.25
1	A	174	GLU	CD-OE1	-5.06	1.20	1.25

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	A	132	ARG	NE-CZ-NH1	12.06	126.33	120.30
1	A	78	ASP	CB-CG-OD2	-9.38	109.85	118.30
1	A	178	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	A	141	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	A	204	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	A	36	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	177	ASP	CB-CG-OD1	7.22	124.79	118.30
1	A	99	ASP	CB-CG-OD1	6.97	124.57	118.30
1	A	177	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	99	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	A	36	ARG	NE-CZ-NH1	6.70	123.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	125	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	A	73	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	78	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	197	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	205	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	215	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	41	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	32	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	178	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	113	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	73	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	123	ALA	N-CA-CB	5.55	117.87	110.10
1	A	56	PHE	CB-CG-CD2	5.48	124.64	120.80
1	A	150	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	148	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	150	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	195	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	197	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	148	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	133	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	27	PHE	CB-CA-C	-5.01	100.39	110.40
1	A	32	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1566	0	1550	17	0
2	A	20	0	0	0	0
3	A	224	0	0	4	0
All	All	1810	0	1550	17	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 5.

All (17) 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:194:LEU:HD13	1:A:198:GLU:HB2	1.62	0.82
1:A:101:GLU:OE2	1:A:132:ARG:HD3	1.80	0.81
1:A:191:PRO:HD2	3:A:1227:HOH:O	1.86	0.74
1:A:99:ASP:OD1	1:A:136:HIS:HD2	1.78	0.65
1:A:33:ASP:CG	1:A:34:PRO:HD2	2.20	0.61
1:A:194:LEU:HD13	1:A:198:GLU:CB	2.31	0.60
1:A:112:HIS:HD2	1:A:113:ASP:OD1	1.87	0.57
1:A:34:PRO:HA	1:A:38:ASN:HB2	1.86	0.56
1:A:151:ARG:HE	1:A:217:ILE:HD13	1.70	0.55
1:A:23:LYS:HD3	1:A:164:ALA:O	2.10	0.51
1:A:190:ALA:HA	3:A:1227:HOH:O	2.14	0.48
1:A:194:LEU:HD22	1:A:194:LEU:HA	1.82	0.45
1:A:106:THR:HG23	3:A:1072:HOH:O	2.17	0.42
1:A:37:GLU:HB3	1:A:39:GLU:HG3	2.02	0.42
1:A:217:ILE:O	1:A:221:GLU:HG3	2.21	0.41
1:A:194:LEU:CD1	1:A:198:GLU:CB	2.99	0.40
1:A:181:GLU:HG3	3:A:1090:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	204/233 (88%)	197 (97%)	6 (3%)	1 (0%)	34	10

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLY

5.3.2 Protein sidechains ⓘ

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	164/186 (88%)	160 (98%)	4 (2%)	57 22

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	133	ARG
1	A	181	GLU
1	A	194	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	81	GLN
1	A	112	HIS
1	A	136	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	SO4	A	1001	-	4,4,4	0.95	0	6,6,6	1.33	1 (16%)
2	SO4	A	1002	-	4,4,4	1.26	1 (25%)	6,6,6	1.44	2 (33%)
2	SO4	A	1003	-	4,4,4	0.86	0	6,6,6	1.55	2 (33%)
2	SO4	A	1004	-	4,4,4	1.12	0	6,6,6	1.71	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	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1004	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	SO4	O2-S	2.23	1.54	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1004	SO4	O2-S-O1	-3.16	99.49	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003	SO4	O2-S-O1	-2.76	100.75	109.50
2	A	1002	SO4	O2-S-O1	-2.31	102.19	109.50
2	A	1003	SO4	O4-S-O3	2.59	119.51	108.98
2	A	1002	SO4	O4-S-O3	2.65	119.75	108.98
2	A	1001	SO4	O4-S-O3	2.74	120.13	108.98
2	A	1004	SO4	O4-S-O3	2.75	120.17	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.