



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 10:25 AM BST

PDB ID : 1G57
Title : CRYSTAL STRUCTURE OF 3,4-DIHYDROXY-2-BUTANONE 4-PHOSPHATE SYNTHASE
Authors : Liao, D.-I.; Calabrese, J.C.; Wawrzak, Z.; Viitanen, P.V.; Jordan, D.B.
Deposited on : 2000-10-30
Resolution : 1.40 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

<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
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) : 2.13

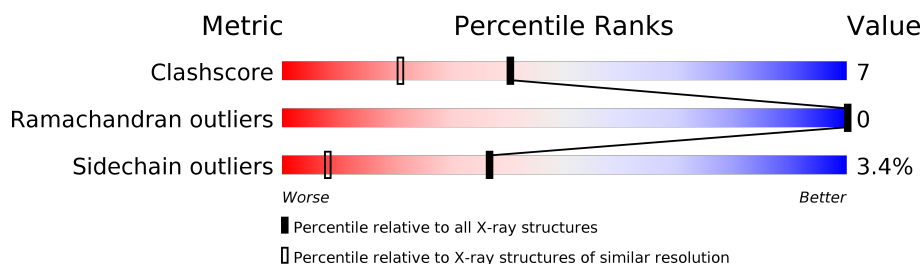
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)

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	217	
1	B	217	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3527 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	205	Total	C	N	O	S	0	0	0
			1529	945	270	301	13			
1	B	209	Total	C	N	O	S	0	0	0
			1558	962	278	305	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	ASN	CLONING ARTIFACT	UNP P0A7J0
B	2	ALA	ASN	CLONING ARTIFACT	UNP P0A7J0

- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs).

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

- Molecule 3 is water.

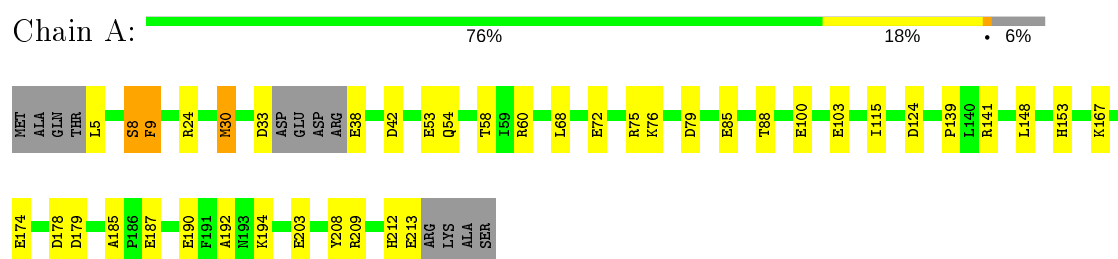
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	246	Total	O	0	0
			246	246		
3	B	190	Total	O	0	0
			190	190		

3 Residue-property plots

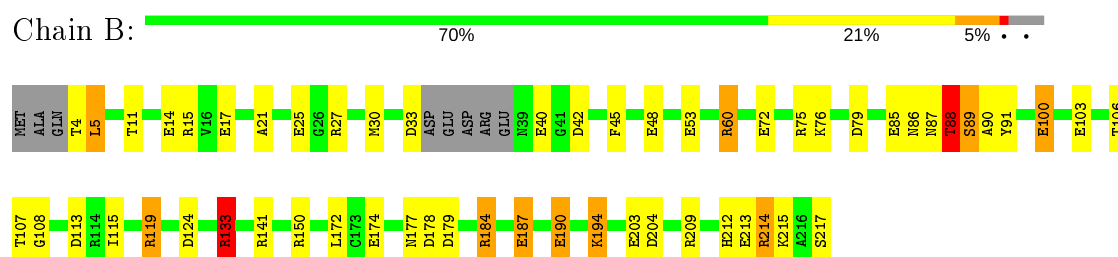
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 3,4-DIHYDROXY-2-BUTANONE 4-PHOSPHATE SYNTHASE



• Molecule 1: 3,4-DIHYDROXY-2-BUTANONE 4-PHOSPHATE SYNTHASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	78.19 Å 78.19 Å 69.62 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 1.40	Depositor
% Data completeness (in resolution range)	100.0 (25.00-1.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.180 , 0.221	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3527	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: CS

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	1.16	10/1549 (0.6%)	1.57	26/2098 (1.2%)
1	B	1.18	12/1578 (0.8%)	1.76	37/2136 (1.7%)
All	All	1.17	22/3127 (0.7%)	1.67	63/4234 (1.5%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	GLU	CD-OE2	8.56	1.35	1.25
1	B	190	GLU	CD-OE2	8.49	1.34	1.25
1	A	213	GLU	CD-OE2	8.12	1.34	1.25
1	B	53	GLU	CD-OE2	8.09	1.34	1.25
1	A	174	GLU	CD-OE2	7.56	1.33	1.25
1	B	203	GLU	CD-OE2	7.29	1.33	1.25
1	A	103	GLU	CD-OE2	7.13	1.33	1.25
1	B	14	GLU	CD-OE2	6.95	1.33	1.25
1	B	187	GLU	CD-OE2	6.75	1.33	1.25
1	B	85	GLU	CD-OE2	6.63	1.32	1.25
1	A	100	GLU	CD-OE2	6.44	1.32	1.25
1	A	38	GLU	CD-OE2	6.14	1.32	1.25
1	B	103	GLU	CD-OE2	6.06	1.32	1.25
1	A	85	GLU	CD-OE2	6.04	1.32	1.25
1	A	190	GLU	CD-OE1	-5.97	1.19	1.25
1	B	100	GLU	CD-OE2	5.45	1.31	1.25
1	B	174	GLU	CD-OE2	5.28	1.31	1.25
1	B	17	GLU	CD-OE2	5.27	1.31	1.25
1	A	53	GLU	CD-OE1	-5.19	1.20	1.25
1	A	187	GLU	CD-OE2	5.16	1.31	1.25
1	B	48	GLU	CD-OE1	-5.14	1.20	1.25
1	B	40	GLU	CD-OE2	5.06	1.31	1.25

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	B	60	ARG	NE-CZ-NH1	14.96	127.78	120.30
1	A	9	PHE	CB-CG-CD1	13.26	130.08	120.80
1	B	27	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	A	141	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	B	209	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	A	178	ASP	CB-CG-OD2	-9.55	109.70	118.30
1	A	33	ASP	CB-CG-OD2	-9.54	109.71	118.30
1	B	42	ASP	CB-CG-OD1	9.47	126.82	118.30
1	B	178	ASP	CB-CG-OD1	9.26	126.63	118.30
1	B	60	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	B	150	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	B	124	ASP	CB-CG-OD2	-8.42	110.72	118.30
1	B	150	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	B	75	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	B	42	ASP	CB-CG-OD2	-8.23	110.89	118.30
1	B	179	ASP	CB-CG-OD1	7.99	125.49	118.30
1	B	141	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	141	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	8	SER	CB-CA-C	7.89	125.09	110.10
1	A	79	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	B	179	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	B	79	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	B	178	ASP	CB-CG-OD2	-7.56	111.49	118.30
1	B	88	THR	N-CA-CB	7.46	124.47	110.30
1	A	33	ASP	CB-CG-OD1	7.06	124.66	118.30
1	A	30	MET	CG-SD-CE	-6.94	89.10	100.20
1	A	24	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	178	ASP	CB-CG-OD1	6.74	124.36	118.30
1	A	53	GLU	OE1-CD-OE2	-6.70	115.26	123.30
1	A	9	PHE	CZ-CE2-CD2	6.67	128.10	120.10
1	A	179	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	91	TYR	CB-CG-CD1	-6.61	117.03	121.00
1	A	42	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	213	GLU	CG-CD-OE2	-6.48	105.34	118.30
1	B	60	ARG	CD-NE-CZ	6.39	132.55	123.60
1	B	213	GLU	OE1-CD-OE2	6.39	130.97	123.30
1	B	124	ASP	CB-CG-OD1	6.27	123.94	118.30
1	B	119	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	9	PHE	CE1-CZ-CE2	-6.16	108.91	120.00
1	A	124	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	B	133	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	45	PHE	CB-CG-CD1	-6.07	116.55	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	MET	CG-SD-CE	-5.96	90.67	100.20
1	A	88	THR	CA-CB-CG2	-5.93	104.10	112.40
1	A	208	TYR	CB-CG-CD1	-5.89	117.47	121.00
1	B	187	GLU	CG-CD-OE1	5.88	130.06	118.30
1	B	60	ARG	CG-CD-NE	-5.86	99.49	111.80
1	B	53	GLU	N-CA-CB	-5.83	100.11	110.60
1	B	187	GLU	CG-CD-OE2	-5.72	106.87	118.30
1	A	9	PHE	CD1-CG-CD2	-5.68	110.91	118.30
1	A	79	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	174	GLU	CG-CD-OE1	5.57	129.44	118.30
1	B	214	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	179	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	B	53	GLU	CB-CG-CD	-5.39	99.64	114.20
1	A	209	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	4	THR	N-CA-CB	5.32	120.42	110.30
1	A	75	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	213	GLU	OE1-CD-OE2	5.06	129.37	123.30
1	B	79	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	204	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	75	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	1529	0	1513	17	0
1	B	1558	0	1550	29	1
2	A	3	0	0	0	0
2	B	1	0	0	0	0
3	A	246	0	0	7	1
3	B	190	0	0	5	0
All	All	3527	0	3063	43	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 7.

All (43) 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:72:GLU:HG3	1:A:76:LYS:HE2	1.23	1.20
1:B:212:HIS:HA	1:B:215:LYS:HE3	1.57	0.86
1:A:9:PHE:CE2	3:A:505:HOH:O	2.29	0.84
1:B:72:GLU:HG3	1:B:76:LYS:HE2	1.62	0.81
1:A:9:PHE:HE2	3:A:505:HOH:O	1.66	0.79
1:A:54:GLN:O	1:A:58:THR:HG23	1.84	0.78
1:B:72:GLU:HG3	1:B:76:LYS:CE	2.12	0.78
1:B:184:ARG:NH1	1:B:187:GLU:OE1	2.24	0.71
1:A:148:LEU:HB2	3:A:720:HOH:O	1.97	0.65
1:B:72:GLU:CG	1:B:76:LYS:HE2	2.28	0.64
1:A:167:LYS:NZ	3:A:610:HOH:O	2.29	0.61
1:B:33:ASP:HB2	3:B:670:HOH:O	2.01	0.61
1:B:72:GLU:O	1:B:76:LYS:HE3	2.01	0.60
1:B:88:THR:HG22	1:B:89:SER:H	1.66	0.60
1:B:90:ALA:HB1	3:B:673:HOH:O	2.01	0.58
1:B:72:GLU:HG3	1:B:76:LYS:HE3	1.86	0.55
1:A:5:LEU:HD21	1:A:185:ALA:HB1	1.88	0.55
1:B:190:GLU:HG2	3:B:617:HOH:O	2.07	0.54
1:B:21:ALA:O	1:B:25:GLU:HG3	2.07	0.54
1:B:177:ASN:ND2	1:B:184:ARG:HH12	2.06	0.54
1:A:9:PHE:CD2	3:A:505:HOH:O	2.57	0.53
1:B:108:GLY:HA2	1:B:113:ASP:HB3	1.92	0.50
1:A:60:ARG:CZ	1:B:60:ARG:CZ	2.90	0.48
1:B:90:ALA:HA	3:B:671:HOH:O	2.13	0.48
1:B:177:ASN:HD21	1:B:184:ARG:NH1	2.11	0.48
1:A:72:GLU:HG3	1:A:76:LYS:CE	2.17	0.47
1:B:106:THR:OG1	1:B:107:THR:N	2.46	0.47
1:A:60:ARG:NH1	1:B:60:ARG:CD	2.78	0.47
1:B:86:ASN:O	1:B:87:ASN:OD1	2.32	0.47
1:B:115:ILE:O	1:B:119:ARG:HG2	2.15	0.46
1:A:9:PHE:CD1	3:A:729:HOH:O	2.69	0.46
1:A:153:HIS:N	3:A:685:HOH:O	2.49	0.45
1:B:172:LEU:HD12	1:B:172:LEU:C	2.37	0.45
1:A:194:LYS:HB2	1:A:194:LYS:HE2	1.58	0.44
1:B:212:HIS:HA	1:B:215:LYS:CE	2.39	0.44
1:B:5:LEU:HA	1:B:5:LEU:HD12	1.65	0.44
1:B:11:THR:O	1:B:15:ARG:HG3	2.18	0.43
1:B:194:LYS:HB2	1:B:194:LYS:HE2	1.42	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:CZ	1:B:60:ARG:NE	2.81	0.42
1:B:194:LYS:HE3	3:B:617:HOH:O	2.19	0.42
1:A:30:MET:HG3	1:A:192:ALA:HB2	2.02	0.42
1:B:133:ARG:HH11	1:B:133:ARG:HD3	1.72	0.40
1:A:68:LEU:O	1:A:139:PRO:HA	2.20	0.40

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:B:214:ARG:NH2	3:A:694:HOH:O 3_764	2.07	0.13

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	201/217 (93%)	199 (99%)	2 (1%)	0	100	100
1	B	205/217 (94%)	204 (100%)	1 (0%)	0	100	100
All	All	406/434 (94%)	403 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	161/171 (94%)	158 (98%)	3 (2%)	57	25
1	B	164/171 (96%)	156 (95%)	8 (5%)	25	3
All	All	325/342 (95%)	314 (97%)	11 (3%)	37	8

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	115	ILE
1	A	212	HIS
1	B	5	LEU
1	B	88	THR
1	B	89	SER
1	B	100	GLU
1	B	133	ARG
1	B	184	ARG
1	B	194	LYS
1	B	217	SER

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	61	HIS
1	A	132	ASN
1	B	132	ASN
1	B	177	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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.