



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:49 PM UTC

PDB ID : 1G57 / pdb_00001g57
Title : CRYSTAL STRUCTURE OF 3,4-DIHYDROXY-2-BUTANONE 4-PHOSPHATE SYNTHASE
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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 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
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

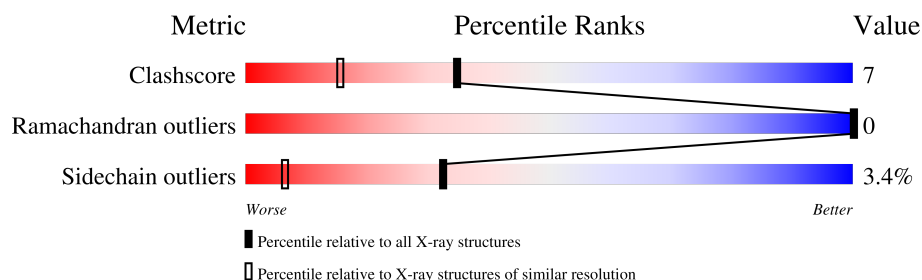
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (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 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	217	 79% 14% • 6%
1	B	217	 72% 19% • • •

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 (CCD ID: CS) (formula: Cs).

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

- 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		

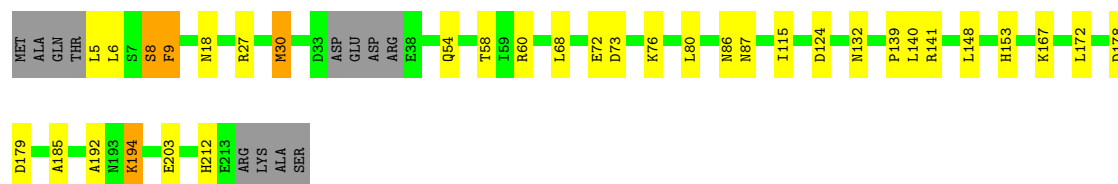
3 Residue-property plots [i](#)

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.

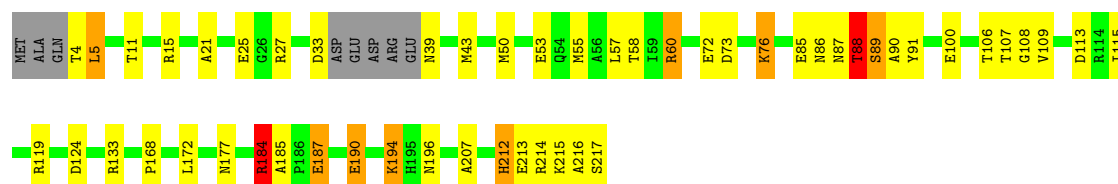
• Molecule 1: 3,4-DIHYDROXY-2-BUTANONE 4-PHOSPHATE SYNTHASE

Chain A: 



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

Chain B: 



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	78.19Å 78.19Å 69.62Å 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	1.32	1/1549 (0.1%)	1.62	23/2098 (1.1%)
1	B	1.35	2/1578 (0.1%)	1.87	39/2136 (1.8%)
All	All	1.34	3/3127 (0.1%)	1.75	62/4234 (1.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	GLU	CD-OE2	5.11	1.35	1.25
1	B	184	ARG	NE-CZ	5.08	1.38	1.33
1	B	190	GLU	CD-OE2	5.08	1.34	1.25

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	THR	N-CA-CB	9.00	124.47	110.87
1	A	141	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	B	53	GLU	CB-CG-CD	-7.62	99.64	112.60
1	A	212	HIS	CA-CB-CG	7.49	121.29	113.80
1	A	8	SER	CB-CA-C	7.07	125.09	110.31
1	B	88	THR	CA-C-N	7.03	129.70	120.28
1	B	88	THR	C-N-CA	7.03	129.70	120.28
1	B	124	ASP	CA-CB-CG	6.92	119.52	112.60
1	B	53	GLU	N-CA-CB	-6.81	100.11	110.12
1	B	216	ALA	CA-C-N	6.81	133.96	121.70
1	B	216	ALA	C-N-CA	6.81	133.96	121.70
1	A	6	LEU	N-CA-CB	-6.70	100.78	110.56
1	B	27	ARG	CA-C-N	-6.53	114.12	121.83
1	B	27	ARG	C-N-CA	-6.53	114.12	121.83
1	A	27	ARG	CA-C-N	-6.47	114.20	121.83
1	A	27	ARG	C-N-CA	-6.47	114.20	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	PRO	N-CA-CB	6.32	106.84	102.35
1	B	60	ARG	NE-CZ-NH1	6.28	127.78	121.50
1	A	9	PHE	CE1-CZ-CE2	-6.16	108.91	120.00
1	B	85	GLU	N-CA-CB	5.94	119.14	109.69
1	A	18	ASN	OD1-CG-ND2	5.87	128.47	122.60
1	B	60	ARG	CD-NE-CZ	5.82	132.55	124.40
1	B	91	TYR	O-C-N	5.75	128.30	122.09
1	B	60	ARG	CG-CD-NE	-5.69	99.49	112.00
1	B	213	GLU	CG-CD-OE2	-5.68	105.34	118.40
1	B	85	GLU	CA-C-O	5.66	127.37	121.15
1	B	39	ASN	CA-C-N	-5.65	115.02	122.99
1	B	39	ASN	C-N-CA	-5.65	115.02	122.99
1	B	212	HIS	N-CA-C	-5.61	105.20	113.61
1	A	179	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	178	ASP	CA-CB-CG	-5.59	107.01	112.60
1	A	9	PHE	CB-CG-CD1	5.52	130.08	120.70
1	A	80	LEU	CB-CA-C	-5.46	104.77	110.17
1	B	196	ASN	CB-CG-ND2	-5.45	108.23	116.40
1	A	73	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	27	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	A	132	ASN	O-C-N	-5.41	116.88	122.94
1	B	124	ASP	N-CA-CB	5.40	117.89	109.85
1	A	30	MET	CG-SD-CE	-5.37	89.10	100.90
1	B	185	ALA	CA-C-O	5.32	123.53	118.63
1	B	216	ALA	O-C-N	5.31	128.84	122.79
1	A	86	ASN	CA-CB-CG	-5.31	107.29	112.60
1	A	140	LEU	CA-C-N	-5.30	115.14	122.30
1	A	140	LEU	C-N-CA	-5.30	115.14	122.30
1	B	43	MET	CB-CA-C	-5.25	101.19	109.80
1	B	109	VAL	CA-C-O	5.25	126.28	120.46
1	B	4	THR	N-CA-CB	5.24	120.42	111.50
1	B	207	ALA	CA-C-O	5.24	126.32	120.82
1	B	58	THR	CA-C-O	5.21	126.07	120.55
1	B	58	THR	OG1-CB-CG2	-5.21	98.89	109.30
1	A	212	HIS	N-CA-CB	5.14	118.09	110.49
1	A	9	PHE	CD1-CG-CD2	-5.12	110.91	118.60
1	B	187	GLU	CG-CD-OE1	5.07	130.06	118.40
1	B	57	LEU	CA-C-O	5.06	125.91	120.55
1	B	212	HIS	CA-C-O	5.06	125.15	119.18
1	A	87	ASN	CA-C-N	-5.03	114.75	122.60
1	A	87	ASN	C-N-CA	-5.03	114.75	122.60
1	A	124	ASP	CB-CA-C	-5.02	102.07	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	ASP	CB-CA-C	-5.01	103.01	110.88
1	B	187	GLU	CG-CD-OE2	-5.01	106.87	118.40
1	B	85	GLU	CA-C-N	-5.00	115.44	122.94
1	B	85	GLU	C-N-CA	-5.00	115.44	122.94

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	18	0
1	B	1558	0	1550	30	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	45	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 (45) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:50:MET:HE2	1:B:55:MET:HA	1.91	0.52
1:B:108:GLY:HA2	1:B:113:ASP:HB3	1.92	0.50
1:B:172:LEU:HD12	1:B:172:LEU:C	2.37	0.49
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:A:172:LEU:C	1:A:172:LEU:HD12	2.42	0.44
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
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

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	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

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%)	50	18
1	B	164/171 (96%)	156 (95%)	8 (5%)	22	3
All	All	325/342 (95%)	314 (97%)	11 (3%)	32	6

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	194	LYS
1	B	5	LEU
1	B	76	LYS
1	B	88	THR
1	B	89	SER
1	B	100	GLU

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Mol	Chain	Res	Type
1	B	184	ARG
1	B	194	LYS
1	B	217	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	132	ASN
1	B	39	ASN
1	B	132	ASN
1	B	177	ASN
1	B	195	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 ⓘ

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.