



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:37 AM UTC

PDB ID : 1G58 / pdb_00001g58
Title : CRYSTAL STRUCTURE OF 3,4-DIHYDROXY-2-BUTANONE 4-PHOSPHATE SYNTHASE GOLD DERIVATIVE
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Deposited on : 2000-10-30
Resolution : 1.55 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

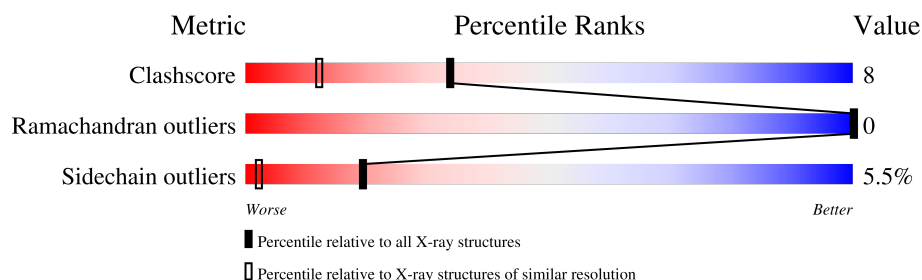
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)

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	
1	B	217	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3225 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	196	Total	C	N	O	S	0	0	0
			1463	907	259	284	13			
1	B	196	Total	C	N	O	S	0	0	0
			1461	906	259	283	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 GOLD ION (CCD ID: AU) (formula: Au).

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

- Molecule 3 is water.

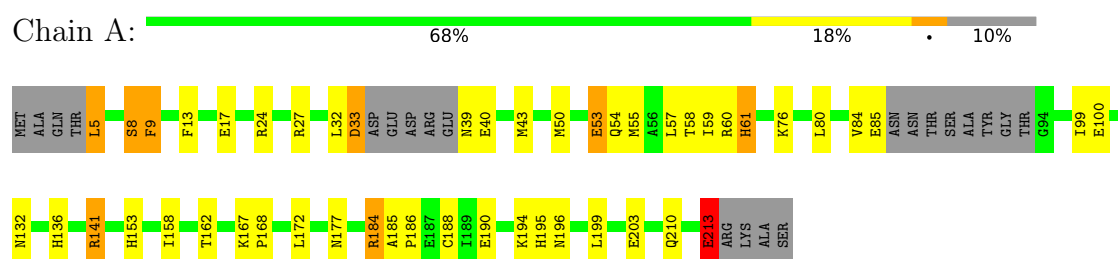
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total	O	0	0
			136	136		
3	B	163	Total	O	0	0
			163	163		

3 Residue-property plots

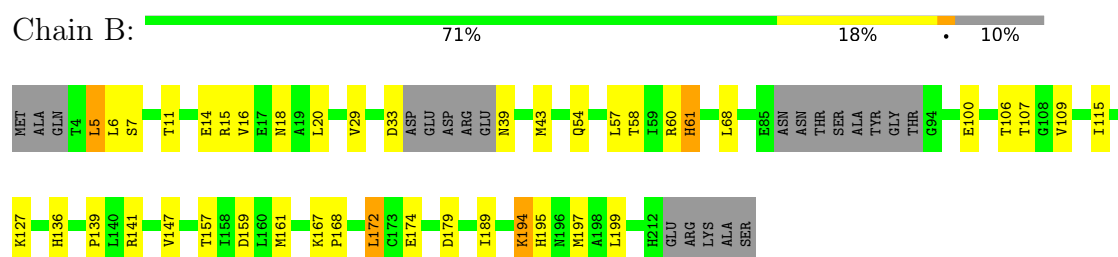
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	78.22Å 78.22Å 69.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 1.55	Depositor
% Data completeness (in resolution range)	90.5 (25.00-1.55)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.185 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3225	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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:
AU

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	4/1481 (0.3%)	1.73	23/2003 (1.1%)
1	B	1.28	1/1479 (0.1%)	1.66	15/2001 (0.7%)
All	All	1.30	5/2960 (0.2%)	1.70	38/4004 (0.9%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	ARG	NE-CZ	5.50	1.39	1.33
1	A	213	GLU	CD-OE2	5.42	1.35	1.25
1	B	141	ARG	CZ-NH1	5.36	1.40	1.32
1	A	190	GLU	CD-OE2	5.09	1.35	1.25
1	A	132	ASN	C-N	-5.03	1.26	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	ASN	OD1-CG-ND2	-11.72	110.88	122.60
1	A	27	ARG	CA-C-N	-8.64	113.40	122.30
1	A	27	ARG	C-N-CA	-8.64	113.40	122.30
1	A	80	LEU	CA-C-O	8.29	126.33	119.36
1	B	141	ARG	NE-CZ-NH2	-8.21	111.81	119.20
1	A	53	GLU	CB-CG-CD	7.16	124.77	112.60
1	B	39	ASN	N-CA-CB	6.86	122.16	110.50
1	B	43	MET	CB-CA-C	-6.71	98.91	109.84
1	A	80	LEU	O-C-N	-6.49	115.09	121.19
1	A	39	ASN	CA-CB-CG	-6.14	106.46	112.60
1	A	61	HIS	CA-CB-CG	-6.03	107.77	113.80
1	B	168	PRO	N-CA-CB	5.99	106.60	102.35
1	A	136	HIS	CA-CB-CG	-5.92	107.88	113.80
1	A	33	ASP	CA-CB-CG	-5.75	106.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	PHE	N-CA-CB	5.69	118.48	110.12
1	B	61	HIS	CA-CB-CG	-5.69	108.11	113.80
1	B	39	ASN	CB-CG-ND2	5.64	124.86	116.40
1	A	196	ASN	N-CA-CB	5.61	120.83	112.30
1	B	174	GLU	CA-C-O	5.57	127.04	120.69
1	B	61	HIS	ND1-CG-CD2	5.56	111.66	106.10
1	B	136	HIS	CA-CB-CG	-5.54	108.26	113.80
1	A	9	PHE	CA-CB-CG	-5.52	108.28	113.80
1	B	18	ASN	OD1-CG-ND2	5.52	128.12	122.60
1	A	24	ARG	CD-NE-CZ	5.51	132.11	124.40
1	B	39	ASN	CB-CA-C	-5.50	99.66	110.10
1	A	195	HIS	CA-CB-CG	-5.37	108.43	113.80
1	B	33	ASP	N-CA-CB	5.25	119.42	110.50
1	A	5	LEU	N-CA-CB	5.19	119.33	110.50
1	B	179	ASP	CA-CB-CG	-5.18	107.42	112.60
1	A	167	LYS	N-CA-C	-5.15	102.68	109.84
1	A	190	GLU	CA-CB-CG	-5.13	103.85	114.10
1	A	13	PHE	CB-CA-C	5.12	119.29	110.79
1	A	53	GLU	CG-CD-OE1	5.10	130.13	118.40
1	A	43	MET	CB-CA-C	-5.04	101.62	109.84
1	A	40	GLU	N-CA-C	5.04	116.63	108.26
1	A	99	ILE	N-CA-C	5.04	117.26	108.95
1	A	141	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	B	60	ARG	CD-NE-CZ	5.03	131.44	124.40

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	1463	0	1458	25	0
1	B	1461	0	1459	20	0
2	A	1	0	0	1	0
2	B	1	0	0	0	0
3	A	136	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	163	0	0	4	0
All	All	3225	0	2917	45	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 8.

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:57:LEU:HD12	1:A:61:HIS:HD2	1.49	0.77
1:A:57:LEU:CD1	1:A:61:HIS:HD2	1.97	0.76
1:B:167:LYS:NZ	3:B:420:HOH:O	2.21	0.73
1:A:54:GLN:O	1:A:58:THR:HG23	1.89	0.72
1:A:203:GLU:HG2	3:A:428:HOH:O	1.89	0.72
1:A:85:GLU:HG2	3:A:353:HOH:O	1.89	0.71
1:B:195:HIS:ND1	3:B:449:HOH:O	2.25	0.69
1:A:158:ILE:O	1:A:162:THR:HG23	1.93	0.68
1:A:188:CYS:SG	2:A:302:AU:AU	2.25	0.64
1:B:54:GLN:O	1:B:58:THR:HG23	2.03	0.58
1:B:172:LEU:HD12	1:B:172:LEU:C	2.30	0.57
1:B:5:LEU:HB3	1:B:189:ILE:HD13	1.86	0.56
1:A:5:LEU:HB2	3:A:375:HOH:O	2.07	0.54
1:A:177:ASN:ND2	1:A:184:ARG:HH12	2.06	0.53
1:B:11:THR:OG1	1:B:14:GLU:HG3	2.08	0.53
1:A:184:ARG:NH2	3:A:366:HOH:O	2.40	0.52
1:B:5:LEU:HB3	1:B:189:ILE:CD1	2.40	0.52
1:B:167:LYS:HE2	3:B:412:HOH:O	2.09	0.51
1:A:8:SER:HB2	1:A:9:PHE:CD1	2.45	0.51
1:A:59:ILE:O	3:A:391:HOH:O	2.20	0.51
1:A:172:LEU:C	1:A:172:LEU:HD12	2.36	0.50
1:B:106:THR:OG1	1:B:107:THR:N	2.45	0.50
1:A:210:GLN:HA	1:A:213:GLU:HG3	1.94	0.49
1:A:57:LEU:CD1	1:A:61:HIS:CD2	2.87	0.48
1:B:57:LEU:HD12	1:B:61:HIS:HD2	1.79	0.48
1:A:141:ARG:HD2	1:A:141:ARG:C	2.39	0.48
1:B:194:LYS:HE3	3:B:388:HOH:O	2.13	0.47
1:A:33:ASP:HB2	1:A:153:HIS:CE1	2.49	0.47
1:B:57:LEU:CD1	1:B:61:HIS:HD2	2.28	0.47
1:A:60:ARG:HG3	1:A:60:ARG:NH1	2.30	0.46
1:A:60:ARG:HA	1:A:60:ARG:HD2	1.70	0.46
1:B:194:LYS:HB2	1:B:194:LYS:HE2	1.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:VAL:C	1:B:197:MET:HE2	2.42	0.45
1:A:57:LEU:HD11	1:A:61:HIS:HD2	1.80	0.45
1:A:50:MET:HE2	1:A:55:MET:HA	1.99	0.43
1:A:57:LEU:HD11	1:A:61:HIS:CD2	2.54	0.43
1:A:185:ALA:N	1:A:186:PRO:HD2	2.34	0.43
1:A:162:THR:HG22	1:A:168:PRO:HB3	2.00	0.43
1:A:199:LEU:C	1:A:199:LEU:HD23	2.44	0.42
1:B:157:THR:O	1:B:161:MET:HG2	2.20	0.41
1:B:147:VAL:HG22	1:B:159:ASP:OD2	2.21	0.41
1:B:6:LEU:CD1	1:B:199:LEU:HD22	2.51	0.41
1:B:16:VAL:O	1:B:20:LEU:HG	2.21	0.41
1:B:68:LEU:O	1:B:139:PRO:HA	2.21	0.41
1:B:11:THR:O	1:B:15:ARG:HG3	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	190/217 (88%)	188 (99%)	2 (1%)	0	100	100
1	B	190/217 (88%)	187 (98%)	3 (2%)	0	100	100
All	All	380/434 (88%)	375 (99%)	5 (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	154/171 (90%)	145 (94%)	9 (6%)	18	2
1	B	154/171 (90%)	146 (95%)	8 (5%)	21	2
All	All	308/342 (90%)	291 (94%)	17 (6%)	19	2

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	17	GLU
1	A	32	LEU
1	A	53	GLU
1	A	76	LYS
1	A	84	VAL
1	A	100	GLU
1	A	194	LYS
1	A	213	GLU
1	B	5	LEU
1	B	7	SER
1	B	100	GLU
1	B	109	VAL
1	B	115	ILE
1	B	127	LYS
1	B	172	LEU
1	B	194	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	132	ASN
1	A	177	ASN
1	B	61	HIS
1	B	132	ASN
1	B	143	GLN
1	B	196	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [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.