



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:33 PM UTC

PDB ID : 2DPL / pdb\_00002dpl  
Title : Crystal Structure of the GMP synthase from *Pyrococcus horikoshii* OT3  
Authors : Asada, Y.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2006-05-12  
Resolution : 1.43 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

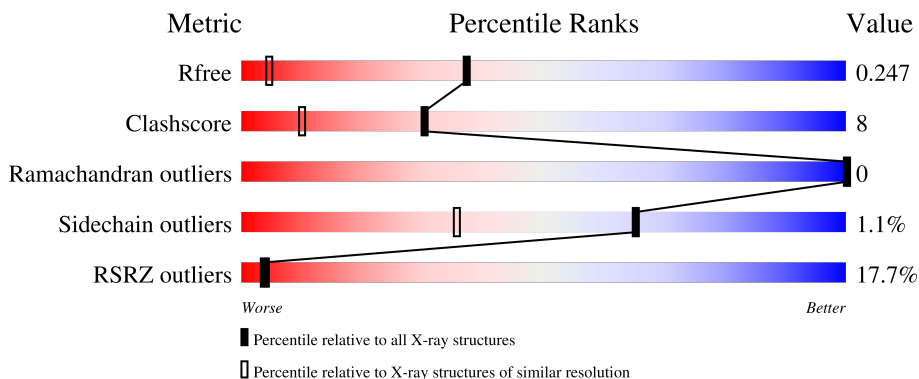
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.43 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))
$R_{free}$	180053	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	308	 8% 80% 13% 7%
1	B	308	 24% 71% 19% 10%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5452 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 GMP synthase [glutamine-hydrolyzing] subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2284	1468	395	416	5	0	3	0
1	B	278	2216	1424	385	403	4	0	3	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	493	Total 493	O 493	0	0
2	B	459	Total 459	O 459	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.40Å 83.33Å 112.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 1.43 29.82 – 1.43	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.82-1.43) 97.7 (29.82-1.43)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.58 (at 1.43Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.236 , 0.249 0.234 , 0.247	Depositor DCC
$R_{free}$ test set	5939 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtrriage
Anisotropy	0.326	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.40	0/2341	0.87	7/3160 (0.2%)
1	B	0.39	0/2270	0.86	2/3064 (0.1%)
All	All	0.40	0/4611	0.86	9/6224 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	LEU	N-CA-C	7.18	120.15	111.82
1	A	44	ILE	N-CA-C	6.59	118.50	112.43
1	A	268	ALA	N-CA-C	-6.33	100.66	110.10
1	A	72	ASP	N-CA-C	5.94	117.56	111.14
1	A	235	LEU	N-CA-C	5.47	118.16	111.82
1	A	159	GLU	CA-C-N	5.38	125.20	119.28
1	A	159	GLU	C-N-CA	5.38	125.20	119.28
1	B	47	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	A	265	THR	N-CA-C	-5.00	101.69	109.24

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	2284	0	2351	30	0
1	B	2216	0	2284	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	493	0	0	13	0
2	B	459	0	0	12	0
All	All	5452	0	4635	77	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 (77) 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:1:MET:HE3	1:A:2:ASP:H	1.28	0.95
1:A:130:ALA:HB3	1:A:131:PRO:HD3	1.62	0.80
1:A:1:MET:CE	1:A:2:ASP:H	1.98	0.76
1:B:238:LYS:HE3	1:B:249:TYR:HB3	1.67	0.74
1:B:85:ASP:HB3	2:B:712:HOH:O	1.89	0.71
1:A:250:LYS:HE2	2:A:550:HOH:O	1.92	0.70
1:B:47:ARG:NH2	2:B:750:HOH:O	2.22	0.69
1:B:211:GLU:HG3	2:B:493:HOH:O	1.95	0.65
1:A:122:GLU:HG2	2:A:695:HOH:O	1.97	0.64
1:A:182:ILE:O	1:A:185:ARG:HG2	1.97	0.64
1:B:69:THR:O	1:B:73:GLU:HB3	1.97	0.64
1:B:161:LEU:HD22	1:B:164:LEU:HD12	1.87	0.57
1:A:238:LYS:NZ	2:A:676:HOH:O	2.36	0.56
1:B:157:LEU:HB3	2:B:718:HOH:O	2.06	0.54
1:A:220:VAL:HG13	1:A:225:LEU:HB2	1.90	0.54
1:B:264:MET:HA	1:B:264:MET:HE2	1.90	0.53
1:B:174:LYS:HE2	1:B:183:TYR:CE1	2.44	0.53
1:B:64:GLU:H	1:B:64:GLU:CD	2.17	0.52
1:A:249:TYR:HE1	2:A:745:HOH:O	1.91	0.52
1:A:130:ALA:HB3	1:A:131:PRO:CD	2.36	0.52
1:A:238:LYS:HE3	2:A:549:HOH:O	2.10	0.51
1:A:58:LEU:HD12	1:A:63:PRO:HG3	1.93	0.51
1:A:62:GLU:HB3	1:A:63:PRO:HD3	1.93	0.51
1:B:38:VAL:O	1:B:42:LYS:HG3	2.11	0.51
1:B:113:GLU:O	1:B:117:LYS:HG3	2.11	0.50
1:B:277:GLN:NE2	2:B:416:HOH:O	2.45	0.50
1:A:185:ARG:NH2	2:A:733:HOH:O	2.33	0.50
1:B:166:LYS:O	1:B:170:ARG:HG3	2.11	0.50
1:A:226:ARG:NE	2:A:759:HOH:O	2.41	0.49
1:A:274:GLU:HA	1:A:277:GLN:HE21	1.78	0.49
1:A:156:LYS:NZ	2:A:750:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:VAL:HG21	1:B:115:VAL:HG21	1.95	0.49
1:A:211:GLU:HG2	2:A:743:HOH:O	2.14	0.48
1:A:131:PRO:HD3	1:A:165:TYR:HA	1.95	0.48
1:B:180:GLU:HA	1:B:183:TYR:CZ	2.49	0.48
1:B:204:GLU:HA	1:B:204:GLU:OE1	2.13	0.48
1:B:190:GLY:N	1:B:191:PRO:HD2	2.29	0.48
1:B:220:VAL:HG13	1:B:225:LEU:HB2	1.96	0.47
2:A:347:HOH:O	1:B:277:GLN:HG2	2.14	0.47
1:A:101:ARG:HD3	2:A:457:HOH:O	2.13	0.47
1:A:1:MET:HE3	1:A:2:ASP:N	2.10	0.47
1:A:242:VAL:HG23	2:A:760:HOH:O	2.14	0.47
1:A:245:ASP:C	1:A:246:ILE:CG2	2.87	0.47
1:B:222:ARG:NH1	2:B:746:HOH:O	2.40	0.47
1:A:27:LEU:HD21	1:A:70:PHE:CG	2.51	0.46
1:B:107:VAL:O	1:B:111:VAL:HG23	2.16	0.46
1:B:12:ARG:HG2	1:B:16:GLU:OE2	2.16	0.45
1:B:68:LYS:HG3	2:B:510:HOH:O	2.14	0.45
1:B:181:LYS:O	1:B:185:ARG:HB3	2.17	0.45
1:B:96:ASP:OD2	1:B:98:GLU:HB2	2.16	0.45
1:B:106:ARG:NH1	2:B:624:HOH:O	2.50	0.45
1:A:22:LYS:HB2	1:A:121:ALA:HA	1.97	0.45
1:A:190:GLY:N	1:A:191:PRO:HD2	2.32	0.45
1:B:64:GLU:CD	1:B:64:GLU:N	2.75	0.45
1:B:86[A]:ARG:HG3	2:B:365:HOH:O	2.15	0.45
1:B:10:LYS:HD3	1:B:13:GLU:OE2	2.17	0.44
1:A:131:PRO:CD	1:A:165:TYR:HA	2.48	0.43
1:B:166:LYS:HA	2:B:720:HOH:O	2.18	0.43
1:B:106:ARG:HH11	1:B:106:ARG:HG2	1.83	0.42
1:B:9:GLU:O	1:B:13:GLU:HG3	2.20	0.42
1:B:62:GLU:HB3	1:B:63:PRO:HD3	2.00	0.42
1:B:170:ARG:CZ	2:B:387:HOH:O	2.68	0.42
1:B:47:ARG:CZ	1:B:47:ARG:HB2	2.48	0.42
1:B:125:ILE:HD13	1:B:158:ILE:HB	2.02	0.42
1:A:245:ASP:C	1:A:246:ILE:HG23	2.45	0.42
1:B:65:PHE:CZ	1:B:181:LYS:HD3	2.55	0.42
1:B:162:ARG:HA	1:B:162:ARG:HD2	1.95	0.42
1:B:243:GLN:OE1	2:B:675:HOH:O	2.21	0.42
1:B:170:ARG:HH11	1:B:170:ARG:HG2	1.86	0.41
1:A:226:ARG:NH2	2:A:759:HOH:O	2.53	0.41
1:B:174:LYS:HG2	1:B:183:TYR:CE2	2.56	0.41
1:A:100:LYS:HE3	1:A:201:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:PHE:HZ	1:B:10:LYS:HZ2	1.68	0.40
1:B:22:LYS:HG2	1:B:47:ARG:HG2	2.03	0.40
1:B:12:ARG:O	1:B:16:GLU:HG3	2.21	0.40
1:B:25:ILE:HB	1:B:125:ILE:HB	2.03	0.40
1:B:234:LEU:HD11	1:B:251:GLU:HB3	2.03	0.40

There are no symmetry-related clashes.

### 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	286/308 (93%)	282 (99%)	4 (1%)	0	100	100
1	B	277/308 (90%)	275 (99%)	2 (1%)	0	100	100
All	All	563/616 (91%)	557 (99%)	6 (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	243/258 (94%)	241 (99%)	2 (1%)	73	48
1	B	236/258 (92%)	233 (99%)	3 (1%)	61	29
All	All	479/516 (93%)	474 (99%)	5 (1%)	65	39

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	LYS
1	A	243	GLN
1	B	47	ARG
1	B	102	LYS
1	B	221	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	154	ASN
1	A	229	GLN
1	A	243	GLN
1	A	277	GLN
1	B	126	GLN
1	B	184	ASN
1	B	243	GLN

### 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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

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

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	287/308 (93%)	0.79	25 (8%) <b>16</b> <b>17</b>	13, 20, 32, 50	3 (1%)
1	B	278/308 (90%)	1.40	75 (26%) <b>1</b> <b>1</b>	14, 27, 45, 53	3 (1%)
All	All	565/616 (91%)	1.09	100 (17%) <b>4</b> <b>4</b>	13, 22, 43, 53	6 (1%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	PRO	6.2
1	B	175	PHE	5.9
1	A	245	ASP	4.8
1	A	244	GLY	4.6
1	B	158	ILE	4.5
1	B	6	PHE	4.5
1	B	155	LEU	4.5
1	B	157	LEU	4.5
1	B	43	ALA	4.4
1	A	249	TYR	4.3
1	B	7	VAL	4.2
1	A	153	LEU	4.1
1	B	123	TYR	3.9
1	A	242	VAL	3.9
1	A	243	GLN	3.8
1	B	129	ILE	3.7
1	A	46	ASP	3.7
1	B	161	LEU	3.6
1	B	109	ILE	3.5
1	B	176	LEU	3.5
1	B	170	ARG	3.5
1	B	178	LEU	3.4
1	A	247	ARG	3.3
1	B	15	ARG	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	246	ILE	3.3
1	B	47	ARG	3.2
1	B	8	GLU	3.2
1	A	154	ASN	3.2
1	B	17	THR	3.2
1	B	182	ILE	3.2
1	B	261	ILE	3.2
1	B	110	GLU	3.2
1	B	74	PHE	3.1
1	B	73	GLU	3.1
1	B	165	TYR	3.1
1	A	130	ALA	3.1
1	B	16	GLU	3.1
1	B	183	TYR	3.0
1	B	167	ASP	3.0
1	B	163	ASP	3.0
1	B	162	ARG	3.0
1	B	117	LYS	3.0
1	B	179	PRO	3.0
1	B	11	VAL	2.9
1	B	164	LEU	2.9
1	A	308	GLU	2.9
1	A	248	ALA	2.9
1	B	262	ASP	2.9
1	B	116	ALA	2.9
1	B	169	VAL	2.9
1	B	29	GLY	2.9
1	B	124	LEU	2.8
1	B	264	MET	2.7
1	B	28	SER	2.7
1	B	113	GLU	2.7
1	B	184	ASN	2.6
1	B	69	THR	2.6
1	B	64	GLU	2.6
1	B	173	ALA	2.5
1	B	44	ILE	2.5
1	B	10	LYS	2.5
1	A	85	ASP	2.5
1	A	236	GLY	2.5
1	B	14	ILE	2.4
1	B	107	VAL	2.4
1	B	221	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	181	LYS	2.4
1	A	27	LEU	2.4
1	B	68	LYS	2.4
1	A	171	GLU	2.4
1	B	98	GLU	2.3
1	B	67	VAL	2.3
1	B	160	PRO	2.3
1	A	12	ARG	2.3
1	B	111	VAL	2.3
1	B	72	ASP	2.3
1	B	49	HIS	2.3
1	B	174	LYS	2.3
1	B	25	ILE	2.3
1	B	21	SER	2.3
1	B	40	ALA	2.2
1	B	9	GLU	2.2
1	B	274	GLU	2.2
1	B	82	ASP	2.2
1	B	236	GLY	2.2
1	B	51	VAL	2.2
1	B	36	ALA	2.2
1	B	18	VAL	2.2
1	B	23	ALA	2.1
1	B	39	LEU	2.1
1	A	99	GLU	2.1
1	A	93	GLY	2.1
1	B	122	GLU	2.1
1	B	12	ARG	2.1
1	A	74	PHE	2.0
1	A	157	LEU	2.0
1	B	171	GLU	2.0
1	A	261	ILE	2.0
1	B	119	ILE	2.0
1	A	20	ASP	2.0

## 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.