



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:45 AM UTC

PDB ID : 1AJZ / pdb_00001ajz
Title : STRUCTURE OF DIHYDROPTEROATE PYROPHOSPHORYLASE
Authors : Achari, A.; Somers, D.O.; Champness, J.N.; Bryant, P.K.; Rosemond, J.;
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Deposited on : 1997-05-13
Resolution : 2.00 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

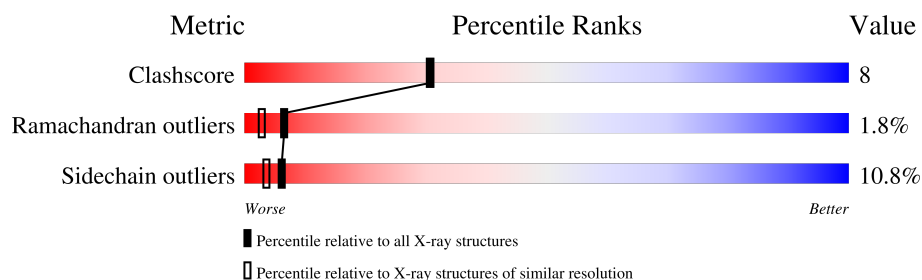
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	282	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2308 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 DIHYDROPTEROATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	282	2147	1348	378	408	13	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

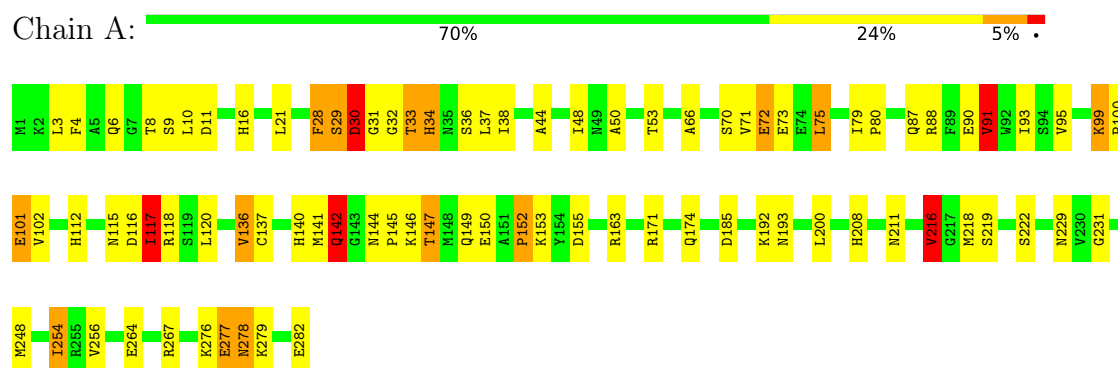
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	151	Total	O	0	0
			151	151		

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: DIHYDROPTEROATE SYNTHASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.02Å 60.20Å 59.80Å 90.00° 114.50° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	91.9 (10.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2308	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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	1.06	4/2184 (0.2%)	1.81	45/2953 (1.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	VAL	CA-CB	6.23	1.63	1.54
1	A	277	GLU	CA-CB	6.16	1.63	1.53
1	A	254	ILE	CA-CB	5.64	1.61	1.54
1	A	279	LYS	CA-CB	5.21	1.61	1.53

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	PHE	O-C-N	10.51	135.69	122.65
1	A	29	SER	O-C-N	8.53	133.74	122.82
1	A	248	MET	CG-SD-CE	-8.36	82.50	100.90
1	A	277	GLU	CB-CG-CD	7.59	125.51	112.60
1	A	91	VAL	CB-CA-C	-7.16	99.55	111.29
1	A	279	LYS	CA-CB-CG	7.05	128.21	114.10
1	A	216	VAL	N-CA-CB	-7.00	99.97	111.45
1	A	147	THR	OG1-CB-CG2	6.92	123.14	109.30
1	A	153	LYS	N-CA-C	-6.68	98.83	109.59
1	A	88	ARG	CB-CG-CD	6.66	126.61	111.30
1	A	50	ALA	N-CA-C	-6.48	105.37	113.28
1	A	29	SER	N-CA-C	6.43	118.60	110.24
1	A	229	ASN	OD1-CG-ND2	6.20	128.80	122.60
1	A	36	SER	N-CA-C	-6.18	105.70	113.18
1	A	117	ILE	CB-CA-C	-6.17	103.04	112.05
1	A	144	ASN	CA-C-N	6.14	125.87	119.05
1	A	144	ASN	C-N-CA	6.14	125.87	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	GLN	CG-CD-NE2	5.95	125.32	116.40
1	A	222	SER	CA-C-O	-5.85	114.32	120.63
1	A	99	LYS	CA-C-N	5.77	125.24	119.24
1	A	99	LYS	C-N-CA	5.77	125.24	119.24
1	A	185	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	144	ASN	N-CA-C	-5.73	101.31	109.62
1	A	267	ARG	CA-CB-CG	-5.70	102.70	114.10
1	A	37	LEU	CA-C-O	-5.62	114.00	120.24
1	A	87	GLN	CG-CD-NE2	5.59	124.78	116.40
1	A	211	ASN	CA-CB-CG	-5.51	107.09	112.60
1	A	185	ASP	CA-C-N	5.49	125.20	119.82
1	A	185	ASP	C-N-CA	5.49	125.20	119.82
1	A	28	PHE	CA-C-N	5.46	128.85	120.82
1	A	28	PHE	C-N-CA	5.46	128.85	120.82
1	A	193	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	34	HIS	N-CA-C	-5.38	99.33	110.80
1	A	229	ASN	N-CA-CB	-5.33	104.08	112.13
1	A	147	THR	N-CA-CB	5.23	118.24	110.29
1	A	222	SER	CB-CA-C	-5.20	101.84	110.68
1	A	95	VAL	CG1-CB-CG2	-5.20	99.37	110.80
1	A	150	GLU	N-CA-C	5.19	116.99	110.24
1	A	264	GLU	CA-C-O	-5.17	115.40	120.82
1	A	79	ILE	N-CA-CB	-5.15	106.43	110.45
1	A	155	ASP	N-CA-C	-5.12	105.59	111.07
1	A	231	GLY	CA-C-N	5.10	124.89	119.28
1	A	231	GLY	C-N-CA	5.10	124.89	119.28
1	A	142	GLN	CA-C-O	5.09	125.63	120.24
1	A	116	ASP	N-CA-C	5.00	116.90	109.25

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	2147	0	2159	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	0	0	0
3	A	151	0	0	3	0
All	All	2308	0	2159	36	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 (36) 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:30:ASP:HB2	1:A:34:HIS:ND1	2.09	0.66
1:A:276:LYS:HZ2	1:A:278:ASN:HD21	1.44	0.66
1:A:71:VAL:HG22	1:A:99:LYS:HD3	1.80	0.64
1:A:44:ALA:O	1:A:48:ILE:HG13	2.00	0.61
1:A:276:LYS:NZ	1:A:278:ASN:HD21	2.00	0.59
1:A:71:VAL:CG1	1:A:101:GLU:HG3	2.35	0.57
1:A:115:ASN:HD22	1:A:137:CYS:HB3	1.70	0.56
1:A:16:HIS:HD2	1:A:53:THR:OG1	1.88	0.55
1:A:93:ILE:H	1:A:112:HIS:CD2	2.24	0.55
1:A:11:ASP:O	1:A:16:HIS:HE1	1.91	0.54
1:A:140:HIS:HD2	1:A:192:LYS:NZ	2.05	0.53
1:A:216:VAL:HG13	1:A:218:MET:HE2	1.92	0.51
1:A:4:PHE:CD1	1:A:9:SER:HB3	2.47	0.50
1:A:3:LEU:O	1:A:9:SER:HA	2.12	0.50
1:A:4:PHE:CE1	1:A:9:SER:HB3	2.47	0.49
1:A:142:GLN:HB3	1:A:152:PRO:HG2	1.96	0.47
1:A:71:VAL:HG11	1:A:101:GLU:HG3	1.96	0.47
1:A:117:ILE:HD11	3:A:331:HOH:O	2.15	0.46
1:A:208:HIS:HD2	3:A:293:HOH:O	1.97	0.46
1:A:141:MET:SD	1:A:145:PRO:HB3	2.56	0.45
1:A:278:ASN:HD22	1:A:278:ASN:H	1.64	0.45
1:A:66:ALA:HB3	1:A:146:LYS:HE3	1.98	0.45
1:A:93:ILE:H	1:A:112:HIS:HD2	1.63	0.45
1:A:276:LYS:NZ	1:A:278:ASN:ND2	2.63	0.45
1:A:99:LYS:HA	1:A:100:PRO:HD3	1.72	0.44
1:A:70:SER:OG	1:A:73:GLU:HG3	2.17	0.44
1:A:72:GLU:HB2	3:A:400:HOH:O	2.18	0.44
1:A:71:VAL:HG12	1:A:75:LEU:HD22	2.00	0.43
1:A:120:LEU:O	1:A:171:ARG:NH2	2.52	0.43
1:A:28:PHE:CE2	1:A:33:THR:HG23	2.54	0.43
1:A:75:LEU:HD13	1:A:102:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:SER:HB2	1:A:256:VAL:HA	2.02	0.42
1:A:117:ILE:HD13	1:A:118:ARG:HG3	2.02	0.42
1:A:16:HIS:CD2	1:A:53:THR:OG1	2.71	0.42
1:A:254:ILE:HG22	1:A:256:VAL:HG13	2.03	0.41
1:A:71:VAL:HG13	1:A:101:GLU:HG3	2.02	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	280/282 (99%)	265 (95%)	10 (4%)	5 (2%)	6 3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	GLY
1	A	30	ASP
1	A	31	GLY
1	A	33	THR
1	A	91	VAL

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	231/231 (100%)	206 (89%)	25 (11%)	6 3

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	THR
1	A	10	LEU
1	A	21	LEU
1	A	29	SER
1	A	30	ASP
1	A	38	ILE
1	A	72	GLU
1	A	75	LEU
1	A	80	PRO
1	A	90	GLU
1	A	91	VAL
1	A	101	GLU
1	A	117	ILE
1	A	136	VAL
1	A	142	GLN
1	A	147	THR
1	A	149	GLN
1	A	152	PRO
1	A	163	ARG
1	A	200	LEU
1	A	216	VAL
1	A	277	GLU
1	A	278	ASN
1	A	282	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	16	HIS
1	A	45	ASN
1	A	49	ASN
1	A	112	HIS
1	A	115	ASN
1	A	140	HIS
1	A	142	GLN

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Mol	Chain	Res	Type
1	A	162	ASN
1	A	208	HIS
1	A	278	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](#)

2 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	283	-	4,4,4	0.58	0	6,6,6	0.58	0
2	SO4	A	284	-	4,4,4	0.34	0	6,6,6	0.80	0

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.