



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 06:45 pm BST

PDB ID : 2CG8
Title : The bifunctional dihydroneopterin aldolase 6-hydroxymethyl-7,8- dihydropterin synthase from *Streptococcus pneumoniae*
Authors : Garcon, A.; Levy, C.; Derrick, J.P.
Deposited on : 2006-02-28
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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) : 2.11

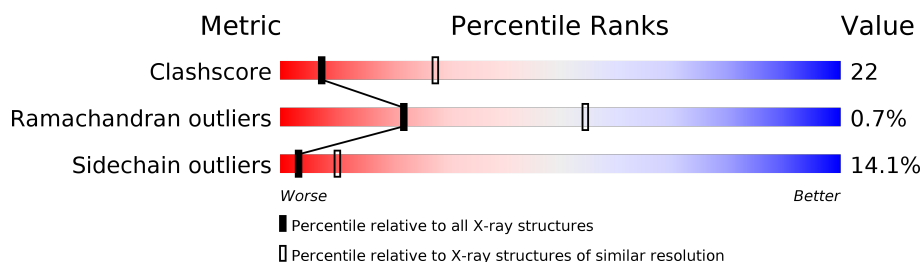
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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	270	
1	B	270	
1	C	270	
1	D	270	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7968 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 DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE.

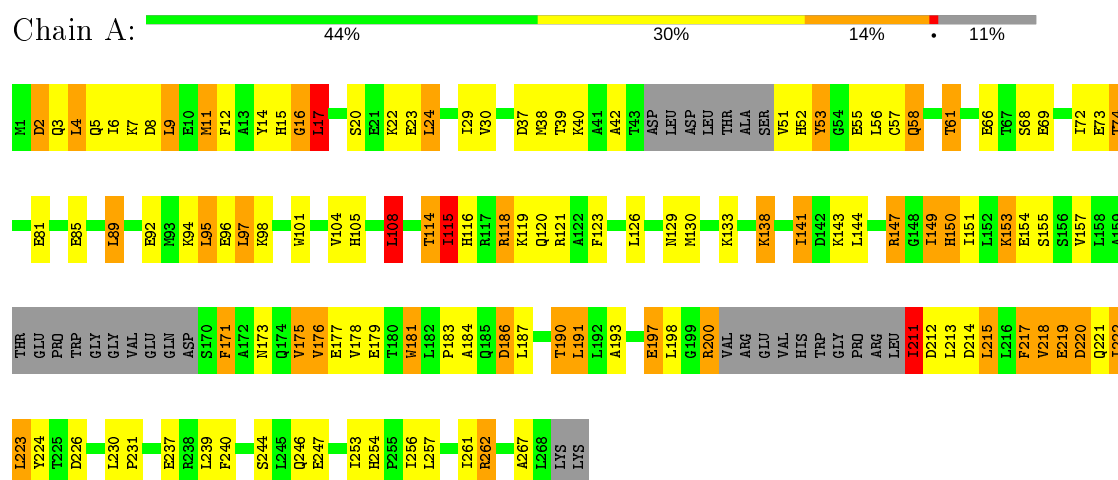
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	1
			1953	1263	321	362	7			
1	B	248	Total	C	N	O	S	0	0	1
			2006	1293	331	375	7			
1	C	249	Total	C	N	O	S	0	0	1
			2011	1299	329	376	7			
1	D	248	Total	C	N	O	S	0	0	2
			1998	1289	331	371	7			

3 Residue-property plots

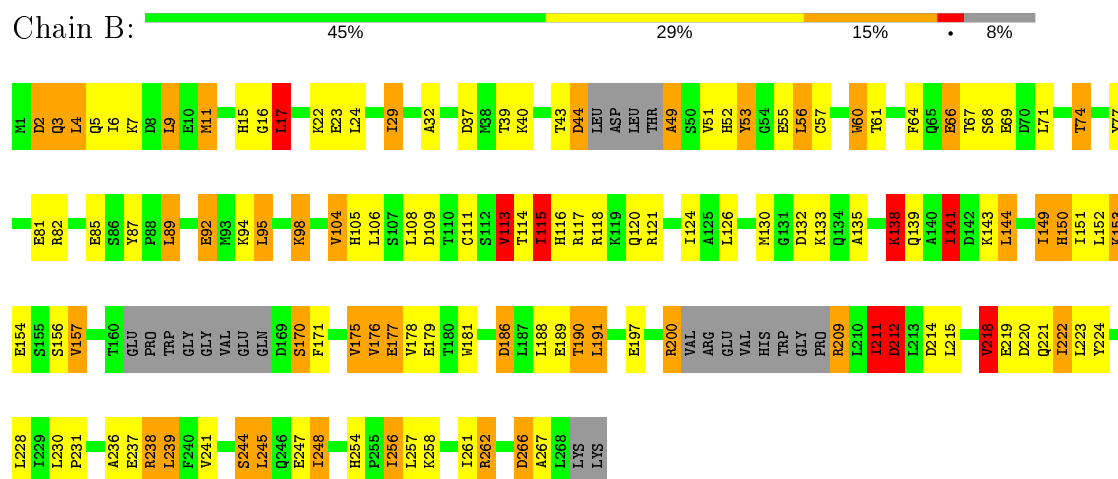
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

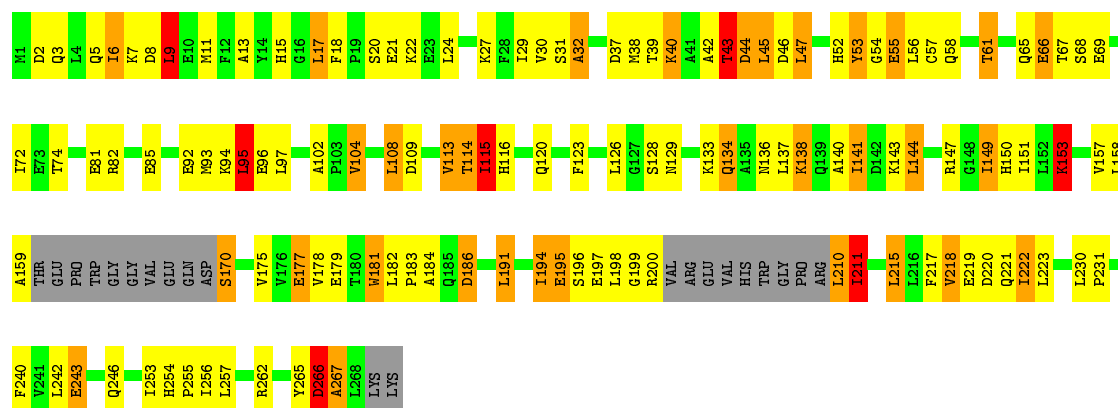
- Molecule 1: DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE



- Molecule 1: DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE

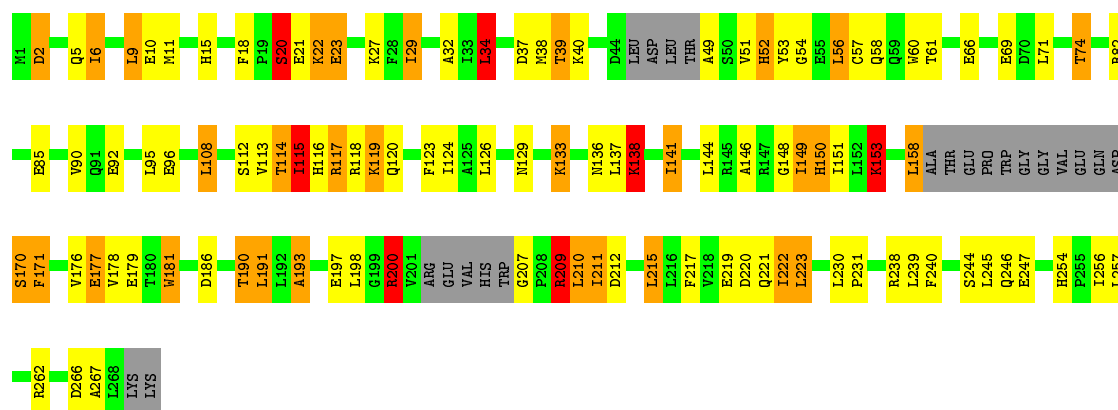


Chain C: 45% 33% 12% 8%



• Molecule 1: DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE

Chain D: 52% 26% 11% 8%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.44Å 149.44Å 238.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.00 – 2.90	Depositor
% Data completeness (in resolution range)	99.8 (127.00-2.90)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7968	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.83	46/1993 (2.3%)	1.65	43/2700 (1.6%)
1	B	1.92	55/2046 (2.7%)	1.63	40/2772 (1.4%)
1	C	1.71	35/2052 (1.7%)	1.53	28/2783 (1.0%)
1	D	1.76	36/2039 (1.8%)	1.54	25/2763 (0.9%)
All	All	1.81	172/8130 (2.1%)	1.59	136/11018 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

The worst 5 of 172 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	TRP	CG-CD1	11.50	1.52	1.36
1	A	181	TRP	CG-CD1	11.42	1.52	1.36
1	A	219	GLU	CD-OE2	11.05	1.37	1.25
1	D	153	LYS	CD-CE	10.99	1.78	1.51
1	C	55	GLU	CD-OE2	10.94	1.37	1.25

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	ARG	NE-CZ-NH2	12.34	126.47	120.30
1	A	2	ASP	CB-CG-OD1	-10.10	109.21	118.30
1	A	220	ASP	CB-CG-OD2	9.90	127.21	118.30
1	D	71	LEU	CB-CG-CD2	-9.81	94.33	111.00
1	B	209	ARG	NE-CZ-NH1	-9.71	115.44	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	266	ASP	Peptide
1	D	223	LEU	Peptide

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	1953	0	1967	94	0
1	B	2006	0	2016	87	0
1	C	2011	0	2026	107	0
1	D	1998	0	2010	88	0
All	All	7968	0	8019	357	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 22.

The worst 5 of 357 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:C:153:LYS:CE	1:C:153:LYS:CD	1.77	1.62
1:A:153:LYS:CD	1:A:153:LYS:CG	1.81	1.58
1:A:17:LEU:CG	1:A:17:LEU:CD1	1.78	1.58
1:D:141:ILE:CD1	1:D:141:ILE:CG1	1.81	1.56
1:D:153:LYS:CD	1:D:153:LYS:CE	1.78	1.56

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	233/270 (86%)	223 (96%)	10 (4%)	0	100	100
1	B	240/270 (89%)	229 (95%)	10 (4%)	1 (0%)	34	66
1	C	243/270 (90%)	223 (92%)	16 (7%)	4 (2%)	9	32
1	D	240/270 (89%)	220 (92%)	18 (8%)	2 (1%)	19	51
All	All	956/1080 (88%)	895 (94%)	54 (6%)	7 (1%)	22	54

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	SER
1	C	266	ASP
1	D	210	LEU
1	D	267	ALA
1	C	134	GLN

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	215/241 (89%)	188 (87%)	27 (13%)	4	13
1	B	221/241 (92%)	188 (85%)	33 (15%)	3	9
1	C	222/241 (92%)	191 (86%)	31 (14%)	3	10
1	D	220/241 (91%)	187 (85%)	33 (15%)	3	9
All	All	878/964 (91%)	754 (86%)	124 (14%)	3	10

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	222	ILE
1	C	95	LEU
1	D	190	THR

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Mol	Chain	Res	Type
1	B	239	LEU
1	C	20	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	254	HIS
1	C	105	HIS
1	D	139	GLN
1	C	15	HIS
1	C	116	HIS

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 carbohydrates 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 [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.