W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2023 – 04:32 AM EDT

PDB ID	:	3GK0
Title	:	Crystal structure of pyridoxal phosphate biosynthetic protein from Burkholderia pseudomallei
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2009-03-09
Resolution	:	2.28 Å(reported)

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

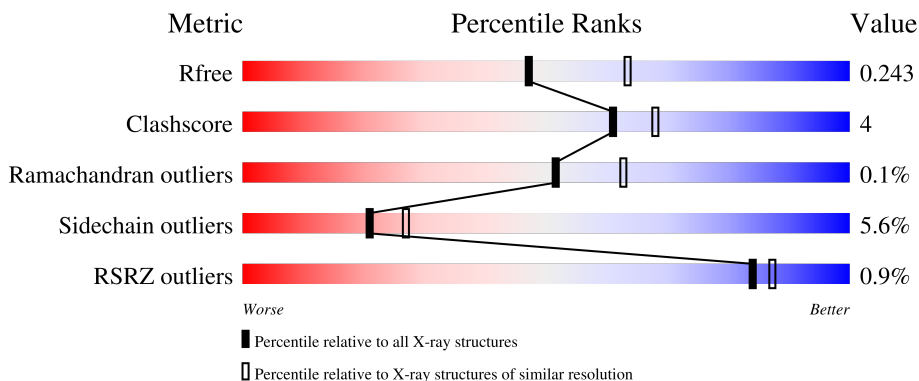|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.28 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	Percentile Ranks	Value
Rfree		0.243
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		5.6%
RSRZ outliers		0.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 <=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	278	% 78% 13% 9%
1	B	278	3% 76% 14% • 9%
1	C	278	76% 10% • 12%
1	D	278	% 79% 9% 12%
1	E	278	78% 9% • 12%

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Mol	Chain	Length	Quality of chain
1	F	278	79% 8% · 12%
1	G	278	82% 6% 12%
1	H	278	77% 10% · 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DXP	C	258	X	X	-	-
3	DXP	G	259	-	X	-	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 15737 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 Pyridoxine 5'-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	2	0
			1911	1190	362	351	8			
1	B	252	Total	C	N	O	S	0	2	0
			1906	1187	358	353	8			
1	C	244	Total	C	N	O	S	0	1	0
			1836	1138	346	343	9			
1	D	246	Total	C	N	O	S	0	1	0
			1843	1144	346	345	8			
1	E	245	Total	C	N	O	S	0	0	0
			1829	1134	345	342	8			
1	F	244	Total	C	N	O	S	0	2	0
			1838	1140	346	343	9			
1	G	245	Total	C	N	O	S	0	1	0
			1825	1133	342	342	8			
1	H	246	Total	C	N	O	S	0	0	0
			1834	1137	346	343	8			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q3JQ80
A	-19	ALA	-	expression tag	UNP Q3JQ80
A	-18	HIS	-	expression tag	UNP Q3JQ80
A	-17	HIS	-	expression tag	UNP Q3JQ80
A	-16	HIS	-	expression tag	UNP Q3JQ80
A	-15	HIS	-	expression tag	UNP Q3JQ80
A	-14	HIS	-	expression tag	UNP Q3JQ80
A	-13	HIS	-	expression tag	UNP Q3JQ80
A	-12	MET	-	expression tag	UNP Q3JQ80
A	-11	GLY	-	expression tag	UNP Q3JQ80
A	-10	THR	-	expression tag	UNP Q3JQ80
A	-9	LEU	-	expression tag	UNP Q3JQ80
A	-8	GLU	-	expression tag	UNP Q3JQ80

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ALA	-	expression tag	UNP Q3JQ80
A	-6	GLN	-	expression tag	UNP Q3JQ80
A	-5	THR	-	expression tag	UNP Q3JQ80
A	-4	GLN	-	expression tag	UNP Q3JQ80
A	-3	GLY	-	expression tag	UNP Q3JQ80
A	-2	PRO	-	expression tag	UNP Q3JQ80
A	-1	GLY	-	expression tag	UNP Q3JQ80
A	0	SER	-	expression tag	UNP Q3JQ80
B	-20	MET	-	expression tag	UNP Q3JQ80
B	-19	ALA	-	expression tag	UNP Q3JQ80
B	-18	HIS	-	expression tag	UNP Q3JQ80
B	-17	HIS	-	expression tag	UNP Q3JQ80
B	-16	HIS	-	expression tag	UNP Q3JQ80
B	-15	HIS	-	expression tag	UNP Q3JQ80
B	-14	HIS	-	expression tag	UNP Q3JQ80
B	-13	HIS	-	expression tag	UNP Q3JQ80
B	-12	MET	-	expression tag	UNP Q3JQ80
B	-11	GLY	-	expression tag	UNP Q3JQ80
B	-10	THR	-	expression tag	UNP Q3JQ80
B	-9	LEU	-	expression tag	UNP Q3JQ80
B	-8	GLU	-	expression tag	UNP Q3JQ80
B	-7	ALA	-	expression tag	UNP Q3JQ80
B	-6	GLN	-	expression tag	UNP Q3JQ80
B	-5	THR	-	expression tag	UNP Q3JQ80
B	-4	GLN	-	expression tag	UNP Q3JQ80
B	-3	GLY	-	expression tag	UNP Q3JQ80
B	-2	PRO	-	expression tag	UNP Q3JQ80
B	-1	GLY	-	expression tag	UNP Q3JQ80
B	0	SER	-	expression tag	UNP Q3JQ80
C	-20	MET	-	expression tag	UNP Q3JQ80
C	-19	ALA	-	expression tag	UNP Q3JQ80
C	-18	HIS	-	expression tag	UNP Q3JQ80
C	-17	HIS	-	expression tag	UNP Q3JQ80
C	-16	HIS	-	expression tag	UNP Q3JQ80
C	-15	HIS	-	expression tag	UNP Q3JQ80
C	-14	HIS	-	expression tag	UNP Q3JQ80
C	-13	HIS	-	expression tag	UNP Q3JQ80
C	-12	MET	-	expression tag	UNP Q3JQ80
C	-11	GLY	-	expression tag	UNP Q3JQ80
C	-10	THR	-	expression tag	UNP Q3JQ80
C	-9	LEU	-	expression tag	UNP Q3JQ80
C	-8	GLU	-	expression tag	UNP Q3JQ80

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ALA	-	expression tag	UNP Q3JQ80
C	-6	GLN	-	expression tag	UNP Q3JQ80
C	-5	THR	-	expression tag	UNP Q3JQ80
C	-4	GLN	-	expression tag	UNP Q3JQ80
C	-3	GLY	-	expression tag	UNP Q3JQ80
C	-2	PRO	-	expression tag	UNP Q3JQ80
C	-1	GLY	-	expression tag	UNP Q3JQ80
C	0	SER	-	expression tag	UNP Q3JQ80
D	-20	MET	-	expression tag	UNP Q3JQ80
D	-19	ALA	-	expression tag	UNP Q3JQ80
D	-18	HIS	-	expression tag	UNP Q3JQ80
D	-17	HIS	-	expression tag	UNP Q3JQ80
D	-16	HIS	-	expression tag	UNP Q3JQ80
D	-15	HIS	-	expression tag	UNP Q3JQ80
D	-14	HIS	-	expression tag	UNP Q3JQ80
D	-13	HIS	-	expression tag	UNP Q3JQ80
D	-12	MET	-	expression tag	UNP Q3JQ80
D	-11	GLY	-	expression tag	UNP Q3JQ80
D	-10	THR	-	expression tag	UNP Q3JQ80
D	-9	LEU	-	expression tag	UNP Q3JQ80
D	-8	GLU	-	expression tag	UNP Q3JQ80
D	-7	ALA	-	expression tag	UNP Q3JQ80
D	-6	GLN	-	expression tag	UNP Q3JQ80
D	-5	THR	-	expression tag	UNP Q3JQ80
D	-4	GLN	-	expression tag	UNP Q3JQ80
D	-3	GLY	-	expression tag	UNP Q3JQ80
D	-2	PRO	-	expression tag	UNP Q3JQ80
D	-1	GLY	-	expression tag	UNP Q3JQ80
D	0	SER	-	expression tag	UNP Q3JQ80
E	-20	MET	-	expression tag	UNP Q3JQ80
E	-19	ALA	-	expression tag	UNP Q3JQ80
E	-18	HIS	-	expression tag	UNP Q3JQ80
E	-17	HIS	-	expression tag	UNP Q3JQ80
E	-16	HIS	-	expression tag	UNP Q3JQ80
E	-15	HIS	-	expression tag	UNP Q3JQ80
E	-14	HIS	-	expression tag	UNP Q3JQ80
E	-13	HIS	-	expression tag	UNP Q3JQ80
E	-12	MET	-	expression tag	UNP Q3JQ80
E	-11	GLY	-	expression tag	UNP Q3JQ80
E	-10	THR	-	expression tag	UNP Q3JQ80
E	-9	LEU	-	expression tag	UNP Q3JQ80
E	-8	GLU	-	expression tag	UNP Q3JQ80

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	ALA	-	expression tag	UNP Q3JQ80
E	-6	GLN	-	expression tag	UNP Q3JQ80
E	-5	THR	-	expression tag	UNP Q3JQ80
E	-4	GLN	-	expression tag	UNP Q3JQ80
E	-3	GLY	-	expression tag	UNP Q3JQ80
E	-2	PRO	-	expression tag	UNP Q3JQ80
E	-1	GLY	-	expression tag	UNP Q3JQ80
E	0	SER	-	expression tag	UNP Q3JQ80
F	-20	MET	-	expression tag	UNP Q3JQ80
F	-19	ALA	-	expression tag	UNP Q3JQ80
F	-18	HIS	-	expression tag	UNP Q3JQ80
F	-17	HIS	-	expression tag	UNP Q3JQ80
F	-16	HIS	-	expression tag	UNP Q3JQ80
F	-15	HIS	-	expression tag	UNP Q3JQ80
F	-14	HIS	-	expression tag	UNP Q3JQ80
F	-13	HIS	-	expression tag	UNP Q3JQ80
F	-12	MET	-	expression tag	UNP Q3JQ80
F	-11	GLY	-	expression tag	UNP Q3JQ80
F	-10	THR	-	expression tag	UNP Q3JQ80
F	-9	LEU	-	expression tag	UNP Q3JQ80
F	-8	GLU	-	expression tag	UNP Q3JQ80
F	-7	ALA	-	expression tag	UNP Q3JQ80
F	-6	GLN	-	expression tag	UNP Q3JQ80
F	-5	THR	-	expression tag	UNP Q3JQ80
F	-4	GLN	-	expression tag	UNP Q3JQ80
F	-3	GLY	-	expression tag	UNP Q3JQ80
F	-2	PRO	-	expression tag	UNP Q3JQ80
F	-1	GLY	-	expression tag	UNP Q3JQ80
F	0	SER	-	expression tag	UNP Q3JQ80
G	-20	MET	-	expression tag	UNP Q3JQ80
G	-19	ALA	-	expression tag	UNP Q3JQ80
G	-18	HIS	-	expression tag	UNP Q3JQ80
G	-17	HIS	-	expression tag	UNP Q3JQ80
G	-16	HIS	-	expression tag	UNP Q3JQ80
G	-15	HIS	-	expression tag	UNP Q3JQ80
G	-14	HIS	-	expression tag	UNP Q3JQ80
G	-13	HIS	-	expression tag	UNP Q3JQ80
G	-12	MET	-	expression tag	UNP Q3JQ80
G	-11	GLY	-	expression tag	UNP Q3JQ80
G	-10	THR	-	expression tag	UNP Q3JQ80
G	-9	LEU	-	expression tag	UNP Q3JQ80
G	-8	GLU	-	expression tag	UNP Q3JQ80

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	ALA	-	expression tag	UNP Q3JQ80
G	-6	GLN	-	expression tag	UNP Q3JQ80
G	-5	THR	-	expression tag	UNP Q3JQ80
G	-4	GLN	-	expression tag	UNP Q3JQ80
G	-3	GLY	-	expression tag	UNP Q3JQ80
G	-2	PRO	-	expression tag	UNP Q3JQ80
G	-1	GLY	-	expression tag	UNP Q3JQ80
G	0	SER	-	expression tag	UNP Q3JQ80
H	-20	MET	-	expression tag	UNP Q3JQ80
H	-19	ALA	-	expression tag	UNP Q3JQ80
H	-18	HIS	-	expression tag	UNP Q3JQ80
H	-17	HIS	-	expression tag	UNP Q3JQ80
H	-16	HIS	-	expression tag	UNP Q3JQ80
H	-15	HIS	-	expression tag	UNP Q3JQ80
H	-14	HIS	-	expression tag	UNP Q3JQ80
H	-13	HIS	-	expression tag	UNP Q3JQ80
H	-12	MET	-	expression tag	UNP Q3JQ80
H	-11	GLY	-	expression tag	UNP Q3JQ80
H	-10	THR	-	expression tag	UNP Q3JQ80
H	-9	LEU	-	expression tag	UNP Q3JQ80
H	-8	GLU	-	expression tag	UNP Q3JQ80
H	-7	ALA	-	expression tag	UNP Q3JQ80
H	-6	GLN	-	expression tag	UNP Q3JQ80
H	-5	THR	-	expression tag	UNP Q3JQ80
H	-4	GLN	-	expression tag	UNP Q3JQ80
H	-3	GLY	-	expression tag	UNP Q3JQ80
H	-2	PRO	-	expression tag	UNP Q3JQ80
H	-1	GLY	-	expression tag	UNP Q3JQ80
H	0	SER	-	expression tag	UNP Q3JQ80

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ —— P ══ O O1

P

O⁻

O4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0
2	E	1	Total 5	O 4	P 1	0	0
2	G	1	Total 5	O 4	P 1	0	0
2	H	1	Total 5	O 4	P 1	0	0

- Molecule 3 is 1-DEOXY-D-XYLULOSE-5-PHOSPHATE (three-letter code: DXP) (formula: $C_5H_{11}O_7P$).

DXP
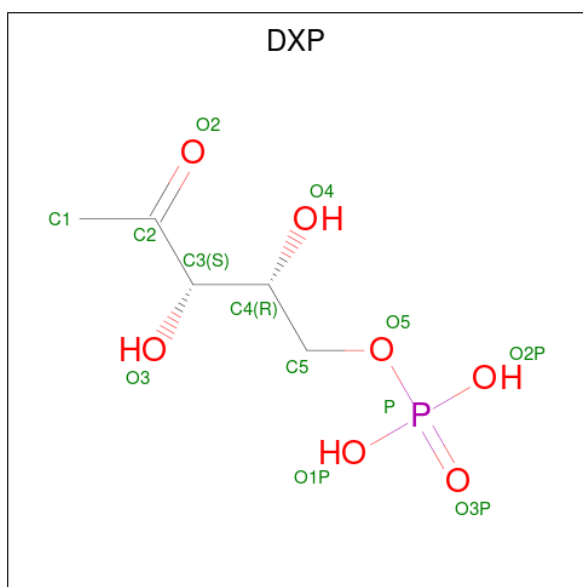
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total 13	C 5	O 7	P 1	0	0
3	F	1	Total 13	C 5	O 7	P 1	0	0
3	G	1	Total 13	C 5	O 7	P 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total 127	O 127	0	0
4	B	121	Total 121	O 121	0	0
4	C	102	Total 102	O 102	0	0
4	D	97	Total 97	O 97	0	0
4	E	98	Total 98	O 98	0	0
4	F	122	Total 122	O 122	0	0
4	G	83	Total 83	O 83	0	0
4	H	101	Total 101	O 101	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

• Molecule 1: Pyridoxine 5'-phosphate synthase
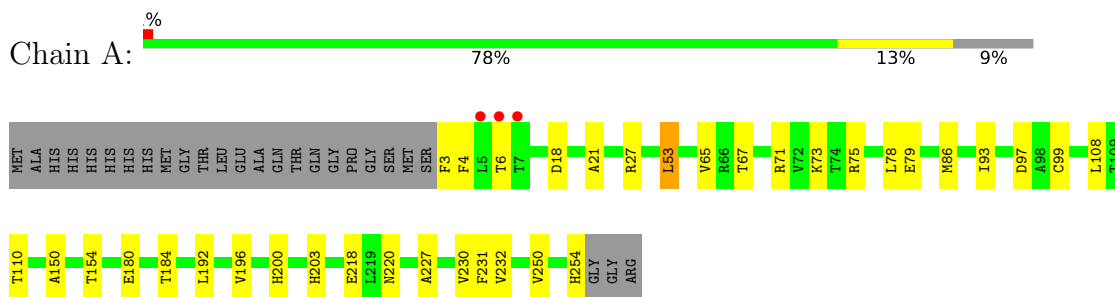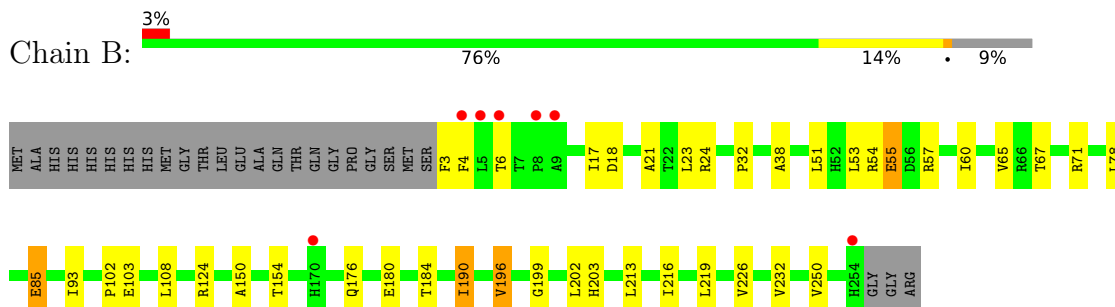
Chain A:

• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain B:

• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain C:

• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain D:

R149 H170 D171 F179 E180 V196 T205 L213 I216 H223 V232 N236 H254 GLY ARG
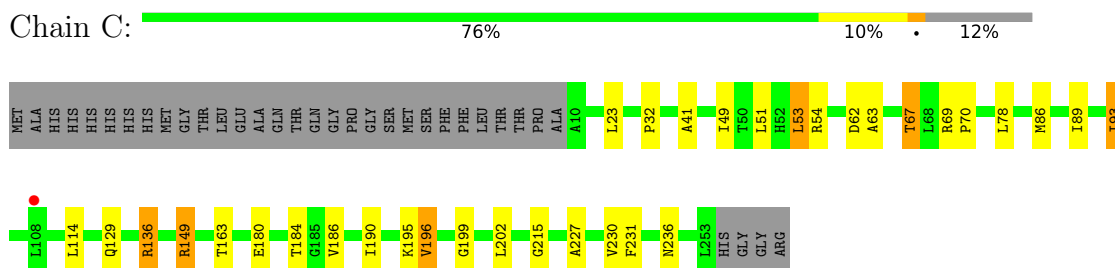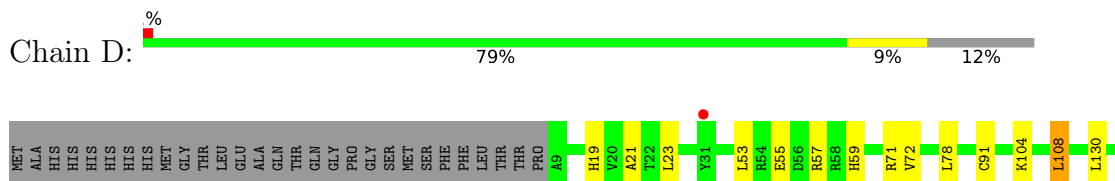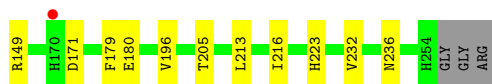
• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain E:

78% 9% · 12%

MET ALA HIS HIS HIS HIS HIS MET GLY THR LEU GLU ALA GLN THR GLN GLY PRO GLY SER MET SER PHE PHE LEU THR THR PRO ALA A10 L23 L51 H52 L53 R54 R57 L78 E79 C80 M86 I93 D97 P102 L108 T109 T110 K128 V135

R136 E145 T163 E178 I182 V186 I190 K195 V196 G199 L202 H203 N236 H254 GLY ARG

• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain F:

79% 8% · 12%

MET ALA HIS HIS HIS HIS HIS MET GLY THR LEU GLU ALA GLN THR GLN GLY PRO GLY SER MET SER PHE PHE LEU THR THR PRO ALA A10 Y31 P32 L51 H52 L53 R54 E55 R58 V65 R71 V72 K73 L78 T83 M86 I93 R149 A150

T154 V186 K195 V196 G199 L202 N206 L213 I216 V232 L253 HIS GLY GLY ARG
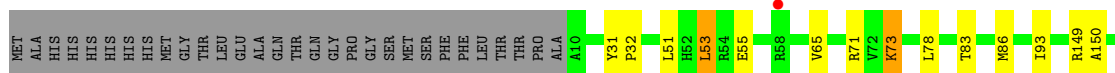
• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain G:

%

82% 6% 12%

MET ALA HIS HIS HIS HIS HIS MET GLY THR LEU GLU ALA GLN THR GLN GLY PRO GLY SER MET SER PHE PHE LEU THR THR PRO ALA A10 L23 L51 H52 L53 R54 E55 D56 R57 V65 L68 L78 A126 R136 H162 T163 Y166 E178 I182

L192 H203 H254 GLY ARG

• Molecule 1: Pyridoxine 5'-phosphate synthase

Chain H:

77% 10% · 12%

MET ALA HIS HIS HIS HIS HIS MET GLY THR LEU GLU ALA GLN THR GLN GLY PRO GLY SER MET SER PHE PHE LEU THR THR PRO A9 D18 A21 T22 L23 V35 L53 R58 H59 D62 V65 L68 R71 L78 I93 L114 C127

R136 L139 R149 T154 G155 A156 H162 D171 F179 V186 V196 G199 L202 L213 I216 A217 E218 L219 N220 N236 H254 GLY GLY ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.09Å 91.86Å 90.02Å 118.48° 116.81° 93.50°	Depositor
Resolution (Å)	46.50 – 2.28 46.50 – 2.28	Depositor EDS
% Data completeness (in resolution range)	94.2 (46.50-2.28) 94.1 (46.50-2.28)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.245 0.185 , 0.243	Depositor DCC
R_{free} test set	4580 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 14.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -l,h+k+l,-k 0.009 for h+k+l,-l,-h 0.439 for l,-h-k-l,h 0.023 for -h-k-l,l,k 0.018 for k,h,-h-k-l 0.009 for -k,-h,-l 0.009 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15737	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, DXP

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	0.45	0/1950	0.60	0/2653
1	B	0.45	0/1945	0.63	0/2648
1	C	0.45	0/1868	0.64	1/2541 (0.0%)
1	D	0.43	0/1876	0.60	0/2555
1	E	0.41	0/1859	0.60	0/2532
1	F	0.45	0/1873	0.62	2/2548 (0.1%)
1	G	0.42	0/1858	0.57	0/2532
1	H	0.44	0/1864	0.60	1/2539 (0.0%)
All	All	0.44	0/15093	0.61	4/20548 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	149	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	149	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	F	149	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	H	149	ARG	NE-CZ-NH1	5.05	122.83	120.30

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1911	0	1911	22	0
1	B	1906	0	1895	27	0
1	C	1836	0	1832	20	1
1	D	1843	0	1828	12	0
1	E	1829	0	1808	15	0
1	F	1838	0	1834	13	0
1	G	1825	0	1799	6	0
1	H	1834	0	1813	20	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	C	13	0	9	5	0
3	F	13	0	9	1	0
3	G	13	0	9	1	0
4	A	127	0	0	4	0
4	B	121	0	0	4	1
4	C	102	0	0	2	0
4	D	97	0	0	2	0
4	E	98	0	0	1	0
4	F	122	0	0	1	0
4	G	83	0	0	1	0
4	H	101	0	0	0	0
All	All	15737	0	14747	132	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 4.

The worst 5 of 132 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:G:178:GLU:O	1:G:182:ILE:HD12	1.68	0.94
1:B:184:THR:HG21	4:B:440:HOH:O	1.74	0.88
1:C:180:GLU:O	1:C:184:THR:HG23	1.82	0.79
1:E:178:GLU:O	1:E:182:ILE:HD12	1.85	0.77
1:H:186:VAL:HG22	1:H:196:VAL:HG21	1.68	0.75

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:C:149:ARG:NH2	4:B:274:HOH:O[1_544]	2.18	0.02

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	252/278 (91%)	246 (98%)	6 (2%)	0	100	100
1	B	252/278 (91%)	246 (98%)	6 (2%)	0	100	100
1	C	243/278 (87%)	237 (98%)	6 (2%)	0	100	100
1	D	245/278 (88%)	238 (97%)	6 (2%)	1 (0%)	34	40
1	E	243/278 (87%)	238 (98%)	5 (2%)	0	100	100
1	F	244/278 (88%)	237 (97%)	7 (3%)	0	100	100
1	G	244/278 (88%)	238 (98%)	6 (2%)	0	100	100
1	H	244/278 (88%)	235 (96%)	9 (4%)	0	100	100
All	All	1967/2224 (88%)	1915 (97%)	51 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	72	VAL

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	190/208 (91%)	180 (95%)	10 (5%)	22	29
1	B	189/208 (91%)	177 (94%)	12 (6%)	18	22
1	C	183/208 (88%)	171 (93%)	12 (7%)	16	20
1	D	182/208 (88%)	173 (95%)	9 (5%)	25	33
1	E	180/208 (86%)	170 (94%)	10 (6%)	21	27
1	F	183/208 (88%)	175 (96%)	8 (4%)	28	37
1	G	179/208 (86%)	171 (96%)	8 (4%)	27	36
1	H	180/208 (86%)	168 (93%)	12 (7%)	16	19
All	All	1466/1664 (88%)	1385 (94%)	81 (6%)	21	27

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	78	LEU
1	H	62	ASP
1	F	196	VAL
1	G	162	HIS
1	H	136	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	223	HIS
1	E	19	HIS
1	F	223	HIS
1	E	200	HIS
1	B	223	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	PO4	E	258	-	4,4,4	0.92	0	6,6,6	0.56	0
2	PO4	B	258	-	4,4,4	0.85	0	6,6,6	0.55	0
2	PO4	H	258	-	4,4,4	0.92	0	6,6,6	0.57	0
3	DXP	C	258	-	11,12,12	2.43	5 (45%)	13,17,17	2.10	5 (38%)
2	PO4	D	258	-	4,4,4	0.83	0	6,6,6	0.40	0
2	PO4	G	258	-	4,4,4	0.96	0	6,6,6	0.64	0
3	DXP	F	258	-	11,12,12	1.97	4 (36%)	13,17,17	2.11	6 (46%)
3	DXP	G	259	-	11,12,12	2.07	3 (27%)	13,17,17	2.13	7 (53%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DXP	C	258	-	1/1/4/4	9/14/14/14	-
3	DXP	G	259	-	-	13/14/14/14	-
3	DXP	F	258	-	-	7/14/14/14	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	258	DXP	C3-C2	-6.35	1.47	1.52
3	G	259	DXP	C3-C2	-3.98	1.49	1.52
3	F	258	DXP	C3-C2	-3.72	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	259	DXP	P-O1P	-3.56	1.41	1.54
3	F	258	DXP	P-O2P	-2.97	1.43	1.54

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	258	DXP	C1-C2-C3	4.35	121.37	118.39
3	C	258	DXP	P-O5-C5	4.12	129.66	118.30
3	G	259	DXP	O3-C3-C2	-3.81	104.92	111.04
3	F	258	DXP	O5-C5-C4	3.73	119.32	109.36
3	F	258	DXP	P-O5-C5	3.59	128.18	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	258	DXP	C4

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	258	DXP	C1-C2-C3-C4
3	C	258	DXP	C1-C2-C3-O3
3	C	258	DXP	O2-C2-C3-C4
3	C	258	DXP	O2-C2-C3-O3
3	C	258	DXP	C2-C3-C4-C5

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	258	DXP	5	0
3	F	258	DXP	1	0
3	G	259	DXP	1	0

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 ⓘ

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, 95th 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^2)	Q<0.9
1	A	252/278 (90%)	0.06	3 (1%)	79 82	18, 25, 39, 52	0
1	B	252/278 (90%)	0.02	7 (2%)	53 59	17, 25, 39, 55	0
1	C	244/278 (87%)	0.03	1 (0%)	92 94	18, 25, 36, 45	0
1	D	246/278 (88%)	0.07	2 (0%)	86 89	18, 28, 38, 46	0
1	E	245/278 (88%)	0.07	1 (0%)	92 94	17, 30, 39, 50	0
1	F	244/278 (87%)	-0.07	1 (0%)	92 94	17, 25, 35, 44	0
1	G	245/278 (88%)	0.00	3 (1%)	79 82	19, 29, 38, 48	0
1	H	246/278 (88%)	-0.01	0	100 100	17, 28, 38, 45	0
All	All	1974/2224 (88%)	0.02	18 (0%)	84 87	17, 27, 38, 55	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	THR	4.3
1	A	6	THR	3.3
1	B	5	LEU	3.1
1	E	135	VAL	3.0
1	B	6	THR	3.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DXP	F	258	13/13	0.89	0.20	48,49,50,50	0
3	DXP	G	259	13/13	0.90	0.20	56,60,63,63	0
2	PO4	B	258	5/5	0.93	0.13	46,46,47,47	0
2	PO4	D	258	5/5	0.93	0.16	49,49,50,51	0
3	DXP	C	258	13/13	0.94	0.17	47,51,53,54	0
2	PO4	H	258	5/5	0.95	0.16	53,54,54,54	0
2	PO4	E	258	5/5	0.97	0.16	37,37,39,40	0
2	PO4	G	258	5/5	0.98	0.11	40,41,41,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.