



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 11:55 AM EDT

PDB ID : 3GK0 / pdb\_00003gk0  
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)

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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

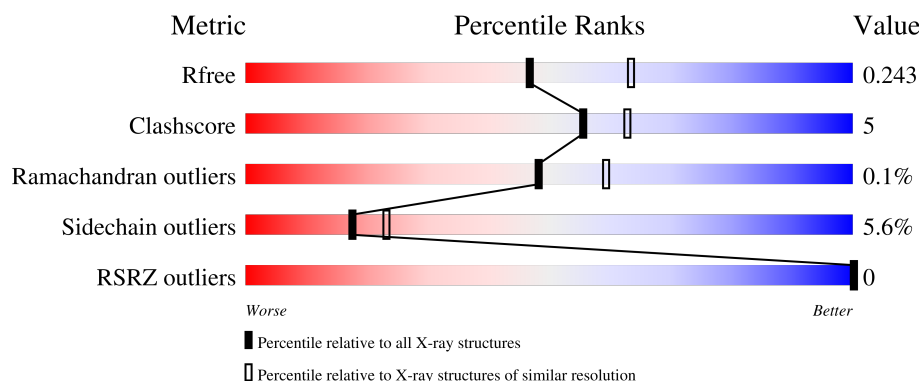
# 1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (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  $\geq 3$ , 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	278	
1	B	278	
1	C	278	
1	D	278	
1	E	278	

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Mol	Chain	Length	Quality of chain
1	F	278	
1	G	278	
1	H	278	

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

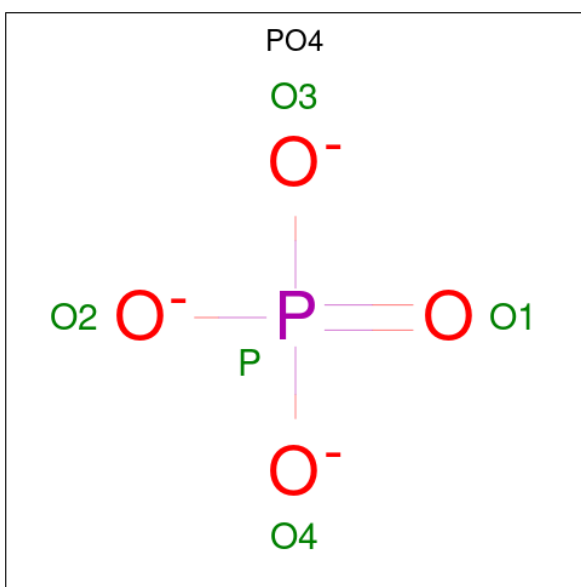
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	ALA	-	expression tag	UNP Q3JQ80
G	-6	GLN	-	expression tag	UNP Q3JQ80
G	-5	THR	-	expression tag	UNP Q3JQ80
G	-4	GLN	-	expression tag	UNP Q3JQ80
G	-3	GLY	-	expression tag	UNP Q3JQ80
G	-2	PRO	-	expression 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

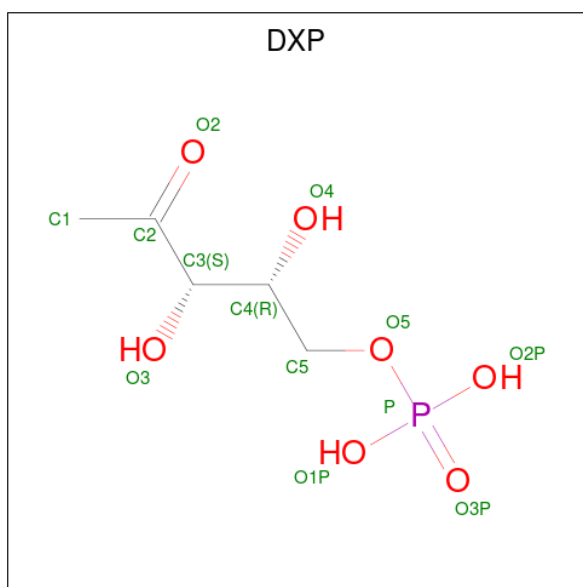
- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).





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

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



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

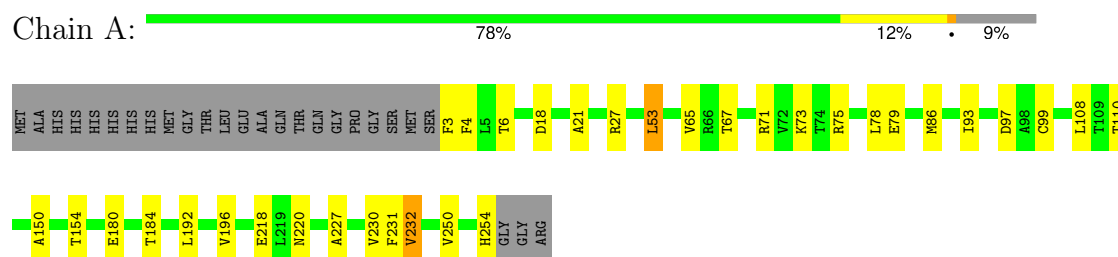
- Molecule 4 is water.

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

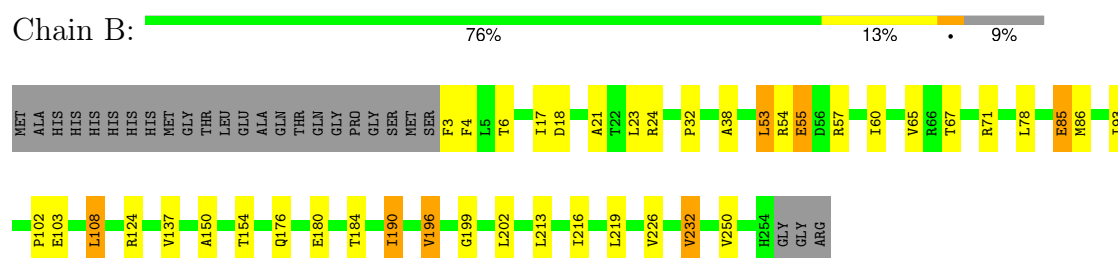
### 3 Residue-property plots

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.

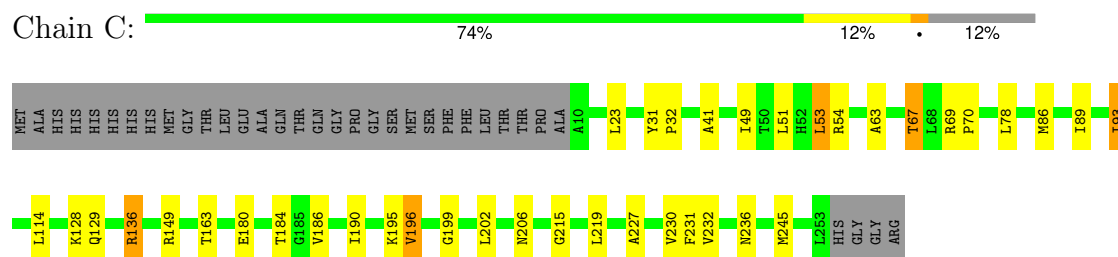
- Molecule 1: Pyridoxine 5'-phosphate synthase



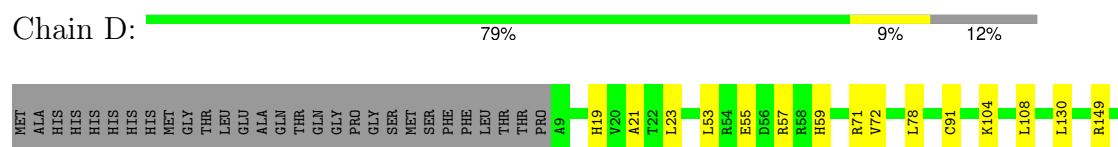
- Molecule 1: Pyridoxine 5'-phosphate synthase



- Molecule 1: Pyridoxine 5'-phosphate synthase



- Molecule 1: Pyridoxine 5'-phosphate synthase





- Molecule 1: Pyridoxine 5'-phosphate synthase

Chain E: 78% 9% 12%



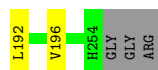
- Molecule 1: Pyridoxine 5'-phosphate synthase

Chain F: 79% 8% 12%



- Molecule 1: Pyridoxine 5'-phosphate synthase

Chain G: 82% 6% 12%



- Molecule 1: Pyridoxine 5'-phosphate synthase

Chain H: 76% 11% 12%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 94.2 (46.50-2.28)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 16.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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	0.97	EDS
Total number of atoms	15737	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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](#)

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	0.62	0/1950	0.79	0/2653
1	B	0.62	0/1945	0.80	1/2648 (0.0%)
1	C	0.63	0/1868	0.78	0/2541
1	D	0.59	0/1876	0.81	0/2555
1	E	0.57	0/1859	0.81	0/2532
1	F	0.62	0/1873	0.79	0/2548
1	G	0.58	0/1858	0.77	0/2532
1	H	0.61	1/1864 (0.1%)	0.79	0/2539
All	All	0.61	1/15093 (0.0%)	0.79	1/20548 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	74	THR	CA-C	5.12	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	VAL	N-CA-C	5.08	115.63	108.36

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	1911	0	1911	21	0
1	B	1906	0	1895	28	0
1	C	1836	0	1832	24	1
1	D	1843	0	1828	12	0
1	E	1829	0	1808	16	0
1	F	1838	0	1834	12	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	3	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	136	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 5.

All (136) 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:F:53:LEU:HD13	1:F:86:MET:HE1	1.57	0.85
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
1:H:139:LEU:HD11	1:H:154:THR:HG21	1.69	0.75
1:H:65:VAL:CG1	1:H:93:ILE:HD13	2.22	0.69
1:H:65:VAL:HG11	1:H:93:ILE:HD13	1.75	0.68
1:B:24:ARG:NH2	4:B:596:HOH:O	2.14	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD13	1:A:86:MET:HE1	1.77	0.67
3:C:258:DXP:C5	3:C:258:DXP:HC13	2.25	0.67
1:B:53:LEU:HD13	1:B:86:MET:HE1	1.78	0.64
1:F:53:LEU:HD13	1:F:86:MET:CE	2.26	0.63
3:F:258:DXP:HC12	3:F:258:DXP:O4	1.98	0.63
1:F:186:VAL:HG22	1:F:196:VAL:HG21	1.80	0.62
1:A:65:VAL:HG12	1:A:93:ILE:HD13	1.80	0.62
1:B:180:GLU:O	1:B:184:THR:HG23	1.99	0.61
1:C:236:ASN:ND2	1:E:236:ASN:ND2	2.49	0.61
1:H:22:THR:OG1	1:H:58:ARG:NH2	2.35	0.60
1:C:63:ALA:O	1:C:67:THR:CG2	2.49	0.60
1:D:19:HIS:ND1	1:D:223:HIS:HD2	1.99	0.60
1:B:65:VAL:HG12	1:B:93:ILE:HD13	1.83	0.60
3:G:259:DXP:HC4	4:G:273:HOH:O	2.02	0.59
1:A:6:THR:HG22	1:D:205:THR:O	2.04	0.58
1:C:53:LEU:HD13	1:C:86:MET:HE1	1.86	0.57
3:C:258:DXP:C5	3:C:258:DXP:C1	2.82	0.57
1:H:154:THR:HG22	1:H:156:ALA:H	1.70	0.57
1:A:230:VAL:HG23	1:A:231:PHE:CD2	2.40	0.57
1:A:6:THR:CG2	1:D:205:THR:O	2.53	0.56
3:C:258:DXP:HC13	3:C:258:DXP:H51	1.88	0.56
3:C:258:DXP:C1	3:C:258:DXP:H52	2.36	0.56
1:D:104:LYS:O	1:D:108:LEU:HD23	2.06	0.55
1:B:23:LEU:HD23	1:B:32:PRO:HG3	1.88	0.55
1:A:18:ASP:O	1:A:21:ALA:HB3	2.07	0.55
1:C:93:ILE:HD12	1:C:93:ILE:O	2.05	0.55
1:H:35:VAL:HG13	1:H:68:LEU:HD13	1.88	0.54
1:C:63:ALA:O	1:C:67:THR:HG23	2.07	0.54
1:A:110:THR:HG21	4:A:506:HOH:O	2.08	0.54
1:B:4:PHE:CD2	1:B:250:VAL:CG1	2.91	0.54
1:A:4:PHE:CD2	1:A:250:VAL:CG1	2.89	0.54
1:G:166:TYR:HB2	1:G:182:ILE:HD11	1.89	0.54
1:C:190:ILE:HD11	1:C:215:GLY:HA3	1.89	0.53
1:F:213:LEU:HB2	1:F:216:ILE:HD12	1.90	0.53
1:A:65:VAL:CG1	1:A:93:ILE:HD13	2.38	0.53
1:C:186:VAL:HG22	1:C:196:VAL:HG21	1.91	0.53
1:G:51:LEU:HD11	1:G:65:VAL:HG22	1.91	0.52
1:C:23:LEU:HD23	1:C:32:PRO:HG3	1.92	0.52
1:A:79:GLU:HG2	1:A:99:CYS:HB3	1.92	0.52
1:B:103:GLU:OE2	4:B:292:HOH:O	2.19	0.52
1:E:199:GLY:HA2	1:E:202:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:ILE:C	1:E:93:ILE:HD12	2.35	0.51
1:A:227:ALA:O	1:A:230:VAL:HG22	2.12	0.50
1:A:184:THR:HG21	4:A:523:HOH:O	2.12	0.50
1:B:190:ILE:HD13	1:B:196:VAL:CG1	2.42	0.50
1:B:199:GLY:HA2	1:B:202:LEU:HD12	1.93	0.49
1:G:51:LEU:CD1	1:G:65:VAL:HG22	2.42	0.49
1:B:226:VAL:HG12	1:E:23:LEU:HD21	1.94	0.49
1:E:145:GLU:CB	4:E:528:HOH:O	2.60	0.49
1:F:65:VAL:CG1	1:F:93:ILE:HD13	2.42	0.49
1:C:53:LEU:HD13	1:C:86:MET:CE	2.43	0.49
1:H:65:VAL:HG12	1:H:93:ILE:HD13	1.95	0.49
1:H:149:ARG:HH11	1:H:149:ARG:HG2	1.78	0.49
1:A:4:PHE:CD2	1:A:250:VAL:HG12	2.48	0.49
1:D:180:GLU:OE1	4:D:260:HOH:O	2.20	0.48
1:B:190:ILE:CD1	1:B:196:VAL:HG13	2.43	0.48
1:C:63:ALA:O	1:C:67:THR:HG22	2.12	0.48
1:B:232:VAL:HG22	1:H:236:ASN:OD1	2.13	0.48
1:F:150:ALA:O	1:F:154:THR:HG23	2.13	0.48
1:E:54:ARG:O	1:E:57:ARG:HD3	2.13	0.48
1:D:55:GLU:O	1:D:57:ARG:NH1	2.47	0.48
1:E:93:ILE:HD12	1:E:93:ILE:O	2.14	0.48
1:B:17:ILE:HD13	1:B:38:ALA:HB2	1.96	0.48
1:B:18:ASP:O	1:B:21:ALA:HB3	2.13	0.47
1:B:150:ALA:O	1:B:154:THR:HG23	2.14	0.47
1:E:97:ASP:OD1	1:E:136:ARG:HD2	2.14	0.47
1:F:199:GLY:HA2	1:F:202:LEU:HD12	1.96	0.47
3:C:258:DXP:HC13	3:C:258:DXP:H52	1.97	0.47
1:A:150:ALA:O	1:A:154:THR:HG23	2.15	0.47
1:C:23:LEU:HD13	1:H:23:LEU:HD22	1.97	0.47
1:C:69:ARG:HB3	1:C:70:PRO:HD3	1.95	0.47
1:B:55:GLU:O	1:B:57:ARG:NH1	2.47	0.46
1:C:136:ARG:HD2	4:C:421:HOH:O	2.15	0.46
1:A:232:VAL:HG22	1:D:236:ASN:OD1	2.16	0.46
1:A:4:PHE:CD2	1:A:250:VAL:HG11	2.50	0.46
1:E:186:VAL:HG13	1:E:196:VAL:HG11	1.98	0.46
1:H:213:LEU:HB2	1:H:216:ILE:HD12	1.97	0.46
1:C:89:ILE:O	1:C:93:ILE:HG23	2.15	0.45
1:F:73:LYS:NZ	4:F:734:HOH:O	2.50	0.45
1:C:227:ALA:O	1:C:230:VAL:HG22	2.16	0.45
1:F:31:TYR:HA	1:F:32:PRO:C	2.42	0.45
1:F:206:ASN:OD1	1:F:206:ASN:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:GLU:H	1:B:85:GLU:CD	2.24	0.45
1:E:53:LEU:HD13	1:E:86:MET:CE	2.46	0.45
1:B:4:PHE:CD2	1:B:250:VAL:HG12	2.52	0.45
1:A:75[A]:ARG:NH1	1:A:97:ASP:OD2	2.47	0.45
1:B:216:ILE:HG21	1:B:219:LEU:HD21	1.98	0.45
1:H:18:ASP:O	1:H:21:ALA:HB3	2.17	0.45
1:A:67:THR:HG23	4:A:446:HOH:O	2.17	0.44
1:C:41:ALA:HB3	1:C:49:ILE:HD11	1.98	0.44
1:E:108:LEU:HD12	1:E:108:LEU:O	2.18	0.44
1:B:3:PHE:HB2	1:H:179:PHE:CD2	2.52	0.44
1:D:91:CYS:SG	1:D:130:LEU:HD23	2.58	0.44
1:B:213:LEU:HB2	1:B:216:ILE:HD12	1.98	0.44
1:E:31:TYR:HA	1:E:32:PRO:C	2.43	0.44
1:C:206:ASN:OD1	1:C:206:ASN:C	2.61	0.43
1:B:6:THR:HG23	1:B:6:THR:O	2.17	0.43
1:G:55:GLU:O	1:G:57:ARG:NH1	2.51	0.43
1:C:236:ASN:ND2	1:E:236:ASN:HD22	2.16	0.43
1:C:230:VAL:HG23	1:C:231:PHE:CD2	2.53	0.43
1:C:199:GLY:HA2	1:C:202:LEU:HD12	2.00	0.43
1:H:186:VAL:HG22	1:H:196:VAL:CG2	2.45	0.43
1:A:3:PHE:HB2	1:D:179:PHE:CD2	2.53	0.43
1:A:180:GLU:O	1:A:184:THR:HG23	2.18	0.43
1:G:54:ARG:O	1:G:57:ARG:HD3	2.19	0.43
1:H:199:GLY:HA2	1:H:202:LEU:HD12	2.01	0.43
1:C:31:TYR:HA	1:C:32:PRO:C	2.43	0.43
1:D:21:ALA:HB3	1:D:59:HIS:HB2	2.00	0.43
1:E:186:VAL:HG12	1:E:190:ILE:HD12	2.01	0.43
1:H:149:ARG:HH11	1:H:149:ARG:CG	2.32	0.43
1:B:60:ILE:HA	4:B:596:HOH:O	2.19	0.42
1:B:190:ILE:CD1	1:B:196:VAL:CG1	2.97	0.42
1:B:4:PHE:CD2	1:B:250:VAL:HG11	2.55	0.42
1:C:54:ARG:NH1	4:C:732:HOH:O	2.52	0.42
1:C:219:LEU:HD12	1:C:245:MET:HE3	2.02	0.42
1:F:55:GLU:OE1	1:F:83:THR:HG21	2.20	0.42
1:D:213:LEU:HB2	1:D:216:ILE:HD12	2.02	0.41
1:H:21:ALA:HB3	1:H:59:HIS:HB2	2.02	0.41
1:B:102:PRO:HB2	1:B:108:LEU:HD23	2.02	0.41
1:A:218:GLU:OE2	1:A:220:ASN:OD1	2.38	0.41
1:H:218:GLU:OE2	1:H:220:ASN:OD1	2.39	0.41
1:H:127:CYS:SG	1:H:154:THR:HG23	2.62	0.40
1:F:186:VAL:HG22	1:F:196:VAL:CG2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ARG:O	1:B:57:ARG:HD3	2.22	0.40
1:D:180:GLU:HG3	4:D:277:HOH:O	2.21	0.40
1:E:102:PRO:HB2	1:E:108:LEU:HB3	2.03	0.40

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%)	30	36
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%)	48	59

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%)	19	25
1	B	189/208 (91%)	177 (94%)	12 (6%)	15	19
1	C	183/208 (88%)	170 (93%)	13 (7%)	12	15
1	D	182/208 (88%)	174 (96%)	8 (4%)	24	33
1	E	180/208 (86%)	171 (95%)	9 (5%)	20	28
1	F	183/208 (88%)	174 (95%)	9 (5%)	21	29
1	G	179/208 (86%)	170 (95%)	9 (5%)	20	28
1	H	180/208 (86%)	168 (93%)	12 (7%)	13	17
All	All	1466/1664 (88%)	1384 (94%)	82 (6%)	17	23

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	53	LEU
1	A	71	ARG
1	A	73	LYS
1	A	78	LEU
1	A	108	LEU
1	A	192	LEU
1	A	196	VAL
1	A	232	VAL
1	A	254	HIS
1	B	53	LEU
1	B	55	GLU
1	B	67	THR
1	B	71	ARG
1	B	78	LEU
1	B	85	GLU
1	B	108	LEU
1	B	124	ARG
1	B	176	GLN

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Mol	Chain	Res	Type
1	B	190	ILE
1	B	196	VAL
1	B	232	VAL
1	C	51	LEU
1	C	53	LEU
1	C	67	THR
1	C	78	LEU
1	C	93	ILE
1	C	114	LEU
1	C	128	LYS
1	C	129	GLN
1	C	136	ARG
1	C	163	THR
1	C	195	LYS
1	C	196	VAL
1	C	232	VAL
1	D	23	LEU
1	D	53	LEU
1	D	71	ARG
1	D	78	LEU
1	D	149	ARG
1	D	171	ASP
1	D	196	VAL
1	D	232	VAL
1	E	51	LEU
1	E	53	LEU
1	E	78	LEU
1	E	93	ILE
1	E	110	THR
1	E	128	LYS
1	E	163	THR
1	E	180	GLU
1	E	195	LYS
1	F	51	LEU
1	F	53	LEU
1	F	71	ARG
1	F	73	LYS
1	F	78	LEU
1	F	128	LYS
1	F	195	LYS
1	F	196	VAL
1	F	232	VAL

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Mol	Chain	Res	Type
1	G	23	LEU
1	G	53	LEU
1	G	72	VAL
1	G	78	LEU
1	G	128	LYS
1	G	136	ARG
1	G	163	THR
1	G	192	LEU
1	G	196	VAL
1	H	23	LEU
1	H	53	LEU
1	H	71	ARG
1	H	78	LEU
1	H	114	LEU
1	H	136	ARG
1	H	149	ARG
1	H	154	THR
1	H	171	ASP
1	H	196	VAL
1	H	230	VAL
1	H	232	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	220	ASN
1	A	223	HIS
1	B	77	ASN
1	B	129	GLN
1	B	223	HIS
1	C	175	GLN
1	C	197	ASN
1	C	223	HIS
1	D	77	ASN
1	D	223	HIS
1	D	254	HIS
1	E	77	ASN
1	E	197	ASN
1	E	200	HIS
1	E	254	HIS
1	F	200	HIS

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Mol	Chain	Res	Type
1	F	223	HIS
1	G	77	ASN
1	H	77	ASN
1	H	152	HIS
1	H	197	ASN
1	H	200	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 oligosaccharides 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	$\# Z  > 2$
3	DXP	F	258	-	12,12,12	1.97	4 (33%)	14,17,17	1.79	5 (35%)
3	DXP	C	258	-	12,12,12	2.41	5 (41%)	14,17,17	2.36	6 (42%)
2	PO4	D	258	-	4,4,4	0.87	0	6,6,6	0.43	0
2	PO4	B	258	-	4,4,4	0.89	0	6,6,6	0.58	0
2	PO4	E	258	-	4,4,4	0.96	0	6,6,6	0.59	0
2	PO4	G	258	-	4,4,4	1.01	0	6,6,6	0.68	0
2	PO4	H	258	-	4,4,4	0.96	0	6,6,6	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DXP	G	259	-	12,12,12	2.13	4 (33%)	14,17,17	2.27	7 (50%)

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	F	258	-	-	7/14/14/14	-
3	DXP	G	259	-	-	13/14/14/14	-
3	DXP	C	258	-	1/1/4/4	8/14/14/14	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	258	DXP	C3-C2	-6.53	1.47	1.52
3	G	259	DXP	C3-C2	-4.11	1.49	1.52
3	F	258	DXP	C3-C2	-3.84	1.49	1.52
3	G	259	DXP	P-O1P	-3.68	1.41	1.54
3	F	258	DXP	P-O2P	-3.07	1.43	1.54
3	F	258	DXP	P-O1P	-2.91	1.44	1.54
3	G	259	DXP	P-O2P	-2.88	1.44	1.54
3	C	258	DXP	P-O2P	-2.87	1.44	1.54
3	C	258	DXP	P-O1P	-2.73	1.44	1.54
3	F	258	DXP	C5-C4	2.50	1.55	1.51
3	C	258	DXP	C5-C4	2.14	1.54	1.51
3	G	259	DXP	C4-C3	-2.12	1.50	1.53
3	C	258	DXP	P-O3P	-2.06	1.44	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	258	DXP	O4-C4-C3	-6.62	100.05	109.67
3	G	259	DXP	O4-C4-C3	-4.14	103.66	109.67
3	G	259	DXP	O3-C3-C2	-3.87	104.92	111.31
3	F	258	DXP	O5-C5-C4	3.73	119.32	109.36
3	C	258	DXP	C1-C2-C3	3.07	121.37	118.13
3	G	259	DXP	O1P-P-O2P	2.70	117.93	107.80
3	F	258	DXP	O3-C3-C2	2.42	115.31	111.31
3	G	259	DXP	C1-C2-C3	2.30	120.55	118.13
3	F	258	DXP	O4-C4-C5	2.28	115.00	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	258	DXP	O1P-P-O5	-2.20	100.93	106.67
3	C	258	DXP	O2P-P-O5	-2.19	100.95	106.67
3	G	259	DXP	O4-C4-C5	-2.19	105.15	109.99
3	G	259	DXP	O1P-P-O5	-2.19	100.96	106.67
3	F	258	DXP	C1-C2-C3	2.14	120.39	118.13
3	C	258	DXP	O2-C2-C3	-2.14	116.37	119.24
3	G	259	DXP	O3-C3-C4	-2.04	104.27	109.46
3	C	258	DXP	O4-C4-C5	2.02	114.43	109.99
3	C	258	DXP	O3-C3-C4	2.01	114.59	109.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	258	DXP	C4

All (28) 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
3	C	258	DXP	O3-C3-C4-C5
3	C	258	DXP	O3-C3-C4-O4
3	F	258	DXP	C2-C3-C4-C5
3	F	258	DXP	C2-C3-C4-O4
3	F	258	DXP	O3-C3-C4-C5
3	F	258	DXP	O3-C3-C4-O4
3	F	258	DXP	C5-O5-P-O2P
3	F	258	DXP	C5-O5-P-O1P
3	F	258	DXP	C5-O5-P-O3P
3	G	259	DXP	C1-C2-C3-C4
3	G	259	DXP	O2-C2-C3-C4
3	G	259	DXP	C2-C3-C4-C5
3	G	259	DXP	O3-C3-C4-C5
3	G	259	DXP	O3-C3-C4-O4
3	G	259	DXP	C3-C4-C5-O5
3	G	259	DXP	O4-C4-C5-O5
3	G	259	DXP	C5-O5-P-O2P
3	G	259	DXP	C5-O5-P-O1P
3	G	259	DXP	C5-O5-P-O3P

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Mol	Chain	Res	Type	Atoms
3	G	259	DXP	O2-C2-C3-O3
3	G	259	DXP	C1-C2-C3-O3
3	C	258	DXP	C2-C3-C4-O4
3	G	259	DXP	C2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 7 short contacts:

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

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	252/278 (90%)	-1.50	0 100 100	15, 25, 39, 52	2 (0%)
1	B	252/278 (90%)	-1.54	0 100 100	16, 25, 39, 55	2 (0%)
1	C	244/278 (87%)	-1.56	0 100 100	18, 25, 36, 45	1 (0%)
1	D	246/278 (88%)	-1.53	0 100 100	16, 28, 38, 46	1 (0%)
1	E	245/278 (88%)	-1.50	0 100 100	17, 30, 39, 50	0
1	F	244/278 (87%)	-1.59	0 100 100	15, 25, 35, 44	2 (0%)
1	G	245/278 (88%)	-1.53	0 100 100	19, 29, 38, 48	1 (0%)
1	H	246/278 (88%)	-1.54	0 100 100	17, 28, 38, 45	0
All	All	1974/2224 (88%)	-1.54	0 100 100	15, 27, 38, 55	9 (0%)

There are no RSRZ outliers to report.

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	DXP	F	258	13/13	0.98	0.05	48,49,50,50	0
2	PO4	D	258	5/5	0.99	0.05	49,49,50,51	0
2	PO4	E	258	5/5	0.99	0.04	37,37,39,40	0
2	PO4	G	258	5/5	0.99	0.03	40,41,41,41	0
2	PO4	H	258	5/5	0.99	0.04	53,54,54,54	0
3	DXP	C	258	13/13	0.99	0.05	47,51,53,54	0
2	PO4	B	258	5/5	0.99	0.03	46,46,47,47	0
3	DXP	G	259	13/13	0.99	0.04	56,60,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.