



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 11:28 PM UTC

PDB ID : 4WY0 / pdb_00004wy0
Title : PdxS (G. stearothermophilus) co-crystallized with R5P in the presence of ammonia.
Authors : Smith, J.L.; Smith, A.M.
Deposited on : 2014-11-14
Resolution : 2.30 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 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)	:	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

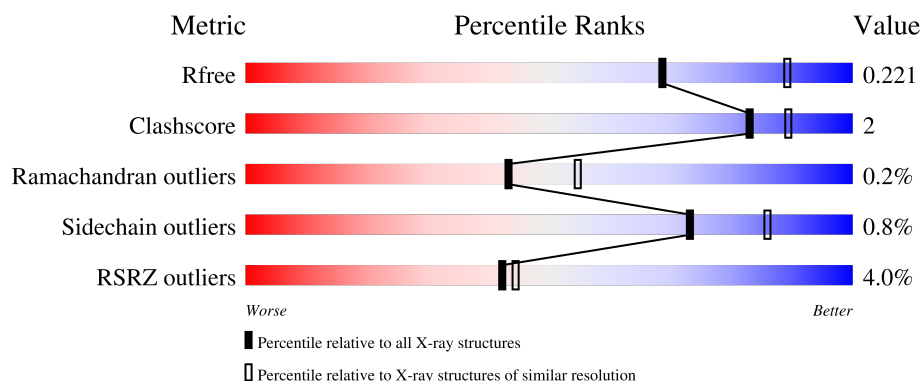
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



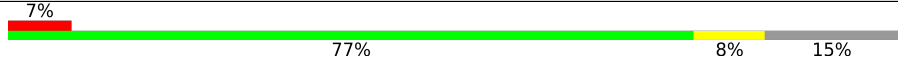
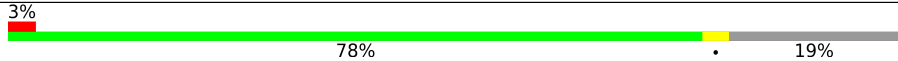
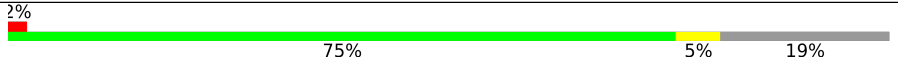
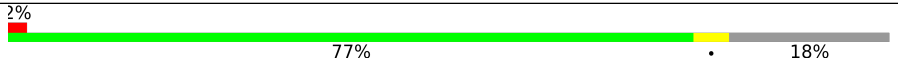
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	305	5% 75% 6% 19%
1	C	305	3% 76% 5% 19%
1	E	305	2% 78% • 19%
1	G	305	5% 76% 9% 16%
1	I	305	3% 78% • 18%

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Mol	Chain	Length	Quality of chain
1	J	305	
1	K	305	
1	L	305	
2	B	305	
2	D	305	
2	H	305	
3	F	304	

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
4	CAC	A	301	-	X	-	-
4	CAC	L	301	-	X	-	-
7	EDO	G	302	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23986 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 Pyridoxal biosynthesis lyase PdxS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	P	S	0	0	0
			1885	1177	332	362	1	13			
1	C	247	Total	C	N	O	P	S	0	0	0
			1866	1165	328	359	1	13			
1	E	247	Total	C	N	O	P	S	0	0	0
			1863	1163	328	359	1	12			
1	G	257	Total	C	N	O	P	S	0	0	0
			1955	1218	348	374	1	14			
1	I	249	Total	C	N	O	P	S	0	0	0
			1884	1176	333	361	1	13			
1	J	245	Total	C	N	O	P	S	0	0	0
			1857	1161	326	357	1	12			
1	K	248	Total	C	N	O	P	S	0	0	0
			1885	1177	332	362	1	13			
1	L	246	Total	C	N	O	P	S	0	0	0
			1858	1162	326	357	1	12			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLU	-	expression tag	UNP Q5L3Y2
A	-8	ASN	-	expression tag	UNP Q5L3Y2
A	-7	LEU	-	expression tag	UNP Q5L3Y2
A	-6	THR	-	expression tag	UNP Q5L3Y2
A	-5	PRO	-	expression tag	UNP Q5L3Y2
A	-4	GLN	-	expression tag	UNP Q5L3Y2
A	-3	HIS	-	expression tag	UNP Q5L3Y2
A	-2	MET	-	expression tag	UNP Q5L3Y2
A	-1	ALA	-	expression tag	UNP Q5L3Y2
A	0	SER	-	expression tag	UNP Q5L3Y2
A	216	THR	ALA	conflict	UNP Q5L3Y2
A	295	ALA	-	expression tag	UNP Q5L3Y2
C	-9	GLU	-	expression tag	UNP Q5L3Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	ASN	-	expression tag	UNP Q5L3Y2
C	-7	LEU	-	expression tag	UNP Q5L3Y2
C	-6	THR	-	expression tag	UNP Q5L3Y2
C	-5	PRO	-	expression tag	UNP Q5L3Y2
C	-4	GLN	-	expression tag	UNP Q5L3Y2
C	-3	HIS	-	expression tag	UNP Q5L3Y2
C	-2	MET	-	expression tag	UNP Q5L3Y2
C	-1	ALA	-	expression tag	UNP Q5L3Y2
C	0	SER	-	expression tag	UNP Q5L3Y2
C	216	THR	ALA	conflict	UNP Q5L3Y2
C	295	ALA	-	expression tag	UNP Q5L3Y2
E	-9	GLU	-	expression tag	UNP Q5L3Y2
E	-8	ASN	-	expression tag	UNP Q5L3Y2
E	-7	LEU	-	expression tag	UNP Q5L3Y2
E	-6	THR	-	expression tag	UNP Q5L3Y2
E	-5	PRO	-	expression tag	UNP Q5L3Y2
E	-4	GLN	-	expression tag	UNP Q5L3Y2
E	-3	HIS	-	expression tag	UNP Q5L3Y2
E	-2	MET	-	expression tag	UNP Q5L3Y2
E	-1	ALA	-	expression tag	UNP Q5L3Y2
E	0	SER	-	expression tag	UNP Q5L3Y2
E	216	THR	ALA	conflict	UNP Q5L3Y2
E	295	ALA	-	expression tag	UNP Q5L3Y2
G	-9	GLU	-	expression tag	UNP Q5L3Y2
G	-8	ASN	-	expression tag	UNP Q5L3Y2
G	-7	LEU	-	expression tag	UNP Q5L3Y2
G	-6	THR	-	expression tag	UNP Q5L3Y2
G	-5	PRO	-	expression tag	UNP Q5L3Y2
G	-4	GLN	-	expression tag	UNP Q5L3Y2
G	-3	HIS	-	expression tag	UNP Q5L3Y2
G	-2	MET	-	expression tag	UNP Q5L3Y2
G	-1	ALA	-	expression tag	UNP Q5L3Y2
G	0	SER	-	expression tag	UNP Q5L3Y2
G	216	THR	ALA	conflict	UNP Q5L3Y2
G	295	ALA	-	expression tag	UNP Q5L3Y2
I	-9	GLU	-	expression tag	UNP Q5L3Y2
I	-8	ASN	-	expression tag	UNP Q5L3Y2
I	-7	LEU	-	expression tag	UNP Q5L3Y2
I	-6	THR	-	expression tag	UNP Q5L3Y2
I	-5	PRO	-	expression tag	UNP Q5L3Y2
I	-4	GLN	-	expression tag	UNP Q5L3Y2
I	-3	HIS	-	expression tag	UNP Q5L3Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	MET	-	expression tag	UNP Q5L3Y2
I	-1	ALA	-	expression tag	UNP Q5L3Y2
I	0	SER	-	expression tag	UNP Q5L3Y2
I	216	THR	ALA	conflict	UNP Q5L3Y2
I	295	ALA	-	expression tag	UNP Q5L3Y2
J	-9	GLU	-	expression tag	UNP Q5L3Y2
J	-8	ASN	-	expression tag	UNP Q5L3Y2
J	-7	LEU	-	expression tag	UNP Q5L3Y2
J	-6	THR	-	expression tag	UNP Q5L3Y2
J	-5	PRO	-	expression tag	UNP Q5L3Y2
J	-4	GLN	-	expression tag	UNP Q5L3Y2
J	-3	HIS	-	expression tag	UNP Q5L3Y2
J	-2	MET	-	expression tag	UNP Q5L3Y2
J	-1	ALA	-	expression tag	UNP Q5L3Y2
J	0	SER	-	expression tag	UNP Q5L3Y2
J	216	THR	ALA	conflict	UNP Q5L3Y2
J	295	ALA	-	expression tag	UNP Q5L3Y2
K	-9	GLU	-	expression tag	UNP Q5L3Y2
K	-8	ASN	-	expression tag	UNP Q5L3Y2
K	-7	LEU	-	expression tag	UNP Q5L3Y2
K	-6	THR	-	expression tag	UNP Q5L3Y2
K	-5	PRO	-	expression tag	UNP Q5L3Y2
K	-4	GLN	-	expression tag	UNP Q5L3Y2
K	-3	HIS	-	expression tag	UNP Q5L3Y2
K	-2	MET	-	expression tag	UNP Q5L3Y2
K	-1	ALA	-	expression tag	UNP Q5L3Y2
K	0	SER	-	expression tag	UNP Q5L3Y2
K	216	THR	ALA	conflict	UNP Q5L3Y2
K	295	ALA	-	expression tag	UNP Q5L3Y2
L	-9	GLU	-	expression tag	UNP Q5L3Y2
L	-8	ASN	-	expression tag	UNP Q5L3Y2
L	-7	LEU	-	expression tag	UNP Q5L3Y2
L	-6	THR	-	expression tag	UNP Q5L3Y2
L	-5	PRO	-	expression tag	UNP Q5L3Y2
L	-4	GLN	-	expression tag	UNP Q5L3Y2
L	-3	HIS	-	expression tag	UNP Q5L3Y2
L	-2	MET	-	expression tag	UNP Q5L3Y2
L	-1	ALA	-	expression tag	UNP Q5L3Y2
L	0	SER	-	expression tag	UNP Q5L3Y2
L	216	THR	ALA	conflict	UNP Q5L3Y2
L	295	ALA	-	expression tag	UNP Q5L3Y2

- Molecule 2 is a protein called Pyridoxal biosynthesis lyase PdxS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total 1955	C 1220	N 351	O 370	S 14	0	0	0
2	D	247	Total 1857	C 1162	N 331	O 352	S 12	0	0	0
2	H	246	Total 1853	C 1160	N 327	O 353	S 13	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLU	-	expression tag	UNP Q5L3Y2
B	-8	ASN	-	expression tag	UNP Q5L3Y2
B	-7	LEU	-	expression tag	UNP Q5L3Y2
B	-6	THR	-	expression tag	UNP Q5L3Y2
B	-5	PRO	-	expression tag	UNP Q5L3Y2
B	-4	GLN	-	expression tag	UNP Q5L3Y2
B	-3	HIS	-	expression tag	UNP Q5L3Y2
B	-2	MET	-	expression tag	UNP Q5L3Y2
B	-1	ALA	-	expression tag	UNP Q5L3Y2
B	0	SER	-	expression tag	UNP Q5L3Y2
B	216	THR	ALA	conflict	UNP Q5L3Y2
B	295	ALA	-	expression tag	UNP Q5L3Y2
D	-9	GLU	-	expression tag	UNP Q5L3Y2
D	-8	ASN	-	expression tag	UNP Q5L3Y2
D	-7	LEU	-	expression tag	UNP Q5L3Y2
D	-6	THR	-	expression tag	UNP Q5L3Y2
D	-5	PRO	-	expression tag	UNP Q5L3Y2
D	-4	GLN	-	expression tag	UNP Q5L3Y2
D	-3	HIS	-	expression tag	UNP Q5L3Y2
D	-2	MET	-	expression tag	UNP Q5L3Y2
D	-1	ALA	-	expression tag	UNP Q5L3Y2
D	0	SER	-	expression tag	UNP Q5L3Y2
D	216	THR	ALA	conflict	UNP Q5L3Y2
D	295	ALA	-	expression tag	UNP Q5L3Y2
H	-9	GLU	-	expression tag	UNP Q5L3Y2
H	-8	ASN	-	expression tag	UNP Q5L3Y2
H	-7	LEU	-	expression tag	UNP Q5L3Y2
H	-6	THR	-	expression tag	UNP Q5L3Y2
H	-5	PRO	-	expression tag	UNP Q5L3Y2
H	-4	GLN	-	expression tag	UNP Q5L3Y2
H	-3	HIS	-	expression tag	UNP Q5L3Y2
H	-2	MET	-	expression tag	UNP Q5L3Y2
H	-1	ALA	-	expression tag	UNP Q5L3Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	SER	-	expression tag	UNP Q5L3Y2
H	216	THR	ALA	conflict	UNP Q5L3Y2
H	295	ALA	-	expression tag	UNP Q5L3Y2

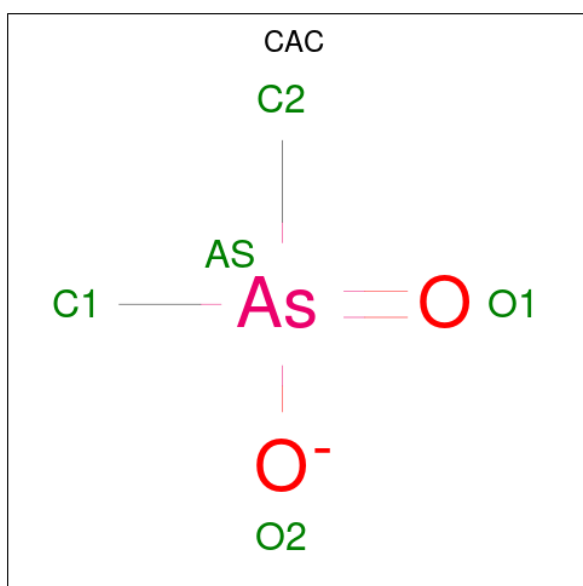
- Molecule 3 is a protein called Pyridoxal biosynthesis lyase PdxS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	248	Total	C	N	O	S	0	0	0
			1877	1177	333	354	13			

There are 11 discrepancies between the modelled and reference sequences:

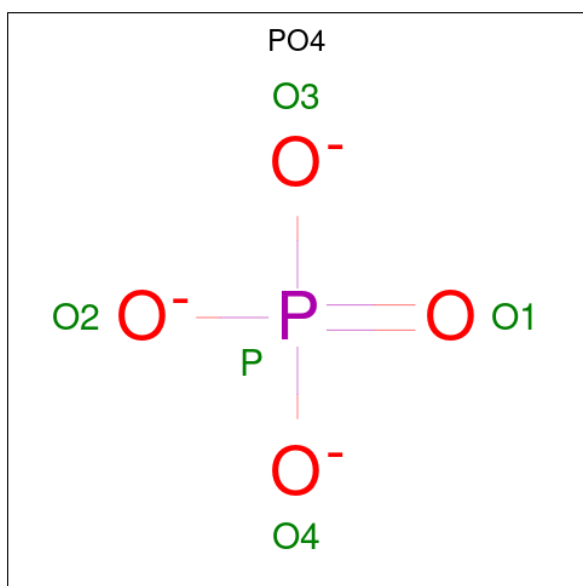
Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	GLU	-	expression tag	UNP Q5L3Y2
F	-8	ASN	-	expression tag	UNP Q5L3Y2
F	-7	LEU	-	expression tag	UNP Q5L3Y2
F	-6	THR	-	expression tag	UNP Q5L3Y2
F	-5	PRO	-	expression tag	UNP Q5L3Y2
F	-4	GLN	-	expression tag	UNP Q5L3Y2
F	-3	HIS	-	expression tag	UNP Q5L3Y2
F	-2	MET	-	expression tag	UNP Q5L3Y2
F	-1	ALA	-	expression tag	UNP Q5L3Y2
F	0	SER	-	expression tag	UNP Q5L3Y2
F	216	THR	ALA	conflict	UNP Q5L3Y2

- Molecule 4 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



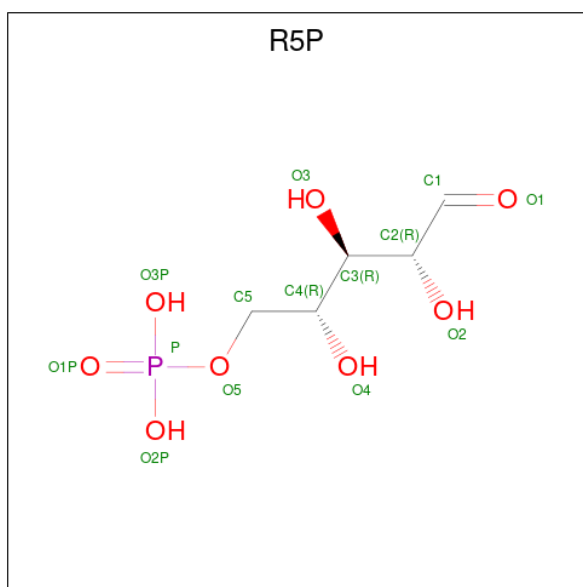
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	C	1	Total	As	C	O	0	0
			5	1	2	2		
4	F	1	Total	As	C	O	0	0
			5	1	2	2		
4	H	1	Total	As	C	O	0	0
			5	1	2	2		
4	L	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



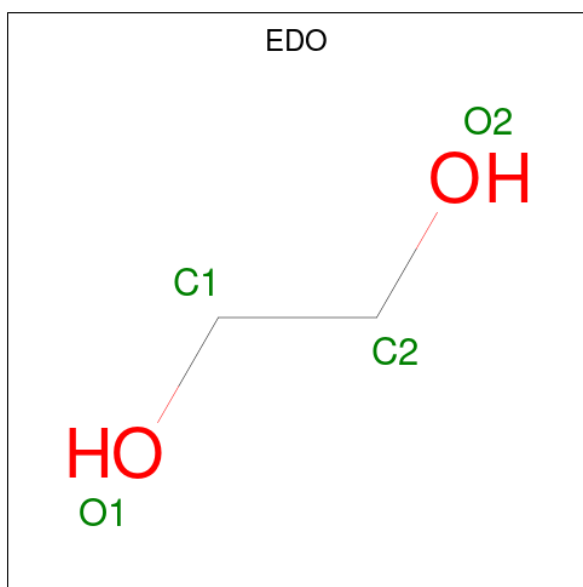
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is RIBOSE-5-PHOSPHATE (CCD ID: R5P) (formula: $C_5H_{11}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	P	0	0
			14	5	8	1		
6	D	1	Total	C	O	P	0	0
			14	5	8	1		
6	E	1	Total	C	O	P	0	0
			14	5	8	1		
6	G	1	Total	C	O	P	0	0
			14	5	8	1		
6	I	1	Total	C	O	P	0	0
			14	5	8	1		
6	J	1	Total	C	O	P	0	0
			14	5	8	1		
6	K	1	Total	C	O	P	0	0
			14	5	8	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

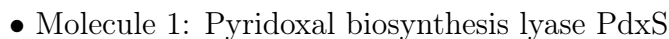
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	115	Total	O	0	0
			115	115		
8	B	114	Total	O	0	0
			114	114		
8	C	96	Total	O	0	0
			96	96		
8	D	119	Total	O	0	0
			119	119		
8	E	102	Total	O	0	0
			102	102		
8	F	69	Total	O	0	0
			69	69		
8	G	123	Total	O	0	0
			123	123		
8	H	109	Total	O	0	0
			109	109		
8	I	106	Total	O	0	0
			106	106		

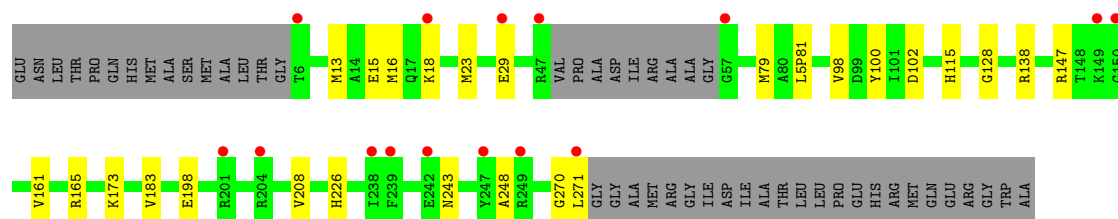
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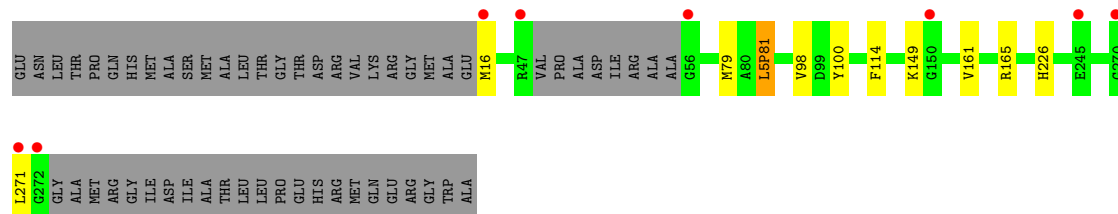
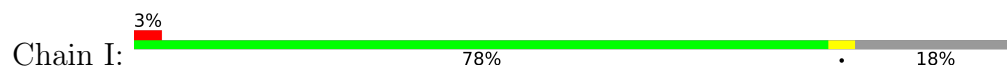
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	94	Total 94	O 94	0	0
8	K	104	Total 104	O 104	0	0
8	L	85	Total 85	O 85	0	0

- Molecule 1: Pyridoxal biosynthesis lyase PdxS

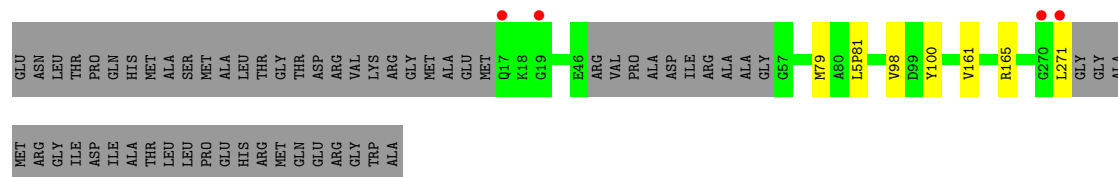
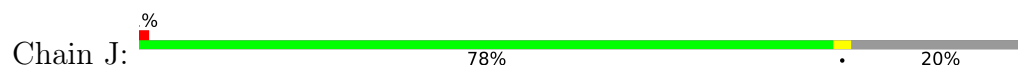




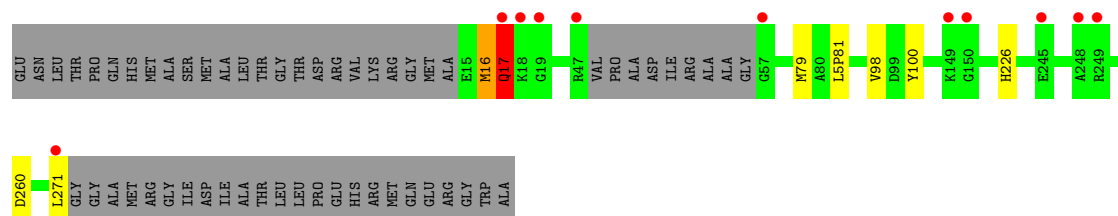
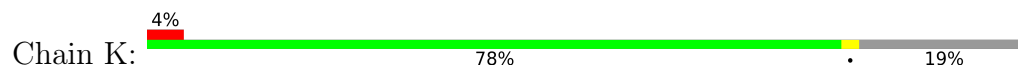
• Molecule 1: Pyridoxal biosynthesis lyase PdxS



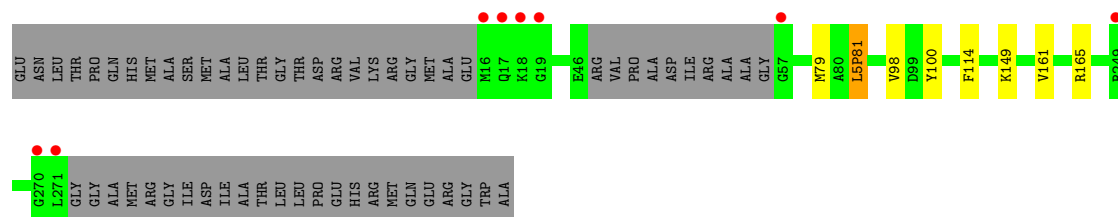
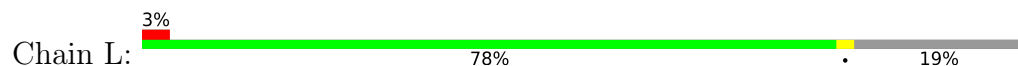
• Molecule 1: Pyridoxal biosynthesis lyase PdxS



• Molecule 1: Pyridoxal biosynthesis lyase PdxS



• Molecule 1: Pyridoxal biosynthesis lyase PdxS



[illegible]

Chain D:

Amino Acid	Frequency (%)
GLU	78%
ASN	78%
LEU	78%
THR	78%
PRO	78%
GLN	78%
HIS	78%
MET	78%
SER	78%
MET	78%
ALA	78%
LEU	78%
THR	78%
GLY	78%
THR	78%
ASP	78%
ARG	78%
VAL	78%
LYS	78%
ARG	78%
GLY	78%
MET	78%
ALA	78%
E15	78%
M16	78%
Q17	78%
K18	78%
G19	78%
R47	78%
VAL	78%
PRO	19%
ASP	19%
ILE	19%
ARG	19%
ALA	19%
ALA	19%
GLY	19%
G57	19%
M79	19%
R91	19%
V98	19%
D99	19%
Y100	19%
R165	19%
H226	19%
T256	19%
G270	19%
LEU	19%
GLY	19%

Chain H:

The sequence logo for Chain H displays the frequency of amino acids at each position. The x-axis represents positions 1 to 100. The y-axis represents the frequency of each amino acid. The legend indicates the following amino acids: GLU, ASN, LEU, THR, PRO, GLN, HIS, MET, ALA, SER, MET, ALA, LEU, THR, GLY, THR, ASP, ARG, VAL, LYS, ARG, GLY, MET, ALA, E16, M16, Q17, K18, G19, K32, L45, E46, ARG, VAL, PRO, ASP, ASP, ILE, ARG, ALA, ALA, GLY, G57, P64, M79, L96, G97, V98, D99, Y100, R137, R138, and V161. The logo shows a high frequency of ALA and GLY in the first 20 positions, followed by a high frequency of MET and ALA in positions 21-40. The frequency of ALA and GLY is high throughout the sequence. The frequency of MET and ALA is high in positions 41-60. The frequency of ALA and GLY is high in positions 61-80. The frequency of MET and ALA is high in positions 81-100.

Position	Amino Acid	Frequency
1	GLU	0.02
2	ASN	0.02
3	LEU	0.02
4	THR	0.02
5	PRO	0.02
6	GLN	0.02
7	HIS	0.02
8	MET	0.02
9	ALA	0.02
10	SER	0.02
11	MET	0.02
12	ALA	0.02
13	LEU	0.02
14	THR	0.02
15	GLY	0.02
16	THR	0.02
17	ASP	0.02
18	ARG	0.02
19	VAL	0.02
20	LYS	0.02
21	ARG	0.02
22	GLY	0.02
23	MET	0.02
24	ALA	0.02
25	E16	0.02
26	M16	0.02
27	Q17	0.02
28	K18	0.02
29	G19	0.02
30	K32	0.02
31	L45	0.02
32	E46	0.02
33	ARG	0.02
34	VAL	0.02
35	PRO	0.02
36	ASP	0.02
37	ASP	0.02
38	ILE	0.02
39	ARG	0.02
40	ALA	0.02
41	ALA	0.02
42	GLY	0.02
43	G57	0.02
44	P64	0.02
45	M79	0.02
46	L96	0.02
47	G97	0.02
48	V98	0.02
49	D99	0.02
50	Y100	0.02
51	R137	0.02
52	R138	0.02
53	V161	0.02

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.68Å 107.20Å 178.22Å 90.00° 92.24° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.30) 99.9 (50.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.222 0.193 , 0.221	Depositor DCC
R_{free} test set	7973 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23986	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EDO, 3ZL, CAC, L5P, PO4, R5P

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	0.54	0/1886	0.70	0/2545
1	C	0.52	0/1867	0.71	0/2520
1	E	0.49	0/1864	0.71	0/2517
1	G	0.54	0/1956	0.74	0/2637
1	I	0.53	0/1885	0.71	0/2543
1	J	0.50	0/1858	0.70	0/2509
1	K	0.50	0/1886	0.69	0/2545
1	L	0.47	0/1859	0.70	0/2511
2	B	0.56	0/1979	0.75	0/2668
2	D	0.52	0/1881	0.70	0/2540
2	H	0.50	0/1877	0.70	0/2534
3	F	0.50	0/1884	0.70	0/2543
All	All	0.52	0/22682	0.71	0/30612

There are no bond length outliers.

There are no bond angle outliers.

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	1885	0	1902	11	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1866	0	1877	10	2
1	E	1863	0	1869	7	2
1	G	1955	0	1978	23	2
1	I	1884	0	1902	7	0
1	J	1857	0	1874	2	0
1	K	1885	0	1902	6	1
1	L	1858	0	1870	6	0
2	B	1955	0	1984	19	0
2	D	1857	0	1875	6	0
2	H	1853	0	1873	13	1
3	F	1877	0	1904	8	2
4	A	5	0	0	0	0
4	C	5	0	0	2	0
4	F	5	0	0	0	0
4	H	5	0	0	2	0
4	L	5	0	0	0	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
5	F	5	0	0	0	0
5	H	5	0	0	0	0
6	B	14	0	9	0	0
6	D	14	0	9	1	0
6	E	14	0	9	1	0
6	G	14	0	9	0	0
6	I	14	0	9	0	0
6	J	14	0	9	0	0
6	K	14	0	9	0	0
7	C	4	0	6	1	0
7	G	8	0	12	10	0
8	A	115	0	0	7	0
8	B	114	0	0	6	0
8	C	96	0	0	3	0
8	D	119	0	0	1	0
8	E	102	0	0	1	0
8	F	69	0	0	1	0
8	G	123	0	0	5	0
8	H	109	0	0	6	0
8	I	106	0	0	2	0
8	J	94	0	0	0	0
8	K	104	0	0	3	0
8	L	85	0	0	1	0
All	All	23986	0	22891	109	6

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 2.

The worst 5 of 109 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:159:GLU:HB2	8:A:414:HOH:O	1.44	1.17
1:G:128:GLY:O	7:G:302:EDO:H22	1.58	1.02
1:K:260:ASP:HB2	8:K:404:HOH:O	1.85	0.77
2:H:19:GLY:HA3	8:H:401:HOH:O	1.88	0.74
1:G:183:VAL:O	7:G:303:EDO:O2	2.05	0.74

The worst 5 of 6 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:A:243:ASN:OD1	1:G:29:GLU:OE2[1_455]	1.55	0.65
1:A:29:GLU:OE2	1:G:243:ASN:OD1[1_455]	1.62	0.58
1:C:266:HIS:NE2	1:K:260:ASP:OD2[2_354]	1.75	0.45
1:E:201:ARG:CG	3:F:260:ASP:OD2[1_565]	1.88	0.32
1:C:259:GLU:OE1	2:H:32:LYS:CD[2_454]	2.13	0.07

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	242/305 (79%)	234 (97%)	7 (3%)	1 (0%)	30	38
1	C	241/305 (79%)	234 (97%)	7 (3%)	0	100	100
1	E	241/305 (79%)	235 (98%)	6 (2%)	0	100	100
1	G	251/305 (82%)	245 (98%)	6 (2%)	0	100	100
1	I	243/305 (80%)	237 (98%)	5 (2%)	1 (0%)	30	38
1	J	239/305 (78%)	234 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	242/305 (79%)	234 (97%)	7 (3%)	1 (0%)	30	38
1	L	240/305 (79%)	236 (98%)	4 (2%)	0	100	100
2	B	256/305 (84%)	250 (98%)	5 (2%)	1 (0%)	30	38
2	D	243/305 (80%)	236 (97%)	6 (2%)	1 (0%)	30	38
2	H	242/305 (79%)	235 (97%)	5 (2%)	2 (1%)	16	20
3	F	243/304 (80%)	236 (97%)	7 (3%)	0	100	100
All	All	2923/3659 (80%)	2846 (97%)	70 (2%)	7 (0%)	43	55

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	16	MET
2	H	17	GLN
1	I	271	LEU
1	K	17	GLN
2	H	18	LYS

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	192/233 (82%)	190 (99%)	2 (1%)	68	82
1	C	189/233 (81%)	188 (100%)	1 (0%)	81	90
1	E	188/233 (81%)	187 (100%)	1 (0%)	81	90
1	G	199/233 (85%)	198 (100%)	1 (0%)	81	90
1	I	191/233 (82%)	190 (100%)	1 (0%)	81	90
1	J	189/233 (81%)	187 (99%)	2 (1%)	65	81
1	K	192/233 (82%)	188 (98%)	4 (2%)	47	66
1	L	188/233 (81%)	187 (100%)	1 (0%)	81	90
2	B	200/234 (86%)	198 (99%)	2 (1%)	68	82
2	D	190/234 (81%)	189 (100%)	1 (0%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	191/234 (82%)	190 (100%)	1 (0%)	81	90
3	F	192/233 (82%)	191 (100%)	1 (0%)	81	90
All	All	2301/2799 (82%)	2283 (99%)	18 (1%)	73	86

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	17	GLN
1	L	98	VAL
1	K	271	LEU
1	G	98	VAL
1	K	16	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	115	HIS
1	J	17	GLN
3	F	17	GLN
1	G	115	HIS
1	G	226	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues 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
1	L5P	A	81	1	20,21,22	1.10	1 (5%)	16,27,29	0.87	0
1	L5P	G	81	1	20,21,22	1.13	1 (5%)	16,27,29	0.88	1 (6%)
1	L5P	K	81	1	20,21,22	1.23	1 (5%)	16,27,29	1.00	1 (6%)
1	L5P	I	81	1	20,21,22	1.10	1 (5%)	16,27,29	1.05	1 (6%)
1	L5P	C	81	1	20,21,22	1.18	2 (10%)	16,27,29	1.06	1 (6%)
1	L5P	L	81	1	20,21,22	1.18	2 (10%)	16,27,29	1.30	2 (12%)
1	L5P	J	81	1	20,21,22	1.22	1 (5%)	16,27,29	1.49	3 (18%)
1	L5P	E	81	1	20,21,22	0.90	0	16,27,29	1.02	1 (6%)
3	3ZL	F	81	3	12,15,16	0.66	0	9,17,19	2.08	4 (44%)

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
1	L5P	A	81	1	-	14/23/25/27	-
1	L5P	G	81	1	-	12/23/25/27	-
1	L5P	K	81	1	-	11/23/25/27	-
1	L5P	I	81	1	-	9/23/25/27	-
1	L5P	C	81	1	-	10/23/25/27	-
1	L5P	L	81	1	-	7/23/25/27	-
1	L5P	J	81	1	-	7/23/25/27	-
1	L5P	E	81	1	-	1/23/25/27	-
3	3ZL	F	81	3	-	2/11/16/18	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	81	L5P	P9-O11	3.76	1.62	1.50
1	I	81	L5P	P9-O11	3.71	1.62	1.50
1	G	81	L5P	P9-O11	3.71	1.62	1.50
1	K	81	L5P	P9-O11	3.70	1.62	1.50
1	C	81	L5P	P9-O11	3.63	1.61	1.50

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	81	L5P	C2-C3-C5	4.16	123.26	116.43
1	L	81	L5P	C2-C3-C5	3.36	121.93	116.43
3	F	81	3ZL	C1-C2-C3	3.35	129.07	122.27
3	F	81	3ZL	C5-C4-N14	-3.21	118.03	125.76
3	F	81	3ZL	O13-C3-C4	-3.15	117.18	121.28

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	81	L5P	C3-C2-NZ-CE
1	A	81	L5P	O4-C3-C5-O13
1	A	81	L5P	O4-C3-C5-C6
1	A	81	L5P	C2-C3-C5-O13
1	A	81	L5P	C2-C3-C5-C6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	81	L5P	1	0
1	C	81	L5P	1	0
1	L	81	L5P	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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
4	CAC	H	302	-	2,4,4	2.24	1 (50%)	4,6,6	1.68	1 (25%)
6	R5P	D	302	-	12,13,13	1.91	1 (8%)	16,18,18	1.02	0
4	CAC	F	302	-	2,4,4	2.80	2 (100%)	4,6,6	2.01	1 (25%)
7	EDO	G	303	-	3,3,3	0.40	0	2,2,2	0.10	0
6	R5P	J	301	-	12,13,13	1.97	1 (8%)	16,18,18	1.01	1 (6%)
6	R5P	E	301	-	12,13,13	1.91	1 (8%)	16,18,18	0.90	0
5	PO4	B	301	-	4,4,4	0.63	0	6,6,6	0.82	0
5	PO4	H	301	-	4,4,4	0.80	0	6,6,6	0.56	0
6	R5P	G	301	-	12,13,13	1.93	1 (8%)	16,18,18	0.81	0
6	R5P	I	301	-	12,13,13	1.91	1 (8%)	16,18,18	0.85	0
5	PO4	F	301	-	4,4,4	0.92	0	6,6,6	0.58	0
6	R5P	B	302	-	12,13,13	1.96	1 (8%)	16,18,18	1.00	0
4	CAC	L	301	-	2,4,4	2.83	2 (100%)	4,6,6	1.67	2 (50%)
4	CAC	A	301	-	2,4,4	2.98	2 (100%)	4,6,6	3.05	2 (50%)
7	EDO	C	302	-	3,3,3	0.49	0	2,2,2	0.33	0
5	PO4	D	301	-	4,4,4	0.86	0	6,6,6	0.59	0
4	CAC	C	301	-	2,4,4	2.39	1 (50%)	4,6,6	2.00	2 (50%)
6	R5P	K	301	-	12,13,13	1.97	1 (8%)	16,18,18	1.05	1 (6%)
7	EDO	G	302	-	3,3,3	0.31	0	2,2,2	0.05	0

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
6	R5P	B	302	-	-	8/15/16/16	-
6	R5P	D	302	-	-	8/15/16/16	-
7	EDO	G	303	-	-	1/1/1/1	-
6	R5P	K	301	-	-	7/15/16/16	-
6	R5P	G	301	-	-	9/15/16/16	-
6	R5P	J	301	-	-	4/15/16/16	-
7	EDO	G	302	-	-	1/1/1/1	-
7	EDO	C	302	-	-	1/1/1/1	-
6	R5P	E	301	-	-	8/15/16/16	-
6	R5P	I	301	-	-	6/15/16/16	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	301	R5P	O1-C1	6.39	1.44	1.20
6	B	302	R5P	O1-C1	6.37	1.44	1.20
6	K	301	R5P	O1-C1	6.35	1.44	1.20
6	E	301	R5P	O1-C1	6.33	1.44	1.20
6	I	301	R5P	O1-C1	6.30	1.43	1.20

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	CAC	O1-AS-C1	-4.83	105.50	111.50
4	F	302	CAC	O1-AS-C2	3.84	116.27	111.50
4	H	302	CAC	O1-AS-C2	-2.71	108.13	111.50
4	C	301	CAC	O1-AS-C1	-2.71	108.13	111.50
4	A	301	CAC	O2-AS-C1	2.69	112.37	105.84

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	302	R5P	C5-O5-P-O2P
6	B	302	R5P	C5-O5-P-O3P
6	D	302	R5P	C1-C2-C3-C4
6	D	302	R5P	O2-C2-C3-O3
6	D	302	R5P	O2-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	302	CAC	2	0
6	D	302	R5P	1	0
7	G	303	EDO	3	0
6	E	301	R5P	1	0
7	C	302	EDO	1	0
4	C	301	CAC	2	0
7	G	302	EDO	7	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 [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, 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	247/305 (80%)	0.18	14 (5%) 29 31	31, 42, 74, 114	0
1	C	246/305 (80%)	0.10	10 (4%) 41 43	32, 43, 71, 116	0
1	E	246/305 (80%)	0.24	7 (2%) 55 57	34, 47, 81, 111	0
1	G	256/305 (83%)	0.20	15 (5%) 28 30	32, 42, 69, 102	0
1	I	248/305 (81%)	0.12	8 (3%) 50 52	32, 43, 72, 105	0
1	J	244/305 (80%)	0.08	4 (1%) 70 72	33, 46, 73, 106	0
1	K	247/305 (80%)	0.22	11 (4%) 38 40	33, 45, 73, 111	0
1	L	245/305 (80%)	0.26	8 (3%) 49 51	37, 49, 78, 107	0
2	B	260/305 (85%)	0.34	21 (8%) 18 19	32, 43, 80, 108	0
2	D	247/305 (80%)	0.14	8 (3%) 50 52	34, 43, 74, 115	0
2	H	246/305 (80%)	0.23	5 (2%) 65 66	35, 48, 79, 96	0
3	F	247/304 (81%)	0.32	7 (2%) 55 57	34, 47, 80, 114	0
All	All	2979/3659 (81%)	0.20	118 (3%) 42 44	31, 45, 77, 116	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	48	VAL	7.8
3	F	271	LEU	7.2
1	K	271	LEU	7.1
1	G	271	LEU	6.3
1	J	271	LEU	5.6

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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
1	L5P	K	81	22/23	0.82	0.15	44,78,85,87	0
1	L5P	E	81	22/23	0.84	0.16	37,87,94,99	0
1	L5P	L	81	22/23	0.86	0.13	44,83,92,95	0
1	L5P	I	81	22/23	0.87	0.14	39,76,85,87	0
1	L5P	J	81	22/23	0.88	0.13	36,77,85,88	0
3	3ZL	F	81	16/17	0.89	0.13	41,58,78,79	0
1	L5P	C	81	22/23	0.90	0.13	39,73,81,83	0
1	L5P	G	81	22/23	0.90	0.11	39,72,76,79	0
1	L5P	A	81	22/23	0.90	0.13	34,81,87,90	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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
5	PO4	B	301	5/5	0.67	0.16	61,62,73,75	0
5	PO4	D	301	5/5	0.69	0.15	76,77,87,93	0
5	PO4	F	301	5/5	0.74	0.14	79,80,85,85	0
5	PO4	H	301	5/5	0.77	0.13	77,81,84,85	0
7	EDO	G	303	4/4	0.81	0.27	89,93,95,99	0
7	EDO	G	302	4/4	0.85	0.28	67,69,69,70	0
4	CAC	A	301	5/5	0.86	0.21	79,86,88,88	0
6	R5P	G	301	14/14	0.87	0.13	63,79,86,86	0
4	CAC	H	302	5/5	0.88	0.15	79,80,86,89	0
6	R5P	J	301	14/14	0.88	0.12	56,75,84,85	0
6	R5P	B	302	14/14	0.89	0.13	57,79,89,90	0
7	EDO	C	302	4/4	0.90	0.28	56,59,61,61	0
6	R5P	K	301	14/14	0.91	0.13	60,79,96,96	0
6	R5P	D	302	14/14	0.91	0.12	55,79,91,92	0
6	R5P	I	301	14/14	0.92	0.11	58,79,101,102	0
6	R5P	E	301	14/14	0.92	0.11	59,75,80,83	0
4	CAC	L	301	5/5	0.92	0.15	75,76,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CAC	C	301	5/5	0.93	0.15	80,81,85,91	0
4	CAC	F	302	5/5	0.93	0.14	67,77,79,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.