



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2023 – 05:42 PM EDT

PDB ID : 4WY0  
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 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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

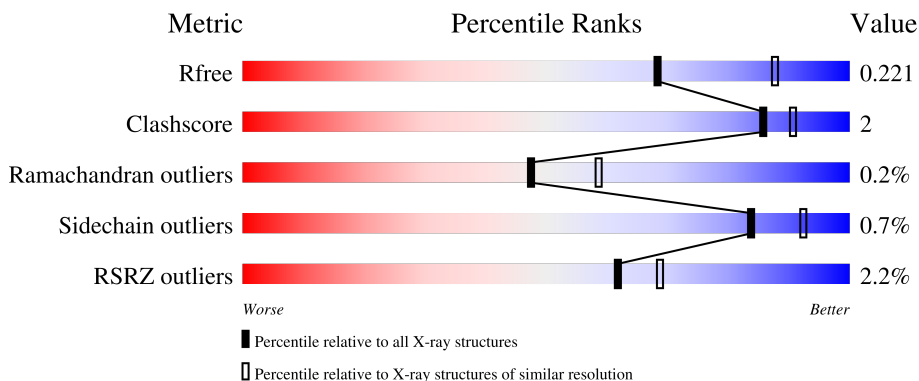
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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  $\geq 3$ , 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	305	 2% 75% 6% 19%
1	C	305	 2% 76% 5% 19%
1	E	305	 3% 78% . 19%
1	G	305	 3% 77% 7% 16%
1	I	305	 % 78% . 18%

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Mol	Chain	Length	Quality of chain
1	J	305	<p>2% 78% 20%</p>
1	K	305	<p>% 79% 19%</p>
1	L	305	<p>% 77% 19%</p>
2	B	305	<p>2% 79% 6% 15%</p>
2	D	305	<p>% 79% 19%</p>
2	H	305	<p>% 75% 5% 19%</p>
3	F	304	<p>2% 77% 18%</p>

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
7	EDO	G	302	-	-	X	X
7	EDO	G	303	-	-	-	X

## 2 Entry composition [i](#)

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

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	C	N	O	S	0	0	0
			1955	1220	351	370	14			
2	D	247	Total	C	N	O	S	0	0	0
			1857	1162	331	352	12			
2	H	246	Total	C	N	O	S	0	0	0
			1853	1160	327	353	13			

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

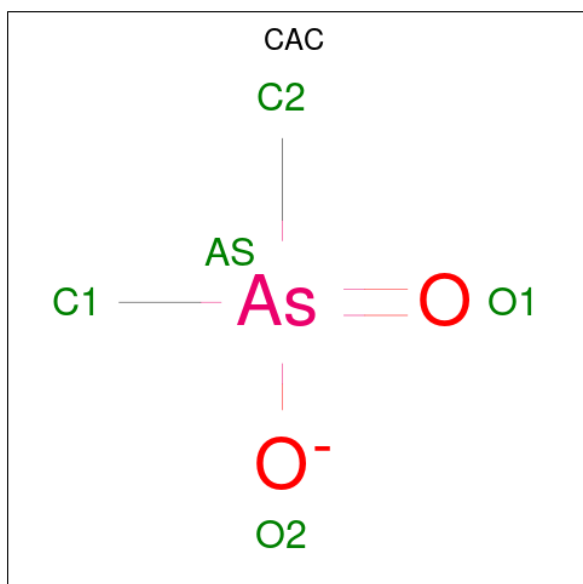
- Molecule 3 is a protein called Pyridoxal biosynthesis lyase PdxS.

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

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

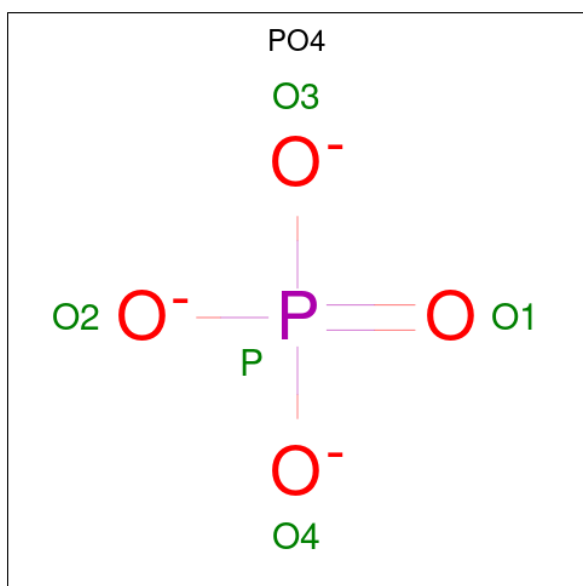
- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula:  $C_2H_6AsO_2$ ).





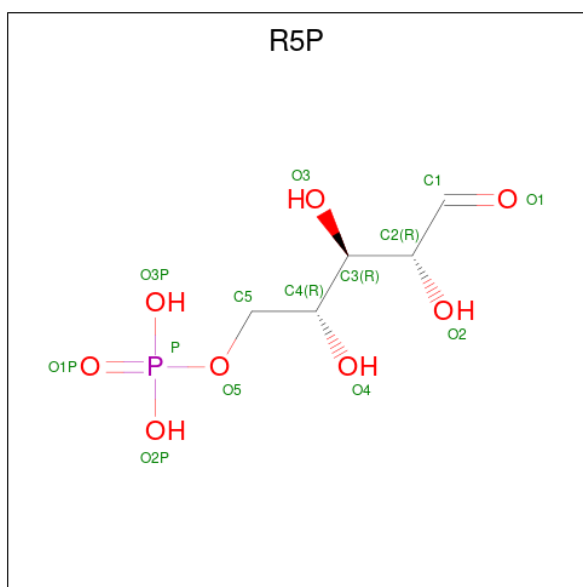
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	C	1	Total	As	C	O	0	0
			5	1	2	2		
4	F	1	Total	As	C	O	0	0
			5	1	2	2		
4	H	1	Total	As	C	O	0	0
			5	1	2	2		
4	L	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



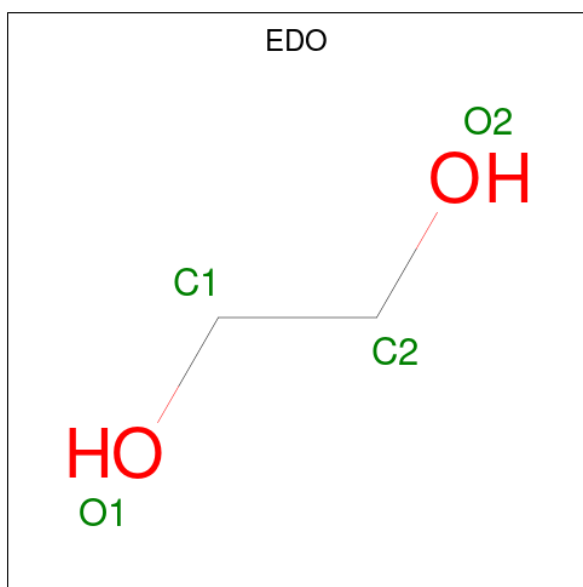
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is RIBOSE-5-PHOSPHATE (three-letter code: R5P) (formula: C<sub>5</sub>H<sub>11</sub>O<sub>8</sub>P).



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 (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 8 is water.

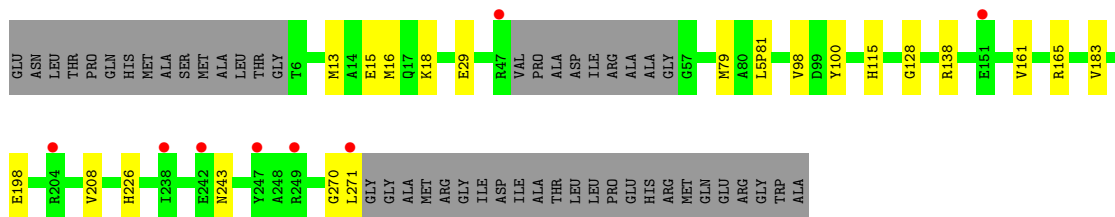
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	115	Total O 115 115	0	0
8	B	114	Total O 114 114	0	0
8	C	96	Total O 96 96	0	0
8	D	119	Total O 119 119	0	0
8	E	102	Total O 102 102	0	0
8	F	69	Total O 69 69	0	0
8	G	123	Total O 123 123	0	0
8	H	109	Total O 109 109	0	0
8	I	106	Total O 106 106	0	0

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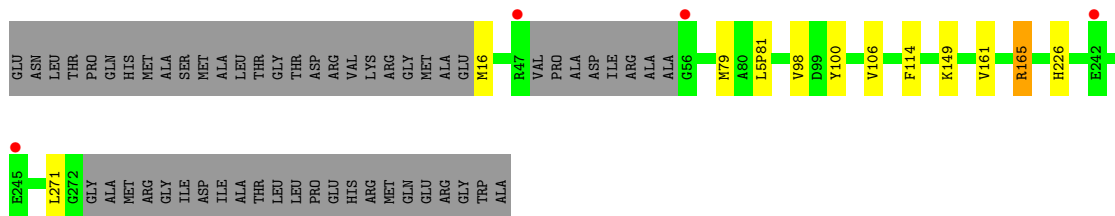
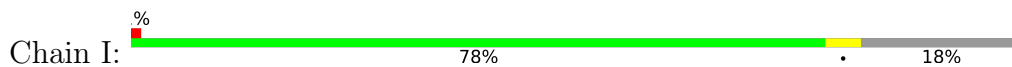
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
8	J	94	Total O 94 94	0	0
8	K	104	Total O 104 104	0	0
8	L	85	Total O 85 85	0	0

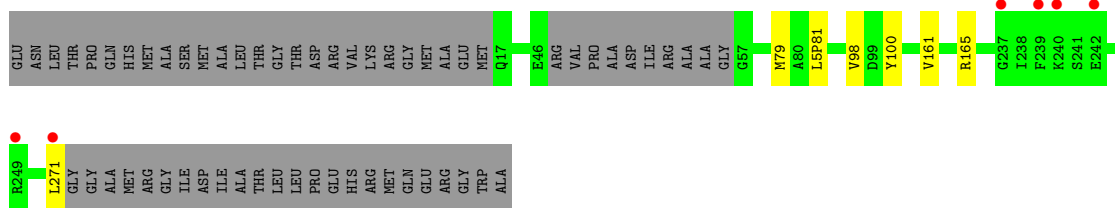
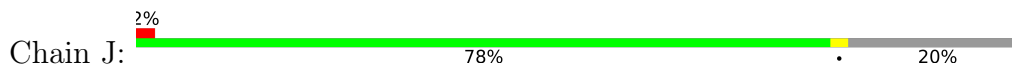




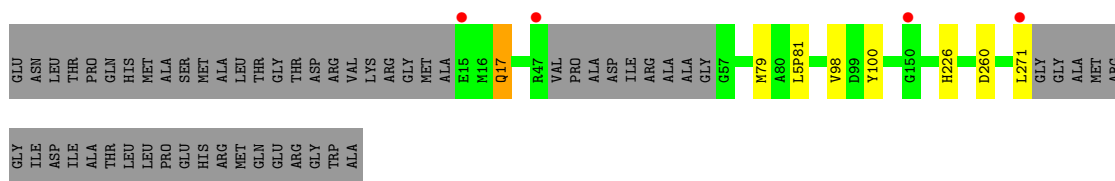
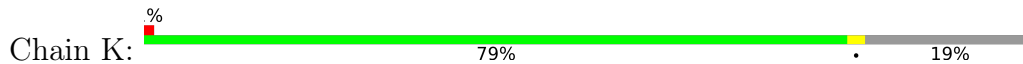
- Molecule 1: Pyridoxal biosynthesis lyase PdxS



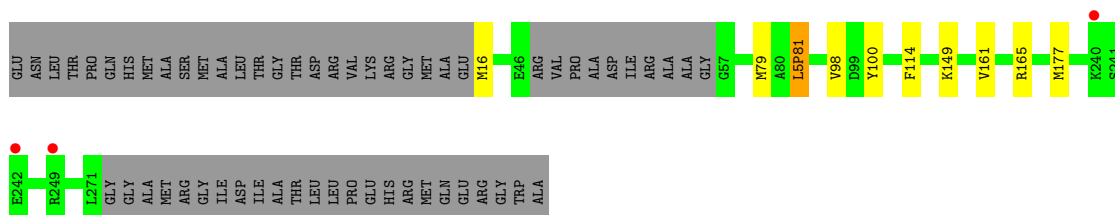
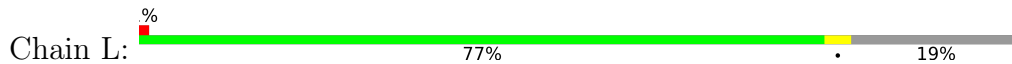
- Molecule 1: Pyridoxal biosynthesis lyase PdxS



- Molecule 1: Pyridoxal biosynthesis lyase PdxS



- Molecule 1: Pyridoxal biosynthesis lyase PdxS





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.68Å 107.20Å 178.22Å 90.00° 92.24° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 47.30 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.30) 99.5 (47.30-2.29)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.29Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.191 , 0.222 0.193 , 0.221	Depositor DCC
$R_{free}$ test set	7970 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtrriage
Anisotropy	0.242	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23986	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage'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.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PO4, L5P, 3ZL, R5P, CAC

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	0.37	0/1886	0.58	0/2545
1	C	0.36	0/1867	0.58	0/2520
1	E	0.35	0/1864	0.58	0/2517
1	G	0.37	0/1956	0.59	0/2637
1	I	0.36	0/1885	0.60	2/2543 (0.1%)
1	J	0.35	0/1858	0.58	0/2509
1	K	0.35	0/1886	0.58	0/2545
1	L	0.32	0/1859	0.57	0/2511
2	B	0.37	0/1979	0.61	0/2668
2	D	0.36	0/1881	0.58	0/2540
2	H	0.34	0/1877	0.57	0/2534
3	F	0.35	0/1884	0.58	1/2543 (0.0%)
All	All	0.35	0/22682	0.58	3/30612 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	165	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	I	165	ARG	NE-CZ-NH2	-5.37	117.62	120.30
3	F	165	ARG	NE-CZ-NH1	5.12	122.86	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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1885	0	1901	11	2
1	C	1866	0	1876	10	2
1	E	1863	0	1869	6	2
1	G	1955	0	1977	20	2
1	I	1884	0	1901	7	0
1	J	1857	0	1873	2	0
1	K	1885	0	1901	4	1
1	L	1858	0	1869	8	0
2	B	1955	0	1984	15	0
2	D	1857	0	1875	4	0
2	H	1853	0	1873	13	1
3	F	1877	0	1903	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	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	85	0	0	2	0
All	All	23986	0	22883	100	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.

All (100) 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
8:A:469:HOH:O	2:B:176:ASN:HB2	1.89	0.72
2:H:18:LYS:O	8:H:401:HOH:O	2.07	0.72
1:I:16:MET:N	8:I:477:HOH:O	2.21	0.71
2:H:138:ARG:HH22	4:H:302:CAC:C2	2.05	0.70
1:G:15:GLU:OE1	1:G:18:LYS:HE3	1.94	0.66
1:C:134:GLU:HG2	4:C:301:CAC:C2	2.25	0.66
1:G:128:GLY:O	7:G:302:EDO:C2	2.38	0.65
1:L:81:L5P:O4	1:L:149:LYS:NZ	2.29	0.65
2:H:46:GLU:C	8:H:508:HOH:O	2.36	0.64
1:C:106:VAL:HG13	8:C:480:HOH:O	2.00	0.61
1:G:15:GLU:HA	1:G:208:VAL:HG21	1.85	0.59
1:L:81:L5P:H18	8:L:470:HOH:O	2.05	0.55
3:F:266:HIS:CD2	8:F:404:HOH:O	2.59	0.55
1:A:190:GLY:O	7:G:303:EDO:H11	2.06	0.55
1:G:115:HIS:HE1	7:G:302:EDO:C1	2.20	0.54
1:E:46:GLU:C	8:E:502:HOH:O	2.47	0.54
8:A:469:HOH:O	2:B:176:ASN:CB	2.50	0.54
1:L:16:MET:N	1:L:100:TYR:HH	2.06	0.54
1:G:15:GLU:HA	1:G:208:VAL:CG2	2.38	0.53
1:C:138:ARG:HH12	4:C:301:CAC:C2	2.21	0.53
1:K:79:MET:HG2	1:K:100:TYR:HB2	1.93	0.51
6:E:301:R5P:O4	6:E:301:R5P:O2	2.24	0.51
2:H:137:ARG:HE	4:H:302:CAC:C2	2.24	0.51
1:G:138:ARG:NH1	7:G:302:EDO:O2	2.43	0.50
1:I:226:HIS:HD2	8:I:452:HOH:O	1.94	0.50
1:G:115:HIS:HE1	7:G:302:EDO:H11	1.77	0.50
2:B:262:GLU:HB3	8:B:405:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:HIS:HD2	8:G:417:HOH:O	1.95	0.49
1:G:13:MET:O	1:G:16:MET:HG2	2.12	0.49
6:D:302:R5P:O4	6:D:302:R5P:O2	2.28	0.48
1:G:115:HIS:CE1	7:G:302:EDO:H11	2.47	0.48
2:H:18:LYS:HB3	8:H:509:HOH:O	2.14	0.47
2:B:60:ARG:NH2	3:F:155:GLY:O	2.40	0.47
1:A:257:HIS:HE1	8:A:403:HOH:O	1.97	0.47
1:A:79:MET:HG2	1:A:100:TYR:HB2	1.96	0.47
2:H:16:MET:O	2:H:18:LYS:N	2.48	0.47
1:C:79:MET:HG2	1:C:100:TYR:HB2	1.97	0.46
8:G:476:HOH:O	1:I:226:HIS:HE1	1.98	0.46
2:H:161:VAL:O	2:H:165:ARG:HG3	2.15	0.46
1:C:81:L5P:NZ	8:C:453:HOH:O	2.30	0.46
2:D:226:HIS:HD2	8:D:470:HOH:O	1.98	0.46
1:A:161:VAL:O	1:A:165:ARG:HG3	2.16	0.46
1:A:213:GLY:O	8:A:414:HOH:O	2.21	0.46
1:C:161:VAL:O	1:C:165:ARG:HG3	2.16	0.45
1:C:226:HIS:HD2	8:C:406:HOH:O	1.98	0.45
1:L:79:MET:HG2	1:L:100:TYR:HB2	1.98	0.45
1:A:190:GLY:O	7:G:303:EDO:C1	2.64	0.45
2:B:19:GLY:HA2	8:B:428:HOH:O	2.16	0.45
1:J:79:MET:HG2	1:J:100:TYR:HB2	1.99	0.45
1:L:161:VAL:O	1:L:165:ARG:HG3	2.17	0.45
1:G:270:GLY:O	1:G:271:LEU:C	2.55	0.44
2:H:18:LYS:C	8:H:401:HOH:O	2.52	0.44
2:B:91:ARG:HB3	3:F:261:TYR:CG	2.53	0.44
2:B:198:GLU:HG2	8:B:497:HOH:O	2.17	0.44
1:E:79:MET:HG2	1:E:100:TYR:HB2	2.00	0.43
1:E:161:VAL:O	1:E:165:ARG:HG3	2.18	0.43
1:G:161:VAL:O	1:G:165:ARG:HG3	2.18	0.43
1:K:260:ASP:CB	8:K:404:HOH:O	2.53	0.43
1:G:115:HIS:CE1	7:G:302:EDO:C1	3.00	0.43
2:B:18:LYS:HB3	8:B:462:HOH:O	2.18	0.43
2:B:79:MET:HG2	2:B:100:TYR:HB2	2.00	0.43
2:H:79:MET:HG2	2:H:100:TYR:HB2	1.99	0.43
2:B:15:GLU:C	2:B:17:GLN:H	2.21	0.43
1:E:114:PHE:CD2	1:G:165:ARG:HD3	2.54	0.43
2:B:161:VAL:O	2:B:165:ARG:HG3	2.19	0.43
1:G:13:MET:HE1	8:G:425:HOH:O	2.19	0.43
2:H:64:PRO:HB3	2:H:96:LEU:HD11	2.01	0.43
3:F:161:VAL:O	3:F:165:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:226:HIS:HD2	8:H:439:HOH:O	2.01	0.43
1:K:226:HIS:HD2	8:K:407:HOH:O	2.02	0.42
1:C:261:TYR:CG	2:D:91:ARG:HB3	2.54	0.42
3:F:91:ARG:HB3	2:H:261:TYR:CG	2.55	0.42
1:G:15:GLU:OE1	1:G:18:LYS:CE	2.64	0.42
2:B:19:GLY:CA	8:B:428:HOH:O	2.67	0.42
1:I:79:MET:HG2	1:I:100:TYR:HB2	2.01	0.42
3:F:79:MET:HG2	3:F:100:TYR:HB2	2.02	0.42
2:B:88:VAL:HG11	3:F:222:ALA:HB3	2.02	0.42
2:D:165:ARG:HD3	1:I:114:PHE:CD2	2.55	0.42
2:B:64:PRO:HG2	3:F:268:SER:HB2	2.00	0.42
1:G:198:GLU:HG2	8:G:501:HOH:O	2.19	0.41
1:A:226:HIS:HD2	8:A:455:HOH:O	2.03	0.41
1:E:165:ARG:HD3	1:L:114:PHE:HD2	1.85	0.41
1:J:161:VAL:O	1:J:165:ARG:HG3	2.20	0.41
1:A:246:LYS:HE2	8:A:489:HOH:O	2.20	0.41
1:A:247:TYR:CD1	1:A:271:LEU:HD13	2.56	0.41
2:D:79:MET:HG2	2:D:100:TYR:HB2	2.03	0.41
1:I:161:VAL:O	1:I:165:ARG:HG3	2.21	0.41
1:L:177:MET:HE1	8:L:447:HOH:O	2.20	0.41
1:G:79:MET:HG2	1:G:100:TYR:HB2	2.02	0.41
1:C:85:GLY:CA	7:C:302:EDO:H21	2.50	0.41
1:E:165:ARG:HD3	1:L:114:PHE:CD2	2.56	0.41
1:A:46:GLU:O	1:A:47:ARG:HG3	2.22	0.40
1:I:106:VAL:CG1	1:I:149:LYS:HZ1	2.34	0.40
2:B:173:LYS:HE3	8:B:493:HOH:O	2.22	0.40
1:C:15:GLU:O	1:C:16:MET:C	2.58	0.40

All (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
1:E:201:ARG:CD	3:F:260:ASP:OD2[1_565]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/305 (79%)	234 (97%)	7 (3%)	1 (0%)	34	42
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%)	34	42
1	J	239/305 (78%)	234 (98%)	5 (2%)	0	100	100
1	K	242/305 (79%)	234 (97%)	7 (3%)	1 (0%)	34	42
1	L	240/305 (79%)	236 (98%)	4 (2%)	0	100	100
2	B	256/305 (84%)	250 (98%)	5 (2%)	1 (0%)	34	42
2	D	243/305 (80%)	236 (97%)	6 (2%)	1 (0%)	34	42
2	H	242/305 (79%)	235 (97%)	5 (2%)	2 (1%)	19	23
3	F	243/304 (80%)	236 (97%)	7 (3%)	0	100	100
All	All	2923/3659 (80%)	2846 (97%)	70 (2%)	7 (0%)	47	58

All (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
1	A	16	MET
2	B	16	MET

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/233 (82%)	190 (99%)	2 (1%)	76	87
1	C	189/233 (81%)	188 (100%)	1 (0%)	88	95
1	E	188/233 (81%)	187 (100%)	1 (0%)	88	95
1	G	199/233 (85%)	198 (100%)	1 (0%)	88	95
1	I	191/233 (82%)	190 (100%)	1 (0%)	88	95
1	J	189/233 (81%)	187 (99%)	2 (1%)	73	86
1	K	192/233 (82%)	189 (98%)	3 (2%)	62	78
1	L	188/233 (81%)	187 (100%)	1 (0%)	88	95
2	B	200/234 (86%)	199 (100%)	1 (0%)	88	95
2	D	190/234 (81%)	189 (100%)	1 (0%)	88	95
2	H	191/234 (82%)	190 (100%)	1 (0%)	88	95
3	F	192/233 (82%)	191 (100%)	1 (0%)	88	95
All	All	2301/2799 (82%)	2285 (99%)	16 (1%)	84	92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	98	VAL
2	B	98	VAL
1	C	98	VAL
2	D	98	VAL
1	E	98	VAL
3	F	98	VAL
1	G	98	VAL
2	H	98	VAL
1	I	98	VAL
1	J	98	VAL
1	J	271	LEU
1	K	17	GLN
1	K	98	VAL

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Mol	Chain	Res	Type
1	K	271	LEU
1	L	98	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	17	GLN
1	G	115	HIS
1	G	226	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](#)

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	E	81	1	18,21,22	0.90	0	13,27,29	0.95	1 (7%)
1	L5P	J	81	1	18,21,22	1.21	1 (5%)	13,27,29	1.00	2 (15%)
1	L5P	I	81	1	18,21,22	1.12	1 (5%)	13,27,29	1.07	1 (7%)
1	L5P	A	81	1	18,21,22	1.11	1 (5%)	13,27,29	1.01	1 (7%)
1	L5P	L	81	1	18,21,22	1.17	1 (5%)	13,27,29	0.89	0
1	L5P	C	81	1	18,21,22	1.18	1 (5%)	13,27,29	1.19	2 (15%)
1	L5P	K	81	1	18,21,22	1.22	1 (5%)	13,27,29	1.05	1 (7%)
3	3ZL	F	81	3	13,15,16	0.99	1 (7%)	8,17,19	2.66	4 (50%)
1	L5P	G	81	1	18,21,22	1.14	1 (5%)	13,27,29	1.19	1 (7%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	L5P	E	81	1	-	1/23/25/27	-
1	L5P	J	81	1	-	7/23/25/27	-
1	L5P	I	81	1	-	9/23/25/27	-
1	L5P	A	81	1	-	14/23/25/27	-
1	L5P	L	81	1	-	7/23/25/27	-
1	L5P	C	81	1	-	10/23/25/27	-
1	L5P	K	81	1	-	10/23/25/27	-
3	3ZL	F	81	3	-	2/11/16/18	-
1	L5P	G	81	1	-	11/23/25/27	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	81	L5P	P9-O11	3.61	1.62	1.50
1	I	81	L5P	P9-O11	3.56	1.62	1.50
1	G	81	L5P	P9-O11	3.55	1.62	1.50
1	K	81	L5P	P9-O11	3.55	1.62	1.50
1	C	81	L5P	P9-O11	3.47	1.61	1.50
1	A	81	L5P	P9-O11	3.46	1.61	1.50
1	L	81	L5P	P9-O11	3.29	1.61	1.50
3	F	81	3ZL	C4-N14	2.75	1.42	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	81	3ZL	C1-C2-C3	5.26	129.07	120.38
1	G	81	L5P	C2-NZ-CE	-3.50	107.79	113.33
3	F	81	3ZL	O13-C3-C4	-3.29	117.18	121.18
3	F	81	3ZL	C5-C4-N14	-3.29	118.03	125.81
3	F	81	3ZL	CE-NZ-C1	2.59	132.92	123.66
1	C	81	L5P	P9-O8-C7	2.46	125.06	118.30
1	K	81	L5P	P9-O8-C7	2.44	125.01	118.30
1	E	81	L5P	P9-O8-C7	2.27	124.54	118.30
1	A	81	L5P	C2-NZ-CE	-2.26	109.75	113.33
1	J	81	L5P	P9-O8-C7	2.24	124.45	118.30
1	C	81	L5P	C2-NZ-CE	-2.17	109.89	113.33
1	I	81	L5P	P9-O8-C7	2.14	124.19	118.30
1	J	81	L5P	O12-P9-O8	2.08	112.26	106.73

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
1	A	81	L5P	C3-C5-C6-O14
1	A	81	L5P	C3-C5-C6-C7
1	A	81	L5P	O13-C5-C6-O14
1	A	81	L5P	O13-C5-C6-C7
1	A	81	L5P	C7-O8-P9-O12
1	A	81	L5P	C7-O8-P9-O11
1	A	81	L5P	C7-O8-P9-O10
1	C	81	L5P	C3-C5-C6-O14
1	C	81	L5P	C3-C5-C6-C7
1	C	81	L5P	O13-C5-C6-O14
1	C	81	L5P	O13-C5-C6-C7
1	C	81	L5P	C7-O8-P9-O12
3	F	81	3ZL	O-C-CA-CB
1	G	81	L5P	O4-C3-C5-O13
1	G	81	L5P	O13-C5-C6-O14
1	G	81	L5P	C5-C6-C7-O8
1	G	81	L5P	O14-C6-C7-O8
1	G	81	L5P	C7-O8-P9-O12
1	G	81	L5P	C7-O8-P9-O11
1	G	81	L5P	C7-O8-P9-O10
1	I	81	L5P	O-C1-CA-CB
1	I	81	L5P	O4-C3-C5-O13
1	I	81	L5P	C7-O8-P9-O12
1	I	81	L5P	C7-O8-P9-O11
1	I	81	L5P	C7-O8-P9-O10
1	J	81	L5P	O-C1-CA-CB
1	J	81	L5P	C7-O8-P9-O12
1	J	81	L5P	C7-O8-P9-O11
1	J	81	L5P	C7-O8-P9-O10
1	K	81	L5P	O-C1-CA-CB
1	K	81	L5P	C3-C2-NZ-CE
1	K	81	L5P	O4-C3-C5-O13
1	K	81	L5P	O13-C5-C6-C7
1	K	81	L5P	C7-O8-P9-O12
1	K	81	L5P	C7-O8-P9-O10
1	L	81	L5P	O-C1-CA-CB

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Mol	Chain	Res	Type	Atoms
1	L	81	L5P	C7-O8-P9-O10
1	J	81	L5P	CG-CD-CE-NZ
1	E	81	L5P	CG-CD-CE-NZ
1	G	81	L5P	CG-CD-CE-NZ
1	A	81	L5P	CG-CD-CE-NZ
1	L	81	L5P	CG-CD-CE-NZ
1	L	81	L5P	NZ-C2-C3-O4
3	F	81	3ZL	CD-CE-NZ-C1
1	C	81	L5P	CG-CD-CE-NZ
1	C	81	L5P	NZ-C2-C3-O4
1	K	81	L5P	C7-O8-P9-O11
1	L	81	L5P	C7-O8-P9-O11
1	I	81	L5P	C3-C2-NZ-CE
1	L	81	L5P	C7-O8-P9-O12
1	I	81	L5P	CG-CD-CE-NZ
1	I	81	L5P	O4-C3-C5-C6
1	I	81	L5P	C2-C3-C5-C6
1	J	81	L5P	NZ-C2-C3-O4
1	G	81	L5P	O13-C5-C6-C7
1	J	81	L5P	O13-C5-C6-C7
1	L	81	L5P	O13-C5-C6-C7
1	K	81	L5P	C3-C5-C6-C7
1	C	81	L5P	C7-O8-P9-O11
1	K	81	L5P	CD-CE-NZ-C2
1	A	81	L5P	C3-C2-NZ-CE
1	C	81	L5P	C3-C2-NZ-CE
1	G	81	L5P	CD-CE-NZ-C2
1	C	81	L5P	C7-O8-P9-O10
1	K	81	L5P	O13-C5-C6-O14
1	A	81	L5P	NZ-C2-C3-O4
1	G	81	L5P	C3-C5-C6-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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
5	PO4	B	301	-	4,4,4	0.59	0	6,6,6	0.78	0
7	EDO	G	302	-	3,3,3	0.33	0	2,2,2	0.02	0
6	R5P	D	302	-	12,13,13	1.82	1 (8%)	17,18,18	0.98	0
5	PO4	H	301	-	4,4,4	0.76	0	6,6,6	0.53	0
7	EDO	C	302	-	3,3,3	0.52	0	2,2,2	0.31	0
4	CAC	C	301	-	0,4,4	-	-	0,6,6	-	-
6	R5P	G	301	-	12,13,13	1.85	1 (8%)	17,18,18	0.86	0
6	R5P	K	301	-	12,13,13	1.89	1 (8%)	17,18,18	1.00	1 (5%)
6	R5P	E	301	-	12,13,13	1.82	1 (8%)	17,18,18	0.88	0
5	PO4	F	301	-	4,4,4	0.87	0	6,6,6	0.54	0
4	CAC	L	301	-	0,4,4	-	-	0,6,6	-	-
6	R5P	B	302	-	12,13,13	1.88	1 (8%)	17,18,18	1.05	0
4	CAC	H	302	-	0,4,4	-	-	0,6,6	-	-
6	R5P	J	301	-	12,13,13	1.88	1 (8%)	17,18,18	1.02	1 (5%)
4	CAC	F	302	-	0,4,4	-	-	0,6,6	-	-
7	EDO	G	303	-	3,3,3	0.43	0	2,2,2	0.04	0
5	PO4	D	301	-	4,4,4	0.81	0	6,6,6	0.56	0
6	R5P	I	301	-	12,13,13	1.83	1 (8%)	17,18,18	0.85	0
4	CAC	A	301	-	0,4,4	-	-	0,6,6	-	-

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
7	EDO	G	303	-	-	1/1/1/1	-
6	R5P	B	302	-	-	8/14/16/16	-
7	EDO	G	302	-	-	1/1/1/1	-
6	R5P	I	301	-	-	6/14/16/16	-
6	R5P	G	301	-	-	9/14/16/16	-
6	R5P	K	301	-	-	7/14/16/16	-
6	R5P	D	302	-	-	8/14/16/16	-
6	R5P	E	301	-	-	7/14/16/16	-
7	EDO	C	302	-	-	1/1/1/1	-
6	R5P	J	301	-	-	4/14/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	301	R5P	O1-C1	6.09	1.44	1.19
6	B	302	R5P	O1-C1	6.07	1.44	1.19
6	K	301	R5P	O1-C1	6.05	1.44	1.19
6	E	301	R5P	O1-C1	6.03	1.44	1.19
6	I	301	R5P	O1-C1	6.01	1.43	1.19
6	G	301	R5P	O1-C1	6.00	1.43	1.19
6	D	302	R5P	O1-C1	5.99	1.43	1.19

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	301	R5P	O3P-P-O5	-2.02	101.36	106.73
6	K	301	R5P	O2P-P-O5	-2.01	101.39	106.73

There are no chirality outliers.

All (52) 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
6	E	301	R5P	C1-C2-C3-C4
6	E	301	R5P	O2-C2-C3-O3
6	E	301	R5P	O2-C2-C3-C4
6	G	301	R5P	C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
6	G	301	R5P	O4-C4-C5-O5
6	G	301	R5P	C5-O5-P-O2P
6	G	301	R5P	C5-O5-P-O3P
6	I	301	R5P	C3-C4-C5-O5
6	I	301	R5P	O4-C4-C5-O5
6	J	301	R5P	C3-C4-C5-O5
6	J	301	R5P	O4-C4-C5-O5
6	K	301	R5P	C1-C2-C3-O3
6	K	301	R5P	C1-C2-C3-C4
6	K	301	R5P	O2-C2-C3-O3
6	K	301	R5P	O2-C2-C3-C4
6	B	302	R5P	O3-C3-C4-C5
6	G	301	R5P	O3-C3-C4-C5
6	B	302	R5P	C2-C3-C4-C5
6	G	301	R5P	C2-C3-C4-C5
6	B	302	R5P	O3-C3-C4-O4
6	G	301	R5P	O3-C3-C4-O4
6	B	302	R5P	C2-C3-C4-O4
6	G	301	R5P	C2-C3-C4-O4
7	G	302	EDO	O1-C1-C2-O2
7	G	303	EDO	O1-C1-C2-O2
6	I	301	R5P	C2-C3-C4-O4
6	K	301	R5P	C2-C3-C4-O4
6	B	302	R5P	C5-O5-P-O1P
6	G	301	R5P	C5-O5-P-O1P
6	E	301	R5P	C1-C2-C3-O3
6	K	301	R5P	C2-C3-C4-C5
6	E	301	R5P	C4-C5-O5-P
6	J	301	R5P	C4-C5-O5-P
6	E	301	R5P	C3-C4-C5-O5
7	C	302	EDO	O1-C1-C2-O2
6	D	302	R5P	C2-C3-C4-O4
6	B	302	R5P	C4-C5-O5-P
6	D	302	R5P	C5-O5-P-O1P
6	K	301	R5P	O3-C3-C4-O4
6	I	301	R5P	O3-C3-C4-O4
6	D	302	R5P	C1-C2-C3-O3
6	E	301	R5P	O4-C4-C5-O5
6	D	302	R5P	C2-C3-C4-C5
6	I	301	R5P	C2-C3-C4-C5
6	J	301	R5P	O3-C3-C4-C5
6	D	302	R5P	O3-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
6	I	301	R5P	O3-C3-C4-C5

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	302	EDO	7	0
6	D	302	R5P	1	0
7	C	302	EDO	1	0
4	C	301	CAC	2	0
6	E	301	R5P	1	0
4	H	302	CAC	2	0
7	G	303	EDO	3	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	247/305 (80%)	-0.17	7 (2%) 53 60	31, 42, 74, 114	0
1	C	246/305 (80%)	-0.16	7 (2%) 53 60	32, 43, 71, 116	0
1	E	246/305 (80%)	-0.09	9 (3%) 41 48	34, 47, 81, 111	0
1	G	256/305 (83%)	-0.17	8 (3%) 49 56	32, 42, 69, 102	0
1	I	248/305 (81%)	-0.12	4 (1%) 72 77	32, 43, 72, 105	0
1	J	244/305 (80%)	-0.16	6 (2%) 57 64	33, 46, 73, 106	0
1	K	247/305 (80%)	-0.14	4 (1%) 72 77	33, 45, 73, 111	0
1	L	245/305 (80%)	-0.11	3 (1%) 79 83	37, 49, 78, 107	0
2	B	260/305 (85%)	-0.04	7 (2%) 54 62	32, 43, 80, 108	0
2	D	247/305 (80%)	-0.17	4 (1%) 72 77	34, 43, 74, 115	0
2	H	246/305 (80%)	-0.18	2 (0%) 86 89	35, 48, 79, 96	0
3	F	247/304 (81%)	-0.04	6 (2%) 59 66	34, 47, 80, 114	0
All	All	2979/3659 (81%)	-0.13	67 (2%) 62 69	31, 45, 77, 116	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	56	GLY	5.8
1	A	271	LEU	5.3
1	K	271	LEU	4.7
1	E	56	GLY	4.6
1	E	242	GLU	3.9
3	F	242	GLU	3.9
1	J	242	GLU	3.8
1	A	17	GLN	3.7
3	F	48	VAL	3.7
1	A	242	GLU	3.3
2	H	18	LYS	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	17	GLN	3.2
1	J	271	LEU	3.1
1	C	266	HIS	2.9
1	I	56	GLY	2.9
1	A	18	LYS	2.9
1	I	47	ARG	2.9
1	L	249	ARG	2.7
1	L	242	GLU	2.7
1	G	151	GLU	2.7
1	L	240	LYS	2.7
2	D	17	GLN	2.7
2	D	16	MET	2.7
1	E	266	HIS	2.6
1	E	236	SER	2.6
1	G	238	ILE	2.6
1	A	47	ARG	2.6
1	I	242	GLU	2.6
1	G	249	ARG	2.5
2	B	272	GLY	2.5
1	K	47	ARG	2.5
2	B	262	GLU	2.5
1	J	240	LYS	2.5
1	K	15	GLU	2.5
2	D	242	GLU	2.5
1	K	150	GLY	2.5
2	B	239	PHE	2.4
1	C	270	GLY	2.4
1	J	249	ARG	2.3
1	I	245	GLU	2.3
1	A	159	GLU	2.3
1	G	242	GLU	2.3
1	E	237	GLY	2.3
1	E	262	GLU	2.3
1	C	249	ARG	2.3
1	G	204	ARG	2.3
3	F	150	GLY	2.2
1	C	16	MET	2.2
1	A	151	GLU	2.2
2	B	18	LYS	2.2
1	G	247	TYR	2.2
1	E	201	ARG	2.2
1	C	15	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	242	GLU	2.2
1	E	57	GLY	2.2
1	J	239	PHE	2.1
3	F	240	LYS	2.1
1	C	17	GLN	2.1
2	B	242	GLU	2.1
1	G	47	ARG	2.0
2	B	72	ASN	2.0
2	B	271	LEU	2.0
3	F	65	THR	2.0
1	G	271	LEU	2.0
1	J	237	GLY	2.0
3	F	16	MET	2.0
2	D	73	ALA	2.0

## 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, 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(Å <sup>2</sup> )	Q<0.9
1	L5P	E	81	22/23	0.89	0.16	37,87,94,99	0
1	L5P	I	81	22/23	0.90	0.13	39,76,85,87	0
1	L5P	J	81	22/23	0.91	0.13	36,77,85,88	0
1	L5P	K	81	22/23	0.92	0.12	44,78,85,87	0
1	L5P	L	81	22/23	0.92	0.15	44,83,92,95	0
1	L5P	C	81	22/23	0.93	0.13	39,73,81,83	0
3	3ZL	F	81	16/17	0.94	0.15	41,58,78,79	0
1	L5P	G	81	22/23	0.94	0.12	39,72,76,79	0
1	L5P	A	81	22/23	0.95	0.13	34,81,87,90	0

## 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(Å <sup>2</sup> )	Q<0.9
7	EDO	G	303	4/4	0.48	1.15	89,93,95,99	0
7	EDO	G	302	4/4	0.68	0.72	67,69,69,70	0
5	PO4	D	301	5/5	0.76	0.17	76,77,87,93	0
5	PO4	B	301	5/5	0.82	0.17	61,62,73,75	0
4	CAC	H	302	5/5	0.91	0.14	79,80,86,89	0
6	R5P	B	302	14/14	0.92	0.19	57,79,89,90	0
6	R5P	K	301	14/14	0.92	0.20	60,79,96,96	0
6	R5P	J	301	14/14	0.93	0.19	56,75,84,85	0
5	PO4	H	301	5/5	0.93	0.11	77,81,84,85	0
7	EDO	C	302	4/4	0.93	0.33	56,59,61,61	0
6	R5P	D	302	14/14	0.93	0.18	55,79,91,92	0
6	R5P	G	301	14/14	0.93	0.23	63,79,86,86	0
6	R5P	I	301	14/14	0.94	0.19	58,79,101,102	0
5	PO4	F	301	5/5	0.94	0.11	79,80,85,85	0
4	CAC	A	301	5/5	0.95	0.12	79,86,88,88	0
6	R5P	E	301	14/14	0.96	0.17	59,75,80,83	0
4	CAC	F	302	5/5	0.96	0.10	67,77,79,80	0
4	CAC	C	301	5/5	0.96	0.12	80,81,85,91	0
4	CAC	L	301	5/5	0.96	0.09	75,76,81,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.