



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2025 – 10:18 am BST

PDB ID : 9FXR / pdb\_00009fxr  
Title : Crystal structure of trans-o-hydroxybenzylidenepyruvate hydratase-aldolase from *Pseudomonas fluorescens* N3 bound to pyruvate  
Authors : Milani, M.; Ferrara, S.  
Deposited on : 2024-07-02  
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](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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

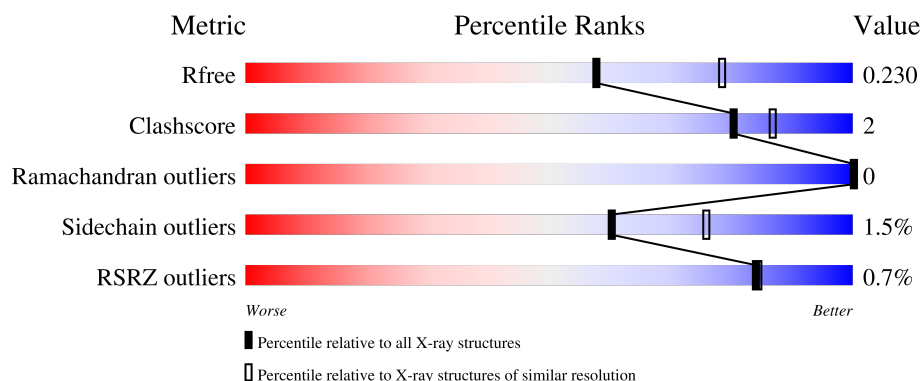
# 1 Overall quality at a glance

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))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (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	346	<div> <div>88%</div> <div>6% • 6%</div> </div>
1	B	346	<div> <div>88%</div> <div>5% • 6%</div> </div>
1	C	346	<div> <div>87%</div> <div>6% • 6%</div> </div>
1	D	346	<div> <div>88%</div> <div>6% • 6%</div> </div>
1	H	346	<div> <div>86%</div> <div>7% • 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	J	346	<div><div>%</div><div><div></div></div><div>88%</div><div>5% • 5%</div></div>
1	L	346	<div><div></div><div>88%</div><div>5% • 6%</div></div>
1	N	346	<div><div>%</div><div><div></div></div><div>86%</div><div>7% • 6%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22153 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 Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	2	0
			2545	1618	434	478	15			
1	B	325	Total	C	N	O	S	0	1	0
			2528	1607	429	477	15			
1	C	325	Total	C	N	O	S	0	1	0
			2528	1607	429	477	15			
1	D	325	Total	C	N	O	S	0	1	0
			2528	1607	429	477	15			
1	H	325	Total	C	N	O	S	0	2	0
			2534	1611	430	478	15			
1	J	327	Total	C	N	O	S	0	2	0
			2552	1622	435	480	15			
1	L	325	Total	C	N	O	S	0	1	0
			2528	1607	429	477	15			
1	N	326	Total	C	N	O	S	0	2	0
			2543	1617	432	479	15			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP C3KFM9
A	-10	ARG	-	expression tag	UNP C3KFM9
A	-9	GLY	-	expression tag	UNP C3KFM9
A	-8	SER	-	expression tag	UNP C3KFM9
A	-7	HIS	-	expression tag	UNP C3KFM9
A	-6	HIS	-	expression tag	UNP C3KFM9
A	-5	HIS	-	expression tag	UNP C3KFM9
A	-4	HIS	-	expression tag	UNP C3KFM9
A	-3	HIS	-	expression tag	UNP C3KFM9
A	-2	HIS	-	expression tag	UNP C3KFM9
A	-1	GLY	-	expression tag	UNP C3KFM9
A	0	SER	-	expression tag	UNP C3KFM9
B	-11	MET	-	initiating methionine	UNP C3KFM9

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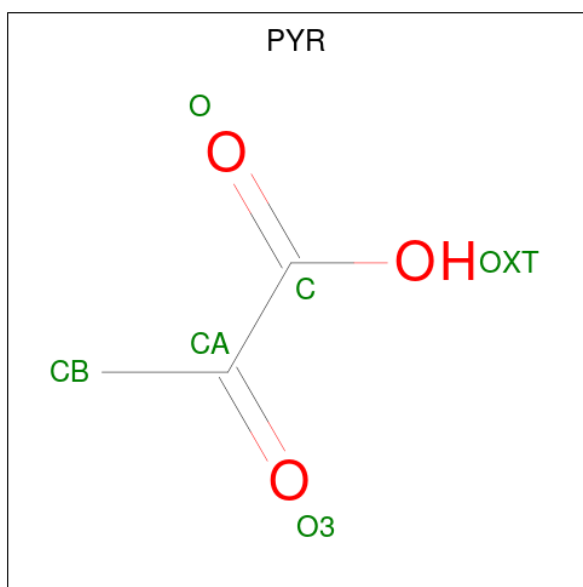
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	ARG	-	expression tag	UNP C3KFM9
B	-9	GLY	-	expression tag	UNP C3KFM9
B	-8	SER	-	expression tag	UNP C3KFM9
B	-7	HIS	-	expression tag	UNP C3KFM9
B	-6	HIS	-	expression tag	UNP C3KFM9
B	-5	HIS	-	expression tag	UNP C3KFM9
B	-4	HIS	-	expression tag	UNP C3KFM9
B	-3	HIS	-	expression tag	UNP C3KFM9
B	-2	HIS	-	expression tag	UNP C3KFM9
B	-1	GLY	-	expression tag	UNP C3KFM9
B	0	SER	-	expression tag	UNP C3KFM9
C	-11	MET	-	initiating methionine	UNP C3KFM9
C	-10	ARG	-	expression tag	UNP C3KFM9
C	-9	GLY	-	expression tag	UNP C3KFM9
C	-8	SER	-	expression tag	UNP C3KFM9
C	-7	HIS	-	expression tag	UNP C3KFM9
C	-6	HIS	-	expression tag	UNP C3KFM9
C	-5	HIS	-	expression tag	UNP C3KFM9
C	-4	HIS	-	expression tag	UNP C3KFM9
C	-3	HIS	-	expression tag	UNP C3KFM9
C	-2	HIS	-	expression tag	UNP C3KFM9
C	-1	GLY	-	expression tag	UNP C3KFM9
C	0	SER	-	expression tag	UNP C3KFM9
D	-11	MET	-	initiating methionine	UNP C3KFM9
D	-10	ARG	-	expression tag	UNP C3KFM9
D	-9	GLY	-	expression tag	UNP C3KFM9
D	-8	SER	-	expression tag	UNP C3KFM9
D	-7	HIS	-	expression tag	UNP C3KFM9
D	-6	HIS	-	expression tag	UNP C3KFM9
D	-5	HIS	-	expression tag	UNP C3KFM9
D	-4	HIS	-	expression tag	UNP C3KFM9
D	-3	HIS	-	expression tag	UNP C3KFM9
D	-2	HIS	-	expression tag	UNP C3KFM9
D	-1	GLY	-	expression tag	UNP C3KFM9
D	0	SER	-	expression tag	UNP C3KFM9
H	-11	MET	-	initiating methionine	UNP C3KFM9
H	-10	ARG	-	expression tag	UNP C3KFM9
H	-9	GLY	-	expression tag	UNP C3KFM9
H	-8	SER	-	expression tag	UNP C3KFM9
H	-7	HIS	-	expression tag	UNP C3KFM9
H	-6	HIS	-	expression tag	UNP C3KFM9
H	-5	HIS	-	expression tag	UNP C3KFM9

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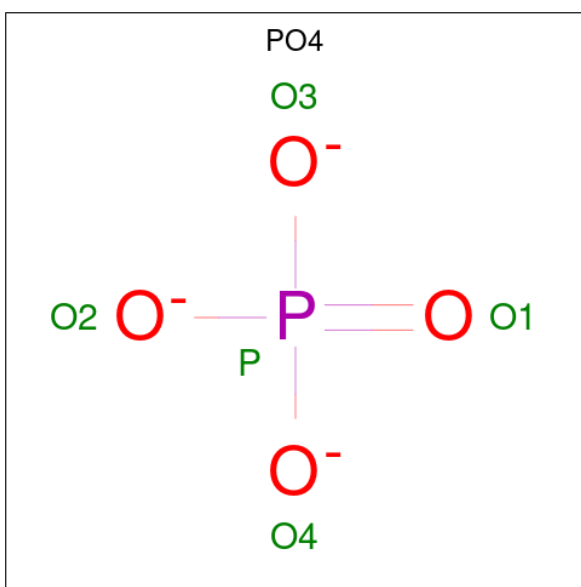
Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	HIS	-	expression tag	UNP C3KFM9
H	-3	HIS	-	expression tag	UNP C3KFM9
H	-2	HIS	-	expression tag	UNP C3KFM9
H	-1	GLY	-	expression tag	UNP C3KFM9
H	0	SER	-	expression tag	UNP C3KFM9
J	-11	MET	-	initiating methionine	UNP C3KFM9
J	-10	ARG	-	expression tag	UNP C3KFM9
J	-9	GLY	-	expression tag	UNP C3KFM9
J	-8	SER	-	expression tag	UNP C3KFM9
J	-7	HIS	-	expression tag	UNP C3KFM9
J	-6	HIS	-	expression tag	UNP C3KFM9
J	-5	HIS	-	expression tag	UNP C3KFM9
J	-4	HIS	-	expression tag	UNP C3KFM9
J	-3	HIS	-	expression tag	UNP C3KFM9
J	-2	HIS	-	expression tag	UNP C3KFM9
J	-1	GLY	-	expression tag	UNP C3KFM9
J	0	SER	-	expression tag	UNP C3KFM9
L	-11	MET	-	initiating methionine	UNP C3KFM9
L	-10	ARG	-	expression tag	UNP C3KFM9
L	-9	GLY	-	expression tag	UNP C3KFM9
L	-8	SER	-	expression tag	UNP C3KFM9
L	-7	HIS	-	expression tag	UNP C3KFM9
L	-6	HIS	-	expression tag	UNP C3KFM9
L	-5	HIS	-	expression tag	UNP C3KFM9
L	-4	HIS	-	expression tag	UNP C3KFM9
L	-3	HIS	-	expression tag	UNP C3KFM9
L	-2	HIS	-	expression tag	UNP C3KFM9
L	-1	GLY	-	expression tag	UNP C3KFM9
L	0	SER	-	expression tag	UNP C3KFM9
N	-11	MET	-	initiating methionine	UNP C3KFM9
N	-10	ARG	-	expression tag	UNP C3KFM9
N	-9	GLY	-	expression tag	UNP C3KFM9
N	-8	SER	-	expression tag	UNP C3KFM9
N	-7	HIS	-	expression tag	UNP C3KFM9
N	-6	HIS	-	expression tag	UNP C3KFM9
N	-5	HIS	-	expression tag	UNP C3KFM9
N	-4	HIS	-	expression tag	UNP C3KFM9
N	-3	HIS	-	expression tag	UNP C3KFM9
N	-2	HIS	-	expression tag	UNP C3KFM9
N	-1	GLY	-	expression tag	UNP C3KFM9
N	0	SER	-	expression tag	UNP C3KFM9

- Molecule 2 is PYRUVIC ACID (CCD ID: PYR) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			6	3	3		
2	B	1	Total	C	O	0	1
			6	3	3		
2	C	1	Total	C	O	0	1
			6	3	3		
2	D	1	Total	C	O	0	1
			6	3	3		
2	H	1	Total	C	O	0	1
			6	3	3		
2	J	1	Total	C	O	0	1
			6	3	3		
2	L	1	Total	C	O	0	1
			6	3	3		
2	N	1	Total	C	O	0	1
			6	3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	N	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	208	Total	O	0	0
			208	208		
5	B	228	Total	O	0	0
			228	228		
5	C	199	Total	O	0	0
			199	199		
5	D	189	Total	O	0	0
			189	189		

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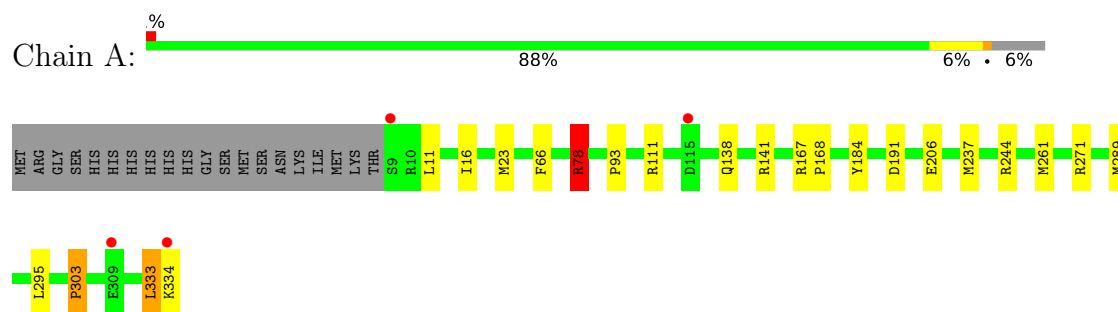
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	225	Total 225	O 225	0	0
5	J	220	Total 220	O 220	0	0
5	L	230	Total 230	O 230	0	0
5	N	237	Total 237	O 237	0	0

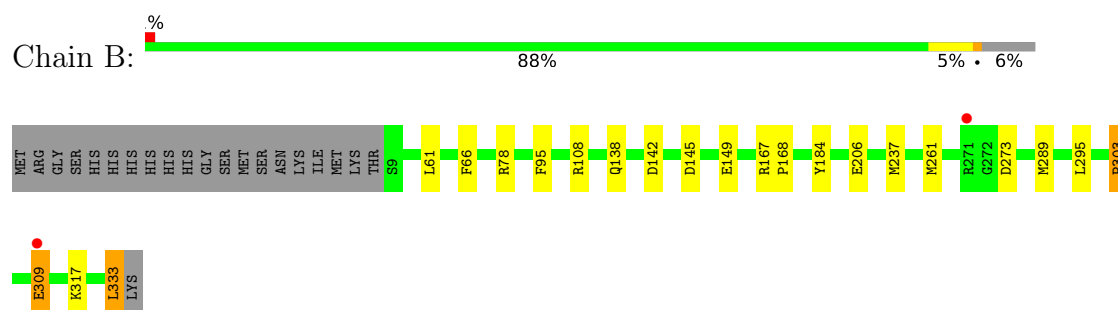
### 3 Residue-property plots [i](#)

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.

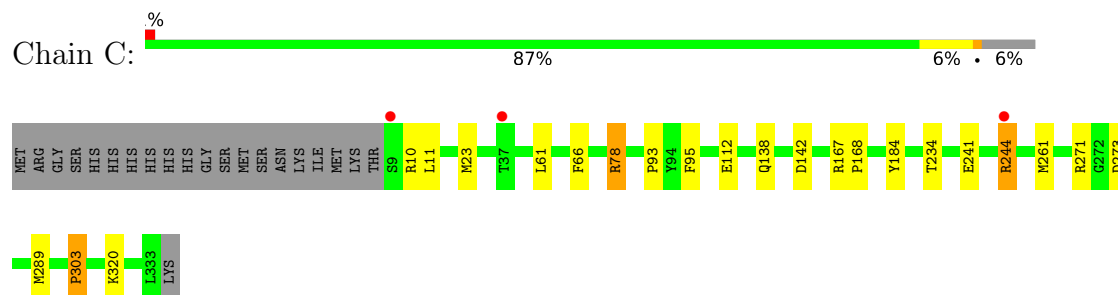
- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase



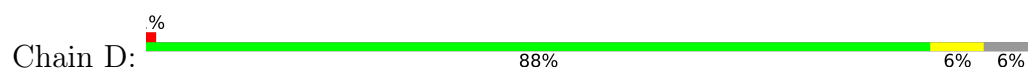
- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase



- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase



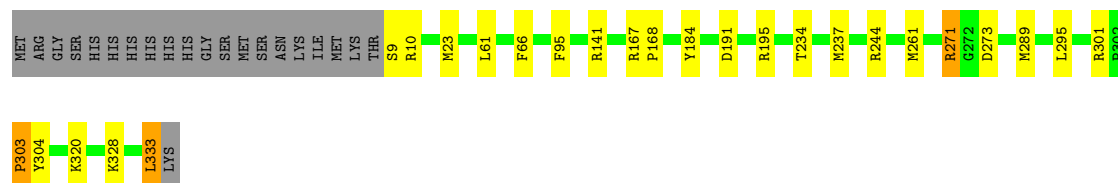
- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase





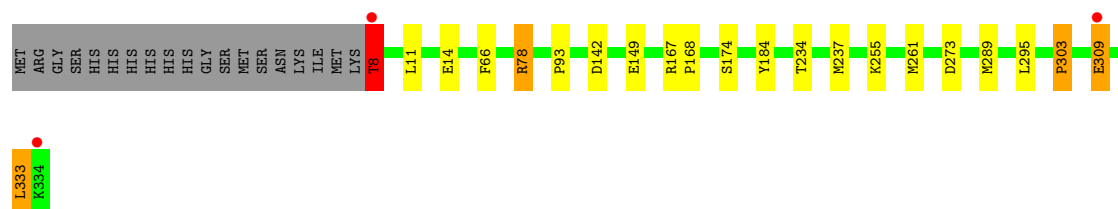
- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase

Chain H: 86% 7% • 6%



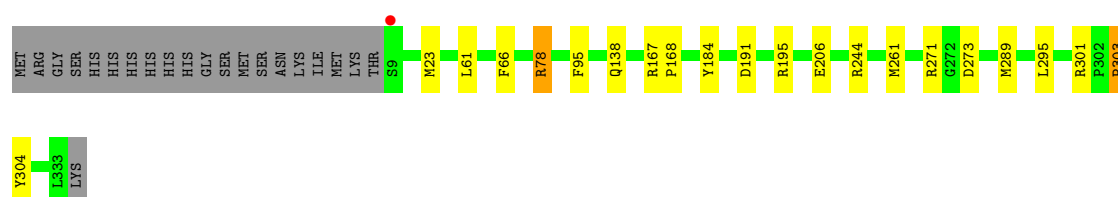
- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase

Chain J: 88% 5% • 5%



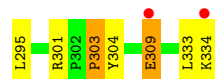
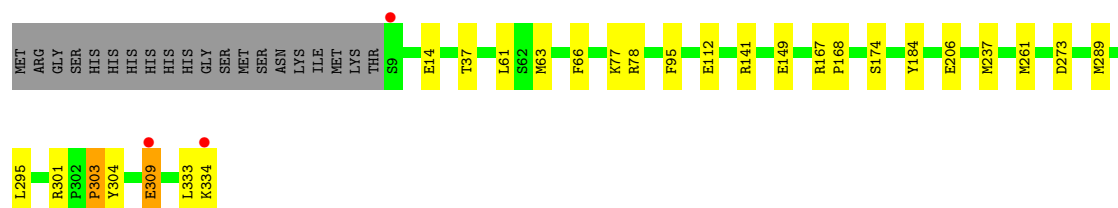
- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase

Chain L: 88% 5% • 6%



- Molecule 1: Trans-O-hydroxybenzylidenepyruvate hydratase-aldolase

Chain N: 86% 7% • 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.17Å 200.36Å 144.47Å 90.00° 133.81° 90.00°	Depositor
Resolution (Å)	104.47 – 2.30 104.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.3 (104.47-2.30) 89.3 (104.47-2.30)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.200 , 0.226 0.205 , 0.230	Depositor DCC
$R_{free}$ test set	9031 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.56$ , $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.000 for -h,-h-2*1,1/2*h-1/2*k 0.000 for -h,h+2*1,1/2*h+1/2*k 0.000 for -h-2*1,k,h+1 0.033 for k,h,-1/2*h-1/2*k-l 0.036 for -k,-h,-1/2*h+1/2*k-l 0.000 for -k,h+2*1,-1/2*h+1/2*k 0.000 for -h-2*1,-h,1/2*h+1/2*k+1 0.000 for -h-2*1,h,1/2*h-1/2*k+1 0.000 for k,-h-2*1,-1/2*h-1/2*k 0.000 for -h-2*1,-k,l 0.027 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	22153	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0677e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PO4, KPI, GOL, PYR

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	0.69	2/2595 (0.1%)	1.09	10/3530 (0.3%)
1	B	0.62	0/2575	1.03	4/3505 (0.1%)
1	C	0.62	0/2575	1.04	5/3505 (0.1%)
1	D	0.60	0/2575	1.03	5/3505 (0.1%)
1	H	0.62	0/2584	1.06	7/3517 (0.2%)
1	J	0.68	2/2602 (0.1%)	1.10	10/3540 (0.3%)
1	L	0.62	0/2575	1.06	6/3505 (0.2%)
1	N	0.63	0/2593	1.06	5/3528 (0.1%)
All	All	0.64	4/20674 (0.0%)	1.06	52/28135 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	2
1	H	0	2
1	J	0	2
1	L	0	3
1	N	0	2
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	78[A]	ARG	C-O	9.28	1.34	1.24
1	J	78[B]	ARG	C-O	9.28	1.34	1.24
1	A	78[A]	ARG	C-O	8.90	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78[B]	ARG	C-O	8.90	1.34	1.24

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	303	PRO	N-CA-CB	-10.23	91.34	102.60
1	J	78[A]	ARG	CA-C-O	10.04	131.20	120.55
1	J	78[B]	ARG	CA-C-O	10.04	131.20	120.55
1	A	78[A]	ARG	CA-C-O	9.91	131.33	120.63
1	A	78[B]	ARG	CA-C-O	9.91	131.33	120.63

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain
1	A	78[A]	ARG	Sidechain
1	A	78[B]	ARG	Sidechain
1	B	78	ARG	Sidechain
1	C	78	ARG	Sidechain

## 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	2545	0	2494	11	0
1	B	2528	0	2468	15	0
1	C	2528	0	2468	10	0
1	D	2528	0	2468	12	0
1	H	2534	0	2476	13	0
1	J	2552	0	2501	11	0
1	L	2528	0	2468	10	0
1	N	2543	0	2489	16	0
2	A	6	0	0	0	0
2	B	6	0	0	1	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	6	0	0	0	0
2	J	6	0	0	0	0
2	L	6	0	0	0	0
2	N	6	0	0	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	H	10	0	0	0	0
3	L	10	0	0	0	0
4	A	6	0	8	1	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
4	H	6	0	8	0	0
4	J	6	0	8	0	0
4	L	6	0	8	0	0
4	N	6	0	8	0	0
5	A	208	0	0	1	0
5	B	228	0	0	5	0
5	C	199	0	0	3	0
5	D	189	0	0	5	0
5	H	225	0	0	5	0
5	J	220	0	0	2	0
5	L	230	0	0	3	0
5	N	237	0	0	4	0
All	All	22153	0	19896	100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 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:C:241:GLU:OE1	1:C:244:ARG:NH1	2.15	0.79
1:C:138:GLN:HG3	5:C:672:HOH:O	1.82	0.77
1:L:138:GLN:HG3	5:L:698:HOH:O	1.87	0.74
1:D:138:GLN:HG3	5:D:667:HOH:O	1.88	0.72
2:N:401[B]:PYR:OXT	5:N:501:HOH:O	2.12	0.68

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/346 (94%)	318 (98%)	6 (2%)	0	100	100
1	B	322/346 (93%)	316 (98%)	6 (2%)	0	100	100
1	C	322/346 (93%)	316 (98%)	6 (2%)	0	100	100
1	D	322/346 (93%)	316 (98%)	6 (2%)	0	100	100
1	H	323/346 (93%)	319 (99%)	4 (1%)	0	100	100
1	J	325/346 (94%)	318 (98%)	7 (2%)	0	100	100
1	L	322/346 (93%)	317 (98%)	5 (2%)	0	100	100
1	N	324/346 (94%)	319 (98%)	5 (2%)	0	100	100
All	All	2584/2768 (93%)	2539 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	261/278 (94%)	254 (97%)	7 (3%)	40	57
1	B	259/278 (93%)	254 (98%)	5 (2%)	52	69
1	C	259/278 (93%)	257 (99%)	2 (1%)	79	89
1	D	259/278 (93%)	257 (99%)	2 (1%)	79	89
1	H	260/278 (94%)	256 (98%)	4 (2%)	60	76
1	J	262/278 (94%)	256 (98%)	6 (2%)	45	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	259/278 (93%)	256 (99%)	3 (1%)	67	81
1	N	261/278 (94%)	258 (99%)	3 (1%)	70	83
All	All	2080/2224 (94%)	2048 (98%)	32 (2%)	60	76

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	303	PRO
1	N	149	GLU
1	C	271	ARG
1	B	333	LEU
1	N	303	PRO

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	N	199	ASN
1	N	205	HIS
1	H	281	ASN
1	J	138	GLN
1	J	205	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

23 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	GOL	A	403	-	5,5,5	0.10	0	5,5,5	0.30	0
4	GOL	J	402	-	5,5,5	0.11	0	5,5,5	0.18	0
4	GOL	D	402	-	5,5,5	0.09	0	5,5,5	0.25	0
2	PYR	H	401[B]	-	5,5,5	1.24	0	3,6,6	1.95	1 (33%)
4	GOL	H	404	-	5,5,5	0.17	0	5,5,5	0.32	0
3	PO4	B	402	-	4,4,4	1.46	1 (25%)	6,6,6	0.48	0
3	PO4	L	403	-	4,4,4	0.53	0	6,6,6	0.55	0
2	PYR	L	401[B]	-	5,5,5	1.56	1 (20%)	3,6,6	1.67	1 (33%)
4	GOL	B	403	-	5,5,5	0.14	0	5,5,5	0.26	0
4	GOL	L	404	-	5,5,5	0.09	0	5,5,5	0.30	0
4	GOL	N	402	-	5,5,5	0.16	0	5,5,5	0.41	0
2	PYR	D	401[B]	-	5,5,5	1.25	0	3,6,6	2.05	2 (66%)
3	PO4	L	402	-	4,4,4	0.52	0	6,6,6	0.64	0
2	PYR	J	401[B]	-	5,5,5	2.13	2 (40%)	3,6,6	1.67	1 (33%)
4	GOL	C	403	-	5,5,5	0.13	0	5,5,5	0.27	0
3	PO4	H	403	-	4,4,4	0.86	0	6,6,6	0.60	0
2	PYR	N	401[B]	-	5,5,5	2.14	2 (40%)	3,6,6	1.69	1 (33%)
3	PO4	C	402	-	4,4,4	0.93	0	6,6,6	0.54	0
3	PO4	H	402	-	4,4,4	0.90	0	6,6,6	0.57	0
2	PYR	B	401[B]	-	5,5,5	1.72	1 (20%)	3,6,6	1.56	1 (33%)
3	PO4	A	402	-	4,4,4	0.70	0	6,6,6	0.65	0
2	PYR	C	401[B]	-	5,5,5	1.01	0	3,6,6	2.18	2 (66%)
2	PYR	A	401[B]	-	5,5,5	1.18	0	3,6,6	1.69	1 (33%)

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
2	PYR	N	401[B]	-	-	0/4/4/4	-
2	PYR	B	401[B]	-	-	0/4/4/4	-
2	PYR	D	401[B]	-	-	0/4/4/4	-
4	GOL	J	402	-	-	2/4/4/4	-
4	GOL	L	404	-	-	1/4/4/4	-
4	GOL	D	402	-	-	3/4/4/4	-
2	PYR	C	401[B]	-	-	0/4/4/4	-
2	PYR	H	401[B]	-	-	0/4/4/4	-
2	PYR	J	401[B]	-	-	0/4/4/4	-
4	GOL	C	403	-	-	0/4/4/4	-
4	GOL	H	404	-	-	2/4/4/4	-
4	GOL	A	403	-	-	2/4/4/4	-
4	GOL	N	402	-	-	0/4/4/4	-
2	PYR	L	401[B]	-	-	0/4/4/4	-
4	GOL	B	403	-	-	0/4/4/4	-
2	PYR	A	401[B]	-	-	0/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	401[B]	PYR	CB-CA	-3.26	1.43	1.50
2	N	401[B]	PYR	CA-C	-3.01	1.43	1.54
2	N	401[B]	PYR	OXT-C	-2.94	1.22	1.30
3	B	402	PO4	P-O1	2.87	1.57	1.50
2	B	401[B]	PYR	CA-C	-2.57	1.44	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401[B]	PYR	OXT-C-CA	3.01	122.20	113.97
2	C	401[B]	PYR	OXT-C-CA	2.86	121.78	113.97
2	N	401[B]	PYR	O3-CA-CB	2.60	125.51	119.73
2	D	401[B]	PYR	OXT-C-CA	2.50	120.82	113.97
2	C	401[B]	PYR	OXT-C-O	-2.40	118.12	123.61

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	GOL	C1-C2-C3-O3
4	D	402	GOL	O1-C1-C2-C3
4	D	402	GOL	C1-C2-C3-O3
4	H	404	GOL	C1-C2-C3-O3
4	J	402	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	GOL	1	0
2	N	401[B]	PYR	1	0
2	B	401[B]	PYR	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	325/346 (93%)	-0.31	4 (1%) 76 76	12, 22, 40, 79	1 (0%)
1	B	324/346 (93%)	-0.29	2 (0%) 85 86	11, 21, 39, 70	0
1	C	324/346 (93%)	-0.26	3 (0%) 81 81	14, 23, 40, 69	0
1	D	324/346 (93%)	-0.28	2 (0%) 85 86	13, 23, 41, 71	0
1	H	324/346 (93%)	-0.27	0 100 100	11, 23, 41, 69	1 (0%)
1	J	326/346 (94%)	-0.22	3 (0%) 81 81	13, 22, 38, 90	1 (0%)
1	L	324/346 (93%)	-0.27	1 (0%) 90 90	14, 22, 42, 62	0
1	N	325/346 (93%)	-0.27	3 (0%) 81 81	12, 22, 39, 88	1 (0%)
All	All	2596/2768 (93%)	-0.27	18 (0%) 84 84	11, 22, 41, 90	4 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	334	LYS	4.6
1	J	8	THR	4.5
1	N	334	LYS	4.4
1	A	334	LYS	3.1
1	N	9	SER	2.9

### 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	KPI	J	183[A]	14/15	0.88	0.12	15,17,23,24	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KPI	N	183[A]	14/15	0.88	0.12	14,19,23,26	5
1	KPI	A	183[A]	14/15	0.89	0.12	14,17,22,25	5
1	KPI	B	183[A]	14/15	0.89	0.13	15,19,25,30	5
1	KPI	L	183[A]	14/15	0.91	0.11	14,18,23,27	5
1	KPI	D	183[A]	14/15	0.91	0.11	17,21,27,33	5
1	KPI	C	183[A]	14/15	0.92	0.11	17,19,23,27	5
1	KPI	H	183[A]	14/15	0.93	0.11	15,19,23,26	5

## 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, 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
2	PYR	J	401[B]	6/6	0.55	0.35	12,13,18,18	6
2	PYR	N	401[B]	6/6	0.57	0.34	16,16,22,22	6
2	PYR	C	401[B]	6/6	0.59	0.32	17,18,24,26	6
2	PYR	D	401[B]	6/6	0.71	0.28	11,12,15,15	6
2	PYR	A	401[B]	6/6	0.73	0.29	10,10,12,14	6
2	PYR	H	401[B]	6/6	0.75	0.22	15,17,20,22	6
2	PYR	B	401[B]	6/6	0.77	0.25	14,15,18,19	6
2	PYR	L	401[B]	6/6	0.79	0.21	11,12,14,15	6
4	GOL	A	403	6/6	0.83	0.17	30,35,36,39	6
4	GOL	L	404	6/6	0.84	0.19	26,29,33,40	6
4	GOL	J	402	6/6	0.85	0.15	29,36,38,40	6
4	GOL	B	403	6/6	0.87	0.16	32,34,35,40	6
4	GOL	D	402	6/6	0.88	0.18	27,31,33,35	6
4	GOL	N	402	6/6	0.88	0.10	20,21,21,24	6
3	PO4	B	402	5/5	0.89	0.17	56,56,63,64	0
4	GOL	C	403	6/6	0.91	0.13	26,28,29,34	6
3	PO4	H	402	5/5	0.92	0.18	59,64,68,69	0
3	PO4	H	403	5/5	0.92	0.14	57,60,68,69	0
4	GOL	H	404	6/6	0.92	0.12	23,27,28,28	6
3	PO4	L	403	5/5	0.92	0.15	48,49,56,64	0
3	PO4	A	402	5/5	0.92	0.14	56,60,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	C	402	5/5	0.92	0.17	55,56,63,64	0
3	PO4	L	402	5/5	0.94	0.11	63,77,86,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.