



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:12 am GMT

PDB ID : 3OOH  
Title : Crystal structure of E. Coli purine nucleoside phosphorylase with PO4  
Authors : Mikleusevic, G.; Stefanic, Z.; Narzyk, M.; Wielgus-Kutrowska, B.; Bzowska, A.; Luic, M.  
Deposited on : 2010-08-31  
Resolution : 2.90 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

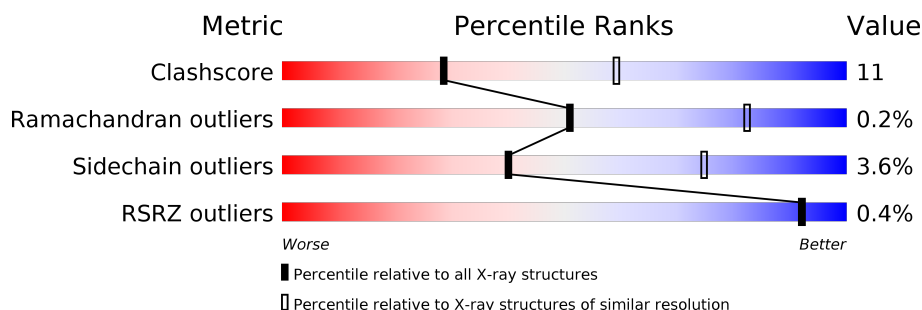
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	237	
1	B	237	
1	C	237	
1	D	237	
1	E	237	
1	F	237	
1	G	237	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	237	
1	I	237	
1	J	237	
1	K	237	
1	L	237	
1	M	237	
1	N	237	
1	O	237	
1	P	237	
1	Q	237	
1	R	237	

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
2	PO4	B	300	-	-	-	X
2	PO4	K	300	-	-	-	X
2	PO4	N	300	-	-	X	-
2	PO4	R	238	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33579 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 Purine nucleoside phosphorylase deoD-type.

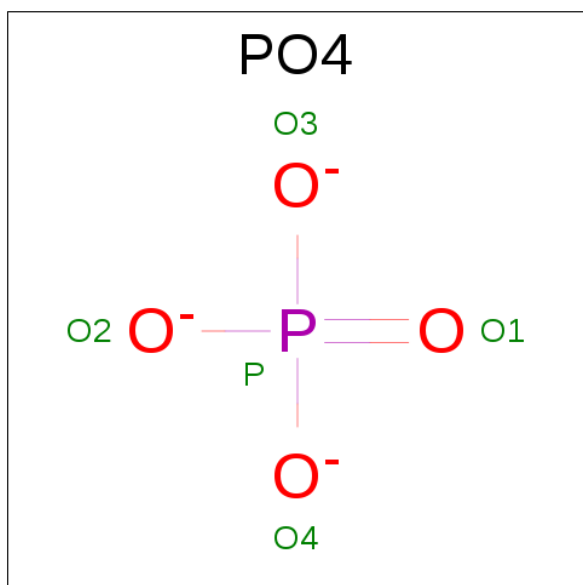
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1797	1135	308	339	15			
1	B	237	Total	C	N	O	S	0	0	0
			1797	1135	308	339	15			
1	C	237	Total	C	N	O	S	0	0	0
			1795	1134	307	339	15			
1	D	237	Total	C	N	O	S	0	0	0
			1795	1134	307	339	15			
1	E	237	Total	C	N	O	S	0	0	0
			1797	1135	308	339	15			
1	F	237	Total	C	N	O	S	0	0	0
			1790	1130	306	339	15			
1	G	237	Total	C	N	O	S	0	0	0
			1797	1135	308	339	15			
1	H	237	Total	C	N	O	S	0	0	0
			1797	1135	308	339	15			
1	I	237	Total	C	N	O	S	0	0	0
			1795	1134	307	339	15			
1	J	237	Total	C	N	O	S	0	0	0
			1793	1133	307	338	15			
1	K	237	Total	C	N	O	S	0	0	0
			1797	1135	308	339	15			
1	L	237	Total	C	N	O	S	0	0	0
			1790	1130	306	339	15			
1	M	237	Total	C	N	O	S	0	0	0
			1797	1135	308	339	15			
1	N	237	Total	C	N	O	S	0	0	0
			1797	1135	308	339	15			
1	O	237	Total	C	N	O	S	0	0	0
			1795	1134	307	339	15			
1	P	237	Total	C	N	O	S	0	0	0
			1791	1132	306	338	15			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	237	Total	C	N	O	S	0	0	0
			1797	1135	308	339	15			
1	R	237	Total	C	N	O	S	0	0	0
			1794	1133	307	339	15			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	M	1	Total	O	P	0	0
			5	4	1		
2	N	1	Total	O	P	0	0
			5	4	1		
2	O	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		
2	Q	1	Total	O	P	0	0
			5	4	1		
2	R	1	Total	O	P	0	0
			5	4	1		
2	R	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total	O	0	0
			75	75		
3	B	60	Total	O	0	0
			60	60		
3	C	62	Total	O	0	0
			62	62		
3	D	50	Total	O	0	0
			50	50		
3	E	60	Total	O	0	0
			60	60		

*Continued on next page...*

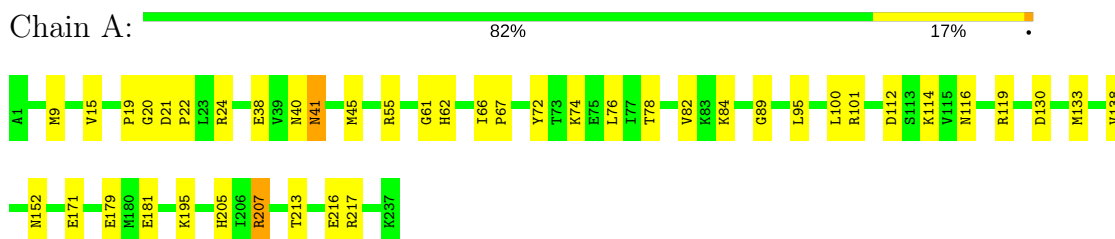
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	78	Total 78	O 78	0	0
3	G	56	Total 56	O 56	0	0
3	H	39	Total 39	O 39	0	0
3	I	52	Total 52	O 52	0	0
3	J	52	Total 52	O 52	0	0
3	K	76	Total 76	O 76	0	0
3	L	77	Total 77	O 77	0	0
3	M	58	Total 58	O 58	0	0
3	N	70	Total 70	O 70	0	0
3	O	58	Total 58	O 58	0	0
3	P	74	Total 74	O 74	0	0
3	Q	78	Total 78	O 78	0	0
3	R	78	Total 78	O 78	0	0

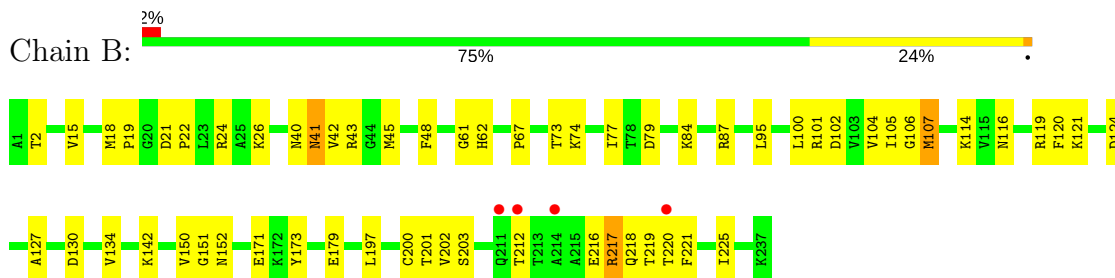
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

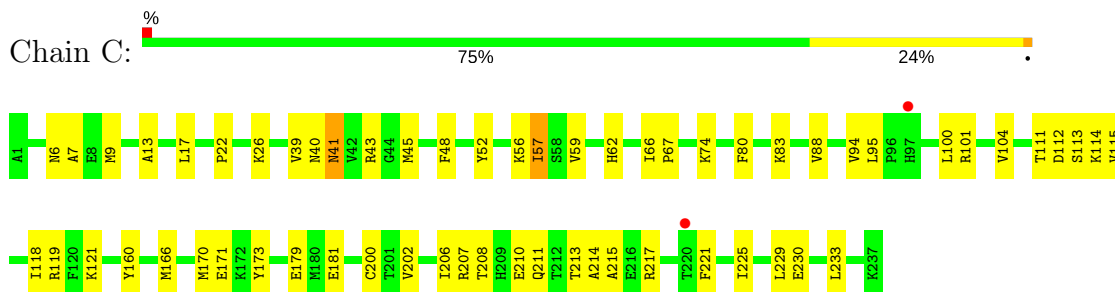
#### • Molecule 1: Purine nucleoside phosphorylase deoD-type



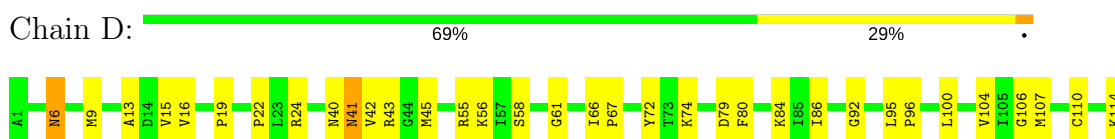
#### • Molecule 1: Purine nucleoside phosphorylase deoD-type



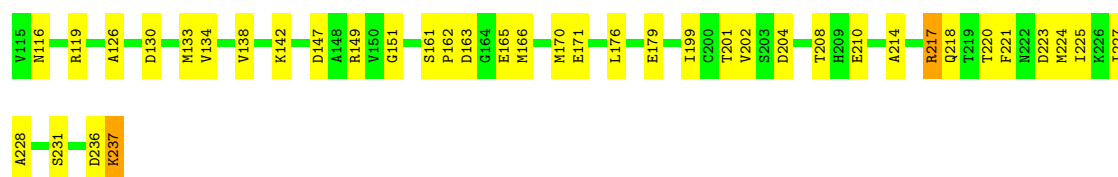
#### • Molecule 1: Purine nucleoside phosphorylase deoD-type



#### • Molecule 1: Purine nucleoside phosphorylase deoD-type

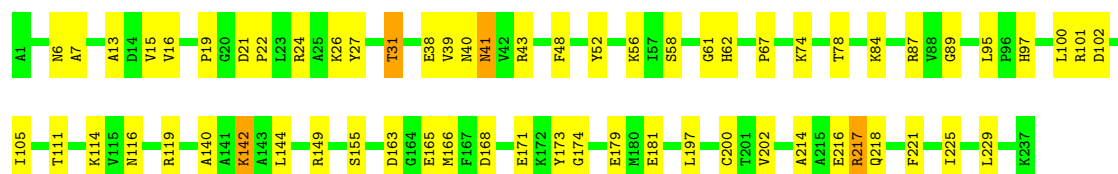






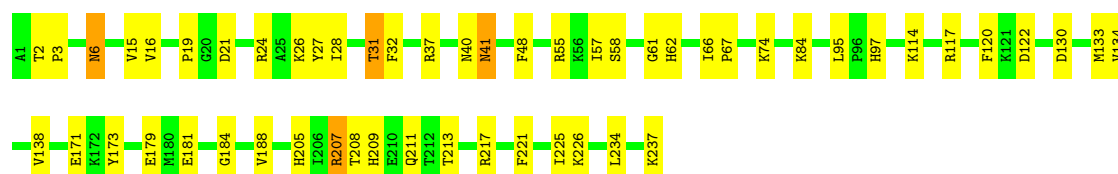
- Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain E: 73% 25%



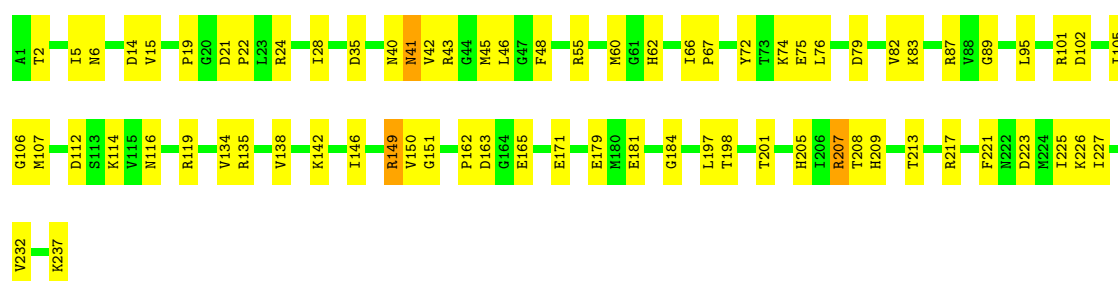
- Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain F: 77% 21%



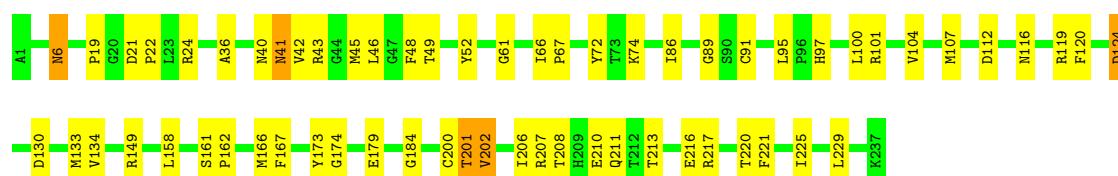
- Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain G: 69% 30%

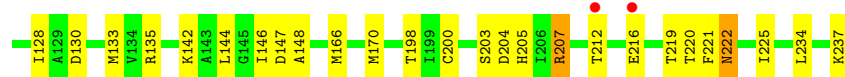
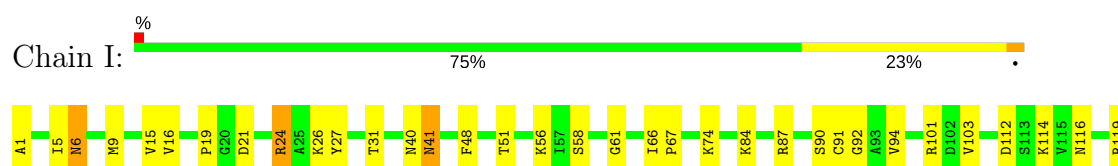


- Molecule 1: Purine nucleoside phosphorylase deoD-type

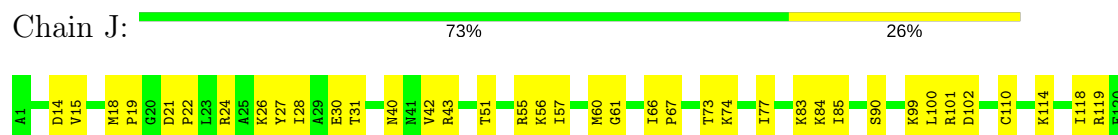
Chain H: 74% 24%



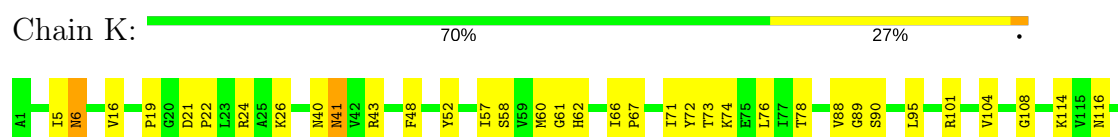
- Molecule 1: Purine nucleoside phosphorylase deoD-type



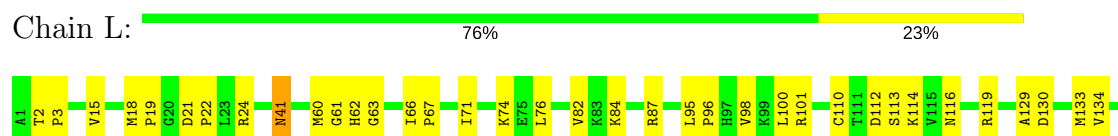
- Molecule 1: Purine nucleoside phosphorylase deoD-type



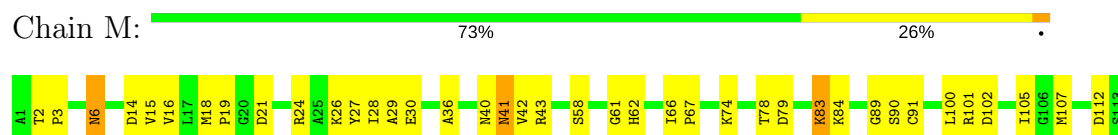
- Molecule 1: Purine nucleoside phosphorylase deoD-type



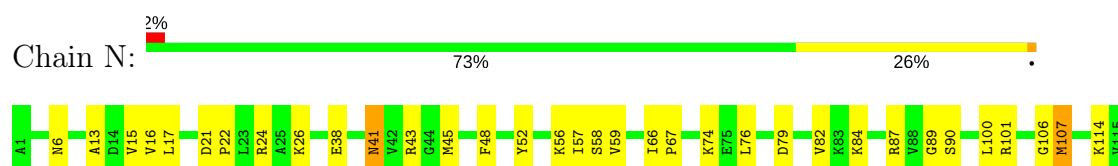
- Molecule 1: Purine nucleoside phosphorylase deoD-type



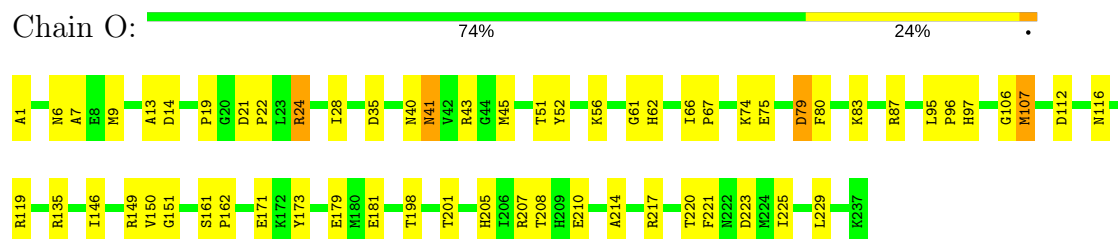
- Molecule 1: Purine nucleoside phosphorylase deoD-type



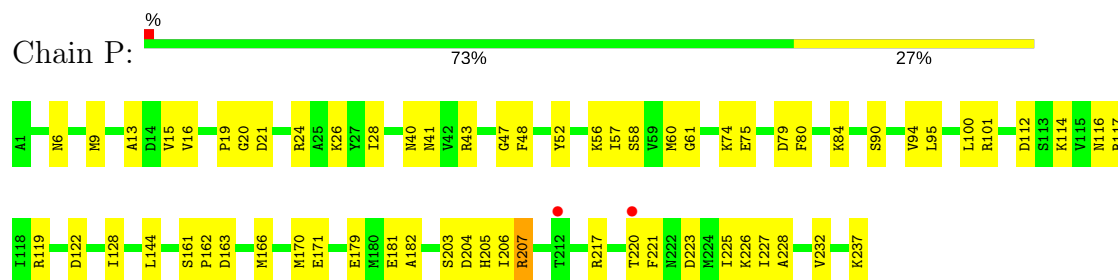
- Molecule 1: Purine nucleoside phosphorylase deoD-type



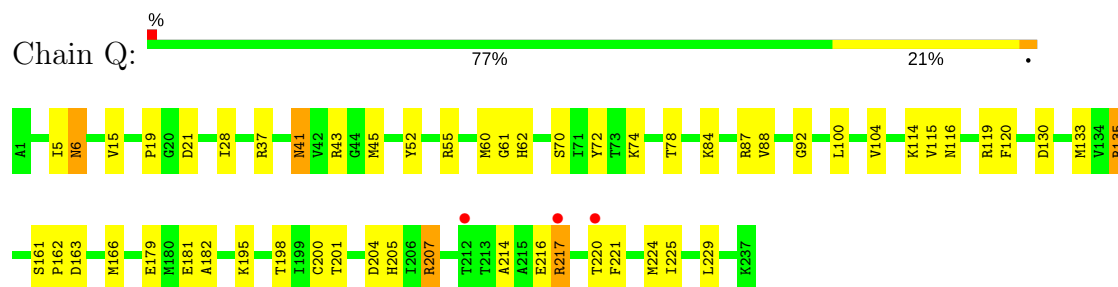
- Molecule 1: Purine nucleoside phosphorylase deoD-type



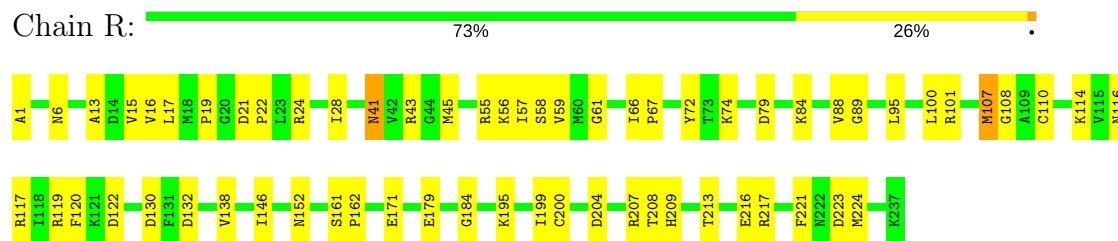
- Molecule 1: Purine nucleoside phosphorylase deoD-type



- Molecule 1: Purine nucleoside phosphorylase deoD-type



- Molecule 1: Purine nucleoside phosphorylase deoD-type



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.45Å 165.92Å 135.38Å 90.00° 99.69° 90.00°	Depositor
Resolution (Å)	48.16 – 2.90 48.16 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.16-2.90) 98.9 (48.16-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.164 , 0.211 0.154 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	33579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.23	0/1826	0.41	0/2461
1	B	0.23	0/1826	0.40	0/2461
1	C	0.23	0/1824	0.40	0/2459
1	D	0.23	0/1824	0.41	0/2459
1	E	0.24	0/1826	0.40	0/2461
1	F	0.23	0/1819	0.41	0/2454
1	G	0.23	0/1826	0.42	0/2461
1	H	0.23	0/1826	0.40	0/2461
1	I	0.23	0/1824	0.40	0/2459
1	J	0.23	0/1822	0.40	0/2456
1	K	0.23	0/1826	0.40	0/2461
1	L	0.23	0/1819	0.41	0/2454
1	M	0.23	0/1826	0.40	0/2461
1	N	0.22	0/1826	0.41	0/2461
1	O	0.23	0/1824	0.40	0/2459
1	P	0.23	0/1820	0.40	0/2454
1	Q	0.23	0/1826	0.40	0/2461
1	R	0.23	0/1823	0.41	0/2458
All	All	0.23	0/32833	0.41	0/44261

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	1797	0	1802	37	0
1	B	1797	0	1802	42	0
1	C	1795	0	1795	45	0
1	D	1795	0	1795	48	0
1	E	1797	0	1802	48	0
1	F	1790	0	1782	38	0
1	G	1797	0	1802	50	0
1	H	1797	0	1802	45	0
1	I	1795	0	1795	42	0
1	J	1793	0	1796	42	0
1	K	1797	0	1802	51	0
1	L	1790	0	1782	37	0
1	M	1797	0	1802	45	0
1	N	1797	0	1802	42	0
1	O	1795	0	1795	41	0
1	P	1791	0	1789	43	0
1	Q	1797	0	1802	38	0
1	R	1794	0	1793	42	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	10	0	0	0	0
2	L	10	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	2	0
2	O	5	0	0	0	0
2	P	5	0	0	1	0
2	Q	5	0	0	0	0
2	R	10	0	0	0	0
3	A	75	0	0	4	0
3	B	60	0	0	0	0
3	C	62	0	0	2	0
3	D	50	0	0	1	0
3	E	60	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	78	0	0	1	0
3	G	56	0	0	1	0
3	H	39	0	0	2	0
3	I	52	0	0	1	0
3	J	52	0	0	0	0
3	K	76	0	0	2	0
3	L	77	0	0	0	0
3	M	58	0	0	0	0
3	N	70	0	0	0	0
3	O	58	0	0	1	0
3	P	74	0	0	0	0
3	Q	78	0	0	2	0
3	R	78	0	0	1	0
All	All	33579	0	32340	709	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 11.

The worst 5 of 709 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:52:TYR:HB3	1:C:57:ILE:HD11	1.41	1.01
1:N:149:ARG:HG3	1:N:149:ARG:HH11	1.30	0.93
1:H:201:THR:HG21	1:H:220:THR:HB	1.51	0.91
1:N:101:ARG:HB3	1:N:220:THR:HG21	1.53	0.88
1:Q:88:VAL:HB	1:Q:224:MET:HE3	1.58	0.84

There are no symmetry-related clashes.

## 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	235/237 (99%)	220 (94%)	15 (6%)	0	100	100
1	B	235/237 (99%)	224 (95%)	8 (3%)	3 (1%)	14	43
1	C	235/237 (99%)	223 (95%)	11 (5%)	1 (0%)	38	72
1	D	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
1	E	235/237 (99%)	221 (94%)	13 (6%)	1 (0%)	38	72
1	F	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
1	G	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
1	H	235/237 (99%)	220 (94%)	14 (6%)	1 (0%)	38	72
1	I	235/237 (99%)	221 (94%)	14 (6%)	0	100	100
1	J	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
1	K	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
1	L	235/237 (99%)	221 (94%)	14 (6%)	0	100	100
1	M	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
1	N	235/237 (99%)	222 (94%)	11 (5%)	2 (1%)	20	54
1	O	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
1	P	235/237 (99%)	226 (96%)	9 (4%)	0	100	100
1	Q	235/237 (99%)	220 (94%)	14 (6%)	1 (0%)	38	72
1	R	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
All	All	4230/4266 (99%)	4006 (95%)	215 (5%)	9 (0%)	51	82

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	217	ARG
1	H	202	VAL
1	B	217	ARG
1	B	127	ALA
1	Q	182	ALA

### 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	188/188 (100%)	184 (98%)	4 (2%)	59	86
1	B	188/188 (100%)	180 (96%)	8 (4%)	33	68
1	C	187/188 (100%)	183 (98%)	4 (2%)	59	86
1	D	187/188 (100%)	176 (94%)	11 (6%)	23	55
1	E	188/188 (100%)	181 (96%)	7 (4%)	39	74
1	F	186/188 (99%)	177 (95%)	9 (5%)	30	64
1	G	188/188 (100%)	177 (94%)	11 (6%)	23	55
1	H	188/188 (100%)	178 (95%)	10 (5%)	26	60
1	I	187/188 (100%)	182 (97%)	5 (3%)	50	82
1	J	187/188 (100%)	184 (98%)	3 (2%)	68	90
1	K	188/188 (100%)	182 (97%)	6 (3%)	44	78
1	L	186/188 (99%)	183 (98%)	3 (2%)	68	90
1	M	188/188 (100%)	180 (96%)	8 (4%)	33	68
1	N	188/188 (100%)	181 (96%)	7 (4%)	39	74
1	O	187/188 (100%)	179 (96%)	8 (4%)	33	68
1	P	186/188 (99%)	182 (98%)	4 (2%)	57	86
1	Q	188/188 (100%)	180 (96%)	8 (4%)	33	68
1	R	187/188 (100%)	180 (96%)	7 (4%)	39	74
All	All	3372/3384 (100%)	3249 (96%)	123 (4%)	40	75

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	24	ARG
1	I	222	ASN
1	Q	179	GLU
1	H	104	VAL
1	H	201	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	116	ASN
1	K	6	ASN
1	Q	41	ASN
1	H	211	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	I	222	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
2	PO4	A	238	-	4,4,4	0.74	0	6,6,6	0.41	0
2	PO4	A	300	-	4,4,4	0.79	0	6,6,6	0.35	0
2	PO4	B	300	-	4,4,4	0.72	0	6,6,6	0.42	0
2	PO4	C	300	-	4,4,4	0.77	0	6,6,6	0.37	0
2	PO4	D	300	-	4,4,4	0.78	0	6,6,6	0.31	0
2	PO4	E	300	-	4,4,4	0.69	0	6,6,6	0.44	0
2	PO4	F	300	-	4,4,4	0.76	0	6,6,6	0.41	0
2	PO4	G	300	-	4,4,4	0.75	0	6,6,6	0.39	0
2	PO4	H	238	-	4,4,4	0.76	0	6,6,6	0.37	0
2	PO4	H	300	-	4,4,4	0.72	0	6,6,6	0.40	0
2	PO4	I	300	-	4,4,4	0.75	0	6,6,6	0.38	0
2	PO4	J	300	-	4,4,4	0.71	0	6,6,6	0.46	0
2	PO4	K	238	-	4,4,4	0.73	0	6,6,6	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	K	300	-	4,4,4	0.72	0	6,6,6	0.40	0
2	PO4	L	238	-	4,4,4	0.73	0	6,6,6	0.43	0
2	PO4	L	300	-	4,4,4	0.74	0	6,6,6	0.36	0
2	PO4	M	300	-	4,4,4	0.76	0	6,6,6	0.40	0
2	PO4	N	300	-	4,4,4	0.75	0	6,6,6	0.38	0
2	PO4	O	300	-	4,4,4	0.68	0	6,6,6	0.44	0
2	PO4	P	300	-	4,4,4	0.72	0	6,6,6	0.42	0
2	PO4	Q	300	-	4,4,4	0.73	0	6,6,6	0.39	0
2	PO4	R	238	-	4,4,4	0.73	0	6,6,6	0.40	0
2	PO4	R	300	-	4,4,4	0.76	0	6,6,6	0.41	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
2	PO4	A	238	-	-	0/0/0/0	0/0/0/0
2	PO4	A	300	-	-	0/0/0/0	0/0/0/0
2	PO4	B	300	-	-	0/0/0/0	0/0/0/0
2	PO4	C	300	-	-	0/0/0/0	0/0/0/0
2	PO4	D	300	-	-	0/0/0/0	0/0/0/0
2	PO4	E	300	-	-	0/0/0/0	0/0/0/0
2	PO4	F	300	-	-	0/0/0/0	0/0/0/0
2	PO4	G	300	-	-	0/0/0/0	0/0/0/0
2	PO4	H	238	-	-	0/0/0/0	0/0/0/0
2	PO4	H	300	-	-	0/0/0/0	0/0/0/0
2	PO4	I	300	-	-	0/0/0/0	0/0/0/0
2	PO4	J	300	-	-	0/0/0/0	0/0/0/0
2	PO4	K	238	-	-	0/0/0/0	0/0/0/0
2	PO4	K	300	-	-	0/0/0/0	0/0/0/0
2	PO4	L	238	-	-	0/0/0/0	0/0/0/0
2	PO4	L	300	-	-	0/0/0/0	0/0/0/0
2	PO4	M	300	-	-	0/0/0/0	0/0/0/0
2	PO4	N	300	-	-	0/0/0/0	0/0/0/0
2	PO4	O	300	-	-	0/0/0/0	0/0/0/0
2	PO4	P	300	-	-	0/0/0/0	0/0/0/0
2	PO4	Q	300	-	-	0/0/0/0	0/0/0/0
2	PO4	R	238	-	-	0/0/0/0	0/0/0/0
2	PO4	R	300	-	-	0/0/0/0	0/0/0/0

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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	PO4	1	0
2	N	300	PO4	2	0
2	P	300	PO4	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	237/237 (100%)	-0.60	0 <b>100</b> <b>100</b>	10, 20, 30, 54	0
1	B	237/237 (100%)	-0.44	4 (1%) 70 68	9, 18, 54, 76	0
1	C	237/237 (100%)	-0.57	2 (0%) 86 85	9, 16, 47, 77	0
1	D	237/237 (100%)	-0.62	0 <b>100</b> <b>100</b>	9, 18, 48, 70	0
1	E	237/237 (100%)	-0.66	0 <b>100</b> <b>100</b>	9, 15, 37, 74	0
1	F	237/237 (100%)	-0.78	0 <b>100</b> <b>100</b>	9, 15, 25, 43	0
1	G	237/237 (100%)	-0.72	0 <b>100</b> <b>100</b>	9, 18, 30, 53	0
1	H	237/237 (100%)	-0.59	0 <b>100</b> <b>100</b>	10, 19, 48, 76	0
1	I	237/237 (100%)	-0.53	2 (0%) 86 85	11, 20, 45, 69	0
1	J	237/237 (100%)	-0.53	0 <b>100</b> <b>100</b>	10, 19, 43, 62	0
1	K	237/237 (100%)	-0.44	1 (0%) 92 92	11, 20, 52, 72	0
1	L	237/237 (100%)	-0.79	0 <b>100</b> <b>100</b>	9, 16, 27, 40	0
1	M	237/237 (100%)	-0.54	0 <b>100</b> <b>100</b>	12, 23, 36, 48	0
1	N	237/237 (100%)	-0.51	4 (1%) 70 68	11, 20, 54, 96	0
1	O	237/237 (100%)	-0.60	0 <b>100</b> <b>100</b>	11, 18, 38, 52	0
1	P	237/237 (100%)	-0.50	2 (0%) 86 85	13, 24, 50, 64	0
1	Q	237/237 (100%)	-0.52	3 (1%) 77 76	12, 20, 56, 89	0
1	R	237/237 (100%)	-0.68	0 <b>100</b> <b>100</b>	11, 19, 31, 52	0
All	All	4266/4266 (100%)	-0.59	18 (0%) 92 92	9, 19, 41, 96	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	215	ALA	7.0
1	B	212	THR	3.4
1	I	212	THR	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	N	212	THR	3.0
1	P	220	THR	2.8

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	R	238	5/5	0.86	0.29	5.80	34,35,50,66	0
2	PO4	K	300	5/5	0.86	0.20	4.50	41,42,66,81	0
2	PO4	B	300	5/5	0.91	0.20	2.20	30,40,47,68	0
2	PO4	L	238	5/5	0.98	0.18	1.90	21,21,24,30	0
2	PO4	A	238	5/5	0.95	0.20	1.88	41,47,50,71	0
2	PO4	E	300	5/5	0.88	0.21	1.69	30,36,41,62	0
2	PO4	H	238	5/5	0.96	0.20	1.55	40,43,46,57	0
2	PO4	D	300	5/5	0.92	0.19	1.22	26,29,37,55	0
2	PO4	K	238	5/5	0.94	0.16	1.18	38,39,56,56	0
2	PO4	J	300	5/5	0.94	0.17	0.75	26,30,47,53	0
2	PO4	C	300	5/5	0.98	0.14	0.69	22,24,29,37	0
2	PO4	O	300	5/5	0.90	0.17	0.37	21,30,33,67	0
2	PO4	H	300	5/5	0.93	0.14	0.06	30,32,32,59	0
2	PO4	Q	300	5/5	0.96	0.13	-0.21	26,26,31,50	0
2	PO4	M	300	5/5	0.99	0.12	-0.47	19,19,25,28	0
2	PO4	R	300	5/5	0.99	0.11	-0.68	14,16,19,19	0
2	PO4	P	300	5/5	0.97	0.12	-0.96	24,33,36,43	0
2	PO4	A	300	5/5	0.99	0.10	-1.05	10,12,17,17	0
2	PO4	N	300	5/5	0.99	0.09	-1.12	20,20,26,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	I	300	5/5	0.97	0.10	-1.48	19,21,26,39	0
2	PO4	F	300	5/5	0.99	0.10	-1.66	10,12,14,16	0
2	PO4	G	300	5/5	0.99	0.08	-1.68	15,17,20,22	0
2	PO4	L	300	5/5	1.00	0.09	-2.62	12,12,14,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.