wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2023 – 11:11 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

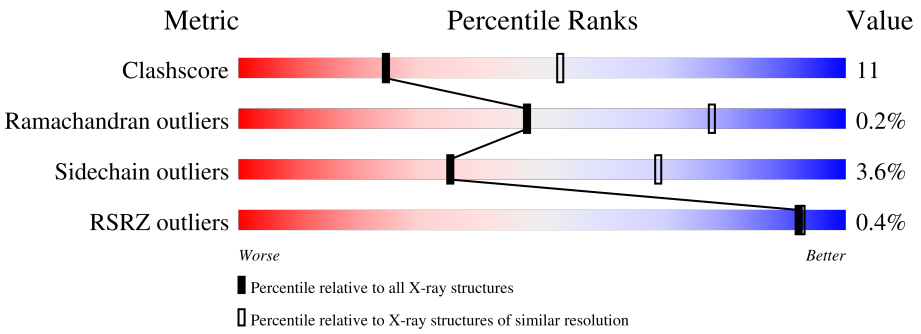
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	82% 17% •
1	B	237	2% 75% 24% •
1	C	237	% 75% 24% •
1	D	237	69% 29% •
1	E	237	73% 25% •
1	F	237	77% 21% •

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Mol	Chain	Length	Quality of chain
1	G	237	69% 30% •
1	H	237	74% 24% •
1	I	237	% 75% 23% •
1	J	237	73% 26%
1	K	237	70% 27% •
1	L	237	76% 23%
1	M	237	73% 26% •
1	N	237	% 73% 26% •
1	O	237	74% 24% •
1	P	237	% 73% 27%
1	Q	237	% 77% 21% •
1	R	237	73% 26% •

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	N	300	-	-	X	-

2 Entry composition (i)

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

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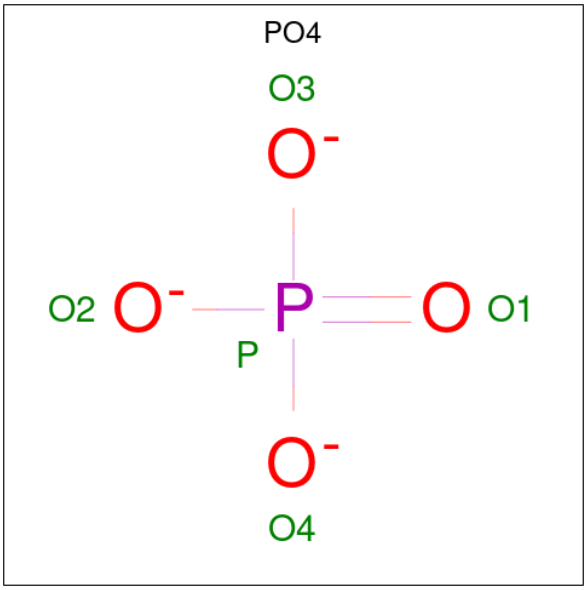
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	237	1797	1135	308	339	15	0	0	0
1	R	237	1794	1133	307	339	15	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

- Molecule 3 is water.

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

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

3 Residue-property plots (i)

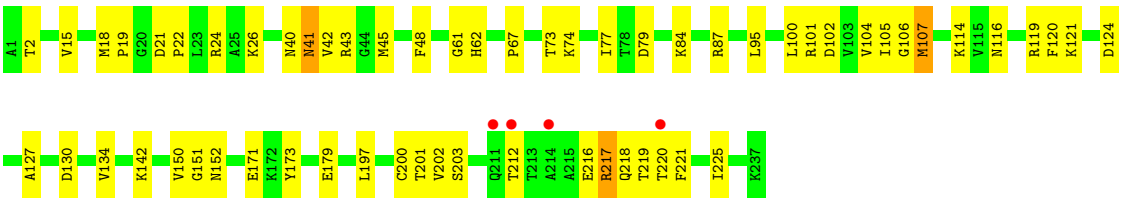
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Purine nucleoside phosphorylase deoD-type

Chain A: 82% 17%

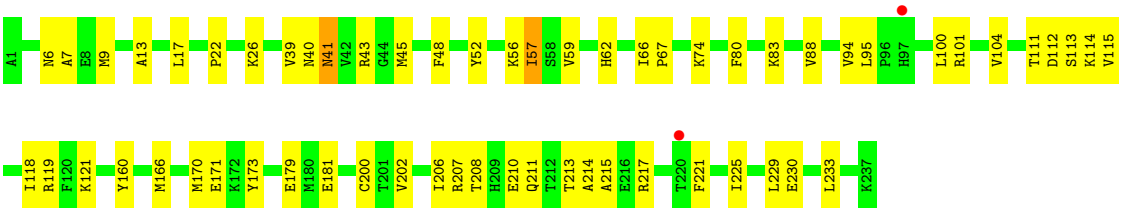
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain B: 2% 75% 24%



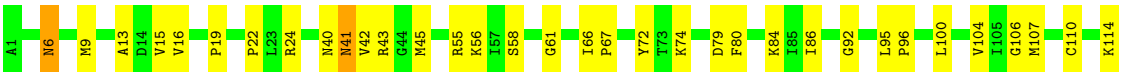
• Molecule 1: Purine nucleoside phosphorylase deoD-type

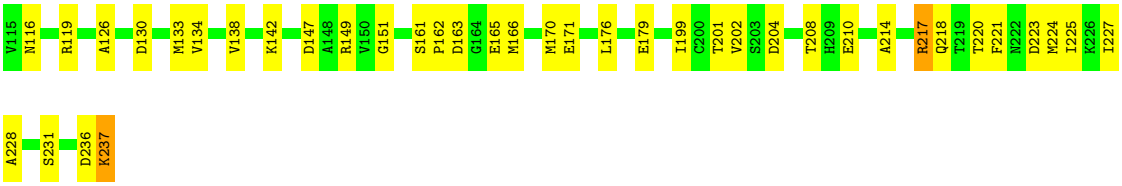
Chain C: % 75% 24%



• Molecule 1: Purine nucleoside phosphorylase deoD-type

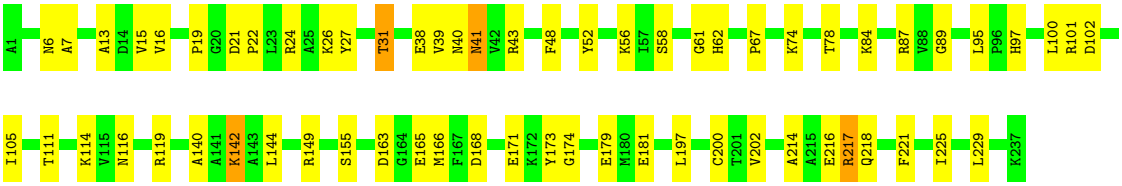
Chain D: 69% 29%





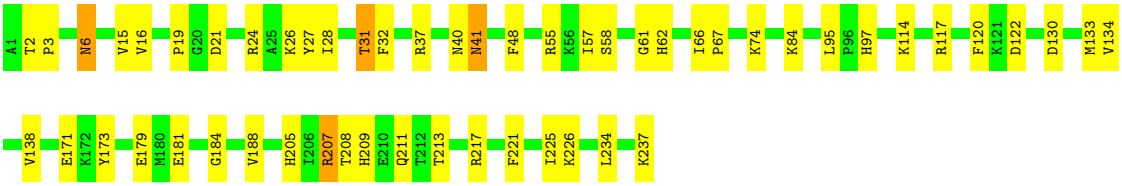
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain E:



• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain F:

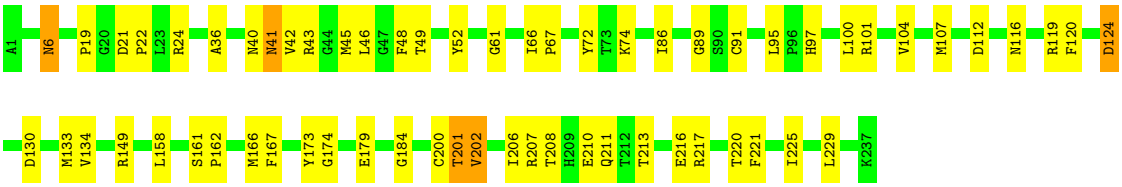


• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain G:

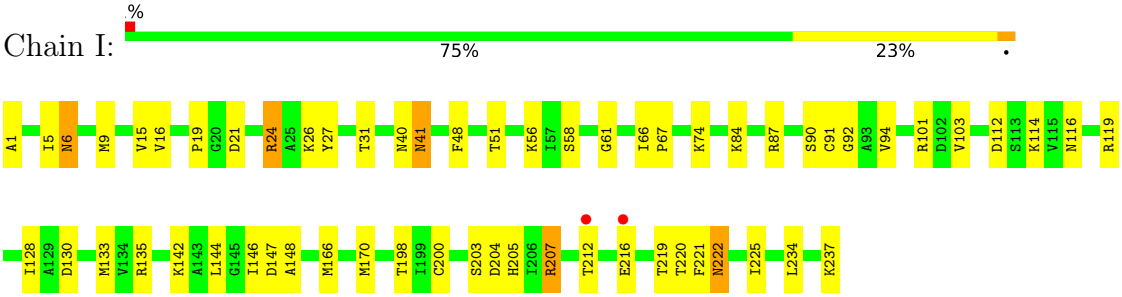
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain H:



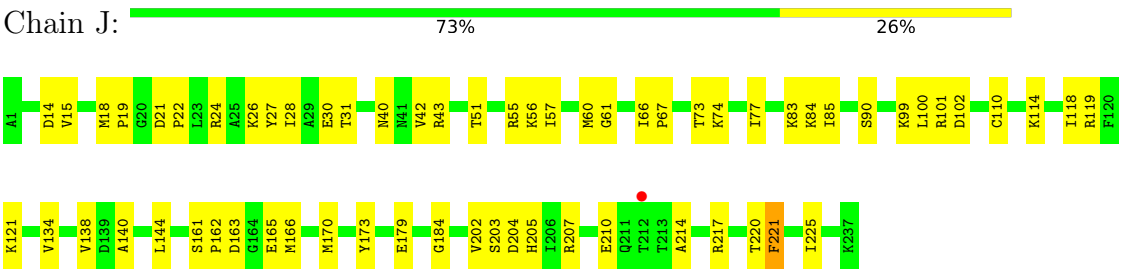
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain I:



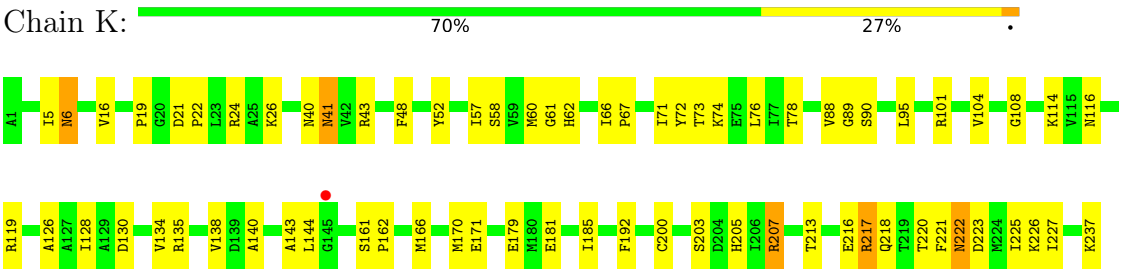
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain J:



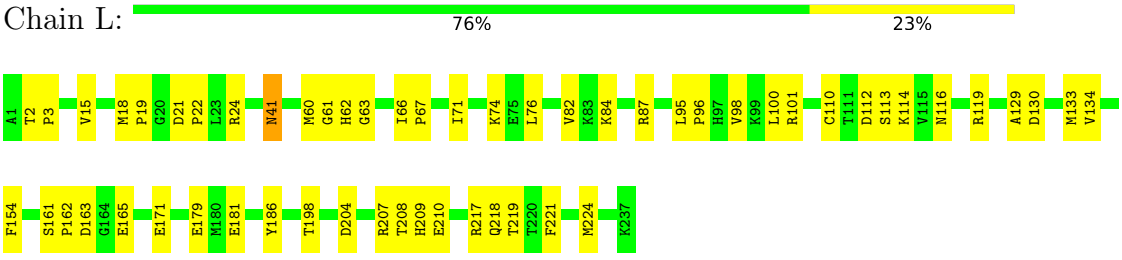
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain K:



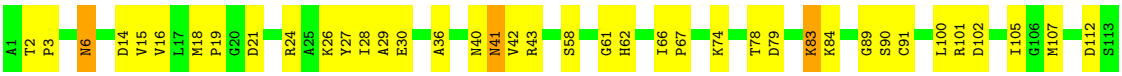
• Molecule 1: Purine nucleoside phosphorylase deoD-type

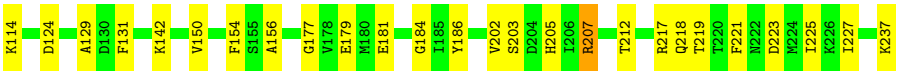
Chain L:



• Molecule 1: Purine nucleoside phosphorylase deoD-type

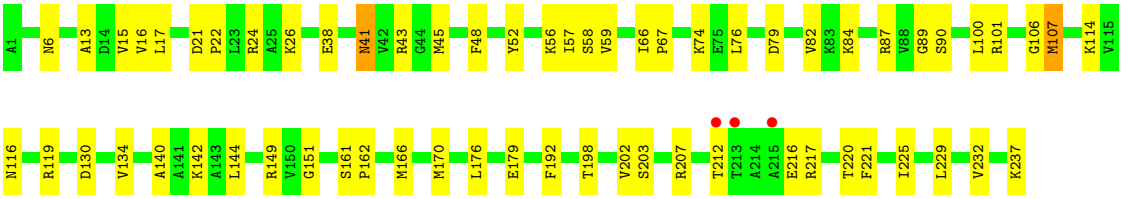
Chain M:





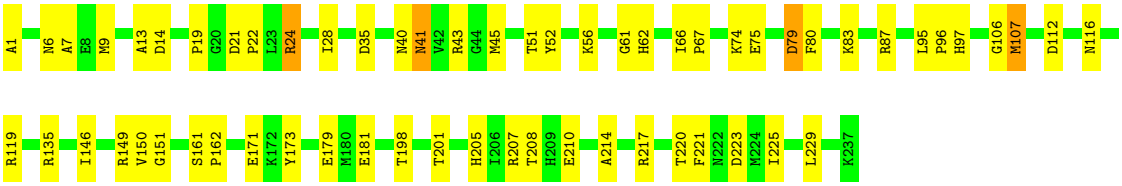
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain N:



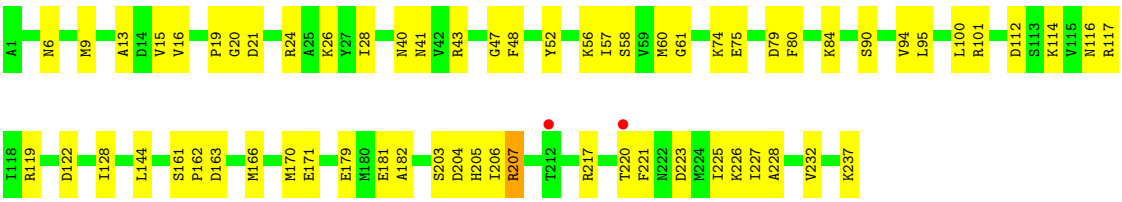
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain O:



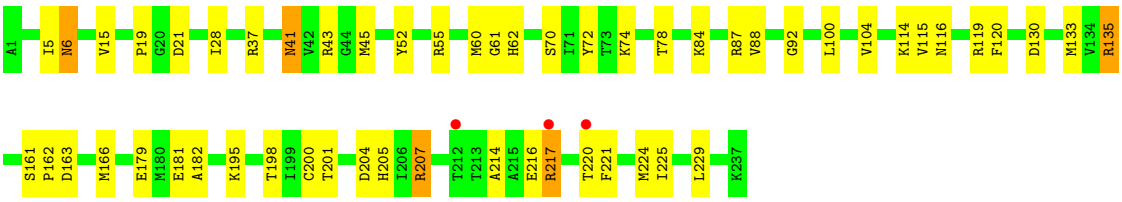
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain P:



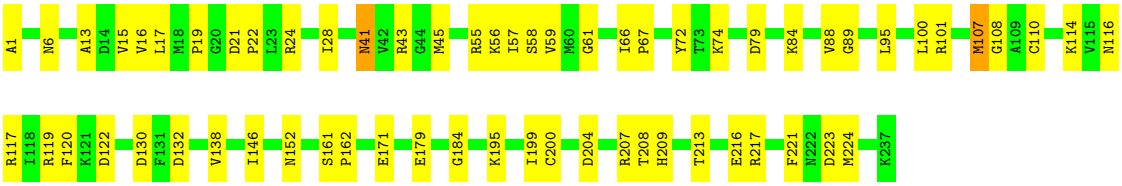
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain Q:



• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain R:


A1
N6
A13
D14
V15
V16
L17
M18
P19
G20
D21
P22
L23
R24
I28
M41
V42
R43
G44
M45
R55
K56
I57
S58
V59
M60
G61
I66
P67
Y72
T73
K74
D79
K84
V88
G89
L95
L100
R101
M107
G108
A109
C110
K114
V115
N116
R117
I118
R119
F120
K121
D122
D130
F131
D132
V138
I146
N152
S161
P162
E171
E179
G184
K195
I199
C200
D204
R207
T208
H209
T213
E216
R217
F221
N222
D223
M224
K237

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.164 , 0.211 0.162 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

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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%)	12	37
1	C	235/237 (99%)	223 (95%)	11 (5%)	1 (0%)	34	66
1	D	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
1	E	235/237 (99%)	221 (94%)	13 (6%)	1 (0%)	34	66
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%)	34	66
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%)	17	48
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%)	34	66
1	R	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
All	All	4230/4266 (99%)	4006 (95%)	215 (5%)	9 (0%)	47	78

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 (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	188/188 (100%)	184 (98%)	4 (2%)	53	81
1	B	188/188 (100%)	180 (96%)	8 (4%)	29	62
1	C	187/188 (100%)	183 (98%)	4 (2%)	53	81
1	D	187/188 (100%)	176 (94%)	11 (6%)	19	49
1	E	188/188 (100%)	181 (96%)	7 (4%)	34	68
1	F	186/188 (99%)	177 (95%)	9 (5%)	25	58
1	G	188/188 (100%)	177 (94%)	11 (6%)	19	49
1	H	188/188 (100%)	178 (95%)	10 (5%)	22	54
1	I	187/188 (100%)	182 (97%)	5 (3%)	44	77
1	J	187/188 (100%)	184 (98%)	3 (2%)	62	86
1	K	188/188 (100%)	182 (97%)	6 (3%)	39	73
1	L	186/188 (99%)	183 (98%)	3 (2%)	62	86
1	M	188/188 (100%)	180 (96%)	8 (4%)	29	62
1	N	188/188 (100%)	181 (96%)	7 (4%)	34	68
1	O	187/188 (100%)	179 (96%)	8 (4%)	29	62
1	P	186/188 (99%)	182 (98%)	4 (2%)	52	81
1	Q	188/188 (100%)	180 (96%)	8 (4%)	29	62
1	R	187/188 (100%)	180 (96%)	7 (4%)	34	68
All	All	3372/3384 (100%)	3249 (96%)	123 (4%)	35	69

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

Mol	Chain	Res	Type
1	H	104	VAL
1	Q	55	ARG
1	J	221	PHE
1	Q	41	ASN
1	R	57	ILE

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

Mol	Chain	Res	Type
1	K	218	GLN
1	N	40	ASN
1	L	6	ASN
1	M	6	ASN

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Mol	Chain	Res	Type
1	N	211	GLN

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 monosaccharides 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	G	300	-	4,4,4	0.91	0	6,6,6	0.42	0
2	PO4	K	300	-	4,4,4	0.85	0	6,6,6	0.45	0
2	PO4	A	238	-	4,4,4	0.87	0	6,6,6	0.45	0
2	PO4	J	300	-	4,4,4	0.85	0	6,6,6	0.52	0
2	PO4	H	238	-	4,4,4	0.90	0	6,6,6	0.41	0
2	PO4	I	300	-	4,4,4	0.88	0	6,6,6	0.42	0
2	PO4	B	300	-	4,4,4	0.85	0	6,6,6	0.46	0
2	PO4	N	300	-	4,4,4	0.89	0	6,6,6	0.41	0
2	PO4	R	300	-	4,4,4	0.92	0	6,6,6	0.45	0
2	PO4	Q	300	-	4,4,4	0.86	0	6,6,6	0.43	0
2	PO4	K	238	-	4,4,4	0.87	0	6,6,6	0.44	0
2	PO4	O	300	-	4,4,4	0.79	0	6,6,6	0.49	0
2	PO4	L	300	-	4,4,4	0.90	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	R	238	-	4,4,4	0.86	0	6,6,6	0.44	0
2	PO4	D	300	-	4,4,4	0.89	0	6,6,6	0.33	0
2	PO4	A	300	-	4,4,4	0.94	0	6,6,6	0.38	0
2	PO4	C	300	-	4,4,4	0.91	0	6,6,6	0.41	0
2	PO4	E	300	-	4,4,4	0.83	0	6,6,6	0.49	0
2	PO4	F	300	-	4,4,4	0.93	0	6,6,6	0.45	0
2	PO4	L	238	-	4,4,4	0.87	0	6,6,6	0.48	0
2	PO4	P	300	-	4,4,4	0.86	0	6,6,6	0.47	0
2	PO4	M	300	-	4,4,4	0.92	0	6,6,6	0.44	0
2	PO4	H	300	-	4,4,4	0.84	0	6,6,6	0.44	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	N	300	PO4	2	0
2	A	300	PO4	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	237/237 (100%)	-0.60	0	100	100	10, 20, 30, 54	0
1	B	237/237 (100%)	-0.44	4 (1%)	70	69	9, 18, 54, 76	0
1	C	237/237 (100%)	-0.57	2 (0%)	86	86	9, 16, 47, 77	0
1	D	237/237 (100%)	-0.62	0	100	100	9, 18, 48, 70	0
1	E	237/237 (100%)	-0.66	0	100	100	9, 15, 37, 74	0
1	F	237/237 (100%)	-0.78	0	100	100	9, 15, 25, 43	0
1	G	237/237 (100%)	-0.72	0	100	100	9, 18, 30, 53	0
1	H	237/237 (100%)	-0.59	0	100	100	10, 19, 48, 76	0
1	I	237/237 (100%)	-0.53	2 (0%)	86	86	11, 20, 45, 69	0
1	J	237/237 (100%)	-0.52	1 (0%)	92	93	10, 19, 43, 62	0
1	K	237/237 (100%)	-0.44	1 (0%)	92	93	11, 20, 52, 72	0
1	L	237/237 (100%)	-0.79	0	100	100	9, 16, 27, 40	0
1	M	237/237 (100%)	-0.54	0	100	100	12, 23, 36, 48	0
1	N	237/237 (100%)	-0.51	3 (1%)	77	77	11, 20, 54, 96	0
1	O	237/237 (100%)	-0.60	0	100	100	11, 18, 38, 52	0
1	P	237/237 (100%)	-0.49	2 (0%)	86	86	13, 24, 50, 64	0
1	Q	237/237 (100%)	-0.52	3 (1%)	77	77	12, 20, 56, 89	0
1	R	237/237 (100%)	-0.67	0	100	100	11, 19, 31, 52	0
All	All	4266/4266 (100%)	-0.59	18 (0%)	92	93	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	3.3
1	I	212	THR	3.2

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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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	K	300	5/5	0.86	0.20	41,42,66,81	0
2	PO4	R	238	5/5	0.86	0.29	34,35,50,66	0
2	PO4	E	300	5/5	0.88	0.21	30,36,41,62	0
2	PO4	O	300	5/5	0.90	0.17	21,30,33,67	0
2	PO4	B	300	5/5	0.91	0.20	30,40,47,68	0
2	PO4	H	300	5/5	0.93	0.14	30,32,32,59	0
2	PO4	D	300	5/5	0.93	0.19	26,29,37,55	0
2	PO4	J	300	5/5	0.94	0.17	26,30,47,53	0
2	PO4	K	238	5/5	0.94	0.17	38,39,56,56	0
2	PO4	A	238	5/5	0.95	0.20	41,47,50,71	0
2	PO4	Q	300	5/5	0.96	0.13	26,26,31,50	0
2	PO4	H	238	5/5	0.96	0.20	40,43,46,57	0
2	PO4	I	300	5/5	0.97	0.10	19,21,26,39	0
2	PO4	P	300	5/5	0.97	0.12	24,33,36,43	0
2	PO4	C	300	5/5	0.98	0.14	22,24,29,37	0
2	PO4	L	238	5/5	0.98	0.18	21,21,24,30	0
2	PO4	N	300	5/5	0.99	0.10	20,20,26,31	0
2	PO4	F	300	5/5	0.99	0.10	10,12,14,16	0
2	PO4	G	300	5/5	0.99	0.08	15,17,20,22	0
2	PO4	A	300	5/5	0.99	0.10	10,12,17,17	0
2	PO4	R	300	5/5	0.99	0.11	14,16,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	M	300	5/5	0.99	0.12	19,19,25,28	0
2	PO4	L	300	5/5	1.00	0.09	12,12,14,15	0

6.5 Other polymers (i)

There are no such residues in this entry.