



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:01 AM GMT

PDB ID : 2P4S  
Title : Structure of Purine Nucleoside Phosphorylase from *Anopheles gambiae* in complex with DADMe-ImmH  
Authors : Rinaldo-Matthis, A.; Almo, S.C.; Schramm, V.L.  
Deposited on : 2007-03-13  
Resolution : 2.20 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

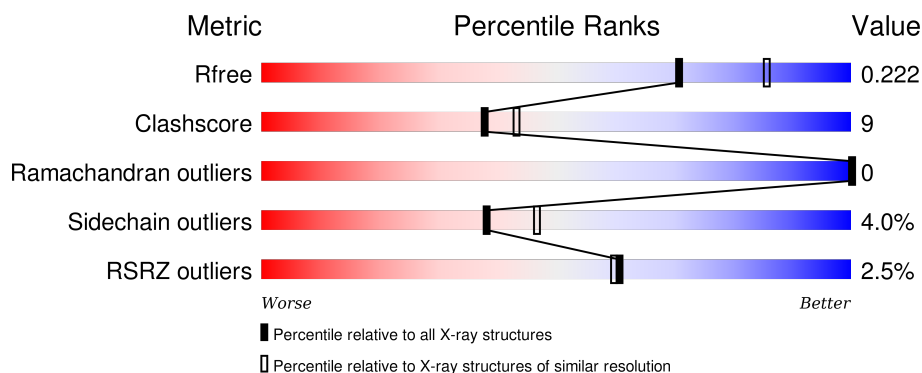
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	373	<div> <div>66%</div> <div>9%</div> <div>24%</div> </div>
1	B	373	<div> <div>3%</div> <div>61%</div> <div>12%</div> <div>••</div> <div>24%</div> </div>
1	C	373	<div> <div>2%</div> <div>62%</div> <div>11%</div> <div>••</div> <div>24%</div> </div>

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	A	504	-	-	-	X
3	DIH	A	401	X	-	-	-
3	DIH	B	403	X	-	-	-
3	DIH	C	402	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6986 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2182	1381	376	403	22			
1	B	282	Total	C	N	O	S	0	0	0
			2182	1381	376	403	22			
1	C	282	Total	C	N	O	S	0	0	0
			2182	1381	376	403	22			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP A4Q998
A	2	GLY	-	EXPRESSION TAG	UNP A4Q998
A	3	SER	-	EXPRESSION TAG	UNP A4Q998
A	4	SER	-	EXPRESSION TAG	UNP A4Q998
A	5	HIS	-	EXPRESSION TAG	UNP A4Q998
A	6	HIS	-	EXPRESSION TAG	UNP A4Q998
A	7	HIS	-	EXPRESSION TAG	UNP A4Q998
A	8	HIS	-	EXPRESSION TAG	UNP A4Q998
A	9	HIS	-	EXPRESSION TAG	UNP A4Q998
A	10	HIS	-	EXPRESSION TAG	UNP A4Q998
A	11	SER	-	EXPRESSION TAG	UNP A4Q998
A	12	SER	-	EXPRESSION TAG	UNP A4Q998
A	13	GLY	-	EXPRESSION TAG	UNP A4Q998
A	14	LEU	-	EXPRESSION TAG	UNP A4Q998
A	15	VAL	-	EXPRESSION TAG	UNP A4Q998
A	16	PRO	-	EXPRESSION TAG	UNP A4Q998
A	17	ARG	-	EXPRESSION TAG	UNP A4Q998
A	18	GLY	-	EXPRESSION TAG	UNP A4Q998
A	19	SER	-	EXPRESSION TAG	UNP A4Q998
A	20	HIS	-	EXPRESSION TAG	UNP A4Q998
B	1	MET	-	EXPRESSION TAG	UNP A4Q998
B	2	GLY	-	EXPRESSION TAG	UNP A4Q998
B	3	SER	-	EXPRESSION TAG	UNP A4Q998

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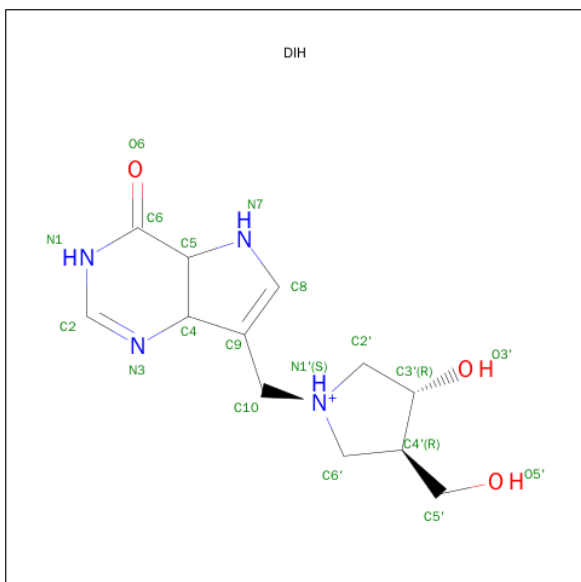
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	EXPRESSION TAG	UNP A4Q998
B	5	HIS	-	EXPRESSION TAG	UNP A4Q998
B	6	HIS	-	EXPRESSION TAG	UNP A4Q998
B	7	HIS	-	EXPRESSION TAG	UNP A4Q998
B	8	HIS	-	EXPRESSION TAG	UNP A4Q998
B	9	HIS	-	EXPRESSION TAG	UNP A4Q998
B	10	HIS	-	EXPRESSION TAG	UNP A4Q998
B	11	SER	-	EXPRESSION TAG	UNP A4Q998
B	12	SER	-	EXPRESSION TAG	UNP A4Q998
B	13	GLY	-	EXPRESSION TAG	UNP A4Q998
B	14	LEU	-	EXPRESSION TAG	UNP A4Q998
B	15	VAL	-	EXPRESSION TAG	UNP A4Q998
B	16	PRO	-	EXPRESSION TAG	UNP A4Q998
B	17	ARG	-	EXPRESSION TAG	UNP A4Q998
B	18	GLY	-	EXPRESSION TAG	UNP A4Q998
B	19	SER	-	EXPRESSION TAG	UNP A4Q998
B	20	HIS	-	EXPRESSION TAG	UNP A4Q998
C	1	MET	-	EXPRESSION TAG	UNP A4Q998
C	2	GLY	-	EXPRESSION TAG	UNP A4Q998
C	3	SER	-	EXPRESSION TAG	UNP A4Q998
C	4	SER	-	EXPRESSION TAG	UNP A4Q998
C	5	HIS	-	EXPRESSION TAG	UNP A4Q998
C	6	HIS	-	EXPRESSION TAG	UNP A4Q998
C	7	HIS	-	EXPRESSION TAG	UNP A4Q998
C	8	HIS	-	EXPRESSION TAG	UNP A4Q998
C	9	HIS	-	EXPRESSION TAG	UNP A4Q998
C	10	HIS	-	EXPRESSION TAG	UNP A4Q998
C	11	SER	-	EXPRESSION TAG	UNP A4Q998
C	12	SER	-	EXPRESSION TAG	UNP A4Q998
C	13	GLY	-	EXPRESSION TAG	UNP A4Q998
C	14	LEU	-	EXPRESSION TAG	UNP A4Q998
C	15	VAL	-	EXPRESSION TAG	UNP A4Q998
C	16	PRO	-	EXPRESSION TAG	UNP A4Q998
C	17	ARG	-	EXPRESSION TAG	UNP A4Q998
C	18	GLY	-	EXPRESSION TAG	UNP A4Q998
C	19	SER	-	EXPRESSION TAG	UNP A4Q998
C	20	HIS	-	EXPRESSION TAG	UNP A4Q998

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



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

- Molecule 3 is 3-HYDROXY-4-HYDROXYMETHYL-1-(4-OXO-4,4A,5,7A-TETRAHYDRO-3H-PYRROLO[3,2-D]PYRIMIDIN-7-YLMETHYL)-PYRROLIDINIUM (three-letter code: DIH) (formula:  $C_{12}H_{19}N_4O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	12	4	3		
3	C	1	Total	C	N	O	0	0
			19	12	4	3		
3	B	1	Total	C	N	O	0	0
			19	12	4	3		

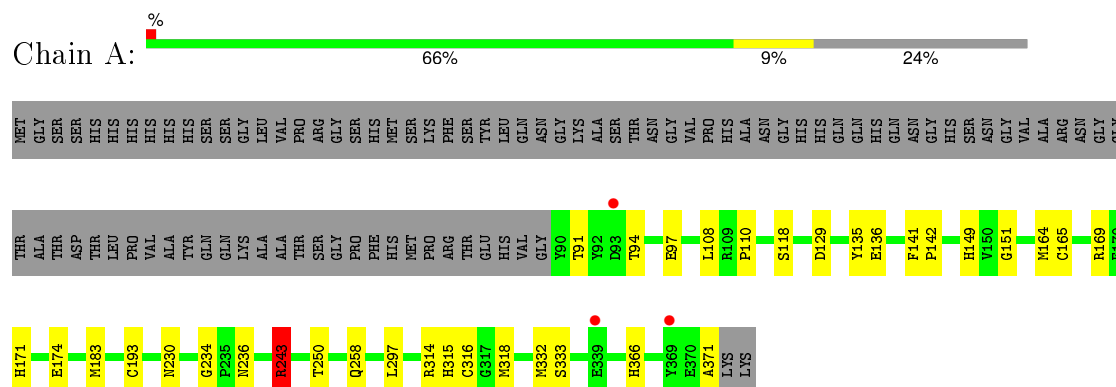
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	136	Total	O	0	0
			136	136		
4	B	95	Total	O	0	0
			95	95		
4	C	132	Total	O	0	0
			132	132		

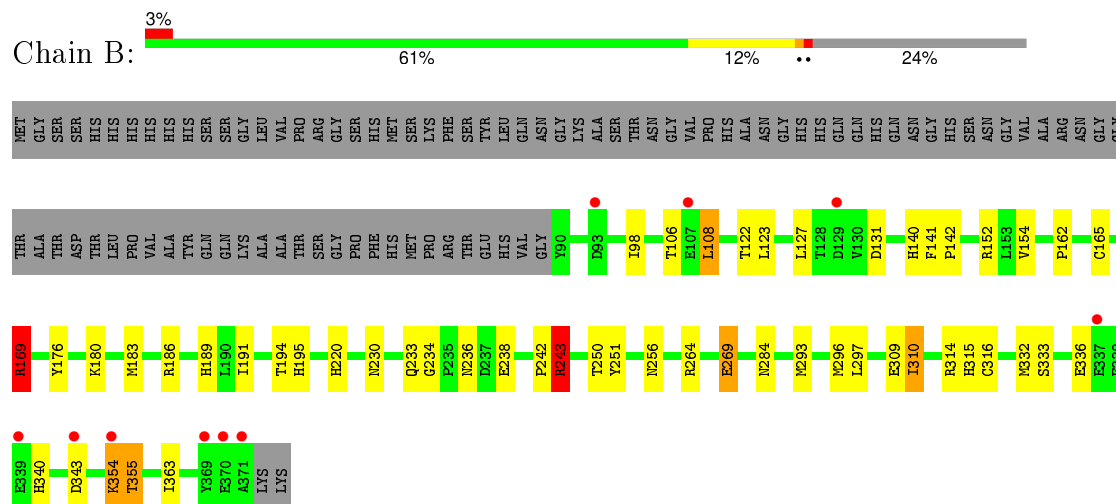
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

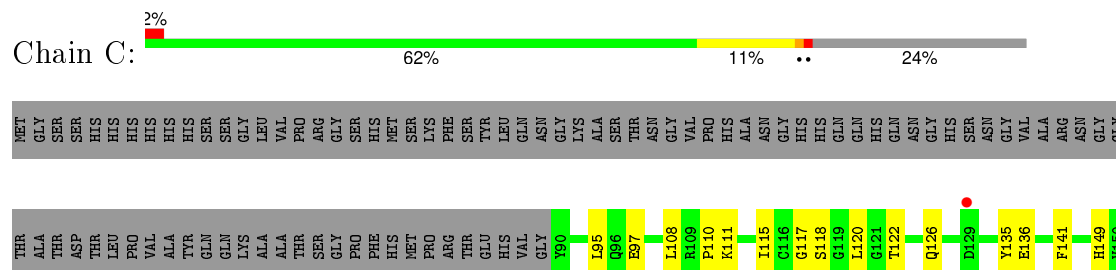
#### • Molecule 1: Purine nucleoside phosphorylase



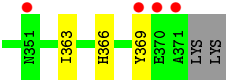
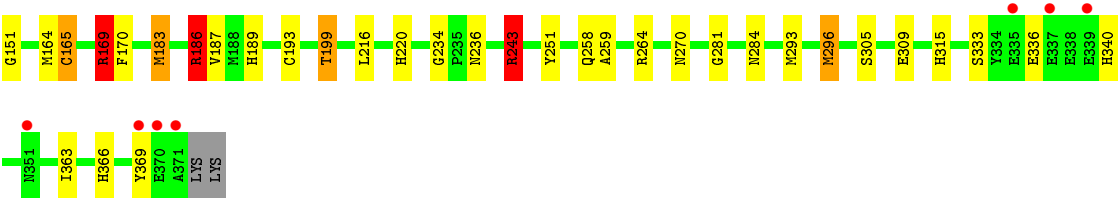
#### • Molecule 1: Purine nucleoside phosphorylase



#### • Molecule 1: Purine nucleoside phosphorylase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.72Å 106.72Å 240.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.9 (8.00-2.20) 93.9 (8.00-2.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.175 , 0.217 0.182 , 0.222	Depositor DCC
$R_{free}$ test set	3300 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.48 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 65412 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6986	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, DIH

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	0.94	3/2230 (0.1%)	0.79	4/3017 (0.1%)
1	B	0.98	3/2230 (0.1%)	0.88	4/3017 (0.1%)
1	C	1.00	3/2230 (0.1%)	0.97	10/3017 (0.3%)
All	All	0.97	9/6690 (0.1%)	0.88	18/9051 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	316	CYS	CB-SG	-10.65	1.64	1.82
1	B	316	CYS	CB-SG	-8.98	1.67	1.82
1	B	165	CYS	CB-SG	-8.97	1.67	1.82
1	C	165	CYS	CB-SG	-6.84	1.70	1.82
1	B	238	GLU	CB-CG	-6.13	1.40	1.52
1	A	165	CYS	CB-SG	-5.72	1.72	1.81
1	C	97	GLU	CB-CG	5.37	1.62	1.52
1	A	136	GLU	CG-CD	5.04	1.59	1.51
1	C	369	TYR	CD2-CE2	-5.01	1.31	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	ARG	NE-CZ-NH2	-19.52	110.54	120.30
1	B	169	ARG	NE-CZ-NH2	-16.58	112.01	120.30
1	C	186	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	C	169	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	B	169	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	C	186	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	C	243	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	243	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	C	169	ARG	CG-CD-NE	-8.01	94.99	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	243	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	169	ARG	CG-CD-NE	-6.57	98.00	111.80
1	A	316	CYS	CB-CA-C	-5.75	98.89	110.40
1	B	243	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	243	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	318	MET	CG-SD-CE	5.52	109.04	100.20
1	C	186	ARG	CD-NE-CZ	5.37	131.12	123.60
1	C	264	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	C	186	ARG	CG-CD-NE	5.29	122.91	111.80

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	2182	0	2145	28	0
1	B	2182	0	2145	46	0
1	C	2182	0	2145	51	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	19	0	17	0	0
3	B	19	0	17	0	0
3	C	19	0	17	0	0
4	A	136	0	0	6	0
4	B	95	0	0	13	0
4	C	132	0	0	10	0
All	All	6986	0	6486	120	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 9.

All (120) 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:136:GLU:HG2	4:C:611:HOH:O	1.59	1.01
1:C:126:GLN:HG2	4:C:633:HOH:O	1.67	0.93
1:C:183:MET:CE	1:C:187:VAL:CG2	2.51	0.88
1:B:186:ARG:HH12	1:B:315:HIS:HD2	1.22	0.88
1:C:281:GLY:HA3	4:C:608:HOH:O	1.73	0.86
1:C:120:LEU:HD13	1:C:199:THR:HG23	1.59	0.84
1:A:149:HIS:HD2	1:A:169:ARG:H	1.22	0.84
1:C:183:MET:CE	1:C:187:VAL:HG21	2.07	0.84
1:C:183:MET:HE2	1:C:187:VAL:HG23	1.60	0.83
1:B:250:THR:CG2	1:B:310:ILE:HD11	2.12	0.78
1:C:186:ARG:HH12	1:C:315:HIS:HD2	1.30	0.78
1:B:106:THR:HG23	1:B:131:ASP:OD2	1.84	0.78
1:C:164:MET:HE3	1:C:193:CYS:SG	2.24	0.77
1:B:250:THR:HG21	1:B:310:ILE:HD11	1.69	0.74
1:C:164:MET:CE	1:C:193:CYS:SG	2.77	0.73
1:C:183:MET:CE	1:C:187:VAL:HG23	2.15	0.73
1:B:142:PRO:HD3	1:B:183:MET:CE	2.20	0.71
1:B:250:THR:CG2	1:B:310:ILE:CD1	2.69	0.70
1:A:164:MET:HE3	1:A:193:CYS:SG	2.33	0.69
1:C:149:HIS:HD2	1:C:169:ARG:H	1.40	0.69
1:B:106:THR:HG22	1:B:108:LEU:H	1.56	0.69
1:C:117:GLY:H	1:C:199:THR:HG22	1.57	0.68
1:C:183:MET:HE1	1:C:187:VAL:HG21	1.75	0.68
1:B:189:HIS:HD2	4:B:550:HOH:O	1.77	0.67
1:B:234:GLY:O	1:B:243:ARG:NH2	2.26	0.67
1:A:230:ASN:HB2	4:A:638:HOH:O	1.97	0.65
1:C:236:ASN:HD21	1:C:315:HIS:CE1	2.15	0.65
1:B:236:ASN:HD21	1:B:315:HIS:CE1	2.15	0.65
1:C:110:PRO:HG2	1:C:164:MET:HE2	1.79	0.63
1:B:220:HIS:HD2	1:B:251:TYR:OH	1.81	0.63
1:B:233:GLN:HB2	4:B:589:HOH:O	2.01	0.60
1:B:233:GLN:CB	4:B:589:HOH:O	2.50	0.60
1:B:220:HIS:HE1	4:C:508:HOH:O	1.85	0.60
1:A:236:ASN:HD21	1:A:315:HIS:HE2	1.50	0.59
1:B:142:PRO:HD3	1:B:183:MET:HE1	1.83	0.59
1:B:194:THR:OG1	1:B:195:HIS:HD2	1.84	0.59
1:C:183:MET:HE1	1:C:187:VAL:CG2	2.29	0.59
1:B:195:HIS:HE1	4:B:541:HOH:O	1.85	0.58
1:B:108:LEU:HD23	1:B:162:PRO:HB3	1.85	0.58
1:B:98:ILE:HD11	1:B:140:HIS:HB2	1.86	0.58
1:B:142:PRO:HD3	1:B:183:MET:HE3	1.85	0.58
1:A:164:MET:CE	1:A:193:CYS:SG	2.91	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PRO:HD3	1:A:183:MET:HE1	1.85	0.58
1:C:189:HIS:HD2	4:C:530:HOH:O	1.87	0.58
1:B:186:ARG:HH12	1:B:315:HIS:CD2	2.13	0.57
1:B:340:HIS:HD2	4:B:574:HOH:O	1.88	0.57
1:C:122:THR:HG23	4:C:592:HOH:O	2.05	0.57
1:C:115:ILE:O	1:C:199:THR:HB	2.05	0.57
1:B:233:GLN:HG3	4:B:589:HOH:O	2.04	0.56
1:A:234:GLY:O	1:A:243:ARG:NH2	2.36	0.56
1:A:149:HIS:CD2	1:A:169:ARG:H	2.13	0.56
1:B:189:HIS:CD2	4:B:550:HOH:O	2.56	0.55
1:C:164:MET:HE1	1:C:193:CYS:SG	2.45	0.55
1:C:220:HIS:HD2	1:C:251:TYR:OH	1.89	0.55
1:A:91:THR:HG23	1:A:94:THR:H	1.72	0.55
1:A:118:SER:OG	1:A:149:HIS:HE1	1.89	0.54
1:C:186:ARG:HH12	1:C:315:HIS:CD2	2.20	0.54
1:B:176:TYR:CD1	1:B:180:LYS:HD3	2.44	0.52
1:C:234:GLY:O	1:C:243:ARG:NH2	2.39	0.52
1:A:258:GLN:HG2	1:A:366:HIS:CG	2.45	0.51
1:C:270:ASN:HB3	4:C:512:HOH:O	2.09	0.51
1:C:149:HIS:CD2	1:C:169:ARG:H	2.26	0.51
1:C:169:ARG:HD2	1:C:305:SER:HB2	1.93	0.50
1:C:169:ARG:HD3	1:C:309:GLU:OE2	2.11	0.50
1:A:171:HIS:HE1	2:A:503:PO4:O2	1.94	0.50
1:A:332:MET:HA	4:A:515:HOH:O	2.11	0.49
1:B:152:ARG:HD2	4:B:566:HOH:O	2.11	0.49
1:C:366:HIS:HD2	4:C:634:HOH:O	1.95	0.49
1:C:110:PRO:CG	1:C:164:MET:HE2	2.41	0.49
1:B:236:ASN:HD21	1:B:315:HIS:HE1	1.58	0.49
1:C:186:ARG:NH1	1:C:315:HIS:HD2	2.06	0.49
1:B:355:THR:HG23	4:B:573:HOH:O	2.12	0.48
1:B:242:PRO:O	1:B:315:HIS:HE1	1.96	0.48
1:C:135:TYR:CE2	1:C:151:GLY:HA2	2.48	0.48
1:C:169:ARG:NH2	1:C:199:THR:O	2.27	0.48
1:C:186:ARG:HH22	1:C:315:HIS:CD2	2.32	0.48
1:C:183:MET:HE3	1:C:187:VAL:HG21	1.93	0.47
1:C:236:ASN:HD21	1:C:315:HIS:HE1	1.58	0.47
1:A:94:THR:O	1:A:97:GLU:HB2	2.15	0.47
1:C:111:LYS:HE2	4:C:555:HOH:O	2.16	0.46
4:A:552:HOH:O	1:C:296:MET:CE	2.63	0.46
1:C:95:LEU:CD2	1:C:183:MET:HG2	2.46	0.46
1:A:297:LEU:HD22	1:B:293:MET:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:HIS:HE1	4:B:522:HOH:O	1.98	0.46
1:A:250:THR:HG23	1:A:314:ARG:HG3	1.97	0.46
1:A:243:ARG:HA	1:A:243:ARG:HD3	1.60	0.45
1:A:314:ARG:HA	1:A:314:ARG:HD2	1.76	0.45
1:A:142:PRO:CD	1:A:183:MET:HE1	2.47	0.45
1:C:118:SER:OG	1:C:149:HIS:HE1	2.00	0.45
1:C:258:GLN:HG2	1:C:366:HIS:CG	2.51	0.45
1:A:171:HIS:HD2	1:A:174:GLU:OE2	1.99	0.44
1:A:110:PRO:HG2	1:A:164:MET:HE2	1.99	0.44
1:A:230:ASN:ND2	4:A:601:HOH:O	2.34	0.44
1:B:142:PRO:CD	1:B:183:MET:HE3	2.47	0.44
1:C:340:HIS:HE1	4:C:529:HOH:O	2.00	0.44
1:B:242:PRO:O	1:B:315:HIS:CE1	2.71	0.43
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.84	0.43
1:B:354:LYS:HE3	1:B:354:LYS:HB2	1.53	0.43
1:B:191:ILE:O	4:B:585:HOH:O	2.21	0.43
4:A:511:HOH:O	1:C:220:HIS:HE1	2.00	0.43
1:A:250:THR:HG23	1:A:314:ARG:CG	2.49	0.43
1:B:332:MET:HA	4:B:531:HOH:O	2.18	0.43
1:C:333:SER:OG	1:C:336:GLU:HG3	2.19	0.42
1:B:169:ARG:HD3	1:B:309:GLU:OE2	2.19	0.42
1:C:149:HIS:HD2	1:C:169:ARG:N	2.14	0.42
1:B:122:THR:HG23	4:B:535:HOH:O	2.18	0.42
1:B:230:ASN:HD21	1:C:284:ASN:HD21	1.66	0.42
1:C:111:LYS:HA	1:C:111:LYS:HD3	1.82	0.42
1:C:259:ALA:HB2	1:C:363:ILE:HD11	2.02	0.41
1:B:250:THR:HG23	1:B:314:ARG:HG3	2.03	0.41
1:A:230:ASN:HD21	1:B:284:ASN:ND2	2.19	0.41
1:B:333:SER:OG	1:B:336:GLU:HG3	2.20	0.41
1:B:127:LEU:HD12	1:B:154:VAL:HG12	2.04	0.40
1:C:169:ARG:HG3	1:C:170:PHE:N	2.37	0.40
1:A:135:TYR:CE2	1:A:151:GLY:HA2	2.56	0.40
1:A:110:PRO:HG2	1:A:164:MET:CE	2.51	0.40
1:B:264:ARG:HA	1:B:269:GLU:HG3	2.03	0.40
1:A:371:ALA:C	4:A:633:HOH:O	2.59	0.40
1:B:230:ASN:HD21	1:C:284:ASN:ND2	2.19	0.40
1:B:297:LEU:HD22	1:C:293:MET:HG3	2.04	0.40

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	280/373 (75%)	276 (99%)	4 (1%)	0	100	100
1	B	280/373 (75%)	273 (98%)	7 (2%)	0	100	100
1	C	280/373 (75%)	277 (99%)	3 (1%)	0	100	100
All	All	840/1119 (75%)	826 (98%)	14 (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	234/306 (76%)	229 (98%)	5 (2%)	61	74
1	B	234/306 (76%)	221 (94%)	13 (6%)	26	29
1	C	234/306 (76%)	224 (96%)	10 (4%)	35	43
All	All	702/918 (76%)	674 (96%)	28 (4%)	38	47

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	129	ASP
1	A	141	PHE
1	A	243	ARG
1	A	333	SER

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Mol	Chain	Res	Type
1	B	108	LEU
1	B	123	LEU
1	B	141	PHE
1	B	169	ARG
1	B	243	ARG
1	B	256	ASN
1	B	269	GLU
1	B	296	MET
1	B	310	ILE
1	B	343	ASP
1	B	354	LYS
1	B	355	THR
1	B	363	ILE
1	C	108	LEU
1	C	141	PHE
1	C	165	CYS
1	C	169	ARG
1	C	183	MET
1	C	186	ARG
1	C	199	THR
1	C	216	LEU
1	C	243	ARG
1	C	296	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	171	HIS
1	A	236	ASN
1	A	256	ASN
1	B	189	HIS
1	B	195	HIS
1	B	220	HIS
1	B	236	ASN
1	B	256	ASN
1	B	284	ASN
1	B	315	HIS
1	B	340	HIS
1	B	351	ASN
1	C	149	HIS
1	C	189	HIS

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Mol	Chain	Res	Type
1	C	220	HIS
1	C	236	ASN
1	C	270	ASN
1	C	284	ASN
1	C	315	HIS
1	C	340	HIS
1	C	366	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

7 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
3	DIH	A	401	-	18,21,21	2.54	6 (33%)	15,30,30	2.25	5 (33%)
2	PO4	A	503	-	4,4,4	0.82	0	6,6,6	0.28	0
2	PO4	A	504	-	4,4,4	0.33	0	6,6,6	0.26	0
3	DIH	B	403	-	18,21,21	2.40	6 (33%)	15,30,30	2.18	4 (26%)
2	PO4	B	501	-	4,4,4	0.49	0	6,6,6	0.26	0
3	DIH	C	402	-	18,21,21	2.63	4 (22%)	15,30,30	2.33	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	C	502	-	4,4,4	0.82	0	6,6,6	0.28	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
3	DIH	A	401	-	2/2/7/11	0/6/41/41	0/3/3/3
2	PO4	A	503	-	-	0/0/0/0	0/0/0/0
2	PO4	A	504	-	-	0/0/0/0	0/0/0/0
3	DIH	B	403	-	2/2/7/11	0/6/41/41	0/3/3/3
2	PO4	B	501	-	-	0/0/0/0	0/0/0/0
3	DIH	C	402	-	2/2/7/11	0/6/41/41	0/3/3/3
2	PO4	C	502	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	DIH	C5-N7	-9.60	1.34	1.46
3	A	401	DIH	C5-N7	-8.25	1.36	1.46
3	B	403	DIH	C5-N7	-8.24	1.36	1.46
3	C	402	DIH	C4-N3	-2.64	1.37	1.46
3	A	401	DIH	C4-N3	-2.50	1.38	1.46
3	B	403	DIH	C5-C6	-2.33	1.48	1.53
3	C	402	DIH	C5-C6	-2.31	1.48	1.53
3	B	403	DIH	C4-N3	-2.15	1.39	1.46
3	B	403	DIH	O6-C6	2.01	1.27	1.23
3	B	403	DIH	C2-N3	2.04	1.33	1.29
3	A	401	DIH	C2'-N1'	2.21	1.50	1.47
3	A	401	DIH	C8-N7	2.32	1.36	1.33
3	A	401	DIH	C2-N3	2.49	1.34	1.29
3	B	403	DIH	C8-N7	2.85	1.37	1.33
3	C	402	DIH	C2-N3	2.97	1.35	1.29
3	A	401	DIH	O6-C6	3.57	1.30	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	DIH	C4-C9-C8	-5.23	105.18	110.53
3	C	402	DIH	C4-C9-C8	-4.73	105.69	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	DIH	C4-C9-C8	-4.56	105.87	110.53
3	A	401	DIH	O5'-C5'-C4'	-2.22	106.56	111.45
3	C	402	DIH	C10-N1'-C2'	-2.10	109.96	113.61
3	A	401	DIH	C6'-C4'-C3'	2.14	107.18	103.82
3	B	403	DIH	C6'-C4'-C3'	2.17	107.23	103.82
3	C	402	DIH	C6'-C4'-C3'	2.70	108.07	103.82
3	B	403	DIH	C2'-N1'-C6'	2.74	107.74	104.19
3	A	401	DIH	C10-N1'-C6'	2.97	118.77	113.61
3	C	402	DIH	C10-N1'-C6'	3.25	119.26	113.61
3	C	402	DIH	C2'-N1'-C6'	3.26	108.41	104.19
3	B	403	DIH	C10-C9-C4	4.28	128.55	122.83
3	C	402	DIH	C10-C9-C4	4.35	128.66	122.83
3	A	401	DIH	C10-C9-C4	4.43	128.75	122.83

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	402	DIH	C4
3	C	402	DIH	C5
3	A	401	DIH	C4
3	A	401	DIH	C5
3	B	403	DIH	C4
3	B	403	DIH	C5

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	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	282/373 (75%)	-0.64	3 (1%) 82 82	12, 23, 38, 50	0
1	B	282/373 (75%)	-0.45	10 (3%) 48 46	14, 25, 42, 49	0
1	C	282/373 (75%)	-0.67	8 (2%) 56 55	13, 20, 35, 55	0
All	All	846/1119 (75%)	-0.59	21 (2%) 61 60	12, 22, 40, 55	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	371	ALA	5.8
1	C	369	TYR	5.0
1	B	369	TYR	4.1
1	A	369	TYR	4.1
1	C	371	ALA	3.5
1	C	337	GLU	3.4
1	C	339	GLU	3.2
1	C	351	ASN	3.1
1	B	370	GLU	3.1
1	B	337	GLU	3.0
1	B	107	GLU	3.0
1	C	129	ASP	2.9
1	B	354	LYS	2.9
1	B	93	ASP	2.6
1	B	343	ASP	2.6
1	A	93	ASP	2.6
1	C	335	GLU	2.5
1	B	129	ASP	2.5
1	A	339	GLU	2.5
1	C	370	GLU	2.2
1	B	339	GLU	2.0

## 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	A	504	5/5	0.93	0.12	3.89	81,81,83,83	0
3	DIH	A	401	19/19	0.98	0.07	-0.36	12,14,18,18	0
3	DIH	B	403	19/19	0.98	0.06	-0.83	14,17,19,22	0
3	DIH	C	402	19/19	0.98	0.06	-1.00	15,17,20,21	0
2	PO4	B	501	5/5	0.99	0.05	-1.48	18,19,20,21	0
2	PO4	C	502	5/5	0.99	0.05	-1.68	14,14,18,20	0
2	PO4	A	503	5/5	0.99	0.05	-2.06	16,16,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.