



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2017 – 08:03 PM EDT

PDB ID : 3K8Q  
Title : Crystal structure of human purine nucleoside phosphorylase in complex with SerMe-Immucillin H  
Authors : Ho, M.; Almo, S.C.; Scharmm, V.L.  
Deposited on : unknown  
Resolution : 2.50 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
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) : rb-20030345

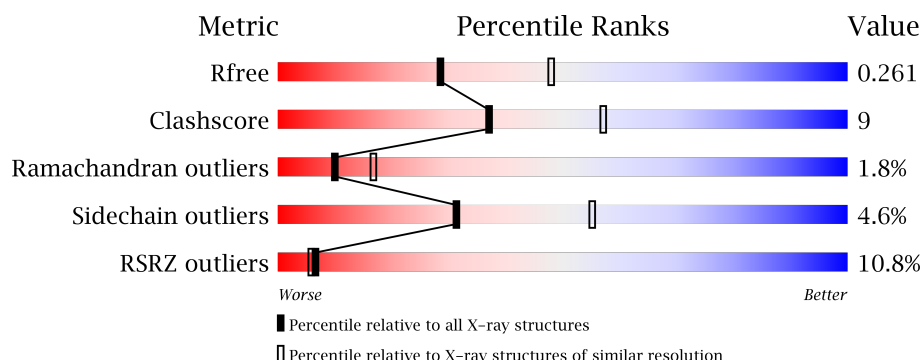
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	289	<div> <div>11%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2305 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.

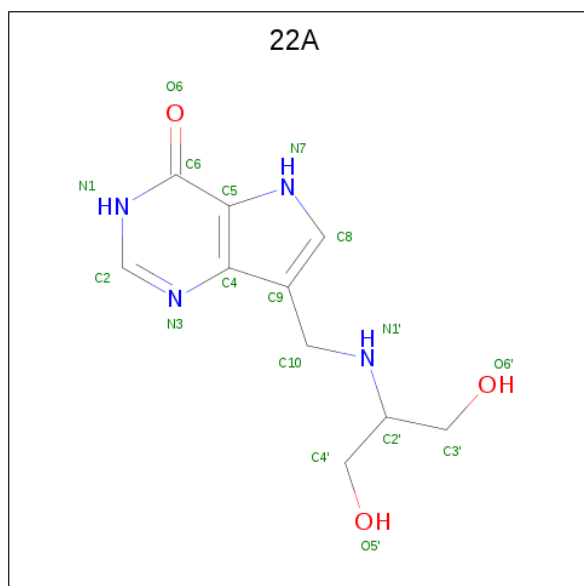
- Molecule 1 is a protein called Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	1	0
			2246	1427	394	409	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	SER	GLY	ENGINEERED	UNP P00491

- Molecule 2 is 7-([2-hydroxy-1-(hydroxymethyl)ethyl]amino)methyl)-3,5-dihydro-4H-pyrrolo[3,2-d]pyrimidin-4-one (three-letter code: 22A) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	10	4	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: 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	A	1	Total	O	P	0	0
			5	4	1		

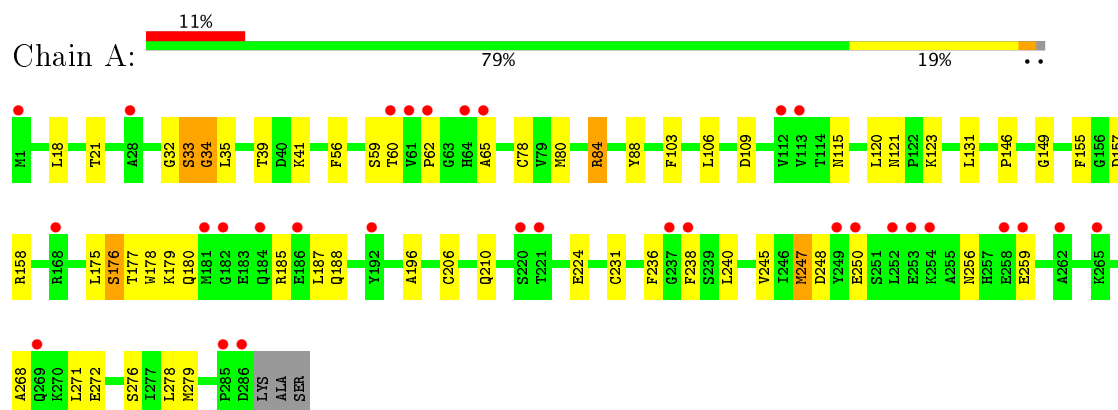
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		

### 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 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.97Å 142.97Å 168.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 29.06 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.50) 99.3 (29.06-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, $R_{free}$	0.222 , 0.262 0.224 , 0.261	Depositor DCC
$R_{free}$ test set	1175 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k- 2/3*l,2/3*h-2/3*k+1/3*l 0.014 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3* k+1/3*l 0.008 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3* *k+1/3*l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2305	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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, 22A

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	0.79	1/2301 (0.0%)	0.76	1/3113 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	CYS	CB-SG	-5.76	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ASP	CB-CG-OD1	5.78	123.50	118.30

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	2246	0	2225	40	0
2	A	17	0	14	0	0
3	A	10	0	0	0	0
4	A	32	0	0	0	0
All	All	2305	0	2239	40	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 (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:CYS:HB3	1:A:247:MET:CE	1.66	1.23
1:A:206:CYS:HB3	1:A:247:MET:HE1	1.27	1.15
1:A:206:CYS:HB3	1:A:247:MET:HE2	1.50	0.91
1:A:35:LEU:HD11	1:A:272:GLU:CG	2.06	0.85
1:A:35:LEU:HD11	1:A:272:GLU:HG2	1.59	0.83
1:A:206:CYS:CB	1:A:247:MET:CE	2.56	0.78
1:A:131:LEU:HD11	1:A:236:PHE:CE1	2.18	0.78
1:A:131:LEU:HD11	1:A:236:PHE:HE1	1.50	0.77
1:A:206:CYS:CB	1:A:247:MET:HE2	2.16	0.71
1:A:59:SER:HB2	1:A:65:ALA:HB2	1.76	0.66
1:A:39:THR:HG22	1:A:80:MET:HE2	1.79	0.63
1:A:35:LEU:O	1:A:35:LEU:HG	2.01	0.61
1:A:32:GLY:O	1:A:34:GLY:N	2.40	0.53
1:A:158[B]:ARG:HE	1:A:158[B]:ARG:HA	1.74	0.53
1:A:103:PHE:O	1:A:106:LEU:HB2	2.10	0.52
1:A:41:LYS:HE2	1:A:272:GLU:OE1	2.10	0.51
1:A:35:LEU:HD11	1:A:272:GLU:HG3	1.87	0.51
1:A:35:LEU:HD22	1:A:271:LEU:HB3	1.93	0.51
1:A:158[B]:ARG:HE	1:A:158[B]:ARG:CA	2.23	0.50
1:A:84:ARG:NH1	1:A:224:GLU:OE2	2.45	0.50
1:A:185:ARG:HH21	1:A:188:GLN:HE21	1.59	0.49
1:A:120:LEU:HD23	1:A:245:VAL:HG21	1.93	0.49
1:A:32:GLY:HA3	1:A:115:ASN:HA	1.95	0.49
1:A:32:GLY:O	1:A:33:SER:C	2.51	0.47
1:A:35:LEU:CD1	1:A:272:GLU:HG3	2.44	0.47
1:A:240:LEU:HD22	1:A:271:LEU:HD11	1.96	0.47
1:A:238:PHE:HE1	1:A:271:LEU:HD22	1.80	0.46
1:A:158[B]:ARG:NE	1:A:158[B]:ARG:HA	2.31	0.45
1:A:155:PHE:O	1:A:231:CYS:HA	2.17	0.45
1:A:256:ASN:ND2	1:A:259:GLU:H	2.15	0.45
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.87	0.42
1:A:175:LEU:HD13	1:A:187:LEU:HD23	2.02	0.42
1:A:88:TYR:HB3	1:A:196:ALA:O	2.19	0.42
1:A:60:THR:O	1:A:62:PRO:HD3	2.19	0.42
1:A:149:GLY:O	1:A:158[A]:ARG:NH1	2.51	0.42
1:A:121:ASN:OD1	1:A:123:LYS:HG2	2.20	0.42
1:A:176:SER:O	1:A:178:TRP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:SER:HA	1:A:179:LYS:HD3	2.03	0.41
1:A:88:TYR:C	1:A:88:TYR:CD1	2.95	0.41
1:A:276:SER:O	1:A:279:MET:HB2	2.21	0.40

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	285/289 (99%)	269 (94%)	11 (4%)	5 (2%)	10 17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	177	THR
1	A	176	SER
1	A	268	ALA
1	A	34	GLY

### 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	239/240 (100%)	228 (95%)	11 (5%)	31 55

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	56	PHE
1	A	84	ARG
1	A	146	PRO
1	A	157	ASP
1	A	180	GLN
1	A	210	GLN
1	A	247	MET
1	A	248	ASP
1	A	250	GLU
1	A	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	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](#)

3 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	22A	A	290	-	17,18,18	1.02	1 (5%)	9,24,24	3.58	6 (66%)
3	PO4	A	291	-	4,4,4	1.01	0	6,6,6	0.89	0
3	PO4	A	292	-	4,4,4	0.99	0	6,6,6	0.60	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	22A	A	290	-	-	0/7/9/9	0/2/2/2
3	PO4	A	291	-	-	0/0/0/0	0/0/0/0
3	PO4	A	292	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	290	22A	C6-C5	2.67	1.46	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	290	22A	N3-C2-N1	-7.28	122.51	128.86
2	A	290	22A	C5-C4-N3	-3.74	120.58	124.92
2	A	290	22A	C6-C5-C4	-3.54	117.33	120.84
2	A	290	22A	C9-C10-N1'	-2.05	106.75	112.83
2	A	290	22A	C10-N1'-C2'	3.68	119.65	114.11
2	A	290	22A	C2-N1-C6	3.92	122.46	115.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	286/289 (98%)	0.46	31 (10%) 6 6	47, 67, 98, 106	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	PRO	5.5
1	A	181	MET	4.9
1	A	286	ASP	4.6
1	A	258	GLU	4.5
1	A	61	VAL	4.0
1	A	65	ALA	3.7
1	A	253	GLU	3.6
1	A	265	LYS	3.5
1	A	182	GLY	3.4
1	A	64	HIS	3.2
1	A	252	LEU	3.1
1	A	184	GLN	3.0
1	A	269	GLN	2.9
1	A	250	GLU	2.7
1	A	254	LYS	2.6
1	A	168	ARG	2.6
1	A	221	THR	2.5
1	A	60	THR	2.4
1	A	285	PRO	2.3
1	A	28	ALA	2.3
1	A	238	PHE	2.3
1	A	186	GLU	2.2
1	A	113	VAL	2.2
1	A	249	TYR	2.2
1	A	262	ALA	2.2
1	A	237	GLY	2.2
1	A	220	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	259	GLU	2.1
1	A	112	VAL	2.1
1	A	1	MET	2.0
1	A	192	TYR	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( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	292	5/5	0.96	0.16	0.13	85,86,87,88	0
3	PO4	A	291	5/5	0.99	0.22	0.11	63,63,66,68	0
2	22A	A	290	17/17	0.97	0.17	-0.22	61,63,74,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.