



# wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 03:22 AM GMT

PDB ID : 1D6N  
Title : TERNARY COMPLEX STRUCTURE OF HUMAN HGPRTASE, PRPP, MG2+, AND THE INHIBITOR HPP REVEALS THE INVOLVEMENT OF THE FLEXIBLE LOOP IN SUBSTRATE BINDING  
Authors : Balendiran, G.K.  
Deposited on : 1999-10-14  
Resolution : 2.70 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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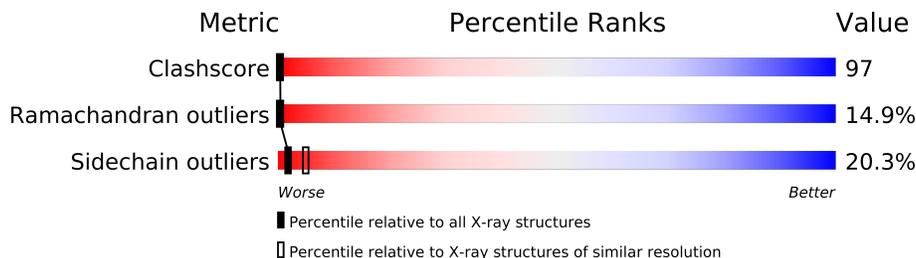
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	
1	B	214	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3490 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (HYPOXANTHINE-GUANINEPHOSPHORIBOSYLTRANSFERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1686	1076	282	318	10	0	0	0
1	B	214	1686	1076	282	318	10	0	0	0

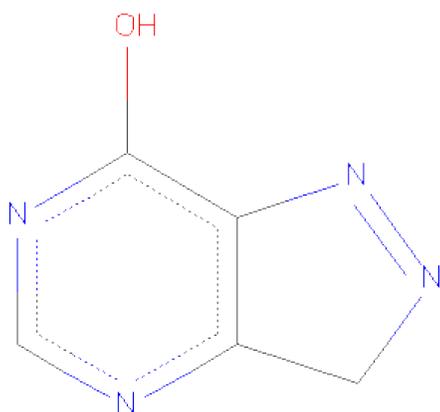
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ALA	LYS	ENGINEERED	UNP P00492
A	102	GLY	LYS	CONFLICT	UNP P00492
B	68	ALA	LYS	ENGINEERED	UNP P00492
B	102	GLY	LYS	CONFLICT	UNP P00492

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

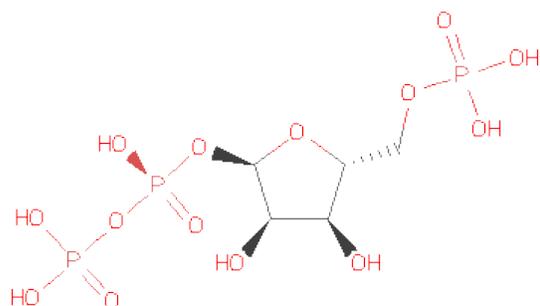
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	B	1	1	1	0	0
2	A	1	1	1	0	0

- Molecule 3 is 3H-PYRAZOLO[4,3-D]PYRIMIDIN-7-OL (three-letter code: PPO) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	10	5	4	1	0	0
3	B	1	10	5	4	1	0	0

- Molecule 4 is ALPHA-PHOSPHORIBOSYLPYROPHOSPHORICACID (three-letter code: PRP) (formula:  $C_5H_{13}O_{14}P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	A	1	22	5	14	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	B	1	22	5	14	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	28	Total	O	0	0
			28	28		

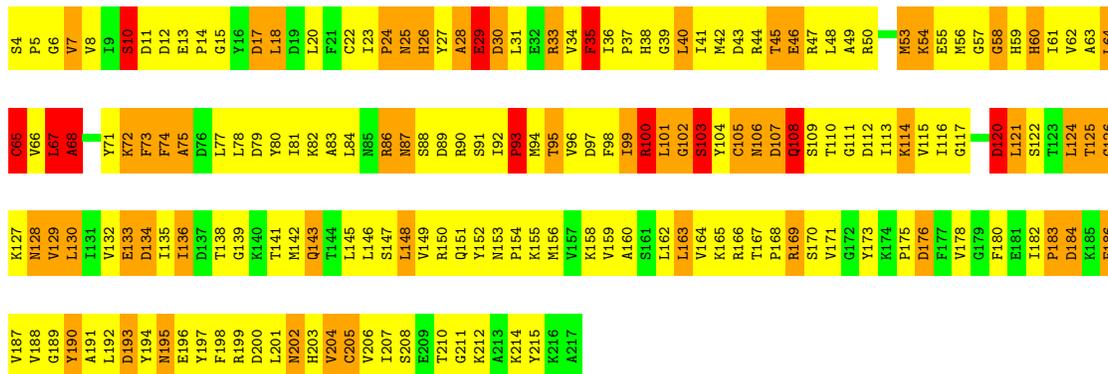
### 3 Residue-property plots

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

Note EDS was not executed.

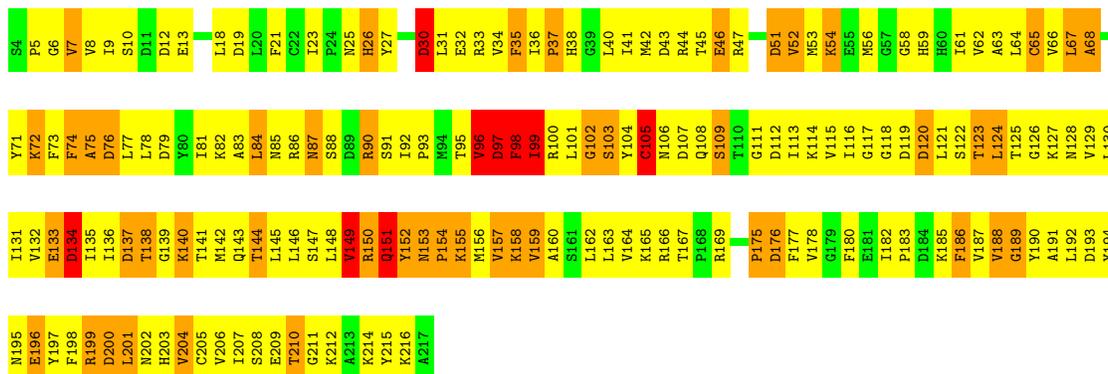
- Molecule 1: PROTEIN (HYPOXANTHINE-GUANINEPHOSPHORIBOSYLTRANSFERASE)

Chain A:



- Molecule 1: PROTEIN (HYPOXANTHINE-GUANINEPHOSPHORIBOSYLTRANSFERASE)

Chain B:



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.56Å 65.85Å 51.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.174 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	3.0	wwPDB-VP

## 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: MG, PPO, PRP

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	0.60	1/1719 (0.1%)	1.05	19/2324 (0.8%)
1	B	0.92	6/1719 (0.3%)	1.43	19/2324 (0.8%)
All	All	0.77	7/3438 (0.2%)	1.25	38/4648 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	5
All	All	0	12

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	CYS	CB-SG	-23.27	1.42	1.82
1	B	105	CYS	C-N	-13.68	1.02	1.34
1	B	109	SER	C-N	-8.09	1.15	1.34
1	B	151	GLN	CA-CB	-7.46	1.37	1.53
1	B	108	GLN	C-N	-6.47	1.19	1.34

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	CYS	O-C-N	-28.23	77.53	122.70
1	B	97	ASP	CB-CG-OD2	17.88	134.39	118.30
1	B	97	ASP	CB-CG-OD1	-17.59	102.47	118.30
1	B	133	GLU	O-C-N	17.57	150.82	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	CYS	CA-C-N	14.19	148.41	117.20

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	LEU	Mainchain
1	A	103	SER	Mainchain
1	A	67	LEU	Peptide
1	A	68	ALA	Peptide
1	A	99	ILE	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1686	0	1687	350	0
1	B	1686	0	1684	333	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	3	1	0
3	B	10	0	3	1	0
4	A	22	0	6	14	0
4	B	22	0	7	7	0
5	A	24	0	0	4	0
5	B	28	0	0	8	0
All	All	3490	0	3390	663	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 97.

The worst 5 of 663 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:64:LEU:CD2	1:A:124:LEU:HD21	1.50	1.41
1:A:65:CYS:SG	1:A:74:PHE:CD1	2.29	1.24

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:191:ALA:O	1:B:192:LEU:HD22	1.05	1.21
1:A:191:ALA:O	1:A:192:LEU:HD22	1.39	1.18
1:A:65:CYS:SG	1:A:132:VAL:HB	1.84	1.17

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	212/214 (99%)	131 (62%)	53 (25%)	28 (13%)	0	0
1	B	212/214 (99%)	130 (61%)	47 (22%)	35 (16%)	0	0
All	All	424/428 (99%)	261 (62%)	100 (24%)	63 (15%)	0	0

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	10	SER
1	A	29	GLU
1	A	40	LEU
1	A	46	GLU

### 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	187/187 (100%)	145 (78%)	42 (22%)	1	4
1	B	187/187 (100%)	153 (82%)	34 (18%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	374/374 (100%)	298 (80%)	76 (20%)	<b>2</b> <b>5</b>

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	LEU
1	B	19	ASP
1	B	196	GLU
1	A	169	ARG
1	A	186	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	B	26	HIS
1	B	128	ASN
1	A	151	GLN
1	B	59	HIS

### 5.3.3 RNA [i](#)

There are no RNA chains 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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	PPO	A	300	-	11,11,11	3.96	4 (36%)	14,15,15	2.41	3 (21%)
4	PRP	A	312	2	22,22,22	2.82	12 (54%)	35,35,35	4.17	20 (57%)
3	PPO	B	301	-	11,11,11	4.12	6 (54%)	14,15,15	2.37	3 (21%)
4	PRP	B	314	2	22,22,22	3.33	11 (50%)	35,35,35	4.90	20 (57%)

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	PPO	A	300	-	-	0/0/6/6	0/0/2/2
4	PRP	A	312	2	-	0/16/33/33	0/1/1/1
3	PPO	B	301	-	-	0/0/6/6	0/0/2/2
4	PRP	B	314	2	-	0/16/33/33	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	314	PRP	PA-O3A	-11.54	1.39	1.59
3	A	300	PPO	C9-C4	-9.71	1.37	1.50
3	B	301	PPO	C9-C4	-9.56	1.37	1.50
3	A	300	PPO	C9-N8	-7.02	1.38	1.46
4	A	312	PRP	PA-O3A	-6.90	1.47	1.59

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	314	PRP	O3A-PA-O1	20.27	154.72	103.48
4	A	312	PRP	O3A-PA-O1	15.65	143.03	103.48
4	A	312	PRP	PA-O3A-PB	11.30	164.81	131.68
4	B	314	PRP	O3B-PB-O1B	-8.64	82.19	110.44
4	A	312	PRP	O3B-PB-O3A	8.11	143.60	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.