



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2IU3 / pdb_00002iu3
Title : Crystal structures of transition state analogue inhibitors of inosine monophosphate cyclohydrolase
Authors : Xu, L.; Chong, Y.; Hwang, I.; D'Onofrio, A.; Amore, K.; Beardsley, G.P.; Li, C.; Olson, A.J.; Boger, D.L.; Wilson, I.A.
Deposited on : 2006-05-27
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

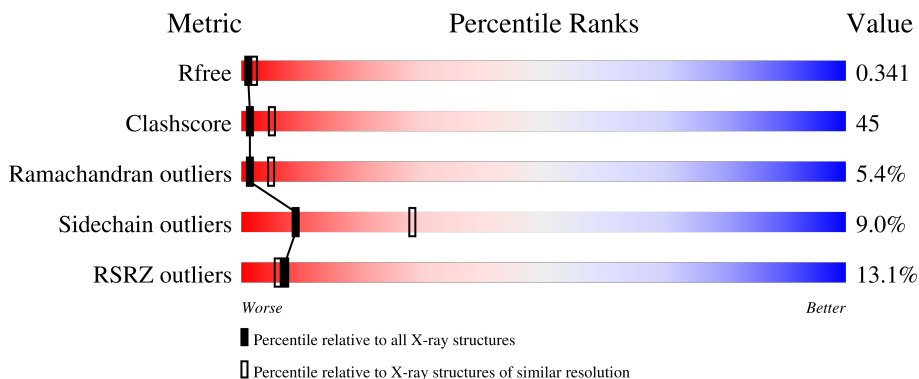
1 Overall quality at a glance

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))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. 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	593	
1	B	593	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9145 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.

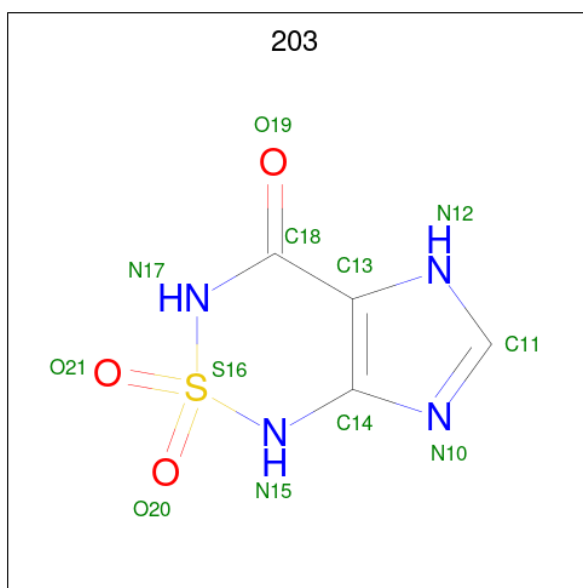
- Molecule 1 is a protein called BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	590	Total 4523	C 2852	N 801	O 851	S 19	0	1	0
1	B	590	Total 4511	C 2843	N 800	O 849	S 19	0	0	0

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 3 is 1,5-DIHYDROIMIDAZO[4,5-C][1,2,6]THIADIAZIN-4(3H)-ONE 2,2-DIOXIDE (CCD ID: 203) (formula: C₄H₄N₄O₃S).



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

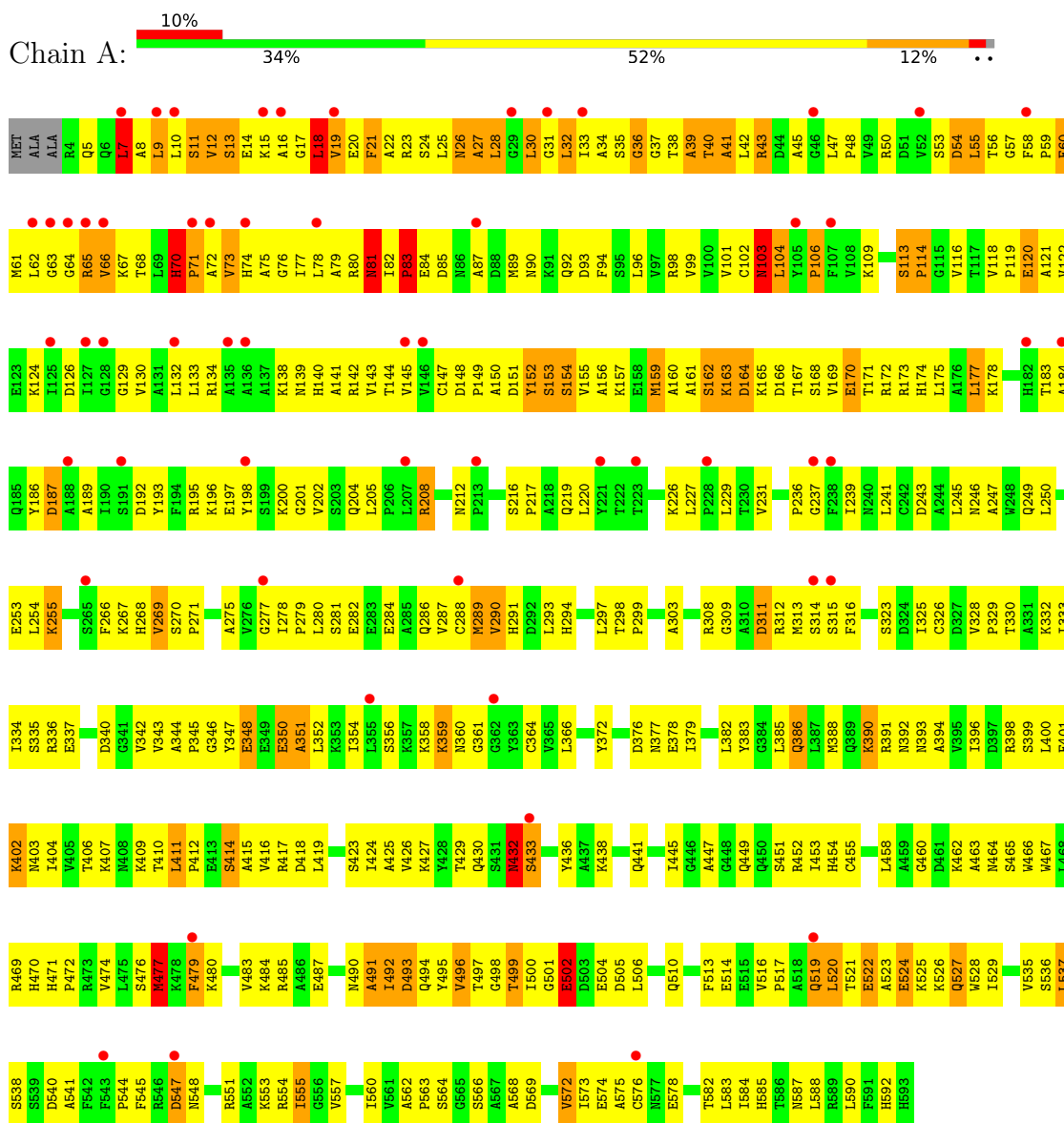
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	45	Total	O	0	0
			45	45		

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: BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH



• Molecule 1: BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	387.00Å 57.00Å 62.10Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	35.20 – 2.90 35.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.5 (35.20-2.90) 91.6 (35.20-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.85Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.300 0.285 , 0.341	Depositor DCC
R_{free} test set	1210 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtrriage
Anisotropy	0.315	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.027 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9145	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: K, 203

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	0.74	6/4608 (0.1%)	1.14	25/6249 (0.4%)
1	B	0.70	5/4595 (0.1%)	1.14	36/6230 (0.6%)
All	All	0.72	11/9203 (0.1%)	1.14	61/12479 (0.5%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	MET	SD-CE	6.70	1.96	1.79
1	A	527	GLN	CD-OE1	5.96	1.34	1.23
1	B	490	ASN	CG-OD1	5.79	1.34	1.23
1	B	139	ASN	CG-OD1	5.61	1.34	1.23
1	B	256	GLN	CD-OE1	5.44	1.33	1.23

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ALA	N-CA-C	-14.51	94.86	113.72
1	B	514	GLU	N-CA-C	-10.29	100.14	111.36
1	A	514	GLU	N-CA-C	-10.16	99.89	110.97
1	B	26	ASN	N-CA-C	-8.76	101.73	111.28
1	A	7	LEU	N-CA-C	8.72	122.62	109.63

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	4523	0	4570	457	0
1	B	4511	0	4561	393	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	12	0	4	1	0
4	A	52	0	0	2	0
4	B	45	0	0	3	0
All	All	9145	0	9135	816	4

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 45.

The worst 5 of 816 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:510:GLN:HE21	1:A:516:VAL:HG21	1.19	1.04
1:B:485:ARG:HG2	1:B:485:ARG:HH11	1.22	1.04
1:A:379:ILE:HG12	1:A:388:MET:HG3	1.34	1.04
1:A:510:GLN:NE2	1:A:516:VAL:HG21	1.76	1.00
1:B:479:PHE:HA	1:B:513:PHE:HA	1.46	0.97

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:O	1:B:47:LEU:O[2_656]	1.94	0.26
1:B:46:GLY:O	1:B:48:PRO:C[2_656]	2.02	0.18
1:B:46:GLY:CA	1:B:49:VAL:O[2_656]	2.07	0.13
1:B:46:GLY:O	1:B:48:PRO:CA[2_656]	2.11	0.09

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	589/593 (99%)	464 (79%)	90 (15%)	35 (6%)	1	4
1	B	588/593 (99%)	484 (82%)	75 (13%)	29 (5%)	1	6
All	All	1177/1186 (99%)	948 (80%)	165 (14%)	64 (5%)	1	5

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	18	LEU
1	A	19	VAL
1	A	40	THR
1	A	66	VAL

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	485/485 (100%)	439 (90%)	46 (10%)	8	26
1	B	484/485 (100%)	443 (92%)	41 (8%)	10	31
All	All	969/970 (100%)	882 (91%)	87 (9%)	9	28

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	157	LYS
1	B	338	VAL
1	B	170	GLU
1	B	282	GLU
1	B	399	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	454	HIS
1	B	464	ASN
1	B	527	GLN
1	A	371	ASN
1	A	294	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	203	B	1595	-	10,13,13	6.63	5 (50%)	8,20,20	8.21	7 (87%)

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	203	B	1595	-	-	-	0/1/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1595	203	O20-S16	16.52	1.65	1.43
3	B	1595	203	O21-S16	10.57	1.57	1.43
3	B	1595	203	C13-C18	4.63	1.55	1.41
3	B	1595	203	C11-N12	4.58	1.42	1.35
3	B	1595	203	C13-N12	2.45	1.41	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1595	203	O21-S16-O20	-17.17	97.97	118.87
3	B	1595	203	C11-N12-C13	-11.31	93.89	106.59
3	B	1595	203	N12-C11-N10	7.54	121.73	112.98
3	B	1595	203	C18-C13-N12	-4.88	121.81	131.14
3	B	1595	203	O19-C18-C13	-3.85	117.98	127.26

There are no chirality outliers.

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
3	B	1595	203	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	590/593 (99%)	1.08	57 (9%) 13 11	22, 43, 66, 74	1 (0%)
1	B	590/593 (99%)	1.21	97 (16%) 4 3	27, 46, 63, 72	0
All	All	1180/1186 (99%)	1.15	154 (13%) 7 6	22, 45, 65, 74	1 (0%)

The worst 5 of 154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	LEU	4.9
1	A	31	GLY	4.8
1	B	46	GLY	4.8
1	B	43	ARG	4.5
1	A	72	ALA	4.2

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 oligosaccharides 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(\AA^2)	Q<0.9
2	K	A	1594	1/1	0.65	0.17	56,56,56,56	0
3	203	B	1595	12/12	0.67	0.16	68,71,74,74	0
2	K	B	1594	1/1	0.93	0.07	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.