



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 09:38 pm BST

PDB ID : 2IU3
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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

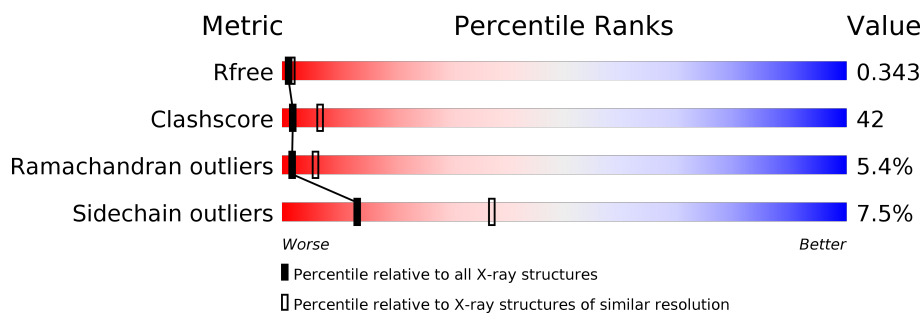
1 Overall quality at a glance

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	593	 36% 55% 8% ..
1	B	593	 39% 53% 7% ..

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.

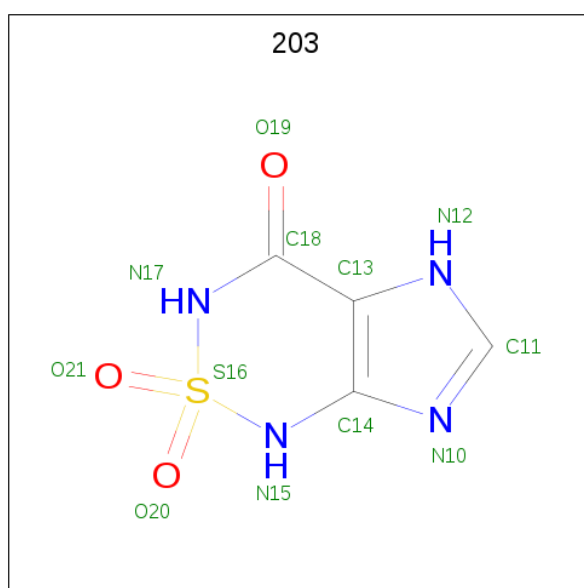
- Molecule 1 is a protein called BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH.

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

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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



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

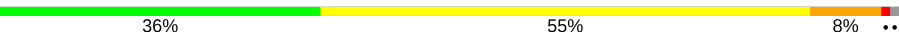
- Molecule 4 is water.

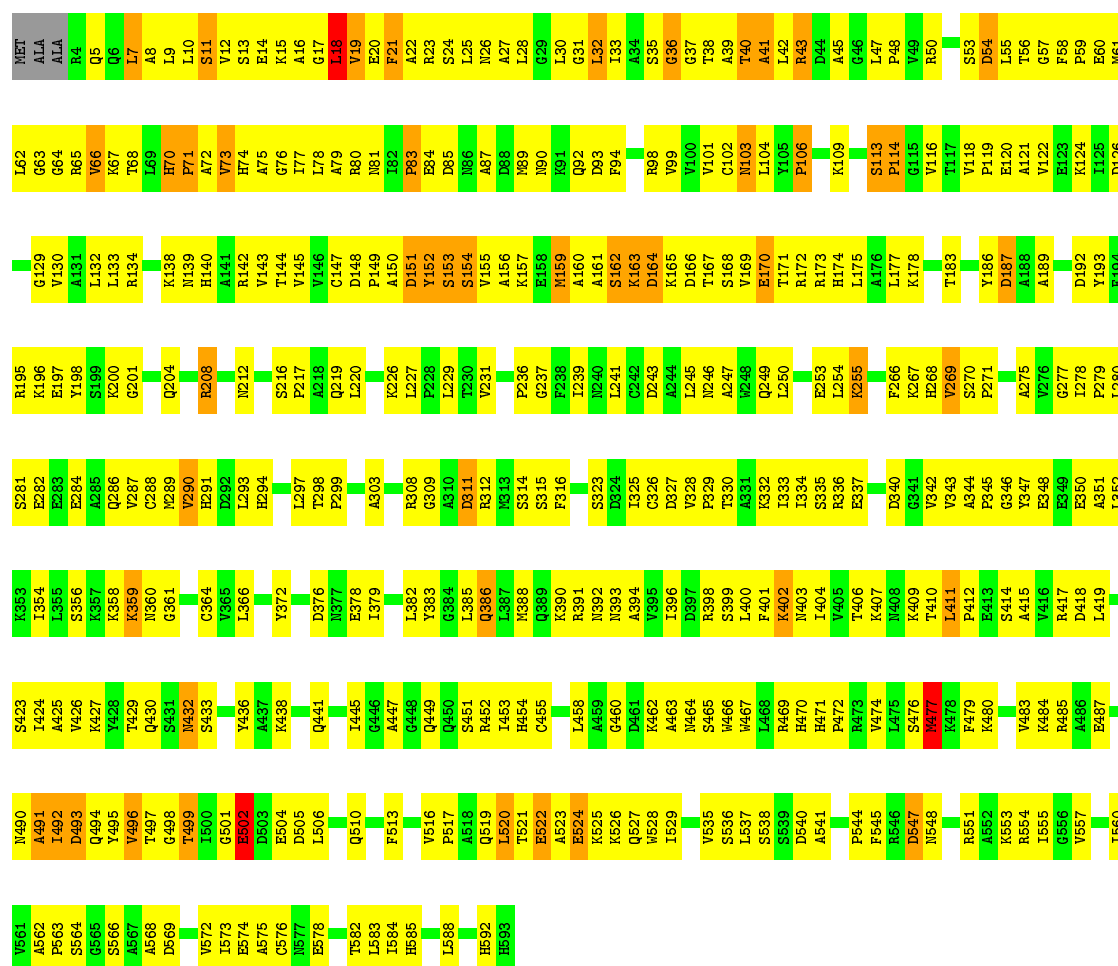
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	45	Total	O	0	0
			45	45		

3 Residue-property plots

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. 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. 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

Chain A: 



• Molecule 1: BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH

Chain B: 



R589	Q519	T456	L382	K295	E197	G129	G64
L590	L520	L457	L383	T296	L198	G130	R65
F591	E522	A459	G384	T298	S199	A131	V66
H592	E523	G460	L387	P299	V202	L132	K67
H593	E524	D461	K388	P302	S203	L133	T68
	K525	K462	L389	S302	Q204	L134	
	K526	A463	K390	A303	L205	R134	
	Q527	M464	K391	S307	P206		P71
	M528	S465	N392	R308		K138	A72
		K466	K393			K139	V73
	L532	M467	L394	D311		H140	H74
	T533	L468	L395	R312		A141	A75
	A534	R469	T396	K313		R142	
	V535	K470	D397	N314		V143	G76
	S536	H471	K398	S314		T144	L78
	L537	P472	S399	S315			A79
	S538	R473	L400	F316		G147	R80
	S539	V474	F401			D148	N81
	D540	L475	K402	T320		P149	I82
		A541	N403	D324		A150	P83
	F542	M477	L404	L325		D151	E84
	F543	K478	V405	L326		Y152	D85
	F544	F479	T406	V328		S153	N86
	F545	K480	K407			S154	A87
	R546		N408			V155	D88
	D547		K409	A331		A156	M89
	N548	K484	T410	K332		K157	N90
	V549	R485	L411	L333		E158	X91
	D550	A486	P412	L334		M159	Q92
	R551	E487		S335			
	A552	V488	V416			S162	S95
	K553	S489	R417	V338		K163	L96
	R554	M490	D418			D164	V97
	I555	A491		G341		K165	R98
				V342		D166	
	G556		T424	V343		T167	V99
	V557	Q494	A425			S168	
		Y495	V426			A257	C102
	I560	V496	K427	G346		V169	
		T497	T428	E347		E170	Y105
	S564	G498	T429	E348		T171	P106
	G565	T499	Q430	E349		R172	F107
	S566	L500	A431	E350		R173	V108
	A567	G501	N432	A351		H174	K109
	A568	E502	S433	L352		L175	T110
	D569	S503				A176	V111
	E570	E504	Y436			L177	S112
	V571	S505	A437	S356		K178	S113
	V572	L506	K438	K357			P114
	L573	V507		R358		T183	G115
	E574	K508	T445	K359		A184	V116
	A575	N509	Q446	N360		E282	T117
	C576	Q510		G361		E283	V118
	N577	A511	Q449	G362			P119
	E578	M512	Q450	V363		Q286	E120
	L579	F513	S451	L366		V237	A121
		E514	R452				V122
	T582		T453	D375		E291	E123
	L584		R454	D376		D292	F124
			C455			L293	R125
						F294	K126

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 35.13 – 2.87	Depositor EDS
% Data completeness (in resolution range)	91.5 (35.20-2.90) 90.9 (35.13-2.87)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.300 0.286 , 0.343	Depositor DCC
R_{free} test set	1210 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h-2*k,l	Xtriage
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

Xtriage'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: 203, K

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	0.61	0/4608	0.75	1/6249 (0.0%)
1	B	0.59	0/4595	0.75	0/6230
All	All	0.60	0/9203	0.75	1/12479 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ALA	N-CA-C	-5.98	94.86	111.00

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	434	0
1	B	4511	0	4561	363	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	763	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 42.

The worst 5 of 763 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	5
1	B	588/593 (99%)	484 (82%)	75 (13%)	29 (5%)	2	8
All	All	1177/1186 (99%)	948 (80%)	165 (14%)	64 (5%)	2	6

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	SER

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

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	485/485 (100%)	450 (93%)	35 (7%)	14	39
1	B	484/485 (100%)	446 (92%)	38 (8%)	12	34
All	All	969/970 (100%)	896 (92%)	73 (8%)	13	37

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	GLU
1	B	54	ASP
1	B	483	VAL
1	B	9	LEU
1	B	60	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	464	ASN
1	B	5	GLN
1	B	494	GLN
1	A	510	GLN
1	B	70	HIS

5.3.3 RNA ⓘ

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](#)

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	-	6,13,13	7.86	4 (66%)	5,20,20	8.02	5 (100%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1595	203	O20-S16	15.37	1.65	1.43
3	B	1595	203	O21-S16	9.84	1.57	1.43
3	B	1595	203	C14-N15	4.30	1.42	1.37
3	B	1595	203	C13-C18	4.06	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1595	203	O21-S16-O20	-16.63	97.97	118.85
3	B	1595	203	C11-N12-C13	-4.78	93.89	102.99
3	B	1595	203	O19-C18-C13	-3.27	117.98	124.37
3	B	1595	203	O19-C18-N17	2.75	124.53	120.82
3	B	1595	203	C13-C18-N17	2.03	117.49	113.95

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.