



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 01:36 PM GMT

PDB ID : 4GDY
Title : Kynurenine Aminotransferase II inhibitors
Authors : Pandit, J.
Deposited on : 2012-08-01
Resolution : 2.89 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

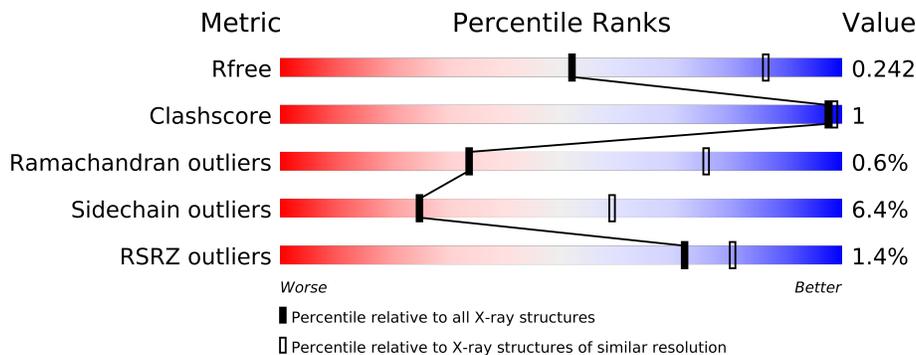
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 2.89 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	439	
1	B	439	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6880 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 Kynurenine/alpha-aminoadipateaminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	415	3245	2083	543	602	17	0	0	0
1	B	428	3344	2145	561	620	18	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

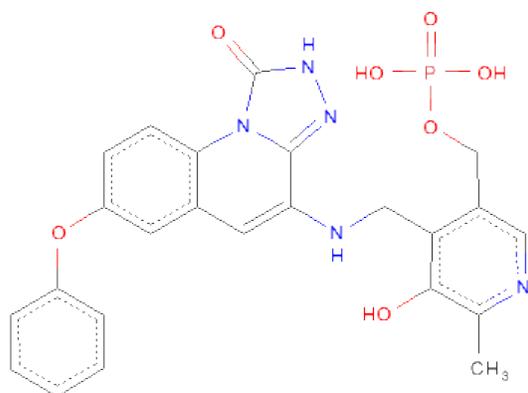
Chain	Residue	Modelled	Actual	Comment	Reference
A	240	SER	LYS	ENGINEERED MUTATION	UNP Q8N5Z0
A	241	GLY	PHE	ENGINEERED MUTATION	UNP Q8N5Z0
A	426	LEU	-	EXPRESSION TAG	UNP Q8N5Z0
A	427	VAL	-	EXPRESSION TAG	UNP Q8N5Z0
A	428	PRO	-	EXPRESSION TAG	UNP Q8N5Z0
A	429	ARG	-	EXPRESSION TAG	UNP Q8N5Z0
A	430	GLY	-	EXPRESSION TAG	UNP Q8N5Z0
A	431	SER	-	EXPRESSION TAG	UNP Q8N5Z0
A	432	LEU	-	EXPRESSION TAG	UNP Q8N5Z0
A	433	GLU	-	EXPRESSION TAG	UNP Q8N5Z0
A	434	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
A	435	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
A	436	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
A	437	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
A	438	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
A	439	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
B	240	SER	LYS	ENGINEERED MUTATION	UNP Q8N5Z0
B	241	GLY	PHE	ENGINEERED MUTATION	UNP Q8N5Z0
B	426	LEU	-	EXPRESSION TAG	UNP Q8N5Z0
B	427	VAL	-	EXPRESSION TAG	UNP Q8N5Z0
B	428	PRO	-	EXPRESSION TAG	UNP Q8N5Z0
B	429	ARG	-	EXPRESSION TAG	UNP Q8N5Z0
B	430	GLY	-	EXPRESSION TAG	UNP Q8N5Z0
B	431	SER	-	EXPRESSION TAG	UNP Q8N5Z0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	432	LEU	-	EXPRESSION TAG	UNP Q8N5Z0
B	433	GLU	-	EXPRESSION TAG	UNP Q8N5Z0
B	434	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
B	435	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
B	436	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
B	437	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
B	438	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
B	439	HIS	-	EXPRESSION TAG	UNP Q8N5Z0

- Molecule 2 is (5-HYDROXY-6-METHYL-4-[[[(1-OXO-7-PHENOXY-1,2-DIHYDRO[1,2,4]TRIAZOLO[4,3-A]QUINOLIN-4-YL)AMINO]METHYL}PYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (three-letter code: 0X1) (formula: C₂₄H₂₂N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	37	24	5	7	1	0	0
2	B	1	37	24	5	7	1	0	0

- Molecule 3 is water.

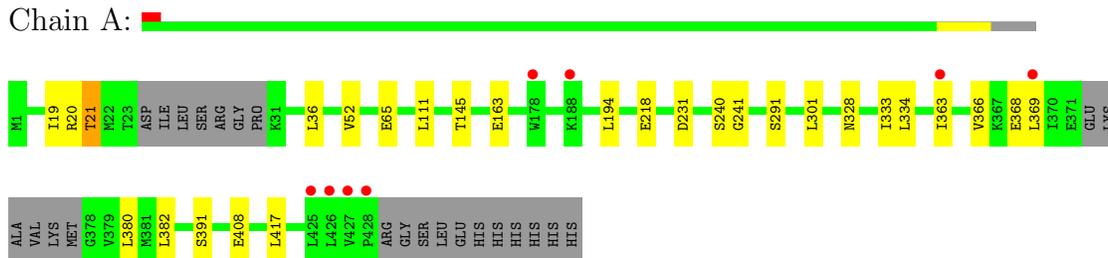
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	94	94	94	0	0
3	B	123	123	123	0	0

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.

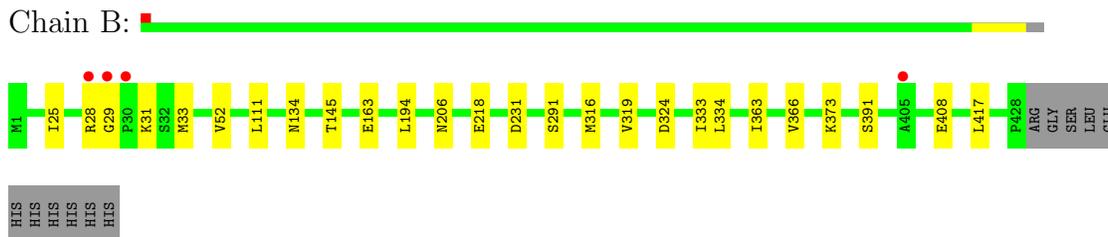
- Molecule 1: Kynurenine/alpha-aminoadipateaminotransferase, mitochondrial

Chain A:



- Molecule 1: Kynurenine/alpha-aminoadipateaminotransferase, mitochondrial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.46Å 116.46Å 115.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.85 – 2.89 38.12 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (100.85-2.89) 99.8 (38.12-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.61 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.171 , 0.240 0.171 , 0.242	Depositor DCC
R_{free} test set	1049 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.2	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 20510 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6880	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: 0X1

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	0.49	0/3324	0.70	1/4514 (0.0%)
1	B	0.48	0/3426	0.71	0/4653
All	All	0.48	0/6750	0.71	1/9167 (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	20	ARG	C-N-CA	5.61	135.73	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	3245	0	0	0	0
1	B	3344	0	0	2	0
2	A	37	0	20	1	0
2	B	37	0	20	2	0
3	A	94	0	0	0	0
3	B	123	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6880	0	40	5	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 1.

All (5) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:134:ASN:N	3:B:606:HOH:O	2.48	0.47
1:B:206:ASN:ND2	3:B:722:HOH:O	2.50	0.43
2:A:501:OX1:N19	2:A:501:OX1:O24	2.51	0.43
2:B:501:OX1:N19	2:B:501:OX1:O24	2.51	0.42
2:B:501:OX1:O36	2:B:501:OX1:H3	2.20	0.41

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	409/439 (93%)	388 (95%)	19 (5%)	2 (0%)	38	79
1	B	426/439 (97%)	404 (95%)	19 (4%)	3 (1%)	30	72
All	All	835/878 (95%)	792 (95%)	38 (5%)	5 (1%)	33	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	B	28	ARG
1	B	25	ILE
1	B	29	GLY
1	A	241	GLY

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	361/382 (94%)	335 (93%)	26 (7%)	21	51
1	B	372/382 (97%)	351 (94%)	21 (6%)	30	66
All	All	733/764 (96%)	686 (94%)	47 (6%)	25	59

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	21	THR
1	A	36	LEU
1	A	52	VAL
1	A	65	GLU
1	A	111	LEU
1	A	145	THR
1	A	163	GLU
1	A	194	LEU
1	A	218	GLU
1	A	231	ASP
1	A	240	SER
1	A	291	SER
1	A	301	LEU
1	A	328	ASN
1	A	333	ILE
1	A	334	LEU
1	A	363	ILE
1	A	366	VAL
1	A	368	GLU
1	A	369	LEU
1	A	380	LEU
1	A	382	LEU
1	A	391	SER
1	A	408	GLU
1	A	417	LEU
1	B	31	LYS
1	B	33	MET
1	B	52	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	111	LEU
1	B	145	THR
1	B	163	GLU
1	B	194	LEU
1	B	218	GLU
1	B	231	ASP
1	B	291	SER
1	B	316	MET
1	B	319	VAL
1	B	324	ASP
1	B	333	ILE
1	B	334	LEU
1	B	363	ILE
1	B	366	VAL
1	B	373	LYS
1	B	391	SER
1	B	408	GLU
1	B	417	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

2 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	0X1	A	501	-	41,41,41	3.57	7 (17%)	56,60,60	1.71	7 (12%)
2	0X1	B	501	-	41,41,41	3.81	7 (17%)	56,60,60	2.02	9 (16%)

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	0X1	A	501	-	-	0/15/15/15	0/2/5/5
2	0X1	B	501	-	-	0/15/15/15	0/2/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	0X1	C25-N35	22.39	1.39	1.31
2	A	501	0X1	C25-N35	20.66	1.38	1.31
2	B	501	0X1	C15-C12	4.50	1.49	1.42
2	B	501	0X1	C6-C8	-4.35	1.38	1.41
2	A	501	0X1	C8-N20	4.18	1.42	1.40
2	A	501	0X1	C15-C12	3.91	1.48	1.42
2	A	501	0X1	C6-C8	-3.69	1.38	1.41
2	A	501	0X1	C10-C11	-3.61	1.38	1.40
2	A	501	0X1	C12-N37	-3.51	1.29	1.33
2	B	501	0X1	C12-N37	-3.20	1.30	1.33
2	B	501	0X1	C10-C11	-2.95	1.38	1.40
2	A	501	0X1	C12-N20	-2.76	1.36	1.42
2	B	501	0X1	C12-N20	-2.70	1.36	1.42
2	B	501	0X1	C13-C5	-2.15	1.49	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	0X1	N35-C25-N20	-8.41	102.53	109.04
2	A	501	0X1	N35-C25-N20	-7.24	103.44	109.04
2	B	501	0X1	C25-N20-C8	-5.92	127.84	134.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	0X1	C25-N20-C12	5.70	108.58	103.20
2	A	501	0X1	C25-N20-C8	-4.56	129.47	134.97
2	A	501	0X1	C25-N20-C12	4.19	107.16	103.20
2	B	501	0X1	C25-N35-N37	3.53	112.53	110.58
2	B	501	0X1	C13-C5-C10	2.78	123.84	120.31
2	A	501	0X1	C1-C6-C8	2.74	120.75	118.78
2	A	501	0X1	C25-N35-N37	2.57	112.00	110.58
2	B	501	0X1	C14-C15-N19	2.51	127.19	122.10
2	A	501	0X1	C14-C15-N19	2.37	126.92	122.10
2	B	501	0X1	O21-P27-O26	-2.24	100.47	106.65
2	A	501	0X1	O26-C17-C7	-2.06	105.07	109.26
2	B	501	0X1	C14-C6-C8	2.03	120.25	118.78
2	B	501	0X1	O23-P27-O21	2.02	115.48	107.61

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

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	415/439 (94%)	-0.24	8 (1%) 64 72	26, 50, 92, 133	0
1	B	428/439 (97%)	-0.48	4 (0%) 81 88	20, 39, 70, 102	0
All	All	843/878 (96%)	-0.36	12 (1%) 72 80	20, 44, 82, 133	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	PRO	4.3
1	A	363	ILE	3.6
1	B	30	PRO	3.5
1	A	425	LEU	3.2
1	A	427	VAL	2.8
1	B	405	ALA	2.6
1	A	426	LEU	2.5
1	A	188	LYS	2.5
1	A	369	LEU	2.4
1	B	29	GLY	2.4
1	B	28	ARG	2.1
1	A	178	TRP	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	OX1	A	501	37/37	0.15	-0.36	33,36,45,48	0
2	OX1	B	501	37/37	0.13	-0.59	30,41,48,49	0

6.5 Other polymers

There are no such residues in this entry.