

Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 10:22 PM EST

PDB ID : 2PXH

Title : Crystal structure of a bipyridylalanyl-tRNA synthetase

Authors : Liu, W.; Xie, J.; Schultz, P.G.

Deposited on : 2007-05-14

Resolution : 1.97 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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) 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 : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

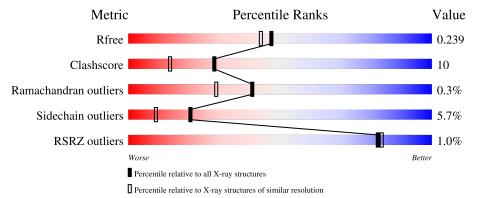
 $Validation\ Pipeline\ (wwPDB-VP) \quad : \quad 2.36$

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.97 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 <=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	Λ	914	81%	14%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2748 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 Tyrosyl-tRNA synthetase.

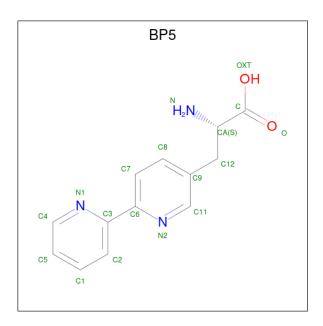
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	306	Total 2452	C 1570	N 412	O 458	S 12	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLY	TYR	engineered mutation	UNP Q57834
A	65	TYR	LEU	engineered mutation	UNP Q57834
A	70	ALA	HIS	engineered mutation	UNP Q57834
A	155	GLU	GLN	engineered mutation	UNP Q57834
A	158	GLY	ASP	engineered mutation	UNP Q57834
A	159	TRP	ILE	engineered mutation	UNP Q57834
A	162	SER	LEU	engineered mutation	UNP Q57834
A	307	LEU	-	expression tag	UNP Q57834
A	308	GLU	-	expression tag	UNP Q57834
A	309	HIS	-	expression tag	UNP Q57834
A	310	HIS	-	expression tag	UNP Q57834
A	311	HIS	-	expression tag	UNP Q57834
A	312	HIS	-	expression tag	UNP Q57834
A	313	HIS	-	expression tag	UNP Q57834
A	314	HIS	-	expression tag	UNP Q57834

• Molecule 2 is 3-(2,2'-BIPYRIDIN-5-YL)-L-ALANINE (three-letter code: BP5) (formula: $C_{13}H_{13}N_3O_2$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	Λ	1	Total	С	N	О	0	0
2	Λ	1	18	13	3	2	0	U

• Molecule 3 is water.

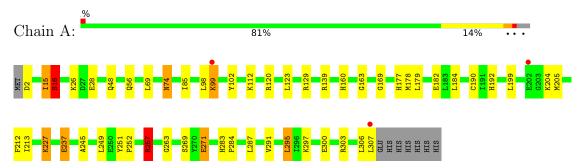
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	278	Total O 278 278	0	0



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: Tyrosyl-tRNA synthetase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	100.84Å 100.84Å 71.07Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.25 - 1.97	Depositor
rtesolution (A)	41.12 - 1.90	EDS
% Data completeness	99.7 (71.25-1.97)	Depositor
(in resolution range)	99.6 (41.12-1.90)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	1.67 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D.	0.191 , 0.242	Depositor
R, R_{free}	0.190 , 0.239	DCC
R_{free} test set	1493 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37, 49.5	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2748	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



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: BP5

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		
IVIOI	Chain	$\mathbf{AIN} \mid \mathbf{RMSZ} \mid \# Z > 5$		RMSZ	# Z > 5	
1	A	0.78	0/2494	0.82	3/3349 (0.1%)	

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	257	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	16	SER	N-CA-C	6.41	128.31	111.00
1	A	15	ILE	C-N-CA	5.36	135.09	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ILE	Peptide

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	2452	0	2516	49	0
2	A	18	0	7	0	0
3	A	278	0	0	23	0
All	All	2748	0	2523	49	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 10.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A	A	Interatomic	Clash	
Atom-1	Atom-2	${\rm distance}\ ({\rm \AA})$	overlap (Å)	
1:A:306:LEU:O	1:A:307:LEU:HG	1.26	1.26	
1:A:306:LEU:O	1:A:307:LEU:CG	2.13	0.96	
1:A:48:GLN:CD	3:A:561:HOH:O	2.09	0.91	
1:A:257:ARG:HD3	1:A:263:GLY:O	1.85	0.76	
1:A:56:GLN:NE2	1:A:99:LYS:O	2.19	0.76	
1:A:120:ARG:NH2	3:A:404:HOH:O	2.19	0.75	
1:A:26:LYS:NZ	1:A:28:GLU:O	2.20	0.74	
1:A:257:ARG:CD	1:A:263:GLY:O	2.36	0.73	
1:A:307:LEU:HD11	3:A:515:HOH:O	1.93	0.69	
1:A:120:ARG:NH2	3:A:315:HOH:O	2.27	0.68	
1:A:237:GLU:H	1:A:237:GLU:CD	1.97	0.66	
1:A:74:ASN:HD21	1:A:139:ARG:H	1.41	0.66	
1:A:98:LEU:O	3:A:545:HOH:O	2.14	0.65	
1:A:48:GLN:NE2	3:A:448:HOH:O	2.29	0.64	
1:A:129:ARG:HH12	1:A:182:GLU:CD	2.01	0.64	
1:A:227:LYS:HE3	3:A:475:HOH:O	1.98	0.63	
1:A:245:ALA:HA	1:A:249:LEU:HD22	1.82	0.62	
1:A:2:ASP:N	3:A:506:HOH:O	2.35	0.59	
1:A:48:GLN:OE1	3:A:561:HOH:O	2.17	0.58	
1:A:257:ARG:HD2	1:A:263:GLY:O	2.05	0.56	
1:A:163:GLY:HA2	3:A:491:HOH:O	2.04	0.56	
1:A:129:ARG:NH2	1:A:182:GLU:OE2	2.36	0.55	
1:A:297:LYS:HE3	3:A:425:HOH:O	2.05	0.54	
1:A:129:ARG:NH1	1:A:182:GLU:OE2	2.38	0.54	
1:A:120:ARG:HD2	3:A:508:HOH:O	2.10	0.52	
1:A:48:GLN:HG3	3:A:561:HOH:O	2.10	0.52	
1:A:48:GLN:CG	3:A:561:HOH:O	2.53	0.51	
1:A:102:TYR:HE1	3:A:545:HOH:O	1.95	0.49	
1:A:205:MET:HE1	3:A:435:HOH:O	2.13	0.48	

Continued on next page...



Continued from previous page...

A + 1	A4 0	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ (\mathring{\rm A})$	overlap (Å)
1:A:120:ARG:CZ	3:A:315:HOH:O	2.59	0.48
1:A:205:MET:HG3	1:A:212:PHE:HB3	1.95	0.48
1:A:177:HIS:HB3	1:A:190:CYS:SG	2.55	0.47
1:A:251:TYR:HA	1:A:252:PRO:C	2.35	0.47
1:A:99:LYS:HA	3:A:545:HOH:O	2.14	0.47
1:A:269:SER:OG	1:A:271:GLU:HG2	2.15	0.46
1:A:120:ARG:NE	3:A:315:HOH:O	2.48	0.46
1:A:199:LEU:HD11	1:A:213:ILE:HG13	1.99	0.45
1:A:306:LEU:C	1:A:307:LEU:HG	2.22	0.45
1:A:160:HIS:HB2	1:A:184:LEU:HD22	1.98	0.45
1:A:205:MET:CE	3:A:435:HOH:O	2.65	0.45
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.52	0.45
1:A:303:ARG:HD3	3:A:401:HOH:O	2.16	0.44
1:A:74:ASN:ND2	1:A:139:ARG:H	2.14	0.44
1:A:99:LYS:HB2	3:A:535:HOH:O	2.17	0.44
1:A:85:ILE:HD12	3:A:526:HOH:O	2.18	0.44
1:A:129:ARG:HG2	1:A:179:LEU:HD21	2.00	0.43
1:A:291:VAL:O	1:A:295:LEU:HB2	2.20	0.42
1:A:271:GLU:CD	1:A:271:GLU:H	2.25	0.40
1:A:169:GLY:O	1:A:192:HIS:HA	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	304/314 (97%)	301 (99%)	2 (1%)	1 (0%)	41 29	

All (1) Ramachandran outliers are listed below:

\mathbf{Mol}	Chain	Res	Type
1	A	16	SER



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	Analysed Rotameric		Percentiles	
1	A	265/273 (97%)	250 (94%)	15 (6%)	20 9	

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	69	LEU
1	A	74	ASN
1	A	99	LYS
1	A	112	LYS
1	A	123	LEU
1	A	178	MET
1	A	204	LYS
1	A	227	LYS
1	A	237	GLU
1	A	257	ARG
1	A	271	GLU
1	A	287	LEU
1	A	295	LEU
1	A	300	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	75	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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).

Mal	Type	Chain	Pos	Link	Bond lengths		В	ond ang	eles	
IVIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BP5	A	308	-	18,19,19	1.56	2 (11%)	24,25,25	1.52	5 (20%)

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	BP5	A	308	-	-	6/12/12/12	0/2/2/2

All (2) bond length outliers are listed below:

Mo	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
2	A	308	BP5	C3-C6	-4.70	1.38	1.49
2	A	308	BP5	C12-C9	2.87	1.58	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	308	BP5	C4-N1-C3	2.97	121.39	117.23
2	A	308	BP5	C7-C8-C9	-2.61	117.43	121.03

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	308	BP5	C12-C9-C11	-2.51	117.33	121.64
2	A	308	BP5	C2-C3-N1	-2.24	118.92	122.26
2	A	308	BP5	C2-C3-C6	2.06	124.89	121.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	308	BP5	CA-C12-C9-C11
2	A	308	BP5	CA-C12-C9-C8
2	A	308	BP5	N1-C3-C6-C7
2	A	308	BP5	C2-C3-C6-C7
2	A	308	BP5	N1-C3-C6-N2
2	A	308	BP5	C2-C3-C6-N2

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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>	$\# \mathrm{RSRZ}{>}2$		$OWAB(Å^2)$	Q<0.9	
1	A	306/314 (97%)	-0.07	3 (0%)	82	83	18, 28, 43, 51	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	LEU	3.7
1	A	99	LYS	2.7
1	A	202	GLU	2.3

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 monosaccharides 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, 95^{th} 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.

\mathbb{N}	Iol	\mathbf{Type}	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
	2	BP5	A	308	18/18	0.97	0.11	16,20,23,25	0



6.5 Other polymers (i)

There are no such residues in this entry.

