

# wwPDB X-ray Structure Validation Summary Report (i)

#### Sep 24, 2023 – 02:39 AM EDT

PDB ID : 5KR4

Title : Directed Evolution of Transaminases By Ancestral Reconstruction. Using Old

Proteins for New Chemistries

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Deposited on : 2016-07-06

Resolution : 2.00 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 (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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35.1

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)

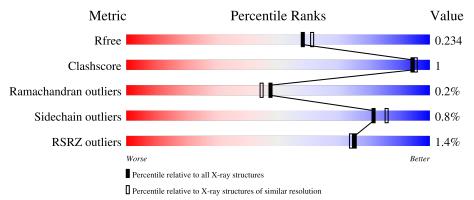
Validation Pipeline (wwPDB-VP) : 2.35.1

## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	Similar resolution
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	A	479	92%	• 5%
1	В	479	90%	5% 5%



## 2 Entry composition (i)

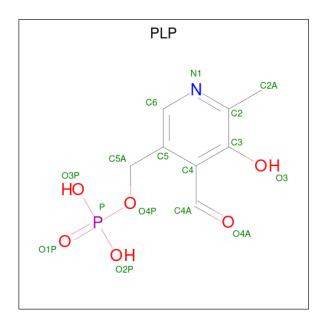
There are 4 unique types of molecules in this entry. The entry contains 7504 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-aminobutyrate transaminase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	457	Total 3504	C 2227	N 608	O 653	S 16	0	2	0
1	В	457	Total 3511	C 2230	N 609	O 657	S 15	0	3	0

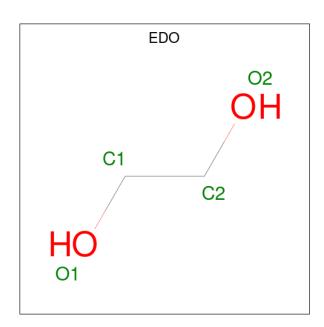
• Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
2	Λ	1	Total	С	N	О	Р	0	0	
	A	1	15	8	1	5	1	0	. 0	
9	D	1	Total	С	N	О	Р	0	0	
2	Б	1	15	8	1	5	1	0	U	

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

### • Molecule 4 is water.

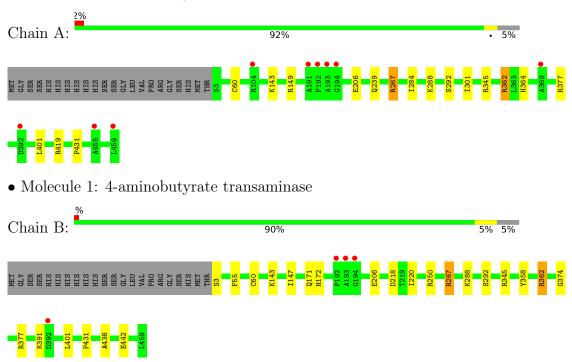
$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	215	Total O 215 215	0	0
4	В	232	Total O 232 232	0	0



# 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: 4-aminobutyrate transaminase





# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	67.05Å 121.78Å 125.63Å	Donogitor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	45.80 - 2.00	Depositor	
rtesolution (A)	45.84 - 2.00	EDS	
% Data completeness	99.2 (45.80-2.00)	Depositor	
(in resolution range)	99.2 (45.84-2.00)	EDS	
$R_{merge}$	0.16	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.93 (at 2.00Å)	Xtriage	
Refinement program	REFMAC 5.8.0155	Depositor	
Ρ. Р.	0.192 , 0.224	Depositor	
$R, R_{free}$	0.201 , $0.234$	DCC	
$R_{free}$ test set	3542 reflections (5.07%)	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage	
Anisotropy	0.131	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.37, 42.2	EDS	
L-test for twinning <sup>2</sup>	$< L >=0.45, < L^2>=0.28$	Xtriage	
Estimated twinning fraction	0.032 for -h,l,k	Xtriage	
$F_o, F_c$ correlation	0.93	EDS	
Total number of atoms	7504	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: PLP, EDO

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	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.65	0/3589	0.79	8/4870 (0.2%)	
1	В	0.67	0/3596	0.81	9/4881~(0.2%)	
All	All	0.66	0/7185	0.80	$17/9751 \ (0.2\%)$	

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	267	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	A	267	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	267	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	В	345	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	В	267	ARG	NE-CZ-NH1	7.49	124.05	120.30

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	3504	0	3439	10	2
1	В	3511	0	3440	7	2
2	A	15	0	6	1	0
2	В	15	0	7	0	0

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	Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
	3	A	12	0	18	1	0
ſ	4	A	215	0	0	7	0
	4	В	232	0	0	0	0
	All	All	7504	0	6910	18	2

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 1.

The worst 5 of 18 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
2:A:501:PLP:O1P	4:A:601:HOH:O	2.07	0.71
1:B:374:GLY:HA2	1:B:391:LYS:HD3	1.79	0.63
1:A:267:ARG:NH2	1:A:431:PRO:O	2.43	0.51
1:B:267:ARG:NH2	1:B:431:PRO:O	2.45	0.49
1:A:362:ARG:HD2	4:A:780:HOH:O	2.13	0.48

All (2) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:239:GLN:OE1	1:B:442[A]:GLU:OE1[3_654]	1.77	0.43
1:A:239:GLN:NE2	1:B:442[A]:GLU:OE2[3_654]	2.09	0.11

## 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	457/479 (95%)	438 (96%)	18 (4%)	1 (0%)	47	44
1	В	458/479 (96%)	438 (96%)	19 (4%)	1 (0%)	47	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	915/958 (96%)	876 (96%)	37 (4%)	2 (0%)	47 44	

#### All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	LYS
1	В	288	LYS

#### 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	356/373~(95%)	355 (100%)	1 (0%)	92 95
1	В	357/373~(96%)	351 (98%)	6 (2%)	60 65
All	All	713/746 (96%)	706 (99%)	7 (1%)	81 81

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	206	GLU
1	В	218[A]	ASP
1	В	401	LEU
1	В	218[B]	ASP
1	В	55	PHE

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	171	GLN
1	В	171	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)

5 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	Iol Type Chain Res		Res	Link	Вс	Bond lengths			Bond angles		
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
3	EDO	A	502	-	3,3,3	0.58	0	2,2,2	0.73	0	
3	EDO	A	504	-	3,3,3	0.53	0	2,2,2	0.55	0	
2	PLP	В	500	-	15,15,16	3.13	5 (33%)	20,22,23	2.61	6 (30%)	
3	EDO	A	503	-	3,3,3	0.54	0	2,2,2	0.56	0	
2	PLP	A	501	-	15,15,16	2.56	5 (33%)	20,22,23	2.38	8 (40%)	

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	EDO	A	502	-	-	1/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
2	PLP	В	500	-	-	2/6/6/8	0/1/1/1
3	EDO	A	503	-	-	1/1/1/1	-
2	PLP	A	501	-	-	1/6/6/8	0/1/1/1



The worst	5	of	10	bond	length	outliers	are	listed	below:
TIIC WOLDS	$\mathbf{O}$	$\circ$	10	Olla	10115011	Outilitie	COL C	IIDUCA	OCIOW.

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
2	В	500	PLP	C3-C2	9.50	1.50	1.40
2	A	501	PLP	C3-C2	7.19	1.48	1.40
2	В	500	PLP	C5-C4	4.92	1.45	1.40
2	A	501	PLP	C5-C4	3.95	1.44	1.40
2	В	500	PLP	P-O2P	-3.16	1.42	1.54

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	500	PLP	O2P-P-O4P	7.07	125.55	106.73
2	В	500	PLP	O4P-P-O1P	-5.52	90.99	106.47
2	A	501	PLP	O4P-P-O1P	-5.38	91.39	106.47
2	A	501	PLP	O2P-P-O4P	4.97	119.97	106.73
2	A	501	PLP	O3-C3-C2	4.40	127.09	117.49

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	500	PLP	C5A-O4P-P-O3P
3	A	503	EDO	O1-C1-C2-O2
3	A	504	EDO	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2
2	A	501	PLP	C5A-O4P-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	EDO	1	0
2	A	501	PLP	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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	457/479 (95%)	0.01	9 (1%) 65 63	12, 20, 38, 56	0
1	В	457/479 (95%)	-0.08	4 (0%) 84 83	12, 18, 34, 50	0
All	All	914/958 (95%)	-0.04	13 (1%) 75 74	12, 19, 36, 56	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	194	GLY	4.3
1	A	193	ALA	3.9
1	В	193	ALA	3.3
1	A	459	LEU	3.2
1	A	392	ASP	3.2

## 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 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.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	EDO	A	504	4/4	0.77	0.18	32,35,36,36	0
2	PLP	A	501	15/16	0.83	0.47	8,11,11,12	15
3	EDO	A	502	4/4	0.85	0.14	25,26,26,29	0
2	PLP	В	500	15/16	0.85	0.39	8,11,12,13	15
3	EDO	A	503	4/4	0.92	0.28	33,33,33,35	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

