

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

Aug 7, 2023 – 06:01 pm BST

PDB ID	:	7QYG
Title	:	Structure of the transaminase TR2
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		Alfonso, J.; Plou, F.J.; Jaeger, K.E.; Smits, S.H.; Ferrer, M.; Guallar, V.
Deposited on	:	2022-01-28
Resolution	:	3.60  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:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.34
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)	:	2.34

# 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 3.60 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	А	465	33%	46%	•	16%
1	В	465	6%	40%	6%	16%
1	С	465	34%	44%	6%	16%
1	D	465	38%	41%	5%	16%



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# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 24079 atoms, of which 12003 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.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	Δ	380	Total	С	Η	Ν	0	$\mathbf{S}$	0	0 0	0
1	Л	309	6017	1917	3000	525	558	17	0		0
1	В	380	Total	С	Η	Ν	0	S	0	0	0
1	I D	369	6005	1914	2992	524	558	17	0	0	0
1	C	201	Total	С	Η	Ν	0	S	0	0	0
	- 591	6052	1926	3019	530	560	17	0	0		
1 D	280	Total	С	Н	Ν	0	S	0	0	0	
	389	6005	1914	2992	524	558	17		U	0	

• Molecule 1 is a protein called Aminotransferase TR2.

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	458	LEU	-	expression tag	UNP A0A3G5BC54
А	459	GLU	-	expression tag	UNP A0A3G5BC54
А	460	HIS	-	expression tag	UNP A0A3G5BC54
А	461	HIS	-	expression tag	UNP A0A3G5BC54
А	462	HIS	-	expression tag	UNP A0A3G5BC54
А	463	HIS	-	expression tag	UNP A0A3G5BC54
А	464	HIS	-	expression tag	UNP A0A3G5BC54
А	465	HIS	-	expression tag	UNP A0A3G5BC54
В	458	LEU	-	expression tag	UNP A0A3G5BC54
В	459	GLU	-	expression tag	UNP A0A3G5BC54
В	460	HIS	-	expression tag	UNP A0A3G5BC54
В	461	HIS	-	expression tag	UNP A0A3G5BC54
В	462	HIS	-	expression tag	UNP A0A3G5BC54
В	463	HIS	-	expression tag	UNP A0A3G5BC54
В	464	HIS	-	expression tag	UNP A0A3G5BC54
В	465	HIS	-	expression tag	UNP A0A3G5BC54
С	458	LEU	-	expression tag	UNP A0A3G5BC54
С	459	GLU	-	expression tag	UNP A0A3G5BC54
С	460	HIS	-	expression tag	UNP A0A3G5BC54
С	461	HIS	-	expression tag	UNP A0A3G5BC54
С	462	HIS	-	expression tag	UNP A0A3G5BC54

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Chain	Residue	Modelled	Actual	Comment	Reference
С	463	HIS	-	expression tag	UNP A0A3G5BC54
С	464	HIS	-	expression tag	UNP A0A3G5BC54
С	465	HIS	-	expression tag	UNP A0A3G5BC54
D	458	LEU	-	expression tag	UNP A0A3G5BC54
D	459	GLU	-	expression tag	UNP A0A3G5BC54
D	460	HIS	-	expression tag	UNP A0A3G5BC54
D	461	HIS	-	expression tag	UNP A0A3G5BC54
D	462	HIS	-	expression tag	UNP A0A3G5BC54
D	463	HIS	-	expression tag	UNP A0A3G5BC54
D	464	HIS	-	expression tag	UNP A0A3G5BC54
D	465	HIS	-	expression tag	UNP A0A3G5BC54

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# 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: Aminotransferase TR2















# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	60.78Å 166.63Å 209.82Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	49.09 - 3.60	Depositor
Resolution (A)	49.09 - 3.60	EDS
% Data completeness	94.2 (49.09-3.60)	Depositor
(in resolution range)	94.2 (49.09-3.60)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.15 (at 3.57 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17	Depositor
B B.	0.345 , $0.422$	Depositor
II, II, <i>free</i>	0.345 , $0.422$	DCC
$R_{free}$ test set	1994 reflections $(8.28\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	113.7	Xtriage
Anisotropy	0.935	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , $67.8$	EDS
L-test for $twinning^2$	$ < L >=0.41, < L^2>=0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	24079	wwPDB-VP
Average B, all atoms $(Å^2)$	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.

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



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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).

Mal	Chain	Bo	nd lengths	Bond angles		
10101	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.36	0/3086	0.57	0/4176	
1	В	0.37	0/3082	0.59	0/4172	
1	С	0.41	1/3102~(0.0%)	0.61	1/4197~(0.0%)	
1	D	0.45	5/3082~(0.2%)	0.60	2/4172~(0.0%)	
All	All	0.40	6/12352~(0.0%)	0.59	3/16717~(0.0%)	

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

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	384	GLU	CD-OE1	-7.81	1.17	1.25
1	D	384	GLU	CG-CD	-6.36	1.42	1.51
1	D	261	GLU	CB-CG	-6.03	1.40	1.52
1	D	261	GLU	CD-OE1	-5.65	1.19	1.25
1	D	261	GLU	CG-CD	5.24	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	285	MET	CG-SD-CE	7.90	112.84	100.20
1	D	384	GLU	OE1-CD-OE2	-5.87	116.25	123.30
1	С	439	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	143	TYR	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	А	3017	3000	3000	209	0
1	В	3013	2992	2992	198	0
1	С	3033	3019	3018	228	0
1	D	3013	2992	2992	210	0
All	All	12076	12003	12002	826	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 34.

The worst 5 of 826 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:B:128:ILE:HD13	1:B:258:ILE:CD1	1.66	1.25
1:B:128:ILE:HD13	1:B:258:ILE:HD11	1.15	1.09
1:D:347:ILE:HD11	1:D:348:GLU:OE2	1.51	1.09
1:D:347:ILE:CD1	1:D:348:GLU:OE2	2.03	1.06
1:B:128:ILE:CD1	1:B:258:ILE:CD1	2.35	1.05

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	Ρ	$\mathbf{erc}$	entiles
1	А	387/465~(83%)	287 (74%)	75 (19%)	25~(6%)		1	16
1	В	387/465~(83%)	285 (74%)	71 (18%)	31 (8%)		1	11
1	С	389/465~(84%)	272 (70%)	87 (22%)	30 (8%)		1	12
1	D	387/465~(83%)	287 (74%)	78 (20%)	22 (6%)		1	18
All	All	1550/1860 (83%)	1131 (73%)	311 (20%)	108 (7%)		1	14

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	313	GLU
1	В	101	SER
1	В	236	ILE
1	В	243	TRP
1	В	266	PHE

#### 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	Perce	ntiles
1	А	315/377~(84%)	308~(98%)	7 (2%)	52	77
1	В	314/377~(83%)	305~(97%)	9~(3%)	42	72
1	С	316/377~(84%)	307~(97%)	9(3%)	43	72
1	D	314/377~(83%)	310 (99%)	4 (1%)	69	86
All	All	1259/1508~(84%)	1230 (98%)	29 (2%)	50	76

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	В	240	ASP
1	D	304	SER
1	С	126	ASP
1	С	442	LYS
1	С	99	GLU



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	С	113	ASN
1	С	220	ASN
1	D	368	HIS
1	D	155	HIS
1	D	276	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)

There are no ligands in this entry.

#### 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>2	$OWAB(Å^2)$	Q<0.9
1	А	389/465~(83%)	0.42	39 (10%) 7 4	77, 125, 171, 205	0
1	В	389/465~(83%)	0.22	30 (7%) 13 8	79, 120, 161, 198	0
1	С	391/465~(84%)	0.61	56 (14%) 2 2	78, 138, 172, 206	0
1	D	389/465~(83%)	0.66	54 (13%) 2 2	82, 134, 183, 208	0
All	All	1558/1860~(83%)	0.48	179 (11%) 4 3	77, 128, 174, 208	0

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	163	SER	14.9
1	С	411	LYS	12.4
1	D	175	ASP	9.8
1	D	163	SER	9.2
1	С	233	GLY	9.0

### 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)

There are no ligands in this entry.



## 6.5 Other polymers (i)

There are no such residues in this entry.

