



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:11 PM UTC

PDB ID : 4W1Y / pdb_00004w1y
Title : Crystal structure of Escherichia coli Tryptophanase in 'semi-holo' form
Authors : Goldgur, Y.
Deposited on : 2014-08-13
Resolution : 3.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

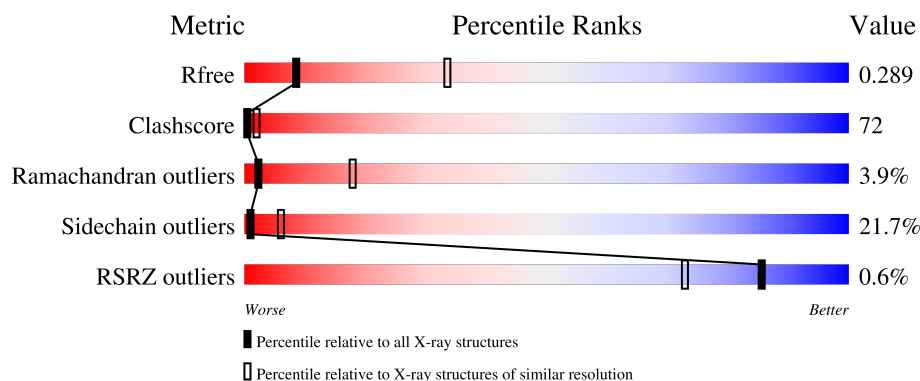
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

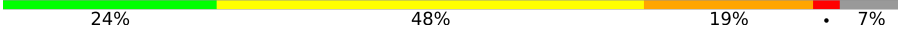
The reported resolution of this entry is 3.20 Å.

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	467	
2	B	467	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6957 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 Tryptophanase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	P	S	0	0	0
			3428	2181	575	650	1	21			

- Molecule 2 is a protein called Tryptophanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	433	Total	C	N	O	S	0	0	0
			3412	2175	575	641	21			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total 42	O 42	0	0
4	B	65	Total 65	O 65	0	0

T455	E395	A319	Y258	S197	Y134
Y456	I396	V320	K259	M198	PHE
E457	G397	Y323	Y260	S199	PHE
P458	S398		A261	A200	ASP
K459	PHE		D262	G201	THR
V460	LEU	M326	M263	G202	THR
L461	LEU	M327	L264	Q203	GLN
R462	GLY	L328	A265	P204	GLY
H463	ARG	D329	M266	V205	HIS
F464	ASP	W330	S267	S206	SER
T465	PRO	L331	A268	L207	GLN
A466	LYS	A332	K269	A208	ILE
K467	THR	Y333	K270	N209	ASN
L468	GLY	R334	D271	L210	GLY
K469	LYS	I335	A272	K211	
E470	GLN	A336	M273	A212	
V471	LEU	Q337	V274	M213	
	PRO	V338	P275	M214	
	C413	Q339	M276	I216	V153
	P414	Y340	G277	I216	Y154
	A415	L341	G278	A217	I155
	E416		L279	K218	K156
	L417	Q353	L280	K219	E157
	L418	Q354	C281	Y220	F159
	B419	A355	M282	D221	D160
	L420	G356	K283	I222	T161
	T421	G357	D284	P223	G162
	I422	H358	D285	V224	V163
	P423	A359	S286	V225	R164
	R424	A360	F287	M226	Y165
	A425	F361	F288	D227	D166
	T426	V362	D289	S228	F167
	Y427	D363	V290	A229	K168
	T428	A364	Y291	R230	G169
	Q429		T292	F231	N170
	T430	L367	E293	A232	F171
	H431	L368	C294	E233	D172
	M432		R295	M234	L173
	D433	I371	T296	A235	E174
	F434	P372	L297	Y236	G175
	I435		C298		L176
	I436	Q375	V299	K239	E177
	B437	F376	V300	Q240	R178
	M438	P377	Q301	R241	G179
	F439	A378	E302	E242	I180
	K440	Q379	GLY	A243	E181
	H441	A380	PHE	E244	E182
	V442	L381	PRO	Y245	V183
	K443	A382	THR	K246	G184
	E444	C383	TYR	D247	
	M445	E384	GLY	W248	M187
	A446	L385	G309	T249	V188
	A447	Y386	L310	I250	P189
	N448	K387	E311	E251	Y190
	I449	V388		Q252	I191
	K450	A389	A314	I253	V192
	G451		M315	T254	A193
	L452	R392	E316	R255	T194
	T453	A393	R317	E256	I195
	F454	V394	L318	T257	T196

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.97Å 109.97Å 238.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (15.00-3.20) 94.0 (15.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.214 , 0.290 0.212 , 0.289	Depositor DCC
R_{free} test set	1207 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	86.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6957	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, LLP

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	1.27	16/3473 (0.5%)	1.53	57/4692 (1.2%)
2	B	1.35	13/3478 (0.4%)	1.62	66/4694 (1.4%)
All	All	1.31	29/6951 (0.4%)	1.58	123/9386 (1.3%)

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	A	0	1
2	B	0	2
All	All	0	3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	422	ILE	CA-CB	-12.26	1.43	1.54
1	A	396	ILE	CA-CB	7.06	1.64	1.54
1	A	417	LEU	CA-C	6.52	1.61	1.52
2	B	423	PRO	N-CA	-6.37	1.39	1.47
2	B	108	ILE	CA-C	6.18	1.60	1.52

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	183	VAL	N-CA-C	12.73	122.21	111.90
1	A	22	THR	N-CA-C	10.26	125.10	108.99
2	B	108	ILE	N-CA-C	10.25	121.07	110.72
2	B	74	TYR	N-CA-C	-10.02	100.37	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	17	GLU	CA-C-N	9.85	129.95	119.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	453	THR	Peptide
2	B	162	GLY	Peptide
2	B	309	GLY	Peptide

5.2 Too-close contacts

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	3428	0	3371	446	0
2	B	3412	0	3395	546	1
3	B	10	0	0	1	0
4	A	42	0	0	29	0
4	B	65	0	0	41	0
All	All	6957	0	6766	975	1

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 72.

The worst 5 of 975 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)
2:B:22:THR:CG2	2:B:27:ARG:HH11	1.02	1.58
2:B:22:THR:CG2	2:B:27:ARG:HG3	1.39	1.52
2:B:450:LYS:HB2	2:B:470:GLU:CD	1.31	1.51
2:B:375:GLN:HE21	2:B:471:VAL:CG1	1.26	1.46
1:A:170:ASN:CB	1:A:209:ASN:ND2	1.79	1.45

All (1) 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)
2:B:103:ARG:NH1	2:B:301:GLN:O[8_665]	2.16	0.04

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	430/467 (92%)	331 (77%)	81 (19%)	18 (4%)	2	16
2	B	425/467 (91%)	327 (77%)	83 (20%)	15 (4%)	3	20
All	All	855/934 (92%)	658 (77%)	164 (19%)	33 (4%)	2	18

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	LEU
2	B	246	LYS
1	A	157	GLU
1	A	238	ILE
2	B	243	ALA

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	356/385 (92%)	275 (77%)	81 (23%)	1	5
2	B	358/386 (93%)	284 (79%)	74 (21%)	1	7
All	All	714/771 (93%)	559 (78%)	155 (22%)	1	6

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	209	ASN
2	B	371	ILE
2	B	220	TYR
2	B	269	LYS
2	B	441	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	64	GLN
2	B	133	ASN
2	B	101	GLN
2	B	152	ASN
1	A	198	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	LLP	A	270	1	23,24,25	2.18	6 (26%)	25,32,34	2.52	7 (28%)

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
1	LLP	A	270	1	-	4/16/17/19	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	LLP	O3-C3	-6.65	1.21	1.36
1	A	270	LLP	C4-C4'	3.31	1.53	1.46
1	A	270	LLP	C2-N1	3.17	1.39	1.33
1	A	270	LLP	C6-N1	2.91	1.40	1.34
1	A	270	LLP	C4'-NZ	2.67	1.36	1.27

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	LLP	OP4-C5'-C5	7.27	122.98	109.36
1	A	270	LLP	C4-C3-C2	7.13	124.16	120.14
1	A	270	LLP	CE-NZ-C4'	-3.47	107.62	118.72
1	A	270	LLP	OP3-P-OP1	3.04	122.68	110.83
1	A	270	LLP	C3-C2-N1	-2.65	117.62	120.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	270	LLP	C4-C5-C5'-OP4
1	A	270	LLP	C6-C5-C5'-OP4
1	A	270	LLP	C4-C4'-NZ-CE
1	A	270	LLP	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	270	LLP	5	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	$\# Z > 2$
3	SO4	B	500	-	4,4,4	0.24	0	6,6,6	0.58	0
3	SO4	B	501	-	4,4,4	0.28	0	6,6,6	0.22	0

There are no bond length outliers.

There are no bond angle outliers.

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	501	SO4	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, 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	434/467 (92%)	-0.55	1 (0%) 91 85	50, 82, 120, 126	0
2	B	433/467 (92%)	-0.39	4 (0%) 81 64	48, 82, 129, 170	0
All	All	867/934 (92%)	-0.47	5 (0%) 85 73	48, 82, 121, 170	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	302	GLU	3.3
1	A	377	PRO	2.4
2	B	468	LEU	2.2
2	B	471	VAL	2.1
2	B	395	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	A	270	24/25	0.96	0.08	63,73,78,80	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	501	5/5	0.85	0.13	184,184,184,185	0
3	SO4	B	500	5/5	0.93	0.11	110,110,111,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.