



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 09:41 PM UTC

PDB ID : 2WEU / pdb_00002weu
Title : Crystal structure of tryptophan 5-halogenase (PyrH) complex with substrate tryptophan
Authors : Leang, K.; Zhu, X.; Naismith, J.H.
Deposited on : 2009-04-01
Resolution : 1.70 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 ⓘ 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	:	FAILED
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

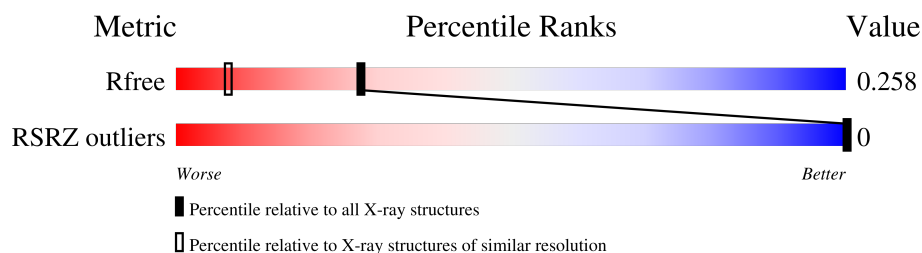
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

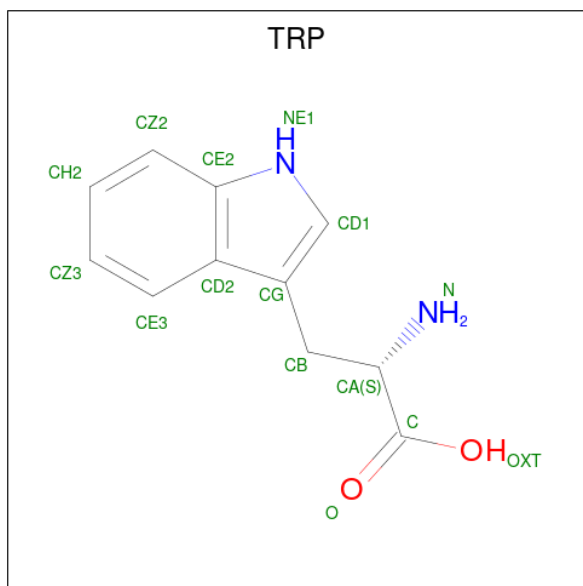
There are 3 unique types of molecules in this entry. The entry contains 17519 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRYPTOPHAN 5-HALOGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	2	0
			3987	2537	697	733	20			
1	B	499	Total	C	N	O	S	0	0	0
			4012	2549	706	738	19			
1	C	499	Total	C	N	O	S	0	1	0
			4013	2549	705	740	19			
1	D	498	Total	C	N	O	S	0	0	0
			3995	2540	699	737	19			

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	393	Total	O	0	0
			393	393		
3	B	368	Total	O	0	0
			368	368		
3	C	365	Total	O	0	0
			365	365		
3	D	326	Total	O	0	0
			326	326		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	142.70Å 141.08Å 122.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.50 – 1.70 100.33 – 1.70	Depositor EDS
% Data completeness (in resolution range)	88.5 (100.50-1.70) 88.5 (100.33-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.215 , 0.248 0.224 , 0.258	Depositor DCC
R_{free} test set	13712 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.240 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17519	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

4 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	TRP	A	1512	-	15,16,16	0.96	0	18,22,22	0.65	0
2	TRP	B	1512	-	15,16,16	0.82	0	18,22,22	0.68	0
2	TRP	C	1512	-	15,16,16	0.99	1 (6%)	18,22,22	0.69	0
2	TRP	D	1512	-	15,16,16	1.17	1 (6%)	18,22,22	0.81	0

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	TRP	A	1512	-	-	3/8/8/8	0/2/2/2
2	TRP	B	1512	-	-	2/8/8/8	0/2/2/2
2	TRP	C	1512	-	-	2/8/8/8	0/2/2/2
2	TRP	D	1512	-	-	2/8/8/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1512	TRP	OXT-C	-2.21	1.23	1.30
2	C	1512	TRP	OXT-C	-2.11	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1512	TRP	OXT-C-CA-CB
2	C	1512	TRP	OXT-C-CA-CB
2	B	1512	TRP	O-C-CA-CB
2	A	1512	TRP	O-C-CA-CB
2	A	1512	TRP	OXT-C-CA-CB
2	C	1512	TRP	O-C-CA-CB
2	D	1512	TRP	O-C-CA-CB
2	A	1512	TRP	CA-CB-CG-CD1
2	D	1512	TRP	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	494/511 (96%)	-1.17	0 100 100	9, 14, 23, 29	2 (0%)
1	B	499/511 (97%)	-1.13	0 100 100	6, 14, 24, 31	0
1	C	499/511 (97%)	-1.13	0 100 100	4, 14, 24, 30	1 (0%)
1	D	498/511 (97%)	-1.16	0 100 100	8, 14, 23, 30	0
All	All	1990/2044 (97%)	-1.14	0 100 100	4, 14, 23, 31	3 (0%)

There are no RSRZ outliers to report.

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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
2	TRP	A	1512	15/15	0.99	0.03	9,9,11,11	0
2	TRP	B	1512	15/15	0.99	0.03	9,10,11,12	0
2	TRP	C	1512	15/15	0.99	0.03	9,10,11,11	0
2	TRP	D	1512	15/15	1.00	0.02	9,10,11,12	0

5.5 Other polymers [i](#)

There are no such residues in this entry.