wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2026 – 09:06 am GMT

PDB ID	:	34LU / pdb_000034lu
Title	:	Trp-5-Hal - Consensus designed artificial tryptophan-5-halogenase
Authors	:	Richmond, D.T.; Crow, A.
Deposited on	:	2026-09-21
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 (i)) were used in the production of this report:

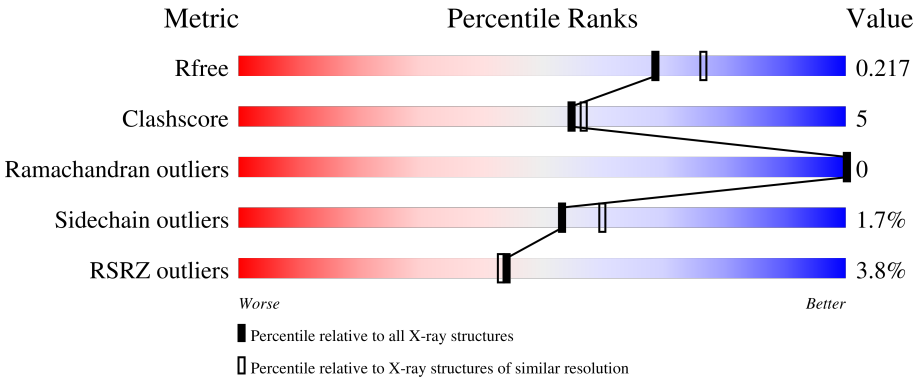
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	514	3% 89% 10%
1	B	514	4% 87% 11%
1	C	514	4% 89% 8%
1	D	514	4% 86% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17228 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 Tryp-5-FDH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			4064	2585	706	757	16			
1	B	511	Total	C	N	O	S	0	0	0
			4064	2585	706	757	16			
1	C	505	Total	C	N	O	S	0	0	0
			4023	2562	697	748	16			
1	D	498	Total	C	N	O	S	0	0	0
			3975	2533	690	736	16			

- Molecule 2 is water.

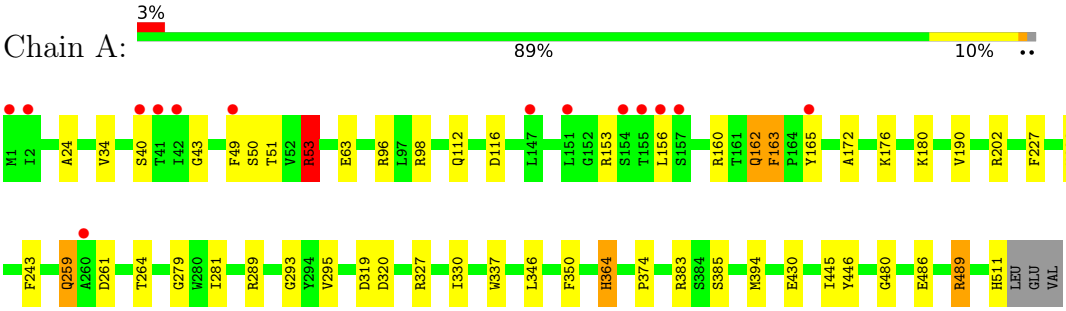
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	306	Total	O	0	0
			306	306		
2	B	282	Total	O	0	0
			282	282		
2	C	276	Total	O	0	0
			276	276		
2	D	238	Total	O	0	0
			238	238		

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.

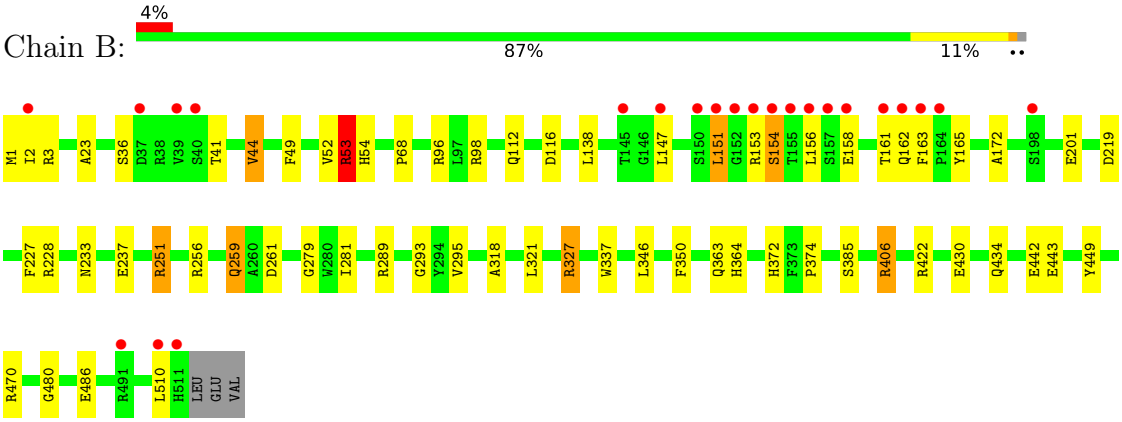
• Molecule 1: Tryp-5-FDH

Chain A:



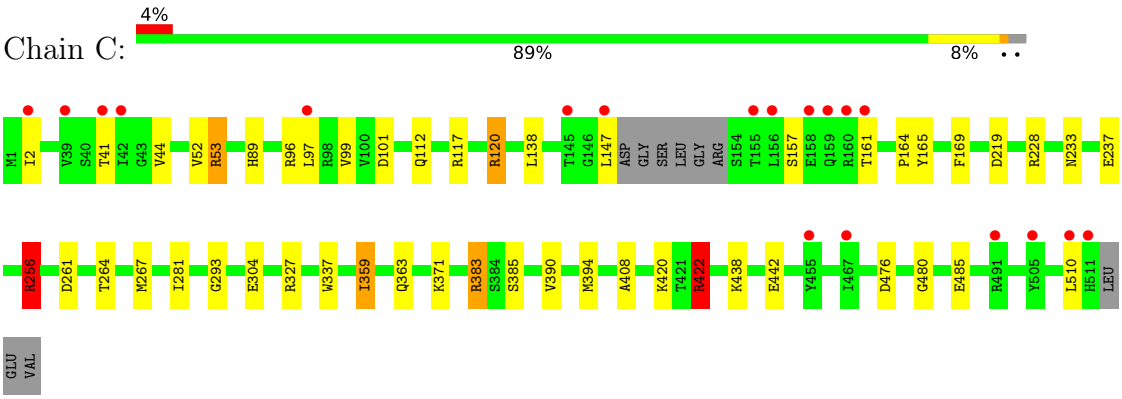
• Molecule 1: Tryp-5-FDH

Chain B:



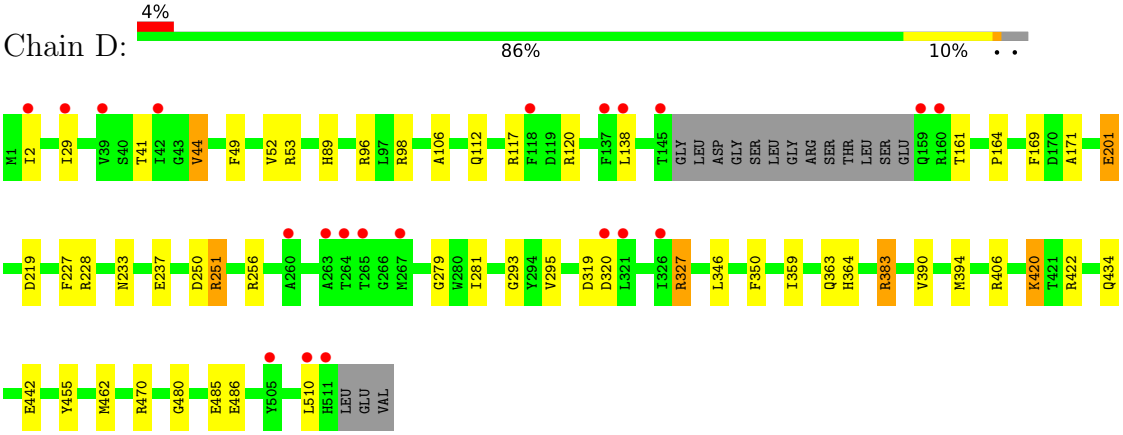
• Molecule 1: Tryp-5-FDH

Chain C:



• Molecule 1: Tryp-5-FDH

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.07Å 140.83Å 89.19Å 90.00° 110.14° 90.00°	Depositor
Resolution (Å)	71.98 – 2.00 71.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (71.98-2.00) 97.3 (71.98-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.174 , 0.212 0.182 , 0.217	Depositor DCC
R_{free} test set	6866 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 36.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17228	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

5 Model quality

5.1 Standard geometry

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	0.62	1/4173 (0.0%)	0.99	7/5665 (0.1%)
1	B	0.62	0/4173	1.00	8/5665 (0.1%)
1	C	0.59	0/4131	0.97	4/5608 (0.1%)
1	D	0.57	0/4083	0.98	11/5543 (0.2%)
All	All	0.60	1/16560 (0.0%)	0.99	30/22481 (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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	6
1	D	0	3
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	HIS	CG-CD2	-5.19	1.30	1.35

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	422	ARG	CD-NE-CZ	7.13	134.38	124.40
1	C	164	PRO	CB-CA-C	6.80	119.89	111.12
1	D	164	PRO	CB-CA-C	6.47	119.47	111.12
1	B	261	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	327	ARG	CG-CD-NE	-5.88	99.06	112.00

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	ARG	Sidechain
1	A	383	ARG	Sidechain
1	A	53	ARG	Sidechain
1	B	251	ARG	Sidechain
1	B	53	ARG	Sidechain

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	4064	0	3909	39	0
1	B	4064	0	3909	53	0
1	C	4023	0	3869	33	0
1	D	3975	0	3821	35	0
2	A	306	0	0	12	0
2	B	282	0	0	14	0
2	C	276	0	0	7	0
2	D	238	0	0	8	0
All	All	17228	0	15508	151	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 5.

The worst 5 of 151 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:D:44:VAL:HG22	2:D:607:HOH:O	1.59	1.02
1:B:23:ALA:O	1:B:153:ARG:NH1	1.97	0.98
1:D:406:ARG:HD2	2:D:604:HOH:O	1.67	0.95
1:C:97:LEU:HD13	2:C:800:HOH:O	1.76	0.85
1:A:53:ARG:HG2	1:A:53:ARG:HH21	1.44	0.82

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	509/514 (99%)	500 (98%)	9 (2%)	0	100	100
1	B	509/514 (99%)	497 (98%)	12 (2%)	0	100	100
1	C	501/514 (98%)	493 (98%)	8 (2%)	0	100	100
1	D	494/514 (96%)	483 (98%)	11 (2%)	0	100	100
All	All	2013/2056 (98%)	1973 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	423/426 (99%)	416 (98%)	7 (2%)	53	60
1	B	423/426 (99%)	415 (98%)	8 (2%)	50	56
1	C	419/426 (98%)	412 (98%)	7 (2%)	53	60
1	D	413/426 (97%)	406 (98%)	7 (2%)	53	60
All	All	1678/1704 (98%)	1649 (98%)	29 (2%)	53	60

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

Mol	Chain	Res	Type
1	B	430	GLU
1	D	420	LYS
1	C	147	LEU

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Mol	Chain	Res	Type
1	D	53	ARG
1	C	120	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	364	HIS
1	D	112	GLN
1	D	434	GLN
1	D	244	GLN
1	B	159	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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

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	A	511/514 (99%)	-0.01	14 (2%)	56	55	21, 33, 58, 93	0
1	B	511/514 (99%)	0.14	23 (4%)	38	37	21, 34, 67, 117	0
1	C	505/514 (98%)	0.15	19 (3%)	44	43	22, 36, 68, 122	0
1	D	498/514 (96%)	0.34	21 (4%)	40	39	24, 40, 68, 104	0
All	All	2025/2056 (98%)	0.16	77 (3%)	44	43	21, 36, 67, 122	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	PHE	6.8
1	B	151	LEU	6.6
1	C	147	LEU	5.0
1	C	156	LEU	4.8
1	B	154	SER	4.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.