



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2026 – 06:31 PM EDT

PDB ID : 5WIO / pdb_00005wio
Title : TraE protein in complex with 4-(1H-pyrrol-1-yl)pyridine-2-carboxylic acid
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Deposited on : 2017-07-19
Resolution : 2.52 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:

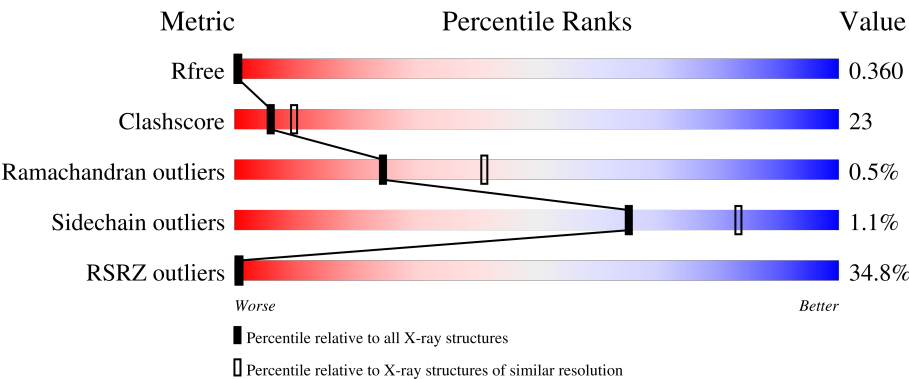
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	112.91Å 125.53Å 110.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.48 – 2.52 39.48 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.48-2.52) 99.6 (39.48-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.300 , 0.356 0.309 , 0.360	Depositor DCC
R_{free} test set	2000 reflections (6.04%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4472	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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.

3 Model quality [i](#)

3.1 Standard geometry [i](#)

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

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	0.39	0/1193	0.73	1/1618 (0.1%)
1	B	0.38	0/1181	0.83	5/1602 (0.3%)
1	C	0.40	0/1132	0.80	4/1539 (0.3%)
1	D	0.35	0/1032	0.87	4/1407 (0.3%)
All	All	0.38	0/4538	0.81	14/6166 (0.2%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	VAL	N-CA-C	9.32	122.15	113.20
1	D	206	LEU	N-CA-C	7.91	119.68	111.14
1	B	181	ARG	N-CA-C	7.87	122.16	110.52
1	D	116	TYR	N-CA-C	-7.52	103.08	111.28
1	C	228	ASN	CA-C-N	5.86	125.83	120.03

There are no chirality outliers.

There are no planarity outliers.

3.2 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	1167	0	1136	32	0
1	B	1155	0	1121	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1106	0	1045	63	0
1	D	1013	0	920	66	0
2	A	14	7	0	2	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
All	All	4465	7	4222	198	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 23.

The worst 5 of 198 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:C:113:TYR:OH	1:C:152:GLY:O	1.56	1.22
1:D:173:ALA:O	1:D:198:ILE:HG23	1.50	1.10
1:C:113:TYR:OH	1:C:152:GLY:HA2	1.61	0.99
1:C:113:TYR:OH	1:C:152:GLY:C	2.07	0.97
1:C:113:TYR:OH	1:C:152:GLY:CA	2.15	0.94

There are no symmetry-related clashes.

3.3 Torsion angles [i](#)

3.3.1 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	141/163 (86%)	137 (97%)	3 (2%)	1 (1%)	18	32
1	B	140/163 (86%)	137 (98%)	3 (2%)	0	100	100
1	C	137/163 (84%)	133 (97%)	3 (2%)	1 (1%)	18	32
1	D	130/163 (80%)	126 (97%)	3 (2%)	1 (1%)	16	29
All	All	548/652 (84%)	533 (97%)	12 (2%)	3 (0%)	24	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	217	PRO
1	D	139	SER
1	A	217	PRO

3.3.2 Protein sidechains

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	128/147 (87%)	127 (99%)	1 (1%)	73	88
1	B	127/147 (86%)	127 (100%)	0	100	100
1	C	117/147 (80%)	117 (100%)	0	100	100
1	D	102/147 (69%)	98 (96%)	4 (4%)	28	52
All	All	474/588 (81%)	469 (99%)	5 (1%)	65	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ASP
1	D	135	GLU
1	D	198	ILE
1	D	199	MET
1	D	206	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	212	GLN
1	C	186	ASN
1	C	105	GLN
1	B	162	ASN
1	C	145	ASN

3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

4.1 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	143/163 (87%)	1.07	20 (13%) 6 5	39, 56, 84, 96	0
1	B	142/163 (87%)	1.30	28 (19%) 3 2	40, 61, 82, 87	0
1	C	139/163 (85%)	2.07	65 (46%) 0 0	64, 87, 101, 108	0
1	D	134/163 (82%)	2.43	81 (60%) 0 0	70, 94, 111, 132	0
All	All	558/652 (85%)	1.71	194 (34%) 1 1	39, 75, 104, 132	0

The worst 5 of 194 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	152	GLY	6.9
1	C	151	LEU	6.0
1	D	219	GLY	5.8
1	D	225	TYR	5.7
1	D	137	TYR	5.5

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

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

4.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

4.4 Other polymers [i](#)

There are no such residues in this entry.