wwPDB X-ray Structure Validation Summary Report (i)

Sep 25, 2023 – 09:50 AM EDT

PDB ID	:	5WIP
Title	:	TraE protein in complex with 2-(2-furyl)isonicotinic acid
Authors	:	Casu, B.; Arya, T.; Bessette, B.; Baron, C.
Deposited on	:	2017-07-19
Resolution	:	2.62 Å(reported)

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

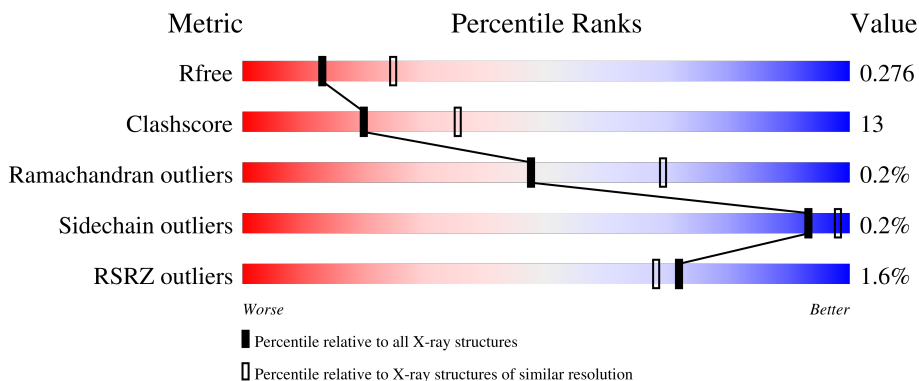|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.62 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	Percentile Ranks	Value
Rfree		0.276
Clashscore		13
Ramachandran outliers		0.2%
Sidechain outliers		0.2%
RSRZ outliers		1.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	163	72% 16% 12%
1	B	163	67% 20% 12%
1	C	163	% 58% 26% 17%
1	D	163	5% 52% 31% 17%

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4659 atoms, of which 6 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 Conjugal transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	0	0
			1168	736	206	223	3			
1	B	143	Total	C	N	O	S	0	1	0
			1177	742	208	224	3			
1	C	136	Total	C	N	O	S	0	0	0
			1088	691	185	209	3			
1	D	135	Total	C	N	O	S	0	0	0
			1060	673	183	202	2			

- Molecule 2 is 2-(furan-2-yl)pyridine-4-carboxylic acid (three-letter code: XXO) (formula: $C_{10}H_7NO_3$).
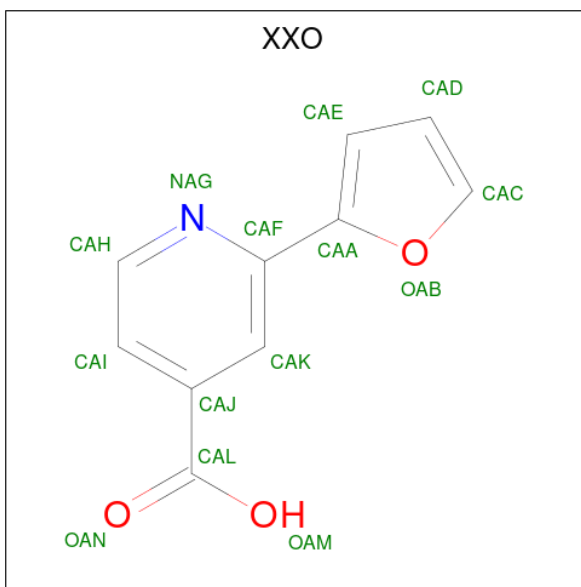
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			20	10	6	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total 66	O 66	0	0
3	B	55	Total 55	O 55	0	0
3	C	12	Total 12	O 12	0	0
3	D	13	Total 13	O 13	0	0

3 Residue-property plots ⓘ

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.
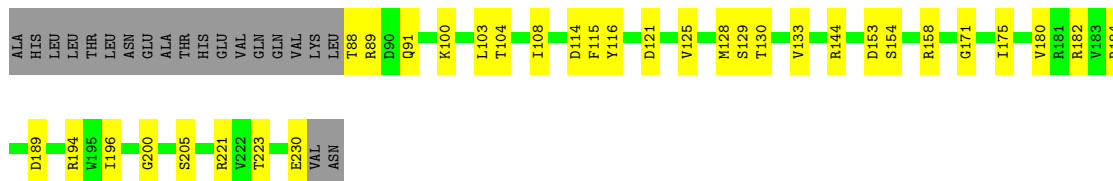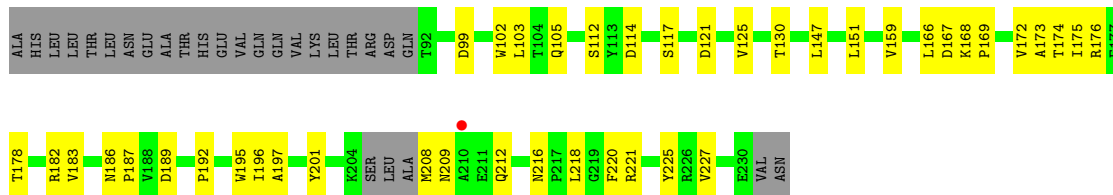
• Molecule 1: Conjugal transfer protein

Chain A:
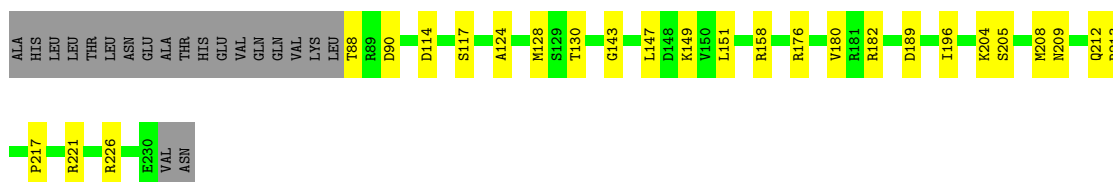
• Molecule 1: Conjugal transfer protein

Chain B:

• Molecule 1: Conjugal transfer protein

Chain C:

• Molecule 1: Conjugal transfer protein

Chain D:

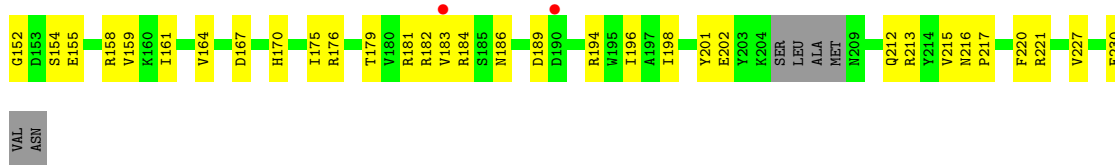G152 D153 S154 E155 R158 V159 K160 I161 V164 D167 H170 I175 R176 T179 V180 R181 R182 V183 R184 S185 N186 D189 D190 R194 W195 I196 A197 I198 Y201 E202 Y203 K204 SER LEU ALA MET N209 Q212 R213 Y214 V215 N216 P217 F220 R221 V227 E230

VAL ASN
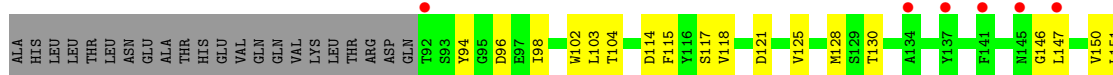
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	112.39Å 124.09Å 109.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.65 – 2.62 41.65 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.1 (41.65-2.62) 95.1 (41.65-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.217 , 0.274 0.219 , 0.276	Depositor DCC
R_{free} test set	2000 reflections (6.76%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.7	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4659	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

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

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	0.32	0/1194	0.43	0/1619
1	B	0.29	0/1203	0.42	0/1630
1	C	0.29	0/1113	0.43	0/1513
1	D	0.46	0/1084	0.43	0/1475
All	All	0.35	0/4594	0.43	0/6237

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1168	0	1139	19	0
1	B	1177	0	1151	20	0
1	C	1088	0	1037	29	0
1	D	1060	0	998	43	0
2	A	14	6	0	0	0
3	A	66	0	0	1	0
3	B	55	0	0	1	0
3	C	12	0	0	1	0
3	D	13	0	0	0	0
All	All	4653	6	4325	111	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 13.

The worst 5 of 111 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:202:GLU:OE2	1:D:221:ARG:NH1	1.72	1.22
1:B:88:THR:HG22	1:B:205:SER:HA	1.38	1.04
1:D:104:THR:HB	1:D:161:ILE:HD13	1.36	1.04
1:D:155:GLU:HB3	1:D:183:VAL:HG12	1.55	0.86
1:A:124:ALA:O	1:A:128:MET:HG3	1.79	0.82

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	139 (99%)	2 (1%)	0	100	100
1	B	142/163 (87%)	141 (99%)	1 (1%)	0	100	100
1	C	132/163 (81%)	129 (98%)	2 (2%)	1 (1%)	19	36
1	D	131/163 (80%)	125 (95%)	6 (5%)	0	100	100
All	All	546/652 (84%)	534 (98%)	11 (2%)	1 (0%)	47	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	187	PRO

5.3.2 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	129/147 (88%)	129 (100%)	0	100	100
1	B	130/147 (88%)	130 (100%)	0	100	100
1	C	118/147 (80%)	118 (100%)	0	100	100
1	D	111/147 (76%)	110 (99%)	1 (1%)	78	90
All	All	488/588 (83%)	487 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	96	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

1 ligand 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	$\#\|Z\| > 2$
2	XXO	A	301	-	11,15,15	4.54	7 (63%)	15,20,20	1.37	2 (13%)

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	XXO	A	301	-	-	4/6/8/8	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	XXO	CAI-CAH	7.14	1.53	1.38
2	A	301	XXO	CAK-CAJ	7.04	1.49	1.39
2	A	301	XXO	CAF-NAG	6.79	1.49	1.35
2	A	301	XXO	CAI-CAJ	-6.15	1.28	1.39
2	A	301	XXO	CAK-CAF	-4.36	1.32	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	XXO	CAI-CAH-NAG	-3.17	120.02	123.96
2	A	301	XXO	CAH-NAG-CAF	2.02	120.06	117.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	XXO	CAK-CAJ-CAL-OAN
2	A	301	XXO	CAI-CAJ-CAL-OAM
2	A	301	XXO	CAI-CAJ-CAL-OAN
2	A	301	XXO	CAK-CAJ-CAL-OAM

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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%)	-0.32	0	100	100	25, 41, 59, 81	0
1	B	143/163 (87%)	-0.28	0	100	100	30, 43, 65, 84	0
1	C	136/163 (83%)	-0.02	1 (0%)	87	85	44, 66, 82, 103	0
1	D	135/163 (82%)	0.21	8 (5%)	22	17	40, 69, 96, 110	0
All	All	557/652 (85%)	-0.11	9 (1%)	72	68	25, 54, 84, 110	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	210	ALA	3.8
1	D	183	VAL	2.8
1	D	92	THR	2.3
1	D	137	TYR	2.3
1	D	190	ASP	2.2

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 monosaccharides in this entry.

6.4 Ligands ⓘ

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	XXO	A	301	14/14	0.92	0.37	42,54,75,84	4

6.5 Other polymers ⓘ

There are no such residues in this entry.