



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 07:00 am BST

PDB ID : 1E9S
Title : Bacterial conjugative coupling protein TrwBdeltaN70. Unbound monoclinic form.
Authors : Gomis-Rueth, F.X.; Moncalian, G.; Cabezon, E.; de la Cruz, F.; Coll, M.
Deposited on : 2000-10-26
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

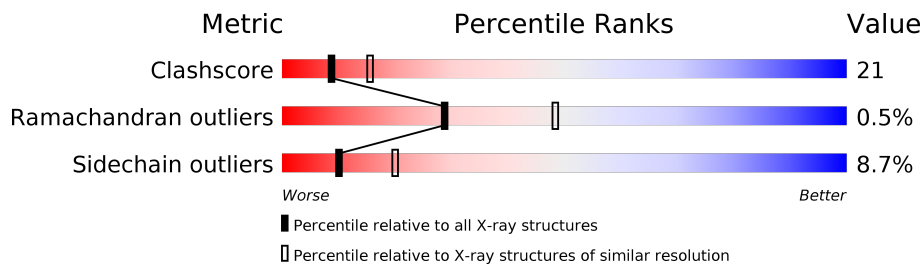
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)





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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	437	66% 28% . .
1	B	437	64% 27% 5% .
1	D	437	61% 30% 5% 5%
1	E	437	63% 28% 7% .
1	F	437	64% 29% 5% .
1	G	437	57% 36% 5% .
1	H	437	57% 36% . .
1	I	437	60% 33% . .

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Mol	Chain	Length	Quality of chain
1	J	437	 60% 33% . .
1	K	437	 56% 36% . .
1	L	437	 55% 38% 5% .
1	M	437	 59% 33% 5% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 41513 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 CONJUGAL TRANSFER PROTEIN TRWB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	Total 3353	C 2118	N 602	O 623	S 10	0	0	0
1	B	422	Total 3318	C 2097	N 596	O 615	S 10	0	0	0
1	D	417	Total 3279	C 2075	N 586	O 608	S 10	0	0	0
1	E	425	Total 3340	C 2110	N 600	O 620	S 10	0	0	0
1	F	427	Total 3348	C 2114	N 602	O 622	S 10	0	0	0
1	G	427	Total 3352	C 2116	N 603	O 623	S 10	0	0	0
1	H	424	Total 3329	C 2103	N 598	O 618	S 10	0	0	0
1	I	424	Total 3328	C 2102	N 598	O 618	S 10	0	0	0
1	J	424	Total 3328	C 2102	N 598	O 618	S 10	0	0	0
1	K	422	Total 3316	C 2096	N 595	O 615	S 10	0	0	0
1	L	426	Total 3344	C 2112	N 601	O 621	S 10	0	0	0
1	M	425	Total 3332	C 2104	N 599	O 619	S 10	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	157	Total 157	O 157	0	0
2	B	135	Total 135	O 135	0	0

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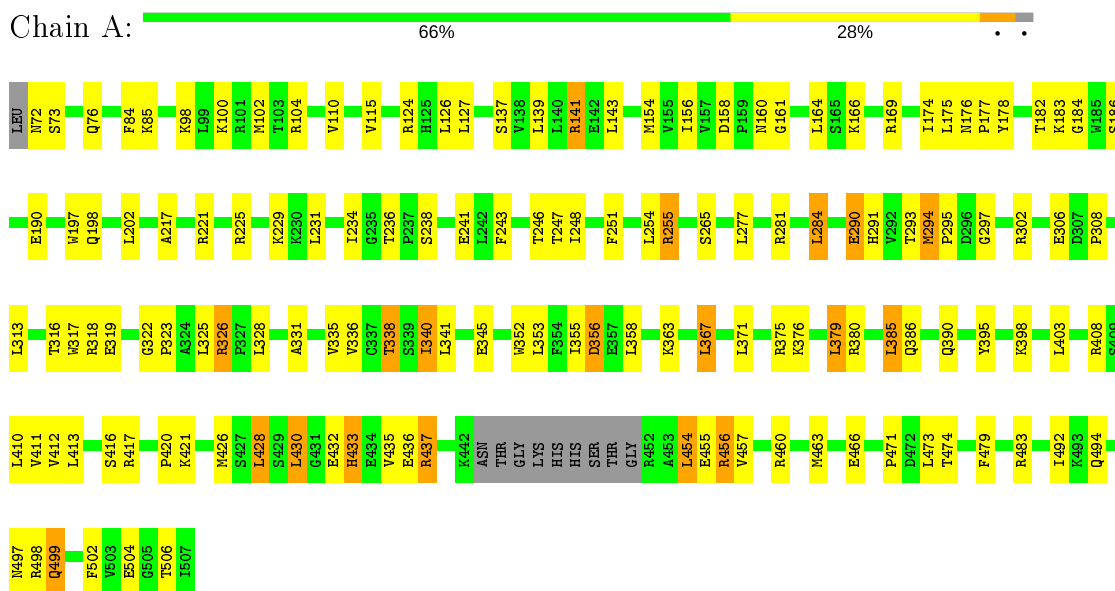
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	139	Total 139	O 139	0	0
2	E	133	Total 133	O 133	0	0
2	F	193	Total 193	O 193	0	0
2	G	167	Total 167	O 167	0	0
2	H	124	Total 124	O 124	0	0
2	I	113	Total 113	O 113	0	0
2	J	102	Total 102	O 102	0	0
2	K	84	Total 84	O 84	0	0
2	L	86	Total 86	O 86	0	0
2	M	113	Total 113	O 113	0	0

3 Residue-property plots [i](#)

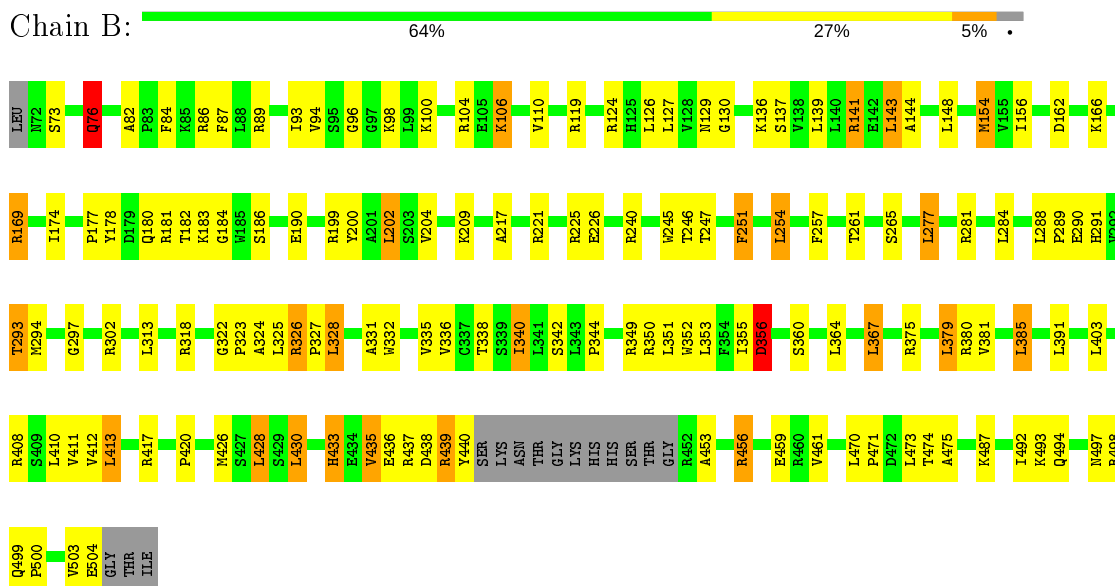
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

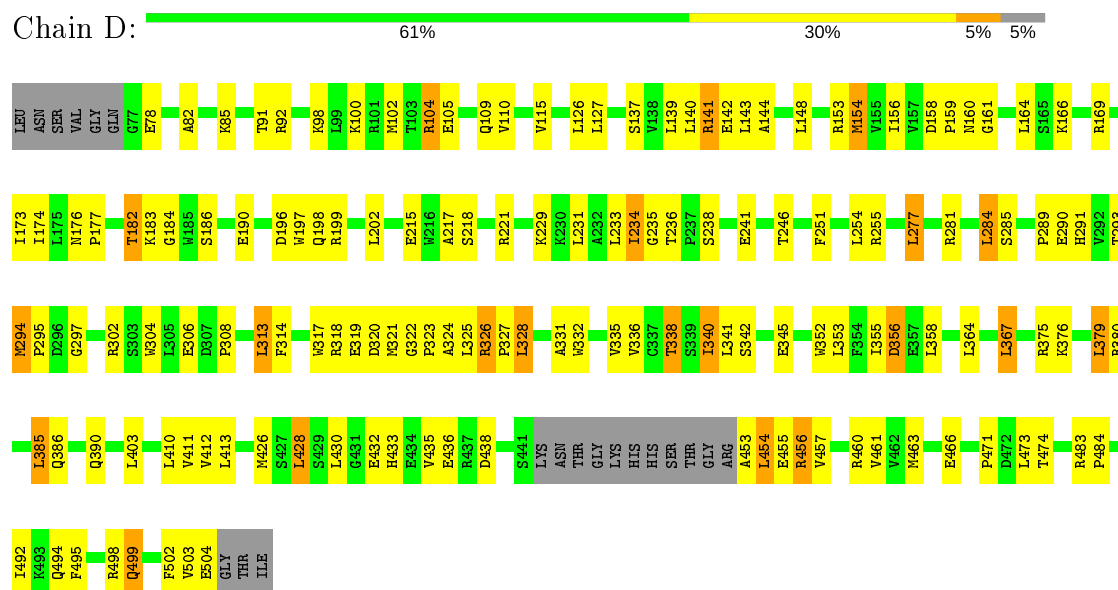
- Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB



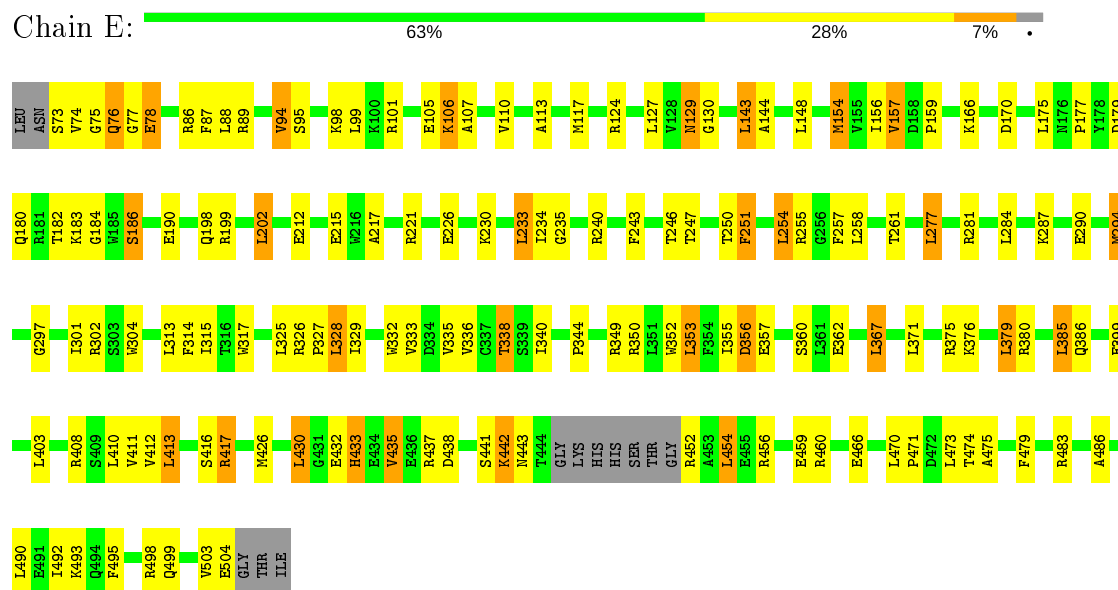
- Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB



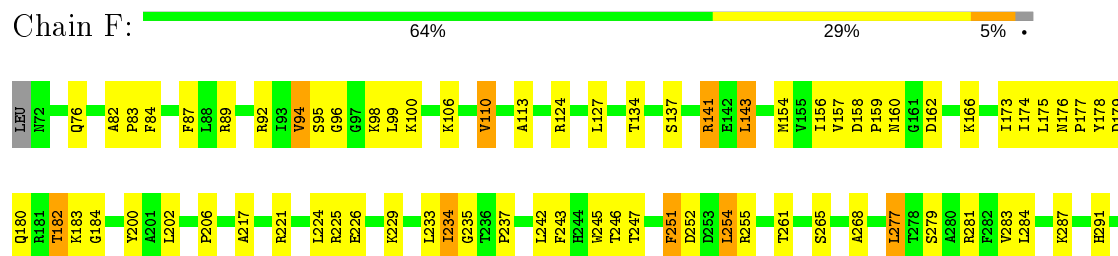
- Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB



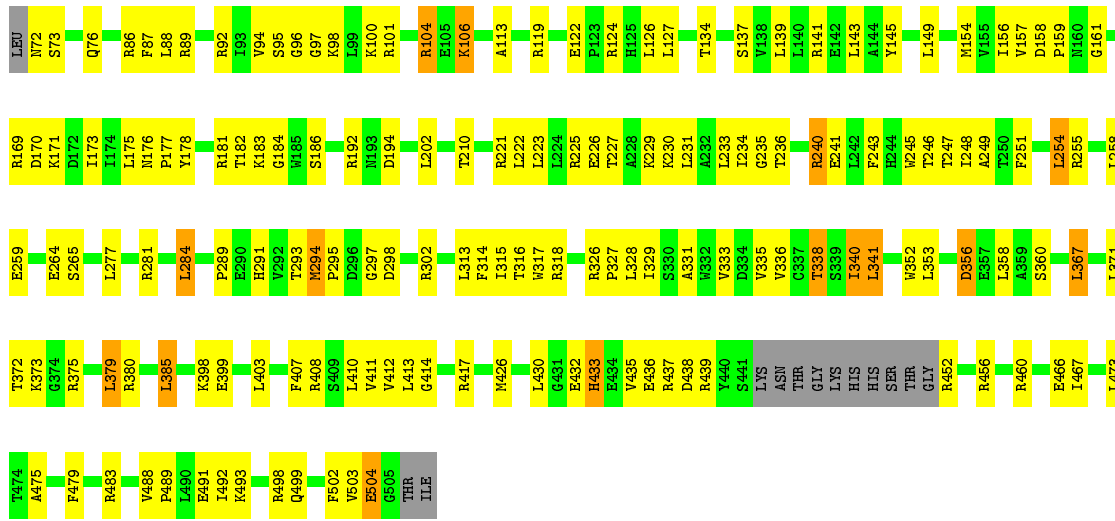
- Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB



- Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

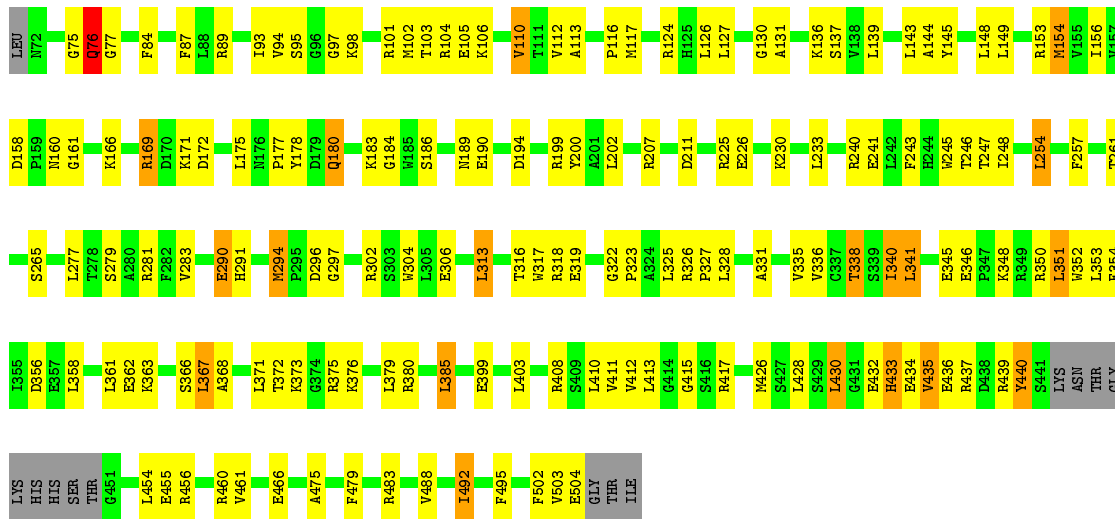


Chain I:  60% 33%



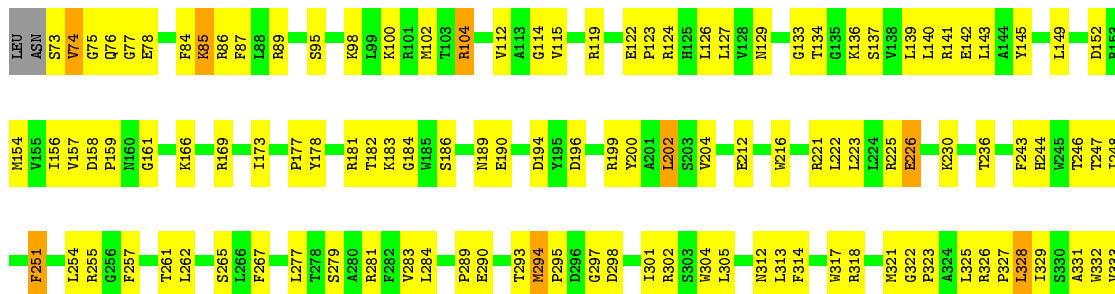
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

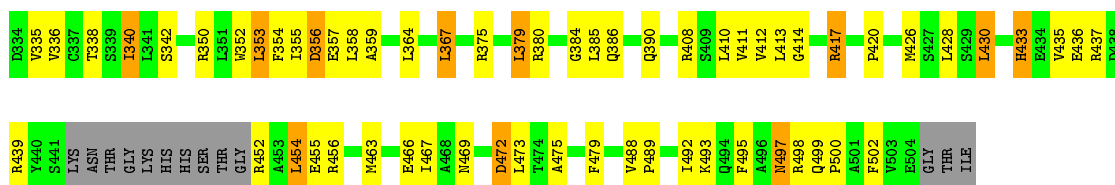
Chain J:  60% 33%



• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

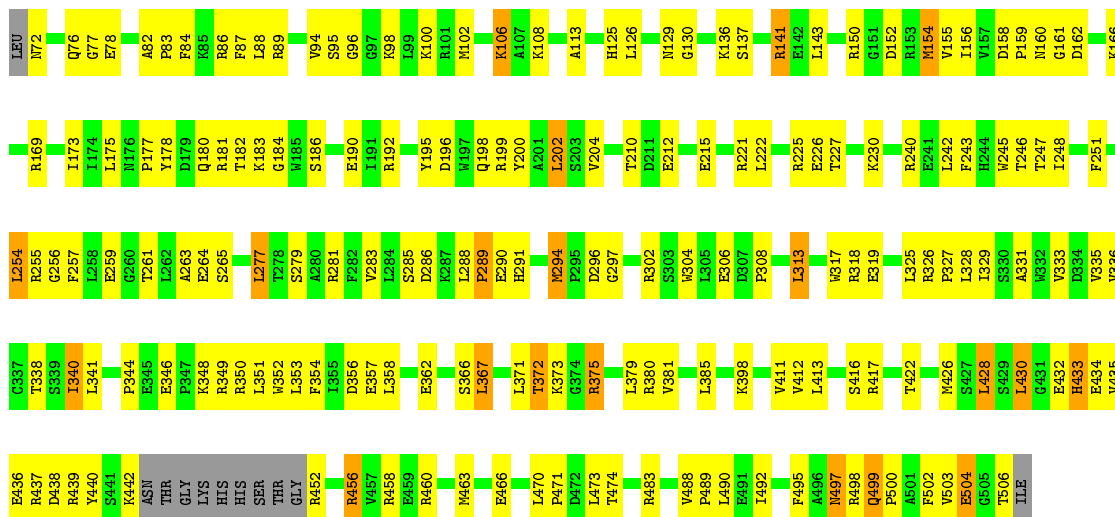
Chain K:  56% 36%





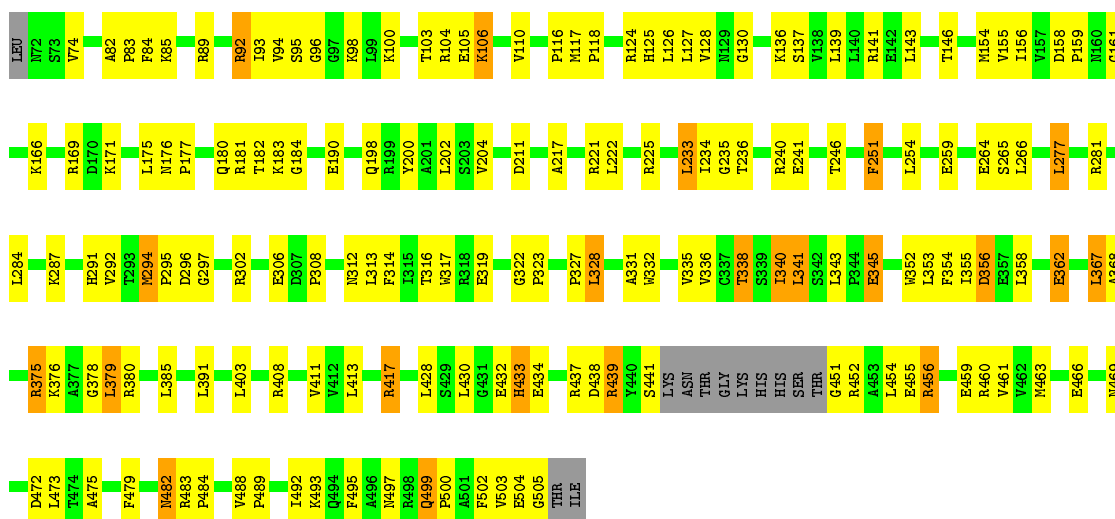
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain L: 55% 38% 5%



• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain M: 59% 33% 5%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.40Å 153.40Å 162.50Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	97.2 (50.00-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	41513	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.42	0/3418	0.67	1/4617 (0.0%)
1	B	0.42	0/3383	0.66	0/4572
1	D	0.41	0/3344	0.69	1/4520 (0.0%)
1	E	0.41	0/3405	0.66	1/4601 (0.0%)
1	F	0.42	0/3413	0.69	1/4611 (0.0%)
1	G	0.41	0/3417	0.66	0/4617
1	H	0.40	0/3394	0.65	1/4587 (0.0%)
1	I	0.39	0/3393	0.66	0/4585
1	J	0.40	0/3393	0.64	0/4585
1	K	0.40	0/3381	0.63	0/4569
1	L	0.40	0/3409	0.65	0/4606
1	M	0.41	0/3397	0.64	0/4590
All	All	0.41	0/40747	0.66	5/55060 (0.0%)

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	F	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	F	157	VAL	N-CA-C	-5.22	96.91	111.00
1	D	104	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	E	157	VAL	N-CA-C	-5.10	97.22	111.00
1	H	157	VAL	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	200	TYR	Sidechain

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	3353	0	3385	109	0
1	B	3318	0	3346	140	0
1	D	3279	0	3307	111	0
1	E	3340	0	3371	141	0
1	F	3348	0	3377	123	0
1	G	3352	0	3380	150	0
1	H	3329	0	3356	145	0
1	I	3328	0	3354	137	0
1	J	3328	0	3354	142	0
1	K	3316	0	3345	191	0
1	L	3344	0	3374	173	0
1	M	3332	0	3357	161	0
2	A	157	0	0	9	0
2	B	135	0	0	7	0
2	D	139	0	0	10	0
2	E	133	0	0	8	0
2	F	193	0	0	9	0
2	G	167	0	0	10	0
2	H	124	0	0	8	0
2	I	113	0	0	8	0
2	J	102	0	0	6	0
2	K	84	0	0	5	0
2	L	86	0	0	4	0
2	M	113	0	0	4	0
All	All	41513	0	40306	1647	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 21.

The worst 5 of 1647 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:J:76:GLN:HG2	1:J:77:GLY:H	1.07	1.16
1:I:106:LYS:HD3	1:I:106:LYS:H	1.04	1.15
1:E:127:LEU:HD11	1:E:385:LEU:HD22	1.27	1.09
1:J:492:ILE:HD13	1:J:492:ILE:H	1.14	1.08
1:F:372:THR:HG22	1:F:373:LYS:HG3	1.40	1.03

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	423/437 (97%)	407 (96%)	15 (4%)	1 (0%)	47	68
1	B	418/437 (96%)	397 (95%)	19 (4%)	2 (0%)	29	48
1	D	413/437 (94%)	395 (96%)	15 (4%)	3 (1%)	22	39
1	E	421/437 (96%)	401 (95%)	16 (4%)	4 (1%)	15	28
1	F	423/437 (97%)	401 (95%)	20 (5%)	2 (0%)	29	48
1	G	423/437 (97%)	410 (97%)	12 (3%)	1 (0%)	47	68
1	H	420/437 (96%)	398 (95%)	20 (5%)	2 (0%)	29	48
1	I	420/437 (96%)	398 (95%)	20 (5%)	2 (0%)	29	48
1	J	420/437 (96%)	402 (96%)	16 (4%)	2 (0%)	29	48
1	K	418/437 (96%)	401 (96%)	15 (4%)	2 (0%)	29	48
1	L	422/437 (97%)	405 (96%)	14 (3%)	3 (1%)	22	39
1	M	421/437 (96%)	403 (96%)	15 (4%)	3 (1%)	22	39
All	All	5042/5244 (96%)	4818 (96%)	197 (4%)	27 (0%)	29	48

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	356	ASP

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Mol	Chain	Res	Type
1	E	76	GLN
1	E	356	ASP
1	G	356	ASP
1	H	76	GLN

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	356/364 (98%)	323 (91%)	33 (9%)	9 17
1	B	352/364 (97%)	316 (90%)	36 (10%)	7 14
1	D	348/364 (96%)	317 (91%)	31 (9%)	9 19
1	E	355/364 (98%)	327 (92%)	28 (8%)	12 24
1	F	355/364 (98%)	324 (91%)	31 (9%)	10 20
1	G	356/364 (98%)	324 (91%)	32 (9%)	9 19
1	H	353/364 (97%)	325 (92%)	28 (8%)	12 24
1	I	353/364 (97%)	326 (92%)	27 (8%)	13 25
1	J	353/364 (97%)	318 (90%)	35 (10%)	8 15
1	K	352/364 (97%)	329 (94%)	23 (6%)	17 33
1	L	355/364 (98%)	322 (91%)	33 (9%)	9 17
1	M	353/364 (97%)	323 (92%)	30 (8%)	10 21
All	All	4241/4368 (97%)	3874 (91%)	367 (9%)	10 20

5 of 367 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	277	LEU
1	H	296	ASP
1	M	202	LEU
1	G	296	ASP
1	G	430	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	180	GLN
1	I	291	HIS
1	M	180	GLN
1	H	291	HIS
1	H	497	ASN

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 carbohydrates 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.