



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1S6M / pdb_00001s6m
Title : Conjugative Relaxase Trwc In Complex With Orit DNA. Metal-Bound Structure
Authors : Guasch, A.; Lucas, M.; Moncalian, G.; Cabezas, M.; Perez-Luque, R.; Gomis-Ruth, F.X.; de la Cruz, F.; Coll, M.
Deposited on : 2004-01-26
Resolution : 2.28 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

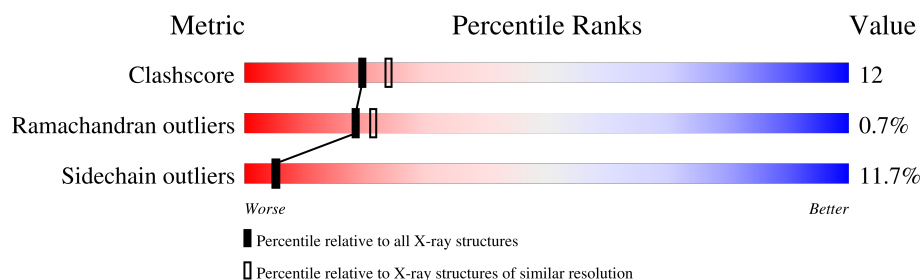
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	25	
2	A	293	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2951 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 DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	25	Total	C	N	O	P	3	0	0
			512	244	95	149	24			

- Molecule 2 is a protein called TrwC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	288	Total	C	N	O	Se	24	0	0
			2276	1402	430	440	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q47673
A	5	MSE	MET	modified residue	UNP Q47673
A	70	MSE	MET	modified residue	UNP Q47673
A	169	MSE	MET	modified residue	UNP Q47673

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	39	Total	O	0	0
			39	39		
4	A	123	Total	O	0	0
			123	123		

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. 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.

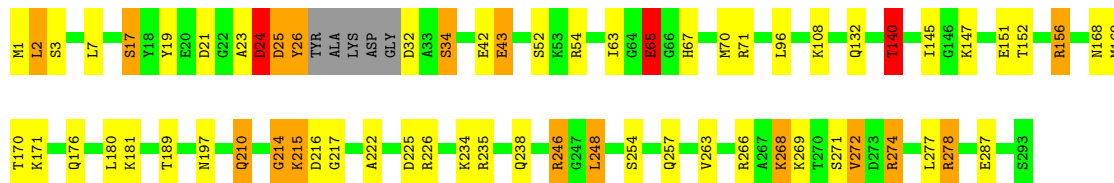
• Molecule 1: DNA (25-MER)

Chain B: 



• Molecule 2: TrwC

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.73Å 92.73Å 208.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.85 – 2.28	Depositor
% Data completeness (in resolution range)	(Not available) (43.85-2.28)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.206 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2951	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	B	0.54	0/574	2.21	46/885 (5.2%)
2	A	0.61	4/2304 (0.2%)	1.12	20/3086 (0.6%)
All	All	0.60	4/2878 (0.1%)	1.43	66/3971 (1.7%)

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	B	0	14

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	26	TYR	CB-CG	11.36	1.76	1.51
2	A	26	TYR	CA-CB	6.43	1.66	1.53
2	A	26	TYR	CA-C	6.39	1.66	1.52
2	A	26	TYR	CD1-CE1	5.62	1.55	1.38

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	DC	C2'-C3'-O3'	-18.16	84.26	111.50
1	B	6	DC	C2'-C3'-O3'	-16.90	86.15	111.50
2	A	25	ASP	N-CA-C	-16.56	92.55	112.92
1	B	20	DT	C2'-C3'-O3'	-13.81	90.79	111.50
2	A	24	ASP	N-CA-C	11.71	125.06	108.54
1	B	10	DA	C2'-C3'-O3'	-9.74	96.88	111.50
1	B	18	DT	C2'-C3'-O3'	-9.40	97.40	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	DG	C2'-C3'-O3'	-9.14	97.78	111.50
1	B	23	DT	C2'-C3'-O3'	-9.14	97.79	111.50
1	B	3	DG	N9-C1'-C2'	9.09	127.13	113.50
2	A	26	TYR	N-CA-C	9.01	136.23	111.00
1	B	19	DA	C4-N9-C1'	-8.73	113.95	127.05
1	B	19	DA	C8-N9-C1'	8.23	139.39	127.05
1	B	19	DA	C2'-C3'-O3'	-8.21	99.19	111.50
1	B	14	DT	C2'-C3'-O3'	-8.00	99.50	111.50
2	A	26	TYR	CA-CB-CG	7.97	128.25	113.90
1	B	19	DA	N9-C1'-C2'	7.71	125.07	113.50
1	B	6	DC	N1-C1'-C2'	7.65	124.98	113.50
1	B	4	DC	C2'-C3'-O3'	-7.56	100.16	111.50
1	B	16	DC	N1-C1'-C2'	7.54	124.81	113.50
1	B	16	DC	C2'-C3'-O3'	-7.54	100.19	111.50
1	B	18	DT	N1-C1'-C2'	7.43	124.65	113.50
1	B	12	DG	C2'-C3'-O3'	-7.27	100.59	111.50
2	A	71	ARG	N-CA-C	7.12	121.27	112.58
1	B	5	DA	N9-C1'-C2'	7.10	124.16	113.50
1	B	10	DA	N9-C1'-C2'	7.01	124.02	113.50
1	B	19	DA	C4'-C3'-O3'	-6.96	99.56	110.00
1	B	17	DG	C2'-C3'-O3'	-6.96	101.06	111.50
1	B	9	DA	N9-C1'-C2'	6.92	123.88	113.50
1	B	5	DA	C4-N9-C1'	-6.89	116.72	127.05
1	B	5	DA	C2'-C3'-O3'	-6.83	101.25	111.50
2	A	181	LYS	N-CA-C	-6.66	97.68	108.41
1	B	5	DA	C8-N9-C1'	6.64	137.01	127.05
2	A	216	ASP	N-CA-C	-6.60	105.26	113.38
1	B	1	DG	N9-C1'-C2'	6.49	123.24	113.50
1	B	15	DG	C2'-C3'-O3'	-6.47	101.79	111.50
2	A	274	ARG	N-CA-C	6.42	118.28	111.28
1	B	7	DC	C2'-C3'-O3'	-6.35	101.98	111.50
2	A	145	ILE	N-CA-C	6.28	117.16	108.12
2	A	263	VAL	N-CA-C	6.17	116.33	110.53
2	A	140	THR	N-CA-C	6.14	119.25	111.69
2	A	271	SER	N-CA-C	6.12	117.94	110.41
1	B	8	DG	N9-C1'-C2'	6.09	122.64	113.50
1	B	23	DT	N1-C1'-C2'	6.09	122.64	113.50
1	B	24	DC	C2'-C3'-O3'	-6.05	102.42	111.50
1	B	20	DT	N1-C1'-C2'	6.01	122.51	113.50
1	B	3	DG	C2'-C3'-O3'	-5.95	102.58	111.50
2	A	222	ALA	N-CA-C	5.91	118.51	111.71
1	B	9	DA	C2'-C3'-O3'	-5.88	102.68	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	DG	N9-C1'-C2'	5.87	122.30	113.50
1	B	23	DT	C4'-C3'-O3'	-5.77	101.35	110.00
1	B	21	DT	C2'-C3'-O3'	-5.59	103.12	111.50
1	B	22	DG	C2'-C3'-O3'	-5.59	103.12	111.50
2	A	65	GLU	N-CA-C	5.56	122.64	110.80
2	A	217	GLY	N-CA-C	-5.54	107.35	115.72
2	A	214	GLY	N-CA-C	5.50	126.22	113.18
2	A	156	ARG	N-CA-C	5.48	119.27	112.58
1	B	22	DG	N9-C1'-C2'	5.48	121.72	113.50
1	B	13	DG	N9-C1'-C2'	5.45	121.67	113.50
1	B	11	DA	C2'-C3'-O3'	-5.42	103.36	111.50
1	B	2	DC	N1-C1'-C2'	5.33	121.50	113.50
2	A	21	ASP	N-CA-C	5.32	117.74	109.60
2	A	26	TYR	N-CA-CB	-5.24	101.60	110.50
1	B	6	DC	C4'-C3'-O3'	-5.21	102.18	110.00
2	A	225	ASP	N-CA-C	5.11	118.00	110.59
1	B	4	DC	N1-C1'-C2'	5.01	121.01	113.50

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	DG	Sidechain
1	B	13	DG	Sidechain
1	B	15	DG	Sidechain
1	B	17	DG	Sidechain
1	B	19	DA	Sidechain
1	B	2	DC	Sidechain
1	B	20	DT	Sidechain
1	B	21	DT	Sidechain
1	B	22	DG	Sidechain
1	B	23	DT	Sidechain
1	B	24	DC	Sidechain
1	B	5	DA	Sidechain
1	B	8	DG	Sidechain
1	B	9	DA	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	B	512	0	283	22	0
2	A	2276	0	2259	40	0
3	A	1	0	0	0	0
4	A	123	0	0	6	0
4	B	39	0	0	1	0
All	All	2951	0	2542	61	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 12.

All (61) 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)
2:A:26:TYR:CB	2:A:26:TYR:CG	1.76	1.68
2:A:23:ALA:HB3	2:A:151:GLU:HB2	1.29	1.07
2:A:140:THR:HG21	2:A:170:THR:OG1	1.77	0.84
2:A:25:ASP:O	2:A:26:TYR:CG	2.33	0.81
2:A:23:ALA:CB	2:A:151:GLU:HB2	2.15	0.72
2:A:63:ILE:HD13	2:A:70:MSE:SE	2.40	0.71
2:A:63:ILE:HD11	2:A:169:MSE:SE	2.42	0.70
1:B:17:DG:H2''	1:B:18:DT:O5'	1.92	0.68
2:A:214:GLY:O	2:A:215:LYS:HG3	1.94	0.68
2:A:25:ASP:HB3	2:A:26:TYR:CD1	2.31	0.66
1:B:8:DG:H21	1:B:10:DA:H2	1.44	0.64
1:B:12:DG:H2''	1:B:13:DG:O5'	1.97	0.64
1:B:17:DG:C2'	1:B:18:DT:O5'	2.47	0.62
1:B:8:DG:H2''	1:B:9:DA:O5'	2.00	0.61
2:A:26:TYR:HD1	2:A:151:GLU:OE2	1.84	0.60
1:B:1:DG:H2''	1:B:2:DC:H5'	1.83	0.60
1:B:13:DG:H2'	1:B:14:DT:H71	1.83	0.58
2:A:23:ALA:HB2	2:A:152:THR:HG23	1.85	0.58
2:A:25:ASP:C	2:A:26:TYR:CG	2.82	0.57
2:A:268:LYS:NZ	4:A:569:HOH:O	2.37	0.57
1:B:13:DG:H2''	1:B:14:DT:O5'	2.05	0.56
1:B:17:DG:H2''	1:B:18:DT:C5'	2.35	0.56
2:A:26:TYR:CG	2:A:26:TYR:HB3	2.22	0.55
1:B:10:DA:C4	1:B:12:DG:H1'	2.42	0.54
1:B:12:DG:C2'	1:B:13:DG:O5'	2.56	0.53
1:B:1:DG:H2''	1:B:2:DC:C5'	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:171:LYS:NZ	4:A:615:HOH:O	2.40	0.51
1:B:5:DA:H2''	1:B:6:DC:O4'	2.10	0.51
2:A:168:ASN:ND2	2:A:180:LEU:H	2.09	0.51
1:B:25:DT:O4'	1:B:25:DT:O2	2.26	0.51
2:A:25:ASP:O	2:A:26:TYR:CD2	2.65	0.50
2:A:43:GLU:HG3	4:A:615:HOH:O	2.12	0.50
2:A:63:ILE:HD11	2:A:169:MSE:CE	2.42	0.49
2:A:234:LYS:HE3	4:A:577:HOH:O	2.11	0.49
2:A:235:ARG:HH11	2:A:238:GLN:HE21	1.61	0.48
2:A:17:SER:C	2:A:19:TYR:H	2.22	0.48
1:B:15:DG:C2'	1:B:16:DC:O5'	2.63	0.47
2:A:254:SER:OG	2:A:257:GLN:HG3	2.15	0.47
2:A:210:GLN:NE2	4:A:558:HOH:O	2.47	0.46
1:B:21:DT:C2	2:A:1:MSE:HE1	2.51	0.46
1:B:24:DC:C2'	1:B:25:DT:OP2	2.64	0.46
2:A:2:LEU:HD13	2:A:189:THR:HG23	1.97	0.46
2:A:54:ARG:NH2	2:A:63:ILE:O	2.49	0.45
1:B:25:DT:P	4:B:28:HOH:O	2.74	0.45
2:A:246:ARG:HB2	2:A:248:LEU:HD22	1.99	0.45
2:A:268:LYS:HE2	2:A:268:LYS:HB2	1.51	0.45
1:B:8:DG:C2'	1:B:9:DA:O5'	2.66	0.44
2:A:63:ILE:CD1	2:A:70:MSE:SE	3.12	0.44
1:B:1:DG:C2'	1:B:2:DC:O5'	2.65	0.43
2:A:156:ARG:HG3	2:A:272:VAL:HG11	2.01	0.43
1:B:15:DG:H2''	1:B:16:DC:C5'	2.50	0.42
2:A:23:ALA:HB3	2:A:151:GLU:CB	2.22	0.42
2:A:34:SER:HA	2:A:147:LYS:O	2.19	0.42
2:A:26:TYR:CG	2:A:26:TYR:HB2	2.22	0.42
2:A:272:VAL:HG21	2:A:277:LEU:HD22	2.01	0.42
2:A:24:ASP:OD2	2:A:24:ASP:N	2.52	0.42
1:B:24:DC:H2''	1:B:25:DT:OP2	2.20	0.41
2:A:2:LEU:HD22	2:A:3:SER:N	2.36	0.41
2:A:19:TYR:OH	2:A:52:SER:HA	2.21	0.41
2:A:235:ARG:HH11	2:A:238:GLN:NE2	2.19	0.40
2:A:278:ARG:NH1	4:A:582:HOH:O	2.54	0.40

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	
2	A	284/293 (97%)	275 (97%)	7 (2%)	2 (1%)	18	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	65	GLU
2	A	215	LYS

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	
2	A	231/230 (100%)	204 (88%)	27 (12%)	5	5

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	LEU
2	A	7	LEU
2	A	17	SER
2	A	24	ASP
2	A	32	ASP
2	A	34	SER
2	A	42	GLU
2	A	43	GLU
2	A	65	GLU

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Mol	Chain	Res	Type
2	A	67	HIS
2	A	96	LEU
2	A	108	LYS
2	A	132	GLN
2	A	140	THR
2	A	176	GLN
2	A	197	ASN
2	A	210	GLN
2	A	226	ARG
2	A	246	ARG
2	A	248	LEU
2	A	266	ARG
2	A	268	LYS
2	A	269	LYS
2	A	272	VAL
2	A	274	ARG
2	A	278	ARG
2	A	287	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	67	HIS
2	A	76	GLN
2	A	129	GLN
2	A	132	GLN
2	A	168	ASN
2	A	176	GLN
2	A	197	ASN
2	A	205	GLN
2	A	218	ASN
2	A	238	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - 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.

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.