



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 11:56 am GMT

PDB ID : 2W2H
Title : Structural basis of transcription activation by the Cyclin T1-Tat-TAR RNA complex from EIAV
Authors : Anand, K.; Geyer, M.
Deposited on : 2008-10-30
Resolution : 3.25 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
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

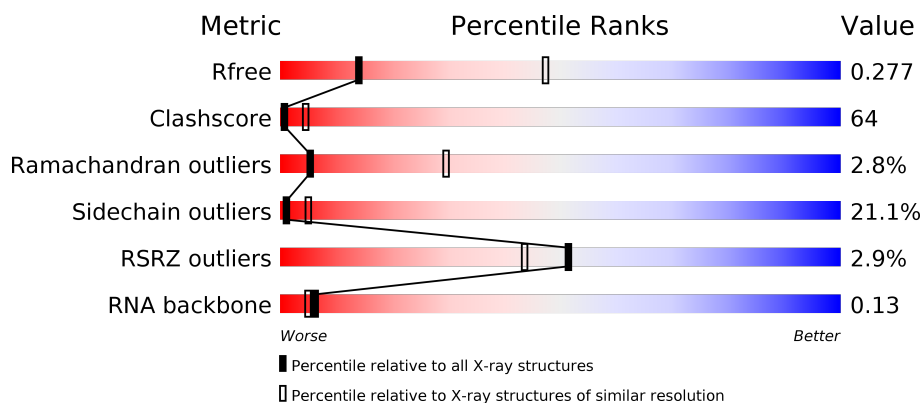
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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.



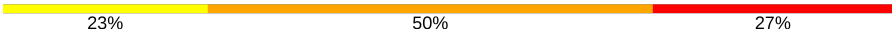
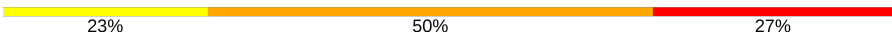
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1008 (3.30-3.22)
Clashscore	122126	1066 (3.30-3.22)
Ramachandran outliers	120053	1046 (3.30-3.22)
Sidechain outliers	120020	1045 (3.30-3.22)
RSRZ outliers	108989	1993 (3.32-3.20)
RNA backbone	2636	1017 (3.70-2.82)

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. 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 $\leq 5\%$. 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	264	 3% 35% 52% 13%
1	B	264	 3% 38% 43% 14%
2	C	29	 3% 17% 62% 21%
2	D	29	 24% 52% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	R	22	
3	S	22	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MN	R	1025	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5593 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 CYCLIN-T1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	7	0	0
			2102	1338	373	381	10			
1	B	260	Total	C	N	O	S	11	0	0
			2084	1329	367	378	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ARG	GLN	conflict	UNP Q9XT26
A	110	THR	ALA	conflict	UNP Q9XT26
A	256	TRP	ARG	conflict	UNP Q9XT26
B	77	ARG	GLN	conflict	UNP Q9XT26
B	110	THR	ALA	conflict	UNP Q9XT26
B	256	TRP	ARG	conflict	UNP Q9XT26

- Molecule 2 is a protein called PROTEIN TAT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	29	Total	C	N	O	0	0	0
			233	150	41	42			
2	D	29	Total	C	N	O	0	0	0
			230	148	40	42			

- Molecule 3 is a RNA chain called 5'-R(*GP*CP*UP*CP*AP*GP*AP*UP*CP*UP *GP*C P*GP*GP*UP*CP*UP*GP*AP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	22	Total	C	N	O	P	0	0	0
			468	208	80	158	22			
3	S	22	Total	C	N	O	P	0	0	0
			468	208	80	158	22			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	3	Total	O	0	0
			3	3		

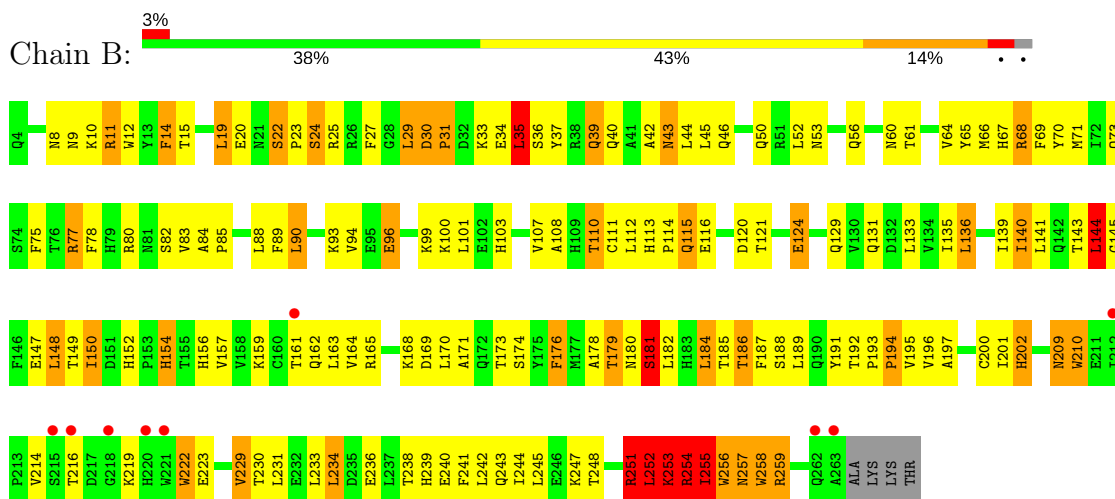
3 Residue-property plots

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 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.

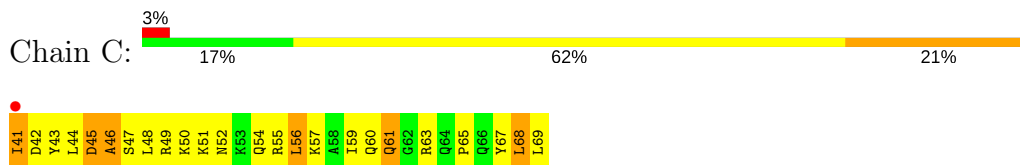
• Molecule 1: CYCLIN-T1



• Molecule 1: CYCLIN-T1



• Molecule 2: PROTEIN TAT



- Molecule 2: PROTEIN TAT

Chain D:  24% 52% 24%



- Molecule 3: 5'-R(*GP*CP*UP*CP*AP*GP*AP*UP*CP*UP *GP*CP*GP*GP*UP*CP*UP*GP*AP*GP*C)-3'

Chain R:  23% 50% 27%



- Molecule 3: 5'-R(*GP*CP*UP*CP*AP*GP*AP*UP*CP*UP *GP*CP*GP*GP*UP*CP*UP*GP*AP*GP*C)-3'

Chain S:  23% 50% 27%



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	149.46Å 149.46Å 129.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 3.25 29.93 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.93-3.25) 99.9 (29.93-3.25)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.243 , 0.278 0.241 , 0.277	Depositor DCC
R_{free} test set	1191 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å ²)	103.9	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 99.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.429 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5593	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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.

5 Model quality

5.1 Standard geometry

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

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	0.68	2/2153 (0.1%)	0.84	3/2934 (0.1%)
1	B	0.65	1/2135 (0.0%)	0.82	4/2910 (0.1%)
2	C	0.72	0/235	1.22	2/312 (0.6%)
2	D	0.77	0/232	1.30	2/309 (0.6%)
3	R	1.35	5/521 (1.0%)	2.54	46/808 (5.7%)
3	S	1.30	4/521 (0.8%)	2.45	44/808 (5.4%)
All	All	0.83	12/5797 (0.2%)	1.37	101/8081 (1.2%)

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	3
2	C	0	2
2	D	0	2
All	All	0	10

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	3	G	OP3-P	-11.21	1.47	1.61
3	S	3	G	OP3-P	-11.15	1.47	1.61
1	A	5	ARG	CZ-NH1	7.42	1.42	1.33
3	S	13	U	N1-C2	-6.74	1.32	1.38
3	R	16	G	C5-C6	-6.62	1.35	1.42

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	16	G	C1'-O4'-C4'	-15.57	97.45	109.90
3	R	16	G	N1-C6-O6	15.47	129.18	119.90
3	S	16	G	C1'-O4'-C4'	-15.46	97.53	109.90
3	R	16	G	C4-C5-N7	13.58	116.23	110.80
1	A	5	ARG	NE-CZ-NH2	-13.51	113.55	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	LEU	Peptide
1	A	263	ALA	Peptide
1	A	264	ALA	Peptide
1	B	252	LEU	Peptide
1	B	253	LYS	Peptide

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	2102	0	2044	219	0
1	B	2084	0	2036	228	0
2	C	233	0	239	84	0
2	D	230	0	230	80	0
3	R	468	0	237	73	0
3	S	468	0	237	79	0
4	A	1	0	0	0	0
4	R	1	0	0	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
All	All	5593	0	5023	680	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 64.

The worst 5 of 680 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:B:252:LEU:HD13	1:B:254:ARG:HG2	1.24	1.16
1:B:254:ARG:HD2	1:B:255:ILE:HG12	1.31	1.12
1:B:180:ASN:HB3	1:B:184:LEU:HD11	1.29	1.12
1:A:180:ASN:HB3	1:A:184:LEU:HD11	1.30	1.09
2:C:55:ARG:NH2	3:R:12:C:H42	1.49	1.09

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	261/264 (99%)	200 (77%)	55 (21%)	6 (2%)	7	34
1	B	258/264 (98%)	196 (76%)	52 (20%)	10 (4%)	3	21
2	C	27/29 (93%)	21 (78%)	6 (22%)	0	100	100
2	D	27/29 (93%)	21 (78%)	6 (22%)	0	100	100
All	All	573/586 (98%)	438 (76%)	119 (21%)	16 (3%)	5	29

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	181	SER
1	B	255	ILE
1	B	258	TRP
1	A	181	SER
1	A	26	ARG

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	225/241 (93%)	178 (79%)	47 (21%)	1	5
1	B	226/241 (94%)	176 (78%)	50 (22%)	1	4
2	C	22/26 (85%)	19 (86%)	3 (14%)	4	18
2	D	21/26 (81%)	17 (81%)	4 (19%)	1	7
All	All	494/534 (92%)	390 (79%)	104 (21%)	1	5

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	11	ARG
1	B	61	THR
1	B	259	ARG
1	B	14	PHE
1	B	24	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	HIS
1	A	156	HIS
1	B	152	HIS
1	A	109	HIS
1	A	115	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	21/22 (95%)	10 (47%)	1 (4%)
3	S	22/22 (100%)	12 (54%)	3 (13%)
All	All	43/44 (97%)	22 (51%)	4 (9%)

5 of 22 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	4	C
3	R	5	U
3	R	11	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	R	12	C
3	R	14	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	R	16	G
3	S	3	G
3	S	16	G
3	S	22	A

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](#)

Of 2 ligands modelled in this entry, 2 are 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 [i](#)

6.1 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	263/264 (99%)	-0.22	8 (3%)	50	42	65, 121, 242, 282	10 (3%)
1	B	260/264 (98%)	-0.17	9 (3%)	44	35	64, 120, 239, 269	11 (4%)
2	C	29/29 (100%)	-0.17	1 (3%)	45	36	100, 125, 165, 186	0
2	D	29/29 (100%)	-0.27	0	100	100	94, 118, 151, 181	0
3	R	22/22 (100%)	-0.40	0	100	100	92, 149, 202, 208	0
3	S	22/22 (100%)	-0.46	0	100	100	105, 148, 196, 215	0
All	All	625/630 (99%)	-0.21	18 (2%)	51	43	64, 124, 238, 282	21 (3%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	GLN	5.6
1	A	218	GLY	5.0
1	B	220	HIS	4.2
1	A	217	ASP	4.1
1	A	220	HIS	4.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
4	MN	R	1025	1/1	0.39	0.41	351,351,351,351	0
4	MN	A	1268	1/1	0.45	0.34	344,344,344,344	0

6.5 Other polymers [i](#)

There are no such residues in this entry.