



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:44 AM UTC

PDB ID : 4ERD / pdb_00004erd
Title : Crystal structure of the C-terminal domain of Tetrahymena telomerase protein p65 in complex with stem IV of telomerase RNA
Authors : Singh, M.; Wang, Z.; Koo, B.-K.; Patel, A.; Cascio, D.; Collins, K.; Feigon, J.
Deposited on : 2012-04-19
Resolution : 2.59 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) : 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

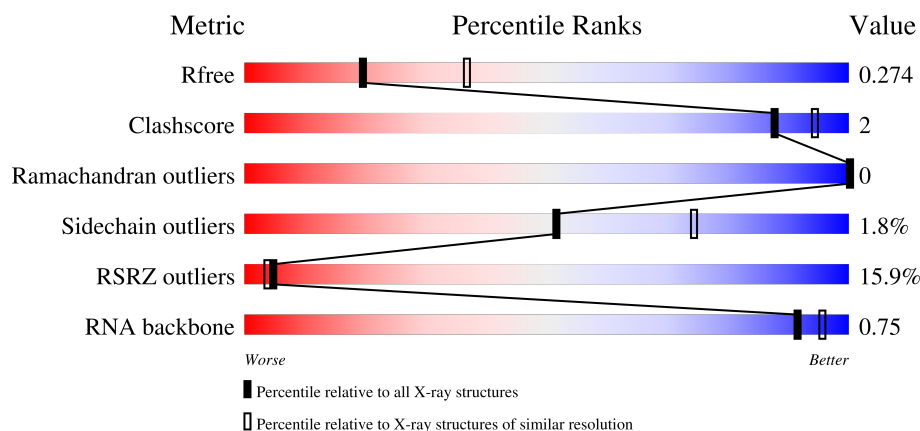
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)
RNA backbone	3983	1011 (2.82-2.34)

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 $\leq 5\%$. 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	129	7% 79% 20%
1	B	129	22% 76% 8% 16%
2	C	22	9% 82% 14% 5%
2	D	22	86% 14%

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
3	K	A	601	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2742 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 Telomerase associated protein p65.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	Se	0	0	0
			868	558	153	152	3	2			
1	B	108	Total	C	N	O	S	Se	0	0	0
			913	587	159	162	3	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	MSE	-	expression tag	UNP Q6JXI6
A	368	HIS	-	expression tag	UNP Q6JXI6
A	369	HIS	-	expression tag	UNP Q6JXI6
A	370	HIS	-	expression tag	UNP Q6JXI6
A	371	HIS	-	expression tag	UNP Q6JXI6
A	372	HIS	-	expression tag	UNP Q6JXI6
A	373	HIS	-	expression tag	UNP Q6JXI6
A	374	SER	-	expression tag	UNP Q6JXI6
B	367	MSE	-	expression tag	UNP Q6JXI6
B	368	HIS	-	expression tag	UNP Q6JXI6
B	369	HIS	-	expression tag	UNP Q6JXI6
B	370	HIS	-	expression tag	UNP Q6JXI6
B	371	HIS	-	expression tag	UNP Q6JXI6
B	372	HIS	-	expression tag	UNP Q6JXI6
B	373	HIS	-	expression tag	UNP Q6JXI6
B	374	SER	-	expression tag	UNP Q6JXI6

- Molecule 2 is a RNA chain called 5'-R(P*GP*GP*UP*CP*GP*AP*CP*AP*UP*CP*UP*UP*CP*GP*GP*AP*UP*GP*GP*AP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	P	0	0	0
			469	209	83	155	22			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	22	Total 469	C 209	N 83	O 155	P 22	0	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

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

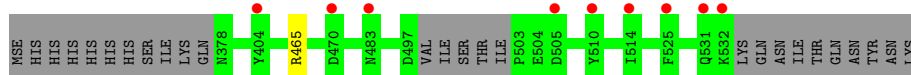
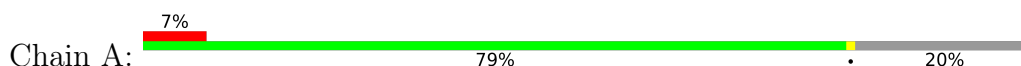
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	4	Total 4	O 4	0	0
4	C	4	Total 4	O 4	0	0
4	D	4	Total 4	O 4	0	0

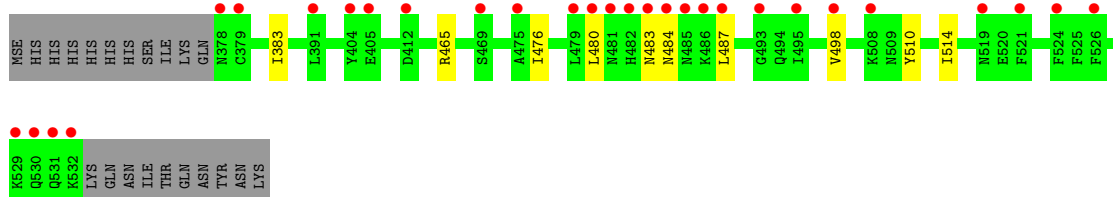
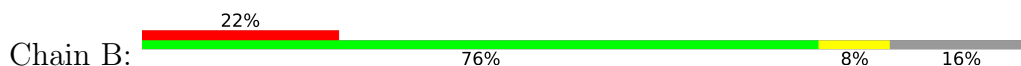
3 Residue-property plots [i](#)

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.

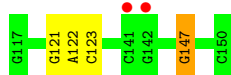
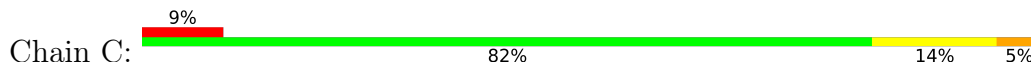
- Molecule 1: Telomerase associated protein p65



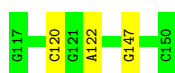
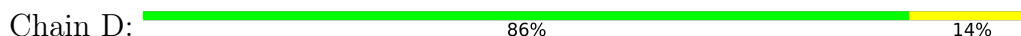
- Molecule 1: Telomerase associated protein p65



- Molecule 2: 5'-R(P*GP*GP*UP*CP*GP*AP*CP*AP*UP*CP*UP*UP*CP*GP*GP*AP*UP*GP*GP*AP*CP*C)-3'



- Molecule 2: 5'-R(P*GP*GP*UP*CP*GP*AP*CP*AP*UP*CP*UP*UP*CP*GP*GP*AP*UP*GP*GP*AP*CP*C)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.83Å 88.83Å 119.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.64 – 2.59 64.64 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.0 (64.64-2.59) 96.3 (64.64-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.220 , 0.272 (Not available) , 0.274	Depositor DCC
R_{free} test set	875 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 78.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2742	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/892	0.65	0/1189
1	B	0.25	0/928	0.68	0/1240
2	C	0.08	0/523	0.24	0/813
2	D	0.13	0/523	0.31	0/813
All	All	0.21	0/2866	0.55	0/4055

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 [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	868	0	879	1	0
1	B	913	0	922	8	0
2	C	469	0	238	4	0
2	D	469	0	238	2	0
3	A	1	0	0	0	0
4	A	10	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
All	All	2742	0	2277	10	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 2.

All (10) 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:C:147:G:H1	2:D:120:C:H5	1.38	0.71
1:A:465:ARG:NH1	2:D:122:A:N7	2.44	0.66
1:B:465:ARG:NH2	2:C:121:G:O6	2.29	0.65
1:B:465:ARG:NH1	2:C:122:A:N7	2.53	0.57
1:B:514:ILE:HD12	2:C:121:G:C6	2.43	0.54
1:B:483:ASN:OD1	1:B:484:ASN:ND2	2.41	0.53
1:B:383:ILE:HG12	1:B:498:VAL:HG12	1.95	0.48
1:B:510:TYR:O	1:B:514:ILE:HG12	2.15	0.47
1:B:476:ILE:HG23	1:B:487:LEU:HD21	2.00	0.43
1:B:487:LEU:HB3	1:B:498:VAL:HG23	2.03	0.41

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	101/129 (78%)	101 (100%)	0	0	100	100
1	B	106/129 (82%)	102 (96%)	4 (4%)	0	100	100
All	All	207/258 (80%)	203 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	B	55/118 (47%)	54 (98%)	1 (2%)	51 74

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

Mol	Chain	Res	Type
1	B	480	LEU

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	21/22 (95%)	2 (9%)	0
2	D	21/22 (95%)	1 (4%)	0
All	All	42/44 (95%)	3 (7%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	123	C
2	C	147	G
2	D	147	G

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry

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

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 [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	99/129 (76%)	0.67	9 (9%) 15 12	32, 50, 80, 108	0
1	B	106/129 (82%)	1.35	29 (27%) 1 1	44, 71, 139, 173	0
2	C	22/22 (100%)	0.32	2 (9%) 15 12	44, 59, 86, 96	0
2	D	22/22 (100%)	-0.01	0 100 100	38, 61, 65, 70	0
All	All	249/302 (82%)	0.87	40 (16%) 5 4	32, 61, 108, 173	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	532	LYS	4.9
1	B	475	ALA	4.2
1	A	532	LYS	3.9
1	B	482	HIS	3.9
1	B	529	LYS	3.8
1	B	481	ASN	3.7
1	B	378	ASN	3.6
1	B	469	SER	3.5
1	A	510	TYR	3.4
1	B	405	GLU	3.2
1	A	470	ASP	3.2
1	B	479	LEU	3.2
1	A	525	PHE	3.0
1	B	379	CYS	3.0
1	B	519	ASN	3.0
1	B	483	ASN	2.9
2	C	141	C	2.9
1	B	530	GLN	2.7
1	A	505	ASP	2.7
1	B	524	PHE	2.7
1	B	480	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	486	LYS	2.6
1	B	484	ASN	2.5
1	B	404	TYR	2.5
1	B	495	ILE	2.5
1	B	487	LEU	2.5
1	B	508	LYS	2.4
1	B	531	GLN	2.4
1	B	521	PHE	2.4
1	A	483	ASN	2.4
2	C	142	G	2.2
1	B	526	PHE	2.2
1	B	391	LEU	2.2
1	A	531	GLN	2.2
1	A	404	TYR	2.2
1	B	412	ASP	2.2
1	B	493	GLY	2.1
1	A	514	ILE	2.1
1	B	485	ASN	2.1
1	B	498	VAL	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	K	A	601	1/1	0.76	0.45	134,134,134,134	0

6.5 Other polymers ⓘ

There are no such residues in this entry.