



Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2026 – 08:12 PM EDT

PDB ID : 11GZ / pdb_000011gz
Title : TEP1 TIR/DUF4062 domain
Authors : Osinski, A.; Tomchick, D.R.; Tagliabracci, V.S.
Deposited on : 2026-02-23
Resolution : 2.44 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

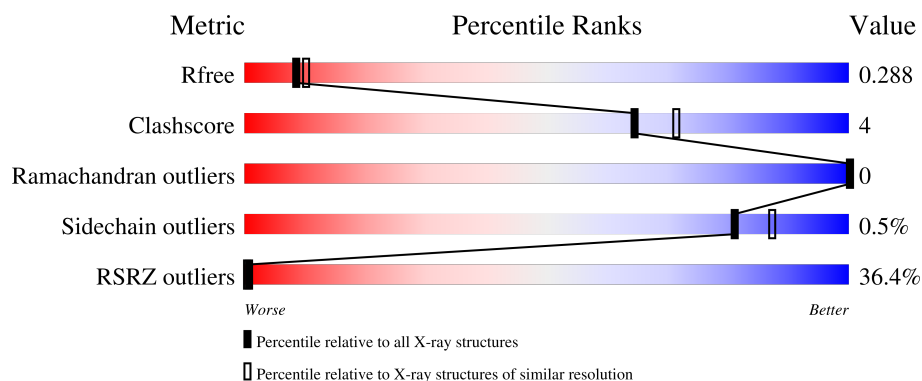
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	220	<div> <div>36%</div> <div>91%</div> <div>9%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3702 atoms, of which 1761 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.

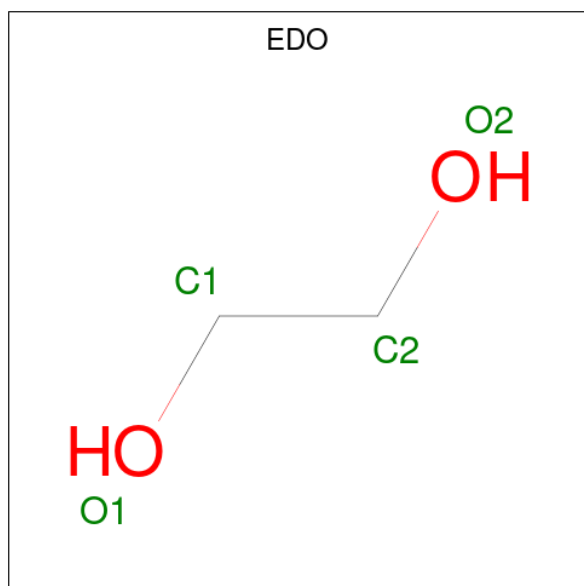
- Molecule 1 is a protein called Telomerase protein component 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	220	Total	C	H	N	O	S	0	0	0
			3540	1133	1749	328	323	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	894	SER	-	expression tag	UNP Q99973

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

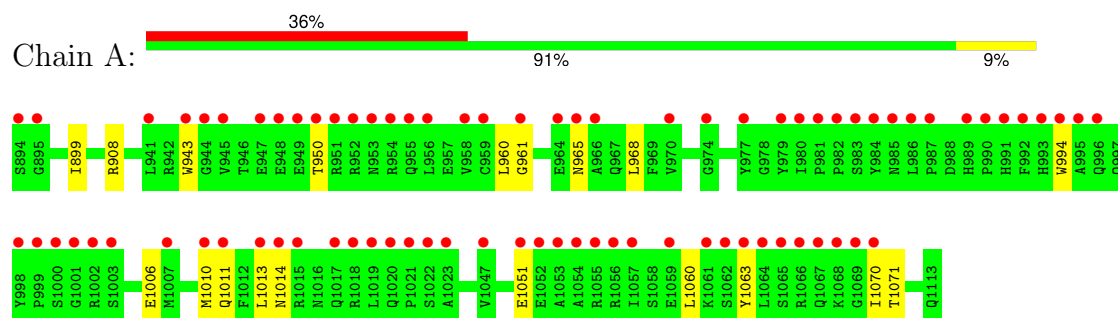
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total	O	0	0
			137	137		

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 protein component 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	132.76Å 132.76Å 132.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.03 – 2.44 40.03 – 2.44	Depositor EDS
% Data completeness (in resolution range)	97.1 (40.03-2.44) 97.3 (40.03-2.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419, BUSTER	Depositor
R, R_{free}	0.236 , 0.287 0.237 , 0.288	Depositor DCC
R_{free} test set	1505 reflections (9.70%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3702	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: EDO, SO4

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	0.39	0/1837	0.42	0/2486

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	1791	1749	1749	14	0
2	A	8	12	12	0	0
3	A	5	0	0	0	0
4	A	137	0	0	1	0
All	All	1941	1761	1761	14	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 4.

All (14) 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:A:1010:MET:HE1	1:A:1063:TYR:CE1	2.24	0.71
1:A:960:LEU:HD22	1:A:1011:GLN:HB2	1.78	0.65
1:A:1013:LEU:HD11	1:A:1070:ILE:HG21	1.87	0.56
1:A:960:LEU:HD22	1:A:1011:GLN:CB	2.39	0.53
1:A:943:TRP:HA	1:A:950:THR:HG23	1.96	0.47
1:A:1010:MET:HE1	1:A:1063:TYR:HE1	1.78	0.47
1:A:908:ARG:NH2	4:A:1305:HOH:O	2.48	0.46
1:A:961:GLY:O	1:A:965:ASN:ND2	2.51	0.44
1:A:994:TRP:NE1	1:A:1011:GLN:OE1	2.51	0.44
1:A:994:TRP:CD1	1:A:994:TRP:H	2.36	0.43
1:A:899:ILE:HD12	1:A:968:LEU:HD11	2.01	0.43
1:A:1051:GLU:H	1:A:1051:GLU:HG2	1.65	0.43
1:A:1014:ASN:OD1	1:A:1014:ASN:C	2.64	0.41
1:A:1006:GLU:CG	1:A:1060:LEU:HD22	2.51	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	218/220 (99%)	214 (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	A	191/191 (100%)	190 (100%)	1 (0%)	81 87

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

Mol	Chain	Res	Type
1	A	1071	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	965	ASN
1	A	1024	GLN
1	A	1067	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are 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	EDO	A	1201	-	3,3,3	0.27	0	2,2,2	0.25	0
3	SO4	A	1202	-	4,4,4	0.78	0	6,6,6	0.40	0
2	EDO	A	1203	-	3,3,3	0.31	0	2,2,2	0.17	0

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	EDO	A	1201	-	-	1/1/1/1	-
2	EDO	A	1203	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	EDO	O1-C1-C2-O2
2	A	1203	EDO	O1-C1-C2-O2

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

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	220/220 (100%)	1.29	80 (36%) 1 0	20, 63, 149, 177	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	980	ILE	5.5
1	A	1021	PRO	5.3
1	A	982	PRO	5.1
1	A	979	TYR	4.7
1	A	945	VAL	4.4
1	A	1001	GLY	4.3
1	A	998	TYR	4.3
1	A	981	PRO	4.2
1	A	1053	ALA	4.2
1	A	1064	LEU	4.1
1	A	1003	SER	3.9
1	A	977	TYR	3.8
1	A	1013	LEU	3.8
1	A	1022	SER	3.7
1	A	956	LEU	3.6
1	A	987	PRO	3.5
1	A	992	PHE	3.5
1	A	1069	GLY	3.5
1	A	1067	GLN	3.5
1	A	1014	ASN	3.4
1	A	1010	MET	3.4
1	A	1054	ALA	3.4
1	A	954	ARG	3.4
1	A	943	TRP	3.4
1	A	989	HIS	3.3
1	A	1070	ILE	3.3
1	A	986	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	3.3
1	A	1017	GLN	3.3
1	A	990	PRO	3.2
1	A	985	ASN	3.2
1	A	1023	ALA	3.2
1	A	1063	TYR	3.2
1	A	994	TRP	3.1
1	A	1055	ARG	3.1
1	A	941	LEU	3.1
1	A	1002	ARG	3.0
1	A	1018	ARG	3.0
1	A	1066	ARG	3.0
1	A	953	ASN	3.0
1	A	991	HIS	3.0
1	A	1051	GLU	2.9
1	A	947	GLU	2.9
1	A	955	GLN	2.9
1	A	995	ALA	2.9
1	A	895	GLY	2.9
1	A	958	VAL	2.8
1	A	1019	LEU	2.8
1	A	1068	LYS	2.8
1	A	961	GLY	2.8
1	A	983	SER	2.7
1	A	964	GLU	2.7
1	A	974	GLY	2.7
1	A	999	PRO	2.7
1	A	894	SER	2.7
1	A	984	TYR	2.7
1	A	959	CYS	2.6
1	A	996	GLN	2.5
1	A	966	ALA	2.5
1	A	1011	GLN	2.5
1	A	1015	ARG	2.5
1	A	1061	LYS	2.5
1	A	944	GLY	2.4
1	A	965	ASN	2.4
1	A	949	GLU	2.4
1	A	948	GLU	2.4
1	A	951	ARG	2.3
1	A	1062	SER	2.3
1	A	1000	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	950	THR	2.3
1	A	1057	ILE	2.2
1	A	1056	ARG	2.2
1	A	1020	GLN	2.2
1	A	970	VAL	2.2
1	A	952	ARG	2.2
1	A	1059	GLU	2.1
1	A	1065	SER	2.1
1	A	1007	MET	2.1
1	A	1052	GLU	2.1
1	A	1047	VAL	2.1

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(\AA^2)	Q<0.9
2	EDO	A	1203	4/4	0.80	0.21	96,117,139,139	0
2	EDO	A	1201	4/4	0.83	0.22	59,75,80,91	0
3	SO4	A	1202	5/5	0.91	0.16	30,36,59,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.