wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	10CR / pdb_000010cr
Title	:	Crystal structure of the complex between human PTPRD and TeNT
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Deposited on	:	2026-01-12
Resolution	:	2.98 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 (i) 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 (1)) were used in the production of this report:

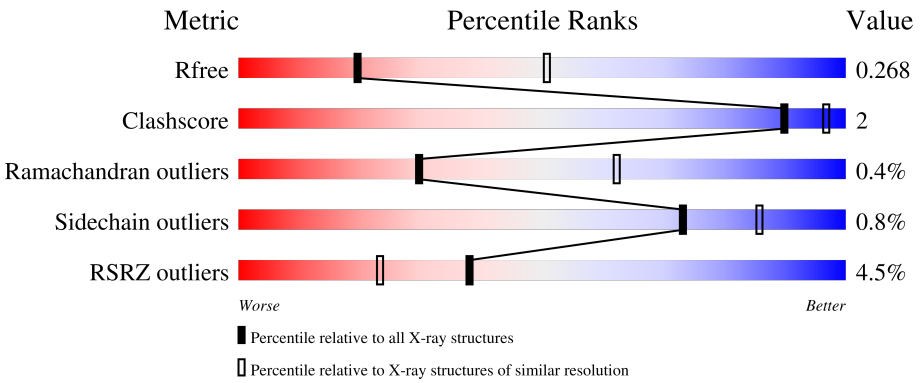
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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 <=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	886	4%, 90%, 5%, 5%
2	B	310	3%, 64%, 5%, 31%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8483 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 Tetanus toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	842	6809	4369	1099	1317	24	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	PHE	TYR	conflict	UNP P04958
A	443F	ALA	-	linker	UNP P04958
A	443G	SER	-	linker	UNP P04958
A	443H	LEU	-	linker	UNP P04958
A	443I	VAL	-	linker	UNP P04958
A	443J	PRO	-	linker	UNP P04958
A	443K	ARG	-	linker	UNP P04958
A	443L	GLY	-	linker	UNP P04958
A	443M	SER	-	linker	UNP P04958
A	443N	GLY	-	linker	UNP P04958
A	443O	SER	-	linker	UNP P04958
A	871	LEU	-	expression tag	UNP P04958
A	872	PRO	-	expression tag	UNP P04958
A	873	GLU	-	expression tag	UNP P04958
A	874	THR	-	expression tag	UNP P04958
A	875	GLY	-	expression tag	UNP P04958
A	876	GLY	-	expression tag	UNP P04958
A	877	LEU	-	expression tag	UNP P04958
A	878	GLU	-	expression tag	UNP P04958
A	879	HIS	-	expression tag	UNP P04958
A	880	HIS	-	expression tag	UNP P04958
A	881	HIS	-	expression tag	UNP P04958
A	882	HIS	-	expression tag	UNP P04958
A	883	HIS	-	expression tag	UNP P04958
A	884	HIS	-	expression tag	UNP P04958

- Molecule 2 is a protein called Receptor-type tyrosine-protein phosphatase delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	214	1662	1026	305	325	6	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	322	GLY	-	expression tag	UNP P23468
B	323	THR	-	expression tag	UNP P23468
B	324	LYS	-	expression tag	UNP P23468
B	325	HIS	-	expression tag	UNP P23468
B	326	HIS	-	expression tag	UNP P23468
B	327	HIS	-	expression tag	UNP P23468
B	328	HIS	-	expression tag	UNP P23468
B	329	HIS	-	expression tag	UNP P23468
B	330	HIS	-	expression tag	UNP P23468

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is water.

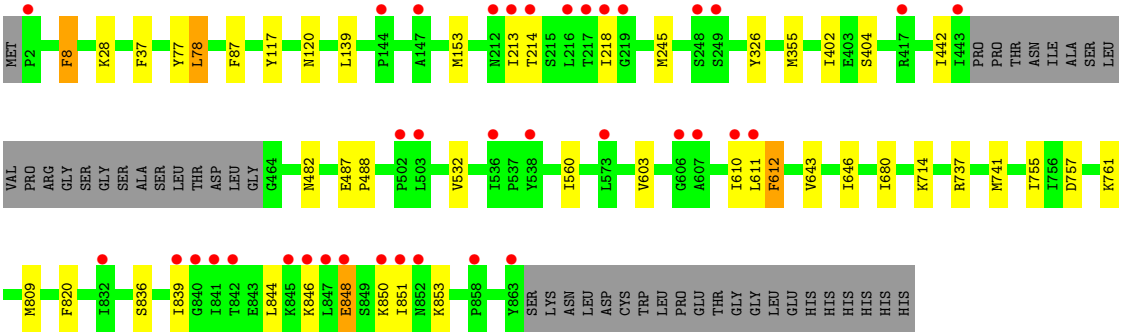
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	8	8	8	0	0
4	B	3	3	3	0	0

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.

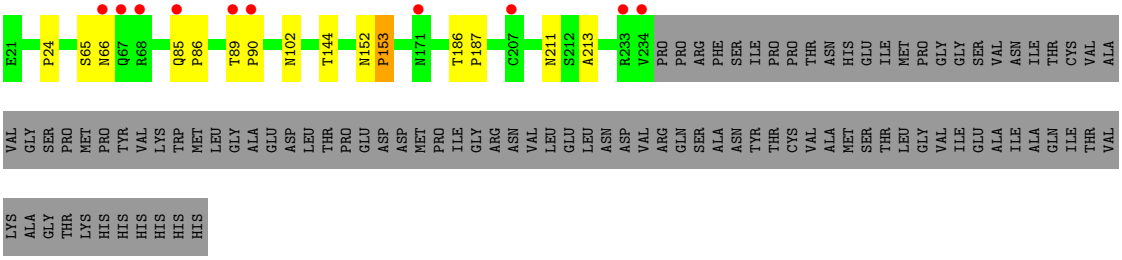
- Molecule 1: Tetanus toxin

Chain A:



- Molecule 2: Receptor-type tyrosine-protein phosphatase delta

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.24Å 94.87Å 246.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.53 – 2.98 88.53 – 2.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (88.53-2.98) 99.9 (88.53-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.237 , 0.279 0.219 , 0.268	Depositor DCC
R_{free} test set	1784 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 25.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8483	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN

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	0.45	0/6948	0.86	0/9402
2	B	0.48	0/1691	0.86	1/2292 (0.0%)
All	All	0.45	0/8639	0.86	1/11694 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	153	PRO	N-CA-C	-5.83	102.00	110.80

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	6809	0	6803	24	0
2	B	1662	0	1650	8	0
3	A	1	0	0	0	0
4	A	8	0	0	0	0
4	B	3	0	0	0	0
All	All	8483	0	8453	31	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.

The worst 5 of 31 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:B:24:PRO:HG3	2:B:102:ASN:HB2	1.79	0.63
2:B:89:THR:HB	2:B:90:PRO:HD3	1.84	0.60
1:A:78:LEU:HD11	1:A:87:PHE:HB2	1.86	0.58
2:B:152:ASN:HB3	2:B:153:PRO:HD3	1.90	0.53
1:A:560:ILE:HG12	1:A:737:ARG:HH12	1.74	0.52

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	838/886 (95%)	802 (96%)	32 (4%)	4 (0%)	24	58
2	B	212/310 (68%)	196 (92%)	16 (8%)	0	100	100
All	All	1050/1196 (88%)	998 (95%)	48 (5%)	4 (0%)	30	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	846	LYS
1	A	844	LEU
1	A	612	PHE
1	A	848	GLU

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	773/810 (95%)	767 (99%)	6 (1%)	73	86
2	B	185/267 (69%)	183 (99%)	2 (1%)	65	82
All	All	958/1077 (89%)	950 (99%)	8 (1%)	73	86

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	144	THR
2	B	66	ASN
1	A	848	GLU
1	A	442	ILE
1	A	850	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	ASN
1	A	328	GLN
1	A	339	GLN
2	B	66	ASN
2	B	85	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)

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 (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	842/886 (95%)	0.35	37 (4%)	39	24	46, 66, 92, 148	0
2	B	214/310 (69%)	0.28	10 (4%)	36	22	45, 58, 79, 115	0
All	All	1056/1196 (88%)	0.34	47 (4%)	38	23	45, 65, 91, 148	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	847	LEU	6.6
2	B	234	VAL	6.2
1	A	848	GLU	6.0
1	A	611	LEU	5.4
1	A	213	ILE	5.3

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)

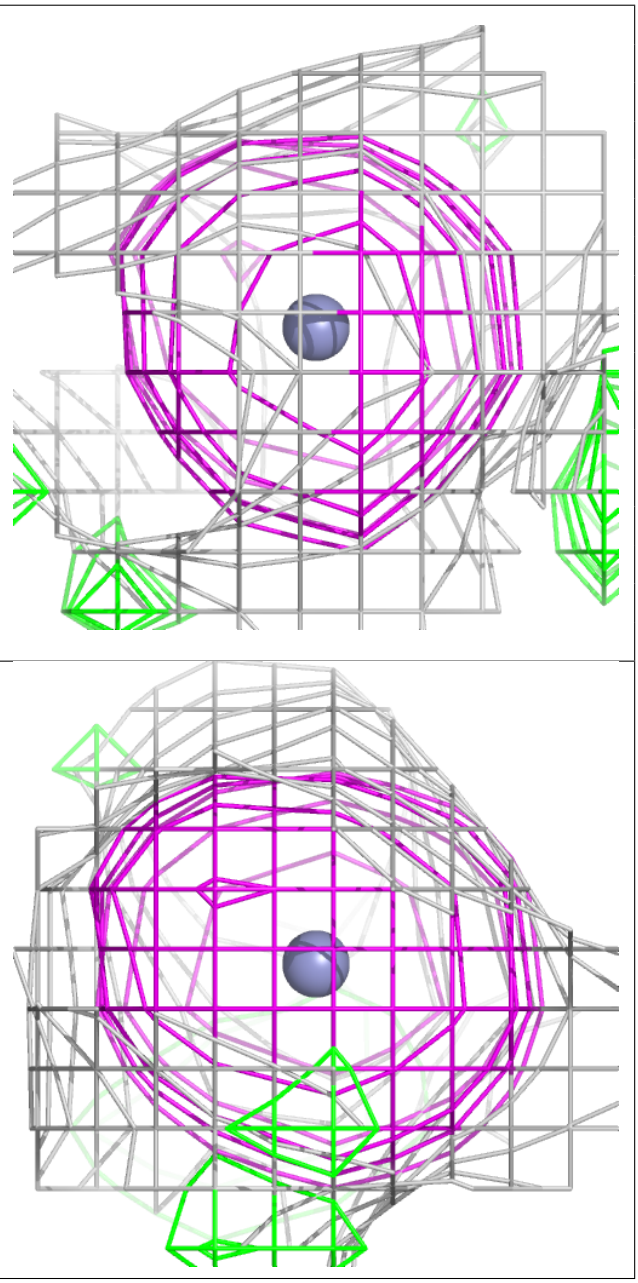
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	A	901	1/1	0.94	0.28	39,39,39,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ZN A 901:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.