



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:54 PM UTC

PDB ID : 2CM3 / pdb_00002cm3
Title : Structure of Protein Tyrosine Phosphatase 1B (C2)
Authors : Ala, P.J.; Gonneville, L.; Hillman, M.C.; Becker-Pasha, M.; Wei, M.; Reid, B.G.; Klabe, R.; Yue, E.W.; Wayland, B.; Douty, B.; Combs, A.P.; Polam, P.; Wasserman, Z.; Bower, M.; Burn, T.C.; Hollis, G.F.; Wynn, R.
Deposited on : 2006-05-04
Resolution : 2.10 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
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

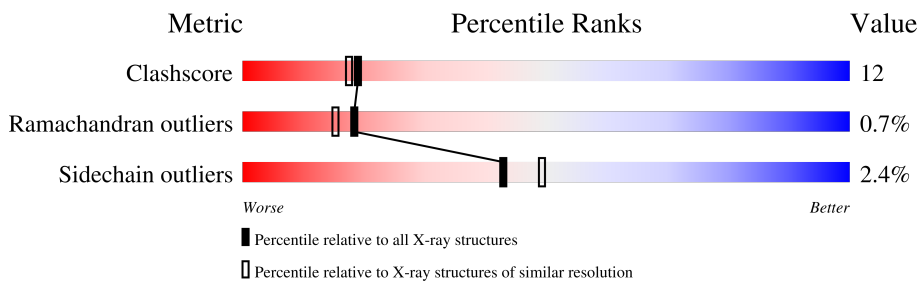
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	A	304	
1	B	304	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4983 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 TYROSINE-PROTEIN PHOSPHATASE NON-RECEPTOR TYPE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	1
			2237	1421	389	413	14			
1	B	275	Total	C	N	O	S	0	0	1
			2237	1421	389	413	14			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total	O	0	0
			244	244		
3	B	263	Total	O	0	0
			263	263		

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.85Å 95.50Å 70.75Å 90.00° 109.66° 90.00°	Depositor
Resolution (Å)	7.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.233 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4983	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: CA

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	0.54	1/2289 (0.0%)	1.00	9/3088 (0.3%)
1	B	0.52	1/2289 (0.0%)	0.98	6/3088 (0.2%)
All	All	0.53	2/4578 (0.0%)	0.99	15/6176 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	PHE	C-N	-5.60	1.25	1.33
1	A	280	PHE	C-N	-5.47	1.25	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	SER	CA-C-N	10.23	130.53	119.28
1	A	205	SER	C-N-CA	10.23	130.53	119.28
1	A	66	TYR	N-CA-C	7.13	121.29	109.46
1	B	75	GLU	N-CA-C	6.65	118.18	111.07
1	B	66	TYR	N-CA-C	6.38	120.28	110.20
1	A	32	CYS	N-CA-C	-6.09	103.13	110.44
1	B	177	THR	N-CA-C	5.99	120.71	113.17
1	A	215	CYS	N-CA-C	-5.62	98.84	110.80
1	B	211	VAL	N-CA-C	-5.55	102.42	109.58
1	B	259	GLY	N-CA-C	5.48	123.19	115.30
1	B	151	SER	N-CA-C	5.39	117.16	111.28
1	A	262	GLN	N-CA-C	5.36	119.80	113.16
1	A	120	LYS	N-CA-C	5.32	119.77	113.28
1	A	179	TRP	N-CA-C	-5.21	103.08	109.65
1	A	54	HIS	N-CA-C	5.04	118.69	112.54

There are no chirality outliers.

There are no planarity outliers.

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	A	2237	0	2213	52	0
1	B	2237	0	2213	53	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	244	0	0	5	0
3	B	263	0	0	4	0
All	All	4983	0	4426	105	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 (105) 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:40:ASN:HD21	1:A:64:ASN:HD21	1.15	0.92
1:A:114:MET:SD	1:A:119:LEU:HG	2.23	0.79
1:A:15:SER:O	1:A:19:ILE:HG12	1.81	0.79
1:B:153:TYR:HE2	1:B:155:VAL:HG23	1.50	0.77
1:B:153:TYR:CE2	1:B:155:VAL:HG23	2.24	0.72
1:B:32:CYS:HB2	3:B:2008:HOH:O	1.89	0.71
1:B:150:LYS:HD3	1:B:153:TYR:CZ	2.26	0.70
1:A:40:ASN:ND2	1:A:64:ASN:HD21	1.90	0.69
1:B:246:ILE:HD11	1:B:271:TYR:CE1	2.28	0.69
1:B:40:ASN:HD21	1:B:64:ASN:HD21	1.43	0.66
1:B:153:TYR:HE2	1:B:155:VAL:CG2	2.07	0.66
1:B:23:ILE:HD13	1:B:250:LEU:HD23	1.79	0.64
1:A:23:ILE:HD13	1:A:250:LEU:HD23	1.80	0.64
1:B:40:ASN:ND2	1:B:64:ASN:HD21	1.96	0.63
1:B:39:LYS:HE3	3:B:2051:HOH:O	1.99	0.63
1:A:152:TYR:CD2	1:A:190:SER:HB2	2.34	0.63
1:B:82:ILE:HG13	1:B:210:PRO:HB2	1.81	0.62
1:B:279:LYS:O	1:B:280:PHE:HB2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLN:NE2	3:B:2131:HOH:O	2.31	0.62
1:A:199:ARG:NH2	1:A:233:LEU:HD13	2.16	0.61
1:B:79:ARG:NH1	1:B:204:LEU:HD13	2.15	0.60
1:A:89:PRO:HD3	3:A:2051:HOH:O	2.00	0.60
1:A:165:THR:OG1	1:A:167:GLU:HG3	2.02	0.59
1:A:75:GLU:HG2	3:A:2098:HOH:O	2.01	0.59
1:A:115:GLU:O	1:A:116:LYS:HB2	2.02	0.59
1:A:87:PRO:HG3	1:A:95:PHE:CD2	2.39	0.57
1:B:140:LEU:HD23	1:B:162:ASN:HA	1.86	0.57
1:B:133:MET:C	1:B:134:ILE:HD12	2.31	0.56
1:A:97:GLU:OE2	1:A:101:GLU:OE2	2.23	0.56
1:B:260:LEU:O	1:B:261:ILE:HB	2.04	0.56
1:A:194:PHE:O	1:A:198:VAL:HG23	2.06	0.55
1:A:270:SER:O	1:A:274:VAL:HG23	2.06	0.54
1:B:144:LEU:HA	1:B:158:LEU:HD23	1.90	0.54
1:A:22:ASP:O	1:A:26:GLU:HG3	2.07	0.54
1:B:165:THR:O	1:B:166:GLN:HB2	2.09	0.53
1:A:234:LEU:HB3	1:A:244:VAL:CG2	2.39	0.52
1:A:150:LYS:HD2	1:A:153:TYR:CZ	2.45	0.52
1:B:245:ASP:O	1:B:249:VAL:HG23	2.10	0.51
1:B:238:ARG:NH1	1:B:244:VAL:HA	2.26	0.51
1:B:15:SER:O	1:B:19:ILE:HG12	2.10	0.51
1:A:28:SER:HB3	3:A:2027:HOH:O	2.11	0.51
1:B:112:ARG:HH11	1:B:112:ARG:HG3	1.75	0.51
1:B:59:LEU:HB2	1:B:65:ASP:HA	1.93	0.51
1:A:255:LYS:HE3	3:A:2236:HOH:O	2.12	0.50
1:A:115:GLU:CD	1:A:221:ARG:HH12	2.19	0.49
1:B:72:ILE:HG13	1:B:256:PHE:HB2	1.95	0.49
1:B:22:ASP:OD2	1:B:26:GLU:OE1	2.31	0.48
1:B:258:MET:HG2	3:B:2071:HOH:O	2.14	0.48
1:A:12:LYS:C	1:A:14:GLY:H	2.22	0.48
1:A:265:ASP:HB2	3:A:2242:HOH:O	2.13	0.48
1:B:229:ASP:O	1:B:233:LEU:HD22	2.14	0.48
1:B:196:PHE:O	1:B:200:GLU:HG3	2.13	0.47
1:A:83:LEU:HD11	1:A:226:CYS:SG	2.55	0.47
1:A:234:LEU:HB3	1:A:244:VAL:HG21	1.95	0.47
1:B:79:ARG:HD2	1:B:229:ASP:OD2	2.15	0.47
1:B:161:GLU:HG3	1:B:168:THR:HG22	1.97	0.47
1:B:79:ARG:NH1	1:B:229:ASP:OD2	2.48	0.46
1:A:227:LEU:HD11	1:A:246:ILE:HG13	1.97	0.46
1:B:61:GLN:CD	1:B:64:ASN:O	2.59	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:HH11	1:A:33:ARG:HG2	1.80	0.46
1:A:111:ASN:HD21	1:A:121:CYS:HB3	1.79	0.46
1:B:272:LEU:HD22	1:B:276:GLU:HG2	1.98	0.46
1:A:132:GLU:OE1	1:A:132:GLU:N	2.39	0.45
1:A:224:THR:HG23	1:A:270:SER:OG	2.16	0.45
1:A:127:GLN:O	1:A:128:LYS:HD2	2.16	0.45
1:A:141:LYS:HB2	1:A:163:LEU:HD21	1.98	0.45
1:A:119:LEU:HD23	1:A:119:LEU:C	2.41	0.45
1:B:83:LEU:HD11	1:B:226:CYS:SG	2.57	0.45
1:B:275:ILE:O	1:B:278:ALA:HB3	2.17	0.45
1:A:260:LEU:O	1:A:261:ILE:HB	2.17	0.45
1:B:276:GLU:OE1	1:B:276:GLU:HA	2.17	0.44
1:B:197:LYS:HD2	1:B:197:LYS:HA	1.75	0.44
1:B:246:ILE:HG13	1:B:247:LYS:N	2.32	0.44
1:A:136:GLU:HA	1:A:136:GLU:OE1	2.18	0.44
1:A:150:LYS:HD2	1:A:153:TYR:CE1	2.53	0.44
1:B:21:GLN:NE2	1:B:21:GLN:HA	2.33	0.44
1:B:65:ASP:C	1:B:65:ASP:OD1	2.61	0.44
1:B:163:LEU:O	1:B:166:GLN:NE2	2.47	0.44
1:A:115:GLU:O	1:A:116:LYS:CB	2.65	0.44
1:B:204:LEU:HD23	1:B:211:VAL:HB	2.00	0.44
1:B:184:VAL:HG21	1:B:269:PHE:HB2	1.99	0.44
1:A:150:LYS:HB2	1:A:153:TYR:O	2.18	0.43
1:B:87:PRO:HG3	1:B:95:PHE:CD2	2.52	0.43
1:B:264:ALA:O	1:B:267:LEU:HB3	2.18	0.43
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.81	0.43
1:B:186:GLU:HG3	1:B:187:SER:N	2.32	0.43
1:A:184:VAL:HG21	1:A:269:PHE:HB2	2.01	0.43
1:A:152:TYR:OH	1:A:193:ASN:HB3	2.20	0.42
1:A:47:ARG:HG2	1:A:47:ARG:HH11	1.85	0.42
1:A:115:GLU:OE1	1:A:221:ARG:NH2	2.48	0.42
1:A:20:TYR:O	1:A:23:ILE:HB	2.20	0.41
1:A:162:ASN:O	1:A:166:GLN:N	2.54	0.41
1:A:197:LYS:HD3	1:A:197:LYS:HA	1.86	0.41
1:B:249:VAL:O	1:B:252:GLU:HB3	2.20	0.41
1:B:72:ILE:HD13	1:B:83:LEU:HD13	2.01	0.41
1:B:112:ARG:HG3	1:B:112:ARG:NH1	2.36	0.41
1:B:155:VAL:HG22	1:B:174:PHE:CD1	2.56	0.41
1:A:77:ALA:CB	1:A:230:THR:HG23	2.51	0.41
1:A:115:GLU:HB2	1:A:120:LYS:CG	2.49	0.41
1:B:260:LEU:O	1:B:261:ILE:CB	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:HE2	1:A:182:PHE:CZ	2.56	0.40
1:A:145:ILE:HD13	1:A:145:ILE:HA	1.85	0.40
1:A:161:GLU:HG3	1:A:167:GLU:O	2.21	0.40
1:A:246:ILE:HG23	1:A:271:TYR:CZ	2.56	0.40
1:B:26:GLU:O	1:B:27:ALA:C	2.63	0.40

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	273/304 (90%)	253 (93%)	18 (7%)	2 (1%)	18	15
1	B	273/304 (90%)	257 (94%)	14 (5%)	2 (1%)	18	15
All	All	546/608 (90%)	510 (93%)	32 (6%)	4 (1%)	18	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
1	B	280	PHE
1	A	261	ILE
1	B	261	ILE

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	248/277 (90%)	242 (98%)	6 (2%)	43	49
1	B	248/277 (90%)	242 (98%)	6 (2%)	43	49
All	All	496/554 (90%)	484 (98%)	12 (2%)	43	49

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	28	SER
1	A	41	LYS
1	A	139	ASN
1	A	193	ASN
1	A	233	LEU
1	B	139	ASN
1	B	186	GLU
1	B	233	LEU
1	B	246	ILE
1	B	247	LYS
1	B	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	21	GLN
1	A	40	ASN
1	A	61	GLN
1	A	111	ASN
1	A	139	ASN
1	A	157	GLN
1	B	21	GLN
1	B	40	ASN
1	B	44	ASN
1	B	102	GLN
1	B	139	ASN
1	B	166	GLN

5.3.3 RNA ⓘ

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 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

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.