



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:43 PM GMT

PDB ID : 1C87
Title : CRYSTAL STRUCTURE OF PROTEIN TYROSINE PHOSPHATASE 1B
COMPLEXED WITH 2-(OXALYL-AMINO-4,7-DIHYDRO-5H-THIENO[2,3
-C]PYRAN-3-CARBOXYLIC ACID
Authors : Iversen, L.F.; Andersen, H.S.; Mortensen, S.B.; Moller, N.P.
Deposited on : 2000-04-16
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

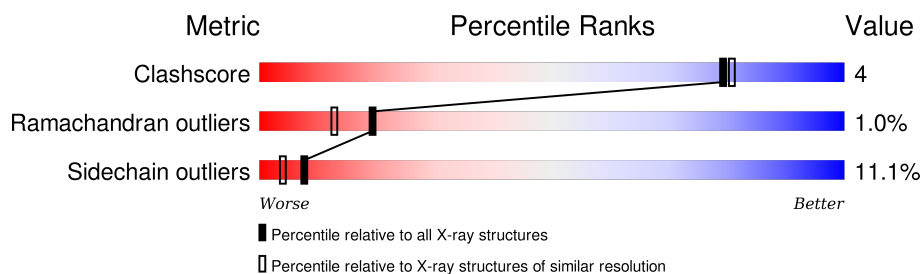
1 Overall quality at a glance

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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	298	 71% 21% 6% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2628 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.

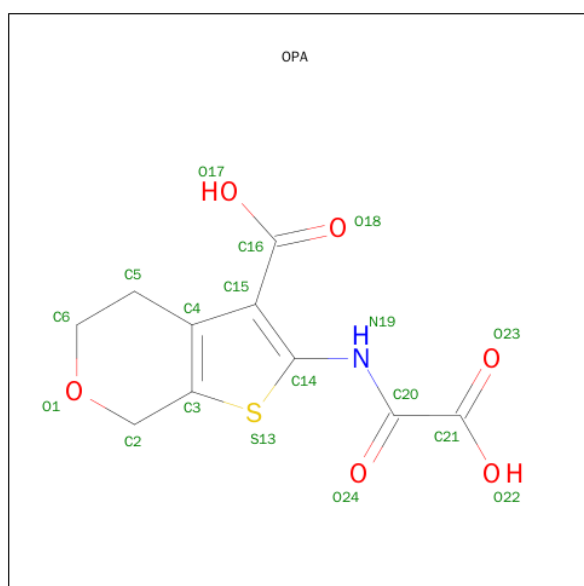
- Molecule 1 is a protein called PROTEIN (PROTEIN-TYROSINE PHOSPHATASE 1B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2427	1535	418	458	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	THR	SER	CONFLICT	UNP P18031
A	252	ASP	GLU	CONFLICT	UNP P18031

- Molecule 2 is 2-(OXALYL-AMINO)-4,7-DIHYDRO-5H-THIENO[2,3-C]PYRAN-3-CARBOXYLIC ACID (three-letter code: OPA) (formula: C₁₀H₉NO₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			18	10	1	6	1		

- Molecule 3 is water.

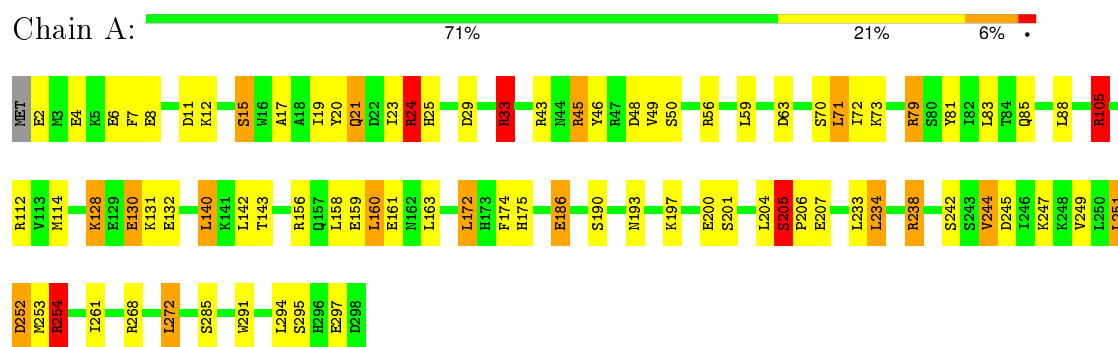
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	183	Total 183	O 183	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: PROTEIN (PROTEIN-TYROSINE PHOSPHATASE 1B)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.90 Å 87.90 Å 103.09 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.10	Depositor
% Data completeness (in resolution range)	98.4 (6.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.194 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2628	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: OPA

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	1.24	13/2482 (0.5%)	1.66	40/3345 (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	9

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	SER	CB-OG	8.07	1.52	1.42
1	A	21	GLN	CG-CD	6.04	1.65	1.51
1	A	285	SER	CB-OG	5.92	1.50	1.42
1	A	186	GLU	CG-CD	5.84	1.60	1.51
1	A	50	SER	CB-OG	5.80	1.49	1.42
1	A	24	ARG	NE-CZ	5.55	1.40	1.33
1	A	252	ASP	CB-CG	5.52	1.63	1.51
1	A	161	GLU	CD-OE1	-5.33	1.19	1.25
1	A	190	SER	CB-OG	5.22	1.49	1.42
1	A	15	SER	CB-OG	5.18	1.49	1.42
1	A	70	SER	CB-OG	5.08	1.48	1.42
1	A	201	SER	CB-OG	5.06	1.48	1.42
1	A	50	SER	C-O	-5.06	1.13	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ARG	NE-CZ-NH1	15.99	128.29	120.30
1	A	254	ARG	NE-CZ-NH2	-12.70	113.95	120.30
1	A	33	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	A	268	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	A	79	ARG	NE-CZ-NH2	-10.99	114.81	120.30
1	A	43	ARG	NE-CZ-NH1	10.89	125.75	120.30
1	A	24	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	A	81	TYR	CB-CG-CD1	-9.19	115.49	121.00
1	A	25	HIS	CA-CB-CG	-8.93	98.43	113.60
1	A	56	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	A	252	ASP	CB-CG-OD2	8.48	125.93	118.30
1	A	156	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	79	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	A	160	LEU	CB-CG-CD2	7.16	123.17	111.00
1	A	132	GLU	CB-CA-C	-7.09	96.22	110.40
1	A	238	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	A	70	SER	CB-CA-C	-6.47	97.81	110.10
1	A	140	LEU	CB-CG-CD1	6.35	121.80	111.00
1	A	8	GLU	CB-CA-C	6.09	122.59	110.40
1	A	33	ARG	NH1-CZ-NH2	6.08	126.09	119.40
1	A	234	LEU	CB-CG-CD1	5.99	121.19	111.00
1	A	114	MET	CG-SD-CE	-5.88	90.79	100.20
1	A	21	GLN	CB-CG-CD	5.79	126.64	111.60
1	A	43	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	244	VAL	CA-CB-CG1	5.67	119.41	110.90
1	A	297	GLU	N-CA-CB	5.66	120.79	110.60
1	A	29	ASP	N-CA-CB	-5.56	100.59	110.60
1	A	200	GLU	N-CA-CB	-5.45	100.80	110.60
1	A	156	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	114	MET	CA-CB-CG	-5.37	104.17	113.30
1	A	112	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	245	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	130	GLU	CB-CA-C	-5.25	99.90	110.40
1	A	143	THR	OG1-CB-CG2	-5.21	98.02	110.00
1	A	48	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	252	ASP	N-CA-CB	5.09	119.77	110.60
1	A	193	ASN	CB-CA-C	5.09	120.57	110.40
1	A	24	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	253	MET	CG-SD-CE	-5.06	92.10	100.20
1	A	45	ARG	NE-CZ-NH2	5.02	122.81	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	204	LEU	Peptide
1	A	205	SER	Peptide
1	A	238	ARG	Sidechain
1	A	24	ARG	Sidechain
1	A	254	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	46	TYR	Sidechain
1	A	79	ARG	Sidechain

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	2427	0	2381	17	0
2	A	18	0	7	0	0
3	A	183	0	0	0	0
All	All	2628	0	2388	17	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 (17) 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:45:ARG:H	1:A:85:GLN:HE22	1.50	0.57
1:A:17:ALA:O	1:A:21:GLN:HG3	2.06	0.56
1:A:2:GLU:HG3	1:A:4:GLU:H	1.74	0.52
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.75	0.52
1:A:45:ARG:H	1:A:85:GLN:NE2	2.07	0.52
1:A:7:PHE:CZ	1:A:272:LEU:HD13	2.48	0.48
1:A:6:GLU:CD	1:A:247:LYS:HZ2	2.18	0.47
1:A:205:SER:O	1:A:207:GLU:N	2.48	0.46
1:A:71:LEU:HD13	1:A:73:LYS:HB2	1.98	0.45
1:A:291:TRP:O	1:A:295:SER:HB3	2.16	0.45
1:A:172:LEU:HB3	1:A:174:PHE:CE1	2.51	0.45
1:A:23:ILE:HG23	1:A:251:LEU:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:SER:O	1:A:19:ILE:HG12	2.19	0.43
1:A:128:LYS:HE2	1:A:128:LYS:HB3	1.75	0.42
1:A:142:LEU:HA	1:A:159:GLU:O	2.21	0.41
1:A:83:LEU:N	1:A:83:LEU:HD12	2.36	0.41
1:A:20:TYR:CE2	1:A:24:ARG:HD2	2.56	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	295/298 (99%)	280 (95%)	12 (4%)	3 (1%)	19 13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	261	ILE
1	A	206	PRO

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	270/271 (100%)	240 (89%)	30 (11%)	8 4

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	12	LYS
1	A	33	ARG
1	A	49	VAL
1	A	59	LEU
1	A	71	LEU
1	A	72	ILE
1	A	88	LEU
1	A	105	ARG
1	A	128	LYS
1	A	130	GLU
1	A	131	LYS
1	A	140	LEU
1	A	158	LEU
1	A	160	LEU
1	A	163	LEU
1	A	172	LEU
1	A	175	HIS
1	A	186	GLU
1	A	197	LYS
1	A	205	SER
1	A	233	LEU
1	A	234	LEU
1	A	244	VAL
1	A	249	VAL
1	A	251	LEU
1	A	252	ASP
1	A	254	ARG
1	A	272	LEU
1	A	294	LEU

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

Mol	Chain	Res	Type
1	A	61	GLN
1	A	85	GLN
1	A	111	ASN
1	A	139	ASN
1	A	175	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	OPA	A	301	-	10,19,19	1.60	2 (20%)	3,27,27	2.93	1 (33%)

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	OPA	A	301	-	-	0/2/19/19	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	OPA	C15-C14	-2.88	1.34	1.41
2	A	301	OPA	C15-C4	3.34	1.47	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	301	OPA	C6-C5-C4	-4.85	102.98	110.62

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.