

Full wwPDB X-ray Structure Validation Report (i)

Jan 18, 2024 – 12:31 AM EST

PDB ID : 7GTP

Title : PanDDA Analysis group deposition – Crystal structure of PTP1B in complex

with FMOPL000688a

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Deposited on : 2024-01-03

Resolution : 2.47 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 (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: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

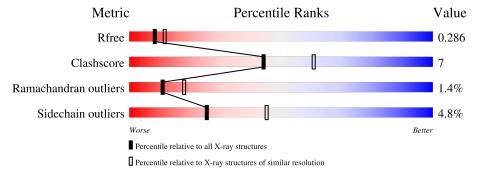
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 2.47 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	Similar resolution
Medit	$(\# {\rm Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)

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%

Mol	Chain	Length	Quality of chain			
1	A	321	77%	14%	• 79	%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5088 atoms, of which 2423 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.

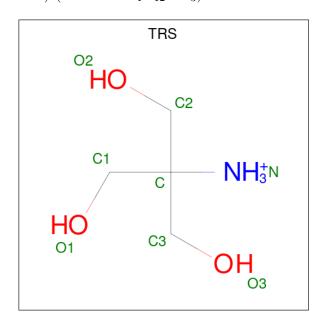
• Molecule 1 is a protein called Tyrosine-protein phosphatase non-receptor type 1.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	A	297	Total 4829	C 1538	H 2402	N 418	O 456	S 15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	SER	CYS	engineered mutation	UNP P18031
A	92	VAL	CYS	engineered mutation	UNP P18031

• Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).

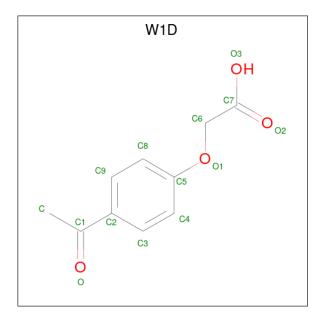


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	Λ	1	Total	С	Н	N	О	0	0
	Α	1	20	4	12	1	3		U

• Molecule 3 is (4-acetylphenoxy)acetic acid (three-letter code: W1D) (formula: $C_{10}H_{10}O_4$)



(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
3	A	1	Total 23	C 10	H 9	O 4	0	0

• Molecule 4 is water.

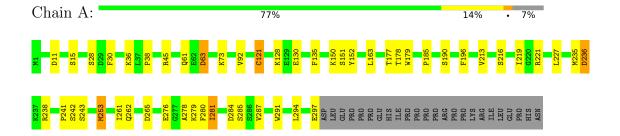
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	214	Total O 216 216	0	4



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. 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. 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: Tyrosine-protein phosphatase non-receptor type 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	90.10Å 90.10Å 107.17Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	78.03 - 2.47	Depositor
resolution (A)	78.03 - 2.47	EDS
% Data completeness	100.0 (78.03-2.47)	Depositor
(in resolution range)	99.9 (78.03-2.47)	EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.04 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.196 , 0.252	Depositor
it, it free	0.264 , 0.286	DCC
R_{free} test set	725 reflections (3.92%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30, 50.2	EDS
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5088	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: TRS, W1D

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).

Т	- 1	Chain	Bond	$\mathbf{lengths}$	Bond angles		
101	Mol Ch	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	1	A	0.69	0/2482	0.77	0/3345	

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	2427	2402	2393	31	2
2	A	8	12	12	1	2
3	A	14	9	0	0	0
4	A	216	0	0	8	1
All	All	2665	2423	2405	32	3

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 7.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	$overlap(\AA)$
1:A:196:PHE:CE2	1:A:291:TRP:CZ3	2.61	0.89
1:A:73:LYS:HE3	4:A:563:HOH:O	1.80	0.81
1:A:73:LYS:HE2	4:A:506:HOH:O	1.95	0.66
2:A:401:TRS:O1	4:A:506:HOH:O	2.14	0.65
1:A:128:LYS:NZ	4:A:509:HOH:O	2.30	0.64
1:A:92:VAL:HG12	1:A:135:PHE:CE1	2.34	0.62
1:A:38:PRO:HD2	4:A:543:HOH:O	2.00	0.60
1:A:280:PHE:CE2	1:A:285:SER:HA	2.40	0.56
1:A:227:LEU:HB2	1:A:253:MET:HE1	1.88	0.55
1:A:196:PHE:HE2	1:A:291:TRP:CZ3	2.18	0.55
1:A:61:GLN:OE1	1:A:63:ASP:HB3	2.08	0.53
1:A:276:GLU:O	1:A:279:LYS:HG3	2.09	0.52
1:A:196:PHE:CE2	1:A:291:TRP:HZ3	2.21	0.51
1:A:151:SER:OG	1:A:297:GLU:HA	2.11	0.51
1:A:163:LEU:O	4:A:507:HOH:O	2.18	0.48
1:A:45:ARG:NH2	1:A:121:CYS:HA	2.28	0.48
1:A:28:SER:HB3	1:A:30:PHE:CE2	2.48	0.48
1:A:227:LEU:HD13	1:A:253:MET:HE2	1.97	0.46
1:A:219:ILE:HD12	1:A:262:GLN:NE2	2.30	0.46
1:A:235:MET:HE1	1:A:278:ALA:HB1	1.99	0.45
1:A:284:ASP:O	1:A:287:VAL:HG12	2.17	0.45
1:A:92:VAL:CG1	1:A:135:PHE:CE1	2.99	0.45
1:A:280:PHE:HB2	1:A:287:VAL:CG1	2.45	0.45
1:A:280:PHE:HB2	1:A:287:VAL:HG11	2.00	0.44
1:A:179:TRP:CE2	1:A:185:PRO:HD3	2.52	0.44
1:A:36:LYS:HD2	4:A:628:HOH:O	2.20	0.41
1:A:179:TRP:CE2	1:A:221:ARG:HG2	2.55	0.41
1:A:152:TYR:O	1:A:177:THR:OG1	2.28	0.41
1:A:278:ALA:C	1:A:280:PHE:H	2.24	0.41
1:A:236:ASP:CG	1:A:281:ILE:HG23	2.40	0.41
1:A:235:MET:HG2	1:A:241:PRO:HA	2.02	0.41
1:A:294:LEU:HB3	4:A:615:HOH:O	2.20	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:130:GLU:OE2	2:A:401:TRS:O2[4_565]	1.76	0.44
1:A:130:GLU:OE2	2:A:401:TRS:HO2[4_565]	1.45	0.15
4:A:521:HOH:O	4:A:651:HOH:O[3_454]	2.19	0.01



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	295/321 (92%)	276 (94%)	15 (5%)	4 (1%)	11 18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	261	ILE
1	A	243	SER
1	A	281	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.

ľ	Mol	Chain	Analysed	Analysed Rotameric		Percentiles	
	1	A	270/294 (92%)	257 (95%)	13 (5%)	25	45

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	15	SER
1	A	121	CYS
1	A	150	LYS
1	A	178	THR
1	A	190	SER
1	A	213	VAL

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Mol	Chain	Res	Type
1	A	216	SER
1	A	236	ASP
1	A	238	ARG
1	A	242	SER
1	A	253	MET
1	A	265	ASP

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	Trme	Chain	Dag	Link	Bond lengths			В	ond ang	cles
IVIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	W1D	A	402	-	14,14,14	1.51	2 (14%)	18,18,18	1.56	3 (16%)
2	TRS	A	401	-	7,7,7	0.31	0	9,9,9	0.49	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
3	W1D	A	402	-	-	4/9/9/9	0/1/1/1
2	TRS	A	401	-	-	3/9/9/9	-

All (2) bond length outliers are listed below:

	Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
	3	A	402	W1D	C6-C7	4.42	1.62	1.50
İ	3	A	402	W1D	C8-C5	2.05	1.42	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	402	W1D	C8-C5-C4	-3.05	115.47	120.18
3	A	402	W1D	C6-O1-C5	2.08	121.32	117.67
3	A	402	W1D	C9-C2-C3	-2.05	115.66	118.59

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	TRS	C1-C-C2-O2
2	A	401	TRS	C3-C-C2-O2
2	A	401	TRS	N-C-C2-O2
3	A	402	W1D	C-C1-C2-C3
3	A	402	W1D	C-C1-C2-C9
3	A	402	W1D	O-C1-C2-C9
3	A	402	W1D	O-C1-C2-C3

There are no ring outliers.

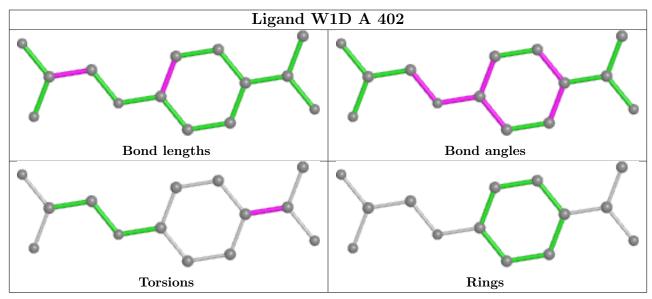
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	TRS	1	2

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is



within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

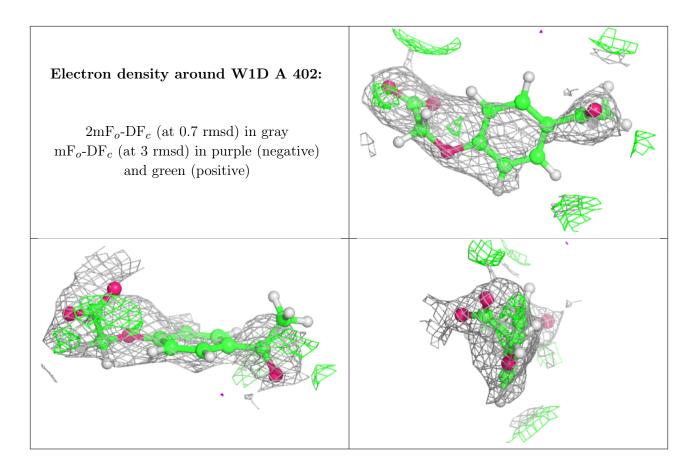
Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.





6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

