



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:41 PM GMT

PDB ID : 2B07
Title : Crystal structure of PTP1B with Tricyclic Thiophene inhibitor.
Authors : Moretto, A.F.; Kirincich, S.J.; Xu, W.X.; Smith, M.J.; Wan, Z.K.; Wilson, D.P.; Follows, B.C.; Binnun, E.; Joseph-McCarthy, D.; Foreman, K.; Erbe, D.V.; Zhang, Y.L.; Tam, S.K.; Tam, S.Y.; Lee, J.
Deposited on : 2005-09-13
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

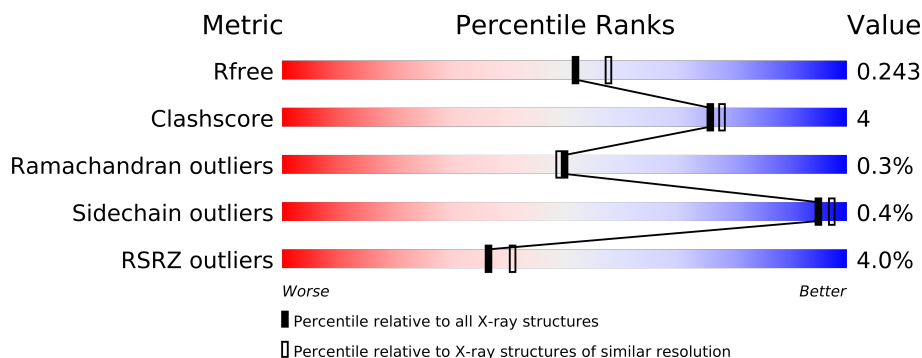
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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))
R_{free}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	299	

2 Entry composition i

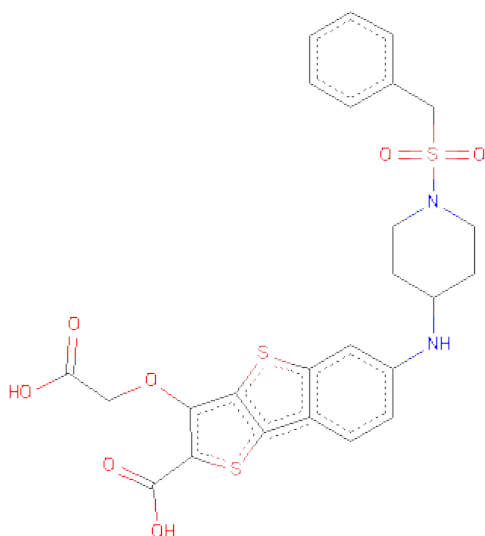
There are 3 unique types of molecules in this entry. The entry contains 2639 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			Total	C	N	O	S			
1	A	297	2426	1535	418	457	16	0	0	0

- Molecule 2 is 6-{[1-(BENZYLSULFONYL)PIPERIDIN-4-YL]AMINO}-3-(CARBOXYMETHOXY)THIENO[3,2-B][1]BENZOTHIOPHENE-2-CARBOXYLICACID (three-letter code: 598) (formula: C₂₅H₂₄N₂O₇S₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	37	25	2	7	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	176	Total	O	0	0
			176	176		

i

- Molecule 1: Tyrosine-protein phosphatase, non-receptor type 1

Amino Acid	Relative Abundance (%)	Modification
Met	~1	None
E2	~1	None
M3	~1	None
E6	~1	None
I10	~1	None
D11	~1	None
K12	~1	None
D22	~1	None
H25	~1	None
R33	~1	None
R47	~1	None
Q61	~1	None
E62	~1	None
D63	~1	None
L83	~1	None
R105	~1	None
G106	~1	None
V107	~1	None
V108	~1	None
M109	~1	None
E115	~1	None
K120	~1	None
L140	~1	None
M162	~1	None
E170	~1	None
H176	~1	None
E186	~1	None
H214	~1	None
C226	~1	None
M235	~1	None
P241	~1	None
T246	~1	None
V249	~1	None
M253	~1	None
T261	~1	None
R262	~1	None
L267	~1	None
E283	~1	None
D286	~1	None
Leu	~1	None

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.24Å 88.24Å 104.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.63 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.10) 96.6 (19.63-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.09Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.241 0.209 , 0.243	Depositor DCC
R_{free} test set	1309 reflections (4.87%)	DCC
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.7	EDS
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 26939 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2639	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 598

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	0.46	0/2481	0.53	0/3344

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	HIS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2426	0	2381	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	37	0	22	1	0
3	A	176	0	0	1	0
All	All	2639	0	2403	19	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (19) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:MET:CE	1:A:246:ILE:HD11	1.77	1.14
1:A:3:MET:HE2	1:A:246:ILE:HD11	1.66	0.78
1:A:3:MET:HE1	1:A:246:ILE:HD11	1.65	0.77
1:A:3:MET:CE	1:A:246:ILE:CD1	2.63	0.72
1:A:186:GLU:HG3	3:A:386:HOH:O	1.96	0.65
1:A:6:GLU:O	1:A:10:ILE:HG13	1.97	0.64
1:A:3:MET:HE2	1:A:246:ILE:CD1	2.30	0.57
1:A:3:MET:HE3	1:A:246:ILE:HD11	1.82	0.51
1:A:105:ARG:NH1	1:A:170:GLU:HB3	2.29	0.48
1:A:105:ARG:HG3	1:A:105:ARG:O	2.16	0.45
1:A:3:MET:HB2	1:A:3:MET:HE2	1.81	0.44
1:A:140:LEU:HD23	1:A:162:ASN:HA	1.99	0.44
1:A:262:GLN:HG3	2:A:301:598:S18	2.58	0.43
1:A:109:MET:HG2	1:A:175:HIS:CD2	2.53	0.43
1:A:235:MET:HG3	1:A:241:PRO:HA	2.00	0.43
1:A:115:GLU:HB2	1:A:120:LYS:HG3	2.01	0.42
1:A:249:VAL:O	1:A:253:MET:HG3	2.19	0.42
1:A:2:GLU:OE1	1:A:2:GLU:HA	2.20	0.41
1:A:83:LEU:HD11	1:A:226:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	295/299 (99%)	288 (98%)	6 (2%)	1 (0%)	50	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	ILE

5.3.2 Protein sidechains ⓘ

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	270/272 (99%)	269 (100%)	1 (0%)	95	97

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

Mol	Chain	Res	Type
1	A	105	ARG

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

5.3.3 RNA ⓘ

There are no RNA chains 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	598	A	301	-	41,41,41	1.99	8 (19%)	55,60,60	3.49	7 (12%)

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	598	A	301	-	-	0/19/34/34	0/2/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	598	S44-N32	9.15	1.73	1.63
2	A	301	598	C33-N32	3.27	1.51	1.47
2	A	301	598	C31-N32	2.91	1.51	1.47
2	A	301	598	C4-C5	-2.76	1.37	1.40
2	A	301	598	C2-C6	2.59	1.56	1.49
2	A	301	598	C21-C19	2.40	1.41	1.37
2	A	301	598	O60-S44	2.31	1.45	1.43
2	A	301	598	C24-C23	2.09	1.41	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	598	C2-C3-C4	-21.34	110.04	119.29
2	A	301	598	C21-C19-C20	-7.73	119.18	123.24
2	A	301	598	C45-S44-N32	-5.70	100.73	107.16
2	A	301	598	O8-C6-C2	-5.49	113.03	123.11
2	A	301	598	C20-C19-S18	5.14	114.10	111.69
2	A	301	598	C2-S1-C5	-3.27	89.91	91.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	598	C20-C5-C4	2.91	115.01	109.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	297/299 (99%)	0.02	12 (4%) 36 41	36, 49, 70, 82	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	LYS	4.5
1	A	62	GLU	3.7
1	A	293	GLU	3.2
1	A	63	ASP	3.1
1	A	22	ASP	2.8
1	A	25	HIS	2.5
1	A	33	ARG	2.4
1	A	267	LEU	2.3
1	A	47	ARG	2.1
1	A	61	GLN	2.0
1	A	298	ASP	2.0
1	A	107	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	598	A	301	37/37	0.16	1.06	51,57,74,75	0

6.5 Other polymers ⓘ

There are no such residues in this entry.