

wwPDB X-ray Structure Validation Summary Report (i)

Nov 3, 2020 – 02:07 PM EST

PDB ID	:	5RX1
Title	:	INPP5D PanDDA analysis group deposition – Crystal Structure of the phos-
		phatase and C2 domains of SHIP1 in complex with $Z2466069494$
Authors	:	Bradshaw, W.J.; Newman, J.A.; von Delft, F.; Arrowsmith, C.H.; Edwards,
		A.M.; Bountra, C.; Gileadi, O.
Deposited on	:	2020-10-30
Resolution	:	1.31 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 following versions of software and data (see references (1)) were used in the production of this report:

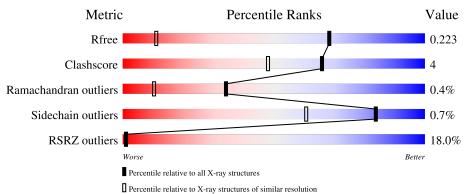
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 1.31 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	$\begin{array}{l} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1611 (1.34-1.30)
Clashscore	141614	1667 (1.34-1.30)
Ramachandran outliers	138981	1615 (1.34-1.30)
Sidechain outliers	138945	1615 (1.34-1.30)
RSRZ outliers	127900	1580 (1.34-1.30)

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 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	
			18%	_
1	А	463	92%	7%•



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2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4743 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.

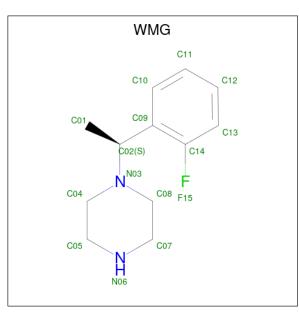
• Molecule 1 is a protein called Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	460	Total 4260	C 2695	N 727	0 818	S 20	0	33	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	394	SER	-	expression tag	UNP Q92835
А	395	MET	-	expression tag	UNP Q92835

• Molecule 2 is 1-[(1S)-1-(2-fluorophenyl)ethyl]piperazine (three-letter code: WMG) (formula: $C_{12}H_{17}FN_2$).

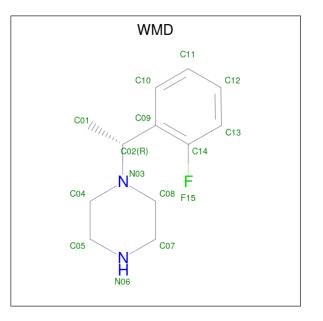


Mol	Chain	Residues	Α	ton	ıs		ZeroOcc	AltConf
2	А	1	Total 15	C 12	F 1	N 2	0	0

• Molecule 3 is 1-[(1R)-1-(2-fluorophenyl)ethyl] piperazine (three-letter code: WMD) (formula:

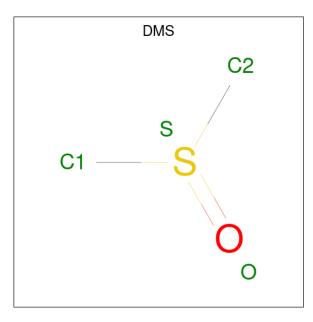


$\mathrm{C}_{12}\mathrm{H}_{17}\mathrm{FN}_2).$



Mol	Chain	Residues	A	aton	ıs		ZeroOcc	AltConf
3	А	1	Total 15	C 12	F 1	N 2	0	0

• Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0

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Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
4	А	1	Total 4	С 2	0 1	S 1	0	0

• Molecule 5 is water.

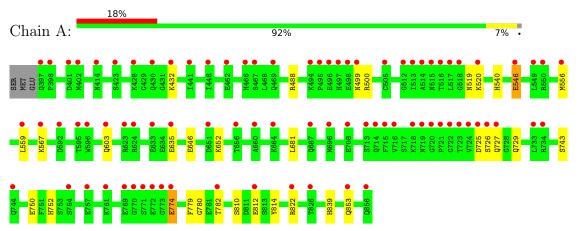
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	437	Total O 441 441	0	8



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: Phosphatidylinositol 3,4,5-trisphosphate 5-phosphatase 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	62.67Å 79.21Å 89.50Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.12 – 1.31	Depositor
Resolution (A)	43.08 - 1.31	EDS
% Data completeness	100.0 (43.12-1.31)	Depositor
(in resolution range)	$100.0 \ (43.08-1.31)$	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.56 (at 1.31 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
D D	0.175 , 0.197	Depositor
R, R_{free}	0.202 , 0.223	DCC
R_{free} test set	5335 reflections (4.97%)	wwPDB-VP
Wilson B-factor $(Å^2)$	14.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 41.6	EDS
L-test for twinning ²	$ \langle L \rangle = 0.51, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4743	wwPDB-VP
Average B, all atoms $(Å^2)$	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: DMS, WMG, WMD

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	
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.77	0/4358	0.88	2/5885~(0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	488	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	А	500	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	А	4260	0	4157	34	0
2	А	15	0	0	0	0
3	А	15	0	0	0	0
4	А	12	0	18	0	0
5	А	441	0	0	9	1
All	All	4743	0	4175	34	1

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.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HD2	5:A:1258:HOH:O	1.50	1.10
1:A:810:SER:OG	1:A:812:GLU:HG2	1.73	0.88
1:A:774:GLU:HB3	5:A:1375:HOH:O	1.79	0.82
1:A:546[A]:GLU:CD	1:A:546[A]:GLU:H	1.90	0.75
1:A:546[C]:GLU:H	1:A:546[C]:GLU:CD	1.90	0.75

The worst 5 of 34 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
5:A:1010:HOH:O	5:A:1246:HOH:O[4_455]	1.81	0.39

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	А	524/463~(113%)	511 (98%)	11 (2%)	2~(0%)	34	10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	726	SER
1	А	780	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

I	Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
	1	А	479/417~(115%)	474 (99%)	5 (1%)	76 47	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	546[A]	GLU
1	А	546[B]	GLU
1	А	546[C]	GLU
1	А	743	SER
1	А	774	GLU

Some side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such side chains are listed below:

Mol	Chain	Res	Type
1	А	515	ASN
1	А	752	HIS
1	А	519	ASN
1	А	508	ASN
1	А	616	HIS

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)

5 ligands are modelled in this entry.



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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	l Type Chain Res Link		Tiple	Bond lengths			Bond angles			
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	DMS	А	903	-	3,3,3	0.53	0	3,3,3	0.62	0
4	DMS	А	904	-	3,3,3	0.36	0	3,3,3	0.55	0
4	DMS	А	905	-	$3,\!3,\!3$	0.20	0	3,3,3	0.28	0
3	WMD	А	902	-	16,16,16	2.41	3 (18%)	19,21,21	1.35	3 (15%)
2	WMG	А	901	-	16,16,16	2.38	3 (18%)	19,21,21	1.51	3 (15%)

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	WMD	А	902	-	-	3/8/16/16	0/2/2/2
2	WMG	А	901	-	-	2/8/16/16	0/2/2/2

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	902	WMD	C02-N03	-8.47	1.28	1.48
2	А	901	WMG	C02-N03	-8.24	1.28	1.48
2	А	901	WMG	C04-N03	-2.64	1.42	1.47
3	А	902	WMD	C04-N03	-2.55	1.42	1.47
2	А	901	WMG	C08-N03	-2.24	1.42	1.47

The worst 5 of 6 bond length outliers are listed below:

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	901	WMG	C13-C14-C09	-3.44	119.89	123.72
3	А	902	WMD	C09-C02-N03	2.41	116.14	110.89
3	А	902	WMD	C13-C14-C09	-2.40	121.05	123.72
2	А	901	WMG	C07-C08-N03	2.31	114.00	109.92
2	А	901	WMG	C01-C02-C09	-2.29	106.71	112.72

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
3	А	902	WMD	N03-C02-C09-C10
3	А	902	WMD	N03-C02-C09-C14
2	А	901	WMG	N03-C02-C09-C10
2	А	901	WMG	N03-C02-C09-C14
3	А	902	WMD	C01-C02-N03-C04

All (5) torsion outliers are listed below:

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, 95^{th} 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	А	460/463~(99%)	1.07	83 (18%)	1	1	9, 16, 46, 84	45 (9%)

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	771	SER	15.5
1	А	559[A]	LEU	15.0
1	А	448[A]	ILE	14.9
1	А	505[A]	CYS	12.6
1	А	556[A]	MET	11.4

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 monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	WMD	А	902	15/15	0.50	0.34	$26,\!28,\!29,\!30$	15
2	WMG	А	901	15/15	0.71	0.23	17,18,20,20	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	DMS	А	905	4/4	0.98	0.07	$15,\!15,\!15,\!17$	0
4	DMS	А	903	4/4	0.98	0.08	16,18,18,19	0
4	DMS	А	904	4/4	0.98	0.06	$16,\!18,\!18,\!19$	0

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6.5 Other polymers (i)

There are no such residues in this entry.

