

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	4ZZX
Title	:	Structure of PARP2 catalytic domain bound to an isoindolinone inhibitor
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Deposited on	:	2015-04-15
Resolution	:	1.65 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

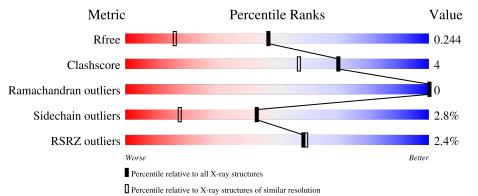
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 1.65 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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% 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					
1	А	363	89%	6% • •				
1	В	363	3% 89%	6% • •				

Validation Pipeline (wwPDB-VP) : 2.36



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5927 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.

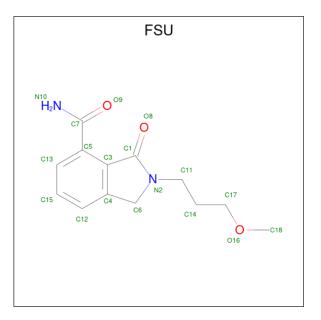
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	351	Total	С	Ν	0	\mathbf{S}	0	1	0
	A	591	2799	1781	482	517	19	0	L	0
1	D	349	Total	С	Ν	0	S	0	0	0
	D	049	2780	1770	480	511	19	0	0	0

• Molecule 1 is a protein called POLY [ADP-RIBOSE] POLYMERASE 2.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	GLY	-	expression tag	UNP Q9UGN5
А	222	PRO	-	expression tag	UNP Q9UGN5
В	221	GLY	-	expression tag	UNP Q9UGN5
В	222	PRO	-	expression tag	UNP Q9UGN5

• Molecule 2 is 2-(3-methoxypropyl)-3-oxo-2,3-dihydro-1H-isoindole-4-carboxamide (three-letter code: FSU) (formula: $C_{13}H_{16}N_2O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C N O 18 13 2 3	0	0
2	В	1	Total C N O 18 13 2 3	0	0

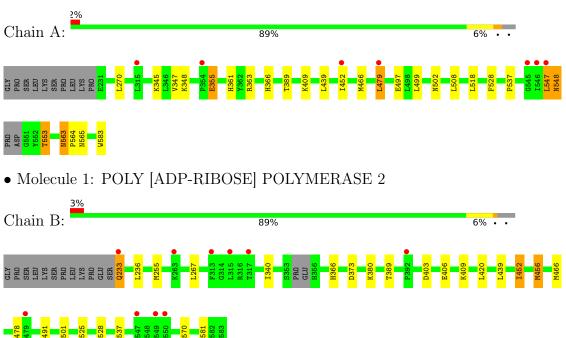
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	163	Total O 163 163	0	0
3	В	149	Total O 149 149	0	0



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: POLY [ADP-RIBOSE] POLYMERASE 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	72.46Å 72.74Å 141.34Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.67 - 1.65	Depositor
Resolution (A)	41.53 - 1.65	EDS
% Data completeness	99.5 (30.67 - 1.65)	Depositor
(in resolution range)	99.5 (41.53 - 1.65)	EDS
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.26 (at 1.65 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.213 , 0.244	Depositor
It, Itfree	0.212 , 0.244	DCC
R_{free} test set	4478 reflections (5.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	18.4	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 24.3	EDS
L-test for $twinning^2$	$< L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	0.070 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5927	wwPDB-VP
Average B, all atoms $(Å^2)$	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.82% 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: FSU

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	Bo	nd lengths	Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.51	1/2861~(0.0%)	0.62	0/3862
1	В	0.51	0/2839	0.61	0/3833
All	All	0.51	1/5700~(0.0%)	0.61	0/7695

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	583	TRP	CD2-CE2	5.15	1.47	1.41

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	А	2799	0	2810	20	0
1	В	2780	0	2792	20	0
2	А	18	0	16	0	0
2	В	18	0	16	0	0
3	А	163	0	0	3	0
3	В	149	0	0	6	0
All	All	5927	0	5634	40	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.

The worst 5 of 40 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:B:456:MET:HA	1:B:456:MET:HE3	1.29	1.10
1:B:456:MET:HA	1:B:456:MET:CE	1.90	1.01
1:B:406:GLU:HG3	1:B:570:ARG:HH12	1.42	0.83
1:A:479:LEU:H	1:A:479:LEU:HD12	1.53	0.73
1:A:563:ASN:HD22	1:A:565:ASN:H	1.36	0.72

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	Perce	\mathbf{ntiles}
1	А	348/363~(96%)	344~(99%)	4 (1%)	0	100	100
1	В	345/363~(95%)	338~(98%)	7 (2%)	0	100	100
All	All	693/726~(96%)	682~(98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	А	306/316~(97%)	297~(97%)	9~(3%)	42 16
1	В	303/316~(96%)	295~(97%)	8 (3%)	46 21
All	All	609/632~(96%)	592~(97%)	17 (3%)	43 18

5 of 17 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	452	ILE
1	В	525	SER
1	А	553	THR
1	А	563	ASN
1	В	233	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	510	GLN
1	В	366	HIS
1	А	563	ASN
1	А	548	ASN
1	В	233	GLN

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	Trune	Chain	Dec	Link	Bo	ond leng	\mathbf{ths}	В	ond ang	les
10101	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	FSU	А	1584	-	$19,\!19,\!19$	1.93	3 (15%)	22,26,26	<mark>3.39</mark>	8 (36%)
2	FSU	В	1584	-	19,19,19	2.00	3 (15%)	22,26,26	<mark>3.54</mark>	9 (40%)

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	FSU	А	1584	-	-	2/9/21/21	0/2/2/2
2	FSU	В	1584	-	-	2/9/21/21	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	1584	FSU	C6-N2	-7.20	1.36	1.46
2	А	1584	FSU	C6-N2	-6.20	1.37	1.46
2	А	1584	FSU	C6-C4	-3.88	1.45	1.50
2	А	1584	FSU	08-C1	3.49	1.29	1.22
2	В	1584	FSU	C6-C4	-3.23	1.46	1.50

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1584	FSU	C3-C1-N2	10.97	114.69	106.41
2	А	1584	FSU	C3-C1-N2	9.53	113.60	106.41
2	А	1584	FSU	C4-C6-N2	8.48	106.47	102.46
2	В	1584	FSU	C4-C6-N2	7.28	105.90	102.46
2	В	1584	FSU	C5-C3-C1	6.37	139.59	131.92

There are no chirality outliers.

All (4) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	А	1584	FSU	C3-C5-C7-O9
2	А	1584	FSU	C3-C5-C7-N10
2	В	1584	FSU	C3-C5-C7-O9
2	В	1584	FSU	C3-C5-C7-N10

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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	351/363~(96%)	-0.02	7 (1%) 65 67	10, 19, 31, 50	0
1	В	349/363~(96%)	-0.02	10 (2%) 51 52	9, 20, 34, 56	0
All	All	700/726~(96%)	-0.02	17 (2%) 59 59	9, 19, 33, 56	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	315	LEU	6.1
1	А	315	LEU	5.4
1	А	479	LEU	4.4
1	В	550	ASP	4.3
1	А	354	PRO	4.2

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
2	FSU	А	1584	18/18	0.94	0.09	$12,\!14,\!24,\!25$	0
2	FSU	В	1584	18/18	0.95	0.08	11,12,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.

