



# Full wwPDB X-ray Structure Validation Report ⓘ

May 2, 2017 – 05:22 PM EDT

PDB ID : 5V7W  
Title : Crystal structure of human PARP14 bound to 2-{[(1-methylpiperidin-4-yl)methyl]amino}-5,6,7,8-tetrahydro[1]benzothieno[2,3-d]pyrimidin-4(3H)-one inhibitor  
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Deposited on : 2017-03-20  
Resolution : 2.65 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029077

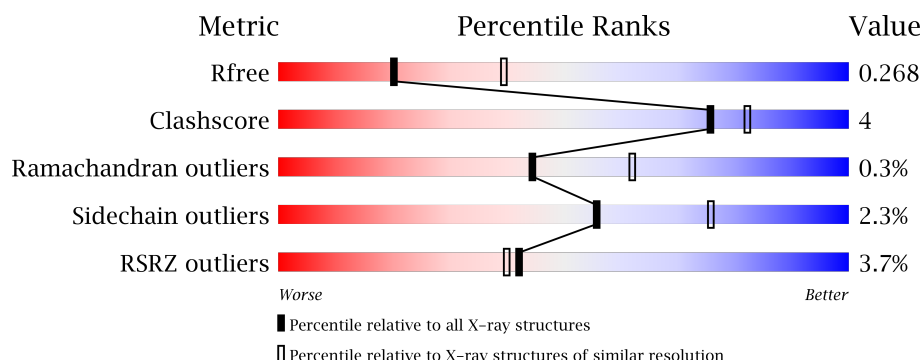
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	194	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>13%</div> </div> </div>
1	B	194	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>••</div> <div>8%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3001 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.

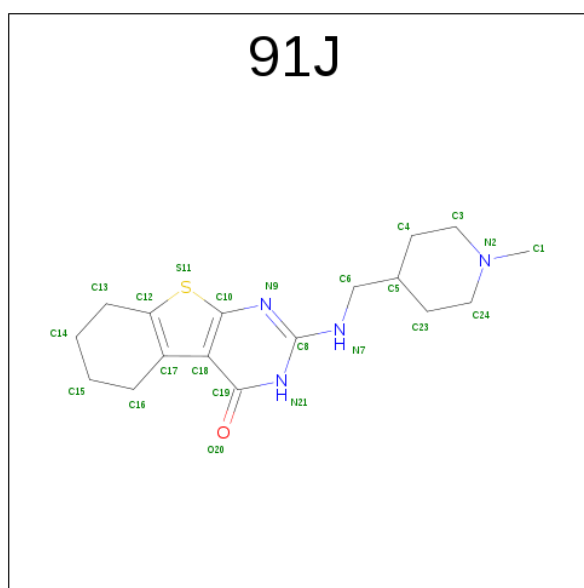
- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1378	871	241	262	4			
1	B	178	Total	C	N	O	S	0	0	0
			1445	913	254	273	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1608	GLY	-	expression tag	UNP Q460N5
A	1609	GLY	-	expression tag	UNP Q460N5
B	1608	GLY	-	expression tag	UNP Q460N5
B	1609	GLY	-	expression tag	UNP Q460N5

- Molecule 2 is 2-[[[(1-methylpiperidin-4-yl)methyl]amino]-5,6,7,8-tetrahydro[1]benzothieno[2,3-d]pyrimidin-4(3H)-one (three-letter code: 91J) (formula: C<sub>17</sub>H<sub>24</sub>N<sub>4</sub>OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	17	4	1	1		
2	B	1	Total	C	N	O	S	0	0
			23	17	4	1	1		

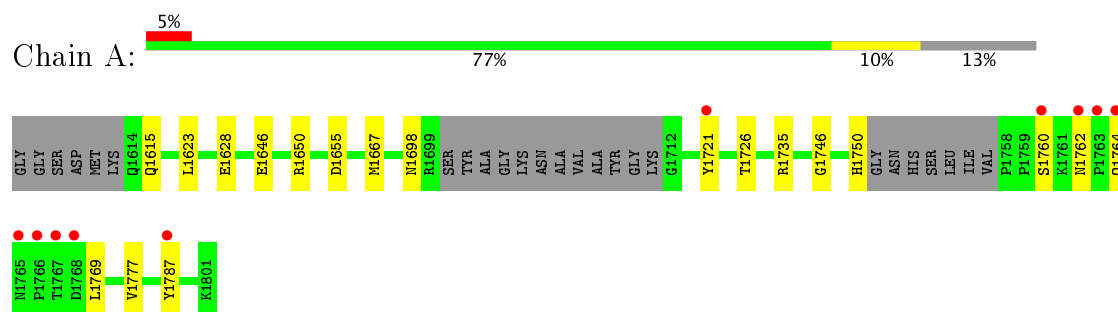
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total	O	0	0
			64	64		
3	B	68	Total	O	0	0
			68	68		

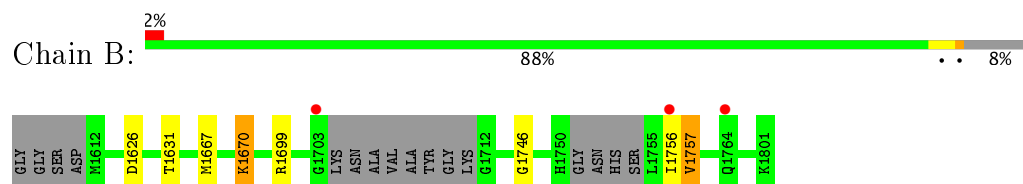
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 14



- Molecule 1: Poly [ADP-ribose] polymerase 14



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.05Å 144.91Å 83.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.45 – 2.65 41.75 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.45-2.65) 99.9 (41.75-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.204 , 0.266 0.205 , 0.268	Depositor DCC
$R_{free}$ test set	757 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3001	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.35 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5455e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 91J

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	0.36	0/1417	0.50	0/1926
1	B	0.35	0/1485	0.50	0/2017
All	All	0.35	0/2902	0.50	0/3943

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 ⓘ

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	1378	0	1290	13	0
1	B	1445	0	1357	7	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
3	A	64	0	0	1	0
3	B	68	0	0	1	0
All	All	3001	0	2647	20	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 (20) 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:1750:HIS:HD2	1:A:1777:VAL:HG23	1.56	0.69
1:B:1667:MET:HE3	1:B:1746:GLY:HA3	1.82	0.61
1:A:1750:HIS:CD2	1:A:1777:VAL:HG23	2.36	0.59
1:A:1667:MET:CE	1:A:1746:GLY:HA3	2.32	0.59
1:A:1667:MET:HE3	1:A:1746:GLY:HA3	1.84	0.59
1:B:1667:MET:CE	1:B:1746:GLY:HA3	2.33	0.58
1:A:1646:GLU:CD	1:A:1735:ARG:HD3	2.28	0.54
1:B:1626:ASP:HB2	3:B:2006:HOH:O	2.10	0.52
1:A:1667:MET:HE3	1:A:1746:GLY:CA	2.42	0.48
1:A:1760:SER:HA	1:A:1769:LEU:HA	1.97	0.47
1:A:1667:MET:CE	1:A:1746:GLY:CA	2.93	0.46
1:B:1667:MET:HE3	1:B:1746:GLY:CA	2.44	0.45
1:A:1628:GLU:OE1	1:A:1650:ARG:NH1	2.50	0.45
1:B:1670:LYS:HG3	1:B:1670:LYS:O	2.17	0.43
1:A:1762:ASN:HD21	1:A:1764:GLN:HB2	1.84	0.42
1:B:1756:ILE:O	1:B:1757:VAL:O	2.37	0.42
1:A:1762:ASN:ND2	1:A:1764:GLN:HB2	2.34	0.42
1:B:1667:MET:CE	1:B:1746:GLY:CA	2.96	0.41
1:A:1615:GLN:HA	1:A:1655:ASP:HB2	2.03	0.41
1:A:1787:TYR:HB2	3:A:2042:HOH:O	2.22	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	163/194 (84%)	160 (98%)	3 (2%)	0	100	100
1	B	172/194 (89%)	165 (96%)	6 (4%)	1 (1%)	28	43
All	All	335/388 (86%)	325 (97%)	9 (3%)	1 (0%)	44	62



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1757	VAL

### 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	151/169 (89%)	147 (97%)	4 (3%)	51	72
1	B	157/169 (93%)	154 (98%)	3 (2%)	62	80
All	All	308/338 (91%)	301 (98%)	7 (2%)	56	76

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1623	LEU
1	A	1698	ASN
1	A	1721	TYR
1	A	1726	THR
1	B	1631	THR
1	B	1670	LYS
1	B	1699	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1630	ASN
1	A	1695	ASN
1	A	1698	ASN
1	A	1750	HIS
1	A	1762	ASN
1	A	1764	GLN
1	B	1750	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 ⓘ

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	91J	A	1901	-	23,26,26	1.23	3 (13%)	23,37,37	2.32	6 (26%)
2	91J	B	1901	-	23,26,26	1.25	3 (13%)	23,37,37	2.26	6 (26%)

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	91J	A	1901	-	-	0/5/22/22	0/4/4/4
2	91J	B	1901	-	-	0/5/22/22	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	91J	C8-N7	2.06	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1901	91J	C8-N7	2.38	1.38	1.34
2	B	1901	91J	C13-C12	2.76	1.52	1.50
2	A	1901	91J	C13-C12	2.77	1.52	1.50
2	B	1901	91J	C17-C18	2.96	1.47	1.41
2	A	1901	91J	C17-C18	3.03	1.47	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1901	91J	C18-C19-N21	-5.36	118.97	124.12
2	A	1901	91J	C18-C19-N21	-5.29	119.04	124.12
2	A	1901	91J	N9-C8-N21	-3.49	120.95	126.23
2	B	1901	91J	N9-C8-N21	-3.33	121.19	126.23
2	A	1901	91J	C14-C13-C12	-2.63	109.06	113.56
2	A	1901	91J	C6-N7-C8	-2.62	119.42	123.43
2	B	1901	91J	C5-C6-N7	-2.27	108.72	112.81
2	B	1901	91J	N7-C8-N9	2.15	121.12	117.19
2	A	1901	91J	C19-N21-C8	3.21	120.93	115.18
2	B	1901	91J	C19-N21-C8	3.23	120.96	115.18
2	B	1901	91J	C8-N9-C10	5.62	121.51	115.14
2	A	1901	91J	C8-N9-C10	5.73	121.63	115.14

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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	169/194 (87%)	-0.01	10 (5%)	23 21	32, 46, 92, 139	0
1	B	178/194 (91%)	-0.14	3 (1%)	70 70	30, 42, 82, 94	0
All	All	347/388 (89%)	-0.08	13 (3%)	42 40	30, 44, 86, 139	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1766	PRO	7.1
1	A	1764	GLN	6.7
1	A	1763	PRO	5.4
1	A	1767	THR	4.8
1	A	1762	ASN	4.7
1	A	1765	ASN	4.0
1	B	1703	GLY	3.6
1	A	1787	TYR	3.6
1	B	1756	ILE	2.4
1	A	1768	ASP	2.3
1	A	1760	SER	2.2
1	B	1764	GLN	2.1
1	A	1721	TYR	2.1

### 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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	91J	A	1901	23/23	0.95	0.17	-0.15	48,53,71,80	0
2	91J	B	1901	23/23	0.97	0.15	-0.66	39,42,51,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.