

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 17, 2020 – 12:30 am BST

PDB ID : 6G8R

Title: SP140 PHD-Bromodomain complex with scFv

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Deposited on : 2018-04-09

Resolution : 2.74 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 : 2.11

buster-report : 1.1.7 (2018)

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)

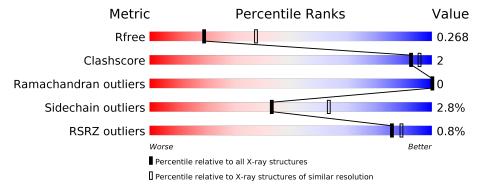
Validation Pipeline (wwPDB-VP) : 2.11

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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		
1	A	250	85%	6%	9%
2	В	198	79%	17	%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3063 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 single-chain variable fragment.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	227	Total	С	N	О	S	0	0	0
1	A	221	1724	1088	287	341	8	0	0	

• Molecule 2 is a protein called Nuclear body protein SP 140.

$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	${f AltConf}$	Trace			
2	В	164	Total 1316	C 835	N 223	O 240	S 18	0	0	0	

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	686	SER	_	expression tag	UNP Q13342
В	863	SER	-	expression tag	UNP Q13342
В	864	SER	-	expression tag	UNP Q13342
В	865	LYS	-	expression tag	UNP Q13342
В	866	GLY	-	expression tag	UNP Q13342
В	867	GLY	-	expression tag	UNP Q13342
В	868	TYR	_	expression tag	UNP Q13342
В	869	GLY	-	expression tag	UNP Q13342
В	870	LEU	-	expression tag	UNP Q13342
В	871	ASN	-	expression tag	UNP Q13342
В	872	ASP	-	expression tag	UNP Q13342
В	873	ILE	_	expression tag	UNP Q13342
В	874	PHE	-	expression tag	UNP Q13342
В	875	GLU	-	expression tag	UNP Q13342
В	876	ALA	-	expression tag	UNP Q13342
В	877	GLN	-	expression tag	UNP Q13342
В	878	LYS	-	expression tag	UNP Q13342
В	879	ILE	-	expression tag	UNP Q13342
В	880	GLU	=	expression tag	UNP Q13342
В	881	TRP	_	expression tag	UNP Q13342

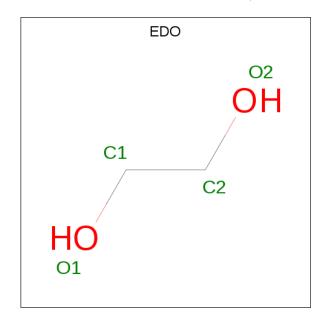
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Chain	Residue	Modelled	Actual	Comment	Reference
В	882	HIS	_	expression tag	UNP Q13342
В	883	GLU	_	expression tag	UNP Q13342

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
4	В	2	Total Zn 2 2	0	0

• Molecule 5 is water.

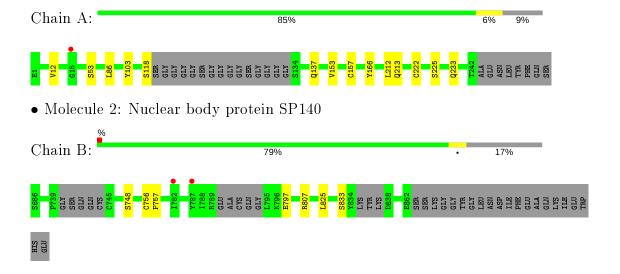
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	В	9	Total O 9 9	0	0



# 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: single-chain variable fragment





# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 61 2 2	Depositor	
Cell constants	89.20Å 89.20Å 343.35Å	D : 4	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	64.11 - 2.74	Depositor	
resolution (A)	64.03 - 2.74	EDS	
% Data completeness	99.5 (64.11-2.74)	Depositor	
(in resolution range)	99.6 (64.03-2.74)	EDS	
$R_{merge}$	0.23	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.78 (at 2.73Å)	Xtriage	
Refinement program	REFMAC 5.8.0257	Depositor	
$R, R_{free}$	0.215 , $0.249$	Depositor	
It, It free	0.225 , $0.268$	DCC	
$R_{free}$ test set	1140 reflections $(5.12\%)$	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	70.0	Xtriage	
Anisotropy	0.581	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32, 48.7	EDS	
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
$F_o$ , $F_c$ correlation	0.94	EDS	
Total number of atoms	3063	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: ZN, EDO

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.66	0/1762	0.75	0/2386	
2	В	0.65	0/1346	0.71	0/1809	
All	All	0.65	0/3108	0.73	0/4195	

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	1724	0	1658	6	0
2	В	1316	0	1208	3	0
3	A	8	0	12	0	0
4	В	2	0	0	0	0
5	A	4	0	0	0	0
5	В	9	0	0	0	0
All	All	3063	0	2878	9	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 2.

The worst 5 of 9 close contacts within the same asymmetric unit are listed below, sorted by their



clash magnitude.

Atom-1	Atom-2	$egin{array}{ll}  ext{Interatomic} \  ext{distance} \ ( ext{\AA}) \end{array}$	Clash overlap (Å)
1:A:12:VAL:HG21	1:A:86:LEU:HD13	1.78	0.65
1:A:166:TYR:HB3	1:A:225:SER:HB2	1.96	0.48
1:A:153:VAL:CG2	1:A:212:LEU:HD12	2.45	0.47
2:B:756:CYS:HB3	2:B:757:PRO:CD	2.44	0.47
1:A:212:LEU:HD23	1:A:213:GLN:N	2.31	0.45

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	Percentiles	
1	A	223/250~(89%)	209 (94%)	14 (6%)	0	100	100	
2	В	156/198~(79%)	149 (96%)	7 (4%)	0	100	100	
All	All	379/448 (85%)	358 (94%)	21 (6%)	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	A	186/200 (93%)	180 (97%)	6 (3%)	39 59		
2	В	140/180 (78%)	137 (98%)	3 (2%)	53 72		

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
All	All	326/380 (86%)	317 (97%)	9 (3%)	43 63		

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	CYS
2	В	833	SER
2	В	748	SER
1	A	137	GLN
1	A	233	GLN

Some 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 carbohydrates in this entry.

### 5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	Tuna	Chain	Dog	Link	B	Bond lengths			Bond angles		
MIOI	Type	Chain	Chain   Res   Li	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
3	EDO	A	301	-	3,3,3	0.09	0	2,2,2	0.25	0	
3	EDO	A	302	-	3,3,3	0.07	0	2,2,2	0.21	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	EDO	A	301	-	_	1/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	_

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	EDO	O1-C1-C2-O2
3	A	301	EDO	O1-C1-C2-O2

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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	$227/250 \ (90\%)$	0.08	1 (0%) 92 95	73, 85, 101, 114	0
2	В	164/198~(82%)	0.30	2 (1%) 79 83	72, 84, 103, 120	0
All	All	391/448 (87%)	0.17	3 (0%) 86 89	72, 85, 102, 120	0

#### All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	GLY	2.3
2	В	782	ILE	2.1
2	В	787	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. 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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
3	EDO	A	302	4/4	0.86	0.26	85,85,85,86	0
3	EDO	A	301	4/4	0.94	0.40	87,88,89,89	0

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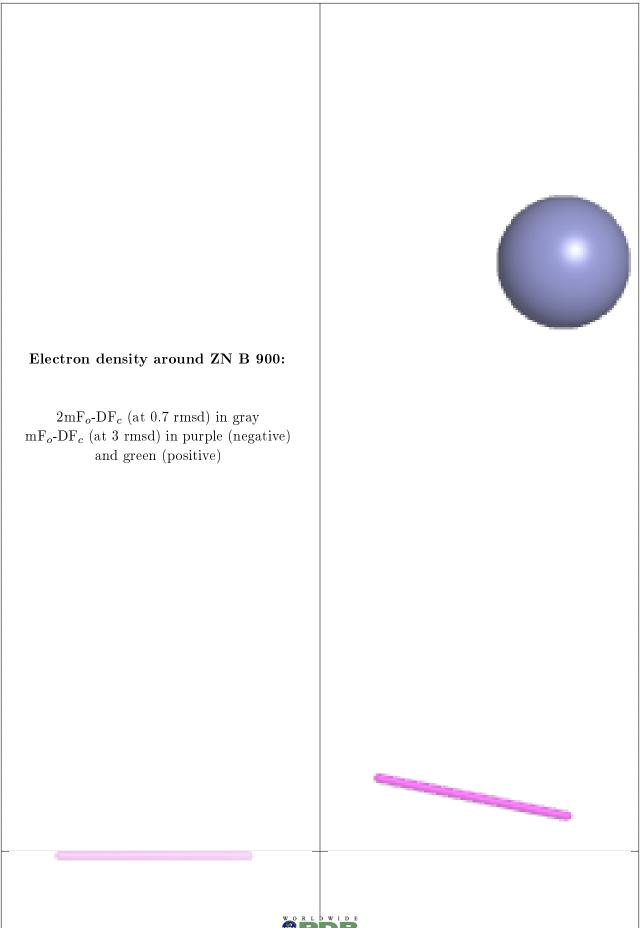


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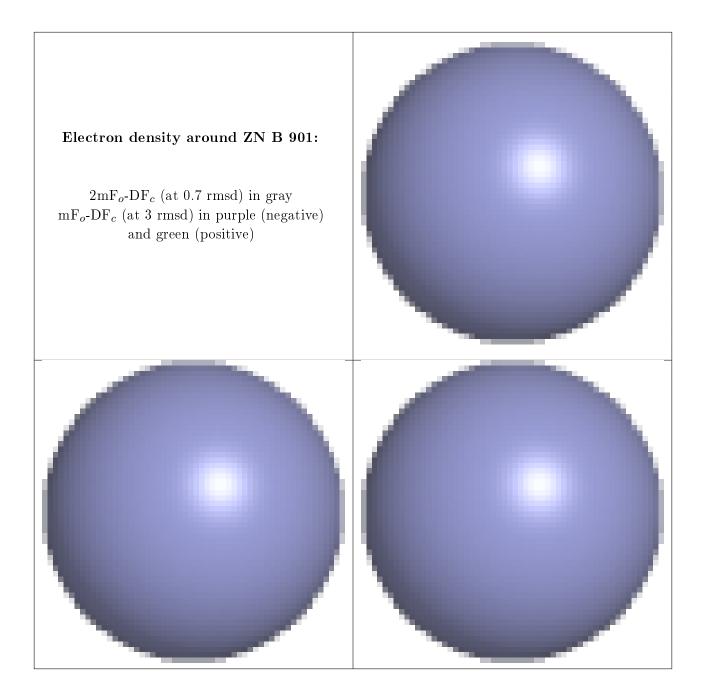
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
4	ZN	В	900	1/1	1.00	0.18	73,73,73,73	0
4	ZN	В	901	1/1	1.00	0.20	72,72,72,72	0

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)

There are no such residues in this entry.

