

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

#### May 16, 2020 - 07:40 am BST

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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 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:

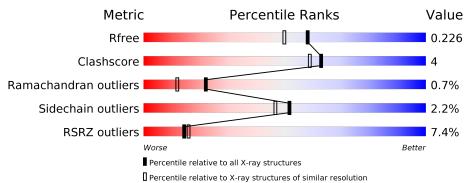
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 1.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847(1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	L	214	88%	8% ••
2	Н	225	87%	• • 8%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3498 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 nivolumab light chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	L	211	Total 1626	C 1017	N 277	O 328	$\frac{S}{4}$	0	0	0

• Molecule 2 is a protein called nivolumab heavy chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Н	208	Total 1561	C 982	N 267	O 306	S 6	0	0	0

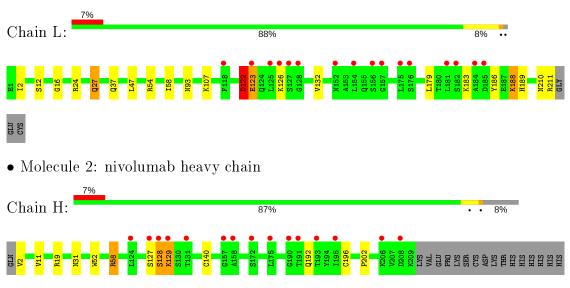
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	161	Total O 161 161	0	0
3	Н	150	Total O 150 150	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: nivolumab light chain



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	88.34Å 88.34Å 215.24Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	31.18 - 1.90	Depositor
	31.18 - 1.90	EDS
% Data completeness	99.9(31.18-1.90)	Depositor
(in resolution range)	99.5(31.18-1.90)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$6.20 (at 1.91 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
$R, R_{free}$	0.196 , $0.226$	Depositor
III, IIIfree	0.200 , $0.226$	DCC
$R_{free}$ test set	2006 reflections $(5.02\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	24.1	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38 , $56.6$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.47, \langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3498	wwPDB-VP
Average B, all atoms $(Å^2)$	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



 $<sup>^1 {\</sup>rm Intensities}$  estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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	Mol Chain		lengths	Bond angles		
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	L	0.39	0/1662	0.59	0/2260	
2	Н	0.37	0/1598	0.55	0/2177	
All	All	0.38	0/3260	0.57	0/4437	

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	L	1626	0	1582	17	1
2	Н	1561	0	1527	10	1
3	Н	150	0	0	7	2
3	L	161	0	0	4	1
All	All	3498	0	3109	27	3

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 (27) 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)
2:H:192:GLN:OE1	3:H:301:HOH:O	1.86	0.93

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		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:H:58:ARG:NH1	3:H:302:HOH:O	2.21	0.72
1:L:210:ASN:O	1:L:211:ARG:HG2	1.93	0.69
1:L:122:ASP:HB2	1:L:123:GLU:HG3	1.75	0.67
2:H:2:VAL:N	3:H:304:HOH:O	2.29	0.65
1:L:24:ARG:NE	3:L:301:HOH:O	2.05	0.62
1:L:132:VAL:HG13	1:L:179:LEU:HB3	1.82	0.61
2:H:58:ARG:HD3	3:H:394:HOH:O	2.05	0.56
1:L:24:ARG:NH2	3:L:301:HOH:O	2.39	0.56
2:H:58:ARG:NH1	3:H:308:HOH:O	2.39	0.56
1:L:27:GLN:HG2	3:L:321:HOH:O	2.08	0.54
2:H:58:ARG:HD2	3:H:356:HOH:O	2.11	0.51
1:L:188:LYS:HB3	1:L:189:HIS:CE1	2.46	0.50
2:H:31:ASN:HB3	3:H:317:HOH:O	2.12	0.49
1:L:186:TYR:O	1:L:186:TYR:CG	2.67	0.47
1:L:2:ILE:HG12	1:L:27:GLN:HE21	1.79	0.47
2:H:128:SER:OG	2:H:129:LYS:N	2.48	0.47
1:L:93:ASN:HB2	3:L:406:HOH:O	2.15	0.45
1:L:122:ASP:N	1:L:122:ASP:OD1	2.43	0.45
1:L:123:GLU:O	1:L:126:LYS:HB2	2.18	0.44
2:H:140:CYS:CB	2:H:196:CYS:HG	2.32	0.42
2:H:11:VAL:HG21	2:H:202:PRO:HB3	2.01	0.42
1:L:37:GLN:HB2	1:L:47:LEU:HD11	2.03	0.41
1:L:54:ARG:HG2	1:L:58:ILE:HB	2.03	0.41
1:L:123:GLU:HG3	1:L:123:GLU:H	1.28	0.41
1:L:12:SER:OG	1:L:107:LYS:HE3	2.21	0.40
1:L:122:ASP:HB2	1:L:123:GLU:H	1.48	0.40

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All (3) 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	${f Interatomic}\ {f distance}\ ({ m \AA})$	Clash overlap (Å)
3:L:304:HOH:O	3:H:317:HOH:O[12_555]	1.82	0.38
3:H:399:HOH:O	3:H:399:HOH:O[7_555]	1.89	0.31
1:L:16:GLY:O	2:H:19:ARG:NH2[5_555]	2.07	0.13



### 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	Percer	ntiles
1	L	209/214~(98%)	199~(95%)	9~(4%)	1 (0%)	29	18
2	Η	206/225~(92%)	199~(97%)	5(2%)	2(1%)	15	6
All	All	415/439~(94%)	398~(96%)	14 (3%)	3~(1%)	22	12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	122	ASP
2	Н	128	SER
2	Н	129	LYS

#### 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	L	184/186~(99%)	179~(97%)	5(3%)	44 38	
2	Н	175/192~(91%)	172 (98%)	3 (2%)	60 57	
All	All	359/378~(95%)	351~(98%)	8 (2%)	52 47	

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	122	ASP
1	L	123	GLU

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Mol	Chain	Res	Type
1	L	183	LYS
1	L	188	LYS
2	Н	52	TRP
2	Н	58	ARG
2	Н	127	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	L	27	GLN
1	L	155	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 carbohydrates in this entry.

### 5.6 Ligand geometry (i)

There are no ligands in this entry.

#### 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 $>2$	$OWAB(Å^2)$	Q<0.9
1	L	211/214~(98%)	0.05	16 (7%) 13 15	15, 25, 62, 73	0
2	Н	208/225~(92%)	0.12	15 (7%) 15 17	14, 32, 61, 72	0
All	All	419/439~(95%)	0.08	31 (7%) 14 16	14, 28, 63, 73	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Н	190	GLY	5.4
2	Н	172	SER	5.1
1	L	128	GLY	4.8
1	L	175	LEU	4.8
1	L	184	ALA	4.2
2	Н	191	THR	3.8
2	Н	158	ALA	3.5
1	L	126	LYS	3.4
1	L	127	SER	3.3
2	Н	193	THR	3.2
2	Н	195	ILE	3.1
1	L	181	LEU	3.1
2	Н	127	SER	3.0
1	L	125	LEU	2.9
2	Н	208	ASP	2.9
1	L	157	GLY	2.8
2	Н	128	SER	2.7
1	L	152	ASN	2.6
2	Н	129	LYS	2.6
2	Н	206	LYS	2.5
2	Н	175	LEU	2.4
1	L	118	PHE	2.4
1	L	185	ASP	2.4
1	L	123	GLU	2.3

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Mol	Chain	$\mathbf{Res}$	Type	RSRZ
2	Н	124	LEU	2.3
1	L	154	LEU	2.3
1	L	182	SER	2.2
1	L	176	SER	2.2
1	L	156	SER	2.2
2	Н	157	GLY	2.1
2	Н	131	THR	2.0

### 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)

There are no ligands in this entry.

### 6.5 Other polymers (i)

There are no such residues in this entry.

