



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 08:34 AM BST

PDB ID : 6W00  
Title : Crystal structure of Fab239 in complex with NPNA2 peptide from circumsporozoite protein  
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Deposited on : 2020-02-28  
Resolution : 1.85 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

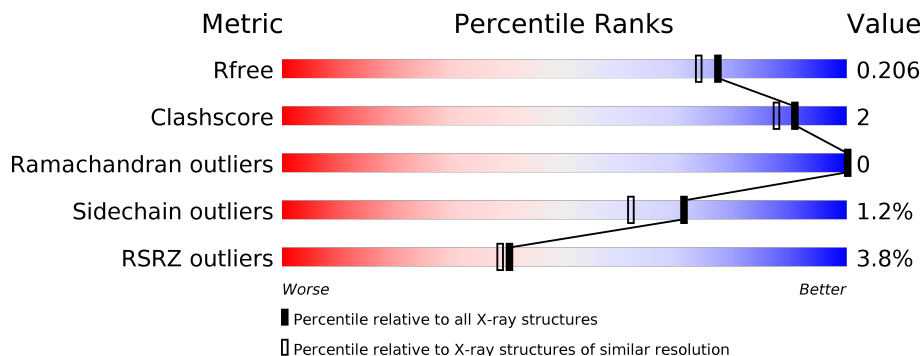
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 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  $\leq 5\%$ . 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	G	58	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 97%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 100%; text-align: center; font-size: small;">100%</div> </div>
2	L	215	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 100%; text-align: center; font-size: small;">92% 8%</div> </div>
3	H	224	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 100%; text-align: center; font-size: small;">95% 5%</div> </div>
4	P	9	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 100%; text-align: center; font-size: small;">100%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7837 atoms, of which 3663 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 Immunoglobulin G-binding protein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
1	G	58	882	282	433	71	96	0	1	0

- Molecule 2 is a protein called Fab239 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	L	215	3226	1029	1577	279	336	5	0	2	0

- Molecule 3 is a protein called Fab239 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	H	224	3273	1055	1605	283	323	7	0	0	0

- Molecule 4 is a protein called NPNA2 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
4	P	9	107	34	48	12	13	0	0	0

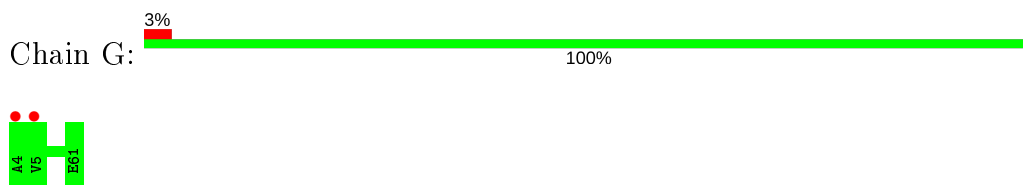
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	42	Total	O	0	0
			42	42		
5	L	155	Total	O	0	0
			155	155		
5	H	143	Total	O	0	0
			143	143		
5	P	9	Total	O	0	0
			9	9		

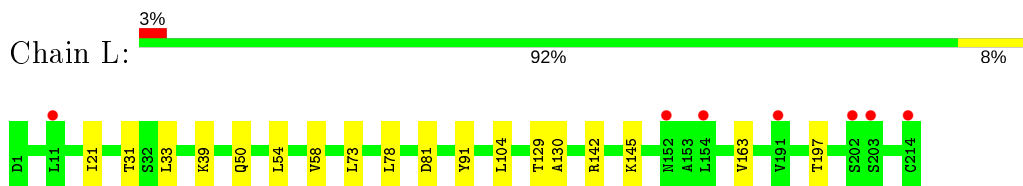
### 3 Residue-property plots [i](#)

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.

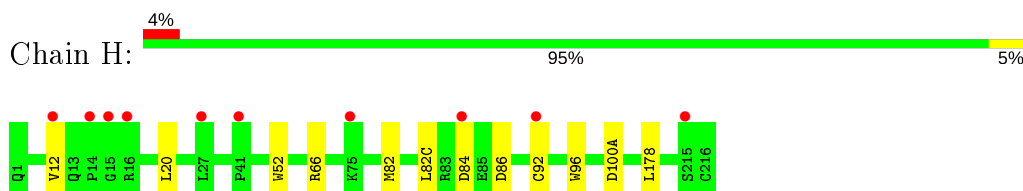
- Molecule 1: Immunoglobulin G-binding protein G



- Molecule 2: Fab239 light chain



- Molecule 3: Fab239 heavy chain



- Molecule 4: NPNA2 peptide



There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.52Å 121.52Å 82.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 1.85 48.95 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.95-1.85) 99.9 (48.95-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 1.86Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.187 , 0.206 0.187 , 0.206	Depositor DCC
$R_{free}$ test set	2577 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	G	0.38	0/455	0.52	0/619
2	L	0.40	0/1684	0.57	0/2292
3	H	0.46	0/1710	0.62	0/2332
4	P	0.38	0/58	0.51	0/81
All	All	0.43	0/3907	0.59	0/5324

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	G	449	433	432	0	0
2	L	1649	1577	1575	9	0
3	H	1668	1605	1603	5	0
4	P	59	48	51	0	0
5	G	42	0	0	0	0
5	H	143	0	0	0	0
5	L	155	0	0	0	0
5	P	9	0	0	0	0
All	All	4174	3663	3661	13	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.

All (13) 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:L:142:ARG:NH2	2:L:163[A]:VAL:HG21	2.05	0.72
3:H:66:ARG:NH1	3:H:86:ASP:OD2	2.30	0.61
2:L:39:LYS:NZ	2:L:81:ASP:OD1	2.41	0.54
2:L:21:ILE:HD11	2:L:73:LEU:HD23	1.92	0.50
3:H:20:LEU:HG	3:H:82:MET:HE2	1.95	0.48
2:L:129:THR:HG22	2:L:130:ALA:N	2.28	0.47
2:L:78:LEU:HD21	2:L:104:LEU:HD21	1.97	0.47
3:H:178:LEU:HD12	3:H:178:LEU:C	2.36	0.46
2:L:145:LYS:HB3	2:L:197:THR:HB	1.98	0.46
2:L:54:LEU:HD22	2:L:58:VAL:HB	1.98	0.45
2:L:91:TYR:CE2	3:H:100(A):ASP:HA	2.53	0.42
3:H:12:VAL:HG21	3:H:82(C):LEU:HD13	2.02	0.42
2:L:31:THR:O	2:L:50:GLN:HA	2.21	0.41

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	G	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
2	L	215/215 (100%)	208 (97%)	7 (3%)	0	100	100
3	H	222/224 (99%)	219 (99%)	3 (1%)	0	100	100
4	P	7/9 (78%)	7 (100%)	0	0	100	100
All	All	501/506 (99%)	490 (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	G	47/47 (100%)	47 (100%)	0	100	100
2	L	185/189 (98%)	184 (100%)	1 (0%)	88	86
3	H	182/190 (96%)	178 (98%)	4 (2%)	52	36
4	P	6/6 (100%)	6 (100%)	0	100	100
All	All	420/432 (97%)	415 (99%)	5 (1%)	71	62

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

Mol	Chain	Res	Type
2	L	33	LEU
3	H	52	TRP
3	H	84	ASP
3	H	92	CYS
3	H	96	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	81	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](#)

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

### 6.1 Protein, DNA and RNA chains

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	G	58/58 (100%)	0.34	2 (3%) 45 42	14, 21, 38, 49	0
2	L	215/215 (100%)	0.44	7 (3%) 46 44	11, 20, 36, 45	0
3	H	224/224 (100%)	0.45	10 (4%) 33 32	12, 20, 34, 47	0
4	P	8/9 (88%)	0.30	0 100 100	13, 14, 17, 21	0
All	All	505/506 (99%)	0.43	19 (3%) 40 38	11, 20, 36, 49	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	154	LEU	4.7
3	H	27	LEU	4.1
3	H	16	ARG	3.5
1	G	5	VAL	3.2
2	L	214	CYS	3.2
3	H	215	SER	3.0
1	G	4	ALA	2.9
2	L	11	LEU	2.9
2	L	152	ASN	2.9
3	H	41	PRO	2.7
3	H	12	VAL	2.7
3	H	92	CYS	2.6
2	L	202	SER	2.6
3	H	84	ASP	2.4
3	H	75	LYS	2.4
3	H	14	PRO	2.3
2	L	191	VAL	2.1
3	H	15	GLY	2.0
2	L	203	SER	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 monosaccharides 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.