

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

#### May 18, 2023 – 02:08 PM JST

PDB ID	:	8HN6
Title	:	Crystal structure of monoclonal antibody complexed with SARS-CoV-2 RBD
Authors	:	Qi, J.; Chen, Y.
Deposited on	:	2022-12-07
Resolution	:	2.07  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* 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 (1)) were used in the production of this report:

MolProbity		4 02h-467
Mon robity	·	1.020-101
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
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)	:	2.32.2

# 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 2.07 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	Δ	117		
	A	117	92%	7% •
	a		2%	
1	C	117	96%	•
			3%	
2	В	108	90%	8% •
			5%	
2	D	108	88%	11% •
			22%	
3	$\mathbf{E}$	195	89%	11% •
			14%	
3	F	195	88%	12%



#### 8HN6

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7012 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 Heavy chain of monoclonal antibody 3G10.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	116	Total	С	Ν	0	S	0	0	0
1	Л	110	882	553	149	174	6	0		
1	С	117	Total	С	Ν	0	S	0	0	0
		117	887	556	150	175	6		0	U

• Molecule 2 is a protein called Light chain of monoclonal antibody 3G10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	108	Total	С	Ν	Ο	S	0	0	0
	В 108		833	533	137	160	3	0	0	0
9	а	108	Total	С	Ν	0	S	0	0	0
	D	108	827	527	137	160	3	0	0	0

• Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Е	195	Total 1533	C 979	N 257	O 289	S 8	0	1	0
3	F	195	Total 1545	C 990	N 257	O 290	S 8	0	1	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	57	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 57 & 57 \end{array}$	0	0
4	В	71	Total O 71 71	0	0
4	Ε	107	Total O 107 107	0	0
4	С	87	Total O 87 87	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	64	$\begin{array}{cc} \text{Total} & \text{O} \\ 64 & 64 \end{array}$	0	0
4	F	119	Total O 119 119	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: Heavy chain of monoclonal antibody 3G10







• Molecule 3: Spike protein S1





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	98.68Å 105.73Å 209.76Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	26.43 - 2.07	Depositor
Resolution (A)	28.65 - 2.07	EDS
% Data completeness	99.6 (26.43-2.07)	Depositor
(in resolution range)	99.9(28.65 - 2.07)	EDS
$R_{merge}$	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.03 (at 2.06 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R R.	0.192 , $0.214$	Depositor
II, II, <i>free</i>	0.192 , $0.215$	DCC
$R_{free}$ test set	3120 reflections $(4.66%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	35.5	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.37, $46.3$	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7012	wwPDB-VP
Average B, all atoms $(Å^2)$	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.02% 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>&</sup>lt;sup>1</sup>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).

Mal	Chain	Bond	lengths	Bond angles		
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.43	0/899	0.65	0/1218	
1	С	0.51	0/904	0.63	0/1225	
2	В	0.43	0/853	0.72	1/1158~(0.1%)	
2	D	0.47	0/846	0.73	2/1149~(0.2%)	
3	Е	0.44	0/1578	0.58	0/2149	
3	F	0.44	0/1592	0.63	0/2169	
All	All	0.45	0/6672	0.65	3/9068~(0.0%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	D	95	PRO	N-CA-C	-6.02	96.45	112.10
2	D	90	LEU	CB-CG-CD2	5.92	121.06	111.00
2	В	95	PRO	N-CA-C	-5.75	97.15	112.10

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	882	0	852	7	0
1	С	887	0	857	3	0
2	В	833	0	823	10	0
2	D	827	0	816	10	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
3	Ε	1533	0	1451	15	0	
3	F	1545	0	1457	17	0	
4	А	57	0	0	0	0	
4	В	71	0	0	1	0	
4	С	87	0	0	0	0	
4	D	64	0	0	1	0	
4	Е	107	0	0	0	0	
4	F	119	0	0	2	0	
All	All	7012	0	6256	53	0	

Continued from previous page...

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 (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:12:VAL:HG22	1:A:16:GLU:HB2	1.73	0.71
3:E:362:VAL:HG13	3:E:527:PRO:HD2	1.73	0.69
2:D:22:THR:HG22	2:D:72:THR:HG22	1.75	0.68
3:F:377:PHE:CD1	3:F:434:ILE:HG12	2.30	0.66
2:B:24:ARG:NH1	3:F:374:PHE:O	2.29	0.66
1:C:30:SER:HB3	1:C:73:ASN:ND2	2.14	0.62
3:E:386:LYS:HE3	3:E:390:LEU:HD21	1.80	0.62
3:F:362:VAL:HG13	3:F:527:PRO:HD2	1.81	0.62
3:E:362:VAL:HG13	3:E:526:GLY:HA2	1.83	0.60
3:F:372:ALA:C	3:F:374:PHE:H	2.05	0.59
2:D:94:TYR:O	2:D:96:VAL:N	2.36	0.58
3:E:443:SER:O	3:E:444:LYS:HE2	2.04	0.57
1:A:50:VAL:HG21	2:B:94:TYR:CZ	2.39	0.57
2:B:94:TYR:O	2:B:96:VAL:N	2.37	0.57
3:F:364:ASP:O	3:F:367:VAL:HG22	2.05	0.56
2:D:45:LYS:HD2	4:D:227:HOH:O	2.06	0.56
3:F:377:PHE:HD1	3:F:434:ILE:HG12	1.72	0.55
3:E:364:ASP:O	3:E:367:VAL:HG22	2.07	0.54
1:A:12:VAL:HG11	1:A:85:LEU:HD13	1.88	0.54
3:F:376:THR:HG22	4:F:669:HOH:O	2.08	0.53
2:D:34:ALA:HB2	2:D:91:LEU:HD21	1.91	0.53
3:E:368:LEU:HD22	3:E:377:PHE:HE2	1.73	0.52
3:F:371:SER:O	3:F:372:ALA:HB3	2.09	0.52
2:D:94:TYR:C	2:D:96:VAL:N	2.65	0.49
3:E:368:LEU:HD22	3:E:377:PHE:CE2	2.49	0.47



	A + 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.96	0.47
3:F:357:ARG:NH1	3:F:359:SER:OG	2.44	0.47
3:F:391:CYS:HB3	3:F:522:ALA:HB1	1.97	0.46
3:F:354:ASN:O	3:F:398:ASP:HA	2.15	0.46
2:B:2:ILE:CD1	2:B:27:GLN:HB2	2.46	0.46
2:D:95:PRO:HG2	4:F:718:HOH:O	2.16	0.46
3:E:503:VAL:HG12	2:D:0:MET:CE	2.48	0.44
3:E:376:THR:HG23	2:D:3:GLN:OE1	2.17	0.44
3:F:372:ALA:C	3:F:374:PHE:N	2.70	0.44
1:A:47:TRP:CG	2:B:96:VAL:HB	2.54	0.43
1:C:29:VAL:HG13	1:C:34:MET:HG3	2.00	0.43
2:B:7:PHE:HA	2:B:8:PRO:C	2.39	0.43
2:D:37:GLN:HB2	2:D:47:LEU:HD11	2.00	0.43
3:F:368:LEU:O	3:F:371:SER:HB3	2.18	0.43
3:F:369:TYR:HA	3:F:374:PHE:CD2	2.53	0.43
1:A:33:TYR:HB3	2:B:94:TYR:OH	2.19	0.43
3:E:374:PHE:O	3:E:375:SER:C	2.57	0.43
1:C:100:SER:HB3	3:F:455:LEU:HD11	2.01	0.42
1:A:50:VAL:HG21	2:B:94:TYR:CE1	2.54	0.42
3:E:412:PRO:HG3	3:E:429:PHE:HB3	2.02	0.42
2:B:27:GLN:NE2	4:B:205:HOH:O	2.52	0.41
3:E:503:VAL:HG12	2:D:0:MET:HE1	2.01	0.41
1:A:66:ARG:HG2	1:A:83:ASN:O	2.19	0.41
3:E:342:PHE:CZ	3:E:368:LEU:HD11	2.55	0.41
3:E:354:ASN:O	3:E:398:ASP:HA	2.21	0.40
3:F:412:PRO:HG3	3:F:429:PHE:HB3	2.02	0.40
3:E:376:THR:O	3:E:434:ILE:HA	2.22	0.40
3:F:379:CYS:HA	3:F:432:CYS:HA	2.04	0.40

Continued from previous page..

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	А	114/117~(97%)	113~(99%)	1 (1%)	0	100 100
1	С	115/117~(98%)	113~(98%)	2~(2%)	0	100 100
2	В	106/108~(98%)	101~(95%)	4 (4%)	1 (1%)	17 8
2	D	106/108~(98%)	100 (94%)	6~(6%)	0	100 100
3	Е	194/195~(100%)	183~(94%)	9~(5%)	2(1%)	15 6
3	F	194/195~(100%)	185 (95%)	9~(5%)	0	100 100
All	All	829/840 (99%)	795 (96%)	31 (4%)	3 (0%)	34 25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Е	375	SER
3	Е	373	SER
2	В	95	PRO

#### 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	Perce	ntiles
1	А	95/95~(100%)	95~(100%)	0	100	100
1	С	95/95~(100%)	95~(100%)	0	100	100
2	В	92/92~(100%)	90~(98%)	2 (2%)	52	46
2	D	91/92~(99%)	91 (100%)	0	100	100
3	Е	167/168~(99%)	167 (100%)	0	100	100
3	F	168/168~(100%)	168 (100%)	0	100	100
All	All	708/710~(100%)	706 (100%)	2(0%)	92	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	93	SER
2	В	94	TYR



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	13	GLN
2	В	3	GLN
1	С	73	ASN
3	F	343	ASN
3	F	450	ASN

#### 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 (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 $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	116/117~(99%)	0.63	13 (11%) 5 5	29, 40, 62, 90	0
1	С	117/117 (100%)	0.21	2 (1%) 70 71	26, 33, 50, 78	0
2	В	108/108~(100%)	0.05	3 (2%) 53 56	25, 33, 50, 69	0
2	D	108/108 (100%)	0.25	5 (4%) 32 33	27, 37, 58, 78	0
3	Ε	195/195~(100%)	1.04	42 (21%) 0 0	28, 40, 90, 121	0
3	F	195/195~(100%)	0.76	28 (14%) 2 2	25, 36, 79, 100	0
All	All	839/840 (99%)	0.57	93 (11%) 5 5	25, 37, 73, 121	0

All (93) RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
3	Е	333	THR	8.2
2	D	94	TYR	7.8
3	Е	372	ALA	7.4
3	Е	519	HIS	6.9
2	В	94	TYR	6.8
1	А	117	SER	6.6
3	Е	374	PHE	6.2
3	F	333	THR	5.7
3	Е	518	LEU	5.7
3	Е	345	THR	5.4
3	F	335	LEU	5.4
3	F	518	LEU	5.4
3	Е	521	PRO	5.3
3	Е	527	PRO	5.0
3	F	527	PRO	4.9
3	F	519	HIS	4.7
3	Е	346	ARG	4.7
1	А	13	GLN	4.1
3	Е	520	ALA	4.1



Mol	Chain	Res	Type	RSRZ
3	F	334	ASN	4.0
3	F	517	LEU	3.9
3	Е	371	SER	3.9
3	F	367	VAL	3.8
1	А	100	SER	3.8
1	С	118	ALA	3.8
3	Е	523	THR	3.7
3	Е	368	LEU	3.6
3	F	343	ASN	3.5
3	F	370	ASN	3.5
1	А	11	LEU	3.5
3	F	520	ALA	3.4
3	Ε	335	LEU	3.4
3	E	455	LEU	3.3
3	Ε	369	TYR	3.3
3	F	374	PHE	3.3
3	F	526	GLY	3.3
3	Ε	492	LEU	3.2
3	F	362	VAL	3.2
1	А	115	VAL	3.2
1	А	116	SER	3.1
3	Е	366	SER	3.0
3	Е	513	LEU	3.0
2	D	95	PRO	3.0
3	Е	517	LEU	3.0
3	Е	522	ALA	3.0
1	А	37	VAL	2.9
3	Е	441	LEU	2.9
3	Е	389	ASP	2.8
1	С	117	SER	2.8
2	D	107	LYS	2.8
3	Е	377	PHE	2.7
3	F	441	LEU	2.7
3	F	478	THR	2.7
3	F	341	VAL	2.6
3	F	369	TYR	2.6
3	Е	370	ASN	2.6
2	D	1	ASP	2.6
3	Ε	376	THR	2.6
3	Е	367	VAL	2.5
1	А	86	ARG	2.5
1	А	12	VAL	2.5

Continued from previous page...



Mol	Chain	Res	Type	RSRZ
3	Е	526	GLY	2.5
2	В	95	PRO	2.5
1	А	65	GLY	2.5
3	Е	525	CYS	2.5
3	Е	512	VAL	2.5
3	Е	479	PRO	2.5
1	А	14	PRO	2.5
3	Е	444	LYS	2.5
1	А	15	GLY	2.5
3	Е	364	ASP	2.5
3	F	521	PRO	2.5
3	Е	343	ASN	2.4
3	Е	360	ASN	2.4
3	F	440[A]	ASN	2.4
1	А	74	SER	2.4
3	Е	478	THR	2.4
3	F	444	LYS	2.4
3	Е	491	PRO	2.3
3	Е	334	ASN	2.3
3	F	372	ALA	2.3
3	F	445	VAL	2.3
3	F	522	ALA	2.3
3	Е	453	TYR	2.3
3	F	364	ASP	2.2
2	D	96	VAL	2.1
2	В	107	LYS	2.1
3	F	373	SER	2.1
3	F	455	LEU	2.1
3	Е	449	TYR	2.1
3	Е	452	LEU	2.1
3	F	433	VAL	2.0
3	Е	396	TYR	2.0

Continued from previous page...

### 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.

