



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:41 PM UTC

PDB ID : 6XC2 / pdb\_00006xc2  
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing antibody CC12.1  
Authors : Yuan, M.; Liu, H.; Wu, N.C.; Zhu, X.; Wilson, I.A.  
Deposited on : 2020-06-08  
Resolution : 3.11 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](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.

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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

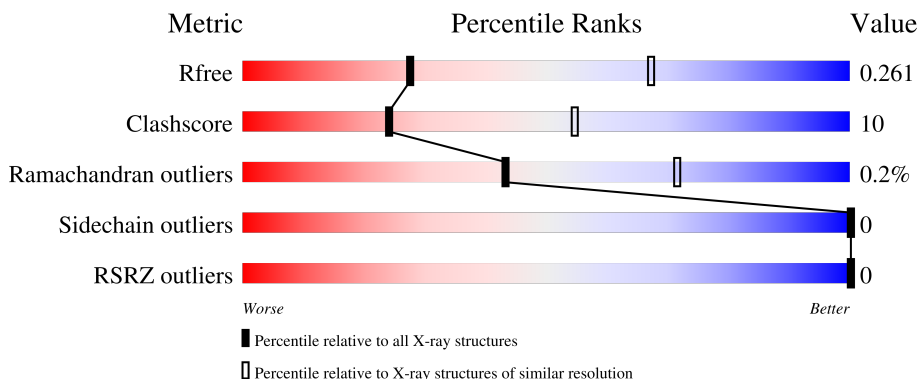
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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))
$R_{free}$	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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  $\geq 3$ , 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	A	231	
1	Z	231	
2	L	217	
2	Y	217	
3	H	220	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	X	220	 75% 21% ..

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9584 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	193	1537	987	256	286	8	0	0	0
1	Z	193	1537	987	256	286	8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	SER	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2
Z	542	SER	-	expression tag	UNP P0DTC2
Z	543	GLY	-	expression tag	UNP P0DTC2
Z	544	HIS	-	expression tag	UNP P0DTC2
Z	545	HIS	-	expression tag	UNP P0DTC2
Z	546	HIS	-	expression tag	UNP P0DTC2
Z	547	HIS	-	expression tag	UNP P0DTC2
Z	548	HIS	-	expression tag	UNP P0DTC2
Z	549	HIS	-	expression tag	UNP P0DTC2

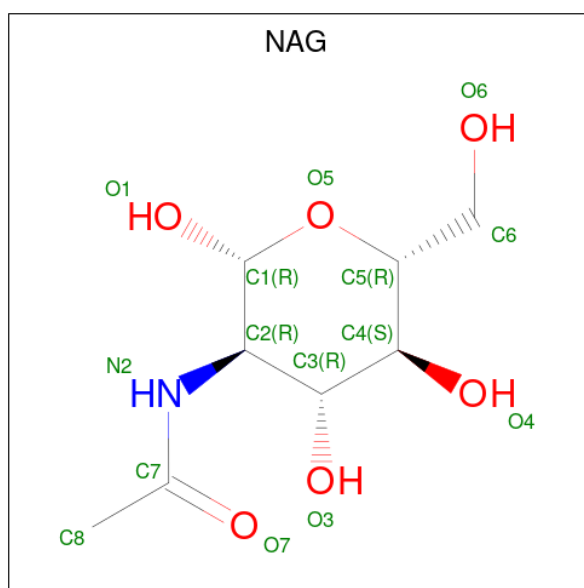
- Molecule 2 is a protein called CC12.1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	215	1650	1041	273	331	5	0	0	0
2	Y	215	1650	1041	273	331	5	0	0	0

- Molecule 3 is a protein called CC12.1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	215	Total	C	N	O	S	0	0	0
			1591	1001	266	318	6			
3	X	215	Total	C	N	O	S	0	0	0
			1591	1001	266	318	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	Z	1	Total	C	N	O	0	0
			14	8	1	5		





- Molecule 3: CC12.1 heavy chain

Chain H: 74% 23% ..



- Molecule 3: CC12.1 heavy chain

Chain X: 75% 21% ..



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.70Å 143.49Å 81.47Å 90.00° 118.68° 90.00°	Depositor
Resolution (Å)	40.34 – 3.11 40.34 – 3.11	Depositor EDS
% Data completeness (in resolution range)	88.3 (40.34-3.11) 88.3 (40.34-3.11)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.213 , 0.267 0.214 , 0.261	Depositor DCC
$R_{free}$ test set	1293 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.8	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.004 for -h-l,k,h 0.004 for l,k,-h-l 0.417 for h,-k,-h-l 0.019 for -h-l,-k,l 0.022 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9584	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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

### 5.1 Standard geometry

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

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	0.14	0/1580	0.36	0/2149
1	Z	0.14	0/1580	0.35	0/2149
2	L	0.16	0/1688	0.40	0/2293
2	Y	0.17	0/1688	0.41	0/2293
3	H	0.16	0/1625	0.42	0/2214
3	X	0.17	0/1625	0.43	0/2214
All	All	0.16	0/9786	0.40	0/13312

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	2
2	Y	0	1
3	H	0	2
3	X	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	127	PRO	Peptide
3	H	96	LEU	Peptide
2	L	29	ILE	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	L	93	SER	Peptide
2	Y	29	ILE	Peptide

## 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	1537	0	1458	36	0
1	Z	1537	0	1458	32	0
2	L	1650	0	1615	36	0
2	Y	1650	0	1615	41	0
3	H	1591	0	1565	40	0
3	X	1591	0	1565	35	0
4	A	14	0	13	0	0
4	Z	14	0	13	0	0
All	All	9584	0	9302	188	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 10.

The worst 5 of 188 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:Y:36:TYR:CE1	2:Y:89:GLN:OE1	2.08	1.07
2:Y:36:TYR:CZ	2:Y:89:GLN:OE1	2.23	0.90
2:Y:12:SER:OG	2:Y:142:TYR:OH	1.94	0.84
2:Y:36:TYR:OH	2:Y:89:GLN:OE1	2.00	0.79
3:X:127:PRO:HG3	3:X:139:LEU:HB3	1.64	0.79

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	189/231 (82%)	176 (93%)	13 (7%)	0	100	100
1	Z	189/231 (82%)	174 (92%)	15 (8%)	0	100	100
2	L	213/217 (98%)	204 (96%)	9 (4%)	0	100	100
2	Y	213/217 (98%)	201 (94%)	12 (6%)	0	100	100
3	H	211/220 (96%)	204 (97%)	6 (3%)	1 (0%)	24	55
3	X	211/220 (96%)	203 (96%)	7 (3%)	1 (0%)	24	55
All	All	1226/1336 (92%)	1162 (95%)	62 (5%)	2 (0%)	43	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	97	ASP
3	X	97	ASP

### 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	168/203 (83%)	168 (100%)	0	100	100
1	Z	168/203 (83%)	168 (100%)	0	100	100
2	L	188/190 (99%)	188 (100%)	0	100	100
2	Y	188/190 (99%)	188 (100%)	0	100	100
3	H	180/185 (97%)	180 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	X	180/185 (97%)	180 (100%)	0	100	100
All	All	1072/1156 (93%)	1072 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	Y	90	GLN
1	Z	501	ASN
1	Z	334	ASN
2	L	90	GLN
1	Z	498	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
4	NAG	Z	601	1	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	A	601	1	14,14,15	0.27	0	17,19,21	0.45	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
4	NAG	Z	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	O5-C5-C6-O6
4	Z	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	Z	601	NAG	C4-C5-C6-O6

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	193/231 (83%)	-1.45	0 100 100	51, 73, 106, 122	0
1	Z	193/231 (83%)	-1.43	0 100 100	51, 74, 103, 113	0
2	L	215/217 (99%)	-1.52	0 100 100	49, 69, 89, 112	0
2	Y	215/217 (99%)	-1.48	0 100 100	47, 71, 90, 102	0
3	H	215/220 (97%)	-1.48	0 100 100	45, 61, 91, 123	0
3	X	215/220 (97%)	-1.45	0 100 100	43, 64, 90, 120	0
All	All	1246/1336 (93%)	-1.47	0 100 100	43, 69, 94, 123	0

There are no RSRZ outliers to report.

### 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 oligosaccharides 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	Z	601	14/15	0.97	0.06	85,92,109,115	0
4	NAG	A	601	14/15	0.98	0.06	88,98,106,111	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.