



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 04:11 PM JST

PDB ID : 9II9
Title : Crystal structure of SARS-CoV-2 neutralizing antibody K4-66
Authors : Kimura, T.K.; Hashiguchi, T.
Deposited on : 2024-06-19
Resolution : 2.90 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 ⓘ 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

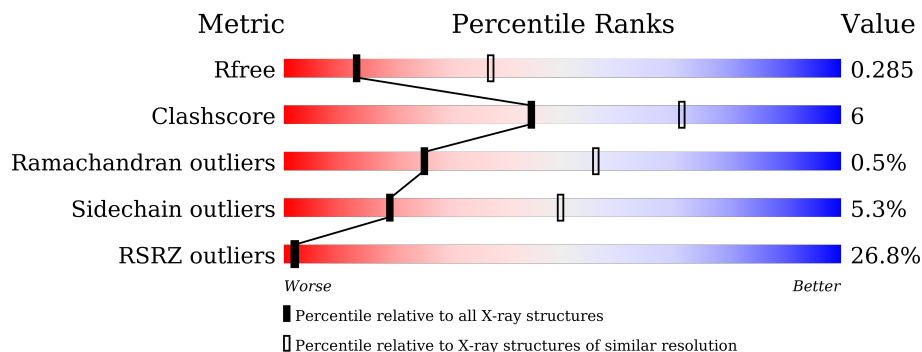
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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 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 $\leq 5\%$. 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	218	 7% 86% 14%
1	C	218	 61% 87% 8% .
2	B	214	 % 84% 14% ..
2	D	214	 35% 79% 18% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5784 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 antigen-binding fragments (Fabs).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1577	994	273	304	6	0	0	0
1	C	209	1208	742	219	243	4	0	0	0

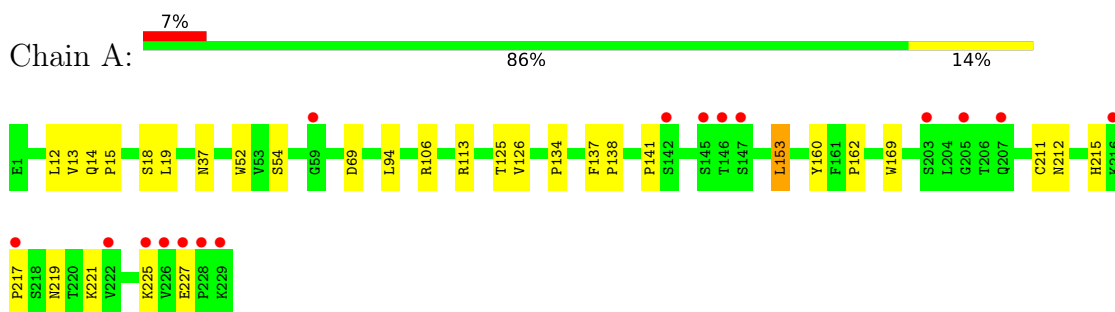
- Molecule 2 is a protein called antigen-binding fragments (Fabs).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	1608	1003	269	331	5	0	0	0
2	D	208	1391	862	239	285	5	0	0	0

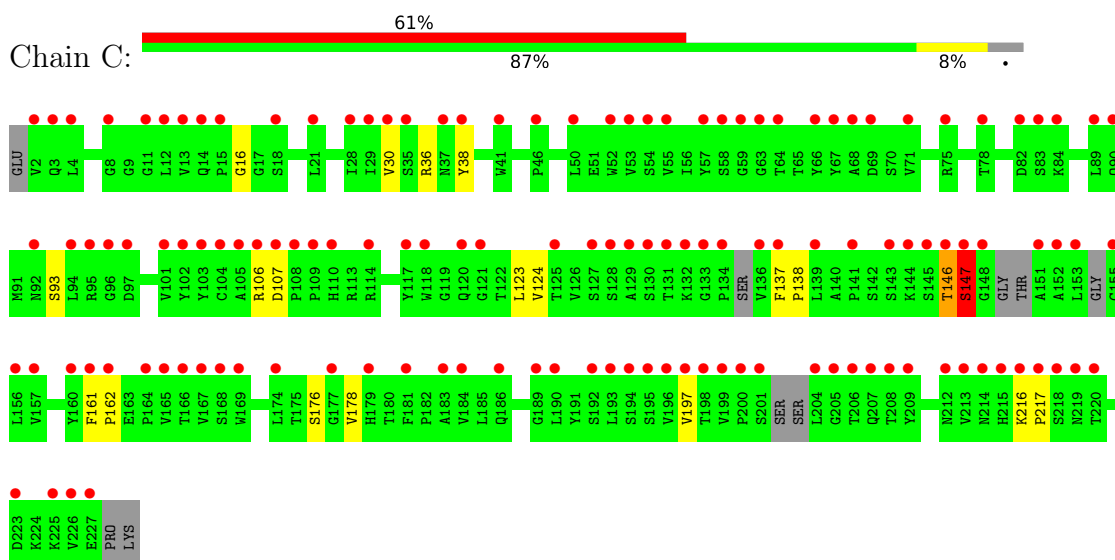
3 Residue-property plots [i](#)

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.

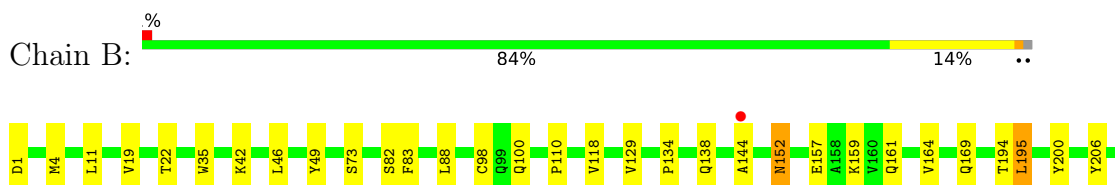
- Molecule 1: antigen-binding fragments (Fabs)

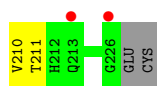


- Molecule 1: antigen-binding fragments (Fabs)

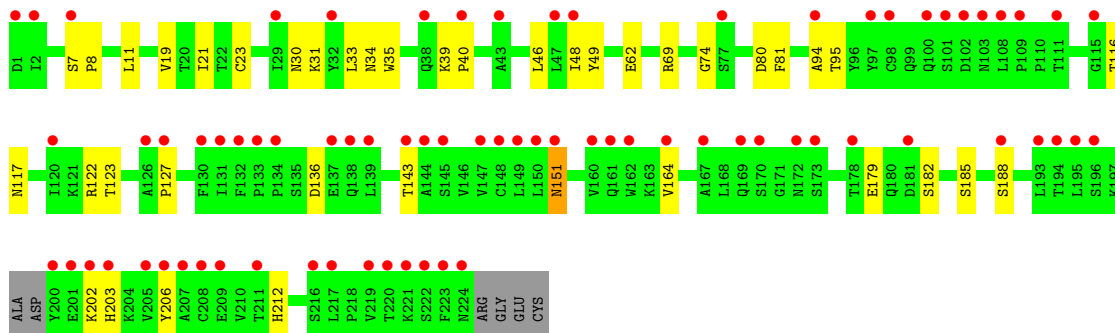
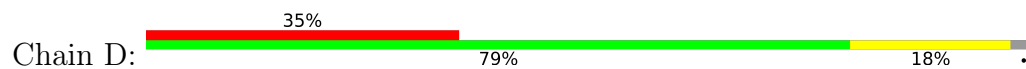


- Molecule 2: antigen-binding fragments (Fabs)





- Molecule 2: antigen-binding fragments (Fabs)



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	147.45Å 147.45Å 154.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 2.90 49.41 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.41-2.90) 100.0 (49.41-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.81Å)	Xtriage
Refinement program	REFMAC 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.262 , 0.288 0.266 , 0.285	Depositor DCC
R_{free} test set	1993 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	80.6	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 71.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for -h,l,k 0.014 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5784	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.28	0/1615	0.53	0/2209
1	C	0.25	0/1227	0.48	0/1698
2	B	0.28	0/1641	0.49	0/2236
2	D	0.26	0/1417	0.50	0/1948
All	All	0.27	0/5900	0.50	0/8091

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
1	C	0	2
2	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	146	THR	Peptide
1	C	216	LYS	Peptide
2	D	202	LYS	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	1577	0	1486	20	0
1	C	1208	0	822	10	0
2	B	1608	0	1539	17	0
2	D	1391	0	1143	19	0
All	All	5784	0	4990	64	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 6.

The worst 5 of 64 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:B:157:GLU:N	2:B:157:GLU:OE1	2.19	0.75
1:A:215:HIS:CD2	1:A:217:PRO:HD2	2.24	0.71
2:B:129:VAL:HG21	2:B:210:VAL:HG11	1.73	0.70
2:D:8:PRO:HG2	2:D:21:ILE:HG22	1.73	0.70
1:A:134:PRO:HB3	1:A:160:TYR:HB3	1.73	0.68

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	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
1	C	199/218 (91%)	173 (87%)	24 (12%)	2 (1%)	13	40
2	B	210/214 (98%)	201 (96%)	8 (4%)	1 (0%)	25	56
2	D	204/214 (95%)	186 (91%)	17 (8%)	1 (0%)	25	56
All	All	829/864 (96%)	768 (93%)	57 (7%)	4 (0%)	25	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	203	HIS
1	C	147	SER
2	B	152	ASN
1	C	217	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	Percentiles	
1	A	162/183 (88%)	152 (94%)	10 (6%)	15	43
1	C	66/183 (36%)	64 (97%)	2 (3%)	36	71
2	B	182/190 (96%)	174 (96%)	8 (4%)	24	57
2	D	121/190 (64%)	113 (93%)	8 (7%)	14	39
All	All	531/746 (71%)	503 (95%)	28 (5%)	19	49

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	82	SER
2	D	185	SER
2	B	195	LEU
2	D	143	THR
2	B	194	THR

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

Mol	Chain	Res	Type
2	B	169	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](#)

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, 95th 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	A	218/218 (100%)	0.17	16 (7%) 22 19	40, 56, 90, 139	0
1	C	209/218 (95%)	2.59	133 (63%) 0 0	96, 140, 181, 247	0
2	B	212/214 (99%)	-0.09	3 (1%) 73 68	39, 59, 92, 110	0
2	D	208/214 (97%)	1.51	75 (36%) 1 1	60, 102, 185, 234	0
All	All	847/864 (98%)	1.03	227 (26%) 2 2	39, 82, 171, 247	0

The worst 5 of 227 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	GLY	9.0
2	D	1	ASP	8.3
2	D	224	ASN	8.1
1	C	194	SER	7.6
1	C	151	ALA	7.2

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.