



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 07:00 AM UTC

PDB ID : 8KGZ / pdb_00008kgz
Title : Crystal structure of single-chain Fv antibody against antigen peptide from SARS-CoV2 S-spike protein
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Deposited on : 2023-08-20
Resolution : 2.21 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	:	4-5-2 with Phenix2.0
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

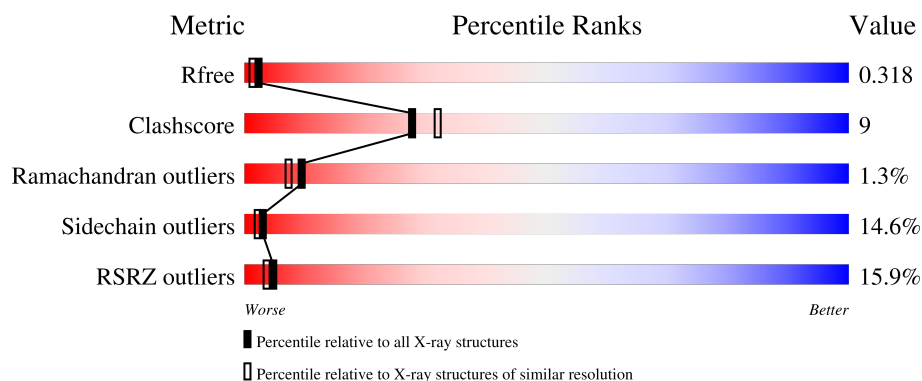
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	412	9% 41% 12% • • 44%
1	B	412	8% 42% 11% • 44%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3483 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 Thioredoxin 1,scFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1693	1049	285	354	5			
1	B	232	Total	C	N	O	S	0	0	0
			1686	1043	285	353	5			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	GLY	-	linker	UNP P0AA25
A	-22	SER	-	linker	UNP P0AA25
A	-21	GLY	-	linker	UNP P0AA25
A	-20	SER	-	linker	UNP P0AA25
A	-19	GLY	-	linker	UNP P0AA25
A	-18	HIS	-	linker	UNP P0AA25
A	-17	MET	-	linker	UNP P0AA25
A	-16	HIS	-	linker	UNP P0AA25
A	-15	HIS	-	linker	UNP P0AA25
A	-14	HIS	-	linker	UNP P0AA25
A	-13	HIS	-	linker	UNP P0AA25
A	-12	HIS	-	linker	UNP P0AA25
A	-11	HIS	-	linker	UNP P0AA25
A	-10	SER	-	linker	UNP P0AA25
A	-9	SER	-	linker	UNP P0AA25
A	-8	GLY	-	linker	UNP P0AA25
A	-7	LEU	-	linker	UNP P0AA25
A	-6	VAL	-	linker	UNP P0AA25
A	-5	PRO	-	linker	UNP P0AA25
A	-4	ARG	-	linker	UNP P0AA25
A	-3	GLY	-	linker	UNP P0AA25
A	-2	SER	-	linker	UNP P0AA25
A	-1	GLY	-	linker	UNP P0AA25
B	-23	GLY	-	linker	UNP P0AA25
B	-22	SER	-	linker	UNP P0AA25

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	GLY	-	linker	UNP P0AA25
B	-20	SER	-	linker	UNP P0AA25
B	-19	GLY	-	linker	UNP P0AA25
B	-18	HIS	-	linker	UNP P0AA25
B	-17	MET	-	linker	UNP P0AA25
B	-16	HIS	-	linker	UNP P0AA25
B	-15	HIS	-	linker	UNP P0AA25
B	-14	HIS	-	linker	UNP P0AA25
B	-13	HIS	-	linker	UNP P0AA25
B	-12	HIS	-	linker	UNP P0AA25
B	-11	HIS	-	linker	UNP P0AA25
B	-10	SER	-	linker	UNP P0AA25
B	-9	SER	-	linker	UNP P0AA25
B	-8	GLY	-	linker	UNP P0AA25
B	-7	LEU	-	linker	UNP P0AA25
B	-6	VAL	-	linker	UNP P0AA25
B	-5	PRO	-	linker	UNP P0AA25
B	-4	ARG	-	linker	UNP P0AA25
B	-3	GLY	-	linker	UNP P0AA25
B	-2	SER	-	linker	UNP P0AA25
B	-1	GLY	-	linker	UNP P0AA25

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	54	Total	O	0	0
			54	54		
2	B	50	Total	O	0	0
			50	50		

- Molecule 1: Thioredoxin 1,scFv





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.21Å 77.75Å 61.35Å 90.00° 112.25° 90.00°	Depositor
Resolution (Å)	55.79 – 2.21 55.79 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.79-2.21) 99.9 (55.79-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.269 , 0.321 0.281 , 0.318	Depositor DCC
R_{free} test set	1227 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	8.4	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	3483	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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

5.1 Standard geometry

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	0.85	0/1722	1.26	3/2344 (0.1%)
1	B	0.85	0/1714	1.26	3/2333 (0.1%)
All	All	0.85	0/3436	1.26	6/4677 (0.1%)

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	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	THR	CA-CB-OG1	-7.87	97.80	109.60
1	A	223	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	B	220	VAL	CA-C-O	5.36	123.86	119.47
1	B	191	TYR	N-CA-CB	5.25	118.44	110.14
1	B	37	PRO	N-CA-CB	-5.20	97.79	103.25

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ARG	Sidechain
1	A	94	ARG	Sidechain
1	B	137	ARG	Sidechain
1	B	94	ARG	Sidechain

5.2 Too-close contacts

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	1693	0	1639	32	1
1	B	1686	0	1632	29	0
2	A	54	0	0	2	0
2	B	50	0	0	2	0
All	All	3483	0	3271	60	1

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 9.

The worst 5 of 60 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)
1:A:41:LYS:HB2	1:A:44:GLN:OE1	1.42	1.16
1:A:223:ARG:NH1	1:A:244:ASP:OD2	2.04	0.90
1:A:41:LYS:HB2	1:A:44:GLN:CD	2.00	0.86
1:A:223:ARG:HH12	1:A:244:ASP:CG	1.88	0.80
1:A:57:ILE:HD11	1:A:101:THR:HA	1.72	0.72

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:NZ	1:A:128:ASP:OD1[2_656]	1.74	0.46

5.3 Torsion angles

5.3.1 Protein backbone

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	228/412 (55%)	209 (92%)	18 (8%)	1 (0%)	30	33
1	B	228/412 (55%)	209 (92%)	14 (6%)	5 (2%)	5	3
All	All	456/824 (55%)	418 (92%)	32 (7%)	6 (1%)	9	7

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	PRO
1	B	39	LEU
1	B	202	PRO
1	B	146	GLY
1	B	69	PRO

5.3.2 Protein sidechains ⓘ

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	189/328 (58%)	159 (84%)	30 (16%)	2	2
1	B	188/328 (57%)	163 (87%)	25 (13%)	4	3
All	All	377/656 (58%)	322 (85%)	55 (15%)	3	2

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	B	71	LYS
1	B	257	SER
1	B	185	SER
1	A	257	SER

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

Mol	Chain	Res	Type
1	A	166	GLN

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Mol	Chain	Res	Type
1	A	231	ASN
1	A	241	GLN
1	B	166	GLN
1	B	241	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	232/412 (56%)	1.06	39 (16%)	4 3	2, 11, 44, 78	0
1	B	232/412 (56%)	1.03	35 (15%)	5 4	2, 10, 43, 104	0
All	All	464/824 (56%)	1.04	74 (15%)	5 4	2, 11, 44, 104	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	GLY	12.8
1	B	38	SER	9.9
1	A	38	SER	8.4
1	B	146	GLY	8.1
1	A	146	GLY	7.9

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.