



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 8DCE / pdb_00008dce
Title : SARS-CoV-2 Receptor-Binding Domain SPEEDesign Immunogen 1 Bound to C144 scFv
Authors : Tang, W.K.; Tolia, N.H.
Deposited on : 2022-06-16
Resolution : 2.00 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
Xtrriage (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

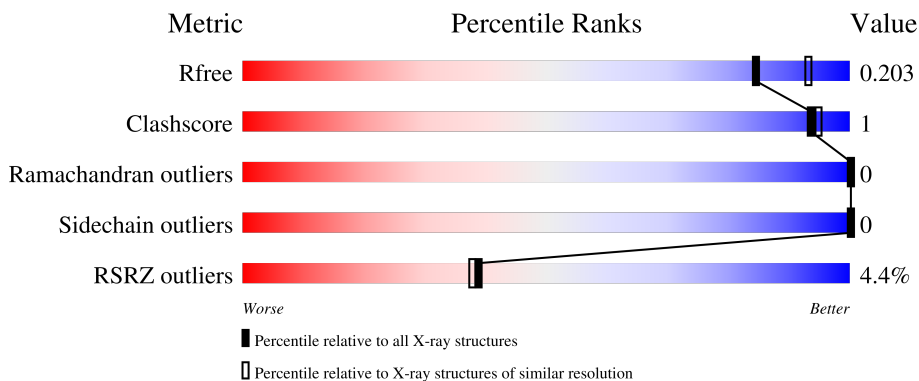
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	H	276	 2% 86% 12%
2	A	210	 6% 88% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6811 atoms, of which 3195 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 C144 scFv.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	H	242	3579	1147	1738	312	375	7	0	0	0

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	A	194	3006	995	1457	254	292	8	0	1	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	GLU	-	expression tag	UNP P0DTC2
A	331	THR	-	expression tag	UNP P0DTC2
A	332	GLY	-	expression tag	UNP P0DTC2
A	333	MET	THR	engineered mutation	UNP P0DTC2
A	348	PRO	ALA	engineered mutation	UNP P0DTC2
A	362	TYR	VAL	engineered mutation	UNP P0DTC2
A	363	TYR	ALA	engineered mutation	UNP P0DTC2
A	394	GLN	ASN	engineered mutation	UNP P0DTC2
A	396	PHE	TYR	engineered mutation	UNP P0DTC2
A	468	THR	ILE	engineered mutation	UNP P0DTC2
A	519	ASP	HIS	engineered mutation	UNP P0DTC2
A	522	PRO	ALA	engineered mutation	UNP P0DTC2
A	527	THR	-	expression tag	UNP P0DTC2
A	528	GLY	-	expression tag	UNP P0DTC2
A	529	GLY	-	expression tag	UNP P0DTC2
A	530	GLY	-	expression tag	UNP P0DTC2
A	531	GLY	-	expression tag	UNP P0DTC2
A	532	SER	-	expression tag	UNP P0DTC2
A	533	LYS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
A	537	HIS	-	expression tag	UNP P0DTC2
A	538	HIS	-	expression tag	UNP P0DTC2
A	539	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	157	Total O 157 157	0	0
3	A	69	Total O 69 69	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	81.63Å 97.31Å 141.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.78 – 2.00 19.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.78-2.00) 99.7 (19.78-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.01Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.177 , 0.203 0.178 , 0.203	Depositor DCC
R_{free} test set	2000 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtrriage
Anisotropy	0.461	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6811	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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	H	0.13	0/1882	0.32	0/2552
2	A	0.11	0/1603	0.27	0/2183
All	All	0.12	0/3485	0.30	0/4735

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	H	1841	1738	1740	3	0
2	A	1549	1457	1450	6	0
3	A	69	0	0	0	0
3	H	157	0	0	0	0
All	All	3616	3195	3190	9	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 1.

The worst 5 of 9 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:A:357:ARG:NH2	2:A:394:GLN:OE1	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:ILE:HD11	1:H:85:LEU:HD13	1.90	0.53
2:A:394:GLN:NE2	2:A:516:GLU:OE1	2.43	0.52
1:H:184:ASP:OD1	1:H:185:VAL:N	2.42	0.51
2:A:353:TRP:CE2	2:A:466:ARG:HG2	2.46	0.51

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	H	238/276 (86%)	228 (96%)	10 (4%)	0	100	100
2	A	193/210 (92%)	185 (96%)	8 (4%)	0	100	100
All	All	431/486 (89%)	413 (96%)	18 (4%)	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	H	200/214 (94%)	200 (100%)	0	100	100
2	A	171/181 (94%)	171 (100%)	0	100	100
All	All	371/395 (94%)	371 (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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	13	GLN
1	H	195	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	H	242/276 (87%)	-0.30	6 (2%) 58 58	25, 34, 55, 91	0
2	A	194/210 (92%)	0.22	13 (6%) 24 22	28, 50, 87, 104	1 (0%)
All	All	436/486 (89%)	-0.07	19 (4%) 39 38	25, 38, 79, 104	1 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	466	ARG	4.9
2	A	449	TYR	4.7
1	H	123	GLN	4.1
1	H	179	THR	3.5
2	A	445	VAL	3.2

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 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.