



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2022 – 06:02 PM EDT

PDB ID : 8DCE
Title : SARS-CoV-2 Receptor-Binding Domain SPEEDesign Immunogen 1 Bound to C144 scFv
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Deposited on : 2022-06-16
Resolution : 2.00 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 ⓘ 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	:	2.29
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)	:	2.29

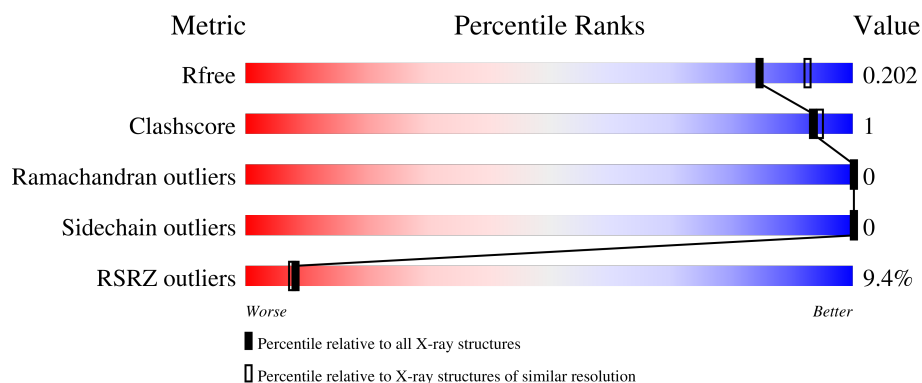
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>•</div> <div>12%</div> </div> </div>
2	A	210	<div> <div>14%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>8%</div> </div> </div>

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
1	H	242	Total	C	H	N	O	S	0	0	0
			3579	1147	1738	312	375	7			

- Molecule 2 is a protein called Spike protein S1.

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

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

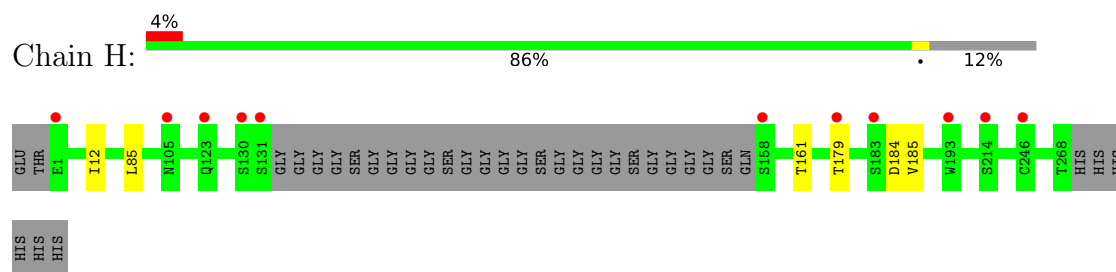
- Molecule 3 is water.

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

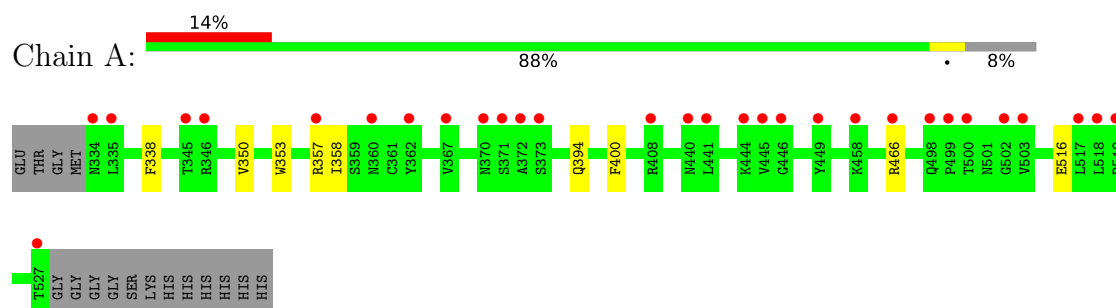
3 Residue-property plots [i](#)

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: C144 scFv



- Molecule 2: Spike protein S1



4 Data and refinement statistics

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) 99.8 (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)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.177 , 0.203 0.176 , 0.202	Depositor DCC
R_{free} test set	2000 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

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	H	0.27	0/1882	0.53	0/2552
2	A	0.26	0/1603	0.49	0/2183
All	All	0.26	0/3485	0.51	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

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.

All (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
1:H:161:THR:HB	1:H:179:THR:OG1	2.17	0.45
2:A:338:PHE:CE1	2:A:358:ILE:HD12	2.53	0.43
2:A:350:VAL:HA	2:A:400:PHE:HB2	2.00	0.42
2:A:353:TRP:CZ2	2:A:466:ARG:HG3	2.57	0.40

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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. There are no such sidechains identified.

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

6.1 Protein, DNA and RNA chains

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%)	0.17	11 (4%) 33 32	23, 31, 49, 83	0
2	A	194/210 (92%)	0.79	30 (15%) 2 1	26, 45, 80, 99	1 (0%)
All	All	436/486 (89%)	0.44	41 (9%) 8 8	23, 35, 73, 99	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	445	VAL	9.6
1	H	131	SER	7.3
2	A	518	LEU	5.2
2	A	372	ALA	5.1
2	A	346	ARG	4.8
2	A	334	ASN	4.8
2	A	527	THR	4.6
2	A	345	THR	4.5
2	A	362	TYR	4.3
2	A	517	LEU	4.1
2	A	519	ASP	3.8
2	A	503	VAL	3.7
2	A	502	GLY	3.7
2	A	500	THR	3.6
2	A	449	TYR	3.5
2	A	466	ARG	3.4
2	A	446	GLY	3.3
1	H	158	SER	3.2
1	H	123	GLN	3.2
2	A	371	SER	3.1
2	A	373	SER	3.1
2	A	335	LEU	3.1
2	A	440	ASN	3.0
2	A	408	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	A	367	VAL	2.8
1	H	193	TRP	2.7
1	H	214	SER	2.7
1	H	105	ASN	2.5
2	A	458	LYS	2.5
2	A	360	ASN	2.5
1	H	183	SER	2.4
2	A	357	ARG	2.4
2	A	444	LYS	2.4
1	H	179	THR	2.4
1	H	130	SER	2.4
2	A	441	LEU	2.3
1	H	1	GLU	2.3
2	A	370	ASN	2.2
2	A	499	PRO	2.2
2	A	498	GLN	2.2
1	H	246	CYS	2.1

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.