Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2026 – 02:54 PM JST

PDB ID	:	9UMI / pdb_00009umi
Title	:	Crystal structure of the SARS-CoV-2 spike protein HR1 in complex with a designed peptide inhibitor dP-S2FI-22 at 1.95 angstrom resolution
Authors	:	Wang, K.; Chen, J.; Dong, Y.; Ye, S.
Deposited on	:	2025-04-22
Resolution	:	1.95 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:

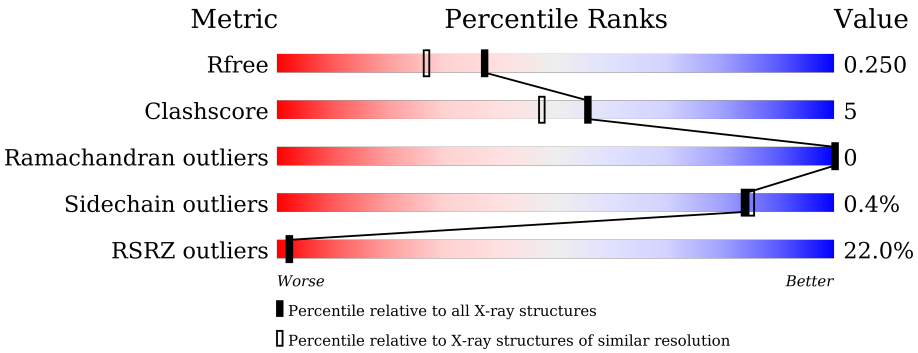
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 <=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	121	19% 83% 7% 9%
1	C	121	18% 86% 5% 9%
1	E	121	22% 78% 11% • 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5598 atoms, of which 2622 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 dP-S2FI-22 peptide,Spike protein S2'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	H	N	O	0	2	0
			1707	518	869	148	172			
1	C	110	Total	C	H	N	O	0	4	0
			1745	529	889	151	176			
1	E	108	Total	C	H	N	O	0	3	0
			1695	513	864	149	169			

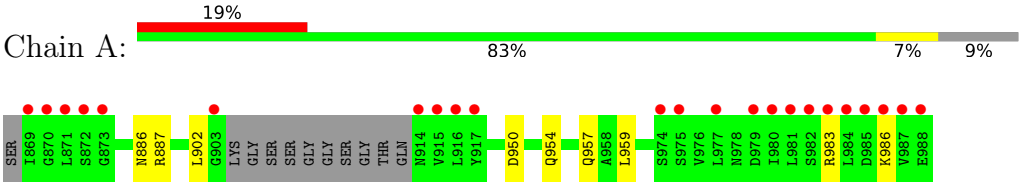
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	154	Total	O	0	0
			154	154		
2	C	153	Total	O	0	0
			153	153		
2	E	144	Total	O	0	0
			144	144		

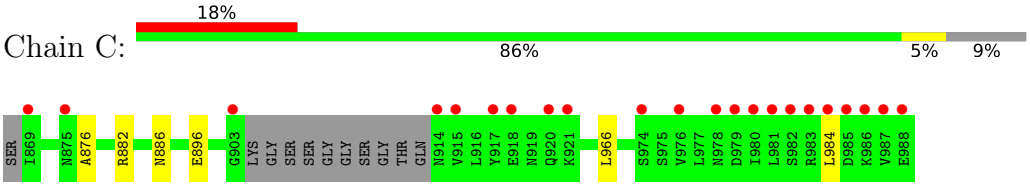
3 Residue-property plots (i)

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.

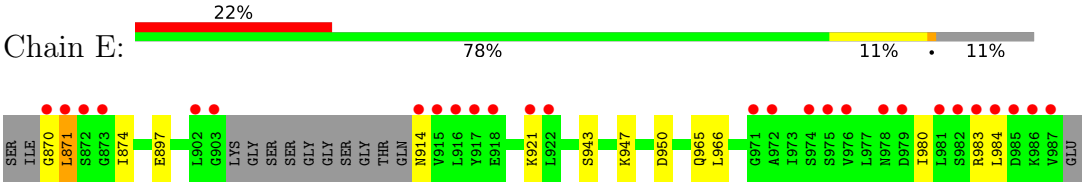
- Molecule 1: dP-S2FI-22 peptide,Spike protein S2'



- Molecule 1: dP-S2FI-22 peptide,Spike protein S2'



- Molecule 1: dP-S2FI-22 peptide,Spike protein S2'



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	146.00Å 42.22Å 67.30Å 90.00° 106.89° 90.00°	Depositor
Resolution (Å)	35.30 – 1.95 35.30 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.3 (35.30-1.95) 96.2 (35.30-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.215 , 0.252 0.216 , 0.250	Depositor DCC
R_{free} test set	1440 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5598	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.23	0/845	0.27	0/1138
1	C	0.23	0/869	0.25	0/1168
1	E	0.22	0/841	0.28	0/1132
All	All	0.23	0/2555	0.27	0/3438

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	A	838	869	869	10	0
1	C	856	889	889	7	0
1	E	831	864	864	12	0
2	A	154	0	0	6	0
2	C	153	0	0	4	3
2	E	144	0	0	5	0
All	All	2976	2622	2622	24	3

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 5.

All (24) 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:C:896[A]:GLU:OE1	2:C:1001:HOH:O	1.88	0.91
1:E:980:ILE:O	2:E:1001:HOH:O	1.94	0.85
1:C:896[B]:GLU:OE2	2:C:1002:HOH:O	1.96	0.82
1:C:984:LEU:HD23	1:E:983:ARG:HH21	1.47	0.77
1:C:882[A]:ARG:NH2	2:C:1003:HOH:O	2.19	0.76
1:A:957:GLN:NE2	2:A:1002:HOH:O	2.21	0.73
1:E:897:GLU:OE1	2:E:1002:HOH:O	2.11	0.67
1:E:871:LEU:O	1:E:965:GLN:NE2	2.28	0.66
1:A:886[A]:ASN:OD1	2:A:1001:HOH:O	2.13	0.65
1:E:914:ASN:N	2:E:1005:HOH:O	2.33	0.61
1:E:871:LEU:HB3	1:E:874:ILE:HD12	1.85	0.56
1:A:959:LEU:HD23	1:C:876:ALA:HB2	1.92	0.51
1:A:902:LEU:HD12	1:E:921:LYS:HD3	1.93	0.51
1:C:886[A]:ASN:OD1	2:C:1004:HOH:O	2.20	0.49
1:C:966:LEU:HD13	1:E:966:LEU:HD21	1.94	0.49
1:A:957:GLN:NE2	2:A:1015:HOH:O	2.45	0.49
1:A:887:ARG:NH2	2:A:1012:HOH:O	2.41	0.48
1:E:870:GLY:N	2:E:1009:HOH:O	2.50	0.44
1:A:950:ASP:O	1:A:954:GLN:HG3	2.19	0.43
1:A:954:GLN:NE2	2:A:1008:HOH:O	2.37	0.42
1:E:950:ASP:OD1	2:E:1003:HOH:O	2.21	0.42
1:A:983:ARG:NH2	1:E:984:LEU:HD23	2.35	0.41
1:A:986:LYS:NZ	2:A:1006:HOH:O	2.35	0.41
1:E:943:SER:O	1:E:947:LYS:HG3	2.21	0.41

All (3) 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)
2:C:1008:HOH:O	2:C:1035:HOH:O[2_555]	1.97	0.23
2:C:1125:HOH:O	2:C:1139:HOH:O[2_555]	2.12	0.08
2:C:1129:HOH:O	2:C:1129:HOH:O[2_555]	2.17	0.03

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	108/121 (89%)	108 (100%)	0	0	100	100
1	C	110/121 (91%)	110 (100%)	0	0	100	100
1	E	107/121 (88%)	106 (99%)	1 (1%)	0	100	100
All	All	325/363 (90%)	324 (100%)	1 (0%)	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	A	97/102 (95%)	97 (100%)	0	100	100
1	C	99/102 (97%)	99 (100%)	0	100	100
1	E	96/102 (94%)	95 (99%)	1 (1%)	68	67
All	All	292/306 (95%)	291 (100%)	1 (0%)	84	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	871	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	957	GLN
1	E	965	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

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, 95^{th} 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	110/121 (90%)	0.72	23 (20%)	2	2	12, 27, 79, 90	2 (1%)
1	C	110/121 (90%)	0.82	22 (20%)	3	3	16, 29, 88, 100	4 (3%)
1	E	108/121 (89%)	1.01	27 (25%)	2	1	17, 33, 82, 107	3 (2%)
All	All	328/363 (90%)	0.85	72 (21%)	2	2	12, 30, 84, 107	9 (2%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	915	VAL	6.7
1	E	987	VAL	6.4
1	C	914	ASN	6.2
1	C	869	ILE	6.0
1	A	869	ILE	5.9
1	E	872	SER	5.7
1	E	873	GLY	5.5
1	A	914	ASN	4.9
1	A	984	LEU	4.8
1	A	903	GLY	4.8
1	A	917	TYR	4.8
1	C	976	VAL	4.7
1	C	985	ASP	4.7
1	E	914	ASN	4.6
1	C	917	TYR	4.4
1	E	871	LEU	4.4
1	E	917	TYR	4.4
1	A	987	VAL	4.3
1	E	986	LYS	4.1
1	C	988	GLU	4.1
1	C	915	VAL	4.0
1	A	977	LEU	3.9
1	E	983	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	870	GLY	3.6
1	C	982	SER	3.6
1	A	986	LYS	3.5
1	C	980	ILE	3.5
1	C	984	LEU	3.5
1	C	979	ASP	3.4
1	E	985	ASP	3.3
1	C	987	VAL	3.3
1	E	984	LEU	3.3
1	A	872	SER	3.3
1	E	981	LEU	3.2
1	E	902	LEU	3.2
1	A	983	ARG	3.1
1	A	871	LEU	3.0
1	A	982	SER	3.0
1	E	915	VAL	3.0
1	A	988	GLU	2.9
1	E	903	GLY	2.9
1	C	974	SER	2.9
1	A	916	LEU	2.9
1	C	903	GLY	2.9
1	C	978	ASN	2.8
1	A	980	ILE	2.8
1	A	979	ASP	2.8
1	E	982	SER	2.8
1	E	979[A]	ASP	2.8
1	C	981	LEU	2.7
1	C	983	ARG	2.7
1	E	978	ASN	2.7
1	E	916	LEU	2.7
1	E	918	GLU	2.6
1	E	921	LYS	2.6
1	C	986	LYS	2.6
1	A	981	LEU	2.6
1	A	974	SER	2.6
1	E	974	SER	2.6
1	A	985	ASP	2.4
1	E	972	ALA	2.4
1	A	870	GLY	2.4
1	E	976	VAL	2.3
1	C	918	GLU	2.3
1	A	975	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	920	GLN	2.3
1	E	922	LEU	2.3
1	C	921	LYS	2.2
1	E	971	GLY	2.1
1	A	873	GLY	2.1
1	C	875	ASN	2.1
1	E	975	SER	2.0

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.