Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2026 – 02:53 PM JST

PDB ID	:	9UM0 / pdb_00009um0
Title	:	Crystal structure of the SARS-CoV-2 spike protein HR1 in complex with a designed peptide inhibitor dP-S2FI-01 at 2.2 angstrom resolution
Authors	:	Wang, K.; Dong, Y.; Ye, S.
Deposited on	:	2025-04-21
Resolution	:	2.20 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:

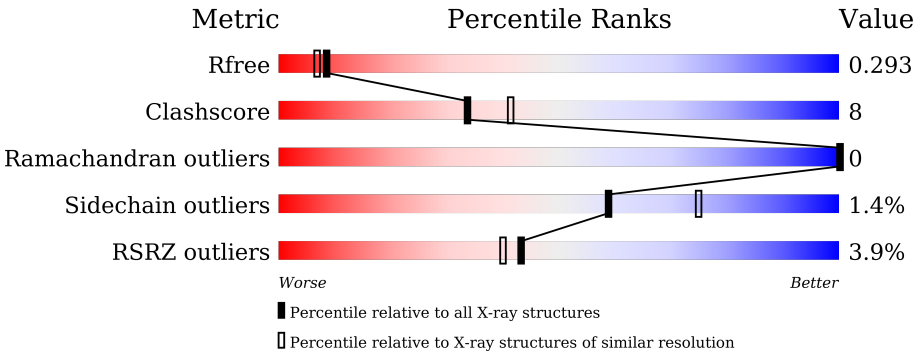
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 <=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	78	5% 83% 13% ·
1	C	78	3% 88% 12%
1	E	78	4% 83% 15% ·
2	B	36	78% 14% 8%
2	D	36	8% 69% 31%
2	F	36	3% 67% 19% · 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2688 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 Spike protein S2'.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	75	Total 567	C 351	N 99	O 117	0	0	0
1	C	78	Total 589	C 363	N 103	O 123	0	0	0
1	E	77	Total 583	C 360	N 102	O 121	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	911	SER	-	expression tag	UNP P0DTC2
C	911	SER	-	expression tag	UNP P0DTC2
E	911	SER	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called designed peptide inhibitor dP-S2FI-01.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	33	Total 256	C 160	N 47	O 49	0	0	0
2	D	36	Total 277	C 174	N 51	O 52	0	0	0
2	F	32	Total 252	C 158	N 46	O 48	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total 39	O 39	0	0
3	B	22	Total 22	O 22	0	0

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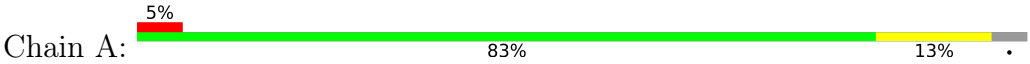
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	31	Total O 31 31	0	0
3	D	22	Total O 22 22	0	0
3	E	38	Total O 38 38	0	0
3	F	12	Total O 12 12	0	0

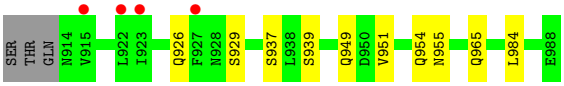
3 Residue-property plots

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: Spike protein S2'

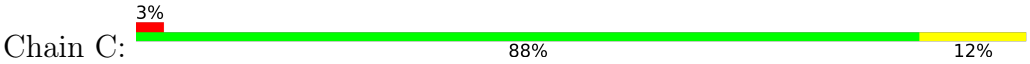
Chain A:

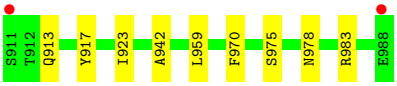




• Molecule 1: Spike protein S2'

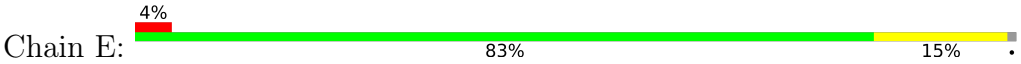
Chain C:

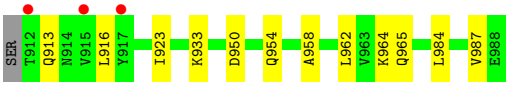




• Molecule 1: Spike protein S2'

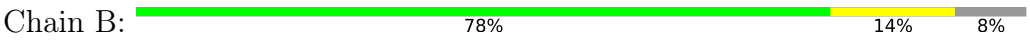
Chain E:





• Molecule 2: designed peptide inhibitor dP-S2FI-01

Chain B:

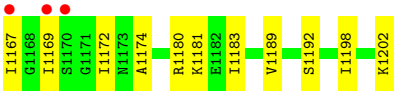




• Molecule 2: designed peptide inhibitor dP-S2FI-01

Chain D:

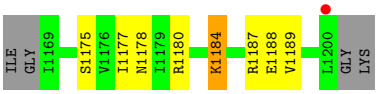




• Molecule 2: designed peptide inhibitor dP-S2FI-01

Chain F:


3%
67%
19%
11%


ILE
GLY
I1169
S1175
V1176
I1177
N1178
I1179
R1180
K1184
R1187
E1188
V1189
L1200
GLY
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.27Å 59.13Å 90.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.21 – 2.20 42.21 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.5 (42.21-2.20) 90.5 (42.21-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.238 , 0.292 0.239 , 0.293	Depositor DCC
R_{free} test set	822 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2688	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.28% 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	0.06	0/569	0.15	0/767
1	C	0.06	0/591	0.17	0/797
1	E	0.06	0/585	0.17	0/789
2	B	0.09	0/255	0.19	0/339
2	D	0.13	0/276	0.32	0/366
2	F	0.07	0/251	0.20	0/334
All	All	0.07	0/2527	0.19	0/3392

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	567	0	580	10	0
1	C	589	0	600	10	0
1	E	583	0	595	11	0
2	B	256	0	281	6	0
2	D	277	0	308	13	0
2	F	252	0	278	8	0
3	A	39	0	0	2	0
3	B	22	0	0	3	0
3	C	31	0	0	1	0
3	D	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	38	0	0	0	0
3	F	12	0	0	1	0
All	All	2688	0	2642	40	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 8.

All (40) 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:D:1202:LYS:NZ	3:D:1302:HOH:O	2.27	0.67
1:C:917:TYR:HD1	1:E:916:LEU:HD21	1.61	0.64
2:B:1191:LYS:NZ	3:B:1301:HOH:O	2.31	0.64
2:B:1187:ARG:NH1	3:B:1301:HOH:O	2.29	0.64
1:A:937:SER:HB3	2:F:1189:VAL:HG11	1.80	0.63
2:B:1198:ILE:HD13	1:C:923:ILE:HG12	1.81	0.62
1:A:984:LEU:HD23	1:C:983:ARG:HH21	1.65	0.61
1:C:978:ASN:ND2	3:C:1002:HOH:O	2.33	0.61
2:D:1169:ILE:HG21	1:E:962:LEU:HD12	1.84	0.60
2:D:1169:ILE:HG23	1:E:965:GLN:HB2	1.84	0.57
2:F:1180:ARG:HH22	2:F:1187:ARG:HH12	1.52	0.57
1:C:942:ALA:HB1	2:D:1183:ILE:HG23	1.88	0.56
2:F:1180:ARG:NH2	2:F:1187:ARG:HH12	2.04	0.55
1:C:917:TYR:CD1	1:E:916:LEU:HD21	2.41	0.53
1:E:984:LEU:HA	1:E:987:VAL:HG12	1.92	0.52
1:A:965:GLN:NE2	3:A:1002:HOH:O	2.33	0.51
2:D:1172:ILE:HG23	1:E:958:ALA:HB1	1.93	0.51
1:C:959:LEU:HD23	2:D:1174:ALA:HB2	1.92	0.51
2:D:1189:VAL:HG13	1:E:933:LYS:HB3	1.92	0.51
1:A:951:VAL:HG21	2:F:1177:ILE:HB	1.92	0.51
2:F:1178:ASN:O	3:F:1301:HOH:O	2.19	0.50
1:A:954:GLN:NE2	1:A:955:ASN:OD1	2.46	0.49
2:D:1169:ILE:HG22	2:D:1172:ILE:HD13	1.93	0.49
1:A:954:GLN:HE22	2:F:1175:SER:H	1.61	0.49
2:D:1180:ARG:HH21	2:D:1181:LYS:NZ	2.11	0.47
1:C:970:PHE:HE2	2:D:1169:ILE:HD11	1.79	0.47
1:C:913:GLN:HE22	1:E:913:GLN:HG3	1.80	0.47
1:E:950:ASP:O	1:E:954:GLN:HG3	2.14	0.47
2:F:1184:LYS:O	2:F:1188:GLU:HG3	2.15	0.47
1:A:939:SER:HB2	3:B:1301:HOH:O	2.16	0.46
1:A:949:GLN:HG3	2:B:1177:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1178:ASN:C	2:B:1178:ASN:HD22	2.24	0.46
2:D:1198:ILE:HD13	1:E:923:ILE:HG12	2.00	0.44
2:D:1172:ILE:HD12	2:D:1172:ILE:N	2.33	0.43
1:A:954:GLN:NE2	2:F:1175:SER:OG	2.52	0.43
2:D:1169:ILE:HG22	2:D:1172:ILE:CD1	2.49	0.43
1:A:926:GLN:NE2	3:A:1001:HOH:O	2.27	0.42
1:E:964:LYS:HD3	1:E:964:LYS:HA	1.63	0.42
1:C:975:SER:HA	1:C:978:ASN:HD22	1.85	0.42
2:B:1187:ARG:O	2:B:1191:LYS:HG2	2.21	0.41

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	73/78 (94%)	73 (100%)	0	0	100	100
1	C	76/78 (97%)	76 (100%)	0	0	100	100
1	E	75/78 (96%)	75 (100%)	0	0	100	100
2	B	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
2	D	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
2	F	30/36 (83%)	30 (100%)	0	0	100	100
All	All	319/342 (93%)	317 (99%)	2 (1%)	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	65/68 (96%)	64 (98%)	1 (2%)	57 73
1	C	68/68 (100%)	68 (100%)	0	100 100
1	E	67/68 (98%)	67 (100%)	0	100 100
2	B	29/31 (94%)	29 (100%)	0	100 100
2	D	31/31 (100%)	29 (94%)	2 (6%)	15 18
2	F	29/31 (94%)	28 (97%)	1 (3%)	32 44
All	All	289/297 (97%)	285 (99%)	4 (1%)	59 75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	929	SER
2	D	1167	ILE
2	D	1192	SER
2	F	1184	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	954	GLN
2	B	1178	ASN
1	C	914	ASN
1	C	920	GLN
1	C	954	GLN
1	C	978	ASN
2	F	1178	ASN

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	75/78 (96%)	0.46	4 (5%) 32 29	13, 26, 40, 53	0
1	C	78/78 (100%)	0.24	2 (2%) 57 54	11, 22, 38, 62	0
1	E	77/78 (98%)	0.38	3 (3%) 43 40	18, 26, 49, 55	0
2	B	33/36 (91%)	0.38	0 100 100	17, 28, 45, 46	0
2	D	36/36 (100%)	0.68	3 (8%) 17 15	24, 37, 50, 52	0
2	F	32/36 (88%)	0.97	1 (3%) 51 48	27, 37, 49, 53	0
All	All	331/342 (96%)	0.45	13 (3%) 43 40	11, 27, 47, 62	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	988	GLU	3.4
1	A	927	PHE	3.3
2	D	1170	SER	3.3
2	D	1167	ILE	3.0
2	F	1200	LEU	3.0
1	A	915	VAL	2.8
1	A	922	LEU	2.8
1	E	917	TYR	2.5
1	E	912	THR	2.5
1	A	923	ILE	2.3
1	C	911	SER	2.2
2	D	1169	ILE	2.1
1	E	915	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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.