



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:52 PM UTC

PDB ID : 5K6I / pdb_00005k6i
Title : Crystal structure of prefusion-stabilized RSV F single-chain 9-10 DS-Cav1 A149C-Y458C, S46G-E92D-S215P-K465Q variant.
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Deposited on : 2016-05-24
Resolution : 2.92 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

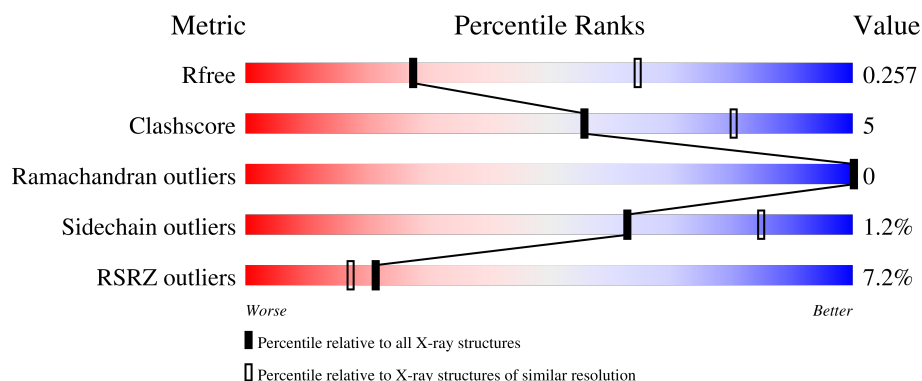
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	F	445	7% 87% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3527 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	445	Total	C	N	O	S	0	4	0
			3462	2178	578	681	25			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	GLY	SER	engineered mutation	UNP P03420
F	92	ASP	GLU	engineered mutation	UNP P03420
F	102	ALA	PRO	engineered mutation	UNP P03420
F	143	GLY	-	linker	UNP P03420
F	144	SER	-	linker	UNP P03420
F	149	CYS	ALA	engineered mutation	UNP P03420
F	155	CYS	SER	engineered mutation	UNP P03420
F	190	PHE	SER	engineered mutation	UNP P03420
F	207	LEU	VAL	engineered mutation	UNP P03420
F	215	PRO	SER	engineered mutation	UNP P03420
F	290	CYS	SER	engineered mutation	UNP P03420
F	373	ARG	LEU	engineered mutation	UNP P03420
F	379	VAL	ILE	engineered mutation	UNP P03420
F	447	VAL	MET	engineered mutation	UNP P03420
F	458	CYS	TYR	engineered mutation	UNP P03420
F	465	GLN	LYS	engineered mutation	UNP P03420

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

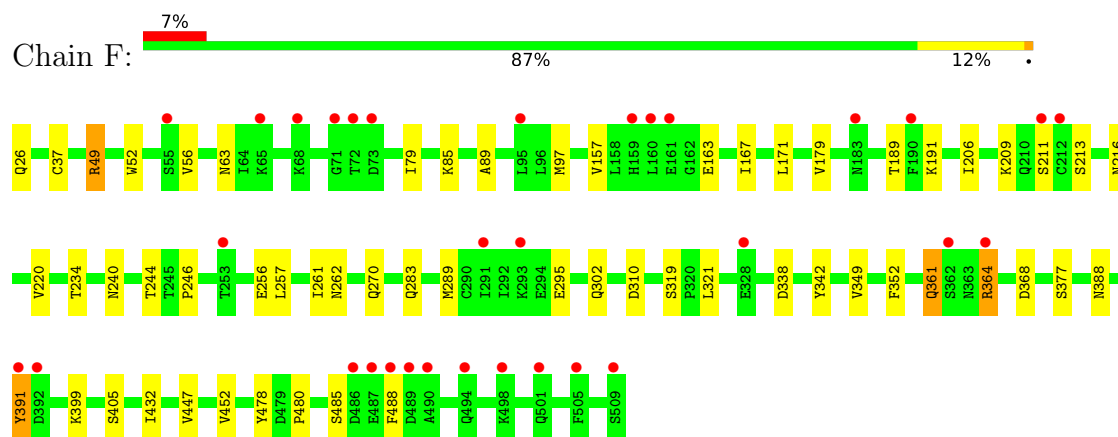
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	22	Total	O	0	0
			22	22		

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: Fusion glycoprotein F0



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	169.56 Å 169.56 Å 169.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.03 – 2.92 47.03 – 2.92	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.03-2.92) 93.9 (47.03-2.92)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.91 Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.220 , 0.253 0.229 , 0.257	Depositor DCC
R_{free} test set	1005 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3527	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PO4, NAG, ZN

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	F	0.28	2/3526 (0.1%)	0.43	8/4780 (0.2%)

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	F	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	364[A]	ARG	CA-C	5.88	1.59	1.52
1	F	364[B]	ARG	CA-C	5.88	1.59	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	364[A]	ARG	CA-C-O	7.72	130.90	121.56
1	F	364[B]	ARG	CA-C-O	7.72	130.90	121.56
1	F	364[A]	ARG	N-CA-C	7.24	121.37	110.14
1	F	364[B]	ARG	N-CA-C	7.24	121.37	110.14
1	F	364[A]	ARG	CA-C-N	-5.99	114.62	122.94
1	F	364[A]	ARG	C-N-CA	-5.99	114.62	122.94
1	F	364[B]	ARG	CA-C-N	-5.99	114.62	122.94
1	F	364[B]	ARG	C-N-CA	-5.99	114.62	122.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	361	GLN	Peptide

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	F	3462	0	3499	33	0
2	F	2	0	0	0	0
3	F	8	0	12	0	0
4	F	5	0	0	1	0
5	F	28	0	26	0	0
6	F	22	0	0	4	0
All	All	3527	0	3537	33	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 5.

All (33) 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:F:49:ARG:NH1	1:F:368:ASP:OD1	1.91	1.03
1:F:270:GLN:NE2	6:F:701:HOH:O	1.87	1.01
1:F:352:PHE:O	6:F:702:HOH:O	2.00	0.80
1:F:256:GLU:OE2	6:F:703:HOH:O	2.07	0.72
1:F:478:TYR:O	1:F:480:PRO:HD3	1.93	0.69
1:F:63:ASN:HB2	1:F:295:GLU:HG2	1.75	0.67
1:F:49:ARG:HH11	1:F:368:ASP:CG	1.99	0.64
1:F:364[B]:ARG:HH11	1:F:364[B]:ARG:HB3	1.65	0.61
1:F:56:VAL:HB	1:F:189:THR:HG22	1.87	0.55
1:F:310:ASP:OD1	1:F:364[B]:ARG:NH2	2.42	0.53
1:F:206:ILE:HG23	1:F:213:SER:HB3	1.92	0.52
1:F:157:VAL:HG12	1:F:163:GLU:HG2	1.92	0.52
1:F:79:ILE:HG12	1:F:220:VAL:HG22	1.93	0.51
1:F:85:LYS:NZ	4:F:605:PO4:O1	2.41	0.51
1:F:97:MET:HE3	1:F:289:MET:HG3	1.93	0.50
1:F:240:ASN:HB2	1:F:244:THR:HG22	1.94	0.49
1:F:89:ALA:HB1	1:F:234:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:CYS:SG	1:F:319:SER:HB3	2.56	0.46
1:F:405:SER:HB2	1:F:452:VAL:HG21	1.98	0.45
1:F:246:PRO:HB3	1:F:283:GLN:HA	1.99	0.44
1:F:171:LEU:HD13	1:F:191:LYS:HB2	1.98	0.43
1:F:399:LYS:HG3	1:F:485:SER:HB2	2.01	0.43
1:F:209:LYS:NZ	1:F:211:SER:O	2.51	0.42
1:F:432:ILE:HD11	1:F:447:VAL:HG22	2.01	0.42
1:F:216:ASN:ND2	6:F:707:HOH:O	2.51	0.42
1:F:338:ASP:O	1:F:342:TYR:OH	2.31	0.42
1:F:349:VAL:HG23	1:F:377:SER:HA	2.02	0.42
1:F:37:CYS:HB2	1:F:321:LEU:HD13	2.02	0.42
1:F:257:LEU:O	1:F:261:ILE:HG13	2.20	0.41
1:F:388:ASN:HB3	1:F:391:TYR:CE2	2.55	0.41
1:F:52:TRP:CE3	1:F:302:GLN:HG2	2.55	0.41
1:F:167:ILE:HG22	1:F:179:VAL:HG21	2.03	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	F	447/445 (100%)	434 (97%)	13 (3%)	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	F	410/406 (101%)	405 (99%)	5 (1%)	63 85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	26	GLN
1	F	49	ARG
1	F	262	ASN
1	F	391	TYR
1	F	488	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	197	ASN
1	F	202	GLN
1	F	240	ASN
1	F	277	ASN
1	F	361	GLN
1	F	380	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](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	F	605	-	4,4,4	0.97	0	6,6,6	0.47	0
5	NAG	F	606	1	14,14,15	0.25	0	17,19,21	0.48	0
3	EDO	F	603	-	3,3,3	0.43	0	2,2,2	0.37	0
5	NAG	F	607	1	14,14,15	0.24	0	17,19,21	0.39	0
3	EDO	F	604	-	3,3,3	0.43	0	2,2,2	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	F	607	1	-	2/6/23/26	0/1/1/1
5	NAG	F	606	1	-	1/6/23/26	0/1/1/1
3	EDO	F	603	-	-	0/1/1/1	-
3	EDO	F	604	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	607	NAG	C8-C7-N2-C2
5	F	607	NAG	O7-C7-N2-C2
5	F	606	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	605	PO4	1	0

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	F	445/445 (100%)	0.45	32 (7%)	21 17	31, 74, 131, 185	4 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	73	ASP	6.0
1	F	159	HIS	4.8
1	F	505	PHE	4.5
1	F	494	GLN	4.4
1	F	183	ASN	4.2
1	F	392	ASP	4.1
1	F	291	ILE	3.7
1	F	55	SER	3.3
1	F	72	THR	3.3
1	F	328	GLU	3.2
1	F	212	CYS	3.1
1	F	509	SER	3.1
1	F	488	PHE	3.0
1	F	489	ASP	3.0
1	F	68	LYS	2.9
1	F	486	ASP	2.9
1	F	95	LEU	2.7
1	F	362	SER	2.6
1	F	391	TYR	2.6
1	F	293	LYS	2.6
1	F	487	GLU	2.6
1	F	71	GLY	2.5
1	F	501	GLN	2.4
1	F	190	PHE	2.4
1	F	364[A]	ARG	2.3
1	F	161	GLU	2.3
1	F	498	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	490	ALA	2.2
1	F	160	LEU	2.2
1	F	211	SER	2.2
1	F	65	LYS	2.1
1	F	253	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	F	607	14/15	0.25	0.17	161,172,178,179	0
5	NAG	F	606	14/15	0.32	0.18	130,156,164,166	0
3	EDO	F	603	4/4	0.56	0.24	104,110,110,112	0
3	EDO	F	604	4/4	0.72	0.24	110,114,119,120	0
4	PO4	F	605	5/5	0.83	0.19	195,197,199,199	0
2	ZN	F	601	1/1	0.91	0.13	134,134,134,134	0
2	ZN	F	602	1/1	0.98	0.09	139,139,139,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.