



wwPDB EM Validation Summary Report ⓘ

Feb 20, 2025 – 06:07 pm GMT

PDB ID : 9HVW
EMDB ID : EMD-52444
Title : Respiratory Syncytial Virus Fusion protein in the postfusion conformation in complex with monoclonal antibody 131-2a Fab
Authors : Snijder, J.
Deposited on : 2025-01-02
Resolution : 3.10 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

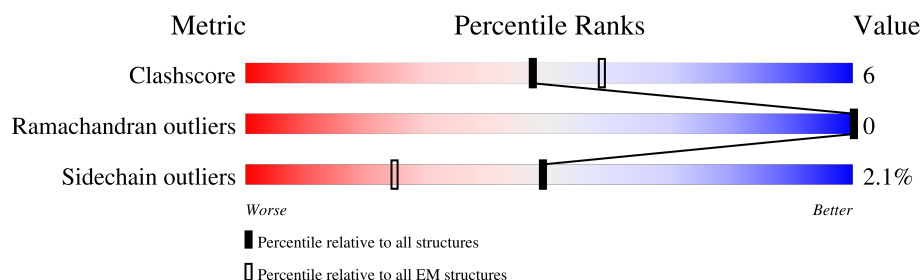
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	80	62% 10% 28%
1	B	80	64% 9% 28%
1	C	80	64% 9% 28%
2	D	511	38% 10% 52%
2	E	511	39% 10% 51%
2	F	511	40% 8% 52%
3	H	120	78% 21% .
4	L	111	83% 16% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8950 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	A	58	Total	C	N	O	S	0	0
			465	298	73	92	2		
1	B	58	Total	C	N	O	S	0	0
			465	298	73	92	2		
1	C	58	Total	C	N	O	S	0	0
			465	298	73	92	2		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	variant	UNP P03420
A	103	ALA	THR	conflict	UNP P03420
A	105	SER	ASN	conflict	UNP P03420
B	102	ALA	PRO	variant	UNP P03420
B	103	ALA	THR	conflict	UNP P03420
B	105	SER	ASN	conflict	UNP P03420
C	102	ALA	PRO	variant	UNP P03420
C	103	ALA	THR	conflict	UNP P03420
C	105	SER	ASN	conflict	UNP P03420

- Molecule 2 is a protein called Fusion glycoprotein F1, Probable N-acetylmuramidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	246	Total	C	N	O	S	0	0
			1916	1202	318	379	17		
2	E	252	Total	C	N	O	S	0	0
			1959	1226	326	390	17		
2	F	246	Total	C	N	O	S	0	0
			1916	1202	318	379	17		

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	152	ILE	VAL	conflict	UNP P03420
D	379	VAL	ILE	conflict	UNP P03420
D	384	ILE	VAL	conflict	UNP P03420
D	447	VAL	MET	conflict	UNP P03420
D	516	LEU	-	linker	UNP P03420
D	517	ILE	-	linker	UNP P03420
D	518	LYS	-	linker	UNP P03420
D	519	ARG	-	linker	UNP P03420
D	520	MET	-	linker	UNP P03420
D	521	LYS	-	linker	UNP P03420
D	522	GLN	-	linker	UNP P03420
D	523	ILE	-	linker	UNP P03420
D	524	GLU	-	linker	UNP P03420
D	525	ASP	-	linker	UNP P03420
D	526	LYS	-	linker	UNP P03420
D	527	ILE	-	linker	UNP P03420
D	528	GLU	-	linker	UNP P03420
D	529	GLU	-	linker	UNP P03420
D	530	ILE	-	linker	UNP P03420
D	531	GLU	-	linker	UNP P03420
D	532	SER	-	linker	UNP P03420
D	533	LYS	-	linker	UNP P03420
D	534	GLN	-	linker	UNP P03420
D	535	LYS	-	linker	UNP P03420
D	536	LYS	-	linker	UNP P03420
D	537	ILE	-	linker	UNP P03420
D	538	GLU	-	linker	UNP P03420
D	539	ASN	-	linker	UNP P03420
D	540	GLU	-	linker	UNP P03420
D	541	ILE	-	linker	UNP P03420
D	542	ALA	-	linker	UNP P03420
D	543	ARG	-	linker	UNP P03420
D	544	ILE	-	linker	UNP P03420
D	545	LYS	-	linker	UNP P03420
D	546	LYS	-	linker	UNP P03420
E	152	ILE	VAL	conflict	UNP P03420
E	379	VAL	ILE	conflict	UNP P03420
E	384	ILE	VAL	conflict	UNP P03420
E	447	VAL	MET	conflict	UNP P03420
E	516	LEU	-	linker	UNP P03420
E	517	ILE	-	linker	UNP P03420
E	518	LYS	-	linker	UNP P03420
E	519	ARG	-	linker	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
E	520	MET	-	linker	UNP P03420
E	521	LYS	-	linker	UNP P03420
E	522	GLN	-	linker	UNP P03420
E	523	ILE	-	linker	UNP P03420
E	524	GLU	-	linker	UNP P03420
E	525	ASP	-	linker	UNP P03420
E	526	LYS	-	linker	UNP P03420
E	527	ILE	-	linker	UNP P03420
E	528	GLU	-	linker	UNP P03420
E	529	GLU	-	linker	UNP P03420
E	530	ILE	-	linker	UNP P03420
E	531	GLU	-	linker	UNP P03420
E	532	SER	-	linker	UNP P03420
E	533	LYS	-	linker	UNP P03420
E	534	GLN	-	linker	UNP P03420
E	535	LYS	-	linker	UNP P03420
E	536	LYS	-	linker	UNP P03420
E	537	ILE	-	linker	UNP P03420
E	538	GLU	-	linker	UNP P03420
E	539	ASN	-	linker	UNP P03420
E	540	GLU	-	linker	UNP P03420
E	541	ILE	-	linker	UNP P03420
E	542	ALA	-	linker	UNP P03420
E	543	ARG	-	linker	UNP P03420
E	544	ILE	-	linker	UNP P03420
E	545	LYS	-	linker	UNP P03420
E	546	LYS	-	linker	UNP P03420
F	152	ILE	VAL	conflict	UNP P03420
F	379	VAL	ILE	conflict	UNP P03420
F	384	ILE	VAL	conflict	UNP P03420
F	447	VAL	MET	conflict	UNP P03420
F	516	LEU	-	linker	UNP P03420
F	517	ILE	-	linker	UNP P03420
F	518	LYS	-	linker	UNP P03420
F	519	ARG	-	linker	UNP P03420
F	520	MET	-	linker	UNP P03420
F	521	LYS	-	linker	UNP P03420
F	522	GLN	-	linker	UNP P03420
F	523	ILE	-	linker	UNP P03420
F	524	GLU	-	linker	UNP P03420
F	525	ASP	-	linker	UNP P03420
F	526	LYS	-	linker	UNP P03420

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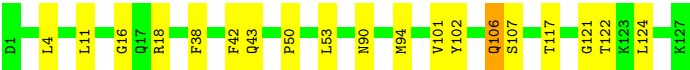
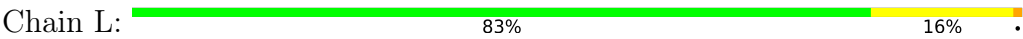
Chain	Residue	Modelled	Actual	Comment	Reference
F	527	ILE	-	linker	UNP P03420
F	528	GLU	-	linker	UNP P03420
F	529	GLU	-	linker	UNP P03420
F	530	ILE	-	linker	UNP P03420
F	531	GLU	-	linker	UNP P03420
F	532	SER	-	linker	UNP P03420
F	533	LYS	-	linker	UNP P03420
F	534	GLN	-	linker	UNP P03420
F	535	LYS	-	linker	UNP P03420
F	536	LYS	-	linker	UNP P03420
F	537	ILE	-	linker	UNP P03420
F	538	GLU	-	linker	UNP P03420
F	539	ASN	-	linker	UNP P03420
F	540	GLU	-	linker	UNP P03420
F	541	ILE	-	linker	UNP P03420
F	542	ALA	-	linker	UNP P03420
F	543	ARG	-	linker	UNP P03420
F	544	ILE	-	linker	UNP P03420
F	545	LYS	-	linker	UNP P03420
F	546	LYS	-	linker	UNP P03420

- Molecule 3 is a protein called 131-2a heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	120	Total	C	N	O	S	0	0
			927	586	151	186	4		

- Molecule 4 is a protein called 131-2a light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	111	Total	C	N	O	S	0	0
			837	529	141	164	3		



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	394000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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	A	0.27	0/470	0.47	0/633
1	B	0.29	0/470	0.51	0/633
1	C	0.27	0/470	0.47	0/633
2	D	0.31	0/1945	0.61	2/2639 (0.1%)
2	E	0.29	0/1989	0.60	2/2699 (0.1%)
2	F	0.30	0/1945	0.57	2/2639 (0.1%)
3	H	0.31	0/949	0.60	0/1285
4	L	0.30	0/857	0.60	0/1160
All	All	0.30	0/9095	0.58	6/12321 (0.0%)

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
3	H	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	263	ASP	CB-CG-OD1	9.54	126.88	118.30
2	E	368	ASP	CB-CG-OD1	8.08	125.57	118.30
2	D	368	ASP	CB-CG-OD2	7.35	124.92	118.30
2	F	368	ASP	CB-CG-OD2	6.97	124.58	118.30
2	F	392	ASP	CB-CG-OD2	6.26	123.93	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	111	PHE	Peptide

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	A	465	0	472	7	0
1	B	465	0	472	4	0
1	C	465	0	472	5	0
2	D	1916	0	1911	30	0
2	E	1959	0	1952	31	0
2	F	1916	0	1911	22	0
3	H	927	0	885	15	0
4	L	837	0	812	11	0
All	All	8950	0	8887	103	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 6.

The worst 5 of 103 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:F:422:CYS:HA	2:F:451:SER:O	1.75	0.87
4:L:102:TYR:O	4:L:121:GLY:HA2	1.82	0.79
3:H:18:SER:HA	3:H:91:LEU:O	1.83	0.78
2:E:422:CYS:HA	2:E:451:SER:O	1.84	0.77
4:L:4:LEU:HD11	4:L:106:GLN:HB3	1.75	0.67

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 PDB entries followed by that with respect to all EM entries.

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	54/80 (68%)	54 (100%)	0	0	100	100
1	B	54/80 (68%)	53 (98%)	1 (2%)	0	100	100
1	C	54/80 (68%)	54 (100%)	0	0	100	100
2	D	242/511 (47%)	231 (96%)	11 (4%)	0	100	100
2	E	250/511 (49%)	233 (93%)	17 (7%)	0	100	100
2	F	242/511 (47%)	233 (96%)	9 (4%)	0	100	100
3	H	118/120 (98%)	108 (92%)	10 (8%)	0	100	100
4	L	109/111 (98%)	104 (95%)	5 (5%)	0	100	100
All	All	1123/2004 (56%)	1070 (95%)	53 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	53/71 (75%)	52 (98%)	1 (2%)	52	75
1	B	53/71 (75%)	51 (96%)	2 (4%)	28	59
1	C	53/71 (75%)	52 (98%)	1 (2%)	52	75
2	D	229/462 (50%)	224 (98%)	5 (2%)	47	71
2	E	234/462 (51%)	230 (98%)	4 (2%)	56	78
2	F	229/462 (50%)	223 (97%)	6 (3%)	41	68
3	H	101/101 (100%)	99 (98%)	2 (2%)	50	74
4	L	92/92 (100%)	91 (99%)	1 (1%)	70	84
All	All	1044/1792 (58%)	1022 (98%)	22 (2%)	49	72

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	228	ASN
2	F	439	CYS
2	F	409	SER
2	F	443	SER
2	D	309	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	L	44	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.