



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:57 PM UTC

PDB ID : 9SHD / pdb_00009shd
Title : Structure of vaccinia virus A26 (residues 1-397) in complex with Fab 10M2146
Authors : Battini, L.; Guardado-Calvo, P.
Deposited on : 2025-08-26
Resolution : 1.90 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
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

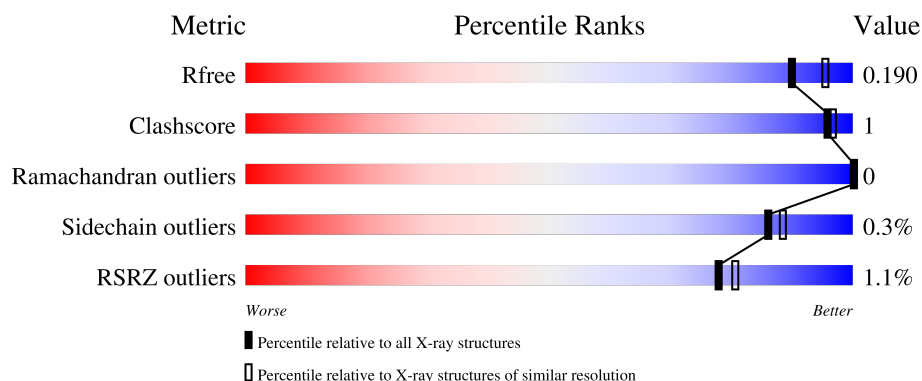
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	H	228	0% 97% 2%
2	L	214	0% 97% 3%
3	K	123	4% 93% 6%
4	H0Z0	457	76% 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8303 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 Heavy chain of Fab 10M2146.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	224	Total	C	N	O	S	0	0	0
			1707	1091	279	331	6			

- Molecule 2 is a protein called Light chain of Fab 10M2146.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1646	1033	274	333	6			

- Molecule 3 is a protein called Anti-Fab VHH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	120	Total	C	N	O	S	0	5	0
			952	591	166	189	6			

- Molecule 4 is a protein called Envelop protein OPG153.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H0Z0	349	Total	C	N	O	S	0	11	0
			2931	1885	491	541	14			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H0Z0	398	GLY	-	expression tag	UNP P24758
H0Z0	399	SER	-	expression tag	UNP P24758
H0Z0	400	GLY	-	expression tag	UNP P24758
H0Z0	401	LEU	-	expression tag	UNP P24758
H0Z0	402	VAL	-	expression tag	UNP P24758
H0Z0	403	PRO	-	expression tag	UNP P24758
H0Z0	404	ARG	-	expression tag	UNP P24758
H0Z0	405	ILE	-	expression tag	UNP P24758

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Chain	Residue	Modelled	Actual	Comment	Reference
H0Z0	406	GLY	-	expression tag	UNP P24758
H0Z0	407	SER	-	expression tag	UNP P24758
H0Z0	408	GLY	-	expression tag	UNP P24758
H0Z0	409	SER	-	expression tag	UNP P24758
H0Z0	410	ALA	-	expression tag	UNP P24758
H0Z0	411	GLY	-	expression tag	UNP P24758
H0Z0	412	TRP	-	expression tag	UNP P24758
H0Z0	413	SER	-	expression tag	UNP P24758
H0Z0	414	HIS	-	expression tag	UNP P24758
H0Z0	415	PRO	-	expression tag	UNP P24758
H0Z0	416	GLN	-	expression tag	UNP P24758
H0Z0	417	PHE	-	expression tag	UNP P24758
H0Z0	418	GLU	-	expression tag	UNP P24758
H0Z0	419	LYS	-	expression tag	UNP P24758
H0Z0	420	GLY	-	expression tag	UNP P24758
H0Z0	421	GLY	-	expression tag	UNP P24758
H0Z0	422	GLY	-	expression tag	UNP P24758
H0Z0	423	SER	-	expression tag	UNP P24758
H0Z0	424	GLY	-	expression tag	UNP P24758
H0Z0	425	GLY	-	expression tag	UNP P24758
H0Z0	426	GLY	-	expression tag	UNP P24758
H0Z0	427	SER	-	expression tag	UNP P24758
H0Z0	428	GLY	-	expression tag	UNP P24758
H0Z0	429	GLY	-	expression tag	UNP P24758
H0Z0	430	GLY	-	expression tag	UNP P24758
H0Z0	431	SER	-	expression tag	UNP P24758
H0Z0	432	TRP	-	expression tag	UNP P24758
H0Z0	433	SER	-	expression tag	UNP P24758
H0Z0	434	HIS	-	expression tag	UNP P24758
H0Z0	435	PRO	-	expression tag	UNP P24758
H0Z0	436	GLN	-	expression tag	UNP P24758
H0Z0	437	PHE	-	expression tag	UNP P24758
H0Z0	438	GLU	-	expression tag	UNP P24758
H0Z0	439	LYS	-	expression tag	UNP P24758
H0Z0	440	GLY	-	expression tag	UNP P24758
H0Z0	441	THR	-	expression tag	UNP P24758
H0Z0	442	GLY	-	expression tag	UNP P24758
H0Z0	443	GLY	-	expression tag	UNP P24758
H0Z0	444	LEU	-	expression tag	UNP P24758
H0Z0	445	ASN	-	expression tag	UNP P24758
H0Z0	446	ASP	-	expression tag	UNP P24758
H0Z0	447	ILE	-	expression tag	UNP P24758

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Chain	Residue	Modelled	Actual	Comment	Reference
H0Z0	448	PHE	-	expression tag	UNP P24758
H0Z0	449	GLU	-	expression tag	UNP P24758
H0Z0	450	ALA	-	expression tag	UNP P24758
H0Z0	451	GLN	-	expression tag	UNP P24758
H0Z0	452	LYS	-	expression tag	UNP P24758
H0Z0	453	ILE	-	expression tag	UNP P24758
H0Z0	454	GLU	-	expression tag	UNP P24758
H0Z0	455	TRP	-	expression tag	UNP P24758
H0Z0	456	HIS	-	expression tag	UNP P24758
H0Z0	457	GLU	-	expression tag	UNP P24758

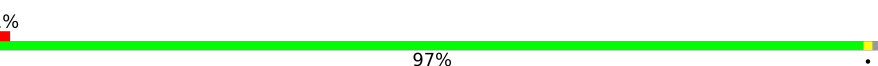
- Molecule 5 is water.

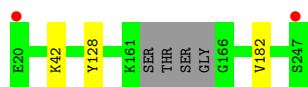
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	237	Total O 237 237	0	0
5	L	283	Total O 283 283	0	0
5	K	112	Total O 112 112	0	0
5	H0Z0	435	Total O 435 435	0	0

3 Residue-property plots [i](#)

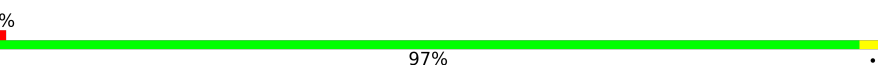
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

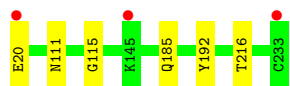
- Molecule 1: Heavy chain of Fab 10M2146

Chain H:  97%

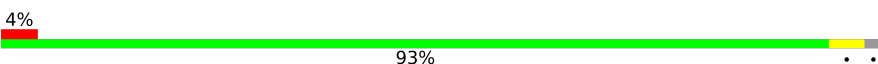


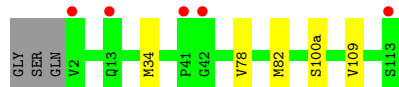
- Molecule 2: Light chain of Fab 10M2146

Chain L:  97%



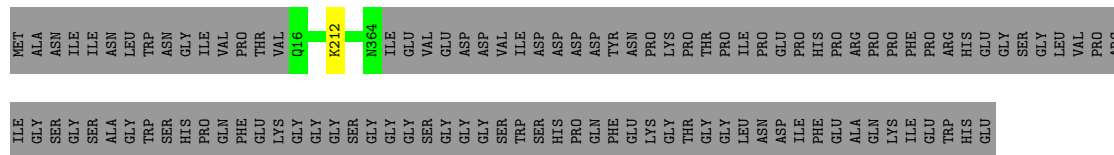
- Molecule 3: Anti-Fab VHH

Chain K:  93%



- Molecule 4: Envelop protein OPG153

Chain H0Z0:  76% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	122.46Å 157.82Å 141.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.93 – 1.90 39.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.93-1.90) 100.0 (39.93-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.158 , 0.190 0.158 , 0.190	Depositor DCC
R_{free} test set	5432 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8303	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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 [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	H	0.34	0/1756	0.52	0/2394
2	L	0.42	0/1681	0.61	0/2280
3	K	0.35	0/977	0.55	0/1320
4	H0Z0	0.42	0/3027	0.58	0/4091
All	All	0.39	0/7441	0.57	0/10085

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 [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	H	1707	0	1663	2	0
2	L	1646	0	1604	4	0
3	K	952	0	904	3	0
4	H0Z0	2931	0	0	0	0
5	H	237	0	0	1	0
5	H0Z0	435	0	0	0	0
5	K	112	0	0	0	0
5	L	283	0	0	0	0
All	All	8303	0	4171	7	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 (7) 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:L:20:GLU:OE2	2:L:115:GLY:N	2.26	0.64
2:L:185:GLN:HG3	2:L:192:TYR:CZ	2.36	0.60
2:L:216:THR:HG22	3:K:100(a):SER:O	2.15	0.47
1:H:128:TYR:CD2	2:L:111:ASN:HA	2.52	0.43
1:H:42:LYS:HD2	5:H:380:HOH:O	2.18	0.43
3:K:82[A]:MET:HE1	3:K:109:VAL:HG21	2.00	0.42
3:K:34:MET:HG3	3:K:78:VAL:HG11	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	H	220/228 (96%)	218 (99%)	2 (1%)	0	100	100
2	L	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
3	K	123/123 (100%)	120 (98%)	3 (2%)	0	100	100
4	H0Z0	358/457 (78%)	352 (98%)	6 (2%)	0	100	100
All	All	913/1022 (89%)	894 (98%)	19 (2%)	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	192/195 (98%)	191 (100%)	1 (0%)	81	84
2	L	186/186 (100%)	186 (100%)	0	100	100
3	K	101/98 (103%)	101 (100%)	0	100	100
4	H0Z0	325/401 (81%)	324 (100%)	1 (0%)	86	88
All	All	804/880 (91%)	802 (100%)	2 (0%)	86	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	182	VAL
4	H0Z0	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	231	ASN
2	L	56	GLN
3	K	81	GLN
3	K	82(A)	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	224/228 (98%)	-0.30	2 (0%) 81 83	18, 26, 44, 71	0
2	L	214/214 (100%)	-0.42	3 (1%) 73 76	17, 22, 40, 88	0
3	K	120/123 (97%)	-0.13	5 (4%) 40 43	15, 27, 54, 78	5 (4%)
4	H0Z0	349/457 (76%)	-0.57	0 100 100	10, 22, 37, 56	11 (3%)
All	All	907/1022 (88%)	-0.41	10 (1%) 78 80	10, 24, 42, 88	16 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	2	VAL	4.8
3	K	113	SER	4.4
1	H	20	GLU	3.6
2	L	233	CYS	3.0
3	K	13	GLN	2.8
2	L	145	LYS	2.6
3	K	41	PRO	2.6
3	K	42	GLY	2.5
1	H	247	SER	2.4
2	L	20	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.