



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:45 AM UTC

PDB ID : 9QT3 / pdb_00009qt3
Title : Structure of vaccinia virus A26 (residues 1-397) in complex with Fab 8M2110
Authors : Guardado-Calvo, P.; Battini, L.
Deposited on : 2025-04-07
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure 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/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

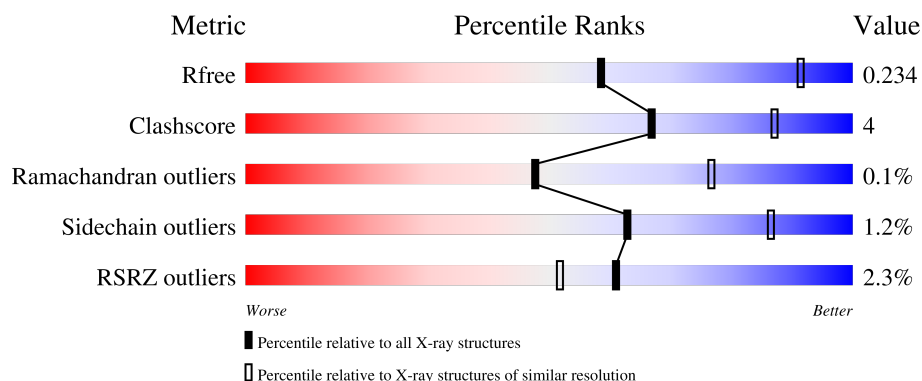
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	A	457	 2% 68% 7% 24%
1	E	457	 2% 70% 6% 24%
1	I	457	 % 68% 7% 25%
1	M	457	 % 67% 9% 23%
2	B	225	 2% 87% 11% .

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Mol	Chain	Length	Quality of chain
2	F	225	4% 88% 9% .
2	J	225	4% 83% 14% .
2	N	225	5% 80% 18% .
3	C	214	94% 5%
3	G	214	% 91% 8%
3	K	214	94% 6%
3	O	214	2% 93% 7%
4	D	123	2% 83% 15% .
4	H	123	3% 81% 15% ..
4	L	123	% 88% 9% ..
4	P	123	7% 84% 11% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28702 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 Envelop protein OPG153.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2849	1830	482	523	14			
1	E	346	Total	C	N	O	S	0	0	0
			2849	1830	482	523	14			
1	I	345	Total	C	N	O	S	0	0	0
			2843	1827	481	521	14			
1	M	350	Total	C	N	O	S	0	0	0
			2880	1848	487	531	14			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	GLY	-	expression tag	UNP P24758
A	399	SER	-	expression tag	UNP P24758
A	400	GLY	-	expression tag	UNP P24758
A	401	LEU	-	expression tag	UNP P24758
A	402	VAL	-	expression tag	UNP P24758
A	403	PRO	-	expression tag	UNP P24758
A	404	ARG	-	expression tag	UNP P24758
A	405	ILE	-	expression tag	UNP P24758
A	406	GLY	-	expression tag	UNP P24758
A	407	SER	-	expression tag	UNP P24758
A	408	GLY	-	expression tag	UNP P24758
A	409	SER	-	expression tag	UNP P24758
A	410	ALA	-	expression tag	UNP P24758
A	411	GLY	-	expression tag	UNP P24758
A	412	TRP	-	expression tag	UNP P24758
A	413	SER	-	expression tag	UNP P24758
A	414	HIS	-	expression tag	UNP P24758
A	415	PRO	-	expression tag	UNP P24758
A	416	GLN	-	expression tag	UNP P24758
A	417	PHE	-	expression tag	UNP P24758
A	418	GLU	-	expression tag	UNP P24758

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Chain	Residue	Modelled	Actual	Comment	Reference
A	419	LYS	-	expression tag	UNP P24758
A	420	GLY	-	expression tag	UNP P24758
A	421	GLY	-	expression tag	UNP P24758
A	422	GLY	-	expression tag	UNP P24758
A	423	SER	-	expression tag	UNP P24758
A	424	GLY	-	expression tag	UNP P24758
A	425	GLY	-	expression tag	UNP P24758
A	426	GLY	-	expression tag	UNP P24758
A	427	SER	-	expression tag	UNP P24758
A	428	GLY	-	expression tag	UNP P24758
A	429	GLY	-	expression tag	UNP P24758
A	430	GLY	-	expression tag	UNP P24758
A	431	SER	-	expression tag	UNP P24758
A	432	TRP	-	expression tag	UNP P24758
A	433	SER	-	expression tag	UNP P24758
A	434	HIS	-	expression tag	UNP P24758
A	435	PRO	-	expression tag	UNP P24758
A	436	GLN	-	expression tag	UNP P24758
A	437	PHE	-	expression tag	UNP P24758
A	438	GLU	-	expression tag	UNP P24758
A	439	LYS	-	expression tag	UNP P24758
A	440	GLY	-	expression tag	UNP P24758
A	441	THR	-	expression tag	UNP P24758
A	442	GLY	-	expression tag	UNP P24758
A	443	GLY	-	expression tag	UNP P24758
A	444	LEU	-	expression tag	UNP P24758
A	445	ASN	-	expression tag	UNP P24758
A	446	ASP	-	expression tag	UNP P24758
A	447	ILE	-	expression tag	UNP P24758
A	448	PHE	-	expression tag	UNP P24758
A	449	GLU	-	expression tag	UNP P24758
A	450	ALA	-	expression tag	UNP P24758
A	451	GLN	-	expression tag	UNP P24758
A	452	LYS	-	expression tag	UNP P24758
A	453	ILE	-	expression tag	UNP P24758
A	454	GLU	-	expression tag	UNP P24758
A	455	TRP	-	expression tag	UNP P24758
A	456	HIS	-	expression tag	UNP P24758
A	457	GLU	-	expression tag	UNP P24758
E	398	GLY	-	expression tag	UNP P24758
E	399	SER	-	expression tag	UNP P24758
E	400	GLY	-	expression tag	UNP P24758

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Chain	Residue	Modelled	Actual	Comment	Reference
E	401	LEU	-	expression tag	UNP P24758
E	402	VAL	-	expression tag	UNP P24758
E	403	PRO	-	expression tag	UNP P24758
E	404	ARG	-	expression tag	UNP P24758
E	405	ILE	-	expression tag	UNP P24758
E	406	GLY	-	expression tag	UNP P24758
E	407	SER	-	expression tag	UNP P24758
E	408	GLY	-	expression tag	UNP P24758
E	409	SER	-	expression tag	UNP P24758
E	410	ALA	-	expression tag	UNP P24758
E	411	GLY	-	expression tag	UNP P24758
E	412	TRP	-	expression tag	UNP P24758
E	413	SER	-	expression tag	UNP P24758
E	414	HIS	-	expression tag	UNP P24758
E	415	PRO	-	expression tag	UNP P24758
E	416	GLN	-	expression tag	UNP P24758
E	417	PHE	-	expression tag	UNP P24758
E	418	GLU	-	expression tag	UNP P24758
E	419	LYS	-	expression tag	UNP P24758
E	420	GLY	-	expression tag	UNP P24758
E	421	GLY	-	expression tag	UNP P24758
E	422	GLY	-	expression tag	UNP P24758
E	423	SER	-	expression tag	UNP P24758
E	424	GLY	-	expression tag	UNP P24758
E	425	GLY	-	expression tag	UNP P24758
E	426	GLY	-	expression tag	UNP P24758
E	427	SER	-	expression tag	UNP P24758
E	428	GLY	-	expression tag	UNP P24758
E	429	GLY	-	expression tag	UNP P24758
E	430	GLY	-	expression tag	UNP P24758
E	431	SER	-	expression tag	UNP P24758
E	432	TRP	-	expression tag	UNP P24758
E	433	SER	-	expression tag	UNP P24758
E	434	HIS	-	expression tag	UNP P24758
E	435	PRO	-	expression tag	UNP P24758
E	436	GLN	-	expression tag	UNP P24758
E	437	PHE	-	expression tag	UNP P24758
E	438	GLU	-	expression tag	UNP P24758
E	439	LYS	-	expression tag	UNP P24758
E	440	GLY	-	expression tag	UNP P24758
E	441	THR	-	expression tag	UNP P24758
E	442	GLY	-	expression tag	UNP P24758

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Chain	Residue	Modelled	Actual	Comment	Reference
E	443	GLY	-	expression tag	UNP P24758
E	444	LEU	-	expression tag	UNP P24758
E	445	ASN	-	expression tag	UNP P24758
E	446	ASP	-	expression tag	UNP P24758
E	447	ILE	-	expression tag	UNP P24758
E	448	PHE	-	expression tag	UNP P24758
E	449	GLU	-	expression tag	UNP P24758
E	450	ALA	-	expression tag	UNP P24758
E	451	GLN	-	expression tag	UNP P24758
E	452	LYS	-	expression tag	UNP P24758
E	453	ILE	-	expression tag	UNP P24758
E	454	GLU	-	expression tag	UNP P24758
E	455	TRP	-	expression tag	UNP P24758
E	456	HIS	-	expression tag	UNP P24758
E	457	GLU	-	expression tag	UNP P24758
I	398	GLY	-	expression tag	UNP P24758
I	399	SER	-	expression tag	UNP P24758
I	400	GLY	-	expression tag	UNP P24758
I	401	LEU	-	expression tag	UNP P24758
I	402	VAL	-	expression tag	UNP P24758
I	403	PRO	-	expression tag	UNP P24758
I	404	ARG	-	expression tag	UNP P24758
I	405	ILE	-	expression tag	UNP P24758
I	406	GLY	-	expression tag	UNP P24758
I	407	SER	-	expression tag	UNP P24758
I	408	GLY	-	expression tag	UNP P24758
I	409	SER	-	expression tag	UNP P24758
I	410	ALA	-	expression tag	UNP P24758
I	411	GLY	-	expression tag	UNP P24758
I	412	TRP	-	expression tag	UNP P24758
I	413	SER	-	expression tag	UNP P24758
I	414	HIS	-	expression tag	UNP P24758
I	415	PRO	-	expression tag	UNP P24758
I	416	GLN	-	expression tag	UNP P24758
I	417	PHE	-	expression tag	UNP P24758
I	418	GLU	-	expression tag	UNP P24758
I	419	LYS	-	expression tag	UNP P24758
I	420	GLY	-	expression tag	UNP P24758
I	421	GLY	-	expression tag	UNP P24758
I	422	GLY	-	expression tag	UNP P24758
I	423	SER	-	expression tag	UNP P24758
I	424	GLY	-	expression tag	UNP P24758

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Chain	Residue	Modelled	Actual	Comment	Reference
I	425	GLY	-	expression tag	UNP P24758
I	426	GLY	-	expression tag	UNP P24758
I	427	SER	-	expression tag	UNP P24758
I	428	GLY	-	expression tag	UNP P24758
I	429	GLY	-	expression tag	UNP P24758
I	430	GLY	-	expression tag	UNP P24758
I	431	SER	-	expression tag	UNP P24758
I	432	TRP	-	expression tag	UNP P24758
I	433	SER	-	expression tag	UNP P24758
I	434	HIS	-	expression tag	UNP P24758
I	435	PRO	-	expression tag	UNP P24758
I	436	GLN	-	expression tag	UNP P24758
I	437	PHE	-	expression tag	UNP P24758
I	438	GLU	-	expression tag	UNP P24758
I	439	LYS	-	expression tag	UNP P24758
I	440	GLY	-	expression tag	UNP P24758
I	441	THR	-	expression tag	UNP P24758
I	442	GLY	-	expression tag	UNP P24758
I	443	GLY	-	expression tag	UNP P24758
I	444	LEU	-	expression tag	UNP P24758
I	445	ASN	-	expression tag	UNP P24758
I	446	ASP	-	expression tag	UNP P24758
I	447	ILE	-	expression tag	UNP P24758
I	448	PHE	-	expression tag	UNP P24758
I	449	GLU	-	expression tag	UNP P24758
I	450	ALA	-	expression tag	UNP P24758
I	451	GLN	-	expression tag	UNP P24758
I	452	LYS	-	expression tag	UNP P24758
I	453	ILE	-	expression tag	UNP P24758
I	454	GLU	-	expression tag	UNP P24758
I	455	TRP	-	expression tag	UNP P24758
I	456	HIS	-	expression tag	UNP P24758
I	457	GLU	-	expression tag	UNP P24758
M	398	GLY	-	expression tag	UNP P24758
M	399	SER	-	expression tag	UNP P24758
M	400	GLY	-	expression tag	UNP P24758
M	401	LEU	-	expression tag	UNP P24758
M	402	VAL	-	expression tag	UNP P24758
M	403	PRO	-	expression tag	UNP P24758
M	404	ARG	-	expression tag	UNP P24758
M	405	ILE	-	expression tag	UNP P24758
M	406	GLY	-	expression tag	UNP P24758

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Chain	Residue	Modelled	Actual	Comment	Reference
M	407	SER	-	expression tag	UNP P24758
M	408	GLY	-	expression tag	UNP P24758
M	409	SER	-	expression tag	UNP P24758
M	410	ALA	-	expression tag	UNP P24758
M	411	GLY	-	expression tag	UNP P24758
M	412	TRP	-	expression tag	UNP P24758
M	413	SER	-	expression tag	UNP P24758
M	414	HIS	-	expression tag	UNP P24758
M	415	PRO	-	expression tag	UNP P24758
M	416	GLN	-	expression tag	UNP P24758
M	417	PHE	-	expression tag	UNP P24758
M	418	GLU	-	expression tag	UNP P24758
M	419	LYS	-	expression tag	UNP P24758
M	420	GLY	-	expression tag	UNP P24758
M	421	GLY	-	expression tag	UNP P24758
M	422	GLY	-	expression tag	UNP P24758
M	423	SER	-	expression tag	UNP P24758
M	424	GLY	-	expression tag	UNP P24758
M	425	GLY	-	expression tag	UNP P24758
M	426	GLY	-	expression tag	UNP P24758
M	427	SER	-	expression tag	UNP P24758
M	428	GLY	-	expression tag	UNP P24758
M	429	GLY	-	expression tag	UNP P24758
M	430	GLY	-	expression tag	UNP P24758
M	431	SER	-	expression tag	UNP P24758
M	432	TRP	-	expression tag	UNP P24758
M	433	SER	-	expression tag	UNP P24758
M	434	HIS	-	expression tag	UNP P24758
M	435	PRO	-	expression tag	UNP P24758
M	436	GLN	-	expression tag	UNP P24758
M	437	PHE	-	expression tag	UNP P24758
M	438	GLU	-	expression tag	UNP P24758
M	439	LYS	-	expression tag	UNP P24758
M	440	GLY	-	expression tag	UNP P24758
M	441	THR	-	expression tag	UNP P24758
M	442	GLY	-	expression tag	UNP P24758
M	443	GLY	-	expression tag	UNP P24758
M	444	LEU	-	expression tag	UNP P24758
M	445	ASN	-	expression tag	UNP P24758
M	446	ASP	-	expression tag	UNP P24758
M	447	ILE	-	expression tag	UNP P24758
M	448	PHE	-	expression tag	UNP P24758

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

- Molecule 2 is a protein called Heavy chain of Fab 8M2110.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1648	1046	272	323	7			
2	F	219	Total	C	N	O	S	0	0	0
			1648	1046	272	323	7			
2	J	219	Total	C	N	O	S	0	0	0
			1648	1046	272	323	7			
2	N	219	Total	C	N	O	S	0	0	0
			1648	1046	272	323	7			

- Molecule 3 is a protein called Light chain of Fab 8M2110.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1642	1026	273	338	5			
3	G	213	Total	C	N	O	S	0	0	0
			1642	1026	273	338	5			
3	K	213	Total	C	N	O	S	0	0	0
			1642	1026	273	338	5			
3	O	213	Total	C	N	O	S	0	0	0
			1642	1026	273	338	5			

- Molecule 4 is a protein called Anti-Fab VHH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	120	Total	C	N	O	S	0	0	0
			922	572	162	184	4			
4	H	120	Total	C	N	O	S	0	0	0
			922	572	162	184	4			

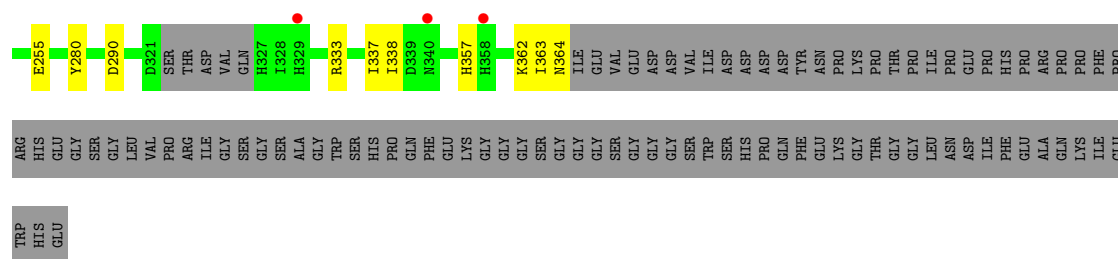
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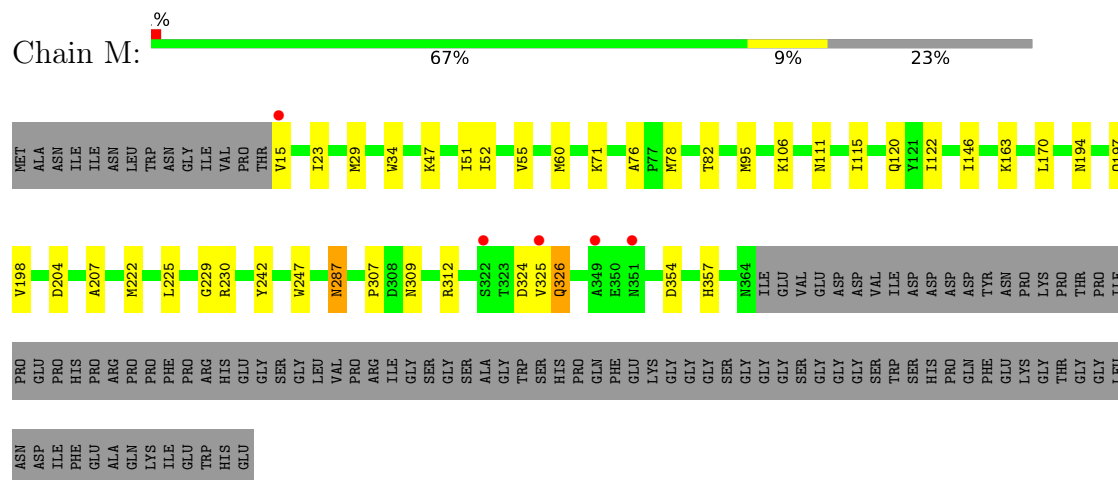
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	120	Total	C	N	O	S	0	0	0
			922	572	162	184	4			
4	P	120	Total	C	N	O	S	0	0	0
			922	572	162	184	4			

- Molecule 5 is water.

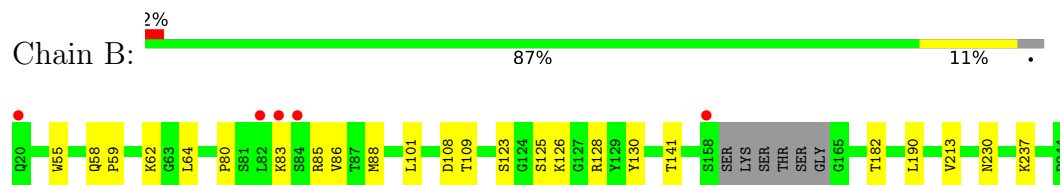
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total	O	0	0
			66	66		
5	B	26	Total	O	0	0
			26	26		
5	C	48	Total	O	0	0
			48	48		
5	D	5	Total	O	0	0
			5	5		
5	E	75	Total	O	0	0
			75	75		
5	F	20	Total	O	0	0
			20	20		
5	G	41	Total	O	0	0
			41	41		
5	H	10	Total	O	0	0
			10	10		
5	I	11	Total	O	0	0
			11	11		
5	J	17	Total	O	0	0
			17	17		
5	K	28	Total	O	0	0
			28	28		
5	L	5	Total	O	0	0
			5	5		
5	M	42	Total	O	0	0
			42	42		
5	N	9	Total	O	0	0
			9	9		
5	O	25	Total	O	0	0
			25	25		
5	P	5	Total	O	0	0
			5	5		



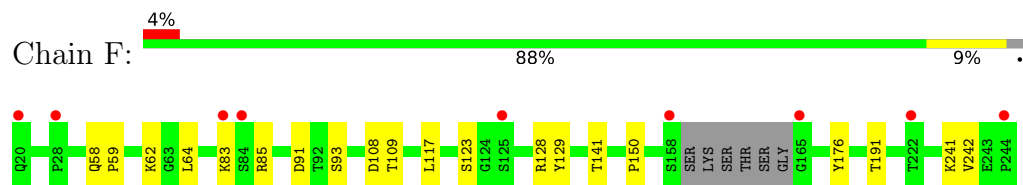
• Molecule 1: Envelop protein OPG153



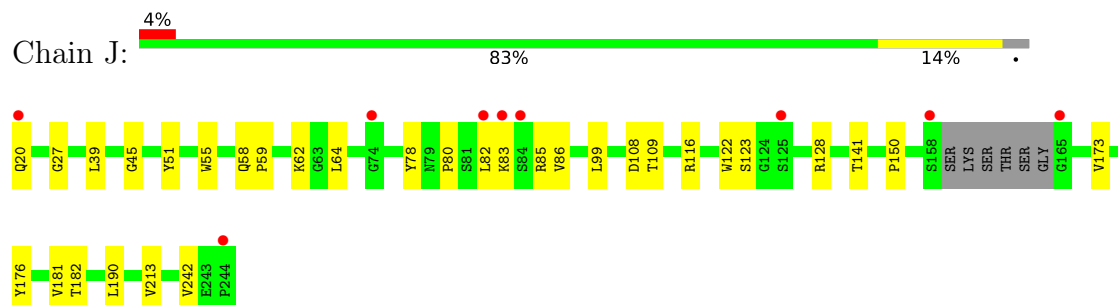
• Molecule 2: Heavy chain of Fab 8M2110



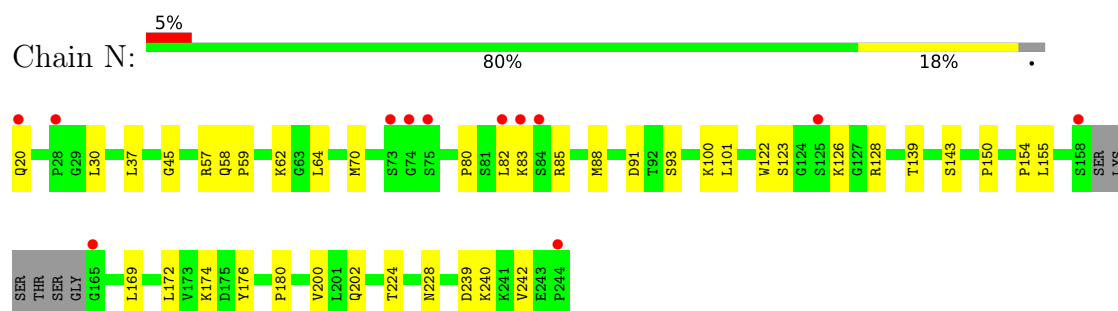
• Molecule 2: Heavy chain of Fab 8M2110



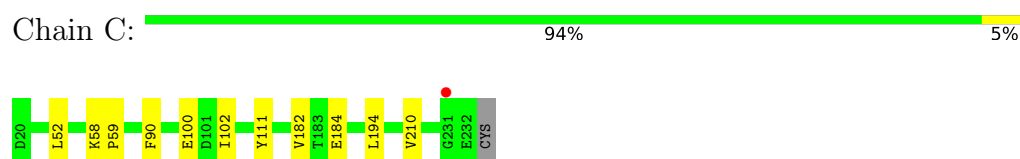
• Molecule 2: Heavy chain of Fab 8M2110



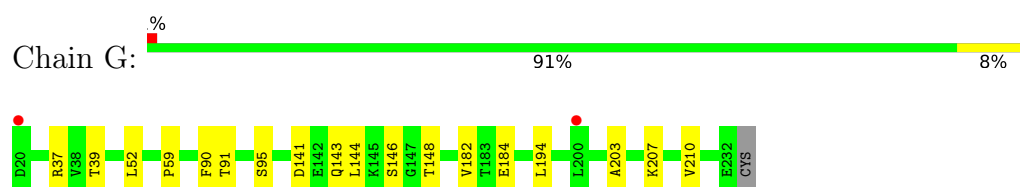
- Molecule 2: Heavy chain of Fab 8M2110



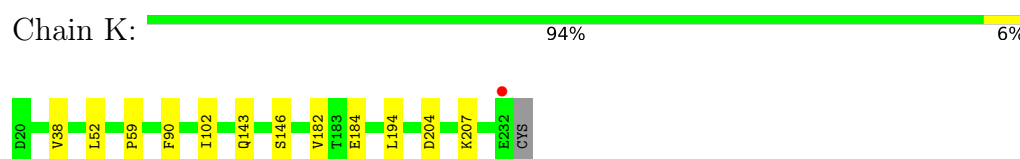
- Molecule 3: Light chain of Fab 8M2110



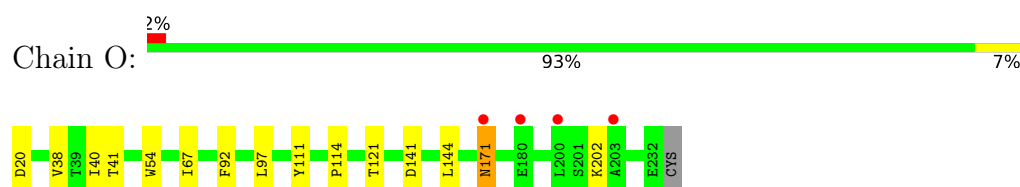
- Molecule 3: Light chain of Fab 8M2110



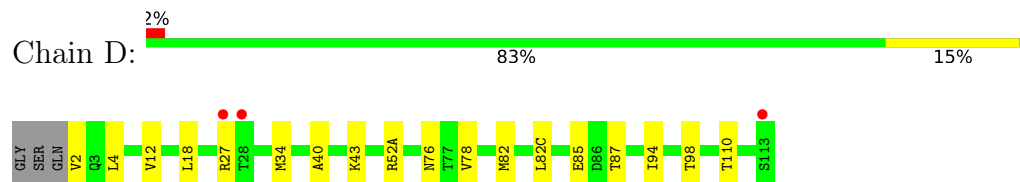
- Molecule 3: Light chain of Fab 8M2110



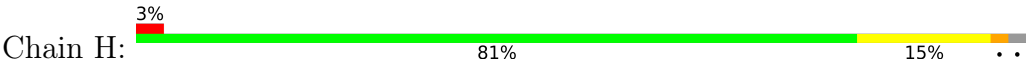
- Molecule 3: Light chain of Fab 8M2110



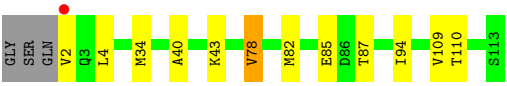
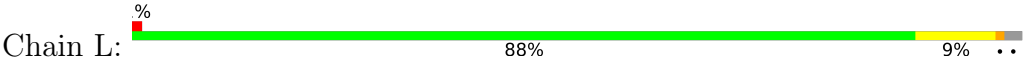
- Molecule 4: Anti-Fab VHH



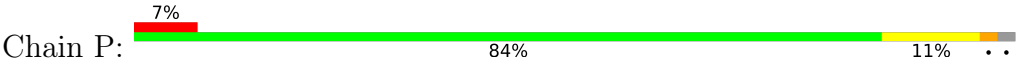
- Molecule 4: Anti-Fab VHH



● Molecule 4: Anti-Fab VHH



● Molecule 4: Anti-Fab VHH



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.41Å 119.41Å 632.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.08 – 2.90 39.08 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.08-2.90) 99.9 (39.08-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.201 , 0.236 0.198 , 0.234	Depositor DCC
R_{free} test set	6018 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	28702	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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	A	0.09	0/2917	0.27	0/3939
1	E	0.09	0/2917	0.27	0/3939
1	I	0.09	0/2911	0.26	0/3931
1	M	0.08	0/2949	0.26	0/3985
2	B	0.09	0/1691	0.28	0/2306
2	F	0.10	0/1691	0.30	0/2306
2	J	0.10	0/1691	0.28	0/2306
2	N	0.10	0/1691	0.30	0/2306
3	C	0.09	0/1678	0.29	0/2282
3	G	0.09	0/1678	0.29	0/2282
3	K	0.09	0/1678	0.28	0/2282
3	O	0.09	0/1678	0.29	0/2282
4	D	0.10	0/941	0.28	0/1272
4	H	0.09	0/941	0.28	0/1272
4	L	0.10	0/941	0.29	0/1272
4	P	0.08	0/941	0.26	0/1272
All	All	0.09	0/28934	0.28	0/39234

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	A	2849	0	2789	20	0
1	E	2849	0	2789	14	0
1	I	2843	0	2784	18	0
1	M	2880	0	2818	25	0
2	B	1648	0	1617	13	0
2	F	1648	0	1617	11	0
2	J	1648	0	1617	18	0
2	N	1648	0	1617	23	0
3	C	1642	0	1572	5	0
3	G	1642	0	1572	9	0
3	K	1642	0	1572	5	0
3	O	1642	0	1572	10	0
4	D	922	0	869	14	0
4	H	922	0	869	11	0
4	L	922	0	869	7	0
4	P	922	0	869	10	0
5	A	66	0	0	0	0
5	B	26	0	0	1	0
5	C	48	0	0	0	0
5	D	5	0	0	1	0
5	E	75	0	0	0	0
5	F	20	0	0	0	0
5	G	41	0	0	0	0
5	H	10	0	0	0	0
5	I	11	0	0	0	0
5	J	17	0	0	0	0
5	K	28	0	0	0	0
5	L	5	0	0	0	0
5	M	42	0	0	0	0
5	N	9	0	0	0	0
5	O	25	0	0	0	0
5	P	5	0	0	0	0
All	All	28702	0	27412	206	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 4.

The worst 5 of 206 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)
3:K:204:ASP:HA	3:K:207:LYS:HE2	1.71	0.73
4:H:4:LEU:HD21	4:H:94:ILE:HG13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:40:ALA:HB3	4:L:43:LYS:HD2	1.73	0.70
2:B:59:PRO:HB2	2:B:62:LYS:HD2	1.73	0.70
2:B:80:PRO:HA	2:B:83:LYS:HB2	1.74	0.69

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	342/457 (75%)	333 (97%)	9 (3%)	0	100	100
1	E	342/457 (75%)	333 (97%)	9 (3%)	0	100	100
1	I	341/457 (75%)	333 (98%)	8 (2%)	0	100	100
1	M	348/457 (76%)	334 (96%)	12 (3%)	2 (1%)	21	51
2	B	215/225 (96%)	208 (97%)	7 (3%)	0	100	100
2	F	215/225 (96%)	207 (96%)	8 (4%)	0	100	100
2	J	215/225 (96%)	207 (96%)	8 (4%)	0	100	100
2	N	215/225 (96%)	206 (96%)	9 (4%)	0	100	100
3	C	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
3	G	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
3	K	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
3	O	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
4	D	118/123 (96%)	118 (100%)	0	0	100	100
4	H	118/123 (96%)	118 (100%)	0	0	100	100
4	L	118/123 (96%)	118 (100%)	0	0	100	100
4	P	118/123 (96%)	118 (100%)	0	0	100	100
All	All	3549/4076 (87%)	3452 (97%)	95 (3%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	325	VAL
1	M	326	GLN

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 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	311/401 (78%)	306 (98%)	5 (2%)	55	83
1	E	311/401 (78%)	310 (100%)	1 (0%)	86	96
1	I	310/401 (77%)	309 (100%)	1 (0%)	86	96
1	M	315/401 (79%)	312 (99%)	3 (1%)	68	89
2	B	188/193 (97%)	186 (99%)	2 (1%)	65	88
2	F	188/193 (97%)	186 (99%)	2 (1%)	65	88
2	J	188/193 (97%)	186 (99%)	2 (1%)	65	88
2	N	188/193 (97%)	186 (99%)	2 (1%)	65	88
3	C	188/189 (100%)	186 (99%)	2 (1%)	65	88
3	G	188/189 (100%)	187 (100%)	1 (0%)	81	93
3	K	188/189 (100%)	186 (99%)	2 (1%)	65	88
3	O	188/189 (100%)	186 (99%)	2 (1%)	65	88
4	D	96/98 (98%)	96 (100%)	0	100	100
4	H	96/98 (98%)	90 (94%)	6 (6%)	16	45
4	L	96/98 (98%)	94 (98%)	2 (2%)	47	77
4	P	96/98 (98%)	90 (94%)	6 (6%)	16	45
All	All	3135/3524 (89%)	3096 (99%)	39 (1%)	63	86

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	287	ASN
4	P	82	MET

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Mol	Chain	Res	Type
2	N	200	VAL
3	O	171	ASN
4	P	82(B)	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	83	GLN
3	O	43	GLN
2	J	20	GLN
4	P	81	GLN
1	M	164	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, 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	A	346/457 (75%)	-0.30	7 (2%) 65 56	23, 33, 52, 104	0
1	E	346/457 (75%)	-0.31	7 (2%) 65 56	22, 31, 52, 103	0
1	I	345/457 (75%)	0.22	4 (1%) 76 69	34, 56, 86, 116	0
1	M	350/457 (76%)	-0.24	5 (1%) 73 65	24, 34, 60, 93	0
2	B	219/225 (97%)	-0.06	5 (2%) 61 52	24, 40, 70, 90	0
2	F	219/225 (97%)	0.03	9 (4%) 41 33	27, 40, 70, 92	0
2	J	219/225 (97%)	0.10	9 (4%) 41 33	29, 44, 78, 110	0
2	N	219/225 (97%)	0.22	12 (5%) 30 24	28, 42, 75, 112	0
3	C	213/214 (99%)	-0.27	1 (0%) 87 83	21, 32, 70, 108	0
3	G	213/214 (99%)	-0.21	2 (0%) 81 75	23, 35, 69, 81	0
3	K	213/214 (99%)	-0.21	1 (0%) 87 83	27, 35, 73, 94	0
3	O	213/214 (99%)	0.01	4 (1%) 66 58	28, 42, 77, 90	0
4	D	120/123 (97%)	0.11	3 (2%) 58 48	34, 44, 65, 97	0
4	H	120/123 (97%)	0.23	4 (3%) 49 40	34, 52, 75, 97	0
4	L	120/123 (97%)	-0.09	1 (0%) 82 77	30, 39, 61, 77	0
4	P	120/123 (97%)	0.51	8 (6%) 24 19	44, 59, 87, 98	0
All	All	3595/4076 (88%)	-0.06	82 (2%) 61 52	21, 40, 74, 116	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	322	SER	5.8
1	I	15	VAL	5.2
2	B	83	LYS	4.9
2	N	158	SER	4.8
1	I	358	HIS	4.6

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.