



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:07 PM UTC

PDB ID : 8V5P / pdb_00008v5p
Title : Crystal Structure of the C-terminal domain of the VZV gE ectodomain in complex with the Fab of human antibody 5A2
Authors : Harshbarger, W.; Malito, E.
Deposited on : 2023-11-30
Resolution : 4.33 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

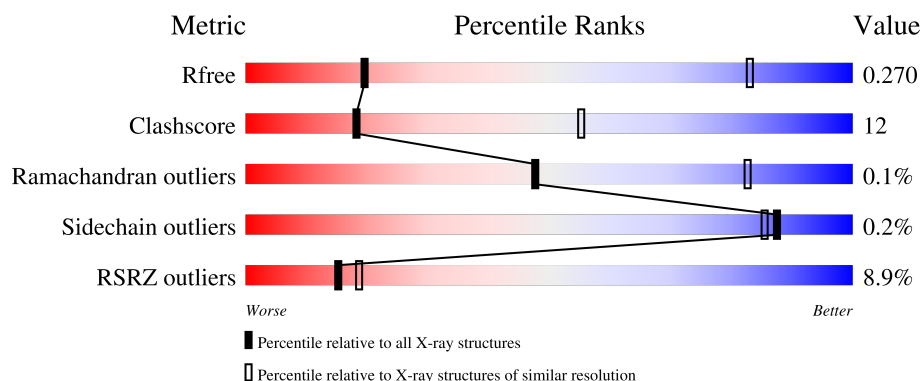
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.33 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	1059 (4.76-3.90)
Clashscore	190562	1105 (4.76-3.90)
Ramachandran outliers	187476	1007 (4.76-3.90)
Sidechain outliers	187428	1022 (4.80-3.88)
RSRZ outliers	180081	1056 (4.76-3.90)

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	254	3% 49% 20% 31%
1	C	254	4% 47% 22% 31%
1	D	254	2% 48% 21% 31%
1	G	254	2% 46% 22% 31%
2	E	242	17% 71% 18% 12%

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Mol	Chain	Length	Quality of chain
2	F	242	3% 72% 15% 12%
2	H	242	2% 70% 17% 12%
2	J	242	7% 60% 29% 12%
3	I	210	5% 77% 23%
3	L	210	4% 73% 27%
3	X	210	16% 73% 27%
3	Y	210	31% 77% 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18368 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 Envelope glycoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1396	899	230	256	11			
1	D	175	Total	C	N	O	S	0	0	0
			1396	899	230	256	11			
1	G	175	Total	C	N	O	S	0	0	0
			1396	899	230	256	11			
1	C	175	Total	C	N	O	S	0	0	0
			1396	899	230	256	11			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	MET	-	initiating methionine	UNP A0A1B1JEP3
A	272	GLY	-	expression tag	UNP A0A1B1JEP3
A	273	THR	-	expression tag	UNP A0A1B1JEP3
A	274	VAL	-	expression tag	UNP A0A1B1JEP3
A	275	ASN	-	expression tag	UNP A0A1B1JEP3
A	276	LYS	-	expression tag	UNP A0A1B1JEP3
A	277	PRO	-	expression tag	UNP A0A1B1JEP3
A	278	VAL	-	expression tag	UNP A0A1B1JEP3
A	279	VAL	-	expression tag	UNP A0A1B1JEP3
A	280	GLY	-	expression tag	UNP A0A1B1JEP3
A	281	VAL	-	expression tag	UNP A0A1B1JEP3
A	282	LEU	-	expression tag	UNP A0A1B1JEP3
A	283	MET	-	expression tag	UNP A0A1B1JEP3
A	284	GLY	-	expression tag	UNP A0A1B1JEP3
A	285	PHE	-	expression tag	UNP A0A1B1JEP3
A	286	GLY	-	expression tag	UNP A0A1B1JEP3
A	287	ILE	-	expression tag	UNP A0A1B1JEP3
A	288	ILE	-	expression tag	UNP A0A1B1JEP3
A	289	THR	-	expression tag	UNP A0A1B1JEP3
A	290	GLY	-	expression tag	UNP A0A1B1JEP3
A	291	THR	-	expression tag	UNP A0A1B1JEP3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	292	LEU	-	expression tag	UNP A0A1B1JEP3
A	293	ARG	-	expression tag	UNP A0A1B1JEP3
A	294	ILE	-	expression tag	UNP A0A1B1JEP3
A	295	THR	-	expression tag	UNP A0A1B1JEP3
A	296	ASN	-	expression tag	UNP A0A1B1JEP3
A	297	PRO	-	expression tag	UNP A0A1B1JEP3
A	298	VAL	-	expression tag	UNP A0A1B1JEP3
A	299	ARG	-	expression tag	UNP A0A1B1JEP3
A	300	ALA	-	expression tag	UNP A0A1B1JEP3
A	517	GLY	-	expression tag	UNP A0A1B1JEP3
A	518	SER	-	expression tag	UNP A0A1B1JEP3
A	519	HIS	-	expression tag	UNP A0A1B1JEP3
A	520	HIS	-	expression tag	UNP A0A1B1JEP3
A	521	HIS	-	expression tag	UNP A0A1B1JEP3
A	522	HIS	-	expression tag	UNP A0A1B1JEP3
A	523	HIS	-	expression tag	UNP A0A1B1JEP3
A	524	HIS	-	expression tag	UNP A0A1B1JEP3
D	271	MET	-	initiating methionine	UNP A0A1B1JEP3
D	272	GLY	-	expression tag	UNP A0A1B1JEP3
D	273	THR	-	expression tag	UNP A0A1B1JEP3
D	274	VAL	-	expression tag	UNP A0A1B1JEP3
D	275	ASN	-	expression tag	UNP A0A1B1JEP3
D	276	LYS	-	expression tag	UNP A0A1B1JEP3
D	277	PRO	-	expression tag	UNP A0A1B1JEP3
D	278	VAL	-	expression tag	UNP A0A1B1JEP3
D	279	VAL	-	expression tag	UNP A0A1B1JEP3
D	280	GLY	-	expression tag	UNP A0A1B1JEP3
D	281	VAL	-	expression tag	UNP A0A1B1JEP3
D	282	LEU	-	expression tag	UNP A0A1B1JEP3
D	283	MET	-	expression tag	UNP A0A1B1JEP3
D	284	GLY	-	expression tag	UNP A0A1B1JEP3
D	285	PHE	-	expression tag	UNP A0A1B1JEP3
D	286	GLY	-	expression tag	UNP A0A1B1JEP3
D	287	ILE	-	expression tag	UNP A0A1B1JEP3
D	288	ILE	-	expression tag	UNP A0A1B1JEP3
D	289	THR	-	expression tag	UNP A0A1B1JEP3
D	290	GLY	-	expression tag	UNP A0A1B1JEP3
D	291	THR	-	expression tag	UNP A0A1B1JEP3
D	292	LEU	-	expression tag	UNP A0A1B1JEP3
D	293	ARG	-	expression tag	UNP A0A1B1JEP3
D	294	ILE	-	expression tag	UNP A0A1B1JEP3
D	295	THR	-	expression tag	UNP A0A1B1JEP3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	296	ASN	-	expression tag	UNP A0A1B1JEP3
D	297	PRO	-	expression tag	UNP A0A1B1JEP3
D	298	VAL	-	expression tag	UNP A0A1B1JEP3
D	299	ARG	-	expression tag	UNP A0A1B1JEP3
D	300	ALA	-	expression tag	UNP A0A1B1JEP3
D	517	GLY	-	expression tag	UNP A0A1B1JEP3
D	518	SER	-	expression tag	UNP A0A1B1JEP3
D	519	HIS	-	expression tag	UNP A0A1B1JEP3
D	520	HIS	-	expression tag	UNP A0A1B1JEP3
D	521	HIS	-	expression tag	UNP A0A1B1JEP3
D	522	HIS	-	expression tag	UNP A0A1B1JEP3
D	523	HIS	-	expression tag	UNP A0A1B1JEP3
D	524	HIS	-	expression tag	UNP A0A1B1JEP3
G	271	MET	-	initiating methionine	UNP A0A1B1JEP3
G	272	GLY	-	expression tag	UNP A0A1B1JEP3
G	273	THR	-	expression tag	UNP A0A1B1JEP3
G	274	VAL	-	expression tag	UNP A0A1B1JEP3
G	275	ASN	-	expression tag	UNP A0A1B1JEP3
G	276	LYS	-	expression tag	UNP A0A1B1JEP3
G	277	PRO	-	expression tag	UNP A0A1B1JEP3
G	278	VAL	-	expression tag	UNP A0A1B1JEP3
G	279	VAL	-	expression tag	UNP A0A1B1JEP3
G	280	GLY	-	expression tag	UNP A0A1B1JEP3
G	281	VAL	-	expression tag	UNP A0A1B1JEP3
G	282	LEU	-	expression tag	UNP A0A1B1JEP3
G	283	MET	-	expression tag	UNP A0A1B1JEP3
G	284	GLY	-	expression tag	UNP A0A1B1JEP3
G	285	PHE	-	expression tag	UNP A0A1B1JEP3
G	286	GLY	-	expression tag	UNP A0A1B1JEP3
G	287	ILE	-	expression tag	UNP A0A1B1JEP3
G	288	ILE	-	expression tag	UNP A0A1B1JEP3
G	289	THR	-	expression tag	UNP A0A1B1JEP3
G	290	GLY	-	expression tag	UNP A0A1B1JEP3
G	291	THR	-	expression tag	UNP A0A1B1JEP3
G	292	LEU	-	expression tag	UNP A0A1B1JEP3
G	293	ARG	-	expression tag	UNP A0A1B1JEP3
G	294	ILE	-	expression tag	UNP A0A1B1JEP3
G	295	THR	-	expression tag	UNP A0A1B1JEP3
G	296	ASN	-	expression tag	UNP A0A1B1JEP3
G	297	PRO	-	expression tag	UNP A0A1B1JEP3
G	298	VAL	-	expression tag	UNP A0A1B1JEP3
G	299	ARG	-	expression tag	UNP A0A1B1JEP3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	300	ALA	-	expression tag	UNP A0A1B1JEP3
G	517	GLY	-	expression tag	UNP A0A1B1JEP3
G	518	SER	-	expression tag	UNP A0A1B1JEP3
G	519	HIS	-	expression tag	UNP A0A1B1JEP3
G	520	HIS	-	expression tag	UNP A0A1B1JEP3
G	521	HIS	-	expression tag	UNP A0A1B1JEP3
G	522	HIS	-	expression tag	UNP A0A1B1JEP3
G	523	HIS	-	expression tag	UNP A0A1B1JEP3
G	524	HIS	-	expression tag	UNP A0A1B1JEP3
C	271	MET	-	initiating methionine	UNP A0A1B1JEP3
C	272	GLY	-	expression tag	UNP A0A1B1JEP3
C	273	THR	-	expression tag	UNP A0A1B1JEP3
C	274	VAL	-	expression tag	UNP A0A1B1JEP3
C	275	ASN	-	expression tag	UNP A0A1B1JEP3
C	276	LYS	-	expression tag	UNP A0A1B1JEP3
C	277	PRO	-	expression tag	UNP A0A1B1JEP3
C	278	VAL	-	expression tag	UNP A0A1B1JEP3
C	279	VAL	-	expression tag	UNP A0A1B1JEP3
C	280	GLY	-	expression tag	UNP A0A1B1JEP3
C	281	VAL	-	expression tag	UNP A0A1B1JEP3
C	282	LEU	-	expression tag	UNP A0A1B1JEP3
C	283	MET	-	expression tag	UNP A0A1B1JEP3
C	284	GLY	-	expression tag	UNP A0A1B1JEP3
C	285	PHE	-	expression tag	UNP A0A1B1JEP3
C	286	GLY	-	expression tag	UNP A0A1B1JEP3
C	287	ILE	-	expression tag	UNP A0A1B1JEP3
C	288	ILE	-	expression tag	UNP A0A1B1JEP3
C	289	THR	-	expression tag	UNP A0A1B1JEP3
C	290	GLY	-	expression tag	UNP A0A1B1JEP3
C	291	THR	-	expression tag	UNP A0A1B1JEP3
C	292	LEU	-	expression tag	UNP A0A1B1JEP3
C	293	ARG	-	expression tag	UNP A0A1B1JEP3
C	294	ILE	-	expression tag	UNP A0A1B1JEP3
C	295	THR	-	expression tag	UNP A0A1B1JEP3
C	296	ASN	-	expression tag	UNP A0A1B1JEP3
C	297	PRO	-	expression tag	UNP A0A1B1JEP3
C	298	VAL	-	expression tag	UNP A0A1B1JEP3
C	299	ARG	-	expression tag	UNP A0A1B1JEP3
C	300	ALA	-	expression tag	UNP A0A1B1JEP3
C	517	GLY	-	expression tag	UNP A0A1B1JEP3
C	518	SER	-	expression tag	UNP A0A1B1JEP3
C	519	HIS	-	expression tag	UNP A0A1B1JEP3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	520	HIS	-	expression tag	UNP A0A1B1JEP3
C	521	HIS	-	expression tag	UNP A0A1B1JEP3
C	522	HIS	-	expression tag	UNP A0A1B1JEP3
C	523	HIS	-	expression tag	UNP A0A1B1JEP3
C	524	HIS	-	expression tag	UNP A0A1B1JEP3

- Molecule 2 is a protein called 5A2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1616	1026	271	315	4			
2	E	214	Total	C	N	O	S	0	0	0
			1616	1026	271	315	4			
2	J	214	Total	C	N	O	S	0	0	0
			1616	1026	271	315	4			
2	F	214	Total	C	N	O	S	0	0	0
			1616	1026	271	315	4			

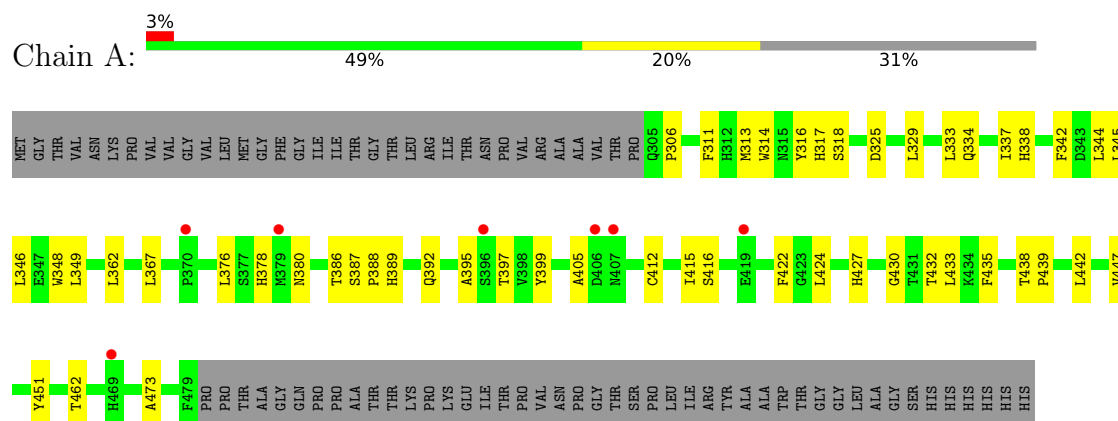
- Molecule 3 is a protein called 5A2 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1580	995	260	320	5			
3	Y	210	Total	C	N	O	S	0	0	0
			1580	995	260	320	5			
3	X	210	Total	C	N	O	S	0	0	0
			1580	995	260	320	5			
3	I	210	Total	C	N	O	S	0	0	0
			1580	995	260	320	5			

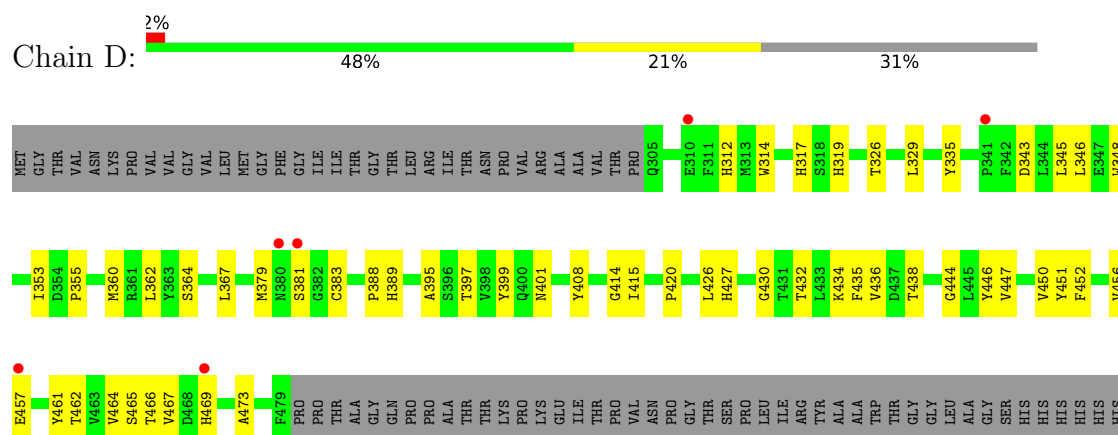
3 Residue-property plots [i](#)

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.

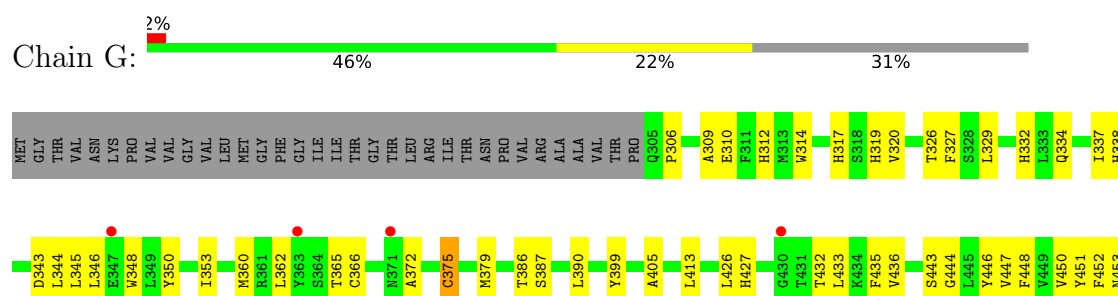
• Molecule 1: Envelope glycoprotein E

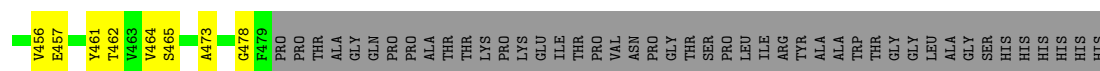


• Molecule 1: Envelope glycoprotein E

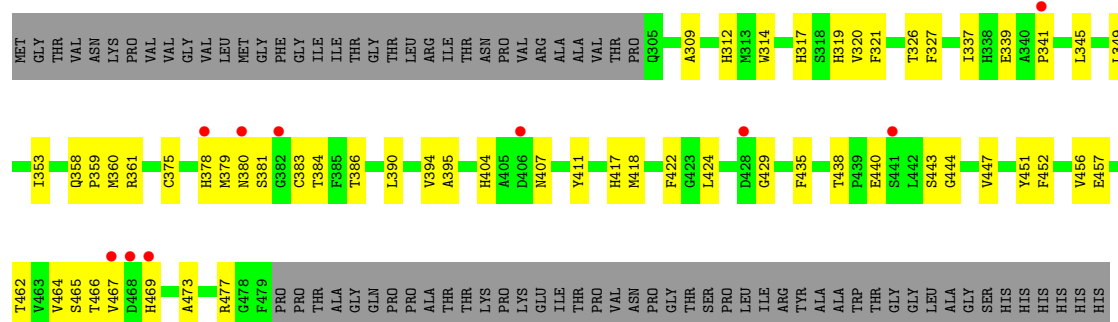


• Molecule 1: Envelope glycoprotein E

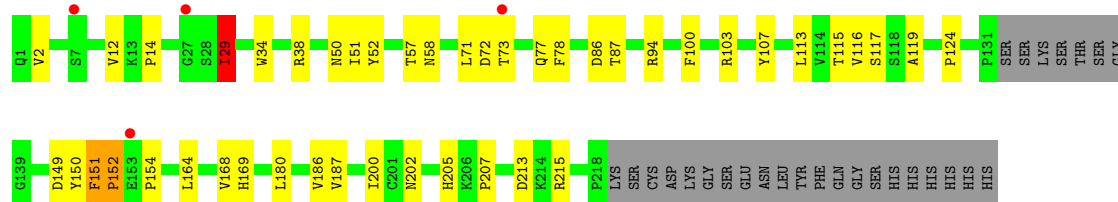




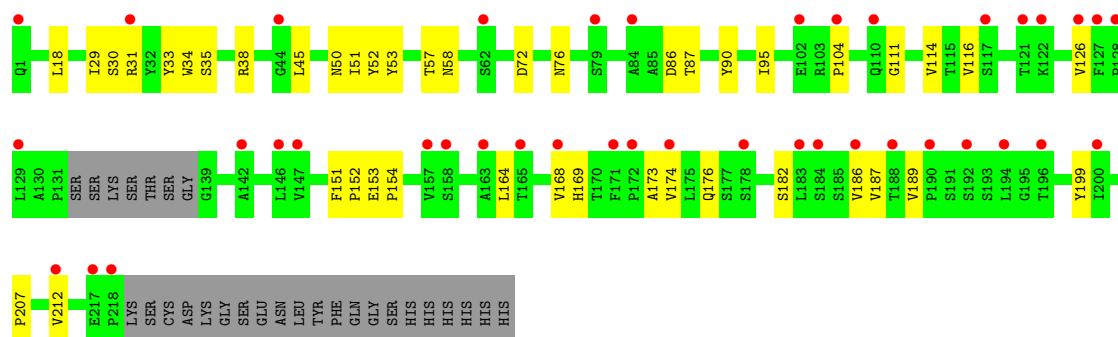
• Molecule 1: Envelope glycoprotein E



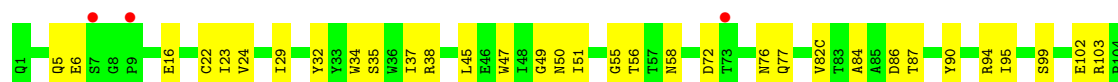
• Molecule 2: 5A2 Fab heavy chain

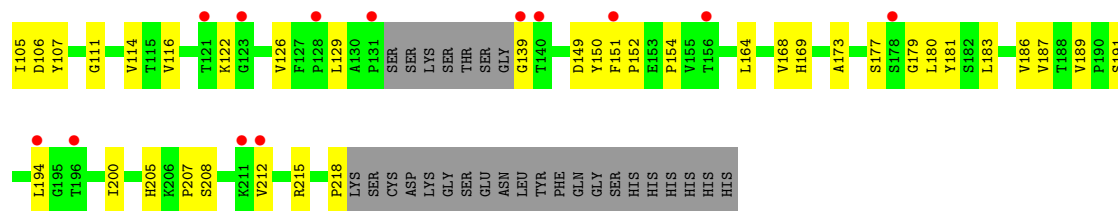


• Molecule 2: 5A2 Fab heavy chain

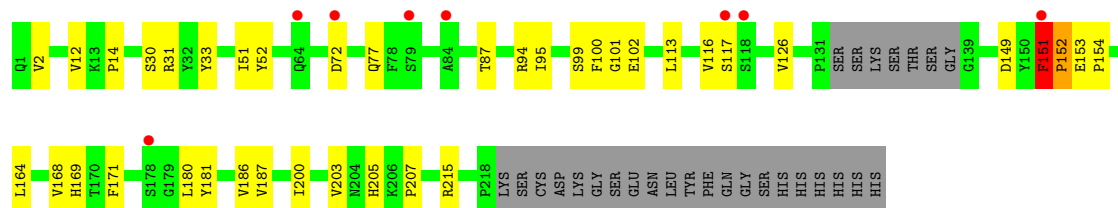
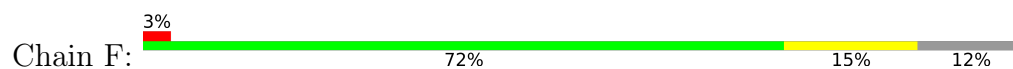


• Molecule 2: 5A2 Fab heavy chain

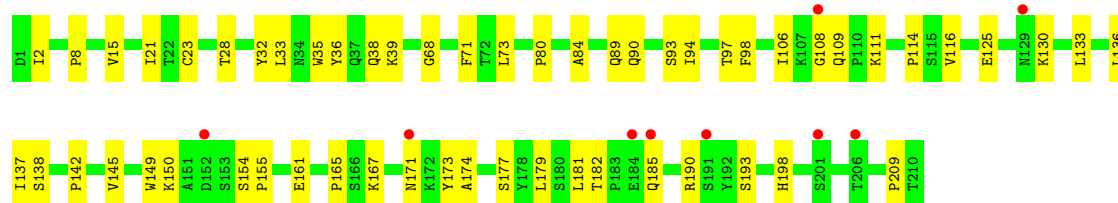
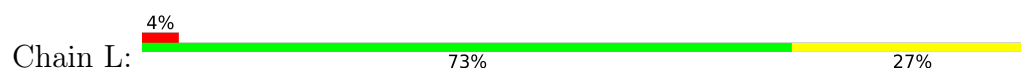




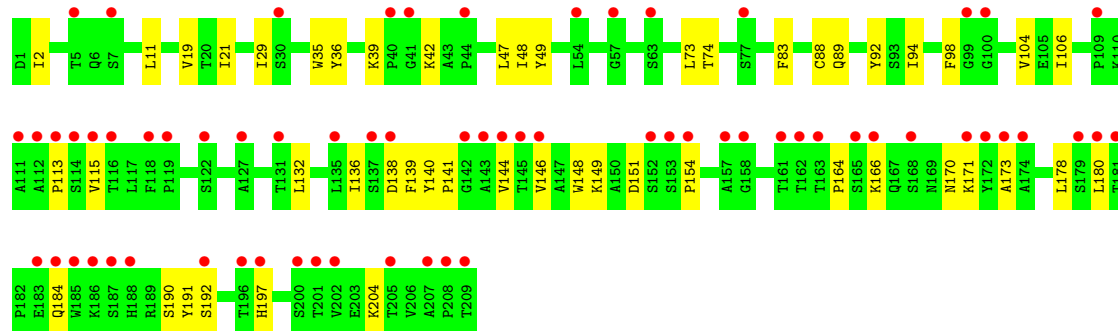
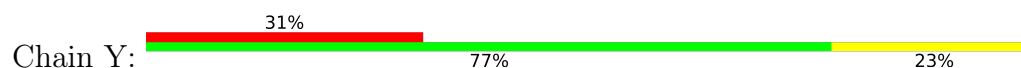
• Molecule 2: 5A2 Fab heavy chain



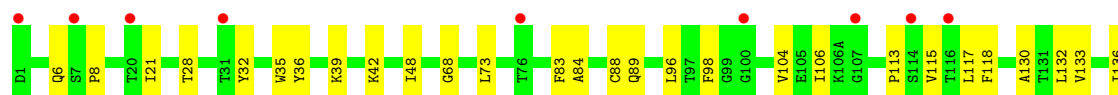
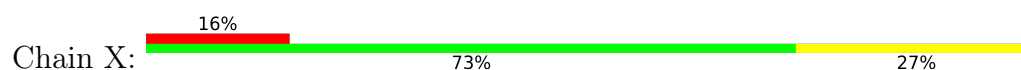
• Molecule 3: 5A2 Fab Light Chain

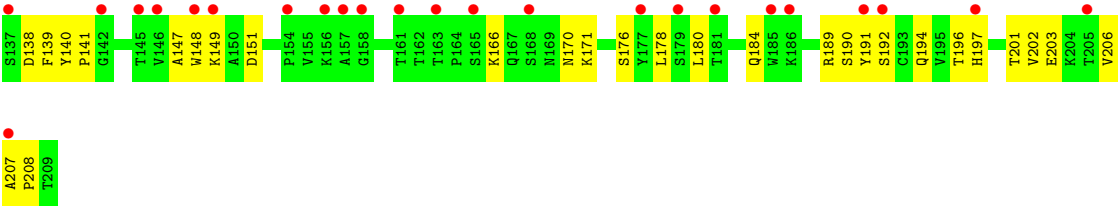


• Molecule 3: 5A2 Fab Light Chain

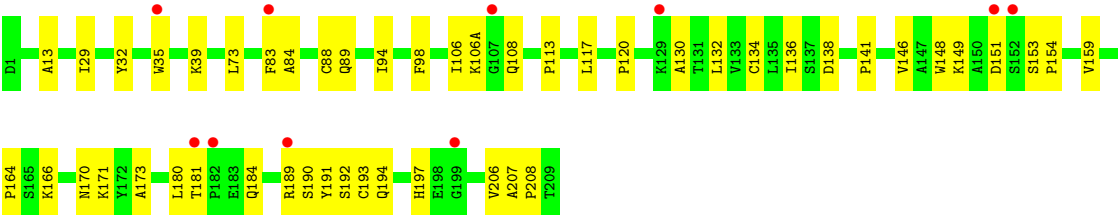
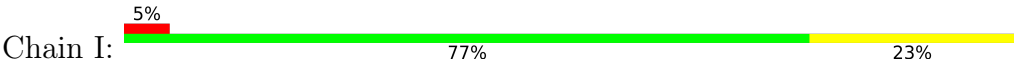


• Molecule 3: 5A2 Fab Light Chain





● Molecule 3: 5A2 Fab Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	274.82Å 274.82Å 128.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.80 – 4.33 45.80 – 4.33	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.80-4.33) 97.3 (45.80-4.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.222 , 0.272 0.222 , 0.270	Depositor DCC
R_{free} test set	1999 reflections (5.97%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 106.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	18368	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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	0.19	0/1444	0.53	0/1974
1	C	0.20	0/1444	0.59	0/1974
1	D	0.17	0/1444	0.50	0/1974
1	G	0.19	0/1444	0.54	0/1974
2	E	0.12	0/1657	0.36	0/2268
2	F	0.13	0/1657	0.42	0/2268
2	H	0.14	0/1657	0.46	2/2268 (0.1%)
2	J	0.16	0/1657	0.47	0/2268
3	I	0.13	0/1618	0.45	0/2208
3	L	0.15	0/1618	0.44	0/2208
3	X	0.14	0/1618	0.41	0/2208
3	Y	0.12	0/1618	0.37	0/2208
All	All	0.15	0/18876	0.46	2/25800 (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
1	C	0	1
2	F	0	1
2	H	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	152	PRO	CA-C-N	6.25	128.83	120.58
2	H	152	PRO	C-N-CA	6.25	128.83	120.58

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	429	GLY	Peptide
2	F	151	PHE	Peptide
2	H	151	PHE	Peptide
2	H	29	ILE	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	A	1396	0	1297	39	0
1	C	1396	0	1297	42	0
1	D	1396	0	1297	40	0
1	G	1396	0	1297	47	0
2	E	1616	0	1594	26	0
2	F	1616	0	1594	23	0
2	H	1616	0	1594	30	0
2	J	1616	0	1594	52	0
3	I	1580	0	1553	44	0
3	L	1580	0	1553	38	0
3	X	1580	0	1553	47	0
3	Y	1580	0	1553	44	0
All	All	18368	0	17776	437	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 12.

The worst 5 of 437 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:I:164:PRO:HG3	3:I:173:ALA:H	1.33	0.93
1:A:397:THR:HG21	1:A:430:GLY:HA3	1.56	0.88
3:X:83:PHE:HB3	3:X:166:LYS:HD2	1.58	0.85
3:L:150:LYS:HB2	3:L:193:SER:HB3	1.58	0.84
3:L:133:LEU:HD11	3:L:149:TRP:HE1	1.42	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	173/254 (68%)	148 (86%)	25 (14%)	0	100	100
1	C	173/254 (68%)	142 (82%)	31 (18%)	0	100	100
1	D	173/254 (68%)	151 (87%)	22 (13%)	0	100	100
1	G	173/254 (68%)	153 (88%)	20 (12%)	0	100	100
2	E	210/242 (87%)	195 (93%)	15 (7%)	0	100	100
2	F	210/242 (87%)	198 (94%)	10 (5%)	2 (1%)	12	47
2	H	210/242 (87%)	194 (92%)	15 (7%)	1 (0%)	24	62
2	J	210/242 (87%)	198 (94%)	12 (6%)	0	100	100
3	I	208/210 (99%)	194 (93%)	14 (7%)	0	100	100
3	L	208/210 (99%)	195 (94%)	13 (6%)	0	100	100
3	X	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
3	Y	208/210 (99%)	195 (94%)	13 (6%)	0	100	100
All	All	2364/2824 (84%)	2159 (91%)	202 (8%)	3 (0%)	48	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	29	ILE
2	F	151	PHE
2	F	152	PRO

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	154/216 (71%)	153 (99%)	1 (1%)	78	80
1	C	154/216 (71%)	154 (100%)	0	100	100
1	D	154/216 (71%)	153 (99%)	1 (1%)	78	80
1	G	154/216 (71%)	152 (99%)	2 (1%)	61	72
2	E	184/209 (88%)	184 (100%)	0	100	100
2	F	184/209 (88%)	184 (100%)	0	100	100
2	H	184/209 (88%)	184 (100%)	0	100	100
2	J	184/209 (88%)	184 (100%)	0	100	100
3	I	179/179 (100%)	179 (100%)	0	100	100
3	L	179/179 (100%)	179 (100%)	0	100	100
3	X	179/179 (100%)	179 (100%)	0	100	100
3	Y	179/179 (100%)	179 (100%)	0	100	100
All	All	2068/2416 (86%)	2064 (100%)	4 (0%)	87	85

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

Mol	Chain	Res	Type
1	A	412	CYS
1	D	383	CYS
1	G	366	CYS
1	G	375	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	338	HIS
1	C	392	GLN
3	X	37	GLN
1	C	407	ASN
3	L	171	ASN

5.3.3 RNA ⓘ

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 [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	A	175/254 (68%)	0.50	7 (4%) 42 36	17, 60, 133, 174	0
1	C	175/254 (68%)	0.62	10 (5%) 29 28	19, 67, 127, 207	0
1	D	175/254 (68%)	0.63	6 (3%) 48 38	30, 71, 133, 180	0
1	G	175/254 (68%)	0.67	4 (2%) 61 48	31, 75, 127, 169	0
2	E	214/242 (88%)	1.22	40 (18%) 3 7	64, 131, 222, 235	0
2	F	214/242 (88%)	0.54	8 (3%) 45 37	21, 66, 112, 132	0
2	H	214/242 (88%)	0.45	4 (1%) 66 52	24, 72, 111, 134	0
2	J	214/242 (88%)	1.01	16 (7%) 20 23	57, 127, 182, 202	0
3	I	210/210 (100%)	0.55	10 (4%) 35 32	19, 52, 96, 156	0
3	L	210/210 (100%)	0.51	9 (4%) 40 34	19, 53, 97, 128	0
3	X	210/210 (100%)	1.08	33 (15%) 5 9	47, 121, 194, 215	0
3	Y	210/210 (100%)	1.61	66 (31%) 1 4	69, 176, 223, 259	0
All	All	2396/2824 (84%)	0.79	213 (8%) 15 19	17, 82, 198, 259	0

The worst 5 of 213 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	184	GLU	5.9
2	E	142	ALA	5.4
2	E	129	LEU	4.6
2	E	128	PRO	4.6
2	E	217	GLU	4.5

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.