



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 12, 2025 – 10:06 AM EST

PDB ID : 9CQD
Title : Antibody 2B11 bound to the central conserved domain of RSV G
Authors : Juarez, M.G.; DuBois, R.M.
Deposited on : 2024-07-19
Resolution : 3.10 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	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

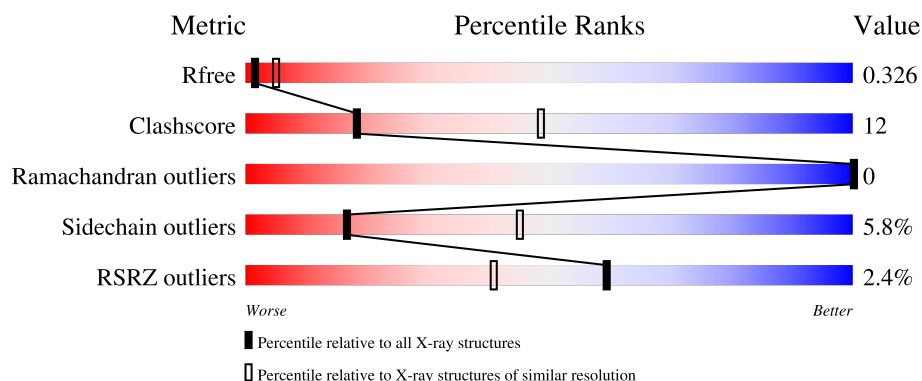
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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	49	<div> <div>47%</div> <div>12%</div> <div>•</div> <div>37%</div> </div>
1	M	49	<div> <div>35%</div> <div>16%</div> <div>•</div> <div>45%</div> </div>
1	N	49	<div>2%</div> <div> <div>51%</div> <div>10%</div> <div>•</div> <div>37%</div> </div>

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	U	49	
1	V	49	
1	j	49	
2	B	261	
2	H	261	
2	J	261	
2	L	261	
2	P	261	
2	R	261	
2	X	261	
2	Z	261	
3	F	220	
3	G	220	
3	I	220	
3	K	220	
3	O	220	
3	Q	220	
3	W	220	
3	Y	220	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25772 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 Mature secreted glycoprotein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	27	Total	C	N	O	S	0	0	0
			221	145	37	35	4			
1	N	31	Total	C	N	O	S	0	0	0
			253	164	43	42	4			
1	S	30	Total	C	N	O	S	0	0	0
			245	160	42	39	4			
1	T	30	Total	C	N	O	S	0	0	0
			245	160	42	39	4			
1	U	30	Total	C	N	O	S	0	0	0
			245	160	42	39	4			
1	V	29	Total	C	N	O	S	0	0	0
			236	154	40	38	4			
1	j	32	Total	C	N	O	S	0	0	0
			261	168	45	44	4			
1	A	31	Total	C	N	O	S	0	0	0
			254	166	44	40	4			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	155	MET	-	initiating methionine	UNP P03423
M	156	GLY	-	expression tag	UNP P03423
M	198	HIS	-	expression tag	UNP P03423
M	199	HIS	-	expression tag	UNP P03423
M	200	HIS	-	expression tag	UNP P03423
M	201	HIS	-	expression tag	UNP P03423
M	202	HIS	-	expression tag	UNP P03423
M	203	HIS	-	expression tag	UNP P03423
N	155	MET	-	initiating methionine	UNP P03423
N	156	GLY	-	expression tag	UNP P03423
N	198	HIS	-	expression tag	UNP P03423
N	199	HIS	-	expression tag	UNP P03423
N	200	HIS	-	expression tag	UNP P03423

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	201	HIS	-	expression tag	UNP P03423
N	202	HIS	-	expression tag	UNP P03423
N	203	HIS	-	expression tag	UNP P03423
S	155	MET	-	initiating methionine	UNP P03423
S	156	GLY	-	expression tag	UNP P03423
S	198	HIS	-	expression tag	UNP P03423
S	199	HIS	-	expression tag	UNP P03423
S	200	HIS	-	expression tag	UNP P03423
S	201	HIS	-	expression tag	UNP P03423
S	202	HIS	-	expression tag	UNP P03423
S	203	HIS	-	expression tag	UNP P03423
T	155	MET	-	initiating methionine	UNP P03423
T	156	GLY	-	expression tag	UNP P03423
T	198	HIS	-	expression tag	UNP P03423
T	199	HIS	-	expression tag	UNP P03423
T	200	HIS	-	expression tag	UNP P03423
T	201	HIS	-	expression tag	UNP P03423
T	202	HIS	-	expression tag	UNP P03423
T	203	HIS	-	expression tag	UNP P03423
U	155	MET	-	initiating methionine	UNP P03423
U	156	GLY	-	expression tag	UNP P03423
U	198	HIS	-	expression tag	UNP P03423
U	199	HIS	-	expression tag	UNP P03423
U	200	HIS	-	expression tag	UNP P03423
U	201	HIS	-	expression tag	UNP P03423
U	202	HIS	-	expression tag	UNP P03423
U	203	HIS	-	expression tag	UNP P03423
V	155	MET	-	initiating methionine	UNP P03423
V	156	GLY	-	expression tag	UNP P03423
V	198	HIS	-	expression tag	UNP P03423
V	199	HIS	-	expression tag	UNP P03423
V	200	HIS	-	expression tag	UNP P03423
V	201	HIS	-	expression tag	UNP P03423
V	202	HIS	-	expression tag	UNP P03423
V	203	HIS	-	expression tag	UNP P03423
j	155	MET	-	initiating methionine	UNP P03423
j	156	GLY	-	expression tag	UNP P03423
j	198	HIS	-	expression tag	UNP P03423
j	199	HIS	-	expression tag	UNP P03423
j	200	HIS	-	expression tag	UNP P03423
j	201	HIS	-	expression tag	UNP P03423
j	202	HIS	-	expression tag	UNP P03423

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
j	203	HIS	-	expression tag	UNP P03423
A	155	MET	-	initiating methionine	UNP P03423
A	156	GLY	-	expression tag	UNP P03423
A	198	HIS	-	expression tag	UNP P03423
A	199	HIS	-	expression tag	UNP P03423
A	200	HIS	-	expression tag	UNP P03423
A	201	HIS	-	expression tag	UNP P03423
A	202	HIS	-	expression tag	UNP P03423
A	203	HIS	-	expression tag	UNP P03423

- Molecule 2 is a protein called Fab 2B11 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1605	1021	267	309	8			
2	J	210	Total	C	N	O	S	0	0	0
			1566	998	260	300	8			
2	L	216	Total	C	N	O	S	0	0	0
			1601	1017	267	309	8			
2	P	214	Total	C	N	O	S	0	0	0
			1592	1014	265	305	8			
2	R	217	Total	C	N	O	S	0	0	0
			1611	1024	268	310	9			
2	X	219	Total	C	N	O	S	0	0	0
			1627	1033	271	315	8			
2	Z	215	Total	C	N	O	S	0	0	0
			1599	1018	266	307	8			
2	H	115	Total	C	N	O	S	0	0	0
			870	552	149	163	6			

- Molecule 3 is a protein called Fab 2B11 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	208	Total	C	N	O	S	0	0	0
			1578	984	267	323	4			
3	G	104	Total	C	N	O	S	0	0	0
			767	477	131	157	2			
3	I	199	Total	C	N	O	S	0	0	0
			1509	939	256	310	4			
3	K	209	Total	C	N	O	S	0	0	0
			1565	973	266	322	4			
3	O	206	Total	C	N	O	S	0	0	0
			1553	966	265	318	4			

Continued on next page...

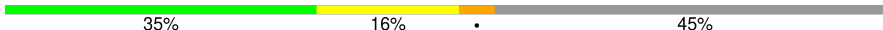
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	211	Total	C	N	O	S	0	0	0
			1584	985	267	328	4			
3	W	211	Total	C	N	O	S	0	0	0
			1593	993	270	326	4			
3	Y	212	Total	C	N	O	S	0	0	0
			1592	989	270	329	4			

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.

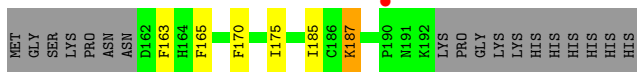
- Molecule 1: Mature secreted glycoprotein G

Chain M: 




- Molecule 1: Mature secreted glycoprotein G

Chain N: 



- Molecule 1: Mature secreted glycoprotein G

Chain S: 



- Molecule 1: Mature secreted glycoprotein G

Chain T: 



- Molecule 1: Mature secreted glycoprotein G

Chain U: 



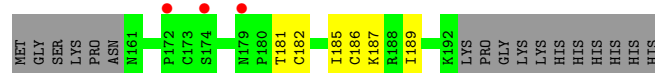
- Molecule 1: Mature secreted glycoprotein G

Chain V: 



- Molecule 1: Mature secreted glycoprotein G

Chain j: 



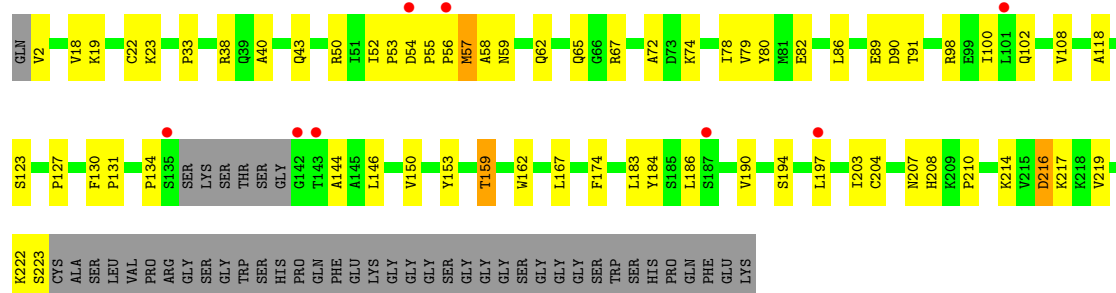
- Molecule 1: Mature secreted glycoprotein G

Chain A: 



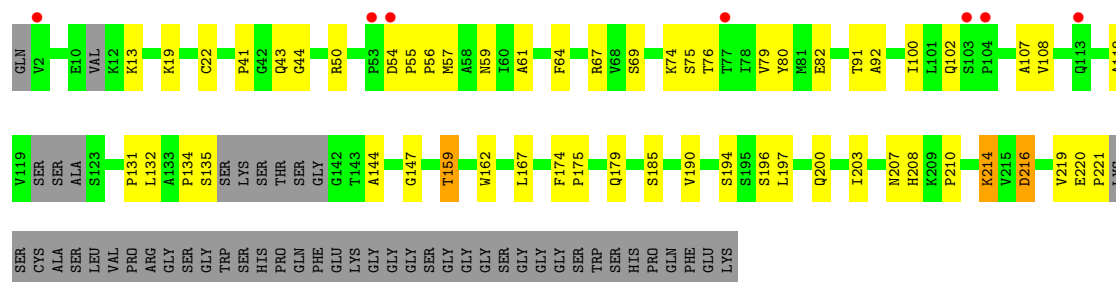
- Molecule 2: Fab 2B11 Heavy Chain

Chain B: 



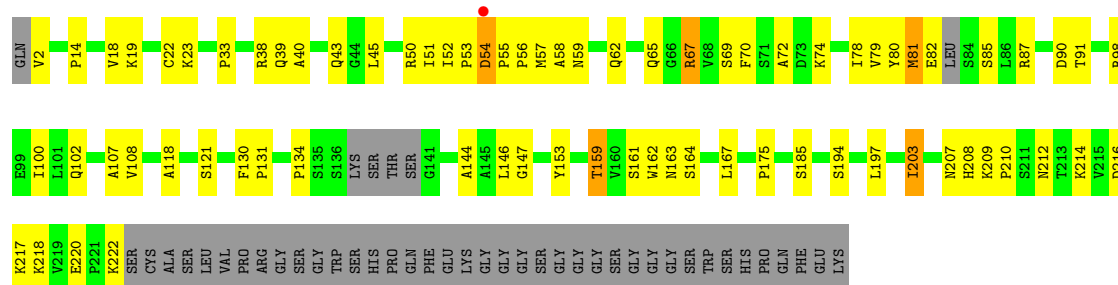
- Molecule 2: Fab 2B11 Heavy Chain

Chain J: 

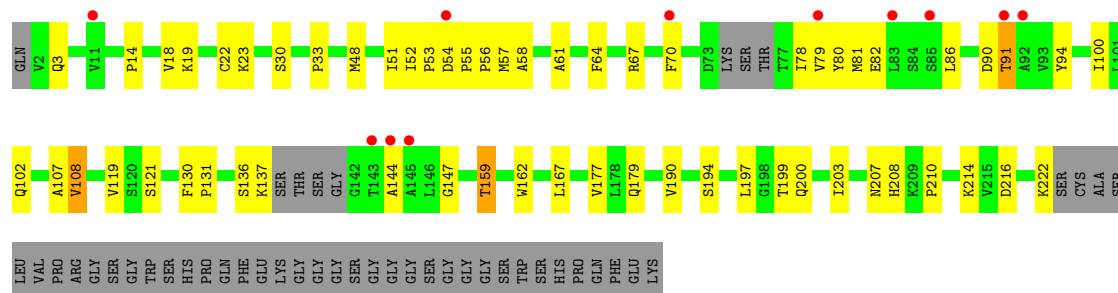


- Molecule 2: Fab 2B11 Heavy Chain

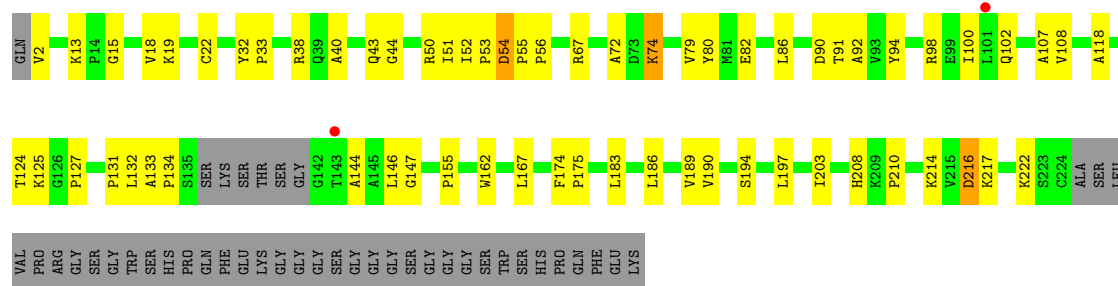
Chain L: 



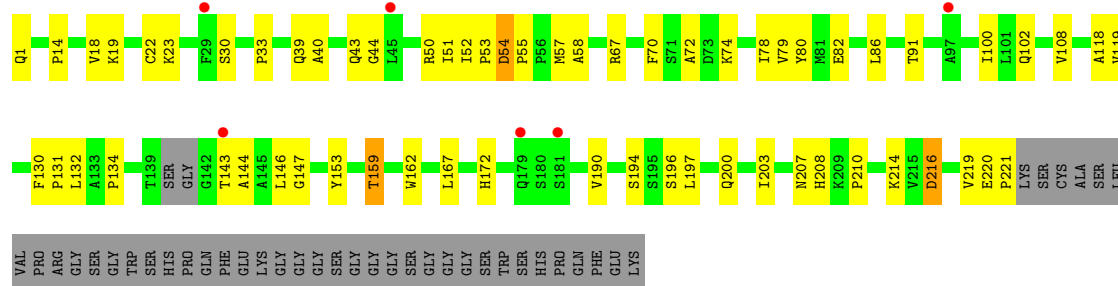
- Molecule 2: Fab 2B11 Heavy Chain



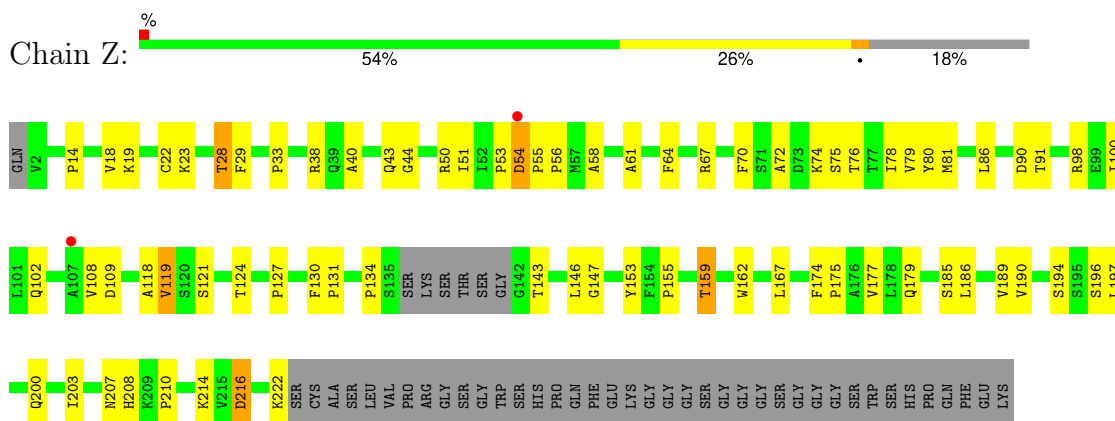
- Molecule 2: Fab 2B11 Heavy Chain



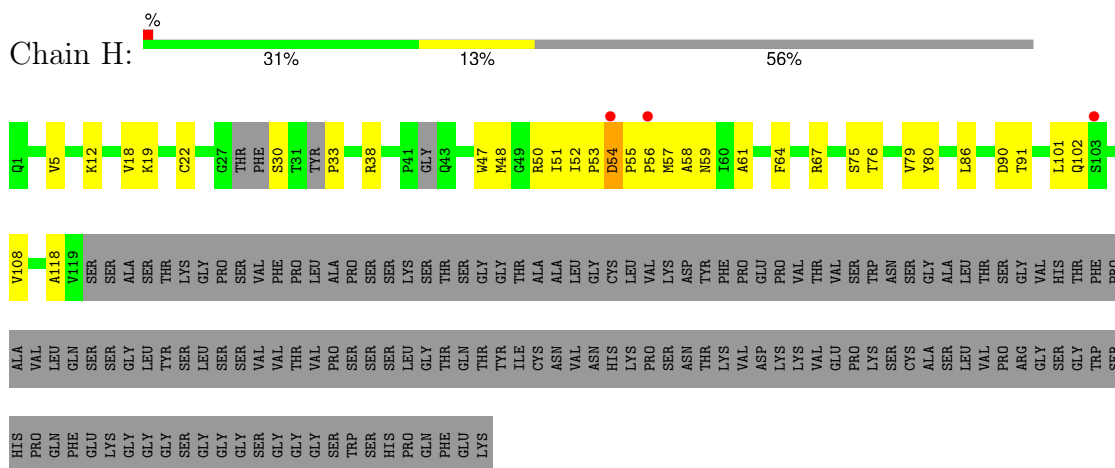
- Molecule 2: Fab 2B11 Heavy Chain



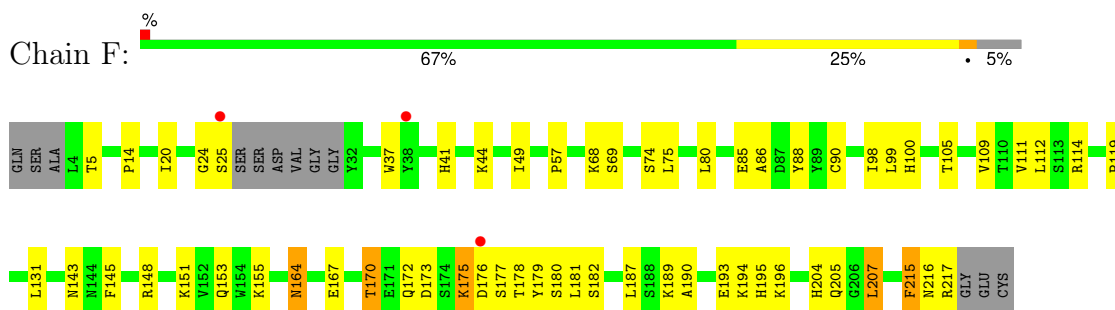
- Molecule 2: Fab 2B11 Heavy Chain



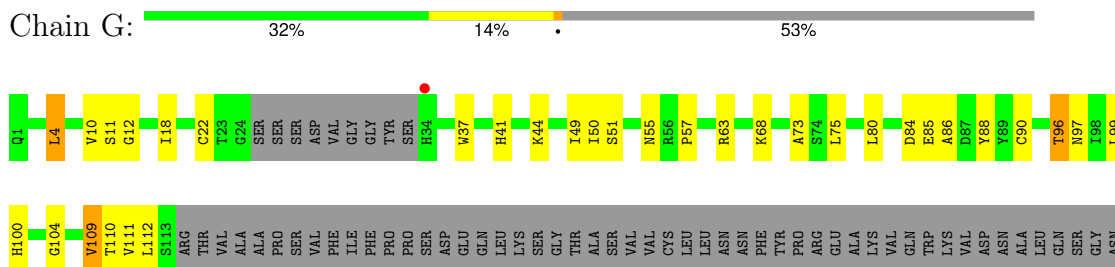
- Molecule 2: Fab 2B11 Heavy Chain



- Molecule 3: Fab 2B11 Light Chain



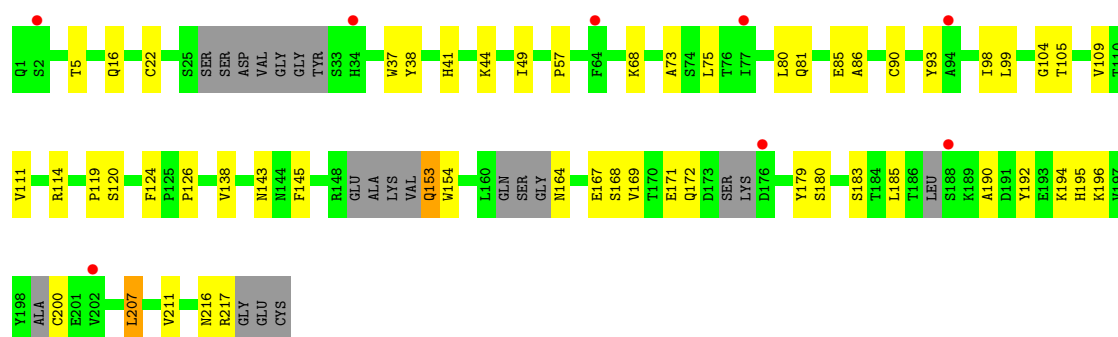
- Molecule 3: Fab 2B11 Light Chain



SER	GLN	GLU	SER	VAL	THR	GLU	GLN	ASP	SER	LYS	SER	ASP	SER	THR	TYR	SER	LEU	SER	SER	THR	THR	LEU	THR	LEU	SER	LYS	ALA	ALA	ASP	TYR	GLU	LYS	HIS	LYS	VAL	TYR	ALA	ALA	CYS	GLY	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLY	CYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

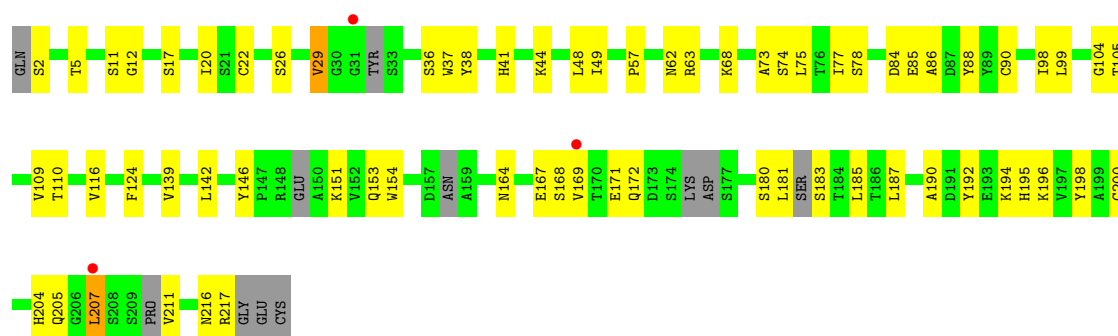
• Molecule 3: Fab 2B11 Light Chain

Chain I:  4% 66% 24% 10%



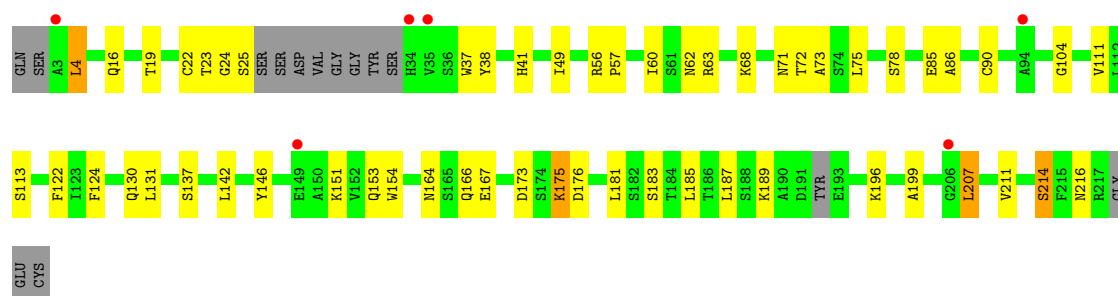
• Molecule 3: Fab 2B11 Light Chain

Chain K:  64% 30% 5%



• Molecule 3: Fab 2B11 Light Chain

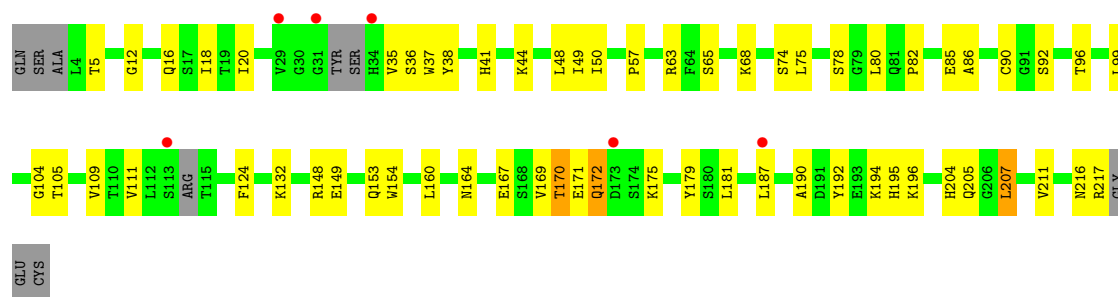
Chain O:  3% 69% 23% 6%



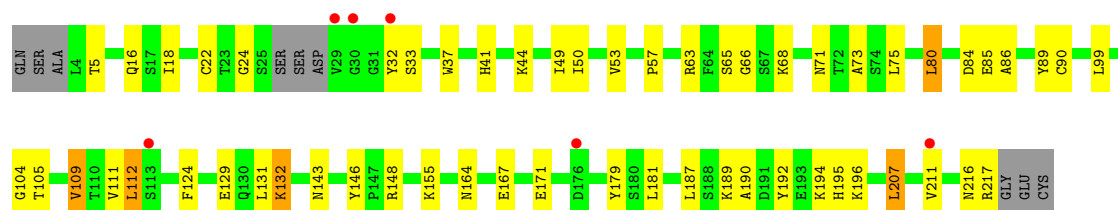
• Molecule 3: Fab 2B11 Light Chain

Chain Q:  3% 68% 26% 5%

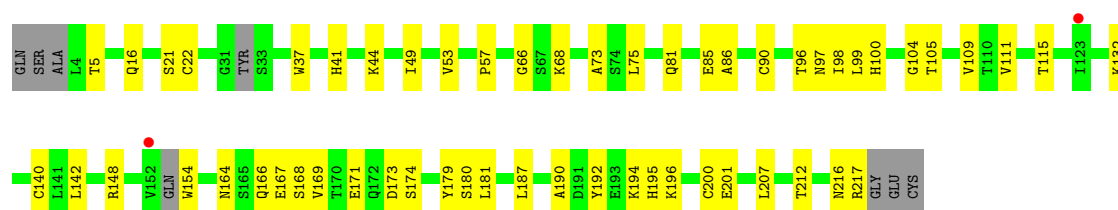




• Molecule 3: Fab 2B11 Light Chain



• Molecule 3: Fab 2B11 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.65Å 184.34Å 161.24Å 90.00° 96.88° 90.00°	Depositor
Resolution (Å)	80.04 – 3.10 80.04 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (80.04-3.10) 99.1 (80.04-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.292 , 0.324 0.291 , 0.326	Depositor DCC
R_{free} test set	2061 reflections (2.64%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	25772	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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

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	0.47	0/263	0.64	0/356
1	M	0.42	0/229	0.57	0/311
1	N	0.42	0/262	0.61	0/356
1	S	0.43	0/254	0.61	0/345
1	T	0.51	0/254	0.71	0/345
1	U	0.54	0/254	0.66	0/345
1	V	0.42	0/245	0.67	0/334
1	j	0.51	0/270	0.62	0/367
2	B	0.35	0/1645	0.54	0/2243
2	H	0.37	0/887	0.58	0/1199
2	J	0.39	0/1604	0.57	0/2185
2	L	0.40	0/1640	0.55	0/2234
2	P	0.35	0/1631	0.56	0/2222
2	R	0.37	0/1651	0.53	0/2251
2	X	0.35	0/1667	0.56	0/2273
2	Z	0.36	0/1639	0.53	0/2235
3	F	0.33	0/1612	0.52	0/2192
3	G	0.33	0/783	0.50	0/1065
3	I	0.32	0/1537	0.51	0/2084
3	K	0.38	0/1592	0.55	0/2156
3	O	0.34	0/1584	0.51	0/2152
3	Q	0.31	0/1616	0.54	0/2196
3	W	0.32	0/1627	0.54	0/2212
3	Y	0.31	0/1624	0.52	0/2206
All	All	0.36	0/26370	0.55	0/35864

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 ⓘ

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	254	0	244	12	0
1	M	221	0	205	10	0
1	N	253	0	235	6	0
1	S	245	0	231	6	0
1	T	245	0	231	10	0
1	U	245	0	231	12	0
1	V	236	0	218	8	0
1	j	261	0	241	0	0
2	B	1605	0	1602	41	0
2	H	870	0	873	28	0
2	J	1566	0	1558	32	0
2	L	1601	0	1593	40	0
2	P	1592	0	1589	41	0
2	R	1611	0	1607	41	0
2	X	1627	0	1625	48	0
2	Z	1599	0	1597	44	0
3	F	1578	0	1528	44	0
3	G	767	0	745	22	0
3	I	1509	0	1452	32	0
3	K	1565	0	1512	44	0
3	O	1553	0	1509	37	0
3	Q	1584	0	1529	40	0
3	W	1593	0	1543	35	0
3	Y	1592	0	1539	36	0
All	All	25772	0	25237	582	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 582 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:14:PRO:HG2	2:L:121:SER:HB3	1.60	0.83
3:O:85:GLU:HG2	3:O:111:VAL:H	1.45	0.81
2:Z:14:PRO:HG2	2:Z:121:SER:HB3	1.62	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:131:PRO:HG3	2:L:217:LYS:HE2	1.66	0.78
3:Q:171:GLU:HG3	3:Q:179:TYR:HE1	1.50	0.77

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	29/49 (59%)	27 (93%)	2 (7%)	0	100	100
1	M	25/49 (51%)	23 (92%)	2 (8%)	0	100	100
1	N	29/49 (59%)	26 (90%)	3 (10%)	0	100	100
1	S	28/49 (57%)	25 (89%)	3 (11%)	0	100	100
1	T	28/49 (57%)	28 (100%)	0	0	100	100
1	U	28/49 (57%)	24 (86%)	4 (14%)	0	100	100
1	V	27/49 (55%)	25 (93%)	2 (7%)	0	100	100
1	j	30/49 (61%)	28 (93%)	2 (7%)	0	100	100
2	B	212/261 (81%)	198 (93%)	14 (7%)	0	100	100
2	H	107/261 (41%)	99 (92%)	8 (8%)	0	100	100
2	J	202/261 (77%)	187 (93%)	15 (7%)	0	100	100
2	L	210/261 (80%)	195 (93%)	15 (7%)	0	100	100
2	P	208/261 (80%)	196 (94%)	12 (6%)	0	100	100
2	R	213/261 (82%)	197 (92%)	16 (8%)	0	100	100
2	X	215/261 (82%)	198 (92%)	17 (8%)	0	100	100
2	Z	211/261 (81%)	195 (92%)	16 (8%)	0	100	100
3	F	204/220 (93%)	194 (95%)	10 (5%)	0	100	100
3	G	100/220 (46%)	93 (93%)	7 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	185/220 (84%)	176 (95%)	9 (5%)	0	100	100
3	K	195/220 (89%)	183 (94%)	12 (6%)	0	100	100
3	O	200/220 (91%)	192 (96%)	8 (4%)	0	100	100
3	Q	205/220 (93%)	192 (94%)	13 (6%)	0	100	100
3	W	207/220 (94%)	196 (95%)	11 (5%)	0	100	100
3	Y	206/220 (94%)	194 (94%)	12 (6%)	0	100	100
All	All	3304/4240 (78%)	3091 (94%)	213 (6%)	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 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	30/46 (65%)	28 (93%)	2 (7%)	13	40
1	M	26/46 (56%)	23 (88%)	3 (12%)	4	19
1	N	30/46 (65%)	28 (93%)	2 (7%)	13	40
1	S	29/46 (63%)	28 (97%)	1 (3%)	32	62
1	T	29/46 (63%)	27 (93%)	2 (7%)	13	39
1	U	29/46 (63%)	28 (97%)	1 (3%)	32	62
1	V	28/46 (61%)	26 (93%)	2 (7%)	12	39
1	j	31/46 (67%)	25 (81%)	6 (19%)	1	5
2	B	183/215 (85%)	171 (93%)	12 (7%)	14	41
2	H	96/215 (45%)	91 (95%)	5 (5%)	19	48
2	J	178/215 (83%)	170 (96%)	8 (4%)	23	53
2	L	182/215 (85%)	162 (89%)	20 (11%)	5	21
2	P	181/215 (84%)	169 (93%)	12 (7%)	14	41
2	R	184/215 (86%)	174 (95%)	10 (5%)	18	47
2	X	186/215 (86%)	177 (95%)	9 (5%)	21	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	182/215 (85%)	170 (93%)	12 (7%)	14	41
3	F	183/191 (96%)	173 (94%)	10 (6%)	18	47
3	G	88/191 (46%)	85 (97%)	3 (3%)	32	62
3	I	176/191 (92%)	169 (96%)	7 (4%)	27	58
3	K	181/191 (95%)	172 (95%)	9 (5%)	20	50
3	O	180/191 (94%)	172 (96%)	8 (4%)	24	54
3	Q	184/191 (96%)	175 (95%)	9 (5%)	21	51
3	W	184/191 (96%)	172 (94%)	12 (6%)	14	41
3	Y	185/191 (97%)	177 (96%)	8 (4%)	25	55
All	All	2965/3616 (82%)	2792 (94%)	173 (6%)	17	45

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	187	LEU
2	X	108	VAL
2	R	52	ILE
3	W	80	LEU
3	Y	68	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	40	GLN
2	J	39	GLN
3	W	143	ASN
3	Q	39	GLN
3	F	16	GLN

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 [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	31/49 (63%)	0.36	0	100	100	30, 66, 83, 85	0
1	M	27/49 (55%)	0.33	0	100	100	47, 65, 73, 93	0
1	N	31/49 (63%)	0.56	1 (3%)	50	31	43, 62, 85, 93	0
1	S	30/49 (61%)	0.20	1 (3%)	49	30	43, 66, 83, 85	0
1	T	30/49 (61%)	0.31	1 (3%)	49	30	49, 63, 75, 85	0
1	U	30/49 (61%)	0.34	1 (3%)	49	30	55, 75, 89, 96	0
1	V	29/49 (59%)	-0.00	0	100	100	48, 68, 80, 86	0
1	j	32/49 (65%)	0.70	3 (9%)	15	9	40, 69, 93, 101	0
2	B	216/261 (82%)	0.21	8 (3%)	45	27	31, 68, 104, 125	0
2	H	115/261 (44%)	0.29	3 (2%)	57	38	47, 73, 96, 125	0
2	J	210/261 (80%)	0.37	7 (3%)	49	30	36, 84, 113, 121	0
2	L	216/261 (82%)	0.34	1 (0%)	87	75	39, 82, 109, 129	0
2	P	214/261 (81%)	0.49	11 (5%)	34	20	30, 85, 109, 120	0
2	R	217/261 (83%)	0.19	2 (0%)	81	66	32, 68, 104, 132	0
2	X	219/261 (83%)	0.20	6 (2%)	56	36	40, 69, 114, 137	0
2	Z	215/261 (82%)	0.24	2 (0%)	81	66	44, 80, 108, 128	0
3	F	208/220 (94%)	0.22	3 (1%)	73	56	29, 65, 91, 112	0
3	G	104/220 (47%)	0.10	1 (0%)	79	64	34, 62, 84, 91	0
3	I	199/220 (90%)	0.35	8 (4%)	43	25	30, 86, 120, 133	0
3	K	209/220 (95%)	0.33	3 (1%)	73	56	37, 81, 111, 136	0
3	O	206/220 (93%)	0.30	6 (2%)	54	34	24, 81, 122, 139	0
3	Q	211/220 (95%)	0.10	6 (2%)	55	35	27, 60, 102, 137	0
3	W	211/220 (95%)	0.23	6 (2%)	55	35	36, 75, 109, 126	0
3	Y	212/220 (96%)	0.28	2 (0%)	81	66	30, 73, 110, 124	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3422/4240 (80%)	0.28	82 (2%) 59 41	24, 73, 112, 139	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	W	29	VAL	4.1
2	P	143	THR	4.0
3	Q	173	ASP	3.8
3	I	2	SER	3.7
2	P	54	ASP	3.5

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.