



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 10:00 PM UTC

PDB ID : 2FJF / pdb_00002fjf
Title : Structure of the G6 Fab, a phage derived VEGF binding Fab
Authors : Wiesmann, C.
Deposited on : 2006-01-02
Resolution : 2.65 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
Xtrriage (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

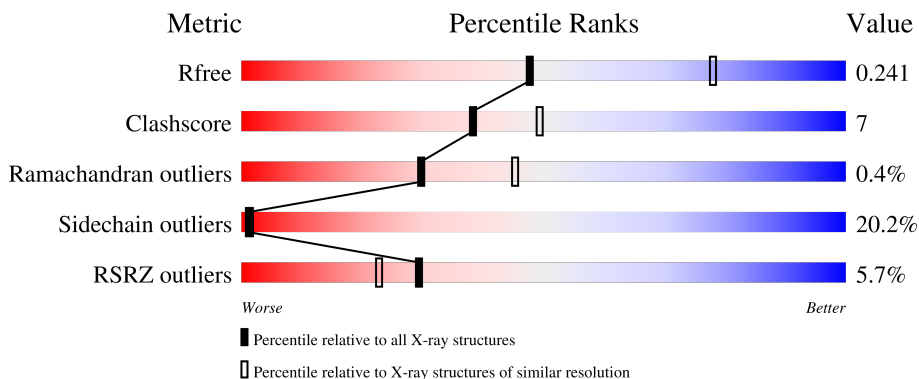
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	214	
1	C	214	
1	E	214	
1	G	214	
1	J	214	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	L	214	 16% 73% 21% . .
1	M	214	 29% 68% 25% 6% .
1	O	214	 7% 70% 24% 5% .
1	Q	214	 3% 65% 29% 5% .
1	S	214	 2% 67% 26% 6% .
1	U	214	 6% 66% 27% 5% .
1	W	214	 6% 64% 33% . .
2	B	227	 % 69% 25% . .
2	D	227	 3% 77% 17% . .
2	F	227	 2% 70% 23% . .
2	H	227	 11% 71% 21% . .
2	I	227	 % 67% 25% . .
2	K	227	 % 71% 22% . .
2	N	227	 31% 72% 19% 5% .
2	P	227	 % 75% 16% . .
2	R	227	 % 68% 23% . .
2	T	227	 % 67% 24% 5% .
2	V	227	 % 69% 22% 5% .
2	X	227	 % 69% 24% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 39642 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 Light Chain of a VEGF binding Antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	1617	1014	268	330	5	0	0	0
1	A	211	1617	1014	268	330	5	0	0	0
1	C	211	1617	1014	268	330	5	0	0	0
1	E	211	1617	1014	268	330	5	0	0	0
1	G	211	1617	1014	268	330	5	0	0	0
1	J	211	1617	1014	268	330	5	0	0	0
1	M	211	1617	1014	268	330	5	0	0	0
1	O	211	1617	1014	268	330	5	0	0	0
1	Q	211	1617	1014	268	330	5	0	0	0
1	S	211	1617	1014	268	330	5	0	0	0
1	U	211	1617	1014	268	330	5	0	0	0
1	W	211	1617	1014	268	330	5	0	0	0

- Molecule 2 is a protein called Heavy Chain of a VEGF binding Antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	218	1633	1044	267	315	7	0	0	0
2	B	218	1633	1044	267	315	7	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	F	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	I	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	K	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	N	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	P	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	R	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	T	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	V	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			
2	X	218	Total	C	N	O	S	0	0	0
			1633	1044	267	315	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	22	Total	O	0	0
			22	22		
3	H	44	Total	O	0	0
			44	44		
3	A	17	Total	O	0	0
			17	17		
3	B	28	Total	O	0	0
			28	28		
3	C	10	Total	O	0	0
			10	10		
3	D	30	Total	O	0	0
			30	30		
3	E	14	Total	O	0	0
			14	14		
3	F	30	Total	O	0	0
			30	30		
3	G	53	Total	O	0	0
			53	53		

Continued on next page...

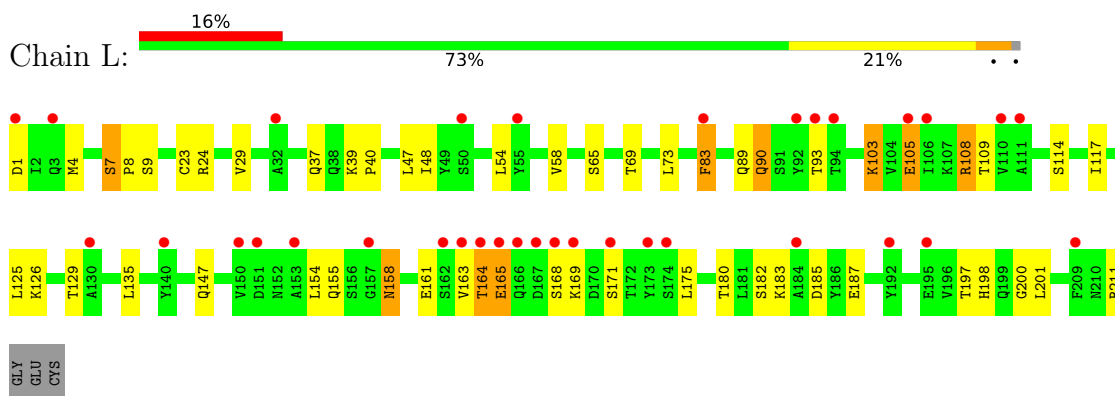
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	52	Total 52	O 52	0	0
3	J	35	Total 35	O 35	0	0
3	K	53	Total 53	O 53	0	0
3	M	17	Total 17	O 17	0	0
3	N	24	Total 24	O 24	0	0
3	O	31	Total 31	O 31	0	0
3	P	52	Total 52	O 52	0	0
3	Q	15	Total 15	O 15	0	0
3	R	21	Total 21	O 21	0	0
3	S	9	Total 9	O 9	0	0
3	T	15	Total 15	O 15	0	0
3	U	16	Total 16	O 16	0	0
3	V	28	Total 28	O 28	0	0
3	W	5	Total 5	O 5	0	0
3	X	21	Total 21	O 21	0	0

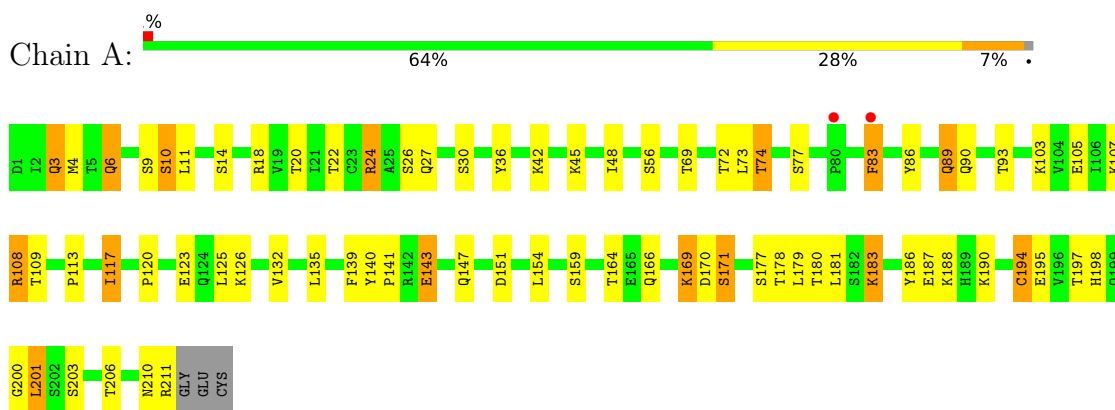
3 Residue-property plots [i](#)

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.

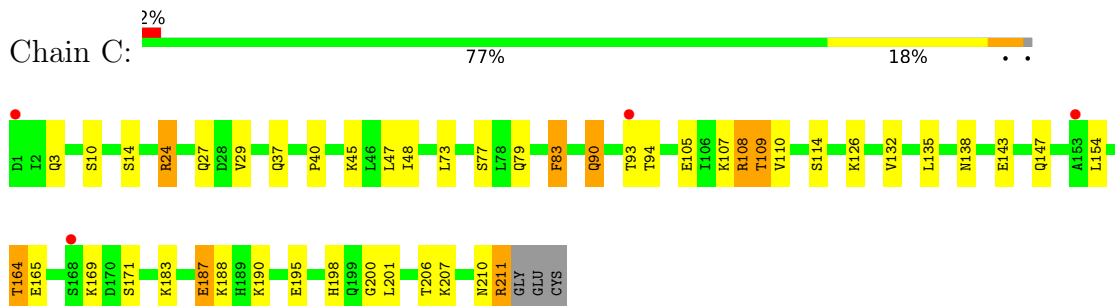
- Molecule 1: Light Chain of a VEGF binding Antibody



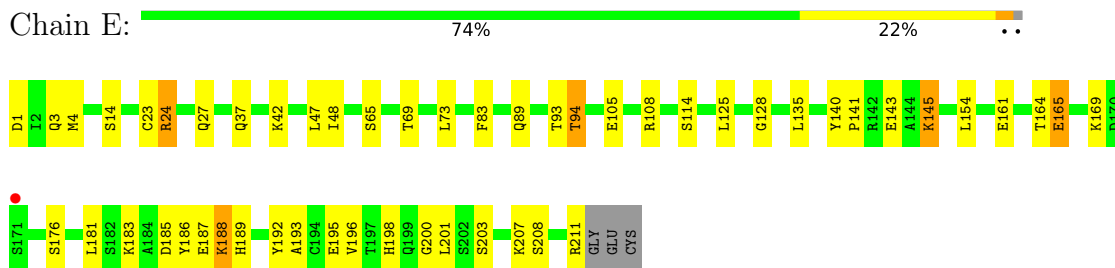
- Molecule 1: Light Chain of a VEGF binding Antibody



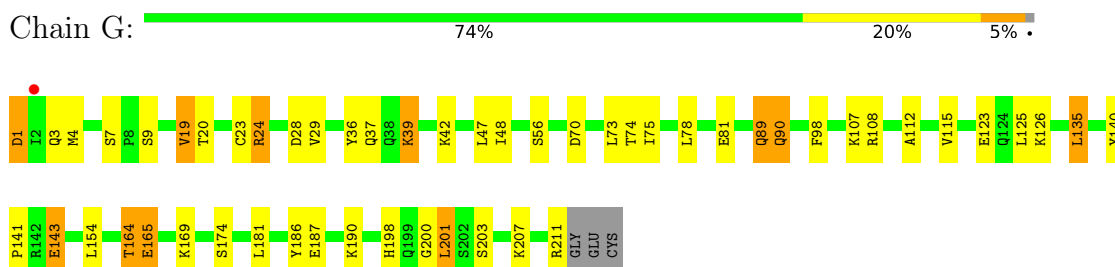
- Molecule 1: Light Chain of a VEGF binding Antibody



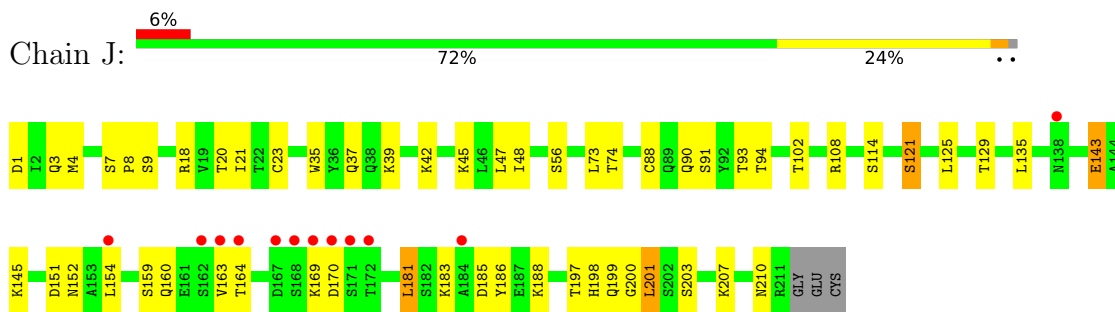
- Molecule 1: Light Chain of a VEGF binding Antibody



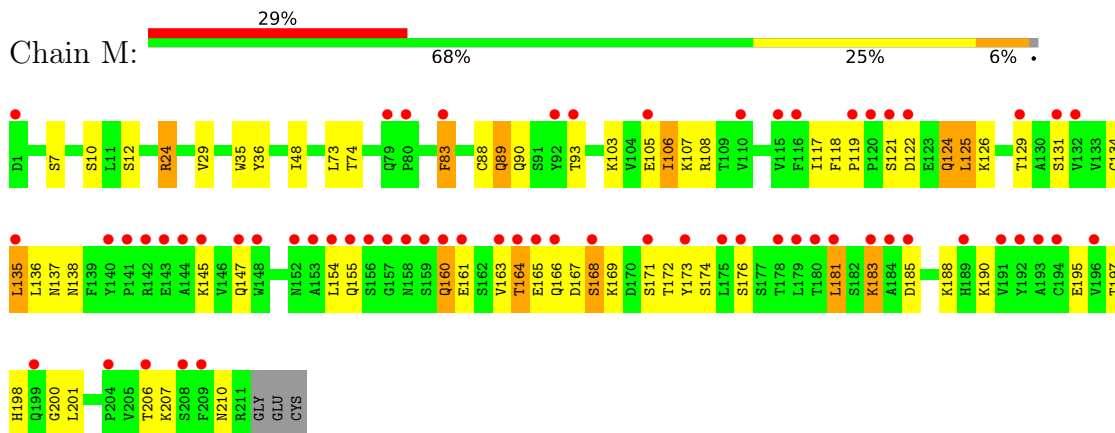
- Molecule 1: Light Chain of a VEGF binding Antibody



- Molecule 1: Light Chain of a VEGF binding Antibody

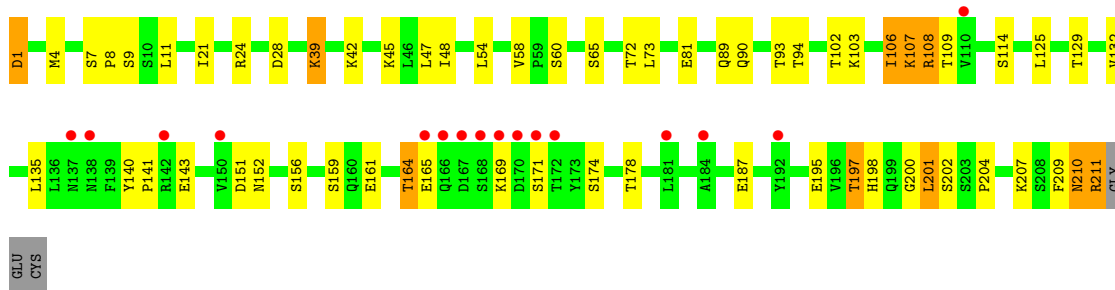


- Molecule 1: Light Chain of a VEGF binding Antibody

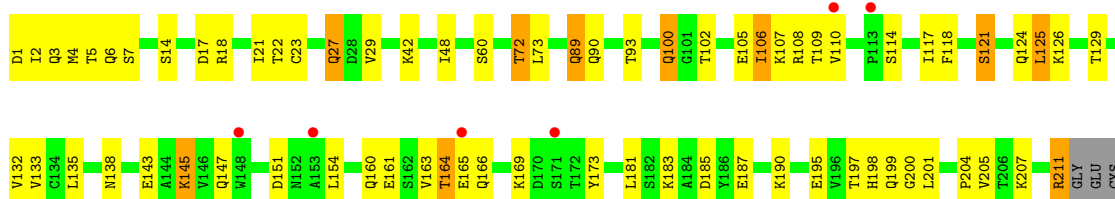


- Molecule 1: Light Chain of a VEGF binding Antibody

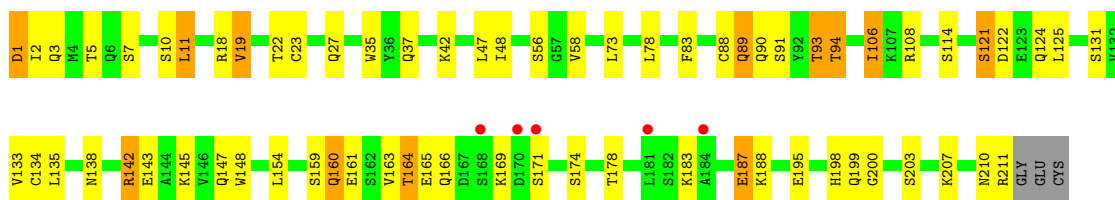


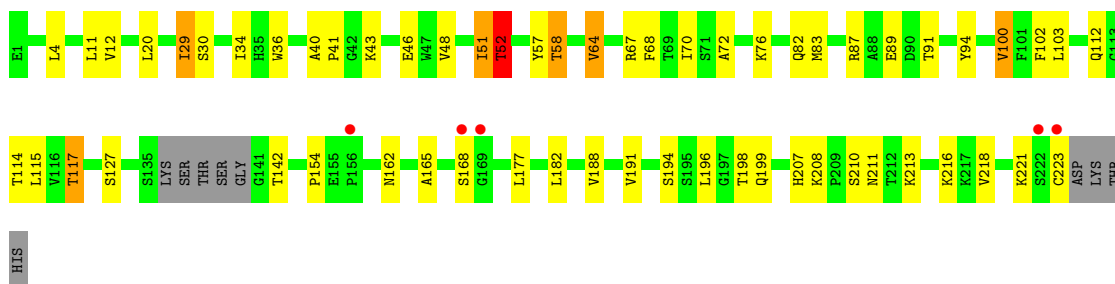


- Molecule 1: Light Chain of a VEGF binding Antibody

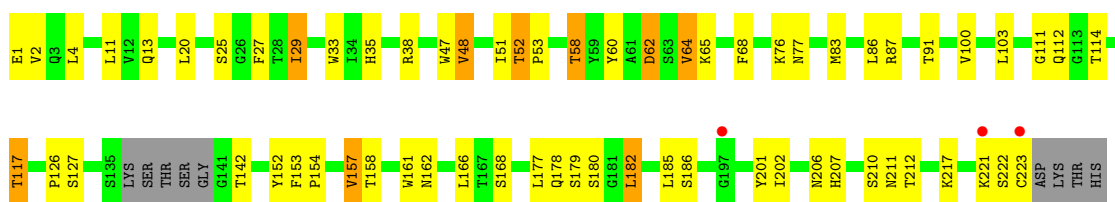


- Molecule 1: Light Chain of a VEGF binding Antibody

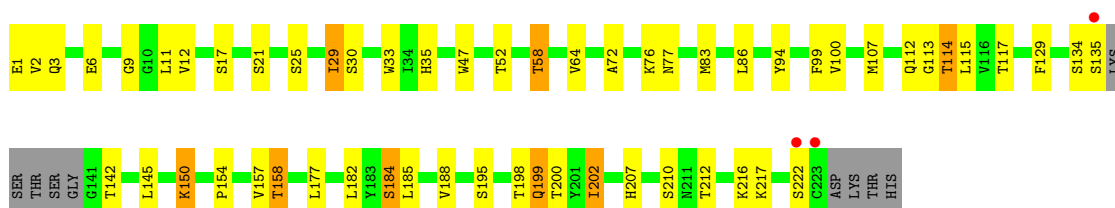




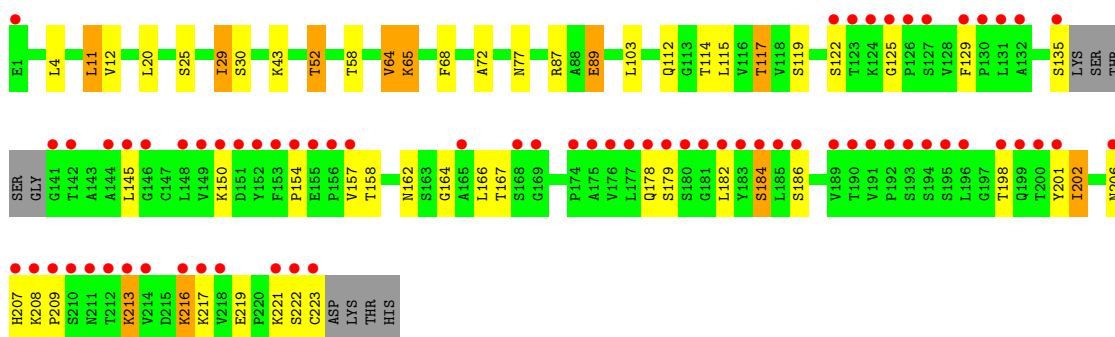
• Molecule 2: Heavy Chain of a VEGF binding Antibody



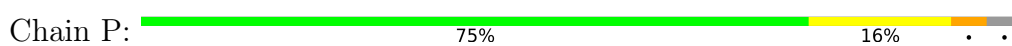
• Molecule 2: Heavy Chain of a VEGF binding Antibody

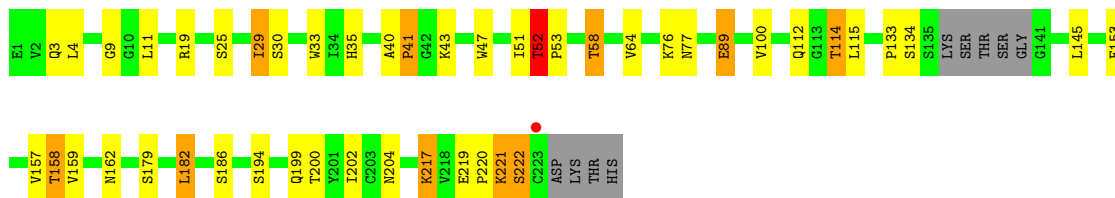


• Molecule 2: Heavy Chain of a VEGF binding Antibody

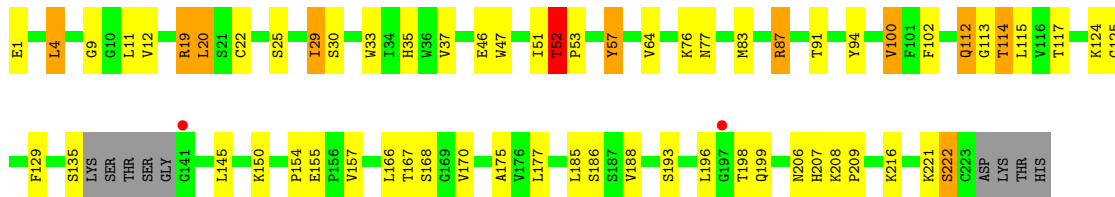


• Molecule 2: Heavy Chain of a VEGF binding Antibody

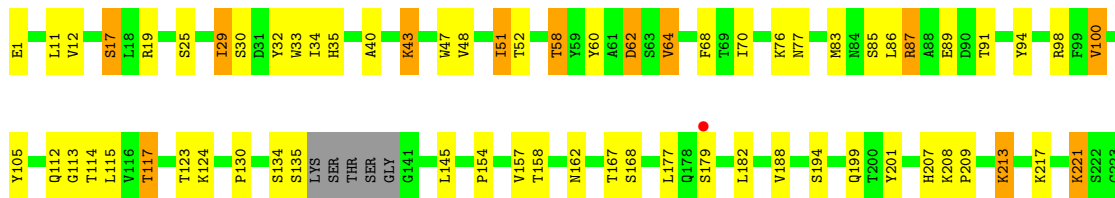




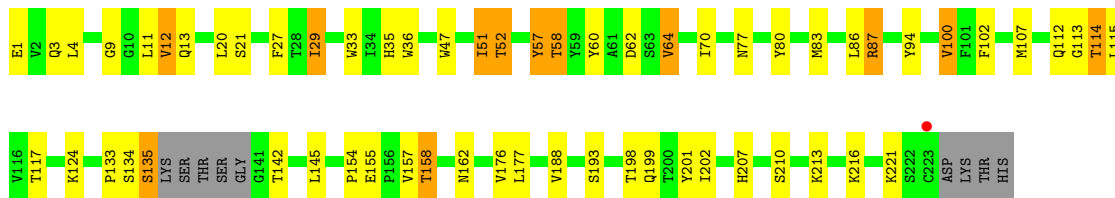
● Molecule 2: Heavy Chain of a VEGF binding Antibody



● Molecule 2: Heavy Chain of a VEGF binding Antibody

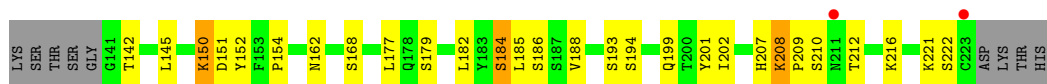


● Molecule 2: Heavy Chain of a VEGF binding Antibody



● Molecule 2: Heavy Chain of a VEGF binding Antibody





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	274.92Å 192.23Å 154.11Å 90.00° 117.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 20.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.65) 99.6 (20.00-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.64Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.199 , 0.248 0.194 , 0.241	Depositor DCC
R_{free} test set	4490 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtrriage
Anisotropy	0.205	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	39642	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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	0.49	0/1653	0.84	0/2248
1	C	0.46	0/1653	0.85	0/2248
1	E	0.47	0/1653	0.85	2/2248 (0.1%)
1	G	0.53	0/1653	0.83	0/2248
1	J	0.50	0/1653	0.87	0/2248
1	L	0.49	0/1653	0.85	0/2248
1	M	0.52	0/1653	0.88	0/2248
1	O	0.49	0/1653	0.85	0/2248
1	Q	0.48	0/1653	0.85	0/2248
1	S	0.45	0/1653	0.81	0/2248
1	U	0.48	0/1653	0.83	0/2248
1	W	0.47	0/1653	0.86	0/2248
2	B	0.55	1/1677 (0.1%)	0.89	0/2290
2	D	0.52	1/1677 (0.1%)	0.86	0/2290
2	F	0.53	0/1677	0.91	1/2290 (0.0%)
2	H	0.56	1/1677 (0.1%)	0.89	0/2290
2	I	0.59	0/1677	0.88	0/2290
2	K	0.53	0/1677	0.87	2/2290 (0.1%)
2	N	0.50	0/1677	0.85	1/2290 (0.0%)
2	P	0.54	0/1677	0.88	2/2290 (0.1%)
2	R	0.50	0/1677	0.86	1/2290 (0.0%)
2	T	0.51	0/1677	0.88	0/2290
2	V	0.51	0/1677	0.88	0/2290
2	X	0.52	0/1677	0.85	1/2290 (0.0%)
All	All	0.51	3/39960 (0.0%)	0.86	10/54456 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	83	MET	SD-CE	-5.33	1.66	1.79
2	H	83	MET	SD-CE	-5.33	1.66	1.79
2	D	83	MET	SD-CE	-5.20	1.66	1.79

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	94	THR	CB-CA-C	6.49	117.66	108.76
1	E	128	GLY	N-CA-C	5.64	121.79	115.08
2	X	151	ASP	N-CA-C	5.56	117.41	110.91
2	K	3	GLN	N-CA-C	5.39	116.71	108.52
2	P	3	GLN	N-CA-C	5.33	116.39	108.60

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	1617	0	1573	25	0
1	C	1617	0	1573	13	0
1	E	1617	0	1573	15	0
1	G	1617	0	1573	25	0
1	J	1617	0	1573	17	0
1	L	1617	0	1573	16	0
1	M	1617	0	1573	20	0
1	O	1617	0	1573	22	0
1	Q	1617	0	1573	21	0
1	S	1617	0	1573	26	0
1	U	1617	0	1573	26	0
1	W	1617	0	1573	17	0
2	B	1633	0	1592	17	0
2	D	1633	0	1592	13	0
2	F	1633	0	1592	22	0
2	H	1633	0	1592	28	0
2	I	1633	0	1592	32	0
2	K	1633	0	1592	25	0
2	N	1633	0	1592	29	0
2	P	1633	0	1592	19	0
2	R	1633	0	1592	28	0
2	T	1633	0	1592	32	0
2	V	1633	0	1592	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	1633	0	1592	23	0
3	A	17	0	0	1	0
3	B	28	0	0	0	0
3	C	10	0	0	0	0
3	D	30	0	0	0	0
3	E	14	0	0	0	0
3	F	30	0	0	2	0
3	G	53	0	0	3	0
3	H	44	0	0	3	0
3	I	52	0	0	2	0
3	J	35	0	0	2	0
3	K	53	0	0	2	0
3	L	22	0	0	0	0
3	M	17	0	0	0	0
3	N	24	0	0	0	0
3	O	31	0	0	3	0
3	P	52	0	0	2	0
3	Q	15	0	0	0	0
3	R	21	0	0	1	0
3	S	9	0	0	1	0
3	T	15	0	0	2	0
3	U	16	0	0	2	0
3	V	28	0	0	2	0
3	W	5	0	0	0	0
3	X	21	0	0	1	0
All	All	39642	0	37980	529	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 7.

The worst 5 of 529 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:R:19:ARG:HG3	2:R:19:ARG:HH11	1.22	0.99
1:S:83:PHE:CE1	1:S:106:ILE:HD11	2.00	0.96
2:X:35:HIS:HD2	2:X:47:TRP:HE1	1.13	0.93
2:I:52:THR:HG21	3:I:265:HOH:O	1.72	0.90
1:E:83:PHE:HZ	1:E:165:GLU:HG2	1.39	0.86

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	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
1	C	209/214 (98%)	203 (97%)	4 (2%)	2 (1%)	12	20
1	E	209/214 (98%)	199 (95%)	10 (5%)	0	100	100
1	G	209/214 (98%)	205 (98%)	4 (2%)	0	100	100
1	J	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
1	L	209/214 (98%)	199 (95%)	9 (4%)	1 (0%)	24	39
1	M	209/214 (98%)	197 (94%)	9 (4%)	3 (1%)	9	14
1	O	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
1	Q	209/214 (98%)	199 (95%)	8 (4%)	2 (1%)	12	20
1	S	209/214 (98%)	201 (96%)	6 (3%)	2 (1%)	12	20
1	U	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
1	W	209/214 (98%)	197 (94%)	11 (5%)	1 (0%)	24	39
2	B	214/227 (94%)	206 (96%)	8 (4%)	0	100	100
2	D	214/227 (94%)	203 (95%)	10 (5%)	1 (0%)	24	39
2	F	214/227 (94%)	203 (95%)	9 (4%)	2 (1%)	14	24
2	H	214/227 (94%)	204 (95%)	10 (5%)	0	100	100
2	I	214/227 (94%)	205 (96%)	9 (4%)	0	100	100
2	K	214/227 (94%)	206 (96%)	8 (4%)	0	100	100
2	N	214/227 (94%)	201 (94%)	13 (6%)	0	100	100
2	P	214/227 (94%)	204 (95%)	8 (4%)	2 (1%)	14	24
2	R	214/227 (94%)	203 (95%)	9 (4%)	2 (1%)	14	24
2	T	214/227 (94%)	204 (95%)	8 (4%)	2 (1%)	14	24
2	V	214/227 (94%)	207 (97%)	7 (3%)	0	100	100
2	X	214/227 (94%)	206 (96%)	8 (4%)	0	100	100
All	All	5076/5292 (96%)	4859 (96%)	197 (4%)	20 (0%)	30	45

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	109	THR
2	P	222	SER
2	F	221	LYS
1	M	183	LYS
1	Q	138	ASN

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	A	186/188 (99%)	137 (74%)	49 (26%)	0	0
1	C	186/188 (99%)	150 (81%)	36 (19%)	1	2
1	E	186/188 (99%)	157 (84%)	29 (16%)	2	3
1	G	186/188 (99%)	158 (85%)	28 (15%)	3	4
1	J	186/188 (99%)	151 (81%)	35 (19%)	1	2
1	L	186/188 (99%)	152 (82%)	34 (18%)	2	2
1	M	186/188 (99%)	141 (76%)	45 (24%)	1	0
1	O	186/188 (99%)	149 (80%)	37 (20%)	1	1
1	Q	186/188 (99%)	142 (76%)	44 (24%)	1	0
1	S	186/188 (99%)	141 (76%)	45 (24%)	1	0
1	U	186/188 (99%)	141 (76%)	45 (24%)	1	0
1	W	186/188 (99%)	135 (73%)	51 (27%)	0	0
2	B	179/187 (96%)	140 (78%)	39 (22%)	1	1
2	D	179/187 (96%)	152 (85%)	27 (15%)	3	4
2	F	179/187 (96%)	144 (80%)	35 (20%)	1	2
2	H	179/187 (96%)	144 (80%)	35 (20%)	1	2
2	I	179/187 (96%)	146 (82%)	33 (18%)	1	2
2	K	179/187 (96%)	148 (83%)	31 (17%)	2	2
2	N	179/187 (96%)	143 (80%)	36 (20%)	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	179/187 (96%)	154 (86%)	25 (14%)	3	5
2	R	179/187 (96%)	142 (79%)	37 (21%)	1	1
2	T	179/187 (96%)	140 (78%)	39 (22%)	1	1
2	V	179/187 (96%)	147 (82%)	32 (18%)	2	2
2	X	179/187 (96%)	140 (78%)	39 (22%)	1	1
All	All	4380/4500 (97%)	3494 (80%)	886 (20%)	1	1

5 of 886 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	52	THR
1	Q	110	VAL
2	X	188	VAL
1	W	6	GLN
2	N	145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
2	V	39	GLN
2	V	162	ASN
2	X	207	HIS
1	J	89	GLN
1	J	37	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 [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	211/214 (98%)	0.13	2 (0%) 81 78	5, 11, 14, 17	0
1	C	211/214 (98%)	-0.06	4 (1%) 66 61	5, 11, 14, 16	0
1	E	211/214 (98%)	-0.08	1 (0%) 87 85	7, 11, 13, 15	0
1	G	211/214 (98%)	-0.45	1 (0%) 87 85	4, 10, 14, 17	0
1	J	211/214 (98%)	0.03	12 (5%) 29 23	6, 10, 13, 18	0
1	L	211/214 (98%)	0.86	34 (16%) 4 3	5, 11, 14, 16	0
1	M	211/214 (98%)	1.19	63 (29%) 1 0	7, 10, 13, 16	0
1	O	211/214 (98%)	0.02	16 (7%) 20 15	6, 11, 14, 17	0
1	Q	211/214 (98%)	0.31	6 (2%) 55 48	6, 11, 13, 15	0
1	S	211/214 (98%)	0.09	5 (2%) 59 53	7, 11, 13, 15	0
1	U	211/214 (98%)	0.21	13 (6%) 26 20	7, 11, 14, 15	0
1	W	211/214 (98%)	0.53	13 (6%) 26 20	7, 10, 13, 14	0
2	B	218/227 (96%)	-0.39	2 (0%) 81 78	6, 10, 14, 20	0
2	D	218/227 (96%)	-0.23	6 (2%) 55 48	5, 10, 14, 19	0
2	F	218/227 (96%)	-0.09	5 (2%) 61 54	6, 10, 14, 19	0
2	H	218/227 (96%)	0.23	26 (11%) 9 7	5, 10, 14, 20	0
2	I	218/227 (96%)	-0.54	3 (1%) 73 69	6, 10, 14, 22	0
2	K	218/227 (96%)	-0.43	3 (1%) 73 69	5, 10, 15, 22	0
2	N	218/227 (96%)	1.05	70 (32%) 1 0	4, 11, 13, 22	0
2	P	218/227 (96%)	-0.64	1 (0%) 87 85	5, 10, 14, 22	0
2	R	218/227 (96%)	-0.27	2 (0%) 81 78	6, 10, 13, 23	0
2	T	218/227 (96%)	-0.35	1 (0%) 87 85	6, 10, 14, 21	0
2	V	218/227 (96%)	-0.41	1 (0%) 87 85	3, 10, 14, 22	0
2	X	218/227 (96%)	0.12	3 (1%) 73 69	6, 10, 13, 22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5148/5292 (97%)	0.03	293 (5%) 29 23	3, 10, 14, 23	0

The worst 5 of 293 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	122	SER	14.3
2	N	179	SER	7.1
2	N	123	THR	6.9
1	M	157	GLY	6.9
1	J	168	SER	6.5

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.