



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 08:23 AM EDT

PDB ID : 2FJF  
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](mailto:validation@mail.wwpdb.org)

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<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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

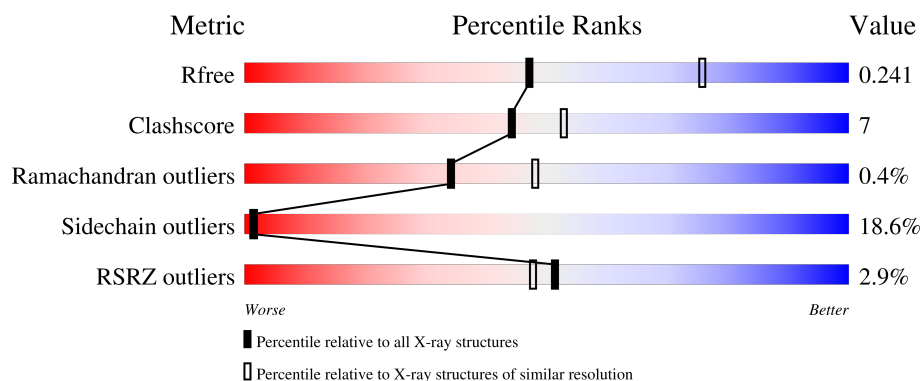
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>6%</div> </div> </div>
1	C	214	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>..</div> </div> </div>
1	E	214	<div> <div></div> <div> <div></div> <div>73%</div> <div>21%</div> <div>..</div> </div> </div>
1	G	214	<div> <div></div> <div> <div></div> <div>75%</div> <div>18%</div> <div>5%</div> </div> </div>
1	J	214	<div> <div></div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	L	214	
1	M	214	
1	O	214	
1	Q	214	
1	S	214	
1	U	214	
1	W	214	
2	B	227	
2	D	227	
2	F	227	
2	H	227	
2	I	227	
2	K	227	
2	N	227	
2	P	227	
2	R	227	
2	T	227	
2	V	227	
2	X	227	

## 2 Entry composition

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
1	L	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	A	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	C	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	E	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	G	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	J	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	M	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	O	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	Q	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	S	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	U	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			
1	W	211	Total	C	N	O	S	0	0	0
			1617	1014	268	330	5			

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

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

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

- Molecule 3 is water.

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

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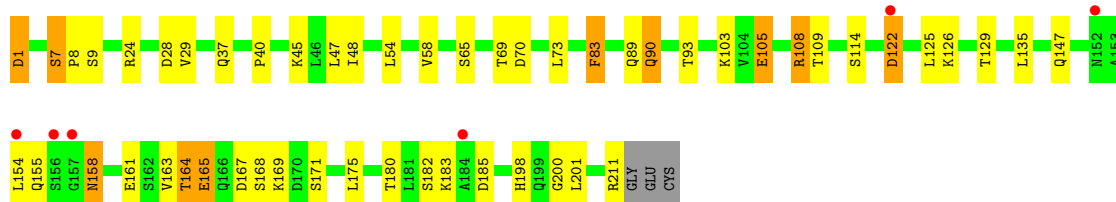
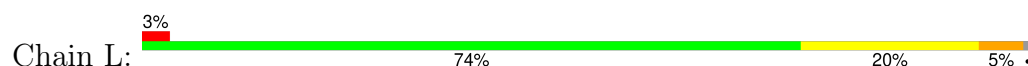
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	52	Total 52	O 52	0	0
3	J	35	Total 35	O 35	0	0
3	K	53	Total 53	O 53	0	0
3	M	17	Total 17	O 17	0	0
3	N	24	Total 24	O 24	0	0
3	O	31	Total 31	O 31	0	0
3	P	52	Total 52	O 52	0	0
3	Q	15	Total 15	O 15	0	0
3	R	21	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

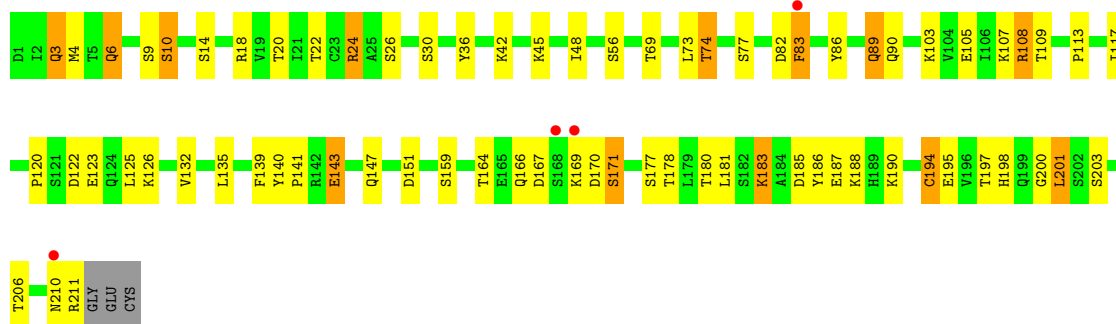
### 3 Residue-property plots [i](#)

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.

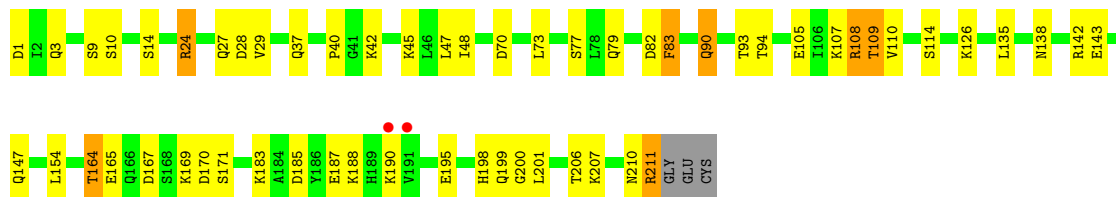
- Molecule 1: Light Chain of a VEGF binding Antibody



- Molecule 1: Light Chain of a VEGF binding Antibody

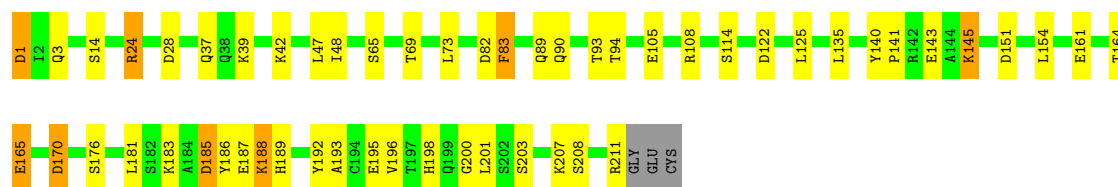


- Molecule 1: Light Chain of a VEGF binding Antibody



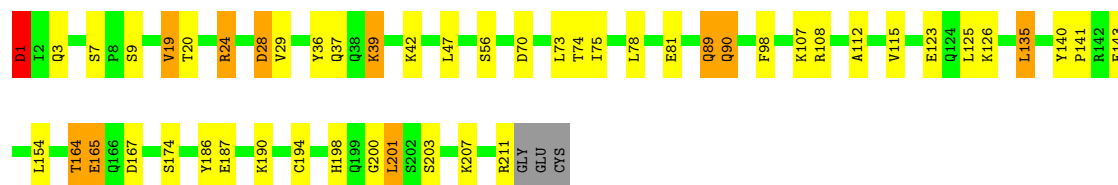
- Molecule 1: Light Chain of a VEGF binding Antibody

Chain E:  73% 21% . .



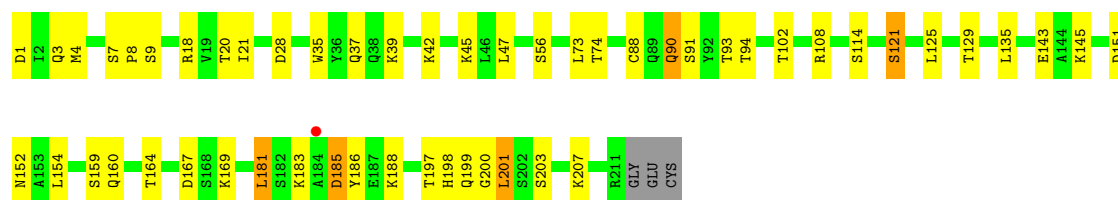
- Molecule 1: Light Chain of a VEGF binding Antibody

Chain G:  75% 18% 5% .



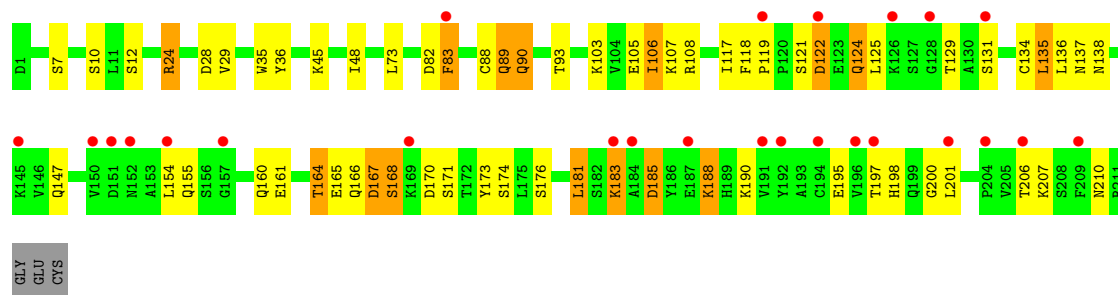
- Molecule 1: Light Chain of a VEGF binding Antibody

Chain J:  74% 22% . .



- Molecule 1: Light Chain of a VEGF binding Antibody

Chain M:  12% 69% 23% 7% .



- Molecule 1: Light Chain of a VEGF binding Antibody

Chain O:  69% 25% . .







- 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



GLY  
GLU  
CYS

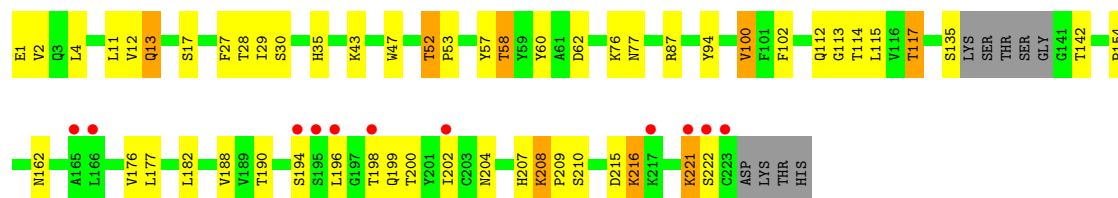
- Molecule 1: Light Chain of a VEGF binding Antibody



CYS

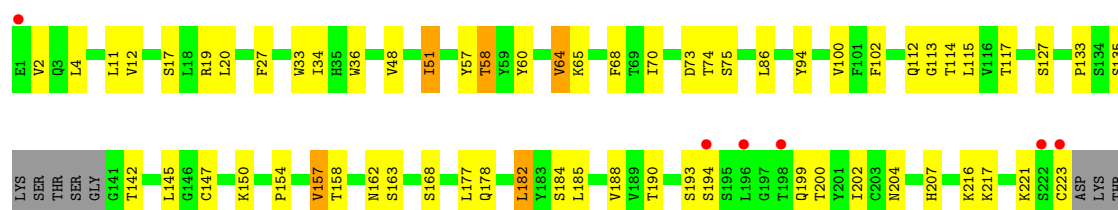
- Molecule 2: Heavy Chain of a VEGF binding Antibody

Chain H: 5% 72% 21% . .



- Molecule 2: Heavy Chain of a VEGF binding Antibody

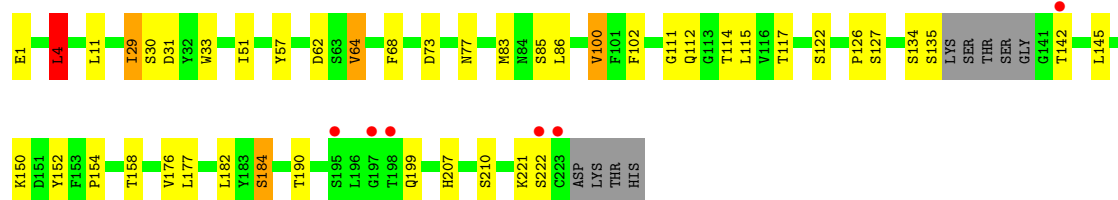
Chain B: 3% 68% 26% . .



HIS

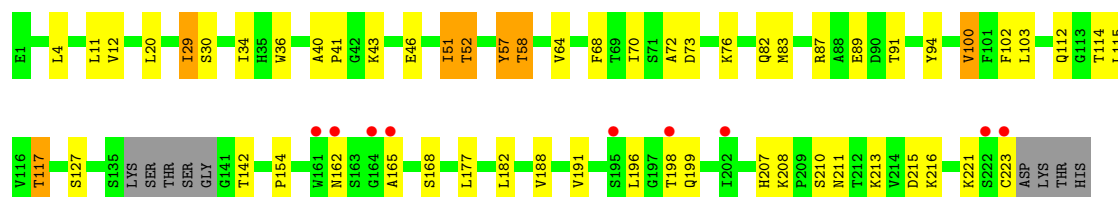
- Molecule 2: Heavy Chain of a VEGF binding Antibody

Chain D: 3% 76% 18% . .

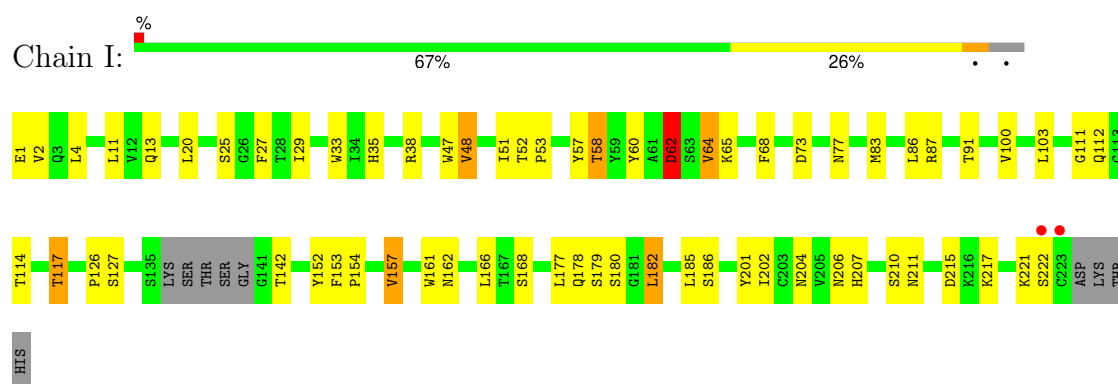


- Molecule 2: Heavy Chain of a VEGF binding Antibody

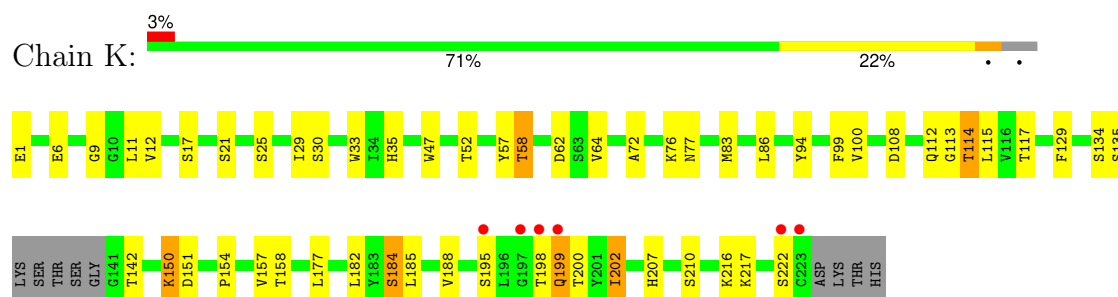
Chain F: 4% 71% 22% . .



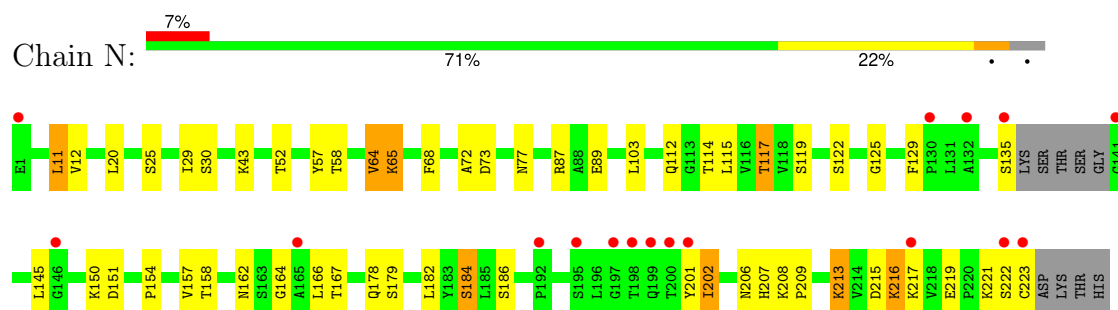
- Molecule 2: Heavy Chain of a VEGF binding Antibody



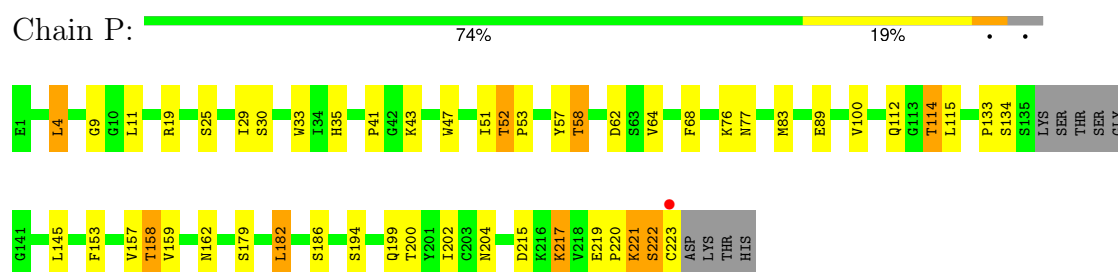
• Molecule 2: Heavy Chain of a VEGF binding Antibody



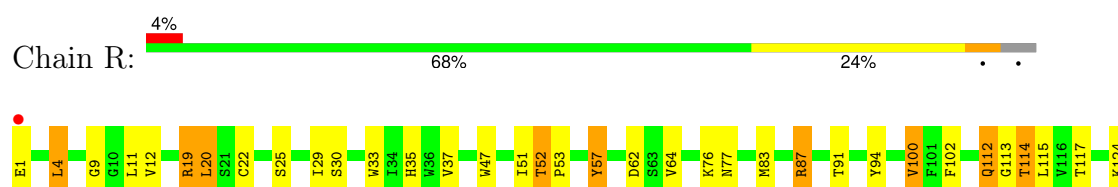
• Molecule 2: Heavy Chain of a VEGF binding Antibody

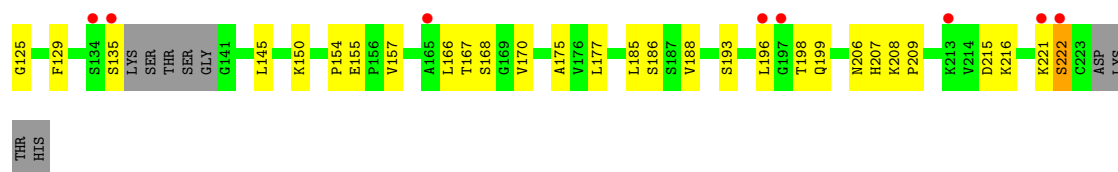


• Molecule 2: Heavy Chain of a VEGF binding Antibody

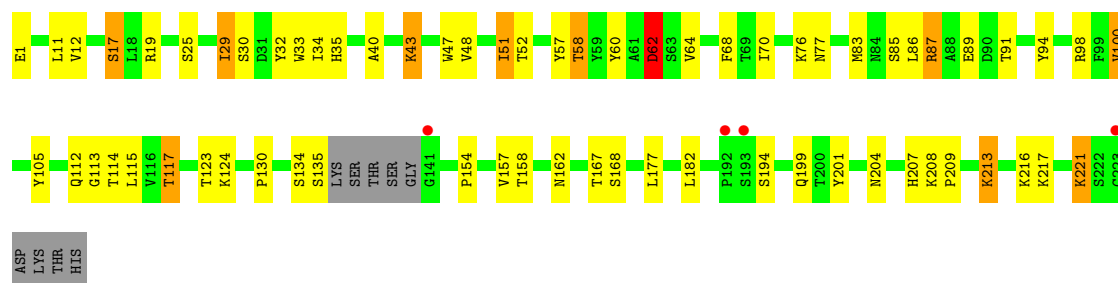


• Molecule 2: Heavy Chain of a VEGF binding Antibody

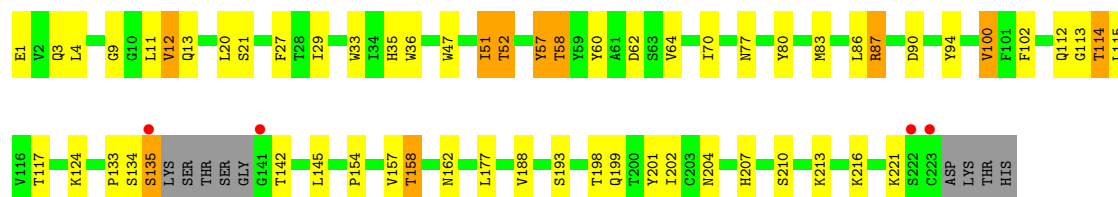




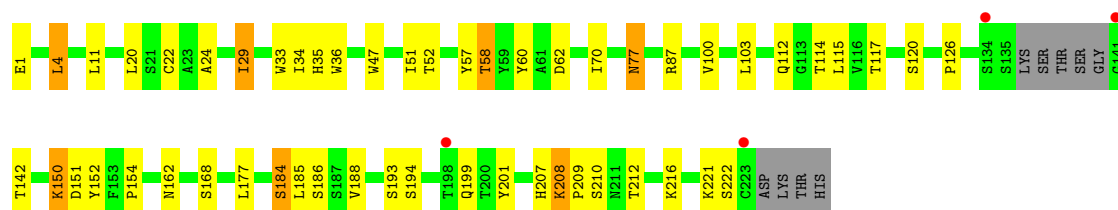
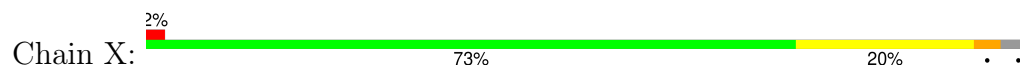
- Molecule 2: Heavy Chain of a VEGF binding Antibody



- 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, $\alpha$ , $\beta$ , $\gamma$	274.92Å 192.23Å 154.11Å 90.00° 117.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 29.96 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.65) 99.8 (29.96-2.65)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.64Å)	Xtriage
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 (2.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	39642	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.41	0/1653	0.72	4/2248 (0.2%)
1	C	0.39	0/1653	0.75	7/2248 (0.3%)
1	E	0.39	0/1653	0.75	7/2248 (0.3%)
1	G	0.44	0/1653	0.75	3/2248 (0.1%)
1	J	0.44	0/1653	0.76	3/2248 (0.1%)
1	L	0.42	0/1653	0.72	5/2248 (0.2%)
1	M	0.42	0/1653	0.75	6/2248 (0.3%)
1	O	0.41	0/1653	0.75	5/2248 (0.2%)
1	Q	0.38	0/1653	0.72	6/2248 (0.3%)
1	S	0.37	0/1653	0.70	3/2248 (0.1%)
1	U	0.39	0/1653	0.72	5/2248 (0.2%)
1	W	0.39	0/1653	0.72	5/2248 (0.2%)
2	B	0.44	0/1677	0.73	0/2290
2	D	0.42	0/1677	0.74	4/2290 (0.2%)
2	F	0.42	0/1677	0.76	2/2290 (0.1%)
2	H	0.44	0/1677	0.76	2/2290 (0.1%)
2	I	0.48	0/1677	0.76	3/2290 (0.1%)
2	K	0.43	0/1677	0.73	3/2290 (0.1%)
2	N	0.42	0/1677	0.73	3/2290 (0.1%)
2	P	0.45	0/1677	0.75	3/2290 (0.1%)
2	R	0.42	0/1677	0.73	2/2290 (0.1%)
2	T	0.43	0/1677	0.73	1/2290 (0.0%)
2	V	0.42	0/1677	0.74	2/2290 (0.1%)
2	X	0.40	0/1677	0.71	2/2290 (0.1%)
All	All	0.42	0/39960	0.74	86/54456 (0.2%)

There are no bond length outliers.

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	28	ASP	CB-CG-OD2	7.48	125.03	118.30
2	I	73	ASP	CB-CG-OD2	7.28	124.85	118.30
2	H	62	ASP	CB-CG-OD2	7.21	124.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	17	ASP	CB-CG-OD2	6.90	124.51	118.30
2	P	62	ASP	CB-CG-OD2	6.63	124.27	118.30

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	1617	0	1573	25	0
1	C	1617	0	1573	13	0
1	E	1617	0	1573	14	0
1	G	1617	0	1573	23	0
1	J	1617	0	1573	14	0
1	L	1617	0	1573	15	0
1	M	1617	0	1573	21	0
1	O	1617	0	1573	22	0
1	Q	1617	0	1573	19	0
1	S	1617	0	1573	26	0
1	U	1617	0	1573	26	0
1	W	1617	0	1573	16	0
2	B	1633	0	1592	17	0
2	D	1633	0	1592	12	0
2	F	1633	0	1592	21	0
2	H	1633	0	1592	26	0
2	I	1633	0	1592	30	0
2	K	1633	0	1592	23	0
2	N	1633	0	1592	28	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	33	0
2	X	1633	0	1592	22	0
3	A	17	0	0	1	0
3	B	28	0	0	0	0
3	C	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	508	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 508 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 ⓘ

### 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	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
1	C	209/214 (98%)	203 (97%)	4 (2%)	2 (1%)	15	23
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%)	29	43
1	M	209/214 (98%)	197 (94%)	9 (4%)	3 (1%)	11	16
1	O	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
1	Q	209/214 (98%)	199 (95%)	8 (4%)	2 (1%)	15	23
1	S	209/214 (98%)	201 (96%)	6 (3%)	2 (1%)	15	23
1	U	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
1	W	209/214 (98%)	197 (94%)	11 (5%)	1 (0%)	29	43
2	B	214/227 (94%)	206 (96%)	8 (4%)	0	100	100
2	D	214/227 (94%)	203 (95%)	10 (5%)	1 (0%)	29	43
2	F	214/227 (94%)	203 (95%)	9 (4%)	2 (1%)	17	26
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%)	17	26
2	R	214/227 (94%)	203 (95%)	9 (4%)	2 (1%)	17	26
2	T	214/227 (94%)	204 (95%)	8 (4%)	2 (1%)	17	26
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%)	34	48

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 ⓘ

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%)	145 (78%)	41 (22%)	1	0
1	C	186/188 (99%)	148 (80%)	38 (20%)	1	1
1	E	186/188 (99%)	155 (83%)	31 (17%)	2	2
1	G	186/188 (99%)	160 (86%)	26 (14%)	3	4
1	J	186/188 (99%)	153 (82%)	33 (18%)	2	1
1	L	186/188 (99%)	155 (83%)	31 (17%)	2	2
1	M	186/188 (99%)	147 (79%)	39 (21%)	1	1
1	O	186/188 (99%)	151 (81%)	35 (19%)	1	1
1	Q	186/188 (99%)	150 (81%)	36 (19%)	1	1
1	S	186/188 (99%)	148 (80%)	38 (20%)	1	1
1	U	186/188 (99%)	144 (77%)	42 (23%)	1	0
1	W	186/188 (99%)	141 (76%)	45 (24%)	0	0
2	B	179/187 (96%)	138 (77%)	41 (23%)	1	0
2	D	179/187 (96%)	153 (86%)	26 (14%)	3	3
2	F	179/187 (96%)	147 (82%)	32 (18%)	2	1
2	H	179/187 (96%)	147 (82%)	32 (18%)	2	1
2	I	179/187 (96%)	150 (84%)	29 (16%)	2	2
2	K	179/187 (96%)	151 (84%)	28 (16%)	2	2
2	N	179/187 (96%)	145 (81%)	34 (19%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	179/187 (96%)	154 (86%)	25 (14%)	3	4
2	R	179/187 (96%)	144 (80%)	35 (20%)	1	1
2	T	179/187 (96%)	141 (79%)	38 (21%)	1	1
2	V	179/187 (96%)	150 (84%)	29 (16%)	2	2
2	X	179/187 (96%)	147 (82%)	32 (18%)	2	1
All	All	4380/4500 (97%)	3564 (81%)	816 (19%)	1	1

5 of 816 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	11	LEU
2	R	135	SER
2	X	117	THR
1	O	108	ARG
1	O	9	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	210	ASN
2	R	178	GLN
1	W	198	HIS
2	P	35	HIS
1	Q	137	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	211/214 (98%)	-0.20	4 (1%) 66 63	5, 11, 14, 17	0
1	C	211/214 (98%)	-0.26	2 (0%) 84 83	5, 11, 14, 16	0
1	E	211/214 (98%)	-0.25	0 100 100	7, 11, 13, 15	0
1	G	211/214 (98%)	-0.57	0 100 100	4, 10, 14, 17	0
1	J	211/214 (98%)	-0.41	1 (0%) 91 91	6, 10, 13, 18	0
1	L	211/214 (98%)	0.07	6 (2%) 53 49	5, 11, 14, 16	0
1	M	211/214 (98%)	0.28	25 (11%) 4 3	7, 10, 13, 16	0
1	O	211/214 (98%)	-0.37	2 (0%) 84 83	6, 11, 14, 17	0
1	Q	211/214 (98%)	0.11	10 (4%) 31 28	6, 11, 13, 15	0
1	S	211/214 (98%)	0.14	8 (3%) 40 36	7, 11, 13, 15	0
1	U	211/214 (98%)	-0.18	7 (3%) 46 43	7, 11, 14, 15	0
1	W	211/214 (98%)	0.07	4 (1%) 66 63	7, 10, 13, 14	0
2	B	218/227 (96%)	-0.27	6 (2%) 53 49	6, 10, 14, 20	0
2	D	218/227 (96%)	-0.37	6 (2%) 53 49	5, 10, 14, 19	0
2	F	218/227 (96%)	-0.17	9 (4%) 37 33	6, 10, 14, 19	0
2	H	218/227 (96%)	-0.22	11 (5%) 28 25	5, 10, 14, 20	0
2	I	218/227 (96%)	-0.48	2 (0%) 84 83	6, 10, 14, 22	0
2	K	218/227 (96%)	-0.17	6 (2%) 53 49	5, 10, 15, 22	0
2	N	218/227 (96%)	-0.05	17 (7%) 13 10	4, 11, 13, 22	0
2	P	218/227 (96%)	-0.45	1 (0%) 91 91	5, 10, 14, 22	0
2	R	218/227 (96%)	-0.15	9 (4%) 37 33	6, 10, 13, 23	0
2	T	218/227 (96%)	-0.23	4 (1%) 68 65	6, 10, 14, 21	0
2	V	218/227 (96%)	-0.25	4 (1%) 68 65	3, 10, 14, 22	0
2	X	218/227 (96%)	-0.29	4 (1%) 68 65	6, 10, 13, 22	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5148/5292 (97%)	-0.20	148 (2%)	51	48	3, 10, 14, 23	0

The worst 5 of 148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	223	CYS	8.9
2	N	198	THR	7.9
2	H	223	CYS	6.4
2	F	223	CYS	6.3
2	B	223	CYS	6.3

## 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 monosaccharides 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.