



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:01 pm BST

PDB ID : 2RCS  
Title : IMMUNOGLOBULIN 48G7 GERMLINE FAB-AFFINITY MATURATION  
OF AN ESTEROLYTIC ANTIBODY  
Authors : Wedemayer, G.J.; Wang, L.H.; Patten, P.A.; Schultz, P.G.; Stevens, R.C.  
Deposited on : 1997-05-14  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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)	:	1.13
EDS	:	2.11
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)	:	2.11

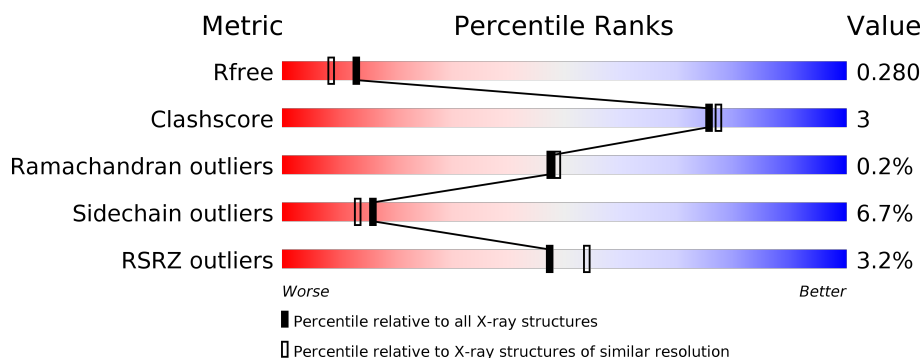
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	L	214	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> <div></div> </div>
2	H	217	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>9%</div> </div> <div></div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4035 atoms, of which 765 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 IMMUNOGLOBULIN 48G7 GERMLINE FAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	214	Total	C	H	N	O	S	0	0	0
			2041	1025	393	277	340	6			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	15	LEU	VAL	CONFLICT	GB 4768677
L	17	GLU	ASP	CONFLICT	GB 4768677
L	20	SER	THR	CONFLICT	GB 4768677
L	21	LEU	ILE	CONFLICT	GB 4768677
L	24	ARG	GLN	CONFLICT	GB 4768677
L	28	GLU	ASP	CONFLICT	GB 4768677
L	30	SER	ASN	CONFLICT	GB 4768677
L	31	GLY	ASN	CONFLICT	GB 4768677
L	34	SER	ASN	CONFLICT	GB 4768677
L	36	LEU	TYR	CONFLICT	GB 4768677
L	41	ASP	GLY	CONFLICT	GB 4768677
L	42	GLY	LYS	CONFLICT	GB 4768677
L	44	ILE	PRO	CONFLICT	GB 4768677
L	46	ARG	LEU	CONFLICT	GB 4768677
L	50	ALA	GLY	CONFLICT	GB 4768677
L	53	THR	ASN	CONFLICT	GB 4768677
L	55	ASP	GLU	CONFLICT	GB 4768677
L	56	SER	THR	CONFLICT	GB 4768677
L	60	LYS	SER	CONFLICT	GB 4768677
L	66	ARG	GLY	CONFLICT	GB 4768677
L	69	SER	THR	CONFLICT	GB 4768677
L	71	TYR	PHE	CONFLICT	GB 4768677
L	72	SER	ILE	CONFLICT	GB 4768677
L	73	LEU	PHE	CONFLICT	GB 4768677
L	79	GLU	GLN	CONFLICT	GB 4768677
L	80	SER	PRO	CONFLICT	GB 4768677
L	83	PHE	ILE	CONFLICT	GB 4768677

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Chain	Residue	Modelled	Actual	Comment	Reference
L	85	ASP	THR	CONFLICT	GB 4768677
L	89	LEU	GLN	CONFLICT	GB 4768677
L	92	ALA	ASP	CONFLICT	GB 4768677
L	93	SER	ASN	CONFLICT	GB 4768677
L	94	TYR	LEU	CONFLICT	GB 4768677
L	96	ARG	LEU	CONFLICT	GB 4768677
L	177	SER	ASN	CONFLICT	GB 4768677

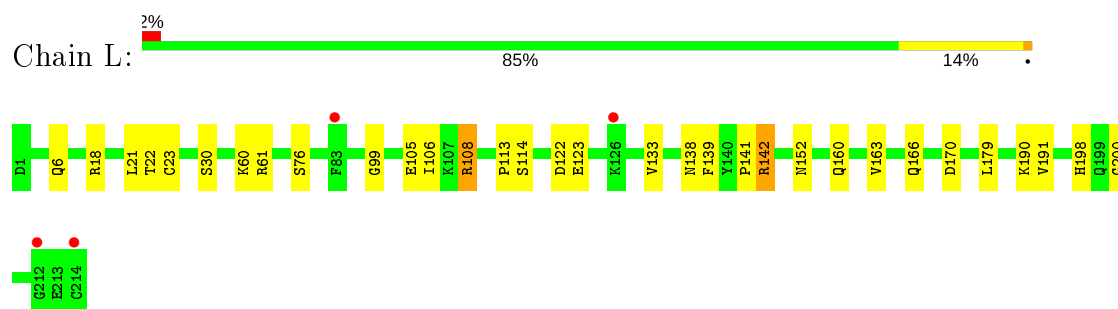
- Molecule 2 is a protein called IMMUNOGLOBULIN 48G7 GERMLINE FAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	217	Total	C	H	N	O	S	372	0	0
			1994	1022	372	267	327	6			

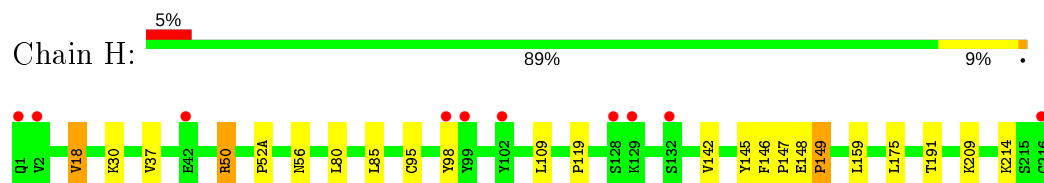
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: IMMUNOGLOBULIN 48G7 GERMLINE FAB



- Molecule 2: IMMUNOGLOBULIN 48G7 GERMLINE FAB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.16Å 75.55Å 86.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-2.10) 95.3 (19.85-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.06 (at 2.09Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.210 , 0.259 0.237 , 0.280	Depositor DCC
$R_{free}$ test set	2436 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.37% 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	L	0.42	0/1680	0.70	0/2273
2	H	0.44	0/1661	0.72	0/2265
All	All	0.43	0/3341	0.71	0/4538

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	L	1648	393	1599	12	1
2	H	1622	372	1590	8	0
All	All	3270	765	3189	20	1

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 3.

All (20) 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:H:50:ARG:HH22	2:H:56:ASN:HD22	1.36	0.73
2:H:18:VAL:HG22	2:H:85:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:VAL:CG2	2:H:85:LEU:HD11	2.28	0.63
1:L:198:HIS:CD2	1:L:200:GLY:H	2.22	0.58
2:H:50:ARG:NH2	2:H:56:ASN:HD22	2.04	0.56
1:L:61:ARG:HB2	1:L:76:SER:O	2.07	0.55
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.91	0.52
1:L:105:GLU:HB2	1:L:166:GLN:HE22	1.75	0.51
1:L:190:LYS:HG3	1:L:191:VAL:H	1.78	0.48
2:H:148:GLU:HG3	2:H:149:PRO:HA	1.97	0.46
1:L:141:PRO:O	1:L:198:HIS:HE1	1.99	0.46
1:L:106:ILE:H	1:L:166:GLN:HE22	1.64	0.45
1:L:190:LYS:HG3	1:L:191:VAL:N	2.31	0.45
1:L:108:ARG:HD2	1:L:170:ASP:O	2.17	0.45
1:L:6:GLN:HE21	1:L:99:GLY:HA3	1.83	0.43
1:L:142:ARG:HH11	1:L:163:VAL:HG11	1.85	0.42
2:H:146:PHE:HA	2:H:147:PRO:HA	1.82	0.42
1:L:22:THR:HG22	1:L:23:CYS:N	2.35	0.41
1:L:113:PRO:HB3	1:L:139:PHE:HB3	2.03	0.41
2:H:30:LYS:HA	2:H:52(A):PRO:HB2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:LYS:HZ3	1:L:114:SER:HG[4_565]	1.30	0.30

## 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	L	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	29	26
2	H	215/217 (99%)	205 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	427/431 (99%)	410 (96%)	16 (4%)	1 (0%)	47	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	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	L	188/188 (100%)	177 (94%)	11 (6%)	19	17
2	H	184/184 (100%)	170 (92%)	14 (8%)	13	10
All	All	372/372 (100%)	347 (93%)	25 (7%)	16	13

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	18	ARG
1	L	21	LEU
1	L	30	SER
1	L	108	ARG
1	L	122	ASP
1	L	123	GLU
1	L	133	VAL
1	L	142	ARG
1	L	152	ASN
1	L	160	GLN
1	L	179	LEU
2	H	18	VAL
2	H	37	VAL
2	H	50	ARG
2	H	80	LEU
2	H	95	CYS
2	H	98	TYR

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Mol	Chain	Res	Type
2	H	109	LEU
2	H	142	VAL
2	H	149	PRO
2	H	159	LEU
2	H	175	LEU
2	H	191	THR
2	H	209	LYS
2	H	214	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	166	GLN
1	L	198	HIS
2	H	56	ASN
2	H	171	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 carbohydrates 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 ⓘ

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, 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	L	214/214 (100%)	0.16	4 (1%) 66 71	7, 19, 36, 68	0
2	H	217/217 (100%)	0.22	10 (4%) 32 38	7, 18, 41, 70	0
All	All	431/431 (100%)	0.19	14 (3%) 47 54	7, 19, 37, 70	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1	GLN	7.9
2	H	216	CYS	7.6
2	H	99	TYR	6.2
1	L	83	PHE	5.8
2	H	2	VAL	4.5
2	H	128	SER	3.8
1	L	212	GLY	3.7
1	L	214	CYS	3.6
2	H	42	GLU	3.4
2	H	98	TYR	3.3
1	L	126	LYS	2.7
2	H	129	LYS	2.4
2	H	102	TYR	2.4
2	H	132	SER	2.2

### 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 carbohydrates 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.