



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:29 am GMT

PDB ID : 2GK0  
Title : Structure of Catalytic Elimination Antibody 13G5 from a twinned crystal in space group C2  
Authors : Debler, E.W.; Wilson, I.A.  
Deposited on : 2006-03-31  
Resolution : 2.45 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)

A user guide is available at

<http://wwpdb.org/validation/2016/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) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

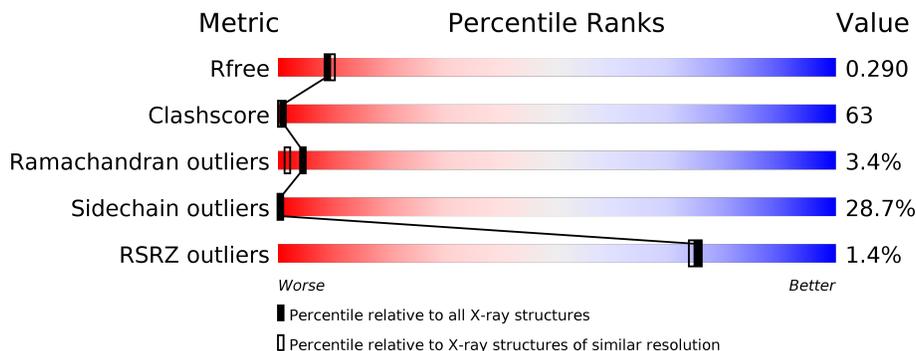
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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. 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	217	<p>2% 18% 62% 20%</p>
1	L	217	<p>2% 26% 51% 23%</p>
2	B	221	<p>2% 19% 57% 21% .</p>
2	H	221	<p>2% 25% 56% 19%</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6692 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 Catalytic elimination antibody 13G5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	217	1683	1053	286	338	6	0	0	0
1	A	217	1683	1053	286	338	6	0	0	0

- Molecule 2 is a protein called Catalytic elimination antibody 13G5 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	221	1649	1043	270	327	9	0	0	0
2	B	216	1606	1012	265	320	9	0	0	0

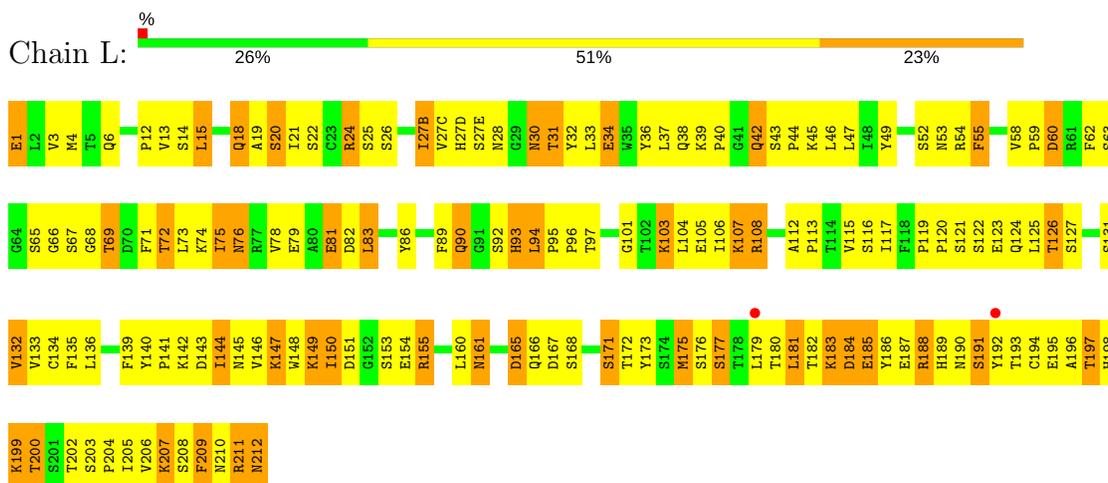
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	17	Total	O	0	0
			17	17		
3	H	24	Total	O	0	0
			24	24		
3	L	18	Total	O	0	0
			18	18		

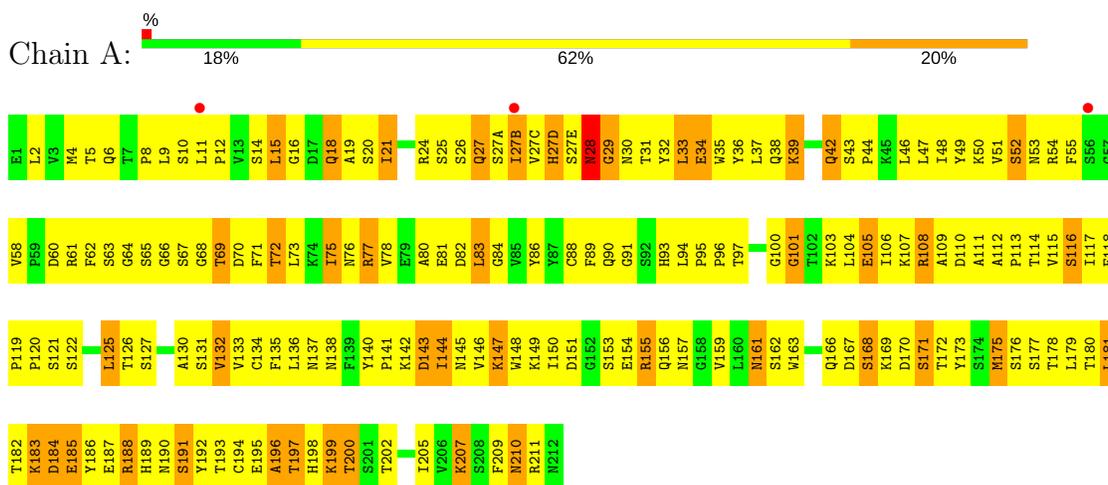
### 3 Residue-property plots [i](#)

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.

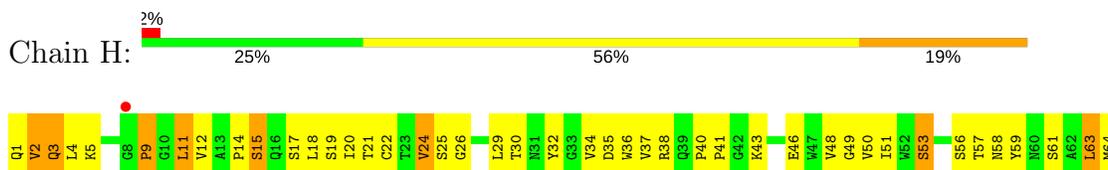
- Molecule 1: Catalytic elimination antibody 13G5 light chain

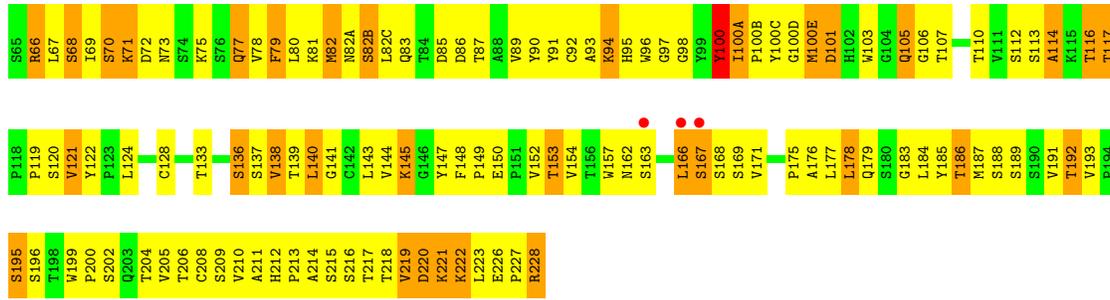


- Molecule 1: Catalytic elimination antibody 13G5 light chain

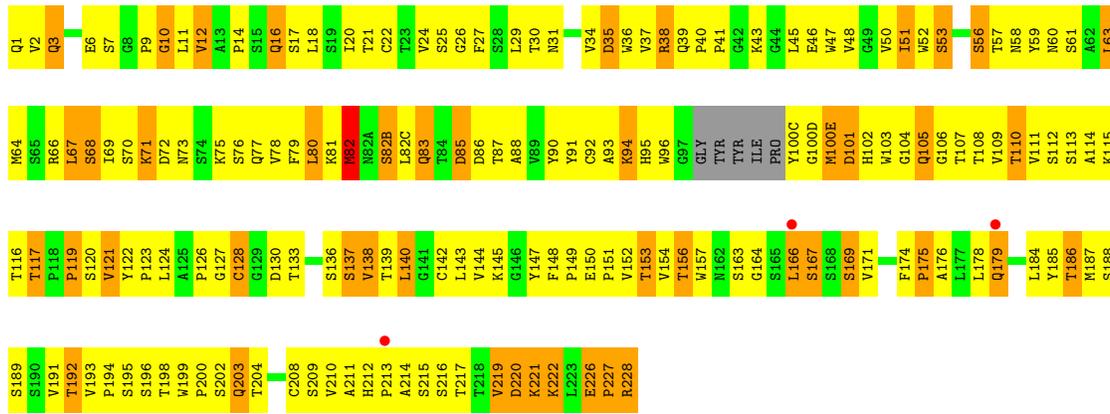


- Molecule 2: Catalytic elimination antibody 13G5 heavy chain





● Molecule 2: Catalytic elimination antibody 13G5 heavy chain



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.88Å 84.62Å 150.07Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	10.00 – 2.45 49.92 – 2.44	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.45) 97.5 (49.92-2.44)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.45Å)	Xtrriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.191 , 0.255 0.227 , 0.290	Depositor DCC
$R_{free}$ test set	1557 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtrriage
Anisotropy	0.377	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 101.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.457 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6692	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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 [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	0.39	0/1722	0.82	1/2337 (0.0%)
1	L	0.40	1/1722 (0.1%)	0.80	0/2337
2	B	0.35	0/1649	0.86	1/2257 (0.0%)
2	H	0.41	2/1696 (0.1%)	0.84	2/2324 (0.1%)
All	All	0.39	3/6789 (0.0%)	0.83	4/9255 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	VAL	CB-CG1	5.33	1.64	1.52
1	L	212	ASN	CG-OD1	5.32	1.35	1.24
2	H	9	PRO	N-CD	5.18	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	100(E)	MET	C-N-CA	7.25	139.83	121.70
2	H	100(E)	MET	C-N-CA	6.79	138.69	121.70
1	A	28	ASN	C-N-CA	5.10	133.00	122.30
2	H	100	TYR	C-N-CA	5.00	134.20	121.70

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	1683	0	1628	242	0
1	L	1683	0	1628	196	0
2	B	1606	0	1564	225	1
2	H	1649	0	1604	191	0
3	A	12	0	0	0	0
3	B	17	0	0	0	0
3	H	24	0	0	0	0
3	L	18	0	0	0	0
All	All	6692	0	6424	819	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 63.

The worst 5 of 819 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)
1:A:94:LEU:HD23	1:A:96:PRO:HD3	1.40	1.01
1:L:115:VAL:HG22	1:L:136:LEU:HG	1.46	0.98
1:A:19:ALA:HB3	1:A:75:ILE:HD12	1.45	0.97
1:A:190:ASN:HA	1:A:211:ARG:HB2	1.47	0.96
2:B:12:VAL:HG23	2:B:111:VAL:HG22	1.46	0.96

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)
2:B:53:SER:O	2:B:56:SER:OG[2_556]	2.05	0.15

## 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	215/217 (99%)	182 (85%)	27 (13%)	6 (3%)	6	3
1	L	215/217 (99%)	186 (86%)	27 (13%)	2 (1%)	20	23
2	B	212/221 (96%)	178 (84%)	24 (11%)	10 (5%)	3	1
2	H	219/221 (99%)	180 (82%)	28 (13%)	11 (5%)	2	1
All	All	861/876 (98%)	726 (84%)	106 (12%)	29 (3%)	4	2

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	68	SER
1	A	101	GLY
2	B	167	SER
1	L	184	ASP
2	H	82	MET

### 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	194/194 (100%)	135 (70%)	59 (30%)	0	0
1	L	194/194 (100%)	134 (69%)	60 (31%)	0	0
2	B	187/191 (98%)	135 (72%)	52 (28%)	0	0
2	H	191/191 (100%)	142 (74%)	49 (26%)	0	0
All	All	766/770 (100%)	546 (71%)	220 (29%)	0	0

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	192	THR
1	A	34	GLU
2	B	156	THR
2	H	202	SER
1	A	14	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	172	HIS
1	A	27	GLN
1	A	189	HIS
2	H	102	HIS
1	A	166	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 [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, 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	217/217 (100%)	-0.14	3 (1%) 75 74	21, 45, 62, 74	0
1	L	217/217 (100%)	-0.29	2 (0%) 84 85	20, 45, 62, 74	0
2	B	216/221 (97%)	-0.20	3 (1%) 75 74	17, 45, 72, 91	0
2	H	221/221 (100%)	-0.23	4 (1%) 69 65	17, 45, 71, 91	0
All	All	871/876 (99%)	-0.22	12 (1%) 75 74	17, 45, 66, 91	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	166	LEU	6.3
2	H	167	SER	5.6
2	H	166	LEU	4.1
2	H	163	SER	3.3
1	A	56	SER	3.0

### 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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.