



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:28 AM GMT

PDB ID : 3ESV  
Title : Crystal structure of the engineered neutralizing antibody M18  
Authors : Monzingo, A.F.; Leysath, C.E.; Barnett, J.; Iverson, B.L.; Georgiou, G.; Robertus, J.D.  
Deposited on : 2008-10-06  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtrriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

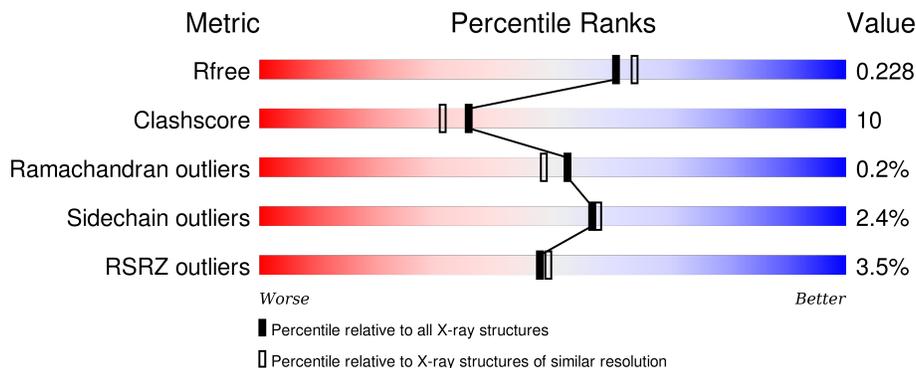
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	F	252	 4% 73% 16% • 9%
1	G	252	 3% 72% 17% • 10%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 3807 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 Antibody M18 light chain and antibody M18 heavy chain linked with a synthetic (GGGS)<sub>4</sub> linker.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	F	229	1762	1105	299	350	8	0	0	1
1	G	228	1759	1103	300	348	8	0	0	1

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	MET	-	EXPRESSION TAG	PDB 3ESV
F	-3	ALA	-	EXPRESSION TAG	PDB 3ESV
F	-2	ASP	-	EXPRESSION TAG	PDB 3ESV
F	-1	TYR	-	EXPRESSION TAG	PDB 3ESV
F	0	LYS	-	EXPRESSION TAG	PDB 3ESV
F	21	VAL	ILE	ENGINEERED	PDB 3ESV
F	46	PHE	LEU	ENGINEERED	PDB 3ESV
F	56	PRO	SER	ENGINEERED	PDB 3ESV
F	76	ASN	SER	ENGINEERED	PDB 3ESV
F	78	LEU	GLN	ENGINEERED	PDB 3ESV
F	94	PRO	LEU	ENGINEERED	PDB 3ESV
F	109	GLY	-	LINKER	PDB 3ESV
F	110	GLY	-	LINKER	PDB 3ESV
F	111	GLY	-	LINKER	PDB 3ESV
F	112	GLY	-	LINKER	PDB 3ESV
F	113	SER	-	LINKER	PDB 3ESV
F	114	GLY	-	LINKER	PDB 3ESV
F	115	GLY	-	LINKER	PDB 3ESV
F	116	GLY	-	LINKER	PDB 3ESV
F	117	GLY	-	LINKER	PDB 3ESV
F	118	SER	-	LINKER	PDB 3ESV
F	119	GLY	-	LINKER	PDB 3ESV
F	120	GLY	-	LINKER	PDB 3ESV
F	121	GLY	-	LINKER	PDB 3ESV

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	122	GLY	-	LINKER	PDB 3ESV
F	123	SER	-	LINKER	PDB 3ESV
F	124	GLY	-	LINKER	PDB 3ESV
F	125	GLY	-	LINKER	PDB 3ESV
F	126	GLY	-	LINKER	PDB 3ESV
F	127	GLY	-	LINKER	PDB 3ESV
F	128	SER	-	LINKER	PDB 3ESV
F	1030	ASN	SER	ENGINEERED	PDB 3ESV
F	1057	SER	THR	ENGINEERED	PDB 3ESV
F	1064	GLU	LYS	ENGINEERED	PDB 3ESV
F	1068	ILE	THR	ENGINEERED	PDB 3ESV
G	-4	MET	-	EXPRESSION TAG	PDB 3ESV
G	-3	ALA	-	EXPRESSION TAG	PDB 3ESV
G	-2	ASP	-	EXPRESSION TAG	PDB 3ESV
G	-1	TYR	-	EXPRESSION TAG	PDB 3ESV
G	0	LYS	-	EXPRESSION TAG	PDB 3ESV
G	21	VAL	ILE	ENGINEERED	PDB 3ESV
G	46	PHE	LEU	ENGINEERED	PDB 3ESV
G	56	PRO	SER	ENGINEERED	PDB 3ESV
G	76	ASN	SER	ENGINEERED	PDB 3ESV
G	78	LEU	GLN	ENGINEERED	PDB 3ESV
G	94	PRO	LEU	ENGINEERED	PDB 3ESV
G	109	GLY	-	LINKER	PDB 3ESV
G	110	GLY	-	LINKER	PDB 3ESV
G	111	GLY	-	LINKER	PDB 3ESV
G	112	GLY	-	LINKER	PDB 3ESV
G	113	SER	-	LINKER	PDB 3ESV
G	114	GLY	-	LINKER	PDB 3ESV
G	115	GLY	-	LINKER	PDB 3ESV
G	116	GLY	-	LINKER	PDB 3ESV
G	117	GLY	-	LINKER	PDB 3ESV
G	118	SER	-	LINKER	PDB 3ESV
G	119	GLY	-	LINKER	PDB 3ESV
G	120	GLY	-	LINKER	PDB 3ESV
G	121	GLY	-	LINKER	PDB 3ESV
G	122	GLY	-	LINKER	PDB 3ESV
G	123	SER	-	LINKER	PDB 3ESV
G	124	GLY	-	LINKER	PDB 3ESV
G	125	GLY	-	LINKER	PDB 3ESV
G	126	GLY	-	LINKER	PDB 3ESV
G	127	GLY	-	LINKER	PDB 3ESV
G	128	SER	-	LINKER	PDB 3ESV

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	1030	ASN	SER	ENGINEERED	PDB 3ESV
G	1057	SER	THR	ENGINEERED	PDB 3ESV
G	1064	GLU	LYS	ENGINEERED	PDB 3ESV
G	1068	ILE	THR	ENGINEERED	PDB 3ESV

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	147	Total O 147 147	0	0
2	G	139	Total O 139 139	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.07Å 54.21Å 61.95Å 71.80° 75.58° 71.25°	Depositor
Resolution (Å)	20.00 – 2.00 31.48 – 2.01	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-2.00) 85.0 (31.48-2.01)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.60 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.194 , 0.229 0.196 , 0.228	Depositor DCC
$R_{free}$ test set	1321 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.1	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 53.7	EDS
Estimated twinning fraction	0.088 for h,h-k,h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 26245 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	F	0.35	0/1802	0.65	0/2440
1	G	0.35	0/1799	0.64	0/2435
All	All	0.35	0/3601	0.64	0/4875

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 [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	F	1762	0	1681	28	0
1	G	1759	0	1684	39	0
2	F	147	0	0	0	0
2	G	139	0	0	0	0
All	All	3807	0	3365	67	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 10.

All (67) 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:G:55:GLN:HE22	1:G:1099:ARG:HH12	1.14	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1050:ARG:HE	1:F:1058:ASN:HD22	1.26	0.82
1:G:1012:VAL:HG11	1:G:1018:VAL:HG12	1.67	0.75
1:G:1083:THR:OG1	1:G:1085:VAL:HG12	1.88	0.73
1:G:1050:ARG:HE	1:G:1058:ASN:HD22	1.37	0.70
1:F:83:ILE:HD11	1:F:106:ILE:HD11	1.75	0.68
1:G:1027:TYR:H	1:G:1027:TYR:HD2	1.41	0.67
1:G:48:ILE:HG12	1:G:54:LEU:HD23	1.78	0.66
1:F:1030:ASN:HA	1:F:1052(A):PRO:HB2	1.79	0.65
1:F:41:ASP:OD1	1:F:43:THR:HG22	1.96	0.65
1:F:1093:ALA:HB3	1:F:1100(B):MET:HG2	1.79	0.64
1:G:14:SER:HA	1:G:107:LYS:HD2	1.79	0.64
1:G:11:LEU:HD21	1:G:19:VAL:HG13	1.80	0.63
1:F:1050:ARG:HE	1:F:1058:ASN:ND2	1.97	0.62
1:F:1006:GLN:HE21	1:F:1104:GLY:HA3	1.66	0.60
1:G:1012:VAL:HG11	1:G:1018:VAL:CG1	2.32	0.59
1:G:1006:GLN:HE21	1:G:1104:GLY:HA3	1.73	0.54
1:G:106:ILE:HG22	1:G:107:LYS:HD3	1.91	0.53
1:G:1039:GLN:O	1:G:1088:ALA:HB1	2.09	0.53
1:G:1030:ASN:HA	1:G:1052(A):PRO:HB2	1.91	0.52
1:G:55:GLN:NE2	1:G:1099:ARG:HH12	1.95	0.52
1:F:1039:GLN:HB2	1:F:1045:LEU:HD23	1.91	0.52
1:F:1094:ARG:HH11	1:F:1094:ARG:HG2	1.75	0.52
1:G:107:LYS:HE2	1:G:108:ARG:CZ	2.40	0.51
1:G:55:GLN:HE22	1:G:1099:ARG:NH1	1.95	0.51
1:F:6:GLN:HE22	1:F:87:PHE:HA	1.75	0.51
1:F:1040:ARG:HB2	1:F:1043:GLN:HB2	1.93	0.50
1:F:59:PRO:HG2	1:F:62:PHE:CD1	2.47	0.50
1:G:46:PHE:CZ	1:G:49:TYR:HB2	2.47	0.50
1:G:48:ILE:HD12	1:G:73:LEU:HD13	1.93	0.50
1:F:1006:GLN:NE2	1:F:1106:GLY:H	2.10	0.50
1:G:1006:GLN:NE2	1:G:1106:GLY:H	2.11	0.48
1:G:107:LYS:HG2	1:G:108:ARG:CG	2.43	0.48
1:G:46:PHE:HZ	1:G:49:TYR:HB2	1.77	0.48
1:F:1012:VAL:HG21	1:F:1082(C):LEU:HD23	1.95	0.48
1:G:6:GLN:HE21	1:G:99:GLY:HA3	1.79	0.47
1:F:80:GLN:O	1:F:83:ILE:HD13	2.14	0.47
1:G:6:GLN:HE22	1:G:87:PHE:HA	1.81	0.46
1:F:1:ASP:C	1:F:1:ASP:OD1	2.54	0.46
1:G:6:GLN:NE2	1:G:101:GLY:H	2.14	0.46
1:G:59:PRO:HG2	1:G:62:PHE:CD1	2.51	0.45
1:G:14:SER:CA	1:G:107:LYS:HD2	2.45	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1087:SER:O	1:G:1088:ALA:HB2	2.17	0.45
1:G:78:LEU:HD11	1:G:104:LEU:HD21	1.99	0.45
1:F:1002:VAL:HA	1:F:1102:TYR:OH	2.17	0.45
1:G:33:LEU:HD21	1:G:88:CYS:HB2	1.99	0.44
1:G:107:LYS:HD3	1:G:107:LYS:N	2.32	0.44
1:F:1038:LYS:HE2	1:F:1040:ARG:HD2	2.00	0.44
1:F:1029:PHE:CD2	1:F:1076:SER:HA	2.53	0.44
1:F:33:LEU:C	1:F:33:LEU:HD13	2.39	0.43
1:F:48:ILE:HG12	1:F:54:LEU:HD23	2.00	0.43
1:G:107:LYS:HG2	1:G:108:ARG:HG3	2.00	0.43
1:F:1093:ALA:CB	1:F:1100(B):MET:HG2	2.47	0.43
1:F:13:ALA:O	1:F:106:ILE:HA	2.19	0.43
1:G:1006:GLN:HE22	1:G:1091:PHE:HA	1.83	0.43
1:G:107:LYS:C	1:G:108:ARG:HG3	2.40	0.42
1:F:1020:ILE:HD11	1:F:1080:MET:HE2	2.01	0.42
1:G:1027:TYR:CD2	1:G:1027:TYR:N	2.84	0.42
1:F:30:ARG:O	1:F:31:ASN:HB2	2.20	0.42
1:G:1042:GLY:O	1:G:1043:GLN:HB2	2.19	0.42
1:G:37:GLN:HB2	1:G:47:LEU:HD11	2.02	0.41
1:G:107:LYS:O	1:G:108:ARG:HG3	2.19	0.41
1:G:33:LEU:HD13	1:G:33:LEU:C	2.41	0.41
1:F:48:ILE:HD12	1:F:73:LEU:HD13	2.01	0.41
1:G:1059:TYR:HB2	1:G:1064:GLU:HG2	2.03	0.41
1:F:6:GLN:HE21	1:F:99:GLY:HA3	1.85	0.41
1:F:6:GLN:NE2	1:F:101:GLY:H	2.20	0.40

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	F	225/252 (89%)	223 (99%)	2 (1%)	0	100 100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	224/252 (89%)	218 (97%)	5 (2%)	1 (0%)	39	33
All	All	449/504 (89%)	441 (98%)	7 (2%)	1 (0%)	52	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	108	ARG

### 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	F	191/201 (95%)	186 (97%)	5 (3%)	54	54
1	G	191/201 (95%)	187 (98%)	4 (2%)	61	63
All	All	382/402 (95%)	373 (98%)	9 (2%)	57	58

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	45	LYS
1	F	1013	LYS
1	F	1082(C)	LEU
1	F	1094	ARG
1	F	1100(B)	MET
1	G	107	LYS
1	G	108	ARG
1	G	1027	TYR
1	G	1094	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	6	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	1006	GLN
1	F	1058	ASN
1	G	6	GLN
1	G	31	ASN
1	G	55	GLN
1	G	76	ASN
1	G	80	GLN
1	G	1006	GLN
1	G	1058	ASN

### 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	F	229/252 (90%)	0.20	9 (3%) 43 45	8, 17, 26, 32	0
1	G	228/252 (90%)	0.15	7 (3%) 52 53	9, 16, 25, 36	0
All	All	457/504 (90%)	0.17	16 (3%) 48 49	8, 16, 26, 36	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	109	GLY	7.6
1	F	109	GLY	4.7
1	G	108	ARG	4.0
1	F	108	ARG	3.6
1	F	1027	TYR	3.2
1	F	1102	TYR	3.0
1	G	77	ASN	2.8
1	F	1113	SER	2.8
1	G	1027	TYR	2.7
1	G	1042	GLY	2.6
1	F	1002	VAL	2.6
1	G	1102	TYR	2.6
1	F	77	ASN	2.4
1	G	107	LYS	2.4
1	F	1098	LEU	2.3
1	F	1074	SER	2.0

### 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.