



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:04 AM GMT

PDB ID : 3H3B  
Title : Crystal structure of the single-chain Fv (scFv) fragment of an anti-ErbB2 antibody chA21 in complex with residues 1-192 of ErbB2 extracellular domain  
Authors : Zhou, H.; Liu, Y.; Niu, L.; Zhu, J.; Teng, M.  
Deposited on : 2009-04-16  
Resolution : 2.45 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.

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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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (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

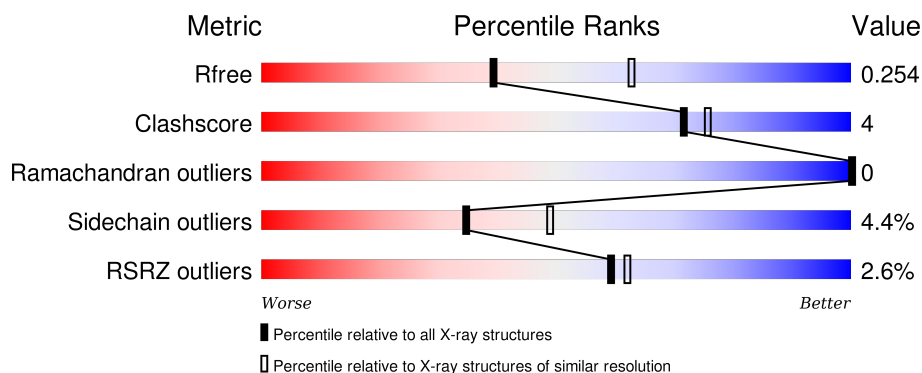
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	194	<div> <div>4%</div> <div>84%14%..</div> </div>
1	B	194	<div> <div>%</div> <div>85%11%..</div> </div>
2	C	259	<div> <div>2%</div> <div>82%8%10%</div> </div>
2	D	259	<div> <div>3%</div> <div>81%8%9%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6907 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 Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	15	2	0
			1522	945	277	289	11			
1	B	189	Total	C	N	O	S	27	2	0
			1499	933	273	282	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P04626
A	0	SER	-	EXPRESSION TAG	UNP P04626
B	-1	GLY	-	EXPRESSION TAG	UNP P04626
B	0	SER	-	EXPRESSION TAG	UNP P04626

- Molecule 2 is a protein called anti-ErbB2 antibody chA21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	234	Total	C	N	O	S	30	0	0
			1816	1152	295	362	7			
2	D	236	Total	C	N	O	S	24	0	0
			1831	1161	298	365	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	48	Total	O	0	0
			48	48		
3	C	54	Total	O	0	0
			54	54		
3	D	69	Total	O	0	0
			69	69		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.18 Å 87.20 Å 108.52 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.45 29.90 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.91-2.45) 99.2 (29.90-2.45)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 2.45 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.255 0.199 , 0.254	Depositor DCC
$R_{free}$ test set	1458 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 29109 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6907	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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

### 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	0.39	1/1556 (0.1%)	0.58	1/2114 (0.0%)
1	B	0.46	0/1530	0.60	0/2077
2	C	0.47	0/1861	0.51	0/2527
2	D	0.50	1/1876 (0.1%)	0.53	0/2546
All	All	0.46	2/6823 (0.0%)	0.55	1/9264 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	51	LYS	CD-CE	-5.48	1.37	1.51
1	A	188	GLU	CD-OE2	-5.17	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLU	OE1-CD-OE2	-5.42	116.80	123.30

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	1522	0	1516	14	0
1	B	1499	0	1500	14	0
2	C	1816	0	1746	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1831	0	1764	14	0
3	A	68	0	0	0	0
3	B	48	0	0	0	0
3	C	54	0	0	2	0
3	D	69	0	0	0	0
All	All	6907	0	6526	55	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 4.

All (55) 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:D:135:GLU:HA	2:D:135:GLU:OE2	1.62	0.98
1:B:87:GLU:OE1	1:B:87:GLU:HA	1.79	0.83
2:D:169:ASN:HD22	2:D:181:TRP:HE1	1.26	0.81
1:B:87:GLU:CA	1:B:87:GLU:OE1	2.30	0.78
2:C:169:ASN:HD22	2:C:181:TRP:HE1	1.31	0.77
1:B:144:THR:O	1:B:181:ARG:HD3	1.90	0.71
2:C:17:GLU:HG3	3:C:264:HOH:O	1.90	0.71
2:C:44:GLN:HE22	2:C:173:LYS:HE3	1.61	0.66
1:B:46:ASN:H	1:B:46:ASN:ND2	1.99	0.61
1:B:46:ASN:H	1:B:46:ASN:HD22	1.47	0.60
2:C:6:GLN:HE22	2:C:93:TYR:HA	1.68	0.59
1:A:152:HIS:HD2	1:A:154:ASN:H	1.52	0.58
2:C:96:GLN:HE22	2:C:99:ASN:H	1.50	0.58
1:A:143:ASP:OD1	1:A:166:ARG:NH2	2.37	0.57
2:D:44:GLN:HE22	2:D:173:LYS:HE3	1.71	0.55
1:B:146:LEU:HB2	1:B:181:ARG:CZ	2.37	0.54
2:D:91:VAL:HG22	2:D:109:ARG:HG3	1.90	0.53
2:D:19:VAL:HG22	2:D:81:ILE:HG12	1.90	0.53
1:A:143:ASP:CG	1:A:166:ARG:HH22	2.11	0.53
2:C:96:GLN:NE2	2:C:98:SER:H	2.07	0.53
2:C:6:GLN:NE2	2:C:94:CYS:H	2.07	0.52
1:A:143:ASP:N	1:A:143:ASP:OD1	2.44	0.49
2:C:44:GLN:NE2	2:C:173:LYS:HE3	2.26	0.48
2:D:96:GLN:NE2	2:D:98:SER:H	2.12	0.47
1:B:107:VAL:HB	1:B:110:ALA:HB3	1.95	0.47
2:C:17:GLU:CG	3:C:264:HOH:O	2.55	0.47
1:A:116:ARG:HH11	1:A:138:GLN:HE21	1.62	0.47
2:D:43:GLN:HB2	2:D:53:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:THR:HA	1:B:32:GLN:NE2	2.30	0.46
1:B:160:THR:HG23	1:B:162:ILE:HD12	1.98	0.46
1:A:57:GLU:HB2	1:A:79:ILE:HG23	1.98	0.46
1:B:141:TYR:HB3	1:B:182:CYS:O	2.15	0.46
2:D:56:TRP:O	2:D:57:ALA:HB3	2.16	0.45
2:C:91:VAL:HG22	2:C:109:ARG:HG3	1.99	0.45
2:D:58:PHE:C	2:D:58:PHE:CD1	2.89	0.44
1:A:153:LYS:H	1:A:153:LYS:CD	2.29	0.44
1:A:32:GLN:HE21	1:A:56:GLN:HE22	1.65	0.44
2:D:135:GLU:OE2	2:D:135:GLU:CA	2.49	0.43
2:C:-2:GLN:N	2:C:-1:PRO:HD3	2.33	0.43
1:A:34:VAL:HG13	1:A:58:VAL:HA	2.01	0.43
1:A:116:ARG:HH11	1:A:138:GLN:NE2	2.17	0.43
2:C:6:GLN:HE21	2:C:105:GLY:HA3	1.83	0.43
1:A:67:ASN:HB3	1:A:69:VAL:HG12	2.00	0.43
1:B:57:GLU:HG3	1:B:79:ILE:HG23	2.00	0.43
2:D:37:ASN:HB2	2:D:57:ALA:HB2	2.00	0.42
1:B:66:HIS:HA	1:B:96:ASP:O	2.19	0.42
2:D:11:LEU:HD22	2:D:13:VAL:HG13	2.01	0.42
1:A:118:LEU:HD22	1:A:120:LEU:HG	2.01	0.42
2:D:96:GLN:HE22	2:D:99:ASN:H	1.67	0.42
2:C:164:THR:HB	2:C:188:SER:HB3	2.01	0.41
2:D:19:VAL:HG22	2:D:81:ILE:CG1	2.51	0.41
1:A:66:HIS:HA	1:A:96:ASP:O	2.21	0.41
1:A:9:MET:O	1:A:12:ARG:HB3	2.21	0.41
1:B:71:GLN:HG2	1:B:117:GLU:HG3	2.03	0.41
1:B:9:MET:O	1:B:12:ARG:HB2	2.21	0.40

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	193/194 (100%)	184 (95%)	9 (5%)	0	100	100
1	B	187/194 (96%)	179 (96%)	8 (4%)	0	100	100
2	C	230/259 (89%)	223 (97%)	7 (3%)	0	100	100
2	D	232/259 (90%)	223 (96%)	9 (4%)	0	100	100
All	All	842/906 (93%)	809 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	174/172 (101%)	162 (93%)	12 (7%)	19	25
1	B	171/172 (99%)	166 (97%)	5 (3%)	50	66
2	C	202/209 (97%)	197 (98%)	5 (2%)	55	72
2	D	204/209 (98%)	193 (95%)	11 (5%)	27	38
All	All	751/762 (99%)	718 (96%)	33 (4%)	35	49

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	3	VAL
1	A	34	VAL
1	A	88	ASP
1	A	108	THR
1	A	118	LEU
1	A	121	ARG
1	A	142	GLN
1	A	153	LYS
1	A	161	LEU
1	A	174	SER
1	A	185	GLU
1	B	46	ASN

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Mol	Chain	Res	Type
1	B	87	GLU
1	B	104	THR
1	B	142	GLN
1	B	161	LEU
2	C	19	VAL
2	C	21	MET
2	C	96	GLN
2	C	184	HIS
2	C	220	LEU
2	D	11	LEU
2	D	14	SER
2	D	51	LYS
2	D	66	ASP
2	D	81	ILE
2	D	96	GLN
2	D	111	GLU
2	D	135	GLU
2	D	139	GLN
2	D	184	HIS
2	D	220	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	68	GLN
1	A	138	GLN
1	A	152	HIS
1	B	32	GLN
1	B	46	ASN
2	C	6	GLN
2	C	43	GLN
2	C	44	GLN
2	C	96	GLN
2	C	169	ASN
2	C	174	ASN
2	C	184	HIS
2	D	43	GLN
2	D	44	GLN
2	D	95	GLN
2	D	96	GLN
2	D	169	ASN

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Mol	Chain	Res	Type
2	D	174	ASN
2	D	184	HIS

### 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 ⓘ

### 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	193/194 (99%)	-0.12	7 (3%)	46	50	14, 22, 33, 36	7 (3%)
1	B	189/194 (97%)	-0.10	2 (1%)	82	84	16, 24, 38, 44	8 (4%)
2	C	234/259 (90%)	-0.03	5 (2%)	67	70	19, 25, 31, 33	9 (3%)
2	D	236/259 (91%)	-0.02	8 (3%)	49	52	15, 24, 36, 39	9 (3%)
All	All	852/906 (94%)	-0.07	22 (2%)	59	62	14, 24, 35, 44	33 (3%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	134	SER	5.4
2	C	-1	PRO	4.4
2	D	112	ILE	3.7
1	B	0	SER	3.5
2	C	-2	GLN	3.2
2	D	113	LYS	3.1
1	A	17	PRO	3.1
1	A	108	THR	2.9
2	D	-1	PRO	2.7
2	D	19	VAL	2.5
1	A	18	GLU	2.4
2	D	86	ALA	2.4
1	A	105	THR	2.3
2	C	89	LEU	2.3
1	A	15	ALA	2.2
2	C	160	GLY	2.2
2	C	152	VAL	2.1
2	D	13	VAL	2.1
1	A	110	ALA	2.1
1	A	154	ASN	2.1
2	D	89	LEU	2.0
1	B	105	THR	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.