



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:20 PM GMT

PDB ID : 1F4W  
Title : CRYSTAL STRUCTURE OF AN ANTI-CARBOHYDRATE ANTIBODY  
DIRECTED AGAINST VIBRIO CHOLERAEE O1 IN COMPLEX WITH  
ANTIGEN  
Authors : Alzari, P.M.; Souchon, H.  
Deposited on : 2000-06-10  
Resolution : 2.30 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

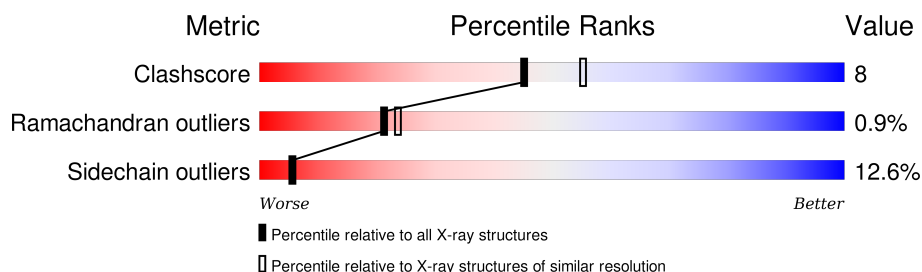
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	210	 69% 27% .
2	H	216	 67% 25% . .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3205 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 S-20-4, FAB FRAGMENT, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	210	Total	C	N	O	S	0	0	0
			1556	977	254	319	6			

- Molecule 2 is a protein called ANTIBODY S-20-4, FAB FRAGMENT, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1598	1011	257	322	8			

- Molecule 3 is water.

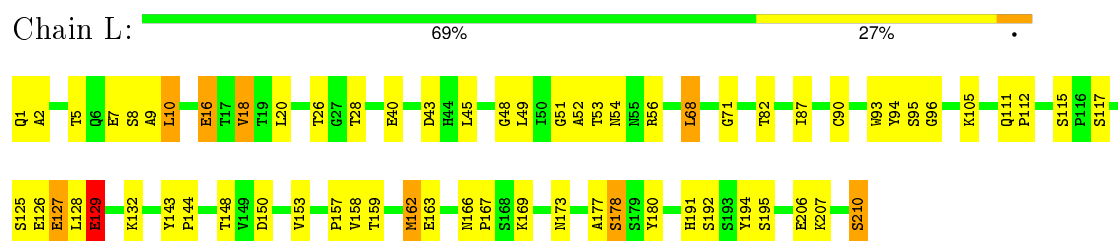
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	23	Total	O	0	0
			23	23		
3	L	28	Total	O	0	0
			28	28		

### 3 Residue-property plots

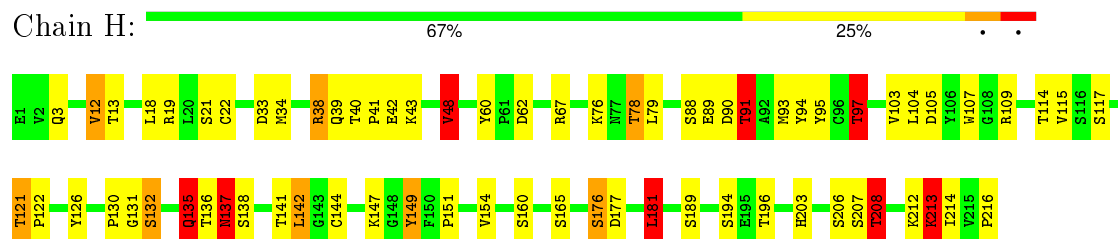
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: ANTIBODY S-20-4, FAB FRAGMENT, LIGHT CHAIN



#### • Molecule 2: ANTIBODY S-20-4, FAB FRAGMENT, HEAVY CHAIN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.67Å 113.32Å 46.21Å 90.00° 100.69° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.197 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

## 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	0.83	0/1592	1.72	16/2180 (0.7%)
2	H	0.88	1/1641 (0.1%)	1.86	40/2252 (1.8%)
All	All	0.86	1/3233 (0.0%)	1.79	56/4432 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
2	H	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	216	PRO	N-CD	5.59	1.55	1.47

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	56	ARG	CD-NE-CZ	20.91	152.87	123.60
2	H	105	ASP	CB-CG-OD1	14.03	130.93	118.30
2	H	38	ARG	NE-CZ-NH1	13.79	127.20	120.30
2	H	38	ARG	NE-CZ-NH2	-11.01	114.79	120.30
2	H	90	ASP	CB-CG-OD2	10.11	127.40	118.30
2	H	95	TYR	CB-CG-CD2	-8.03	116.18	121.00
1	L	18	VAL	CB-CA-C	-7.66	96.85	111.40
2	H	105	ASP	CB-CG-OD2	-7.62	111.44	118.30
2	H	97	THR	CB-CA-C	-7.49	91.38	111.60
1	L	40	GLU	OE1-CD-OE2	-7.45	114.36	123.30
2	H	89	GLU	OE1-CD-OE2	7.24	131.98	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	97	THR	N-CA-CB	7.22	124.02	110.30
2	H	208	THR	N-CA-CB	-7.12	96.76	110.30
2	H	48	VAL	N-CA-CB	-7.09	95.89	111.50
2	H	149	TYR	CB-CG-CD2	-6.96	116.82	121.00
2	H	60	TYR	CB-CG-CD1	-6.94	116.83	121.00
2	H	95	TYR	CB-CG-CD1	6.92	125.16	121.00
1	L	90	CYS	CA-CB-SG	-6.77	101.81	114.00
2	H	21	SER	O-C-N	6.61	133.27	122.70
1	L	150	ASP	CB-CG-OD2	-6.53	112.43	118.30
2	H	181	LEU	CA-CB-CG	6.41	130.05	115.30
2	H	144	CYS	CA-CB-SG	-6.37	102.54	114.00
2	H	94	TYR	CB-CG-CD2	-6.35	117.19	121.00
2	H	121	THR	CA-CB-CG2	6.30	121.22	112.40
2	H	3	GLN	CB-CA-C	6.27	122.94	110.40
1	L	16	GLU	OE1-CD-OE2	6.25	130.81	123.30
2	H	62	ASP	CB-CG-OD2	-6.24	112.69	118.30
2	H	21	SER	CA-CB-OG	-6.20	94.46	111.20
2	H	89	GLU	CG-CD-OE2	-5.93	106.44	118.30
2	H	147	LYS	N-CA-CB	-5.83	100.10	110.60
2	H	213	LYS	CA-CB-CG	5.82	126.21	113.40
2	H	19	ARG	CD-NE-CZ	5.82	131.74	123.60
1	L	8	SER	N-CA-CB	-5.80	101.81	110.50
2	H	126	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	L	125	SER	CB-CA-C	-5.73	99.22	110.10
1	L	7	GLU	OE1-CD-OE2	-5.72	116.44	123.30
2	H	165	SER	N-CA-CB	5.66	118.99	110.50
2	H	12	VAL	O-C-N	-5.64	113.67	122.70
1	L	127	GLU	OE1-CD-OE2	-5.55	116.63	123.30
2	H	48	VAL	CG1-CB-CG2	5.47	119.66	110.90
1	L	129	GLU	CA-CB-CG	5.46	125.42	113.40
1	L	177	ALA	N-CA-CB	5.43	117.70	110.10
2	H	67	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	H	60	TYR	CB-CG-CD2	5.35	124.21	121.00
2	H	181	LEU	CB-CG-CD2	5.33	120.07	111.00
1	L	178	SER	CA-CB-OG	-5.29	96.91	111.20
2	H	91	THR	N-CA-CB	5.29	120.36	110.30
2	H	109	ARG	N-CA-CB	-5.29	101.08	110.60
1	L	90	CYS	N-CA-CB	-5.17	101.30	110.60
2	H	154	VAL	N-CA-CB	5.16	122.85	111.50
2	H	117	SER	CA-CB-OG	-5.15	97.29	111.20
1	L	8	SER	CA-C-O	5.15	130.91	120.10
2	H	48	VAL	CB-CA-C	5.14	121.16	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	33	ASP	CB-CG-OD2	-5.12	113.69	118.30
2	H	62	ASP	CB-CG-OD1	5.06	122.85	118.30
1	L	163	GLU	CA-CB-CG	5.04	124.49	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	39	GLN	Mainchain
1	L	128	LEU	Mainchain

## 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	1556	0	1490	26	0
2	H	1598	0	1517	25	0
3	H	23	0	0	0	0
3	L	28	0	0	1	0
All	All	3205	0	3007	48	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 8.

All (48) 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:L:1:GLN:HG2	1:L:2:ALA:H	1.42	0.85
2:H:196:THR:HG23	2:H:213:LYS:HD3	1.58	0.84
2:H:88:SER:O	2:H:91:THR:HG23	1.87	0.75
1:L:28:THR:HG23	1:L:71:GLY:HA2	1.75	0.67
2:H:122:PRO:HB3	2:H:208:THR:HG21	1.79	0.63
2:H:38:ARG:HD3	2:H:48:VAL:HG21	1.80	0.62
1:L:28:THR:HG23	1:L:71:GLY:CA	2.32	0.60
1:L:192:SER:O	1:L:210:SER:HA	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:PRO:HD3	2:H:142:LEU:HD12	1.85	0.58
2:H:206:SER:OG	2:H:208:THR:HB	2.04	0.58
2:H:151:PRO:O	2:H:203:HIS:HE1	1.87	0.58
1:L:126:GLU:OE2	2:H:212:LYS:NZ	2.38	0.56
1:L:94:TYR:O	1:L:95:SER:HB2	2.06	0.56
2:H:176:SER:O	2:H:177:ASP:HB2	2.06	0.55
1:L:162:MET:HE2	1:L:162:MET:H	1.72	0.54
1:L:166:ASN:O	3:L:228:HOH:O	2.19	0.53
1:L:153:VAL:HG23	1:L:158:VAL:CG2	2.39	0.52
1:L:93:TRP:CH2	1:L:96:GLY:HA2	2.46	0.51
2:H:91:THR:HG22	2:H:115:VAL:H	1.76	0.51
1:L:191:HIS:HB2	1:L:194:TYR:OH	2.11	0.50
1:L:169:LYS:HE3	1:L:173:ASN:OD1	2.11	0.49
2:H:12:VAL:HG12	2:H:13:THR:N	2.27	0.48
1:L:127:GLU:HG2	1:L:132:LYS:O	2.13	0.48
2:H:42:GLU:O	2:H:43:LYS:HB2	2.12	0.48
1:L:93:TRP:CZ2	1:L:96:GLY:HA2	2.48	0.48
1:L:52:ALA:O	1:L:53:THR:HB	2.13	0.48
2:H:142:LEU:HG	2:H:214:ILE:HG21	1.95	0.47
1:L:51:GLY:HA3	2:H:103:VAL:HG22	1.96	0.47
1:L:111:GLN:HB2	1:L:112:PRO:HD2	1.99	0.45
2:H:149:TYR:OH	2:H:181:LEU:HD13	2.17	0.45
2:H:97:THR:HG23	2:H:107:TRP:CG	2.52	0.45
1:L:129:GLU:HA	1:L:129:GLU:OE1	2.18	0.44
1:L:111:GLN:HB2	1:L:112:PRO:CD	2.48	0.44
2:H:97:THR:HG23	2:H:107:TRP:CD1	2.53	0.43
1:L:48:GLY:HA3	2:H:104:LEU:O	2.18	0.43
1:L:166:ASN:HA	1:L:167:PRO:HD3	1.89	0.43
1:L:53:THR:HG21	1:L:68:LEU:HD22	2.01	0.42
1:L:87:ILE:HD12	1:L:105:LYS:HG2	2.01	0.42
2:H:131:GLY:O	2:H:132:SER:C	2.58	0.42
1:L:162:MET:HA	1:L:180:TYR:O	2.20	0.41
1:L:143:TYR:HA	1:L:144:PRO:C	2.40	0.41
2:H:135:GLN:HG3	2:H:135:GLN:H	1.63	0.41
2:H:91:THR:HB	2:H:114:THR:HA	2.01	0.41
2:H:76:LYS:HB2	2:H:78:THR:HG23	2.03	0.41
2:H:40:THR:HB	2:H:41:PRO:HD2	2.03	0.41
2:H:137:ASN:HB2	2:H:138:SER:H	1.63	0.40
1:L:9:ALA:O	1:L:10:LEU:HD13	2.22	0.40
2:H:22:CYS:HB3	2:H:79:LEU:HB3	2.02	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	L	208/210 (99%)	200 (96%)	7 (3%)	1 (0%)	34	41
2	H	214/216 (99%)	203 (95%)	8 (4%)	3 (1%)	14	13
All	All	422/426 (99%)	403 (96%)	15 (4%)	4 (1%)	21	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	43	ASP
2	H	135	GLN
2	H	132	SER
2	H	137	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	172/177 (97%)	149 (87%)	23 (13%)	5	5
2	H	178/186 (96%)	157 (88%)	21 (12%)	6	7
All	All	350/363 (96%)	306 (87%)	44 (13%)	5	5

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	10	LEU

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Mol	Chain	Res	Type
1	L	16	GLU
1	L	18	VAL
1	L	20	LEU
1	L	26	THR
1	L	45	LEU
1	L	49	LEU
1	L	54	ASN
1	L	68	LEU
1	L	82	THR
1	L	115	SER
1	L	117	SER
1	L	129	GLU
1	L	148	THR
1	L	157	PRO
1	L	159	THR
1	L	162	MET
1	L	178	SER
1	L	195	SER
1	L	206	GLU
1	L	207	LYS
1	L	210	SER
2	H	18	LEU
2	H	34	MET
2	H	48	VAL
2	H	78	THR
2	H	91	THR
2	H	93	MET
2	H	97	THR
2	H	121	THR
2	H	135	GLN
2	H	136	THR
2	H	137	ASN
2	H	141	THR
2	H	142	LEU
2	H	160	SER
2	H	176	SER
2	H	181	LEU
2	H	189	SER
2	H	194	SER
2	H	207	SER
2	H	208	THR
2	H	213	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	44	HIS
1	L	54	ASN
1	L	191	HIS
2	H	137	ASN
2	H	203	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.