



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 03:40 AM EST

PDB ID : 1EJO
Title : FAB FRAGMENT OF NEUTRALISING MONOCLONAL ANTIBODY 4C4
COMPLEXED WITH G-H LOOP FROM FMDV.
Authors : Ochoa, W.F.; Kalko, S.G.; Gomes, P.; Fita, I.; Verdaguer, N.
Deposited on : 2000-03-03
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

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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

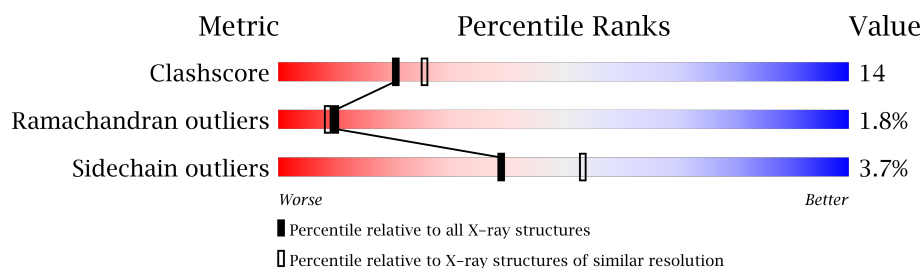
1 Overall quality at a glance

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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (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 ≥ 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	216	 76% 21% .
2	H	220	 71% 24% . . .
3	P	15	 67% 20% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3520 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 IGG2A MONOCLONAL ANTIBODY (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1647	1023	277	341	6			

- Molecule 2 is a protein called IGG2A MONOCLONAL ANTIBODY (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1608	1017	262	320	9			

- Molecule 3 is a protein called FMDV PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	0	0	0
			99	60	18	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	3147	VAL	ILE	CONFLICT	GB 210410
P	3149	THR	ALA	CONFLICT	GB 210410

- Molecule 4 is water.

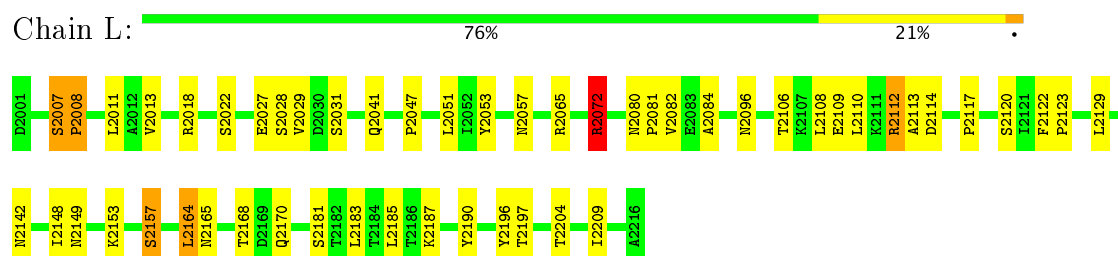
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	103	Total	O	0	0
			103	103		
4	H	56	Total	O	0	0
			56	56		
4	P	7	Total	O	0	0
			7	7		

3 Residue-property plots [i](#)

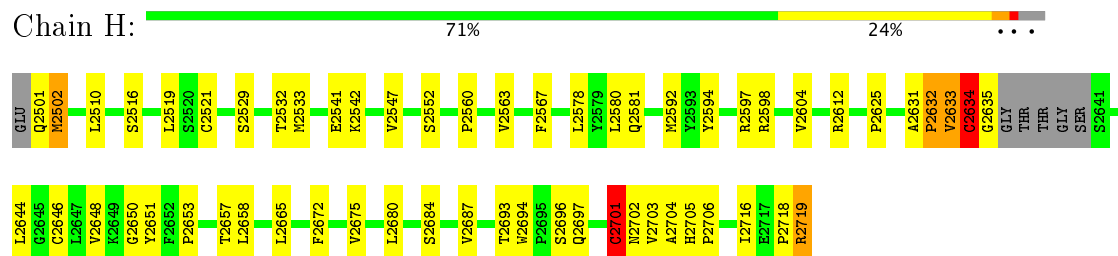
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

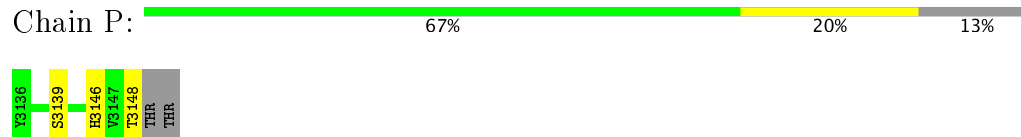
• Molecule 1: IGG2A MONOCLONAL ANTIBODY (LIGHT CHAIN)



• Molecule 2: IGG2A MONOCLONAL ANTIBODY (HEAVY CHAIN)



• Molecule 3: FMDV PEPTIDE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.18 Å 69.33 Å 146.54 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	8.0 (15.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3520	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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	L	0.33	0/1684	0.59	0/2294
2	H	0.38	0/1648	0.71	3/2248 (0.1%)
3	P	0.64	0/100	0.82	0/136
All	All	0.36	0/3432	0.66	3/4678 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2633	VAL	N-CA-C	-11.24	80.65	111.00
2	H	2701	CYS	CA-CB-SG	6.25	125.25	114.00
2	H	2719	ARG	NE-CZ-NH1	-5.32	117.64	120.30

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	L	1647	0	1548	44	0
2	H	1608	0	1560	54	0
3	P	99	0	93	1	0
4	H	56	0	0	1	0
4	L	103	0	0	1	0
4	P	7	0	0	0	0
All	All	3520	0	3201	90	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 14.

All (90) 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:2631:ALA:HB1	2:H:2634:CYS:SG	1.75	1.26
1:L:2007:SER:HB3	1:L:2008:PRO:HD2	1.19	1.13
2:H:2634:CYS:SG	2:H:2694:TRP:HH2	1.89	0.94
2:H:2632:PRO:HB3	4:H:176:HOH:O	1.74	0.85
2:H:2634:CYS:SG	2:H:2694:TRP:CH2	2.67	0.81
2:H:2632:PRO:HD2	2:H:2634:CYS:SG	2.22	0.78
2:H:2701:CYS:SG	2:H:2716:ILE:HD11	2.23	0.78
1:L:2007:SER:HB2	1:L:2022:SER:HB2	1.66	0.77
1:L:2084:ALA:HA	1:L:2110:LEU:HD11	1.67	0.76
1:L:2007:SER:HB3	1:L:2008:PRO:CD	2.09	0.74
2:H:2563:VAL:HG13	2:H:2567:PHE:HB2	1.69	0.73
1:L:2065:ARG:HD2	1:L:2081:PRO:O	1.88	0.72
2:H:2631:ALA:CB	2:H:2634:CYS:SG	2.69	0.72
1:L:2153:LYS:HB2	1:L:2197:THR:HB	1.72	0.71
1:L:2117:PRO:HG2	1:L:2209:ILE:HD12	1.74	0.69
2:H:2631:ALA:HB3	2:H:2719:ARG:HE	1.59	0.67
2:H:2532:THR:HG22	2:H:2598:ARG:HB3	1.78	0.66
1:L:2122:PHE:CD2	2:H:2632:PRO:HA	2.32	0.64
2:H:2631:ALA:HB3	2:H:2719:ARG:NE	2.11	0.64
1:L:2007:SER:CB	1:L:2008:PRO:HD2	2.10	0.64
1:L:2084:ALA:HA	1:L:2110:LEU:CD1	2.30	0.62
1:L:2153:LYS:HA	1:L:2157:SER:O	1.99	0.61
1:L:2112:ARG:HG2	1:L:2113:ALA:H	1.65	0.61
2:H:2634:CYS:HB3	2:H:2719:ARG:H	1.67	0.59
1:L:2112:ARG:HG2	1:L:2113:ALA:N	2.18	0.58
1:L:2183:LEU:HG	1:L:2185:LEU:HD11	1.85	0.58
1:L:2008:PRO:O	1:L:2106:THR:HG23	2.04	0.58
1:L:2018:ARG:HB3	1:L:2080:ASN:ND2	2.20	0.57
1:L:2123:PRO:HB2	2:H:2719:ARG:HH12	1.71	0.55
2:H:2634:CYS:SG	2:H:2718:PRO:HA	2.46	0.55
1:L:2123:PRO:HB2	2:H:2719:ARG:NH1	2.21	0.55
1:L:2047:PRO:HB3	2:H:2594:TYR:CE2	2.42	0.55
1:L:2165:ASN:HD22	1:L:2181:SER:HA	1.71	0.55
2:H:2633:VAL:O	2:H:2635:GLY:N	2.40	0.54
1:L:2122:PHE:CE2	2:H:2632:PRO:HA	2.42	0.54
1:L:2013:VAL:HG11	1:L:2082:VAL:HG21	1.89	0.54
2:H:2632:PRO:C	2:H:2634:CYS:N	2.59	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2560:PRO:HG2	2:H:2563:VAL:HB	1.91	0.52
1:L:2148:ILE:HG12	1:L:2149:ASN:H	1.75	0.52
2:H:2658:LEU:HD13	2:H:2703:VAL:HG22	1.91	0.52
1:L:2110:LEU:H	1:L:2170:GLN:HE22	1.57	0.52
2:H:2658:LEU:CD1	2:H:2702:ASN:O	2.59	0.50
2:H:2703:VAL:HG12	2:H:2704:ALA:N	2.27	0.50
2:H:2510:LEU:HD22	2:H:2653:PRO:HD3	1.93	0.50
1:L:2122:PHE:HD2	2:H:2631:ALA:O	1.94	0.49
2:H:2625:PRO:HB3	2:H:2651:TYR:HB3	1.94	0.49
1:L:2164:LEU:HD12	2:H:2675:VAL:HB	1.93	0.49
1:L:2041:GLN:HB2	1:L:2051:LEU:HD11	1.94	0.49
1:L:2007:SER:O	1:L:2008:PRO:C	2.51	0.49
2:H:2658:LEU:HD12	2:H:2702:ASN:O	2.13	0.49
2:H:2501:GLN:O	2:H:2502:MET:HB2	2.14	0.48
2:H:2632:PRO:HG2	2:H:2634:CYS:HA	1.95	0.47
1:L:2082:VAL:HG12	1:L:2110:LEU:HD21	1.97	0.47
1:L:2072:ARG:HH11	1:L:2072:ARG:CG	2.28	0.47
2:H:2592:MET:HG3	2:H:2612:ARG:CB	2.45	0.46
2:H:2632:PRO:HD3	2:H:2644:LEU:HD23	1.98	0.46
1:L:2164:LEU:CD1	2:H:2675:VAL:HB	2.46	0.46
2:H:2693:THR:HG23	2:H:2697:GLN:OE1	2.17	0.45
2:H:2533:MET:SD	2:H:2597:ARG:HA	2.57	0.45
1:L:2029:VAL:HG12	1:L:2029:VAL:O	2.17	0.44
1:L:2080:ASN:HA	1:L:2081:PRO:HA	1.83	0.44
1:L:2031:SER:HB2	1:L:2096:ASN:OD1	2.17	0.44
2:H:2657:THR:OG1	2:H:2704:ALA:HB3	2.17	0.44
3:P:3146:HIS:O	3:P:3148:THR:HG22	2.17	0.43
2:H:2631:ALA:O	2:H:2632:PRO:O	2.36	0.43
2:H:2650:GLY:HA2	2:H:2680:LEU:HB3	1.99	0.43
2:H:2529:SER:O	2:H:2552:SER:HB2	2.17	0.43
2:H:2510:LEU:HB2	2:H:2653:PRO:HG3	1.99	0.43
1:L:2027:GLU:HG2	1:L:2028:SER:N	2.33	0.43
2:H:2648:VAL:HG22	2:H:2703:VAL:HG21	2.00	0.42
1:L:2164:LEU:O	1:L:2164:LEU:HG	2.19	0.42
1:L:2013:VAL:HG12	1:L:2108:LEU:HD11	2.01	0.42
2:H:2519:LEU:HD12	2:H:2580:LEU:HD23	2.01	0.42
1:L:2114:ASP:HB3	1:L:2204:THR:HG22	2.01	0.41
2:H:2604:VAL:O	2:H:2604:VAL:HG12	2.20	0.41
2:H:2687:VAL:O	2:H:2687:VAL:HG13	2.20	0.41
2:H:2705:HIS:HA	2:H:2706:PRO:HD2	1.94	0.41
2:H:2541:GLU:O	2:H:2542:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2521:CYS:HB3	2:H:2578:LEU:HB3	2.02	0.41
2:H:2658:LEU:HD13	2:H:2703:VAL:CG2	2.51	0.41
2:H:2703:VAL:CG1	2:H:2704:ALA:N	2.83	0.41
2:H:2547:VAL:O	2:H:2560:PRO:HD2	2.21	0.41
2:H:2634:CYS:HG	2:H:2694:TRP:HH2	0.71	0.41
1:L:2129:LEU:O	1:L:2187:LYS:HD3	2.21	0.40
1:L:2165:ASN:ND2	1:L:2181:SER:HA	2.34	0.40
1:L:2190:TYR:HA	1:L:2196:TYR:OH	2.21	0.40
2:H:2567:PHE:HA	2:H:2581:GLN:O	2.22	0.40
1:L:2011:LEU:HD21	4:L:121:HOH:O	2.21	0.40
1:L:2053:TYR:O	1:L:2057:ASN:HB2	2.21	0.40
1:L:2168:THR:HG23	2:H:2672:PHE:CD2	2.57	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	L	214/216 (99%)	203 (95%)	7 (3%)	4 (2%)	9	8
2	H	210/220 (96%)	195 (93%)	11 (5%)	4 (2%)	9	8
3	P	11/15 (73%)	10 (91%)	1 (9%)	0	100	100
All	All	435/451 (96%)	408 (94%)	19 (4%)	8 (2%)	10	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	2008	PRO
2	H	2502	MET
2	H	2632	PRO
2	H	2634	CYS
1	L	2007	SER

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Mol	Chain	Res	Type
1	L	2072	ARG
2	H	2701	CYS
1	L	2142	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	184/189 (97%)	178 (97%)	6 (3%)	43	59
2	H	182/188 (97%)	175 (96%)	7 (4%)	38	52
3	P	11/13 (85%)	10 (91%)	1 (9%)	11	13
All	All	377/390 (97%)	363 (96%)	14 (4%)	39	53

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2072	ARG
1	L	2109	GLU
1	L	2112	ARG
1	L	2120	SER
1	L	2157	SER
1	L	2164	LEU
2	H	2516	SER
2	H	2634	CYS
2	H	2646	CYS
2	H	2665	LEU
2	H	2684	SER
2	H	2696	SER
2	H	2701	CYS
3	P	3139	SER

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	2080	ASN
1	L	2165	ASN
1	L	2170	GLN
1	L	2214	ASN
2	H	2581	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.