



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:43 PM BST

PDB ID : 3J1S
EMDB ID: : EMD-5424
Title : Structure of adeno-associated virus-2 in complex with neutralizing monoclonal antibody A20
Authors : Chapman, M.S.; McCraw, D.M.
Deposited on : 2012-05-23
Resolution : 8.50 Å(reported)
Based on PDB ID : 1LP3

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
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) : trunk27241

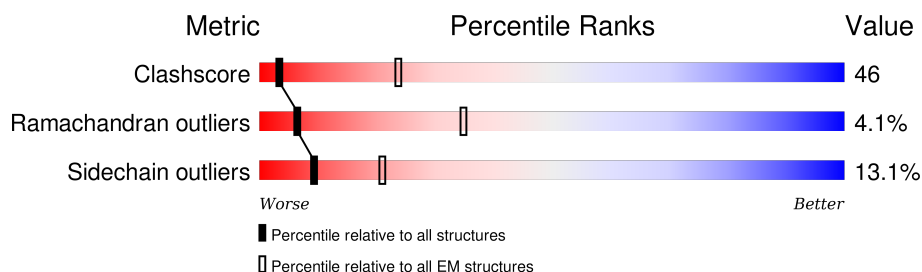
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.50 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	L	214	55% 41% .
2	H	218	56% 38% 6%
3	A	519	37% 47% 15% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7485 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 A20 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	214	Total	C	N	O	S	0	0
			1657	1028	281	341	7		

- Molecule 2 is a protein called A20 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	218	Total	C	N	O	S	0	0
			1676	1063	270	336	7		

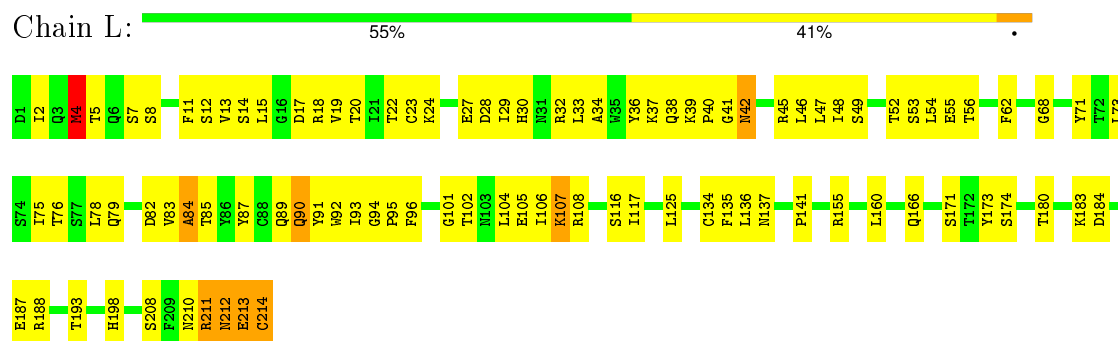
- Molecule 3 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	519	Total	C	N	O	S	0	0
			4152	2612	725	802	13		

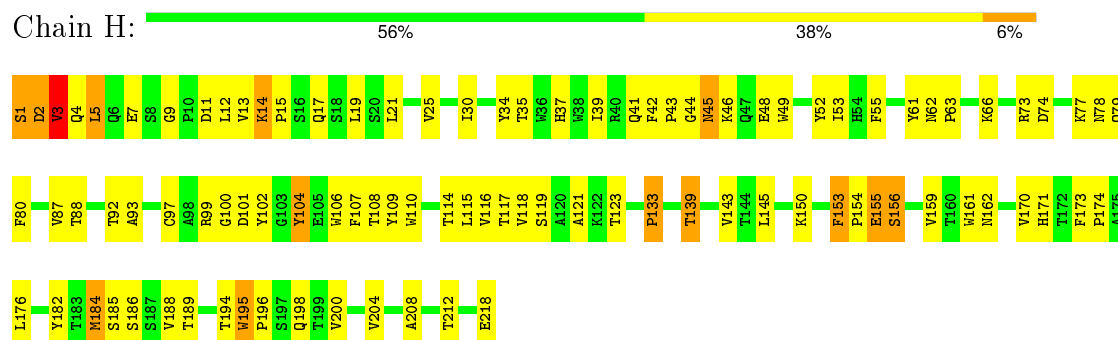
3 Residue-property plots

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. 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. 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.

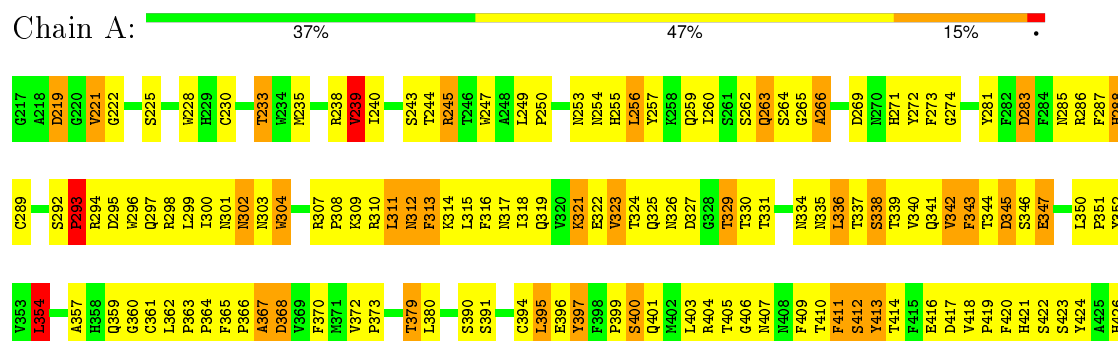
• Molecule 1: A20 light chain



• Molecule 2: A20 heavy chain



• Molecule 3: Capsid protein VP1





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	11898	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Whole image	Depositor
Microscope	FEI Titan Krios	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-4000	Depositor
Magnification	37000	Depositor
Image detector	Gatan Ultrascan CCD	Depositor

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 >2	RMSZ	# Z >2
1	L	0.85	3/1692 (0.2%)	0.96	4/2295 (0.2%)
2	H	0.95	8/1726 (0.5%)	1.18	11/2364 (0.5%)
3	A	0.94	3/4275 (0.1%)	1.06	7/5827 (0.1%)
All	All	0.92	14/7693 (0.2%)	1.07	22/10486 (0.2%)

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	2
3	A	0	3
All	All	0	5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	213	GLU	C-N	14.56	1.67	1.34
2	H	133	PRO	C-N	14.54	1.59	1.33
1	L	211	ARG	C-N	-8.26	1.15	1.34
1	L	212	ASN	C-N	-7.96	1.15	1.34
2	H	2	ASP	N-CA	7.54	1.61	1.46

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	133	PRO	O-C-N	15.73	149.94	123.20
2	H	133	PRO	CA-C-N	-13.60	89.01	116.20
1	L	211	ARG	O-C-N	-10.85	105.34	122.70
3	A	633	LEU	CA-CB-CG	-8.48	95.79	115.30
1	L	4	MET	CG-SD-CE	-6.52	89.76	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	413	TYR	Sidechain
3	A	612	TYR	Sidechain
3	A	730	TYR	Sidechain
1	L	211	ARG	Mainchain
1	L	212	ASN	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	1657	0	1581	145	0
2	H	1676	0	1594	161	0
3	A	4152	0	3904	385	0
All	All	7485	0	7079	674	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 46.

The worst 5 of 674 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:213:GLU:C	1:L:214:CYS:N	1.67	1.45
1:L:107:LYS:CE	1:L:108:ARG:HB3	1.66	1.25
2:H:5:LEU:HD22	2:H:25:VAL:HG12	1.18	1.16
1:L:107:LYS:HE2	1:L:108:ARG:CB	1.76	1.15
2:H:139:THR:CG2	2:H:143:VAL:HG12	1.77	1.14

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 PDB entries followed by that with respect to all EM entries.

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	210/214 (98%)	199 (95%)	9 (4%)	2 (1%)	19	65
2	H	214/218 (98%)	197 (92%)	10 (5%)	7 (3%)	5	40
3	A	517/519 (100%)	402 (78%)	85 (16%)	30 (6%)	2	27
All	All	941/951 (99%)	798 (85%)	104 (11%)	39 (4%)	6	35

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	7	SER
2	H	3	VAL
2	H	5	LEU
2	H	45	ASN
3	A	264	SER

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 PDB entries followed by that with respect to all EM entries.

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	190/190 (100%)	185 (97%)	5 (3%)	54	80
2	H	193/193 (100%)	189 (98%)	4 (2%)	61	84
3	A	459/459 (100%)	358 (78%)	101 (22%)	1	9
All	All	842/842 (100%)	732 (87%)	110 (13%)	9	28

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	427	SER
3	A	460	LEU
3	A	696	PRO
3	A	434	MET
3	A	446	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	312	ASN
3	A	335	ASN
3	A	650	ASN
3	A	297	GLN
3	A	672	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.