



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:56 PM BST

PDB ID : 4AQ5
EMDB ID: : EMD-2071
Title : Gating movement in acetylcholine receptor analysed by time-resolved electron cryo-microscopy (closed class)
Authors : Unwin, N.; Fujiyoshi, Y.
Deposited on : 2012-04-12
Resolution : 6.20 Å(reported)
Based on PDB ID : 2BG9

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

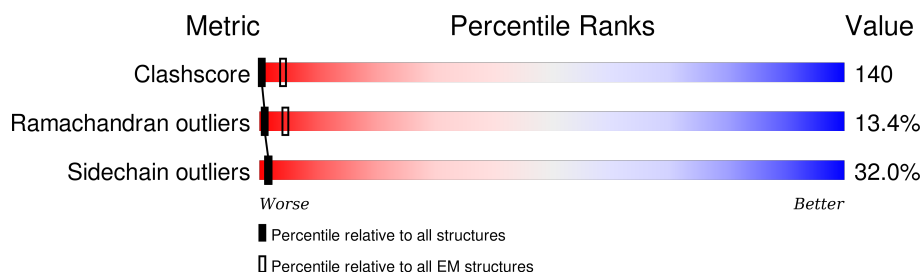
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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	A	461	
1	D	461	
2	B	493	
3	C	522	
4	E	488	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14924 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 ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
1	D	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		

- Molecule 2 is a protein called ACETYLCHOLINE RECEPTOR BETA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	370	Total	C	N	O	S	0	0
			2972	1938	465	554	15		

- Molecule 3 is a protein called ACETYLCHOLINE RECEPTOR DELTA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	370	Total	C	N	O	S	0	1
			2983	1944	489	536	14		

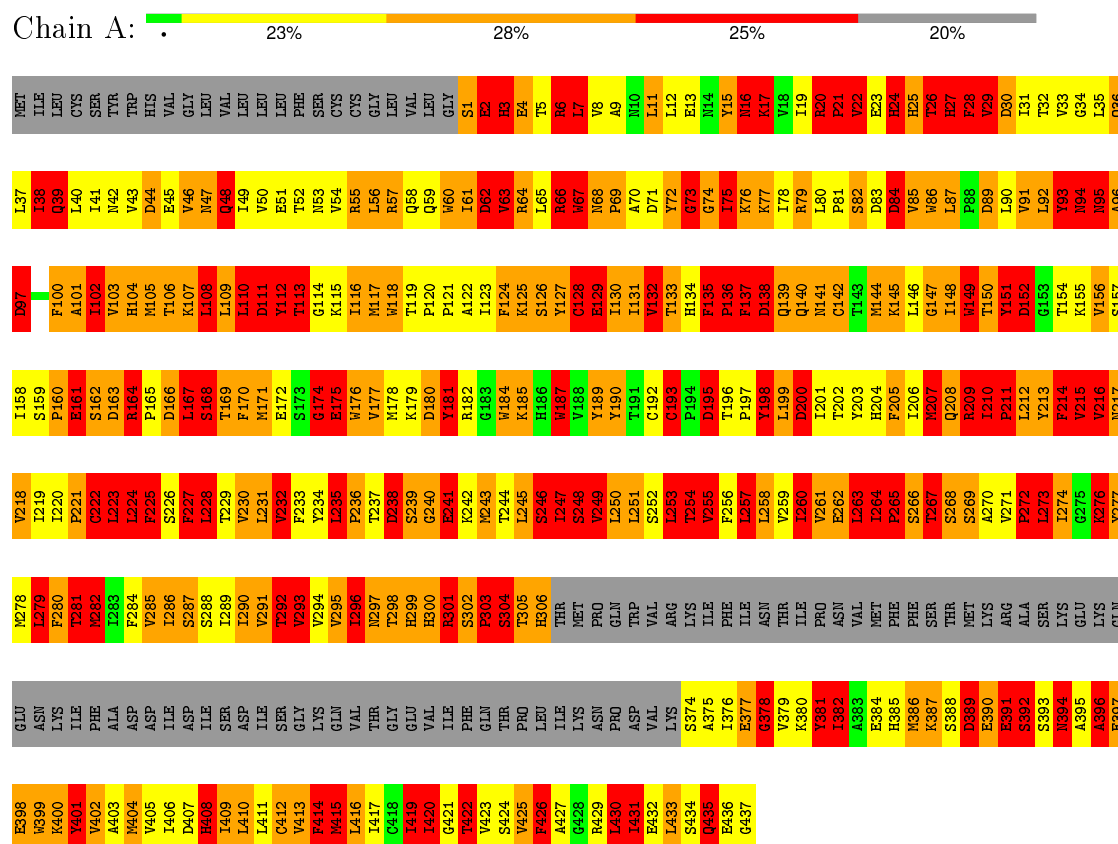
- Molecule 4 is a protein called ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		

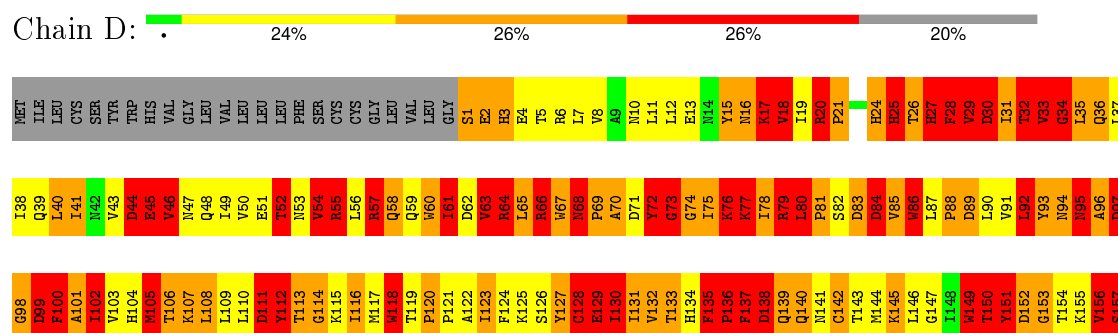
3 Residue-property plots

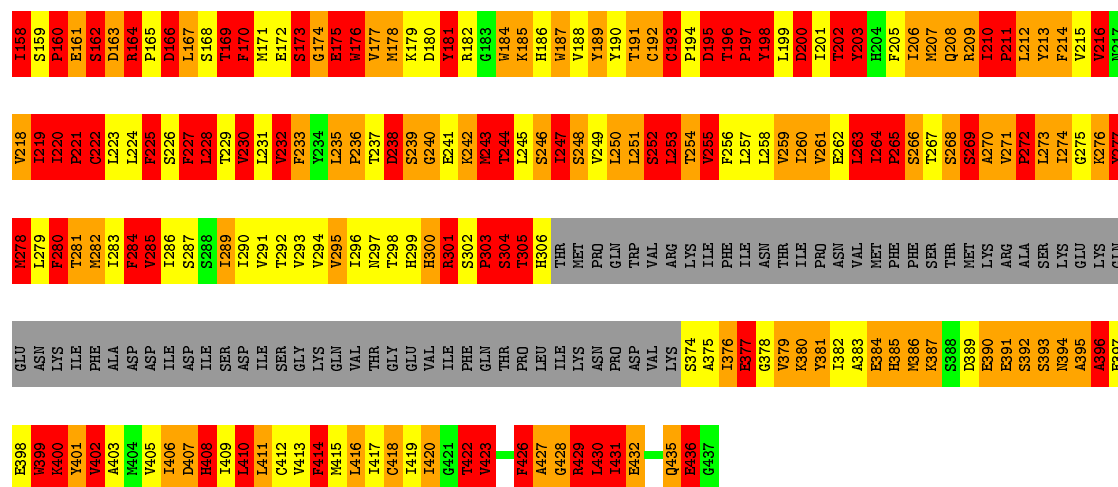
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

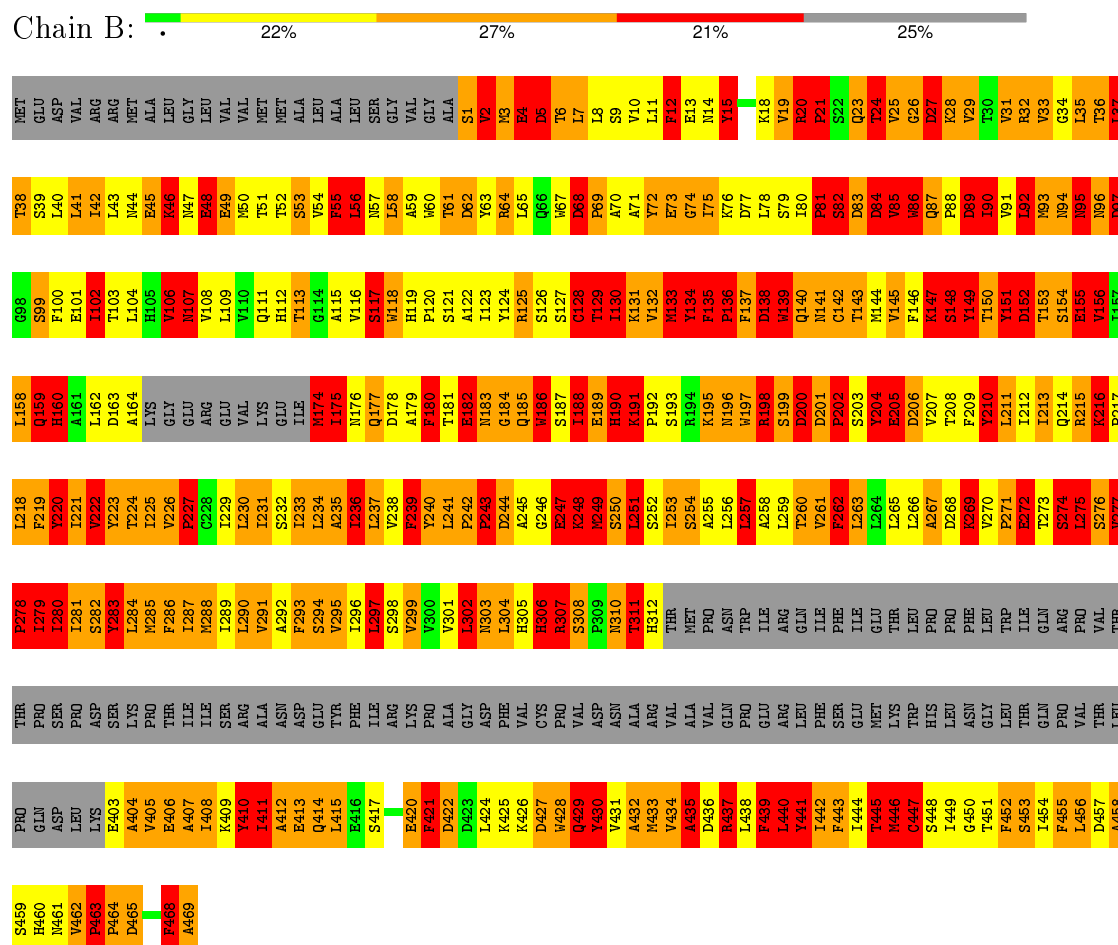


• Molecule 1: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

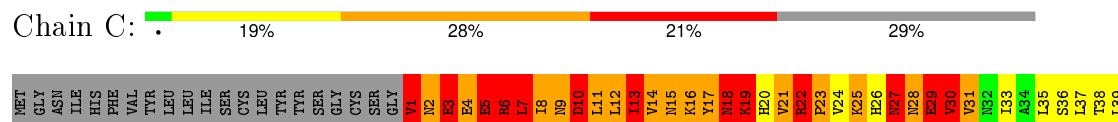




• Molecule 2: ACETYLCHOLINE RECEPTOR BETA SUBUNIT



• Molecule 3: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT



ASP
PRO
ARG
LYS
TYR
VAL
PRO

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH TUBE IMAGE	Depositor
Microscope	JEOL 3000FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	40000	Depositor
Image detector	KODAK SO163 FILM	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	A	1.68	15/3069 (0.5%)	2.70	244/4186 (5.8%)
1	D	1.70	13/3069 (0.4%)	2.80	272/4186 (6.5%)
2	B	1.70	14/3048 (0.5%)	2.78	261/4162 (6.3%)
3	C	1.63	11/3059 (0.4%)	2.83	284/4175 (6.8%)
4	E	1.67	17/3057 (0.6%)	2.80	266/4174 (6.4%)
All	All	1.68	70/15302 (0.5%)	2.78	1327/20883 (6.4%)

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	A	7	116
1	D	6	125
2	B	6	112
3	C	6	125
4	E	12	107
All	All	37	585

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	THR	C-N	-9.22	1.12	1.34
4	E	8	GLU	CB-CG	8.90	1.69	1.52
1	A	118	TRP	CB-CG	8.84	1.66	1.50
1	D	175	GLU	CD-OE1	8.46	1.34	1.25
1	A	222	CYS	CB-SG	-7.49	1.69	1.82

The worst 5 of 1327 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	309	ARG	NE-CZ-NH1	25.87	133.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	307	ARG	NE-CZ-NH2	24.36	132.48	120.30
3	C	277	ARG	NE-CZ-NH2	21.78	131.19	120.30
3	C	17	TYR	CB-CG-CD1	-19.82	109.11	121.00
4	E	17	ARG	NE-CZ-NH2	-18.78	110.91	120.30

5 of 37 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	SER	CA
1	A	209	ARG	CA
1	A	267	THR	CB
1	A	292	THR	CB
1	A	304	SER	CA

5 of 585 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ASN	Mainchain
1	A	24	HIS	Mainchain
1	A	25	HIS	Mainchain
1	A	28	PHE	Mainchain
1	A	3	HIS	Peptide

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	2991	0	3004	897	0
1	D	2991	0	3005	854	0
2	B	2972	0	2951	830	0
3	C	2983	0	2985	848	0
4	E	2987	0	2988	947	0
All	All	14924	0	14933	4181	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 140.

The worst 5 of 4181 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:A:282:MET:CE	1:A:282:MET:SD	2.01	1.46
1:D:86:TRP:CD2	1:D:86:TRP:O	1.71	1.40
2:B:306:HIS:O	2:B:306:HIS:ND1	1.62	1.29
1:A:113:THR:O	1:A:113:THR:CG2	1.76	1.28
1:A:236:PRO:HB3	1:A:299:HIS:CE1	1.69	1.27

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 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	A	366/461 (79%)	260 (71%)	58 (16%)	48 (13%)	0	7
1	D	366/461 (79%)	264 (72%)	56 (15%)	46 (13%)	0	8
2	B	364/493 (74%)	243 (67%)	65 (18%)	56 (15%)	0	5
3	C	364/522 (70%)	252 (69%)	68 (19%)	44 (12%)	0	8
4	E	365/488 (75%)	234 (64%)	80 (22%)	51 (14%)	0	6
All	All	1825/2425 (75%)	1253 (69%)	327 (18%)	245 (13%)	1	7

5 of 245 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	PRO
1	A	24	HIS
1	A	27	HIS
1	A	48	GLN
1	A	76	LYS

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	A	343/427 (80%)	231 (67%)	112 (33%)	0	2
1	D	343/427 (80%)	230 (67%)	113 (33%)	0	2
2	B	340/449 (76%)	235 (69%)	105 (31%)	0	3
3	C	335/475 (70%)	235 (70%)	100 (30%)	0	3
4	E	337/447 (75%)	224 (66%)	113 (34%)	0	2
All	All	1698/2225 (76%)	1155 (68%)	543 (32%)	1	2

5 of 543 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	99	ASP
3	C	442	GLU
4	E	217	LYS
3	C	130	CYS
3	C	249	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	231	ASN
1	D	53	ASN
4	E	206	GLN
3	C	267	GLN
3	C	479	ASN

5.3.3 RNA ⓘ

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.