wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:17 PM BST

PDB ID	:	4BOG
EMDB ID:	:	EMD-2376
Title	:	The structure and super-organization of acetylcholine receptor-rapsyn complexes
Authors	:	Zuber, B.; Unwin, N.
Deposited on	:	2013-05-20
Resolution	:	50.00 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

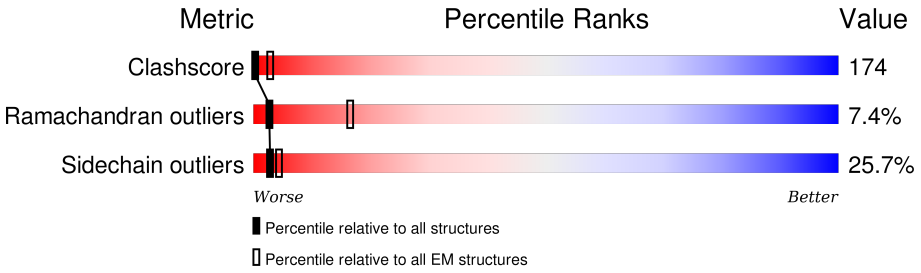
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 50.00 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 <=5%

Mol	Chain	Length	Quality of chain
1	0	493	52% 20% 25%
1	B	493	52% 20% 25%
1	G	493	50% 19% 25%
1	L	493	50% 20% 25%
1	Q	493	52% 20% 25%
1	V	493	51% 20% 25%
2	1	522	48% 19% 29%
2	C	522	48% 19% 29%
2	H	522	49% 19% 29%

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Mol	Chain	Length	Quality of chain
2	M	522	49% 19% 29%
2	R	522	6% 45% 19% 29%
2	W	522	48% 20% 29%
3	2	461	52% 23% 20%
3	A	461	54% 22% 20%
3	D	461	53% 23% 20%
3	F	461	54% 22% 20%
3	I	461	53% 22% 20%
3	K	461	52% 21% 20%
3	N	461	53% 22% 20%
3	P	461	54% 22% 20%
3	S	461	52% 23% 20%
3	U	461	54% 21% 20%
3	X	461	5% 52% 21% 20%
3	Z	461	53% 21% 20%
4	3	505	5% 47% 19% 27%
4	E	505	50% 19% 27%
4	J	505	50% 19% 27%
4	O	505	48% 19% 27%
4	T	505	50% 19% 27%
4	Y	505	49% 19% 27%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 89544 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 BETA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	370	Total	C	N	O	S	0	0
			2972	1938	465	554	15		
1	B	370	Total	C	N	O	S	0	0
			2972	1938	465	554	15		
1	G	370	Total	C	N	O	S	0	0
			2972	1938	465	554	15		
1	L	370	Total	C	N	O	S	0	0
			2972	1938	465	554	15		
1	Q	370	Total	C	N	O	S	0	0
			2972	1938	465	554	15		
1	V	370	Total	C	N	O	S	0	0
			2972	1938	465	554	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	370	Total	C	N	O	S	0	1
			2983	1944	489	536	14		
2	C	370	Total	C	N	O	S	0	1
			2983	1944	489	536	14		
2	H	370	Total	C	N	O	S	0	1
			2983	1944	489	536	14		
2	M	370	Total	C	N	O	S	0	1
			2983	1944	489	536	14		
2	R	370	Total	C	N	O	S	0	1
			2983	1944	489	536	14		
2	W	370	Total	C	N	O	S	0	1
			2983	1944	489	536	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
3	D	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
3	F	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
3	I	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
3	K	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
3	N	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
3	P	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
3	S	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
3	U	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
3	X	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
3	Z	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		

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

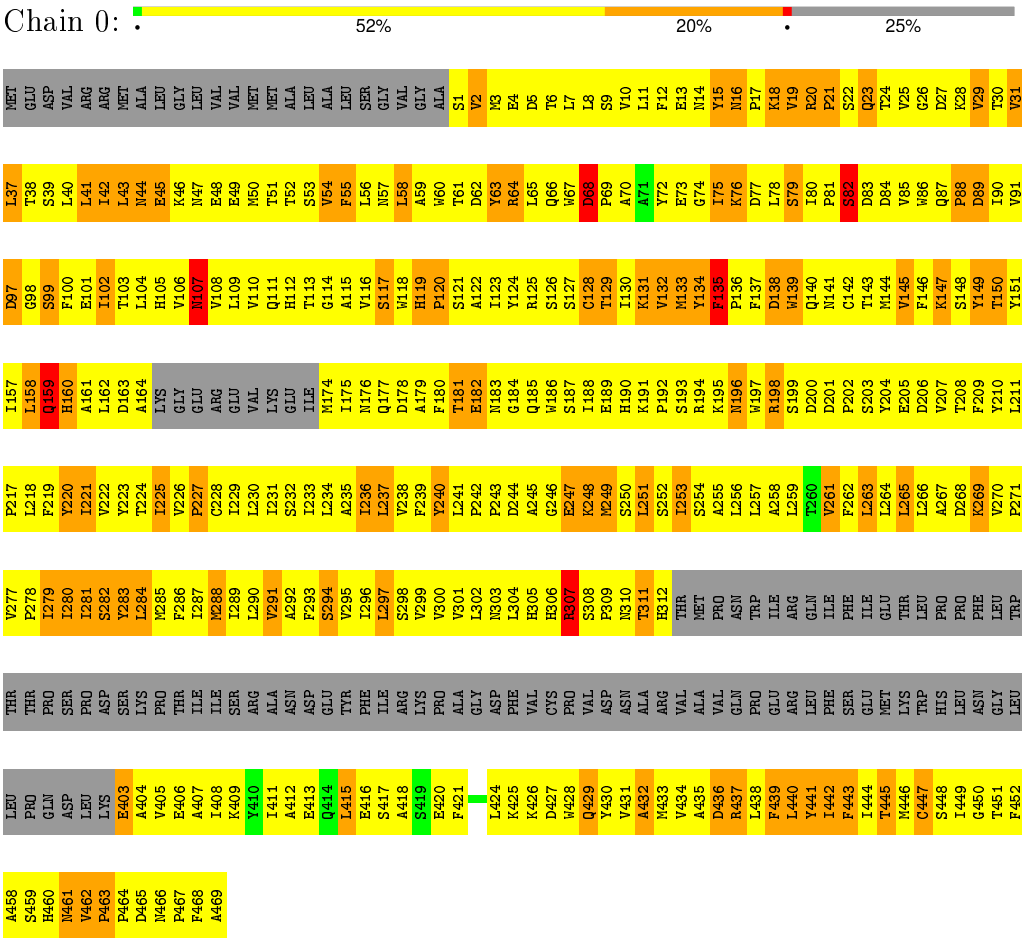
Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		
4	E	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		
4	J	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		
4	O	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		
4	T	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		
4	Y	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		

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 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.

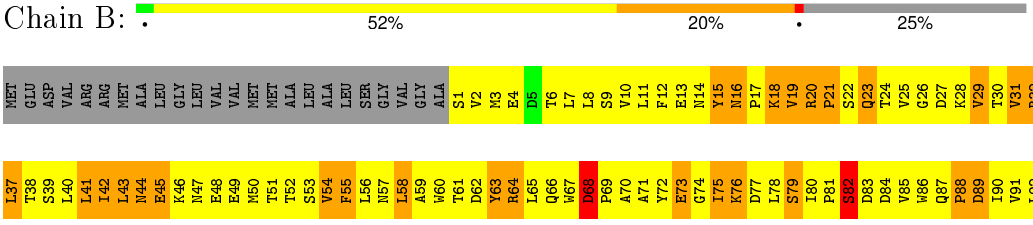
- Molecule 1: ACETYLCHOLINE RECEPTOR BETA SUBUNIT

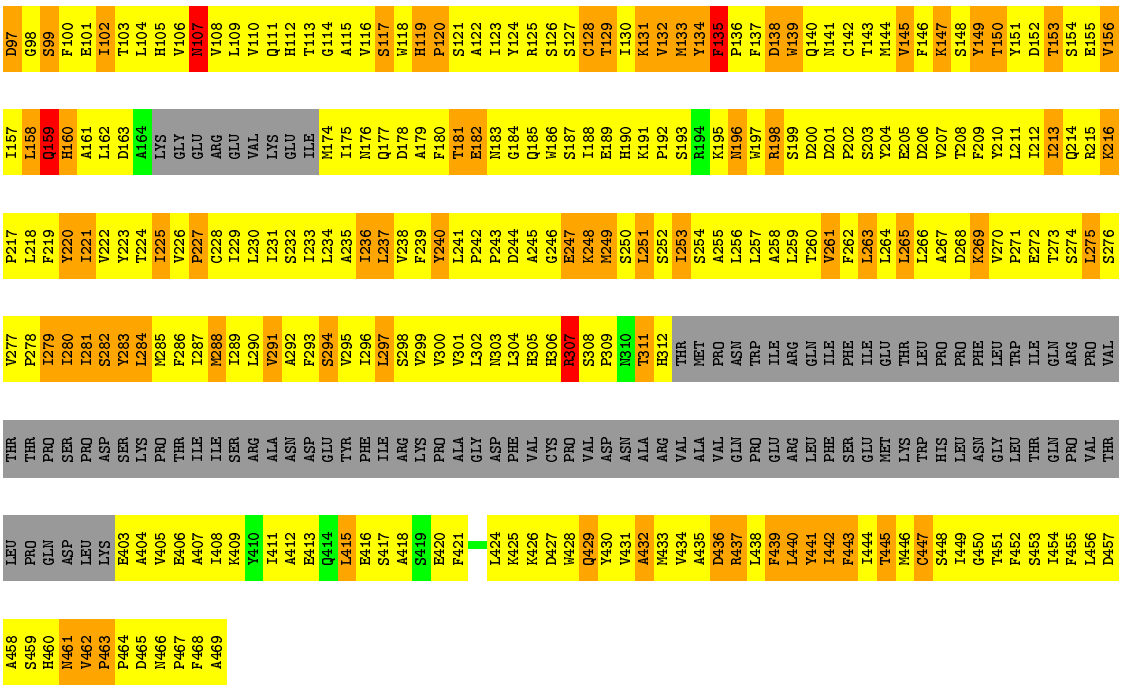
Chain 0:



- Molecule 1: ACETYLCHOLINE RECEPTOR BETA SUBUNIT

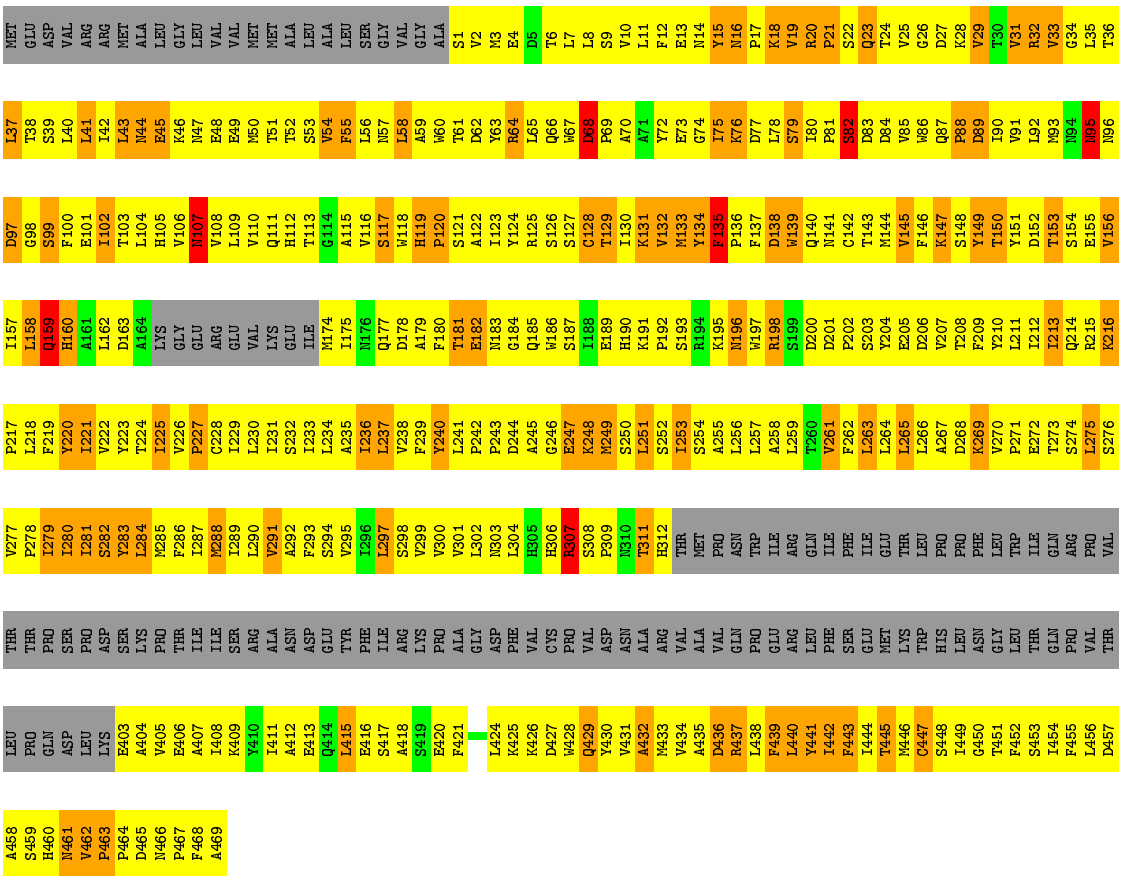
Chain B:





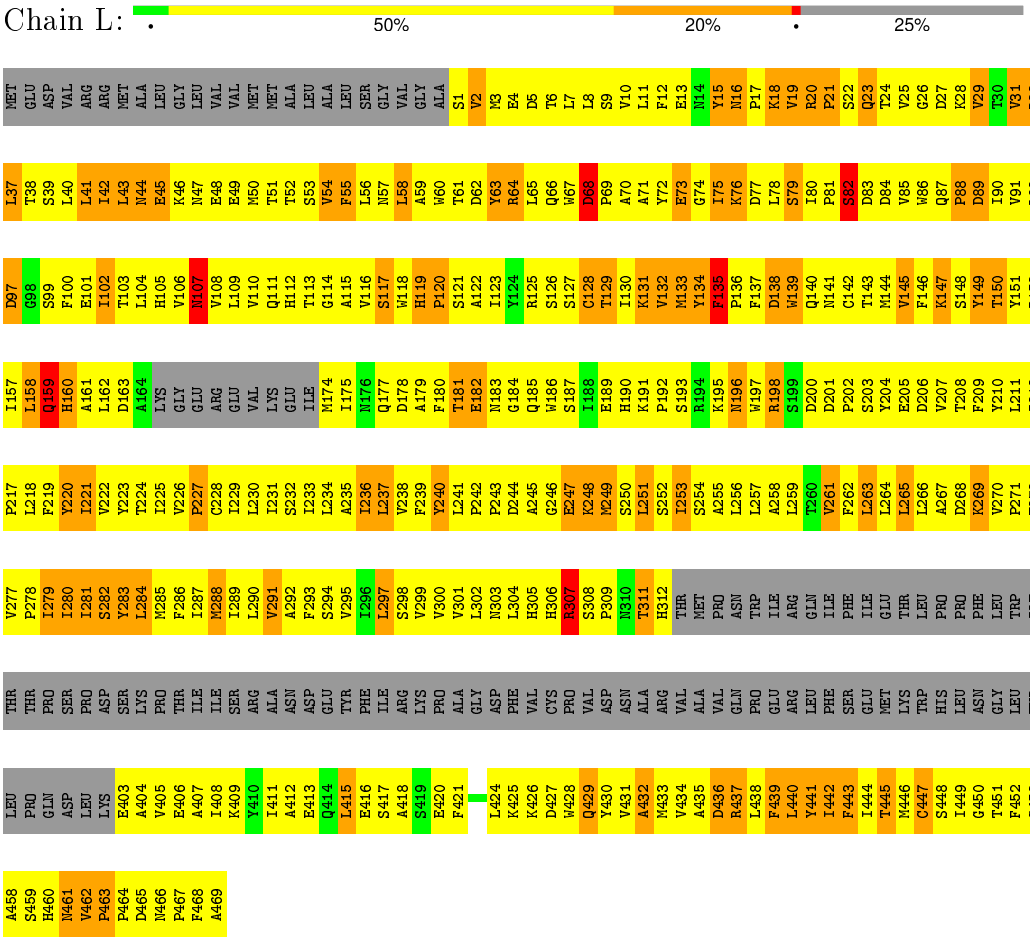
• Molecule 1: ACETYLCHOLINE RECEPTOR BETA SUBUNIT

Chain G:



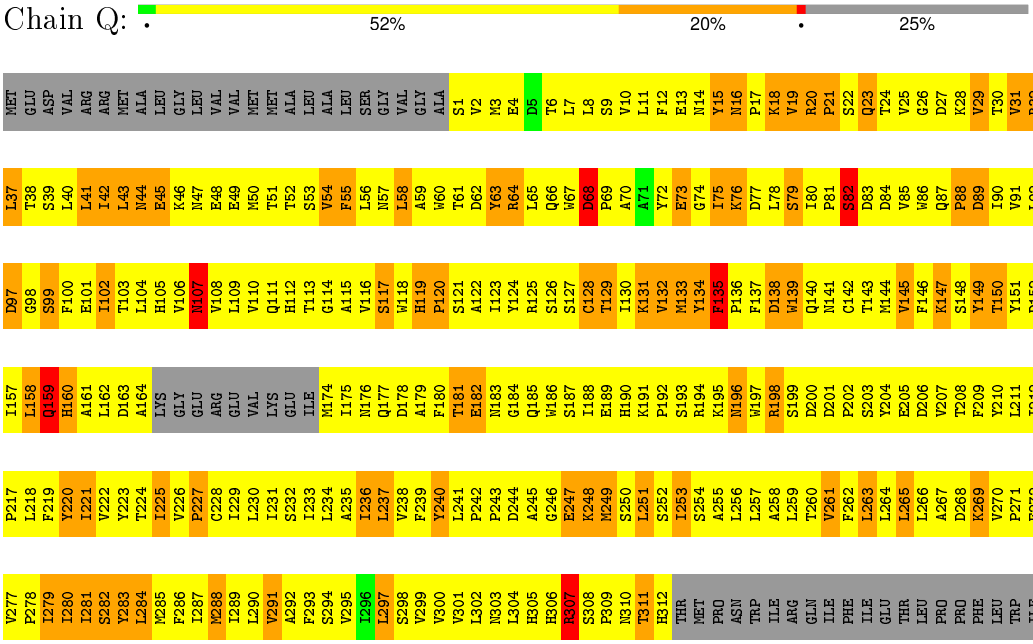
• Molecule 1: ACETYLCHOLINE RECEPTOR BETA SUBUNIT

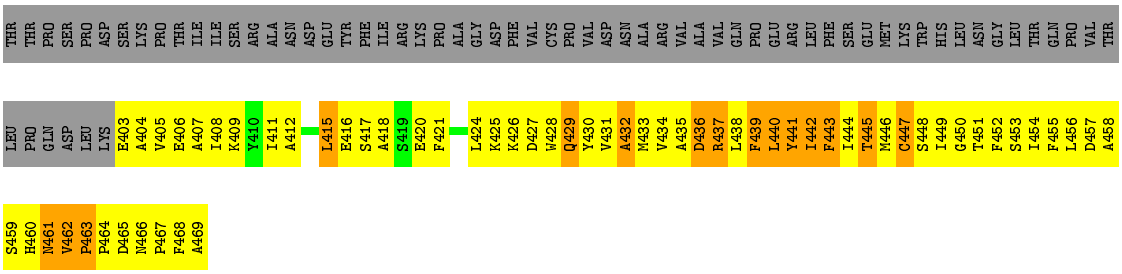
Chain L:



• Molecule 1: ACETYLCHOLINE RECEPTOR BETA SUBUNIT

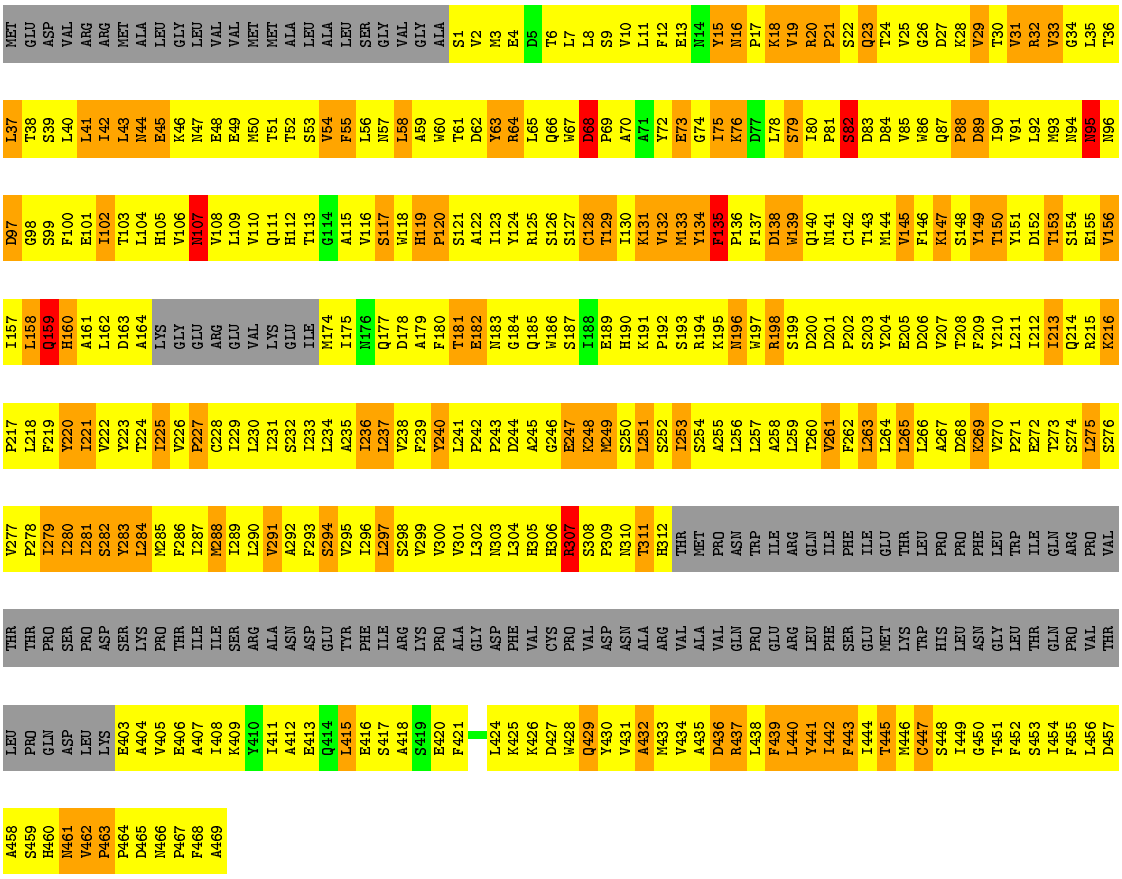
Chain Q:





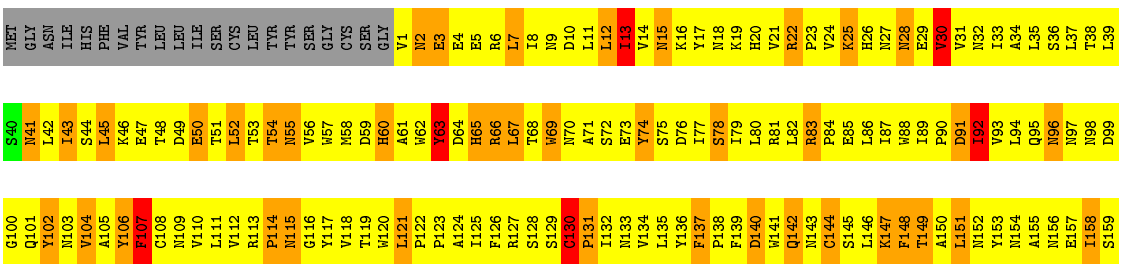
• Molecule 1: ACETYLCHOLINE RECEPTOR BETA SUBUNIT

Chain V: 51% 20% 25%



• Molecule 2: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT

Chain 1: 48% 19% 29%



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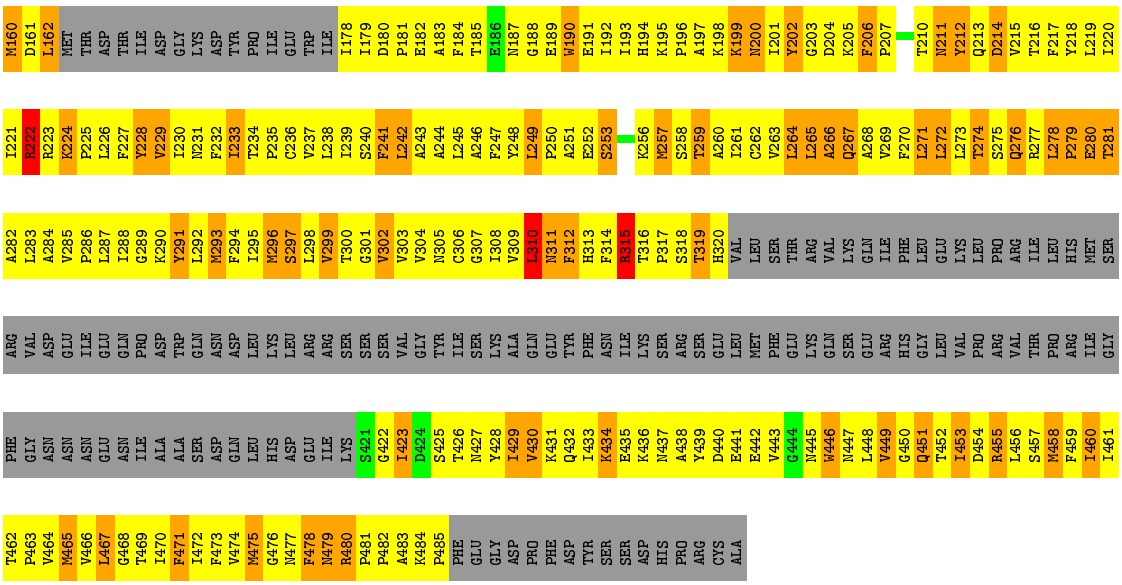
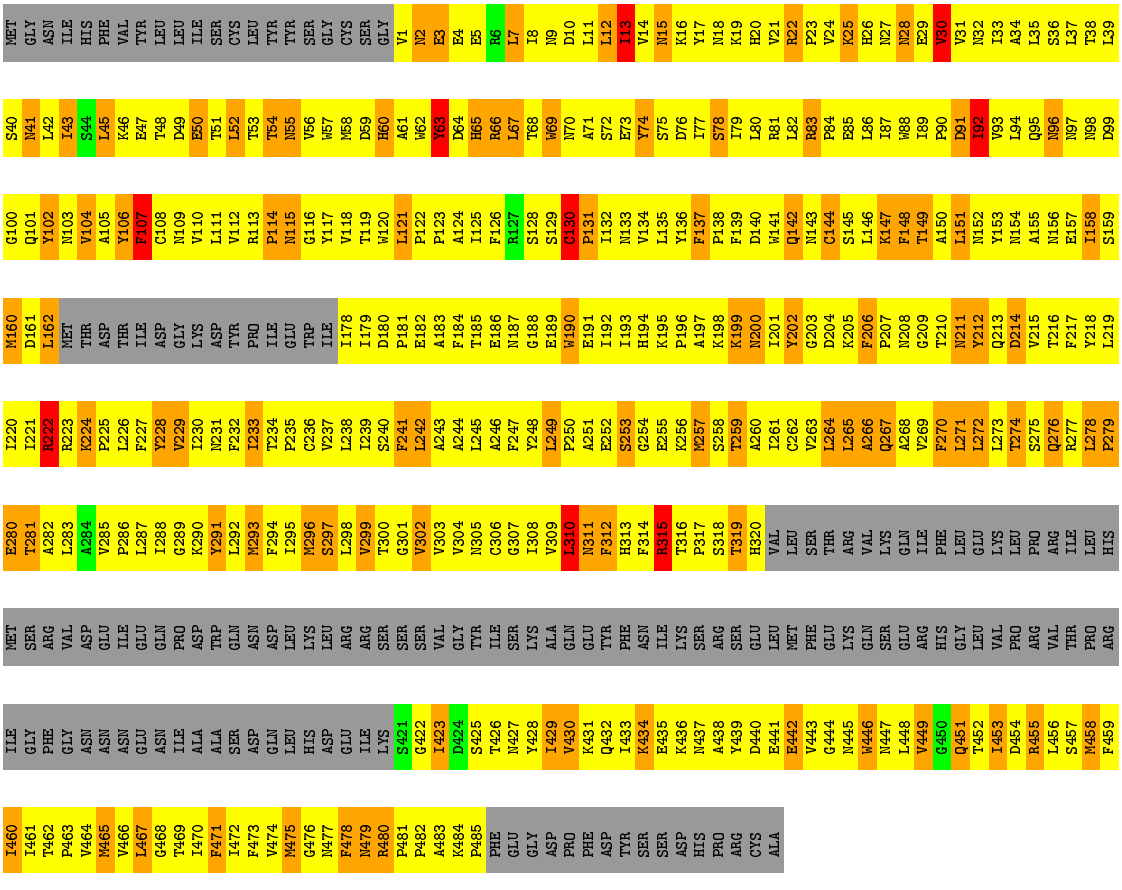


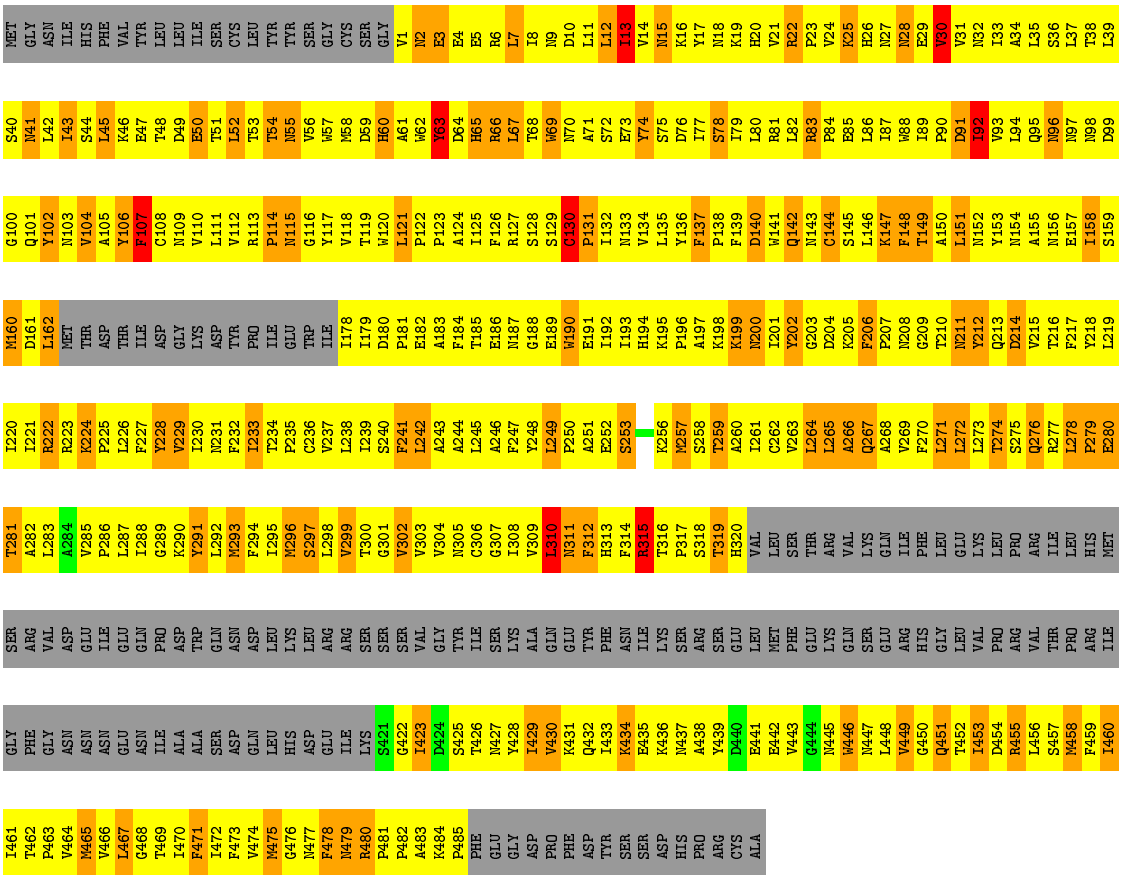
• Molecule 2: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT

Chain C:



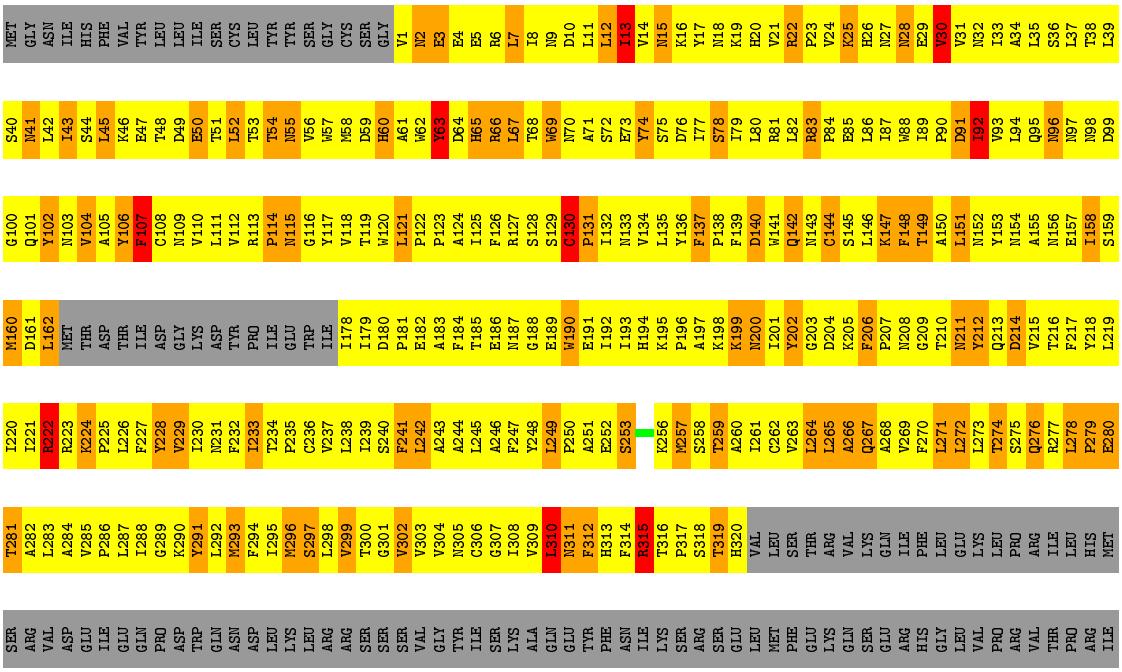
• Molecule 2: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT

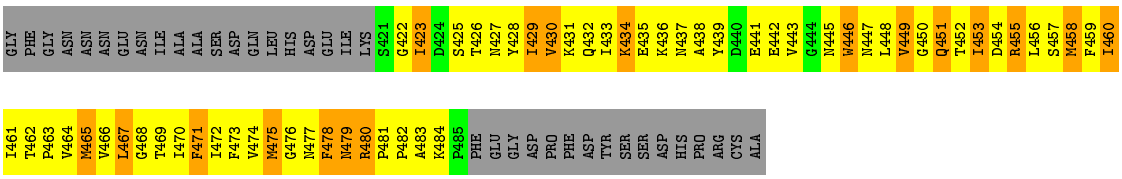
Chain H:



• Molecule 2: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT

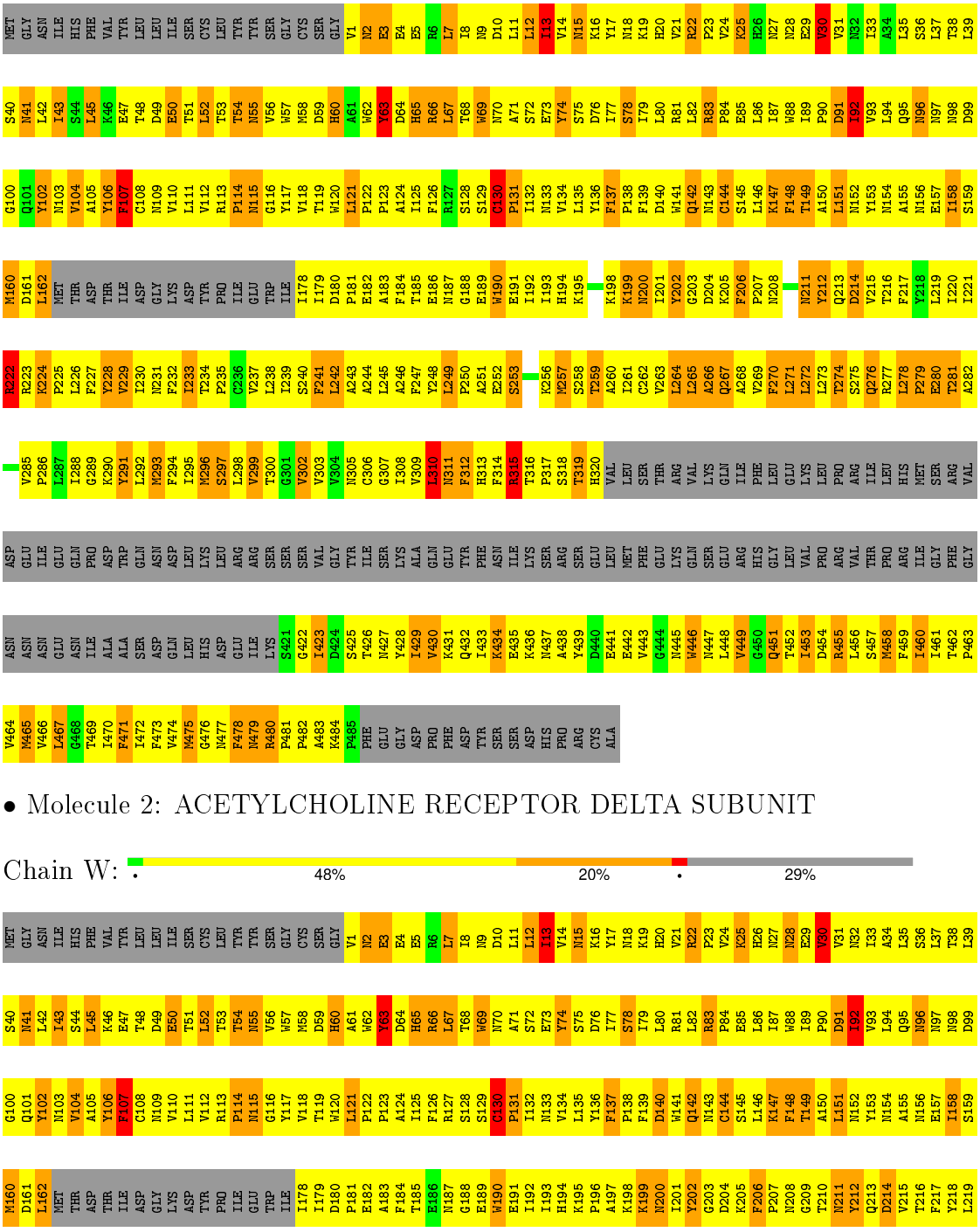
Chain M:





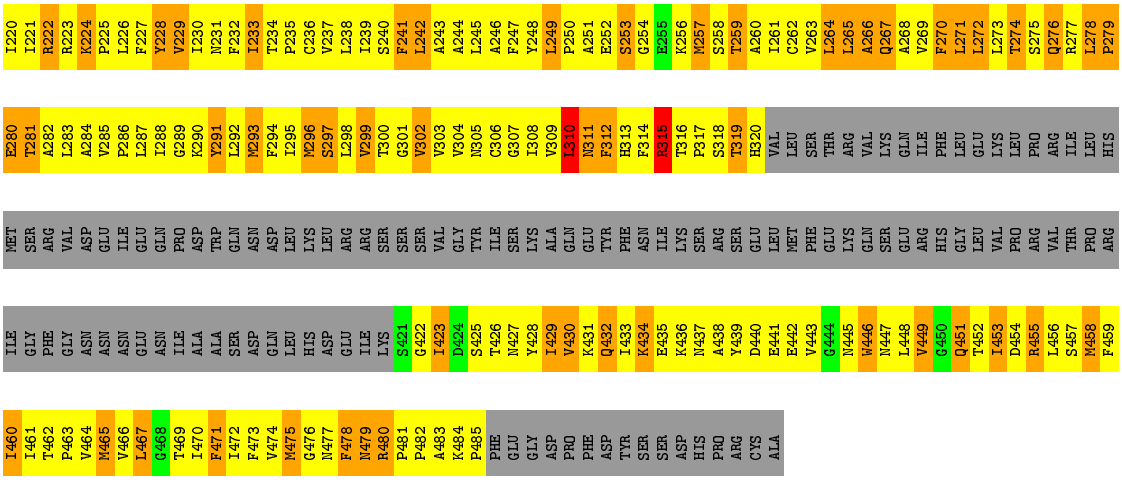
• Molecule 2: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT

Chain R:



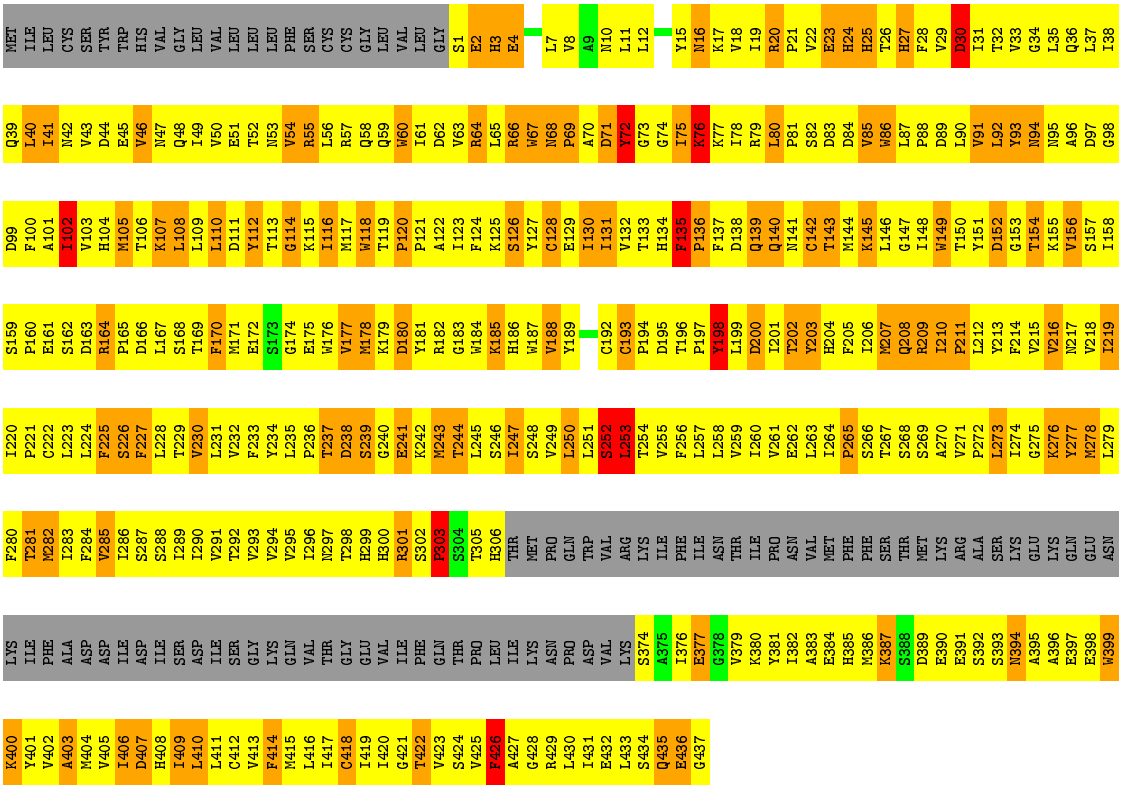
• Molecule 2: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT

Chain W:



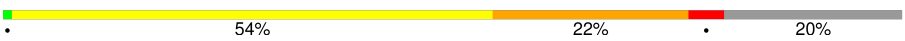
• Molecule 3: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

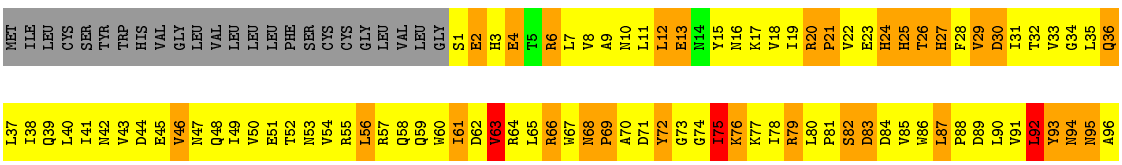
Chain 2:

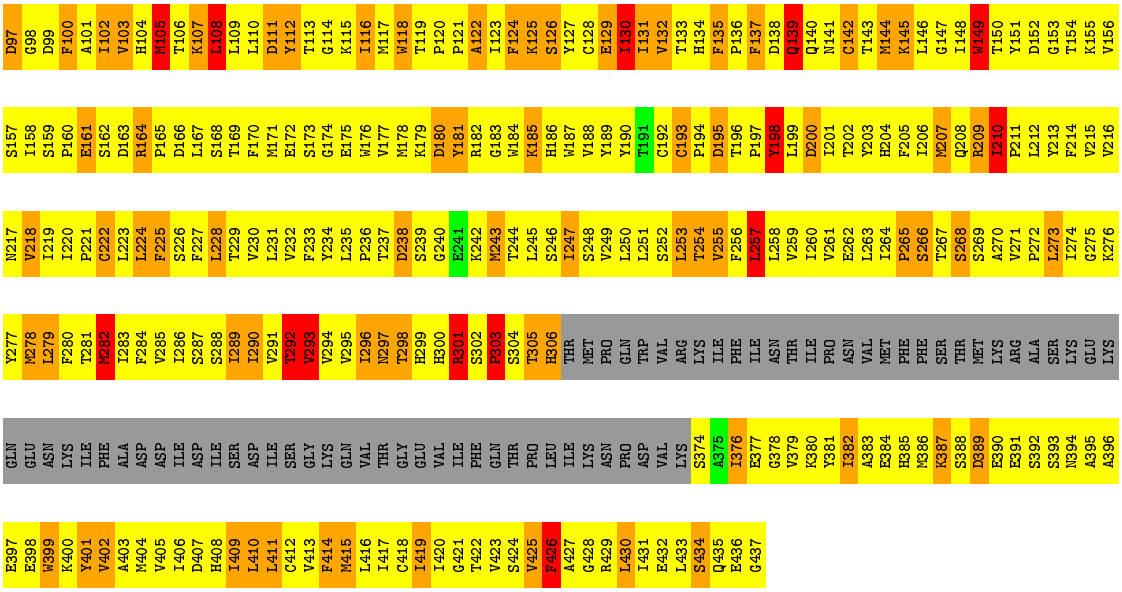


• Molecule 3: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

Chain A:

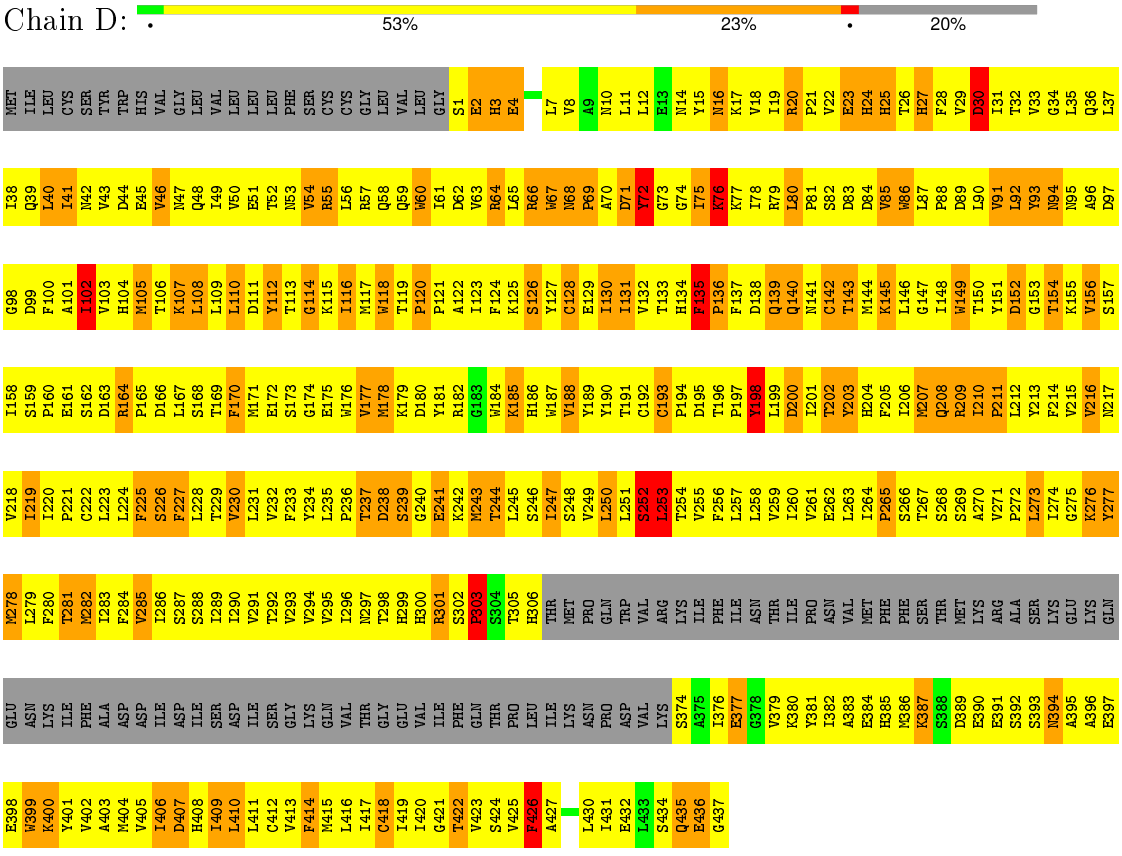






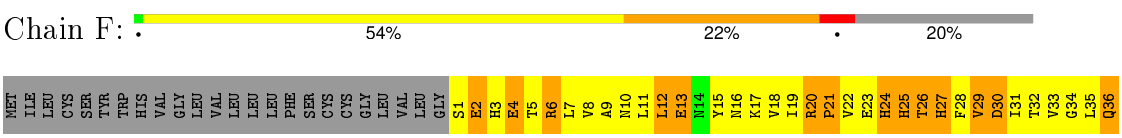
• Molecule 3: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

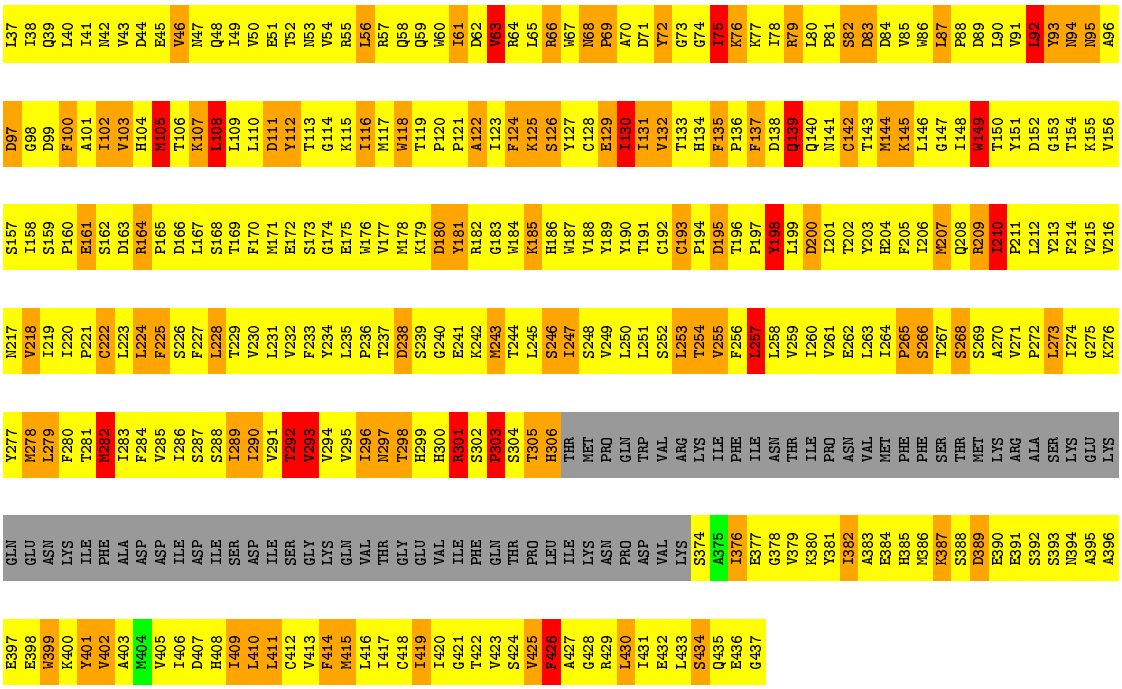
Chain D:



• Molecule 3: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

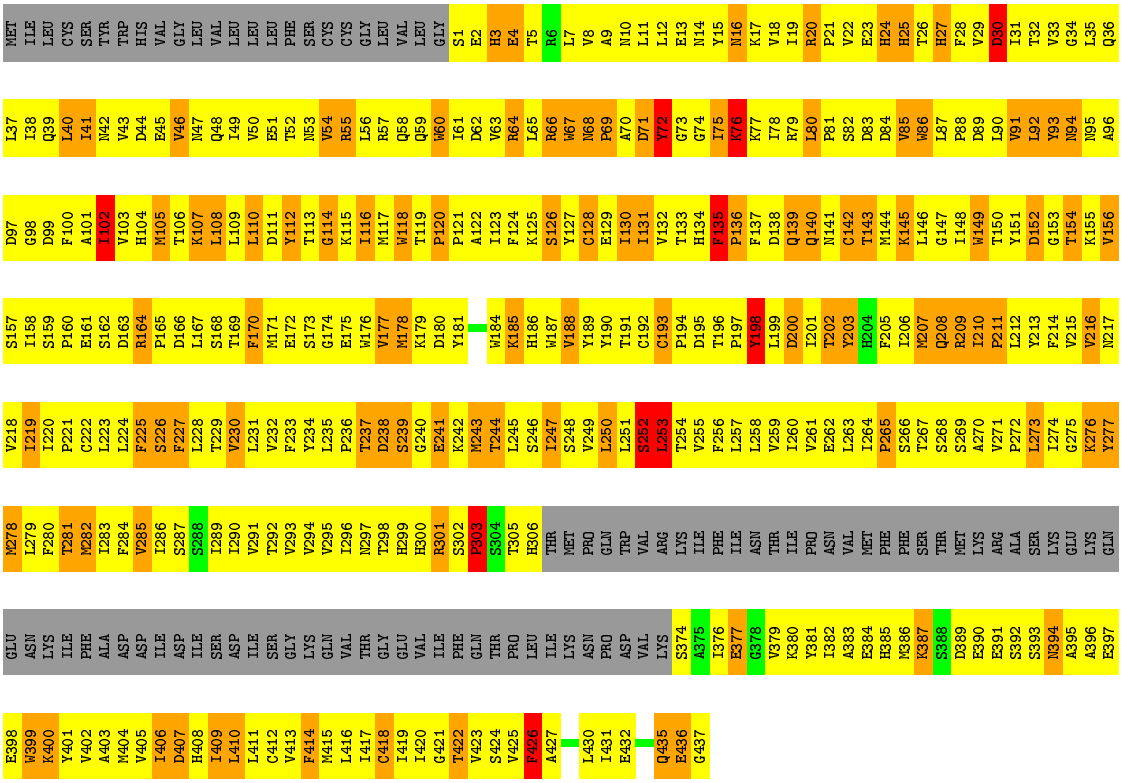
Chain F:





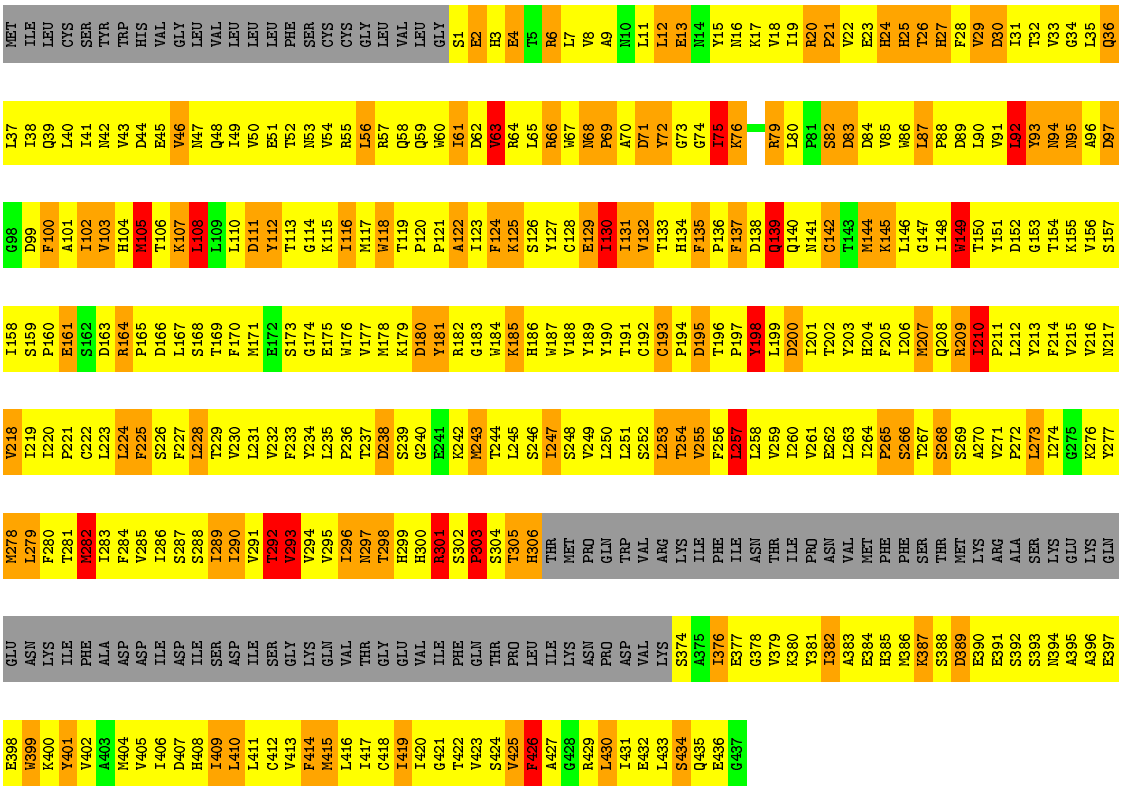
• Molecule 3: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

Chain I:



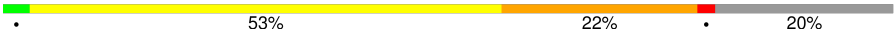
• Molecule 3: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

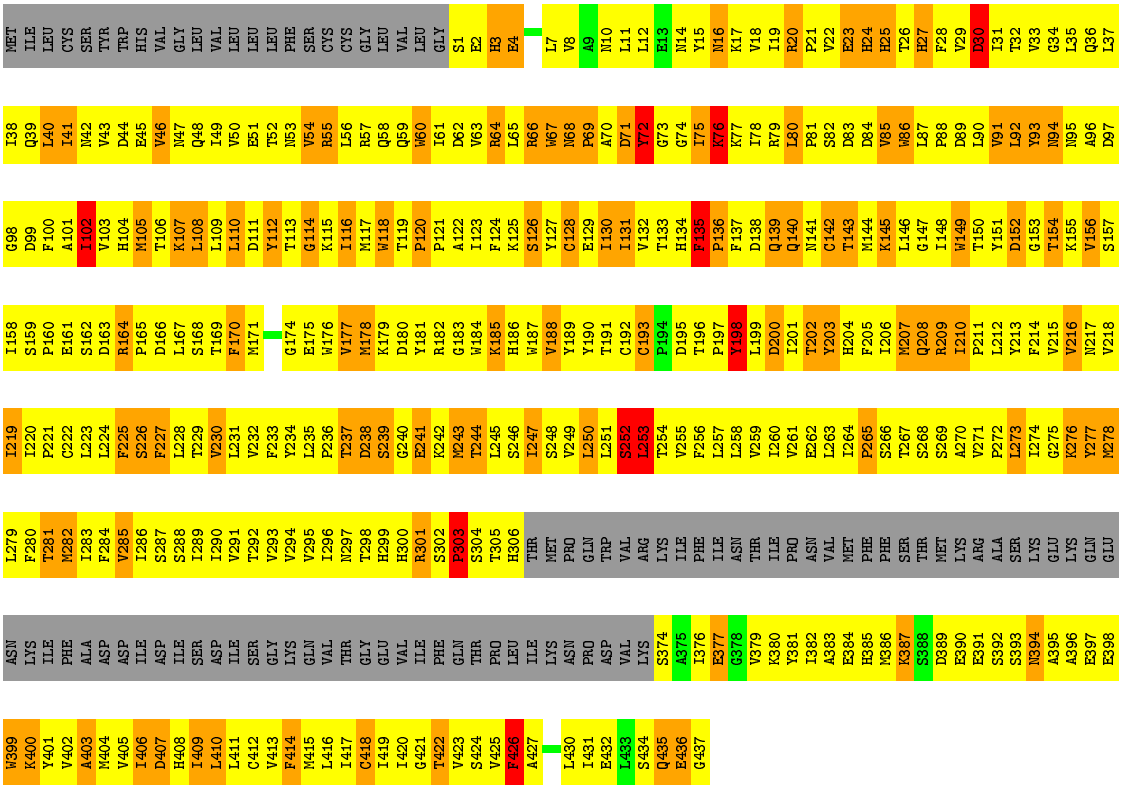
Chain K:



• Molecule 3: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

Chain N:





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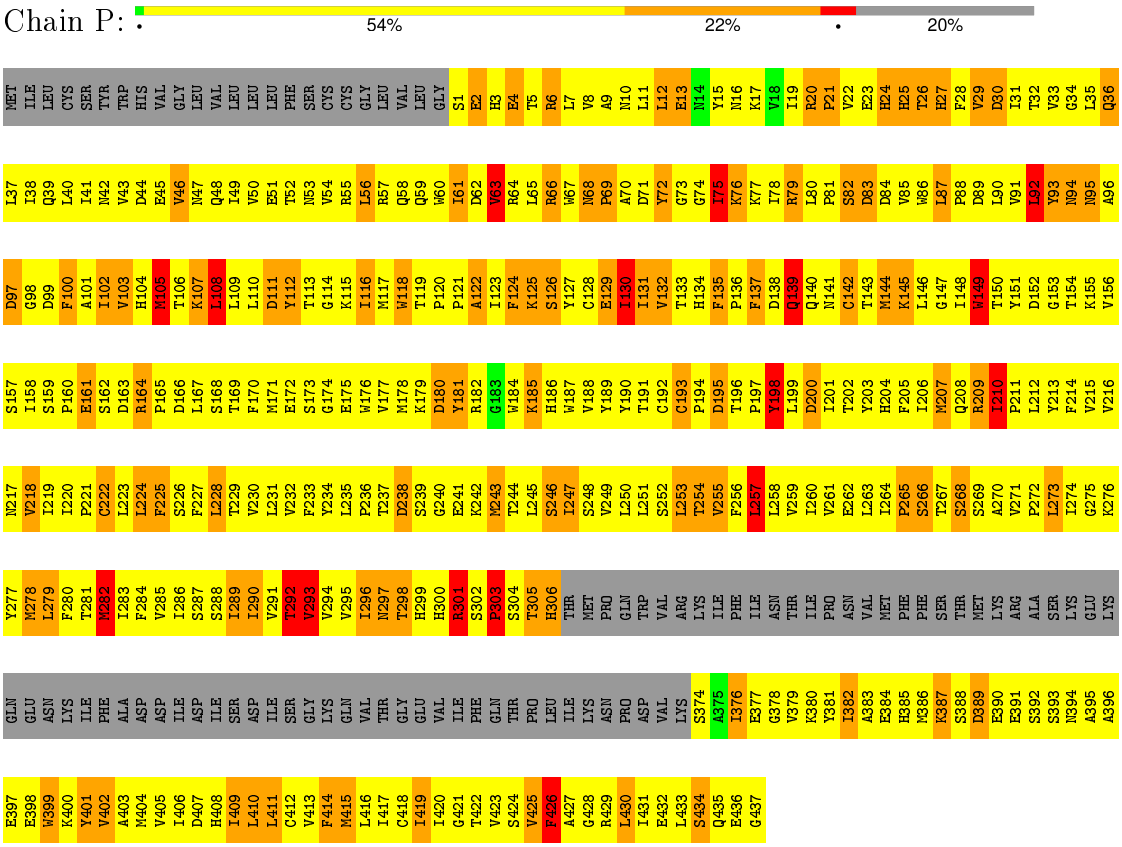
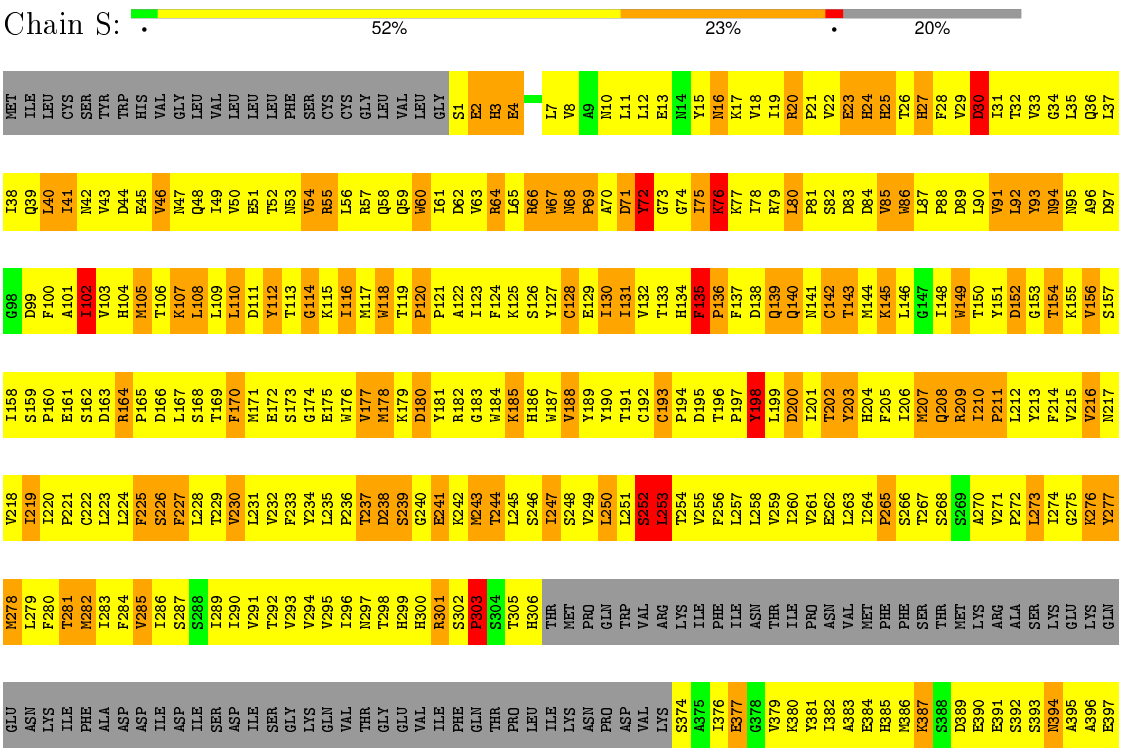
• Molecule 3: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

Chain P:



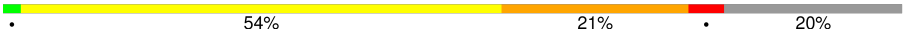
• Molecule 3: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

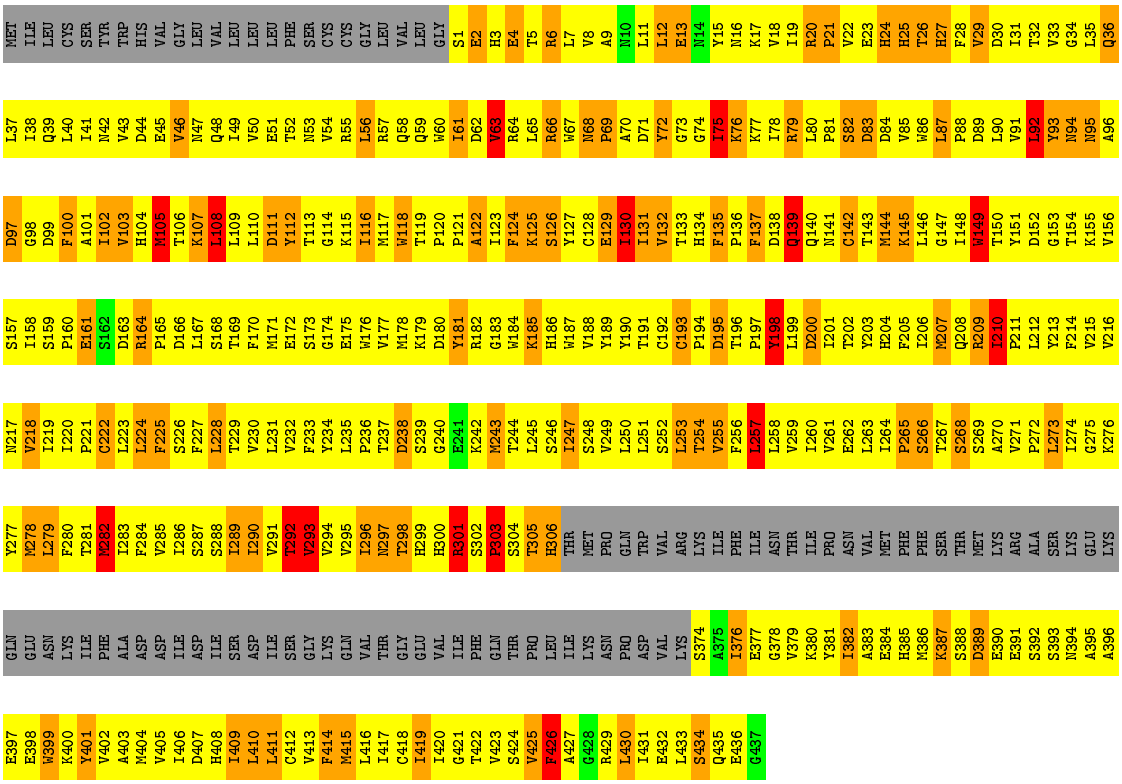
Chain S:

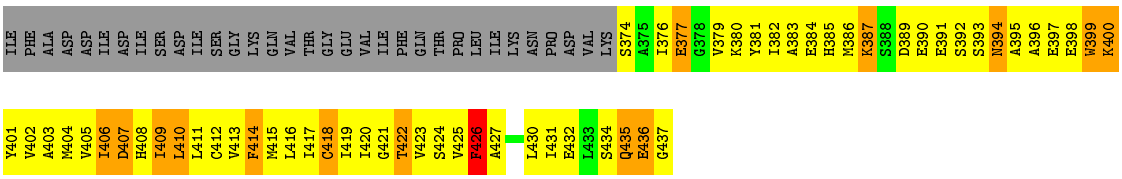


• Molecule 3: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

Chain U:

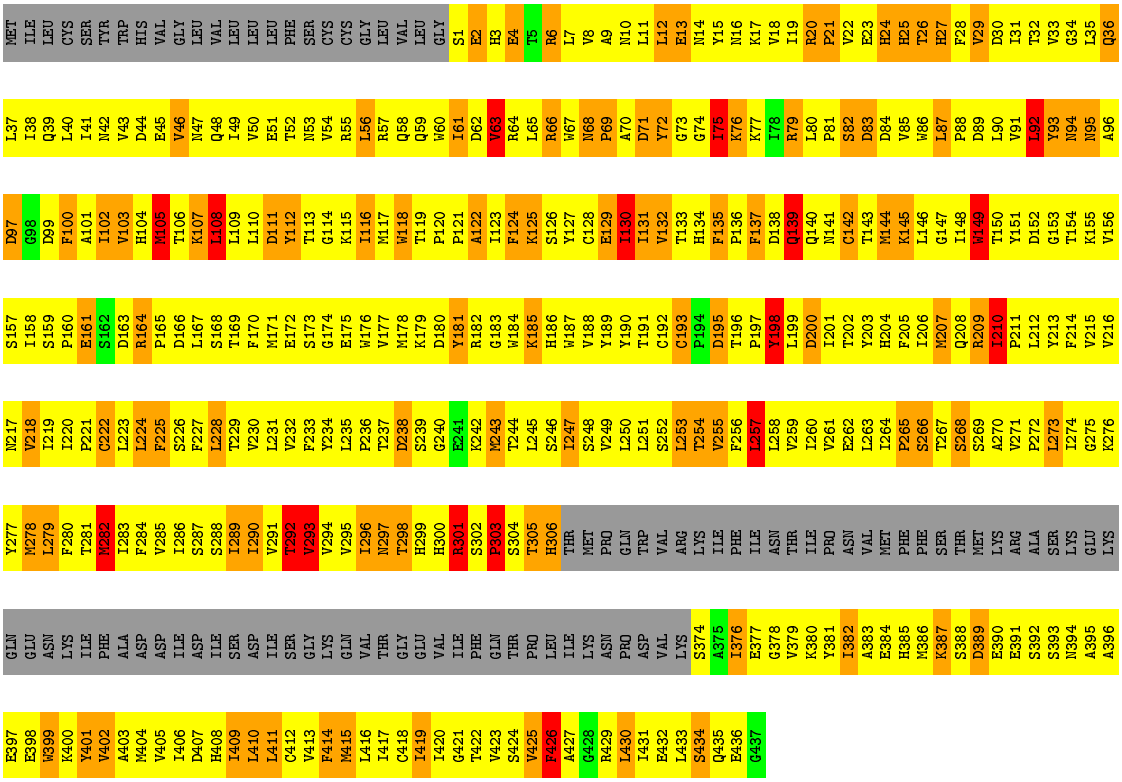






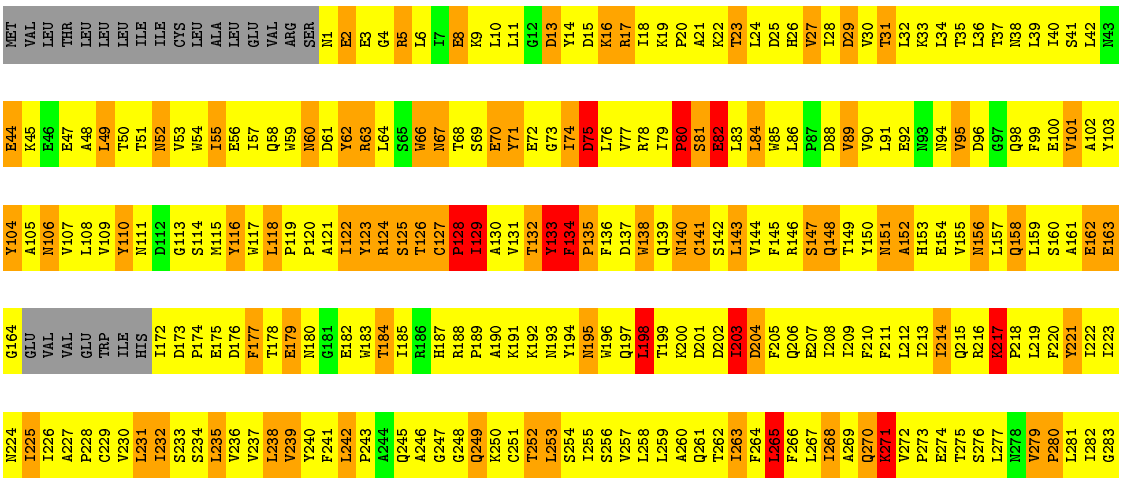
• Molecule 3: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

Chain Z:



• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

Chain 3:



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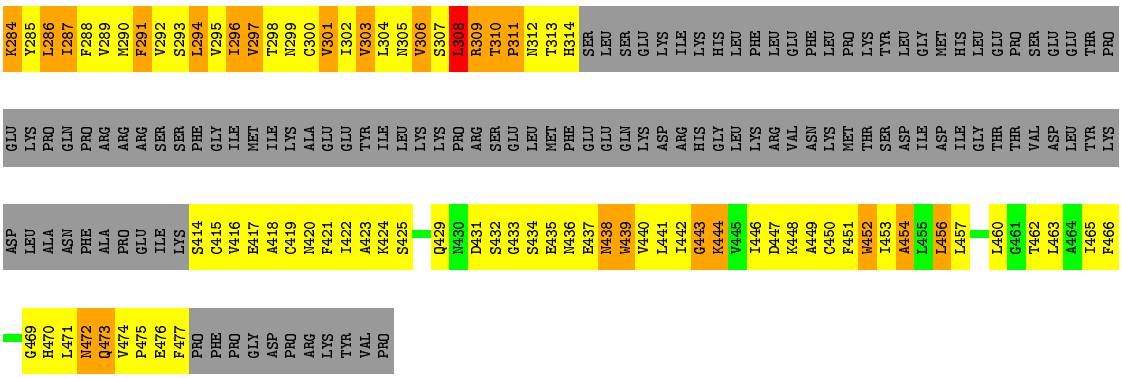
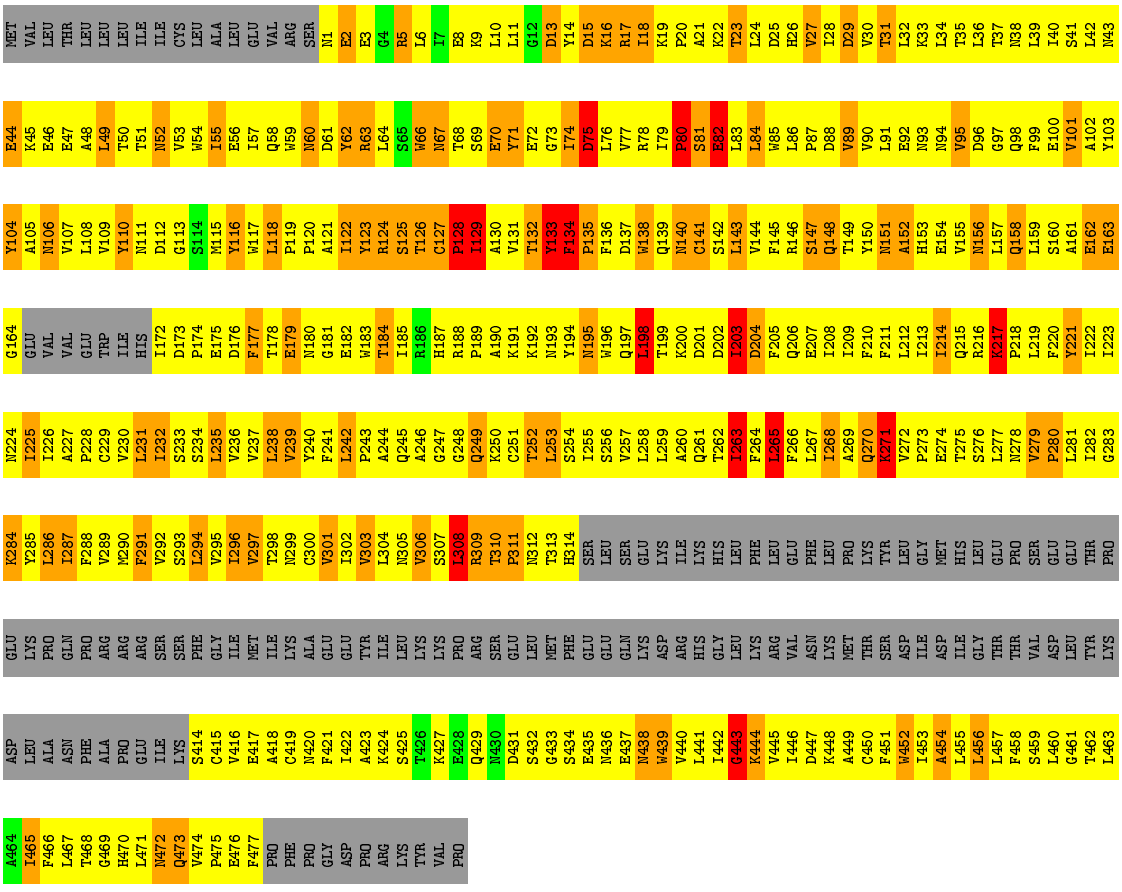
EMDataBank Unified Data Resource for 3DEM



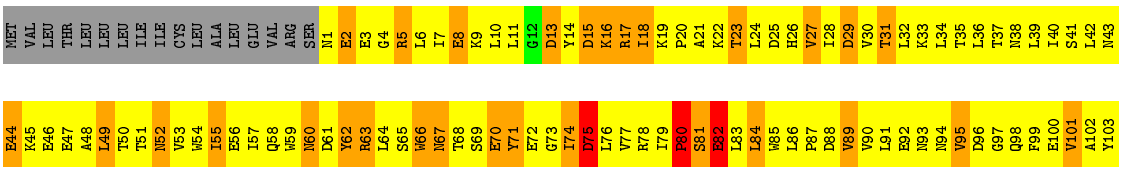
• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

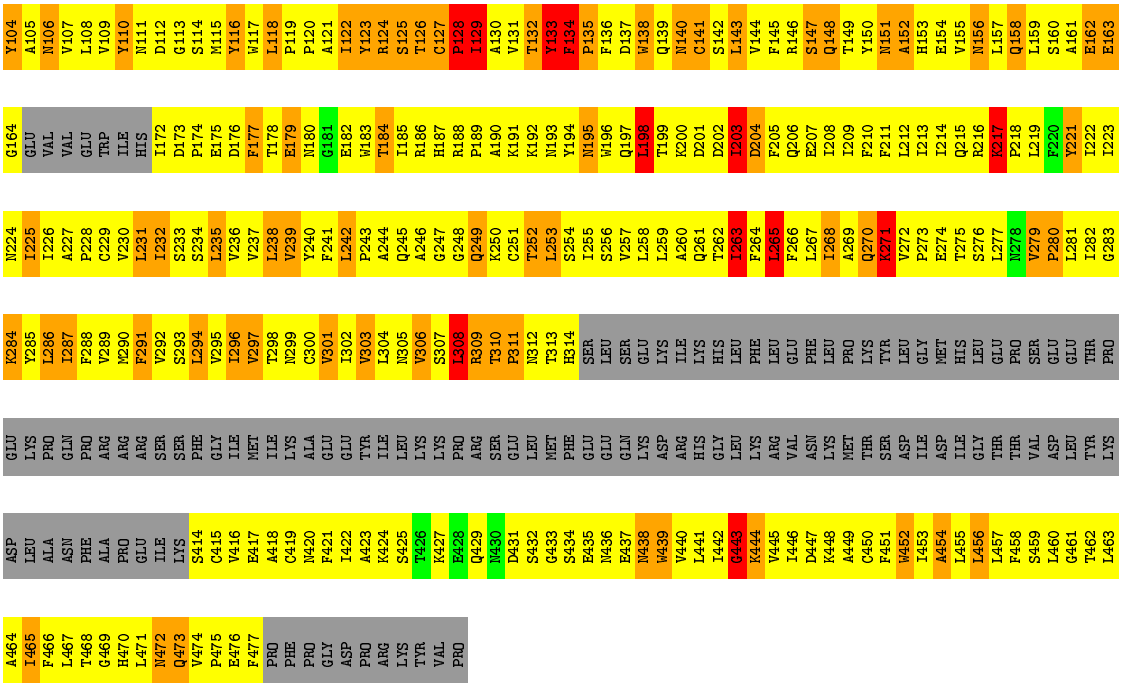
Chain E:



• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

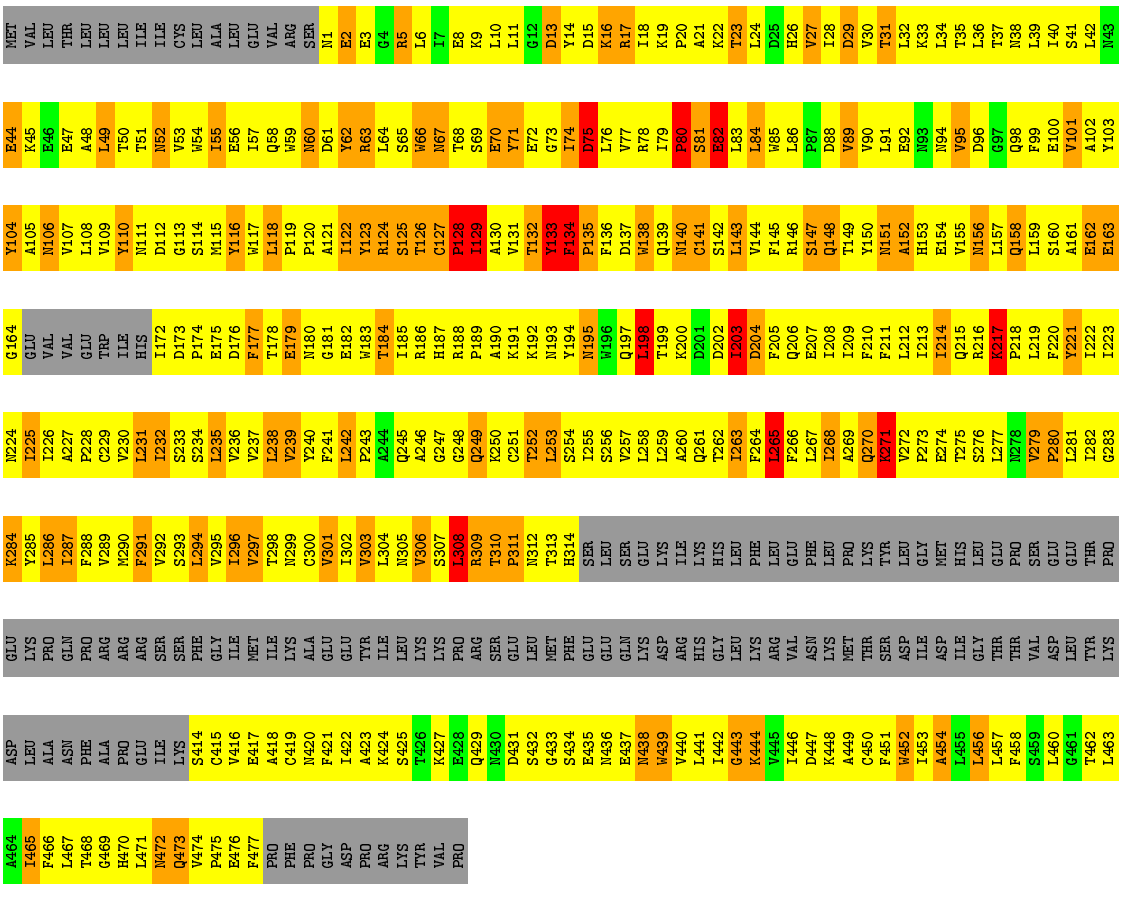
Chain J:





• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

Chain O:



WORLDWIDE PDB PROTEIN DATA BANK
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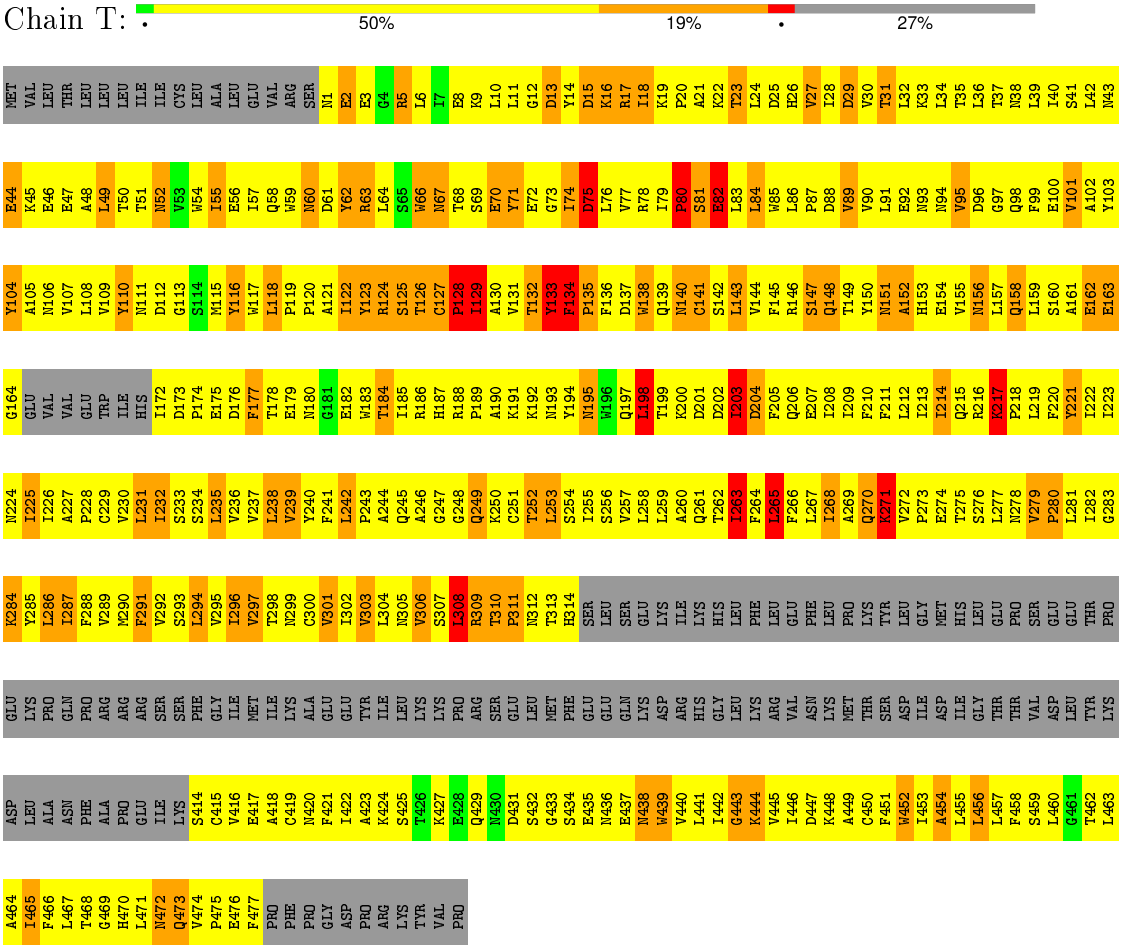
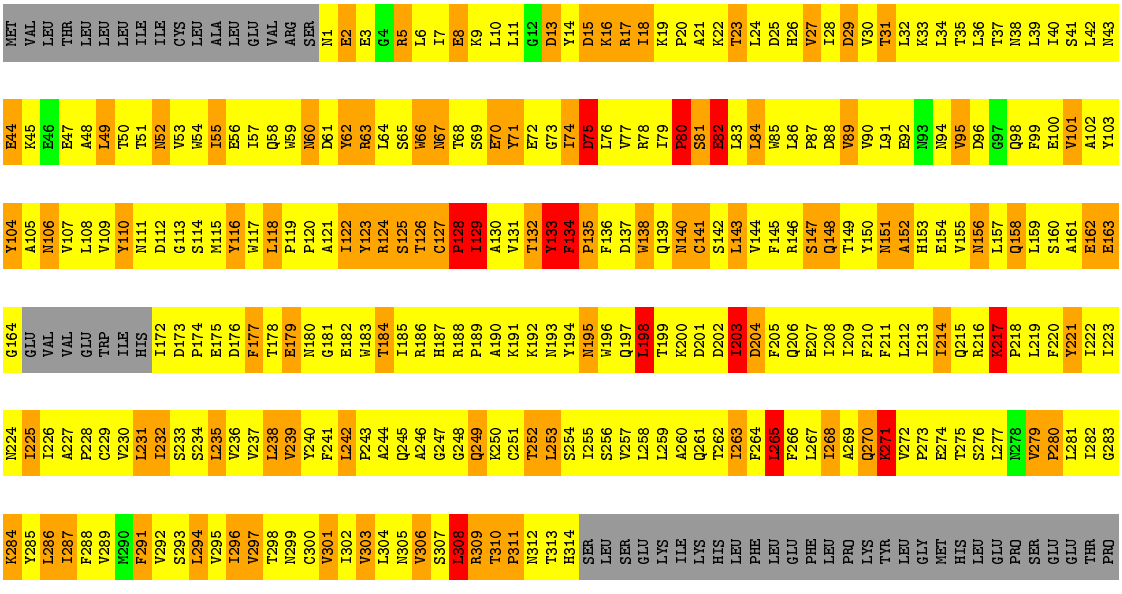
• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

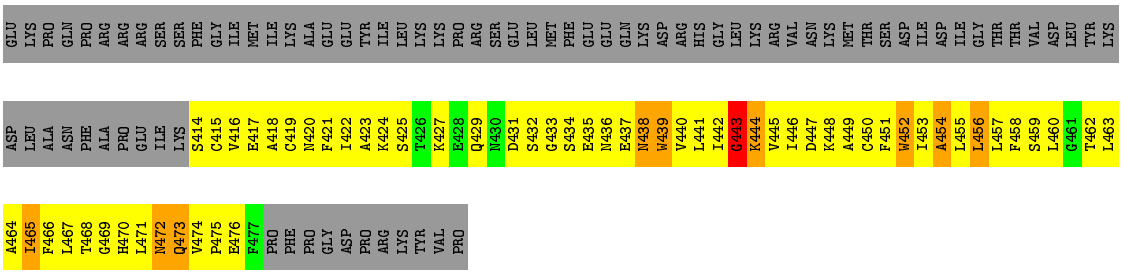
Chain T:



• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

Chain Y:




GLU LYS PRO GLN PRO ARG ARG ARG SER SER PHE GLY ILE MET ILE LYS ALA GLU GLU TYR ILE LEU LYS LYS PRO ARG SER GLU LEU MET PHE GLU GLU GLN LYS ASP ARG HIS GLY LEU LYS ARG VAL ASN LYS MET THR SER ASP ILE ASP ILE GLY THR THR VAL ASP LEU TYR LYS
ASP LEU ALA ASN PHE ALA PRO GLU ILE LYS S414 C415 V416 E417 A418 C419 N420 F421 I422 A423 K424 S425 T426 K427 E428 Q429 M430 D431 S432 G433 S434 E435 N436 E437 N438 W439 V440 L441 I442 G443 K444 V445 I446 D447 K448 A449 C450 F451 W452 I453 A454 L455 L456 L457 F458 S459 L460 G461 T462 L463
A464 T465 F466 L467 T468 G469 H470 L471 N472 Q473 V474 P475 E476 F477 PRO PHE PRO GLY ASP PRO ARG LYS TYR VAL PRO

4 Experimental information (i)

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided, Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	69000	Depositor
Image detector	GATAN US4000	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	0	0.76	2/3048 (0.1%)	0.99	4/4162 (0.1%)
1	B	0.76	2/3048 (0.1%)	0.99	4/4162 (0.1%)
1	G	0.76	2/3048 (0.1%)	0.99	4/4162 (0.1%)
1	L	0.76	2/3048 (0.1%)	0.99	4/4162 (0.1%)
1	Q	0.76	2/3048 (0.1%)	0.99	4/4162 (0.1%)
1	V	0.76	2/3048 (0.1%)	0.99	4/4162 (0.1%)
2	1	0.74	2/3059 (0.1%)	1.03	9/4175 (0.2%)
2	C	0.74	2/3059 (0.1%)	1.03	9/4175 (0.2%)
2	H	0.74	2/3059 (0.1%)	1.03	8/4175 (0.2%)
2	M	0.74	2/3059 (0.1%)	1.03	9/4175 (0.2%)
2	R	0.74	2/3059 (0.1%)	1.03	9/4175 (0.2%)
2	W	0.75	2/3059 (0.1%)	1.03	8/4175 (0.2%)
3	2	0.74	2/3069 (0.1%)	1.01	6/4186 (0.1%)
3	A	0.72	3/3069 (0.1%)	1.03	10/4186 (0.2%)
3	D	0.74	2/3069 (0.1%)	1.01	6/4186 (0.1%)
3	F	0.72	3/3069 (0.1%)	1.03	10/4186 (0.2%)
3	I	0.74	2/3069 (0.1%)	1.01	6/4186 (0.1%)
3	K	0.72	3/3069 (0.1%)	1.03	10/4186 (0.2%)
3	N	0.74	2/3069 (0.1%)	1.01	6/4186 (0.1%)
3	P	0.72	3/3069 (0.1%)	1.03	10/4186 (0.2%)
3	S	0.74	2/3069 (0.1%)	1.01	6/4186 (0.1%)
3	U	0.72	3/3069 (0.1%)	1.03	10/4186 (0.2%)
3	X	0.74	2/3069 (0.1%)	1.01	6/4186 (0.1%)
3	Z	0.72	3/3069 (0.1%)	1.03	10/4186 (0.2%)
4	3	0.73	6/3057 (0.2%)	1.01	9/4174 (0.2%)
4	E	0.73	6/3057 (0.2%)	1.01	9/4174 (0.2%)
4	J	0.73	6/3057 (0.2%)	1.01	9/4174 (0.2%)
4	O	0.73	6/3057 (0.2%)	1.01	9/4174 (0.2%)
4	T	0.73	6/3057 (0.2%)	1.01	9/4174 (0.2%)
4	Y	0.73	6/3057 (0.2%)	1.01	9/4174 (0.2%)
All	All	0.74	90/91812 (0.1%)	1.01	226/125298 (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
2	1	0	2
2	C	0	2
2	H	0	2
2	M	0	2
2	R	0	2
2	W	0	2
3	2	0	2
3	D	0	2
3	I	0	2
3	N	0	2
3	S	0	2
3	X	0	2
All	All	0	24

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	THR	C-N	-8.43	1.14	1.34
1	L	129	THR	C-N	-8.42	1.14	1.34
1	V	129	THR	C-N	-8.42	1.14	1.34
1	0	129	THR	C-N	-8.41	1.14	1.34
1	G	129	THR	C-N	-8.40	1.14	1.34

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	266	ALA	N-CA-CB	10.41	124.67	110.10
2	C	266	ALA	N-CA-CB	10.40	124.66	110.10
2	1	266	ALA	N-CA-CB	10.39	124.64	110.10
2	H	266	ALA	N-CA-CB	10.39	124.64	110.10
2	R	266	ALA	N-CA-CB	10.39	124.64	110.10

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	63	TYR	Sidechain
2	1	74	TYR	Sidechain
3	2	277	TYR	Sidechain
3	2	72	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	C	63	TYR	Sidechain

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	0	2972	0	2952	1088	7802
1	B	2972	0	2952	1083	3661
1	G	2972	0	2953	1088	1593
1	L	2972	0	2953	1094	1307
1	Q	2972	0	2952	1084	5595
1	V	2972	0	2952	1069	4109
2	1	2983	0	2987	1163	7210
2	C	2983	0	2987	1152	3764
2	H	2983	0	2987	1166	6117
2	M	2983	0	2987	1156	7545
2	R	2983	0	2987	1158	1006
2	W	2983	0	2987	1150	4296
3	2	2991	0	3006	1054	5605
3	A	2991	0	3005	1077	8192
3	D	2991	0	3006	1060	5713
3	F	2991	0	3005	1085	5994
3	I	2991	0	3006	1056	3886
3	K	2991	0	3005	1077	1150
3	N	2991	0	3006	1066	3557
3	P	2991	0	3005	1069	5628
3	S	2991	0	3006	1052	3544
3	U	2991	0	3005	1069	5618
3	X	2991	0	3006	1067	746
3	Z	2991	0	3005	1075	4197
4	3	2987	0	2994	1084	1711
4	E	2987	0	2994	1088	5363
4	J	2987	0	2994	1093	6974
4	O	2987	0	2994	1098	2002
4	T	2987	0	2994	1090	3133
4	Y	2987	0	2994	1091	4518
All	All	89544	0	89666	31224	65768

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 174.

The worst 5 of 31224 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)
4:Y:183:TRP:CB	4:Y:216:ARG:HG2	1.33	1.59
4:3:183:TRP:CB	4:3:216:ARG:HG2	1.33	1.56
4:E:183:TRP:CB	4:E:216:ARG:HG2	1.33	1.55
4:J:183:TRP:CB	4:J:216:ARG:HG2	1.33	1.53
1:G:134:TYR:CE1	1:G:213:ILE:HG13	1.44	1.52

The worst 5 of 65768 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:VAL:CG2	3:F:111:ASP:OD1[1_655]	0.03	2.17
3:P:22:VAL:N	3:U:17:LYS:NZ[1_455]	0.05	2.15
3:2:215:VAL:CG2	1:Q:281:ILE:O[1_645]	0.05	2.15
2:1:267:GLN:CD	4:E:237:VAL:CG1[1_655]	0.06	2.14
1:B:106:VAL:CG1	3:F:104:HIS:C[1_655]	0.07	2.13

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	0	364/493 (74%)	274 (75%)	58 (16%)	32 (9%)	1 17
1	B	364/493 (74%)	274 (75%)	58 (16%)	32 (9%)	1 17
1	G	364/493 (74%)	273 (75%)	59 (16%)	32 (9%)	1 17
1	L	364/493 (74%)	273 (75%)	59 (16%)	32 (9%)	1 17
1	Q	364/493 (74%)	274 (75%)	58 (16%)	32 (9%)	1 17
1	V	364/493 (74%)	274 (75%)	58 (16%)	32 (9%)	1 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	364/522 (70%)	289 (79%)	57 (16%)	18 (5%)	3	31
2	C	364/522 (70%)	289 (79%)	57 (16%)	18 (5%)	3	31
2	H	364/522 (70%)	288 (79%)	58 (16%)	18 (5%)	3	31
2	M	364/522 (70%)	288 (79%)	58 (16%)	18 (5%)	3	31
2	R	364/522 (70%)	288 (79%)	58 (16%)	18 (5%)	3	31
2	W	364/522 (70%)	289 (79%)	57 (16%)	18 (5%)	3	31
3	2	366/461 (79%)	294 (80%)	41 (11%)	31 (8%)	1	18
3	A	366/461 (79%)	288 (79%)	50 (14%)	28 (8%)	1	20
3	D	366/461 (79%)	294 (80%)	41 (11%)	31 (8%)	1	18
3	F	366/461 (79%)	288 (79%)	50 (14%)	28 (8%)	1	20
3	I	366/461 (79%)	294 (80%)	41 (11%)	31 (8%)	1	18
3	K	366/461 (79%)	289 (79%)	48 (13%)	29 (8%)	1	19
3	N	366/461 (79%)	293 (80%)	42 (12%)	31 (8%)	1	18
3	P	366/461 (79%)	289 (79%)	49 (13%)	28 (8%)	1	20
3	S	366/461 (79%)	294 (80%)	41 (11%)	31 (8%)	1	18
3	U	366/461 (79%)	288 (79%)	50 (14%)	28 (8%)	1	20
3	X	366/461 (79%)	294 (80%)	41 (11%)	31 (8%)	1	18
3	Z	366/461 (79%)	289 (79%)	48 (13%)	29 (8%)	1	19
4	3	365/505 (72%)	281 (77%)	58 (16%)	26 (7%)	1	22
4	E	365/505 (72%)	281 (77%)	58 (16%)	26 (7%)	1	22
4	J	365/505 (72%)	281 (77%)	58 (16%)	26 (7%)	1	22
4	O	365/505 (72%)	281 (77%)	58 (16%)	26 (7%)	1	22
4	T	365/505 (72%)	281 (77%)	58 (16%)	26 (7%)	1	22
4	Y	365/505 (72%)	281 (77%)	58 (16%)	26 (7%)	1	22
All	All	10950/14652 (75%)	8553 (78%)	1585 (14%)	812 (7%)	3	21

5 of 812 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	2	VAL
1	0	68	ASP
1	0	82	SER
1	0	95	ASN
1	0	131	LYS

5.3.2 Protein sidechains (i)

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	0	340/449 (76%)	262 (77%)	78 (23%)	1 7
1	B	340/449 (76%)	262 (77%)	78 (23%)	1 7
1	G	340/449 (76%)	263 (77%)	77 (23%)	1 8
1	L	340/449 (76%)	262 (77%)	78 (23%)	1 7
1	Q	340/449 (76%)	262 (77%)	78 (23%)	1 7
1	V	340/449 (76%)	262 (77%)	78 (23%)	1 7
2	1	335/475 (70%)	244 (73%)	91 (27%)	0 4
2	C	335/475 (70%)	243 (72%)	92 (28%)	0 4
2	H	335/475 (70%)	244 (73%)	91 (27%)	0 4
2	M	335/475 (70%)	244 (73%)	91 (27%)	0 4
2	R	335/475 (70%)	243 (72%)	92 (28%)	0 4
2	W	335/475 (70%)	243 (72%)	92 (28%)	0 4
3	2	343/427 (80%)	258 (75%)	85 (25%)	1 6
3	A	343/427 (80%)	248 (72%)	95 (28%)	0 4
3	D	343/427 (80%)	258 (75%)	85 (25%)	1 6
3	F	343/427 (80%)	248 (72%)	95 (28%)	0 4
3	I	343/427 (80%)	258 (75%)	85 (25%)	1 6
3	K	343/427 (80%)	248 (72%)	95 (28%)	0 4
3	N	343/427 (80%)	258 (75%)	85 (25%)	1 6
3	P	343/427 (80%)	248 (72%)	95 (28%)	0 4
3	S	343/427 (80%)	258 (75%)	85 (25%)	1 6
3	U	343/427 (80%)	248 (72%)	95 (28%)	0 4
3	X	343/427 (80%)	258 (75%)	85 (25%)	1 6
3	Z	343/427 (80%)	248 (72%)	95 (28%)	0 4
4	3	337/463 (73%)	249 (74%)	88 (26%)	0 5
4	E	337/463 (73%)	249 (74%)	88 (26%)	0 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	J	337/463 (73%)	250 (74%)	87 (26%)	0 5
4	O	337/463 (73%)	249 (74%)	88 (26%)	0 5
4	T	337/463 (73%)	249 (74%)	88 (26%)	0 5
4	Y	337/463 (73%)	249 (74%)	88 (26%)	0 5
All	All	10188/13446 (76%)	7565 (74%)	2623 (26%)	3 6

5 of 2623 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	J	235	LEU
2	M	451	GLN
3	X	281	THR
3	K	30	ASP
1	L	82	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 379 such sidechains are listed below:

Mol	Chain	Res	Type
4	J	148	GLN
2	M	447	ASN
3	X	300	HIS
4	J	197	GLN
1	L	140	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.