



# wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 20, 2017 – 08:57 AM EDT

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 : unknown  
Resolution : 6.20 Å(reported)  
Based on PDB ID : 2BG9

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
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-20029824

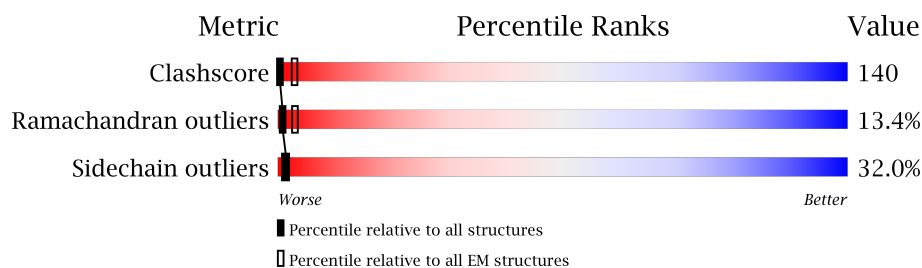
# 1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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  $\leq 5\%$

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		

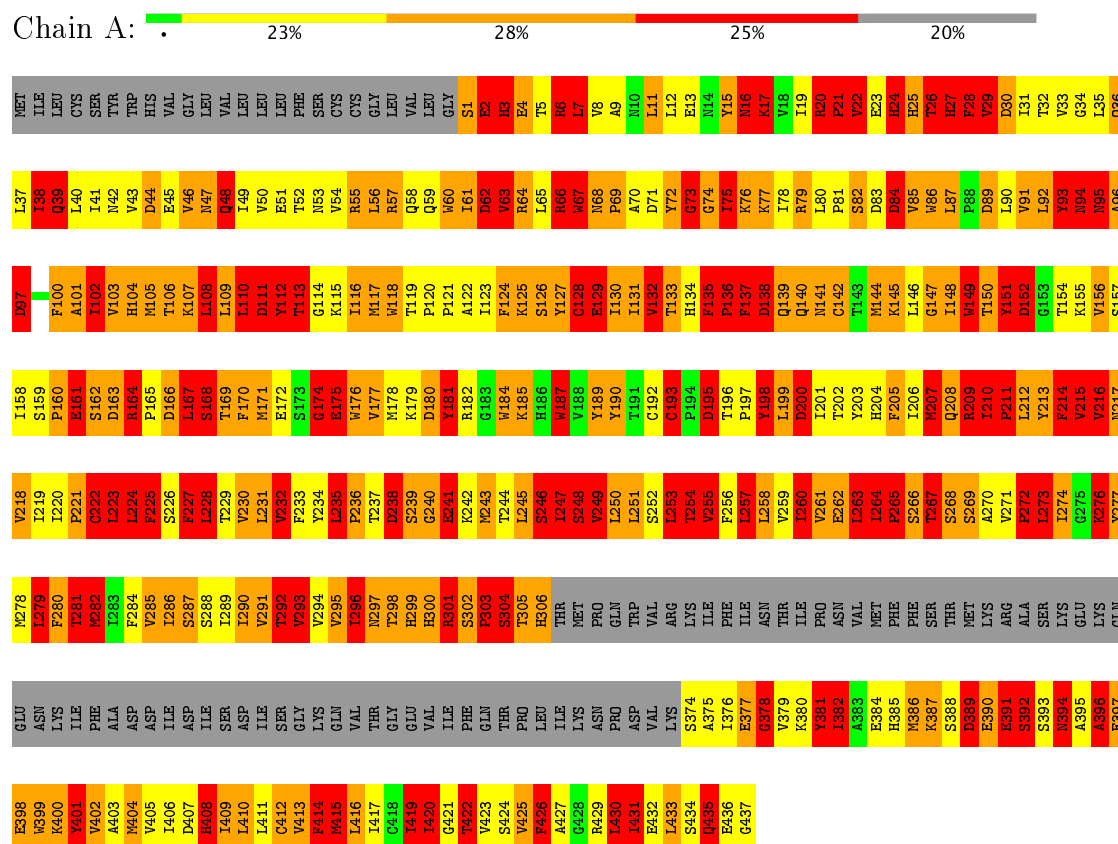
- Molecule 4 is a protein called ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT.

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

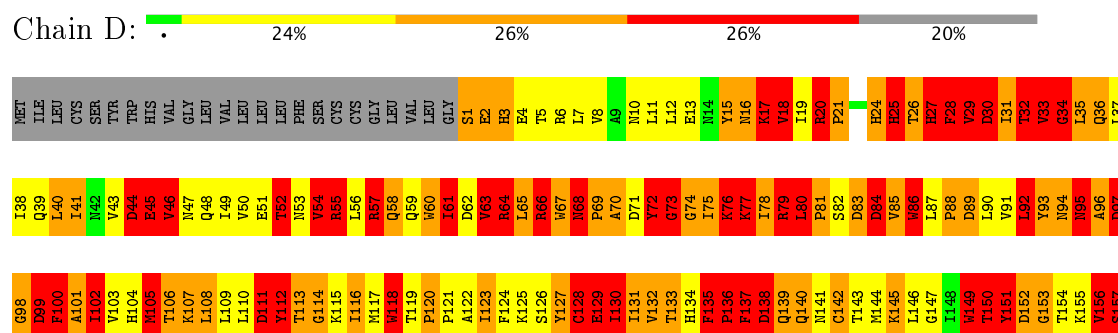
### 3 Residue-property plots

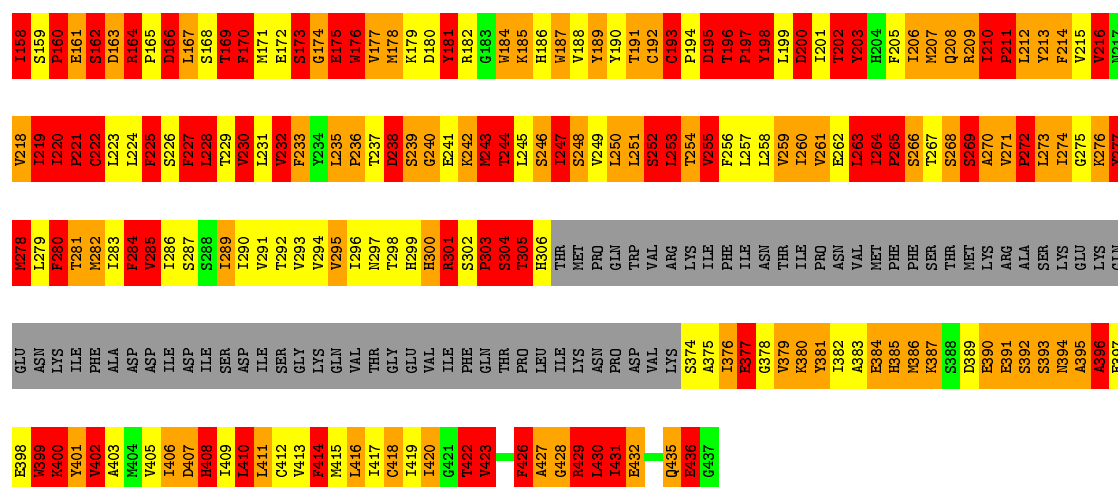
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

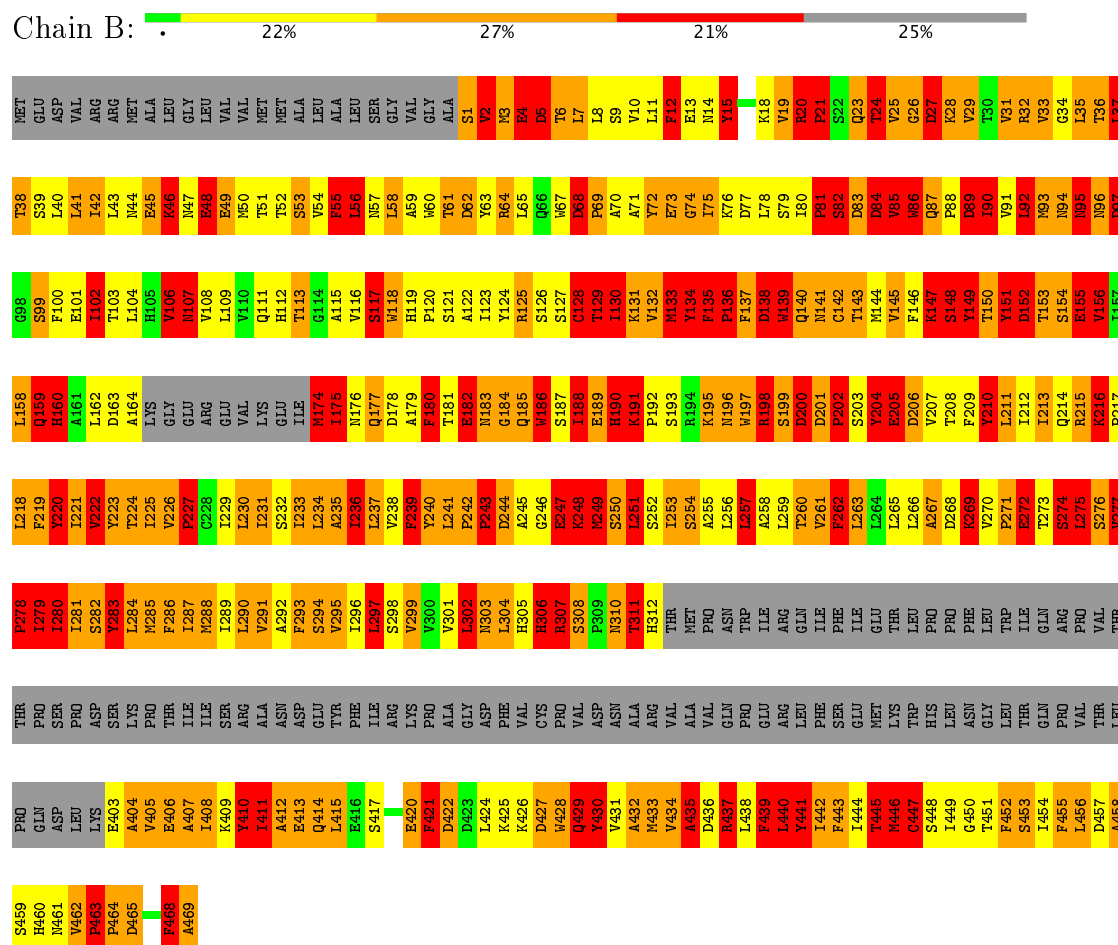


#### • Molecule 1: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

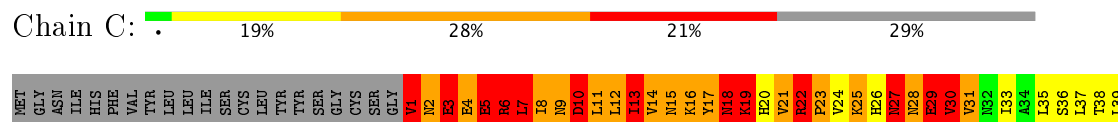




• Molecule 2: ACETYLCHOLINE RECEPTOR BETA SUBUNIT



• Molecule 3: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT



F421	A423	K424	S425	T426	K427	E428	Q429	M430	A431	S432	G433	S434	E435	M436	E437	M438	M439	L440	L441	I442	G443	L444	L445	L446	V447	A448	A449	C450	F451	I452	I453	A454	L455	L456	L457	S458	L460	L463	A464	L465	F466	L467	T468	G469	H470	L471	N472	Q473	V474	F475	F476	P477	P478	C479	T480																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
GLU	GLU	TYR	ILE	LYS	LYS	PRQ	ARG	SER	GLU	LEU	MET	PHE	GLU	GLY	GLY	LYS	ASP	ARG	VAL	ASN	GLY	LYS	LYS	ASP	VAL	LYS	MET	THR	LYS	TYR	LEU	ILE	ASP	GLY	GLY	THR	THR	GLU	THR	LYS	ASP	GLU	LYS	GLY	ALA	PRE	ALA	PRQ	GLU	LYS	ILE	S414	C415	E417	A418	C419	V420																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
V301	I302	V303	I304	N305	V306	S307	L308	T309	P310	C311	N312	H313	SER	LEU	SER	GLU	LYS	ILE	GLU	GLY	HIS	GLY	LEU	PHE	GLU	LEU	PRQ	LYS	TYR	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
D61	Y62	R63	L64	S65	M66	G67	T68	S69	E70	Y71	E72	G73	I74	D75	L76	V77	R78	I79	P80	A81	E82	S83	L84	M85	P86	L87	D88	V89	Y90	L91	E92	N93	L94	N95	G96	D97	Q98	R99	E100	V101	A102	Y103	E104	K105	E106	V107	L108	I109	Y110	N111	G112	D113	S114	M115	I116	W117	F118	Q119	P120	M121																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
A121	I122	Y123	R124	S125	T126	C127	H128	I129	A130	V131	T132	Y133	F134	P135	D136	V137	M138	Q139	N140	C141	S142	L143	V144	F145	R146	S147	Q148	T149	Y150	M151	A152	I153	E154	V155	M156	L157	Q158	L159	S160	E161	E162	E163	G164	VAL	VAL	VAL	TRP	ILE	HIS	I172	D173	P174	E175	D176	F177	T178	E179	P180	M181																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G181	E182	R183	T184	I185	R186	G187	H188	P189	A190	K191	K192	N193	Y194	M195	V196	Q197	L198	T199	K200	D201	D202	L203	D204	F205	P206	L207	I208	L209	F210	F211	L212	I213	I214	Q215	R216	R217	N218	L219	F220	Y221	I222	I223	N224	G225	L226	L227	A228	C229	Y230	F231	I232	S233	S234	L235	T236	V237	T238	V239	Y240																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
F241	L242	P243	A244	Q245	A246	G247	Q248	Q249	K250	C251	T252	L253	S254	L255	S256	V257	L258	L259	A260	Q261	E262	T263	F264	L265	P266	L267	L268	A269	Q270	E271	V272	P273	E274	T275	S276	L277	N278	I279	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

Chain E: . 23% 26% 24% 24%

F421	L422	A423	K424	S425	T426	K427	E428	Q429	N430	D431	S432	G433	S434	E435	M436	E437	N438	N439	N440	L441	T442	G443	R444	V445	L446	L447	L448	K449	C450	F451	F452	L453	A454	L455	L456	L457	F458	S459	L460	L461	A464	T465	F466	L467	G468	G469	H470	L471	M472	Q473	V474	P475	E476	F477	PRO	PHE	PRO	PRO	GLY				
GLU	GLU	TYR	ILE	LEU	LYS	LYS	PRO	ARG	SER	GLU	GLU	LEU	MET	PHE	GLU	GLU	GLN	LYS	ASP	ARG	HIS	GLY	LEU	LEU	LYS	ARG	VAL	ASN	LYS	MET	THR	SER	ASP	ILE	ASP	ILE	GLY	GLY	THR	THR	VAL	ASP	LEU	LYS	ALA	ASN	PHE	PRO	ALA	ARG	ARG	ARG	ILE	SER	SER	PHE	GLY	GLY	ILE	MET	ILE	LYS	ALA
V301	L302	V303	L304	N305	V306	S307	L308	R309	T310	P311	N312	T313	H314	SER	LEU	GLU	SER	GLY	LYS	ASP	LYS	GLY	PHE	LYS	LEU	GLU	GLY	PRO	LYS	TYR	GLU	GLU	GLY	MET	GLY	GLY	PRO	ASP	GLU	LYS	PRO	GLN	ASN	PHE	PRO	ALA	ARG	ARG	ARG	ILE	SER	SER	PHE	GLY	GLY	ILE	MET	ILE	LYS	ALA			
F241	L242	P243	A244	Q245	A246	G247	G248	Q249	K250	C251	L252	L253	S254	L255	S256	V257	L258	L259	A260	T261	T262	L263	F264	L265	F266	L267	L268	A269	Q270	K271	V272	P273	E274	T275	S276	L277	N278	V279	P280	L281	L282	G283	K284	Y285	L286	L287	F288	V289	M290	Y291	V292	S293	L294	V295	L296	V297	L298	C299	N300				
G181	E182	T183	T184	I185	R186	H187	R188	P189	A190	K191	K192	N193	Y194	N195	M196	Q197	L198	T199	K200	D201	T202	L203	D204	F205	Q206	E207	L208	A209	F210	T211	L212	T213	L214	Q215	T216	K217	N218	V219	P220	Y221	L222	L223	N224	L225	L226	A227	F228	G229	Y230	L231	L232	S233	L234	V235	V236	V237	L238	C239	N240				
A121	I122	R123	L124	S125	T126	C127	P128	I129	A130	V131	T132	Y133	F134	P135	F136	D137	M138	Q139	M140	C141	S142	L143	V144	F145	R146	S147	Q148	T149	Y150	M151	A152	H153	E154	V155	M156	L157	Q158	L159	S160	A161	E162	E163	G164	VAL	VAL	VAL	GLU	TRP	ILE	HIS	I172	D173	P174	S175	L176	D177	E178	E179	N180				
D61	Y62	R63	L64	S65	M66	M67	T68	S69	E70	Y71	E72	G73	I74	D75	L76	V77	R78	I79	P80	S81	E82	L83	L84	R85	L86	P87	D88	V89	Y90	L91	E92	N93	N94	V95	D96	G97	Q98	F99	E100	V101	A102	Y103	Y104	A105	N106	V107	L108	Y109	Y110	N111	D112	G113	S114	M115	Y116	W117	L118	P119	N120				
M1	E2	E3	G4	R5	L6	I7	E8	K9	L10	L11	G12	D13	Y14	D15	K16	R17	I18	K19	P20	A21	F22	T23	L24	D25	E26	V27	D28	W29	V30	T31	L32	K33	L34	T35	L36	T37	N38	L39	I40	S41	L42	L43	M44	K45	E46	E47	A48	L49	T50	T51	N52	W53	W54	I55	E56	I57	Q58	W59	N60				

ASP
PRO
ARG
LYS
TYR
VAL
PRO

## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH TUBE IMAGE	Depositor
Microscope	JEOL 3000SFF	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	38500	Depositor
Image detector	KODAK SO-163 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

*Continued on next page...*

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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	6
1	D	366/461 (79%)	264 (72%)	56 (15%)	46 (13%)	0	7
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	7
4	E	365/488 (75%)	234 (64%)	80 (22%)	51 (14%)	0	5
All	All	1825/2425 (75%)	1253 (69%)	327 (18%)	245 (13%)	1	6

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	2
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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	E	3
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	126:THR	C	127:CYS	N	1.19
1	E	306:VAL	C	307:SER	N	1.19
1	E	309:ARG	C	310:THR	N	1.19
1	B	129:THR	C	130:ILE	N	1.12