



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 07:20 AM UTC

PDB ID : 2BG9 / pdb_00002bg9
Title : REFINED STRUCTURE OF THE NICOTINIC ACETYLCHOLINE RE-
CEPTOR AT 4A RESOLUTION.
Authors : Unwin, N.
Deposited on : 2004-12-17
Resolution : 4.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

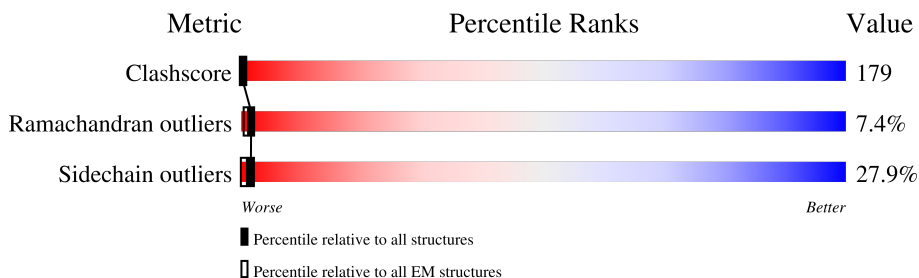
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	370	7% 51% 35% 8%
1	D	370	7% 55% 31% 7%
2	B	370	6% 56% 31% 7%
3	C	369	9% 51% 33% 7%
4	E	370	7% 52% 34% 7%

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 PROTEIN, ALPHA CHAIN.

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 PROTEIN, BETA CHAIN.

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 PROTEIN, DELTA CHAIN.

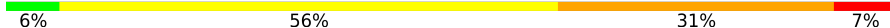
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	369	Total	C	N	O	S	0	0
			2983	1944	488	537	14		

- Molecule 4 is a protein called ACETYLCHOLINE RECEPTOR PROTEIN, GAMMA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	370	Total	C	N	O	S	0	0
			2987	1948	477	552	10		

L245	L246	T305	L433
S246	H306	S305	S434
I247	S374	P302	S435
S248	A375	P303	E436
V249	I376	P304	G437
L250	E377		
L251	G378		
S252	V379		
L253	K380		
T254	L253		
V255	Y381		
F256	I382		
L257	A383		
L258	E384		
V259	H385		
I260	M386		
V261	K387		
E262	S388		
L263	D389		
I264	E390		
P265	E391		
T267	S392		
S268	N393		
S269	A395		
A270	E396		
V271	E397		
P272	E398		
L273	V399		
I274	K400		
G275	Y401		
K276	V402		
Y277	A403		
M278	M404		
L279	I405		
F280	L279		
T281	D407		
M282	H408		
I283	L409		
V284	L410		
L286	L411		
S287	C412		
S288	V413		
I289	F414		
V291	M415		
T292	L416		
V293	I417		
V294	C418		
V295	I419		
V296	I420		
N297	G421		
S298	T422		
H299	V423		
H300	F424		
R301	S425		
S302	V426		
P303	H427		
S304	L430		
	I431		
	E432		

• Molecule 2: ACETYLCHOLINE RECEPTOR PROTEIN, BETA CHAIN

Chain B:  6% 56% 31% 7%

S1	V2	T61	S121	H190	S250	R310	M461
D62	M3	D62	A122	K191	L251	T311	V462
E4	E4	R64	I123	P192	S252	E403	P463
D5	D5	L65	Y124	S193	I253	E404	P464
T6	T6	Q66	K125	R194	S254	A405	D465
L7	L7	W67	S126	K195	A255	V406	M466
L8	L8	D68	S127	R196	L256	E407	P467
S9	S9	P69	C128	W197	L257	L408	F468
L10	L10	A70	T129	I198	A258	K409	A469
L11	L11	I75	K130	S199	T260	Y410	
F12	F12	Y72	V132	D201	F261	A411	
E13	E13	E73	M133	P202	F262	A412	
H14	H14	G74	Y134	S203	L263	E413	
Y15	Y15	I75	P135	Y204	L264	Q414	
M16	M16	K76	P136	E205	L265	E415	
P17	P17	D77	F137	D206	A266	E416	
K18	K18	L78	D138	V207	L267	S417	
E19	E19	S79	W139	T208	D268	A418	
R20	R20	I80	Q140	F209	K269	S419	
P21	P21	P81	M141	Y210	V270	E420	
S22	S22	S82	C142	L211	P271	E421	
Q23	Q23	D83	T143	I212	E272	F422	
T24	T24	D84	M144	I213	T273	L424	
V25	V25	V85	W145	Q214	S274	K425	
G26	G26	W86	F146	R215	L275	K426	
D27	D27	Q87	K147	R216	S276	D427	
K28	K28	P88	S148	P217	W277	W428	
V29	V29	D89	T149	L218	P278	Q429	
T30	T30	I90	Y150	F219	K279	Y430	
V31	V31	V91	D151	Y220	L280	V431	
R32	R32	L92	D152	I221	I281	A432	
V33	V33	M93	T153	V222	S282	K433	
G34	G34	S94	S154	Y223	Y283	V434	
L35	L35	R95	E155	T224	L284	A435	
T36	T36	N96	V156	I225	M285	D436	
L37	L37	D97	I157	V226	F286	R437	
T38	T38	G98	L158	P227	L287	L438	
S39	S39	S99	Q159	C228	M288	F439	
L40	L40	F100	H160	I229	L289	L440	
L41	L41	E101	A161	L230	L290	Y441	
I42	I42	I102	L162	I231	V291	L442	
L43	L43	T103	D163	S232	A292	F443	
N44	N44	L104	A164	I233	F293	T444	
E45	E45	H105	M174	L234	S294	T445	
K46	K46	V106	I175	A235	V295	M446	
N47	N47	M107	Q176	I236	L296	C447	
E48	E48	L108	Q177	L237	L297	S448	
E49	E49	L109	D178	V238	S298	T449	
M50	M50	V110	A179	F239	V299	G450	
T51	T51	Q111	F180	Y240	V300	T451	
T52	T52	H112	T181	L241	V301	F452	
S53	S53	T113	L182	P242	L302	S453	
V54	V54	G114	N183	P243	N303	E454	
F55	F55	A115	G184	D244	L304	F455	
L56	L56	V116	Q185	A245	H305	L456	
N57	N57	S117	W186	G246	H306	D457	
L58	L58	W118	S187	E247	R307	A458	
A59	A59	H119	I188	K248	S308	S459	
W60	W60	P120	E189	M249	P309	H460	

• Molecule 3: ACETYLCHOLINE RECEPTOR PROTEIN, DELTA CHAIN

Chain C:  9% 51% 33% 7%

V1	M2	A61	V1	V1	A260
E3	E3	W62	M2	M2	L261
D4	D4	P63	E3	E3	C262
E5	E5	D64	E4	E4	V263
H6	H6	H65	E5	E5	L264
L7	L7	R66	H6	H6	L265
I8	I8	L67	L7	L7	A266
N9	N9	T68	I8	I8	D267
D10	D10	W69	N9	N9	A268
L11	L11	N70	D10	D10	V269
L12	L12	A71	L11	L11	F270
I13	I13	S72	L12	L12	L271
F14	F14	E73	I13	I13	L272
M15	M15	Y74	F14	F14	L273
K16	K16	S75	M15	M15	T274
Y17	Y17	D76	K16	K16	S275
N18	N18	I77	Y17	Y17	T276
K19	K19	P78	N18	N18	E277
H20	H20	F79	K19	K19	R278
R81	R81	L80	H20	H20	F279
L82	L82	W81	R81	R81	E280
R83	R83	Q82	L82	L82	T281
P84	P84	N143	R83	R83	A282
V24	V24	C144	P84	P84	L283
E25	E25	S145	V24	V24	K284
H26	H26	L146	E25	E25	V285
N27	N27	K147	H26	H26	L286
W28	W28	F148	N27	N27	T287
E29	E29	T149	W28	W28	L288
P90	P90	A150	E29	E29	Q289
D91	D91	L151	P90	P90	Y290
I92	I92	M152	D91	D91	K291
V93	V93	Y153	I92	I92	L292
L94	L94	M154	V93	V93	M293
Q95	Q95	A155	L94	L94	T294
N96	N96	M156	Q95	Q95	L295
L97	L97	E157	N96	N96	M296
N98	N98	I158	L97	L97	S297
D99	D99	S159	N98	N98	L298
G100	G100	M160	D99	D99	V299
Q101	Q101	D161	G100	G100	T300
L42	L42	L162	Q101	Q101	G301
I43	I43	T163	L42	L42	V302
S44	S44	I179	I43	I43	L242
A105	A105	D180	S44	S44	A243
F46	F46	P181	A105	A105	A244
E47	E47	F107	F46	F46	N305
T48	T48	A182	E47	E47	L245
D49	D49	A183	T48	T48	C306
E50	E50	T184	D49	D49	G307
T51	T51	V110	E50	E50	Y248
L111	L111	I111	T51	T51	L249
L112	L112	V112	L111	L111	P250
T53	T53	R113	L112	L112	A251
T54	T54	P114	T53	T53	E252
N55	N55	E189	T54	T54	S253
M115	M115	W190	N55	N55	Q254
V56	V56	E191	M115	M115	E255
Y117	Y117	I192	V56	V56	K256
M58	M58	F193	Y117	Y117	F257
D59	D59	T119	M58	M58	S258
W60	W60	K195	D59	D59	T319

4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 4.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-4.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14924	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.96	9/3069 (0.3%)	1.55	70/4186 (1.7%)
1	D	0.98	13/3069 (0.4%)	1.49	56/4186 (1.3%)
2	B	1.05	18/3048 (0.6%)	1.51	59/4162 (1.4%)
3	C	0.97	12/3059 (0.4%)	1.55	72/4173 (1.7%)
4	E	0.96	12/3057 (0.4%)	1.50	71/4172 (1.7%)
All	All	0.98	64/15302 (0.4%)	1.52	328/20879 (1.6%)

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	D	0	2
3	C	0	2
All	All	0	4

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	THR	C-N	-18.38	1.14	1.34
1	D	208	GLN	C-N	12.69	1.51	1.33
4	E	182	GLU	C-N	12.54	1.44	1.33
3	C	265	LEU	C-N	10.81	1.48	1.33
4	E	306	VAL	C-N	-8.80	1.22	1.33

The worst 5 of 328 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	122	PRO	CA-C-N	13.68	134.60	119.83
3	C	122	PRO	C-N-CA	13.68	134.60	119.83
3	C	460	ILE	N-CA-C	-13.50	100.97	111.90
4	E	238	LEU	N-CA-C	-13.45	96.10	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	441	TYR	N-CA-C	-12.77	97.05	112.89

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

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	3006	1096	0
1	D	2991	0	3006	1086	0
2	B	2972	0	2954	1119	0
3	C	2983	0	2987	1189	0
4	E	2987	0	2994	1113	0
All	All	14924	0	14947	5341	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 179.

The worst 5 of 5341 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:E:183:TRP:CB	4:E:216:ARG:HG2	1.33	1.53
2:B:134:TYR:CE1	2:B:213:ILE:HG13	1.44	1.50
1:A:167:LEU:HD12	1:A:178:MET:CB	1.43	1.47
1:A:167:LEU:CD1	1:A:178:MET:HB2	1.46	1.44
3:C:316:THR:CG2	3:C:447:ASN:HB3	1.53	1.38

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	366/370 (99%)	288 (79%)	50 (14%)	28 (8%)	1	12
1	D	366/370 (99%)	294 (80%)	41 (11%)	31 (8%)	0	11
2	B	364/370 (98%)	274 (75%)	58 (16%)	32 (9%)	0	10
3	C	363/369 (98%)	288 (79%)	57 (16%)	18 (5%)	1	18
4	E	364/370 (98%)	280 (77%)	58 (16%)	26 (7%)	1	14
All	All	1823/1849 (99%)	1424 (78%)	264 (14%)	135 (7%)	1	13

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	27	HIS
1	A	76	LYS
1	A	83	ASP
1	A	102	ILE

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	A	343/343 (100%)	237 (69%)	106 (31%)	0	2
1	D	343/343 (100%)	247 (72%)	96 (28%)	0	3
2	B	340/340 (100%)	261 (77%)	79 (23%)	1	5
3	C	335/335 (100%)	241 (72%)	94 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	337/337 (100%)	238 (71%)	99 (29%)	0	3
All	All	1698/1698 (100%)	1224 (72%)	474 (28%)	1	3

5 of 474 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	214	ASP
4	E	258	LEU
1	D	30	ASP
4	E	235	LEU
4	E	474	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	140	ASN
4	E	153	HIS
4	E	249	GLN
3	C	41	ASN
3	C	20	HIS

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 oligosaccharides 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
2	B	3
3	C	2
4	E	2
1	A	1
1	D	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	312:HIS	C	403:GLU	N	45.08
1	C	320:HIS	C	421:SER	N	45.05
1	E	314:HIS	C	414:SER	N	44.81
1	A	306:HIS	C	374:SER	N	44.46
1	D	306:HIS	C	374:SER	N	43.93