



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 23, 2017 – 07:37 PM EDT

PDB ID : 4BOR
EMDB ID: : EMD-2382
Title : The structure and super-organization of acetylcholine receptor-rapsyn complexes class D
Authors : Zuber, B.; Unwin, N.
Deposited on : unknown
Resolution : 42.00 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

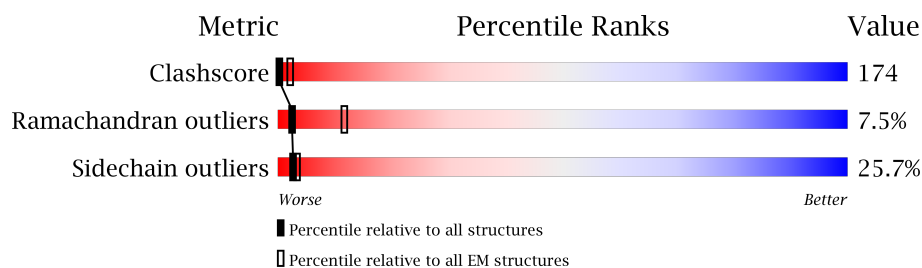
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 42.00 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	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 ≥ 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	6% 50% 20% . 20%
1	D	461	7% 51% 21% . 20%
2	B	493	5% 50% 19% . 25%
3	C	522	7% 43% 19% . 29%
4	E	505	6% 46% 18% . 27%

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		

S159	P160	E161	S162	D163	R164	P165	D166	L167	S168	T169	F170	M171	G174	E175	W176	V177	M178	K179	D180	Y181	L184	K185	H186	W187	V188	Y189	C192	C193	P194	D195	T196	P197	Y198	L199	D200	T201	T202	Y203	H204	F205	T206	M207	S208	R209	L210	P211	L212	L213	F214	V215	K216	Y217	V218	L219	T220	T281			
C222	L223	L224	F225	S226	F227	L228	T229	V230	L231	V232	F233	Y234	L235	P236	T237	D238	S239	G240	E241	K242	M243	T244	L245	S246	L247	V248	V249	L250	L251	S252	L253	T254	F255	T256	P257	L258	V259	L260	V261	E262	L263	L264	P265	S266	T267	S268	S269	A270	L271	P272	L273	L274	G275	K276	Y277	M278	L279	F280	T281
W282	L283	F284	V285	L286	S287	S288	L289	L290	L291	T292	V293	V294	V295	L296	T297	T298	H299	H300	R301	S302	P303	S304	T305	H306	THR	MET	PRO	GLN	TRP	VAL	ARG	LYS	ILE	PHE	ASN	PRO	ASN	VAL	ASN	MET	PHE	SER	THR	LYS	ARG	ALA	SER	L273	L274	G275	K276	Y277	GLN	GLU	ASN	L279	F280	T281	
PHE	ALA	ASP	ASP	ILE	ASP	ILE	SER	ASP	ILE	SER	GLY	LYS	GLN	VAL	THR	GLY	GLU	VAL	ILE	PHE	GLN	THR	PRO	LEU	ILE	LYS	S374	A375	I376	E377	G378	V379	K380	Y381	I382	A383	V384	H385	K386	K387	S388	D389	NET	LYS	E390	E391	S392	S393	N394	A395	A396	E397	E398	W399	K400	Y401			

V402	A403	N404	V405	L406	D407	H408	I409	L410	L411	C412	F413	V414	N415	L416	T417	O418	T419	T420	G421	T422	V423	S424	V425	F426	A427	L430	T431	F432	L433	S434	Q435	E436	C437
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• Molecule 2: ACETYLCHOLINE RECEPTOR BETA SUBUNIT

Chain B: 5% 50% 19% 25%

LEU	PRO	GLN	ASP	LEU	LYS	E403	A404	V405	A406	A407	I408	K409	V410	T411	A412	E413	Q414	L415	E416	S417	A418	S419	E420	F421	L424	K425	K426	D427	W428	Q429	Y430	V431	A432	M433	V434	A435	D436	L437	L438	F439	L440	Y441	I442	F443	T444	T445	M446	Q447	S448	I449	G450	T451	F452	S453	I454	F455	L456	T457							
THR	THR	PRO	SER	PRO	ASP	SER	LYS	PRO	THR	ILE	ILE	SER	ARG	ALA	ALA	ASN	ASP	GLU	TVR	PHE	ILE	ARG	LYS	PRO	ALA	ALA	ASP	PHE	VAL	CYS	PRO	VAL	ASP	ASN	ALA	ARG	VAL	ALA	VAL	GLN	PRO	GLU	GLU	ARG	ARG	LEU	PHE	SER	GLU	MET	LYS	TRP	HIS	LEU	LEU	ASN	GLY	LEU	TRP	ILE	GLN	PRO	ARG	VAL	THR
V277	P278	L279	T280	L281	S282	Y283	L284	M285	F286	L287	M288	L289	L290	V291	A292	F293	S294	V295	L296	L297	S298	V299	V300	V301	L302	N303	L304	H305	H306	R307	S308	F309	N310	T311	H312	THR	MET	PRO	ASN	TRP	ILE	TRP	GLU	TRP	ILE	GLN	ILE	GLU	LYS	TRP	THR	ILE	GLN	ARG	PRO	VAL	THR								
P217	L218	F219	Y220	L221	V222	Y223	T224	L225	V226	P227	C228	I229	L230	L231	S232	L233	L234	A235	L236	L237	V238	F239	Y240	L241	P242	P243	D244	A245	G246	E247	K248	M249	L250	L251	S252	L253	S254	A255	L256	L257	A258	L259	T260	V261	F262	L263	L264	L265	L266	A267	P268	K269	V270	P271	T272	T273	S274	S275	S276						
I157	L158	H159	Q160	L161	D162	D163	L164	LYS	GLY	GLU	ARG	GLU	VAL	LYS	GLY	ILE	M174	I175	H176	Q177	D178	A179	F180	T181	E182	H183	I184	Q185	V186	S187	T188	E189	H190	K191	P192	S193	R194	K195	M196	W197	R198	S199	D200	D201	P202	S203	Y204	E205	D206	V207	T208	F209	Y210	L211	L212	L213	Q214	R215	K216						
D97	G98	S99	F100	E101	I102	T103	H104	H105	V106	M107	V108	L109	V110	Q111	H112	T113	G114	A115	V116	S117	D118	H119	P120	S121	A122	I123	Y124	G125	L126	S127	C128	I129	I130	K131	V132	M133	Y134	F135	P136	F137	D138	M139	Q140	M141	C142	T143	M144	V145	F146	K147	P148	Y149	T150	V151	D152	T153	S154	V155	V156						
L37	T38	S39	L40	L41	L42	L43	M44	E45	K46	M47	E48	E49	M50	T51	T52	S53	V54	F55	L56	H57	L58	A59	P60	D61	T62	R63	L64	L65	Q66	H67	D68	F69	A70	L71	L72	E73	G74	I75	K76	L77	D78	S79	L80	F81	S82	D83	D84	V85	H86	Q87	P88	D89	I90	V91	L92	H93	H94	L95	R96						
MET	GLU	ASP	VAL	ARG	ARG	MET	MET	ALA	LEU	LEU	VAL	VAL	VAL	MET	MET	ALA	LEU	ALA	LEU	SER	GLY	VAL	GLY	ALA	S1	V2	M3	E4	D5	T6	L7	L8	S9	V10	L11	F12	E13	M14	Y15	M16	P17	K18	V19	R20	F21	S22	T23	T24	V25	G26	D27	K28	V29	T30	V31	R32	V33	G34	L35	T36					

A458	S459	H460	N461	V462	P463	P464	D465	M466	P467	F468	A469
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• Molecule 3: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT

Chain C: 7% 43% 19% 29%

WET	GLY	ASN	ILE	PHE	HIS	VAL	TYR	LEU	LEU	ILE	SER	CYS	LEU	TYR	T37	N2	E3	F4	E5	H6	L7	I8	N9	D10	L11	L12	V13	M14	M15	K16	Y17	M18	K19	H20	V21	R22	P23	V24	K25	E26	N27	N28	E29	V30	V31	N32	I33	A34	I35	S36	L37	T38	L39
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I465	G469		PRO
F466	H470		PHE
	L471		PRO
	I472		GLY
	Q473		ASP
	V474		PRO
	P475		ARG
	E476		LYS
	F477		TYR
			VAL
			PRO

4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of tilted images used	3564	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	80213	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.72	3/3069 (0.1%)	1.03	10/4186 (0.2%)
1	D	0.74	2/3069 (0.1%)	1.01	6/4186 (0.1%)
2	B	0.76	2/3048 (0.1%)	0.99	4/4162 (0.1%)
3	C	0.74	2/3059 (0.1%)	1.03	9/4175 (0.2%)
4	E	0.73	6/3057 (0.2%)	1.01	9/4174 (0.2%)
All	All	0.74	15/15302 (0.1%)	1.01	38/20883 (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	D	0	2
3	C	0	2
All	All	0	4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	THR	C-N	-8.41	1.14	1.34
1	A	118	TRP	CB-CG	7.91	1.64	1.50
1	D	208	GLN	C-N	7.57	1.51	1.34
4	E	8	GLU	CB-CG	6.50	1.64	1.52
3	C	265	LEU	C-N	6.16	1.48	1.34

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	266	ALA	N-CA-CB	10.38	124.64	110.10
4	E	198	LEU	CA-CB-CG	7.19	131.83	115.30
3	C	315	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	A	209	ARG	NE-CZ-NH2	6.92	123.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	263	ILE	CG1-CB-CG2	-6.66	96.75	111.40

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	3005	1073	0
1	D	2991	0	3006	1063	0
2	B	2972	0	2952	1078	0
3	C	2983	0	2987	1156	0
4	E	2987	0	2994	1087	0
All	All	14924	0	14944	5194	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 174.

The worst 5 of 5194 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	1.56
2:B:134:TYR:CE1	2:B:213:ILE:HG13	1.44	1.49
1:A:167:LEU:HD12	1:A:178:MET:CB	1.43	1.48
1:A:167:LEU:CD1	1:A:178:MET:HB2	1.46	1.44
3:C:316:THR:CG2	3:C:317:PRO:HD2	1.53	1.37

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	A	366/461 (79%)	288 (79%)	49 (13%)	29 (8%)	1	17
1	D	366/461 (79%)	294 (80%)	41 (11%)	31 (8%)	1	15
2	B	364/493 (74%)	273 (75%)	59 (16%)	32 (9%)	1	15
3	C	364/522 (70%)	289 (79%)	57 (16%)	18 (5%)	2	27
4	E	365/505 (72%)	281 (77%)	58 (16%)	26 (7%)	1	19
All	All	1825/2442 (75%)	1425 (78%)	264 (14%)	136 (8%)	2	18

5 of 136 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

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%)	248 (72%)	95 (28%)	0	3
1	D	343/427 (80%)	258 (75%)	85 (25%)	1	5
2	B	340/449 (76%)	262 (77%)	78 (23%)	1	6
3	C	335/475 (70%)	244 (73%)	91 (27%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	337/463 (73%)	249 (74%)	88 (26%)	0 4
All	All	1698/2241 (76%)	1261 (74%)	437 (26%)	3 4

5 of 437 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	104	VAL
3	C	315	ARG
4	E	217	LYS
3	C	130	CYS
3	C	233	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	200	ASN
1	D	42	ASN
4	E	197	GLN
3	C	231	ASN
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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	129:THR	C	130:ILE	N	1.14