

wwPDB X-ray Structure Validation Summary Report (i)

Dec 4, 2023 – 12:08 am GMT

PDB ID : 2BYN

Title: Crystal structure of apo AChBP from Aplysia californica

Authors: Hansen, S.B.; Sulzenbacher, G.; Huxford, T.; Marchot, P.; Taylor, P.; Bourne,

Υ.

Deposited on : 2005-08-03

Resolution : 2.02 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

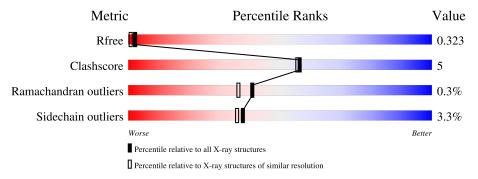
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.02 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	Similar resolution
Metric	$(\# { m Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 <=5%

Mol	Chain	Length	Quality of chain		
1	A	227	85%	7%	• 5%
1	В	227	77%	15%	7%
1	С	227	84%	9%	7%
1	D	227	81%	11%	• 6%
1	Е	227	84%	8%	• 6%



2 Entry composition (i)

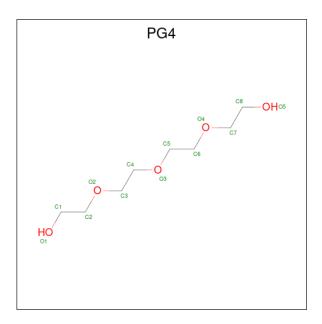
There are 5 unique types of molecules in this entry. The entry contains 9684 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 SOLUBLE ACETYLCHOLINE RECEPTOR.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	A	216	Total	С	N	О	S	0	9	0
1	Λ	210	1786	1128	296	353	9	0	9	U
1	В	211	Total	С	N	О	S	0	6	0
1	Ъ	211	1721	1085	286	341	9	0	0	
1	C	212	Total	С	N	О	S	0	6	0
1		212	1739	1094	294	342	9	0	0	
1	D	213	Total	С	N	О	S	0	3	0
1	D	210	1722	1083	285	346	8	0	3	
1	Е	214	Total	С	N	О	S	0	7	0
1	ינו	214	1752	1106	292	344	10	0	'	

• Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total C 13 8	O 5	0	0

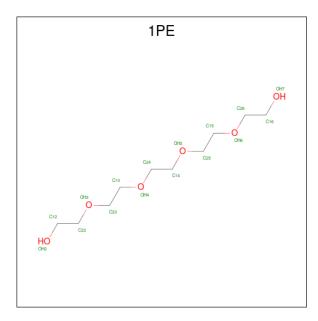
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total C O 13 8 5	0	0
2	D	1	Total C O 13 8 5	0	0
2	Е	1	Total C O 13 8 5	0	0

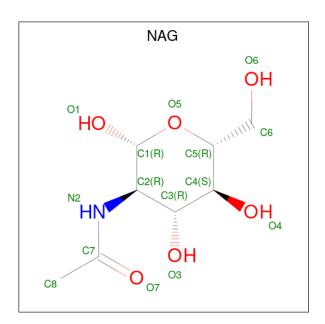
 \bullet Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $\mathrm{C}_{10}\mathrm{H}_{22}\mathrm{O}_6).$



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	С	1	Total C 16 10	O 6	0	0

 \bullet Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Ε	1	Total C N O	0	0

• Molecule 5 is water.

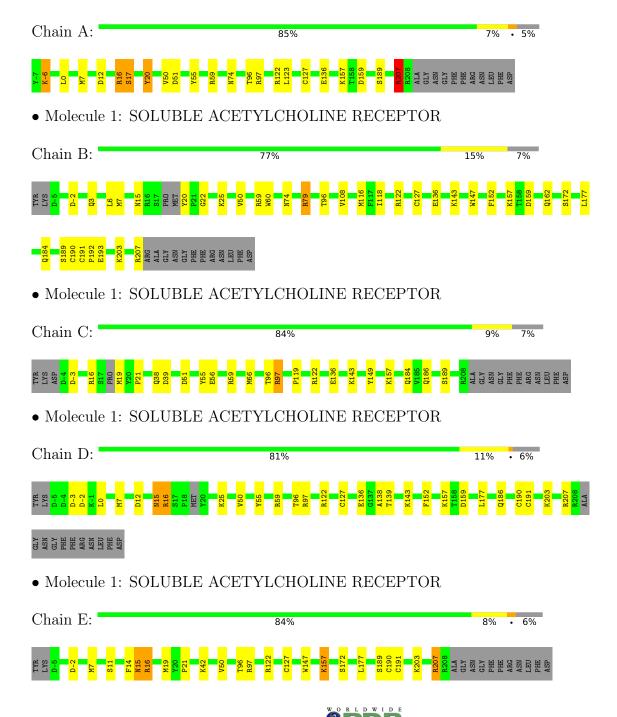
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	186	Total O	0	0
			186 186 Total O		
5	В	189	189 189	0	0
5	С	169	Total O	0	0
			169 169	Ŭ	Ü
5	D	159	Total O	0	0
		100	159 159	Ŭ	Ü
5	E	179	Total O	0	
	Ш	113	179 179	U	U



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: SOLUBLE ACETYLCHOLINE RECEPTOR



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	144.15Å 146.77Å 143.31Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.03 - 2.02	Depositor
Resolution (A)	34.28 - 2.02	EDS
% Data completeness	98.5 (40.03-2.02)	Depositor
(in resolution range)	5.7 (34.28-2.02)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
P. P.	0.169 , 0.202	Depositor
R, R_{free}	0.273 , 0.323	DCC
R_{free} test set	177 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 37.4	EDS
L-test for twinning ¹	$ < L >=$ (Not available), $ =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9684	wwPDB-VP
Average B, all atoms $(Å^2)$	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: (Not available)

Theoretical values of $<|L|>, < L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, 1PE, NAG

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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	RMSZ $ $ # $ Z > 5$		# Z > 5	
1	A	0.62	1/1854 (0.1%)	0.80	$2/2525 \ (0.1\%)$	
1	В	0.63	0/1778	0.74	0/2417	
1	С	0.60	0/1792	0.77	$2/2435 \ (0.1\%)$	
1	D	0.59	0/1768	0.74	0/2409	
1	Е	0.60	0/1816	0.75	0/2471	
All	All	0.61	1/9008 (0.0%)	0.76	$4/12257 \ (0.0\%)$	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(ext{\AA})$
1	A	17	SER	CB-OG	5.13	1.49	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^o)$
1	A	207[A]	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	207[B]	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	С	39	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	С	51	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

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	A	1786	0	1725	18	0
1	В	1721	0	1662	29	0
1	С	1739	0	1682	11	0
1	D	1722	0	1643	21	0
1	Е	1752	0	1700	16	0
2	A	13	0	18	0	0
2	В	13	0	18	1	0
2	D	13	0	18	0	0
2	Е	13	0	18	2	0
3	С	16	0	22	2	0
4	Е	14	0	13	0	0
5	A	186	0	0	3	0
5	В	189	0	0	6	0
5	С	169	0	0	3	0
5	D	159	0	0	2	0
5	Ε	179	0	0	8	0
All	All	9684	0	8519	87	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 5.

The worst 5 of 87 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:B:203[B]:LYS:NZ	5:B:2184:HOH:O	1.66	1.27
1:D:136:GLU:O	1:D:203:LYS:HE3	1.69	0.89
1:B:136:GLU:O	1:B:203[B]:LYS:HE2	1.75	0.86
1:A:59:ARG:NH1	1:A:159:ASP:OD1	2.22	0.73
1:D:7:MET:HG2	5:E:2013:HOH:O	1.89	0.72

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 X-ray entries followed by that with respect to entries of similar resolution.

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	Perce	ntiles
1	A	223/227 (98%)	218 (98%)	5 (2%)	0	100	100
1	В	212/227 (93%)	207 (98%)	5 (2%)	0	100	100
1	С	213/227 (94%)	209 (98%)	3 (1%)	1 (0%)	29	22
1	D	212/227 (93%)	208 (98%)	3 (1%)	1 (0%)	29	22
1	E	219/227 (96%)	210 (96%)	8 (4%)	1 (0%)	29	22
All	All	1079/1135 (95%)	1052 (98%)	24 (2%)	3 (0%)	41	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	16	ARG
1	Е	16	ARG
1	D	16	ARG

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 X-ray entries followed by that with respect to entries of similar resolution.

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	$206/205 \ (100\%)$	197 (96%)	9 (4%)	28 24
1	В	198/205 (97%)	193 (98%)	5 (2%)	47 48
1	C	199/205 (97%)	189 (95%)	10 (5%)	24 19
1	D	197/205~(96%)	192 (98%)	5 (2%)	47 48
1	E	202/205~(98%)	195 (96%)	7 (4%)	36 34
All	All	1002/1025 (98%)	966 (96%)	36 (4%)	38 32

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	157	LYS
1	Е	207[B]	ARG
1	Ε	-2	ASP
1	Ε	16	ARG
1	В	79	ARG



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	184	GLN
1	С	186	GLN
1	Е	63	ASN
1	D	3	GLN
1	В	15	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Tune	Chain	Res	Link	Bo	ond leng	$ ag{ths}$	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PG4	D	401	-	12,12,12	0.55	0	11,11,11	0.68	0
3	1PE	С	401	_	15,15,15	0.53	0	14,14,14	0.30	0
2	PG4	В	401	-	12,12,12	0.50	0	11,11,11	0.80	1 (9%)
2	PG4	A	401	-	12,12,12	0.56	0	11,11,11	0.31	0
4	NAG	E	301	1	14,14,15	0.54	0	17,19,21	1.53	3 (17%)
2	PG4	Е	401	-	12,12,12	0.48	0	11,11,11	0.86	0



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG4	D	401	-	-	8/10/10/10	-
3	1PE	С	401	-	-	7/13/13/13	-
2	PG4	В	401	-	-	7/10/10/10	-
2	PG4	A	401	-	-	8/10/10/10	-
4	NAG	Е	301	1	-	4/6/23/26	0/1/1/1
2	PG4	Е	401	-	-	5/10/10/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	Ε	301	NAG	C2-N2-C7	3.65	128.10	122.90
4	E	301	NAG	C8-C7-N2	3.19	121.50	116.10
4	Е	301	NAG	C1-O5-C5	2.26	115.26	112.19
2	В	401	PG4	C3-O2-C2	2.13	122.51	113.29

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Е	401	PG4	C4-C3-O2-C2
2	В	401	PG4	C4-C3-O2-C2
2	D	401	PG4	C4-C3-O2-C2
2	A	401	PG4	O2-C3-C4-O3
2	В	401	PG4	O2-C3-C4-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	401	1PE	2	0
2	В	401	PG4	1	0
2	Е	401	PG4	2	0



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.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

