



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2RIN / pdb\_00002rin  
Title : ABC-transporter choline binding protein in complex with acetylcholine  
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Deposited on : 2007-10-12  
Resolution : 1.80 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

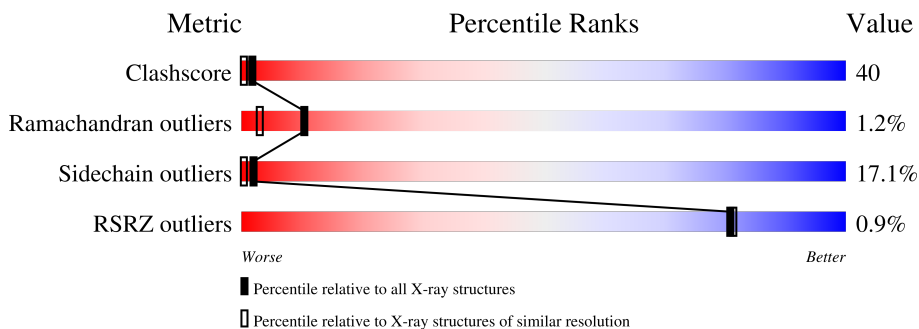
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	298	 33% 49% 13% . .
1	B	298	 35% 45% 15% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACH	A	1	-	-	X	-
2	ACH	B	1	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4616 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.

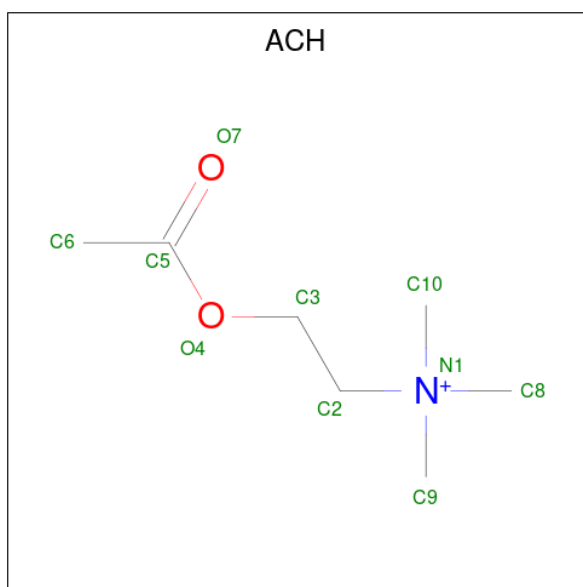
- Molecule 1 is a protein called PUTATIVE GLYCINE BETAIN-BINDING ABC TRANSPORTER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2180	1373	357	441	9	0	0	0
1	B	288	2180	1373	357	441	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ASP	GLY	engineered mutation	UNP Q92N37
A	319	GLU	-	expression tag	UNP Q92N37
A	320	HIS	-	expression tag	UNP Q92N37
A	321	HIS	-	expression tag	UNP Q92N37
A	322	HIS	-	expression tag	UNP Q92N37
A	323	HIS	-	expression tag	UNP Q92N37
A	324	HIS	-	expression tag	UNP Q92N37
A	325	HIS	-	expression tag	UNP Q92N37
B	251	ASP	GLY	engineered mutation	UNP Q92N37
B	319	GLU	-	expression tag	UNP Q92N37
B	320	HIS	-	expression tag	UNP Q92N37
B	321	HIS	-	expression tag	UNP Q92N37
B	322	HIS	-	expression tag	UNP Q92N37
B	323	HIS	-	expression tag	UNP Q92N37
B	324	HIS	-	expression tag	UNP Q92N37
B	325	HIS	-	expression tag	UNP Q92N37

- Molecule 2 is ACETYLCHOLINE (CCD ID: ACH) (formula: C<sub>7</sub>H<sub>16</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	10	7	1	2	0	0
2	B	1	10	7	1	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	120	120	120	0	0
3	B	116	116	116	0	0



L309	L318
A310	GLU
A311	HIS
V312	HIS
K313	HIS
A314	HIS
	HIS
	HIS

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	31.20Å 212.70Å 42.80Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.3 (20.00-1.80) 89.3 (20.00-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.33 (at 1.80Å)	Xtrriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.154 , 0.210 0.143 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	4.5	Xtrriage
Anisotropy	0.923	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 132.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.097 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: ACH

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	0.48	0/2221	1.81	64/3015 (2.1%)
1	B	0.49	0/2221	1.76	48/3015 (1.6%)
All	All	0.49	0/4442	1.79	112/6030 (1.9%)

There are no bond length outliers.

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	LYS	CA-C-N	11.43	138.11	123.14
1	A	148	LYS	C-N-CA	11.43	138.11	123.14
1	B	138	ILE	CA-C-N	9.43	133.30	120.38
1	B	138	ILE	C-N-CA	9.43	133.30	120.38
1	B	104	ASP	CA-CB-CG	9.10	121.70	112.60

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	2180	0	2125	165	0
1	B	2180	0	2125	179	0
2	A	10	0	16	13	0
2	B	10	0	16	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	120	0	0	11	0
3	B	116	0	0	22	0
All	All	4616	0	4282	347	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 40.

The worst 5 of 347 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:B:90:TRP:HB2	1:B:94:MET:HE3	1.53	0.90
1:A:114:LEU:HD11	1:A:261:LEU:HD23	1.54	0.89
1:B:98:ILE:HG23	1:B:102:ARG:HD3	1.56	0.85
1:A:132:ILE:HG22	1:A:219:LEU:HD21	1.57	0.82
1:B:99:ALA:HA	1:B:102:ARG:HE	1.42	0.82

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	Percentiles
1	A	286/298 (96%)	251 (88%)	30 (10%)	5 (2%)	<b>7</b> <b>2</b>
1	B	286/298 (96%)	263 (92%)	21 (7%)	2 (1%)	<b>18</b> <b>8</b>
All	All	572/596 (96%)	514 (90%)	51 (9%)	7 (1%)	<b>10</b> <b>3</b>

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	B	257	LEU

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Mol	Chain	Res	Type
1	B	152	ILE
1	A	139	ALA
1	A	298	SER

### 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	231/240 (96%)	195 (84%)	36 (16%)	<b>2</b> <b>0</b>
1	B	231/240 (96%)	188 (81%)	43 (19%)	<b>1</b> <b>0</b>
All	All	462/480 (96%)	383 (83%)	79 (17%)	<b>2</b> <b>0</b>

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	164	ASP
1	B	225	VAL
1	B	177	GLU
1	B	200	ILE
1	B	276	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	A	289	ASN
1	B	291	GLN
1	B	213	ASN
1	B	262	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ACH	A	1	-	9,9,9	0.79	0	12,12,12	1.18	2 (16%)
2	ACH	B	1	-	9,9,9	0.91	0	12,12,12	1.14	1 (8%)

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	ACH	A	1	-	-	6/7/7/7	-
2	ACH	B	1	-	-	4/7/7/7	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ACH	C3-O4-C5	-2.97	103.89	117.14
2	A	1	ACH	C3-O4-C5	-2.64	105.37	117.14
2	A	1	ACH	C3-C2-N1	-2.00	109.40	115.82

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	ACH	N1-C2-C3-O4
2	B	1	ACH	N1-C2-C3-O4
2	A	1	ACH	C6-C5-O4-C3
2	A	1	ACH	O7-C5-O4-C3
2	B	1	ACH	O7-C5-O4-C3

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	ACH	13	0
2	B	1	ACH	9	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](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	288/298 (96%)	-0.27	4 (1%) 73 73	0, 7, 18, 38	0
1	B	288/298 (96%)	-0.29	1 (0%) 90 90	0, 7, 18, 40	0
All	All	576/596 (96%)	-0.28	5 (0%) 81 81	0, 7, 18, 40	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	GLY	3.2
1	A	299	GLY	3.0
1	A	283	ALA	2.9
1	A	308	GLY	2.4
1	B	292	SER	2.3

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACH	A	1	10/10	0.95	0.06	0,0,13,14	0
2	ACH	B	1	10/10	0.96	0.10	0,19,31,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.