

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 11, 2021 – 01:00 AM EDT

PDB ID : 2RIN

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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.23.2

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)

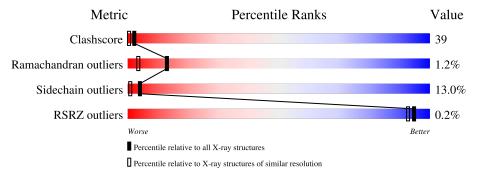
Validation Pipeline (wwPDB-VP) : 2.23.2

### 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 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 >=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% 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	38%	50%	8% •		
1	В	298	41%	49%	7% • •		

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	В	1	-	-	X	-



## 2 Entry composition (i)

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 BETAINE-BINDING ABC TRANS-PORTER PROTEIN.

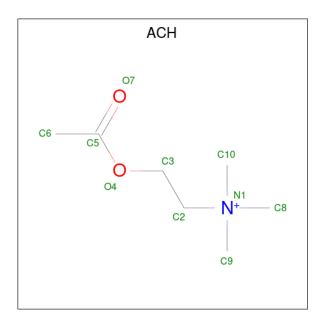
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	288	Total 2180	C 1373	11	O 441	S 9	0	0	0
1	В	288		C 1373		O 441	S 9	0	0	0

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
В	251	ASP	GLY	engineered mutation	UNP Q92N37
В	319	GLU	-	expression tag	UNP Q92N37
В	320	HIS	-	expression tag	UNP Q92N37
В	321	HIS	-	expression tag	UNP Q92N37
В	322	HIS	-	expression tag	UNP Q92N37
В	323	HIS	-	expression tag	UNP Q92N37
В	324	HIS	-	expression tag	UNP Q92N37
В	325	HIS	-	expression tag	UNP Q92N37

• Molecule 2 is ACETYLCHOLINE (three-letter code: ACH) (formula: C<sub>7</sub>H<sub>16</sub>NO<sub>2</sub>).





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

#### • Molecule 3 is water.

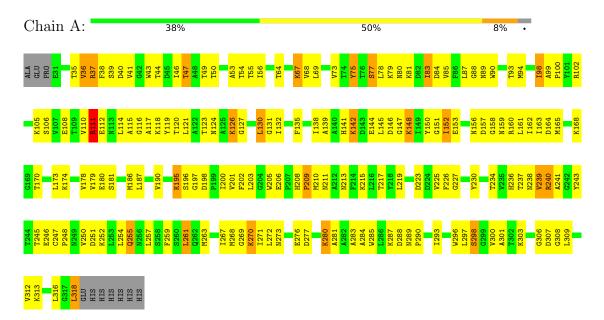
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	120	Total O 120 120	0	0
3	В	116	Total O 116 116	0	0



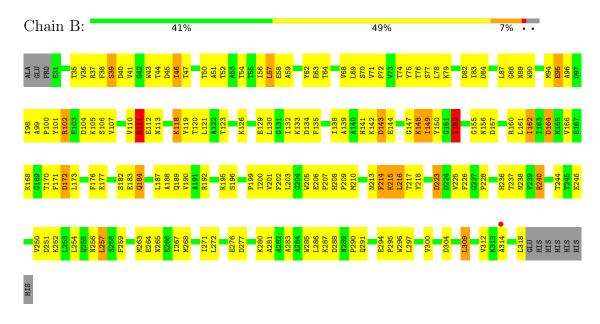
## 3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: PUTATIVE GLYCINE BETAINE-BINDING ABC TRANSPORTER PROTEIN



• Molecule 1: PUTATIVE GLYCINE BETAINE-BINDING ABC TRANSPORTER PROTEIN





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	31.20Å 212.70Å 42.80Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.10^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	20.00 - 1.80	Depositor
resolution (A)	19.12 - 1.80	EDS
% Data completeness	89.3 (20.00-1.80)	Depositor
(in resolution range)	89.4 (19.12-1.80)	EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	5.33  (at  1.80Å)	Xtriage
Refinement program	SHELXL-97	Depositor
$R, R_{free}$	0.154 , $0.210$	Depositor
it, it free	0.143 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	4.5	Xtriage
Anisotropy	0.923	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	$0.37 \; , \; 303.0$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.38, < L^2>=0.22$	Xtriage
Estimated twinning fraction	0.097 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	wwPDB-VP

Xtriage'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>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

### 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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.38	0/2221	1.21	6/3015 (0.2%)	
1	В	0.39	0/2221	1.20	3/3015 (0.1%)	
All	All	0.39	0/4442	1.21	9/6030 (0.1%)	

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	307	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	148	LYS	C-N-CA	6.56	138.11	121.70
1	В	111	ARG	NE-CZ-NH2	6.27	123.43	120.30
1	В	304	ASP	C-N-CA	5.99	134.87	122.30
1	A	75	TYR	CB-CG-CD1	5.54	124.32	121.00

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	В	2180	0	2125	174	0
2	A	10	0	16	13	0
2	В	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	В	116	0	0	22	0
All	All	4616	0	4282	342	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 39.

The worst 5 of 342 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: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
1:A:277:ASP:HB3	1:A:280:LYS:HB2	1.61	0.81

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%)	9 2
1	В	$286/298 \; (96\%)$	263 (92%)	21 (7%)	2 (1%)	22 10
All	All	572/596~(96%)	514 (90%)	51 (9%)	7 (1%)	13 3

5 of 7 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	В	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	n Analysed Rotameric Outliers		Outliers	Percentiles
1	A	231/240 (96%)	201 (87%)	30 (13%)	4 1
1	В	231/240 (96%)	201 (87%)	30 (13%)	4 1
All	All	462/480 (96%)	402 (87%)	60 (13%)	4 1

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	В	216	LEU
1	В	102	ARG
1	В	215	LYS
1	В	309	LEU

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	В	184	GLN
1	В	213	ASN
1	В	291	GLN
1	В	238	ASN
1	A	238	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)

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	True	Chain Res Link Bond lengths		$\operatorname{gths}$	В	ond ang	les			
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	ACH	В	1	-	9,9,9	0.87	0	12,12,12	1.11	1 (8%)
2	ACH	A	1	-	9,9,9	0.76	0	12,12,12	1.15	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	В	1	-	-	4/7/7/7	-
2	ACH	A	1	-	-	6/7/7/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	1	ACH	C3-O4-C5	-2.91	103.89	117.06
2	A	1	ACH	C3-O4-C5	-2.58	105.37	117.06

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	В	1	ACH	N1-C2-C3-O4
2	A	1	ACH	C6-C5-O4-C3
2	В	1	ACH	O7-C5-O4-C3
2	A	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	В	1	ACH	9	0
2	A	1	ACH	13	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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	A	288/298 (96%)	-0.17	0 100 100	0, 7, 18, 38	0
1	В	288/298 (96%)	-0.20	1 (0%) 94 92	0, 7, 18, 40	0
All	All	576/596 (96%)	-0.18	1 (0%) 95 93	0, 7, 18, 40	0

#### All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	314	ALA	2.2

#### 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 monosaccharides 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	ACH	В	1	10/10	0.96	0.14	0,19,31,32	0
2	ACH	A	1	10/10	0.97	0.10	0,0,13,14	0



## 6.5 Other polymers (i)

There are no such residues in this entry.

