WORLDWIDE
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Apr 27, 2024 – 01:00 pm BST

PDB ID	:	2XQA
Title	:	Pentameric ligand gated ion channel GLIC in complex with tetrabutylanti-mony (TBSb)
Authors	:	Hilf, R.J.C.; Bertozzi, C.; Zimmermann, I.; Reiter, A.; Trauner, D.; Dutzler, R.
Deposited on	:	2010-09-01
Resolution	:	3.70 Å(reported)

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

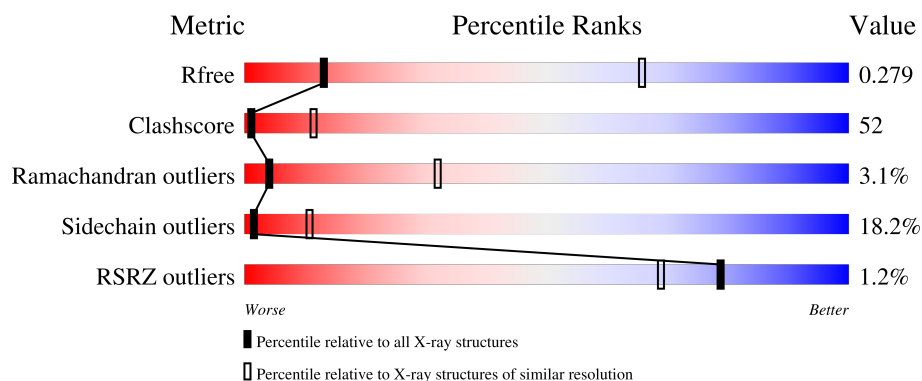|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.70 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	Percentile Ranks	Value
Rfree		0.279
Clashscore		52
Ramachandran outliers		3.1%
Sidechain outliers		18.2%
RSRZ outliers		1.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	317	2% — 32% / 53% / 12% ·
1	B	317	31% / 55% / 12% ·
1	C	317	2% — 33% / 52% / 12% ·
1	D	317	% — 32% / 53% / 12% ··
1	E	317	2% — 33% / 53% / 12% ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 12606 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 GLR4197 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	B	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	C	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	D	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	E	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			

- Molecule 2 is ANTIMONY (III) ION (three-letter code: SB) (formula: Sb).

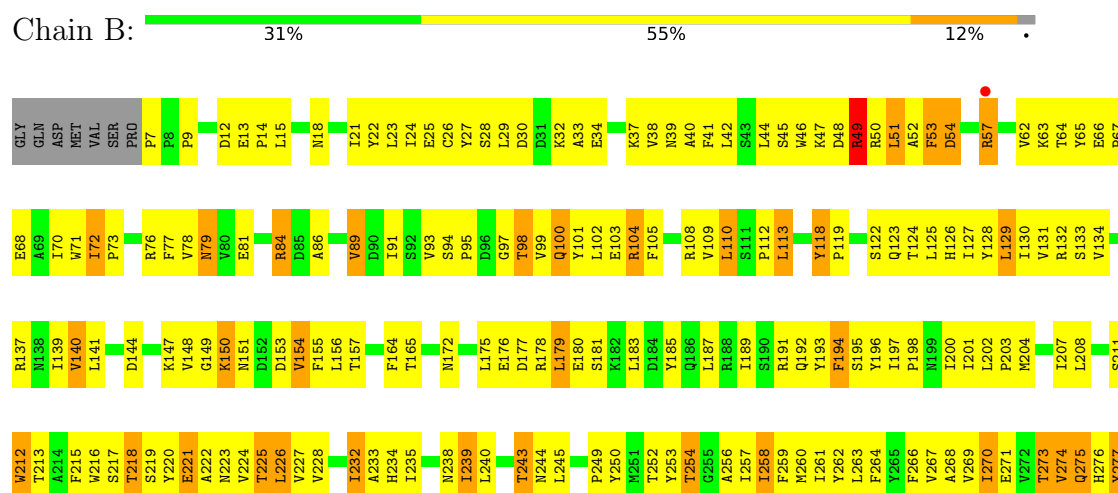| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Sb	0	0
			1	1		

3   Residue-property plots ⓘ

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: GLR4197 PROTEIN

Chain A:

- Molecule 1: GLR4197 PROTEIN

Chain B:

L278 K279 V280 E281 S282 Q283 P284 A285 R286 A287 T291 R292 R295 I296 A297 F298 P299 V300 V301 F302 L303 L304 A305 N306 I307 I308 L309 F313 G314 F316

● Molecule 1: GLR4197 PROTEIN

Chain C:

2%

33%   52%   12%

GLY GLN ASP MET VAL SER PRO P7 P8 P9 I10 A11 D12 E13 P14 L15 N18 I21 Y22 L23 I24 E25 C26 Y27 S28 L29 D30 D31 K32 A33 K37 V38 M39 A40 F41 L42 S43 L44 S45 W46 K47 D48 R49 R50 L51 A52 F53 D54 R57 S58 G59 V60 R61 V62 K63 T64

Y65 E66 P67 E68 A69 I70 W71 I72 P73 R76 F77 V78 N79 V80 E81 R84 D85 A86 D87 V88 V89 D90 I91 S92 V93 S94 P95 D96 G97 T98 V99 Q100 Y101 L102 E103 R104 F105 R108 V109 L110 L113 Y118 P119 S122 Q123 T124 L125 H126 I127 Y128 L129 I130 V131 R132

S133 V134 R137 N138 I139 V140 L141 D144 K147 V148 G149 K150 N151 D152 D153 V154 F155 L156 T157 G158 W159 F164 T165 N172 E176 D177 R178 L179 E180 S181 K182 L183 D184 Y185 I189 S190 R191 Q192 Y193 F194 S195 Y196 I197 P198 N199 I200 I201 L202 P203 M204 I207 L208

F209 I210 S211 W212 T213 A214 F215 W216 S217 T218 S219 Y220 E221 A222 N223 V224 T225 L226 V227 I232 A233 H234 I235 N238 I239 L240 T243 N244 L245 P249 Y250 M251 T252 Y253 T254 A256 I257 I258 F259 M260 I261 Y262 L263 F264 V267 A268 V269 I270 E271 V272 T273 V274 Q275 H276

Y277 L278 K279 V280 E281 S282 Q283 P284 A285 R286 A287 T291 R292 R295 I296 A297 F298 P299 V300 V301 F302 L303 L304 A305 N306 I307 I308 L309 F313 F314 G315 F316

● Molecule 1: GLR4197 PROTEIN

Chain D:

%

32%   53%   12%

GLY GLN ASP MET VAL SER PRO P7 P8 P9 D12 E13 P14 L15 N18 I21 Y22 L23 I24 E25 C26 Y27 S28 L29 D30 D31 K32 A33 E34 K37 V38 N39 A40 F41 L42 S43 L44 S45 W46 K47 D48 R49 R50 L51 A52 F53 D54 R57 R61 V62 K63 T64 Y65 E66

P67 E68 A69 I70 W71 I72 P73 R76 F77 V78 N79 V80 E81 R84 D85 A86 V89 D90 I91 S92 V93 S94 P95 D96 G97 T98 V99 Q100 Y101 L102 E103 R104 F105 R108 V109 L110 L113 Y118 P119 S122 Q123 T124 L125 H126 I127 Y128 L129 I130 V131 R132 S133 V134

R137 N138 I139 V140 L141 A142 V143 D144 L145 E146 K147 V148 G149 K150 N151 D152 D153 V154 F155 L156 T157 G158 W159 F164 T165 A166 N172 D177 R178 L179 E180 S181 Y185 Q186 L187 R188 I189 S190 R191 Q192 Y193 F194 S195 Y196 I197 P198 N199 I200 I201 L202 P203 M204 I207 L208 F209

I210 S211 W212 T213 A214 F215 W216 S217 T218 S219 Y220 E221 A222 N223 V224 T225 L226 V227 V228 S229 I232 A233 H234 I235 N238 I239 L240 V241 E242 T243 N244 L245 P249 Y250 M251 T252 Y253 T254 G255 A256 I257 I258 F259 M260 I261 Y262 L263 F264 V267 A268 V269 I270 E271 V272 T273 V274

Q275 H276 Y277 L278 K279 V280 E281 S282 Q283 P284 A285 R286 A287 A288 S289 I290 T291 R292 R295 I296 A297 F298 P299 V300 V301 F302 L303 L304 A305 N306 I307 I308 L309 F313 F314 G315 F316

● Molecule 1: GLR4197 PROTEIN

Chain E:

2%

33%   53%   12%

GLY GLN ASP MET VAL SER PRO P7 P8 P9 D12 E13 P14 L15 N18 I21 Y22 L23 I24 E25 C26 Y27 S28 L29 D30 D31 K32 A33 E34 K37 V38 N39 A40 F41 L42 S43 L44 S45 W46 K47 D48 R49 R50 L51 A52 F53 D54 R57 S58 G59 V60 R61 V62 K63 T64

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	183.31Å 128.31Å 164.37Å 90.00° 104.04° 90.00°	Depositor
Resolution (Å)	40.20 – 3.70 40.20 – 3.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.20-3.70) 92.4 (40.20-3.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.256 , 0.274 0.259 , 0.279	Depositor DCC
R_{free} test set	2172 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	94.3	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 100.1	EDS
L-test for twinning [2]	$< |L| > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	12606	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]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: SB

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	0.51	0/2589	0.73	2/3535 (0.1%)
1	B	0.53	0/2589	0.73	2/3535 (0.1%)
1	C	0.52	0/2589	0.74	3/3535 (0.1%)
1	D	0.53	0/2589	0.73	3/3535 (0.1%)
1	E	0.53	0/2589	0.73	2/3535 (0.1%)
All	All	0.53	0/12945	0.73	12/17675 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	129	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	129	LEU	CA-CB-CG	5.53	128.02	115.30
1	C	129	LEU	CA-CB-CG	5.53	128.01	115.30
1	D	129	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	129	LEU	CA-CB-CG	5.53	128.01	115.30

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	2521	0	2537	314	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2521	0	2537	316	0
1	C	2521	0	2537	270	0
1	D	2521	0	2537	287	0
1	E	2521	0	2537	264	0
2	E	1	0	0	0	0
All	All	12606	0	12685	1319	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 52.

The worst 5 of 1319 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:A:155:PHE:CE1	1:B:112:PRO:HB3	1.83	1.12
1:B:76:ARG:NH2	1:B:130:ILE:HD12	1.68	1.08
1:D:76:ARG:NH2	1:D:130:ILE:HD12	1.70	1.06
1:A:76:ARG:NH2	1:A:130:ILE:HD12	1.73	1.03
1:A:104:ARG:HH22	1:B:78:VAL:HA	1.20	1.03

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 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	308/317 (97%)	244 (79%)	55 (18%)	9 (3%)	4	32
1	B	308/317 (97%)	245 (80%)	55 (18%)	8 (3%)	5	34
1	C	308/317 (97%)	246 (80%)	51 (17%)	11 (4%)	3	29
1	D	308/317 (97%)	248 (80%)	51 (17%)	9 (3%)	4	32
1	E	308/317 (97%)	243 (79%)	54 (18%)	11 (4%)	3	29
All	All	1540/1585 (97%)	1226 (80%)	266 (17%)	48 (3%)	4	32

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	PHE
1	B	118	TYR
1	B	194	PHE
1	C	118	TYR
1	C	194	PHE

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 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	278/284 (98%)	228 (82%)	50 (18%)	1	11
1	B	278/284 (98%)	227 (82%)	51 (18%)	1	10
1	C	278/284 (98%)	229 (82%)	49 (18%)	2	12
1	D	278/284 (98%)	227 (82%)	51 (18%)	1	10
1	E	278/284 (98%)	226 (81%)	52 (19%)	1	10
All	All	1390/1420 (98%)	1137 (82%)	253 (18%)	1	11

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	100	GLN
1	E	124	THR
1	C	273	THR
1	E	113	LEU
1	E	226	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	172	ASN
1	E	172	ASN
1	D	79	ASN
1	E	275	GLN

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Mol	Chain	Res	Type
1	E	79	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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^2)	Q<0.9
1	A	310/317 (97%)	-0.25	5 (1%)	72	61	57, 98, 154, 227	0
1	B	310/317 (97%)	-0.37	1 (0%)	94	90	59, 98, 154, 227	0
1	C	310/317 (97%)	-0.26	5 (1%)	72	61	58, 98, 154, 227	0
1	D	310/317 (97%)	-0.36	2 (0%)	89	83	59, 98, 154, 227	0
1	E	310/317 (97%)	-0.31	6 (1%)	66	55	58, 99, 154, 227	0
All	All	1550/1585 (97%)	-0.31	19 (1%)	79	69	57, 98, 154, 227	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	316	PHE	4.3
1	A	316	PHE	4.1
1	E	59	GLY	3.8
1	A	59	GLY	3.0
1	E	315	GLY	2.8

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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(Å^2)	Q<0.9
2	SB	E	1316	1/1	0.95	0.44	151,151,151,151	0

6.5   Other polymers (i)

There are no such residues in this entry.