



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4DJI
Title : Structure of glutamate-GABA antiporter GadC
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Deposited on : 2012-02-02
Resolution : 3.19 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

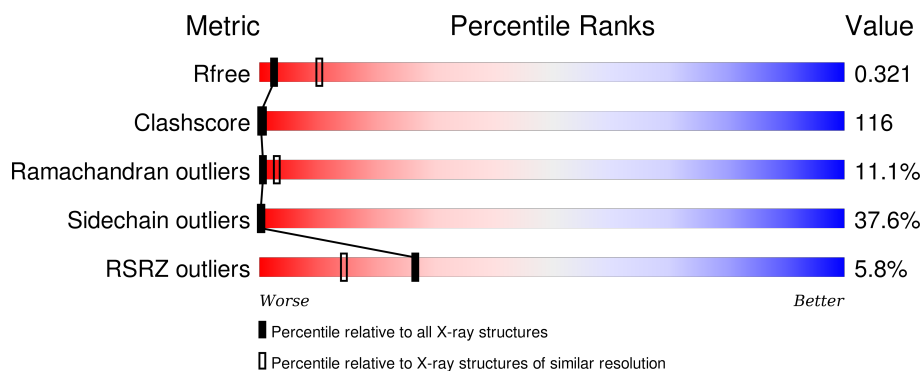
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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))
R_{free}	91344	1115 (3.22-3.14)
Clashscore	102246	1125 (3.20-3.16)
Ramachandran outliers	100387	1105 (3.20-3.16)
Sidechain outliers	100360	1104 (3.20-3.16)
RSRZ outliers	91569	1120 (3.22-3.14)

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 on the lower 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 $\leq 5\%$. 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	511	
1	B	511	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7342 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 Probable glutamate/gamma-aminobutyrate antiporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3732	2493	581	636	22			
1	B	480	Total	C	N	O	S	0	0	0
			3610	2417	556	616	21			

H491	F492	F493	L494	H495	P496	R497	A498	R499	S500	P501	H502	Y503	I504	VAL	MET	ASN	ASP	LYS	LYS	HIS
F431	L432	P433	P434	M435	M436	I437	Q438	G439	D440	S441	T442	D443	M444	Y445	V446	E447	L448	L449	V450	V451
A370	L371	A372	L373	T374	V375	V376	I377	Y378	L379	C380	A381	Y382	F383	M384	L385	F386	I387	G388	Y389	I390
M308	I309	V310	G311	P312	S313	R314	G315	M316	V317	V318	T319	A320	Q321	K322	N323	L324	L325	P326	F329	A330
I246	C247	L248	S249	S250	V251	G252	G253	I256	A257	M258	V259	I260	P261	N263	E264	I265	M266	L267	S268	A269
V246	A186	I187	E188	M189	D190	S191	I192	T193	F194	F195	P196	D197	F198	S199	K200	G201	T203	L204	V205	F146
M124	F125	D126	P127	I128	T129	R130	T131	I132	A133	I136	I137	L138	F139	A140	L141	A142	I143	T144	Q145	G147
A61	A62	E63	M64	A65	T66	V67	D68	G69	W70	E72	G73	G74	F75	A77	V78	V79	S80	N81	T82	L83
MET	ALA	THR	SER	VAL	GLN	THR	GLY	LYS	ALA	L13	T14	L15	G17	F18	F19	A20	I21	T22	A23	S24
																				M25
																				V26
																				M27
																				A28
																				V29
																				Y30
																				E31
																				Y32
																				G33
																				T34
																				F35
																				L37
																				Q38
																				I39
																				A100
																				I101
																				G102
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																				L114
																				S115
																				W53
																				I117
																				F54
																				I55
																				K118
																				W120
																				P121
																				A122
																				L59
																				O60

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.62Å 105.42Å 188.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.52 – 3.19 35.52 – 3.19	Depositor EDS
% Data completeness (in resolution range)	84.2 (35.52-3.19) 84.6 (35.52-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.310 , 0.328 0.304 , 0.321	Depositor DCC
R_{free} test set	1137 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	107.4	Xtriage
Anisotropy	0.971	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 87.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 22474 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.77	0/3826	0.81	9/5222 (0.2%)
1	B	0.70	0/3700	0.79	5/5054 (0.1%)
All	All	0.74	0/7526	0.80	14/10276 (0.1%)

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	A	0	2

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	TYR	CB-CA-C	-8.67	93.07	110.40
1	B	215	MET	CG-SD-CE	8.39	113.62	100.20
1	B	41	SER	CB-CA-C	8.19	125.65	110.10
1	A	234	TYR	N-CA-C	7.97	132.52	111.00
1	A	482	ILE	CB-CA-C	-7.76	96.09	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ILE	Mainchain
1	A	75	VAL	Peptide

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	3732	0	3867	887	0
1	B	3610	0	3738	860	0
All	All	7342	0	7605	1738	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 116.

The worst 5 of 1738 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:157:LYS:HG2	1:A:493:PHE:CD2	1.38	1.57
1:A:117:ILE:HG22	1:A:118:LEU:CD1	1.33	1.55
1:B:395:LYS:CE	1:B:396:HIS:HE1	1.18	1.53
1:A:160:PHE:CE1	1:A:165:LEU:HD23	1.46	1.51
1:A:202:GLY:CA	1:A:434:PRO:HG3	1.05	1.49

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	487/511 (95%)	374 (77%)	59 (12%)	54 (11%)	0 3
1	B	472/511 (92%)	336 (71%)	84 (18%)	52 (11%)	0 3
All	All	959/1022 (94%)	710 (74%)	143 (15%)	106 (11%)	0 3

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	86	ARG
1	A	152	THR
1	A	231	GLY
1	A	280	SER

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	394/414 (95%)	249 (63%)	145 (37%)	0	0
1	B	380/414 (92%)	234 (62%)	146 (38%)	0	0
All	All	774/828 (94%)	483 (62%)	291 (38%)	0	0

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	463	LEU
1	B	67	VAL
1	B	404	ASN
1	A	484	SER
1	B	15	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	145	GLN
1	B	266	ASN
1	B	485	GLN
1	B	124	ASN
1	B	491	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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](#)

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, 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	493/511 (96%)	0.07	23 (4%)	35 22	47, 95, 150, 198	0
1	B	480/511 (93%)	0.19	33 (6%)	20 11	51, 115, 177, 251	0
All	All	973/1022 (95%)	0.13	56 (5%)	26 14	47, 105, 168, 251	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	LYS	5.3
1	B	480	GLU	5.0
1	B	435	ASP	4.8
1	B	196	PRO	4.0
1	B	504	ILE	4.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.