



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 09:36 PM UTC

PDB ID : 4DJI / pdb_00004dji
Title : Structure of glutamate-GABA antiporter GadC
Authors : Ma, D.; Lu, P.L.; Yan, C.Y.; Fan, C.; Yin, P.; Wang, J.W.; Shi, Y.G.
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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
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

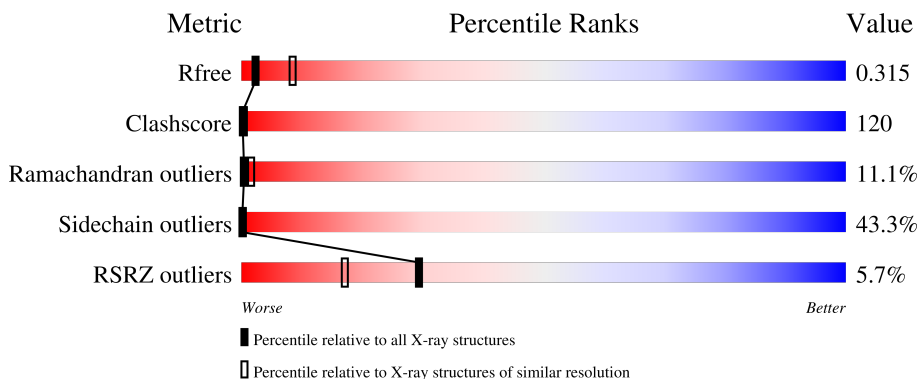
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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 $\leq 5\%$. 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.

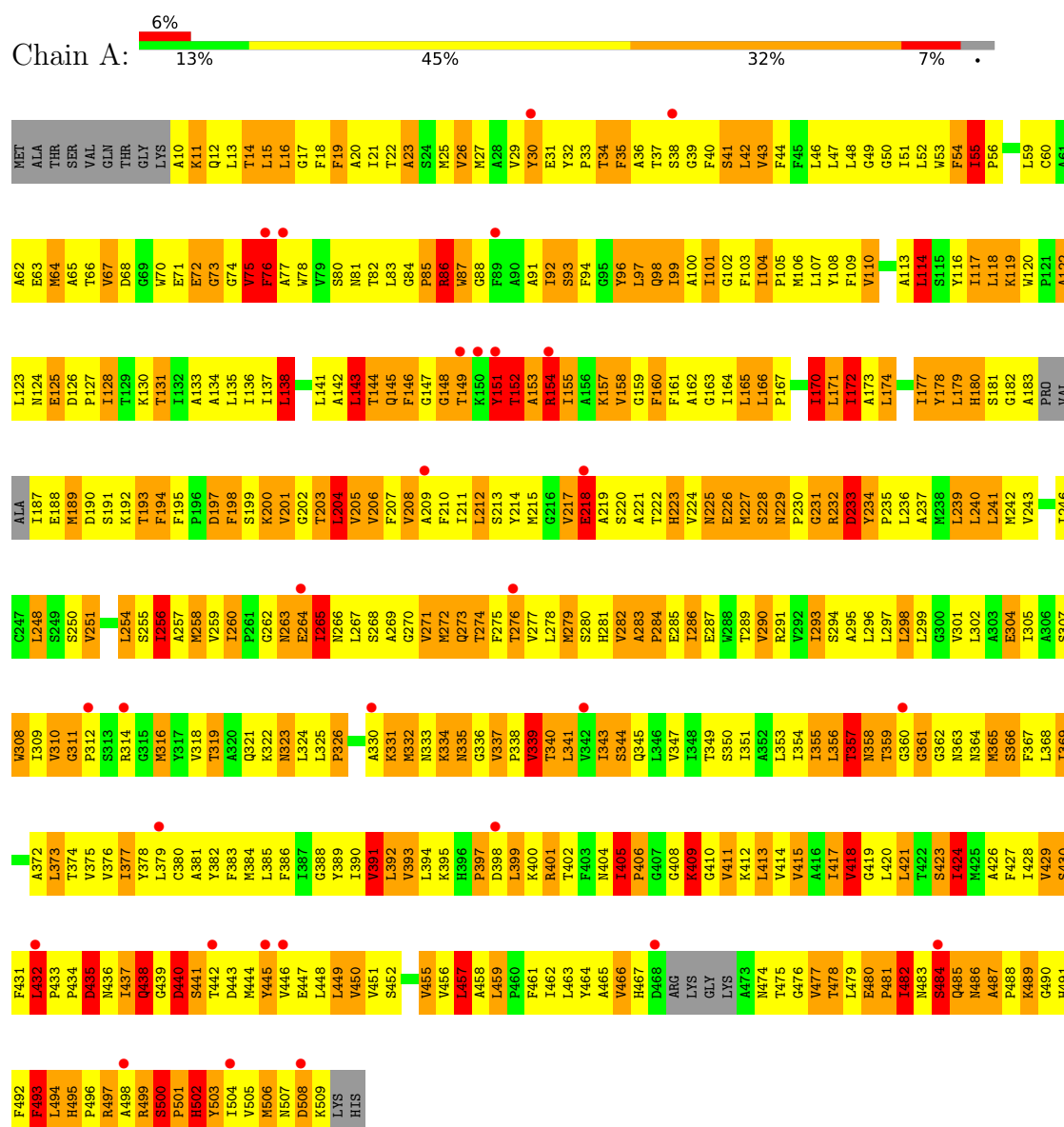
- Molecule 1 is a protein called Probable glutamate/gamma-aminobutyrate antiporter.

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			

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: Probable glutamate/gamma-aminobutyrate antiporter



- Molecule 1: Probable glutamate/gamma-aminobutyrate antiporter



K489	V429	L368	S307	T246	VAL	N124	A61	MET
G490	S430	I369	W308	C247	A186	E125	A62	ALA
H491	F431	A370	I309	L248	I187	E126	E63	THR
F492	L432	L371	V310	S249	E188	P127	M64	SER
F493	P433	A372	G311	S250	M189	T129	A65	VAL
L494	P434	L373	P312	V251	D190	T129	T66	GLN
H495	D435	T374	S313	G252	S191	K130	V67	THR
H496	N436	V375	S314	G253	K192	T131	D68	GLY
R497	I437	V376	G315	L256	T193	I132	G69	LYS
A498	Q438	I377	M316	A257	F194	E71	W70	ALA
R499	G439	I378	Y317	M258	F195	E72	Q12	LYS
S500	D440	L379	V318	V259	D197	G73	L13	L13
P501	S441	C380	T319	V260	F198	G74	T14	T14
H502	T442	A381	A320	L260	S199	W139	L35	L35
Y503	D443	Y382	Q321	P261	K200	A140	V75	V75
VAL	M444	F383	K322	G262	V201	L141	F76	L16
MET	Y445	M384	N323	N263	G202	A142	A77	G17
ASN	V446	L385	L324	E264	T203	L143	W78	F18
ASP	E447	F386	L325	T265	L204	T144	V79	F19
LYS	L448	I387	P326	N266	V205	Q145	N81	A20
LYS	L449	G388	F329	L267	V206	F146	N80	I21
LYS	V450	Y389	A330	S268	F207	G147	T82	T22
HIS	V451	I390	K331	A269	V208	G148	L83	A23
	S452	V391	M332	G270	A209	T149	G84	S24
	F453	L392	N333	M272	F210	K150	P85	M25
	L454	V393	N333	Q273	I211	Y151	F89	V26
	V455	L394	K334	T274	L212	T152	A90	M27
	V456	K395	N335	F275	S213	A153	A91	A28
	L457	H396	G336	T276	Y214	R154	V29	V29
	A458	P397	V337	T277	K215	I155	I92	Y30
	L459	ASP	P338	V277	E216	A156	S93	E31
	P460	LEU	V339	L278	V217	K157	F94	Y32
	F461	LYS	T340	M279	E218	V158	G95	P33
	L462	ARG	L341	H281	A219	G159	Y96	T34
	L463	T402	V342	S280	A221	F161	Q98	F35
	Y464	F403	I343	V282	S220	F160	I99	A36
	A465	M404	S344	A283	T222	A162	S38	T37
	V466	I405	Q345	P284	H223	G163	F45	F45
	H467	L346	L346	E285	V224	I164	F109	L46
	ASP	V347	V347	I286	V224	I165	V110	L47
	ARG	I348	I348	E287	N225	L166	L111	L48
	LYS	T349	T349	V288	E226	L166	G112	L48
	GLY	V411	S350	T289	M227	P167	A113	G49
	LYS	K412	I351	V290	S228	A168	G50	G49
	ALA	L413	A352	R291	N229	F169	I51	I51
	ASN	V414	L353	V292	P230	I170	L114	L52
	T475	V415	I354	I293	G231	L171	S115	L47
	G476	A416	I355	S294	R232	I172	L111	L48
	V477	I417	L356	A295	D233	A173	G12	G49
	T478	V418	T357	L296	Y234	L174	A113	G49
	L479	G419	N358	L297	P235	A175	L114	I51
	E480	L420	T359	L298	L236	A176	S115	I51
	P481	L421	G360	L299	A237	I177	L115	L52
	I482	T422	G361	G300	M238	Y178	Y116	W53
	N483	S423	G362	V301	L239	L179	I117	F54
	S484	I424	N363	L302	L240	H180	K119	I55
	Q485	M425	N364	A303	L241	S181	K119	P56
	N486	A426	M365	E304	M242	G182	W120	V57
	A487	F427	S366	I305	V243	A183	A122	G58
	P488	I428	F367	A306		PRO	L123	C60

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 0.302 , 0.315	Depositor DCC
R_{free} test set	1138 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å ²)	107.4	Xtriage
Anisotropy	0.971	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	1.02	0/3826	1.17	40/5222 (0.8%)
1	B	0.90	0/3700	1.14	39/5054 (0.8%)
All	All	0.96	0/7526	1.16	79/10276 (0.8%)

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 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	234	TYR	N-CA-C	10.27	132.52	109.81
1	A	482	ILE	CB-CA-C	-9.57	96.09	110.82
1	A	234	TYR	CB-CA-C	-8.68	93.07	110.17
1	A	193	THR	N-CA-C	-8.60	102.91	112.72
1	B	42	LEU	CB-CA-C	-8.52	97.84	110.96

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	915	0
1	B	3610	0	3738	881	0
All	All	7342	0	7605	1787	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 120.

The worst 5 of 1787 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%)	01
1	B	472/511 (92%)	336 (71%)	84 (18%)	52 (11%)	01
All	All	959/1022 (94%)	710 (74%)	143 (15%)	106 (11%)	01

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%)	226 (57%)	168 (43%)	0	0
1	B	380/414 (92%)	213 (56%)	167 (44%)	0	0
All	All	774/828 (94%)	439 (57%)	335 (43%)	0	0

5 of 335 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	194	PHE
1	B	353	LEU
1	B	215	MET
1	B	278	LEU
1	B	385	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	266	ASN
1	B	333	ASN
1	B	495	HIS
1	B	323	ASN
1	B	345	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](#)

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%)	0.32	29 (5%)	28 16	47, 95, 150, 198	0
1	B	480/511 (93%)	0.40	26 (5%)	31 18	51, 115, 177, 251	0
All	All	973/1022 (95%)	0.36	55 (5%)	29 17	47, 105, 168, 251	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	504	ILE	5.3
1	B	480	GLU	5.2
1	A	89	PHE	5.1
1	B	502	HIS	5.0
1	B	30	TYR	4.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.