



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 24, 2018 – 10:15 PM EST

PDB ID : 2V36
Title : Crystal structure of gamma-glutamyl transferase from Bacillus subtilis
Authors : Sharath, B.; Prabhune, A.A.; Suresh, C.G.; Wilkinson, A.J.; Brannigan, J.A.
Deposited on : 2007-06-13
Resolution : 1.85 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

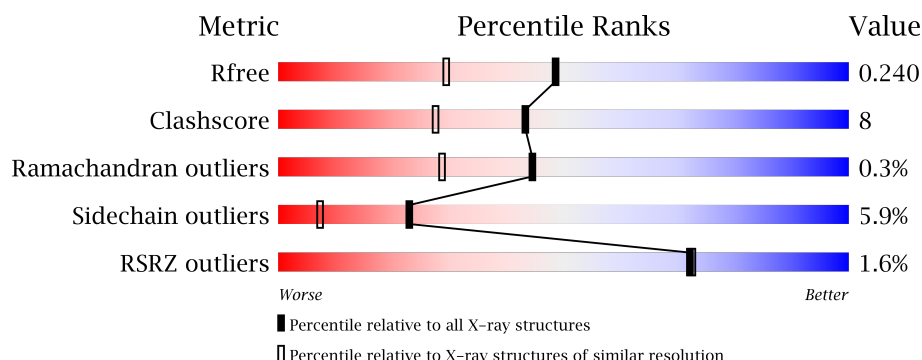
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	100719	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

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	376	<div> <div>2%</div> <div>73%</div> <div>19%</div> <div>• • 5%</div> </div>
1	C	376	<div> <div>%</div> <div>75%</div> <div>16%</div> <div>• • 5%</div> </div>
2	B	193	<div> <div>3%</div> <div>71%</div> <div>16%</div> <div>• • 9%</div> </div>
2	D	193	<div> <div>%</div> <div>70%</div> <div>22%</div> <div>• • 5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8372 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 GAMMA-GLUTAMYLTRANSPEPTIDASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2693	1719	445	519	10			
1	C	357	Total	C	N	O	S	0	0	0
			2670	1702	440	518	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	PRO	LEU	conflict	UNP P54422
C	302	PRO	LEU	conflict	UNP P54422

- Molecule 2 is a protein called GAMMA-GLUTAMYLTRANSPEPTIDASE SMALL CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1297	822	213	258	4			
2	D	183	Total	C	N	O	S	0	0	0
			1363	862	228	268	5			

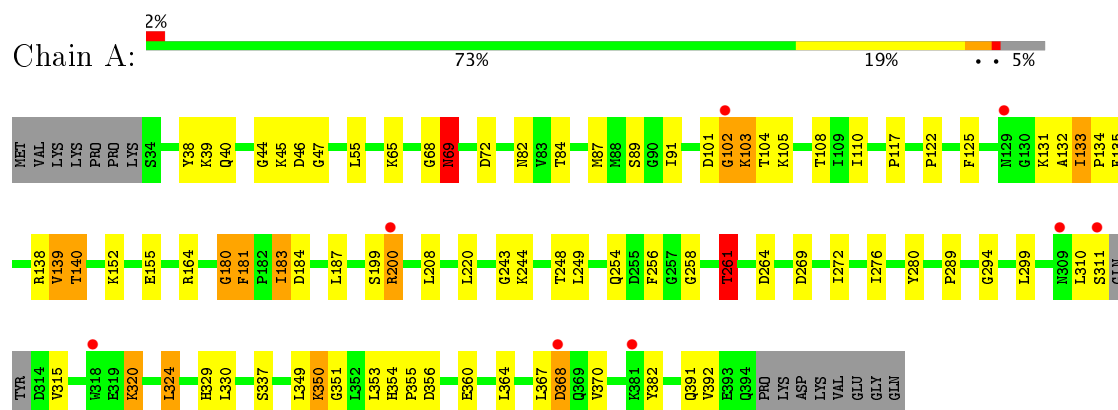
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total	O	0	0
			130	130		
3	B	55	Total	O	0	0
			55	55		
3	C	113	Total	O	0	0
			113	113		
3	D	51	Total	O	0	0
			51	51		

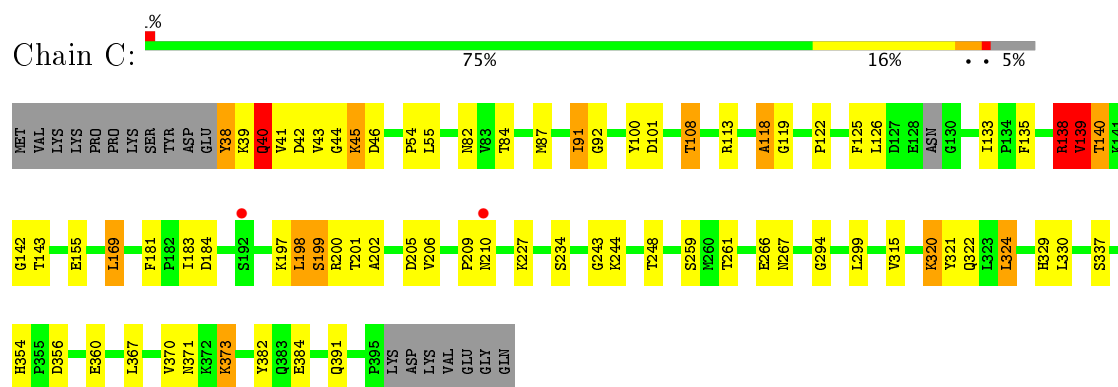
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

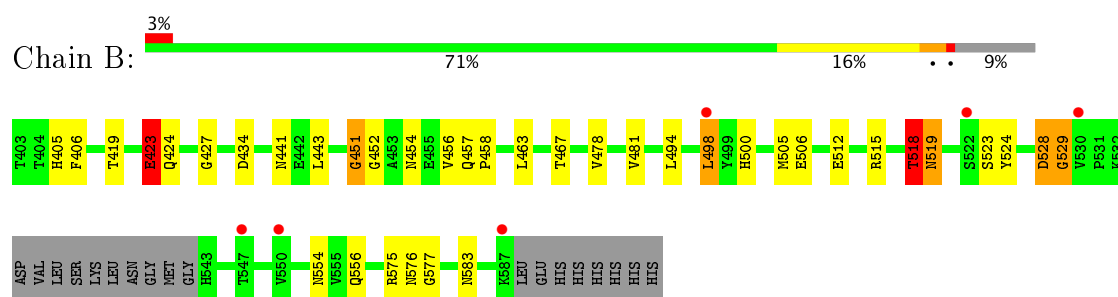
• Molecule 1: GAMMA-GLUTAMYLTRANSPEPTIDASE LARGE CHAIN



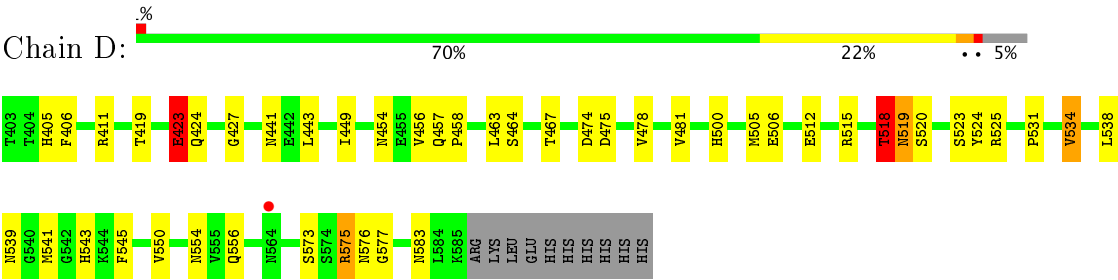
• Molecule 1: GAMMA-GLUTAMYLTRANSPEPTIDASE LARGE CHAIN



• Molecule 2: GAMMA-GLUTAMYLTRANSPEPTIDASE SMALL CHAIN



• Molecule 2: GAMMA-GLUTAMYLTRANSPEPTIDASE SMALL CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.26Å 108.77Å 161.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.17 – 1.85 29.56 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.6 (90.17-1.85) 97.6 (29.56-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.249 0.210 , 0.240	Depositor DCC
R_{free} test set	5336 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8372	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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	0.94	12/2750 (0.4%)	0.99	18/3729 (0.5%)
1	C	0.93	9/2727 (0.3%)	1.01	20/3699 (0.5%)
2	B	0.99	10/1324 (0.8%)	1.01	10/1805 (0.6%)
2	D	0.97	7/1391 (0.5%)	1.13	12/1895 (0.6%)
All	All	0.95	38/8192 (0.5%)	1.03	60/11128 (0.5%)

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	20
1	C	0	18
2	B	0	4
2	D	0	3
All	All	0	45

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	197	LYS	C-N	9.56	1.56	1.34
1	C	384	GLU	C-N	8.49	1.48	1.33
1	A	256	PHE	C-N	-8.33	1.18	1.33
1	A	139	VAL	CB-CG1	-7.91	1.36	1.52
1	C	139	VAL	CB-CG2	-7.87	1.36	1.52

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	575	ARG	NE-CZ-NH1	18.26	129.43	120.30
2	D	575	ARG	NE-CZ-NH2	-17.30	111.65	120.30
1	A	132	ALA	N-CA-C	-12.98	75.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	481	VAL	CG1-CB-CG2	-9.86	95.12	110.90
1	C	138	ARG	NE-CZ-NH1	9.74	125.17	120.30

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	LYS	Peptide
1	A	46	ASP	Peptide
1	A	65	LYS	Peptide
1	A	68	GLY	Peptide
1	A	89	SER	Peptide

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	2693	0	2615	36	0
1	C	2670	0	2577	37	0
2	B	1297	0	1243	28	0
2	D	1363	0	1327	45	0
3	A	130	0	0	2	0
3	B	55	0	0	4	0
3	C	113	0	0	5	0
3	D	51	0	0	1	0
All	All	8372	0	7762	122	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 8.

The worst 5 of 122 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)
2:D:525:ARG:NH1	2:D:550:VAL:HG11	1.53	1.21
2:D:525:ARG:HH12	2:D:550:VAL:HG11	1.19	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:SER:OG	1:C:391:GLN:NE2	2.12	0.83
2:D:525:ARG:NH1	2:D:550:VAL:CG1	2.41	0.82
1:A:329:HIS:HE1	2:B:518:THR:CG2	1.93	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	355/376 (94%)	342 (96%)	13 (4%)	0	100	100
1	C	351/376 (93%)	338 (96%)	12 (3%)	1 (0%)	44	29
2	B	171/193 (89%)	162 (95%)	8 (5%)	1 (1%)	28	13
2	D	181/193 (94%)	175 (97%)	5 (3%)	1 (1%)	28	13
All	All	1058/1138 (93%)	1017 (96%)	38 (4%)	3 (0%)	44	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	423	GLU
2	D	423	GLU
1	C	202	ALA

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	274/312 (88%)	253 (92%)	21 (8%)	15	3
1	C	272/312 (87%)	255 (94%)	17 (6%)	21	6
2	B	139/165 (84%)	133 (96%)	6 (4%)	33	15
2	D	149/165 (90%)	144 (97%)	5 (3%)	42	22
All	All	834/954 (87%)	785 (94%)	49 (6%)	23	7

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	443	LEU
1	C	41	VAL
2	D	443	LEU
2	B	506	GLU
1	C	55	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	583	ASN
1	C	329	HIS
2	D	543	HIS
1	C	40	GLN
1	C	82	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	256:PHE	C	257:GLY	N	1.18

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	359/376 (95%)	0.02	8 (2%) 62 61	7, 16, 31, 39	0
1	C	357/376 (94%)	-0.07	2 (0%) 89 89	8, 17, 30, 38	0
2	B	175/193 (90%)	0.13	6 (3%) 46 43	8, 15, 28, 37	0
2	D	183/193 (94%)	-0.14	1 (0%) 90 91	9, 15, 27, 34	0
All	All	1074/1138 (94%)	-0.02	17 (1%) 72 72	7, 16, 30, 39	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	ASN	5.0
1	A	318	TRP	3.4
1	A	368	ASP	3.1
1	A	311	SER	3.0
2	B	547	THR	2.9

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.