



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6J3I / pdb_00006j3i
Title : Structure of LmbA2991T421A
Authors : Song, Y.
Deposited on : 2019-01-04
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

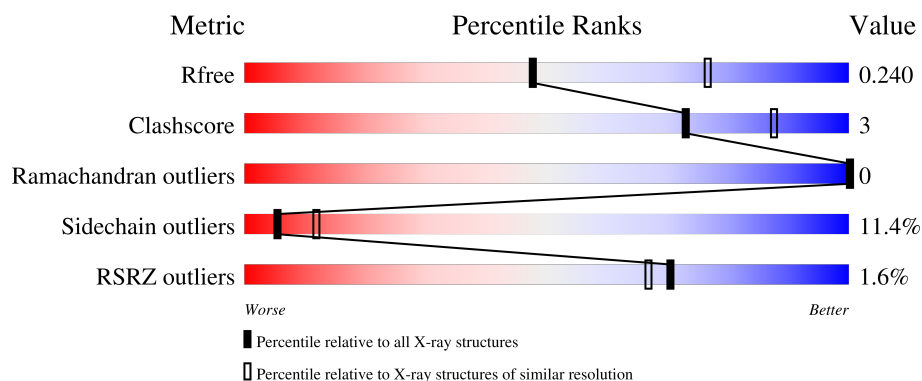
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	617	80% 13% 6%
1	B	617	2% 81% 12% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8749 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4307	2714	778	799	16			
1	B	581	Total	C	N	O	S	0	0	0
			4288	2706	773	793	16			

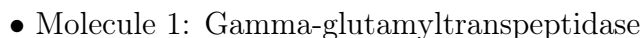
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	ALA	THR	engineered mutation	UNP A0A1B1MKD3
B	421	ALA	THR	engineered mutation	UNP A0A1B1MKD3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	77	Total	O	0	0
			77	77		
2	B	77	Total	O	0	0
			77	77		

- Molecule 1: Gamma-glutamyltranspeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.35Å 113.21Å 116.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.50) 99.7 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.214 , 0.255 (Not available) , 0.240	Depositor DCC
R_{free} test set	2261 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	1.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 15.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8749	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8360e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.61	0/4421	0.95	5/6051 (0.1%)
1	B	0.67	4/4402 (0.1%)	0.95	4/6026 (0.1%)
All	All	0.64	4/8823 (0.0%)	0.95	9/12077 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	GLN	C-O	-6.17	1.15	1.24
1	B	274	GLY	C-O	-5.86	1.16	1.24
1	B	279	GLY	C-O	-5.41	1.19	1.24
1	B	276	TRP	C-O	-5.39	1.17	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	TRP	N-CA-C	-9.05	101.50	112.54
1	A	217	ARG	N-CA-C	7.19	118.76	111.07
1	A	281	VAL	N-CA-CB	6.49	119.36	110.54
1	A	178	ARG	NE-CZ-NH2	6.23	124.81	119.20
1	A	281	VAL	CB-CA-C	-5.90	104.17	112.14
1	A	248	ALA	N-CA-C	5.42	117.19	111.28
1	B	434	VAL	CB-CA-C	-5.23	102.32	110.69
1	B	280	PRO	CA-C-N	5.07	127.41	120.46
1	B	280	PRO	C-N-CA	5.07	127.41	120.46

There are no chirality outliers.

There are no planarity outliers.

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	4307	0	4174	29	0
1	B	4288	0	4158	25	0
2	A	77	0	0	1	0
2	B	77	0	0	0	0
All	All	8749	0	8332	54	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 3.

All (54) 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:178:ARG:HH21	1:A:178:ARG:HG2	1.31	0.92
1:A:157:GLU:O	1:A:161:THR:HB	1.89	0.72
1:B:316:ARG:HA	1:B:320:TYR:CD1	2.31	0.66
1:A:512:HIS:HD2	1:A:537:ASN:OD1	1.81	0.63
1:A:316:ARG:HA	1:A:320:TYR:CD1	2.37	0.58
1:A:442:TRP:HB2	1:A:444:GLN:HE22	1.68	0.57
1:A:539:HIS:HD2	1:A:586:GLU:OE2	1.88	0.56
1:B:512:HIS:HD2	1:B:537:ASN:OD1	1.88	0.56
1:A:543:PHE:O	1:A:552:MET:HB2	2.07	0.55
1:B:486:SER:OG	1:B:510:GLN:NE2	2.40	0.55
1:A:336:TYR:CZ	1:A:340:ARG:HD2	2.42	0.55
1:B:442:TRP:HB2	1:B:444:GLN:HE22	1.73	0.54
1:A:500:THR:HG22	1:A:510:GLN:HG3	1.90	0.54
1:A:6:PRO:HG2	1:A:8:LEU:HD23	1.90	0.54
1:A:30:LEU:HD13	1:A:39:ALA:HB2	1.90	0.54
1:A:178:ARG:HG2	1:A:178:ARG:NH2	2.06	0.51
1:A:176:ALA:O	1:A:178:ARG:NH2	2.43	0.51
1:B:30:LEU:HD13	1:B:39:ALA:HB2	1.92	0.51
1:A:278:GLN:O	1:A:281:VAL:HG22	2.10	0.51
1:A:14:MET:HB3	1:A:603:ALA:HB2	1.94	0.50
1:B:336:TYR:CZ	1:B:340:ARG:HD2	2.46	0.50
1:B:6:PRO:HG2	1:B:8:LEU:HD23	1.94	0.49
1:A:480:ARG:O	1:A:480:ARG:HG3	2.12	0.49
1:A:131:LEU:HD11	1:A:196:LEU:HD11	1.93	0.48
1:A:278:GLN:O	1:A:281:VAL:CG2	2.61	0.48
1:A:235:ASP:OD2	1:A:241:HIS:HD2	1.98	0.47
1:A:512:HIS:CD2	1:A:537:ASN:OD1	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:ARG:O	1:B:480:ARG:HG3	2.15	0.47
1:B:570:GLU:OE2	1:B:573:ARG:NH1	2.48	0.47
1:A:595:ASP:HB3	1:A:598:THR:HG22	1.95	0.46
1:A:228:GLN:HG2	1:A:449:VAL:HA	1.97	0.46
1:B:8:LEU:O	1:B:602:SER:HA	2.16	0.46
1:A:357:PRO:O	1:A:360:ARG:NH2	2.50	0.45
1:A:442:TRP:HB2	1:A:444:GLN:NE2	2.31	0.45
1:B:539:HIS:HD2	1:B:586:GLU:OE2	1.99	0.45
1:B:572:ARG:HH11	1:B:572:ARG:HG2	1.80	0.45
1:B:437:THR:HG23	1:B:485:PRO:HD3	1.98	0.45
1:A:273:ALA:O	1:A:280:PRO:HD3	2.17	0.44
1:B:276:TRP:CD1	1:B:276:TRP:H	2.34	0.44
1:A:61:VAL:HG12	1:A:111:ALA:HA	2.00	0.44
1:B:14:MET:SD	1:B:616:GLY:HA3	2.58	0.43
1:B:120:ARG:HD3	1:B:121:ASP:OD1	2.18	0.43
1:B:235:ASP:OD1	1:B:237:SER:HB3	2.19	0.43
1:B:213:ARG:O	1:B:217:ARG:HB2	2.18	0.42
1:B:282:LEU:C	1:B:282:LEU:HD23	2.44	0.42
1:B:45:PHE:HA	1:B:48:HIS:CD2	2.55	0.42
1:B:296:TYR:O	1:B:301:TYR:CD2	2.73	0.41
1:B:282:LEU:HD23	1:B:282:LEU:O	2.21	0.41
1:B:371:VAL:HG13	1:B:552:MET:HG2	2.01	0.41
1:A:110:GLY:HA2	1:A:253:TRP:CH2	2.56	0.41
1:B:423:HIS:HE1	1:B:425:ASP:OD1	2.03	0.41
1:A:161:THR:HG22	1:A:162:GLU:HB2	2.03	0.41
1:A:145:VAL:HG12	2:A:722:HOH:O	2.21	0.40
1:B:110:GLY:HA2	1:B:253:TRP:CZ3	2.57	0.40

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	579/617 (94%)	565 (98%)	14 (2%)	0	100	100
1	B	577/617 (94%)	561 (97%)	16 (3%)	0	100	100
All	All	1156/1234 (94%)	1126 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	422/457 (92%)	369 (87%)	53 (13%)	4	9
1	B	419/457 (92%)	376 (90%)	43 (10%)	7	14
All	All	841/914 (92%)	745 (89%)	96 (11%)	5	12

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	60	GLU
1	A	65	LEU
1	A	119	LEU
1	A	120	ARG
1	A	127	LEU
1	A	130	VAL
1	A	146	GLU
1	A	161	THR
1	A	178	ARG
1	A	181	GLU
1	A	184	ARG
1	A	188	LEU
1	A	199	VAL
1	A	206	GLU
1	A	228	GLN
1	A	242	THR
1	A	245	LEU

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Mol	Chain	Res	Type
1	A	246	THR
1	A	258	GLU
1	A	281	VAL
1	A	283	LEU
1	A	286	LEU
1	A	288	LEU
1	A	305	LEU
1	A	311	LEU
1	A	316	ARG
1	A	332	LEU
1	A	347	LYS
1	A	353	ARG
1	A	361	THR
1	A	363	ARG
1	A	370	LEU
1	A	371	VAL
1	A	424	LEU
1	A	434	VAL
1	A	437	THR
1	A	444	GLN
1	A	451	GLU
1	A	469	LEU
1	A	477	ARG
1	A	478	ARG
1	A	480	ARG
1	A	491	ASP
1	A	495	VAL
1	A	522	ARG
1	A	552	MET
1	A	557	VAL
1	A	562	ARG
1	A	572	ARG
1	A	579	THR
1	A	598	THR
1	A	610	MET
1	B	30	LEU
1	B	32	ASP
1	B	60	GLU
1	B	65	LEU
1	B	71	GLU
1	B	119	LEU
1	B	127	LEU

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Mol	Chain	Res	Type
1	B	145	VAL
1	B	184	ARG
1	B	188	LEU
1	B	228	GLN
1	B	245	LEU
1	B	258	GLU
1	B	281	VAL
1	B	283	LEU
1	B	286	LEU
1	B	288	LEU
1	B	305	LEU
1	B	310	LYS
1	B	311	LEU
1	B	316	ARG
1	B	332	LEU
1	B	335	GLU
1	B	342	GLU
1	B	353	ARG
1	B	361	THR
1	B	370	LEU
1	B	371	VAL
1	B	424	LEU
1	B	429	ARG
1	B	434	VAL
1	B	437	THR
1	B	444	GLN
1	B	451	GLU
1	B	477	ARG
1	B	478	ARG
1	B	480	ARG
1	B	491	ASP
1	B	495	VAL
1	B	522	ARG
1	B	562	ARG
1	B	579	THR
1	B	610	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	241	HIS

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Mol	Chain	Res	Type
1	A	278	GLN
1	A	423	HIS
1	A	444	GLN
1	A	506	GLN
1	A	510	GLN
1	A	512	HIS
1	A	539	HIS
1	A	611	GLN
1	B	48	HIS
1	B	53	HIS
1	B	140	HIS
1	B	241	HIS
1	B	278	GLN
1	B	367	HIS
1	B	506	GLN
1	B	510	GLN
1	B	512	HIS
1	B	539	HIS
1	B	611	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 [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	583/617 (94%)	0.12	8 (1%) 73 70	14, 23, 42, 56	0
1	B	581/617 (94%)	0.10	11 (1%) 66 62	14, 24, 40, 54	0
All	All	1164/1234 (94%)	0.11	19 (1%) 70 67	14, 23, 40, 56	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	GLY	5.8
1	B	419	GLY	5.0
1	A	409	PRO	4.3
1	A	417	THR	3.7
1	B	418	ARG	3.3
1	A	414	ASP	3.0
1	B	412	ALA	2.7
1	B	373	THR	2.6
1	B	417	THR	2.6
1	A	413	ALA	2.5
1	A	418	ARG	2.5
1	B	416	SER	2.5
1	B	410	ASP	2.4
1	B	413	ALA	2.2
1	A	374	GLY	2.2
1	A	291	PRO	2.2
1	B	187	THR	2.1
1	B	370	LEU	2.1
1	B	335	GLU	2.1

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.