



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:52 am BST

PDB ID : 6J3I
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

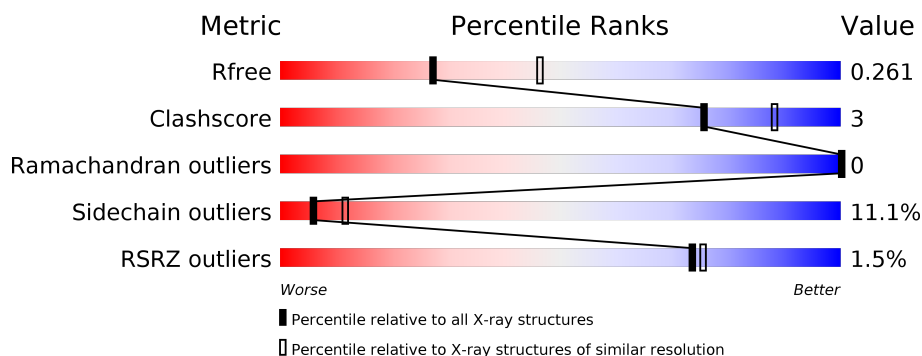
1 Overall quality at a glance

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>
1	B	617	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>

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

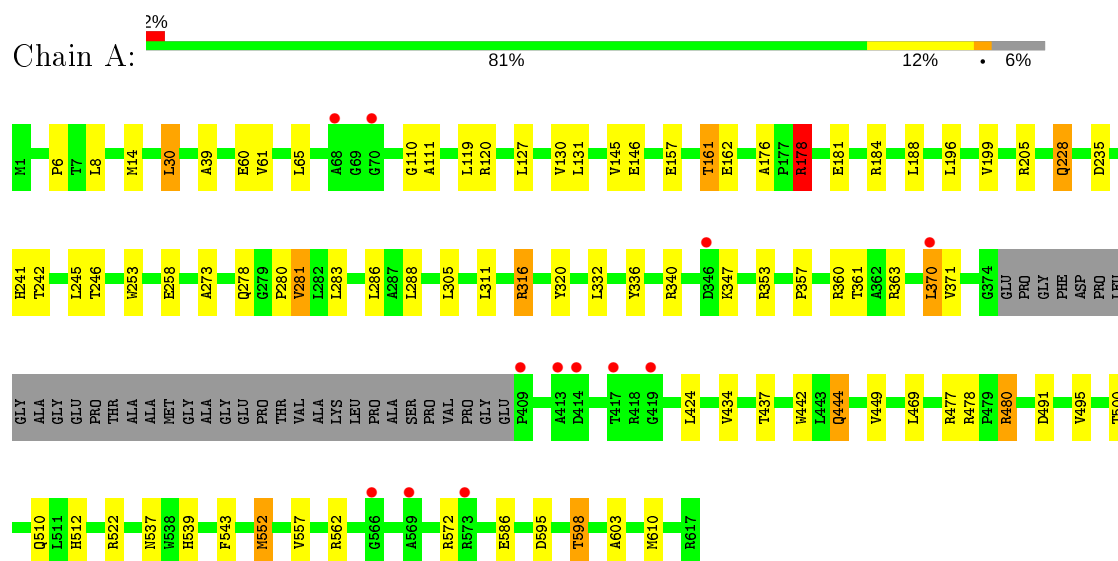
- Molecule 2 is water.

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

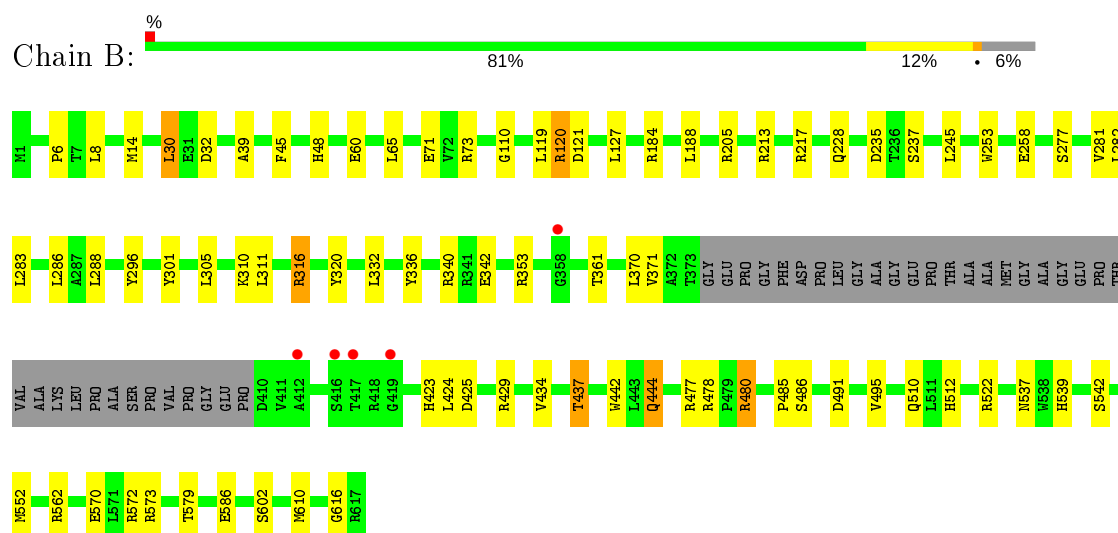
3 Residue-property plots [i](#)

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



• 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 36.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.50) 99.7 (36.69-2.50)	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 0.218 , 0.261	Depositor DCC
R_{free} test set	2261 reflections (5.04%)	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)	0.31 , 18.3	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.42	0/4421	0.76	4/6051 (0.1%)
1	B	0.47	0/4402	0.75	1/6026 (0.0%)
All	All	0.45	0/8823	0.76	5/12077 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ARG	NE-CZ-NH2	9.01	124.81	120.30
1	A	370	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	205	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	205	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	205	ARG	NE-CZ-NH1	5.13	122.86	120.30

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	4307	0	4174	29	0
1	B	4288	0	4158	23	0
2	A	77	0	0	1	0
2	B	77	0	0	0	0
All	All	8749	0	8332	52	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 (52) 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:HG2	1:A:178:ARG:HH21	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:B:512:HIS:HD2	1:B:537:ASN:OD1	1.88	0.56
1:A:539:HIS:HD2	1:A:586:GLU:OE2	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:30:LEU:HD13	1:A:39:ALA:HB2	1.90	0.54
1:A:6:PRO:HG2	1:A:8:LEU:HD23	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:HG3	1:A:480:ARG:O	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
1:B:480:ARG:HG3	1:B:480:ARG:O	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:HG2	1:B:572:ARG:HH11	1.80	0.45
1:B:437:THR:HG23	1:B:485:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:O	1:A:280:PRO:HD3	2.17	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: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:O	1:B:282:LEU:HD23	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%)	372 (88%)	50 (12%)	5	10
1	B	419/457 (92%)	376 (90%)	43 (10%)	7	14
All	All	841/914 (92%)	748 (89%)	93 (11%)	6	11

All (93) 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	228	GLN
1	A	242	THR
1	A	245	LEU
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

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Mol	Chain	Res	Type
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	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	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	73	ARG
1	B	119	LEU
1	B	120	ARG
1	B	127	LEU
1	B	184	ARG
1	B	188	LEU
1	B	228	GLN
1	B	245	LEU
1	B	258	GLU
1	B	277	SER
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

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Mol	Chain	Res	Type
1	B	332	LEU
1	B	342	GLU
1	B	353	ARG
1	B	361	THR
1	B	370	LEU
1	B	424	LEU
1	B	429	ARG
1	B	434	VAL
1	B	437	THR
1	B	444	GLN
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	542	SER
1	B	562	ARG
1	B	579	THR
1	B	610	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	55	ASN
1	A	89	HIS
1	A	241	HIS
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	55	ASN
1	B	278	GLN
1	B	423	HIS
1	B	444	GLN

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Mol	Chain	Res	Type
1	B	506	GLN
1	B	510	GLN
1	B	512	HIS
1	B	539	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 ⓘ

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	583/617 (94%)	-0.08	12 (2%) 63 66	14, 23, 42, 56	0
1	B	581/617 (94%)	-0.11	5 (0%) 84 86	14, 24, 40, 54	0
All	All	1164/1234 (94%)	-0.10	17 (1%) 73 75	14, 23, 40, 56	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	GLY	4.1
1	A	417	THR	3.1
1	B	412	ALA	3.1
1	A	566	GLY	3.0
1	B	416	SER	3.0
1	B	419	GLY	3.0
1	A	346	ASP	2.7
1	A	409	PRO	2.5
1	B	358	GLY	2.2
1	A	70	GLY	2.2
1	A	68	ALA	2.2
1	A	573	ARG	2.2
1	A	414	ASP	2.2
1	A	413	ALA	2.1
1	A	569	ALA	2.1
1	B	417	THR	2.1
1	A	370	LEU	2.0

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 [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.