Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2024 – 01:20 PM JST

PDB ID	:	6J3A
Title	:	Structure of LmbA2991HD
Authors	:	Song, Y.
Deposited on	:	2019-01-04
Resolution	:	2.38 Å(reported)

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

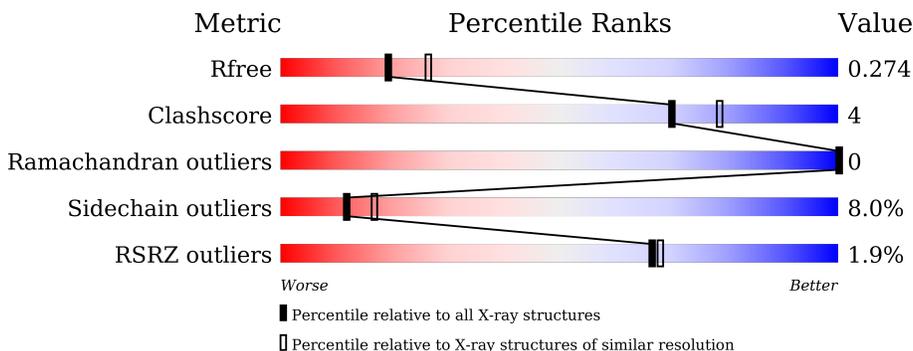|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.38 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	Percentile Ranks	Value
Rfree		0.274
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		8.0%
RSRZ outliers		1.9%

Worse ——— Better

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 <=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	85% · 8% · 6%
1	B	617	79% · 13% · 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8828 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	580	Total	C	N	O	S	0	0	0
			4315	2725	773	801	16			
1	B	580	Total	C	N	O	S	0	0	0
			4306	2719	778	793	16			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total	O	0	0
			110	110		
2	B	97	Total	O	0	0
			97	97		

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: Gamma-glutamyltranspeptidase

Chain A:

• Molecule 1: Gamma-glutamyltranspeptidase

Chain B:
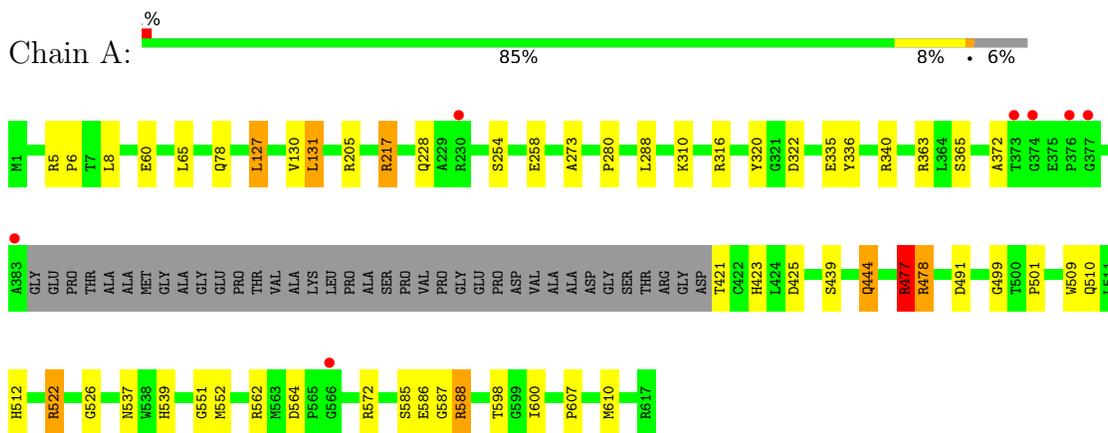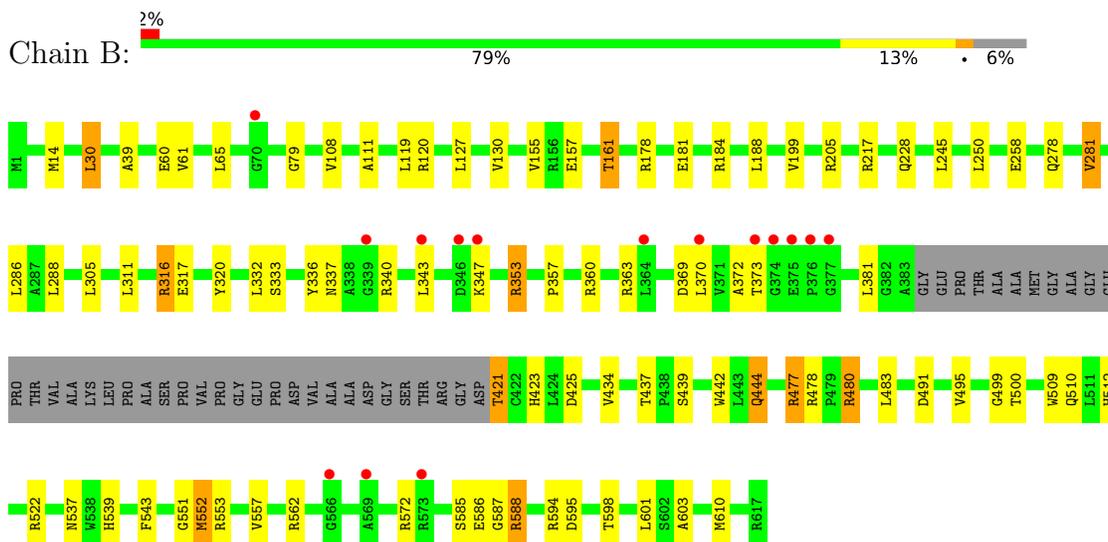
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.44Å 113.18Å 116.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.38 49.87 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.38) 99.3 (49.87-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.224 , 0.267 0.228 , 0.274	Depositor DCC
R_{free} test set	2588 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.899	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 24.9	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8828	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 46.35 % 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 1.1597e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.42	0/4432	0.72	3/6064 (0.0%)
1	B	0.44	0/4423	0.75	2/6053 (0.0%)
All	All	0.43	0/8855	0.73	5/12117 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	205	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	B	205	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	205	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	205	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	477	ARG	NE-CZ-NH2	5.42	123.01	120.30

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	4315	0	4193	25	0
1	B	4306	0	4189	36	0
2	A	110	0	0	2	0
2	B	97	0	0	3	0
All	All	8828	0	8382	61	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 4.

All (61) 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:444:GLN:HE21	1:A:444:GLN:H	1.41	0.67
1:B:539:HIS:HD2	1:B:586:GLU:OE2	1.78	0.66
1:B:442:TRP:HB2	1:B:444:GLN:HE22	1.63	0.63
1:A:336:TYR:CZ	1:A:340:ARG:HD2	2.34	0.62
1:B:594:ARG:HG3	1:B:601:LEU:HD23	1.81	0.61
1:A:372:ALA:HB2	1:A:551:GLY:HA3	1.84	0.60
1:B:278:GLN:O	1:B:281:VAL:HG22	2.02	0.58
1:B:316:ARG:HA	1:B:320:TYR:CD1	2.39	0.57
1:B:512:HIS:HD2	1:B:537:ASN:OD1	1.88	0.56
1:A:273:ALA:O	1:A:280:PRO:HD3	2.06	0.55
1:B:157:GLU:O	1:B:161:THR:HB	2.07	0.55
1:B:372:ALA:HB2	1:B:551:GLY:HA3	1.88	0.55
1:A:444:GLN:HE21	1:A:444:GLN:N	2.05	0.55
1:A:512:HIS:HD2	1:A:537:ASN:OD1	1.91	0.54
1:A:258:GLU:OE2	1:A:478:ARG:NH1	2.40	0.54
1:B:594:ARG:HG3	1:B:601:LEU:CD2	2.38	0.54
1:B:217:ARG:CZ	2:B:701:HOH:O	2.55	0.53
1:B:442:TRP:HB2	1:B:444:GLN:NE2	2.23	0.53
1:B:553:ARG:HD3	2:B:703:HOH:O	2.08	0.53
1:B:421:THR:HB	1:B:439:SER:HB2	1.91	0.52
1:B:421:THR:HG22	1:B:439:SER:OG	2.10	0.51
1:B:423:HIS:HE1	1:B:425:ASP:OD1	1.94	0.51
1:B:333:SER:O	1:B:337:ASN:ND2	2.38	0.50
1:B:217:ARG:HG2	1:B:250:LEU:O	2.11	0.50
1:B:357:PRO:O	1:B:360:ARG:NH2	2.44	0.49
1:A:127:LEU:HD22	1:A:131:LEU:HD23	1.94	0.49
1:A:423:HIS:HE1	1:A:425:ASP:OD1	1.95	0.49
1:B:500:THR:HG22	1:B:510:GLN:HG3	1.95	0.49
1:A:316:ARG:HA	1:A:320:TYR:CD1	2.48	0.48
1:A:322:ASP:O	1:A:477:ARG:HG3	2.12	0.48
1:B:278:GLN:NE2	2:B:702:HOH:O	2.43	0.48
1:A:217:ARG:NH2	1:A:254:SER:OG	2.46	0.48
1:A:499:GLY:HA2	1:A:510:GLN:NE2	2.29	0.48
1:B:278:GLN:O	1:B:281:VAL:CG2	2.61	0.48
1:A:509:TRP:CE3	1:A:587:GLY:HA2	2.49	0.48
1:B:30:LEU:HD13	1:B:39:ALA:HB2	1.95	0.47
1:B:336:TYR:CZ	1:B:340:ARG:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:PRO:HD2	1:A:588:ARG:HB2	1.98	0.46
1:B:595:ASP:HB3	1:B:598:THR:HG22	1.97	0.46
1:B:343:LEU:HB3	1:B:353:ARG:NH2	2.32	0.44
1:B:499:GLY:HA2	1:B:510:GLN:NE2	2.33	0.44
1:B:543:PHE:C	1:B:552:MET:HB2	2.39	0.44
1:B:585:SER:O	1:B:588:ARG:NH1	2.51	0.43
1:B:79:GLY:HA3	1:B:108:VAL:O	2.18	0.43
1:B:317:GLU:OE1	1:B:480:ARG:NH2	2.51	0.43
1:A:60:GLU:HG3	2:A:707:HOH:O	2.18	0.42
1:B:477:ARG:N	1:B:477:ARG:HD2	2.34	0.42
1:A:539:HIS:HD2	1:A:586:GLU:OE2	2.03	0.42
1:B:509:TRP:CE3	1:B:587:GLY:HA2	2.54	0.42
1:A:522:ARG:HB3	1:A:526:GLY:O	2.19	0.42
1:B:14:MET:HB3	1:B:603:ALA:HB2	2.02	0.42
1:B:439:SER:HB3	1:B:483:LEU:HD11	2.01	0.42
1:A:564:ASP:CB	2:A:797:HOH:O	2.68	0.42
1:A:585:SER:O	1:A:588:ARG:NH1	2.52	0.41
1:A:6:PRO:HG2	1:A:8:LEU:HD23	2.00	0.41
1:B:61:VAL:HG12	1:B:111:ALA:HA	2.02	0.41
1:A:598:THR:HG21	1:A:600:ILE:HD12	2.03	0.41
1:A:60:GLU:HG2	1:A:78:GLN:NE2	2.36	0.40
1:A:5:ARG:NH1	1:A:607:PRO:HA	2.36	0.40
1:A:421:THR:HG23	1:A:439:SER:HB2	2.03	0.40
1:B:423:HIS:NE2	1:B:499:GLY:HA3	2.37	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	576/617 (93%)	562 (98%)	14 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	576/617 (93%)	562 (98%)	14 (2%)	0	100	100
All	All	1152/1234 (93%)	1124 (98%)	28 (2%)	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	426/458 (93%)	405 (95%)	21 (5%)	25	38
1	B	424/458 (93%)	377 (89%)	47 (11%)	6	7
All	All	850/916 (93%)	782 (92%)	68 (8%)	12	17

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	127	LEU
1	A	130	VAL
1	A	131	LEU
1	A	217	ARG
1	A	228	GLN
1	A	288	LEU
1	A	310	LYS
1	A	335	GLU
1	A	363	ARG
1	A	365	SER
1	A	444	GLN
1	A	477	ARG
1	A	478	ARG
1	A	491	ASP
1	A	522	ARG
1	A	552	MET
1	A	562	ARG

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Mol	Chain	Res	Type
1	A	572	ARG
1	A	588	ARG
1	A	610	MET
1	B	30	LEU
1	B	60	GLU
1	B	65	LEU
1	B	119	LEU
1	B	120	ARG
1	B	127	LEU
1	B	130	VAL
1	B	155	VAL
1	B	161	THR
1	B	178	ARG
1	B	181	GLU
1	B	184	ARG
1	B	188	LEU
1	B	199	VAL
1	B	228	GLN
1	B	245	LEU
1	B	258	GLU
1	B	281	VAL
1	B	286	LEU
1	B	288	LEU
1	B	305	LEU
1	B	311	LEU
1	B	316	ARG
1	B	332	LEU
1	B	347	LYS
1	B	353	ARG
1	B	363	ARG
1	B	369	ASP
1	B	370	LEU
1	B	373	THR
1	B	381	LEU
1	B	421	THR
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

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Mol	Chain	Res	Type
1	B	495	VAL
1	B	522	ARG
1	B	552	MET
1	B	557	VAL
1	B	562	ARG
1	B	572	ARG
1	B	588	ARG
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	53	HIS
1	A	55	ASN
1	A	89	HIS
1	A	228	GLN
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	B	53	HIS
1	B	241	HIS
1	B	278	GLN
1	B	423	HIS
1	B	444	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 monosaccharides 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 ⓘ

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(Å²)	Q<0.9
1	A	580/617 (94%)	0.10	7 (1%)	79	80	23, 32, 49, 78	0
1	B	580/617 (94%)	0.18	15 (2%)	56	57	23, 32, 51, 78	0
All	All	1160/1234 (94%)	0.14	22 (1%)	66	68	23, 32, 50, 78	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	373	THR	4.8
1	A	383	ALA	4.4
1	A	374	GLY	4.2
1	B	339	GLY	3.8
1	B	573	ARG	3.4
1	A	373	THR	3.4
1	A	376	PRO	3.2
1	B	374	GLY	3.2
1	B	347	LYS	3.0
1	B	569	ALA	3.0
1	A	377	GLY	2.7
1	B	343	LEU	2.5
1	A	566	GLY	2.4
1	B	364	LEU	2.3
1	B	70	GLY	2.3
1	B	370	LEU	2.2
1	B	375	GLU	2.1
1	A	230	ARG	2.1
1	B	377	GLY	2.1
1	B	566	GLY	2.1
1	B	376	PRO	2.0
1	B	346	ASP	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.