



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:10 pm BST

PDB ID : 6HUW  
Title : Crystal structure of CdaA from Bacillus subtilis  
Authors : Tosi, T.; Freemont, P.S.; Grundling, A.  
Deposited on : 2018-10-09  
Resolution : 2.80 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](mailto: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.

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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

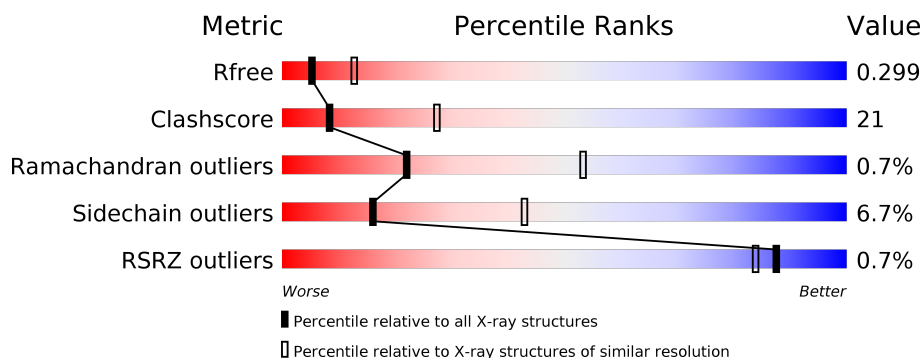
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	183	<div> <div></div> <div> <div></div> <div>48%</div> <div>27%</div> <div>• •</div> <div>20%</div> </div> </div>
1	B	183	<div> <div></div> <div> <div></div> <div>55%</div> <div>23%</div> <div>•</div> <div>21%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2198 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 Diadenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	136	0	0
			1106	692	187	222	5			
1	B	144	Total	C	N	O	S	108	0	0
			1092	683	185	219	5			

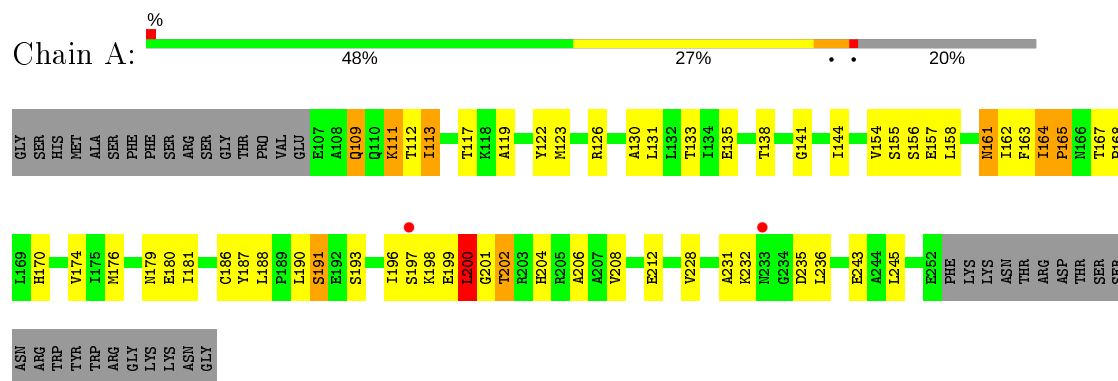
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	GLY	-	expression tag	UNP A0A063XB03
A	92	SER	-	expression tag	UNP A0A063XB03
A	93	HIS	-	expression tag	UNP A0A063XB03
A	94	MET	-	expression tag	UNP A0A063XB03
A	95	ALA	-	expression tag	UNP A0A063XB03
A	96	SER	-	expression tag	UNP A0A063XB03
B	91	GLY	-	expression tag	UNP A0A063XB03
B	92	SER	-	expression tag	UNP A0A063XB03
B	93	HIS	-	expression tag	UNP A0A063XB03
B	94	MET	-	expression tag	UNP A0A063XB03
B	95	ALA	-	expression tag	UNP A0A063XB03
B	96	SER	-	expression tag	UNP A0A063XB03

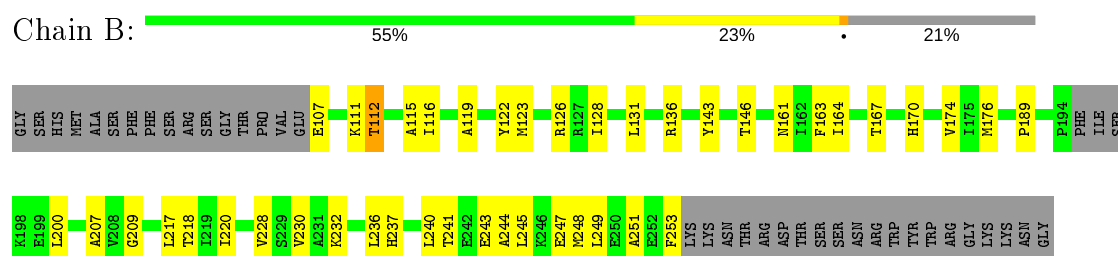
### 3 Residue-property plots [i](#)

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: Diadenylate cyclase



#### • Molecule 1: Diadenylate cyclase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.89 Å 62.89 Å 187.32 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.62 – 2.80 59.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (59.62-2.80) 100.0 (59.62-2.80)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.99 (at 2.81 Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.255 , 0.297 0.260 , 0.299	Depositor DCC
$R_{free}$ test set	446 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.1	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	2198	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 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	1.41	8/1118 (0.7%)	1.08	7/1512 (0.5%)
1	B	0.89	1/1103 (0.1%)	0.85	0/1490
All	All	1.18	9/2221 (0.4%)	0.97	7/3002 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	PRO	N-CD	-17.37	1.23	1.47
1	A	186	CYS	CB-SG	-7.10	1.70	1.82
1	A	130	ALA	C-O	-5.40	1.13	1.23
1	A	122	TYR	CE1-CZ	-5.30	1.31	1.38
1	A	135	GLU	CD-OE2	-5.23	1.19	1.25
1	A	131	LEU	C-O	-5.21	1.13	1.23
1	A	135	GLU	CD-OE1	-5.16	1.20	1.25
1	A	133	THR	C-O	-5.13	1.13	1.23
1	B	115	ALA	C-O	-5.01	1.13	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	A	126	ARG	NE-CZ-NH2	8.57	124.58	120.30
1	A	113	ILE	N-CA-C	-7.34	91.18	111.00
1	A	200	LEU	CA-CB-CG	7.07	131.55	115.30
1	A	164	ILE	N-CA-C	-5.84	95.22	111.00
1	A	111	LYS	N-CA-C	-5.71	95.57	111.00
1	A	131	LEU	CA-CB-CG	5.64	128.28	115.30

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	1106	0	1126	41	0
1	B	1092	0	1110	46	0
All	All	2198	0	2236	82	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 21.

All (82) 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:B:143:TYR:O	1:B:146:THR:HG22	1.14	1.27
1:B:143:TYR:O	1:B:146:THR:CG2	1.90	1.19
1:B:164:ILE:O	1:B:167:THR:HG22	1.55	1.05
1:B:131:LEU:CD1	1:B:220:ILE:HG12	1.87	1.05
1:A:191:SER:OG	1:A:212:GLU:OE2	1.79	0.97
1:B:131:LEU:CD1	1:B:220:ILE:CG1	2.44	0.95
1:B:131:LEU:HD12	1:B:220:ILE:HG13	1.48	0.95
1:B:131:LEU:HD12	1:B:220:ILE:CG1	1.96	0.94
1:A:164:ILE:HG22	1:A:167:THR:HB	1.47	0.94
1:A:168:PRO:HD2	1:B:161:ASN:OD1	1.69	0.91
1:B:131:LEU:HD13	1:B:220:ILE:HG12	1.51	0.90
1:B:207:ALA:HB2	1:B:220:ILE:CD1	2.05	0.86
1:A:167:THR:OG1	1:B:161:ASN:OD1	2.00	0.80
1:B:167:THR:HG23	1:B:170:HIS:HB3	1.63	0.80
1:B:111:LYS:O	1:B:112:THR:OG1	1.99	0.79
1:B:207:ALA:CB	1:B:220:ILE:CD1	2.63	0.77
1:B:207:ALA:HB2	1:B:220:ILE:HD11	1.66	0.77
1:A:161:ASN:ND2	1:B:161:ASN:O	2.18	0.77
1:A:164:ILE:O	1:A:167:THR:HG22	1.86	0.76
1:B:207:ALA:CB	1:B:220:ILE:HD13	2.19	0.73
1:B:167:THR:CG2	1:B:170:HIS:HB3	2.22	0.70
1:A:164:ILE:HG22	1:A:167:THR:CB	2.21	0.69
1:A:190:LEU:N	1:A:190:LEU:HD12	2.08	0.69
1:A:167:THR:OG1	1:B:161:ASN:CG	2.31	0.68
1:A:111:LYS:C	1:A:112:THR:HG23	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLU:O	1:B:107:GLU:HG3	1.94	0.67
1:B:143:TYR:C	1:B:146:THR:HG22	2.10	0.66
1:B:207:ALA:CB	1:B:220:ILE:HD11	2.24	0.65
1:B:228:VAL:O	1:B:240:LEU:HD12	1.96	0.65
1:A:111:LYS:O	1:A:112:THR:HG23	1.98	0.64
1:B:241:THR:OG1	1:B:244:ALA:CB	2.46	0.63
1:B:241:THR:OG1	1:B:244:ALA:HB2	2.01	0.61
1:A:196:ILE:HD11	1:A:208:VAL:HG11	1.83	0.60
1:B:207:ALA:HB2	1:B:220:ILE:HD13	1.80	0.60
1:A:119:ALA:O	1:A:123:MET:HG3	2.01	0.60
1:A:123:MET:CE	1:A:163:PHE:HB2	2.32	0.59
1:A:167:THR:CG2	1:A:170:HIS:HB2	2.32	0.58
1:A:164:ILE:CG2	1:A:167:THR:HB	2.29	0.58
1:A:164:ILE:HG13	1:A:165:PRO:HD2	1.86	0.58
1:A:231:ALA:HB2	1:A:236:LEU:HD23	1.85	0.57
1:B:126:ARG:HB2	1:B:128:ILE:HG13	1.89	0.54
1:B:112:THR:O	1:B:116:ILE:HD12	2.07	0.54
1:A:190:LEU:N	1:A:190:LEU:CD1	2.71	0.53
1:B:230:VAL:O	1:B:236:LEU:HD12	2.09	0.53
1:A:167:THR:OG1	1:B:161:ASN:ND2	2.42	0.52
1:A:123:MET:HE1	1:A:163:PHE:HB2	1.92	0.52
1:A:231:ALA:HA	1:A:235:ASP:O	2.10	0.52
1:A:201:GLY:O	1:A:202:THR:HB	2.11	0.51
1:A:198:LYS:O	1:A:199:GLU:HB3	2.11	0.51
1:B:253:PHE:H	1:B:253:PHE:HD1	1.59	0.50
1:A:228:VAL:HG11	1:A:245:LEU:HD22	1.93	0.49
1:B:241:THR:OG1	1:B:244:ALA:N	2.39	0.49
1:B:247:GLU:O	1:B:248:MET:C	2.51	0.49
1:A:167:THR:HG22	1:A:170:HIS:HB2	1.95	0.48
1:B:119:ALA:HB1	1:B:123:MET:HE2	1.96	0.48
1:A:164:ILE:HG22	1:A:167:THR:CG2	2.44	0.48
1:A:158:LEU:HD23	1:A:181:ILE:HD12	1.97	0.47
1:A:174:VAL:HG13	1:A:181:ILE:HG23	1.97	0.47
1:A:123:MET:HE3	1:A:163:PHE:HB2	1.96	0.46
1:B:207:ALA:HB1	1:B:220:ILE:CD1	2.43	0.46
1:A:154:VAL:HG22	1:A:181:ILE:HG13	1.97	0.46
1:A:113:ILE:O	1:A:117:THR:HG23	2.14	0.46
1:B:164:ILE:O	1:B:167:THR:CG2	2.44	0.46
1:A:204:HIS:O	1:A:208:VAL:HG12	2.17	0.45
1:B:122:TYR:O	1:B:126:ARG:HG2	2.16	0.45
1:B:189:PRO:O	1:B:209:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLN:O	1:A:113:ILE:HG13	2.17	0.44
1:A:188:LEU:HB2	1:A:206:ALA:HB1	1.98	0.44
1:A:197:SER:O	1:A:200:LEU:HG	2.18	0.44
1:B:217:LEU:HD23	1:B:232:LYS:HD3	2.00	0.44
1:B:218:THR:HG22	1:B:220:ILE:HD11	1.99	0.43
1:A:155:SER:HB2	1:A:157:GLU:OE2	2.18	0.43
1:B:237:HIS:O	1:B:240:LEU:HD11	2.18	0.42
1:A:141:GLY:HA2	1:A:144:ILE:HD12	2.01	0.42
1:B:249:LEU:C	1:B:251:ALA:H	2.23	0.42
1:A:157:GLU:CD	1:A:157:GLU:H	2.13	0.42
1:A:154:VAL:HG23	1:A:180:GLU:HA	2.02	0.42
1:B:111:LYS:O	1:B:112:THR:CB	2.67	0.42
1:B:163:PHE:CZ	1:B:174:VAL:HG13	2.55	0.42
1:B:228:VAL:HG11	1:B:245:LEU:HD22	2.02	0.41
1:A:176:MET:HE3	1:A:176:MET:HB3	1.73	0.41
1:B:245:LEU:O	1:B:249:LEU:HB2	2.21	0.40

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	144/183 (79%)	133 (92%)	10 (7%)	1 (1%)	22	53
1	B	140/183 (76%)	130 (93%)	9 (6%)	1 (1%)	22	53
All	All	284/366 (78%)	263 (93%)	19 (7%)	2 (1%)	22	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	112	THR
1	A	202	THR

### 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	120/152 (79%)	108 (90%)	12 (10%)	7	22
1	B	118/152 (78%)	114 (97%)	4 (3%)	37	71
All	All	238/304 (78%)	222 (93%)	16 (7%)	16	43

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	138	THR
1	A	156	SER
1	A	161	ASN
1	A	162	ILE
1	A	179	ASN
1	A	187	TYR
1	A	191	SER
1	A	193	SER
1	A	200	LEU
1	A	232	LYS
1	A	243	GLU
1	B	136	ARG
1	B	176	MET
1	B	200	LEU
1	B	243	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	178	ASN
1	A	233	ASN

### 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	146/183 (79%)	0.20	2 (1%) 75 70	38, 66, 100, 119	29 (19%)
1	B	144/183 (78%)	0.14	0 100 100	39, 72, 109, 137	23 (15%)
All	All	290/366 (79%)	0.17	2 (0%) 87 84	38, 69, 105, 137	52 (17%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	ASN	2.2
1	A	197	SER	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 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.