



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:09 pm BST

PDB ID : 3HR8  
Title : Crystal Structure of Thermotoga maritima RecA  
Authors : Lee, S.; Kim, T.G.; Jeong, E.-Y.; Ban, C.; Jeon, W.-J.; Min, K.I.; Song, K.-M.;  
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Deposited on : 2009-06-09  
Resolution : 1.95 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

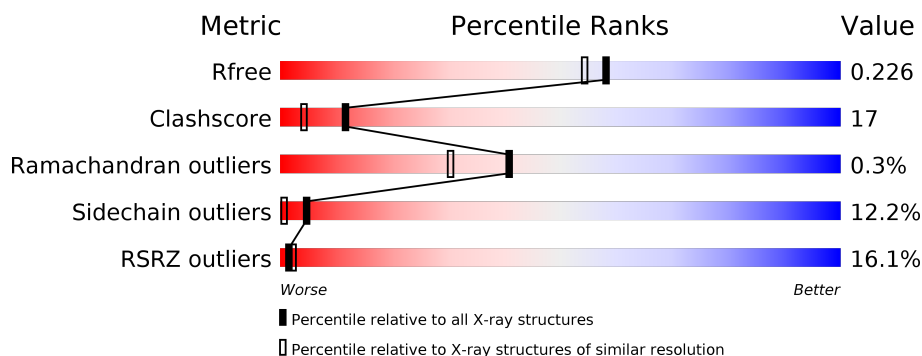
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	356	<div> <div>15%</div> <div>71%</div> <div>21%</div> <div>.</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2918 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 Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2619	1658	452	500	9			

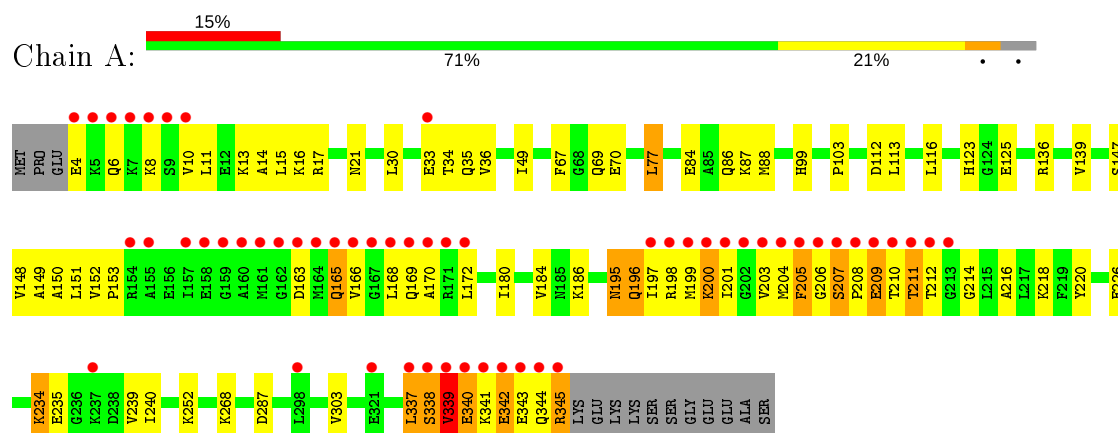
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	299	Total	O	0	0
			299	299		

### 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: Protein recA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.14Å 102.14Å 81.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.49 – 1.95 23.49 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (23.49-1.95) 99.7 (23.49-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 1.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.195 , 0.230 0.192 , 0.226	Depositor DCC
$R_{free}$ test set	1801 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.049 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2918	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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	0.50	0/2653	0.68	1/3571 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	206	GLY	N-CA-C	7.02	130.65	113.10

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	2619	0	2704	93	0
2	A	299	0	0	12	0
All	All	2918	0	2704	93	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 17.

All (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ( $\text{\AA}$ )	Clash overlap ( $\text{\AA}$ )
1:A:200:LYS:HD3	1:A:200:LYS:C	1.65	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASN:OD1	1:A:210:THR:HG23	1.49	1.11
1:A:207:SER:OG	1:A:208:PRO:HD2	1.58	1.03
1:A:211:THR:O	1:A:214:GLY:N	1.95	0.98
1:A:200:LYS:CD	1:A:200:LYS:C	2.34	0.96
1:A:35:GLN:N	1:A:36:VAL:HA	1.78	0.95
1:A:204:MET:HG2	1:A:205:PHE:N	1.85	0.92
1:A:337:LEU:HD13	1:A:338:SER:N	1.86	0.90
1:A:337:LEU:HD13	1:A:338:SER:H	1.39	0.88
1:A:153:PRO:HB3	1:A:169:GLN:HG2	1.55	0.86
1:A:345:ARG:HG3	1:A:345:ARG:HH11	1.41	0.85
1:A:86:GLN:HE22	1:A:112:ASP:H	1.26	0.84
1:A:204:MET:HG2	1:A:205:PHE:H	1.40	0.83
1:A:211:THR:O	1:A:214:GLY:CA	2.29	0.81
1:A:70:GLU:H	1:A:198:ARG:HG3	1.42	0.80
1:A:200:LYS:HD3	1:A:201:ILE:N	1.98	0.79
1:A:338:SER:O	1:A:339:VAL:HG12	1.85	0.77
1:A:200:LYS:HD3	1:A:200:LYS:O	1.85	0.75
1:A:207:SER:CB	1:A:208:PRO:HD2	2.16	0.75
1:A:210:THR:HG21	2:A:417:HOH:O	1.89	0.72
1:A:211:THR:O	1:A:214:GLY:HA3	1.91	0.71
1:A:86:GLN:NE2	1:A:112:ASP:H	1.87	0.70
1:A:35:GLN:N	1:A:36:VAL:CA	2.55	0.69
1:A:197:ILE:HG22	1:A:197:ILE:O	1.92	0.69
1:A:165:GLN:HG3	1:A:168:LEU:HB2	1.75	0.68
1:A:153:PRO:HB3	1:A:169:GLN:CG	2.24	0.68
1:A:207:SER:OG	1:A:208:PRO:CD	2.39	0.67
1:A:209:GLU:HA	2:A:491:HOH:O	1.95	0.66
1:A:13:LYS:HD3	1:A:13:LYS:C	2.16	0.66
1:A:123:HIS:HD2	1:A:125:GLU:HG2	1.61	0.65
1:A:148:VAL:HA	1:A:151:LEU:CD1	2.25	0.65
1:A:35:GLN:H	1:A:36:VAL:HA	1.60	0.63
1:A:169:GLN:HA	1:A:172:LEU:HB2	1.80	0.62
1:A:197:ILE:HG23	1:A:209:GLU:HB3	1.81	0.62
1:A:209:GLU:H	1:A:209:GLU:CD	2.01	0.62
1:A:341:LYS:O	1:A:341:LYS:HG3	1.98	0.62
1:A:70:GLU:N	1:A:198:ARG:HG3	2.15	0.62
1:A:148:VAL:HA	1:A:151:LEU:HD12	1.79	0.62
1:A:4:GLU:HB2	2:A:577:HOH:O	2.00	0.61
1:A:337:LEU:CD1	1:A:338:SER:N	2.60	0.61
1:A:6:GLN:O	1:A:10:VAL:HG23	2.01	0.60
1:A:123:HIS:CD2	1:A:125:GLU:HG2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:SER:CB	1:A:208:PRO:CD	2.79	0.59
1:A:165:GLN:HB2	2:A:651:HOH:O	2.01	0.59
1:A:204:MET:CG	1:A:205:PHE:H	2.03	0.59
1:A:147:SER:O	1:A:151:LEU:HG	2.02	0.59
1:A:200:LYS:HB3	2:A:547:HOH:O	2.04	0.57
1:A:165:GLN:O	1:A:165:GLN:HG2	2.04	0.57
1:A:207:SER:HG	1:A:208:PRO:HD2	1.66	0.57
1:A:200:LYS:CD	1:A:200:LYS:O	2.48	0.56
1:A:345:ARG:HG3	1:A:345:ARG:NH1	2.18	0.56
1:A:195:ASN:HD22	1:A:196:GLN:H	1.51	0.56
1:A:195:ASN:ND2	1:A:196:GLN:H	2.04	0.55
1:A:339:VAL:O	1:A:339:VAL:HG13	2.07	0.54
1:A:99:HIS:HE1	2:A:399:HOH:O	1.90	0.54
1:A:268:LYS:HE3	2:A:482:HOH:O	2.08	0.54
1:A:337:LEU:C	1:A:337:LEU:CD1	2.75	0.54
1:A:136:ARG:CZ	2:A:527:HOH:O	2.57	0.53
1:A:218:LYS:CE	2:A:634:HOH:O	2.58	0.52
1:A:345:ARG:CG	1:A:345:ARG:HH11	2.13	0.52
1:A:86:GLN:HE22	1:A:112:ASP:N	2.03	0.51
1:A:218:LYS:HE2	2:A:634:HOH:O	2.10	0.51
1:A:148:VAL:O	1:A:151:LEU:HB2	2.11	0.51
1:A:180:ILE:O	1:A:184:VAL:HG13	2.11	0.50
1:A:204:MET:CG	1:A:205:PHE:N	2.57	0.50
1:A:340:GLU:O	1:A:342:GLU:OE1	2.30	0.48
1:A:345:ARG:CG	1:A:345:ARG:NH1	2.74	0.48
1:A:165:GLN:CG	1:A:168:LEU:HB2	2.44	0.48
1:A:67:PHE:CZ	1:A:226:GLU:HB2	2.49	0.48
1:A:216:ALA:HB1	1:A:220:TYR:CE2	2.50	0.47
1:A:234:LYS:HE2	1:A:234:LYS:HB3	1.57	0.46
1:A:150:ALA:O	1:A:152:VAL:HG23	2.15	0.46
1:A:139:VAL:HG12	1:A:139:VAL:O	2.16	0.46
1:A:169:GLN:O	1:A:170:ALA:C	2.53	0.45
1:A:49:ILE:CD1	1:A:77:LEU:HD11	2.46	0.45
1:A:235:GLU:HB2	1:A:240:ILE:HD13	1.98	0.45
1:A:34:THR:HA	1:A:35:GLN:HA	1.63	0.45
1:A:149:ALA:HB2	2:A:554:HOH:O	2.17	0.45
1:A:235:GLU:HG3	2:A:619:HOH:O	2.16	0.44
1:A:103:PRO:O	1:A:113:LEU:HD11	2.18	0.44
1:A:172:LEU:HA	1:A:172:LEU:HD23	1.82	0.43
1:A:216:ALA:O	1:A:220:TYR:CD2	2.72	0.43
1:A:69:GLN:HG2	1:A:198:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:HA	1:A:16:LYS:HD3	1.73	0.43
1:A:211:THR:C	1:A:214:GLY:H	2.14	0.42
1:A:87:LYS:HB2	1:A:87:LYS:HE3	1.95	0.42
1:A:84:GLU:O	1:A:88:MET:HG3	2.19	0.42
1:A:200:LYS:HD3	1:A:201:ILE:CA	2.50	0.42
1:A:13:LYS:HD3	1:A:14:ALA:N	2.34	0.41
1:A:8:LYS:HA	1:A:11:LEU:HB3	2.02	0.41
1:A:204:MET:HG2	1:A:205:PHE:HB2	2.03	0.41
1:A:210:THR:HG22	1:A:214:GLY:HA3	2.03	0.40
1:A:337:LEU:HD22	1:A:337:LEU:HA	1.84	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	340/356 (96%)	333 (98%)	6 (2%)	1 (0%)	41	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	VAL

### 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	279/291 (96%)	245 (88%)	34 (12%)	5 1

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	17	ARG
1	A	21	ASN
1	A	30	LEU
1	A	33	GLU
1	A	77	LEU
1	A	116	LEU
1	A	163	ASP
1	A	165	GLN
1	A	166	VAL
1	A	186	LYS
1	A	195	ASN
1	A	196	GLN
1	A	199	MET
1	A	200	LYS
1	A	203	VAL
1	A	205	PHE
1	A	207	SER
1	A	209	GLU
1	A	211	THR
1	A	212	THR
1	A	234	LYS
1	A	239	VAL
1	A	252	LYS
1	A	287	ASP
1	A	303	VAL
1	A	337	LEU
1	A	338	SER
1	A	339	VAL
1	A	340	GLU
1	A	342	GLU
1	A	343	GLU
1	A	344	GLN
1	A	345	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	99	HIS
1	A	120	GLN
1	A	123	HIS
1	A	195	ASN
1	A	196	GLN
1	A	311	ASN
1	A	319	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 ⓘ

### 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, 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	342/356 (96%)	1.16	55 (16%) ⓘ ⓘ	20, 35, 97, 118	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	ILE	17.2
1	A	204	MET	14.1
1	A	205	PHE	14.1
1	A	203	VAL	13.9
1	A	208	PRO	11.6
1	A	207	SER	10.8
1	A	199	MET	10.8
1	A	211	THR	10.4
1	A	210	THR	9.4
1	A	198	ARG	9.1
1	A	212	THR	9.0
1	A	164	MET	8.6
1	A	345	ARG	8.2
1	A	202	GLY	8.1
1	A	5	LYS	8.0
1	A	339	VAL	7.9
1	A	168	LEU	7.7
1	A	165	GLN	7.7
1	A	206	GLY	7.5
1	A	162	GLY	7.4
1	A	200	LYS	7.1
1	A	343	GLU	7.0
1	A	163	ASP	7.0
1	A	161	MET	6.9
1	A	167	GLY	6.8
1	A	338	SER	6.4
1	A	155	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	344	GLN	6.2
1	A	6	GLN	6.0
1	A	342	GLU	5.6
1	A	340	GLU	5.2
1	A	159	GLY	5.0
1	A	7	LYS	4.7
1	A	169	GLN	4.5
1	A	166	VAL	4.3
1	A	341	LYS	4.2
1	A	213	GLY	4.1
1	A	4	GLU	4.0
1	A	209	GLU	3.9
1	A	337	LEU	3.4
1	A	160	ALA	3.4
1	A	33	GLU	3.3
1	A	157	ILE	3.2
1	A	197	ILE	3.1
1	A	10	VAL	3.1
1	A	9	SER	3.0
1	A	8	LYS	2.9
1	A	170	ALA	2.7
1	A	298	LEU	2.7
1	A	171	ARG	2.6
1	A	158	GLU	2.4
1	A	154	ARG	2.3
1	A	172	LEU	2.3
1	A	321	GLU	2.1
1	A	237	LYS	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.