



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:00 pm BST

PDB ID : 5WM0  
Title : Crystal structure of apo wild type peptidylglycine alpha-hydroxylating monooxygenase (PHM) soaked with peptide (peptide not observed)  
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Deposited on : 2017-07-28  
Resolution : 2.40 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

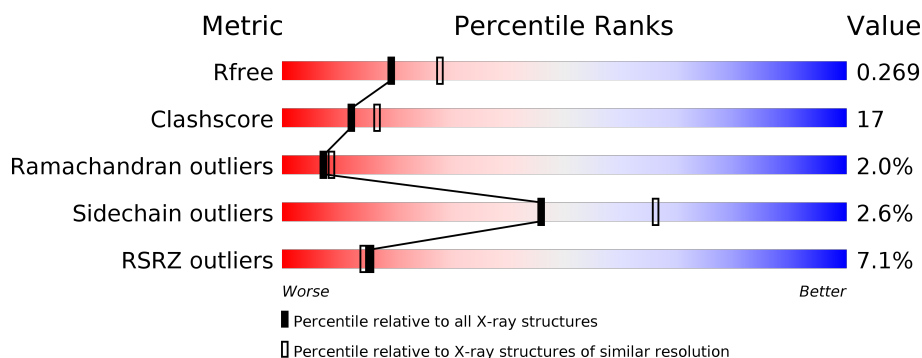
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	976	<div> <div>2%</div> <div>25%</div> <div>6%</div> <div>68%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2445 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.

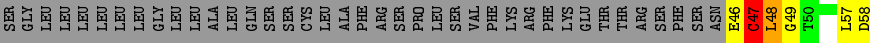
- Molecule 1 is a protein called Peptidyl-glycine alpha-amidating monooxygenase.

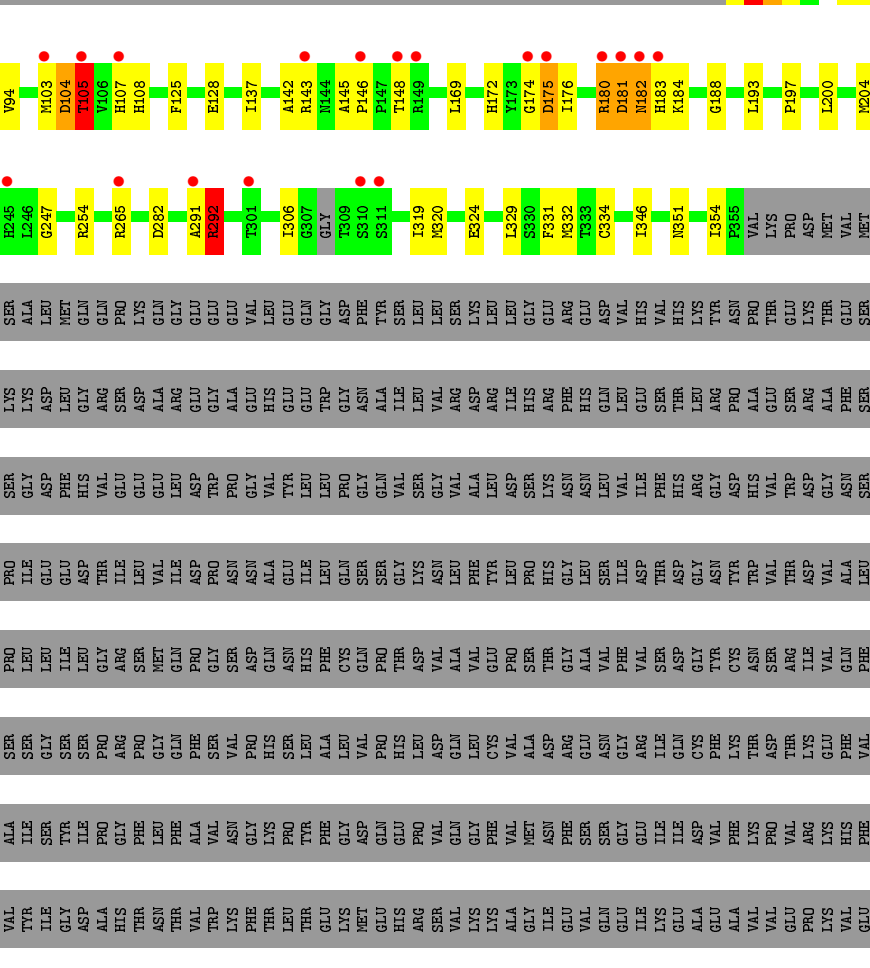
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	1	0
			2418	1541	407	444	26			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	27	Total	O	0	0
			27	27		

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.

- Chain A: 



The following table lists the highlighted residues from the Chain A structure, organized by their position in the sequence (from top to bottom):

Residue	Position
Met	1
Ala	2
Gly	3
Arg	4
Ala	5
Arg	6
Arg	7
Ser	8
Gly	9
Leu	10
Leu	11
Leu	12
Leu	13
Leu	14
Leu	15
Leu	16
Leu	17
Leu	18
Leu	19
Leu	20
Leu	21
Leu	22
Leu	23
Leu	24
Leu	25
Leu	26
Leu	27
Leu	28
Leu	29
Leu	30
Leu	31
Leu	32
Leu	33
Leu	34
Leu	35
Leu	36
Leu	37
Leu	38
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Leu	41
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Leu	43
Leu	44
Leu	45
Leu	46
Leu	47
Leu	48
Leu	49
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Leu	59
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Leu	62
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Leu	86
Leu	87
Leu	88
Leu	89
Leu	90
Leu	91
Leu	92
Leu	93
Leu	94
Leu	95
Leu	96
Leu	97
Leu	98
Leu	99
Leu	100

PRO  
LYS  
PRO  
ALA  
PRO  
SER  
SER

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.10Å 65.93Å 69.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.93 – 2.40 47.93 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.93-2.40) 99.1 (47.93-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.200 , 0.281 0.232 , 0.269	Depositor DCC
$R_{free}$ test set	562 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.7	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	0.93	EDS
Total number of atoms	2445	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% 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	0.88	1/2489 (0.0%)	0.96	2/3385 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	PRO	N-CD	6.37	1.56	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	CYS	CA-CB-SG	-6.17	102.89	114.00
1	A	146	PRO	C-N-CD	5.29	139.50	128.40

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	2418	0	2342	80	0
2	A	27	0	0	4	0
All	All	2445	0	2342	80	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 (80) 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:265:ARG:NH1	1:A:354:ILE:HD11	1.52	1.20
1:A:62:PHE:CE1	1:A:193:LEU:HD12	1.76	1.20
1:A:174:GLY:O	1:A:175:ASP:HB2	1.44	1.16
1:A:227:CYS:SG	1:A:334:CYS:SG	1.36	1.13
1:A:265:ARG:NH1	1:A:354:ILE:CD1	2.11	1.12
1:A:227:CYS:SG	1:A:334:CYS:CB	2.44	1.05
1:A:329:LEU:HD11	1:A:332:MET:HG3	1.44	0.99
1:A:103:MET:O	1:A:143:ARG:NH2	1.97	0.97
1:A:72:THR:HG23	1:A:182:ASN:O	1.65	0.97
1:A:265:ARG:HH11	1:A:354:ILE:HD11	1.20	0.95
1:A:46:GLU:O	1:A:48:LEU:N	2.01	0.93
1:A:105:THR:HG21	1:A:180:ARG:NH1	1.82	0.93
1:A:62:PHE:CZ	1:A:193:LEU:HD12	2.03	0.93
1:A:174:GLY:O	1:A:175:ASP:CB	2.22	0.87
1:A:105:THR:HG23	1:A:180:ARG:HH22	1.37	0.87
1:A:72:THR:CG2	1:A:182:ASN:O	2.27	0.82
1:A:181:ASP:O	2:A:1001:HOH:O	2.01	0.79
1:A:105:THR:HG21	1:A:180:ARG:HH12	1.45	0.78
1:A:105:THR:HG23	1:A:180:ARG:NH2	2.00	0.75
1:A:265:ARG:NH1	1:A:354:ILE:CG1	2.51	0.74
1:A:62:PHE:CZ	1:A:193:LEU:CD1	2.72	0.72
1:A:292:ARG:HD2	1:A:346:ILE:HD13	1.70	0.72
1:A:105:THR:CG2	1:A:180:ARG:HH12	2.05	0.70
1:A:47:CYS:C	1:A:48:LEU:HG	2.12	0.70
1:A:104:ASP:O	1:A:105:THR:HG23	1.92	0.69
1:A:329:LEU:CD1	1:A:332:MET:HG3	2.18	0.69
1:A:231:MET:CE	2:A:1012:HOH:O	2.40	0.69
1:A:108:HIS:HB3	1:A:172:HIS:HB3	1.76	0.67
1:A:292:ARG:HD2	1:A:346:ILE:CD1	2.25	0.66
1:A:94:VAL:HG22	1:A:193:LEU:HD23	1.79	0.65
1:A:105:THR:CG2	1:A:180:ARG:NH1	2.57	0.65
1:A:329:LEU:HD13	1:A:331:PHE:O	1.97	0.65
1:A:265:ARG:HH12	1:A:354:ILE:HG12	1.62	0.65
1:A:265:ARG:HH11	1:A:354:ILE:CD1	1.94	0.64
1:A:66:ILE:HG23	1:A:84:MET:HG3	1.79	0.63
1:A:291:ALA:O	1:A:292:ARG:HB2	1.98	0.63
1:A:265:ARG:HH12	1:A:354:ILE:CD1	2.06	0.63
1:A:265:ARG:NH1	1:A:354:ILE:HG12	2.13	0.63
1:A:231:MET:HE3	2:A:1012:HOH:O	1.99	0.62
1:A:46:GLU:O	1:A:46:GLU:HG3	2.00	0.62
1:A:183:HIS:O	1:A:184:LYS:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD23	1:A:324:GLU:HA	1.82	0.60
1:A:94:VAL:HG22	1:A:193:LEU:CD2	2.32	0.60
1:A:180:ARG:HD3	1:A:183:HIS:ND1	2.17	0.58
1:A:62:PHE:HE1	1:A:193:LEU:HD12	1.56	0.58
1:A:231:MET:HE2	2:A:1012:HOH:O	2.03	0.57
1:A:254:ARG:NH1	1:A:282:ASP:O	2.30	0.56
1:A:76:SER:OG	1:A:176:ILE:N	2.37	0.55
1:A:107:HIS:ND1	1:A:108:HIS:HB2	2.22	0.54
1:A:62:PHE:CE1	1:A:193:LEU:CD1	2.71	0.54
1:A:105:THR:HG22	1:A:175:ASP:O	2.07	0.54
1:A:57:LEU:HG	1:A:62:PHE:HA	1.90	0.53
1:A:243:THR:HG21	1:A:247:GLY:HA3	1.92	0.52
1:A:103:MET:O	1:A:143:ARG:CZ	2.58	0.51
1:A:105:THR:CG2	1:A:180:ARG:NH2	2.72	0.51
1:A:292:ARG:CD	1:A:346:ILE:HD13	2.39	0.50
1:A:105:THR:HG21	1:A:180:ARG:CZ	2.40	0.50
1:A:329:LEU:HD11	1:A:332:MET:CG	2.29	0.50
1:A:265:ARG:HH12	1:A:354:ILE:CG1	2.17	0.49
1:A:103:MET:C	1:A:143:ARG:HH22	2.13	0.49
1:A:329:LEU:HD12	1:A:329:LEU:C	2.34	0.48
1:A:125:PHE:O	1:A:128:GLU:HB2	2.13	0.48
1:A:265:ARG:HG2	1:A:354:ILE:HD11	1.97	0.47
1:A:58:ASP:OD1	1:A:61:ASP:HB2	2.15	0.47
1:A:105:THR:CG2	1:A:180:ARG:CZ	2.93	0.46
1:A:212:THR:O	1:A:306:ILE:HG12	2.16	0.46
1:A:227:CYS:CB	1:A:334:CYS:SG	2.82	0.46
1:A:47:CYS:C	1:A:49:GLY:H	2.18	0.46
1:A:137:ILE:HG23	1:A:204:MET:HE3	1.98	0.46
1:A:236:VAL:HG13	1:A:319:ILE:HG23	1.99	0.44
1:A:93:PHE:CE2	1:A:197:PRO:HA	2.51	0.44
1:A:72:THR:HG21	1:A:182:ASN:HA	2.00	0.44
1:A:175:ASP:O	1:A:176:ILE:HD13	2.19	0.42
1:A:169:LEU:HD21	1:A:188:GLY:HA2	2.02	0.42
1:A:292:ARG:NH1	1:A:351:ASN:OD1	2.53	0.41
1:A:265:ARG:HH11	1:A:354:ILE:CG1	2.27	0.41
1:A:237:PHE:CZ	1:A:320:MET:SD	3.13	0.41
1:A:47:CYS:O	1:A:48:LEU:CB	2.69	0.40
1:A:142:ALA:HB3	1:A:145:ALA:HB3	2.04	0.40
1:A:329:LEU:HD12	1:A:329:LEU:O	2.21	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	306/976 (31%)	278 (91%)	22 (7%)	6 (2%)	<b>7</b> <b>9</b>

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	CYS
1	A	175	ASP
1	A	292	ARG
1	A	105	THR
1	A	148	THR
1	A	181	ASP

### 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	266/841 (32%)	259 (97%)	7 (3%)	<b>46</b> <b>66</b>

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	104	ASP
1	A	105	THR
1	A	180	ARG
1	A	182	ASN

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Mol	Chain	Res	Type
1	A	228	GLN
1	A	292	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	182	ASN
1	A	272	GLN
1	A	316	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	309/976 (31%)	0.01	22 (7%) 16 14	27, 47, 90, 125	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	ASP	5.8
1	A	310	SER	4.8
1	A	311	SER	4.0
1	A	175	ASP	3.5
1	A	180	ARG	3.5
1	A	183	HIS	3.4
1	A	265	ARG	3.3
1	A	48	LEU	3.2
1	A	50	THR	3.0
1	A	182	ASN	2.8
1	A	105	THR	2.8
1	A	143	ARG	2.7
1	A	291	ALA	2.7
1	A	47	CYS	2.7
1	A	103	MET	2.6
1	A	149	ARG	2.6
1	A	174	GLY	2.5
1	A	245	HIS	2.3
1	A	107	HIS	2.3
1	A	148	THR	2.2
1	A	301	THR	2.0
1	A	146	PRO	2.0

### 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.