



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2017 – 07:45 AM EDT

PDB ID : 3I4F  
Title : Structure of putative 3-oxoacyl-reductase from bacillus thuringiensis  
Authors : Ramagopal, U.A.; Kim, J.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX  
Research Center for Structural Genomics (NYSGXRC)  
Deposited on : unknown  
Resolution : 2.39 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

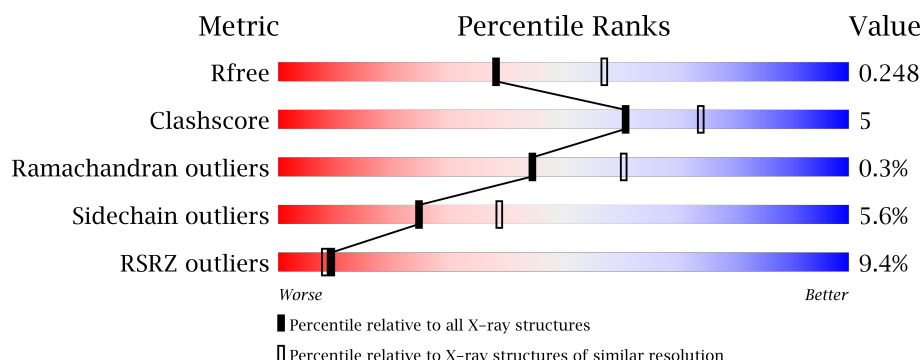
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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. 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	264	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>• 8%</div> </div> </div>
1	B	264	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 8%</div> </div> </div>
1	C	264	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>• 9%</div> </div> </div>
1	D	264	<div> <div>9%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 8%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7541 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 3-oxoacyl-[acyl-carrier protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1865	1186	314	355	10			
1	B	242	Total	C	N	O	S	0	1	0
			1875	1192	314	359	10			
1	C	240	Total	C	N	O	S	0	0	0
			1862	1182	312	358	10			
1	D	242	Total	C	N	O	S	0	0	0
			1879	1192	315	362	10			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	EXPRESSION TAG	UNP C3ERL8
A	33	SER	-	EXPRESSION TAG	UNP C3ERL8
A	34	LEU	-	EXPRESSION TAG	UNP C3ERL8
A	35	GLY	-	EXPRESSION TAG	UNP C3ERL8
A	36	ARG	-	EXPRESSION TAG	UNP C3ERL8
A	288	GLU	-	EXPRESSION TAG	UNP C3ERL8
A	289	GLY	-	EXPRESSION TAG	UNP C3ERL8
A	290	HIS	-	EXPRESSION TAG	UNP C3ERL8
A	291	HIS	-	EXPRESSION TAG	UNP C3ERL8
A	292	HIS	-	EXPRESSION TAG	UNP C3ERL8
A	293	HIS	-	EXPRESSION TAG	UNP C3ERL8
A	294	HIS	-	EXPRESSION TAG	UNP C3ERL8
A	295	HIS	-	EXPRESSION TAG	UNP C3ERL8
B	32	MET	-	EXPRESSION TAG	UNP C3ERL8
B	33	SER	-	EXPRESSION TAG	UNP C3ERL8
B	34	LEU	-	EXPRESSION TAG	UNP C3ERL8
B	35	GLY	-	EXPRESSION TAG	UNP C3ERL8
B	36	ARG	-	EXPRESSION TAG	UNP C3ERL8
B	288	GLU	-	EXPRESSION TAG	UNP C3ERL8
B	289	GLY	-	EXPRESSION TAG	UNP C3ERL8
B	290	HIS	-	EXPRESSION TAG	UNP C3ERL8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	291	HIS	-	EXPRESSION TAG	UNP C3ERL8
B	292	HIS	-	EXPRESSION TAG	UNP C3ERL8
B	293	HIS	-	EXPRESSION TAG	UNP C3ERL8
B	294	HIS	-	EXPRESSION TAG	UNP C3ERL8
B	295	HIS	-	EXPRESSION TAG	UNP C3ERL8
C	32	MET	-	EXPRESSION TAG	UNP C3ERL8
C	33	SER	-	EXPRESSION TAG	UNP C3ERL8
C	34	LEU	-	EXPRESSION TAG	UNP C3ERL8
C	35	GLY	-	EXPRESSION TAG	UNP C3ERL8
C	36	ARG	-	EXPRESSION TAG	UNP C3ERL8
C	288	GLU	-	EXPRESSION TAG	UNP C3ERL8
C	289	GLY	-	EXPRESSION TAG	UNP C3ERL8
C	290	HIS	-	EXPRESSION TAG	UNP C3ERL8
C	291	HIS	-	EXPRESSION TAG	UNP C3ERL8
C	292	HIS	-	EXPRESSION TAG	UNP C3ERL8
C	293	HIS	-	EXPRESSION TAG	UNP C3ERL8
C	294	HIS	-	EXPRESSION TAG	UNP C3ERL8
C	295	HIS	-	EXPRESSION TAG	UNP C3ERL8
D	32	MET	-	EXPRESSION TAG	UNP C3ERL8
D	33	SER	-	EXPRESSION TAG	UNP C3ERL8
D	34	LEU	-	EXPRESSION TAG	UNP C3ERL8
D	35	GLY	-	EXPRESSION TAG	UNP C3ERL8
D	36	ARG	-	EXPRESSION TAG	UNP C3ERL8
D	288	GLU	-	EXPRESSION TAG	UNP C3ERL8
D	289	GLY	-	EXPRESSION TAG	UNP C3ERL8
D	290	HIS	-	EXPRESSION TAG	UNP C3ERL8
D	291	HIS	-	EXPRESSION TAG	UNP C3ERL8
D	292	HIS	-	EXPRESSION TAG	UNP C3ERL8
D	293	HIS	-	EXPRESSION TAG	UNP C3ERL8
D	294	HIS	-	EXPRESSION TAG	UNP C3ERL8
D	295	HIS	-	EXPRESSION TAG	UNP C3ERL8

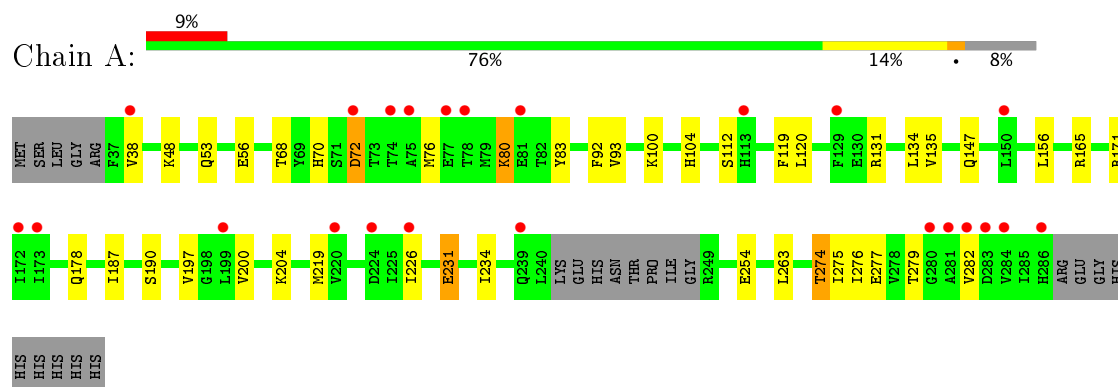
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	18	Total O 18 18	0	0
2	B	19	Total O 19 19	0	0
2	C	10	Total O 10 10	0	0
2	D	13	Total O 13 13	0	0

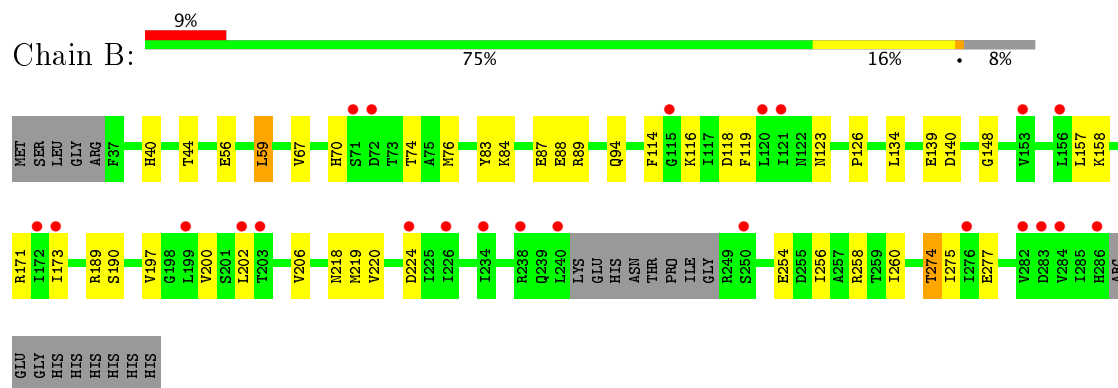
### 3 Residue-property plots [i](#)

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.

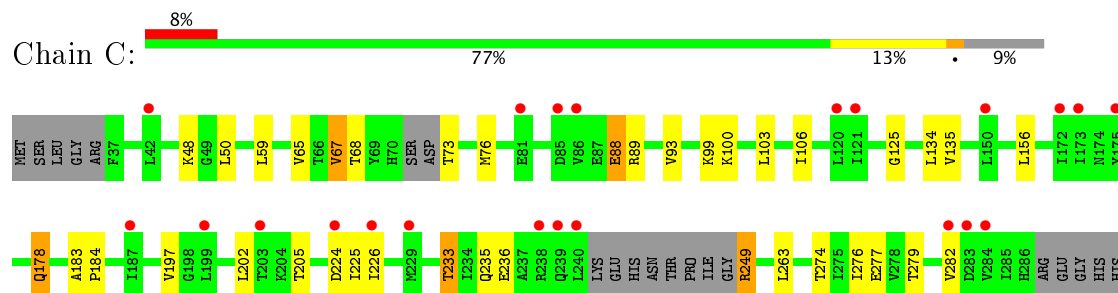
- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



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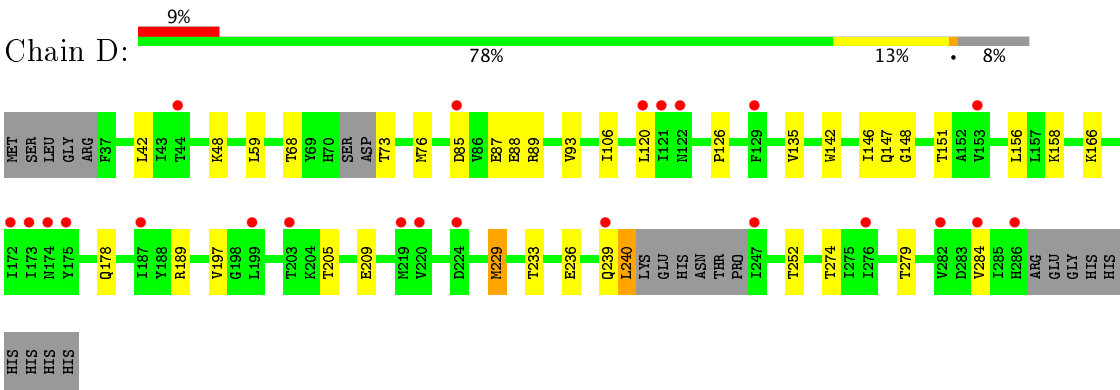
HIS

HIS

HIS

HIS

• Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.42Å 86.59Å 78.41Å 90.00° 97.05° 90.00°	Depositor
Resolution (Å)	27.60 – 2.39 27.06 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.3 (27.60-2.39) 99.3 (27.06-2.39)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.05 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.192 , 0.248 0.193 , 0.248	Depositor DCC
$R_{free}$ test set	1841 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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 36.12 % 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 5.2492e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [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	0.49	0/1899	0.59	0/2567
1	B	0.50	0/1909	0.57	0/2579
1	C	0.49	0/1891	0.58	0/2553
1	D	0.52	0/1908	0.60	0/2574
All	All	0.50	0/7607	0.58	0/10273

There are no bond length outliers.

There are no bond angle outliers.

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	1865	0	1844	27	0
1	B	1875	0	1856	25	0
1	C	1862	0	1847	25	0
1	D	1879	0	1867	19	0
2	A	18	0	0	0	0
2	B	19	0	0	0	0
2	C	10	0	0	0	0
2	D	13	0	0	0	0
All	All	7541	0	7414	78	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 5.



The worst 5 of 78 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:190:SER:HB3	1:C:205:THR:HG21	1.65	0.78
1:D:239:GLN:O	1:D:240:LEU:HB2	1.84	0.78
1:C:249:ARG:HH21	1:C:249:ARG:HG3	1.48	0.78
1:A:178:GLN:HG3	1:A:279:THR:HG21	1.75	0.69
1:B:134:LEU:CD1	1:C:202:LEU:HD11	2.26	0.65

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	239/264 (90%)	229 (96%)	8 (3%)	2 (1%)	22	33
1	B	239/264 (90%)	231 (97%)	8 (3%)	0	100	100
1	C	234/264 (89%)	231 (99%)	2 (1%)	1 (0%)	38	54
1	D	236/264 (89%)	231 (98%)	5 (2%)	0	100	100
All	All	948/1056 (90%)	922 (97%)	23 (2%)	3 (0%)	44	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	72	ASP
1	C	125	GLY

### 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	194/221 (88%)	185 (95%)	9 (5%)	31	49
1	B	196/221 (89%)	186 (95%)	10 (5%)	28	44
1	C	196/221 (89%)	181 (92%)	15 (8%)	15	23
1	D	198/221 (90%)	188 (95%)	10 (5%)	28	44
All	All	784/884 (89%)	740 (94%)	44 (6%)	25	39

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	48	LYS
1	C	88	GLU
1	D	166	LYS
1	C	50	LEU
1	C	73	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	123	ASN
1	B	147	GLN
1	D	70	HIS
1	B	113	HIS
1	C	178	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 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	242/264 (91%)	0.63	23 (9%) 9 8	28, 36, 50, 62	0
1	B	242/264 (91%)	0.60	23 (9%) 9 8	29, 38, 53, 70	0
1	C	240/264 (90%)	0.62	22 (9%) 10 8	27, 37, 50, 52	0
1	D	242/264 (91%)	0.56	23 (9%) 9 8	26, 37, 47, 56	0
All	All	966/1056 (91%)	0.60	91 (9%) 9 8	26, 37, 50, 70	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	SER	4.6
1	D	284	VAL	4.5
1	B	284	VAL	4.3
1	B	286	HIS	4.3
1	D	173	ILE	4.1

### 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.