



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 6, 2016 – 04:58 PM EDT

PDB ID : 5HZ4  
Title : The structural and biochemical characterization of acyl-coa hydrolase mutant Thr60Ala from Staphylococcus aureus.  
Authors : Khandokar, Y.B.; Srivastava, P.; Forwood, J.K.  
Deposited on : 2016-02-02  
Resolution : 2.50 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.

---

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20027107

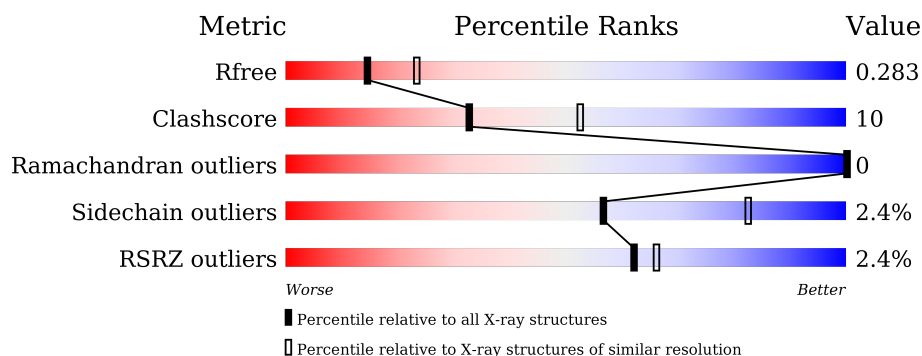
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	179	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	179	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	179	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div></div> <div>9%</div> </div> </div>
1	D	179	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>20%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	179	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>22%</div> <div>•</div> <div>11%</div> </div> </div>
1	F	179	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7691 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 Thioesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1282	809	220	245	8			
1	B	162	Total	C	N	O	S	0	0	0
			1282	809	220	245	8			
1	C	162	Total	C	N	O	S	0	0	0
			1282	809	220	245	8			
1	D	159	Total	C	N	O	S	0	0	0
			1257	795	214	240	8			
1	E	159	Total	C	N	O	S	0	0	0
			1254	793	212	241	8			
1	F	162	Total	C	N	O	S	0	0	0
			1282	809	220	245	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A0H3K033
A	-1	ASN	-	expression tag	UNP A0A0H3K033
A	0	ALA	-	expression tag	UNP A0A0H3K033
A	60	ALA	THR	engineered mutation	UNP A0A0H3K033
B	-2	SER	-	expression tag	UNP A0A0H3K033
B	-1	ASN	-	expression tag	UNP A0A0H3K033
B	0	ALA	-	expression tag	UNP A0A0H3K033
B	60	ALA	THR	engineered mutation	UNP A0A0H3K033
C	-2	SER	-	expression tag	UNP A0A0H3K033
C	-1	ASN	-	expression tag	UNP A0A0H3K033
C	0	ALA	-	expression tag	UNP A0A0H3K033
C	60	ALA	THR	engineered mutation	UNP A0A0H3K033
D	-2	SER	-	expression tag	UNP A0A0H3K033
D	-1	ASN	-	expression tag	UNP A0A0H3K033
D	0	ALA	-	expression tag	UNP A0A0H3K033
D	60	ALA	THR	engineered mutation	UNP A0A0H3K033
E	-2	SER	-	expression tag	UNP A0A0H3K033

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP A0A0H3K033
E	0	ALA	-	expression tag	UNP A0A0H3K033
E	60	ALA	THR	engineered mutation	UNP A0A0H3K033
F	-2	SER	-	expression tag	UNP A0A0H3K033
F	-1	ASN	-	expression tag	UNP A0A0H3K033
F	0	ALA	-	expression tag	UNP A0A0H3K033
F	60	ALA	THR	engineered mutation	UNP A0A0H3K033

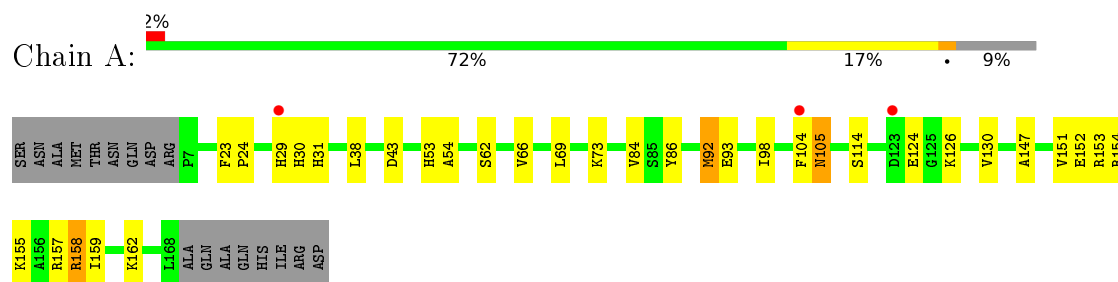
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	8	Total O 8 8	0	0
2	C	11	Total O 11 11	0	0
2	D	9	Total O 9 9	0	0
2	E	6	Total O 6 6	0	0
2	F	9	Total O 9 9	0	0

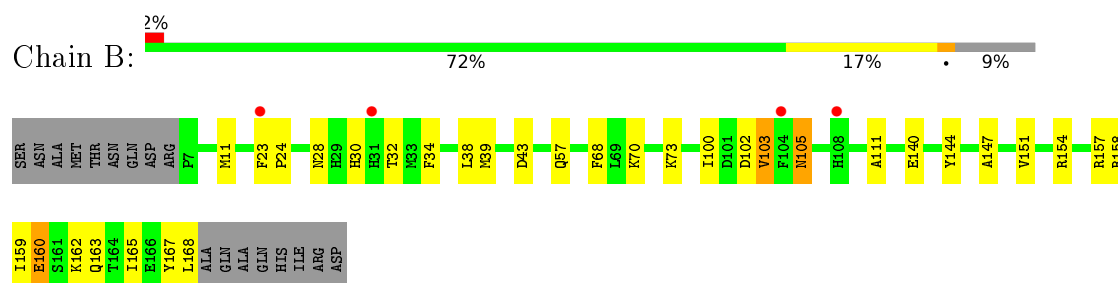
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

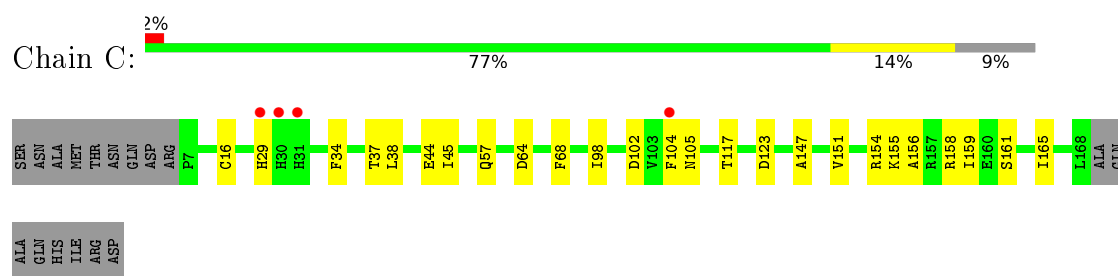
#### • Molecule 1: Thioesterase



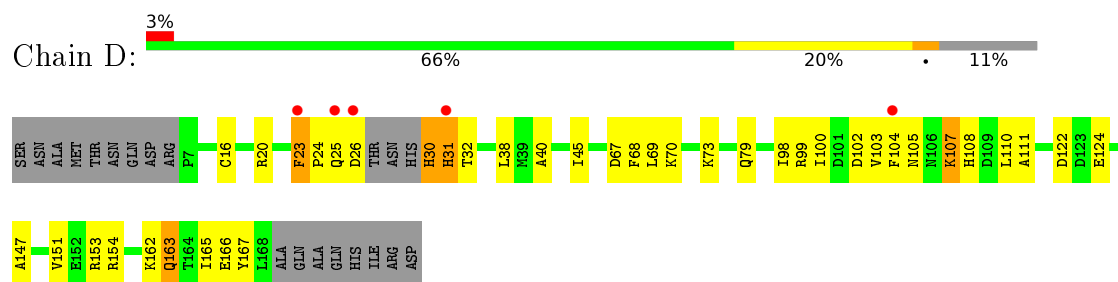
#### • Molecule 1: Thioesterase



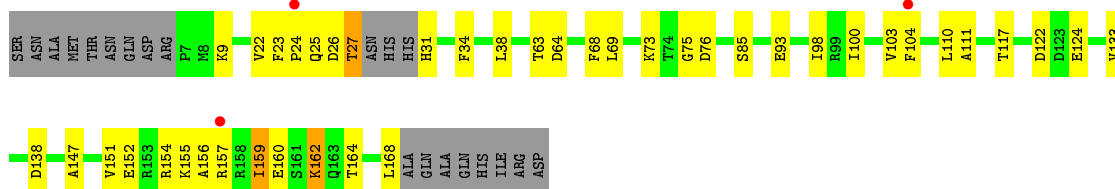
#### • Molecule 1: Thioesterase



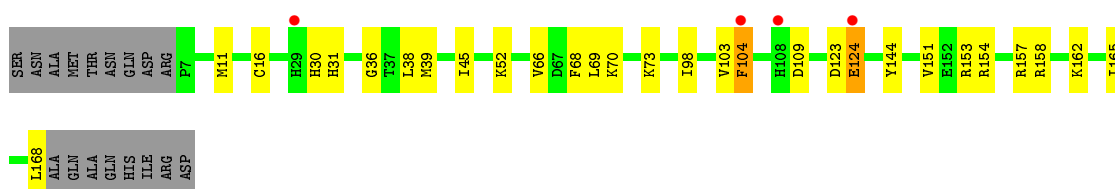
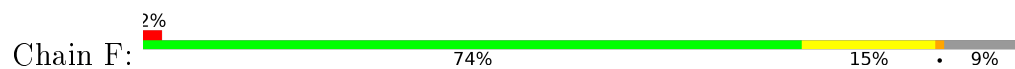
#### • Molecule 1: Thioesterase



## ● Molecule 1: Thioesterase



## ● Molecule 1: Thioesterase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.05Å 128.54Å 84.36Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	31.70 – 2.50 31.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.70-2.50) 99.9 (31.70-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.236 , 0.283 0.236 , 0.283	Depositor DCC
$R_{free}$ test set	1700 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 28.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 35719 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7691	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.53	0/1309	0.71	1/1770 (0.1%)
1	B	0.47	0/1309	0.67	0/1770
1	C	0.48	0/1309	0.67	0/1770
1	D	0.53	0/1282	0.75	2/1731 (0.1%)
1	E	0.57	0/1278	0.74	0/1726
1	F	0.51	0/1309	0.69	1/1770 (0.1%)
All	All	0.52	0/7796	0.71	4/10537 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	123	ASP	CB-CG-OD1	6.03	123.73	118.30
1	D	23	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	A	158	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	23	PHE	CB-CG-CD2	5.03	124.32	120.80

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	1282	0	1263	25	0
1	B	1282	0	1263	27	0
1	C	1282	0	1263	19	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1257	0	1242	37	0
1	E	1254	0	1242	44	0
1	F	1282	0	1263	28	0
2	A	9	0	0	0	0
2	B	8	0	0	0	0
2	C	11	0	0	0	0
2	D	9	0	0	0	0
2	E	6	0	0	0	0
2	F	9	0	0	1	0
All	All	7691	0	7536	158	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 10.

The worst 5 of 158 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:E:23:PHE:HB3	1:E:24:PRO:CD	1.63	1.27
1:E:23:PHE:HB3	1:E:24:PRO:HD3	1.22	1.10
1:D:30:HIS:O	1:D:31:HIS:ND1	1.90	1.04
1:E:23:PHE:CB	1:E:24:PRO:CD	2.34	1.03
1:D:30:HIS:ND1	1:D:30:HIS:O	1.93	1.01

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	160/179 (89%)	157 (98%)	3 (2%)	0	100	100
1	B	160/179 (89%)	159 (99%)	1 (1%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	160/179 (89%)	160 (100%)	0	0	100	100
1	D	155/179 (87%)	152 (98%)	3 (2%)	0	100	100
1	E	155/179 (87%)	154 (99%)	1 (1%)	0	100	100
1	F	160/179 (89%)	159 (99%)	1 (1%)	0	100	100
All	All	950/1074 (88%)	941 (99%)	9 (1%)	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	140/154 (91%)	137 (98%)	3 (2%)	61	85
1	B	140/154 (91%)	136 (97%)	4 (3%)	50	77
1	C	140/154 (91%)	138 (99%)	2 (1%)	74	91
1	D	137/154 (89%)	131 (96%)	6 (4%)	35	60
1	E	137/154 (89%)	134 (98%)	3 (2%)	60	84
1	F	140/154 (91%)	138 (99%)	2 (1%)	74	91
All	All	834/924 (90%)	814 (98%)	20 (2%)	57	82

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	30	HIS
1	D	31	HIS
1	E	159	ILE
1	C	104	PHE
1	C	123	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	30	HIS
1	F	30	HIS
1	C	57	GLN
1	C	21	GLN
1	E	31	HIS

### 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	162/179 (90%)	-0.01	3 (1%) 70 73	22, 42, 71, 80	0
1	B	162/179 (90%)	-0.07	4 (2%) 61 65	28, 44, 69, 86	0
1	C	162/179 (90%)	0.03	4 (2%) 61 65	22, 42, 72, 79	0
1	D	159/179 (88%)	0.03	5 (3%) 52 57	26, 44, 79, 88	0
1	E	159/179 (88%)	0.04	3 (1%) 70 73	23, 45, 77, 83	0
1	F	162/179 (90%)	0.01	4 (2%) 61 65	28, 48, 74, 95	0
All	All	966/1074 (89%)	0.00	23 (2%) 62 66	22, 45, 74, 95	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	PHE	5.3
1	C	104	PHE	4.2
1	A	29	HIS	3.4
1	B	23	PHE	3.3
1	F	29	HIS	3.1

### 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 carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.