



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:33 PM GMT

PDB ID : 4FD3  
Title : Crystal structure of apo-formed ymtOAR1  
Authors : Zhang, Y.; Gao, Y.; Ning, F.; Niu, L.; Teng, M.  
Deposited on : 2012-05-26  
Resolution : 2.60 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

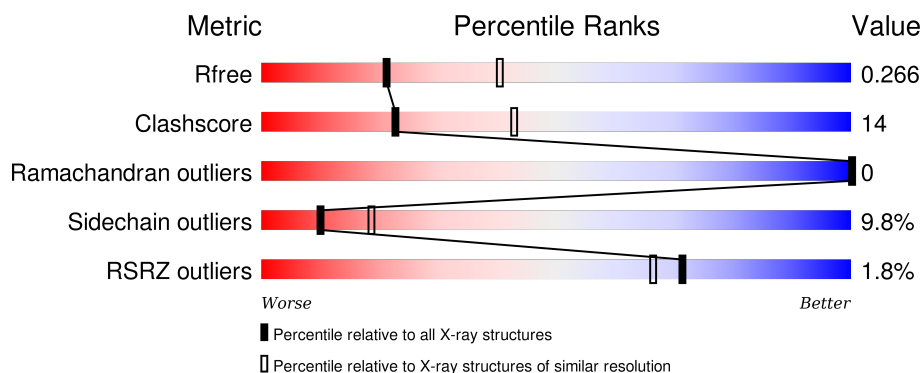
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.



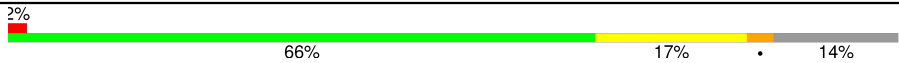
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	286	<div> <div>3%</div> <div>65% 21% 11%</div> </div>
1	B	286	<div> <div>65% 20% 12%</div> </div>
1	C	286	<div> <div>65% 20% 13%</div> </div>
1	D	286	<div> <div>3% 67% 22% 5% 6%</div> </div>
1	E	286	<div> <div>3% 62% 23% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	286	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (2%), green (66%), yellow (17%), and grey (14%). The segments are labeled with their respective percentages: 2%, 66%, 17%, and 14%. The red segment is at the far left, followed by the green segment, then the yellow segment, and finally the grey segment at the far right.

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11328 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	254	Total	C	N	O	S	0	0	0
			1865	1189	320	342	14			
1	B	253	Total	C	N	O	S	0	0	0
			1903	1212	323	353	15			
1	C	250	Total	C	N	O	S	0	0	0
			1878	1198	319	346	15			
1	D	268	Total	C	N	O	S	0	0	0
			1961	1248	338	360	15			
1	E	250	Total	C	N	O	S	0	0	0
			1837	1174	311	337	15			
1	F	246	Total	C	N	O	S	0	0	0
			1820	1161	312	333	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	LEU	-	EXPRESSION TAG	UNP P35731
A	280	GLU	-	EXPRESSION TAG	UNP P35731
A	281	HIS	-	EXPRESSION TAG	UNP P35731
A	282	HIS	-	EXPRESSION TAG	UNP P35731
A	283	HIS	-	EXPRESSION TAG	UNP P35731
A	284	HIS	-	EXPRESSION TAG	UNP P35731
A	285	HIS	-	EXPRESSION TAG	UNP P35731
A	286	HIS	-	EXPRESSION TAG	UNP P35731
B	279	LEU	-	EXPRESSION TAG	UNP P35731
B	280	GLU	-	EXPRESSION TAG	UNP P35731
B	281	HIS	-	EXPRESSION TAG	UNP P35731
B	282	HIS	-	EXPRESSION TAG	UNP P35731
B	283	HIS	-	EXPRESSION TAG	UNP P35731
B	284	HIS	-	EXPRESSION TAG	UNP P35731
B	285	HIS	-	EXPRESSION TAG	UNP P35731
B	286	HIS	-	EXPRESSION TAG	UNP P35731
C	279	LEU	-	EXPRESSION TAG	UNP P35731

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Chain	Residue	Modelled	Actual	Comment	Reference
C	280	GLU	-	EXPRESSION TAG	UNP P35731
C	281	HIS	-	EXPRESSION TAG	UNP P35731
C	282	HIS	-	EXPRESSION TAG	UNP P35731
C	283	HIS	-	EXPRESSION TAG	UNP P35731
C	284	HIS	-	EXPRESSION TAG	UNP P35731
C	285	HIS	-	EXPRESSION TAG	UNP P35731
C	286	HIS	-	EXPRESSION TAG	UNP P35731
D	279	LEU	-	EXPRESSION TAG	UNP P35731
D	280	GLU	-	EXPRESSION TAG	UNP P35731
D	281	HIS	-	EXPRESSION TAG	UNP P35731
D	282	HIS	-	EXPRESSION TAG	UNP P35731
D	283	HIS	-	EXPRESSION TAG	UNP P35731
D	284	HIS	-	EXPRESSION TAG	UNP P35731
D	285	HIS	-	EXPRESSION TAG	UNP P35731
D	286	HIS	-	EXPRESSION TAG	UNP P35731
E	279	LEU	-	EXPRESSION TAG	UNP P35731
E	280	GLU	-	EXPRESSION TAG	UNP P35731
E	281	HIS	-	EXPRESSION TAG	UNP P35731
E	282	HIS	-	EXPRESSION TAG	UNP P35731
E	283	HIS	-	EXPRESSION TAG	UNP P35731
E	284	HIS	-	EXPRESSION TAG	UNP P35731
E	285	HIS	-	EXPRESSION TAG	UNP P35731
E	286	HIS	-	EXPRESSION TAG	UNP P35731
F	279	LEU	-	EXPRESSION TAG	UNP P35731
F	280	GLU	-	EXPRESSION TAG	UNP P35731
F	281	HIS	-	EXPRESSION TAG	UNP P35731
F	282	HIS	-	EXPRESSION TAG	UNP P35731
F	283	HIS	-	EXPRESSION TAG	UNP P35731
F	284	HIS	-	EXPRESSION TAG	UNP P35731
F	285	HIS	-	EXPRESSION TAG	UNP P35731
F	286	HIS	-	EXPRESSION TAG	UNP P35731

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0
2	B	15	Total O 15 15	0	0
2	C	16	Total O 16 16	0	0
2	D	9	Total O 9 9	0	0

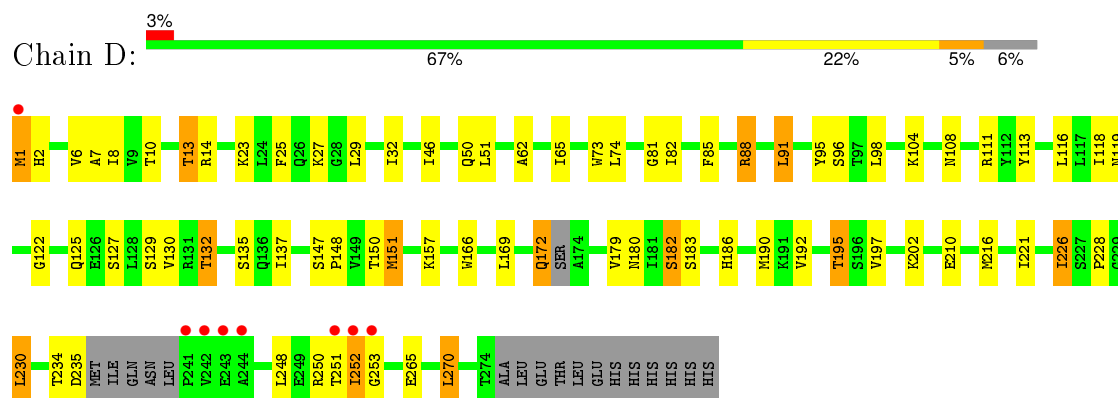
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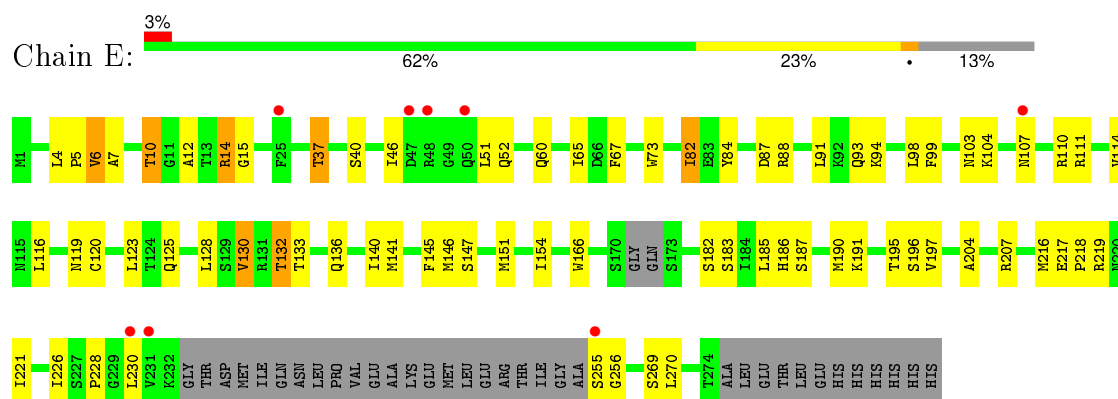
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	9	Total	O	0	0
			9	9		
2	F	9	Total	O	0	0
			9	9		



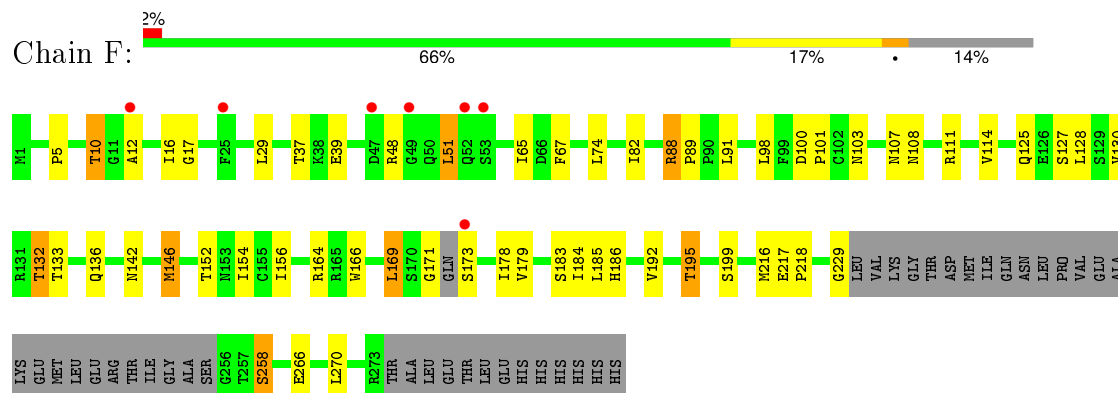
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



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



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## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.83Å 170.83Å 316.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.20 – 2.60 41.08 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.20-2.60) 98.4 (41.08-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.73 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.229 , 0.274 0.225 , 0.266	Depositor DCC
$R_{free}$ test set	3577 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 70628 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11328	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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	0.62	2/1905 (0.1%)	0.64	0/2598
1	B	0.67	0/1944	0.67	1/2644 (0.0%)
1	C	0.62	0/1918	0.69	0/2609
1	D	0.57	0/2002	0.64	0/2727
1	E	0.61	0/1876	0.73	1/2559 (0.0%)
1	F	0.57	0/1859	0.61	0/2532
All	All	0.61	2/11504 (0.0%)	0.66	2/15669 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	GLU	CD-OE2	7.67	1.34	1.25
1	A	120	CYS	CB-SG	-5.02	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	14	ARG	N-CA-C	5.96	127.10	111.00
1	B	122	GLY	N-CA-C	5.38	126.56	113.10

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	1778	61	0
1	B	1903	0	1847	47	0
1	C	1878	0	1815	46	0
1	D	1961	0	1859	63	0
1	E	1837	0	1751	47	0
1	F	1820	0	1744	48	0
2	A	6	0	0	0	0
2	B	15	0	0	0	0
2	C	16	0	0	0	0
2	D	9	0	0	0	0
2	E	9	0	0	2	0
2	F	9	0	0	0	0
All	All	11328	0	10794	300	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 14.

The worst 5 of 300 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:230:LEU:H	1:A:230:LEU:CD1	1.56	1.18
1:C:171:GLY:HA3	1:C:172:GLN:CB	1.71	1.18
1:D:1:MET:H2	1:D:2:HIS:HA	1.07	1.09
1:A:230:LEU:HD12	1:A:230:LEU:N	1.52	1.08
1:D:1:MET:N	1:D:2:HIS:HA	1.58	1.08

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	250/286 (87%)	245 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	249/286 (87%)	242 (97%)	7 (3%)	0	100	100
1	C	244/286 (85%)	240 (98%)	4 (2%)	0	100	100
1	D	262/286 (92%)	253 (97%)	9 (3%)	0	100	100
1	E	244/286 (85%)	239 (98%)	5 (2%)	0	100	100
1	F	240/286 (84%)	230 (96%)	10 (4%)	0	100	100
All	All	1489/1716 (87%)	1449 (97%)	40 (3%)	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	187/250 (75%)	173 (92%)	14 (8%)	17	33
1	B	199/250 (80%)	175 (88%)	24 (12%)	6	11
1	C	194/250 (78%)	176 (91%)	18 (9%)	11	21
1	D	194/250 (78%)	171 (88%)	23 (12%)	6	11
1	E	185/250 (74%)	168 (91%)	17 (9%)	11	21
1	F	185/250 (74%)	169 (91%)	16 (9%)	13	25
All	All	1144/1500 (76%)	1032 (90%)	112 (10%)	10	19

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	195	THR
1	D	88	ARG
1	F	130	VAL
1	C	225	THR
1	D	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	186	HIS
1	C	153	ASN
1	F	136	GLN
1	C	108	ASN
1	C	186	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 [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	254/286 (88%)	-0.15	3 (1%) 81 77	28, 45, 68, 83	0
1	B	253/286 (88%)	-0.32	1 (0%) 93 91	21, 39, 54, 63	0
1	C	250/286 (87%)	-0.39	0 100 100	20, 37, 54, 60	0
1	D	268/286 (93%)	-0.18	8 (2%) 54 47	20, 44, 66, 90	0
1	E	250/286 (87%)	-0.12	8 (3%) 51 44	23, 45, 66, 69	0
1	F	246/286 (86%)	-0.11	7 (2%) 56 49	32, 45, 71, 78	0
All	All	1521/1716 (88%)	-0.21	27 (1%) 71 66	20, 42, 64, 90	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	255	SER	4.0
1	D	241	PRO	3.6
1	D	242	VAL	3.6
1	E	230	LEU	3.5
1	F	53	SER	3.3

### 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.