



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:43 PM GMT

PDB ID : 1YFM  
Title : RECOMBINANT YEAST FUMARASE  
Authors : Weaver, T.M.; Lees, M.R.; Banaszak, L.J.  
Deposited on : 1998-01-07  
Resolution : 2.60 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  
<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

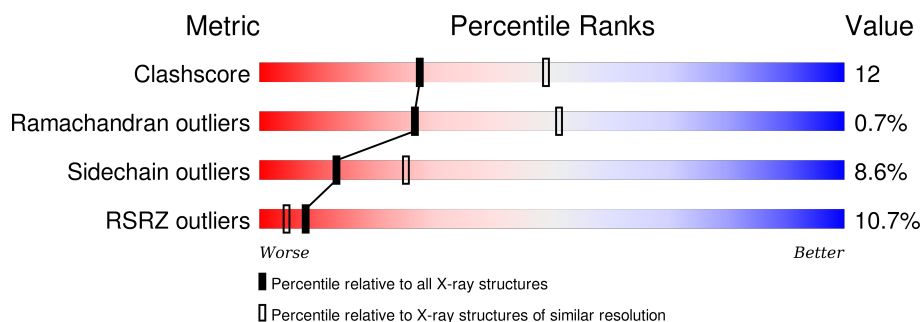
# 1 Overall quality at a glance

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))
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	488	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3439 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 FUMARASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3439	2166	602	656	15			

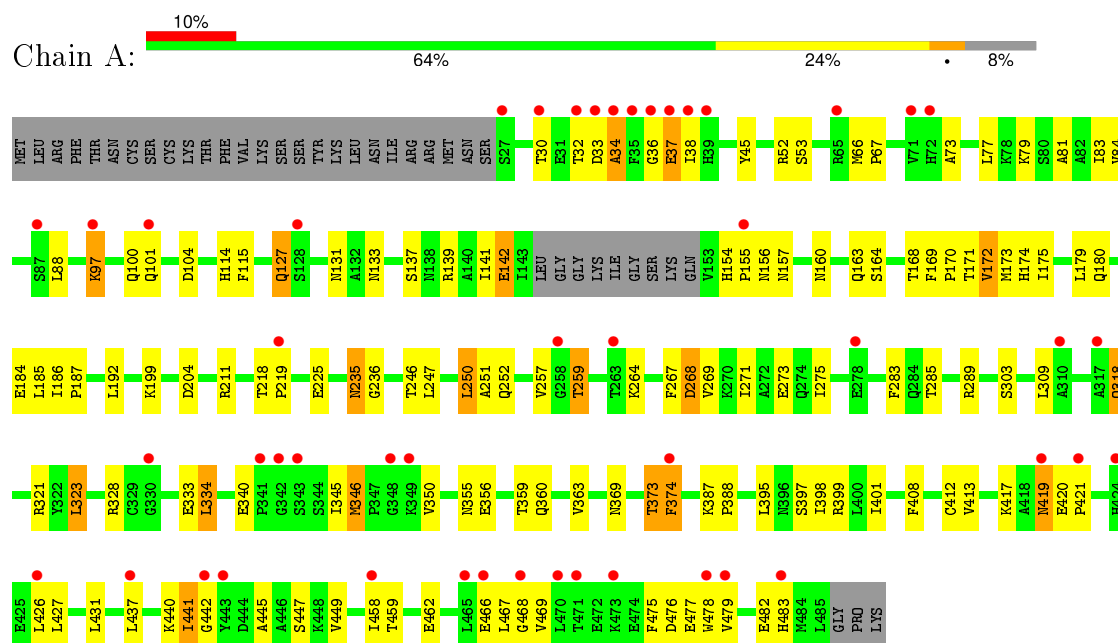
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	ARG	LYS	ENGINEERED	UNP P08417

### 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 ( $RSRZ > 2$ ). 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: FUMARASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.19 Å 95.19 Å 100.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 47.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	60.0 (30.00-2.60) 88.6 (47.59-2.60)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.95 (at 2.61 Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.196 , 0.315 0.300 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 14139 reflections	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	3439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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	0.44	3/3502 (0.1%)	0.68	3/4741 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	THR	C-N	-6.01	1.20	1.34
1	A	468	GLY	C-N	5.81	1.47	1.34
1	A	426	LEU	C-N	5.06	1.45	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	LEU	O-C-N	-6.12	112.90	122.70
1	A	427	LEU	C-N-CA	-5.66	107.55	121.70
1	A	427	LEU	O-C-N	5.11	130.88	122.70

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	3439	0	3441	82	0
All	All	3439	0	3441	82	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 12.

All (82) 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:77:LEU:HD21	1:A:168:THR:HG23	1.39	1.05
1:A:345:ILE:HG23	1:A:346:MET:HG2	1.60	0.83
1:A:139:ARG:NH1	1:A:142:GLU:HG2	2.00	0.77
1:A:139:ARG:HH11	1:A:142:GLU:HG2	1.52	0.74
1:A:33:ASP:HB3	1:A:52:ARG:HH22	1.54	0.72
1:A:38:ILE:HD12	1:A:52:ARG:HG2	1.75	0.69
1:A:133:ASN:ND2	1:A:160:ASN:HB2	2.08	0.69
1:A:269:VAL:O	1:A:273:GLU:HB2	1.97	0.65
1:A:387:LYS:HB2	1:A:388:PRO:HD3	1.76	0.65
1:A:84:VAL:HG21	1:A:271:ILE:HA	1.77	0.65
1:A:37:GLU:CD	1:A:37:GLU:H	2.01	0.64
1:A:73:ALA:HB3	1:A:172:VAL:HG22	1.81	0.62
1:A:257:VAL:HG23	1:A:259:THR:HB	1.82	0.61
1:A:137:SER:O	1:A:141:ILE:HG12	2.00	0.61
1:A:479:VAL:HG13	1:A:479:VAL:O	2.00	0.60
1:A:115:PHE:HA	1:A:131:ASN:HD21	1.66	0.60
1:A:356:GLU:O	1:A:360:GLN:HG3	2.02	0.60
1:A:440:LYS:HD3	1:A:478:TRP:CE2	2.38	0.58
1:A:397:SER:O	1:A:401:ILE:HG13	2.03	0.58
1:A:180:GLN:O	1:A:184:GLU:HB2	2.03	0.58
1:A:458:ILE:HG13	1:A:462:GLU:OE1	2.04	0.57
1:A:53:SER:HB2	1:A:127:GLN:NE2	2.20	0.57
1:A:267:PHE:O	1:A:271:ILE:HG22	2.05	0.56
1:A:466:GLU:HG3	1:A:467:LEU:HD13	1.89	0.54
1:A:374:PHE:N	1:A:374:PHE:CD1	2.75	0.54
1:A:437:LEU:O	1:A:441:ILE:HG22	2.08	0.53
1:A:169:PHE:O	1:A:172:VAL:HG12	2.09	0.53
1:A:441:ILE:HD11	1:A:469:VAL:CG1	2.39	0.53
1:A:225:GLU:OE1	1:A:323:LEU:HD21	2.09	0.52
1:A:475:PHE:O	1:A:479:VAL:HG12	2.10	0.52
1:A:369:ASN:O	1:A:373:THR:HG23	2.09	0.52
1:A:445:ALA:O	1:A:449:VAL:HG23	2.09	0.51
1:A:88:LEU:HD13	1:A:264:LYS:HB2	1.93	0.51
1:A:81:ALA:HB1	1:A:163:GLN:HE22	1.75	0.51
1:A:66:MET:SD	1:A:67:PRO:HD2	2.51	0.51
1:A:32:THR:HG22	1:A:33:ASP:N	2.26	0.51
1:A:133:ASN:HD21	1:A:160:ASN:HB2	1.75	0.51
1:A:97:LYS:NZ	1:A:101:GLN:HE21	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ASN:O	1:A:163:GLN:HG2	2.12	0.50
1:A:355:ASN:HD22	1:A:355:ASN:N	2.09	0.50
1:A:271:ILE:O	1:A:275:ILE:HG13	2.12	0.50
1:A:303:SER:OG	1:A:369:ASN:ND2	2.45	0.50
1:A:83:ILE:HG12	1:A:100:GLN:NE2	2.28	0.49
1:A:441:ILE:HD11	1:A:469:VAL:HG13	1.94	0.49
1:A:441:ILE:HG23	1:A:442:GLY:N	2.28	0.49
1:A:419:ASN:HD22	1:A:421:PRO:HD2	1.78	0.48
1:A:458:ILE:HG23	1:A:462:GLU:HB2	1.94	0.48
1:A:97:LYS:HZ2	1:A:101:GLN:HE21	1.62	0.48
1:A:175:ILE:O	1:A:179:LEU:HG	2.14	0.48
1:A:268:ASP:OD1	1:A:269:VAL:HG23	2.14	0.47
1:A:318:GLN:NE2	1:A:321:ARG:HH21	2.14	0.46
1:A:170:PRO:HA	1:A:173:MET:SD	2.56	0.46
1:A:475:PHE:CE2	1:A:479:VAL:HG11	2.49	0.46
1:A:186:ILE:HB	1:A:187:PRO:HD3	1.97	0.46
1:A:180:GLN:HB3	1:A:398:ILE:HG21	1.98	0.45
1:A:482:GLU:H	1:A:482:GLU:CD	2.21	0.45
1:A:236:GLY:HA3	1:A:309:LEU:HD13	1.98	0.44
1:A:359:THR:O	1:A:363:VAL:HG23	2.18	0.44
1:A:441:ILE:CG2	1:A:442:GLY:N	2.80	0.44
1:A:355:ASN:ND2	1:A:355:ASN:N	2.65	0.44
1:A:420:GLU:HB2	1:A:421:PRO:HD3	2.00	0.43
1:A:250:LEU:HD22	1:A:283:PHE:HB3	1.99	0.43
1:A:211:ARG:HH22	1:A:333:GLU:CD	2.21	0.43
1:A:437:LEU:HB3	1:A:441:ILE:HG21	2.00	0.43
1:A:154:HIS:HA	1:A:155:PRO:HD3	1.88	0.43
1:A:417:LYS:HE2	1:A:417:LYS:HB3	1.79	0.43
1:A:154:HIS:HD2	1:A:157:ASN:CG	2.21	0.43
1:A:408:PHE:O	1:A:412:CYS:HB3	2.18	0.43
1:A:164:SER:O	1:A:168:THR:HB	2.20	0.42
1:A:154:HIS:CD2	1:A:157:ASN:H	2.37	0.42
1:A:199:LYS:HE3	1:A:413:VAL:O	2.18	0.42
1:A:45:TYR:H	1:A:114:HIS:CD2	2.38	0.42
1:A:171:THR:O	1:A:175:ILE:HG13	2.19	0.42
1:A:235:ASN:N	1:A:235:ASN:HD22	2.17	0.42
1:A:459:THR:HG23	1:A:462:GLU:H	1.85	0.42
1:A:77:LEU:CD2	1:A:168:THR:HG23	2.28	0.41
1:A:174:HIS:ND1	1:A:247:LEU:HA	2.35	0.41
1:A:79:LYS:HD2	1:A:104:ASP:HB2	2.02	0.41
1:A:323:LEU:HB3	1:A:334:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:THR:HB	1:A:219:PRO:HD2	2.03	0.40
1:A:34:ALA:C	1:A:36:GLY:H	2.25	0.40
1:A:251:ALA:O	1:A:252:GLN:C	2.59	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	446/488 (91%)	402 (90%)	41 (9%)	3 (1%)	26 51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	441	ILE
1	A	34	ALA
1	A	185	LEU

### 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	373/407 (92%)	341 (91%)	32 (9%)	13 25

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	37	GLU
1	A	97	LYS
1	A	127	GLN
1	A	142	GLU
1	A	156	ASN
1	A	172	VAL
1	A	192	LEU
1	A	204	ASP
1	A	235	ASN
1	A	246	THR
1	A	250	LEU
1	A	259	THR
1	A	268	ASP
1	A	289	ARG
1	A	318	GLN
1	A	323	LEU
1	A	328	ARG
1	A	334	LEU
1	A	340	GLU
1	A	346	MET
1	A	350	VAL
1	A	373	THR
1	A	374	PHE
1	A	395	LEU
1	A	399	ARG
1	A	419	ASN
1	A	431	LEU
1	A	447	SER
1	A	476	ASP
1	A	477	GLU
1	A	483	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	85	ASN
1	A	101	GLN
1	A	114	HIS
1	A	127	GLN
1	A	131	ASN
1	A	138	ASN

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Mol	Chain	Res	Type
1	A	154	HIS
1	A	183	ASN
1	A	191	ASN
1	A	235	ASN
1	A	262	ASN
1	A	318	GLN
1	A	351	ASN
1	A	354	GLN
1	A	355	ASN
1	A	369	ASN
1	A	393	ASN
1	A	419	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	450/488 (92%)	0.86	48 (10%) 8 4	4, 23, 54, 100	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	GLY	7.9
1	A	468	GLY	5.5
1	A	32	THR	5.2
1	A	348	GLY	5.1
1	A	30	THR	4.7
1	A	341	PRO	4.5
1	A	33	ASP	4.2
1	A	317	ALA	3.5
1	A	421	PRO	3.1
1	A	473	LYS	3.0
1	A	37	GLU	3.0
1	A	219	PRO	2.9
1	A	374	PHE	2.9
1	A	34	ALA	2.9
1	A	483	HIS	2.8
1	A	437	LEU	2.8
1	A	155	PRO	2.8
1	A	466	GLU	2.7
1	A	479	VAL	2.7
1	A	71	VAL	2.7
1	A	72	HIS	2.7
1	A	443	TYR	2.7
1	A	39	HIS	2.6
1	A	97	LYS	2.6
1	A	35	PHE	2.5
1	A	458	ILE	2.5
1	A	424	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	349	LYS	2.5
1	A	343	SER	2.5
1	A	465	LEU	2.5
1	A	471	THR	2.5
1	A	310	ALA	2.4
1	A	478	TRP	2.3
1	A	263	THR	2.3
1	A	419	ASN	2.3
1	A	101	GLN	2.2
1	A	38	ILE	2.2
1	A	278	GLU	2.2
1	A	470	LEU	2.2
1	A	128	SER	2.1
1	A	258	GLY	2.1
1	A	426	LEU	2.1
1	A	27	SER	2.1
1	A	65	ARG	2.1
1	A	330	GLY	2.1
1	A	442	GLY	2.1
1	A	87	SER	2.0
1	A	36	GLY	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.