



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 09:07 pm GMT

PDB ID : 5HQP  
Title : Crystal structure of the ERp44-peroxiredoxin 4 complex  
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Deposited on : 2016-01-22  
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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

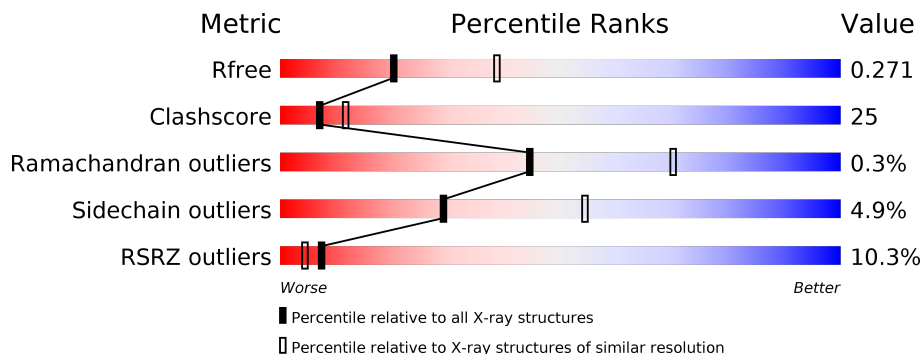
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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	246	<div> <div></div> <div>57% 15% • 26%</div> </div>
1	B	246	<div> <div></div> <div>52% 18% • 29%</div> </div>
2	C	382	<div> <div>5%</div> <div>45% 36% • • 15%</div> </div>
2	D	382	<div> <div>18%</div> <div>21% 29% • 47%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7219 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 Peroxiredoxin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1450	937	241	270	2			
1	B	175	Total	C	N	O	S	0	0	0
			1409	912	235	260	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP Q13162
A	27	ARG	-	expression tag	UNP Q13162
A	28	GLY	-	expression tag	UNP Q13162
A	29	SER	-	expression tag	UNP Q13162
A	30	HIS	-	expression tag	UNP Q13162
A	31	HIS	-	expression tag	UNP Q13162
A	32	HIS	-	expression tag	UNP Q13162
A	33	HIS	-	expression tag	UNP Q13162
A	34	HIS	-	expression tag	UNP Q13162
A	35	HIS	-	expression tag	UNP Q13162
A	36	GLY	-	expression tag	UNP Q13162
A	37	SER	-	expression tag	UNP Q13162
A	51	SER	CYS	engineered mutation	UNP Q13162
A	124	SER	CYS	engineered mutation	UNP Q13162
A	155	GLU	THR	engineered mutation	UNP Q13162
B	26	MET	-	expression tag	UNP Q13162
B	27	ARG	-	expression tag	UNP Q13162
B	28	GLY	-	expression tag	UNP Q13162
B	29	SER	-	expression tag	UNP Q13162
B	30	HIS	-	expression tag	UNP Q13162
B	31	HIS	-	expression tag	UNP Q13162
B	32	HIS	-	expression tag	UNP Q13162
B	33	HIS	-	expression tag	UNP Q13162
B	34	HIS	-	expression tag	UNP Q13162
B	35	HIS	-	expression tag	UNP Q13162

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	GLY	-	expression tag	UNP Q13162
B	37	SER	-	expression tag	UNP Q13162
B	51	SER	CYS	engineered mutation	UNP Q13162
B	124	SER	CYS	engineered mutation	UNP Q13162
B	155	GLU	THR	engineered mutation	UNP Q13162

- Molecule 2 is a protein called Endoplasmic reticulum resident protein 44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	323	Total	C	N	O	S	0	0	0
			2657	1692	452	499	14			
2	D	204	Total	C	N	O	S	0	0	0
			1676	1056	289	321	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP Q9BS26
C	-3	PRO	-	expression tag	UNP Q9BS26
C	-2	LEU	-	expression tag	UNP Q9BS26
C	-1	GLY	-	expression tag	UNP Q9BS26
C	0	SER	-	expression tag	UNP Q9BS26
D	-4	GLY	-	expression tag	UNP Q9BS26
D	-3	PRO	-	expression tag	UNP Q9BS26
D	-2	LEU	-	expression tag	UNP Q9BS26
D	-1	GLY	-	expression tag	UNP Q9BS26
D	0	SER	-	expression tag	UNP Q9BS26

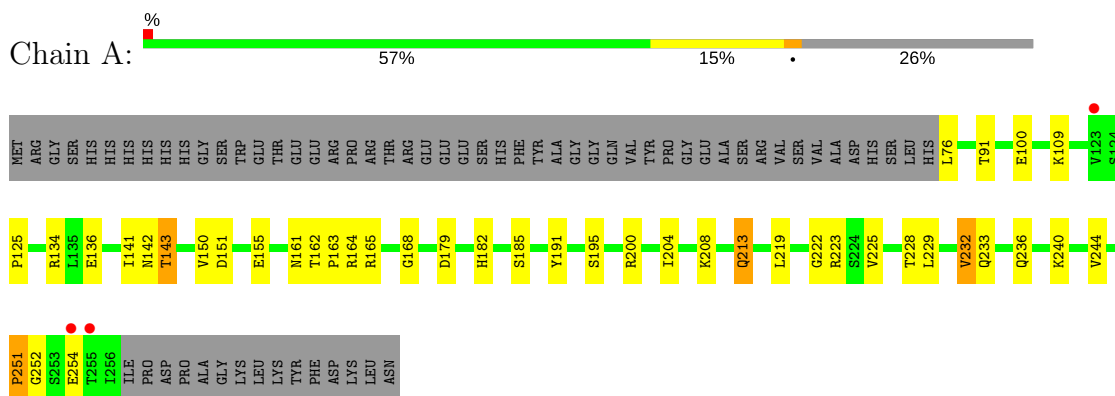
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	8	Total	O	0	0
			8	8		
3	C	8	Total	O	0	0
			8	8		

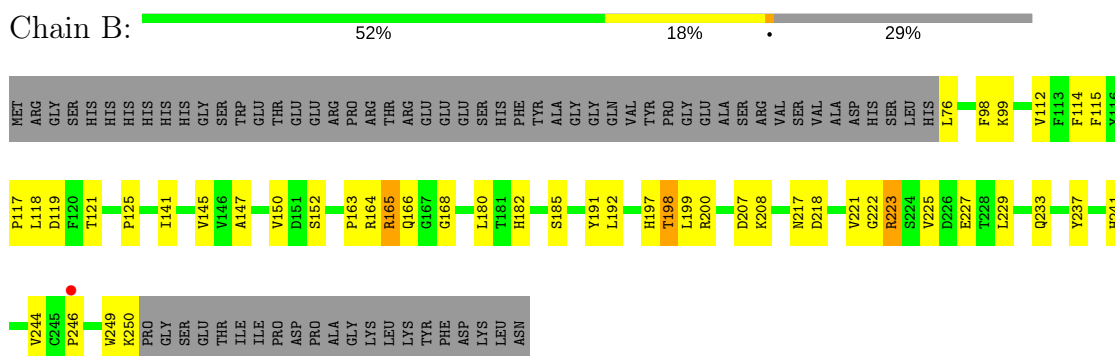
### 3 Residue-property plots [i](#)

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.

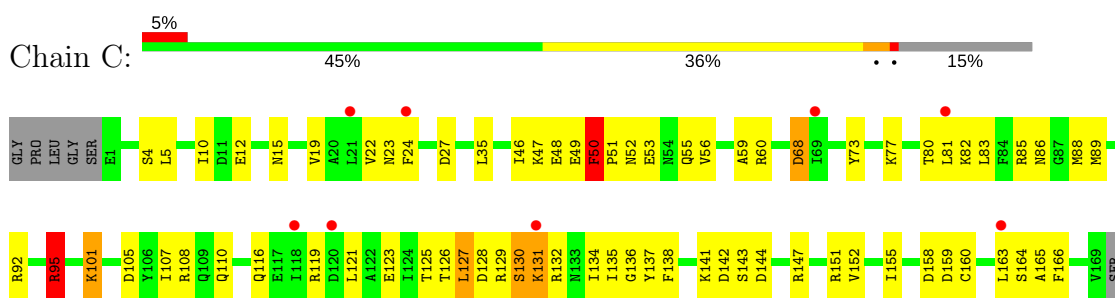
- Molecule 1: Peroxiredoxin-4

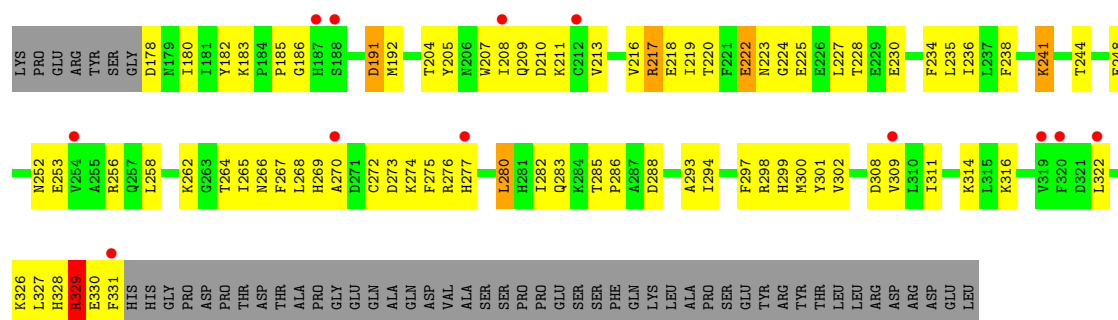


- Molecule 1: Peroxiredoxin-4



- Molecule 2: Endoplasmic reticulum resident protein 44





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.29Å 198.98Å 225.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 2.60 99.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.74-2.60) 93.0 (99.49-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.62Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.235 , 0.272 0.234 , 0.271	Depositor DCC
$R_{free}$ test set	2369 reflections (4.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.3	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 74.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7219	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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	0.33	0/1487	0.59	0/2018
1	B	0.37	0/1445	0.66	0/1960
2	C	0.51	6/2717 (0.2%)	0.68	4/3670 (0.1%)
2	D	0.54	0/1710	0.86	6/2311 (0.3%)
All	All	0.46	6/7359 (0.1%)	0.71	10/9959 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	C	0	2
2	D	0	2
All	All	0	7

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	95	ARG	NE-CZ	-8.90	1.21	1.33
2	C	95	ARG	CZ-NH1	-7.86	1.22	1.33
2	C	95	ARG	CZ-NH2	-6.21	1.25	1.33
2	C	95	ARG	CD-NE	-5.75	1.36	1.46
2	C	329	ARG	CZ-NH2	-5.51	1.25	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	60	ARG	NE-CZ-NH1	-8.86	115.87	120.30
2	C	50	PHE	C-N-CD	-8.20	102.56	120.60
2	D	50	PHE	C-N-CD	-6.48	106.35	120.60
2	D	132	ARG	NE-CZ-NH1	-6.14	117.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	50	PHE	N-CA-C	-6.04	94.70	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	GLY	Peptide
1	A	251	PRO	Peptide
1	A	252	GLY	Peptide
2	C	127	LEU	Peptide
2	C	128	ASP	Peptide

## 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	1450	0	1434	26	0
1	B	1409	0	1395	38	0
2	C	2657	0	2577	139	1
2	D	1676	0	1611	166	1
3	A	11	0	0	0	0
3	B	8	0	0	3	0
3	C	8	0	0	1	0
All	All	7219	0	7017	361	1

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 25.

The worst 5 of 361 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)
2:C:220:THR:HG23	2:C:222:GLU:OE2	1.09	1.22
2:D:44:ASP:OD1	2:D:47:LYS:NZ	1.71	1.20
2:C:220:THR:CG2	2:C:222:GLU:OE2	1.96	1.12
2:D:82:LYS:HZ3	2:D:89:MET:CE	1.64	1.09
2:D:44:ASP:N	2:D:47:LYS:HZ3	1.55	1.04

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:ARG:NH2	2:D:168:ASP:O[5_455]	2.19	0.01

## 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	179/246 (73%)	172 (96%)	7 (4%)	0	100	100
1	B	173/246 (70%)	166 (96%)	7 (4%)	0	100	100
2	C	319/382 (84%)	297 (93%)	20 (6%)	2 (1%)	28	53
2	D	200/382 (52%)	179 (90%)	20 (10%)	1 (0%)	32	58
All	All	871/1256 (69%)	814 (94%)	54 (6%)	3 (0%)	44	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	50	PHE
2	D	67	SER
2	C	52	ASN

### 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	158/213 (74%)	151 (96%)	7 (4%)	33	60
1	B	153/213 (72%)	149 (97%)	4 (3%)	51	78
2	C	293/343 (85%)	277 (94%)	16 (6%)	25	49
2	D	184/343 (54%)	172 (94%)	12 (6%)	20	39
All	All	788/1112 (71%)	749 (95%)	39 (5%)	29	54

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	130	SER
2	C	191	ASP
2	D	182	TYR
2	C	131	LYS
2	C	143	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	16	ASN
2	C	55	GLN
2	D	110	GLN
1	B	236	GLN
2	C	209	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	181/246 (73%)	0.45	3 (1%) 70 65	57, 80, 114, 141	0
1	B	175/246 (71%)	0.57	1 (0%) 89 88	56, 76, 108, 124	0
2	C	323/382 (84%)	0.61	20 (6%) 21 16	59, 106, 170, 211	0
2	D	204/382 (53%)	1.54	67 (32%) 0 0	106, 171, 215, 228	0
All	All	883/1256 (70%)	0.79	91 (10%) 7 4	56, 99, 190, 228	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	57	VAL	11.4
2	D	56	VAL	9.8
2	D	165	ALA	8.1
2	D	19	VAL	7.3
2	D	195	LEU	7.2

### 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.