



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:00 am GMT

PDB ID : 1PSQ  
Title : Structure of a probable thiol peroxidase from *Streptococcus pneumoniae*  
Authors : Kniewel, R.; Buglino, J.; Solorzano, V.; Wu, J.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2003-06-21  
Resolution : 2.30 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.

---

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

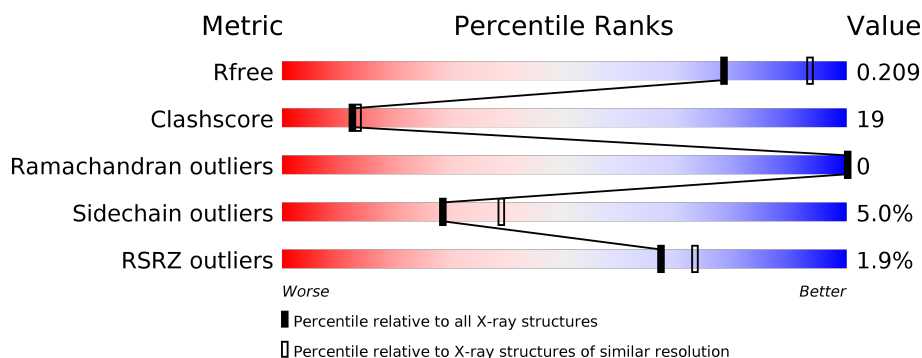
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	163	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>27%</div> <div>•</div> </div> </div>
1	B	163	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>32%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2791 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 probable thiol peroxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	Se	0	0	0
			1269	807	209	248	2	3			
1	B	163	Total	C	N	O	S	Se	0	0	0
			1269	807	209	248	2	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P0A4M5
A	82	MSE	MET	MODIFIED RESIDUE	UNP P0A4M5
A	102	MSE	MET	MODIFIED RESIDUE	UNP P0A4M5
B	1	MSE	MET	MODIFIED RESIDUE	UNP P0A4M5
B	82	MSE	MET	MODIFIED RESIDUE	UNP P0A4M5
B	102	MSE	MET	MODIFIED RESIDUE	UNP P0A4M5

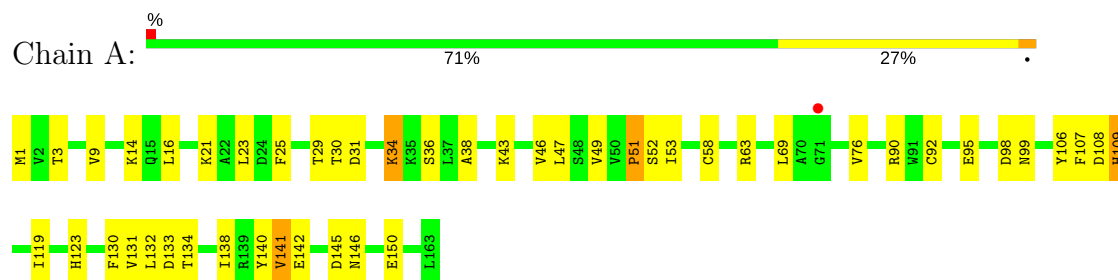
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	133	Total	O	0	0
			133	133		
2	B	120	Total	O	0	0
			120	120		

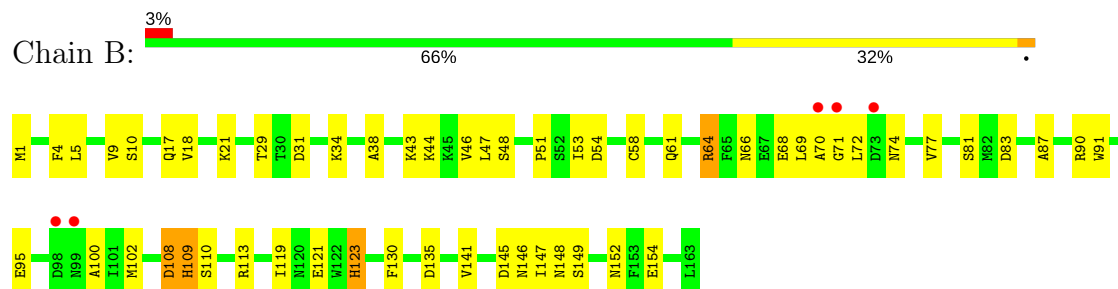
### 3 Residue-property plots [i](#)

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: probable thiol peroxidase



- Molecule 1: probable thiol peroxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.00Å 49.90Å 81.66Å 90.00° 116.85° 90.00°	Depositor
Resolution (Å)	19.80 – 2.30 19.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (19.80-2.30) 90.2 (19.80-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.67 (at 2.30Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.200 , 0.249 0.201 , 0.209	Depositor DCC
$R_{free}$ test set	755 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2791	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.46% 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 [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	0.41	0/1290	0.61	0/1746
1	B	0.41	0/1290	0.61	0/1746
All	All	0.41	0/2580	0.61	0/3492

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	1269	0	1254	38	0
1	B	1269	0	1254	59	0
2	A	133	0	0	13	1
2	B	120	0	0	17	0
All	All	2791	0	2508	95	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 19.

All (95) 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:49:VAL:HG23	2:A:296:HOH:O	1.61	0.97

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ALA:HB1	2:B:199:HOH:O	1.70	0.91
1:A:1:MSE:O	1:A:1:MSE:HE3	1.71	0.89
1:B:5:LEU:H	1:B:148:ASN:HD21	1.27	0.80
1:B:9:VAL:HG11	1:B:119:ILE:HG23	1.62	0.80
1:B:47:LEU:HB2	1:B:130:PHE:HB2	1.64	0.79
1:B:100:ALA:HB1	1:B:102:MSE:HE3	1.66	0.77
1:B:5:LEU:H	1:B:148:ASN:ND2	1.83	0.77
1:B:46:VAL:HG21	1:B:69:LEU:HD13	1.68	0.74
1:B:70:ALA:HA	2:B:174:HOH:O	1.87	0.73
1:A:3:THR:HG22	1:A:146:ASN:HA	1.72	0.71
1:B:9:VAL:CG1	1:B:119:ILE:HG23	2.22	0.70
1:A:133:ASP:HB3	2:A:274:HOH:O	1.92	0.68
1:A:131:VAL:HB	1:A:140:TYR:HB3	1.77	0.67
1:A:29:THR:HG23	1:A:31:ASP:H	1.61	0.65
1:B:9:VAL:HG13	1:B:121:GLU:OE1	1.97	0.64
1:A:108:ASP:O	1:A:109:HIS:HB2	1.97	0.64
1:B:34:LYS:HD3	2:B:280:HOH:O	1.98	0.64
1:A:138:ILE:HG21	1:A:141:VAL:HG13	1.81	0.62
1:A:99:ASN:HB2	2:A:212:HOH:O	2.00	0.62
1:B:90:ARG:NH1	1:B:90:ARG:HB3	2.14	0.61
1:A:107:PHE:O	1:B:123:HIS:HD2	1.84	0.61
1:B:108:ASP:O	1:B:109:HIS:HB2	2.02	0.60
1:B:100:ALA:CB	1:B:102:MSE:HE3	2.31	0.59
1:A:108:ASP:HB2	2:A:188:HOH:O	2.01	0.59
1:A:34:LYS:HE3	2:A:218:HOH:O	2.02	0.59
1:B:53:ILE:HG13	1:B:83:ASP:OD1	2.03	0.59
1:B:5:LEU:N	1:B:148:ASN:HD21	2.00	0.58
1:B:87:ALA:HA	1:B:90:ARG:NH1	2.20	0.57
1:A:9:VAL:HB	1:A:119:ILE:HG23	1.88	0.56
1:B:109:HIS:HE1	2:B:166:HOH:O	1.88	0.56
1:A:3:THR:HG23	2:A:211:HOH:O	2.04	0.56
1:B:4:PHE:HA	1:B:148:ASN:HD21	1.71	0.55
1:A:1:MSE:C	1:A:1:MSE:HE3	2.27	0.55
1:B:51:PRO:HD2	1:B:58:CYS:SG	2.47	0.54
1:B:64:ARG:HG3	1:B:68:GLU:HG3	1.91	0.53
1:B:17:GLN:HB3	2:B:206:HOH:O	2.08	0.53
1:B:4:PHE:HA	1:B:148:ASN:ND2	2.24	0.52
1:B:81:SER:HB2	2:B:271:HOH:O	2.10	0.51
1:A:51:PRO:HD2	1:A:58:CYS:SG	2.51	0.51
1:A:130:PHE:CD2	1:A:141:VAL:HG12	2.46	0.51
1:B:9:VAL:HB	2:B:265:HOH:O	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ILE:CG2	1:A:141:VAL:HG13	2.41	0.50
1:A:30:THR:HG21	2:A:254:HOH:O	2.12	0.50
1:B:18:VAL:HG23	1:B:141:VAL:HG12	1.93	0.50
1:B:66:ASN:O	1:B:70:ALA:HB2	2.12	0.49
1:A:46:VAL:HG21	1:A:69:LEU:HD13	1.93	0.49
1:B:21:LYS:HE2	1:B:135:ASP:O	2.12	0.49
1:B:4:PHE:O	1:B:5:LEU:HB2	2.12	0.49
1:A:142:GLU:HG3	2:A:261:HOH:O	2.12	0.49
1:B:9:VAL:CG1	1:B:10:SER:N	2.76	0.49
1:B:54:ASP:OD1	1:B:90:ARG:NH2	2.46	0.48
1:B:46:VAL:HG21	1:B:69:LEU:CD1	2.38	0.48
1:B:43:LYS:HG2	1:B:74:ASN:ND2	2.29	0.48
1:B:87:ALA:HA	1:B:90:ARG:HH12	1.77	0.48
1:A:47:LEU:HB2	1:A:130:PHE:HB2	1.94	0.48
1:B:100:ALA:HB1	1:B:102:MSE:CE	2.40	0.48
1:B:146:ASN:ND2	1:B:149:SER:HB3	2.28	0.47
1:B:152:ASN:OD1	1:B:154:GLU:HG2	2.14	0.47
1:A:38:ALA:HB2	2:A:226:HOH:O	2.15	0.47
1:B:91:TRP:CE2	1:B:95:GLU:HG3	2.49	0.47
1:A:109:HIS:HE1	2:B:166:HOH:O	1.99	0.46
1:A:1:MSE:HB3	2:A:179:HOH:O	2.14	0.46
1:B:108:ASP:HB3	1:B:110:SER:HB3	1.96	0.46
1:A:16:LEU:HD11	1:A:23:LEU:HG	1.98	0.45
1:A:92:CYS:HB3	1:A:98:ASP:HA	1.98	0.45
1:B:17:GLN:HG2	2:B:237:HOH:O	2.15	0.45
1:B:1:MSE:HG3	1:B:1:MSE:O	2.15	0.45
1:B:29:THR:HG23	1:B:31:ASP:H	1.82	0.45
1:A:52:SER:O	1:A:58:CYS:HB2	2.17	0.45
1:B:43:LYS:HG2	1:B:74:ASN:HD21	1.82	0.44
1:B:9:VAL:CB	2:B:265:HOH:O	2.65	0.44
1:A:63:ARG:NH1	1:A:95:GLU:O	2.51	0.44
1:B:147:ILE:HD12	2:B:265:HOH:O	2.18	0.44
1:A:150:GLU:CD	2:A:268:HOH:O	2.56	0.44
1:B:145:ASP:HB2	2:B:192:HOH:O	2.17	0.43
1:B:108:ASP:C	1:B:110:SER:N	2.72	0.43
1:A:43:LYS:HD2	2:A:217:HOH:O	2.17	0.43
1:B:48:SER:HB2	1:B:61:GLN:HE21	1.82	0.43
1:B:77:VAL:HG13	2:B:200:HOH:O	2.19	0.43
1:B:71:GLY:O	1:B:72:LEU:C	2.57	0.43
1:A:90:ARG:NH2	1:B:90:ARG:NH1	2.66	0.42
1:B:113:ARG:HD2	2:B:231:HOH:O	2.19	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ARG:CZ	1:B:90:ARG:HB3	2.50	0.42
1:A:133:ASP:CG	1:A:134:THR:H	2.23	0.42
1:A:25:PHE:O	1:A:36:SER:HA	2.20	0.42
1:B:44:LYS:HG2	2:B:252:HOH:O	2.19	0.41
1:A:106:TYR:CG	1:A:107:PHE:N	2.88	0.41
1:B:146:ASN:HB3	2:B:275:HOH:O	2.19	0.41
1:A:1:MSE:N	2:A:210:HOH:O	2.41	0.41
1:B:72:LEU:HA	1:B:72:LEU:HD23	1.82	0.41
1:B:91:TRP:CZ2	1:B:95:GLU:HG3	2.56	0.41
1:A:1:MSE:HE2	1:A:145:ASP:CG	2.41	0.41
1:A:108:ASP:O	1:A:109:HIS:CB	2.66	0.40
1:B:4:PHE:HB2	2:B:265:HOH:O	2.22	0.40

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:A:172:HOH:O	2:A:172:HOH:O[2_554]	1.49	0.71

## 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	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
1	B	161/163 (99%)	151 (94%)	10 (6%)	0	100	100
All	All	322/326 (99%)	305 (95%)	17 (5%)	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	139/136 (102%)	129 (93%)	10 (7%)	17	21
1	B	139/136 (102%)	135 (97%)	4 (3%)	48	64
All	All	278/272 (102%)	264 (95%)	14 (5%)	28	39

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	21	LYS
1	A	34	LYS
1	A	51	PRO
1	A	53	ILE
1	A	76	VAL
1	A	109	HIS
1	A	123	HIS
1	A	132	LEU
1	A	141	VAL
1	B	64	ARG
1	B	108	ASP
1	B	109	HIS
1	B	123	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	109	HIS
1	A	120	ASN
1	A	123	HIS
1	B	17	GLN
1	B	74	ASN
1	B	88	GLN
1	B	109	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	123	HIS
1	B	148	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 [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	160/163 (98%)	-0.32	1 (0%) 89 92	9, 19, 30, 33	0
1	B	160/163 (98%)	-0.17	5 (3%) 49 56	10, 19, 30, 39	0
All	All	320/326 (98%)	-0.25	6 (1%) 67 73	9, 19, 30, 39	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	GLY	6.6
1	B	73	ASP	4.2
1	A	71	GLY	3.2
1	B	99	ASN	2.8
1	B	70	ALA	2.6
1	B	98	ASP	2.1

### 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.