



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:08 PM UTC

PDB ID : 4ROB / pdb\_00004rob  
Title : 2.8Å resolution structure of SRPN2 (K198C) from Anopheles gambiae  
Authors : Lovell, S.; Battaile, K.P.; Zhang, X.; Meekins, D.A.; An, C.; Michel, K.  
Deposited on : 2014-10-28  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

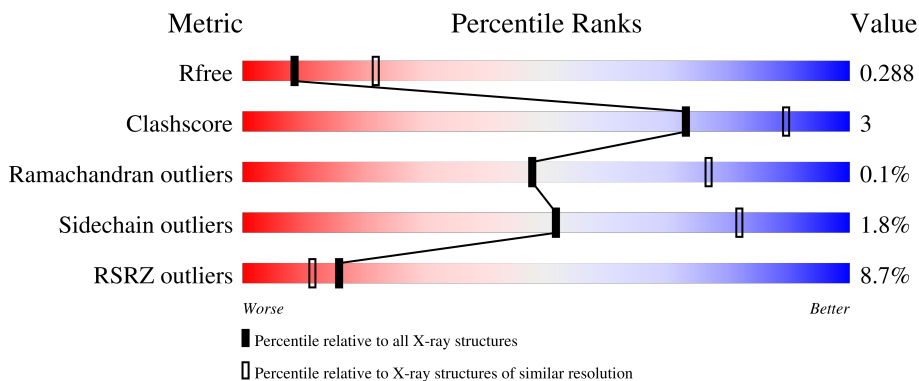
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


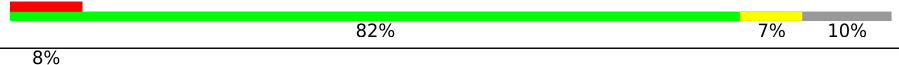
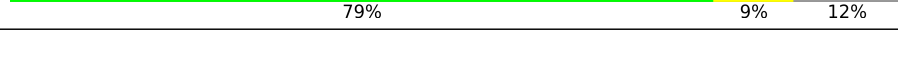
The reported resolution of this entry is 2.80 Å.

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))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	397	 7% 80% 10% 10%
1	B	397	 8% 82% 7% 10%
1	C	397	 8% 79% 9% 12%

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 8402 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 Serpin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	356	Total 2811	C 1808	N 462	O 534	S 7	0	0	0
1	B	356	Total 2822	C 1812	N 467	O 536	S 7	0	0	0
1	C	351	Total 2769	C 1783	N 458	O 522	S 6	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

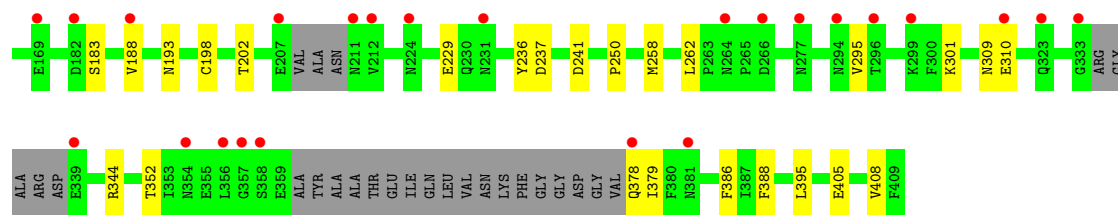
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	expression tag	UNP Q005N3
A	14	GLY	-	expression tag	UNP Q005N3
A	15	HIS	-	expression tag	UNP Q005N3
A	16	HIS	-	expression tag	UNP Q005N3
A	17	HIS	-	expression tag	UNP Q005N3
A	18	HIS	-	expression tag	UNP Q005N3
A	19	HIS	-	expression tag	UNP Q005N3
A	20	HIS	-	expression tag	UNP Q005N3
A	21	GLY	-	expression tag	UNP Q005N3
A	198	CYS	LYS	engineered mutation	UNP Q005N3
B	13	MET	-	expression tag	UNP Q005N3
B	14	GLY	-	expression tag	UNP Q005N3
B	15	HIS	-	expression tag	UNP Q005N3
B	16	HIS	-	expression tag	UNP Q005N3
B	17	HIS	-	expression tag	UNP Q005N3
B	18	HIS	-	expression tag	UNP Q005N3
B	19	HIS	-	expression tag	UNP Q005N3
B	20	HIS	-	expression tag	UNP Q005N3
B	21	GLY	-	expression tag	UNP Q005N3
B	198	CYS	LYS	engineered mutation	UNP Q005N3
C	13	MET	-	expression tag	UNP Q005N3
C	14	GLY	-	expression tag	UNP Q005N3
C	15	HIS	-	expression tag	UNP Q005N3

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<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
C	16	HIS	-	expression tag	UNP Q005N3
C	17	HIS	-	expression tag	UNP Q005N3
C	18	HIS	-	expression tag	UNP Q005N3
C	19	HIS	-	expression tag	UNP Q005N3
C	20	HIS	-	expression tag	UNP Q005N3
C	21	GLY	-	expression tag	UNP Q005N3
C	198	CYS	LYS	engineered mutation	UNP Q005N3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.09Å 167.21Å 90.26Å 90.00° 99.16° 90.00°	Depositor
Resolution (Å)	41.80 – 2.80 41.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (41.80-2.80) 95.4 (41.80-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.81Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.211 , 0.281 0.221 , 0.288	Depositor DCC
$R_{free}$ test set	1562 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtrriage
Anisotropy	0.676	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8402	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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	0.44	0/2875	0.62	0/3911
1	B	0.42	0/2886	0.60	0/3925
1	C	0.40	0/2832	0.60	0/3851
All	All	0.42	0/8593	0.60	0/11687

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	2811	0	2681	20	0
1	B	2822	0	2695	17	0
1	C	2769	0	2633	17	0
All	All	8402	0	8009	53	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 3.

All (53) 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:130:ILE:O	1:A:150:LYS:NZ	1.93	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ILE:O	1:C:150:LYS:NZ	2.01	0.93
1:C:38:ASP:N	1:C:38:ASP:OD1	2.34	0.59
1:C:183:SER:O	1:C:344:ARG:NH1	2.37	0.57
1:B:38:ASP:OD2	1:B:38:ASP:N	2.38	0.56
1:C:258:MET:HE3	1:C:388:PHE:CD1	2.42	0.54
1:A:388:PHE:CZ	1:A:402:GLY:HA3	2.43	0.54
1:B:155:ASN:ND2	1:B:158:GLN:OE1	2.40	0.53
1:C:105:LEU:HD12	1:C:395:LEU:HD13	1.92	0.52
1:B:205:PHE:CZ	1:B:297:LEU:HD12	2.45	0.51
1:B:52:ASN:HB3	1:B:302:PHE:CE2	2.46	0.50
1:B:249:LEU:HD11	1:B:297:LEU:HD11	1.93	0.50
1:C:262:LEU:HD12	1:C:386:PHE:HB3	1.93	0.49
1:C:309:ASN:HD21	1:C:344:ARG:HA	1.77	0.49
1:A:80:SER:OG	1:A:81:ASN:N	2.46	0.48
1:B:327:LEU:N	1:B:328:PRO:HD3	2.28	0.48
1:C:202:THR:HB	1:C:250:PRO:HG2	1.95	0.47
1:A:139:ILE:HD11	1:B:30:GLN:HB3	1.97	0.47
1:A:248:ARG:NH2	1:A:393:GLU:OE2	2.43	0.47
1:C:161:ALA:O	1:C:165:ASN:ND2	2.44	0.47
1:B:229:GLU:HA	1:B:295:VAL:O	2.14	0.47
1:A:63:LEU:HD21	1:A:193:ASN:HB2	1.96	0.46
1:C:99:ARG:HB3	1:C:143:HIS:ND1	2.31	0.46
1:A:236:TYR:CD1	1:A:237:ASP:N	2.84	0.46
1:A:330:LEU:C	1:A:330:LEU:HD23	2.41	0.46
1:C:52:ASN:OD1	1:C:405:GLU:N	2.40	0.45
1:C:229:GLU:HA	1:C:295:VAL:O	2.16	0.45
1:C:48:ASN:O	1:C:49:HIS:ND1	2.49	0.45
1:B:123:ASN:OD1	1:B:124:PHE:N	2.50	0.44
1:A:174:ARG:NH2	1:A:302:PHE:O	2.43	0.43
1:B:208:VAL:O	1:B:210:ASN:N	2.51	0.43
1:A:285:LEU:HA	1:A:288:MET:SD	2.58	0.43
1:B:63:LEU:HD21	1:B:193:ASN:HB2	2.01	0.43
1:A:221:LYS:HG2	1:A:222:PRO:HD2	2.01	0.43
1:A:103:LYS:NZ	1:A:107:GLU:OE2	2.40	0.42
1:A:123:ASN:HB2	1:A:166:TRP:CZ2	2.54	0.42
1:C:301:LYS:HB2	1:C:352:THR:HG23	2.00	0.42
1:B:174:ARG:NH2	1:B:302:PHE:O	2.53	0.42
1:A:171:THR:HG21	1:A:175:LEU:HD12	2.01	0.41
1:C:236:TYR:CD1	1:C:237:ASP:N	2.88	0.41
1:C:130:ILE:CD1	1:C:188:VAL:CG1	2.99	0.41
1:A:309:ASN:OD1	1:A:309:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:TYR:CD1	1:B:236:TYR:C	2.98	0.41
1:A:263:PRO:O	1:A:384:ARG:NH2	2.53	0.41
1:A:263:PRO:HG3	1:A:272:VAL:HG21	2.01	0.41
1:B:319:GLU:C	1:B:321:PHE:H	2.28	0.41
1:C:63:LEU:HD21	1:C:193:ASN:HB2	2.02	0.41
1:A:126:VAL:CG1	1:A:130:ILE:HB	2.51	0.41
1:A:309:ASN:HD21	1:A:344:ARG:HA	1.85	0.41
1:B:296:THR:HB	1:B:381:ASN:HA	2.03	0.41
1:A:92:ASN:O	1:A:93:ASP:C	2.64	0.40
1:B:103:LYS:HE3	1:B:107:GLU:OE2	2.20	0.40
1:B:155:ASN:CG	1:B:158:GLN:HB3	2.46	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	348/397 (88%)	322 (92%)	25 (7%)	1 (0%)	36	66
1	B	348/397 (88%)	327 (94%)	21 (6%)	0	100	100
1	C	341/397 (86%)	314 (92%)	27 (8%)	0	100	100
All	All	1037/1191 (87%)	963 (93%)	73 (7%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	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	300/349 (86%)	296 (99%)	4 (1%)	61	86
1	B	302/349 (86%)	298 (99%)	4 (1%)	61	86
1	C	293/349 (84%)	285 (97%)	8 (3%)	39	74
All	All	895/1047 (86%)	879 (98%)	16 (2%)	51	82

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	SER
1	A	137	GLN
1	A	152	SER
1	A	391	GLU
1	B	38	ASP
1	B	305	SER
1	B	359	GLU
1	B	391	GLU
1	C	38	ASP
1	C	152	SER
1	C	198	CYS
1	C	241	ASP
1	C	310	GLU
1	C	378	GLN
1	C	379	ILE
1	C	408	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	245	GLN
1	A	383	ASN
1	A	406	ASN
1	B	231	ASN

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Mol	Chain	Res	Type
1	C	34	GLN
1	C	91	GLN
1	C	119	ASN
1	C	233	GLN
1	C	307	GLN
1	C	381	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 oligosaccharides 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	356/397 (89%)	0.77	27 (7%)	20   14	14, 35, 59, 73	0
1	B	356/397 (89%)	0.84	33 (9%)	14   10	16, 36, 61, 91	0
1	C	351/397 (88%)	0.94	32 (9%)	15   11	19, 39, 61, 82	0
All	All	1063/1191 (89%)	0.85	92 (8%)	16   11	14, 36, 61, 91	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	ALA	4.4
1	C	358	SER	4.3
1	A	92	ASN	4.3
1	C	154	SER	3.8
1	C	266	ASP	3.6
1	C	357	GLY	3.6
1	B	73	THR	3.6
1	A	357	GLY	3.5
1	C	81	ASN	3.5
1	A	88	SER	3.4
1	C	74	SER	3.4
1	A	324	ASN	3.3
1	B	339	GLU	3.3
1	B	291	ASN	3.3
1	B	322	SER	3.3
1	B	266	ASP	3.2
1	C	299	LYS	3.2
1	B	57	PRO	3.2
1	A	72	ASP	3.2
1	C	211	ASN	3.2
1	A	130	ILE	3.0
1	A	231	ASN	3.0
1	C	333	GLY	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	360	ALA	3.0
1	B	93	ASP	2.9
1	A	218	THR	2.9
1	A	36	GLU	2.9
1	C	231	ASN	2.8
1	A	266	ASP	2.8
1	B	72	ASP	2.8
1	A	112	ASP	2.8
1	B	340	VAL	2.7
1	A	74	SER	2.7
1	B	243	GLY	2.7
1	C	296	THR	2.6
1	B	270	ASN	2.6
1	B	112	ASP	2.6
1	C	310	GLU	2.5
1	C	224	ASN	2.5
1	B	114	LYS	2.5
1	C	97	HIS	2.5
1	B	80	SER	2.5
1	A	402	GLY	2.4
1	B	253	GLY	2.4
1	A	154	SER	2.4
1	B	84	ARG	2.4
1	B	254	ASN	2.4
1	B	83	LYS	2.4
1	B	360	ALA	2.4
1	A	73	THR	2.4
1	C	139	ILE	2.4
1	B	224	ASN	2.3
1	C	264	ASN	2.3
1	A	83	LYS	2.3
1	A	340	VAL	2.3
1	B	409	PHE	2.3
1	A	93	ASP	2.3
1	C	207	GLU	2.3
1	C	71	SER	2.3
1	B	324	ASN	2.2
1	C	294	ASN	2.2
1	C	356	LEU	2.2
1	B	221	LYS	2.2
1	A	275	ARG	2.2
1	B	208	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	129	PHE	2.2
1	C	323	GLN	2.2
1	B	265	PRO	2.2
1	B	210	ASN	2.1
1	C	381	ASN	2.1
1	B	232	GLY	2.1
1	A	41	PHE	2.1
1	A	358	SER	2.1
1	B	229	GLU	2.1
1	B	359	GLU	2.1
1	A	97	HIS	2.1
1	B	211	ASN	2.1
1	C	277	ASN	2.1
1	C	188	VAL	2.1
1	C	182	ASP	2.1
1	C	169	GLU	2.1
1	C	339	GLU	2.1
1	A	80	SER	2.1
1	B	323	GLN	2.1
1	C	378	GLN	2.1
1	C	73	THR	2.1
1	C	212	VAL	2.0
1	C	354	ASN	2.0
1	A	310	GLU	2.0
1	A	87	SER	2.0
1	C	148	LEU	2.0
1	A	117	ASP	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 oligosaccharides 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.