



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2025 – 10:05 AM EST

PDB ID : 9YP2 / pdb\_00009yp2  
Title : Structure of HaCV P domain in complex with Nanobody 7  
Authors : Kara, D.; Pancera, M.; Hansman, G.  
Deposited on : 2025-10-13  
Resolution : 2.09 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

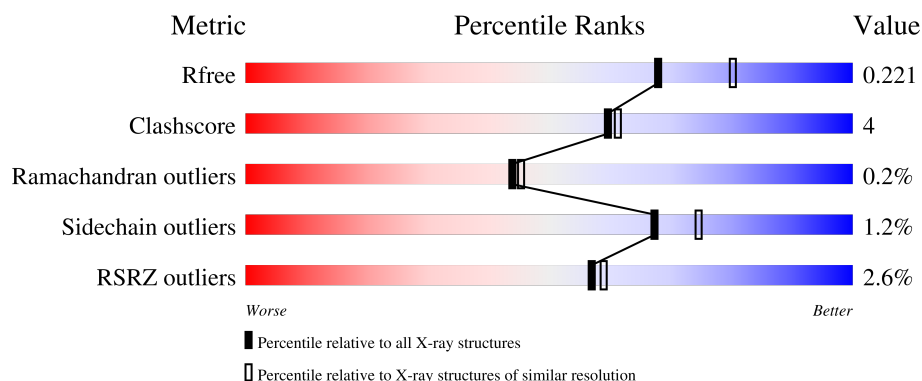
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	339	<div> <div>2%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	B	339	<div> <div>3%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
2	C	111	<div> <div>%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	D	111	<div> <div>5%</div> <div>68%</div> <div>29%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6812 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	1	0
			2398	1516	408	470	4			
1	B	327	Total	C	N	O	S	0	1	0
			2387	1507	407	469	4			

- Molecule 2 is a protein called Nanobody 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	109	Total	C	N	O	S	0	0	0
			836	523	145	165	3			
2	D	107	Total	C	N	O	S	0	0	0
			826	516	143	164	3			

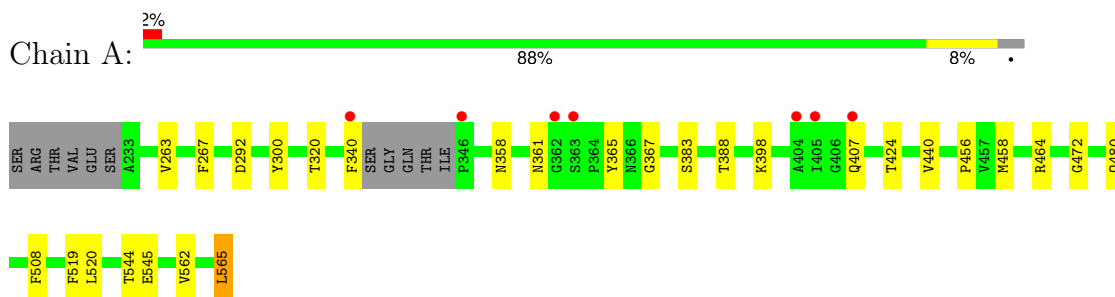
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	177	Total	O	0	0
			177	177		
3	C	31	Total	O	0	0
			31	31		
3	B	149	Total	O	0	0
			149	149		
3	D	8	Total	O	0	0
			8	8		

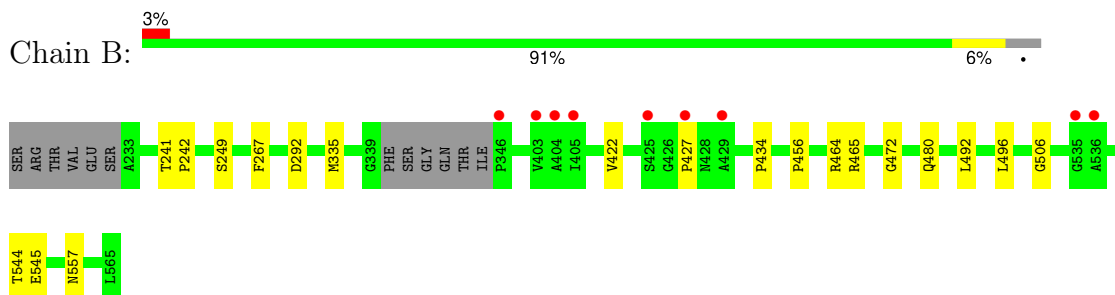
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

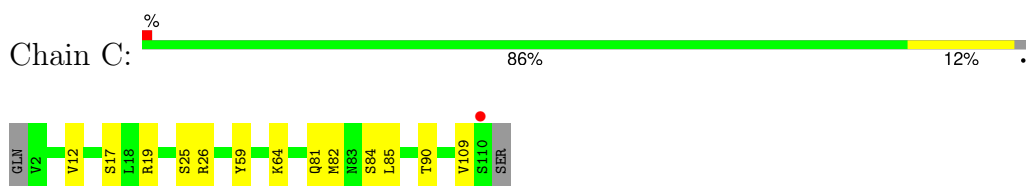
- Molecule 1: Capsid protein



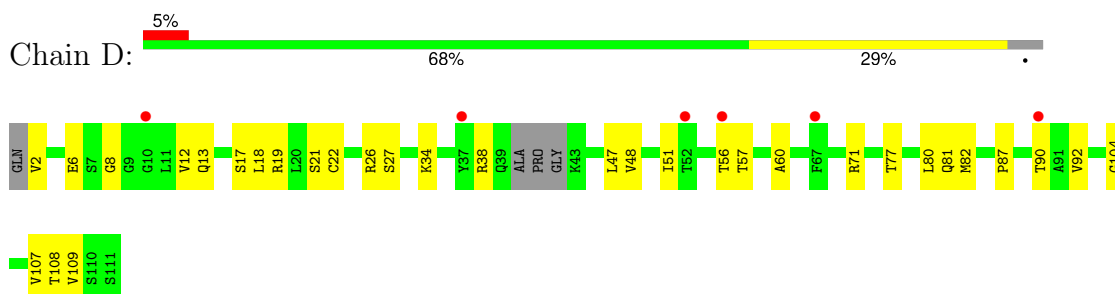
- Molecule 1: Capsid protein



- Molecule 2: Nanobody 7



- Molecule 2: Nanobody 7



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.25Å 73.51Å 59.25Å 90.00° 94.11° 90.00°	Depositor
Resolution (Å)	29.66 – 2.09 29.66 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.66-2.09) 98.6 (29.66-2.09)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.182 , 0.223 0.182 , 0.221	Depositor DCC
$R_{free}$ test set	2702 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 28.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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	0.38	0/2464	0.57	0/3382
1	B	0.36	0/2452	0.53	0/3366
2	C	0.29	0/852	0.48	0/1152
2	D	0.24	0/840	0.42	0/1133
All	All	0.34	0/6608	0.53	0/9033

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	508	PHE	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	2398	0	2308	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2387	0	2299	10	0
2	C	836	0	810	6	0
2	D	826	0	799	22	0
3	A	177	0	0	3	0
3	B	149	0	0	1	0
3	C	31	0	0	0	0
3	D	8	0	0	0	0
All	All	6812	0	6216	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 4.

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)
2:D:38:ARG:HD3	2:D:48:VAL:HG22	1.69	0.75
1:B:545:GLU:OE1	3:B:601:HOH:O	2.10	0.68
1:A:545:GLU:HA	2:D:56:THR:HG21	1.81	0.62
1:A:464:ARG:NH2	1:B:292:ASP:OD1	2.34	0.60
1:A:424:THR:OG1	1:A:480:GLN:OE1	2.13	0.59
2:D:51:ILE:HD12	2:D:57:THR:HG22	1.85	0.58
1:A:292:ASP:OD2	1:B:464:ARG:NH2	2.35	0.58
2:D:38:ARG:HD3	2:D:48:VAL:CG2	2.36	0.55
1:A:300:TYR:CZ	1:A:407:GLN:HB2	2.42	0.54
2:C:82:MET:HE2	2:C:85:LEU:HD21	1.90	0.53
2:D:90:THR:HG22	2:D:109:VAL:H	1.73	0.53
2:D:8:GLY:HA3	2:D:19:ARG:O	2.09	0.51
1:A:519:PHE:CE2	1:A:562:VAL:HG11	2.44	0.51
1:A:520:LEU:HD23	1:A:565:LEU:HD22	1.92	0.51
1:B:335:MET:HG2	1:B:434:PRO:HB3	1.93	0.51
1:A:320:THR:HG22	3:A:716:HOH:O	2.10	0.50
1:A:544:THR:HG23	1:A:545:GLU:HG2	1.94	0.49
2:D:80:LEU:HD12	2:D:82:MET:CG	2.42	0.48
2:D:87:PRO:O	2:D:90:THR:HG23	2.13	0.48
1:B:506:GLY:HA2	1:B:557:ASN:ND2	2.29	0.47
1:A:267:PHE:CE1	1:A:456:PRO:HB2	2.49	0.47
1:A:358:ASN:O	1:A:361:ASN:HB2	2.15	0.47
2:D:90:THR:HG22	2:D:109:VAL:N	2.30	0.46
2:D:92:VAL:HG12	2:D:104:GLY:HA3	1.97	0.46
1:A:340:PHE:HE2	1:A:383:SER:HA	1.81	0.45
2:D:80:LEU:HD12	2:D:82:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:TYR:CZ	1:A:367:GLY:HA2	2.52	0.44
1:B:492:LEU:O	1:B:496:LEU:HG	2.17	0.44
2:D:6:GLU:HA	2:D:21:SER:O	2.18	0.44
1:A:480:GLN:NE2	3:A:616:HOH:O	2.51	0.44
2:C:85:LEU:HB3	2:C:109:VAL:HG21	1.99	0.44
2:C:59:TYR:HB2	2:C:64:LYS:HG3	2.00	0.44
2:D:22:CYS:O	2:D:77:THR:HA	2.18	0.44
2:D:17:SER:O	2:D:18:LEU:HD23	2.18	0.43
2:D:19:ARG:HB2	2:D:81:GLN:NE2	2.34	0.43
1:A:263:VAL:HG21	1:A:458:MET:HE3	1.99	0.43
2:D:12:VAL:HG22	2:D:13:GLN:O	2.19	0.43
1:B:422:VAL:HG11	1:B:480:GLN:HB2	2.01	0.43
2:D:34:LYS:HD2	2:D:71:ARG:HD2	2.01	0.42
2:D:2:VAL:HG22	2:D:26:ARG:HG2	2.02	0.42
2:D:90:THR:CG2	2:D:109:VAL:H	2.33	0.42
1:A:565:LEU:HA	1:A:565:LEU:HD12	1.81	0.42
2:C:25:SER:O	2:C:26:ARG:HD3	2.20	0.42
1:B:241:THR:HB	1:B:242:PRO:HD3	2.02	0.42
2:D:47:LEU:O	2:D:60:ALA:HB2	2.20	0.42
2:C:19:ARG:HG3	2:C:81:GLN:OE1	2.20	0.41
1:B:267:PHE:CE1	1:B:456:PRO:HB2	2.55	0.41
1:B:427:PRO:HB3	1:B:465:ARG:HD2	2.03	0.41
2:D:18:LEU:HD12	2:D:107:VAL:HG22	2.02	0.41
2:D:19:ARG:HB2	2:D:81:GLN:HE22	1.86	0.40
2:C:12:VAL:HG11	2:C:85:LEU:HD13	2.04	0.40
1:A:388:THR:HA	1:A:440:VAL:HG22	2.02	0.40
1:A:398:LYS:HE2	3:A:663:HOH:O	2.21	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	325/339 (96%)	313 (96%)	11 (3%)	1 (0%)	37	37
1	B	324/339 (96%)	308 (95%)	15 (5%)	1 (0%)	37	37
2	C	107/111 (96%)	107 (100%)	0	0	100	100
2	D	103/111 (93%)	101 (98%)	2 (2%)	0	100	100
All	All	859/900 (95%)	829 (96%)	28 (3%)	2 (0%)	44	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	GLY
1	B	472	GLY

### 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	256/265 (97%)	255 (100%)	1 (0%)	89	93
1	B	255/265 (96%)	253 (99%)	2 (1%)	79	84
2	C	88/90 (98%)	85 (97%)	3 (3%)	32	35
2	D	88/90 (98%)	86 (98%)	2 (2%)	45	51
All	All	687/710 (97%)	679 (99%)	8 (1%)	67	74

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	LEU
2	C	17	SER
2	C	84	SER
2	C	90	THR
1	B	249	SER
1	B	544	THR
2	D	27	SER
2	D	108	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	271	ASN
1	A	277	ASN
1	A	539	ASN
2	C	76	ASN
1	B	408	ASN
1	B	409	GLN
1	B	504	GLN
2	D	81	GLN

### 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	328/339 (96%)	-0.34	7 (2%) 63 65	18, 31, 63, 79	1 (0%)
1	B	327/339 (96%)	-0.12	9 (2%) 55 57	18, 33, 65, 89	1 (0%)
2	C	109/111 (98%)	-0.05	1 (0%) 81 82	25, 42, 56, 64	0
2	D	107/111 (96%)	0.87	6 (5%) 31 33	30, 66, 75, 85	0
All	All	871/900 (96%)	-0.07	23 (2%) 57 59	18, 36, 70, 89	2 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	ILE	4.2
1	B	536	ALA	3.9
1	A	363	SER	3.6
1	B	405	ILE	3.5
1	B	427	PRO	2.8
2	D	37	TYR	2.7
1	A	362	GLY	2.7
1	B	404	ALA	2.7
1	B	425	SER	2.5
1	B	535	GLY	2.5
1	A	346	PRO	2.4
2	D	90	THR	2.3
2	D	52	THR	2.3
1	B	346	PRO	2.3
2	D	10	GLY	2.3
2	C	110	SER	2.3
1	B	403	VAL	2.2
2	D	67	PHE	2.2
1	A	407	GLN	2.1
1	A	404	ALA	2.1
1	A	340	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	429	ALA	2.0
2	D	56	THR	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.