



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 PM GMT

PDB ID : 3S37  
Title : Structural basis for the function of two anti-VEGF receptor antibodies  
Authors : Franklin, M.C.  
Deposited on : 2011-05-17  
Resolution : 2.70 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

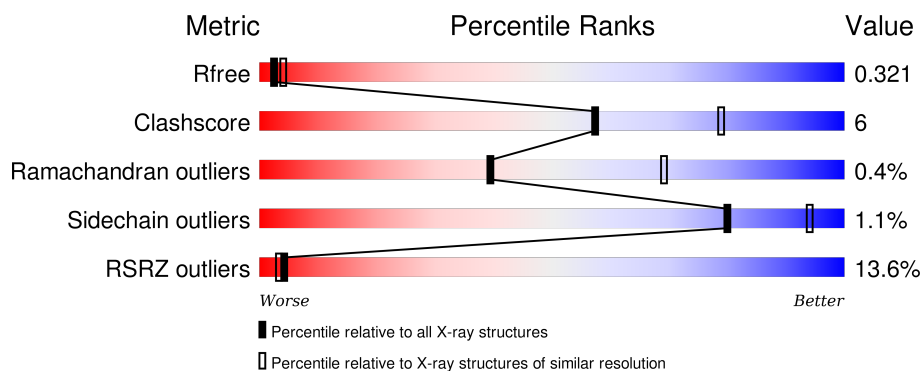
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	L	214	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	H	221	<div> <div>4%</div> <div>75%</div> <div>18%</div> <div>5%</div> </div>
3	X	122	<div> <div>50%</div> <div>75%</div> <div>14%</div> <div>10%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4037 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 1121B Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1616	1016	272	323	5			

- Molecule 2 is a protein called 1121B Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	209	Total	C	N	O	S	0	0	0
			1559	984	262	306	7			

- Molecule 3 is a protein called Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	110	Total	C	N	O	S	0	0	0
			862	543	152	163	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	217	ALA	-	EXPRESSION TAG	UNP P35968
X	218	ASP	-	EXPRESSION TAG	UNP P35968
X	219	PRO	-	EXPRESSION TAG	UNP P35968

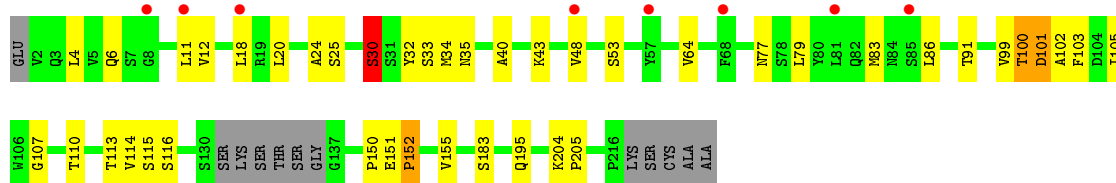
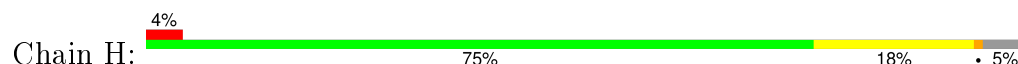
### 3 Residue-property plots [i](#)

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.

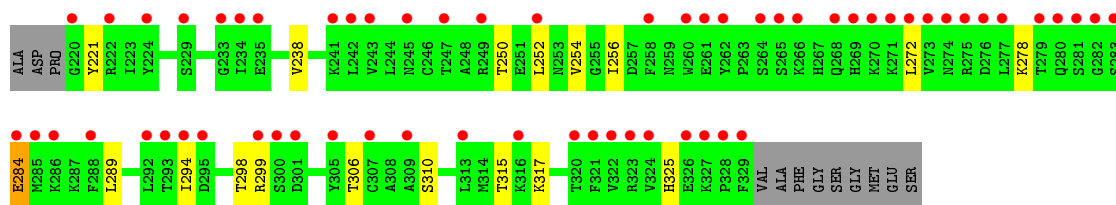
- Molecule 1: 1121B Fab light chain



- Molecule 2: 1121B Fab heavy chain



- Molecule 3: Vascular endothelial growth factor receptor 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.68Å 63.68Å 275.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.46 – 2.70 44.44 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.46-2.70) 99.8 (44.44-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.282 , 0.315 0.281 , 0.321	Depositor DCC
$R_{free}$ test set	831 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.6	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 30.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 16484 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4037	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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

### 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	L	0.27	0/1652	0.46	0/2243
2	H	0.36	1/1595 (0.1%)	0.79	14/2172 (0.6%)
3	X	0.27	0/878	0.46	1/1183 (0.1%)
All	All	0.31	1/4125 (0.0%)	0.61	15/5598 (0.3%)

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
2	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	152	PRO	N-CD	9.92	1.61	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	116	SER	N-CA-CB	-16.05	86.42	110.50
2	H	115	SER	CB-CA-C	-11.44	88.37	110.10
2	H	25	SER	CB-CA-C	-8.93	93.13	110.10
2	H	25	SER	N-CA-C	-8.82	87.19	111.00
2	H	30	SER	N-CA-C	6.66	128.98	111.00
2	H	151	GLU	CB-CA-C	-6.55	97.30	110.40
2	H	151	GLU	N-CA-C	6.32	128.06	111.00
2	H	102	ALA	N-CA-CB	6.30	118.92	110.10
2	H	116	SER	N-CA-C	6.02	127.25	111.00
2	H	24	ALA	CB-CA-C	-5.77	101.45	110.10
2	H	30	SER	C-N-CA	5.65	135.83	121.70
2	H	115	SER	N-CA-C	-5.24	96.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	284	GLU	N-CA-CB	-5.24	101.17	110.60
2	H	152	PRO	CA-N-CD	-5.20	104.23	111.50
2	H	25	SER	N-CA-CB	-5.01	102.99	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	30	SER	Peptide

## 5.2 Too-close contacts

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	L	1616	0	1570	15	0
2	H	1559	0	1527	24	0
3	X	862	0	865	11	0
All	All	4037	0	3962	48	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 6.

All (48) 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:H:100:THR:O	2:H:101:ASP:HB2	1.59	1.02
2:H:30:SER:O	2:H:53:SER:OG	1.90	0.89
3:X:250:THR:HG21	3:X:256:ILE:HD11	1.64	0.80
3:X:221:TYR:HA	3:X:254:VAL:HG22	1.71	0.71
2:H:100:THR:O	2:H:101:ASP:CB	2.38	0.70
1:L:115:VAL:HG21	1:L:196:VAL:HG21	1.75	0.69
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.80	0.62
2:H:32:TYR:HA	3:X:315:THR:HG21	1.87	0.56
2:H:20:LEU:HD11	2:H:110:THR:HG21	1.86	0.56
1:L:29:ILE:HG23	1:L:92:LYS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.43	0.53
2:H:48:VAL:HG13	2:H:64:VAL:HG11	1.91	0.53
1:L:29:ILE:HD13	1:L:90:GLN:HB2	1.90	0.53
3:X:298:THR:HG22	3:X:299:ARG:H	1.74	0.53
2:H:155:VAL:HG11	2:H:183:SER:CB	2.41	0.51
3:X:278:LYS:HD2	3:X:289:LEU:HD22	1.93	0.51
1:L:78:LEU:HD13	1:L:79:GLN:N	2.25	0.51
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.94	0.50
1:L:29:ILE:O	1:L:29:ILE:HG22	2.12	0.50
2:H:4:LEU:HD12	2:H:105:ILE:HG22	1.94	0.49
1:L:36:TYR:CE2	1:L:46:LEU:HD13	2.48	0.49
2:H:6:GLN:HE21	2:H:107:GLY:HA3	1.78	0.49
2:H:86:LEU:HB3	2:H:114:VAL:HG21	1.95	0.48
3:X:252:LEU:HD11	3:X:284:GLU:HA	1.96	0.48
2:H:11:LEU:HD21	2:H:150:PRO:HB3	1.95	0.48
1:L:33:LEU:HD22	1:L:71:PHE:CB	2.44	0.47
2:H:91:THR:HG23	2:H:113:THR:HA	1.97	0.47
2:H:35:ASN:ND2	2:H:99:VAL:HG21	2.30	0.46
1:L:2:ILE:HG21	1:L:90:GLN:NE2	2.31	0.45
1:L:8:PRO:HG2	1:L:11:VAL:HG22	1.99	0.45
2:H:20:LEU:HD11	2:H:110:THR:CG2	2.47	0.45
2:H:12:VAL:HG22	2:H:18:LEU:HD12	2.00	0.44
3:X:250:THR:HG21	3:X:256:ILE:CD1	2.41	0.44
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.99	0.44
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.99	0.44
2:H:30:SER:C	2:H:53:SER:OG	2.55	0.43
2:H:33:SER:HB3	3:X:310:SER:HB2	2.02	0.42
1:L:2:ILE:O	1:L:2:ILE:HG23	2.19	0.41
2:H:99:VAL:HG22	2:H:103:PHE:CD1	2.56	0.41
3:X:306:THR:HG21	3:X:317:LYS:HE3	2.03	0.41
1:L:163:VAL:HG22	1:L:175:LEU:HD12	2.02	0.41
1:L:78:LEU:HD13	1:L:79:GLN:O	2.21	0.41
3:X:272:LEU:HD22	3:X:294:ILE:HG12	2.03	0.41
2:H:34:MET:C	2:H:35:ASN:HD22	2.23	0.41
3:X:238:VAL:HG23	3:X:325:HIS:O	2.22	0.40
1:L:124:GLN:HE22	1:L:131:SER:CB	2.34	0.40
2:H:6:GLN:OE1	2:H:110:THR:HG22	2.22	0.40
2:H:204:LYS:N	2:H:205:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

## 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	L	210/214 (98%)	200 (95%)	10 (5%)	0	100	100
2	H	205/221 (93%)	196 (96%)	7 (3%)	2 (1%)	19	45
3	X	108/122 (88%)	102 (94%)	6 (6%)	0	100	100
All	All	523/557 (94%)	498 (95%)	23 (4%)	2 (0%)	39	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	30	SER
2	H	101	ASP

### 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	L	181/184 (98%)	180 (99%)	1 (1%)	90	97
2	H	176/185 (95%)	172 (98%)	4 (2%)	58	85
3	X	98/107 (92%)	98 (100%)	0	100	100
All	All	455/476 (96%)	450 (99%)	5 (1%)	80	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	90	GLN

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Mol	Chain	Res	Type
2	H	77	ASN
2	H	100	THR
2	H	152	PRO
2	H	195	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	199	GLN
2	H	6	GLN
2	H	35	ASN
2	H	77	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	L	212/214 (99%)	0.15	3 (1%) 78 77	43, 59, 79, 90	0
2	H	209/221 (94%)	0.47	8 (3%) 44 44	48, 75, 119, 144	0
3	X	110/122 (90%)	3.29	61 (55%) 0 0	103, 137, 194, 222	0
All	All	531/557 (95%)	0.93	72 (13%) 4 3	43, 71, 162, 222	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	329	PHE	14.1
3	X	275	ARG	13.0
3	X	269	HIS	11.3
3	X	276	ASP	11.2
3	X	305	TYR	10.7
3	X	270	LYS	8.4
3	X	220	GLY	8.4
3	X	327	LYS	8.0
3	X	234	ILE	7.3
3	X	271	LYS	7.2
3	X	264	SER	7.1
3	X	277	LEU	6.7
3	X	279	THR	6.6
3	X	245	ASN	6.6
3	X	322	VAL	6.4
3	X	265	SER	6.1
3	X	324	VAL	5.9
3	X	323	ARG	5.8
3	X	281	SER	5.7
3	X	294	ILE	5.6
3	X	280	GLN	5.3
3	X	295	ASP	5.2
3	X	268	GLN	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	X	320	THR	5.1
3	X	252	LEU	5.0
3	X	242	LEU	5.0
3	X	247	THR	5.0
3	X	272	LEU	4.7
3	X	328	PRO	4.5
3	X	282	GLY	4.4
3	X	262	TYR	4.4
3	X	313	LEU	4.3
3	X	301	ASP	4.2
2	H	85	SER	4.2
3	X	288	PHE	4.1
3	X	283	SER	4.1
3	X	321	PHE	4.0
3	X	224	TYR	3.9
3	X	274	ASN	3.9
3	X	243	VAL	3.9
2	H	48	VAL	3.8
3	X	233	GLY	3.8
3	X	222	ARG	3.7
3	X	266	LYS	3.5
3	X	273	VAL	3.5
3	X	235	GLU	3.4
3	X	293	THR	3.4
2	H	57	TYR	3.4
3	X	326	GLU	3.2
3	X	229	SER	3.2
3	X	292	LEU	3.0
3	X	241	LYS	3.0
3	X	316	LYS	3.0
2	H	68	PHE	2.9
3	X	299	ARG	2.8
3	X	258	PHE	2.7
3	X	285	MET	2.7
3	X	300	SER	2.6
2	H	18	LEU	2.5
3	X	284	GLU	2.5
1	L	93	ALA	2.3
3	X	309	ALA	2.3
2	H	8	GLY	2.3
3	X	260	TRP	2.2
3	X	261	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	2	ILE	2.1
2	H	11	LEU	2.0
3	X	286	LYS	2.0
3	X	307	CYS	2.0
1	L	94	PHE	2.0
2	H	81	LEU	2.0
3	X	249	ARG	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.