



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:20 am GMT

PDB ID : 4NGH  
Title : Crystal structure of the HIV-1 neutralizing antibody 4E10 Fab fragment in complex with a hydrocarbon-stapled peptide containing the 4e10 epitope on gp41 and a tethered phosphate moiety.  
Authors : Irimia, A.; Wilson, I.A.  
Deposited on : 2013-11-01  
Resolution : 2.68 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	:	1.7.2 (RC1), CSD as538be (2017)
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

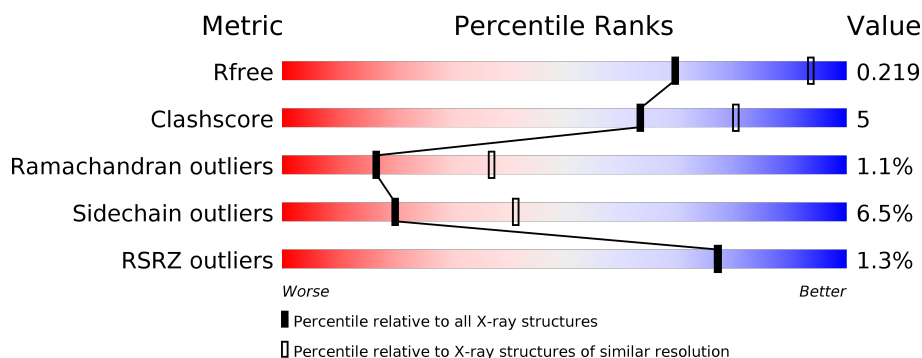
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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	3050 (2.70-2.66)
Clashscore	112137	3418 (2.70-2.66)
Ramachandran outliers	110173	3367 (2.70-2.66)
Sidechain outliers	110143	3367 (2.70-2.66)
RSRZ outliers	101464	3069 (2.70-2.66)

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	215	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>•</div> </div> </div>
2	H	228	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>•</div> </div> </div>
3	P	17	<div> <div></div> <div> <div>71%</div> <div>18%</div> <div>12%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3602 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 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	1	0
			1654	1025	286	338	5			

- Molecule 2 is a protein called FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	228	Total	C	N	O	S	0	0	0
			1690	1069	289	327	5			

- Molecule 3 is a protein called MODIFIED FRAGMENT OF HIV GLYCOPROTEIN (GP41).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	17	Total	C	N	O	P	0	0	0
			162	106	27	28	1			

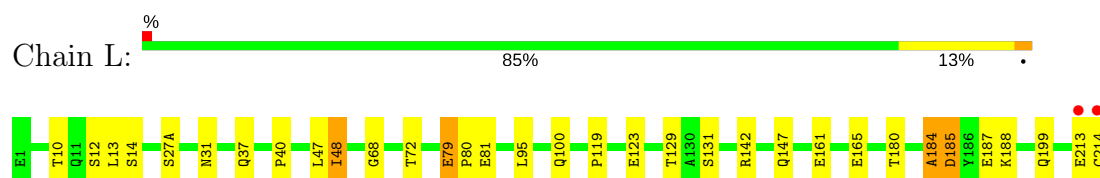
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	35	Total	O	0	0
			35	35		
4	H	57	Total	O	0	0
			57	57		
4	P	4	Total	O	0	0
			4	4		

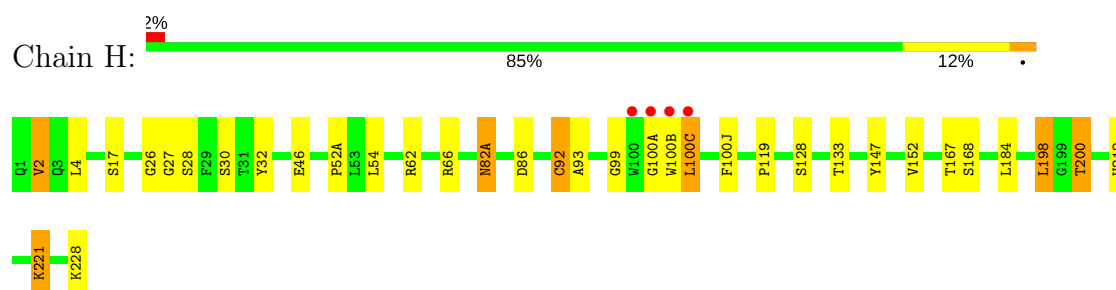
### 3 Residue-property plots [i](#)

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.

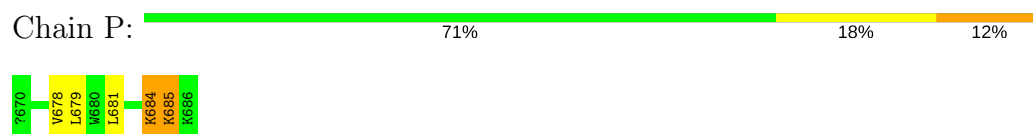
- Molecule 1: FAB LIGHT CHAIN



- Molecule 2: FAB HEAVY CHAIN



- Molecule 3: MODIFIED FRAGMENT OF HIV GLYCOPROTEIN (GP41)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.51Å 226.51Å 42.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.04 – 2.68 49.04 – 2.68	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.04-2.68) 100.0 (49.04-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.37 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.169 , 0.223 0.165 , 0.219	Depositor DCC
$R_{free}$ test set	929 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.3	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	0.96	EDS
Total number of atoms	3602	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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

Bond lengths and bond angles in the following residue types are not validated in this section: DIV, LYV, ACE, MK8

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	0.47	0/1687	0.63	1/2286 (0.0%)
2	H	0.50	0/1733	0.64	0/2366
3	P	1.41	3/124 (2.4%)	1.26	0/161
All	All	0.55	3/3544 (0.1%)	0.67	1/4813 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	685	LYS	C-N	8.40	1.53	1.34
3	P	684	LYS	C-N	6.18	1.48	1.34
3	P	679	LEU	C-N	5.79	1.47	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	184	ALA	N-CA-C	-6.03	94.71	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	1654	0	1599	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1690	0	1679	19	0
3	P	162	0	159	1	0
4	H	57	0	0	0	0
4	L	35	0	0	3	0
4	P	4	0	0	0	0
All	All	3602	0	3437	32	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 5.

All (32) 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:L:213:GLU:HA	1:L:214:CYS:HB3	1.60	0.83
1:L:123[B]:GLU:OE1	2:H:221:LYS:NZ	2.23	0.72
2:H:4:LEU:HD13	2:H:92:CYS:SG	2.41	0.60
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.84	0.60
2:H:66:ARG:NH1	2:H:86:ASP:OD2	2.32	0.60
2:H:128:SER:HA	2:H:133:THR:HG22	1.90	0.54
1:L:199:GLN:HG2	4:L:303:HOH:O	2.09	0.51
2:H:28:SER:HB3	2:H:32:TYR:HE2	1.76	0.51
2:H:200:THR:OG1	2:H:200:THR:O	2.27	0.50
1:L:79:GLU:HG3	1:L:80:PRO:HD2	1.93	0.50
1:L:214:CYS:HA	2:H:228:LYS:HB3	1.94	0.49
2:H:93:ALA:HB1	2:H:100(J):PHE:HB3	1.95	0.49
1:L:31:ASN:OD1	4:L:329:HOH:O	2.20	0.49
2:H:30:SER:HA	2:H:52(A):PRO:HB2	1.96	0.48
2:H:2:VAL:H	2:H:26:GLY:HA3	1.79	0.47
2:H:100(A):GLY:HA2	2:H:100(B):TRP:O	2.15	0.47
2:H:152:VAL:HG22	2:H:212:HIS:HB2	1.97	0.47
1:L:47:LEU:O	1:L:48:ILE:HD12	2.14	0.47
1:L:213:GLU:HA	1:L:214:CYS:CB	2.39	0.46
1:L:119:PRO:HG2	2:H:228:LYS:HE3	1.97	0.46
2:H:46:GLU:CG	2:H:62:ARG:HH21	2.30	0.44
1:L:131:SER:OG	1:L:180:THR:HG22	2.19	0.43
3:P:678:DIV:HB12	3:P:681:MK8:HB	2.01	0.43
2:H:198:LEU:HD12	2:H:198:LEU:HA	1.78	0.43
2:H:119:PRO:HB3	2:H:147:TYR:HB3	2.00	0.43
1:L:185:ASP:HA	1:L:188:LYS:HG3	2.01	0.43
2:H:27:GLY:HA2	2:H:100(C):LEU:HD11	2.01	0.42
1:L:72:THR:HG22	4:L:311:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:184:ALA:HA	1:L:187:GLU:H	1.84	0.42
2:H:17:SER:OG	2:H:82(A):ASN:HB3	2.20	0.42
1:L:12:SER:O	1:L:13:LEU:HD23	2.20	0.41
2:H:28:SER:HB2	2:H:100(C):LEU:HD23	2.03	0.41

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	L	214/215 (100%)	208 (97%)	4 (2%)	2 (1%)	20	43
2	H	226/228 (99%)	216 (96%)	7 (3%)	3 (1%)	14	32
3	P	12/17 (71%)	12 (100%)	0	0	100	100
All	All	452/460 (98%)	436 (96%)	11 (2%)	5 (1%)	17	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	40	PRO
2	H	99	GLY
2	H	100(C)	LEU
2	H	2	VAL
1	L	68	GLY

### 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	L	186/185 (100%)	172 (92%)	14 (8%)	16	34
2	H	187/187 (100%)	178 (95%)	9 (5%)	30	56
3	P	13/13 (100%)	11 (85%)	2 (15%)	3	7
All	All	386/385 (100%)	361 (94%)	25 (6%)	20	41

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	THR
1	L	14	SER
1	L	27(A)	SER
1	L	48	ILE
1	L	79	GLU
1	L	81	GLU
1	L	95	LEU
1	L	100	GLN
1	L	129	THR
1	L	142	ARG
1	L	147	GLN
1	L	161	GLU
1	L	165	GLU
1	L	185	ASP
2	H	54	LEU
2	H	82(A)	ASN
2	H	92	CYS
2	H	167	THR
2	H	168	SER
2	H	184	LEU
2	H	198	LEU
2	H	200	THR
2	H	221	LYS
3	P	684	LYS
3	P	685	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	DIV	P	678	3	3,6,7	0.79	0	3,8,10	1.85	1 (33%)
3	MK8	P	681	3	6,8,9	1.21	1 (16%)	4,10,12	0.30	0
3	LYV	P	683	3	20,20,21	2.11	2 (10%)	22,26,28	3.43	10 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DIV	P	678	3	-	0/3/6/9	0/0/0/0
3	MK8	P	681	3	-	0/6/8/11	0/0/0/0
3	LYV	P	683	3	-	0/21/23/25	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	681	MK8	CB-CA	-2.73	1.51	1.55
3	P	683	LYV	CE-ND	5.77	1.47	1.33
3	P	683	LYV	C2-N1	6.53	1.46	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	683	LYV	OZ1-C2-N1	-3.28	116.76	123.07
3	P	683	LYV	CG-ND-CE	-2.73	117.59	122.84
3	P	683	LYV	O7-CE-ND	-2.38	118.44	122.97
3	P	683	LYV	O-C-CA	-2.30	118.68	125.02
3	P	683	LYV	CZ-CE-ND	2.32	123.87	116.48
3	P	678	DIV	CG1-CB1-CA	2.38	121.01	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	683	LYV	C4-C2-N1	3.14	126.35	115.72
3	P	683	LYV	CZ-N1-C2	3.69	129.35	121.29
3	P	683	LYV	CB-CG-ND	3.96	124.12	111.82
3	P	683	LYV	CB-CA-C	5.18	120.19	111.65
3	P	683	LYV	O1-C5-C4	11.96	118.67	108.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	678	DIV	1	0
3	P	681	MK8	1	0

## 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	L	215/215 (100%)	-0.19	2 (0%) 84 85	31, 52, 90, 136	0
2	H	228/228 (100%)	-0.29	4 (1%) 69 69	26, 41, 79, 150	2 (0%)
3	P	13/17 (76%)	-0.12	0 100 100	35, 43, 80, 92	0
All	All	456/460 (99%)	-0.24	6 (1%) 77 77	26, 46, 88, 150	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	100(C)	LEU	4.9
2	H	100(A)	GLY	4.3
2	H	100(B)	TRP	3.7
1	L	213	GLU	2.8
1	L	214	CYS	2.7
2	H	100	TRP	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DIV	P	678	7/8	0.99	0.12	-	36,44,49,49	0
3	LYV	P	683	21/22	0.88	0.28	-	64,111,129,134	0
3	MK8	P	681	9/10	0.98	0.20	-	42,46,55,59	0

### 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.