



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:30 PM GMT

PDB ID : 5DFV  
Title : CRYSTAL STRUCTURE OF HUMAN CD81 LARGE EXTRACELLULAR  
LOOP IN COMPLEX WITH MURINE FAB FRAGMENT K04  
Authors : Harris, S.F.; Wong, A.; Kuglstatter, A.  
Deposited on : 2015-08-27  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

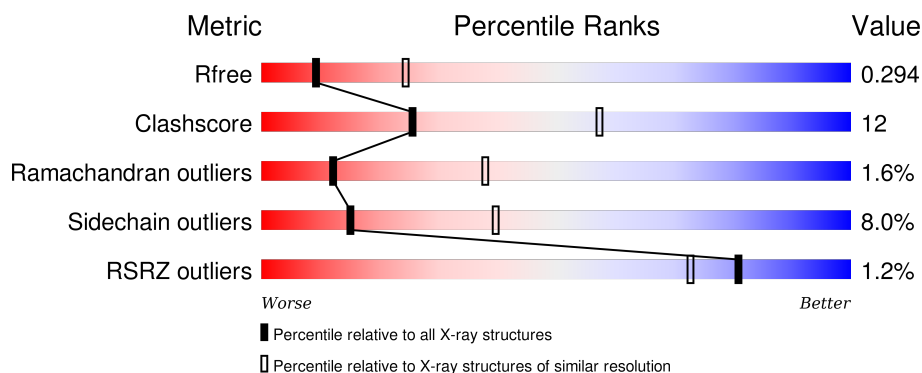
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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	99	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>28%</div> <div>5%</div> <div>11%</div> </div> </div>
1	B	99	<div> <div></div> <div> <div>62%</div> <div>20%</div> <div>5%</div> <div>13%</div> </div> </div>
2	C	222	<div> <div></div> <div> <div>73%</div> <div>21%</div> <div>.</div> <div>.</div> </div> </div>
2	E	222	<div> <div></div> <div> <div>73%</div> <div>19%</div> <div>.</div> <div>.</div> <div>.</div> </div> </div>
3	D	218	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	218	 A horizontal bar chart showing the quality of chain F. The bar is divided into two segments: a green segment representing 77% and a yellow segment representing 21%. A small orange segment is visible at the end of the bar, followed by a black dot.

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7930 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 CD81 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	88	Total	C	N	O	S	0	0	0
			683	425	116	138	4			
1	B	86	Total	C	N	O	S	1	0	0
			657	408	112	133	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	GLY	-	expression tag	UNP P60033
A	111	SER	-	expression tag	UNP P60033
A	202	HIS	LEU	conflict	UNP P60033
A	203	HIS	-	expression tag	UNP P60033
A	204	HIS	-	expression tag	UNP P60033
A	205	HIS	-	expression tag	UNP P60033
A	206	HIS	-	expression tag	UNP P60033
A	207	HIS	-	expression tag	UNP P60033
A	208	HIS	-	expression tag	UNP P60033
B	110	GLY	-	expression tag	UNP P60033
B	111	SER	-	expression tag	UNP P60033
B	202	HIS	LEU	conflict	UNP P60033
B	203	HIS	-	expression tag	UNP P60033
B	204	HIS	-	expression tag	UNP P60033
B	205	HIS	-	expression tag	UNP P60033
B	206	HIS	-	expression tag	UNP P60033
B	207	HIS	-	expression tag	UNP P60033
B	208	HIS	-	expression tag	UNP P60033

- Molecule 2 is a protein called FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	214	Total	C	N	O	S	0	0	0
			1599	1011	268	314	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	214	Total	C	N	O	S	0	0	0
			1599	1011	268	314	6			

- Molecule 3 is a protein called FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	217	Total	C	N	O	S	0	0	0
			1694	1061	284	343	6			
3	F	217	Total	C	N	O	S	0	0	0
			1694	1061	284	343	6			

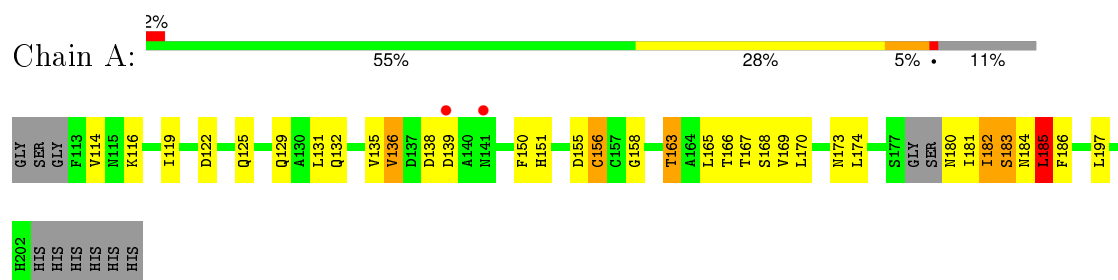
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	O	0	0
			1	1		
4	D	2	Total	O	0	0
			2	2		
4	E	1	Total	O	0	0
			1	1		

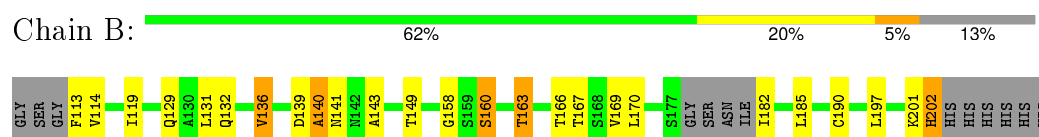
### 3 Residue-property plots [i](#)

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.

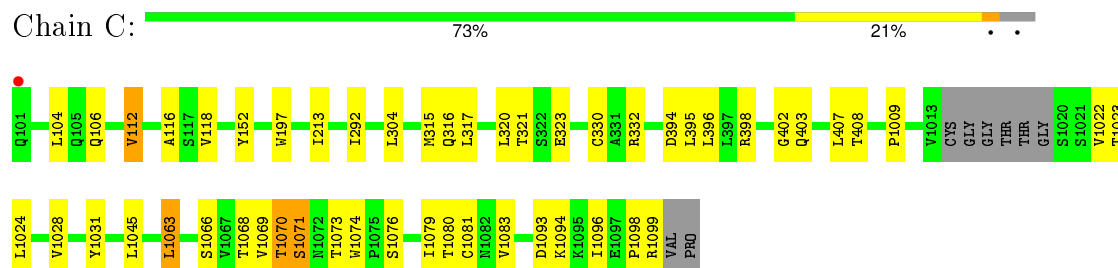
#### • Molecule 1: CD81 antigen



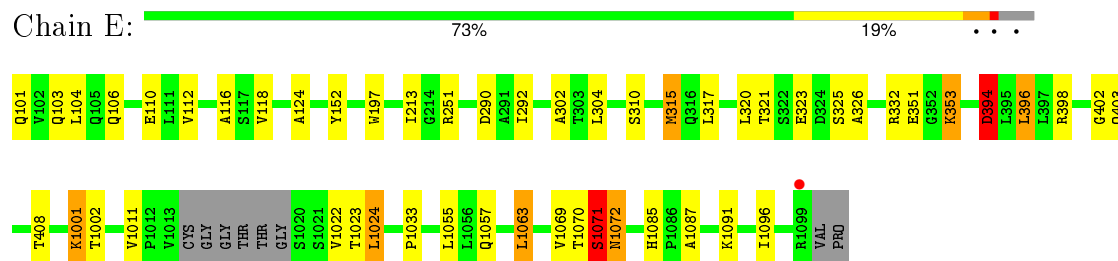
#### • Molecule 1: CD81 antigen



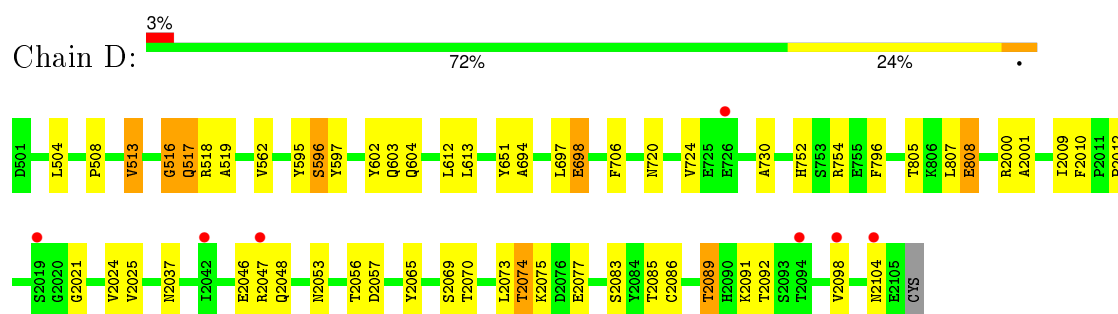
#### • Molecule 2: FAB HEAVY CHAIN



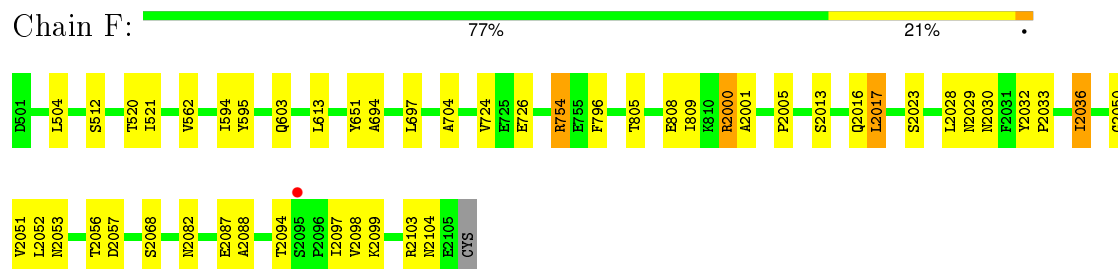
#### • Molecule 2: FAB HEAVY CHAIN



#### • Molecule 3: FAB LIGHT CHAIN



• Molecule 3: FAB LIGHT CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.63Å 94.48Å 94.11Å 90.00° 104.14° 90.00°	Depositor
Resolution (Å)	47.25 – 2.80 45.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.0 (47.25-2.80) 94.0 (45.66-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.239 , 0.291 0.244 , 0.294	Depositor DCC
$R_{free}$ test set	1583 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 29.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30669 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	7930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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	A	0.41	0/691	0.50	0/932
1	B	0.47	1/664 (0.2%)	0.49	1/895 (0.1%)
2	C	0.33	0/1636	0.53	0/2225
2	E	0.36	0/1636	0.57	0/2225
3	D	0.33	0/1736	0.54	0/2358
3	F	0.34	0/1736	0.51	0/2358
All	All	0.36	1/8099 (0.0%)	0.53	1/10993 (0.0%)

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
3	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	PHE	CA-CB	-6.99	1.38	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	PHE	CB-CA-C	-5.01	100.37	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	596	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	A	683	0	663	37	0
1	B	657	0	636	29	0
2	C	1599	0	1587	34	0
2	E	1599	0	1587	51	0
3	D	1694	0	1621	36	0
3	F	1694	0	1619	28	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
All	All	7930	0	7713	194	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 12.

The worst 5 of 194 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:E:118:VAL:HG23	2:E:320:LEU:HD11	1.28	1.15
1:B:167:THR:HG21	2:E:292:ILE:HD11	1.41	1.01
2:E:213:ILE:HD13	2:E:315:MET:HE3	1.44	0.98
2:E:213:ILE:HD13	2:E:315:MET:CE	1.99	0.92
2:C:118:VAL:HG23	2:C:320:LEU:HD11	1.51	0.92

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	A	84/99 (85%)	73 (87%)	6 (7%)	5 (6%)	2	5
1	B	82/99 (83%)	76 (93%)	5 (6%)	1 (1%)	16	47
2	C	210/222 (95%)	195 (93%)	13 (6%)	2 (1%)	19	52
2	E	210/222 (95%)	192 (91%)	16 (8%)	2 (1%)	19	52
3	D	215/218 (99%)	185 (86%)	26 (12%)	4 (2%)	10	32
3	F	215/218 (99%)	203 (94%)	10 (5%)	2 (1%)	21	55
All	All	1016/1078 (94%)	924 (91%)	76 (8%)	16 (2%)	12	38

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ILE
1	A	185	LEU
1	B	140	ALA
3	D	517	GLN
3	D	2001	ALA

### 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	79/87 (91%)	71 (90%)	8 (10%)	9	27
1	B	75/87 (86%)	71 (95%)	4 (5%)	28	61
2	C	180/186 (97%)	169 (94%)	11 (6%)	23	55
2	E	180/186 (97%)	161 (89%)	19 (11%)	8	24
3	D	193/194 (100%)	176 (91%)	17 (9%)	12	35
3	F	193/194 (100%)	180 (93%)	13 (7%)	20	50
All	All	900/934 (96%)	828 (92%)	72 (8%)	15	40

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	2048	GLN

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Mol	Chain	Res	Type
2	E	101	GLN
3	F	2017	LEU
3	D	2053	ASN
3	D	2075	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1077	GLN
3	D	517	GLN
2	E	1085	HIS
2	C	316	GLN
2	E	106	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 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	88/99 (88%)	0.10	2 (2%) 64 52	27, 35, 44, 50	0
1	B	86/99 (86%)	-0.23	0 100 100	22, 32, 41, 42	1 (1%)
2	C	214/222 (96%)	-0.16	1 (0%) 91 88	23, 30, 49, 56	0
2	E	214/222 (96%)	-0.27	1 (0%) 91 88	18, 25, 46, 51	0
3	D	217/218 (99%)	0.08	7 (3%) 51 39	24, 42, 68, 70	0
3	F	217/218 (99%)	-0.24	1 (0%) 91 88	17, 25, 47, 53	0
All	All	1036/1078 (96%)	-0.13	12 (1%) 81 73	17, 32, 58, 70	1 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	2047	ARG	2.9
3	D	2094	THR	2.8
1	A	139	ASP	2.8
1	A	141	ASN	2.8
3	D	2019	SER	2.6

### 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.