Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:20 pm BST

PDB ID	:	6FY3
Title	:	Crystal structure of a V2-directed, RV144 vaccine-like antibody from HIV-1 infection, CAP228-3D, bound to a heterologous V2 peptide
Authors	:	Wibmer, C.K.; Moore, P.L.; Morris, L.
Deposited on	:	2018-03-10
Resolution	:	2.60 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

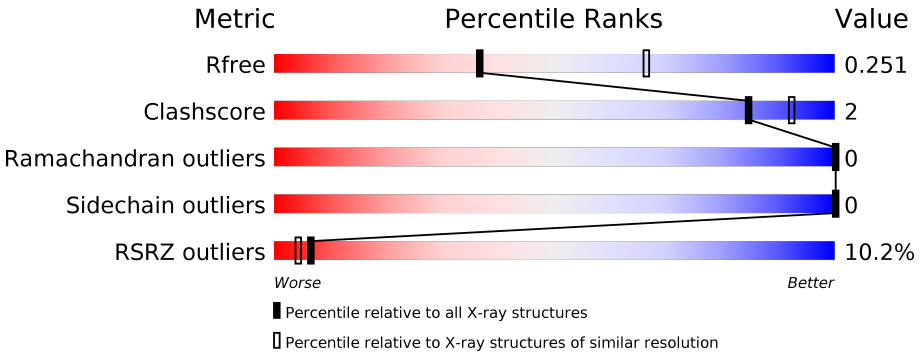
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 >=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 <=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	H	238	8% 88% 7% 5%
1	X	238	12% 69% 5% 25%
2	L	218	% 95%
2	Y	218	17% 89% 7%
3	P	19	68% 11% 21%
3	Z	19	74% 11% 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13013 atoms, of which 6319 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 CAP228-3D Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	X	178	Total	C	H	N	O	S	0	0	0
			2730	887	1349	221	265	8			
1	H	226	Total	C	H	N	O	S	0	0	0
			3394	1096	1681	275	334	8			

- Molecule 2 is a protein called CAP228-3D Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	Y	202	Total	C	H	N	O	S	0	0	0
			2996	955	1462	256	317	6			
2	L	214	Total	C	H	N	O	S	0	0	0
			3168	1008	1546	271	337	6			

- Molecule 3 is a protein called CAP45 V2 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	16	Total	C	H	N	O	0	0	0
			288	93	146	26	23			
3	P	15	Total	C	H	N	O	0	0	0
			269	87	135	25	22			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	14	Total	O	0	0
			14	14		
4	Y	32	Total	O	0	0
			32	32		
4	Z	6	Total	O	0	0
			6	6		
4	H	77	Total	O	0	0
			77	77		

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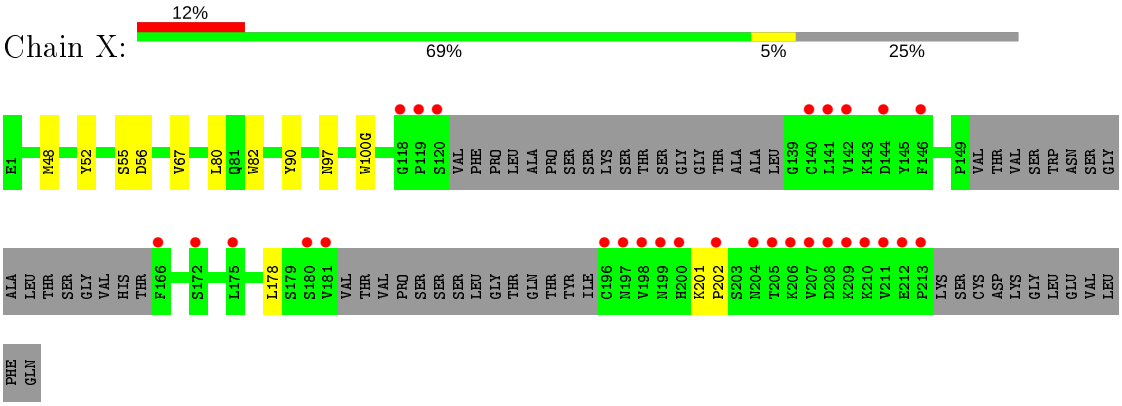
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	35	Total O 35 35	0	0
4	P	4	Total O 4 4	0	0

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.

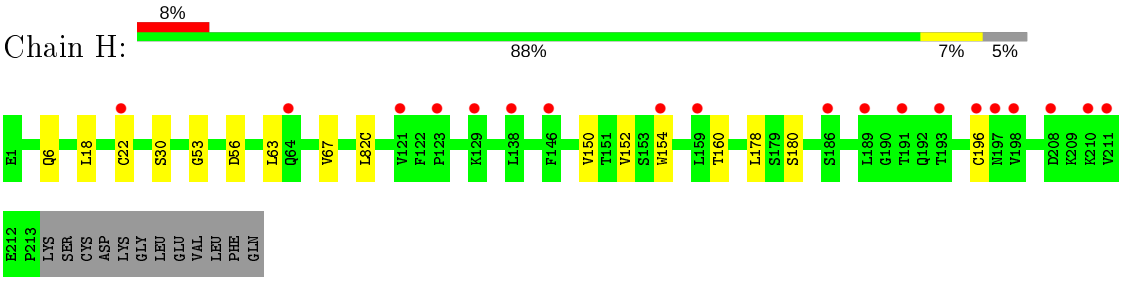
• Molecule 1: CAP228-3D Heavy Chain

Chain X:



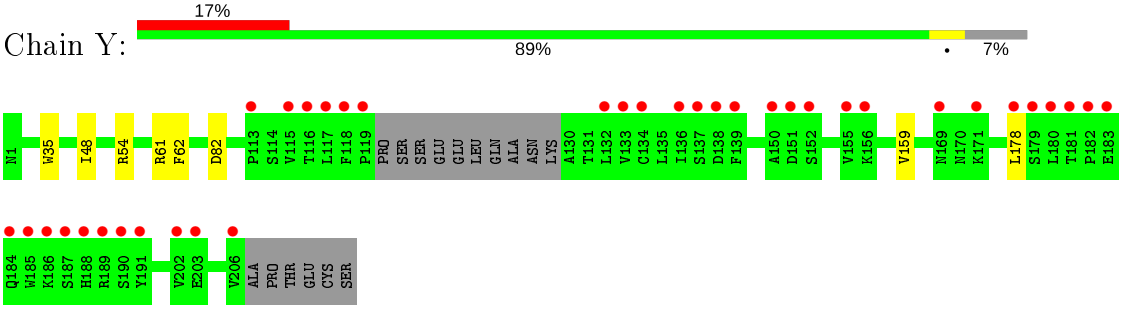
• Molecule 1: CAP228-3D Heavy Chain

Chain H:



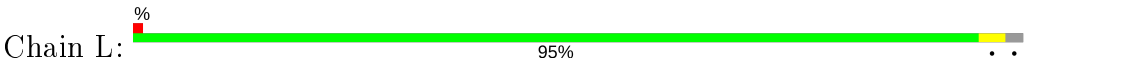
• Molecule 2: CAP228-3D Light Chain

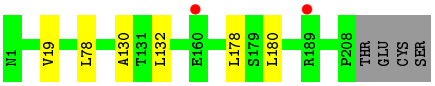
Chain Y:



• Molecule 2: CAP228-3D Light Chain

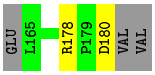
Chain L:





- Molecule 3: CAP45 V2 peptide

Chain Z:



- Molecule 3: CAP45 V2 peptide

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	208.36Å 43.81Å 119.91Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	42.87 – 2.60 42.87 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.87-2.60) 99.4 (42.87-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.21 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.13.2998	Depositor
R, R_{free}	0.220 , 0.250 0.220 , 0.251	Depositor DCC
R_{free} test set	1697 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13013	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	H	0.28	0/1760	0.47	0/2398
1	X	0.26	0/1417	0.45	0/1919
2	L	0.26	0/1663	0.45	0/2271
2	Y	0.26	0/1572	0.47	0/2145
3	P	0.25	0/137	0.44	0/181
3	Z	0.25	0/145	0.36	0/192
All	All	0.27	0/6694	0.46	0/9106

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

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	H	1713	1681	1681	11	0
1	X	1381	1349	1345	8	0
2	L	1622	1546	1546	4	0
2	Y	1534	1462	1461	4	0
3	P	134	135	135	2	0
3	Z	142	146	146	2	0
4	H	77	0	0	0	0
4	L	35	0	0	0	0
4	P	4	0	0	0	0
4	X	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Y	32	0	0	0	0
4	Z	6	0	0	0	0
All	All	6694	6319	6314	29	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 2.

All (29) 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:Y:61:ARG:NH1	2:Y:82:ASP:OD2	2.23	0.71
1:X:56:ASP:OD2	3:Z:178:ARG:NH1	2.37	0.57
1:H:63:LEU:HD13	1:H:67:VAL:HG22	1.88	0.54
1:H:160:THR:O	1:H:160:THR:HG22	2.09	0.52
1:H:18:LEU:HB2	1:H:82(C):LEU:HD11	1.92	0.50
2:Y:54:ARG:NE	2:Y:62:PHE:O	2.34	0.49
1:X:67:VAL:HG12	1:X:82:TRP:CD1	2.47	0.49
2:L:132:LEU:HD12	2:L:178:LEU:HD23	1.94	0.49
3:P:180:ASP:OD1	3:P:180:ASP:N	2.46	0.48
1:X:48:MET:HE1	1:X:80:LEU:HD21	1.96	0.48
1:H:6:GLN:HG2	1:H:22:CYS:SG	2.54	0.47
1:H:152:VAL:HG11	1:H:180:SER:CB	2.45	0.46
1:H:178:LEU:HD12	1:H:178:LEU:C	2.35	0.46
3:Z:180:ASP:OD1	3:Z:180:ASP:N	2.48	0.46
1:H:154:TRP:CZ3	1:H:196:CYS:HB3	2.51	0.46
2:L:130:ALA:HB3	2:L:180:LEU:O	2.17	0.45
2:L:19:VAL:HG13	2:L:78:LEU:HD11	1.99	0.45
1:H:30:SER:HB2	1:H:53:GLY:HA2	2.00	0.44
1:H:63:LEU:HD13	1:H:67:VAL:CG2	2.47	0.44
1:H:150:VAL:CG2	1:H:178:LEU:HD21	2.49	0.43
1:H:56:ASP:OD2	3:P:178:ARG:NH2	2.51	0.43
1:X:178:LEU:HD12	1:X:178:LEU:C	2.38	0.43
1:X:97:ASN:HB3	1:X:100(G):TRP:CD1	2.54	0.42
2:Y:35:TRP:HB2	2:Y:48:ILE:HB	2.02	0.42
1:X:52:TYR:O	1:X:55:SER:N	2.53	0.41
2:Y:159:VAL:HG22	2:Y:178:LEU:HD13	2.02	0.41
1:X:48:MET:HE1	1:X:90:TYR:CD1	2.54	0.41
1:X:201:LYS:N	1:X:202:PRO:CD	2.83	0.41
2:L:19:VAL:CG1	2:L:78:LEU:HD11	2.52	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	H	224/238 (94%)	220 (98%)	4 (2%)	0	100	100
1	X	170/238 (71%)	167 (98%)	3 (2%)	0	100	100
2	L	212/218 (97%)	206 (97%)	6 (3%)	0	100	100
2	Y	198/218 (91%)	193 (98%)	5 (2%)	0	100	100
3	P	13/19 (68%)	13 (100%)	0	0	100	100
3	Z	14/19 (74%)	14 (100%)	0	0	100	100
All	All	831/950 (88%)	813 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	H	193/204 (95%)	193 (100%)	0	100	100
1	X	154/204 (76%)	154 (100%)	0	100	100
2	L	187/191 (98%)	187 (100%)	0	100	100
2	Y	177/191 (93%)	177 (100%)	0	100	100
3	P	13/17 (76%)	13 (100%)	0	100	100
3	Z	14/17 (82%)	14 (100%)	0	100	100
All	All	738/824 (90%)	738 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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^2)	Q<0.9
1	H	226/238 (94%)	0.49	19 (8%) 11 7	12, 45, 125, 163	0
1	X	178/238 (74%)	0.83	29 (16%) 1 1	26, 56, 167, 217	0
2	L	214/218 (98%)	0.18	2 (0%) 84 82	21, 56, 108, 151	0
2	Y	202/218 (92%)	0.97	37 (18%) 1 0	13, 68, 163, 198	0
3	P	15/19 (78%)	0.23	0 100 100	17, 28, 73, 87	0
3	Z	16/19 (84%)	0.12	0 100 100	30, 50, 111, 142	0
All	All	851/950 (89%)	0.59	87 (10%) 6 4	12, 55, 142, 217	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	211	VAL	10.7
1	X	210	LYS	9.5
2	Y	191	TYR	9.3
2	Y	119	PRO	8.7
2	Y	185	TRP	8.4
2	Y	118	PHE	7.0
2	Y	180	LEU	7.0
1	X	196	CYS	6.6
1	X	212	GLU	6.1
1	X	198	VAL	6.0
2	Y	117	LEU	6.0
2	Y	189	ARG	6.0
1	X	208	ASP	5.7
1	X	199	ASN	5.6
1	X	142	VAL	5.5
1	X	213	PRO	5.1
1	X	119	PRO	5.1
1	X	181	VAL	4.9
2	Y	133	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
2	Y	184	GLN	4.8
2	Y	188	HIS	4.6
2	Y	169	ASN	4.6
1	H	22	CYS	4.6
2	Y	186	LYS	4.5
2	Y	181	THR	4.5
2	L	189	ARG	4.4
2	Y	113	PRO	4.4
1	X	205	THR	4.3
2	Y	206	VAL	4.2
1	X	206	LYS	4.2
2	Y	183	GLU	4.1
2	Y	190	SER	4.0
1	X	141	LEU	3.8
1	X	197	ASN	3.7
2	Y	182	PRO	3.6
2	Y	171	LYS	3.6
1	X	209	LYS	3.4
2	Y	150	ALA	3.4
2	Y	151	ASP	3.4
2	Y	152	SER	3.4
1	H	210	LYS	3.4
1	X	180	SER	3.3
1	H	197	ASN	3.3
1	X	118	GLY	3.2
1	X	207	VAL	3.2
1	X	140	CYS	3.1
1	X	175	LEU	3.1
1	H	191	THR	3.1
1	H	121	VAL	3.0
1	X	204	ASN	3.0
1	H	123	PRO	2.9
1	H	159	LEU	2.9
2	Y	116	THR	2.8
2	Y	136	ILE	2.8
1	X	144	ASP	2.8
1	X	202	PRO	2.8
2	Y	156	LYS	2.8
2	Y	179	SER	2.8
1	H	138	LEU	2.8
1	X	200	HIS	2.8
1	H	196	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	Y	134	CYS	2.8
1	X	166	PHE	2.7
1	H	189	LEU	2.7
2	Y	187	SER	2.6
2	Y	178	LEU	2.6
2	Y	203	GLU	2.6
2	L	160	GLU	2.6
1	H	193	THR	2.5
2	Y	115	VAL	2.5
1	X	146	PHE	2.5
1	H	154	TRP	2.5
1	X	172	SER	2.5
1	H	208	ASP	2.4
1	H	129	LYS	2.4
2	Y	137	SER	2.4
1	X	120	SER	2.4
2	Y	138	ASP	2.4
1	H	211	VAL	2.4
2	Y	155	VAL	2.3
2	Y	139	PHE	2.3
1	H	146	PHE	2.2
1	H	198	VAL	2.2
2	Y	132	LEU	2.1
1	H	64	GLN	2.1
1	H	186	SER	2.1
2	Y	202	VAL	2.1

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.