Full wwPDB X-ray Structure Validation Report (i)

Apr 30, 2024 – 08:21 pm BST

PDB ID	:	5AMR
Title	:	Structure of the La Crosse Bunyavirus polymerase in complex with the 3' viral RNA
Authors	:	Reguera, J.; Gerlach, P.; Cusack, S.
Deposited on	:	2015-03-12
Resolution	:	2.57 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

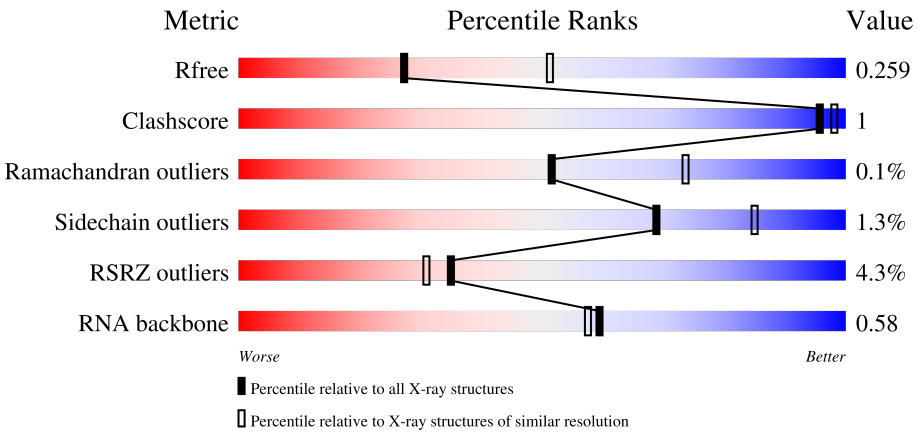
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)
RNA backbone	3102	1075 (2.90-2.26)

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 >=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	A	2264	3% 70% • 27%
2	B	16	75% 25%
3	C	8	75% 12% 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14163 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 RNA POLYMERASE L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1657	13571	8701	2256	2525	89	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A5HC98

- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	16	334	151	56	112	15	0	0	0

- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	8	166	76	31	52	7	0	0	0

- Molecule 4 is water.

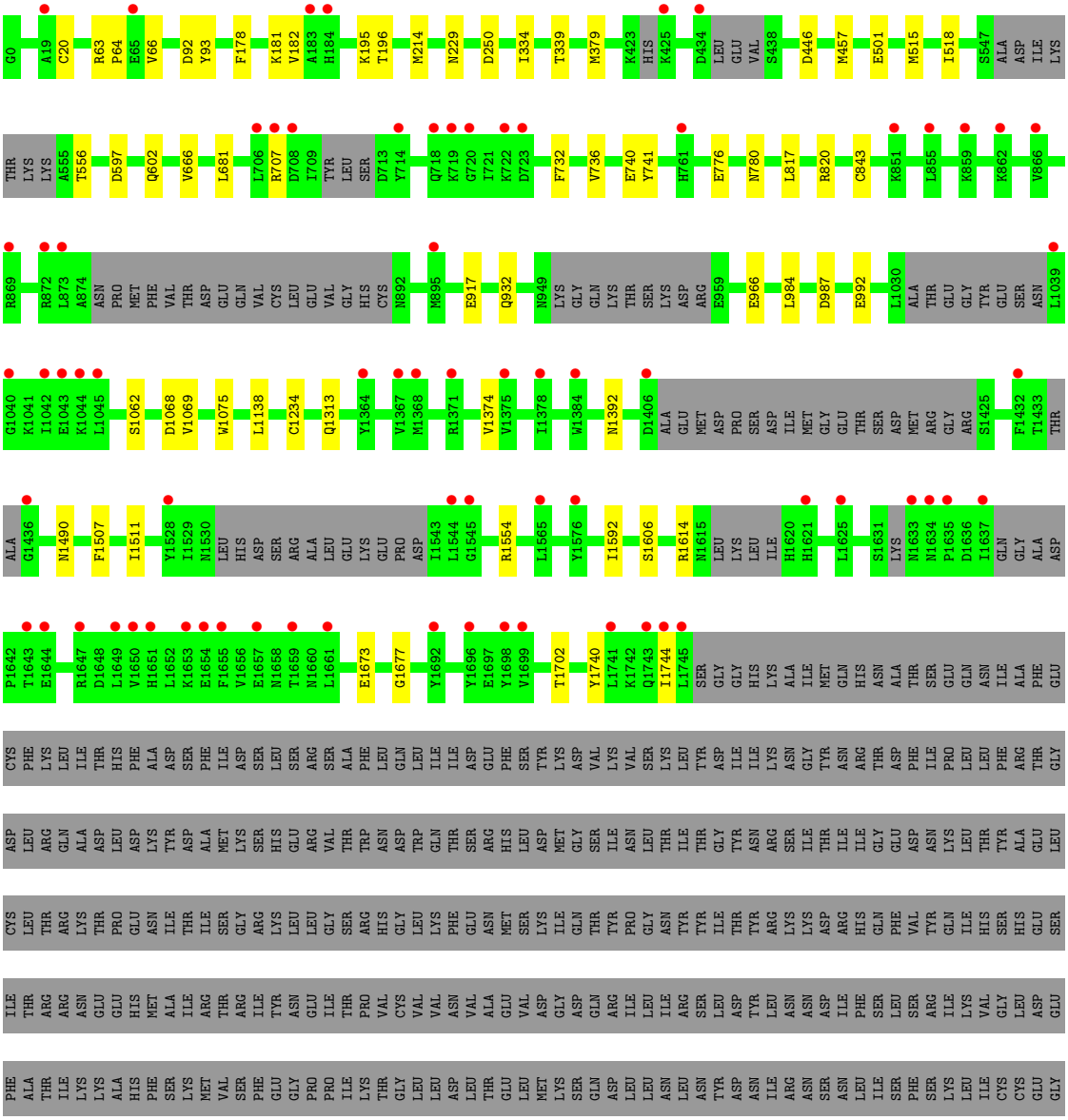
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	87	87	87	0	0
4	B	1	1	1	0	0
4	C	4	4	4	0	0

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: RNA POLYMERASE L

Chain A:



SER ASP ASN ILE ASN ASP GLY LEU GLU PHE LEU SER ASP ASP PRO MET ASN PHE THR GLU GLY GLU ALA ILE HIS SER THR PRO ILE PHE ASN ILE TYR TYR SER LYS ARG GLY GLU ARG HIS MET THR TYR ARG ASN ALA ILE LYS LEU LEU ILE GLU ARG GLU THR LYS ILE PHE GLU

GLU ALA PHE THR PHE SER GLU ASN GLY PHE ILE SER PRO GLU ASN LEU GLY CYS LEU GLU ALA VAL VAL SER LEU ILE LYS LEU LEU LYS THR ASN GLU TRP SER THR VAL ILE ASP LYS CYS ILE HIS ILE CYS LEU ILE LYS ASN GLY MET ASP HIS MET TYR HIS SER PHE ASP VAL

PRO LYS CYS PHE MET GLY ASN PRO ILE THR ARG ASP ILE ASN TRP VAL MET PHE ARG GLU PHE ILE ASN SER LEU PRO GLY THR ASP ILE PRO PRO TRP ASN VAL MET THR GLU ASN PHE LYS LYS LYS CYS ILE ALA LEU ILE ASN SER LYS PHE GLU THR GLN ARG ASP PHE SER GLU

PHE THR LYS LEU MET LYS LYS GLU GLY GLY ARG SER ASN ILE GLU PHE ASP

- Molecule 2: RNA

Chain B: 75% 25%

U1 A9 C10 A11 C12 U13 A14 C15 U16

- Molecule 3: RNA

Chain C: 75% 12% 12%

G9 C10 U11 A16

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.00Å 140.70Å 162.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.66 – 2.57 48.66 – 2.57	Depositor EDS
% Data completeness (in resolution range)	95.3 (48.66-2.57) 94.7 (48.66-2.57)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.204 , 0.252 0.212 , 0.259	Depositor DCC
R_{free} test set	3533 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14163	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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 (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	0.23	0/13841	0.36	0/18649
2	B	0.19	0/372	0.71	0/577
3	C	0.18	0/185	0.69	0/286
All	All	0.23	0/14398	0.38	0/19512

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 (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	13571	0	13652	27	0
2	B	334	0	172	1	0
3	C	166	0	89	2	0
4	A	87	0	0	10	0
4	B	1	0	0	0	0
4	C	4	0	0	2	0
All	All	14163	0	13913	30	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 1.

All (30) 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:A:334:ILE:O	4:A:3025:HOH:O	1.81	0.96
1:A:501:GLU:OE1	4:A:3037:HOH:O	1.82	0.95
1:A:741:TYR:OH	4:A:3046:HOH:O	2.05	0.73
4:A:3080:HOH:O	2:B:12:C:OP1	2.07	0.73
1:A:917:GLU:OE2	4:A:3054:HOH:O	2.10	0.68
3:C:16:A:O3'	4:C:3004:HOH:O	2.11	0.68
3:C:11:U:OP1	4:C:3001:HOH:O	2.13	0.67
1:A:992:GLU:OE1	4:A:3066:HOH:O	2.13	0.65
1:A:1614:ARG:NH1	1:A:1702:THR:OG1	2.36	0.59
1:A:932:GLN:OE1	4:A:3057:HOH:O	2.18	0.54
1:A:20:CYS:SG	1:A:181:LYS:NZ	2.80	0.54
1:A:214:MET:HE3	1:A:1075:TRP:HE1	1.70	0.54
1:A:457:MET:HE3	1:A:681:LEU:HD12	1.90	0.53
1:A:776:GLU:OE2	1:A:780:ASN:ND2	2.43	0.52
1:A:736:VAL:HG22	1:A:740:GLU:HB2	1.93	0.50
1:A:1490:ASN:OD1	4:A:3082:HOH:O	2.20	0.47
1:A:917:GLU:OE1	4:A:3053:HOH:O	2.21	0.46
1:A:1374:VAL:HG22	1:A:1592:ILE:HD12	1.97	0.46
1:A:1068:ASP:OD1	1:A:1069:VAL:N	2.48	0.45
1:A:64:PRO:O	4:A:3004:HOH:O	2.21	0.45
1:A:195:LYS:HG3	1:A:196:THR:HG23	1.99	0.44
1:A:515:MET:HE3	1:A:518:ILE:HB	1.99	0.44
1:A:178:PHE:CZ	1:A:182:VAL:HG21	2.54	0.43
1:A:817:LEU:HD13	1:A:984:LEU:HD11	2.02	0.42
1:A:1507:PHE:CZ	1:A:1511:ILE:HD11	2.55	0.42
1:A:229:ASN:O	1:A:229:ASN:OD1	2.39	0.41
1:A:63:ARG:HB3	1:A:66:VAL:HG23	2.03	0.40
1:A:1740:TYR:CD2	1:A:1744:ILE:HD11	2.56	0.40
1:A:966:GLU:OE1	1:A:966:GLU:N	2.45	0.40
1:A:1673:GLU:O	1:A:1677:GLY:N	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	A	1629/2264 (72%)	1567 (96%)	60 (4%)	2 (0%)	51 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	707	ARG
1	A	1234	CYS

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	A	1535/2087 (74%)	1515 (99%)	20 (1%)	69 85

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ASP
1	A	93	TYR
1	A	250	ASP
1	A	339	THR
1	A	379	MET
1	A	446	ASP
1	A	556	THR
1	A	597	ASP
1	A	602	GLN
1	A	666	VAL
1	A	732	PHE
1	A	820	ARG
1	A	843	CYS
1	A	987	ASP
1	A	1062	SER
1	A	1138	LEU
1	A	1313	GLN
1	A	1392	ASN
1	A	1554	ARG

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Mol	Chain	Res	Type
1	A	1606	SER

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	15/16 (93%)	3 (20%)	0
3	C	7/8 (87%)	1 (14%)	0
All	All	22/24 (91%)	4 (18%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	A
2	B	10	C
2	B	14	A
3	C	16	A

There are no RNA pucker outliers to report.

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 monosaccharides 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, 95th 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	A	1657/2264 (73%)	0.31	72 (4%) 35 31	36, 62, 111, 145	0
2	B	16/16 (100%)	-0.62	0 100 100	49, 57, 62, 66	0
3	C	8/8 (100%)	-0.95	0 100 100	55, 62, 72, 73	0
All	All	1681/2288 (73%)	0.29	72 (4%) 35 31	36, 62, 111, 145	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1039	LEU	6.6
1	A	1745	LEU	6.4
1	A	1436	GLY	6.0
1	A	1042	ILE	5.6
1	A	1544	LEU	5.5
1	A	714	TYR	5.3
1	A	1743	GLN	4.7
1	A	1432	PHE	4.5
1	A	1643	THR	4.4
1	A	1655	PHE	4.3
1	A	872	ARG	4.3
1	A	708	ASP	4.0
1	A	184	HIS	4.0
1	A	1654	GLU	3.9
1	A	1545	GLY	3.8
1	A	1625	LEU	3.8
1	A	1650	VAL	3.7
1	A	719	LYS	3.7
1	A	183	ALA	3.6
1	A	1367	VAL	3.5
1	A	1635	PRO	3.4
1	A	1651	HIS	3.3
1	A	1699	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	866	VAL	3.3
1	A	707	ARG	3.3
1	A	1371	ARG	3.2
1	A	1040	GLY	3.1
1	A	1384	TRP	3.1
1	A	1649	LEU	3.0
1	A	1368	MET	3.0
1	A	1661	LEU	3.0
1	A	1364	TYR	2.9
1	A	1653	LYS	2.9
1	A	722	LYS	2.9
1	A	895	MET	2.8
1	A	851	LYS	2.8
1	A	1634	ASN	2.8
1	A	1698	TYR	2.7
1	A	1657	GLU	2.7
1	A	862	LYS	2.6
1	A	1043	GLU	2.6
1	A	1621	HIS	2.6
1	A	1045	LEU	2.6
1	A	1741	LEU	2.6
1	A	1044	LYS	2.6
1	A	1576	TYR	2.5
1	A	859	LYS	2.5
1	A	720	GLY	2.5
1	A	1375	VAL	2.5
1	A	1644	GLU	2.4
1	A	1378	ILE	2.4
1	A	1406	ASP	2.4
1	A	425	LYS	2.4
1	A	1637	ILE	2.4
1	A	723	ASP	2.4
1	A	761	HIS	2.3
1	A	1633	ASN	2.3
1	A	65	GLU	2.3
1	A	1659	THR	2.3
1	A	855	LEU	2.2
1	A	1565	LEU	2.2
1	A	1744	ILE	2.2
1	A	1696	TYR	2.2
1	A	434	ASP	2.2
1	A	873	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	19	ALA	2.1
1	A	869	ARG	2.1
1	A	1528	TYR	2.1
1	A	1647	ARG	2.1
1	A	706	LEU	2.0
1	A	1692	TYR	2.0
1	A	718	GLN	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 monosaccharides 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.