



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 04:46 am GMT

PDB ID : 1N4L
Title : A DNA analogue of the polypurine tract of HIV-1
Authors : Cote, M.L.; Pflomm, M.; Georgiadis, M.M.
Deposited on : 2002-10-31
Resolution : 2.00 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 : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

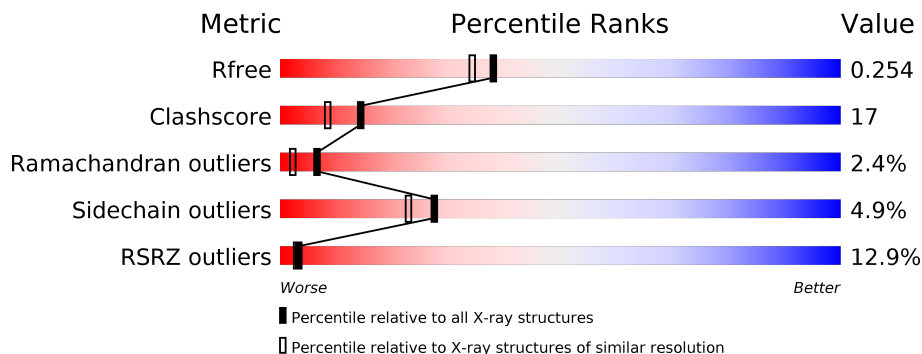
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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. 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	B	16	
2	D	16	
3	A	255	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2834 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 DNA chain called 5'-D(*CP*TP*TP*TP*TP*TP*AP*AP*AP*AP*GP*AP*AP*AP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	16	Total	C	N	O	P	0	16	0
			328	159	63	91	15			

- Molecule 2 is a DNA chain called 5'-D(*CP*TP*TP*TP*TP*TP*CP*TP*TP*TP*TP*AP*AP*AP*AP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	16	Total	C	N	O	P	0	16	0
			322	158	52	97	15			

- Molecule 3 is a protein called Reverse Transcriptase.

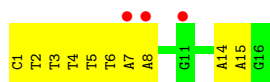
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	255	Total	C	N	O	S	0	0	0
			2039	1311	356	365	7			

- Molecule 4 is water.

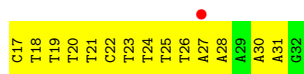
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	O	0	0
			2	2		
4	A	143	Total	O	0	0
			143	143		

i

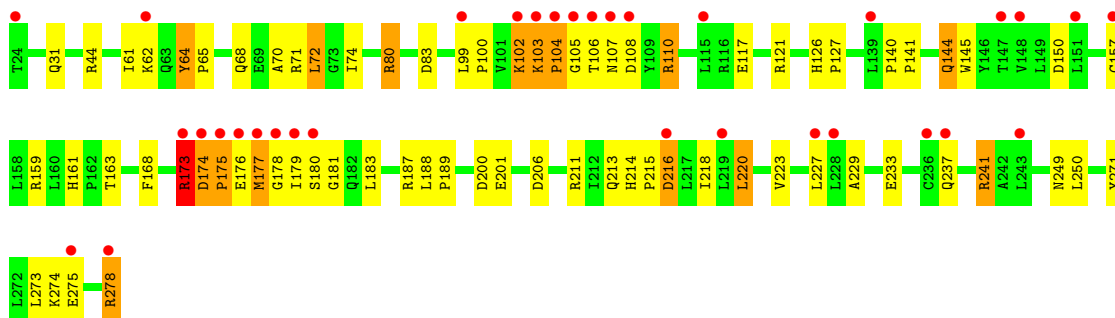
● Molecule 1: 5'-D(*CP*TP*TP*TP*TP*TP*AP*AP*AP*AP*GP*AP*AP*AP*AP*G)-3'



Chain D:  6% 13% 88%



Chain A:  13% 71% 22% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	54.41Å 146.22Å 46.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 19.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (50.00-2.00) 93.8 (19.92-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.91 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.240 , 0.269 0.226 , 0.254	Depositor DCC
R_{free} test set	1249 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2834	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [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	$\# Z > 5$
3	A	0.69	0/2095	1.29	23/2857 (0.8%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	187	ARG	NE-CZ-NH1	9.95	125.28	120.30
3	A	278	ARG	NE-CZ-NH1	9.35	124.97	120.30
3	A	44	ARG	NE-CZ-NH2	8.48	124.54	120.30
3	A	211	ARG	NE-CZ-NH2	-8.30	116.15	120.30
3	A	187	ARG	NE-CZ-NH2	-8.00	116.30	120.30
3	A	278	ARG	CD-NE-CZ	7.85	134.59	123.60
3	A	241	ARG	NE-CZ-NH1	7.57	124.08	120.30
3	A	150	ASP	CB-CG-OD1	7.29	124.86	118.30
3	A	80	ARG	NE-CZ-NH2	7.21	123.91	120.30
3	A	159	ARG	NE-CZ-NH2	-6.59	117.01	120.30
3	A	44	ARG	NE-CZ-NH1	-6.16	117.22	120.30
3	A	83	ASP	CB-CG-OD1	6.09	123.78	118.30
3	A	174	ASP	N-CA-C	-6.04	94.69	111.00
3	A	201	GLU	OE1-CD-OE2	-5.71	116.44	123.30
3	A	216	ASP	CB-CG-OD2	5.69	123.42	118.30
3	A	241	ARG	NH1-CZ-NH2	-5.62	113.22	119.40
3	A	110	ARG	NE-CZ-NH1	5.62	123.11	120.30
3	A	168	PHE	CB-CG-CD1	5.25	124.48	120.80
3	A	173	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	A	200	ASP	CB-CG-OD1	5.18	122.96	118.30
3	A	157	CYS	CA-CB-SG	-5.12	104.79	114.00
3	A	121	ARG	NE-CZ-NH2	-5.11	117.74	120.30
3	A	211	ARG	NE-CZ-NH1	5.07	122.83	120.30

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	B	328	0	183	9	0
2	D	322	0	186	16	0
3	A	2039	0	2056	61	1
4	A	143	0	0	12	0
4	D	2	0	0	0	0
All	All	2834	0	2425	85	1

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 17.

All (85) 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:B:5[B]:DT:H4'	1:B:6[B]:DT:OP1	1.38	1.07
3:A:177:MET:HE1	3:A:178:GLY:HA2	1.14	1.06
1:B:14[B]:DA:H2''	1:B:15[B]:DA:H5'	1.41	1.03
2:D:24[D]:DT:H4'	2:D:25[D]:DT:OP1	1.58	1.02
3:A:278:ARG:HD2	4:A:377:HOH:O	1.58	1.01
2:D:30[D]:DA:H2''	2:D:31[D]:DA:H5'	1.41	0.99
3:A:177:MET:HE1	3:A:178:GLY:CA	1.95	0.96
3:A:177:MET:CE	3:A:178:GLY:HA2	1.93	0.96
3:A:100:PRO:HG2	4:A:366:HOH:O	1.71	0.91
3:A:103:LYS:HB3	3:A:104:PRO:HD3	1.53	0.90
2:D:23[D]:DT:H1'	2:D:24[D]:DT:O5'	1.70	0.90
3:A:161:HIS:HD2	3:A:163:THR:H	1.20	0.89
3:A:278:ARG:CD	4:A:377:HOH:O	2.18	0.86
3:A:177:MET:CE	3:A:178:GLY:CA	2.56	0.79
3:A:103:LYS:CB	3:A:104:PRO:HD3	2.12	0.79
2:D:23[D]:DT:C1'	2:D:24[D]:DT:O5'	2.31	0.79
3:A:177:MET:CE	3:A:178:GLY:N	2.46	0.77
3:A:80:ARG:NH1	4:A:330:HOH:O	2.19	0.76
3:A:174:ASP:HB3	3:A:177:MET:O	1.89	0.72
3:A:177:MET:HE2	3:A:178:GLY:H	1.53	0.72
3:A:161:HIS:CD2	3:A:163:THR:H	2.08	0.70
3:A:177:MET:HE2	3:A:178:GLY:N	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14[B]:DA:C2'	1:B:15[B]:DA:H5'	2.21	0.69
2:D:30[D]:DA:C2'	2:D:31[D]:DA:H5'	2.21	0.68
3:A:61:ILE:HD11	3:A:117:GLU:HG3	1.77	0.67
1:B:5[B]:DT:C4'	1:B:6[B]:DT:OP1	2.28	0.65
3:A:71:ARG:HD2	3:A:175:PRO:HD3	1.81	0.63
3:A:103:LYS:CB	3:A:104:PRO:CD	2.77	0.63
3:A:100:PRO:HD2	4:A:366:HOH:O	1.99	0.62
3:A:103:LYS:HE3	3:A:110:ARG:NH1	2.14	0.62
3:A:220:LEU:HD22	3:A:227:LEU:HD23	1.81	0.62
3:A:179:ILE:HD13	3:A:183:LEU:HD21	1.84	0.60
3:A:103:LYS:HB3	3:A:104:PRO:CD	2.29	0.60
2:D:24[D]:DT:C4'	2:D:25[D]:DT:OP1	2.25	0.60
3:A:206:ASP:HB3	3:A:250:LEU:HD13	1.83	0.60
2:D:25[D]:DT:H1'	2:D:26[D]:DT:H5''	1.83	0.59
3:A:99:LEU:HD12	3:A:99:LEU:N	2.18	0.58
3:A:233:GLU:O	3:A:237:GLN:HG3	2.04	0.57
2:D:27[D]:DA:H2''	2:D:28[D]:DA:C8	2.41	0.56
3:A:100:PRO:CG	4:A:366:HOH:O	2.42	0.56
3:A:100:PRO:CD	4:A:366:HOH:O	2.53	0.56
2:D:23[D]:DT:C2'	2:D:24[D]:DT:O5'	2.55	0.55
2:D:17[D]:DC:H2'	2:D:18[D]:DT:H72	1.90	0.54
2:D:25[D]:DT:H1'	2:D:26[D]:DT:C5'	2.38	0.54
2:D:21[D]:DT:H1'	2:D:22[D]:DC:C6	2.44	0.53
3:A:173:ARG:CZ	3:A:180:SER:O	2.57	0.53
3:A:71:ARG:NH1	4:A:316:HOH:O	2.39	0.52
3:A:216:ASP:HB3	4:A:381:HOH:O	2.08	0.52
1:B:1[B]:DC:H2'	1:B:2[B]:DT:H72	1.90	0.52
3:A:71:ARG:NH1	3:A:175:PRO:HG3	2.27	0.50
3:A:102:LYS:HB2	3:A:105:GLY:O	2.12	0.50
3:A:274:LYS:HG2	3:A:275:GLU:HG3	1.93	0.50
3:A:233:GLU:HG2	3:A:237:GLN:HE21	1.77	0.49
3:A:173:ARG:HA	3:A:173:ARG:HE	1.78	0.48
3:A:70:ALA:HB1	3:A:100:PRO:CG	2.44	0.48
3:A:68:GLN:HG2	3:A:72:LEU:HD22	1.95	0.48
3:A:173:ARG:NH2	3:A:179:ILE:O	2.46	0.48
3:A:278:ARG:HG3	4:A:377:HOH:O	2.13	0.48
1:B:5[B]:DT:C6	1:B:6[B]:DT:H72	2.51	0.46
2:D:26[D]:DT:H2''	2:D:27[D]:DA:O5'	2.15	0.46
1:B:3[B]:DT:H1'	1:B:4[B]:DT:H5'	1.99	0.45
3:A:173:ARG:NH1	3:A:180:SER:O	2.50	0.45
1:B:7[B]:DA:H2''	1:B:8[B]:DA:O5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27[D]:DA:H2''	2:D:28[D]:DA:H8	1.79	0.45
3:A:174:ASP:O	3:A:175:PRO:C	2.54	0.45
3:A:214:HIS:N	3:A:215:PRO:HD3	2.31	0.45
3:A:31:GLN:NE2	3:A:249:ASN:OD1	2.50	0.45
2:D:24[D]:DT:H2''	2:D:25[D]:DT:H71	1.98	0.44
3:A:106:THR:HG23	3:A:107:ASN:OD1	2.17	0.44
3:A:188:LEU:HA	3:A:189:PRO:HD3	1.80	0.44
3:A:213:GLN:HA	3:A:213:GLN:HE21	1.82	0.44
2:D:19[D]:DT:H1'	2:D:20[D]:DT:H5'	1.99	0.43
3:A:74:ILE:HD11	3:A:100:PRO:HB3	2.00	0.43
3:A:237:GLN:O	3:A:241:ARG:HG3	2.19	0.43
3:A:64:TYR:HE2	3:A:99:LEU:HG	1.84	0.42
3:A:177:MET:HE2	3:A:178:GLY:CA	2.41	0.42
3:A:145:TRP:CH2	3:A:233:GLU:HB2	2.55	0.42
3:A:144:GLN:HE21	3:A:144:GLN:HB3	1.61	0.41
3:A:237:GLN:CD	4:A:398:HOH:O	2.58	0.41
1:B:1[B]:DC:N3	3:A:99:LEU:HD23	2.35	0.41
3:A:216:ASP:N	3:A:216:ASP:OD2	2.54	0.41
3:A:218:ILE:HB	3:A:229:ALA:HB3	2.03	0.40
3:A:278:ARG:CG	4:A:377:HOH:O	2.59	0.40
3:A:140:PRO:HA	3:A:141:PRO:HD3	1.88	0.40
3:A:126:HIS:HA	3:A:127:PRO:HD3	1.98	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:271:TYR:OH	3:A:271:TYR:OH[2_665]	2.07	0.13

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
3	A	253/255 (99%)	241 (95%)	6 (2%)	6 (2%)	6 2

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	103	LYS
3	A	175	PRO
3	A	104	PRO
3	A	223	VAL
3	A	108	ASP
3	A	181	GLY

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
3	A	224/224 (100%)	213 (95%)	11 (5%)	27 23

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	62	LYS
3	A	64	TYR
3	A	65	PRO
3	A	72	LEU
3	A	102	LYS
3	A	144	GLN
3	A	173	ARG
3	A	176	GLU
3	A	177	MET
3	A	220	LEU
3	A	273	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	31	GLN
3	A	77	HIS
3	A	79	GLN
3	A	134	ASN
3	A	144	GLN
3	A	161	HIS
3	A	213	GLN
3	A	237	GLN
3	A	245	GLN
3	A	249	ASN
3	A	277	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	24[D]:DT	O3'	25[D]:DT	P	1.34

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, 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	B	16/16 (100%)	1.37	3 (18%) 1 1	46, 69, 72, 72	16 (100%)
2	D	16/16 (100%)	1.25	1 (6%) 20 19	46, 71, 72, 73	16 (100%)
3	A	255/255 (100%)	1.01	33 (12%) 3 3	25, 40, 73, 88	0
All	All	287/287 (100%)	1.04	37 (12%) 3 3	25, 42, 72, 88	32 (11%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	178	GLY	13.4
3	A	106	THR	13.2
3	A	177	MET	11.8
3	A	105	GLY	10.6
3	A	107	ASN	10.3
3	A	175	PRO	8.6
3	A	176	GLU	8.5
3	A	108	ASP	8.0
3	A	104	PRO	7.1
3	A	179	ILE	6.6
3	A	180	SER	6.4
3	A	99	LEU	4.4
3	A	102	LYS	4.0
3	A	174	ASP	4.0
3	A	103	LYS	3.8
1	B	11[B]	DG	3.5
3	A	227	LEU	3.4
3	A	228	LEU	3.3
3	A	173	ARG	2.9
3	A	147	THR	2.7
3	A	237	GLN	2.7
3	A	278	ARG	2.5
3	A	243	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	24	THR	2.4
2	D	27[D]	DA	2.4
3	A	216	ASP	2.3
3	A	115	LEU	2.3
3	A	151	LEU	2.3
3	A	62	LYS	2.2
3	A	157	CYS	2.2
3	A	148	VAL	2.2
3	A	139	LEU	2.1
3	A	236	CYS	2.1
3	A	219	LEU	2.1
3	A	275	GLU	2.1
1	B	7[B]	DA	2.0
1	B	8[B]	DA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.