



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:36 AM GMT

PDB ID : 2DNJ
Title : DNASE I-INDUCED DNA CONFORMATION. 2 ANGSTROMS STRUCTURE OF A DNASE I-OCTAMER COMPLEX
Authors : Lahm, A.; Suck, D.
Deposited on : 1986-10-21
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

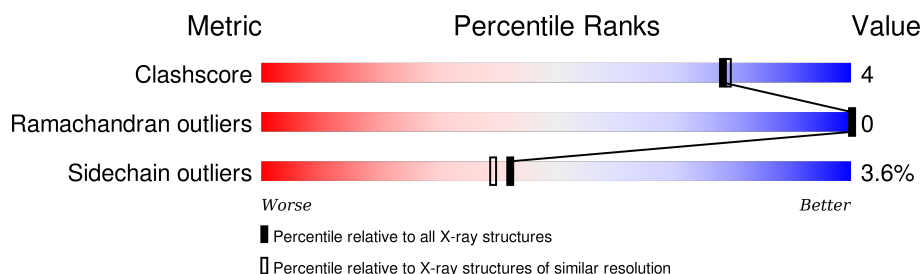
1 Overall quality at a glance

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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	8	
2	C	6	
3	A	260	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2553 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(*GP*CP*GP*AP*TP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	8	Total	C	N	O	P	0	0	0
			161	77	31	46	7			

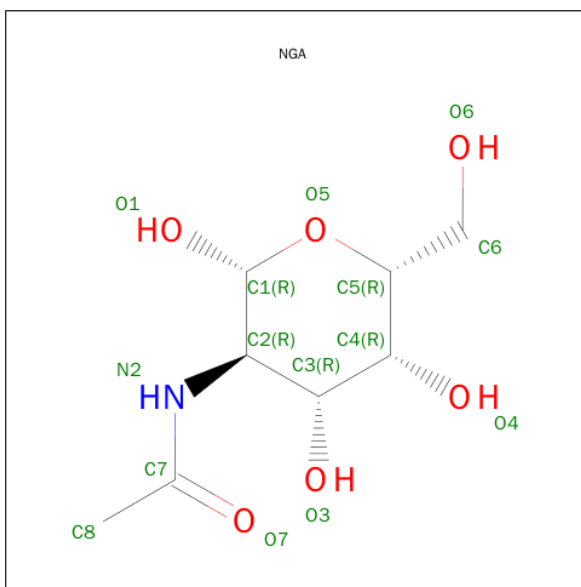
- Molecule 2 is a DNA chain called 5'-D(*GP*CP*GP*AP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	0
			120	58	23	34	5			

- Molecule 3 is a protein called DEOXYRIBONUCLEASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	253	Total	C	N	O	S	0	0	0
			2006	1276	333	391	6			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NGA) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		
5	B	24	Total	O	0	0
			24	24		
5	C	13	Total	O	0	0
			13	13		

3 Residue-property plots

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.

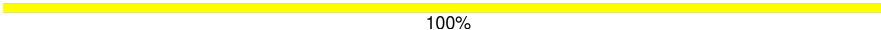
Note EDS was not executed.

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

Chain B: 


G301
C302
G303
A304
T305
C306
G307
C308

- Molecule 2: 5'-D(*GP*CP*GP*AP*TP*C)-3'

Chain C: 

G309
C310
G311
A312
T313
C314

- Molecule 3: DEOXYRIBONUCLEASE I

Chain A: 

L1
A5
R9
R27
I28
V29
R30
V35
L52
E69
F70
L71
R79
R85
Y95
Q96
Y97
D98
D99
GLY
CYS
GLU
SER
CYS
GLY
ASN
D107
S110
R111
E112
Y125
K126
E127
H134
S138
Q156
K157
M166
D172
R187
L220

S224
A230
D234
E244
M245
D251
E256
T260

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	72.90 Å 100.10 Å 92.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	90.2 (6.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2553	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NGA

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	B	2.58	15/180 (8.3%)	3.09	28/276 (10.1%)
2	C	2.86	9/134 (6.7%)	3.35	24/205 (11.7%)
3	A	0.99	1/2051 (0.0%)	1.51	26/2793 (0.9%)
All	All	1.35	25/2365 (1.1%)	1.86	78/3274 (2.4%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	312	DA	P-O5'	11.25	1.71	1.59
3	A	260	THR	C-OXT	10.52	1.43	1.23
2	C	311	DG	P-O5'	9.84	1.69	1.59
1	B	304	DA	P-O5'	8.83	1.68	1.59
1	B	307	DG	P-O5'	8.58	1.68	1.59
1	B	308	DC	C2'-C1'	8.32	1.60	1.52
2	C	310	DC	P-O5'	8.32	1.68	1.59
2	C	310	DC	C2'-C1'	8.18	1.60	1.52
1	B	307	DG	C2'-C1'	7.94	1.60	1.52
2	C	313	DT	P-O5'	7.69	1.67	1.59
1	B	302	DC	P-O5'	7.47	1.67	1.59
1	B	301	DG	C3'-C2'	7.23	1.60	1.52
2	C	310	DC	O3'-P	-6.98	1.52	1.61
1	B	303	DG	C2'-C1'	6.95	1.59	1.52
2	C	314	DC	P-O5'	6.89	1.66	1.59
2	C	314	DC	C2'-C1'	6.86	1.59	1.52
1	B	303	DG	P-O5'	6.86	1.66	1.59
1	B	308	DC	P-O5'	6.77	1.66	1.59
1	B	308	DC	C3'-C2'	6.73	1.60	1.52
1	B	301	DG	C2'-C1'	6.70	1.59	1.52
1	B	305	DT	P-O5'	5.96	1.65	1.59
1	B	303	DG	C5'-C4'	5.50	1.57	1.51
1	B	304	DA	C3'-C2'	5.35	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	DG	N7-C5	5.29	1.42	1.39
2	C	312	DA	C2'-C1'	5.09	1.57	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	310	DC	P-O3'-C3'	15.31	138.07	119.70
3	A	79	ARG	NE-CZ-NH2	-13.25	113.68	120.30
2	C	311	DG	P-O3'-C3'	12.33	134.49	119.70
1	B	308	DC	N1-C2-O2	-11.43	112.04	118.90
3	A	99	ASP	CB-CG-OD2	-11.08	108.33	118.30
3	A	187	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	B	308	DC	C3'-C2'-C1'	-10.09	90.39	102.50
1	B	302	DC	O4'-C1'-N1	10.01	115.01	108.00
1	B	301	DG	C8-N9-C4	-9.95	102.42	106.40
3	A	79	ARG	NE-CZ-NH1	9.78	125.19	120.30
2	C	309	DG	O4'-C1'-C2'	9.40	113.42	105.90
1	B	301	DG	C3'-C2'-C1'	-8.76	91.99	102.50
3	A	27	ARG	NE-CZ-NH2	-8.33	116.14	120.30
3	A	234	ASP	CB-CG-OD1	8.30	125.77	118.30
1	B	307	DG	C8-N9-C4	-8.27	103.09	106.40
1	B	305	DT	P-O3'-C3'	7.97	129.27	119.70
1	B	301	DG	O4'-C1'-N9	7.85	113.50	108.00
3	A	9	ARG	NE-CZ-NH2	-7.80	116.40	120.30
3	A	187	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	308	DC	O4'-C1'-N1	7.39	113.17	108.00
2	C	309	DG	C5-C6-O6	7.26	132.96	128.60
1	B	304	DA	O4'-C1'-C2'	7.11	111.58	105.90
2	C	310	DC	C6-N1-C2	-7.10	117.46	120.30
1	B	308	DC	C6-N1-C1'	7.08	129.30	120.80
3	A	85	ARG	NE-CZ-NH2	7.00	123.80	120.30
3	A	111	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	B	308	DC	N3-C2-O2	6.96	126.77	121.90
2	C	312	DA	P-O3'-C3'	6.95	128.04	119.70
1	B	301	DG	N9-C4-C5	6.94	108.17	105.40
2	C	309	DG	N1-C6-O6	-6.93	115.74	119.90
2	C	310	DC	OP2-P-O3'	6.88	120.33	105.20
1	B	308	DC	C2-N1-C1'	-6.80	111.32	118.80
1	B	305	DT	N3-C2-O2	-6.78	118.23	122.30
1	B	307	DG	C8-N9-C1'	6.74	135.76	127.00
2	C	309	DG	C8-N9-C1'	6.71	135.72	127.00
3	A	166	MET	N-CA-CB	-6.64	98.64	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	310	DC	C4'-C3'-O3'	6.61	126.24	109.70
2	C	313	DT	O4'-C1'-C2'	6.60	111.18	105.90
1	B	303	DG	O4'-C1'-C2'	6.54	111.13	105.90
3	A	30	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	C	309	DG	N3-C4-N9	-6.53	122.08	126.00
3	A	187	ARG	CD-NE-CZ	6.52	132.72	123.60
1	B	301	DG	N7-C8-N9	6.51	116.36	113.10
3	A	251	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	307	DG	N7-C8-N9	6.23	116.22	113.10
3	A	127	GLU	CA-CB-CG	6.23	127.10	113.40
2	C	310	DC	C5-C6-N1	6.19	124.10	121.00
2	C	309	DG	C4'-C3'-C2'	6.18	108.66	103.10
2	C	311	DG	P-O5'-C5'	-6.15	111.06	120.90
3	A	251	ASP	CB-CG-OD2	-5.99	112.91	118.30
3	A	187	ARG	CG-CD-NE	5.93	124.25	111.80
1	B	304	DA	P-O3'-C3'	5.92	126.81	119.70
1	B	307	DG	N9-C4-C5	5.91	107.76	105.40
3	A	134	HIS	N-CA-CB	5.90	121.22	110.60
2	C	311	DG	N7-C8-N9	5.86	116.03	113.10
2	C	310	DC	C6-N1-C1'	5.80	127.76	120.80
3	A	234	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	B	307	DG	C3'-C2'-C1'	-5.79	95.56	102.50
3	A	166	MET	CA-CB-CG	5.79	123.14	113.30
1	B	303	DG	C3'-C2'-C1'	-5.75	95.60	102.50
3	A	98	ASP	CB-CG-OD2	5.74	123.47	118.30
1	B	301	DG	P-O3'-C3'	5.60	126.42	119.70
3	A	172	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	303	DG	C8-N9-C1'	5.41	134.03	127.00
2	C	309	DG	N9-C4-C5	5.37	107.55	105.40
1	B	303	DG	O4'-C1'-N9	5.36	111.75	108.00
2	C	311	DG	C8-N9-C4	-5.29	104.28	106.40
2	C	310	DC	O4'-C1'-N1	5.28	111.70	108.00
1	B	302	DC	O4'-C1'-C2'	5.28	110.12	105.90
2	C	309	DG	C8-N9-C4	-5.23	104.31	106.40
3	A	244	GLU	OE1-CD-OE2	5.21	129.55	123.30
3	A	125	VAL	CG1-CB-CG2	5.18	119.19	110.90
3	A	172	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	306	DC	P-O3'-C3'	5.16	125.90	119.70
2	C	312	DA	C2-N3-C4	-5.09	108.06	110.60
2	C	309	DG	C4-N9-C1'	-5.03	119.96	126.50
2	C	310	DC	N3-C4-N4	5.02	121.52	118.00
3	A	112	GLU	CG-CD-OE1	5.02	128.34	118.30

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	161	0	91	6	0
2	C	120	0	69	0	0
3	A	2006	0	1949	10	0
4	A	14	0	11	0	0
5	A	215	0	0	1	0
5	B	24	0	0	1	0
5	C	13	0	0	1	0
All	All	2553	0	2120	16	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 4.

All (16) 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:301:DG:H8	1:B:301:DG:O5'	1.54	0.88
1:B:301:DG:HO5'	1:B:301:DG:H8	0.89	0.83
1:B:301:DG:O5'	1:B:301:DG:C8	2.34	0.78
3:A:5:ALA:HB2	3:A:166:MET:HG2	1.75	0.68
3:A:125:VAL:HG13	3:A:220:LEU:HB3	1.80	0.64
1:B:301:DG:N3	5:B:559:HOH:O	2.33	0.55
3:A:125:VAL:HG22	3:A:224:SER:OG	2.05	0.55
1:B:304:DA:H2'	1:B:305:DT:C6	2.43	0.54
3:A:29:VAL:HG13	3:A:35:VAL:HG11	1.99	0.45
3:A:156:GLN:HG3	5:A:406:HOH:O	2.17	0.45
3:A:95:TYR:CE2	3:A:157:LYS:HD3	2.52	0.45
5:C:468:HOH:O	3:A:138:SER:HB2	2.18	0.42
3:A:230:ALA:HA	3:A:256:GLU:O	2.19	0.42
3:A:69:GLU:O	3:A:71:LEU:HG	2.20	0.42
3:A:97:TYR:O	3:A:112:GLU:HB3	2.19	0.42
1:B:308:DC:H3'	1:B:308:DC:C6	2.56	0.40

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	
3	A	249/260 (96%)	242 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	224/229 (98%)	216 (96%)	8 (4%)	42	39

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	9	ARG
3	A	52	LEU
3	A	95	TYR
3	A	99	ASP
3	A	110	SER
3	A	125	VAL
3	A	138	SER
3	A	245	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	155	GLN
3	A	161	ASN
3	A	208	ASN
3	A	236	GLN
3	A	243	ASN

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](#)

1 ligand is 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	$\# Z > 2$
4	NGA	A	1000	3	14,14,15	1.67	3 (21%)	15,19,21	5.08	11 (73%)

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
4	NGA	A	1000	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	NGA	C4-C5	-2.33	1.48	1.53
4	A	1000	NGA	C3-C2	2.09	1.57	1.52
4	A	1000	NGA	O5-C1	4.13	1.50	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1000	NGA	O7-C7-C8	-12.64	98.87	122.06
4	A	1000	NGA	O3-C3-C4	-5.92	97.01	110.34
4	A	1000	NGA	C1-O5-C5	-2.09	109.59	112.25
4	A	1000	NGA	O4-C4-C5	2.46	115.75	109.24
4	A	1000	NGA	O5-C5-C6	2.82	113.45	107.35
4	A	1000	NGA	C8-C7-N2	3.12	122.08	116.11
4	A	1000	NGA	C4-C3-C2	4.00	117.44	111.23
4	A	1000	NGA	C6-C5-C4	4.30	123.61	113.02
4	A	1000	NGA	C3-C4-C5	4.44	117.93	110.20
4	A	1000	NGA	O4-C4-C3	5.07	121.75	110.34
4	A	1000	NGA	C2-N2-C7	9.02	134.63	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.