



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:36 PM UTC

PDB ID : 3DNI / pdb_00003dni
Title : CRYSTALLOGRAPHIC REFINEMENT AND STRUCTURE OF DNASE I
AT 2 ANGSTROMS RESOLUTION
Authors : Oefner, C.; Suck, D.
Deposited on : 1992-08-20
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

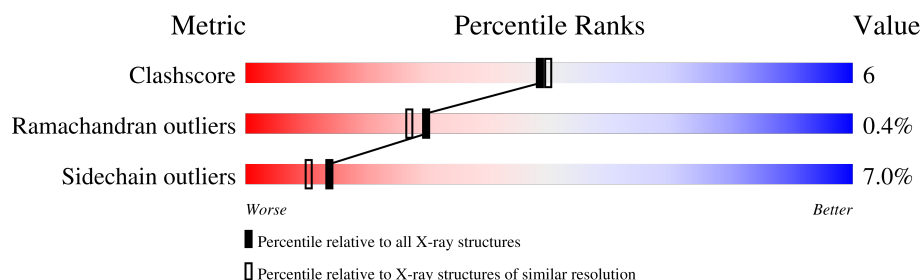
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	260	
2	B	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	2	X	-	-	-
2	MAN	B	6	X	-	-	-

2 Entry composition [i](#)

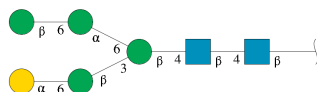
There are 4 unique types of molecules in this entry. The entry contains 2494 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DEOXYRIBONUCLEASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2034	1290	339	397	8			

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	375	Total	O	0	0
			375	375		

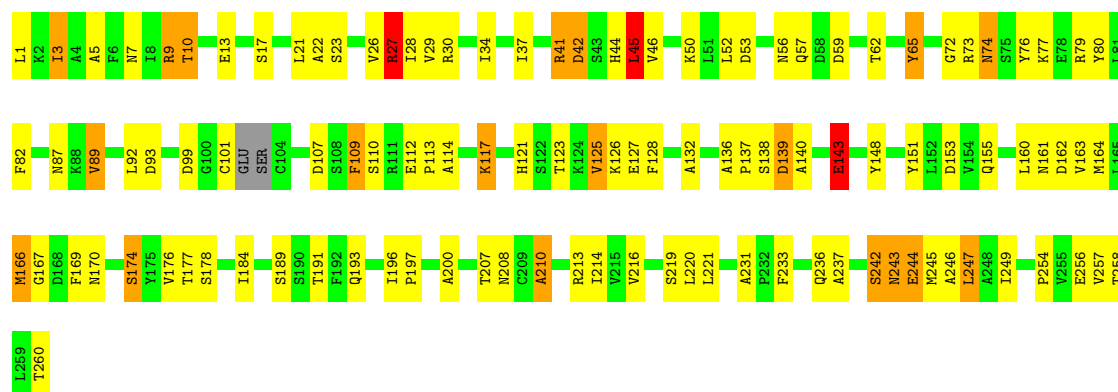
3 Residue-property plots

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. 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. 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: DEOXYRIBONUCLEASE I

Chain A: 



• Molecule 2: alpha-D-galactopyranose-(1-6)-beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.60Å 54.90Å 38.40Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2494	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA, MAN, GLA

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	1.64	12/2079 (0.6%)	2.41	129/2830 (4.6%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	ILE	CA-CB	7.69	1.62	1.53
1	A	163	VAL	C-N	6.37	1.41	1.33
1	A	151	TYR	C-O	6.22	1.31	1.24
1	A	72	GLY	N-CA	6.01	1.51	1.45
1	A	148	TYR	N-CA	5.82	1.53	1.46
1	A	123	THR	CA-CB	5.78	1.62	1.53
1	A	99	ASP	CG-OD2	5.71	1.36	1.25
1	A	125	VAL	C-N	-5.47	1.25	1.33
1	A	27	ARG	CD-NE	5.32	1.53	1.46
1	A	243	ASN	N-CA	5.13	1.52	1.46
1	A	82	PHE	C-N	-5.10	1.26	1.33
1	A	231	ALA	C-N	-5.06	1.26	1.33

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	HIS	CA-CB-CG	20.49	134.29	113.80
1	A	127	GLU	CA-CB-CG	12.55	139.20	114.10
1	A	27	ARG	CD-NE-CZ	-10.98	109.03	124.40
1	A	143	GLU	OE1-CD-OE2	10.37	147.80	122.90
1	A	166	MET	N-CA-CB	-10.30	94.46	111.66
1	A	74	ASN	CA-CB-CG	-10.26	102.34	112.60
1	A	139	ASP	CA-CB-CG	-10.21	102.39	112.60
1	A	9	ARG	CD-NE-CZ	10.21	138.69	124.40
1	A	196	ILE	CA-C-O	-9.79	113.37	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	PHE	CA-CB-CG	9.13	122.93	113.80
1	A	143	GLU	CG-CD-OE1	-9.02	97.65	118.40
1	A	178	SER	O-C-N	8.71	131.15	122.09
1	A	34	ILE	CA-C-O	-8.59	111.26	120.36
1	A	89	VAL	N-CA-CB	-8.49	96.65	112.36
1	A	178	SER	CA-CB-OG	-8.40	94.29	111.10
1	A	73	ARG	NE-CZ-NH1	-8.39	113.11	121.50
1	A	254	PRO	CA-C-O	-8.34	111.49	121.67
1	A	42	ASP	CA-CB-CG	8.33	120.93	112.60
1	A	184	ILE	N-CA-CB	-8.32	101.02	111.41
1	A	166	MET	CA-CB-CG	8.01	130.12	114.10
1	A	178	SER	CA-C-O	-7.89	112.46	120.90
1	A	244	GLU	CB-CG-CD	7.82	125.90	112.60
1	A	256	GLU	O-C-N	7.77	133.25	123.15
1	A	153	ASP	CA-CB-CG	-7.73	104.87	112.60
1	A	93	ASP	O-C-N	7.48	130.87	123.46
1	A	17	SER	CA-CB-OG	-7.28	96.54	111.10
1	A	125	VAL	CB-CA-C	-7.28	100.49	111.33
1	A	236	GLN	CG-CD-NE2	7.24	127.26	116.40
1	A	138	SER	O-C-N	7.06	129.60	122.12
1	A	167	GLY	O-C-N	6.85	133.12	123.67
1	A	56	ASN	O-C-N	6.84	130.77	122.35
1	A	37	ILE	O-C-N	6.79	130.31	123.18
1	A	243	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	A	176	VAL	O-C-N	6.53	129.05	122.71
1	A	27	ARG	NE-CZ-NH2	6.46	125.01	119.20
1	A	260	THR	CA-CB-OG1	-6.44	99.94	109.60
1	A	7	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	A	93	ASP	CA-C-O	-6.39	114.07	121.10
1	A	125	VAL	N-CA-CB	6.38	118.16	110.31
1	A	137	PRO	CA-C-N	6.34	129.07	120.38
1	A	137	PRO	C-N-CA	6.34	129.07	120.38
1	A	99	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	196	ILE	O-C-N	6.28	127.03	121.57
1	A	9	ARG	NE-CZ-NH1	6.22	127.72	121.50
1	A	76	TYR	CA-C-O	-6.16	113.73	120.81
1	A	73	ARG	N-CA-CB	-6.15	101.01	110.42
1	A	77	LYS	CB-CA-C	-6.10	96.63	109.38
1	A	139	ASP	O-C-N	6.08	130.35	122.20
1	A	125	VAL	CA-C-O	-6.06	114.13	121.04
1	A	143	GLU	CB-CA-C	-6.05	101.38	110.88
1	A	77	LYS	CA-CB-CG	6.02	126.14	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ASN	CB-CA-C	6.00	122.35	110.42
1	A	138	SER	CB-CA-C	-5.98	100.51	110.68
1	A	87	ASN	CB-CG-ND2	5.98	125.37	116.40
1	A	45	LEU	N-CA-CB	-5.96	103.18	112.41
1	A	138	SER	CA-CB-OG	-5.91	99.28	111.10
1	A	3	ILE	O-C-N	5.90	129.55	123.18
1	A	245	MET	O-C-N	5.89	129.89	122.23
1	A	184	ILE	CB-CA-C	5.88	119.55	111.31
1	A	79	ARG	NE-CZ-NH1	5.88	127.38	121.50
1	A	44	HIS	CA-CB-CG	-5.86	107.94	113.80
1	A	28	ILE	CA-C-N	5.85	128.14	120.60
1	A	28	ILE	C-N-CA	5.85	128.14	120.60
1	A	73	ARG	NH1-CZ-NH2	5.81	126.85	119.30
1	A	216	VAL	O-C-N	5.76	129.16	123.00
1	A	65	TYR	CA-C-N	5.75	130.99	122.99
1	A	65	TYR	C-N-CA	5.75	130.99	122.99
1	A	76	TYR	N-CA-CB	-5.73	101.31	109.85
1	A	139	ASP	CA-C-O	-5.73	113.60	120.65
1	A	56	ASN	CA-C-O	-5.73	112.96	119.78
1	A	244	GLU	CA-CB-CG	5.73	125.56	114.10
1	A	191	THR	CA-CB-CG2	5.72	120.23	110.50
1	A	110	SER	CA-CB-OG	-5.70	99.69	111.10
1	A	193	GLN	CB-CG-CD	-5.67	102.97	112.60
1	A	41	ARG	CD-NE-CZ	-5.65	116.48	124.40
1	A	110	SER	N-CA-C	-5.64	104.52	111.40
1	A	13	GLU	O-C-N	5.58	127.81	122.07
1	A	140	ALA	O-C-N	5.54	127.85	122.09
1	A	184	ILE	N-CA-C	5.49	115.69	107.51
1	A	210	ALA	N-CA-CB	-5.49	103.84	110.53
1	A	242	SER	CA-CB-OG	-5.46	100.18	111.10
1	A	189	SER	CA-CB-OG	-5.46	100.19	111.10
1	A	76	TYR	CB-CA-C	5.45	118.60	109.89
1	A	107	ASP	CB-CA-C	5.43	118.74	109.72
1	A	132	ALA	CA-C-O	-5.43	114.78	120.80
1	A	123	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	243	ASN	CB-CA-C	5.42	120.06	110.85
1	A	233	PHE	CA-C-O	-5.40	115.01	120.84
1	A	160	LEU	N-CA-CB	-5.38	101.46	110.83
1	A	136	ALA	CB-CA-C	5.38	117.13	109.38
1	A	208	ASN	CB-CA-C	5.38	119.95	111.77
1	A	114	ALA	N-CA-C	-5.37	100.95	109.96
1	A	249	ILE	N-CA-C	-5.34	105.88	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ASN	CA-C-O	-5.33	113.39	119.41
1	A	1	LEU	CB-CA-C	5.32	120.22	110.10
1	A	257	VAL	CA-C-N	-5.32	115.65	123.00
1	A	257	VAL	C-N-CA	-5.32	115.65	123.00
1	A	170	ASN	N-CA-C	-5.32	105.43	112.24
1	A	213	ARG	N-CA-C	5.32	117.28	109.24
1	A	197	PRO	CA-C-N	5.32	129.11	120.60
1	A	197	PRO	C-N-CA	5.32	129.11	120.60
1	A	62	THR	N-CA-CB	5.31	117.77	110.07
1	A	177	THR	CA-CB-CG2	5.29	119.50	110.50
1	A	117	LYS	CG-CD-CE	5.29	123.47	111.30
1	A	57	GLN	CA-CB-CG	5.29	124.68	114.10
1	A	258	THR	CA-C-O	-5.29	114.61	120.38
1	A	13	GLU	CA-C-O	-5.25	115.31	120.82
1	A	174	SER	N-CA-C	5.23	117.89	111.82
1	A	161	ASN	O-C-N	5.23	129.78	122.36
1	A	214	ILE	CA-C-O	-5.21	115.00	120.27
1	A	80	TYR	CA-C-N	-5.21	115.65	122.99
1	A	80	TYR	C-N-CA	-5.21	115.65	122.99
1	A	109	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	236	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	A	46	VAL	O-C-N	5.19	127.30	121.90
1	A	73	ARG	CB-CA-C	5.16	118.08	109.56
1	A	207	THR	CA-C-O	-5.11	115.95	121.87
1	A	29	VAL	O-C-N	5.10	127.04	121.94
1	A	260	THR	CA-CB-CG2	5.09	119.15	110.50
1	A	257	VAL	CA-C-O	-5.08	115.96	121.19
1	A	246	ALA	CA-C-O	5.07	125.92	120.55
1	A	128	PHE	CA-C-N	5.05	130.73	122.81
1	A	128	PHE	C-N-CA	5.05	130.73	122.81
1	A	237	ALA	O-C-N	5.04	127.27	122.07
1	A	163	VAL	CA-C-O	5.04	125.71	120.36
1	A	59	ASP	CA-CB-CG	-5.04	107.56	112.60
1	A	162	ASP	CA-CB-CG	-5.04	107.56	112.60
1	A	53	ASP	O-C-N	5.02	127.24	122.07
1	A	82	PHE	CA-CB-CG	5.02	118.82	113.80

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	A	2034	0	1969	18	0
2	B	83	0	64	5	0
3	A	2	0	0	0	0
4	A	375	0	0	7	2
All	All	2494	0	2033	23	2

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 6.

All (23) 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:B:2:NAG:H4	2:B:3:BMA:O2	1.34	1.08
2:B:2:NAG:C4	2:B:3:BMA:O2	2.15	0.94
4:A:618:HOH:O	2:B:7:BMA:H2	1.72	0.89
1:A:5:ALA:HB2	1:A:166:MET:HG2	1.69	0.75
2:B:3:BMA:O4	2:B:4:BMA:C1	2.38	0.72
2:B:4:BMA:H2	2:B:7:BMA:H62	1.71	0.70
1:A:30:ARG:HD2	4:A:303:HOH:O	1.99	0.62
1:A:9:ARG:NH2	4:A:609:HOH:O	2.33	0.57
1:A:174:SER:HB2	4:A:434:HOH:O	2.08	0.53
1:A:109:PHE:CD1	1:A:143:GLU:HG3	2.46	0.51
1:A:10:THR:HG23	1:A:41:ARG:HH11	1.76	0.51
1:A:92:LEU:HB2	1:A:117:LYS:HD2	1.95	0.48
1:A:243:ASN:O	1:A:247:LEU:HB2	2.14	0.47
1:A:42:ASP:OD2	1:A:45:LEU:HA	2.14	0.47
1:A:155:GLN:NE2	4:A:444:HOH:O	2.48	0.46
1:A:126:LYS:NZ	4:A:606:HOH:O	2.49	0.45
1:A:112:GLU:HA	1:A:113:PRO:HD3	1.84	0.43
1:A:22:ALA:O	1:A:26:VAL:HG23	2.18	0.43
1:A:200:ALA:O	1:A:210:ALA:HB2	2.20	0.41
1:A:3:ILE:CD1	1:A:164:MET:HE1	2.51	0.41
1:A:50:LYS:NZ	4:A:578:HOH:O	2.53	0.41
1:A:52:LEU:HD11	1:A:65:TYR:CE1	2.56	0.41
1:A:27:ARG:HH11	1:A:27:ARG:HD3	1.48	0.40

All (2) 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)
4:A:618:HOH:O	4:A:618:HOH:O[2_556]	1.82	0.38
4:A:368:HOH:O	4:A:368:HOH:O[2_456]	2.10	0.10

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	254/260 (98%)	247 (97%)	6 (2%)	1 (0%)	30 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ASN

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	227/229 (99%)	211 (93%)	16 (7%)	14 10

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR

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Mol	Chain	Res	Type
1	A	21	LEU
1	A	23	SER
1	A	27	ARG
1	A	45	LEU
1	A	89	VAL
1	A	101	CYS
1	A	125	VAL
1	A	139	ASP
1	A	143	GLU
1	A	219	SER
1	A	220	LEU
1	A	221	LEU
1	A	242	SER
1	A	244	GLU
1	A	247	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	96	GLN
1	A	155	GLN
1	A	156	GLN
1	A	159	HIS
1	A	161	ASN
1	A	236	GLN
1	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](#)

7 monosaccharides are 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
2	NAG	B	1	2,1	14,14,15	1.62	2 (14%)	17,19,21	5.39	12 (70%)
2	NAG	B	2	2	14,14,15	2.41	6 (42%)	17,19,21	5.42	9 (52%)
2	BMA	B	3	2	11,11,12	1.21	1 (9%)	15,15,17	3.03	5 (33%)
2	BMA	B	4	2	11,11,12	1.34	2 (18%)	15,15,17	3.51	6 (40%)
2	GLA	B	5	2	11,11,12	2.41	2 (18%)	15,15,17	4.22	7 (46%)
2	MAN	B	6	2	11,11,12	0.82	0	15,15,17	3.16	9 (60%)
2	BMA	B	7	2	11,11,12	2.78	3 (27%)	15,15,17	4.22	9 (60%)

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
2	NAG	B	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	1/1/5/7	3/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	BMA	B	4	2	-	2/2/19/22	0/1/1/1
2	GLA	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	1/1/4/5	2/2/19/22	0/1/1/1
2	BMA	B	7	2	-	2/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	BMA	O2-C2	-8.05	1.26	1.43
2	B	5	GLA	C4-C5	-5.92	1.40	1.53
2	B	2	NAG	C1-C2	4.63	1.58	1.52
2	B	5	GLA	C2-C3	-4.58	1.45	1.52
2	B	2	NAG	O7-C7	4.44	1.33	1.23
2	B	2	NAG	C8-C7	3.93	1.58	1.50
2	B	1	NAG	O5-C1	-3.86	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	BMA	C2-C3	-3.07	1.47	1.52
2	B	3	BMA	O5-C1	-3.06	1.38	1.43
2	B	2	NAG	C4-C3	2.85	1.59	1.52
2	B	1	NAG	O3-C3	2.67	1.49	1.43
2	B	4	BMA	O5-C5	-2.65	1.38	1.43
2	B	7	BMA	C2-C3	2.43	1.56	1.52
2	B	7	BMA	O5-C5	-2.38	1.38	1.43
2	B	2	NAG	O5-C5	-2.26	1.39	1.43
2	B	2	NAG	O3-C3	-2.12	1.37	1.43

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	14.18	131.19	112.19
2	B	1	NAG	O7-C7-C8	-13.00	98.90	122.05
2	B	7	BMA	C1-O5-C5	11.91	128.14	112.19
2	B	1	NAG	C1-O5-C5	11.68	127.84	112.19
2	B	2	NAG	O3-C3-C2	10.20	130.58	109.40
2	B	5	GLA	C3-C4-C5	9.89	128.17	110.23
2	B	5	GLA	C1-O5-C5	9.40	124.78	112.19
2	B	3	BMA	C1-O5-C5	9.06	124.33	112.19
2	B	1	NAG	C2-N2-C7	8.93	134.87	122.90
2	B	4	BMA	C1-O5-C5	7.72	122.53	112.19
2	B	4	BMA	C1-C2-C3	7.47	120.53	109.64
2	B	2	NAG	C8-C7-N2	-7.01	104.50	116.12
2	B	2	NAG	O7-C7-C8	6.81	134.18	122.05
2	B	6	MAN	O3-C3-C2	6.34	122.99	110.05
2	B	7	BMA	O4-C4-C3	5.80	124.04	110.38
2	B	2	NAG	O5-C1-C2	-5.68	102.50	111.29
2	B	1	NAG	C4-C3-C2	5.62	119.25	111.02
2	B	4	BMA	O3-C3-C2	5.49	121.25	110.05
2	B	6	MAN	C1-C2-C3	5.39	117.49	109.64
2	B	7	BMA	C2-C3-C4	-5.28	101.57	110.86
2	B	5	GLA	O4-C4-C5	5.27	122.31	109.32
2	B	5	GLA	O2-C2-C3	4.76	120.00	110.15
2	B	4	BMA	C2-C3-C4	4.46	118.71	110.86
2	B	6	MAN	O2-C2-C3	4.22	118.88	110.15
2	B	6	MAN	C2-C3-C4	4.20	118.25	110.86
2	B	2	NAG	C4-C3-C2	4.08	117.00	111.02
2	B	1	NAG	O5-C5-C6	-4.04	99.79	107.66
2	B	3	BMA	C3-C4-C5	-3.89	103.17	110.23
2	B	2	NAG	C1-C2-N2	-3.85	104.36	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	BMA	O6-C6-C5	3.82	124.35	111.33
2	B	2	NAG	O5-C5-C4	3.71	119.86	110.83
2	B	1	NAG	C8-C7-N2	3.61	122.11	116.12
2	B	7	BMA	O3-C3-C2	-3.48	102.95	110.05
2	B	5	GLA	O3-C3-C2	3.41	117.02	110.05
2	B	2	NAG	O5-C5-C6	3.30	114.09	107.66
2	B	6	MAN	O3-C3-C4	3.23	117.98	110.38
2	B	7	BMA	C3-C4-C5	-3.22	104.39	110.23
2	B	3	BMA	C1-C2-C3	3.14	114.22	109.64
2	B	3	BMA	C2-C3-C4	-3.12	105.37	110.86
2	B	3	BMA	O4-C4-C5	2.95	116.60	109.32
2	B	6	MAN	C1-O5-C5	2.91	116.09	112.19
2	B	1	NAG	C6-C5-C4	2.86	120.03	113.02
2	B	1	NAG	O4-C4-C5	2.74	116.08	109.32
2	B	1	NAG	O3-C3-C2	-2.73	103.74	109.40
2	B	7	BMA	O5-C1-C2	2.60	116.99	110.79
2	B	4	BMA	O2-C2-C1	2.53	115.01	109.22
2	B	6	MAN	O5-C5-C6	2.50	112.53	107.66
2	B	7	BMA	O3-C3-C4	2.49	116.24	110.38
2	B	1	NAG	O4-C4-C3	2.36	115.94	110.38
2	B	6	MAN	O5-C5-C4	2.27	116.36	110.83
2	B	7	BMA	O2-C2-C3	2.27	114.84	110.15
2	B	1	NAG	C3-C4-C5	2.25	114.31	110.23
2	B	5	GLA	O4-C4-C3	-2.20	105.19	110.38
2	B	4	BMA	O2-C2-C3	2.16	114.63	110.15
2	B	5	GLA	O6-C6-C5	2.09	118.46	111.33
2	B	1	NAG	O5-C1-C2	2.05	114.46	111.29
2	B	6	MAN	O6-C6-C5	-2.02	104.47	111.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2	NAG	C3
2	B	6	MAN	C3

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	6	MAN	O5-C5-C6-O6
2	B	6	MAN	C4-C5-C6-O6

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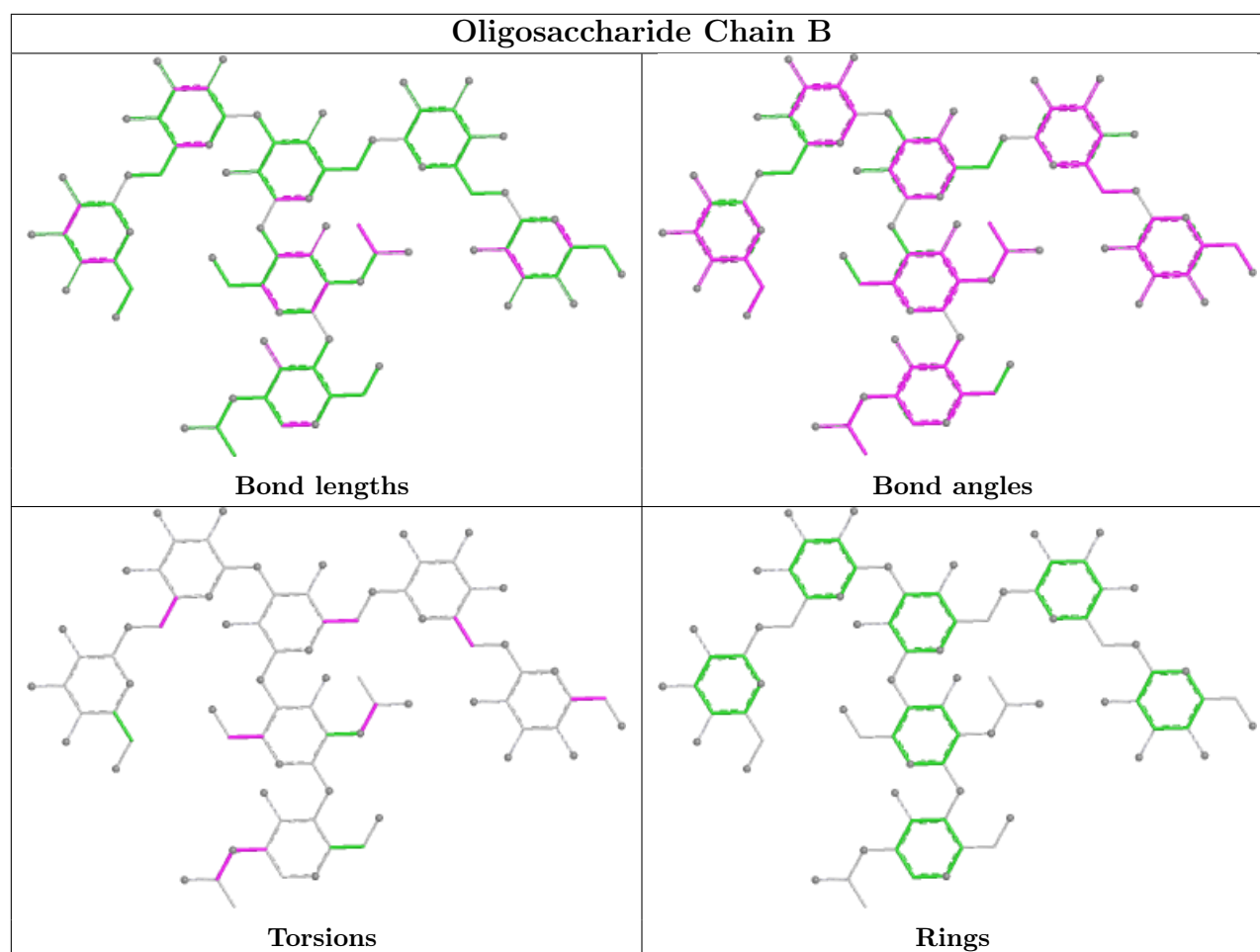
Mol	Chain	Res	Type	Atoms
2	B	4	BMA	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	4	BMA	O5-C5-C6-O6
2	B	7	BMA	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	7	BMA	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C3-C2-N2-C7
2	B	2	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	BMA	3	0
2	B	2	NAG	2	0
2	B	7	BMA	2	0
2	B	4	BMA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.