



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:19 PM UTC

PDB ID : 1DNK / pdb_00001dnk
Title : THE X-RAY STRUCTURE OF THE DNASE I-D(GGTATACC)2 COM-
PLEX AT 2.3 ANGSTROMS RESOLUTION
Authors : Weston, S.A.; Lahm, A.; Suck, D.
Deposited on : 1992-08-10
Resolution : 2.30 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

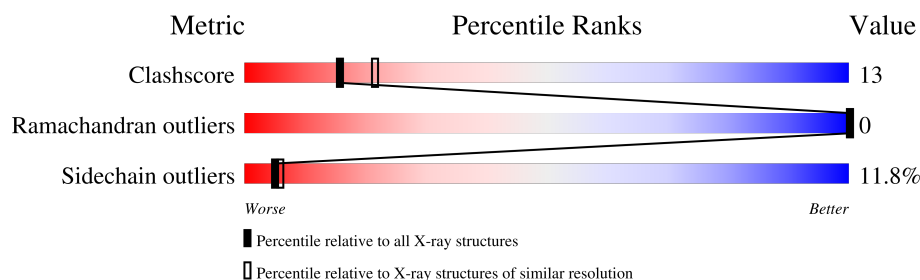
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	B	7	43% 29% 29%
2	C	8	25% 62% 12%
3	A	260	46% 36% 13% • •
4	D	2	50% 50%

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
4	NAG	D	1	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2390 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 DNA (5'-D(*GP*GP*TP*AP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	7	Total	C	N	O	P	0	0	0
			142	69	27	40	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			

- Molecule 3 is a protein called PROTEIN (DEOXYRIBONUCLEASE I (DNASE I) (E.C.3.1.21.1)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	250	Total	C	N	O	S	0	0	0
			1982	1264	330	382	6			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	4	Total	O	0	0
			4	4		
5	A	70	Total	O	0	0
			70	70		

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. 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: DNA (5'-D(*GP*GP*TP*AP*TP*AP*C)-3')

Chain B: 



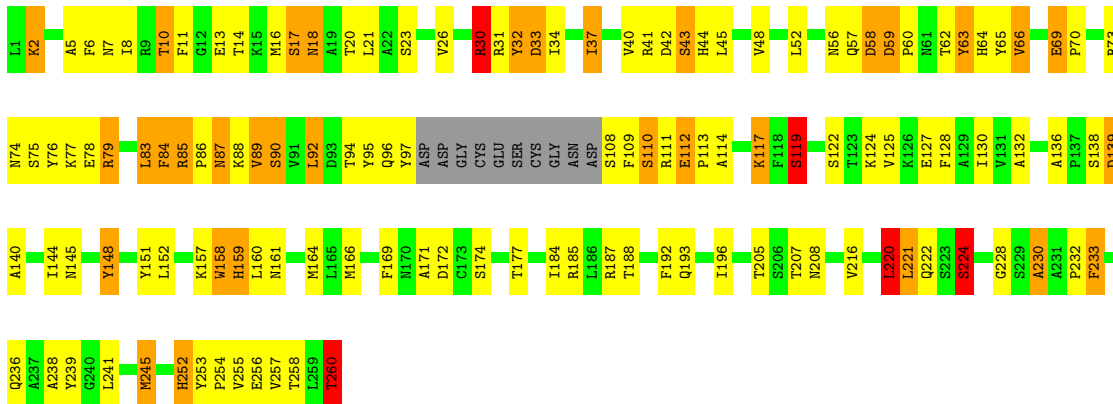
- Molecule 2: DNA (5'-D(*GP*GP*TP*AP*TP*AP*CP*C)-3')

Chain C: 



- Molecule 3: PROTEIN (DEOXYRIBONUCLEASE I (DNASE I) (E.C.3.1.21.1))

Chain A: 



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	51.10Å 108.40Å 62.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, PROLSQ	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2390	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: NAG

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	1.11	0/159	2.08	5/244 (2.0%)
2	C	1.27	0/180	2.18	5/276 (1.8%)
3	A	3.72	2/2027 (0.1%)	2.21	101/2760 (3.7%)
All	All	3.48	2/2366 (0.1%)	2.20	111/3280 (3.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	260	THR	C-OXT	158.53	4.40	1.23
3	A	160	LEU	N-CA	5.37	1.52	1.46

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	18	ASN	OD1-CG-ND2	16.13	138.73	122.60
3	A	169	PHE	CA-CB-CG	15.83	129.63	113.80
3	A	30	ARG	CD-NE-CZ	11.63	140.68	124.40
3	A	89	VAL	N-CA-CB	-9.90	94.63	110.96
3	A	85	ARG	NE-CZ-NH2	9.71	127.94	119.20
3	A	109	PHE	CA-CB-CG	9.38	123.19	113.80
3	A	16	MET	CA-C-N	8.09	131.78	120.29
3	A	16	MET	C-N-CA	8.09	131.78	120.29
3	A	196	ILE	O-C-N	8.06	126.44	121.37
3	A	42	ASP	CA-CB-CG	8.03	120.63	112.60
3	A	224	SER	CB-CA-C	7.72	123.09	109.65
3	A	44	HIS	CA-CB-CG	-7.66	106.14	113.80
3	A	185	ARG	NE-CZ-NH1	7.62	129.12	121.50
2	C	309	DG	P-O3'-C3'	7.46	131.39	120.20
3	A	30	ARG	NE-CZ-NH1	7.43	128.93	121.50
3	A	62	THR	N-CA-C	-7.40	102.58	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	32	TYR	N-CA-C	7.36	121.54	110.14
3	A	92	LEU	O-C-N	7.28	130.34	122.34
2	C	309	DG	C2'-C3'-O3'	-7.25	100.62	111.50
3	A	96	GLN	CA-C-O	-7.10	112.77	120.36
3	A	92	LEU	N-CA-C	-7.05	105.21	114.31
3	A	85	ARG	NE-CZ-NH1	-6.99	114.51	121.50
2	C	309	DG	C3'-C2'-C1'	-6.94	91.19	101.60
3	A	66	VAL	N-CA-C	-6.91	98.17	108.12
3	A	132	ALA	CA-C-O	-6.89	113.16	120.80
3	A	177	THR	CA-C-N	6.87	129.81	120.54
3	A	177	THR	C-N-CA	6.87	129.81	120.54
3	A	66	VAL	CA-C-O	-6.83	113.12	120.36
3	A	128	PHE	CA-CB-CG	6.77	120.57	113.80
1	B	301	DG	C3'-C2'-C1'	-6.62	91.68	101.60
3	A	59	ASP	O-C-N	6.59	128.90	121.32
3	A	159	HIS	CB-CA-C	-6.43	102.60	111.73
3	A	69	GLU	O-C-N	6.40	128.80	121.31
3	A	184	ILE	CA-C-N	6.39	129.13	120.38
3	A	184	ILE	C-N-CA	6.39	129.13	120.38
3	A	73	ARG	NE-CZ-NH2	6.30	124.87	119.20
3	A	69	GLU	CG-CD-OE2	-6.25	104.01	118.40
3	A	139	ASP	CA-CB-CG	-6.23	106.37	112.60
3	A	113	PRO	CA-C-O	6.16	128.37	121.34
3	A	193	GLN	CA-CB-CG	6.16	126.42	114.10
3	A	69	GLU	CG-CD-OE1	6.13	132.49	118.40
3	A	70	PRO	CA-C-O	-6.10	114.07	121.03
3	A	95	TYR	O-C-N	6.05	129.45	123.46
3	A	111	ARG	NE-CZ-NH1	6.02	127.52	121.50
1	B	306	DA	O5'-C5'-C4'	-5.94	101.89	110.80
3	A	34	ILE	CA-C-O	-5.94	113.96	120.43
3	A	63	TYR	N-CA-C	5.88	119.10	108.69
3	A	205	THR	N-CA-CB	5.87	118.23	110.25
3	A	112	GLU	N-CA-CB	5.86	119.64	109.57
3	A	117	LYS	CA-C-O	-5.84	114.01	120.38
3	A	145	ASN	OD1-CG-ND2	5.83	128.43	122.60
3	A	83	LEU	CA-C-O	-5.83	114.33	120.80
3	A	148	TYR	N-CA-C	-5.79	105.05	111.36
3	A	220	LEU	N-CA-C	-5.78	104.62	111.03
3	A	58	ASP	CA-CB-CG	5.72	118.32	112.60
3	A	255	VAL	N-CA-C	-5.72	100.24	108.53
3	A	66	VAL	O-C-N	5.71	129.37	123.20
3	A	158	TRP	CA-C-O	-5.71	112.65	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	18	ASN	CB-CG-ND2	-5.69	107.86	116.40
2	C	315	DC	P-O3'-C3'	5.69	128.73	120.20
3	A	33	ASP	CA-CB-CG	-5.68	106.92	112.60
3	A	122	SER	CA-C-O	-5.64	112.60	119.43
3	A	23	SER	O-C-N	5.63	127.87	122.07
3	A	185	ARG	NE-CZ-NH2	-5.62	114.14	119.20
3	A	208	ASN	OD1-CG-ND2	-5.61	116.99	122.60
3	A	164	MET	CA-C-O	-5.61	114.32	120.43
3	A	161	ASN	CA-C-N	5.59	131.23	122.17
3	A	161	ASN	C-N-CA	5.59	131.23	122.17
1	B	305	DT	O5'-C5'-C4'	-5.59	102.42	110.80
3	A	90	SER	CA-C-O	-5.58	114.59	121.06
3	A	238	ALA	CA-C-O	-5.56	114.66	120.55
3	A	136	ALA	N-CA-C	-5.53	102.81	109.72
3	A	40	VAL	O-C-N	5.52	129.08	122.62
3	A	160	LEU	CB-CA-C	5.52	119.81	109.71
3	A	7	ASN	OD1-CG-ND2	-5.51	117.09	122.60
2	C	311	DT	C3'-C2'-C1'	-5.48	93.39	101.60
3	A	188	THR	CA-CB-OG1	-5.46	101.40	109.60
3	A	192	PHE	N-CA-C	5.46	118.14	109.24
3	A	145	ASN	CA-CB-CG	-5.42	107.18	112.60
3	A	87	ASN	CA-C-O	-5.41	112.19	119.11
3	A	233	PHE	N-CA-CB	5.40	119.60	110.69
3	A	94	THR	CA-C-O	-5.39	115.51	121.33
3	A	17	SER	CB-CA-C	-5.38	101.71	110.85
3	A	128	PHE	CA-C-O	-5.37	114.99	120.89
3	A	119	SER	CB-CA-C	5.36	118.59	109.75
3	A	230	ALA	CA-C-O	-5.36	114.58	120.69
3	A	79	ARG	NE-CZ-NH1	5.33	126.83	121.50
3	A	232	PRO	N-CA-C	-5.33	103.42	111.41
3	A	31	ARG	N-CA-C	-5.32	105.52	112.23
3	A	193	GLN	N-CA-CB	5.30	118.87	110.55
1	B	304	DA	P-O5'-C5'	5.28	127.93	120.00
3	A	157	LYS	CB-CA-C	-5.24	102.66	110.88
3	A	37	ILE	N-CA-CB	5.22	118.35	111.25
3	A	5	ALA	N-CA-C	-5.22	100.40	108.90
3	A	114	ALA	N-CA-C	-5.21	100.75	109.24
3	A	84	PHE	CA-CB-CG	5.17	118.97	113.80
3	A	97	TYR	CA-C-O	-5.17	112.02	120.80
3	A	252	HIS	CA-C-O	-5.16	115.42	121.46
3	A	31	ARG	NE-CZ-NH2	5.13	123.82	119.20
3	A	245	MET	CA-C-N	5.13	127.92	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	245	MET	C-N-CA	5.13	127.92	120.79
1	B	304	DA	C8-N9-C1'	5.13	134.74	127.05
3	A	110	SER	O-C-N	5.06	127.56	122.09
3	A	114	ALA	CA-C-O	-5.06	114.92	120.43
3	A	160	LEU	N-CA-CB	-5.05	102.19	110.68
3	A	57	GLN	N-CA-CB	5.04	118.09	110.28
3	A	127	GLU	CA-C-O	-5.04	114.86	120.66
3	A	238	ALA	O-C-N	5.02	127.45	122.12
3	A	260	THR	N-CA-CB	-5.01	102.98	111.50
3	A	139	ASP	CA-C-N	5.00	126.94	120.44
3	A	139	ASP	C-N-CA	5.00	126.94	120.44

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	142	0	81	2	0
2	C	161	0	92	5	0
3	A	1982	0	1937	53	1
4	D	28	0	22	0	1
5	A	70	0	0	4	0
5	B	3	0	0	0	0
5	C	4	0	0	0	0
All	All	2390	0	2132	58	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 13.

All (58) 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)
3:A:125:VAL:HA	3:A:220:LEU:HD13	1.52	0.91
3:A:84:PHE:O	3:A:86:PRO:HD3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:252:HIS:HB3	5:A:468:HOH:O	1.81	0.78
3:A:63:TYR:OH	3:A:85:ARG:NH1	2.20	0.73
3:A:10:THR:HG23	3:A:41:ARG:HD3	1.76	0.68
3:A:125:VAL:HA	3:A:220:LEU:CD1	2.22	0.68
3:A:20:THR:HG22	3:A:245:MET:HE1	1.79	0.64
3:A:124:LYS:HE3	3:A:260:THR:CG2	2.27	0.64
2:C:314:DA:H2''	2:C:315:DC:O4'	1.98	0.64
3:A:239:TYR:HB2	3:A:241:LEU:HG	1.79	0.64
3:A:58:ASP:HB2	5:A:444:HOH:O	1.98	0.63
3:A:10:THR:HG23	3:A:41:ARG:HH11	1.66	0.60
3:A:230:ALA:HA	3:A:256:GLU:O	2.02	0.59
3:A:216:VAL:HG23	3:A:222:GLN:HG2	1.87	0.56
3:A:74:ASN:O	3:A:77:LYS:NZ	2.36	0.55
3:A:14:THR:O	3:A:17:SER:HB2	2.05	0.55
2:C:313:DT:OP2	3:A:74:ASN:ND2	2.39	0.55
3:A:125:VAL:CA	3:A:220:LEU:HD13	2.32	0.54
1:B:305:DT:H2'	1:B:306:DA:C8	2.42	0.54
3:A:20:THR:HG22	3:A:245:MET:CE	2.37	0.54
3:A:65:TYR:HB3	3:A:83:LEU:HD23	1.90	0.53
3:A:56:ASN:HB3	3:A:60:PRO:HA	1.95	0.49
3:A:48:VAL:O	3:A:52:LEU:HD12	2.13	0.49
3:A:20:THR:CG2	3:A:245:MET:HE1	2.42	0.49
3:A:125:VAL:HG12	3:A:224:SER:OG	2.13	0.49
3:A:59:ASP:OD1	3:A:60:PRO:HD2	2.13	0.49
3:A:253:TYR:N	5:A:468:HOH:O	2.46	0.48
3:A:158:TRP:O	3:A:159:HIS:HB2	2.13	0.48
3:A:33:ASP:OD1	3:A:85:ARG:HD2	2.14	0.48
3:A:124:LYS:HB2	3:A:224:SER:HB2	1.95	0.48
3:A:26:VAL:O	3:A:30:ARG:HG3	2.14	0.47
2:C:316:DC:H5''	3:A:207:THR:HG21	1.96	0.47
3:A:87:ASN:HD21	3:A:88:LYS:NZ	2.14	0.46
3:A:216:VAL:HB	3:A:221:LEU:HD13	1.97	0.46
3:A:130:ILE:HG21	3:A:166:MET:HE2	1.96	0.46
3:A:140:ALA:O	3:A:144:ILE:HG13	2.16	0.46
2:C:313:DT:OP1	2:C:313:DT:H4'	2.16	0.45
3:A:87:ASN:HD21	3:A:88:LYS:HZ3	1.63	0.45
3:A:2:LYS:HB2	3:A:2:LYS:HE3	1.50	0.45
3:A:18:ASN:C	3:A:18:ASN:OD1	2.61	0.44
3:A:32:TYR:O	3:A:85:ARG:NH1	2.51	0.43
3:A:6:PHE:CD2	3:A:8:ILE:HD11	2.54	0.43
3:A:92:LEU:HD11	3:A:119:SER:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:DT:H2''	1:B:306:DA:O5'	2.18	0.42
3:A:233:PHE:O	3:A:253:TYR:HB3	2.19	0.42
2:C:313:DT:H2'	2:C:314:DA:C8	2.55	0.42
3:A:64:HIS:CG	3:A:86:PRO:HG3	2.54	0.42
3:A:130:ILE:CG2	3:A:166:MET:HE2	2.49	0.42
3:A:69:GLU:OE1	3:A:69:GLU:HA	2.20	0.42
3:A:221:LEU:O	3:A:224:SER:N	2.38	0.42
3:A:92:LEU:HD12	3:A:117:LYS:HD2	2.02	0.41
3:A:171:ALA:O	3:A:172:ASP:HB2	2.20	0.41
3:A:148:TYR:O	3:A:151:TYR:HB3	2.20	0.41
3:A:43:SER:O	3:A:79:ARG:NH2	2.53	0.41
3:A:236:GLN:NE2	5:A:406:HOH:O	2.53	0.41
3:A:76:TYR:OH	3:A:78:GLU:OE2	2.35	0.41
3:A:257:VAL:HG22	3:A:258:THR:N	2.36	0.40
3:A:233:PHE:O	3:A:254:PRO:HD2	2.22	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:228:GLY:CA	4:D:2:NAG:O7[4_455]	2.18	0.02

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	246/260 (95%)	229 (93%)	17 (7%)	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	221/229 (96%)	195 (88%)	26 (12%)	5 6

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	2	LYS
3	A	10	THR
3	A	11	PHE
3	A	13	GLU
3	A	21	LEU
3	A	30	ARG
3	A	37	ILE
3	A	43	SER
3	A	45	LEU
3	A	66	VAL
3	A	75	SER
3	A	89	VAL
3	A	90	SER
3	A	108	SER
3	A	110	SER
3	A	112	GLU
3	A	119	SER
3	A	138	SER
3	A	139	ASP
3	A	152	LEU
3	A	174	SER
3	A	187	ARG
3	A	220	LEU
3	A	221	LEU
3	A	224	SER
3	A	260	THR

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

Mol	Chain	Res	Type
3	A	44	HIS
3	A	87	ASN
3	A	96	GLN
3	A	155	GLN
3	A	161	ASN
3	A	170	ASN
3	A	236	GLN
3	A	243	ASN

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 ⓘ

2 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
4	NAG	D	1	4,3	14,14,15	1.52	2 (14%)	17,19,21	9.31	11 (64%)
4	NAG	D	2	4	14,14,15	2.25	5 (35%)	17,19,21	4.52	12 (70%)

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	NAG	D	1	4,3	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C1	4.49	1.51	1.43
4	D	2	NAG	O7-C7	4.42	1.33	1.23
4	D	2	NAG	C8-C7	3.92	1.58	1.50
4	D	2	NAG	O5-C1	3.85	1.50	1.43
4	D	2	NAG	C2-N2	-3.24	1.40	1.46
4	D	1	NAG	C4-C5	-2.09	1.48	1.53
4	D	2	NAG	O5-C5	2.08	1.47	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C2-N2-C7	32.96	167.07	122.90
4	D	1	NAG	O7-C7-C8	-13.03	98.86	122.05
4	D	1	NAG	C1-C2-N2	10.96	127.71	110.43
4	D	2	NAG	C2-N2-C7	10.26	136.66	122.90
4	D	2	NAG	C8-C7-N2	-6.98	104.55	116.12
4	D	2	NAG	O3-C3-C2	-6.82	95.24	109.40
4	D	2	NAG	O7-C7-C8	6.78	134.13	122.05
4	D	2	NAG	O3-C3-C4	5.75	123.93	110.38
4	D	2	NAG	O5-C1-C2	-4.59	104.19	111.29
4	D	1	NAG	O5-C1-C2	-3.82	105.38	111.29
4	D	1	NAG	C4-C3-C2	3.77	116.54	111.02
4	D	1	NAG	O3-C3-C4	-3.68	101.71	110.38
4	D	1	NAG	C8-C7-N2	3.62	122.13	116.12
4	D	2	NAG	O4-C4-C3	3.51	118.66	110.38
4	D	1	NAG	O5-C5-C6	3.31	114.10	107.66
4	D	2	NAG	C3-C4-C5	2.90	115.49	110.23
4	D	1	NAG	C3-C4-C5	2.78	115.28	110.23
4	D	1	NAG	C1-O5-C5	-2.69	108.58	112.19
4	D	2	NAG	C1-O5-C5	-2.69	108.58	112.19
4	D	2	NAG	C4-C3-C2	2.47	114.64	111.02
4	D	1	NAG	O3-C3-C2	2.19	113.95	109.40
4	D	2	NAG	O5-C5-C4	-2.15	105.61	110.83
4	D	2	NAG	C6-C5-C4	-2.10	107.86	113.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	1	NAG	C2

All (2) torsion outliers are listed below:

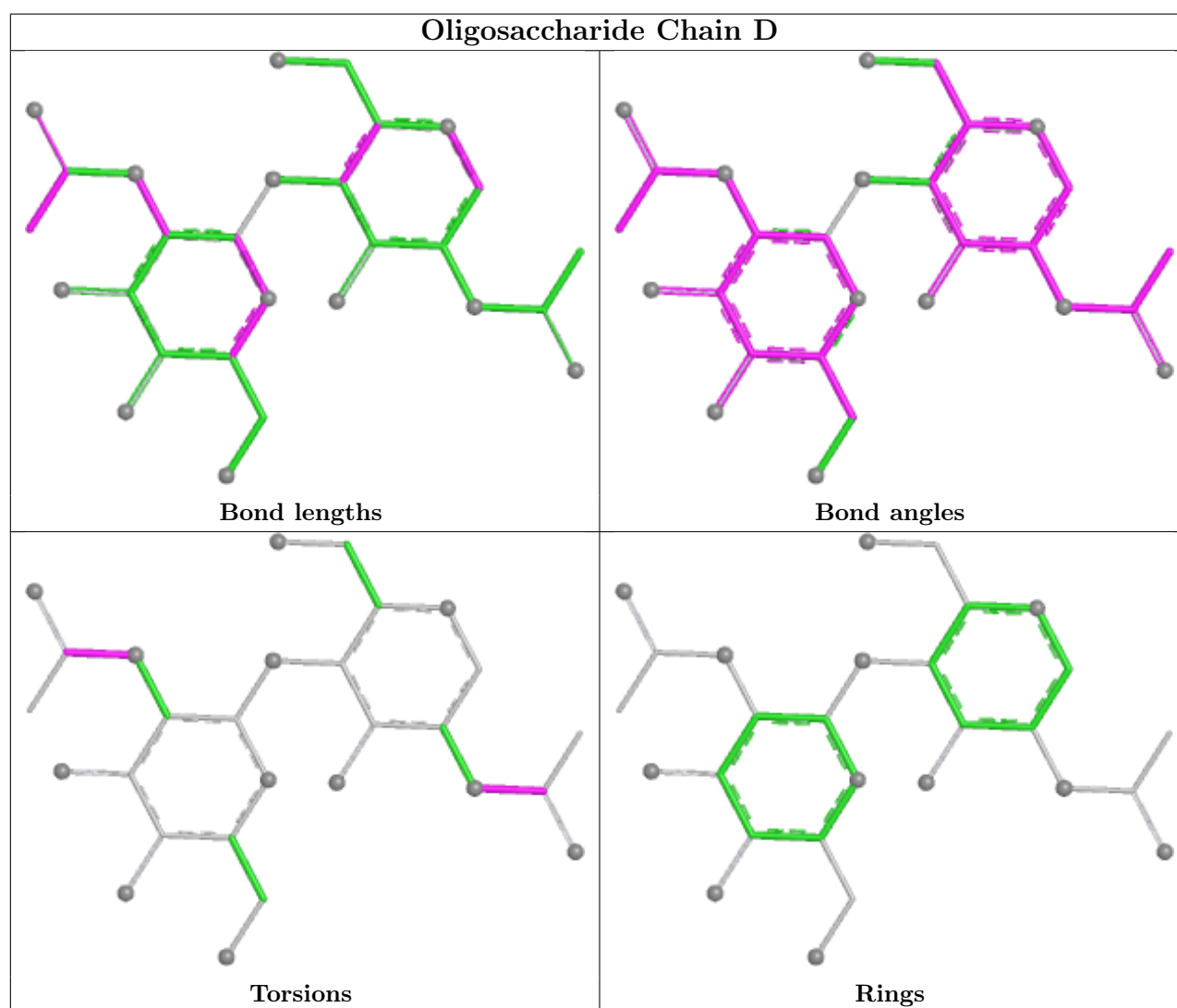
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	0	1

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](#)

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

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.