



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:00 PM UTC

PDB ID : 2WGC / pdb_00002wgc
Title : 2.2 ANGSTROMS RESOLUTION STRUCTURE ANALYSIS OF TWO RE-
FINED N-ACETYLNEURAMINYLLACTOSE-WHEAT GERM AGGLU-
TININ ISOLECTIN COMPLEXES
Authors : Wright, C.S.
Deposited on : 1990-04-03
Resolution : 2.20 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

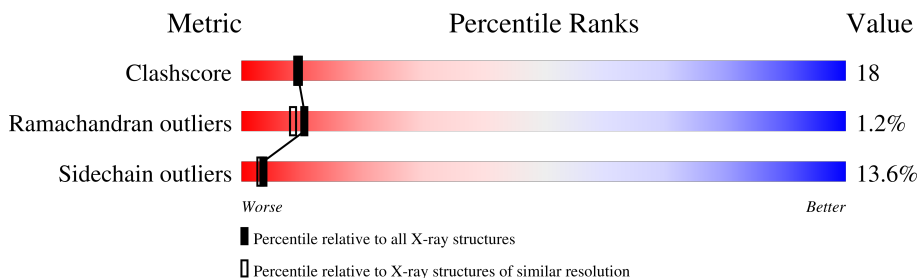
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	171	
1	B	171	
2	C	3	
2	D	3	

2 Entry composition [i](#)

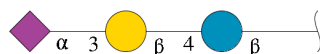
There are 3 unique types of molecules in this entry. The entry contains 2634 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 WHEAT GERM LECTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1159	674	215	236	34			
1	B	171	Total	C	N	O	S	0	0	0
			1154	669	215	236	34			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	D	3	Total	C	N	O	0	0	0
			43	23	1	19			

- Molecule 3 is water.

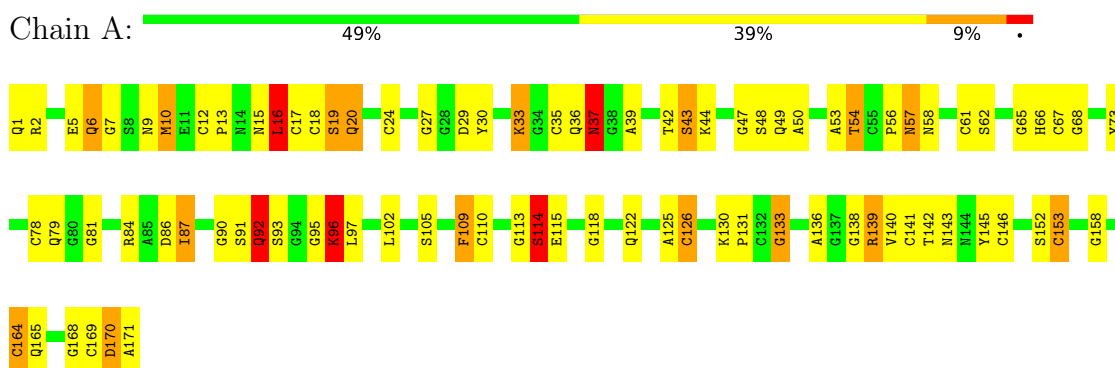
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	120	Total	O	0	0
			120	120		

3 Residue-property plots

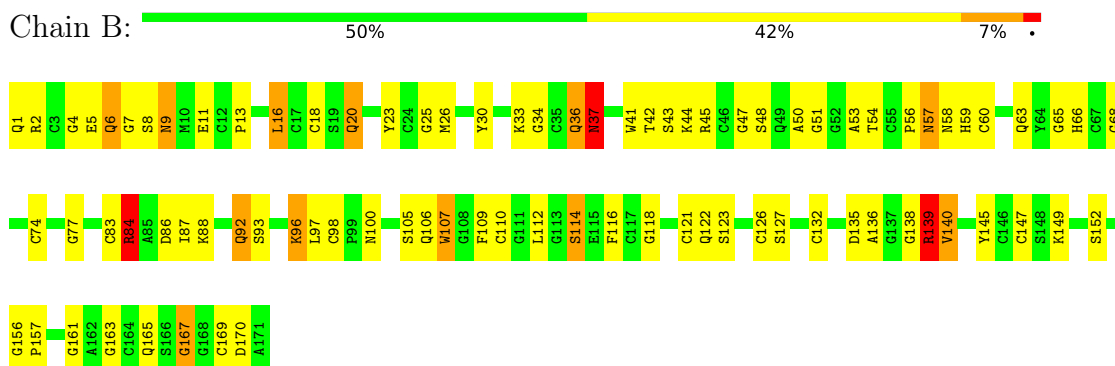
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

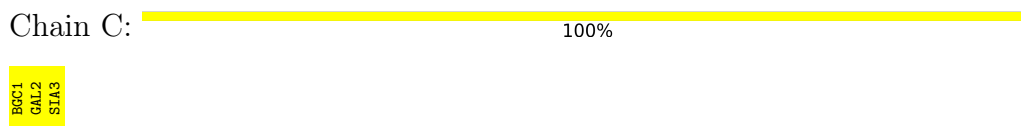
• Molecule 1: WHEAT GERM LECTIN



• Molecule 1: WHEAT GERM LECTIN



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



BGC1
GAL2
SLA3

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	51.44Å 73.35Å 91.68Å 90.00° 97.52° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.153 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2634	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: PCA, GAL, SIA, BGC

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	1.32	3/1175 (0.3%)	2.30	55/1575 (3.5%)
1	B	1.32	1/1168 (0.1%)	2.27	60/1563 (3.8%)
All	All	1.32	4/2343 (0.2%)	2.28	115/3138 (3.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	GLY	N-CA	5.94	1.52	1.44
1	A	16	LEU	N-CA	5.60	1.52	1.46
1	A	13	PRO	N-CD	5.29	1.55	1.47
1	B	68	GLY	N-CA	5.16	1.50	1.45

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ARG	CD-NE-CZ	15.04	145.45	124.40
1	B	57	ASN	CA-CB-CG	10.54	123.14	112.60
1	A	90	GLY	O-C-N	9.61	130.85	122.88
1	B	36	GLN	OE1-CD-NE2	9.20	131.80	122.60
1	A	86	ASP	CA-CB-CG	-9.19	103.41	112.60
1	A	96	LYS	CA-CB-CG	8.54	131.19	114.10
1	B	60	CYS	CA-C-O	-8.04	111.67	120.92
1	A	170	ASP	N-CA-C	-7.94	102.22	112.23
1	A	96	LYS	N-CA-CB	7.77	123.62	110.49
1	A	126	CYS	CA-C-O	-7.69	113.40	121.55
1	B	86	ASP	CA-CB-CG	-7.55	105.05	112.60
1	A	170	ASP	N-CA-CB	7.55	121.93	110.30
1	B	126	CYS	CA-C-O	-7.41	113.44	121.44
1	B	66	HIS	CA-CB-CG	-7.24	106.56	113.80
1	A	109	PHE	CA-CB-CG	-7.24	106.56	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	SER	CB-CA-C	7.11	121.14	109.70
1	B	106	GLN	OE1-CD-NE2	7.00	129.60	122.60
1	B	100	ASN	CA-C-O	-6.97	112.37	121.08
1	A	29	ASP	CA-CB-CG	6.87	119.47	112.60
1	B	107	TRP	N-CA-C	6.84	121.08	112.87
1	B	9	ASN	CA-CB-CG	-6.80	105.80	112.60
1	B	45	ARG	CD-NE-CZ	6.79	133.90	124.40
1	B	20	GLN	OE1-CD-NE2	6.71	129.31	122.60
1	B	139	ARG	CA-CB-CG	6.68	127.46	114.10
1	B	60	CYS	O-C-N	6.65	130.88	123.16
1	B	169	CYS	O-C-N	6.64	130.99	122.89
1	A	133	GLY	CA-C-N	6.52	130.61	120.82
1	A	133	GLY	C-N-CA	6.52	130.61	120.82
1	B	47	GLY	CA-C-N	6.50	133.95	121.54
1	B	47	GLY	C-N-CA	6.50	133.95	121.54
1	B	165	GLN	OE1-CD-NE2	6.46	129.06	122.60
1	B	59	HIS	ND1-CE1-NE2	6.42	114.82	108.40
1	A	113	GLY	N-CA-C	-6.41	105.06	111.85
1	B	16	LEU	N-CA-CB	6.41	119.51	109.83
1	A	153	CYS	O-C-N	6.39	130.49	123.27
1	B	9	ASN	OD1-CG-ND2	6.34	128.94	122.60
1	A	62	SER	CA-CB-OG	-6.32	98.47	111.10
1	B	30	TYR	O-C-N	6.31	130.81	122.36
1	A	44	LYS	CA-C-O	-6.30	114.80	121.99
1	B	84	ARG	NE-CZ-NH1	6.23	127.73	121.50
1	B	43	SER	CA-C-O	-6.22	114.78	121.56
1	A	78	CYS	CA-CB-SG	6.22	128.70	114.40
1	B	109	PHE	CA-C-N	6.13	130.26	121.50
1	B	109	PHE	C-N-CA	6.13	130.26	121.50
1	A	139	ARG	CB-CA-C	6.11	119.82	109.50
1	B	11	GLU	CA-C-N	6.10	129.16	120.49
1	B	11	GLU	C-N-CA	6.10	129.16	120.49
1	B	139	ARG	NH1-CZ-NH2	6.08	127.21	119.30
1	B	53	ALA	CA-C-N	6.07	132.45	122.07
1	B	53	ALA	C-N-CA	6.07	132.45	122.07
1	A	57	ASN	OD1-CG-ND2	6.01	128.61	122.60
1	A	24	CYS	N-CA-C	6.00	119.02	109.24
1	B	13	PRO	CB-CA-C	5.98	118.85	110.60
1	A	27	GLY	CA-C-O	-5.94	116.85	122.13
1	B	42	THR	CA-CB-OG1	-5.92	100.73	109.60
1	A	113	GLY	CA-C-O	5.91	127.12	122.33
1	B	37	ASN	O-C-N	5.89	129.18	123.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ASN	CA-CB-CG	-5.85	106.75	112.60
1	A	15	ASN	CA-CB-CG	5.80	118.40	112.60
1	B	37	ASN	CA-CB-CG	5.79	118.39	112.60
1	B	139	ARG	NE-CZ-NH1	-5.77	115.73	121.50
1	A	168	GLY	CA-C-N	5.77	128.95	120.82
1	A	168	GLY	C-N-CA	5.77	128.95	120.82
1	B	59	HIS	N-CA-C	-5.75	102.79	110.55
1	B	114	SER	CB-CA-C	-5.72	101.25	110.74
1	A	20	GLN	OE1-CD-NE2	5.71	128.31	122.60
1	A	66	HIS	ND1-CG-CD2	5.70	111.80	106.10
1	B	106	GLN	CB-CG-CD	-5.69	102.92	112.60
1	A	54	THR	CA-CB-CG2	5.65	120.10	110.50
1	A	68	GLY	CA-C-N	5.62	131.42	122.59
1	A	68	GLY	C-N-CA	5.62	131.42	122.59
1	A	16	LEU	N-CA-C	-5.60	101.99	110.28
1	A	142	THR	N-CA-C	-5.57	102.51	110.59
1	A	10	MET	CA-C-O	5.57	127.87	121.47
1	A	65	GLY	CA-C-N	5.54	131.50	122.81
1	A	65	GLY	C-N-CA	5.54	131.50	122.81
1	B	147	CYS	CA-C-O	5.52	126.28	120.54
1	A	164	CYS	CA-C-O	-5.49	114.09	120.62
1	A	164	CYS	N-CA-C	-5.48	101.25	109.15
1	B	54	THR	CA-CB-CG2	5.47	119.81	110.50
1	B	114	SER	O-C-N	5.44	128.37	122.11
1	A	169	CYS	O-C-N	5.40	129.64	122.95
1	B	65	GLY	CA-C-N	5.39	131.03	122.62
1	B	65	GLY	C-N-CA	5.39	131.03	122.62
1	B	98	CYS	O-C-N	5.36	128.45	121.64
1	B	127	SER	O-C-N	5.34	128.83	122.26
1	A	84	ARG	CA-C-N	5.33	130.08	122.72
1	A	84	ARG	C-N-CA	5.33	130.08	122.72
1	B	140	VAL	CB-CA-C	5.33	120.03	111.29
1	A	102	LEU	N-CA-C	-5.32	103.36	110.55
1	A	143	ASN	OD1-CG-ND2	5.29	127.89	122.60
1	A	9	ASN	CA-CB-CG	-5.26	107.34	112.60
1	B	50	ALA	CA-C-N	5.25	131.70	121.41
1	B	50	ALA	C-N-CA	5.25	131.70	121.41
1	A	19	SER	CA-CB-OG	5.22	121.55	111.10
1	B	167	GLY	N-CA-C	-5.22	104.58	112.84
1	B	16	LEU	N-CA-C	-5.21	102.67	110.23
1	B	156	GLY	CA-C-N	5.21	125.25	119.32
1	B	156	GLY	C-N-CA	5.21	125.25	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ASN	O-C-N	5.17	130.35	122.03
1	A	114	SER	CB-CA-C	5.15	119.43	110.68
1	A	153	CYS	CA-C-O	-5.14	114.82	120.43
1	A	47	GLY	CA-C-N	5.14	128.53	120.82
1	A	47	GLY	C-N-CA	5.14	128.53	120.82
1	B	41	TRP	CB-CA-C	5.13	119.57	110.85
1	A	84	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	152	SER	N-CA-CB	5.10	119.81	111.08
1	B	84	ARG	NH1-CZ-NH2	-5.08	112.69	119.30
1	A	115	GLU	CG-CD-OE1	5.07	130.07	118.40
1	A	73	TYR	CA-C-N	-5.07	113.49	122.26
1	A	73	TYR	C-N-CA	-5.07	113.49	122.26
1	B	68	GLY	CA-C-N	5.07	130.65	122.29
1	B	68	GLY	C-N-CA	5.07	130.65	122.29
1	B	170	ASP	N-CA-C	-5.05	102.57	110.10
1	A	57	ASN	CA-C-O	-5.00	114.37	120.12

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	1159	0	972	38	0
1	B	1154	0	975	41	0
2	C	43	0	37	0	0
2	D	43	0	37	0	0
3	A	115	0	0	5	0
3	B	120	0	0	8	0
All	All	2634	0	2021	79	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 18.

All (79) 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:92:GLN:HE21	1:B:92:GLN:H	1.25	0.82
1:B:92:GLN:HE22	1:B:122:GLN:HE22	1.31	0.77
1:B:92:GLN:H	1:B:92:GLN:NE2	1.86	0.72
1:A:6:GLN:HE21	1:A:6:GLN:H	1.37	0.71
1:B:2:ARG:O	1:B:7:GLY:HA3	1.93	0.68
1:B:37:ASN:OD1	3:B:356:HOH:O	2.14	0.66
1:A:37:ASN:HD22	1:A:37:ASN:C	2.03	0.66
1:A:164:CYS:HB3	1:A:171:ALA:O	1.96	0.66
1:A:6:GLN:HE22	1:A:36:GLN:HE22	1.45	0.65
1:A:54:THR:HG22	3:A:400:HOH:O	1.98	0.63
1:B:16:LEU:HD22	1:B:26:MET:HG2	1.80	0.63
1:B:20:GLN:NE2	3:B:411:HOH:O	2.33	0.62
1:B:107:TRP:HA	1:B:107:TRP:CE3	2.35	0.62
1:B:83:CYS:HB2	1:B:87:ILE:HD11	1.82	0.61
1:A:56:PRO:HD2	3:A:319:HOH:O	2.02	0.60
1:B:6:GLN:HE22	1:B:36:GLN:HE22	1.49	0.60
1:B:16:LEU:HD13	1:B:25:GLY:HA2	1.83	0.60
1:B:139:ARG:NH1	3:B:410:HOH:O	2.33	0.60
1:B:96:LYS:HD3	3:B:338:HOH:O	2.04	0.57
1:A:7:GLY:O	1:A:10:MET:HB2	2.04	0.56
1:A:61:CYS:O	1:A:79:GLN:N	2.33	0.56
1:B:37:ASN:ND2	3:B:343:HOH:O	2.39	0.56
1:A:2:ARG:O	1:A:7:GLY:HA3	2.06	0.55
1:B:132:CYS:HA	1:B:139:ARG:HG3	1.87	0.55
1:B:107:TRP:CE3	1:B:107:TRP:CA	2.91	0.54
1:A:50:ALA:O	1:A:53:ALA:HB2	2.09	0.53
1:A:133:GLY:O	1:A:136:ALA:N	2.34	0.53
1:B:20:GLN:HG2	3:B:392:HOH:O	2.09	0.53
1:B:135:ASP:HB2	3:B:344:HOH:O	2.08	0.52
1:A:6:GLN:H	1:A:6:GLN:NE2	2.07	0.52
1:B:20:GLN:HB3	1:B:34:GLY:HA3	1.92	0.52
1:A:158:GLY:HA3	3:A:369:HOH:O	2.10	0.51
1:A:17:CYS:HB3	1:A:35:CYS:SG	2.50	0.51
1:B:63:GLN:NE2	3:B:317:HOH:O	2.32	0.50
1:A:92:GLN:HE22	1:A:122:GLN:HE22	1.58	0.50
1:A:93:SER:O	1:A:96:LYS:HG2	2.11	0.50
1:A:92:GLN:NE2	1:A:92:GLN:H	2.10	0.50
1:A:18:CYS:HB2	1:A:37:ASN:HD21	1.78	0.49
1:B:87:ILE:HB	1:B:110:CYS:HB2	1.95	0.49
1:B:107:TRP:CD2	1:B:107:TRP:N	2.79	0.48
1:B:97:LEU:HD23	1:B:123:SER:OG	2.13	0.48
1:A:20:GLN:NE2	3:A:411:HOH:O	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:CYS:O	1:B:84:ARG:HB2	2.13	0.48
1:B:57:ASN:O	1:B:58:ASN:HB2	2.13	0.48
1:A:87:ILE:HB	1:A:110:CYS:HB2	1.96	0.47
1:A:114:SER:O	1:A:118:GLY:HA3	2.14	0.47
1:A:136:ALA:C	1:A:138:GLY:N	2.68	0.47
1:B:136:ALA:C	1:B:138:GLY:H	2.21	0.47
1:B:157:PRO:O	1:B:161:GLY:HA3	2.14	0.47
1:B:107:TRP:HA	1:B:107:TRP:HE3	1.75	0.47
1:B:63:GLN:HB3	1:B:77:GLY:HA3	1.96	0.46
1:A:95:GLY:O	1:A:96:LYS:C	2.59	0.45
1:B:16:LEU:HA	1:B:26:MET:HE2	1.99	0.45
1:A:43:SER:HB3	1:A:67:CYS:O	2.16	0.45
1:B:18:CYS:HB3	1:B:36:GLN:HB2	1.98	0.45
1:A:49:GLN:OE1	1:A:49:GLN:N	2.48	0.45
1:B:118:GLY:O	1:B:121:CYS:HB2	2.17	0.44
1:A:146:CYS:O	1:A:153:CYS:HA	2.18	0.44
1:A:12:CYS:HB2	1:A:16:LEU:O	2.17	0.44
1:A:57:ASN:O	1:A:58:ASN:HB2	2.16	0.44
1:A:141:CYS:HB3	1:A:145:TYR:HB2	2.00	0.43
1:B:92:GLN:NE2	1:B:92:GLN:N	2.62	0.43
1:A:130:LYS:HA	1:A:131:PRO:HD3	1.80	0.43
1:B:149:LYS:HB3	1:B:163:GLY:HA3	2.01	0.42
1:A:105:SER:HA	3:A:380:HOH:O	2.20	0.42
1:A:42:THR:O	1:A:43:SER:C	2.61	0.42
1:A:33:LYS:O	1:A:33:LYS:HD3	2.19	0.42
1:B:16:LEU:HD13	1:B:25:GLY:CA	2.49	0.42
1:A:92:GLN:H	1:A:92:GLN:HE21	1.66	0.42
1:B:105:SER:HB3	1:B:116:PHE:HA	2.02	0.42
1:A:19:SER:HB3	1:A:30:TYR:HA	2.03	0.41
1:B:4:GLY:O	1:B:9:ASN:N	2.50	0.41
1:B:92:GLN:HE21	1:B:92:GLN:N	2.03	0.41
1:B:2:ARG:NH1	1:B:23:TYR:OH	2.54	0.41
1:A:87:ILE:O	1:A:109:PHE:HA	2.21	0.41
1:B:56:PRO:O	1:B:57:ASN:HB2	2.20	0.41
1:B:145:TYR:O	1:B:167:GLY:HA3	2.20	0.41
1:A:33:LYS:HD3	1:A:33:LYS:C	2.46	0.40
1:A:125:ALA:O	1:A:126:CYS:C	2.60	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	
1	A	169/171 (99%)	149 (88%)	18 (11%)	2 (1%)	10	8
1	B	169/171 (99%)	156 (92%)	11 (6%)	2 (1%)	10	8
All	All	338/342 (99%)	305 (90%)	29 (9%)	4 (1%)	10	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	93	SER
1	A	39	ALA
1	A	92	GLN
1	B	51	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	
1	A	118/120 (98%)	101 (86%)	17 (14%)	3	2
1	B	118/120 (98%)	103 (87%)	15 (13%)	4	4
All	All	236/240 (98%)	204 (86%)	32 (14%)	3	3

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	6	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	16	LEU
1	A	33	LYS
1	A	37	ASN
1	A	48	SER
1	A	87	ILE
1	A	91	SER
1	A	92	GLN
1	A	96	LYS
1	A	97	LEU
1	A	114	SER
1	A	139	ARG
1	A	140	VAL
1	A	152	SER
1	A	165	GLN
1	A	170	ASP
1	B	5	GLU
1	B	6	GLN
1	B	8	SER
1	B	33	LYS
1	B	37	ASN
1	B	44	LYS
1	B	48	SER
1	B	84	ARG
1	B	88	LYS
1	B	92	GLN
1	B	96	LYS
1	B	112	LEU
1	B	114	SER
1	B	139	ARG
1	B	140	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	9	ASN
1	A	37	ASN
1	A	63	GLN
1	A	92	GLN
1	B	6	GLN
1	B	9	ASN
1	B	37	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	92	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	A	1	1	7,8,9	1.21	1 (14%)	9,10,12	2.04	3 (33%)
1	PCA	B	1	1	7,8,9	1.00	0	9,10,12	1.61	1 (11%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	O-C	2.80	1.30	1.20

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	PCA	O-C-CA	-4.19	113.99	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	O-C-CA	-4.07	114.30	124.77
1	A	1	PCA	CB-CA-C	2.66	116.30	112.66
1	A	1	PCA	CB-CG-CD	-2.42	100.67	104.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

6 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	BGC	C	1	2	12,12,12	1.28	2 (16%)	17,17,17	1.48	3 (17%)
2	GAL	C	2	2	11,11,12	0.89	0	15,15,17	1.66	4 (26%)
2	SIA	C	3	2	20,20,21	1.20	2 (10%)	21,28,31	2.53	8 (38%)
2	BGC	D	1	2	12,12,12	1.22	1 (8%)	17,17,17	1.09	0
2	GAL	D	2	2	11,11,12	0.90	0	15,15,17	1.50	3 (20%)
2	SIA	D	3	2	20,20,21	1.37	3 (15%)	21,28,31	2.29	6 (28%)

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	BGC	C	1	2	-	1/2/22/22	0/1/1/1
2	GAL	C	2	2	-	1/2/19/22	0/1/1/1
2	SIA	C	3	2	-	3/18/34/38	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	D	1	2	-	2/2/22/22	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	SIA	D	3	2	-	3/18/34/38	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	SIA	O1B-C1	-3.16	1.20	1.30
2	D	3	SIA	O1A-C1	3.06	1.31	1.22
2	C	1	BGC	O2-C2	2.90	1.50	1.43
2	C	3	SIA	O1B-C1	-2.85	1.21	1.30
2	D	1	BGC	O2-C2	2.84	1.50	1.43
2	C	3	SIA	O1A-C1	2.81	1.30	1.22
2	D	3	SIA	C2-C1	2.30	1.55	1.52
2	C	1	BGC	O1-C1	2.12	1.46	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	SIA	O1A-C1-C2	-6.28	109.28	122.85
2	C	3	SIA	O1B-C1-C2	5.24	126.33	112.71
2	C	3	SIA	O1A-C1-C2	-4.65	112.80	122.85
2	C	3	SIA	C5-N5-C10	4.56	133.79	123.11
2	C	3	SIA	O10-C10-N5	4.50	129.94	121.98
2	D	3	SIA	O1B-C1-C2	4.34	123.99	112.71
2	D	3	SIA	O10-C10-N5	3.74	128.59	121.98
2	C	3	SIA	O8-C8-C9	3.54	117.06	109.03
2	C	2	GAL	C1-C2-C3	-3.28	104.86	109.64
2	D	3	SIA	O4-C4-C5	3.28	117.31	109.84
2	C	2	GAL	O3-C3-C4	3.04	117.53	110.38
2	C	2	GAL	C6-C5-C4	2.97	120.32	113.02
2	D	3	SIA	O10-C10-C11	-2.94	116.83	122.05
2	C	3	SIA	C11-C10-N5	-2.86	111.37	116.12
2	C	1	BGC	O4-C4-C3	-2.69	104.04	110.38
2	D	2	GAL	O3-C3-C2	-2.45	105.05	110.05
2	D	2	GAL	C6-C5-C4	2.39	118.89	113.02
2	C	3	SIA	C4-C5-N5	2.39	115.14	110.44
2	D	3	SIA	C6-C5-N5	-2.37	107.13	110.91
2	C	3	SIA	O6-C2-C1	2.26	111.98	107.72
2	C	1	BGC	C3-C4-C5	-2.23	106.20	110.23
2	C	1	BGC	O4-C4-C5	-2.18	103.96	109.32
2	D	2	GAL	O4-C4-C3	-2.12	105.38	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	GAL	O5-C5-C4	-2.12	105.68	110.83

There are no chirality outliers.

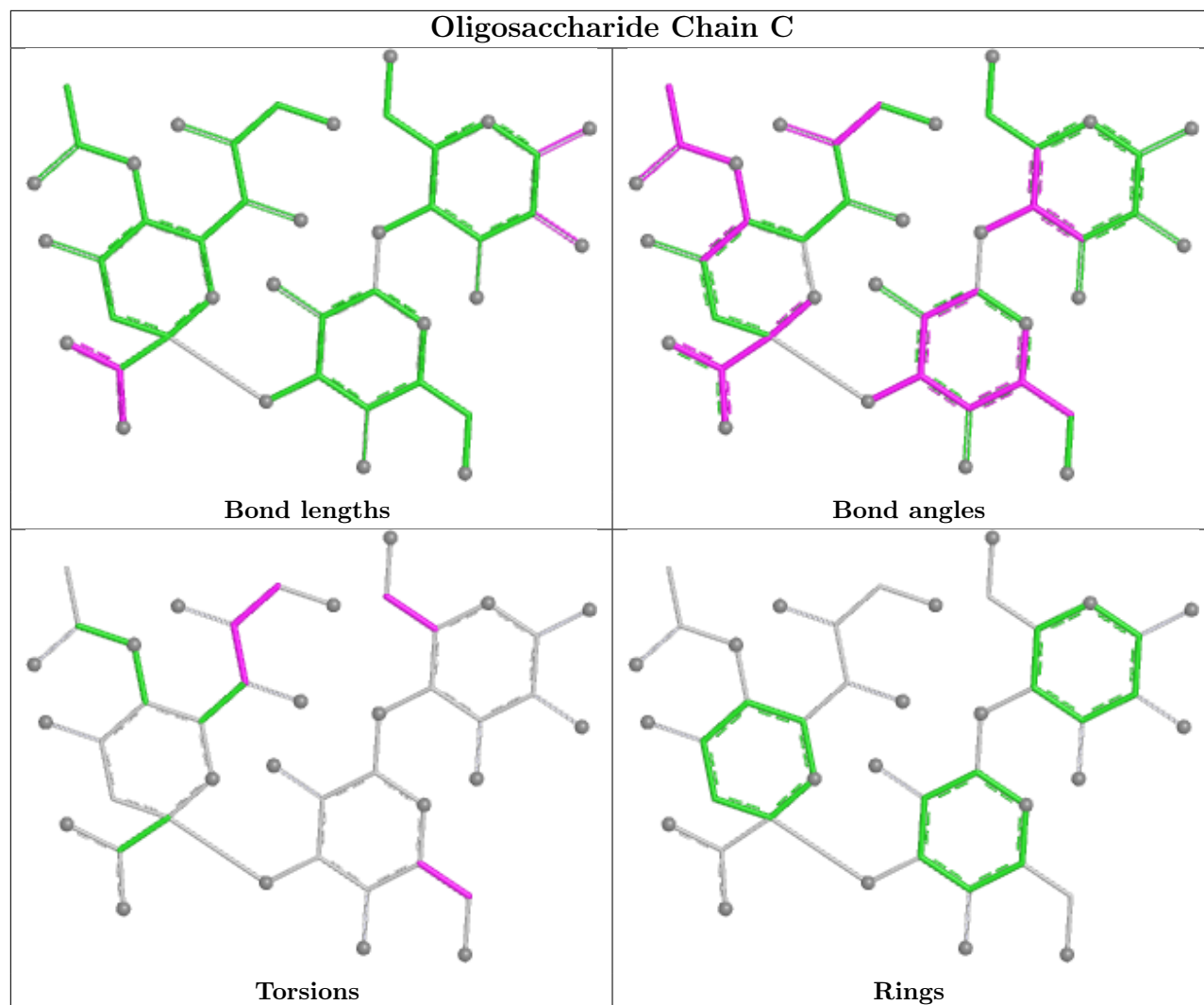
All (10) torsion outliers are listed below:

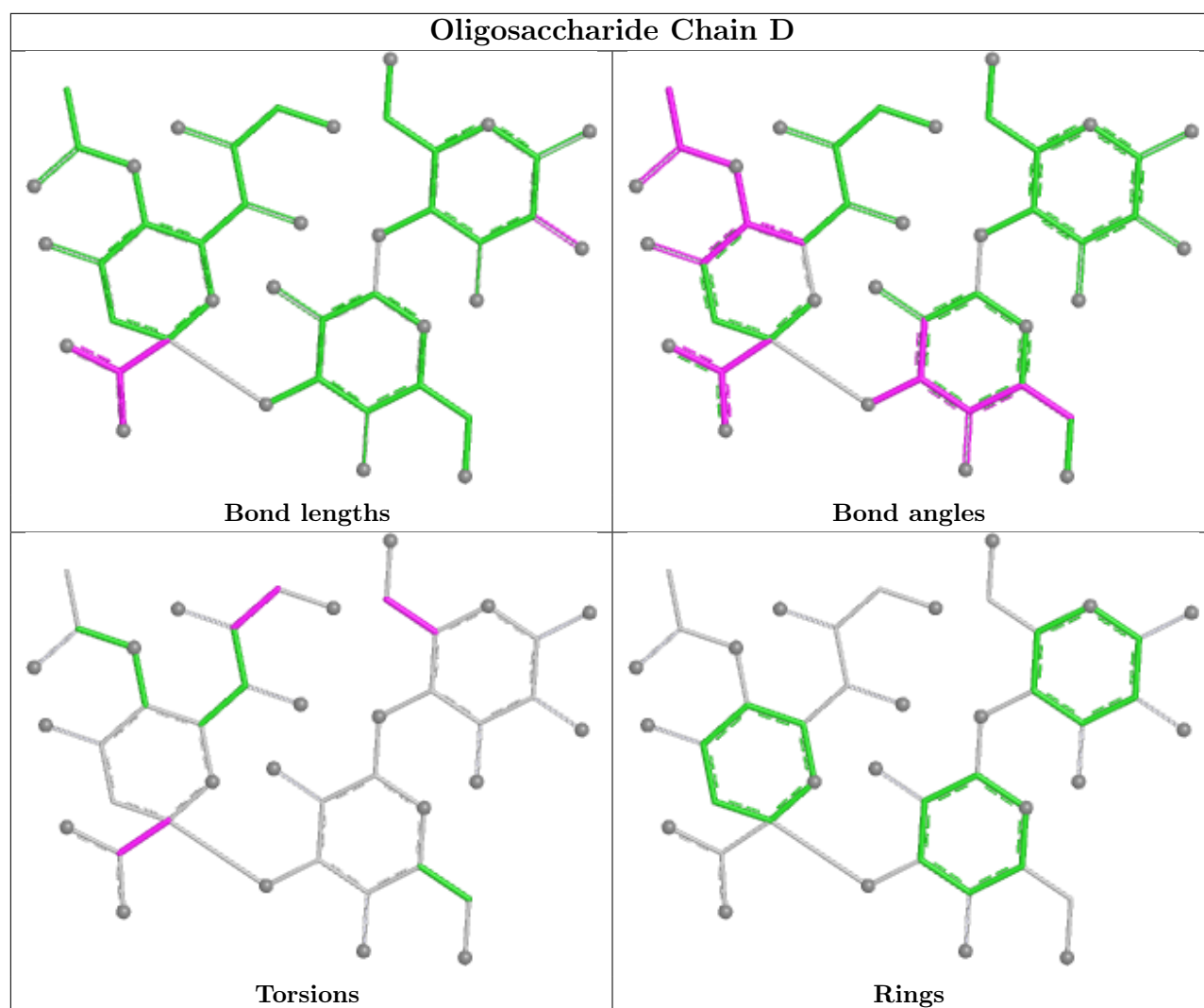
Mol	Chain	Res	Type	Atoms
2	C	3	SIA	O8-C8-C9-O9
2	D	3	SIA	O8-C8-C9-O9
2	C	3	SIA	C7-C8-C9-O9
2	D	1	BGC	C4-C5-C6-O6
2	D	1	BGC	O5-C5-C6-O6
2	D	3	SIA	C7-C8-C9-O9
2	C	1	BGC	O5-C5-C6-O6
2	C	2	GAL	O5-C5-C6-O6
2	D	3	SIA	O1A-C1-C2-O6
2	C	3	SIA	O7-C7-C8-C9

There are no ring outliers.

No monomer is involved in short contacts.

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 [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 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.