



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 07:59 AM BST

PDB ID : 1GYC
Title : CRYSTAL STRUCTURE DETERMINATION AT ROOM TEMPERATURE
OF A LACCASE FROM TRAMETES VERSICOLOR IN ITS OXIDISED
FORM CONTAINING A FULL COMPLEMENT OF COPPER IONS
Authors : Choinowski, T.; Antorini, M.; Piontek, K.
Deposited on : 2002-04-23
Resolution : 1.90 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

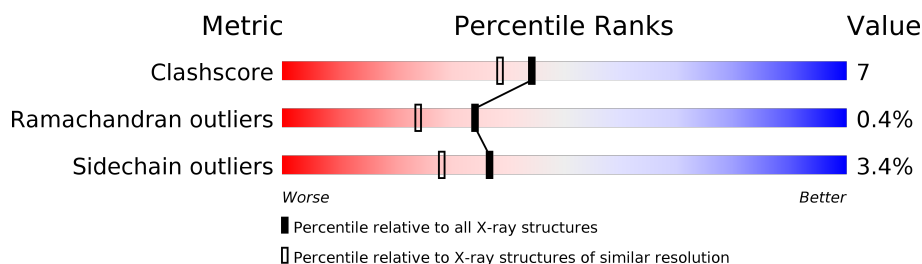
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 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	499	
2	B	2	
2	C	2	
2	D	2	

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
5	IPA	A	1514	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4600 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.

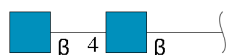
- Molecule 1 is a protein called LACCASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	9	0
			3872	2479	665	720	8			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	VAL	SEE REMARK 999	UNP Q12718
A	31	PHE	VAL	SEE REMARK 999	UNP Q12718
A	49	VAL	ASP	variant	UNP Q12718
A	56	THR	SER	SEE REMARK 999	UNP Q12718
A	259	ILE	VAL	SEE REMARK 999	UNP Q12718
A	343	SER	THR	SEE REMARK 999	UNP Q12718
A	460	GLU	ASP	SEE REMARK 999	UNP Q12718

- Molecule 2 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
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Cu 4 4	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	3	1		
5	A	1	Total	C	O	0	0
			4	3	1		

- Molecule 6 is water.

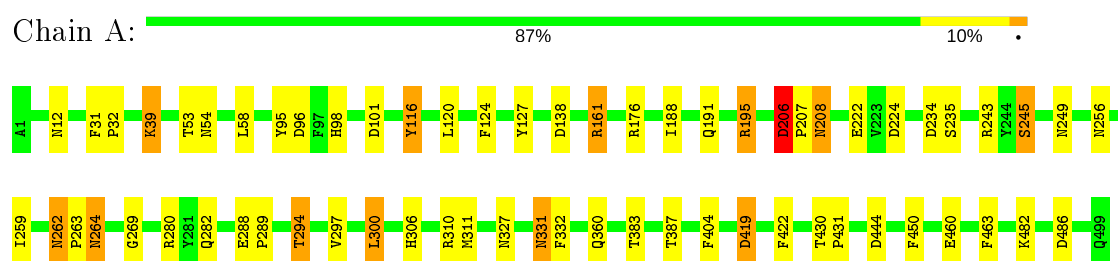
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	590	Total	O	0	0
			590	590		

3 Residue-property plots [i](#)

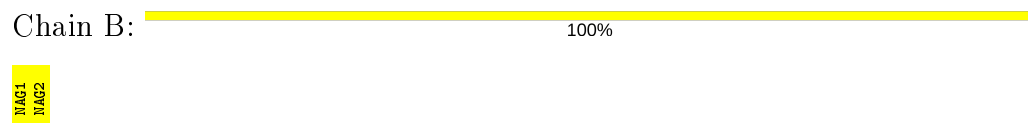
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: LACCASE 2



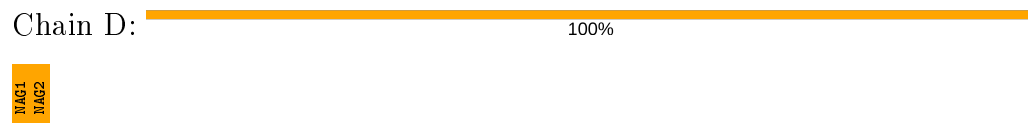
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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 21	Depositor
Cell constants a, b, c, α , β , γ	83.68Å 84.98Å 91.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.90 – 1.90	Depositor
% Data completeness (in resolution range)	99.4 (17.90-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.159 , 0.212	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4600	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: IPA, NAG, CU

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	0.65	0/3992	1.16	18/5485 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	A	195	ARG	CD-NE-CZ	9.46	136.84	123.60
1	A	96	ASP	CB-CG-OD2	7.71	125.24	118.30
1	A	195	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	A	116	TYR	CA-CB-CG	7.24	127.15	113.40
1	A	444	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	224	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	116	TYR	CB-CG-CD1	5.94	124.56	121.00
1	A	96	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	A	161	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	235	SER	N-CA-CB	5.83	119.25	110.50
1	A	245	SER	N-CA-CB	5.82	119.23	110.50
1	A	234	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	419	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	176	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	95	TYR	CB-CG-CD2	-5.26	117.85	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	206	ASP	CB-CG-OD1	5.24	123.01	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300[B]	LEU	Mainchain

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	3872	0	3729	50	0
2	B	28	0	25	0	0
2	C	28	0	24	3	0
2	D	28	0	25	3	0
3	A	4	0	0	0	0
4	A	42	0	39	0	0
5	A	8	0	16	6	0
6	A	590	0	0	9	1
All	All	4600	0	3858	52	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 7.

All (52) 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:A:161:ARG:HH22	5:A:1514:IPA:H2	1.20	1.02
1:A:256:ASN:HD21	1:A:280:ARG:HE	1.16	0.92
1:A:331:ASN:HD22	1:A:332:PHE:H	1.17	0.91
1:A:161:ARG:HH22	5:A:1514:IPA:C2	1.90	0.84
1:A:262:ASN:HD21	1:A:269:GLY:H	1.26	0.79
1:A:161:ARG:NH2	5:A:1514:IPA:H2	1.96	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLN:HG2	1:A:282:GLN:HE21	1.51	0.76
1:A:264:ASN:HD22	1:A:264:ASN:H	1.35	0.73
1:A:256:ASN:ND2	1:A:280:ARG:HE	1.88	0.71
1:A:460:GLU:O	5:A:1514:IPA:H11	1.93	0.68
1:A:306:HIS:HD2	1:A:419:ASP:O	1.81	0.64
1:A:262:ASN:ND2	1:A:269:GLY:H	1.96	0.63
5:A:1513:IPA:H13	6:A:2139:HOH:O	2.00	0.62
1:A:39[B]:LYS:HD3	1:A:127:TYR:HB2	1.82	0.61
1:A:191:GLN:HG2	1:A:282:GLN:NE2	2.13	0.61
1:A:208:ASN:H	1:A:264:ASN:ND2	1.99	0.60
1:A:360:GLN:HG2	6:A:1938:HOH:O	2.02	0.59
1:A:138:ASP:OD2	1:A:195:ARG:HD3	2.04	0.58
1:A:331:ASN:HD22	1:A:332:PHE:N	1.97	0.57
1:A:294:THR:HG22	6:A:1816:HOH:O	2.06	0.56
1:A:188:ILE:HD12	1:A:259:ILE:HD13	1.87	0.55
1:A:206:ASP:HB3	1:A:207:PRO:CD	2.38	0.54
1:A:98:HIS:HD2	6:A:2073:HOH:O	1.91	0.53
5:A:1514:IPA:H12	6:A:1779:HOH:O	2.10	0.51
1:A:430:THR:HB	1:A:431:PRO:HD2	1.94	0.50
1:A:12:ASN:ND2	1:A:53:THR:H	2.08	0.50
1:A:12:ASN:HD21	1:A:54:ASN:H	1.60	0.49
1:A:297:VAL:HG21	2:C:2:NAG:H81	1.94	0.48
1:A:331:ASN:ND2	1:A:332:PHE:H	1.98	0.48
1:A:188:ILE:HD12	1:A:259:ILE:CD1	2.43	0.48
1:A:31:PHE:CD1	1:A:32:PRO:HA	2.48	0.48
1:A:294:THR:HG23	6:A:2013:HOH:O	2.13	0.47
1:A:306:HIS:HE1	6:A:2061:HOH:O	1.98	0.47
1:A:262:ASN:HD22	1:A:263:PRO:HD2	1.80	0.47
1:A:207:PRO:HA	1:A:264:ASN:HD21	1.81	0.46
1:A:12:ASN:ND2	1:A:54:ASN:H	2.14	0.46
1:A:300[B]:LEU:HD13	1:A:300[B]:LEU:C	2.37	0.45
1:A:327:ASN:HB2	2:D:2:NAG:H83	1.99	0.44
1:A:297:VAL:HG21	2:C:2:NAG:C8	2.47	0.44
1:A:311[B]:MET:HE1	6:A:1783:HOH:O	2.17	0.43
1:A:297:VAL:HG11	2:C:2:NAG:H81	2.00	0.43
1:A:12:ASN:HD22	1:A:53:THR:H	1.67	0.43
1:A:264:ASN:H	1:A:264:ASN:ND2	2.10	0.43
1:A:222:GLU:HB3	1:A:245:SER:HB2	2.02	0.42
1:A:206:ASP:HB3	1:A:207:PRO:HD3	2.01	0.42
1:A:311[B]:MET:HE2	6:A:2173:HOH:O	2.21	0.41
1:A:482[B]:LYS:HE3	1:A:486:ASP:OD1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLU:HA	1:A:289:PRO:HD3	1.93	0.41
1:A:383:THR:HG21	2:D:1:NAG:H62	2.01	0.41
1:A:101:ASP:OD1	1:A:101:ASP:N	2.54	0.40
1:A:404:PHE:O	1:A:422:PHE:HA	2.21	0.40
1:A:327:ASN:CB	2:D:2:NAG:H83	2.51	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)
6:A:1709:HOH:O	6:A:2074:HOH:O[2_555]	1.99	0.21

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	506/499 (101%)	494 (98%)	10 (2%)	2 (0%)	34 24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASP
1	A	58	LEU

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	416/407 (102%)	401 (96%)	15 (4%)	35	26

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39[A]	LYS
1	A	39[B]	LYS
1	A	116	TYR
1	A	120	LEU
1	A	124	PHE
1	A	208	ASN
1	A	243	ARG
1	A	249	ASN
1	A	262	ASN
1	A	264	ASN
1	A	294	THR
1	A	331	ASN
1	A	387	THR
1	A	450	PHE
1	A	463	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	47	ASN
1	A	70	GLN
1	A	84	GLN
1	A	98	HIS
1	A	208	ASN
1	A	227	ASN
1	A	237	GLN
1	A	249	ASN
1	A	256	ASN
1	A	262	ASN
1	A	264	ASN
1	A	282	GLN
1	A	306	HIS
1	A	327	ASN
1	A	331	ASN
1	A	336	ASN
1	A	363	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	442	GLN
1	A	478	ASN
1	A	498	ASN
1	A	499	GLN

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 ⓘ

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	NAG	B	1	1,2	14,14,15	1.22	2 (14%)	17,19,21	1.34	2 (11%)
2	NAG	B	2	2	14,14,15	1.21	1 (7%)	17,19,21	1.33	3 (17%)
2	NAG	C	1	1,2	14,14,15	1.20	1 (7%)	17,19,21	0.98	0
2	NAG	C	2	2	14,14,15	1.62	2 (14%)	17,19,21	5.88	8 (47%)
2	NAG	D	1	1,2	14,14,15	1.16	1 (7%)	17,19,21	0.86	0
2	NAG	D	2	2	14,14,15	1.45	1 (7%)	17,19,21	2.62	7 (41%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	5/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	O7-C7	-3.85	1.14	1.23
2	C	1	NAG	O7-C7	-3.82	1.14	1.23
2	C	2	NAG	C2-N2	-3.71	1.40	1.46
2	C	2	NAG	O7-C7	-3.63	1.15	1.23
2	D	1	NAG	O7-C7	-3.42	1.15	1.23
2	B	2	NAG	O7-C7	-3.35	1.15	1.23
2	B	1	NAG	O7-C7	-3.25	1.15	1.23
2	B	1	NAG	C4-C5	2.29	1.57	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C2-N2-C7	20.70	152.37	122.90
2	C	2	NAG	C1-C2-N2	7.31	122.97	110.49
2	C	2	NAG	O7-C7-N2	-6.04	110.85	121.95
2	D	2	NAG	O5-C1-C2	-5.96	101.88	111.29
2	D	2	NAG	C2-N2-C7	4.86	129.83	122.90
2	D	2	NAG	C4-C3-C2	-4.72	104.10	111.02
2	C	2	NAG	O5-C1-C2	-4.47	104.23	111.29
2	C	2	NAG	C4-C3-C2	-4.13	104.97	111.02
2	C	2	NAG	O7-C7-C8	3.13	127.87	122.06
2	C	2	NAG	C8-C7-N2	3.04	121.24	116.10
2	C	2	NAG	C1-O5-C5	2.99	116.25	112.19
2	D	2	NAG	C1-C2-N2	2.83	115.33	110.49
2	B	2	NAG	C8-C7-N2	-2.78	111.39	116.10
2	B	1	NAG	O4-C4-C5	-2.68	102.65	109.30
2	B	1	NAG	O5-C1-C2	-2.38	107.53	111.29
2	D	2	NAG	O5-C5-C4	2.37	116.61	110.83
2	D	2	NAG	C3-C4-C5	2.31	114.36	110.24
2	B	2	NAG	O5-C1-C2	-2.19	107.82	111.29
2	B	2	NAG	O5-C5-C4	-2.16	105.56	110.83
2	D	2	NAG	C6-C5-C4	-2.13	108.01	113.00

There are no chirality outliers.

All (11) torsion outliers are listed below:

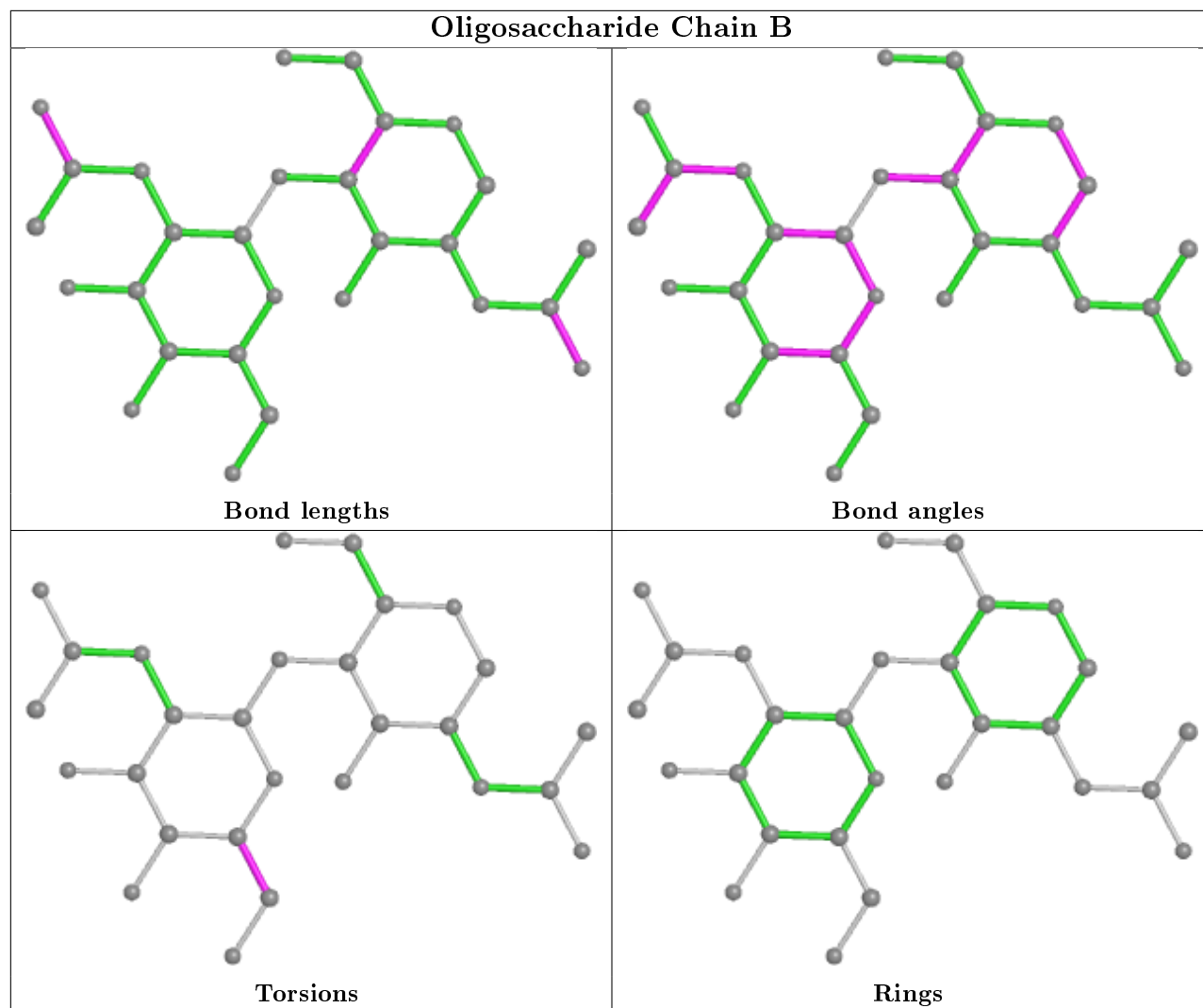
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C3-C2-N2-C7
2	B	2	NAG	O5-C5-C6-O6

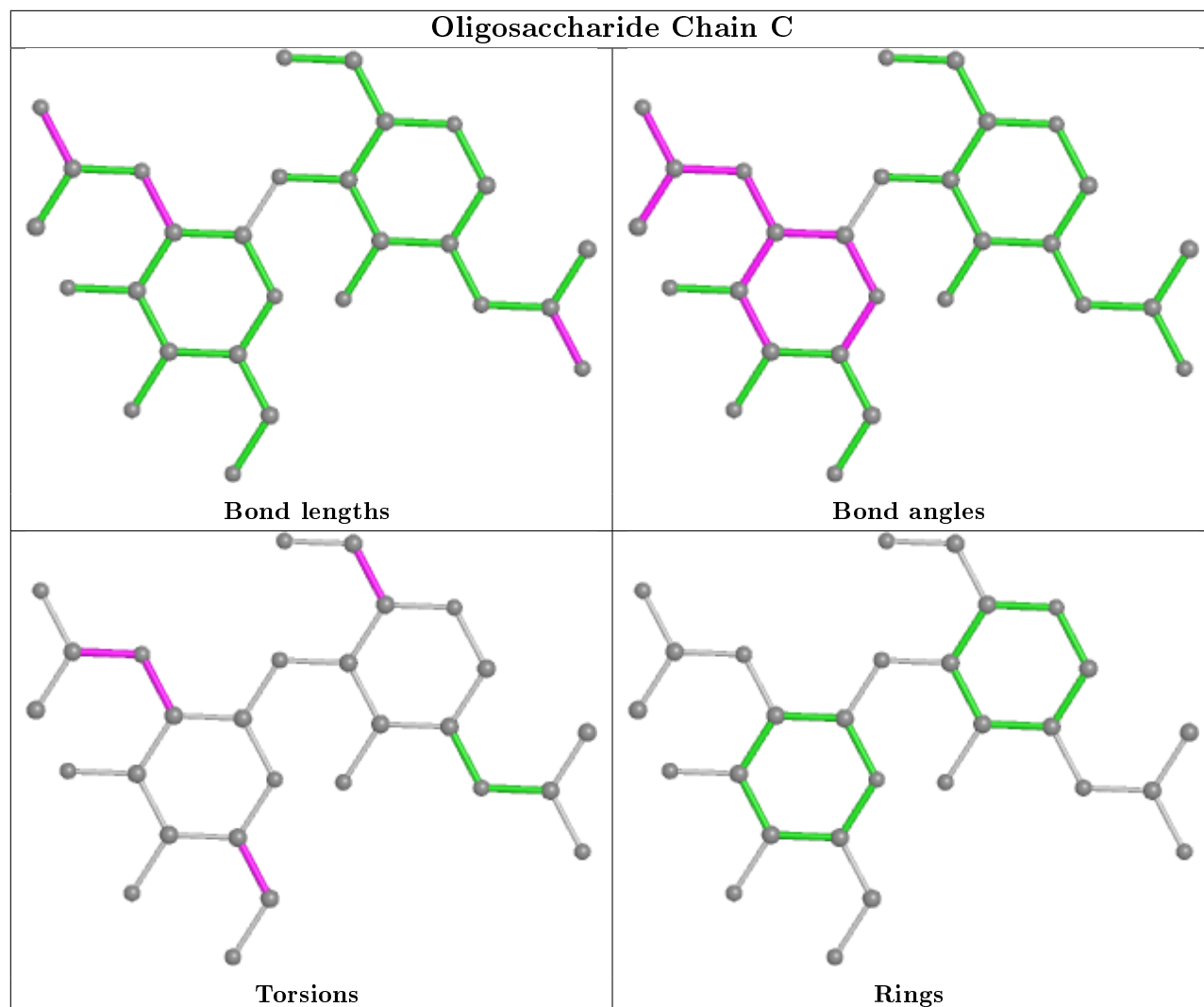
There are no ring outliers.

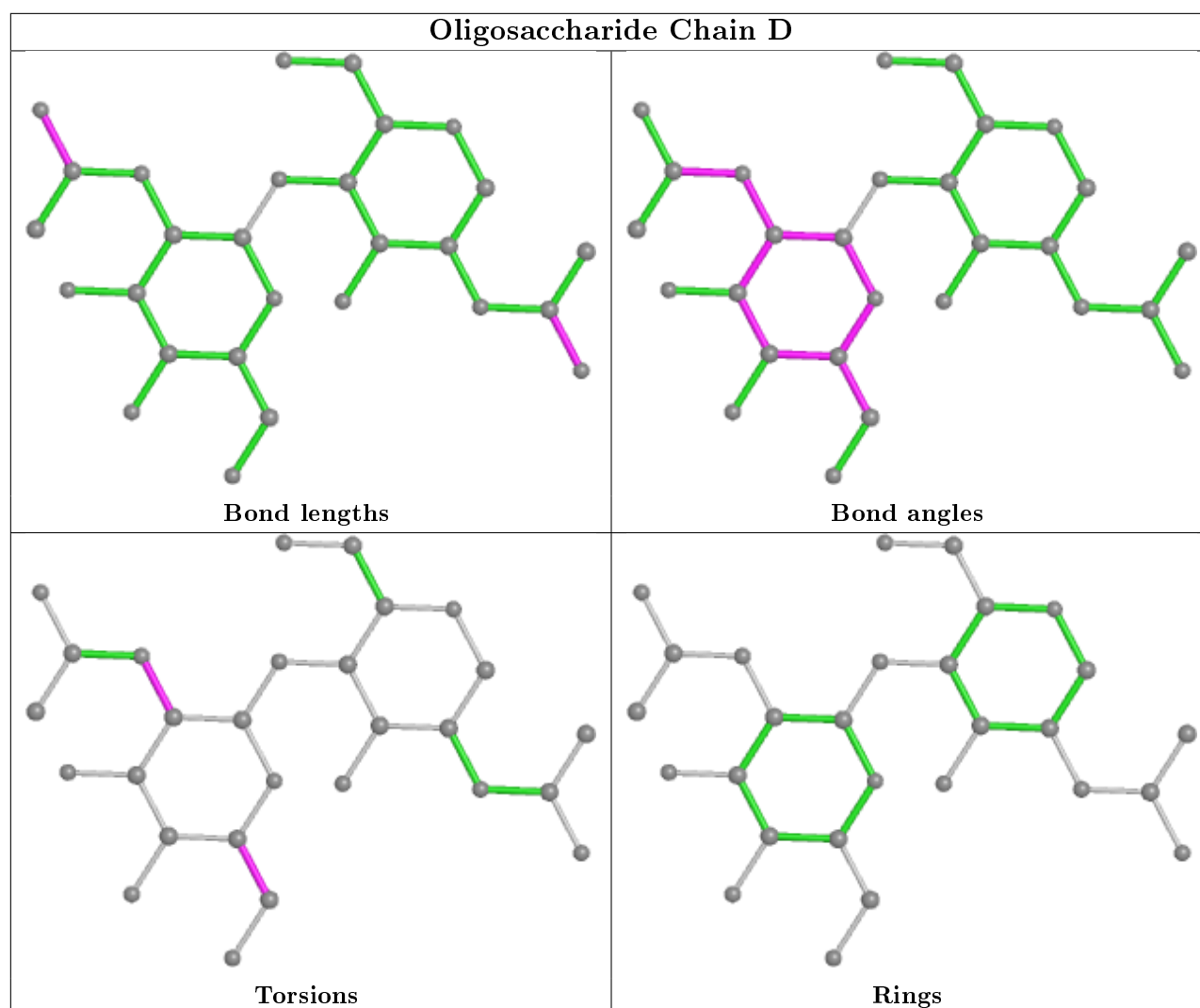
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	D	2	NAG	2	0
2	C	2	NAG	3	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 ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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	A	1512	1	14,14,15	1.25	2 (14%)	17,19,21	1.03	0
5	IPA	A	1513	-	3,3,3	1.09	0	3,3,3	0.95	0
4	NAG	A	1509	1	14,14,15	1.11	1 (7%)	17,19,21	1.13	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	IPA	A	1514	-	3,3,3	1.04	0	3,3,3	0.82	0
4	NAG	A	1508	1	14,14,15	1.35	1 (7%)	17,19,21	1.83	4 (23%)

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	A	1512	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1509	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1508	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1508	NAG	O7-C7	-3.57	1.15	1.23
4	A	1512	NAG	O7-C7	-3.51	1.15	1.23
4	A	1509	NAG	O7-C7	-3.35	1.15	1.23
4	A	1512	NAG	C2-N2	2.18	1.50	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1508	NAG	C4-C3-C2	4.27	117.27	111.02
4	A	1508	NAG	O5-C1-C2	-3.66	105.50	111.29
4	A	1508	NAG	C3-C4-C5	3.18	115.91	110.24
4	A	1509	NAG	C1-O5-C5	-2.29	109.09	112.19
4	A	1509	NAG	O5-C5-C4	-2.28	105.29	110.83
4	A	1509	NAG	O5-C1-C2	-2.14	107.91	111.29
4	A	1508	NAG	C2-N2-C7	-2.13	119.86	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1508	NAG	C8-C7-N2-C2
4	A	1508	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1513	IPA	1	0
5	A	1514	IPA	5	0

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.