



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:35 PM UTC

PDB ID : 1IEX / pdb_00001iex
Title : Crystal structure of barley beta-D-glucan glucohydrolase isoenzyme Exo1 in complex with 4I,4III,4V-S-trithiocellohexaose
Authors : Hrmova, M.; DeGori, R.; Fincher, G.B.; Smith, B.J.; Driguez, H.; Varghese, J.N.
Deposited on : 2001-04-11
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

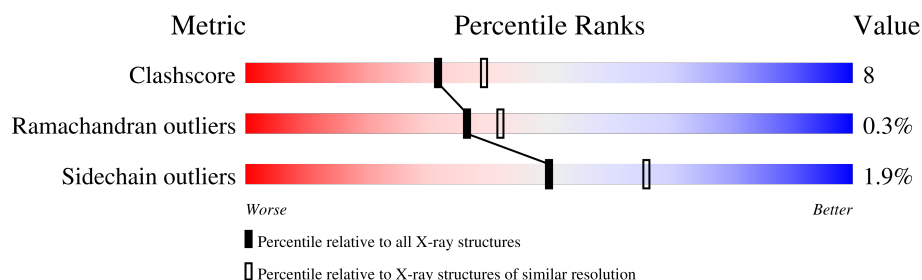
1 Overall quality at a glance

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	605	
2	B	6	
3	C	2	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4987 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.

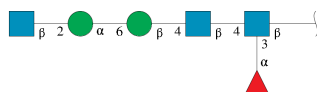
- Molecule 1 is a protein called BETA-D-GLUCAN GLUCOHYDROLASE ISOENZYME EXO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	0	0	0
			4575	2897	789	863	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	LYS	ASN	SEE REMARK 999	GB 4566505

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			74	42	3	29			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	S	0	0	0
			23	12	10	1			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	301	Total	O	0	0
			301	301		

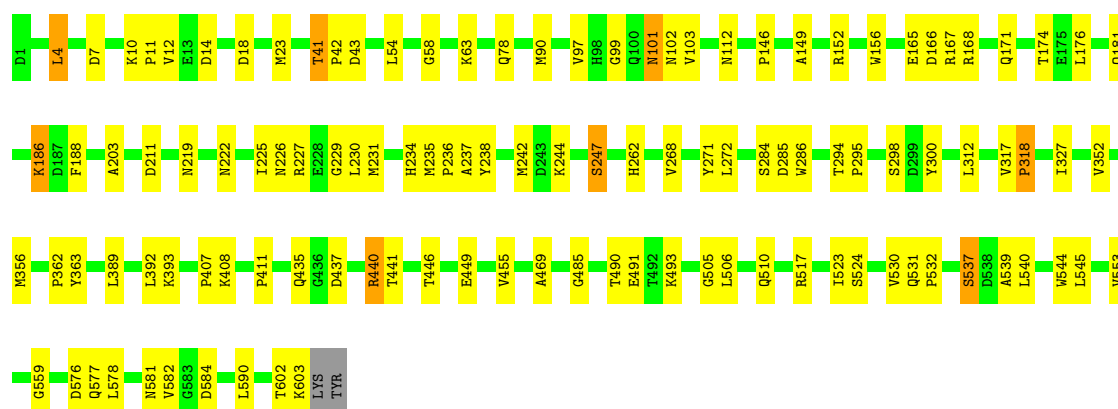
3 Residue-property plots

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: BETA-D-GLUCAN GLUCOHYDROLASE ISOENZYME EXO1

Chain A: 



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

Chain B: 



• Molecule 3: beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.42Å 102.42Å 185.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.20)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.178 , 0.211	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4987	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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, BGC, FUC, SGC, MAN, BMA

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	0.40	0/4672	0.92	17/6345 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ASN	N-CA-C	8.83	123.81	112.34
1	A	545	LEU	CA-C-N	6.93	127.50	119.47
1	A	545	LEU	C-N-CA	6.93	127.50	119.47
1	A	103	VAL	N-CA-C	6.84	118.43	108.58
1	A	112	ASN	N-CA-C	6.80	119.56	111.33
1	A	12	VAL	N-CA-C	6.52	117.21	110.36
1	A	455	VAL	N-CA-C	6.13	116.74	110.05
1	A	247	SER	N-CA-C	5.89	118.66	111.82
1	A	537	SER	N-CA-C	5.63	119.23	110.17
1	A	590	LEU	N-CA-C	-5.55	104.87	111.69
1	A	469	ALA	N-CA-C	5.43	117.62	111.11
1	A	99	GLY	N-CA-C	-5.40	104.60	112.17
1	A	188	PHE	N-CA-C	5.25	117.84	110.23
1	A	23	MET	N-CA-C	5.21	118.44	110.20
1	A	577	GLN	N-CA-C	-5.16	106.99	113.28
1	A	530	VAL	N-CA-C	5.12	119.41	113.42
1	A	578	LEU	N-CA-C	5.08	116.23	109.93

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	4575	0	4564	76	0
2	B	74	0	64	0	0
3	C	23	0	21	1	0
4	A	14	0	13	2	0
5	A	301	0	0	6	0
All	All	4987	0	4662	76	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 8.

All (76) 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:407:PRO:HA	1:A:603:LYS:HD2	1.51	0.93
1:A:352:VAL:HG12	1:A:356:MET:HE3	1.59	0.84
1:A:231:MET:HE1	1:A:271:TYR:CZ	2.16	0.80
1:A:440:ARG:HB2	1:A:440:ARG:HH11	1.53	0.72
1:A:97:VAL:H	1:A:101:ASN:HD21	1.37	0.71
1:A:181:GLN:HE21	1:A:203:ALA:H	1.40	0.70
1:A:408:LYS:H	1:A:603:LYS:CD	2.08	0.67
1:A:181:GLN:HE22	1:A:247:SER:H	1.44	0.66
1:A:156:TRP:HE1	1:A:219:ASN:HD22	1.47	0.63
1:A:11:PRO:HG2	1:A:14:ASP:OD2	2.00	0.62
1:A:41:THR:HG22	1:A:43:ASP:H	1.65	0.62
1:A:437:ASP:HB3	1:A:441:THR:HG21	1.83	0.59
1:A:167:ARG:HH11	1:A:171:GLN:HE22	1.50	0.59
1:A:146:PRO:HB3	1:A:176:LEU:HD23	1.84	0.59
1:A:559:GLY:O	1:A:602:THR:N	2.34	0.57
1:A:435:GLN:CD	1:A:493:LYS:HD3	2.31	0.56
1:A:41:THR:HG22	1:A:43:ASP:N	2.20	0.56
1:A:222:ASN:HB2	4:A:610:NAG:H82	1.86	0.56
1:A:167:ARG:NH1	1:A:171:GLN:HE22	2.03	0.55
1:A:167:ARG:O	1:A:171:GLN:HG3	2.06	0.55
1:A:156:TRP:HE1	1:A:219:ASN:ND2	2.05	0.54
1:A:152:ARG:HD3	5:A:813:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LYS:H	1:A:603:LYS:HD2	1.71	0.54
1:A:181:GLN:NE2	1:A:203:ALA:H	2.05	0.53
1:A:262:HIS:HE1	1:A:285:ASP:H	1.56	0.53
1:A:294:THR:HA	1:A:295:PRO:C	2.34	0.52
1:A:231:MET:HE1	1:A:271:TYR:OH	2.09	0.51
1:A:7:ASP:HB3	1:A:10:LYS:HG2	1.91	0.51
1:A:506:LEU:O	1:A:510:GLN:HG3	2.10	0.51
1:A:58:GLY:H	1:A:102:ASN:ND2	2.09	0.51
1:A:356:MET:SD	5:A:852:HOH:O	2.59	0.51
1:A:146:PRO:HB3	1:A:176:LEU:CD2	2.43	0.49
1:A:285:ASP:OD1	1:A:286:TRP:N	2.42	0.49
1:A:58:GLY:H	1:A:102:ASN:HD21	1.59	0.48
1:A:446:THR:OG1	1:A:449:GLU:HG3	2.12	0.48
1:A:166:ASP:OD1	1:A:168:ARG:HB2	2.14	0.48
1:A:408:LYS:H	1:A:603:LYS:HD3	1.76	0.48
1:A:222:ASN:HB2	4:A:610:NAG:C8	2.44	0.47
1:A:225:ILE:HG12	1:A:226:ASN:N	2.29	0.47
1:A:317:VAL:HB	1:A:318:PRO:HA	1.96	0.47
1:A:97:VAL:H	1:A:101:ASN:ND2	2.08	0.47
1:A:389:LEU:HD11	1:A:553:VAL:HA	1.96	0.47
1:A:238:TYR:O	1:A:242:MET:HG2	2.14	0.47
1:A:362:PRO:HG2	1:A:363:TYR:CD1	2.48	0.47
1:A:225:ILE:HD11	1:A:229:GLY:HA3	1.96	0.47
1:A:235:MET:N	1:A:236:PRO:CD	2.78	0.47
1:A:524:SER:O	1:A:544:TRP:HA	2.15	0.47
1:A:186:LYS:HZ1	1:A:186:LYS:HA	1.79	0.47
1:A:230:LEU:C	1:A:230:LEU:HD13	2.40	0.46
1:A:149:ALA:HB2	1:A:211:ASP:OD2	2.16	0.46
1:A:295:PRO:HG2	1:A:298:SER:HB3	1.98	0.45
1:A:491:GLU:OE2	3:C:1:SGC:S4	2.75	0.45
1:A:165:GLU:HB2	1:A:581:ASN:ND2	2.32	0.45
1:A:284:SER:HB3	1:A:312:LEU:HD23	1.99	0.44
1:A:352:VAL:CG1	1:A:356:MET:HE3	2.41	0.44
1:A:4:LEU:HB3	1:A:18:ASP:CG	2.43	0.43
1:A:300:TYR:HD2	1:A:327:ILE:HD12	1.83	0.43
1:A:485:GLY:HA3	1:A:523:ILE:O	2.19	0.43
1:A:167:ARG:HH11	1:A:171:GLN:NE2	2.15	0.43
1:A:407:PRO:CA	1:A:603:LYS:HD2	2.36	0.42
1:A:174:THR:OG1	1:A:244:LYS:HE3	2.18	0.42
1:A:63:LYS:HD3	1:A:63:LYS:HA	1.81	0.42
1:A:352:VAL:HG12	1:A:356:MET:CE	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ALA:HB3	5:A:782:HOH:O	2.20	0.42
1:A:392:LEU:HD12	1:A:540:LEU:CD2	2.50	0.42
1:A:41:THR:HG23	1:A:42:PRO:HD2	2.03	0.41
1:A:531:GLN:HB2	1:A:532:PRO:HD3	2.01	0.41
1:A:268:VAL:O	1:A:272:LEU:HB3	2.21	0.41
1:A:490:THR:HG22	1:A:491:GLU:HG3	2.02	0.41
1:A:517:ARG:HG2	5:A:915:HOH:O	2.20	0.41
1:A:234:HIS:HD2	5:A:709:HOH:O	2.02	0.41
1:A:411:PRO:HB2	5:A:787:HOH:O	2.19	0.41
1:A:227:ARG:O	1:A:231:MET:HG2	2.21	0.40
1:A:393:LYS:O	1:A:539:ALA:HA	2.21	0.40
1:A:165:GLU:HB2	1:A:581:ASN:HD22	1.85	0.40
1:A:78:GLN:OE1	1:A:90:MET:HG3	2.22	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	601/605 (99%)	573 (95%)	26 (4%)	2 (0%)	36	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	GLY
1	A	584	ASP

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	486/488 (100%)	477 (98%)	9 (2%)	50 66

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	41	THR
1	A	54	LEU
1	A	186	LYS
1	A	318	PRO
1	A	440	ARG
1	A	537	SER
1	A	576	ASP
1	A	582	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	102	ASN
1	A	171	GLN
1	A	181	GLN
1	A	199	ASN
1	A	219	ASN
1	A	234	HIS
1	A	262	HIS
1	A	323	GLN
1	A	371	GLN
1	A	375	GLN
1	A	377	HIS
1	A	510	GLN
1	A	586	HIS

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 ⓘ

8 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	0.66	0	17,19,21	0.70	1 (5%)
2	NAG	B	2	2	14,14,15	0.67	0	17,19,21	0.69	0
2	BMA	B	3	2	11,11,12	0.57	0	15,15,17	0.29	0
2	MAN	B	4	2	11,11,12	0.60	0	15,15,17	0.59	1 (6%)
2	NAG	B	5	2	14,14,15	0.61	0	17,19,21	0.66	0
2	FUC	B	6	2	10,10,11	0.56	0	14,14,16	0.40	0
3	SGC	C	1	3	11,12,12	8.44	9 (81%)	14,17,17	2.11	6 (42%)
3	BGC	C	2	3	11,11,12	3.30	5 (45%)	15,15,17	2.15	4 (26%)

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	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	NAG	B	5	2	-	2/6/23/26	0/1/1/1
2	FUC	B	6	2	-	-	0/1/1/1
3	SGC	C	1	3	-	2/2/22/22	0/1/1/1
3	BGC	C	2	3	-	0/2/19/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	SGC	C3-C4	22.90	1.72	1.53
3	C	1	SGC	C5-C4	13.84	1.64	1.53
3	C	2	BGC	C1-C2	5.80	1.66	1.52
3	C	2	BGC	C2-C3	5.17	1.60	1.52
3	C	2	BGC	C4-C3	4.89	1.65	1.52
3	C	1	SGC	C1-C2	3.94	1.61	1.52
3	C	2	BGC	C4-C5	3.87	1.61	1.53
3	C	1	SGC	C3-C2	3.82	1.62	1.52
3	C	2	BGC	O5-C1	3.32	1.49	1.43
3	C	1	SGC	O5-C1	3.07	1.50	1.42
3	C	1	SGC	O1-C1	2.89	1.48	1.39
3	C	1	SGC	O3-C3	2.84	1.50	1.43
3	C	1	SGC	C6-C5	2.39	1.59	1.51
3	C	1	SGC	O5-C5	2.23	1.49	1.44

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	BGC	C1-O5-C5	6.58	121.01	112.19
3	C	1	SGC	O3-C3-C4	4.22	117.79	109.17
3	C	1	SGC	O3-C3-C2	-3.94	101.10	110.38
3	C	1	SGC	C1-O5-C5	2.93	119.32	113.65
3	C	2	BGC	C6-C5-C4	2.78	119.83	113.02
3	C	1	SGC	C5-C4-S4	-2.17	104.87	110.16
3	C	1	SGC	O5-C5-C4	2.12	111.59	109.50
3	C	1	SGC	C6-C5-C4	2.11	117.17	112.76
2	B	1	NAG	C2-N2-C7	-2.09	120.10	122.90
2	B	4	MAN	C1-O5-C5	2.02	114.89	112.19
3	C	2	BGC	O5-C5-C4	-2.01	105.94	110.83
3	C	2	BGC	O5-C5-C6	-2.00	103.76	107.66

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	NAG	O7-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	5	NAG	C8-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
3	C	1	SGC	O5-C5-C6-O6

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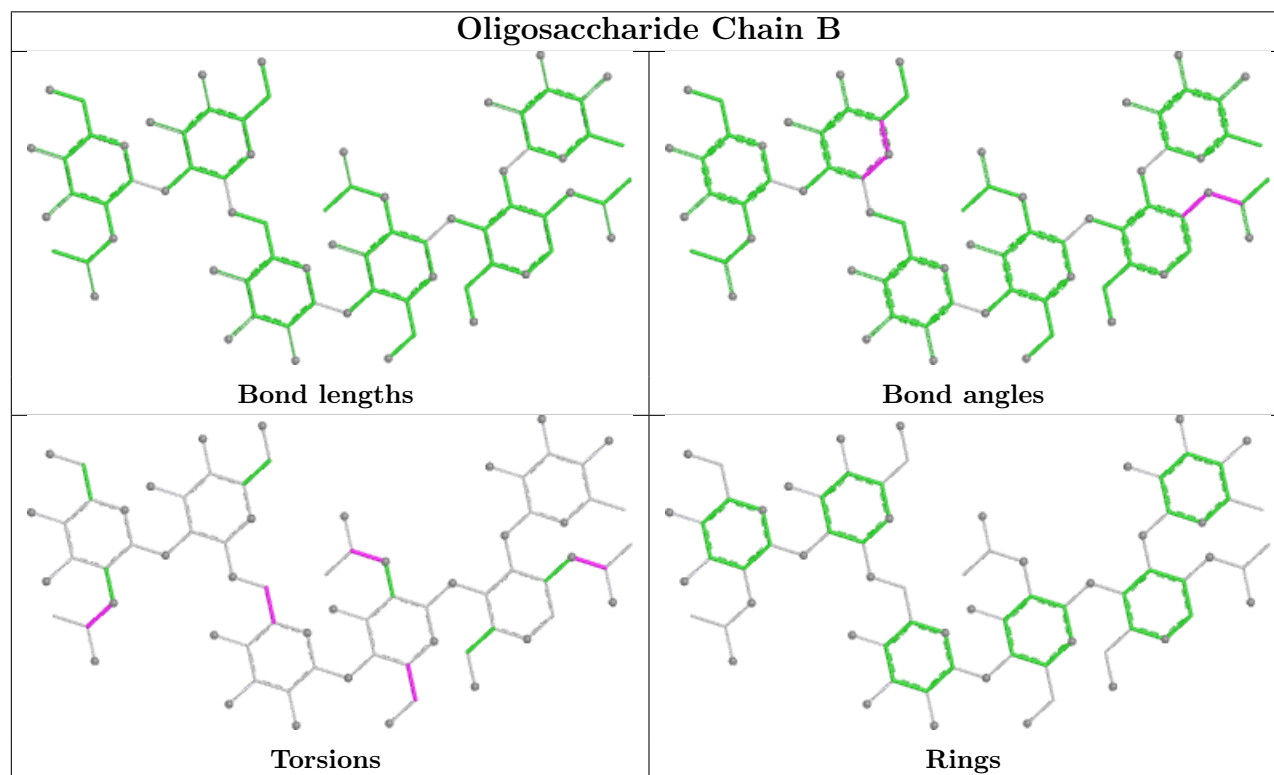
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
3	C	1	SGC	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6

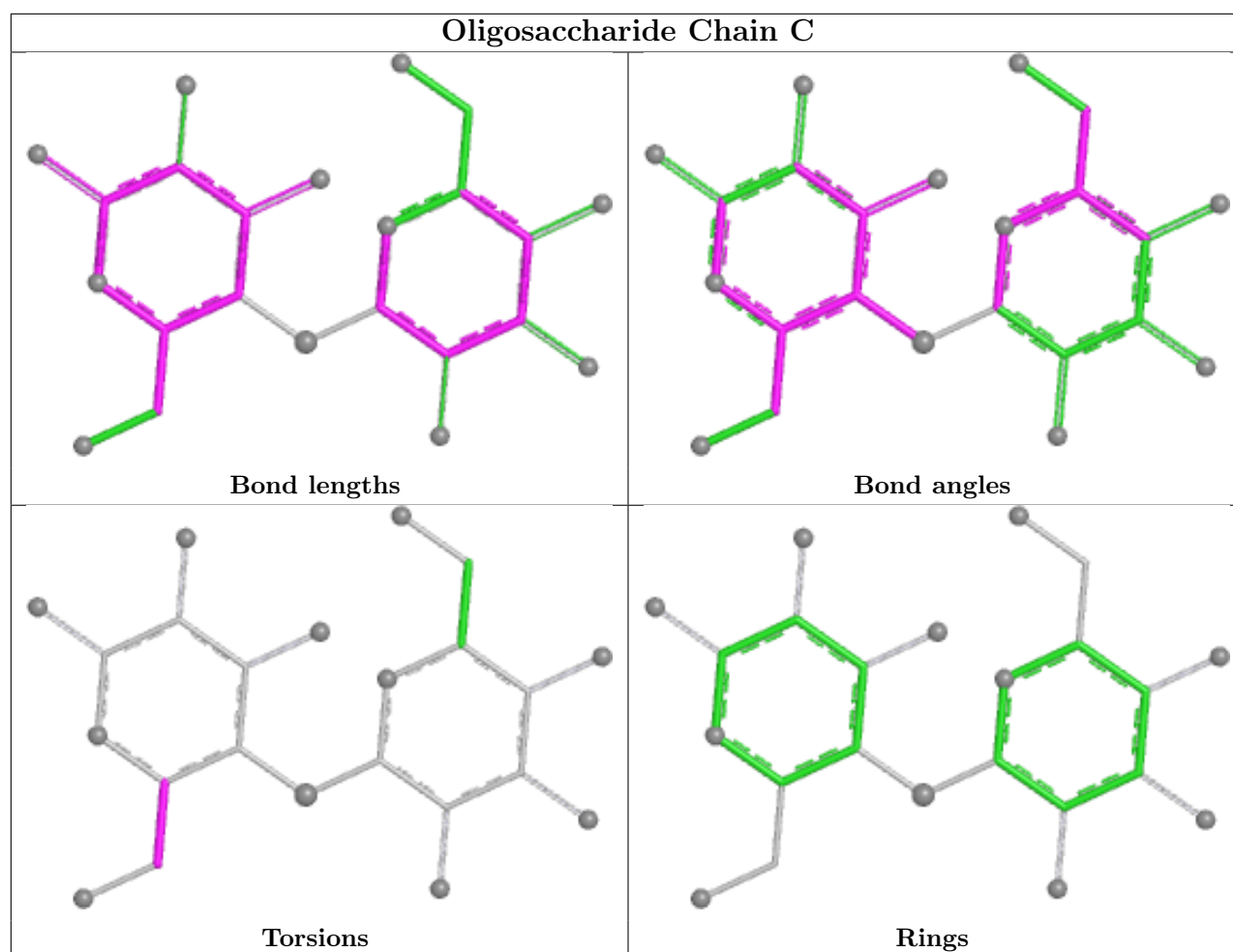
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	SGC	1	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	610	1	14,14,15	0.58	0	17,19,21	0.65	0

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	610	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	610	NAG	C4-C5-C6-O6
4	A	610	NAG	C8-C7-N2-C2
4	A	610	NAG	O5-C5-C6-O6
4	A	610	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	610	NAG	2	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.