



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:52 AM UTC

PDB ID : 1CPU / pdb_00001cpu
Title : SUBSITE MAPPING OF THE ACTIVE SITE OF HUMAN PANCREATIC
ALPHA-AMYLASE USING SUBSTRATES, THE PHARMACOLOGICAL
INHIBITOR ACARBOSE, AND AN ACTIVE SITE VARIANT
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Deposited on : 1999-06-07
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

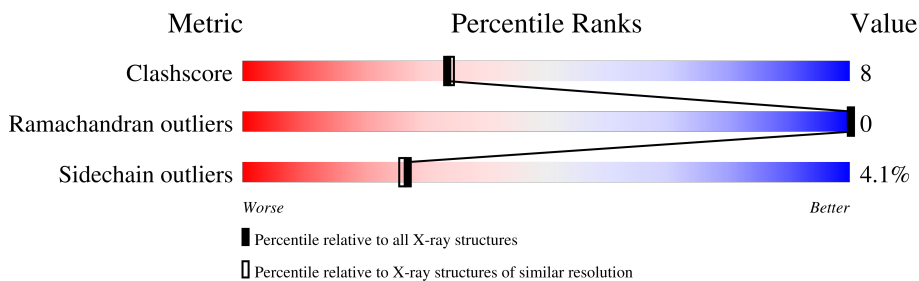
1 Overall quality at a glance

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	496	
2	B	2	
3	C	2	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4277 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 PROTEIN (ALPHA-AMYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3945	2497	696	732	20			

- Molecule 2 is an oligosaccharide called 4-amino-4,6-dideoxy-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			22	12	1	9			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			22	12	10			

- 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		

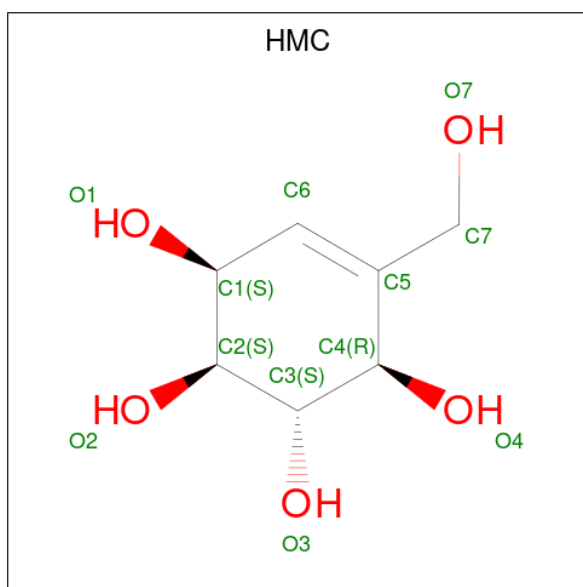
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 5-HYDROXYMETHYL-CHONDURITOL (CCD ID: HMC) (formula: C₇H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	7	4		

- Molecule 8 is water.

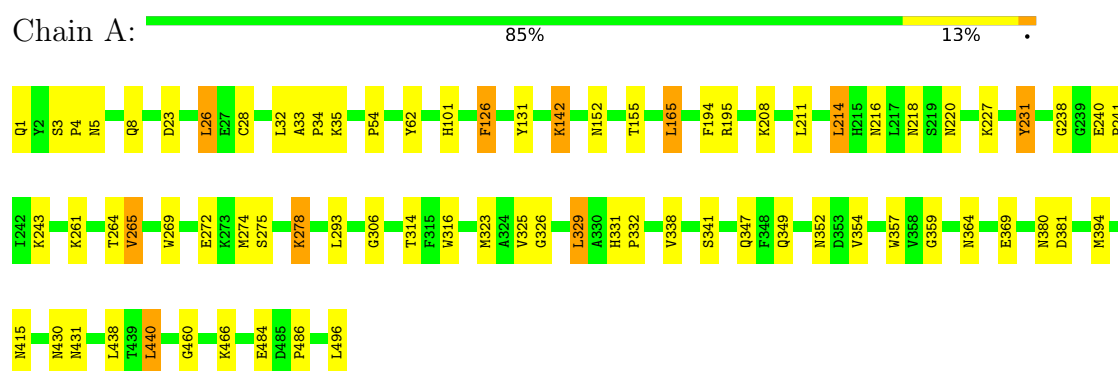
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	261	Total	O	0	0
			261	261		

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: PROTEIN (ALPHA-AMYLASE)



- Molecule 2: 4-amino-4,6-dideoxy-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-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	52.91Å 68.90Å 131.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.8 (8.00-2.00)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4277	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: AGL, GLC, HMC, PCA, CL, NAG, CA

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	0.47	1/4053 (0.0%)	0.83	5/5506 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	484	GLU	CA-C	7.02	1.62	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	GLY	N-CA-C	8.88	125.56	114.37
1	A	359	GLY	CA-C-N	6.30	124.26	119.66
1	A	359	GLY	C-N-CA	6.30	124.26	119.66
1	A	126	PHE	CA-C-N	5.31	126.48	119.84
1	A	126	PHE	C-N-CA	5.31	126.48	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3945	0	3717	60	0
2	B	22	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	22	0	19	0	0
4	A	14	0	13	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	11	0	9	1	0
8	A	261	0	0	5	0
All	All	4277	0	3778	60	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 (60) 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:142:LYS:H	1:A:142:LYS:HD2	1.13	1.06
1:A:142:LYS:HD2	1:A:142:LYS:N	1.72	1.03
1:A:231:TYR:HD2	1:A:293:LEU:HG	1.30	0.96
1:A:142:LYS:H	1:A:142:LYS:CD	1.85	0.90
1:A:314:THR:HG23	1:A:316:TRP:H	1.40	0.87
1:A:325:VAL:O	1:A:329:LEU:HD22	1.82	0.78
1:A:329:LEU:HD22	1:A:329:LEU:H	1.50	0.76
1:A:261:LYS:O	1:A:265:VAL:HG12	1.85	0.76
1:A:8:GLN:H	1:A:8:GLN:CD	1.93	0.75
1:A:231:TYR:CD2	1:A:293:LEU:HG	2.20	0.69
1:A:227:LYS:HA	1:A:227:LYS:HE2	1.76	0.67
1:A:275:SER:O	1:A:278:LYS:HE2	1.96	0.65
1:A:8:GLN:CD	1:A:8:GLN:N	2.55	0.64
1:A:306:GLY:HA3	8:A:632:HOH:O	1.99	0.62
1:A:314:THR:HG21	1:A:316:TRP:HD1	1.68	0.59
1:A:329:LEU:CD2	1:A:394:MET:HB3	2.32	0.58
1:A:329:LEU:HD21	1:A:394:MET:HB3	1.86	0.57
1:A:216:ASN:OD1	1:A:227:LYS:HE3	2.05	0.57
1:A:314:THR:HG22	8:A:677:HOH:O	2.05	0.55
1:A:142:LYS:CE	1:A:155:THR:HG22	2.36	0.55
1:A:369:GLU:HG2	8:A:703:HOH:O	2.06	0.54
1:A:211:LEU:HA	1:A:214:LEU:HD22	1.90	0.54
1:A:347:GLN:HB3	1:A:354:VAL:HG22	1.90	0.53
1:A:460:GLY:O	1:A:496:LEU:HD11	2.10	0.52
1:A:264:THR:HG23	1:A:269:TRP:HB2	1.92	0.51
1:A:23:ASP:HA	1:A:26:LEU:HD21	1.92	0.51
1:A:380:ASN:O	1:A:381:ASP:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLN:O	1:A:352:ASN:ND2	2.46	0.48
1:A:326:GLY:HA2	1:A:329:LEU:HD21	1.95	0.48
1:A:274:MET:HG3	8:A:573:HOH:O	2.14	0.48
1:A:460:GLY:C	1:A:496:LEU:HD11	2.39	0.48
1:A:415:ASN:HB3	1:A:431:ASN:HB3	1.96	0.48
1:A:231:TYR:H	1:A:231:TYR:HD1	1.62	0.47
1:A:142:LYS:HG2	8:A:701:HOH:O	2.15	0.47
1:A:331:HIS:CG	1:A:332:PRO:HD2	2.50	0.47
1:A:274:MET:H	1:A:415:ASN:HD22	1.64	0.46
1:A:240:GLU:HB3	1:A:241:PRO:HD2	1.97	0.46
1:A:3:SER:HA	1:A:4:PRO:HD3	1.86	0.45
1:A:23:ASP:O	1:A:26:LEU:CD2	2.65	0.45
1:A:23:ASP:HA	1:A:26:LEU:CD2	2.46	0.45
1:A:314:THR:HG23	1:A:316:TRP:N	2.20	0.44
1:A:4:PRO:O	1:A:5:ASN:HB2	2.17	0.44
1:A:35:LYS:HD3	1:A:35:LYS:HA	1.87	0.44
1:A:126:PHE:HB2	1:A:131:TYR:HB2	2.00	0.43
1:A:269:TRP:O	1:A:272:GLU:HG3	2.17	0.43
1:A:349:GLN:NE2	1:A:354:VAL:HG11	2.32	0.43
1:A:62:TYR:CD1	1:A:62:TYR:N	2.86	0.43
1:A:274:MET:H	1:A:415:ASN:ND2	2.16	0.43
1:A:194:PHE:O	1:A:231:TYR:HD1	2.02	0.42
1:A:325:VAL:O	1:A:329:LEU:CD2	2.60	0.42
1:A:101:HIS:CD2	1:A:165:LEU:HG	2.54	0.42
1:A:195:ARG:HA	1:A:231:TYR:CD1	2.55	0.41
1:A:438:LEU:HD23	1:A:440:LEU:CD1	2.50	0.41
1:A:33:ALA:HB3	1:A:34:PRO:HD3	2.03	0.41
1:A:54:PRO:HB2	1:A:357:TRP:CE3	2.55	0.41
1:A:430:ASN:O	1:A:486:PRO:HB2	2.20	0.41
1:A:26:LEU:H	1:A:26:LEU:HD22	1.85	0.41
1:A:62:TYR:CD2	7:A:503:HMC:H4	2.56	0.41
1:A:28:CYS:HA	1:A:32:LEU:HB2	2.03	0.40
1:A:218:ASN:OD1	1:A:220:ASN:HB2	2.20	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	494/496 (100%)	483 (98%)	11 (2%)	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	
1	A	418/418 (100%)	401 (96%)	17 (4%)	27	26

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	142	LYS
1	A	152	ASN
1	A	165	LEU
1	A	208	LYS
1	A	214	LEU
1	A	231	TYR
1	A	243	LYS
1	A	265	VAL
1	A	278	LYS
1	A	323	MET
1	A	329	LEU
1	A	338	VAL

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Mol	Chain	Res	Type
1	A	341	SER
1	A	364	ASN
1	A	440	LEU
1	A	466	LYS

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	7	GLN
1	A	15	HIS
1	A	105	ASN
1	A	349	GLN
1	A	350	ASN
1	A	352	ASN
1	A	363	ASN
1	A	415	ASN
1	A	459	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	PCA	A	1	1	6,7,9	1.38	0	7,8,12	1.41	1 (14%)

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	-	0/0/9/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	O-C-CA	-2.21	119.09	124.77

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](#)

4 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	GLC	B	1	2	12,12,12	0.79	0	17,17,17	0.94	1 (5%)
2	AGL	B	2	2,7	10,10,11	1.07	0	12,14,16	1.03	1 (8%)
3	GLC	C	1	3,7	11,11,12	0.98	1 (9%)	15,15,17	1.11	1 (6%)
3	GLC	C	2	3	11,11,12	0.94	0	15,15,17	0.90	1 (6%)

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	GLC	B	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGL	B	2	2,7	-	-	0/1/1/1
3	GLC	C	1	3,7	-	0/2/19/22	0/1/1/1
3	GLC	C	2	3	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	GLC	C2-C3	2.04	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	GLC	C1-O5-C5	3.38	116.72	112.19
3	C	2	GLC	C1-O5-C5	2.38	115.38	112.19
2	B	2	AGL	C1-C2-C3	2.26	112.93	109.64
2	B	1	GLC	C1-O5-C5	2.07	117.66	113.65

There are no chirality outliers.

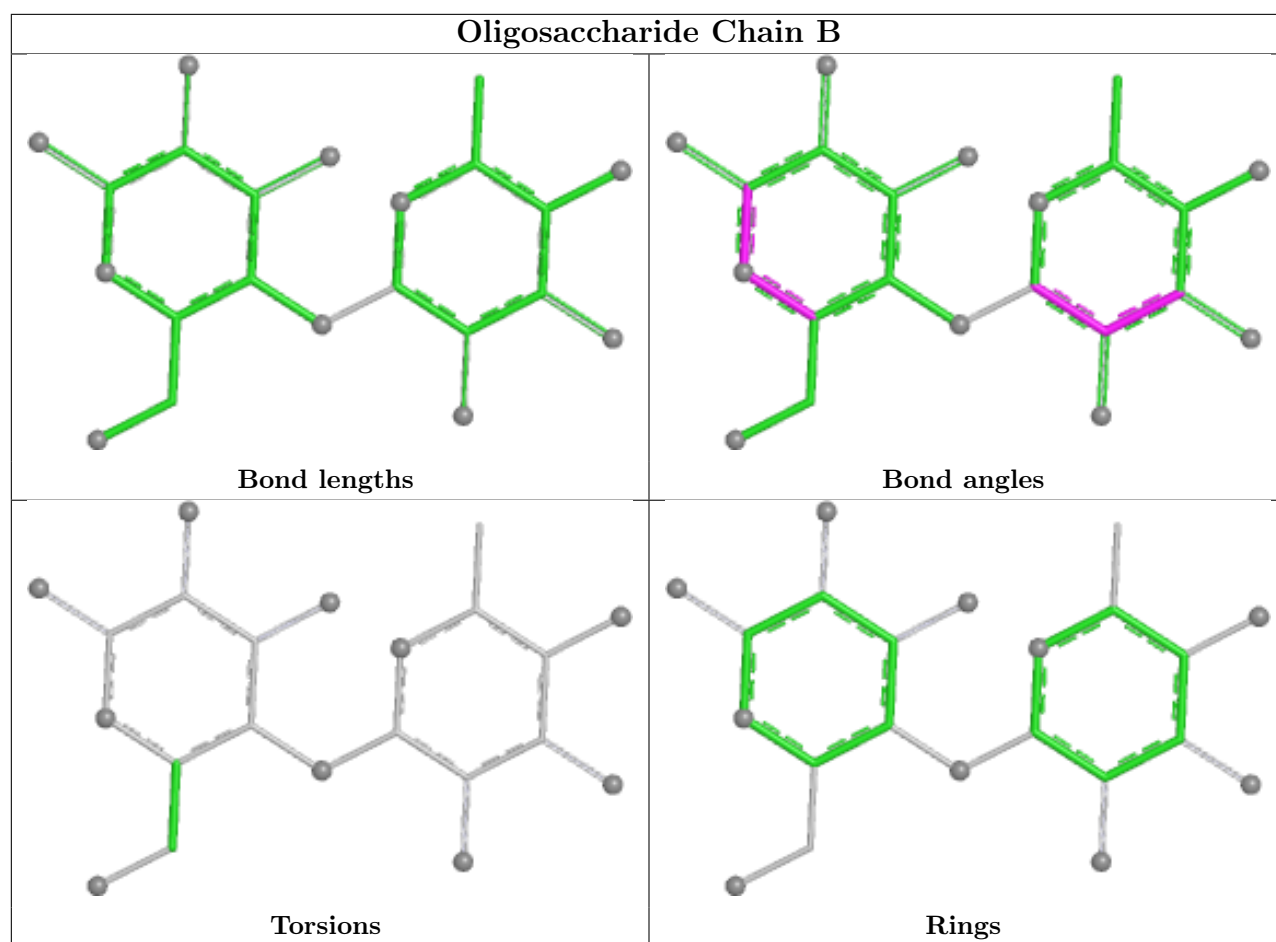
All (1) torsion outliers are listed below:

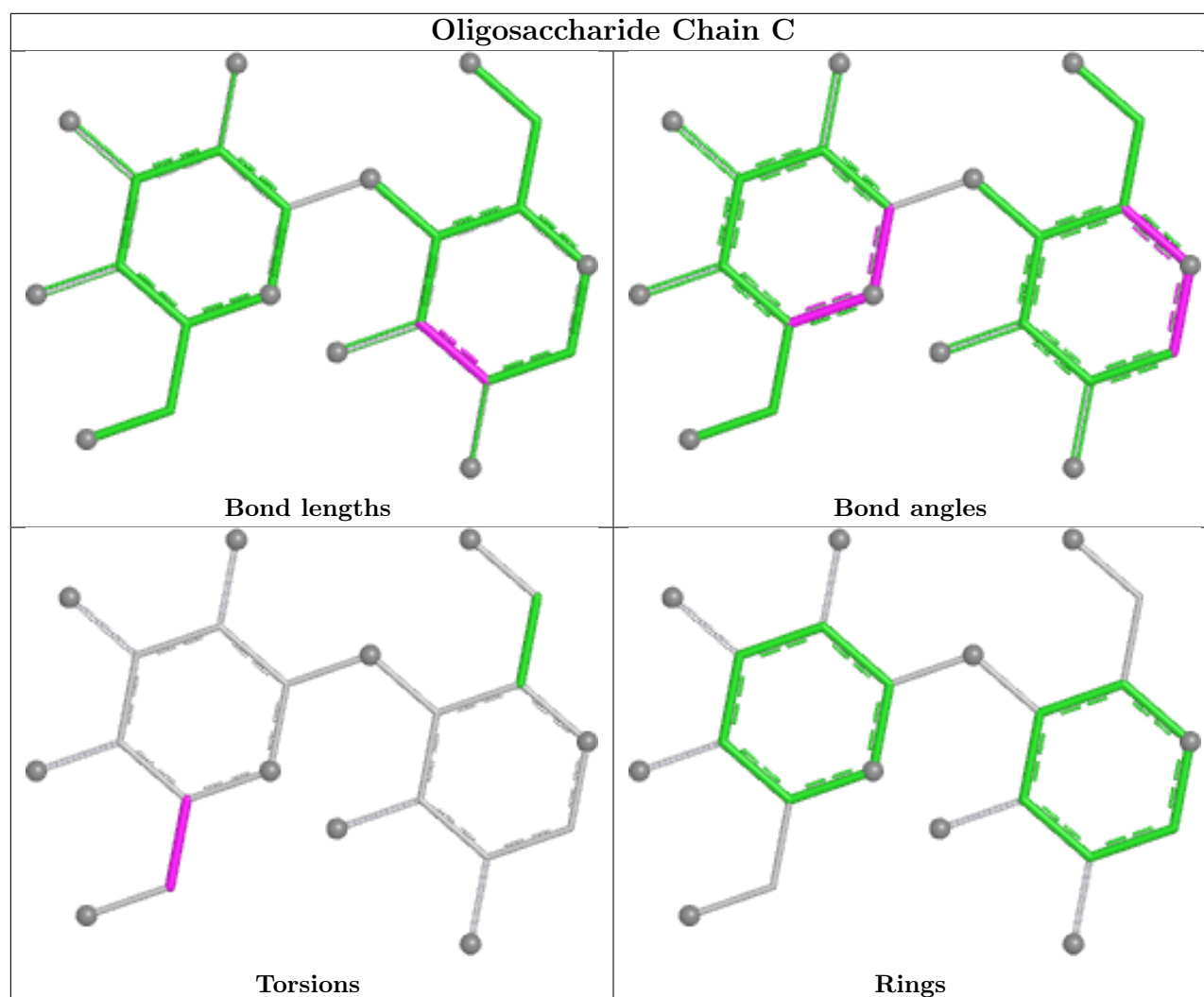
Mol	Chain	Res	Type	Atoms
3	C	2	GLC	O5-C5-C6-O6

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	497	1	14,14,15	0.78	0	17,19,21	1.14	2 (11%)
7	HMC	A	503	3,2	11,11,12	2.76	4 (36%)	10,15,17	1.42	2 (20%)

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	497	1	-	0/6/23/26	0/1/1/1
7	HMC	A	503	3,2	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	503	HMC	C4-C5	7.49	1.57	1.51
7	A	503	HMC	C2-C3	2.94	1.57	1.52
7	A	503	HMC	C6-C5	2.25	1.38	1.33
7	A	503	HMC	C3-C4	2.22	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	503	HMC	C3-C4-C5	2.89	116.22	111.67
4	A	497	NAG	C1-O5-C5	2.80	115.93	112.19
7	A	503	HMC	C1-C6-C5	2.54	128.90	123.11
4	A	497	NAG	C8-C7-N2	-2.07	112.69	116.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	503	HMC	C6-C5-C7-O7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	503	HMC	1	0

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.