



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:50 AM UTC

PDB ID : 2DIJ / pdb_00002dij
Title : COMPLEX OF A Y195F MUTANT CGTASE FROM B. CIRCULANS STRAIN 251 COMPLEXED WITH A MALTONONAOSE INHIBITOR AT PH 9.8 OBTAINED AFTER SOAKING THE CRYSTAL WITH ACARBOSE AND MALTOHEXAOSE
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Deposited on : 1998-05-27
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

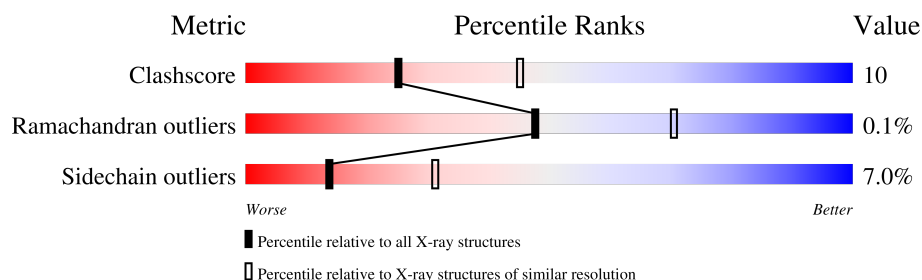
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	686	
2	B	2	
3	C	3	
4	D	5	
5	E	2	
6	F	6	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5603 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 CYCLODEXTRIN GLYCOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5263	3321	900	1026	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	PHE	TYR	engineered mutation	UNP P43379

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



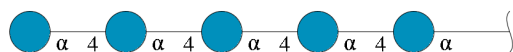
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			23	12	11			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	3	Total	C	O	0	0	0
			34	18	16			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	D	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 5 is an oligosaccharide called alpha-D-quinovopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	E	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 6 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

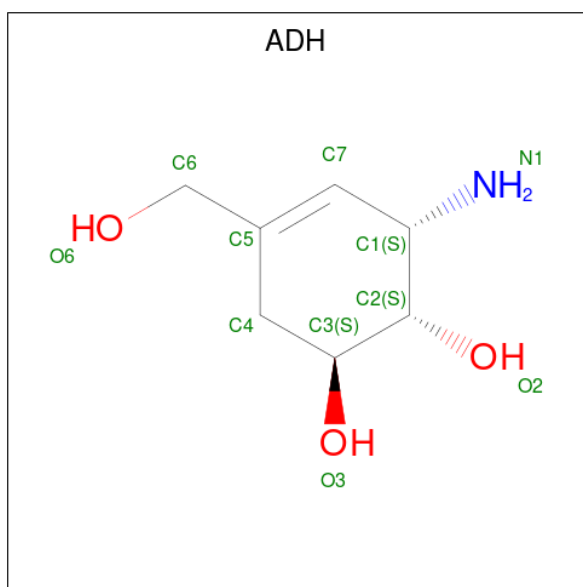


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
6	F	6	Total	C	O	0	0	0
			67	36	31			

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		

- Molecule 8 is 1-AMINO-2,3-DIHYDROXY-5-HYDROXYMETHYL CYCLOHEX-5-ENE (CCD ID: ADH) (formula: C₇H₁₃NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 9 is water.

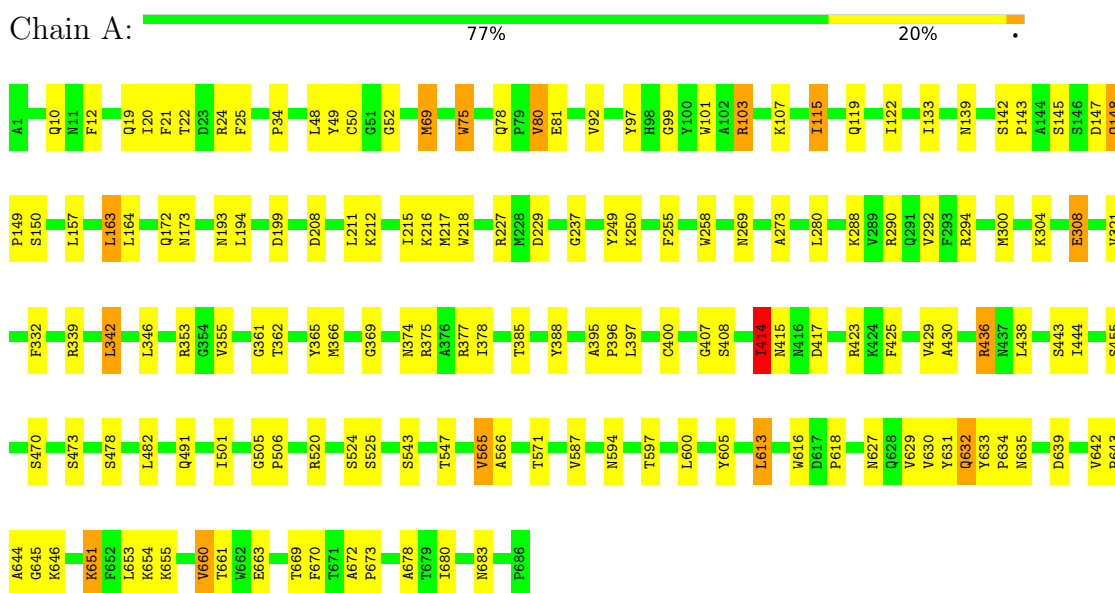
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	126	Total	O	0	0
			126	126		

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: CYCLODEXTRIN GLYCOSYLTRANSFERASE



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



GLC1
GLC2
GLC3
GLC4
GLC5

- Molecule 5: alpha-D-quinovopyranose-(1-4)-alpha-D-glucopyranose

Chain E:  50% 50%

GLC1
G6D2

- Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:  33% 67%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6

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	119.96Å 111.28Å 67.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	94.1 (8.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5603	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: CA, ADH, GLC, G6D

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	0.74	0/5393	1.01	3/7350 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	20	ILE	N-CA-C	5.96	116.45	108.11
1	A	414	ILE	N-CA-C	5.15	114.99	107.88
1	A	292	VAL	N-CA-C	5.10	115.77	110.82

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	5263	0	5025	103	0
2	B	23	0	21	0	0
3	C	34	0	30	1	0
4	D	56	0	48	1	0
5	E	21	0	12	0	0
6	F	67	0	56	4	0
7	A	2	0	0	0	0
8	A	11	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	126	0	0	3	0
All	All	5603	0	5203	104	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 10.

The worst 5 of 104 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:69:MET:HG3	1:A:388:TYR:CE2	2.12	0.84
1:A:670:PHE:CE2	1:A:680:ILE:HD11	2.13	0.84
1:A:75:TRP:CZ2	1:A:227:ARG:HD3	2.18	0.78
1:A:423:ARG:HG3	1:A:423:ARG:HH11	1.49	0.78
1:A:227:ARG:HH21	1:A:229:ASP:HB2	1.51	0.76

There are no symmetry-related clashes.

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	684/686 (100%)	656 (96%)	27 (4%)	1 (0%)	48 70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	629	VAL

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	556/556 (100%)	517 (93%)	39 (7%)	14	31

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	478	SER
1	A	632	GLN
1	A	491	GLN
1	A	543	SER
1	A	653	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	479	ASN
1	A	594	ASN
1	A	681	ASN
1	A	632	GLN
1	A	410	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 ⓘ

18 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	0.34	0	17,17,17	0.69	0
2	GLC	B	2	2	11,11,12	0.42	0	15,15,17	1.04	1 (6%)
3	GLC	C	1	3	12,12,12	0.35	0	17,17,17	0.57	0
3	GLC	C	2	3	11,11,12	0.43	0	15,15,17	0.93	1 (6%)
3	GLC	C	3	3	11,11,12	0.39	0	15,15,17	1.22	1 (6%)
4	GLC	D	1	4	12,12,12	0.36	0	17,17,17	0.62	0
4	GLC	D	2	4	11,11,12	0.45	0	15,15,17	1.65	1 (6%)
4	GLC	D	3	4	11,11,12	0.42	0	15,15,17	0.94	1 (6%)
4	GLC	D	4	4	11,11,12	0.43	0	15,15,17	0.96	1 (6%)
4	GLC	D	5	4	11,11,12	0.37	0	15,15,17	1.13	1 (6%)
5	GLC	E	1	5	12,12,12	0.36	0	17,17,17	0.65	0
5	G6D	E	2	8,5	9,9,11	0.39	0	11,12,16	1.20	1 (9%)
6	GLC	F	1	8,6	12,12,12	0.38	0	17,17,17	1.30	3 (17%)
6	GLC	F	2	6	11,11,12	0.39	0	15,15,17	1.08	1 (6%)
6	GLC	F	3	6	11,11,12	0.43	0	15,15,17	0.92	1 (6%)
6	GLC	F	4	6	11,11,12	0.44	0	15,15,17	0.93	1 (6%)
6	GLC	F	5	6	11,11,12	0.44	0	15,15,17	1.23	1 (6%)
6	GLC	F	6	6	11,11,12	0.37	0	15,15,17	1.43	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
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1
3	GLC	C	1	3	-	0/2/22/22	0/1/1/1
3	GLC	C	2	3	-	0/2/19/22	0/1/1/1
3	GLC	C	3	3	-	2/2/19/22	0/1/1/1
4	GLC	D	1	4	-	2/2/22/22	0/1/1/1
4	GLC	D	2	4	-	0/2/19/22	0/1/1/1
4	GLC	D	3	4	-	0/2/19/22	0/1/1/1
4	GLC	D	4	4	-	0/2/19/22	0/1/1/1
4	GLC	D	5	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	E	1	5	-	0/2/22/22	0/1/1/1
5	G6D	E	2	8,5	-	-	0/1/1/1
6	GLC	F	1	8,6	-	2/2/22/22	0/1/1/1
6	GLC	F	2	6	-	2/2/19/22	0/1/1/1
6	GLC	F	3	6	-	0/2/19/22	0/1/1/1
6	GLC	F	4	6	-	2/2/19/22	0/1/1/1
6	GLC	F	5	6	-	2/2/19/22	0/1/1/1
6	GLC	F	6	6	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	GLC	C1-O5-C5	5.24	119.21	112.19
3	C	3	GLC	C1-O5-C5	3.76	117.23	112.19
6	F	5	GLC	C1-O5-C5	3.68	117.12	112.19
6	F	6	GLC	C1-O5-C5	3.65	117.08	112.19
4	D	5	GLC	C1-O5-C5	3.53	116.91	112.19

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

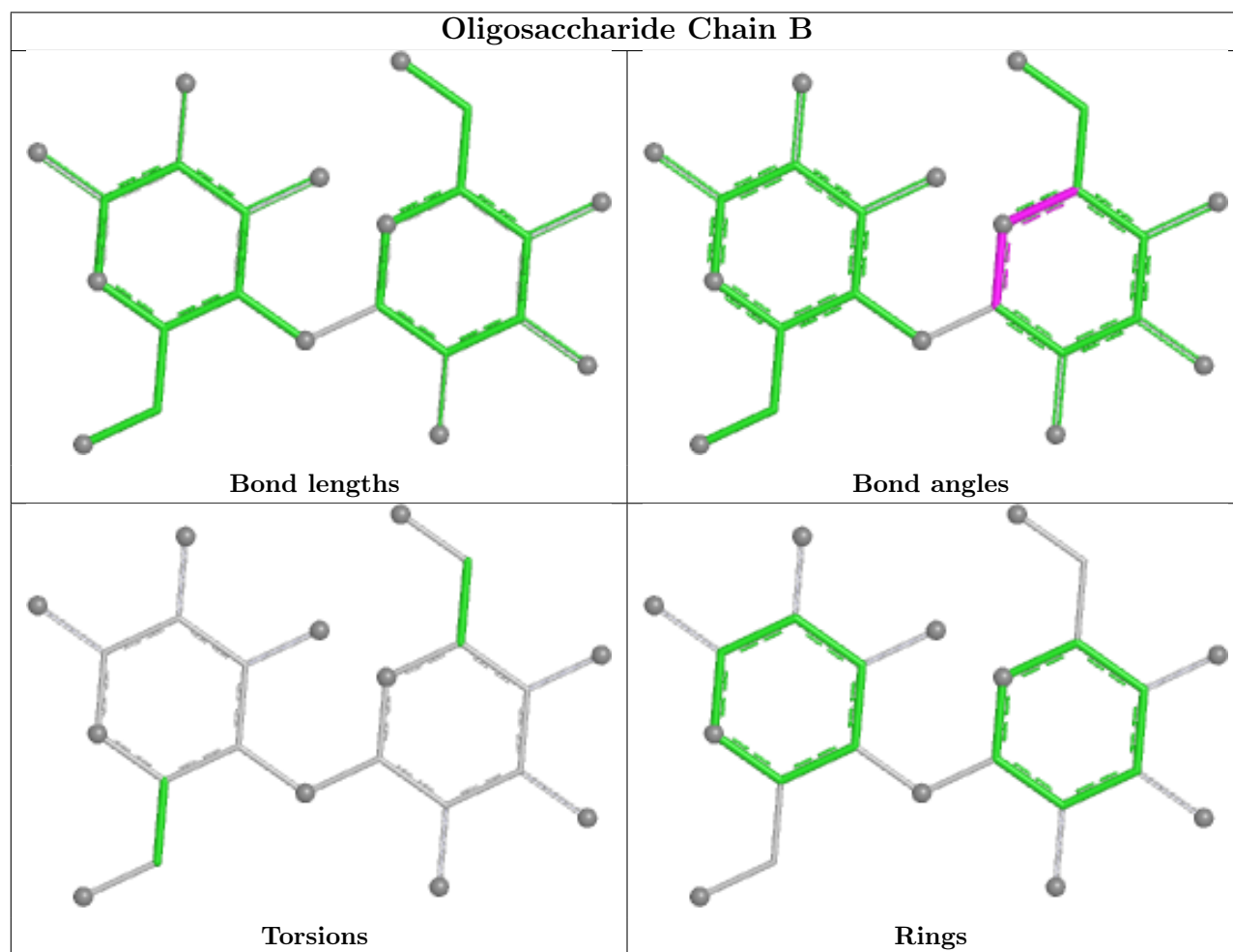
Mol	Chain	Res	Type	Atoms
3	C	3	GLC	O5-C5-C6-O6
6	F	4	GLC	O5-C5-C6-O6
6	F	4	GLC	C4-C5-C6-O6
3	C	3	GLC	C4-C5-C6-O6
6	F	1	GLC	C4-C5-C6-O6

There are no ring outliers.

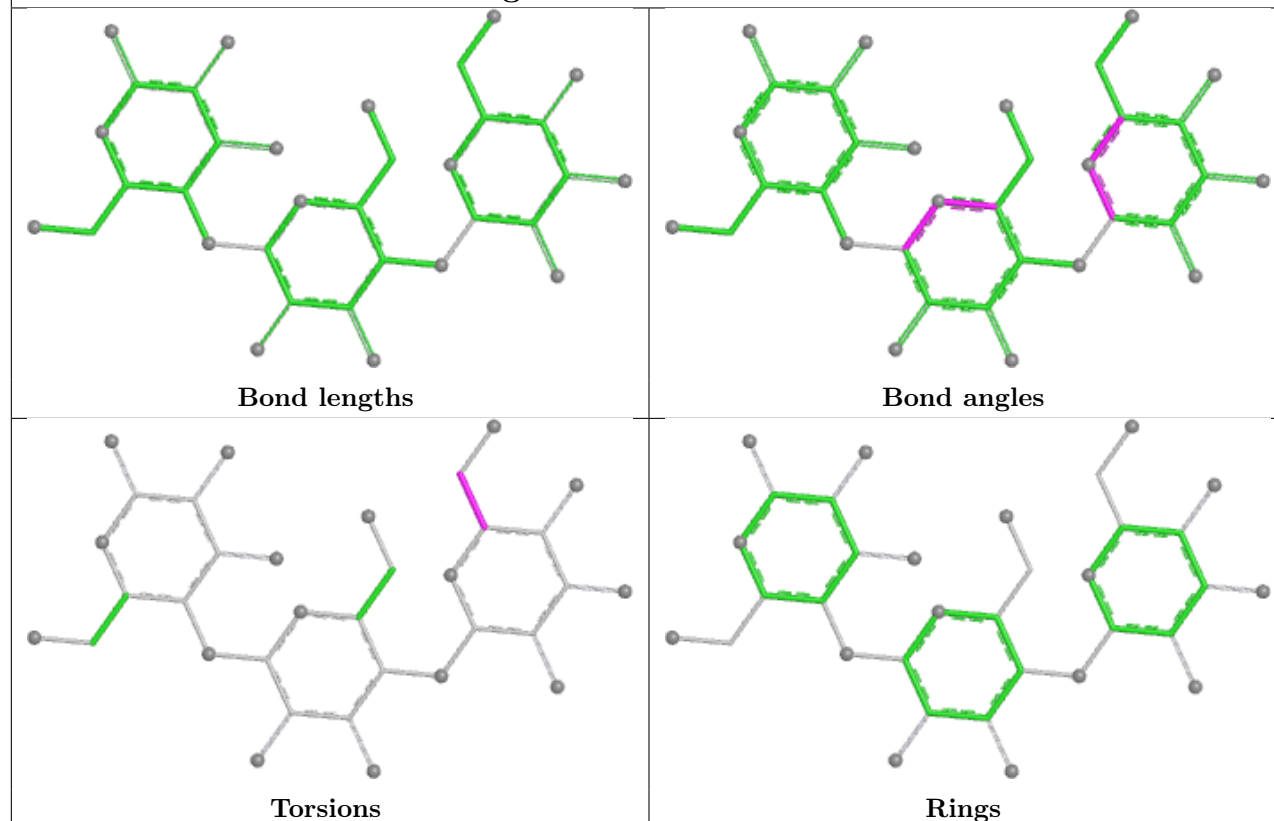
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	GLC	1	0
6	F	1	GLC	1	0
6	F	5	GLC	1	0
6	F	6	GLC	2	0
6	F	4	GLC	1	0
3	C	1	GLC	1	0

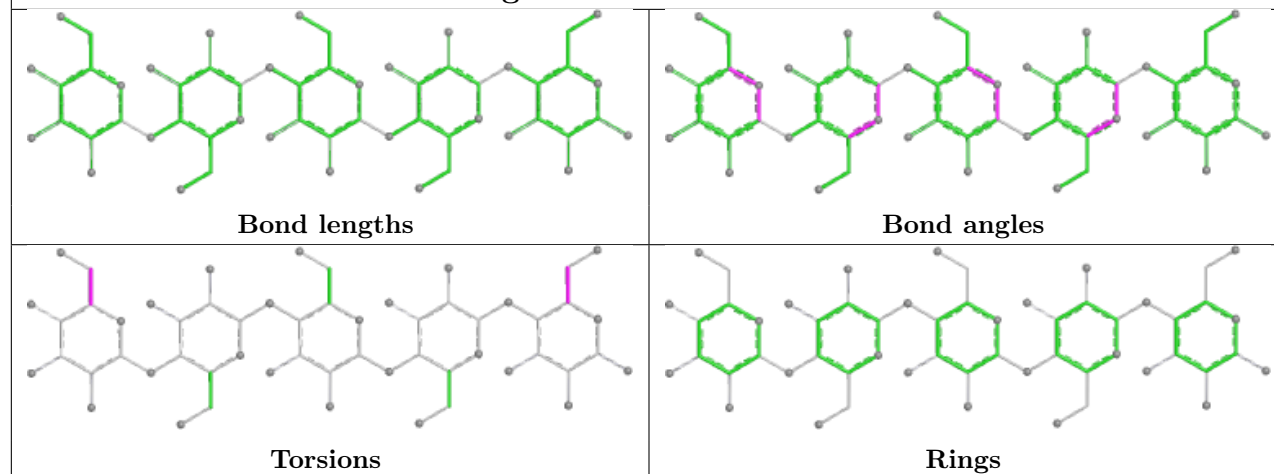
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

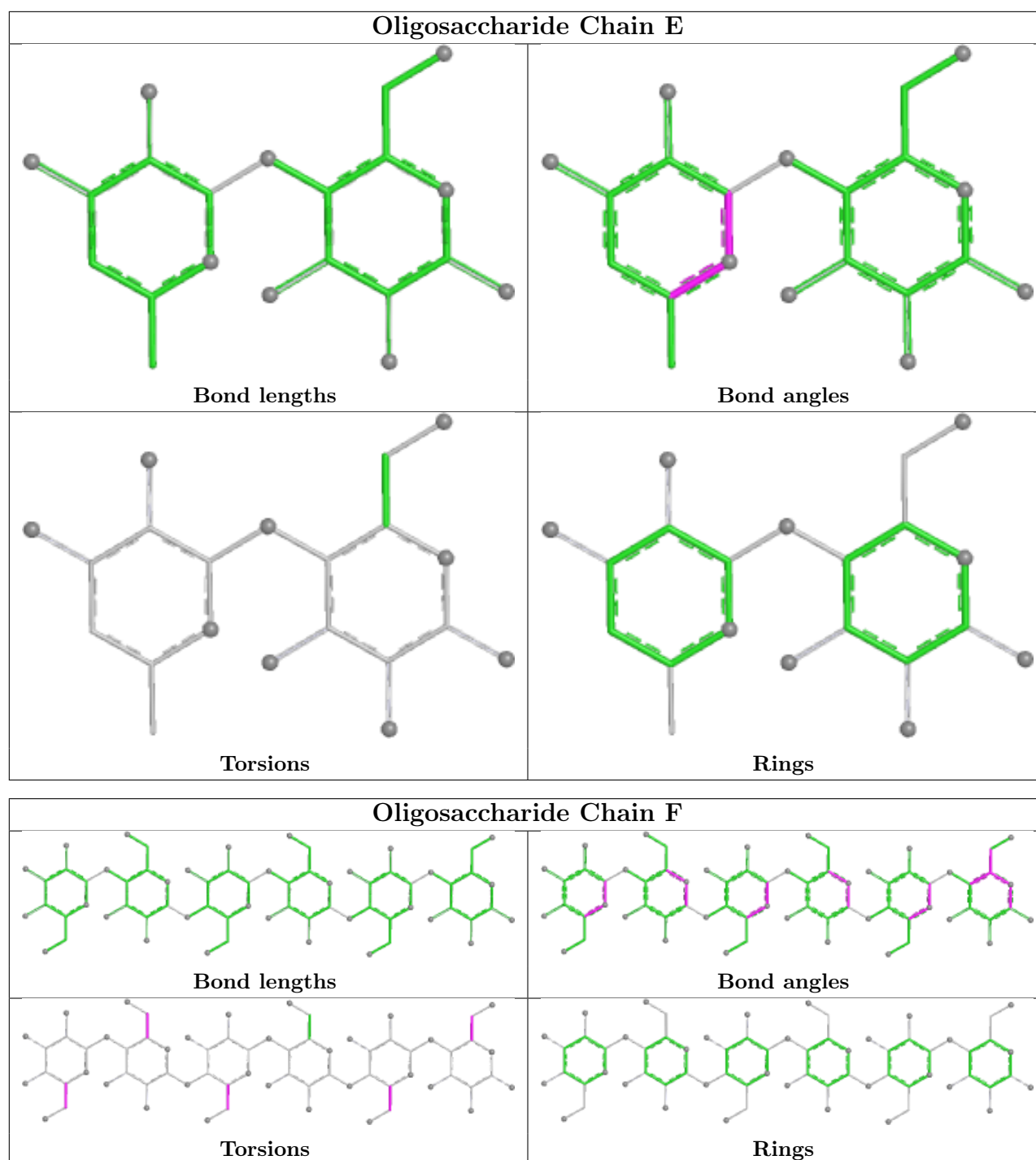


Oligosaccharide Chain C



Oligosaccharide Chain D





5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
8	ADH	A	705	6,5	11,11,11	2.14	3 (27%)	8,15,15	0.93	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
8	ADH	A	705	6,5	-	0/2/18/18	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	705	ADH	C4-C5	-5.19	1.41	1.50
8	A	705	ADH	C1-C7	-3.26	1.42	1.50
8	A	705	ADH	C7-C5	3.03	1.42	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	705	ADH	1	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.