



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2024 – 01:58 AM EST

PDB ID : 6CE0  
Title : Crystal structure of a HIV-1 clade B tier-3 isolate H078.14 UFO-BG Env trimer in complex with broadly neutralizing Fabs PGT124 and 35O22 at 4.6 Angstrom  
Authors : Kumar, S.; Sarkar, A.; Wilson, I.A.  
Deposited on : 2018-02-09  
Resolution : 4.60 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

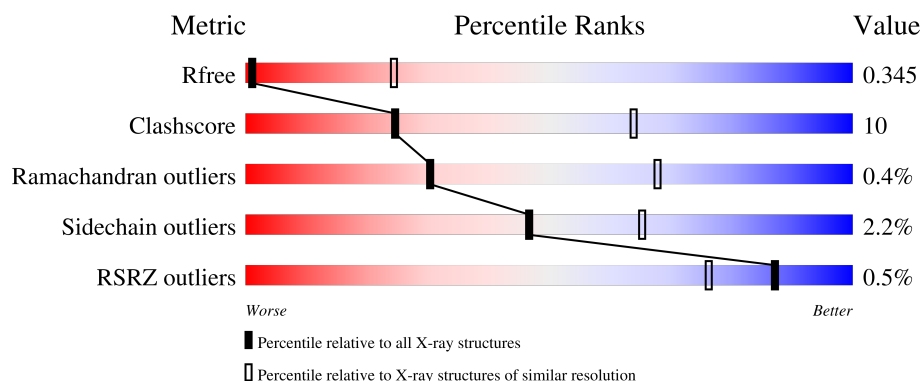
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 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.








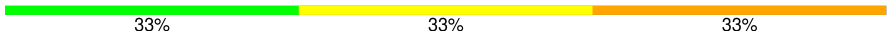
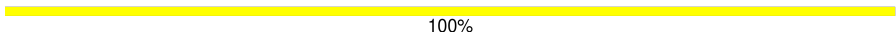
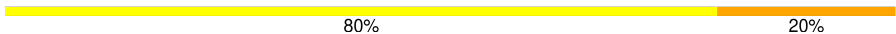

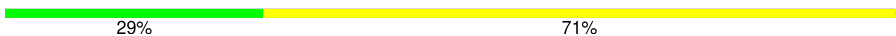
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1068 (5.30-3.90)
Clashscore	180529	1123 (5.30-3.90)
Ramachandran outliers	177936	1015 (5.30-3.90)
Sidechain outliers	177891	1016 (5.32-3.88)
RSRZ outliers	164620	1064 (5.30-3.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	140	<div> <div>81%</div> <div>16%</div> <div>..</div> </div>
2	G	487	<div> <div>66%</div> <div>24%</div> <div>• 8%</div> </div>
3	D	243	<div> <div>82%</div> <div>16%</div> <div>..</div> </div>
4	E	216	<div> <div>84%</div> <div>13%</div> <div>..</div> </div>
5	H	236	<div> <div>72%</div> <div>22%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
6	L	214	 80% 17% ..
7	A	2	 100%
7	C	2	 50% 50%
7	J	2	 50% 50%
8	F	3	 67% 33%
8	K	3	 33% 33% 33%
9	I	5	 100%
9	N	5	 80% 20%
10	M	4	 50% 25% 25%
11	O	7	 29% 71%

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11946 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	137	Total	C	N	O	S	0	0	0
			1086	688	185	206	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	548	ASN	-	linker	UNP Q2N0T3
B	549	PRO	-	linker	UNP Q2N0T3
B	563	ASP	-	linker	UNP Q2N0T3
B	564	TRP	-	linker	UNP Q2N0T3
B	565	LEU	-	linker	UNP Q2N0T3
B	566	PRO	-	linker	UNP Q2N0T3
B	567	ASP	-	linker	UNP Q2N0T3
B	568	MET	-	linker	UNP Q2N0T3
B	569	THR	-	linker	UNP Q2N0T3
B	605	CYS	THR	engineered mutation	UNP Q2N0S5

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	446	Total	C	N	O	S	0	0	0
			3512	2212	616	659	25			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	engineered mutation	UNP A4ZPX1
G	507	GLY	-	expression tag	UNP A4ZPX1
G	508	GLY	-	expression tag	UNP A4ZPX1
G	509	GLY	-	expression tag	UNP A4ZPX1
G	510	GLY	-	expression tag	UNP A4ZPX1
G	511	GLY	-	expression tag	UNP A4ZPX1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	512	SER	-	expression tag	UNP A4ZPX1
G	513	GLY	-	expression tag	UNP A4ZPX1
G	514	GLY	-	expression tag	UNP A4ZPX1
G	515	GLY	-	expression tag	UNP A4ZPX1
G	516	GLY	-	expression tag	UNP A4ZPX1
G	517	SER	-	expression tag	UNP A4ZPX1

- Molecule 3 is a protein called 35O22 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 4 is a protein called 35O22 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 5 is a protein called PGT124 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	226	Total	C	N	O	S	0	0	0
			1720	1093	287	335	5			

- Molecule 6 is a protein called PGT124 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1601	1008	271	317	5			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



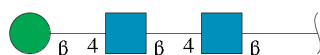
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

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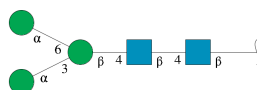
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
8	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



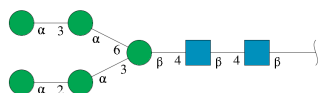
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
9	N	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



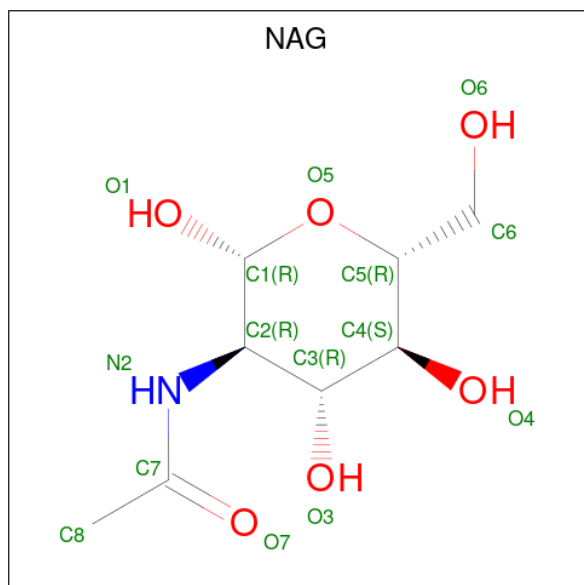
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		

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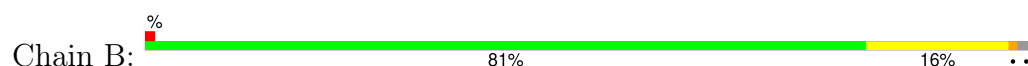
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		



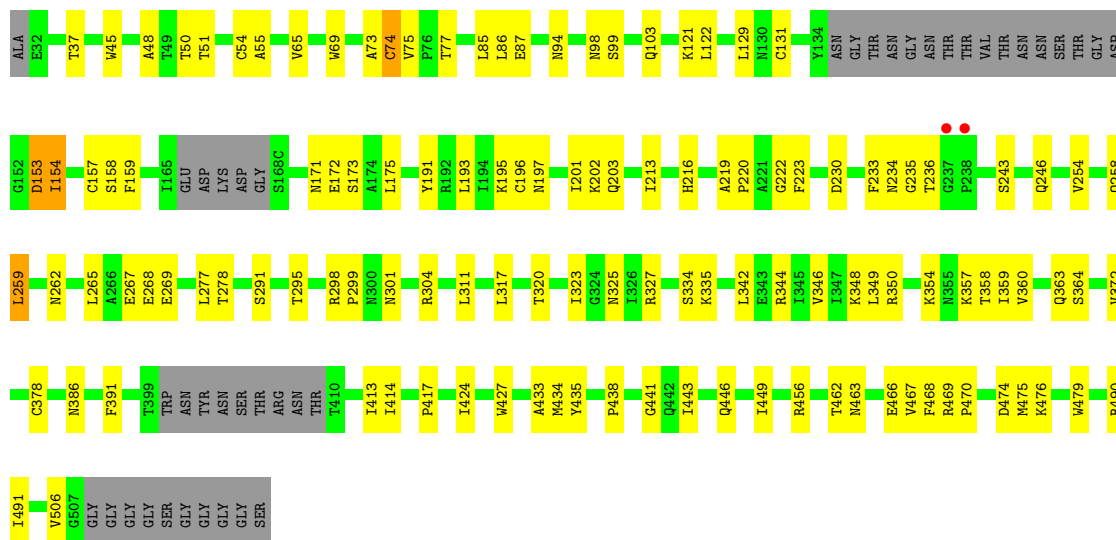
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

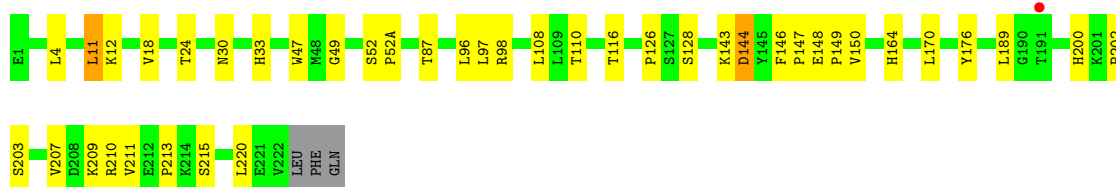
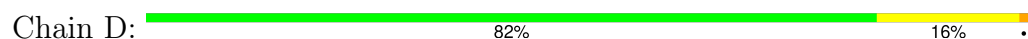
- Molecule 1: Envelope glycoprotein gp160




- Molecule 2: Envelope glycoprotein gp160

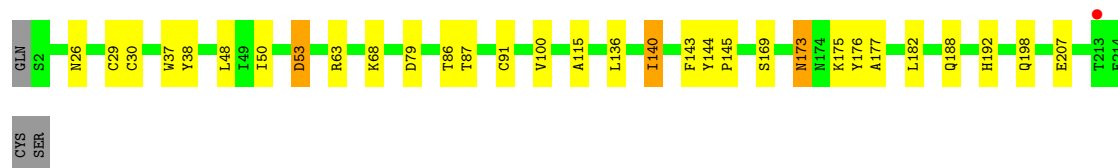


- Molecule 3: 35O22 Heavy chain



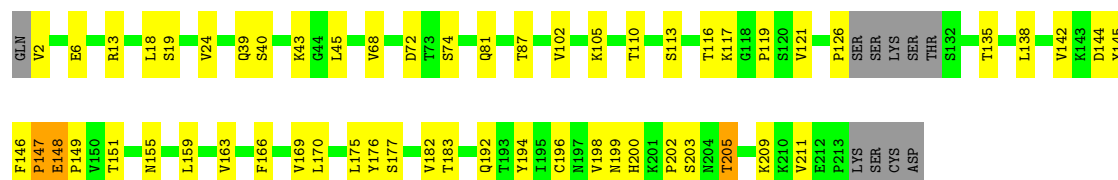
- Molecule 4: 35O22 Light chain

Chain E:  84% 13% ..




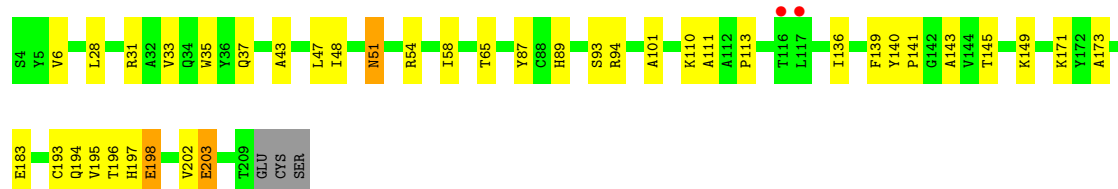
- Molecule 5: PGT124 Heavy chain

Chain H:  72% 22% . .



- Molecule 6: PGT124 Light chain

Chain L:  80% 17% ..



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%



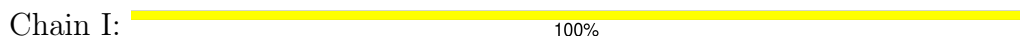
- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



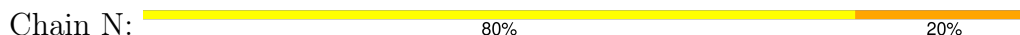
- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.35Å 127.35Å 316.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.87 – 4.60 48.87 – 4.60	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.87-4.60) 96.9 (48.87-4.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 4.64Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.313 , 0.341 0.314 , 0.345	Depositor DCC
$R_{free}$ test set	749 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	181.7	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 658.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.159 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11946	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	274.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG

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	B	0.23	0/1109	0.42	0/1509
2	G	0.24	0/3579	0.44	0/4854
3	D	0.25	0/1860	0.46	0/2533
4	E	0.25	0/1659	0.45	0/2269
5	H	0.25	0/1763	0.48	0/2407
6	L	0.27	0/1644	0.45	0/2246
All	All	0.25	0/11614	0.45	0/15818

There are no bond length outliers.

There are no bond angle outliers.

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	B	1086	0	1055	21	0
2	G	3512	0	3485	83	0
3	D	1813	0	1784	26	0
4	E	1615	0	1544	21	0
5	H	1720	0	1684	40	0
6	L	1601	0	1545	44	0
7	A	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	28	0	25	1	0
7	J	28	0	25	1	0
8	F	39	0	34	2	0
8	K	39	0	34	1	0
9	I	61	0	52	1	0
9	N	61	0	50	6	0
10	M	50	0	43	1	0
11	O	83	0	69	0	0
12	G	182	0	165	7	0
All	All	11946	0	11619	228	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 228 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)
6:L:195:VAL:HG23	6:L:202:VAL:CG2	1.45	1.45
6:L:195:VAL:CG2	6:L:202:VAL:HG23	1.48	1.41
6:L:195:VAL:CG2	6:L:202:VAL:CG2	2.02	1.35
6:L:145:THR:HB	6:L:196:THR:HB	1.19	1.19
6:L:195:VAL:HG23	6:L:202:VAL:HG21	1.28	1.10

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	B	135/140 (96%)	125 (93%)	9 (7%)	1 (1%)	19 56
2	G	438/487 (90%)	404 (92%)	34 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	238/243 (98%)	229 (96%)	8 (3%)	1 (0%)	30	68
4	E	211/216 (98%)	202 (96%)	9 (4%)	0	100	100
5	H	222/236 (94%)	207 (93%)	13 (6%)	2 (1%)	14	51
6	L	209/214 (98%)	196 (94%)	11 (5%)	2 (1%)	13	48
All	All	1453/1536 (95%)	1363 (94%)	84 (6%)	6 (0%)	30	68

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	566	PRO
5	H	148	GLU
6	L	198	GLU
3	D	144	ASP
6	L	6	VAL

### 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	B	117/118 (99%)	117 (100%)	0	100	100
2	G	400/428 (94%)	386 (96%)	14 (4%)	31	52
3	D	203/206 (98%)	201 (99%)	2 (1%)	73	81
4	E	186/189 (98%)	183 (98%)	3 (2%)	58	74
5	H	194/204 (95%)	191 (98%)	3 (2%)	60	75
6	L	177/180 (98%)	171 (97%)	6 (3%)	32	53
All	All	1277/1325 (96%)	1249 (98%)	28 (2%)	47	65

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	11	LEU
6	L	203	GLU

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Mol	Chain	Res	Type
4	E	140	ILE
6	L	89	HIS
4	E	53	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	575	GLN
2	G	103	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 ⓘ

33 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	$\# Z  > 2$
7	NAG	A	1	1,7	14,14,15	0.37	0	17,19,21	0.47	0
7	NAG	A	2	7	14,14,15	0.30	0	17,19,21	0.55	0
7	NAG	C	1	2,7	14,14,15	0.74	1 (7%)	17,19,21	1.28	2 (11%)
7	NAG	C	2	7	14,14,15	0.34	0	17,19,21	0.39	0
8	NAG	F	1	2,8	14,14,15	0.23	0	17,19,21	0.74	1 (5%)
8	NAG	F	2	8	14,14,15	0.20	0	17,19,21	0.47	0
8	BMA	F	3	8	11,11,12	0.76	0	15,15,17	0.67	0
9	NAG	I	1	2,9	14,14,15	0.48	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	I	2	9	14,14,15	0.64	0	17,19,21	0.81	0
9	BMA	I	3	9	11,11,12	0.83	0	15,15,17	1.01	1 (6%)
9	MAN	I	4	9	11,11,12	0.75	0	15,15,17	0.82	1 (6%)
9	MAN	I	5	9	11,11,12	0.68	0	15,15,17	0.98	2 (13%)
7	NAG	J	1	2,7	14,14,15	0.57	0	17,19,21	1.56	2 (11%)
7	NAG	J	2	7	14,14,15	0.39	0	17,19,21	0.62	0
8	NAG	K	1	2,8	14,14,15	0.43	0	17,19,21	0.61	0
8	NAG	K	2	8	14,14,15	0.23	0	17,19,21	0.63	1 (5%)
8	BMA	K	3	8	11,11,12	0.58	0	15,15,17	0.70	0
10	NAG	M	1	2,10	14,14,15	0.55	0	17,19,21	1.36	2 (11%)
10	NAG	M	2	10	14,14,15	0.31	0	17,19,21	0.60	0
10	BMA	M	3	10	11,11,12	0.58	0	15,15,17	0.69	0
10	MAN	M	4	10	11,11,12	0.65	0	15,15,17	1.04	2 (13%)
9	NAG	N	1	2,9	14,14,15	0.56	0	17,19,21	1.95	3 (17%)
9	NAG	N	2	9	14,14,15	0.20	0	17,19,21	0.41	0
9	BMA	N	3	9	11,11,12	0.86	1 (9%)	15,15,17	0.94	0
9	MAN	N	4	9	11,11,12	0.68	0	15,15,17	0.83	1 (6%)
9	MAN	N	5	9	11,11,12	1.08	1 (9%)	15,15,17	0.77	1 (6%)
11	NAG	O	1	2,11	14,14,15	0.32	0	17,19,21	0.48	0
11	NAG	O	2	11	14,14,15	0.31	0	17,19,21	0.53	0
11	BMA	O	3	11	11,11,12	1.42	1 (9%)	15,15,17	1.38	2 (13%)
11	MAN	O	4	11	11,11,12	1.57	3 (27%)	15,15,17	2.24	1 (6%)
11	MAN	O	5	11	11,11,12	0.91	1 (9%)	15,15,17	1.04	2 (13%)
11	MAN	O	6	11	11,11,12	1.34	1 (9%)	15,15,17	1.83	3 (20%)
11	MAN	O	7	11	11,11,12	0.73	1 (9%)	15,15,17	1.26	2 (13%)

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
7	NAG	A	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	2	7	-	3/6/23/26	0/1/1/1
7	NAG	C	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	C	2	7	-	1/6/23/26	0/1/1/1
8	NAG	F	1	2,8	-	1/6/23/26	0/1/1/1
8	NAG	F	2	8	-	0/6/23/26	0/1/1/1
8	BMA	F	3	8	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	I	1	2,9	-	1/6/23/26	0/1/1/1
9	NAG	I	2	9	-	4/6/23/26	0/1/1/1
9	BMA	I	3	9	-	1/2/19/22	0/1/1/1
9	MAN	I	4	9	-	0/2/19/22	0/1/1/1
9	MAN	I	5	9	-	1/2/19/22	0/1/1/1
7	NAG	J	1	2,7	-	3/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
8	NAG	K	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	K	2	8	-	0/6/23/26	0/1/1/1
8	BMA	K	3	8	-	0/2/19/22	0/1/1/1
10	NAG	M	1	2,10	-	6/6/23/26	0/1/1/1
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1
10	BMA	M	3	10	-	0/2/19/22	0/1/1/1
10	MAN	M	4	10	-	0/2/19/22	0/1/1/1
9	NAG	N	1	2,9	-	3/6/23/26	0/1/1/1
9	NAG	N	2	9	-	0/6/23/26	0/1/1/1
9	BMA	N	3	9	-	2/2/19/22	0/1/1/1
9	MAN	N	4	9	-	1/2/19/22	0/1/1/1
9	MAN	N	5	9	-	2/2/19/22	0/1/1/1
11	NAG	O	1	2,11	-	2/6/23/26	0/1/1/1
11	NAG	O	2	11	-	0/6/23/26	0/1/1/1
11	BMA	O	3	11	-	2/2/19/22	0/1/1/1
11	MAN	O	4	11	-	0/2/19/22	0/1/1/1
11	MAN	O	5	11	-	0/2/19/22	0/1/1/1
11	MAN	O	6	11	-	0/2/19/22	0/1/1/1
11	MAN	O	7	11	-	0/2/19/22	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	3	BMA	O3-C3	3.66	1.52	1.43
11	O	4	MAN	C1-C2	3.18	1.59	1.52
9	N	5	MAN	O5-C1	-3.17	1.38	1.43
11	O	6	MAN	C1-C2	3.12	1.59	1.52
11	O	4	MAN	O5-C5	2.96	1.49	1.43

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	4	MAN	C1-O5-C5	7.75	122.58	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	1	NAG	C1-O5-C5	6.25	120.57	112.19
11	O	6	MAN	C1-O5-C5	5.68	119.81	112.19
7	J	1	NAG	C2-N2-C7	4.66	129.15	122.90
10	M	1	NAG	C2-N2-C7	4.43	128.84	122.90

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

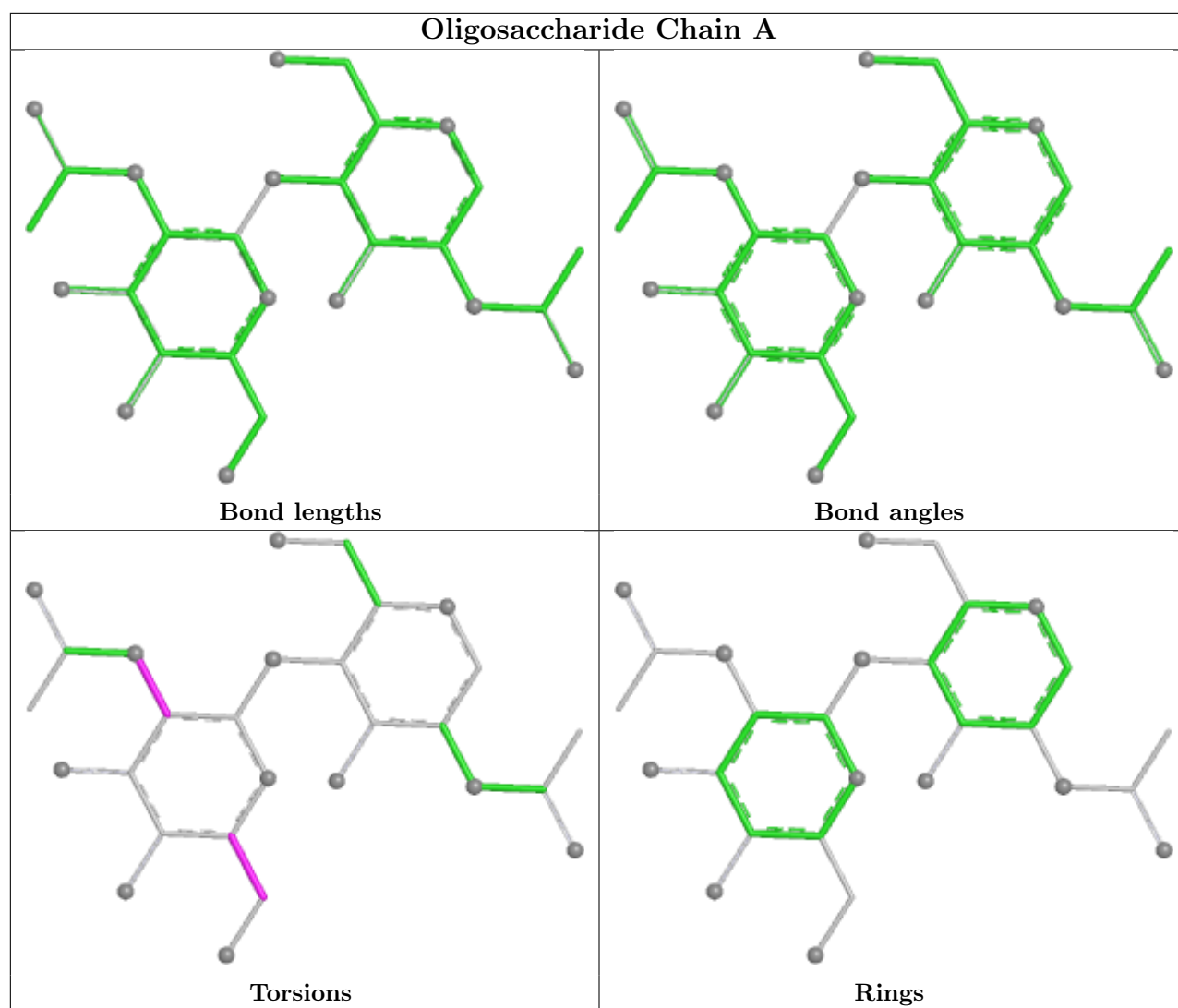
Mol	Chain	Res	Type	Atoms
7	J	1	NAG	C1-C2-N2-C7
9	N	5	MAN	O5-C5-C6-O6
9	N	3	BMA	O5-C5-C6-O6
8	K	1	NAG	C4-C5-C6-O6
11	O	1	NAG	O5-C5-C6-O6

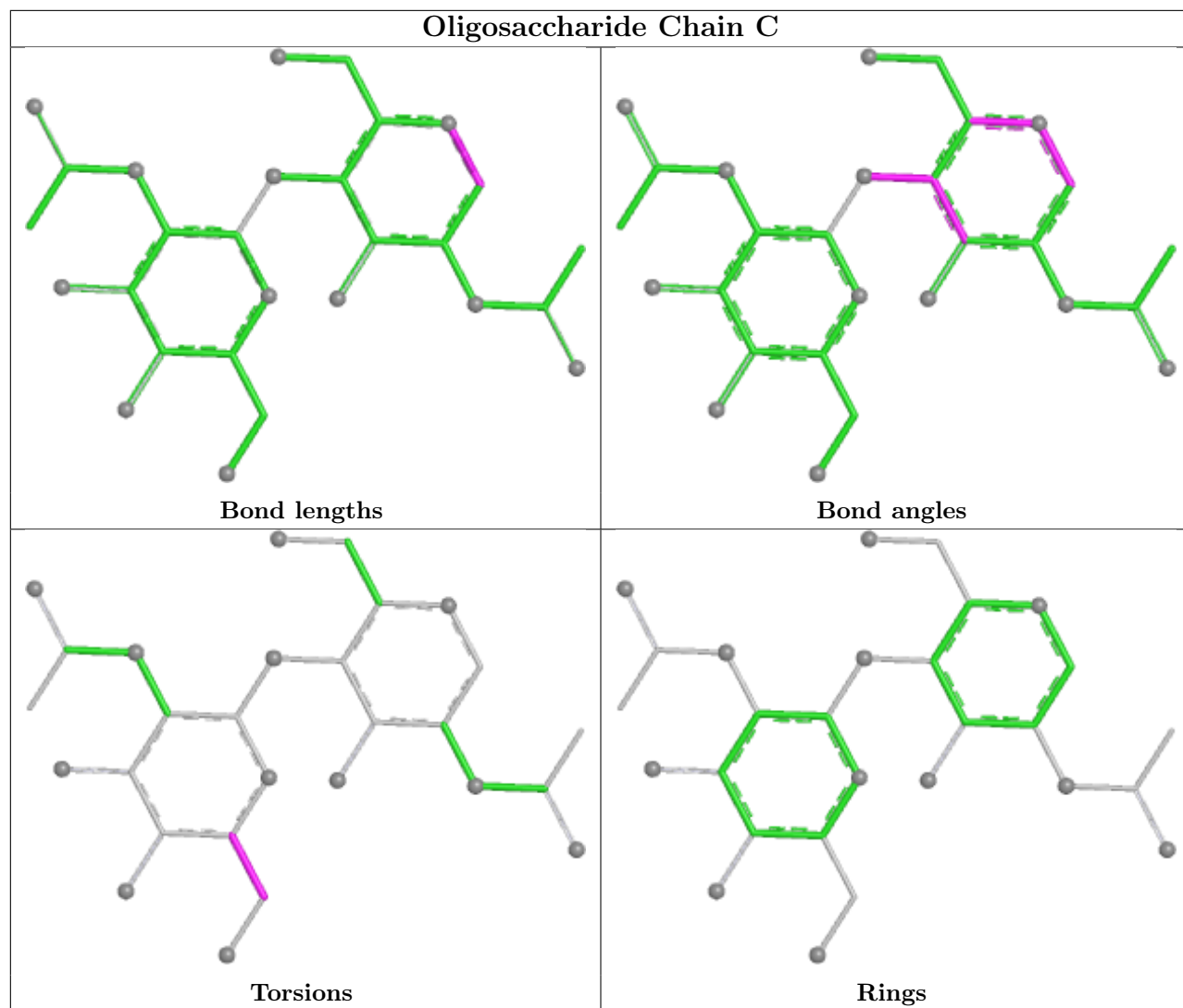
There are no ring outliers.

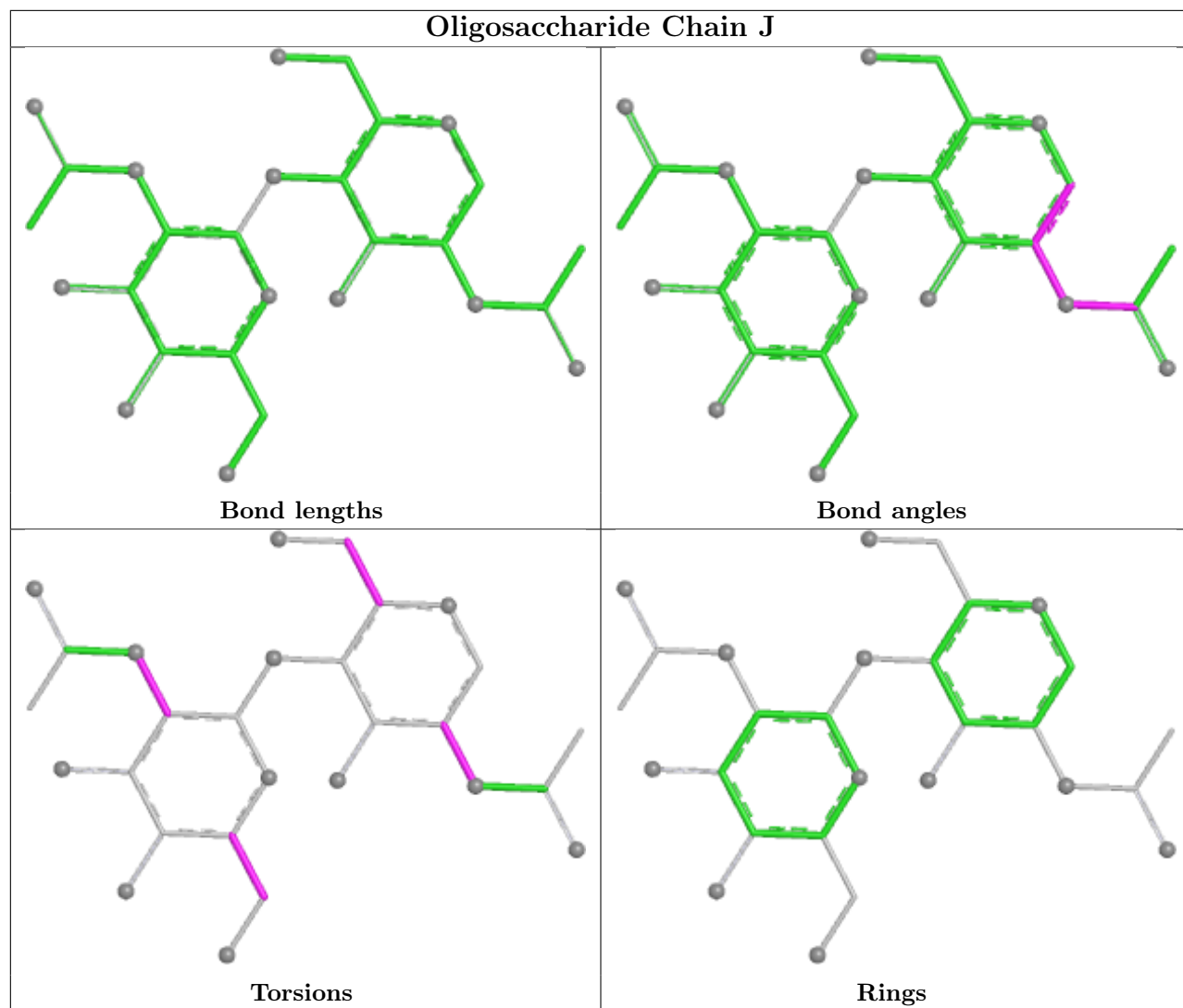
11 monomers are involved in 13 short contacts:

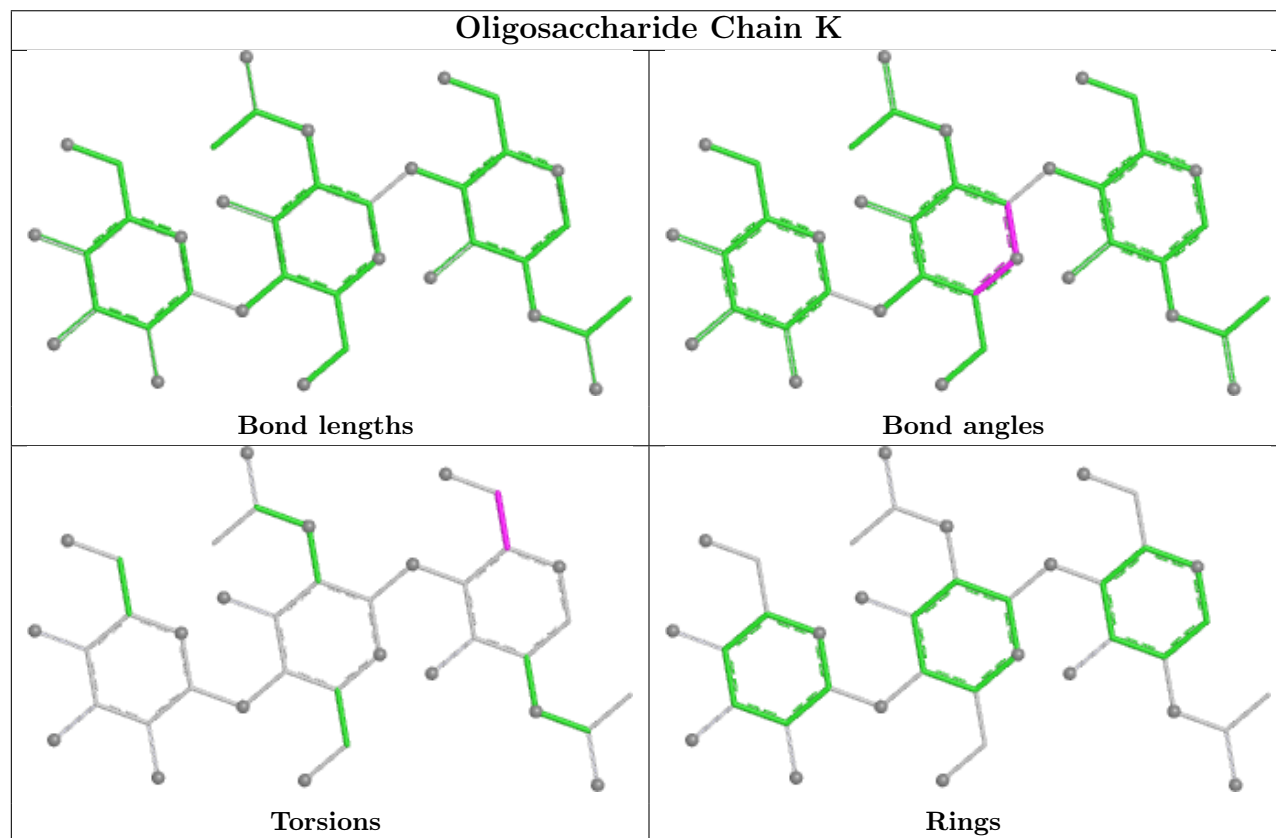
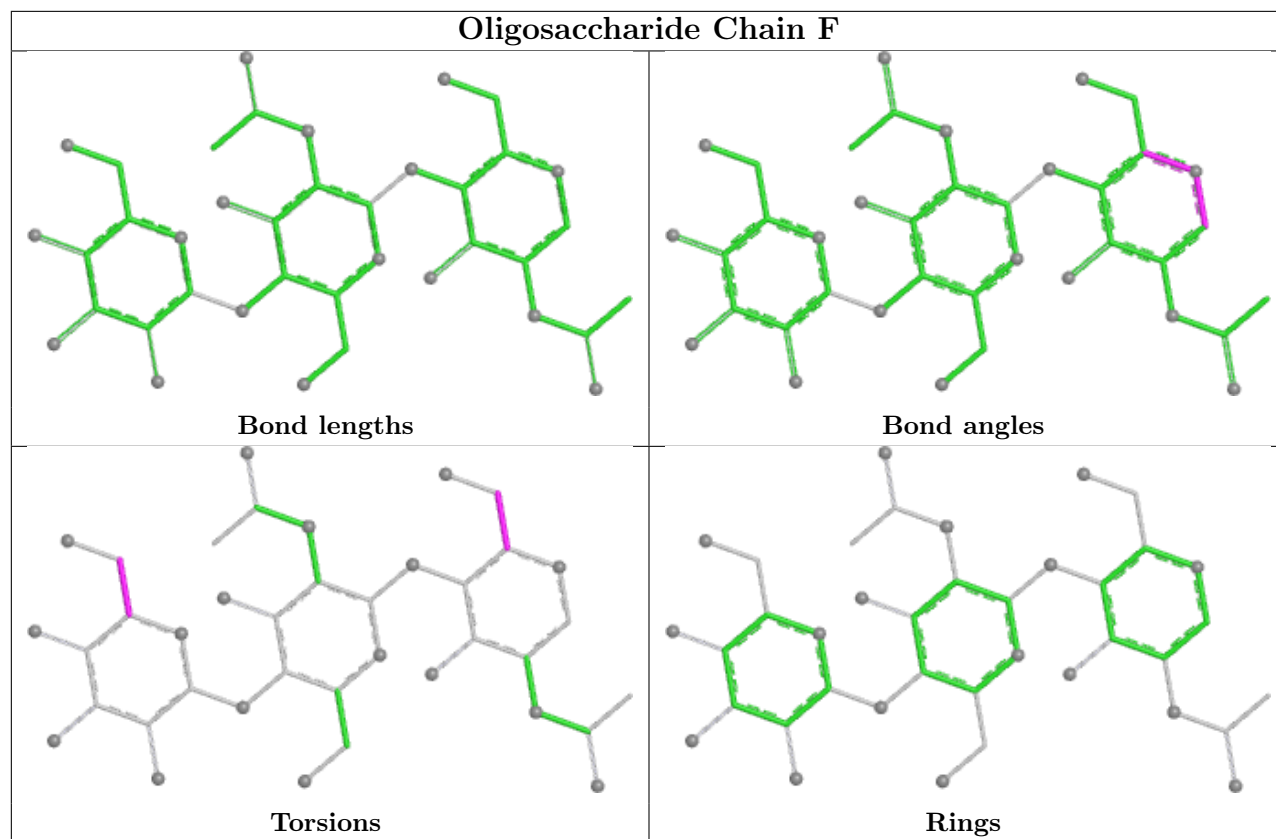
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	1	NAG	1	0
10	M	1	NAG	1	0
9	I	1	NAG	1	0
8	F	1	NAG	2	0
9	I	2	NAG	1	0
7	C	2	NAG	1	0
9	N	2	NAG	4	0
7	C	1	NAG	1	0
9	N	1	NAG	2	0
8	K	2	NAG	1	0
7	J	1	NAG	1	0

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

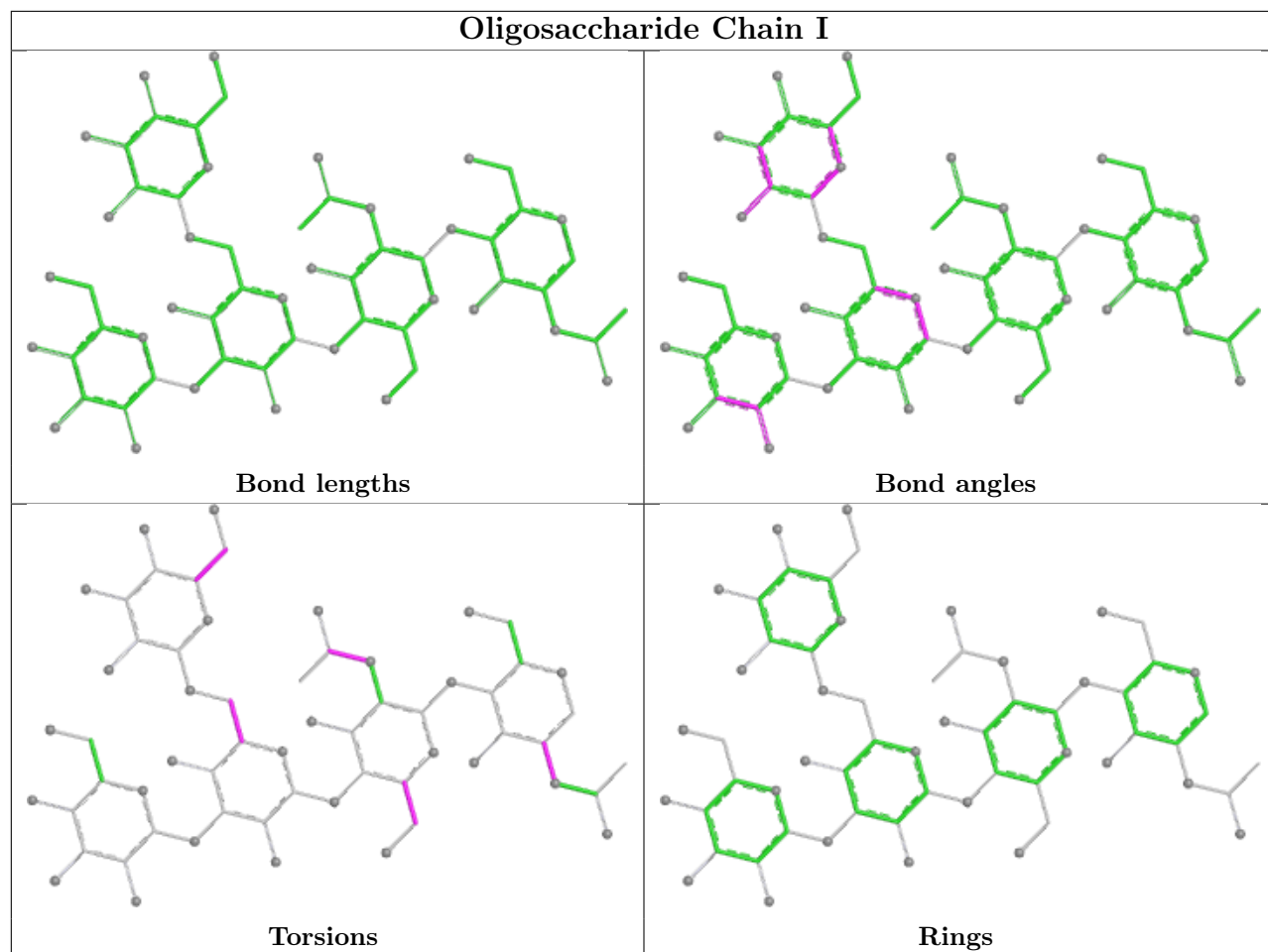


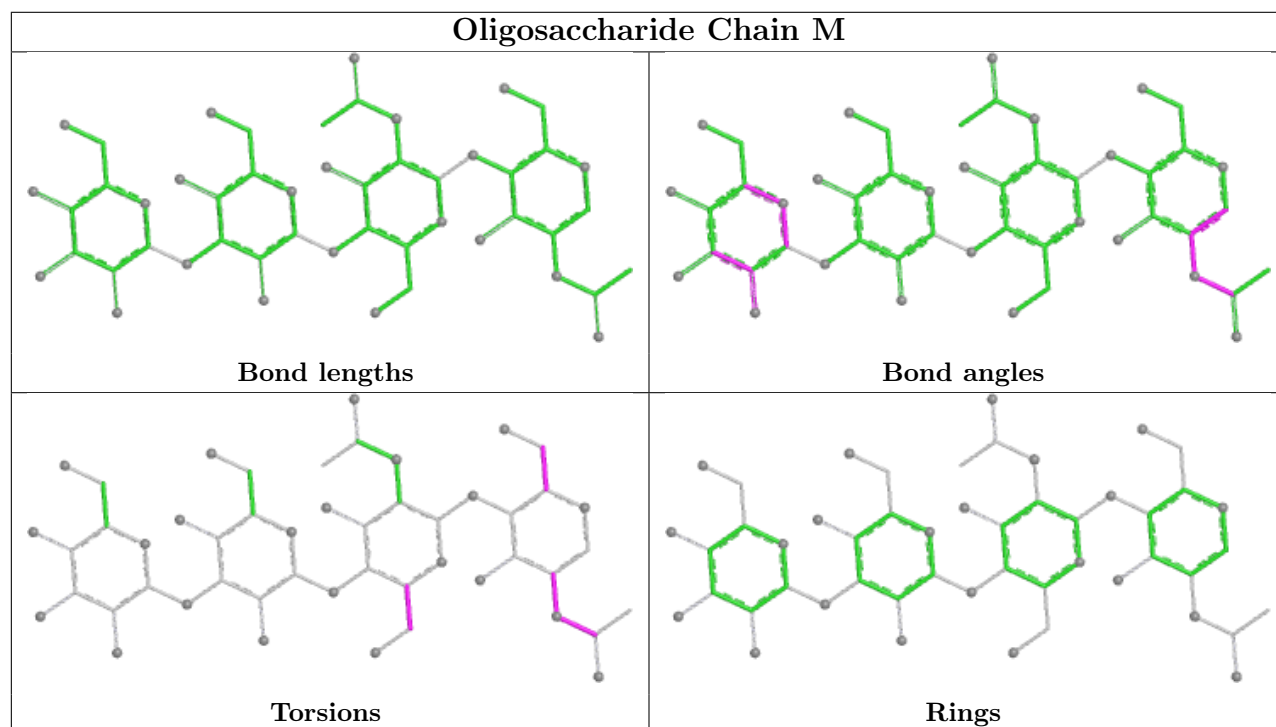
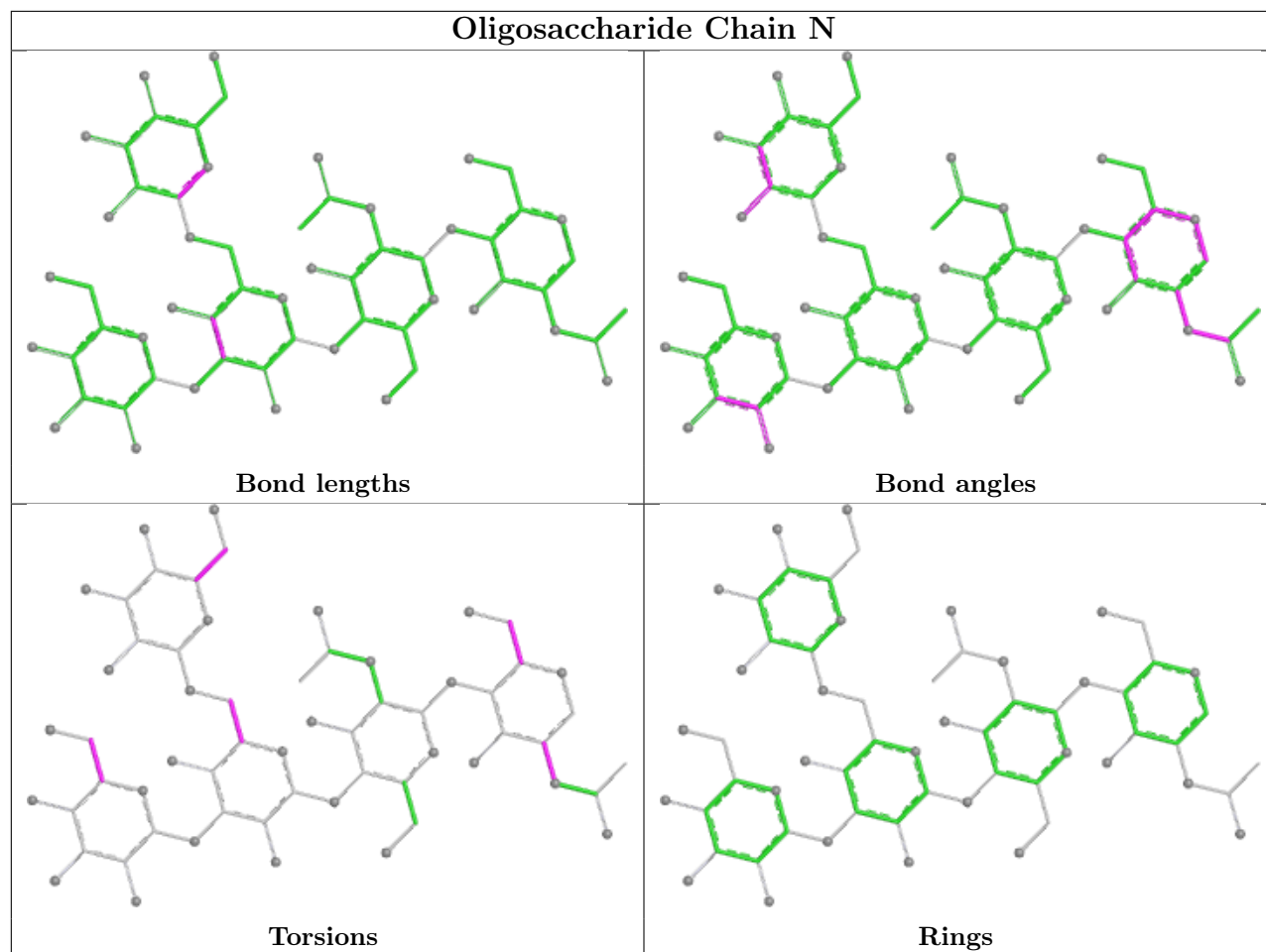


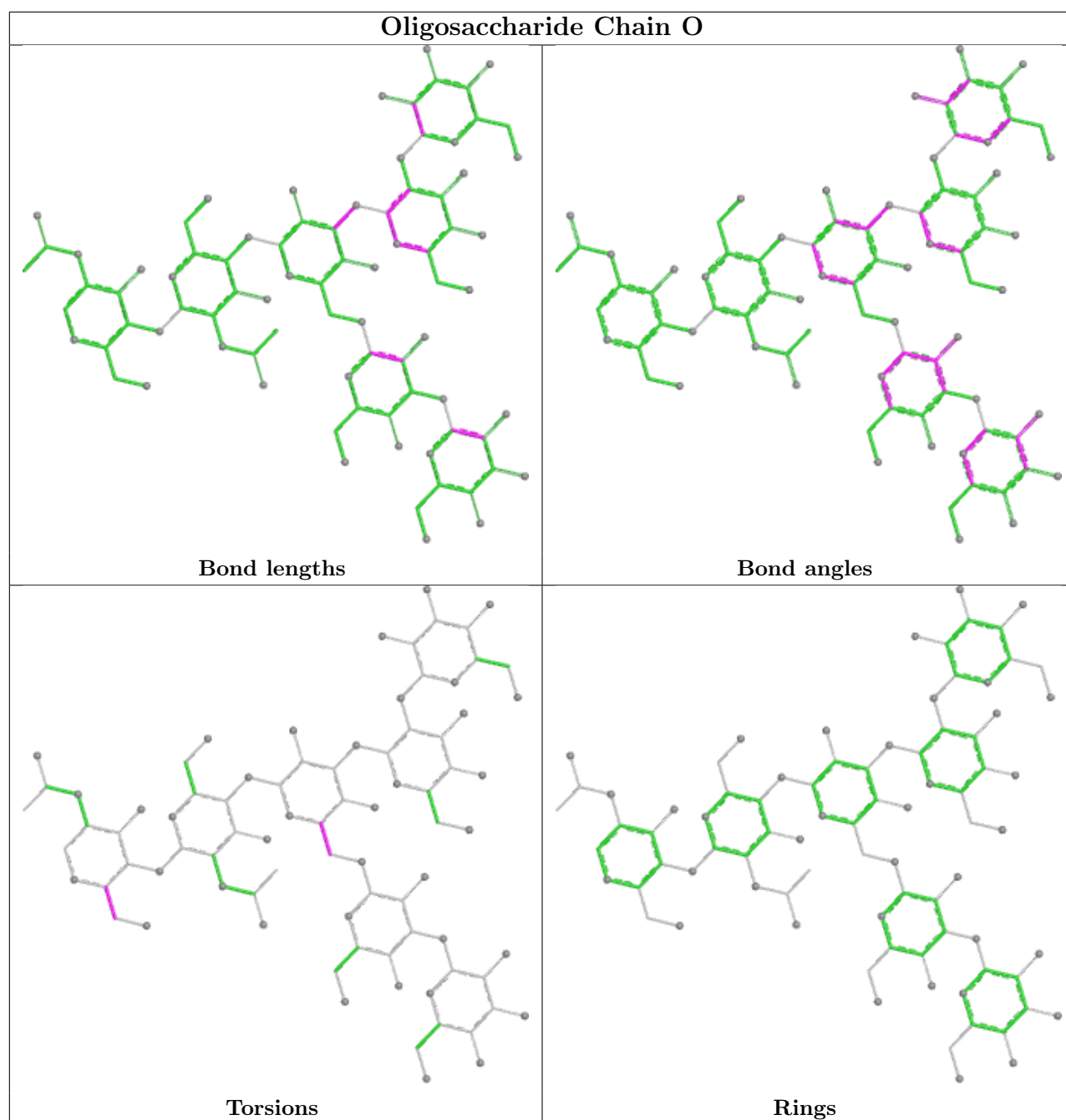












## 5.6 Ligand geometry [i](#)

13 ligands 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
12	NAG	G	610	2	14,14,15	0.32	0	17,19,21	0.39	0
12	NAG	G	606	2	14,14,15	0.26	0	17,19,21	0.69	1 (5%)
12	NAG	G	612	2	14,14,15	0.25	0	17,19,21	0.39	0
12	NAG	G	602	2	14,14,15	0.35	0	17,19,21	0.44	0
12	NAG	G	601	2	14,14,15	0.39	0	17,19,21	0.47	0
12	NAG	G	605	2	14,14,15	0.28	0	17,19,21	0.62	0
12	NAG	G	613	2	14,14,15	0.38	0	17,19,21	0.46	0
12	NAG	G	607	2	14,14,15	0.28	0	17,19,21	0.54	0
12	NAG	G	603	2	14,14,15	0.47	0	17,19,21	0.77	1 (5%)
12	NAG	G	611	2	14,14,15	0.17	0	17,19,21	0.48	0
12	NAG	G	604	2	14,14,15	0.31	0	17,19,21	0.37	0
12	NAG	G	609	2	14,14,15	0.30	0	17,19,21	0.43	0
12	NAG	G	608	2	14,14,15	0.27	0	17,19,21	0.54	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
12	NAG	G	610	2	-	4/6/23/26	0/1/1/1
12	NAG	G	606	2	-	0/6/23/26	0/1/1/1
12	NAG	G	612	2	-	3/6/23/26	0/1/1/1
12	NAG	G	602	2	-	3/6/23/26	0/1/1/1
12	NAG	G	601	2	-	4/6/23/26	0/1/1/1
12	NAG	G	605	2	-	2/6/23/26	0/1/1/1
12	NAG	G	613	2	-	0/6/23/26	0/1/1/1
12	NAG	G	607	2	-	0/6/23/26	0/1/1/1
12	NAG	G	603	2	-	2/6/23/26	0/1/1/1
12	NAG	G	611	2	-	0/6/23/26	0/1/1/1
12	NAG	G	604	2	-	0/6/23/26	0/1/1/1
12	NAG	G	609	2	-	0/6/23/26	0/1/1/1
12	NAG	G	608	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	603	NAG	C1-O5-C5	2.70	115.81	112.19
12	G	606	NAG	C1-O5-C5	2.28	115.25	112.19

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	601	NAG	C4-C5-C6-O6
12	G	602	NAG	O5-C5-C6-O6
12	G	603	NAG	O5-C5-C6-O6
12	G	610	NAG	C4-C5-C6-O6
12	G	610	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	606	NAG	2	0
12	G	602	NAG	1	0
12	G	601	NAG	3	0
12	G	605	NAG	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	B	137/140 (97%)	-0.66	1 (0%) 84 71	181, 225, 304, 320	0
2	G	446/487 (91%)	-0.76	2 (0%) 89 79	142, 236, 306, 372	0
3	D	240/243 (98%)	-0.57	1 (0%) 89 79	158, 270, 425, 444	0
4	E	213/216 (98%)	-0.76	1 (0%) 87 76	183, 292, 389, 429	0
5	H	226/236 (95%)	-0.73	0 100 100	204, 284, 405, 456	0
6	L	211/214 (98%)	-0.60	2 (0%) 81 67	209, 296, 363, 411	0
All	All	1473/1536 (95%)	-0.69	7 (0%) 87 76	142, 264, 389, 456	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	237	GLY	3.8
1	B	664	ASP	3.7
6	L	116	THR	2.8
6	L	117	LEU	2.3
2	G	238	PRO	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	NAG	G	608	14/15	0.88	0.09	352,352,352,352	0
12	NAG	G	607	14/15	0.89	0.08	323,323,323,323	0
12	NAG	G	602	14/15	0.89	0.10	331,331,331,331	0
12	NAG	G	601	14/15	0.91	0.06	360,360,360,360	0
12	NAG	G	612	14/15	0.92	0.13	364,364,364,364	0
12	NAG	G	611	14/15	0.93	0.10	377,377,377,377	0
12	NAG	G	610	14/15	0.96	0.05	345,345,345,345	0
12	NAG	G	613	14/15	0.97	0.09	124,124,124,124	0
12	NAG	G	606	14/15	0.98	0.05	355,355,355,355	0
12	NAG	G	609	14/15	0.98	0.09	371,371,371,371	0
12	NAG	G	605	14/15	0.99	0.04	327,327,327,327	0
12	NAG	G	603	14/15	0.99	0.08	294,294,294,294	0
12	NAG	G	604	14/15	0.99	0.12	379,379,379,379	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.