



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:00 PM UTC

PDB ID : 5U7O / pdb_00005u7o
Title : Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer Bound to Small Molecule HIV-1 Entry Inhibitor BMS-626529 in Complex with Human Antibodies PGT122 and 35O22 at 3.8 Angstrom
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Deposited on : 2016-12-12
Resolution : 3.03 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

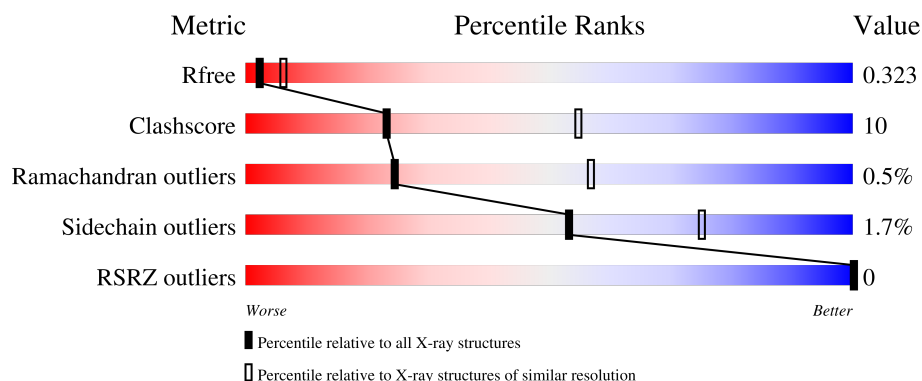
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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.



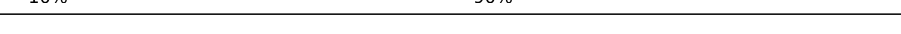
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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 $\leq 5\%$. 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	153	
2	D	243	
3	E	216	
4	G	481	

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Mol	Chain	Length	Quality of chain
5	H	235	
6	L	213	
7	A	7	
8	C	4	
9	F	5	
10	I	2	
10	J	2	
10	K	2	
10	N	2	
10	O	2	
10	Q	2	
10	R	2	
10	S	2	
11	M	6	
12	P	10	
13	T	3	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 12089 atoms, of which 23 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	126	Total	C	N	O	S	0	0	0
			998	632	172	188	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S5
B	605	CYS	THR	engineered mutation	UNP Q2N0S5

- Molecule 2 is a protein called 35O22 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	242	Total	C	N	O	S	0	0	0
			1832	1165	306	353	8			

- Molecule 3 is a protein called 35O22 FAB LIGHT CHAIN.

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

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	444	Total	C	N	O	S	0	0	0
			3485	2188	616	654	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S5
G	501	CYS	ALA	engineered mutation	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	509	ARG	GLU	engineered mutation	UNP Q2N0S5
G	510	ARG	LYS	engineered mutation	UNP Q2N0S5
G	512	ARG	ALA	engineered mutation	UNP Q2N0S5
G	513	ARG	VAL	engineered mutation	UNP Q2N0S5

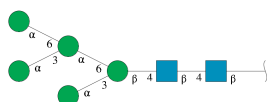
- Molecule 5 is a protein called PGT122 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

- Molecule 6 is a protein called PGT122 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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
7	A	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 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.



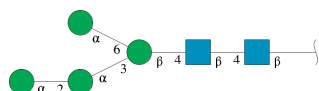
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

-

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

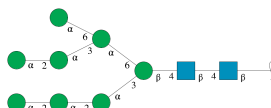


- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



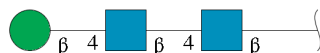
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	M	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
12	P	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 13 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
13	T	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 14 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



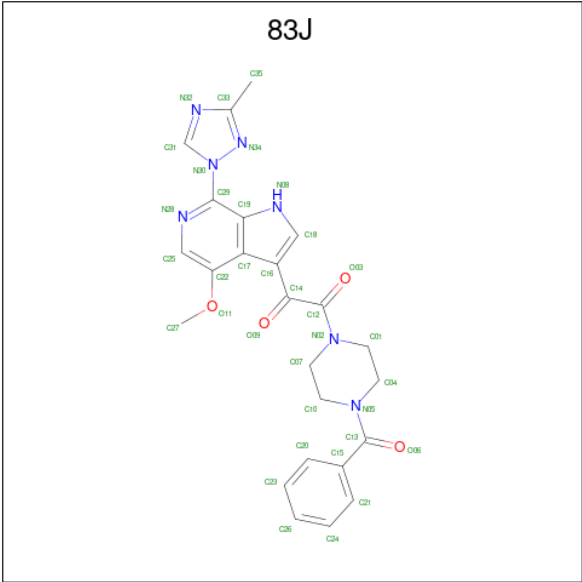
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	O	S	0	0
			5	4	1		
14	G	1	Total	O	S	0	0
			5	4	1		
14	G	1	Total	O	S	0	0
			5	4	1		
14	G	1	Total	O	S	0	0
			5	4	1		
14	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 16 is 1-[4-(benzenecarbonyl)piperazin-1-yl]-2-[4-methoxy-7-(3-methyl-1H-1,2,4-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]ethane-1,2-dione (CCD ID: 83J) (formula: C₂₄H₂₃N₇O₄).



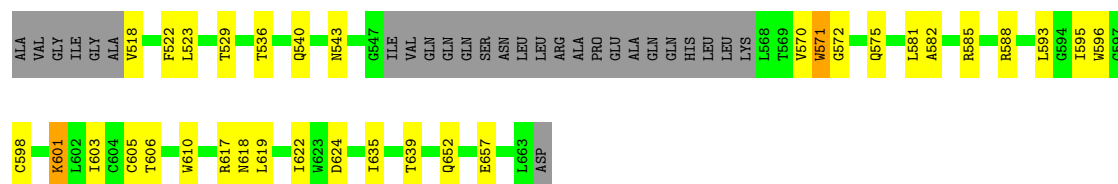
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	G	1	Total	C	H	N	O	0	0
			58	24	23	7	4		

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 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.

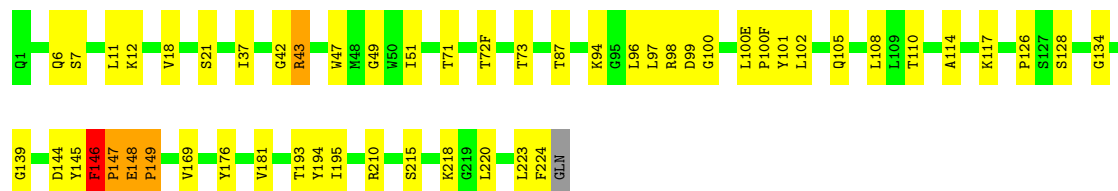
- Molecule 1: Envelope glycoprotein gp160

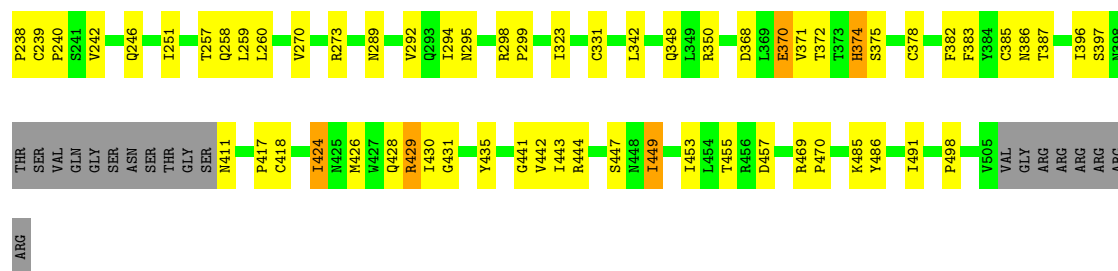
Chain B: 



- Molecule 2: 35O22 FAB HEAVY CHAIN

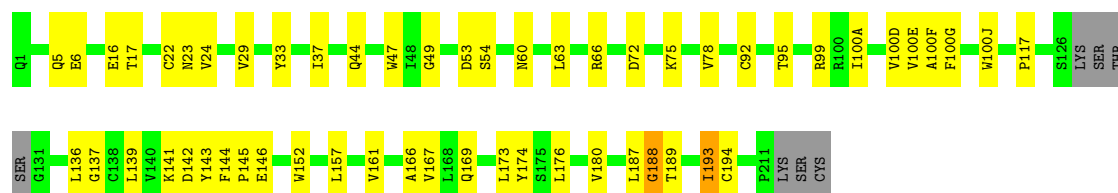
Chain D: 





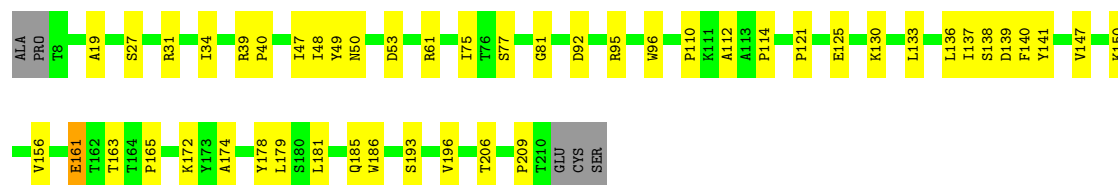
• Molecule 5: PGT122 FAB HEAVY CHAIN

Chain H: 74% 23%



• Molecule 6: PGT122 FAB LIGHT CHAIN

Chain L: 75% 22%



• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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

Chain A: 14% 86%



• Molecule 8: 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

Chain C: 25% 75%



• 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

Chain F:  60% 40%



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

Chain I:  50% 50%



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

Chain J:  100%



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

Chain K:  100%



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

Chain N:  100%



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

Chain O:  100%



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

Chain Q:  100%



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

Chain R:  100%

MAG1
MAG2

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

Chain S:  100%

MAG1
MAG2

- Molecule 11: alpha-D-mannopyranose-(1-2)-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

Chain M:  50%  50%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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

Chain P:  10%  90%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

- Molecule 13: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	131.03Å 131.03Å 311.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.35 – 3.03 41.35 – 3.03	Depositor EDS
% Data completeness (in resolution range)	54.1 (41.35-3.03) 54.2 (41.35-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.272 , 0.325 0.272 , 0.323	Depositor DCC
R_{free} test set	1584 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.189 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12089	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 83J, SO4, NAG, 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	B	0.16	0/1016	0.22	0/1378
2	D	0.08	0/1880	0.23	0/2560
3	E	0.07	0/1659	0.24	0/2269
4	G	0.07	0/3556	0.24	0/4827
5	H	0.07	0/1789	0.23	0/2443
6	L	0.07	0/1619	0.23	0/2217
All	All	0.08	0/11519	0.23	0/15694

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	146	PHE	Peptide
2	D	148	GLU	Peptide

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	998	0	973	27	0
2	D	1832	0	1806	44	0
3	E	1615	0	1542	17	0
4	G	3485	0	3414	90	0
5	H	1742	0	1715	38	0
6	L	1577	0	1518	32	0
7	A	83	0	70	5	0
8	C	50	0	43	1	0
9	F	61	0	52	0	0
10	I	28	0	25	4	0
10	J	28	0	25	0	0
10	K	28	0	25	0	0
10	N	28	0	25	0	0
10	O	28	0	25	0	0
10	Q	28	0	25	0	0
10	R	28	0	25	1	0
10	S	28	0	25	0	0
11	M	72	0	61	0	0
12	P	116	0	97	2	0
13	T	39	0	34	0	0
14	B	5	0	0	1	0
14	G	15	0	0	0	0
14	L	5	0	0	0	0
15	B	42	0	39	1	0
15	G	56	0	52	4	0
15	H	14	0	13	0	0
16	G	35	23	0	1	0
All	All	12066	23	11629	244	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.

All (244) 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)
4:G:426:MET:HE2	4:G:428:GLN:HG3	1.42	1.01
2:D:11:LEU:HD22	2:D:147:PRO:HG3	1.44	0.96
10:I:2:NAG:H3	10:I:2:NAG:H83	1.55	0.89
15:G:633:NAG:H83	15:G:633:NAG:H3	1.56	0.88
7:A:2:NAG:H3	7:A:2:NAG:H83	1.55	0.88
6:L:39:ARG:NH1	6:L:81:GLY:O	2.10	0.83
2:D:114:ALA:HB3	2:D:146:PHE:CE2	2.18	0.79
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.64	0.79
4:G:201:ILE:HD11	4:G:435:TYR:HB2	1.66	0.76
1:B:571:TRP:CE3	1:B:571:TRP:HA	2.23	0.74
1:B:588:ARG:NH2	14:B:701:SO4:O1	2.21	0.73
6:L:47:ILE:HG22	6:L:48:ILE:HG13	1.71	0.73
4:G:65:LYS:HA	4:G:65:LYS:NZ	2.05	0.72
2:D:6:GLN:H	2:D:105:GLN:HE22	1.34	0.72
4:G:65:LYS:HA	4:G:65:LYS:HZ3	1.54	0.72
3:E:127:ALA:H	3:E:128:ASN:HA	1.55	0.72
1:B:536:THR:O	1:B:540:GLN:NE2	2.23	0.71
4:G:170:GLN:HG2	4:G:172:VAL:HG23	1.72	0.71
1:B:571:TRP:HA	1:B:571:TRP:HE3	1.54	0.71
15:B:703:NAG:H4	3:E:53:GLU:HG3	1.73	0.70
3:E:37:GLN:HB2	3:E:47:ILE:HD11	1.72	0.69
6:L:39:ARG:HG3	6:L:40:PRO:HD2	1.77	0.67
5:H:157:LEU:HD21	5:H:180:VAL:HG11	1.78	0.65
2:D:128:SER:HB2	2:D:220:LEU:HB2	1.78	0.65
2:D:114:ALA:HB3	2:D:146:PHE:HE2	1.61	0.65
6:L:19:ALA:HB3	6:L:75:ILE:HB	1.78	0.64
4:G:396:ILE:HG22	4:G:397:SER:H	1.61	0.64
4:G:69:TRP:CD1	4:G:111:LEU:HD13	2.33	0.64
4:G:258:GLN:NE2	4:G:371:VAL:O	2.27	0.64
1:B:529:THR:HG23	2:D:98:ARG:HD2	1.79	0.64
3:E:127:ALA:N	3:E:128:ASN:HA	2.11	0.64
1:B:582:ALA:HB1	4:G:221:ALA:HB3	1.81	0.62
4:G:219:ALA:O	4:G:246:GLN:NE2	2.32	0.62
4:G:68:VAL:HG13	4:G:69:TRP:CD2	2.35	0.61
6:L:150:LYS:HB2	6:L:193:SER:HB2	1.80	0.61
2:D:72(F):THR:HG1	2:D:73:THR:HG1	1.47	0.61
4:G:350:ARG:NH2	4:G:396:ILE:O	2.28	0.61
2:D:146:PHE:CD2	2:D:147:PRO:HD3	2.34	0.61
2:D:87:THR:HG23	2:D:110:THR:HA	1.83	0.61
4:G:368:ASP:OD2	4:G:370:GLU:HG2	2.00	0.61
2:D:99:ASP:OD1	2:D:100:GLY:N	2.34	0.61
4:G:193:LEU:HB2	4:G:196:CYS:SG	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:137:ILE:HD13	6:L:196:VAL:HG11	1.84	0.60
4:G:270:VAL:HG12	4:G:289:ASN:H	1.67	0.60
10:I:2:NAG:H3	10:I:2:NAG:C8	2.30	0.59
7:A:2:NAG:H3	7:A:2:NAG:C8	2.31	0.59
4:G:121:LYS:HD2	4:G:123:THR:HG23	1.85	0.58
4:G:69:TRP:HD1	4:G:111:LEU:HD13	1.69	0.58
4:G:69:TRP:HZ3	4:G:212:PRO:HA	1.68	0.57
4:G:382:PHE:HD2	4:G:424:ILE:HG21	1.69	0.57
6:L:138:SER:HB2	6:L:172:LYS:HE2	1.87	0.57
1:B:581:LEU:HD23	1:B:581:LEU:O	2.05	0.56
4:G:426:MET:CE	4:G:428:GLN:HG3	2.25	0.56
4:G:197:ASN:OD1	4:G:198:THR:HG23	2.05	0.56
5:H:22:CYS:HB3	5:H:78:VAL:HB	1.86	0.56
6:L:181:LEU:HD22	6:L:185:GLN:HG2	1.88	0.56
2:D:117:LYS:NZ	2:D:144:ASP:HB3	2.21	0.55
1:B:605:CYS:HA	4:G:37:THR:HG22	1.89	0.55
4:G:45:TRP:HB3	4:G:491:ILE:HD13	1.87	0.55
6:L:139:ASP:H	6:L:172:LYS:HG3	1.71	0.55
4:G:239:CYS:SG	4:G:242:VAL:HG22	2.46	0.55
5:H:188:GLY:H	5:H:189:THR:HA	1.72	0.55
4:G:183:GLN:HA	4:G:191:TYR:HA	1.90	0.54
4:G:257:THR:HG21	4:G:370:GLU:O	2.07	0.54
4:G:257:THR:O	4:G:259:LEU:N	2.38	0.54
4:G:298:ARG:NH2	4:G:441:GLY:O	2.40	0.54
4:G:292:VAL:HB	4:G:449:ILE:HG23	1.89	0.54
15:G:633:NAG:H3	15:G:633:NAG:C8	2.32	0.54
5:H:117:PRO:HB3	5:H:143:TYR:HB3	1.89	0.54
4:G:292:VAL:HB	4:G:449:ILE:CG2	2.38	0.54
4:G:386:ASN:HB3	4:G:417:PRO:HG2	1.90	0.54
2:D:108:LEU:HD23	2:D:148:GLU:O	2.08	0.53
4:G:50:THR:O	4:G:103:GLN:NE2	2.37	0.53
4:G:382:PHE:CD2	4:G:424:ILE:HG21	2.43	0.53
5:H:100(D):VAL:HA	12:P:2:NAG:H2	1.90	0.53
5:H:137:GLY:HA2	5:H:152:TRP:HH2	1.73	0.53
2:D:126:PRO:HB2	2:D:215:SER:HB2	1.91	0.53
2:D:146:PHE:CG	2:D:147:PRO:HD3	2.44	0.53
3:E:47:ILE:HG22	3:E:48:ILE:HG12	1.90	0.53
6:L:133:LEU:HD12	6:L:179:LEU:HD23	1.91	0.53
6:L:147:VAL:HG22	6:L:196:VAL:HG22	1.91	0.53
4:G:113:ASP:OD1	16:G:659:83J:N08	2.43	0.52
4:G:378:CYS:HB3	4:G:383:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:633:NAG:C1	15:G:633:NAG:H82	2.40	0.52
5:H:167:VAL:HB	6:L:163:THR:HG22	1.91	0.52
4:G:91:GLU:O	4:G:239:CYS:N	2.40	0.52
4:G:215:ILE:HG22	4:G:251:ILE:O	2.09	0.52
4:G:424:ILE:N	4:G:424:ILE:HD13	2.25	0.52
4:G:70:ALA:HB3	4:G:213:ILE:HD11	1.90	0.51
5:H:53:ASP:OD1	5:H:54:SER:N	2.40	0.51
4:G:426:MET:HE2	4:G:428:GLN:CG	2.27	0.51
5:H:47:TRP:O	5:H:60:ASN:ND2	2.44	0.51
6:L:114:PRO:HB3	6:L:140:PHE:HB3	1.92	0.51
2:D:117:LYS:HZ2	2:D:144:ASP:HB3	1.75	0.51
1:B:617:ARG:HB2	1:B:622:ILE:HD11	1.92	0.51
5:H:161:VAL:HG22	5:H:180:VAL:HG22	1.92	0.51
6:L:161:GLU:O	6:L:178:TYR:N	2.35	0.51
2:D:146:PHE:CG	2:D:147:PRO:CD	2.94	0.51
3:E:127:ALA:HB3	3:E:128:ASN:HA	1.92	0.51
10:I:2:NAG:H82	10:I:2:NAG:C1	2.40	0.51
7:A:2:NAG:H82	7:A:2:NAG:C1	2.40	0.51
4:G:429:ARG:O	4:G:429:ARG:HG2	2.10	0.51
2:D:218:LYS:NZ	3:E:210:GLU:OE1	2.31	0.50
4:G:260:LEU:HD21	4:G:453:ILE:HD11	1.94	0.50
8:C:2:NAG:H61	8:C:3:BMA:H2	1.93	0.50
1:B:571:TRP:CZ2	4:G:215:ILE:HD11	2.47	0.50
1:B:601:LYS:HZ2	1:B:601:LYS:HB3	1.77	0.50
2:D:100(E):LEU:HD12	2:D:100(F):PRO:HD2	1.93	0.50
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.48	0.49
1:B:635:ILE:O	1:B:639:THR:HG23	2.12	0.49
1:B:571:TRP:HZ2	4:G:215:ILE:HD11	1.77	0.49
4:G:257:THR:CG2	4:G:375:SER:H	2.25	0.49
5:H:63:LEU:HD22	5:H:66:ARG:HH21	1.78	0.49
1:B:624:ASP:HB3	2:D:99:ASP:O	2.13	0.48
4:G:86:LEU:HB3	4:G:89:VAL:HG21	1.95	0.48
4:G:199:SER:HB2	4:G:431:GLY:C	2.38	0.48
1:B:610:TRP:HE3	4:G:36:VAL:HG22	1.78	0.48
4:G:68:VAL:HG13	4:G:69:TRP:CE2	2.48	0.48
4:G:95:MET:SD	4:G:273:ARG:HD3	2.54	0.48
1:B:529:THR:HG23	2:D:98:ARG:CD	2.43	0.48
2:D:96:LEU:HG	2:D:97:LEU:HG	1.96	0.48
3:E:209:THR:HG23	3:E:210:GLU:HG3	1.96	0.48
4:G:259:LEU:HB2	4:G:374:HIS:CE1	2.48	0.48
1:B:601:LYS:HB3	1:B:601:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:230:ASP:OD2	4:G:233:PHE:HB2	2.14	0.47
6:L:186:TRP:CE2	6:L:209:PRO:HG3	2.49	0.47
2:D:12:LYS:HG3	2:D:18:VAL:HB	1.96	0.47
2:D:145:TYR:HE2	2:D:148:GLU:HA	1.80	0.47
4:G:121:LYS:HD3	4:G:201:ILE:O	2.13	0.47
4:G:385:CYS:HA	4:G:418:CYS:HA	1.97	0.47
2:D:101:TYR:HD1	3:E:46:LEU:HD23	1.80	0.47
5:H:139:LEU:HD21	5:H:141:LYS:HB2	1.97	0.47
5:H:188:GLY:N	5:H:189:THR:HA	2.30	0.46
2:D:147:PRO:O	2:D:149:PRO:CD	2.63	0.46
4:G:258:GLN:HG2	4:G:470:PRO:HB2	1.97	0.46
4:G:294:ILE:HG22	4:G:447:SER:O	2.15	0.46
3:E:27(C):CYS:HA	3:E:28:CYS:HA	1.53	0.46
4:G:92:GLU:HA	4:G:238:PRO:HA	1.98	0.46
6:L:193:SER:OG	6:L:206:THR:HG22	2.16	0.46
1:B:595:ILE:HG13	1:B:596:TRP:CD1	2.50	0.46
5:H:72:ASP:OD2	5:H:75:LYS:HD2	2.15	0.46
1:B:593:LEU:HG	1:B:598:CYS:O	2.15	0.46
6:L:121:PRO:HD3	6:L:133:LEU:HD23	1.98	0.46
1:B:603:ILE:O	1:B:603:ILE:HG13	2.14	0.46
4:G:131:CYS:HA	4:G:157:CYS:HA	1.98	0.46
5:H:187:LEU:HD13	5:H:188:GLY:N	2.31	0.46
4:G:429:ARG:HD3	4:G:429:ARG:C	2.40	0.46
4:G:84:ILE:HD12	4:G:84:ILE:N	2.30	0.45
4:G:98:ASN:ND2	4:G:486:TYR:O	2.49	0.45
4:G:457:ASP:OD1	4:G:457:ASP:N	2.50	0.45
2:D:94:LYS:HB3	2:D:102:LEU:HB3	1.98	0.45
4:G:122:LEU:HD11	4:G:203:GLN:HB2	1.98	0.45
1:B:522:PHE:CD1	1:B:543:ASN:HB2	2.52	0.45
2:D:147:PRO:O	2:D:149:PRO:HD3	2.17	0.45
3:E:96:CYS:SG	3:E:97:VAL:N	2.89	0.45
10:R:1:NAG:H61	10:R:2:NAG:N2	2.31	0.45
2:D:6:GLN:N	2:D:105:GLN:HE22	2.09	0.44
5:H:5:GLN:NE2	5:H:6:GLU:O	2.49	0.44
5:H:49:GLY:HA2	6:L:96:TRP:HZ3	1.82	0.44
6:L:112:ALA:HB3	6:L:141:TYR:H	1.82	0.44
4:G:69:TRP:CZ3	4:G:212:PRO:HA	2.52	0.44
4:G:428:GLN:O	4:G:429:ARG:HB3	2.18	0.44
6:L:125:GLU:HG2	6:L:130:LYS:O	2.18	0.44
1:B:523:LEU:O	4:G:86:LEU:HD22	2.17	0.44
1:B:610:TRP:CD2	4:G:498:PRO:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:146:PHE:O	2:D:147:PRO:C	2.60	0.44
4:G:123:THR:N	4:G:124:PRO:HD2	2.33	0.44
5:H:146:GLU:OE2	5:H:166:ALA:HB3	2.18	0.44
1:B:585:ARG:HH21	4:G:491:ILE:C	2.25	0.44
2:D:145:TYR:CZ	2:D:176:TYR:HB2	2.53	0.44
2:D:11:LEU:HD22	2:D:147:PRO:CG	2.32	0.43
2:D:220:LEU:HG	2:D:224:PHE:HE1	1.83	0.43
5:H:99:ARG:HD3	5:H:100(J):TRP:CZ3	2.52	0.43
5:H:100(D):VAL:O	5:H:100(F):ALA:N	2.47	0.43
5:H:136:LEU:HD23	5:H:137:GLY:N	2.32	0.43
5:H:100(A):ILE:HD13	5:H:100(E):VAL:HG22	2.00	0.43
6:L:112:ALA:HB3	6:L:141:TYR:N	2.33	0.43
5:H:37:ILE:N	5:H:37:ILE:HD12	2.33	0.43
5:H:193:ILE:HD13	5:H:194:CYS:N	2.33	0.43
6:L:27:SER:HA	6:L:31:ARG:CZ	2.48	0.43
2:D:7:SER:HB3	2:D:21:SER:OG	2.18	0.43
2:D:51:ILE:HD13	2:D:71:THR:HG23	2.01	0.43
4:G:215:ILE:HG23	4:G:215:ILE:O	2.19	0.43
7:A:1:NAG:H61	7:A:2:NAG:C7	2.48	0.43
6:L:34:ILE:HD13	6:L:50:ASN:H	1.84	0.43
2:D:139:GLY:HA3	2:D:181:VAL:HA	1.99	0.43
4:G:417:PRO:HB3	5:H:100(G):PHE:CE1	2.53	0.43
4:G:227:LYS:HE3	4:G:485:LYS:HD3	2.00	0.43
4:G:299:PRO:HA	4:G:442:VAL:HG13	2.01	0.43
5:H:169:GLN:HG2	6:L:161:GLU:HG2	2.01	0.43
2:D:146:PHE:O	2:D:147:PRO:O	2.37	0.42
3:E:4:LEU:HB3	3:E:99:GLY:HA2	2.01	0.42
4:G:455:THR:OG1	4:G:469:ARG:O	2.31	0.42
5:H:137:GLY:HA2	5:H:152:TRP:CH2	2.53	0.42
6:L:92:ASP:HB3	6:L:95:ARG:HB2	2.01	0.42
2:D:134:GLY:HA2	2:D:223:LEU:HD13	2.01	0.42
4:G:270:VAL:HG23	4:G:348:GLN:HG3	2.01	0.42
4:G:342:LEU:HD23	4:G:342:LEU:HA	1.88	0.42
5:H:144:PHE:HA	5:H:145:PRO:HA	1.80	0.42
1:B:618:ASN:OD1	1:B:619:LEU:N	2.45	0.42
3:E:49:TYR:CD2	3:E:50:GLU:HG3	2.54	0.42
4:G:443:ILE:HD12	4:G:443:ILE:HA	1.93	0.42
5:H:33:TYR:HB2	5:H:95:THR:O	2.20	0.42
5:H:166:ALA:HB1	5:H:174:TYR:HB3	2.02	0.42
6:L:49:TYR:O	6:L:53:ASP:HB2	2.19	0.42
6:L:61:ARG:HD2	6:L:77:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:117:LYS:HB3	4:G:118:PRO:HD3	2.02	0.42
3:E:49:TYR:HD2	3:E:50:GLU:HG3	1.85	0.42
15:G:633:NAG:C8	15:G:633:NAG:C1	2.98	0.42
1:B:606:THR:OG1	4:G:36:VAL:O	2.29	0.41
4:G:71:THR:O	4:G:72:HIS:HB3	2.18	0.41
5:H:6:GLU:OE2	5:H:92:CYS:HB3	2.19	0.41
5:H:16:GLU:HG2	5:H:17:THR:H	1.84	0.41
6:L:156:VAL:HG11	6:L:179:LEU:HD11	2.02	0.41
1:B:572:GLY:O	1:B:575:GLN:NE2	2.53	0.41
2:D:145:TYR:CE1	2:D:176:TYR:HB2	2.56	0.41
2:D:42:GLY:O	2:D:43:ARG:HB2	2.20	0.41
4:G:170:GLN:HG2	4:G:172:VAL:CG2	2.44	0.41
5:H:47:TRP:N	6:L:96:TRP:O	2.47	0.41
5:H:176:LEU:HD12	5:H:176:LEU:C	2.46	0.41
6:L:39:ARG:CG	6:L:40:PRO:HD2	2.49	0.41
2:D:193:THR:HG22	2:D:195:ILE:HG13	2.02	0.41
5:H:24:VAL:HG21	5:H:29:VAL:HG12	2.03	0.41
2:D:37:ILE:HD12	2:D:37:ILE:N	2.36	0.41
3:E:81:GLU:H	3:E:81:GLU:CD	2.29	0.41
5:H:44:GLN:OE1	5:H:44:GLN:N	2.54	0.41
10:I:2:NAG:C8	10:I:2:NAG:C1	2.98	0.41
2:D:169:VAL:O	2:D:176:TYR:HA	2.21	0.41
5:H:6:GLU:OE1	5:H:6:GLU:N	2.53	0.41
6:L:165:PRO:HA	6:L:174:ALA:O	2.21	0.41
3:E:89:CYS:SG	3:E:90:SER:N	2.94	0.41
4:G:444:ARG:HH12	12:P:1:NAG:C8	2.33	0.41
5:H:142:ASP:HA	5:H:173:LEU:HB3	2.03	0.41
6:L:136:LEU:N	6:L:136:LEU:HD22	2.36	0.41
7:A:2:NAG:C8	7:A:2:NAG:C1	2.98	0.41
2:D:194:TYR:O	2:D:210:ARG:HD2	2.21	0.41
4:G:108:ILE:O	4:G:112:TRP:HD1	2.04	0.41
4:G:155:LYS:O	4:G:175:LEU:HD12	2.21	0.40
4:G:258:GLN:HE22	4:G:372:THR:C	2.29	0.40
4:G:430:ILE:HG22	4:G:431:GLY:H	1.86	0.40
4:G:323:ILE:HD12	4:G:323:ILE:N	2.36	0.40
3:E:39:PRO:HA	3:E:40:PRO:HD3	1.98	0.40
4:G:295:ASN:O	4:G:331:CYS:HA	2.22	0.40
4:G:411:ASN:ND2	4:G:411:ASN:O	2.55	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	B	122/153 (80%)	114 (93%)	8 (7%)	0	100	100
2	D	240/243 (99%)	223 (93%)	14 (6%)	3 (1%)	9	35
3	E	211/216 (98%)	196 (93%)	15 (7%)	0	100	100
4	G	434/481 (90%)	396 (91%)	36 (8%)	2 (0%)	24	57
5	H	224/235 (95%)	209 (93%)	14 (6%)	1 (0%)	30	61
6	L	206/213 (97%)	186 (90%)	19 (9%)	1 (0%)	24	57
All	All	1437/1541 (93%)	1324 (92%)	106 (7%)	7 (0%)	24	57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	149	PRO
2	D	146	PHE
4	G	240	PRO
2	D	147	PRO
4	G	374	HIS
5	H	188	GLY
6	L	110	PRO

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	107/129 (83%)	101 (94%)	6 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	205/206 (100%)	204 (100%)	1 (0%)	81	86
3	E	186/189 (98%)	184 (99%)	2 (1%)	65	80
4	G	394/428 (92%)	384 (98%)	10 (2%)	42	69
5	H	198/205 (97%)	196 (99%)	2 (1%)	68	81
6	L	177/181 (98%)	176 (99%)	1 (1%)	78	85
All	All	1267/1338 (95%)	1245 (98%)	22 (2%)	53	75

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	518	VAL
1	B	570	VAL
1	B	571	TRP
1	B	601	LYS
1	B	652	GLN
1	B	657	GLU
2	D	43	ARG
3	E	11	VAL
3	E	53	GLU
4	G	65	LYS
4	G	123	THR
4	G	153	GLU
4	G	202	THR
4	G	217	TYR
4	G	370	GLU
4	G	387	THR
4	G	424	ILE
4	G	429	ARG
4	G	449	ILE
5	H	23	ASN
5	H	193	ILE
6	L	161	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	543	ASN
1	B	607	ASN
2	D	199	ASN

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Mol	Chain	Res	Type
4	G	425	ASN
4	G	462	ASN
5	H	39	GLN
6	L	95(C)	ASN
6	L	109	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 ⓘ

51 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	7,4	14,14,15	0.25	0	17,19,21	0.45	0
7	NAG	A	2	7	14,14,15	0.26	0	17,19,21	0.64	0
7	BMA	A	3	7	11,11,12	0.63	0	15,15,17	0.70	0
7	MAN	A	4	7	11,11,12	0.67	0	15,15,17	1.19	2 (13%)
7	MAN	A	5	7	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
7	MAN	A	6	7	11,11,12	0.64	0	15,15,17	1.07	2 (13%)
7	MAN	A	7	7	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
8	NAG	C	1	8,4	14,14,15	0.25	0	17,19,21	0.40	0
8	NAG	C	2	8	14,14,15	0.23	0	17,19,21	0.43	0
8	BMA	C	3	8	11,11,12	0.50	0	15,15,17	0.80	0
8	MAN	C	4	8	11,11,12	0.67	0	15,15,17	1.01	2 (13%)
9	NAG	F	1	4,9	14,14,15	0.21	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	F	2	9	14,14,15	0.23	0	17,19,21	0.44	0
9	BMA	F	3	9	11,11,12	0.58	0	15,15,17	0.69	0
9	MAN	F	4	9	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
9	MAN	F	5	9	11,11,12	0.63	0	15,15,17	1.09	2 (13%)
10	NAG	I	1	10,4	14,14,15	0.27	0	17,19,21	0.44	0
10	NAG	I	2	10	14,14,15	0.24	0	17,19,21	0.58	0
10	NAG	J	1	10,4	14,14,15	0.23	0	17,19,21	0.48	0
10	NAG	J	2	10	14,14,15	0.22	0	17,19,21	0.43	0
10	NAG	K	1	10,4	14,14,15	0.23	0	17,19,21	0.41	0
10	NAG	K	2	10	14,14,15	0.22	0	17,19,21	0.43	0
11	NAG	M	1	4,11	14,14,15	0.26	0	17,19,21	0.53	0
11	NAG	M	2	11	14,14,15	0.29	0	17,19,21	0.42	0
11	BMA	M	3	11	11,11,12	0.64	0	15,15,17	0.74	0
11	MAN	M	4	11	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
11	MAN	M	5	11	11,11,12	0.71	0	15,15,17	1.09	2 (13%)
11	MAN	M	6	11	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
10	NAG	N	1	10,4	14,14,15	0.27	0	17,19,21	0.53	0
10	NAG	N	2	10	14,14,15	0.22	0	17,19,21	0.42	0
10	NAG	O	1	10,4	14,14,15	0.21	0	17,19,21	0.44	0
10	NAG	O	2	10	14,14,15	0.23	0	17,19,21	0.44	0
12	NAG	P	1	4,12	14,14,15	0.21	0	17,19,21	0.42	0
12	MAN	P	10	12	11,11,12	0.70	0	15,15,17	0.95	1 (6%)
12	NAG	P	2	12	14,14,15	0.22	0	17,19,21	0.43	0
12	BMA	P	3	12	11,11,12	0.67	0	15,15,17	0.93	0
12	MAN	P	4	12	11,11,12	0.67	0	15,15,17	1.03	2 (13%)
12	MAN	P	5	12	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
12	MAN	P	6	12	11,11,12	0.57	0	15,15,17	1.14	2 (13%)
12	MAN	P	7	12	11,11,12	0.71	0	15,15,17	0.93	1 (6%)
12	MAN	P	8	12	11,11,12	0.68	0	15,15,17	1.08	2 (13%)
12	MAN	P	9	12	11,11,12	0.71	0	15,15,17	1.11	2 (13%)
10	NAG	Q	1	10,4	14,14,15	0.22	0	17,19,21	0.42	0
10	NAG	Q	2	10	14,14,15	0.23	0	17,19,21	0.45	0
10	NAG	R	1	10,4	14,14,15	0.23	0	17,19,21	0.54	0
10	NAG	R	2	10	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	S	1	10,4	14,14,15	0.25	0	17,19,21	0.42	0
10	NAG	S	2	10	14,14,15	0.24	0	17,19,21	0.52	0
13	NAG	T	1	13,4	14,14,15	0.22	0	17,19,21	0.49	0
13	NAG	T	2	13	14,14,15	0.23	0	17,19,21	0.42	0
13	BMA	T	3	13	11,11,12	0.56	0	15,15,17	0.78	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
7	NAG	A	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	4/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	0/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
7	MAN	A	7	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	2/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
8	MAN	C	4	8	-	1/2/19/22	0/1/1/1
9	NAG	F	1	4,9	-	2/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
9	BMA	F	3	9	-	1/2/19/22	0/1/1/1
9	MAN	F	4	9	-	1/2/19/22	0/1/1/1
9	MAN	F	5	9	-	0/2/19/22	0/1/1/1
10	NAG	I	1	10,4	-	4/6/23/26	0/1/1/1
10	NAG	I	2	10	-	5/6/23/26	0/1/1/1
10	NAG	J	1	10,4	-	4/6/23/26	0/1/1/1
10	NAG	J	2	10	-	1/6/23/26	0/1/1/1
10	NAG	K	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1
11	NAG	M	1	4,11	-	0/6/23/26	0/1/1/1
11	NAG	M	2	11	-	1/6/23/26	0/1/1/1
11	BMA	M	3	11	-	0/2/19/22	0/1/1/1
11	MAN	M	4	11	-	2/2/19/22	0/1/1/1
11	MAN	M	5	11	-	0/2/19/22	1/1/1/1
11	MAN	M	6	11	-	0/2/19/22	0/1/1/1
10	NAG	N	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	N	2	10	-	2/6/23/26	0/1/1/1
10	NAG	O	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	O	2	10	-	2/6/23/26	0/1/1/1
12	NAG	P	1	4,12	-	0/6/23/26	0/1/1/1
12	MAN	P	10	12	-	0/2/19/22	0/1/1/1
12	NAG	P	2	12	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BMA	P	3	12	-	0/2/19/22	0/1/1/1
12	MAN	P	4	12	-	0/2/19/22	0/1/1/1
12	MAN	P	5	12	-	0/2/19/22	0/1/1/1
12	MAN	P	6	12	-	1/2/19/22	0/1/1/1
12	MAN	P	7	12	-	2/2/19/22	0/1/1/1
12	MAN	P	8	12	-	0/2/19/22	0/1/1/1
12	MAN	P	9	12	-	0/2/19/22	1/1/1/1
10	NAG	Q	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	Q	2	10	-	2/6/23/26	0/1/1/1
10	NAG	R	1	10,4	-	4/6/23/26	0/1/1/1
10	NAG	R	2	10	-	0/6/23/26	0/1/1/1
10	NAG	S	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	2/6/23/26	0/1/1/1
13	NAG	T	1	13,4	-	4/6/23/26	0/1/1/1
13	NAG	T	2	13	-	2/6/23/26	0/1/1/1
13	BMA	T	3	13	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	6	MAN	C1-O5-C5	3.13	116.38	112.19
12	P	9	MAN	C1-O5-C5	3.13	116.38	112.19
7	A	4	MAN	C1-O5-C5	3.01	116.23	112.19
11	M	5	MAN	C1-O5-C5	3.01	116.22	112.19
7	A	6	MAN	C1-O5-C5	2.70	115.80	112.19
9	F	5	MAN	C1-O5-C5	2.64	115.73	112.19
7	A	7	MAN	C1-O5-C5	2.64	115.72	112.19
12	P	8	MAN	C1-O5-C5	2.57	115.64	112.19
11	M	4	MAN	O2-C2-C3	-2.54	104.90	110.15
9	F	4	MAN	C1-O5-C5	2.49	115.52	112.19
11	M	4	MAN	C1-O5-C5	2.47	115.50	112.19
12	P	4	MAN	C1-O5-C5	2.45	115.46	112.19
8	C	4	MAN	C1-O5-C5	2.39	115.39	112.19
12	P	5	MAN	C1-O5-C5	2.37	115.36	112.19
11	M	6	MAN	C1-O5-C5	2.33	115.31	112.19
7	A	5	MAN	C1-O5-C5	2.32	115.29	112.19
12	P	5	MAN	O2-C2-C3	-2.31	105.38	110.15
7	A	4	MAN	O2-C2-C3	-2.26	105.47	110.15
11	M	5	MAN	O2-C2-C3	-2.21	105.56	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	9	MAN	O2-C2-C3	-2.21	105.58	110.15
7	A	7	MAN	O2-C2-C3	-2.19	105.62	110.15
12	P	6	MAN	O2-C2-C3	-2.18	105.63	110.15
7	A	6	MAN	O2-C2-C3	-2.17	105.67	110.15
9	F	5	MAN	O2-C2-C3	-2.17	105.67	110.15
7	A	5	MAN	O2-C2-C3	-2.16	105.67	110.15
8	C	4	MAN	O2-C2-C3	-2.15	105.69	110.15
9	F	4	MAN	O2-C2-C3	-2.15	105.71	110.15
12	P	10	MAN	O2-C2-C3	-2.14	105.71	110.15
11	M	6	MAN	O2-C2-C3	-2.13	105.73	110.15
12	P	4	MAN	O2-C2-C3	-2.11	105.77	110.15
12	P	7	MAN	O2-C2-C3	-2.10	105.80	110.15
12	P	8	MAN	O2-C2-C3	-2.04	105.94	110.15

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	2	NAG	O5-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
10	S	2	NAG	O5-C5-C6-O6
12	P	2	NAG	O5-C5-C6-O6
7	A	3	BMA	C4-C5-C6-O6
10	N	1	NAG	O5-C5-C6-O6
10	O	1	NAG	O5-C5-C6-O6
10	S	2	NAG	C4-C5-C6-O6
10	R	1	NAG	O5-C5-C6-O6
10	S	1	NAG	O5-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
8	C	2	NAG	C4-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
10	Q	2	NAG	O5-C5-C6-O6
13	T	1	NAG	O5-C5-C6-O6
10	R	1	NAG	C4-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6
13	T	1	NAG	C4-C5-C6-O6
10	O	1	NAG	C4-C5-C6-O6
10	Q	2	NAG	C4-C5-C6-O6
13	T	2	NAG	O5-C5-C6-O6
10	N	1	NAG	C4-C5-C6-O6
12	P	2	NAG	C4-C5-C6-O6
10	O	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	1	NAG	C4-C5-C6-O6
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
10	I	1	NAG	C8-C7-N2-C2
10	I	1	NAG	O7-C7-N2-C2
10	I	2	NAG	C8-C7-N2-C2
10	I	2	NAG	O7-C7-N2-C2
10	J	1	NAG	C8-C7-N2-C2
10	J	1	NAG	O7-C7-N2-C2
13	T	1	NAG	C8-C7-N2-C2
13	T	1	NAG	O7-C7-N2-C2
10	K	2	NAG	O5-C5-C6-O6
10	S	1	NAG	C4-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
11	M	4	MAN	O5-C5-C6-O6
11	M	4	MAN	C4-C5-C6-O6
10	K	1	NAG	O5-C5-C6-O6
7	A	1	NAG	C4-C5-C6-O6
10	N	2	NAG	C4-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
10	I	1	NAG	C4-C5-C6-O6
10	J	1	NAG	O5-C5-C6-O6
13	T	3	BMA	O5-C5-C6-O6
10	J	1	NAG	C4-C5-C6-O6
10	O	2	NAG	C4-C5-C6-O6
10	N	2	NAG	O5-C5-C6-O6
13	T	2	NAG	C4-C5-C6-O6
9	F	4	MAN	O5-C5-C6-O6
10	I	1	NAG	O5-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
8	C	4	MAN	O5-C5-C6-O6
12	P	6	MAN	O5-C5-C6-O6
9	F	1	NAG	O5-C5-C6-O6
10	K	2	NAG	C4-C5-C6-O6
12	P	7	MAN	O5-C5-C6-O6
12	P	7	MAN	C4-C5-C6-O6
11	M	2	NAG	O5-C5-C6-O6
10	K	1	NAG	C4-C5-C6-O6
10	I	2	NAG	O5-C5-C6-O6
7	A	2	NAG	C3-C2-N2-C7
10	I	2	NAG	C3-C2-N2-C7
10	R	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
12	P	2	NAG	C3-C2-N2-C7
9	F	3	BMA	C4-C5-C6-O6
7	A	2	NAG	C1-C2-N2-C7
10	I	2	NAG	C1-C2-N2-C7
10	R	1	NAG	C1-C2-N2-C7
12	P	2	NAG	C1-C2-N2-C7

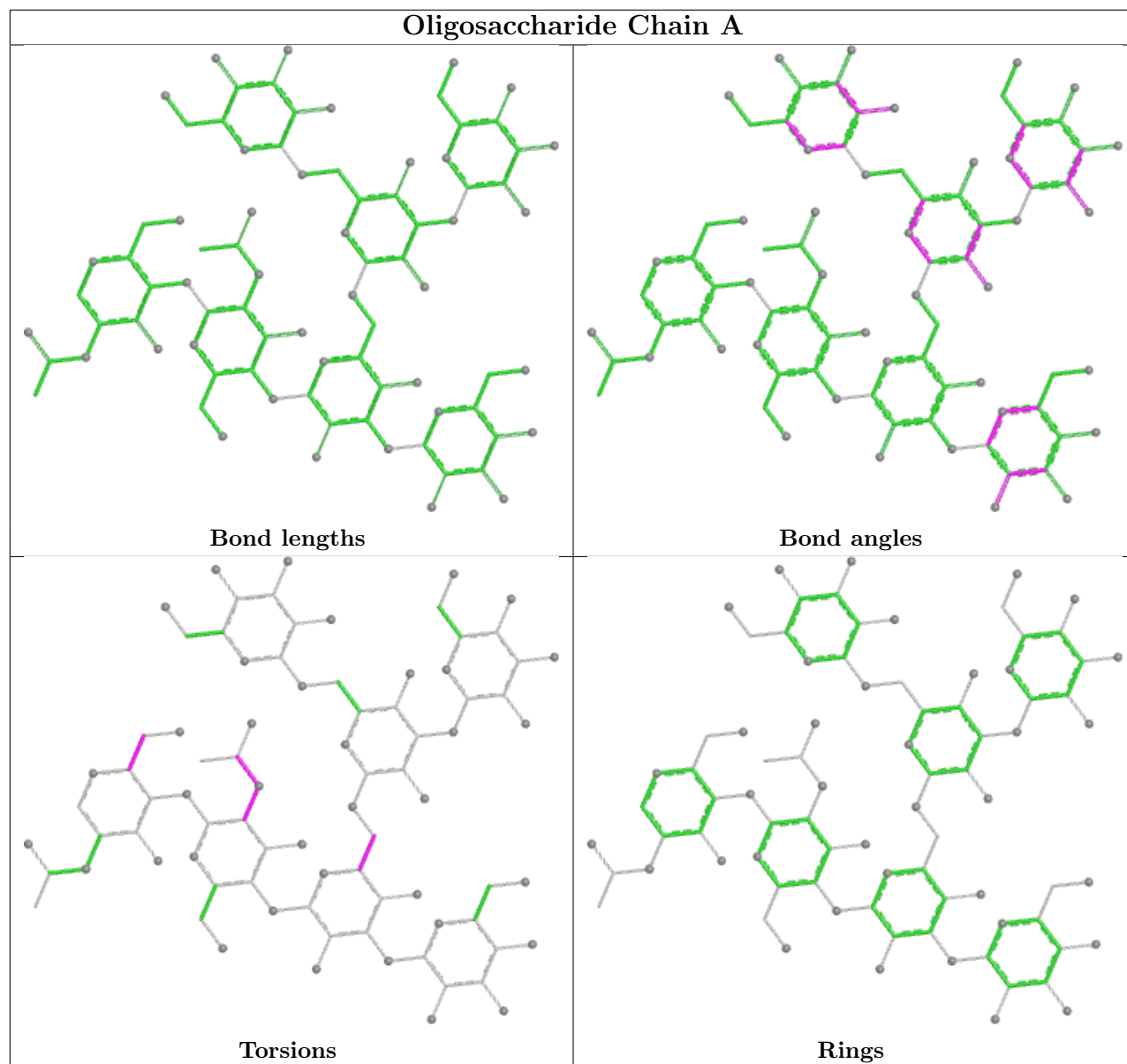
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	P	9	MAN	C1-C2-C3-C4-C5-O5
11	M	5	MAN	C1-C2-C3-C4-C5-O5

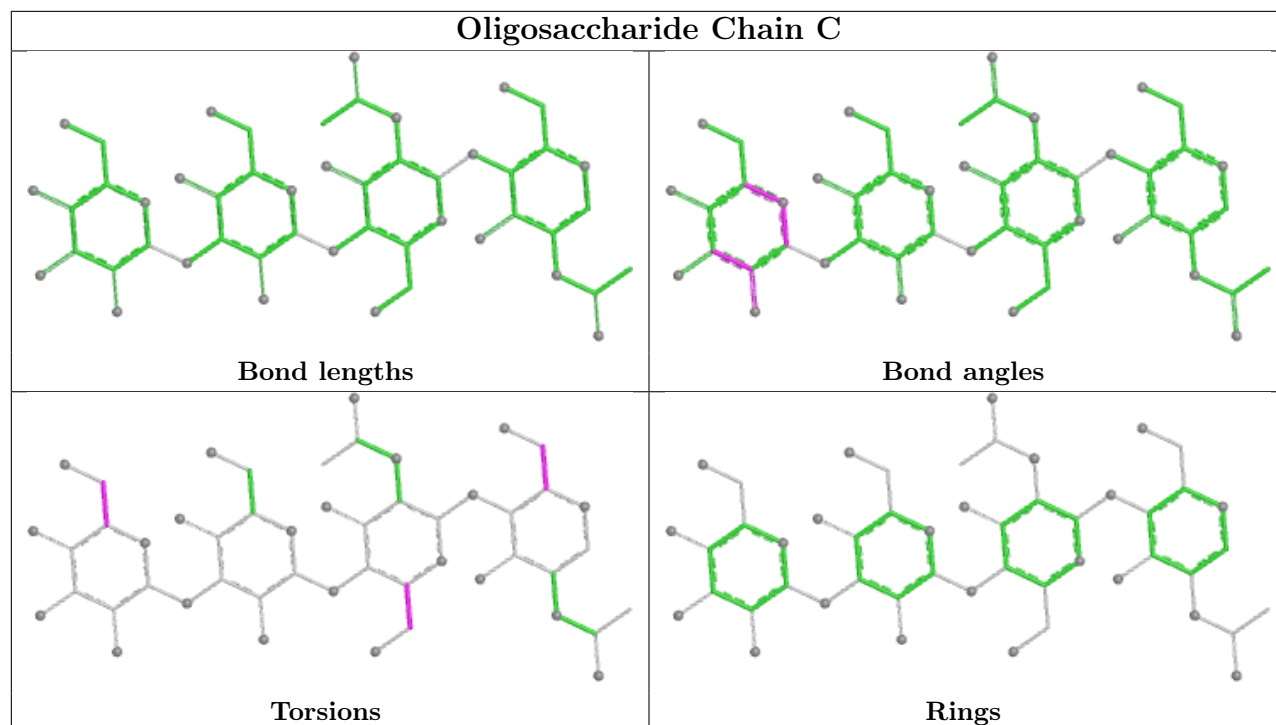
9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	P	1	NAG	1	0
10	I	2	NAG	4	0
10	R	2	NAG	1	0
10	R	1	NAG	1	0
8	C	2	NAG	1	0
8	C	3	BMA	1	0
12	P	2	NAG	1	0
7	A	1	NAG	1	0
7	A	2	NAG	5	0

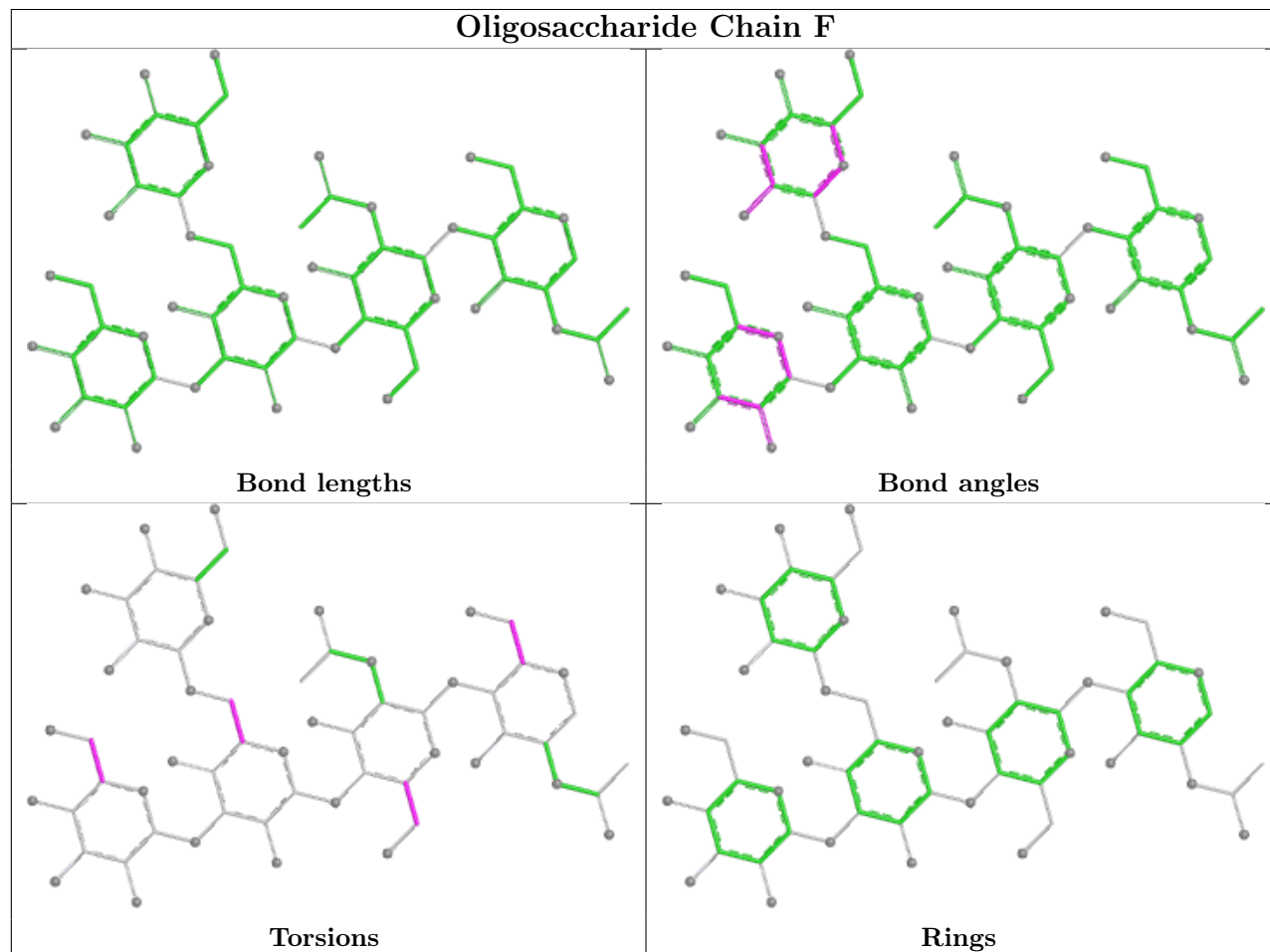
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

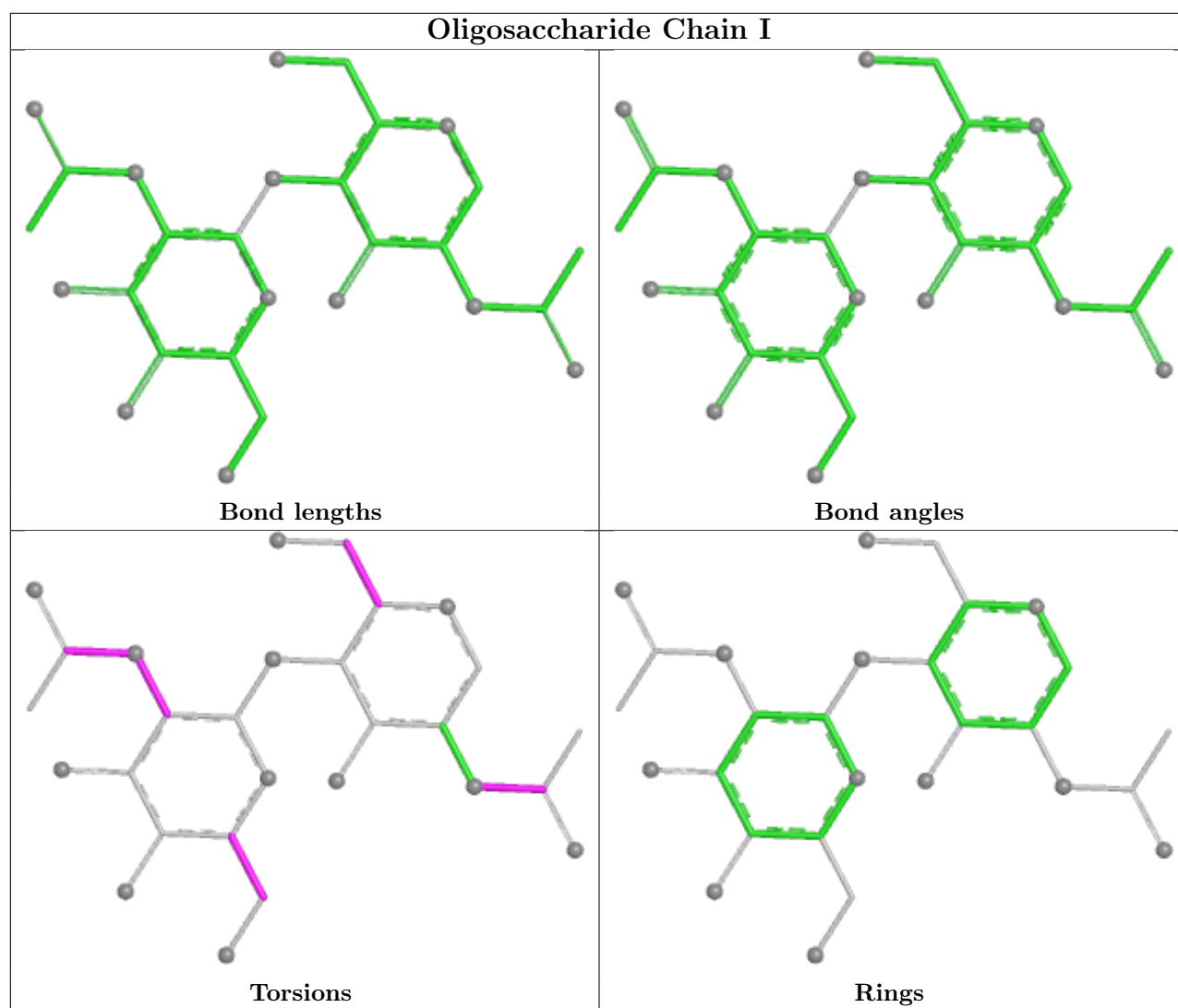


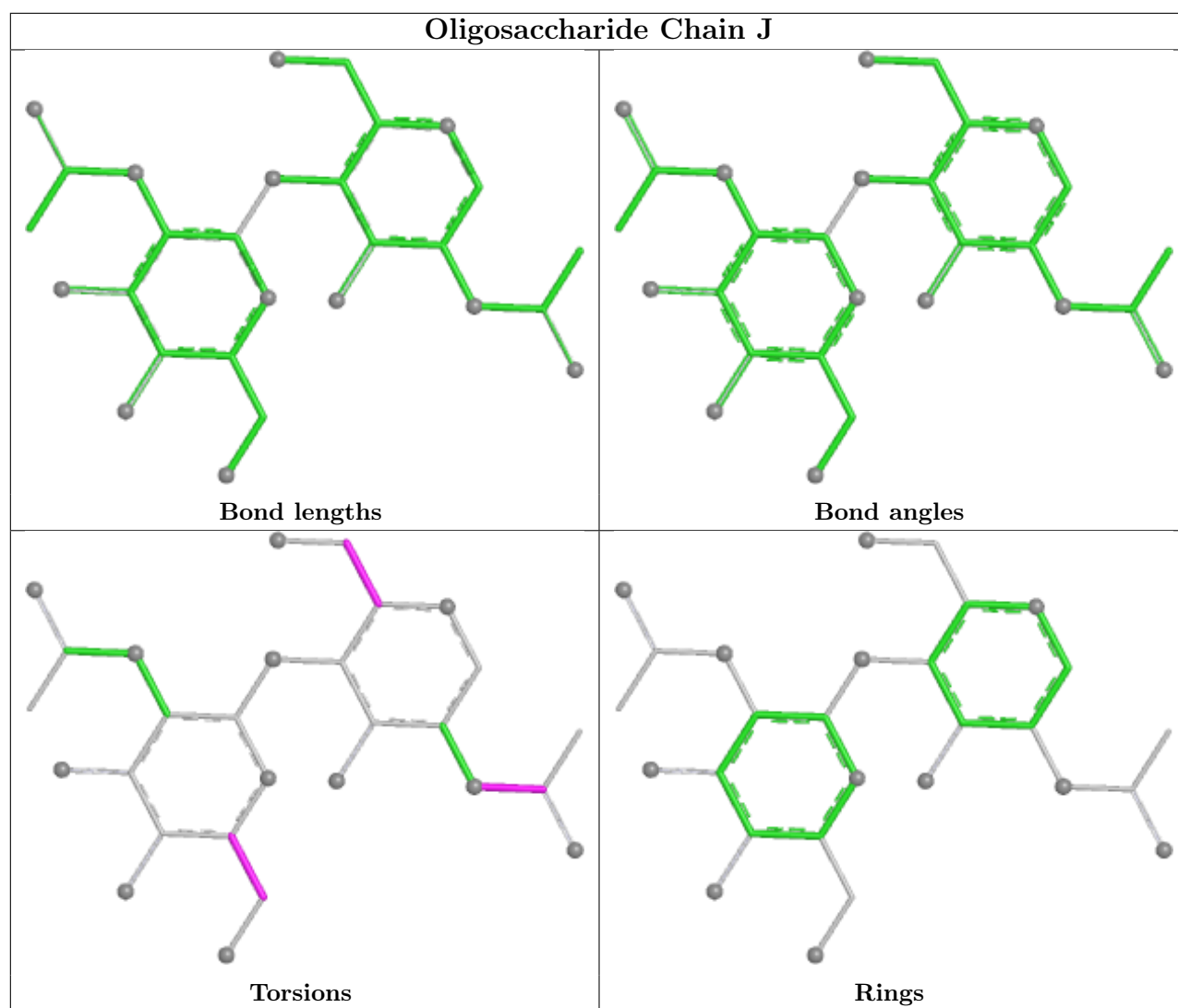
Oligosaccharide Chain C

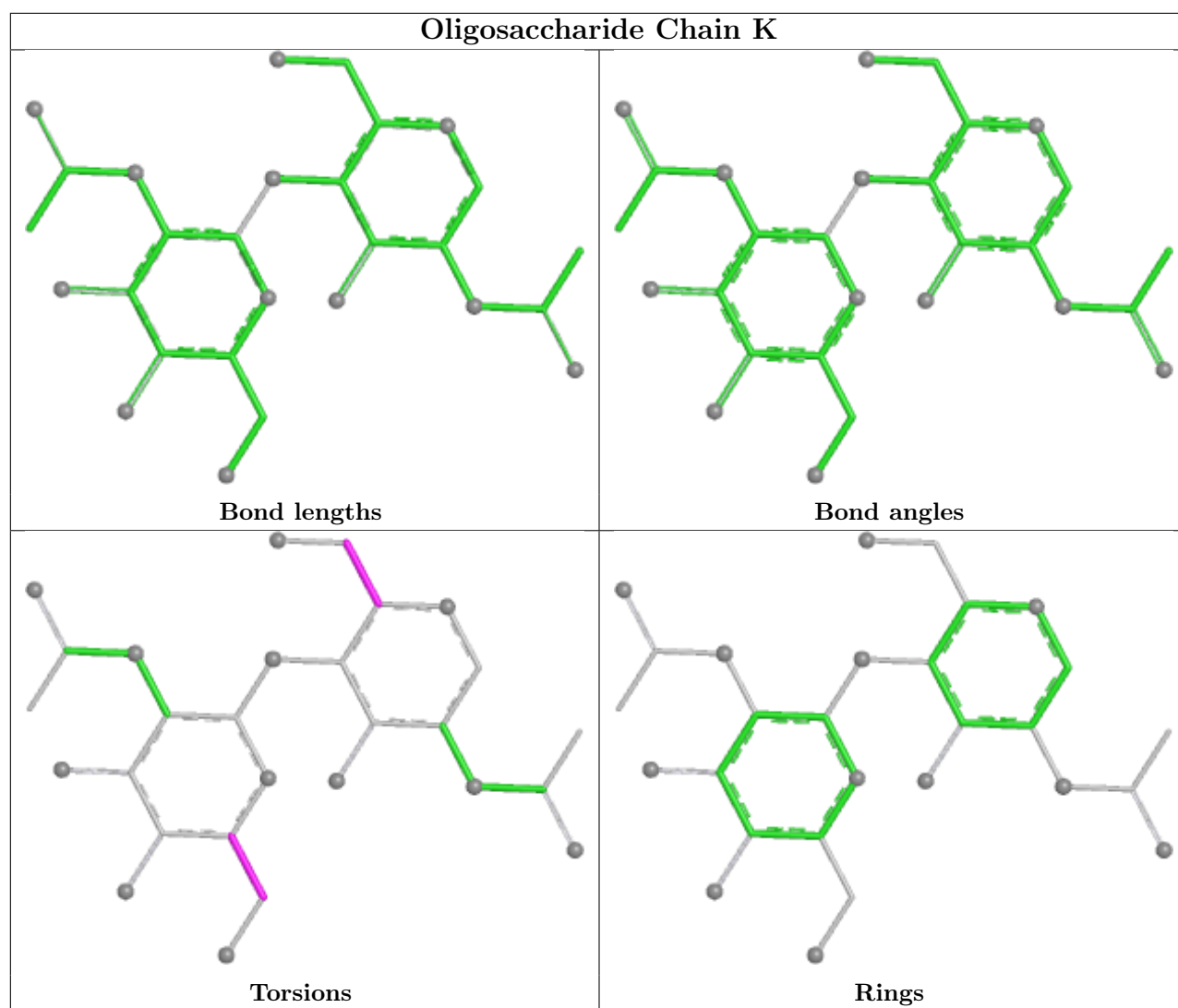


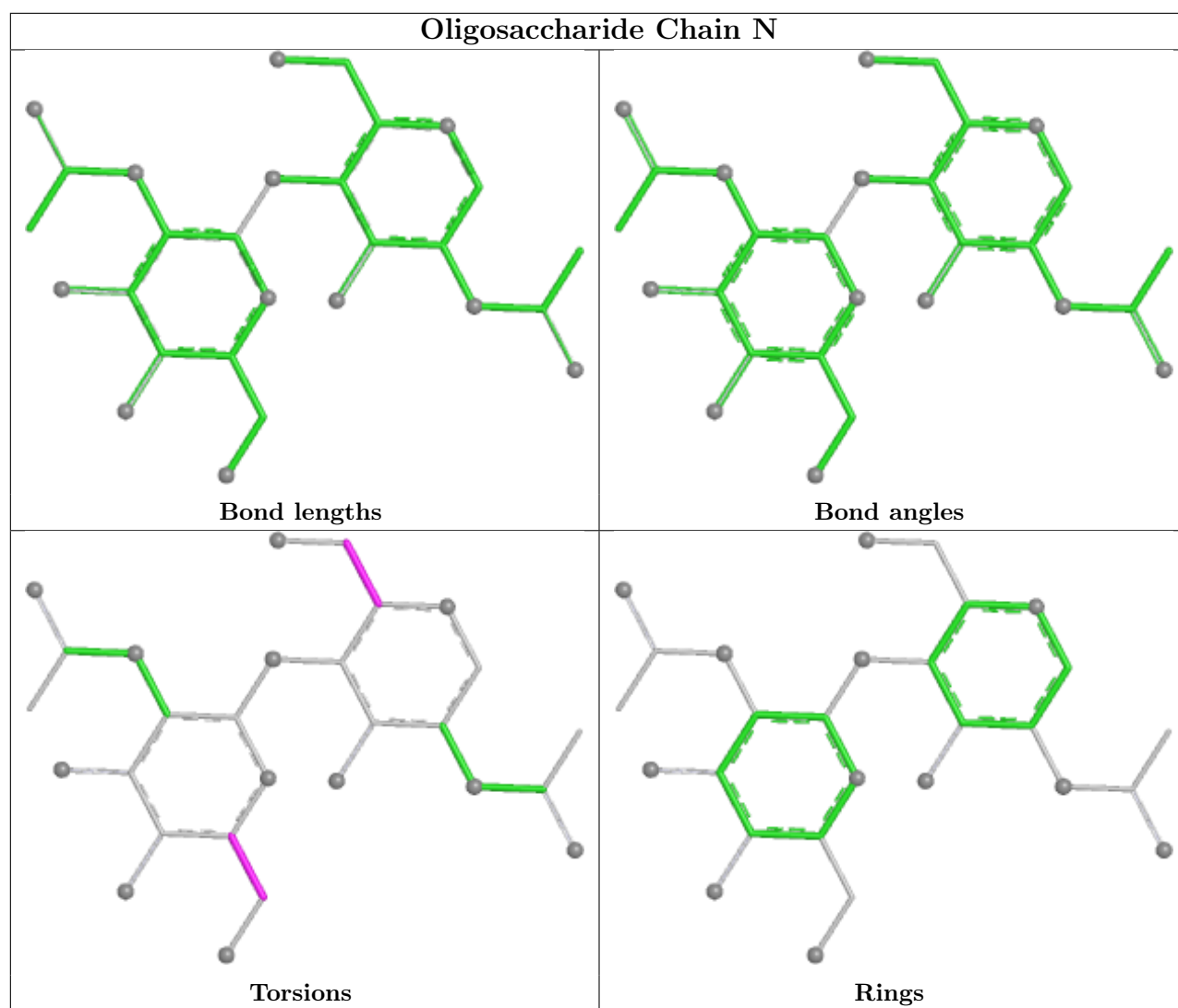
Oligosaccharide Chain F

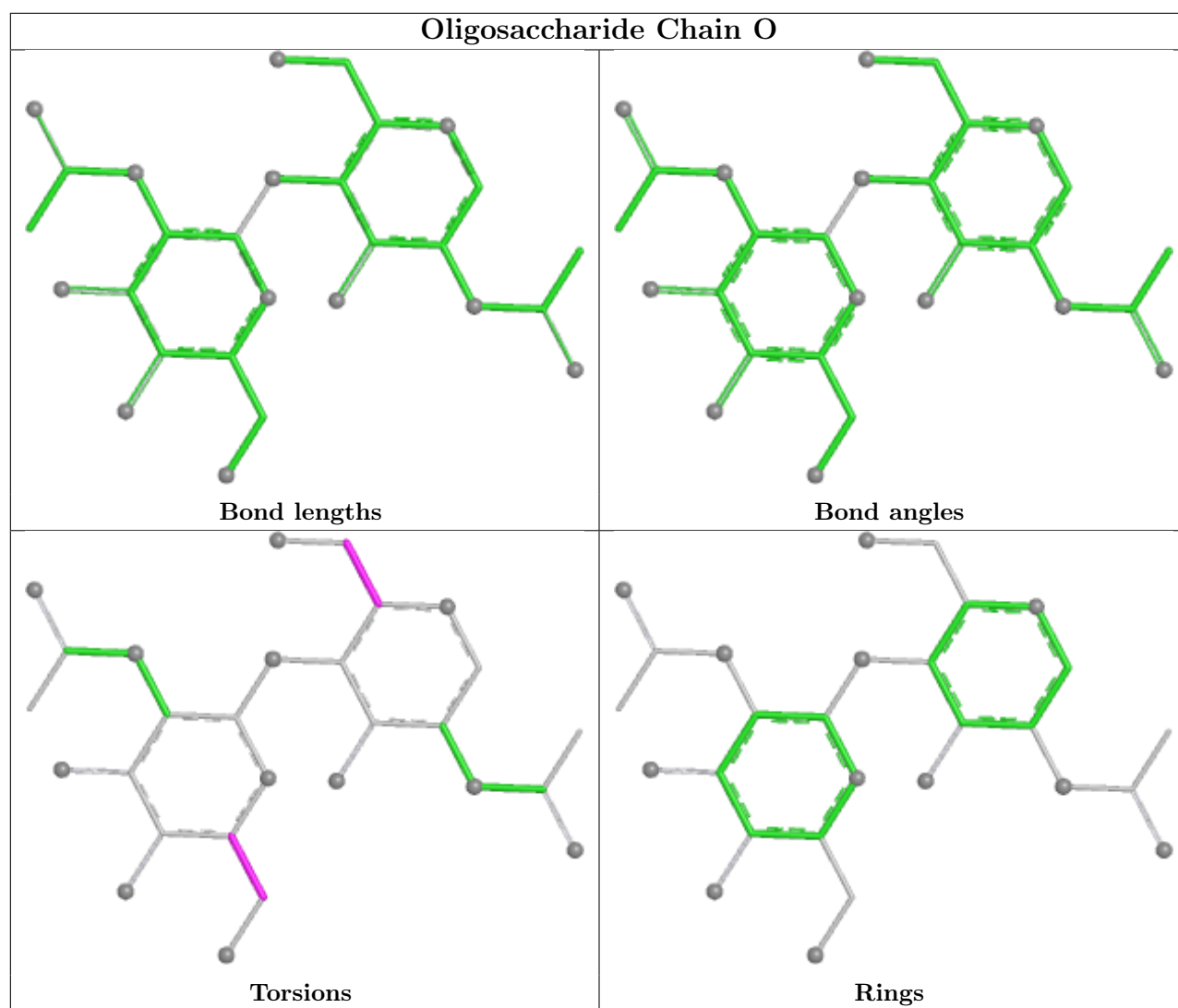


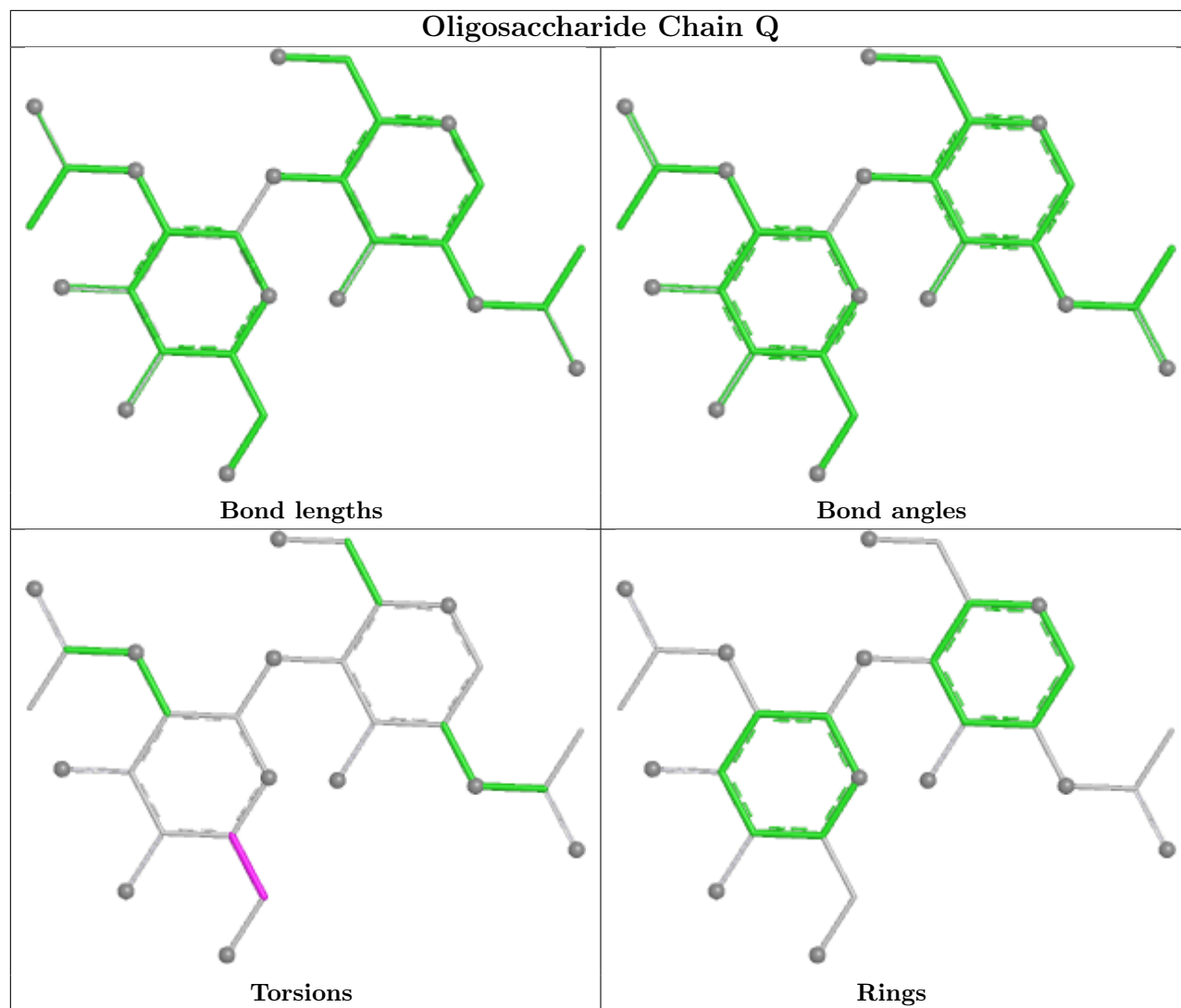


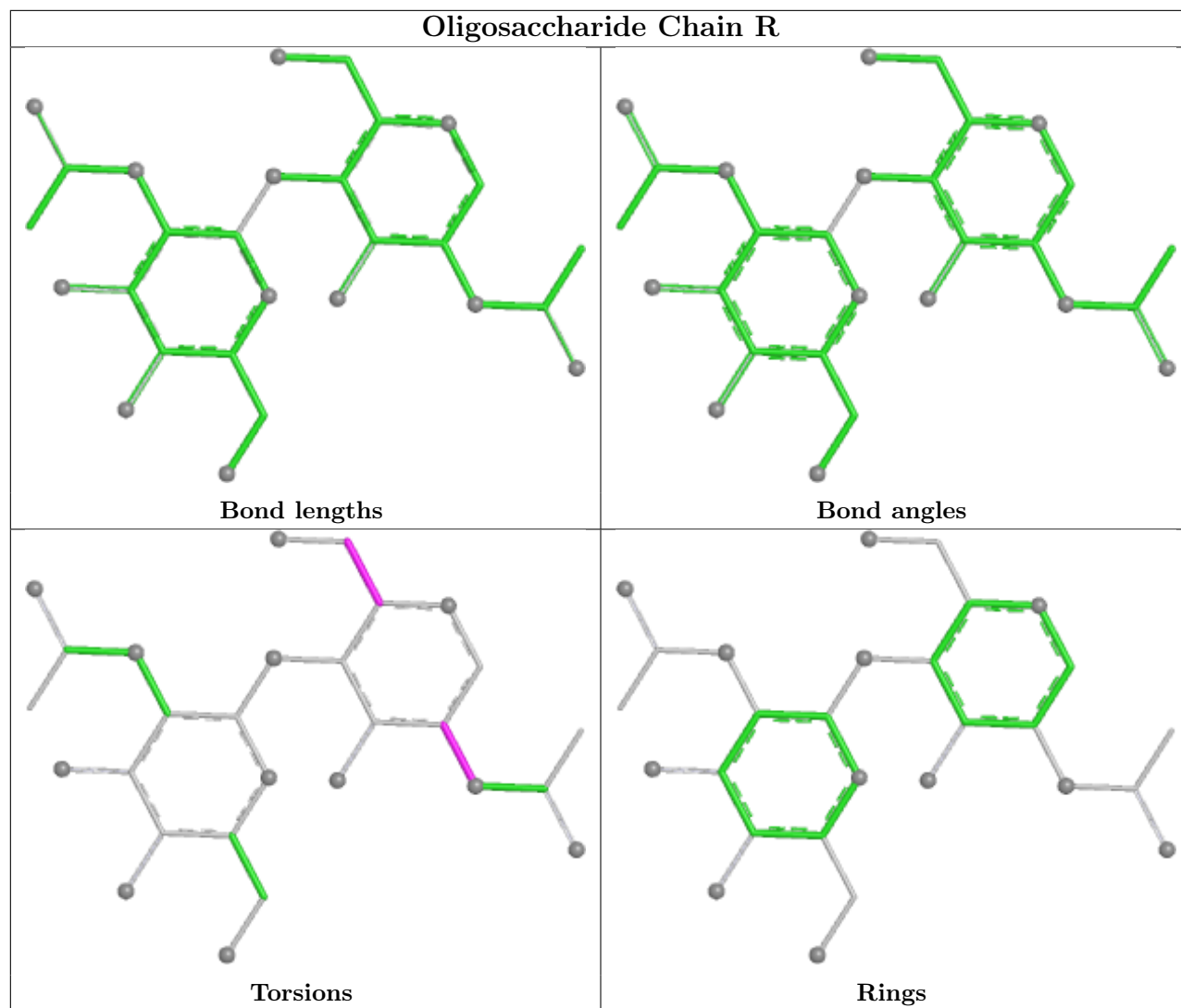


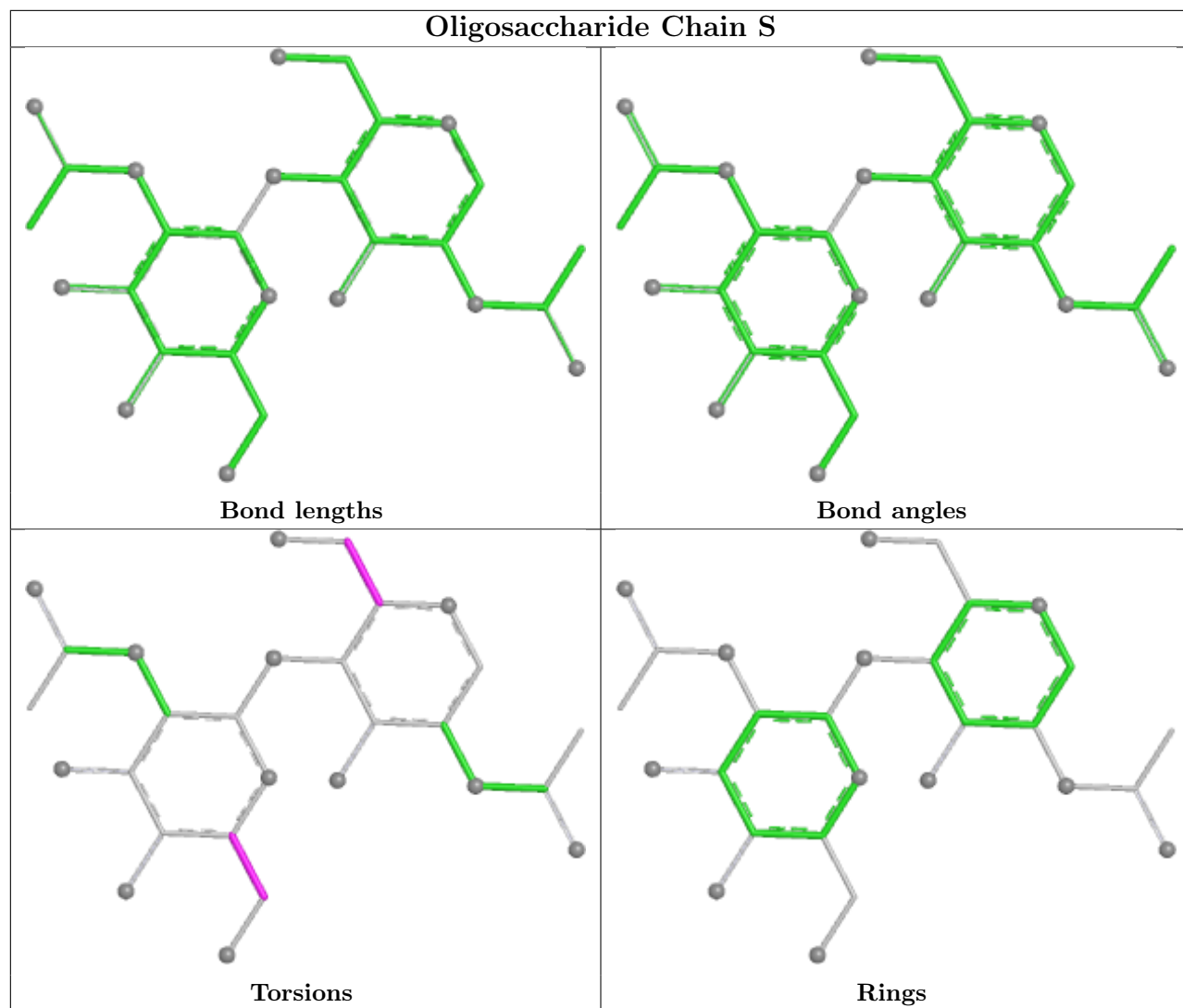




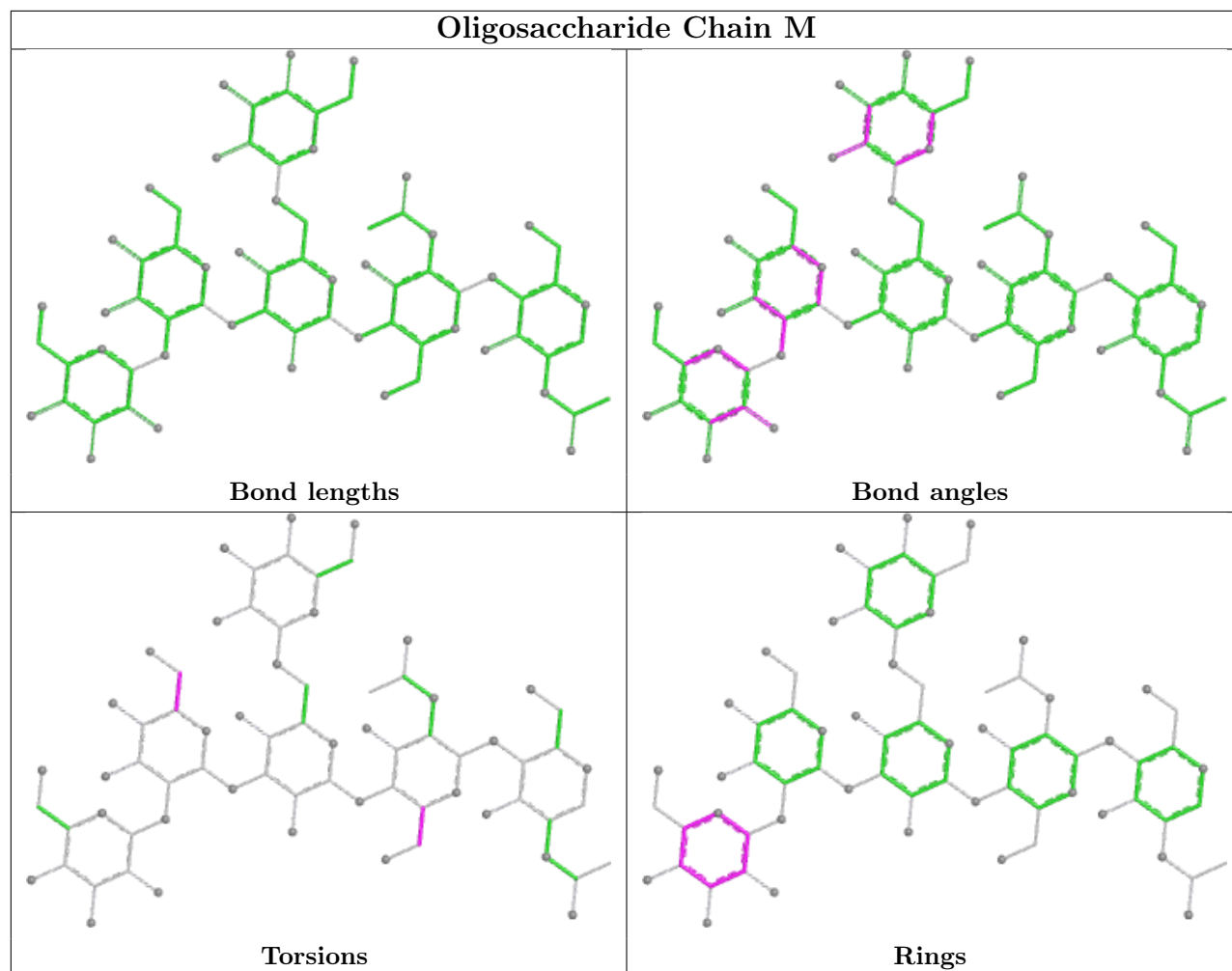


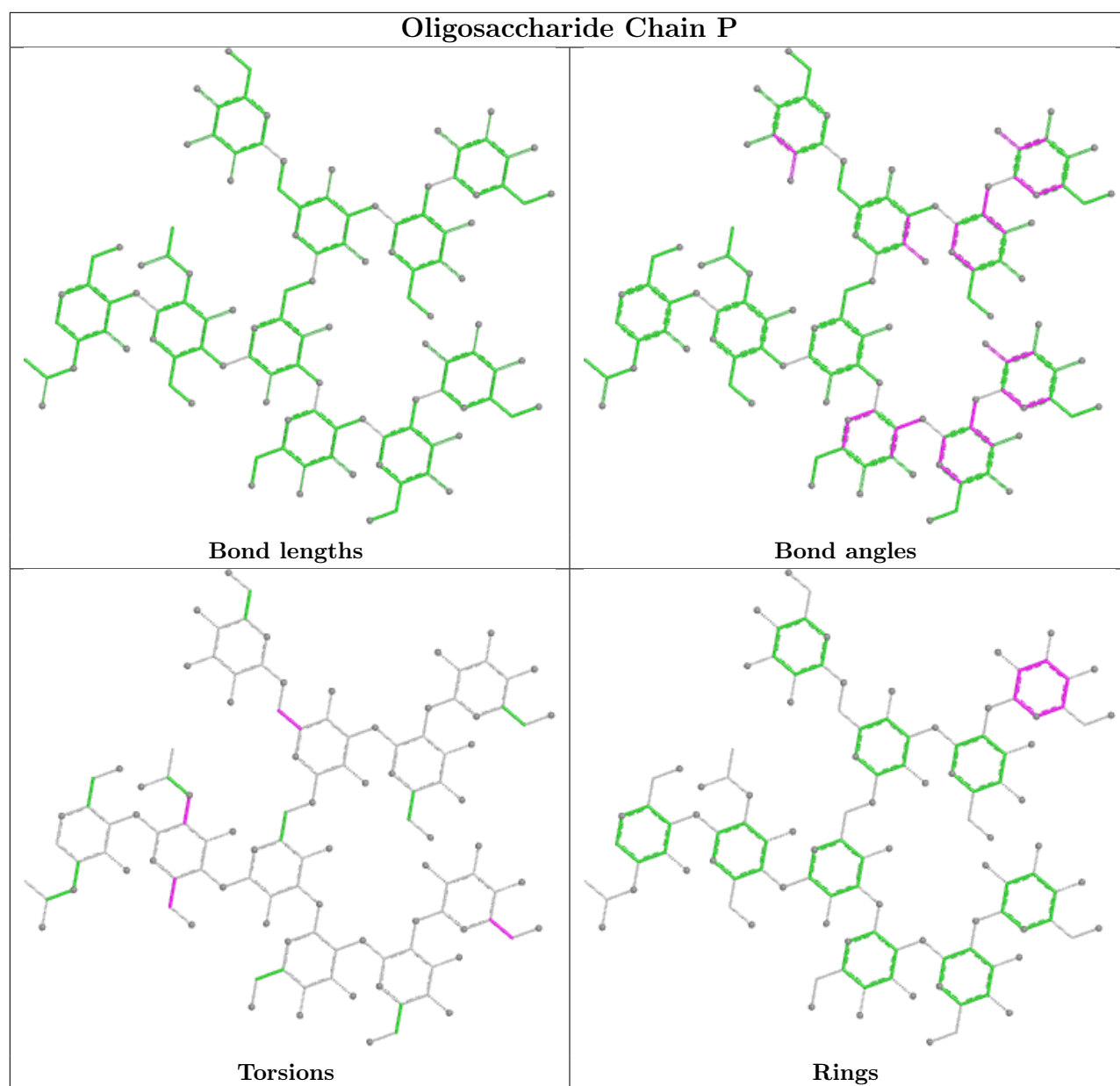


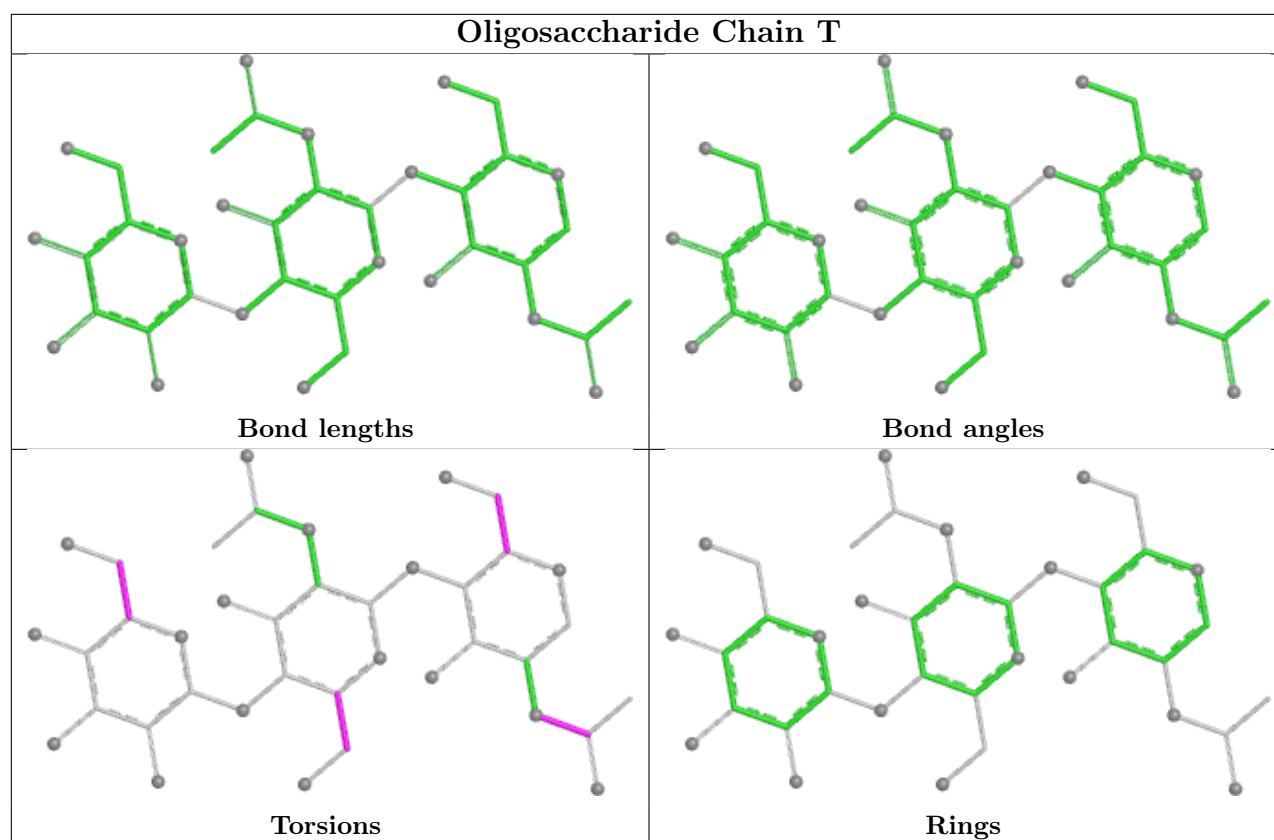




Oligosaccharide Chain M







5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
15	NAG	H	301	5	14,14,15	0.23	0	17,19,21	0.42	0
15	NAG	G	648	4	14,14,15	0.19	0	17,19,21	0.42	0
14	SO4	B	701	-	4,4,4	0.24	0	6,6,6	0.07	0
15	NAG	B	704	1	14,14,15	0.23	0	17,19,21	0.44	0
15	NAG	G	611	4	14,14,15	0.19	0	17,19,21	0.44	0
15	NAG	B	703	1	14,14,15	0.21	0	17,19,21	0.40	0
14	SO4	G	602	-	4,4,4	0.23	0	6,6,6	0.08	0
14	SO4	G	601	-	4,4,4	0.24	0	6,6,6	0.07	0
14	SO4	L	301	-	4,4,4	0.23	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	SO4	G	603	-	4,4,4	0.23	0	6,6,6	0.07	0
15	NAG	B	702	1	14,14,15	0.22	0	17,19,21	0.44	0
15	NAG	G	633	4	14,14,15	0.25	0	17,19,21	0.60	0
16	83J	G	659	-	39,39,39	2.23	10 (25%)	52,56,56	2.52	14 (26%)
15	NAG	G	658	4	14,14,15	0.21	0	17,19,21	0.41	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
15	NAG	H	301	5	-	2/6/23/26	0/1/1/1
15	NAG	G	648	4	-	4/6/23/26	0/1/1/1
15	NAG	B	704	1	-	0/6/23/26	0/1/1/1
15	NAG	G	611	4	-	2/6/23/26	0/1/1/1
15	NAG	B	703	1	-	2/6/23/26	0/1/1/1
15	NAG	G	633	4	-	6/6/23/26	0/1/1/1
16	83J	G	659	-	-	3/26/36/36	0/5/5/5
15	NAG	B	702	1	-	2/6/23/26	0/1/1/1
15	NAG	G	658	4	-	1/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	659	83J	C12-N02	6.63	1.46	1.34
16	G	659	83J	C13-N05	5.86	1.47	1.34
16	G	659	83J	C18-N08	-5.61	1.28	1.37
16	G	659	83J	C19-N08	-4.20	1.30	1.37
16	G	659	83J	C16-C14	3.55	1.52	1.45
16	G	659	83J	C29-N30	3.31	1.45	1.41
16	G	659	83J	C15-C13	2.46	1.54	1.50
16	G	659	83J	O11-C22	2.17	1.40	1.37
16	G	659	83J	O03-C12	-2.09	1.18	1.23
16	G	659	83J	O09-C14	-2.08	1.18	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	659	83J	C19-N08-C18	7.73	115.59	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	659	83J	C33-N34-N30	7.20	108.06	102.40
16	G	659	83J	N34-C33-N32	-5.56	108.07	115.24
16	G	659	83J	C31-N32-C33	5.26	107.85	102.88
16	G	659	83J	C19-C17-C16	-4.58	104.58	106.74
16	G	659	83J	C16-C18-N08	-4.53	107.15	110.22
16	G	659	83J	C07-N02-C01	4.18	121.21	112.68
16	G	659	83J	C17-C19-N08	-3.24	105.51	107.76
16	G	659	83J	O11-C22-C17	3.20	120.37	115.84
16	G	659	83J	C29-N30-C31	-3.10	125.51	129.09
16	G	659	83J	C01-C04-N05	-3.00	104.46	110.42
16	G	659	83J	C29-N30-N34	2.65	126.66	121.59
16	G	659	83J	N30-C31-N32	-2.26	108.20	110.81
16	G	659	83J	C14-C12-N02	2.09	120.76	118.56

There are no chirality outliers.

All (22) torsion outliers are listed below:

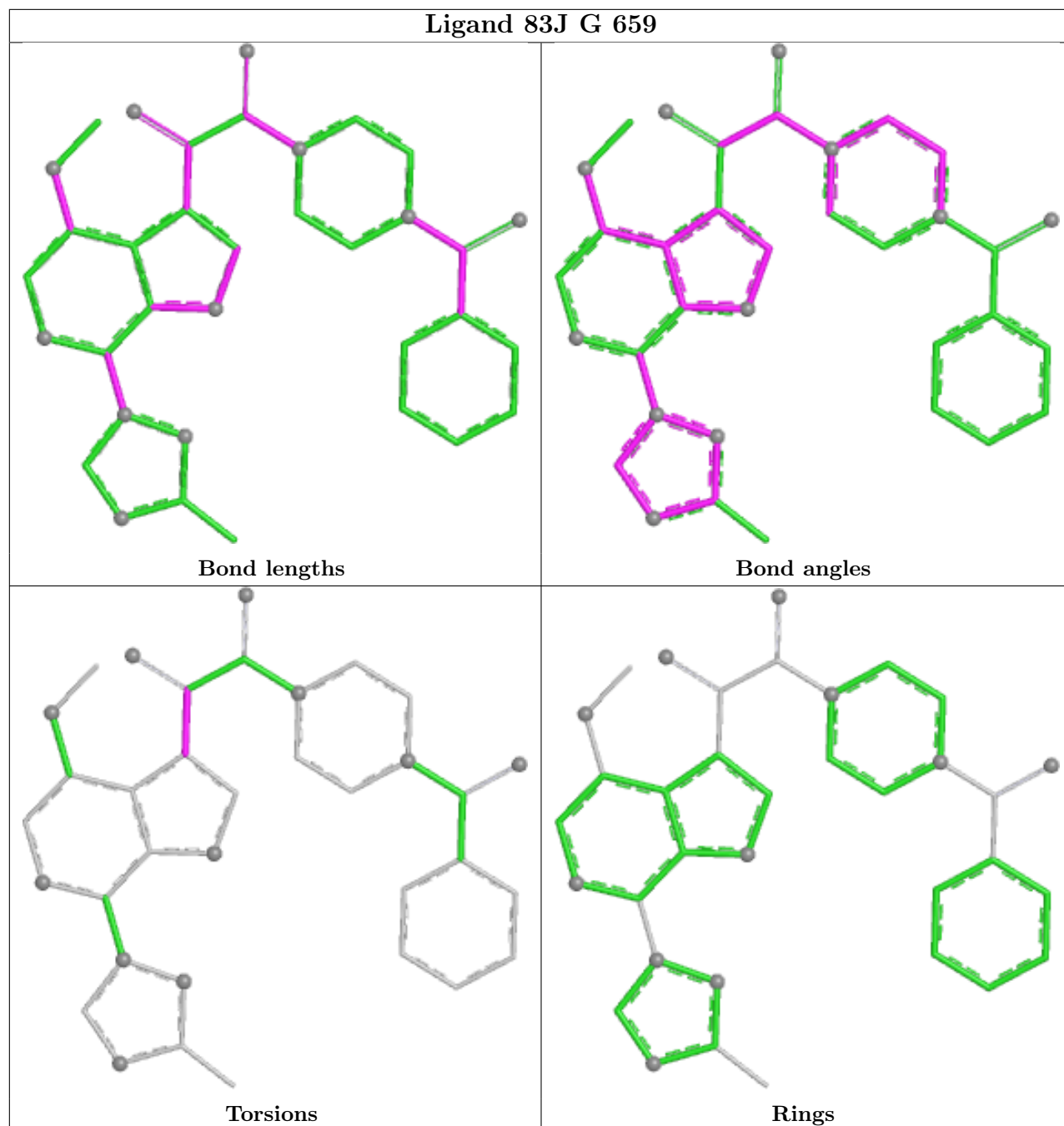
Mol	Chain	Res	Type	Atoms
15	B	702	NAG	O5-C5-C6-O6
15	G	633	NAG	O5-C5-C6-O6
15	H	301	NAG	O5-C5-C6-O6
15	B	702	NAG	C4-C5-C6-O6
15	B	703	NAG	O5-C5-C6-O6
15	G	648	NAG	C4-C5-C6-O6
15	G	611	NAG	O5-C5-C6-O6
15	G	648	NAG	O5-C5-C6-O6
15	G	633	NAG	C4-C5-C6-O6
15	H	301	NAG	C4-C5-C6-O6
15	G	633	NAG	C8-C7-N2-C2
15	G	633	NAG	O7-C7-N2-C2
15	G	648	NAG	C8-C7-N2-C2
15	G	648	NAG	O7-C7-N2-C2
15	B	703	NAG	C4-C5-C6-O6
15	G	611	NAG	C4-C5-C6-O6
15	G	633	NAG	C3-C2-N2-C7
16	G	659	83J	O09-C14-C16-C17
16	G	659	83J	O09-C14-C16-C18
15	G	633	NAG	C1-C2-N2-C7
15	G	658	NAG	C4-C5-C6-O6
16	G	659	83J	C12-C14-C16-C18

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	701	SO4	1	0
15	B	703	NAG	1	0
15	G	633	NAG	4	0
16	G	659	83J	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95th 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 ²)	Q<0.9
1	B	126/153 (82%)	-1.66	0 100 100	19, 80, 131, 154	0
2	D	242/243 (99%)	-1.37	0 100 100	64, 170, 267, 297	0
3	E	213/216 (98%)	-1.20	0 100 100	94, 177, 274, 310	0
4	G	444/481 (92%)	-1.70	0 100 100	37, 81, 134, 168	0
5	H	228/235 (97%)	-1.59	0 100 100	64, 107, 166, 216	0
6	L	208/213 (97%)	-1.68	0 100 100	41, 84, 131, 167	0
All	All	1461/1541 (94%)	-1.55	0 100 100	19, 105, 232, 310	0

There are no RSRZ outliers to report.

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](#)

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, 95th 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 ²)	Q<0.9
7	NAG	A	1	14/15	-	-	65,99,119,120	0
7	NAG	A	2	14/15	-	-	86,112,131,152	0
7	BMA	A	3	11/12	-	-	47,107,126,129	0
7	MAN	A	4	11/12	-	-	106,117,127,134	0
7	MAN	A	5	11/12	-	-	65,125,138,139	0
7	MAN	A	6	11/12	-	-	93,114,130,130	0

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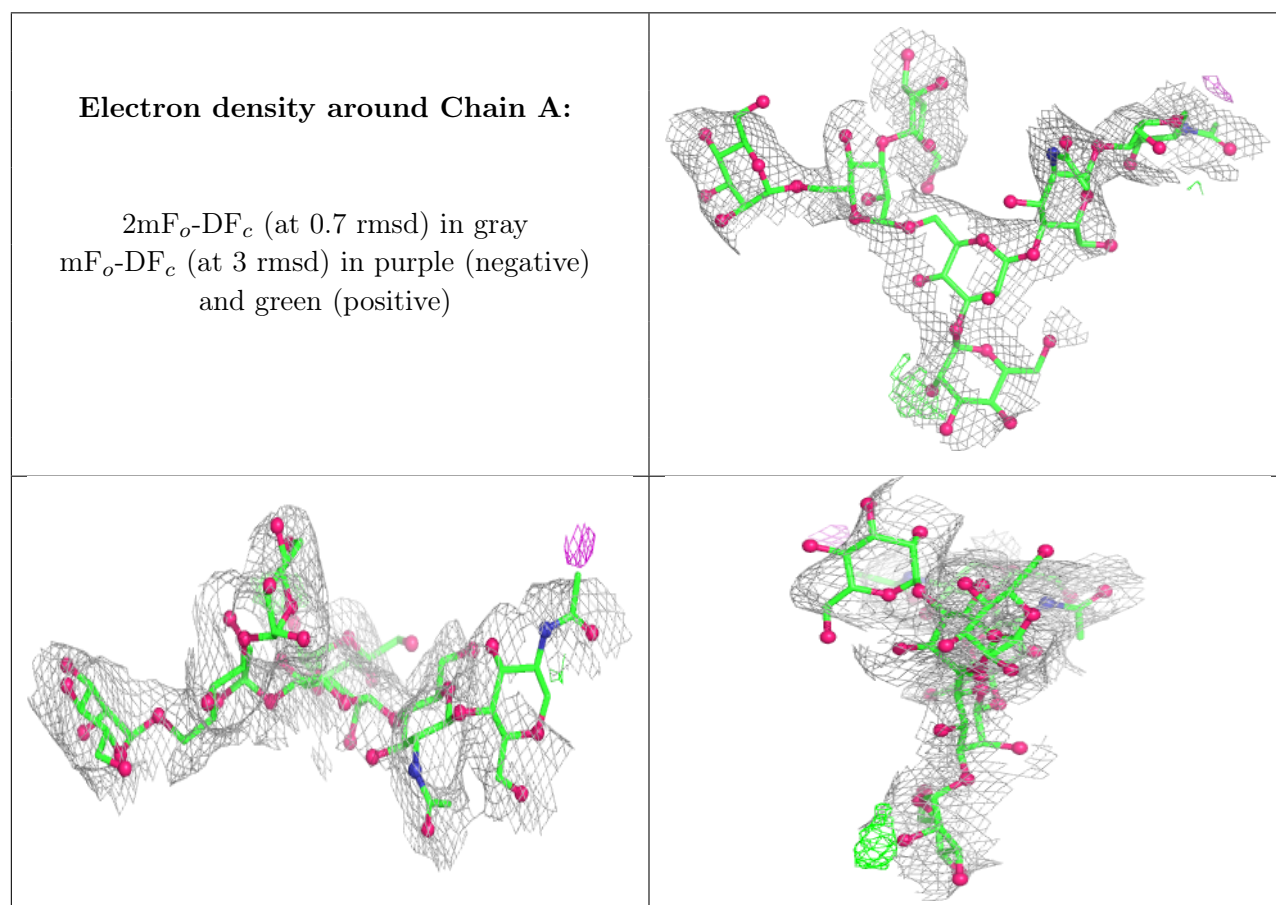
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MAN	A	7	11/12	-	-	91,109,155,165	0
8	NAG	C	1	14/15	-	-	79,113,139,153	0
8	NAG	C	2	14/15	-	-	95,108,130,130	0
8	BMA	C	3	11/12	-	-	94,130,150,161	0
8	MAN	C	4	11/12	-	-	124,145,173,184	0
9	NAG	F	1	14/15	-	-	50,70,88,88	0
9	NAG	F	2	14/15	-	-	52,76,107,113	0
9	BMA	F	3	11/12	-	-	85,110,118,118	0
9	MAN	F	4	11/12	-	-	95,110,131,134	0
9	MAN	F	5	11/12	-	-	110,119,132,140	0
13	BMA	T	3	11/12	0.97	0.03	123,137,155,162	0
10	NAG	N	2	14/15	0.98	0.04	58,96,115,120	0
11	MAN	M	5	11/12	0.98	0.04	109,127,147,157	0
11	MAN	M	6	11/12	0.98	0.04	105,149,161,167	0
12	MAN	P	10	11/12	0.98	0.03	96,105,121,129	0
10	NAG	J	2	14/15	0.98	0.03	108,121,149,154	0
10	NAG	N	1	14/15	0.99	0.02	73,94,104,107	0
10	NAG	I	2	14/15	0.99	0.02	86,122,136,143	0
10	NAG	O	2	14/15	0.99	0.04	98,136,164,165	0
10	NAG	Q	1	14/15	0.99	0.03	71,119,151,155	0
10	NAG	Q	2	14/15	0.99	0.03	61,102,140,141	0
10	NAG	R	2	14/15	0.99	0.03	105,119,132,141	0
10	NAG	S	2	14/15	0.99	0.03	104,146,161,162	0
11	BMA	M	3	11/12	0.99	0.02	53,122,140,143	0
11	MAN	M	4	11/12	0.99	0.03	102,137,160,161	0
10	NAG	J	1	14/15	0.99	0.02	57,105,125,152	0
10	NAG	I	1	14/15	0.99	0.04	48,89,117,118	0
12	NAG	P	1	14/15	0.99	0.03	60,102,117,128	0
12	BMA	P	3	11/12	0.99	0.03	77,110,119,129	0
12	MAN	P	6	11/12	0.99	0.03	82,105,118,119	0
12	MAN	P	7	11/12	0.99	0.02	77,100,107,109	0
12	MAN	P	9	11/12	0.99	0.03	64,120,146,153	0
10	NAG	K	1	14/15	0.99	0.02	105,122,154,165	0
13	NAG	T	1	14/15	0.99	0.02	30,108,125,131	0
13	NAG	T	2	14/15	0.99	0.03	101,130,140,154	0
10	NAG	K	2	14/15	0.99	0.03	105,121,159,162	0
12	MAN	P	5	11/12	1.00	0.03	86,93,112,122	0
10	NAG	S	1	14/15	1.00	0.02	83,114,128,145	0
10	NAG	R	1	14/15	1.00	0.02	72,103,113,125	0
12	MAN	P	8	11/12	1.00	0.02	81,105,130,145	0
11	NAG	M	1	14/15	1.00	0.02	18,60,85,99	0
11	NAG	M	2	14/15	1.00	0.03	57,90,102,110	0

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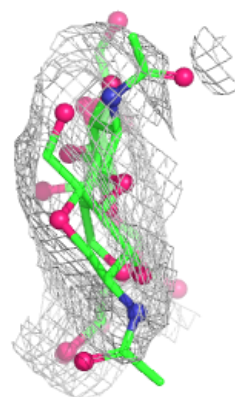
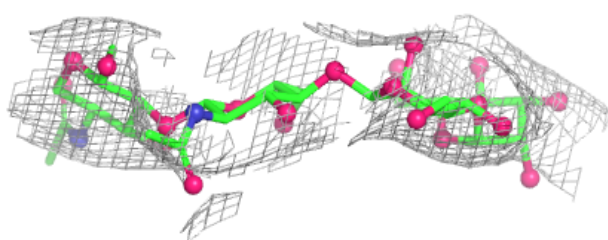
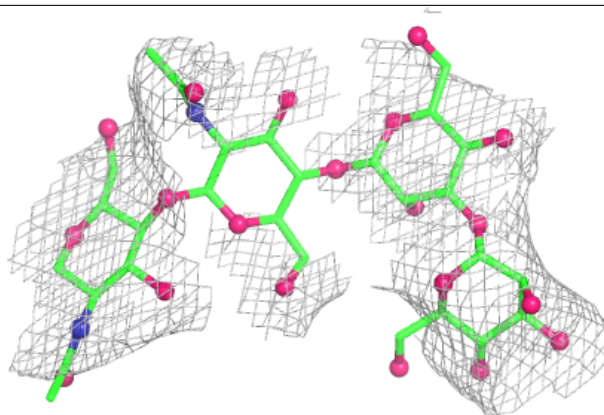
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	NAG	P	2	14/15	1.00	0.02	54,105,114,122	0
10	NAG	O	1	14/15	1.00	0.02	18,63,85,86	0
12	MAN	P	4	11/12	1.00	0.02	39,74,90,92	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

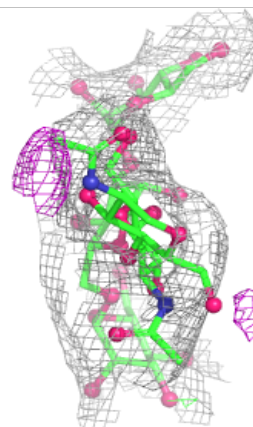
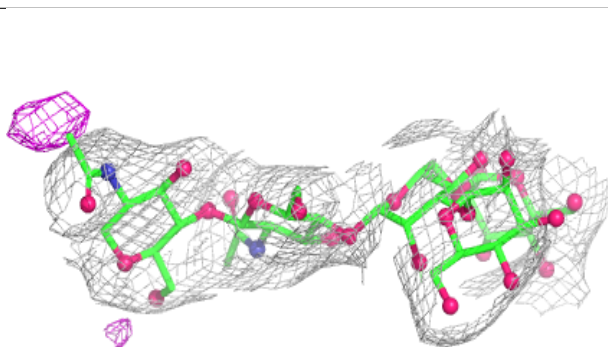
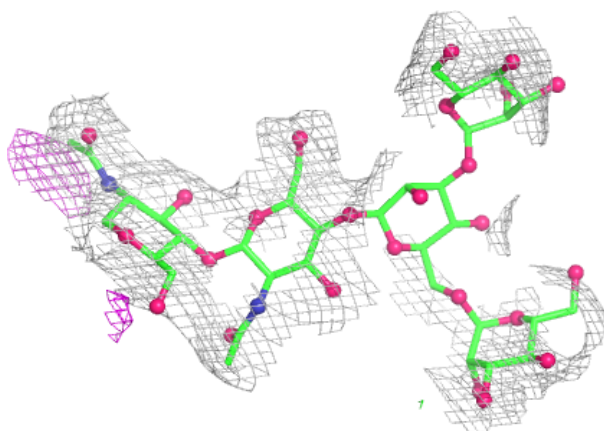


Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

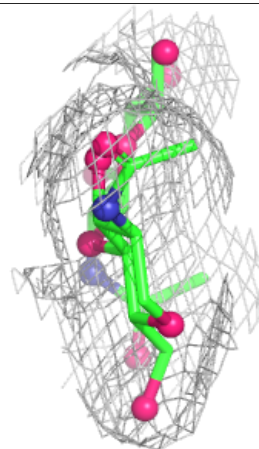
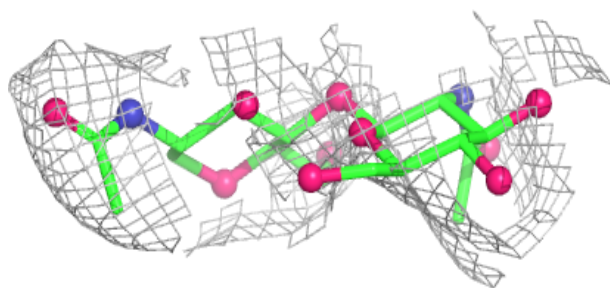
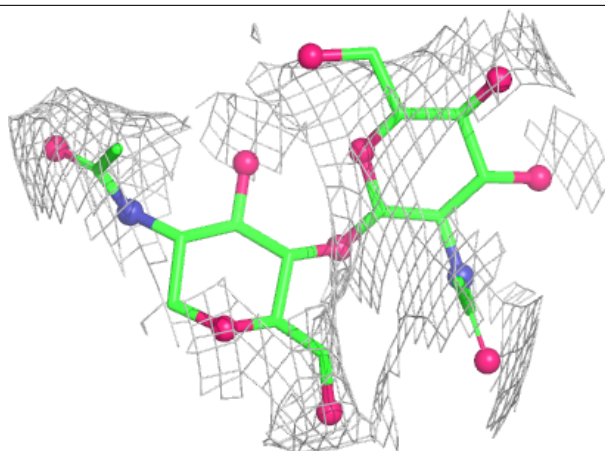
**Electron density around Chain F:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



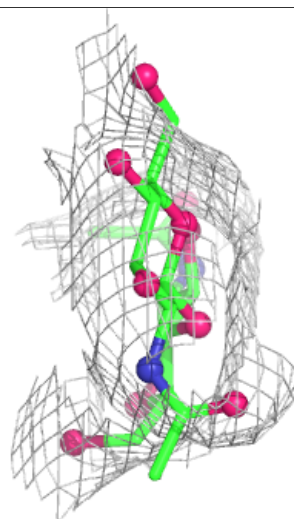
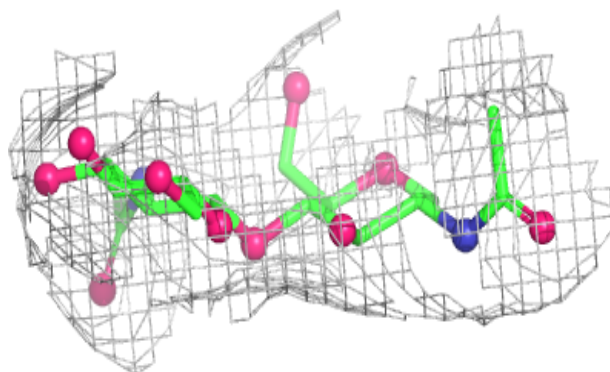
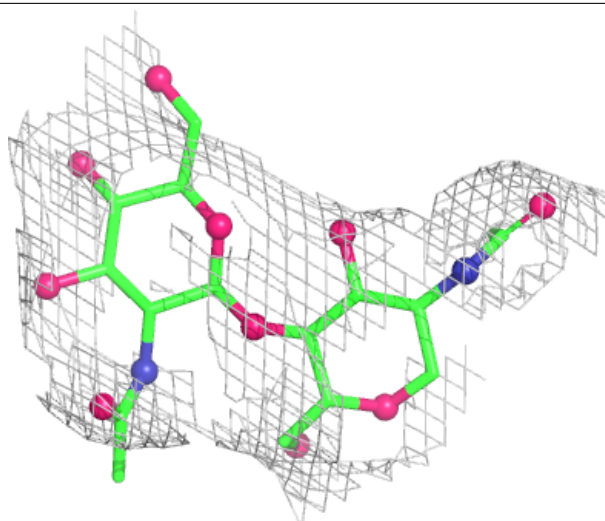
Electron density around Chain I:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



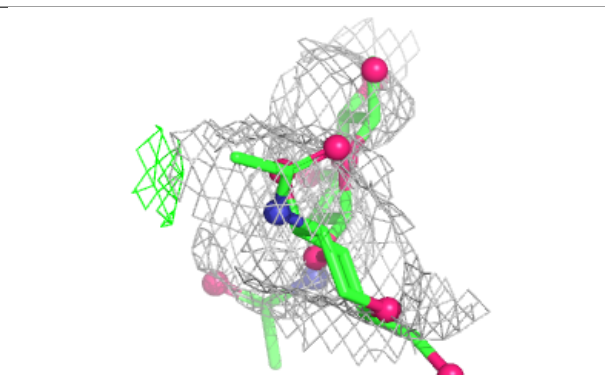
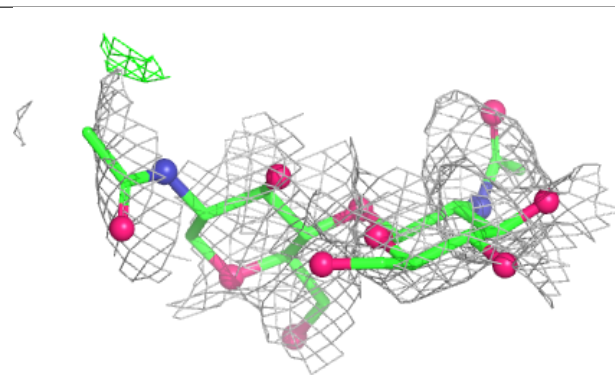
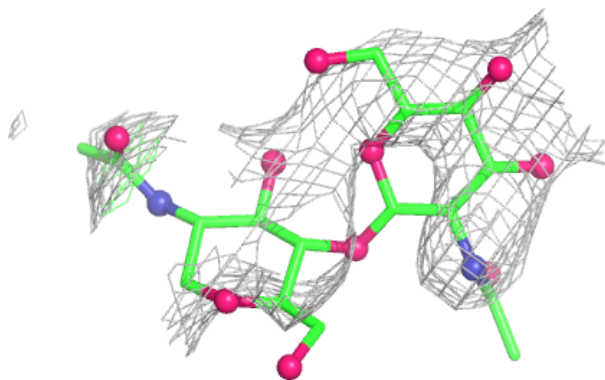
Electron density around Chain J:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

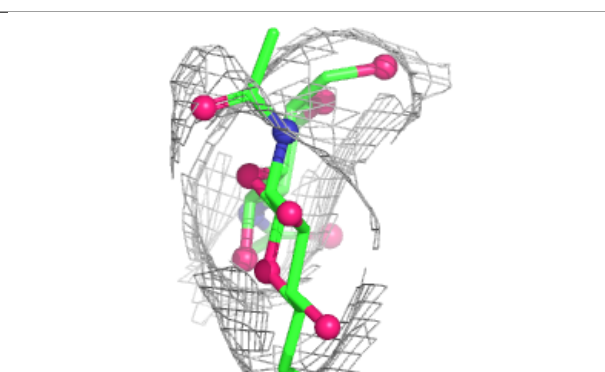
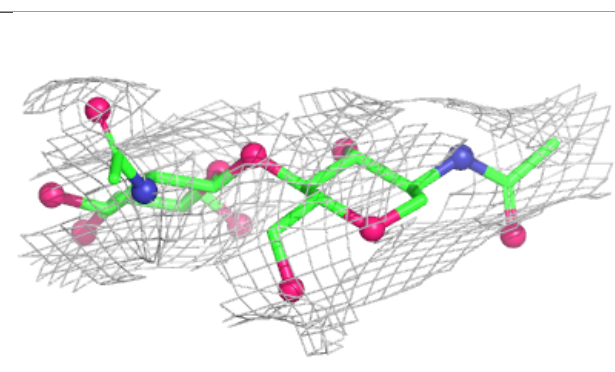
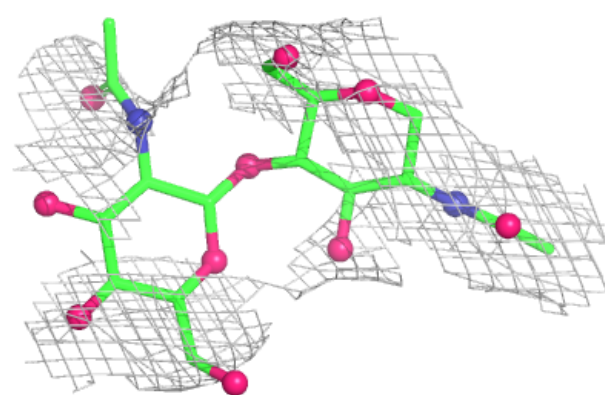


Electron density around Chain K:

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and green (positive)

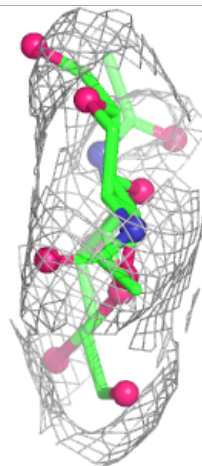
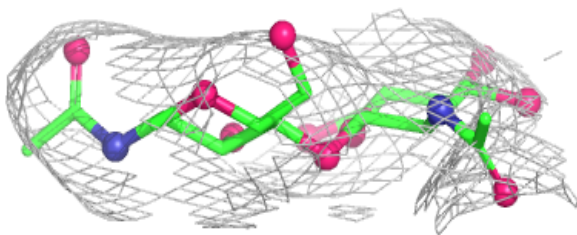
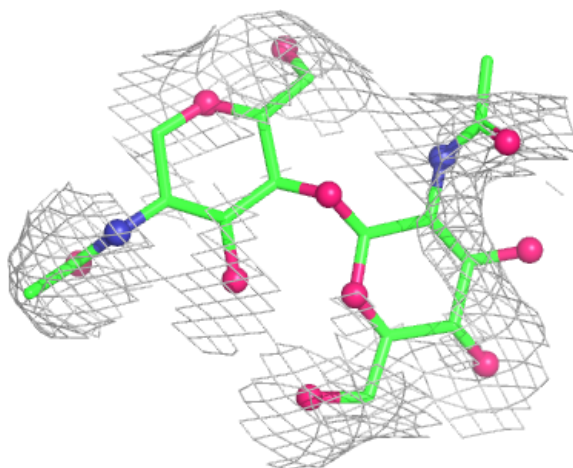
**Electron density around Chain N:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



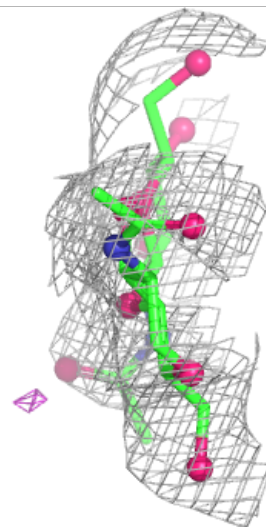
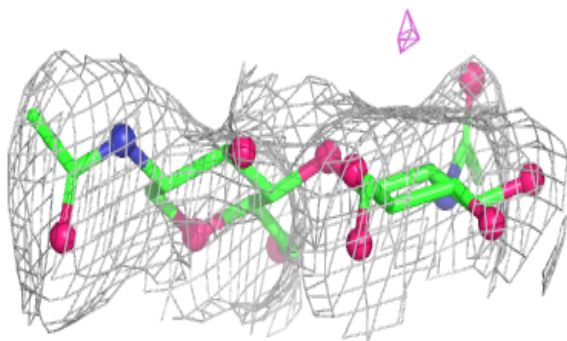
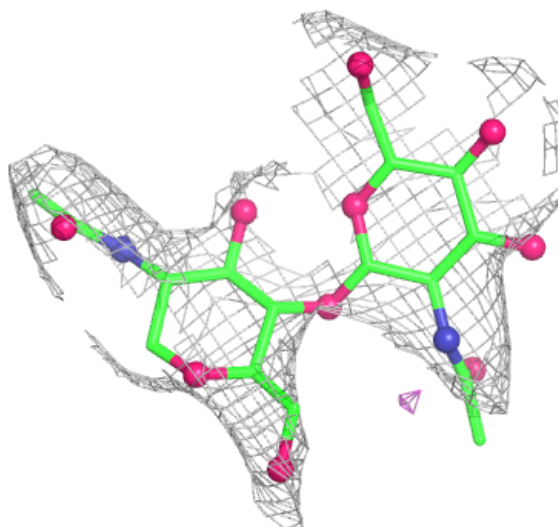
Electron density around Chain O:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



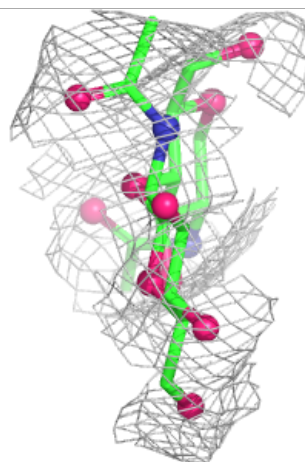
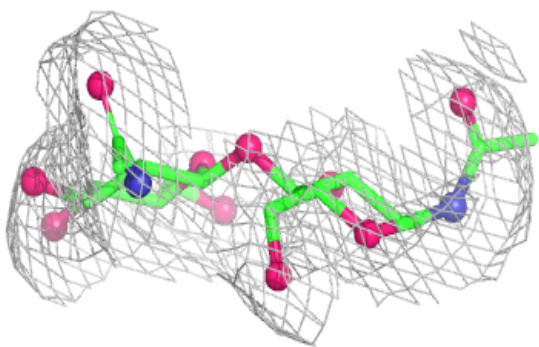
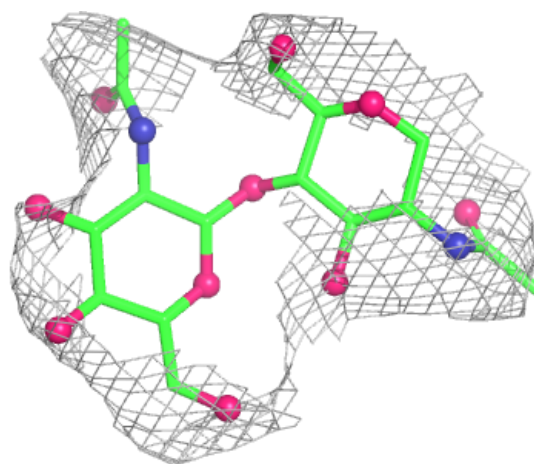
Electron density around Chain Q:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



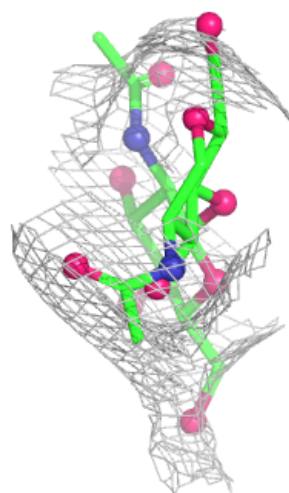
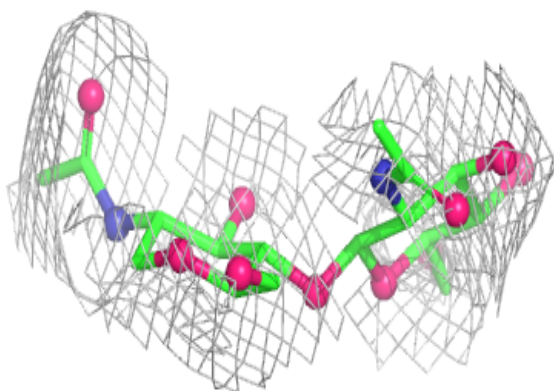
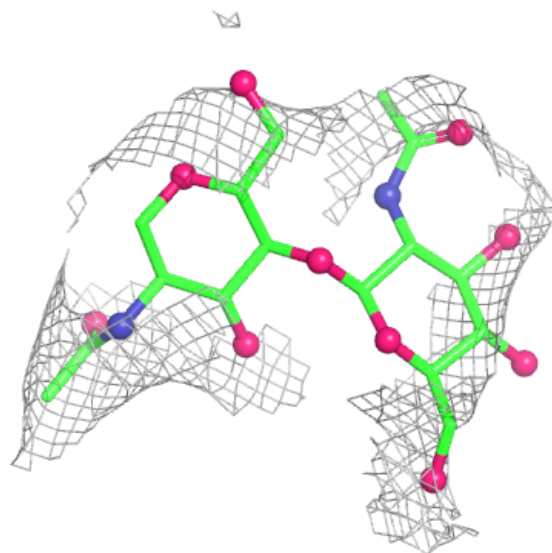
Electron density around Chain R:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



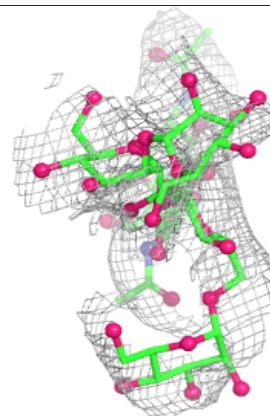
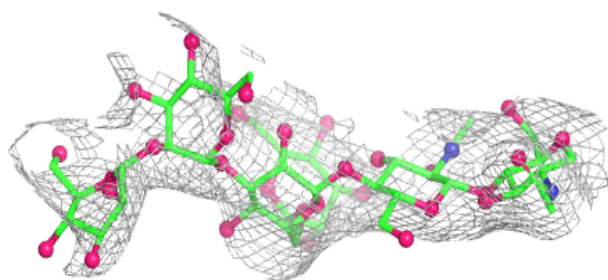
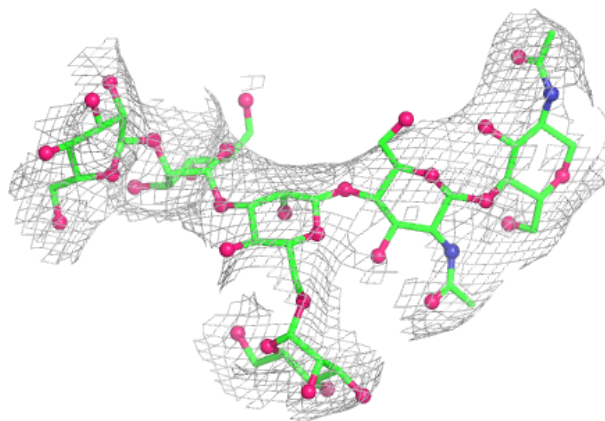
Electron density around Chain S:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



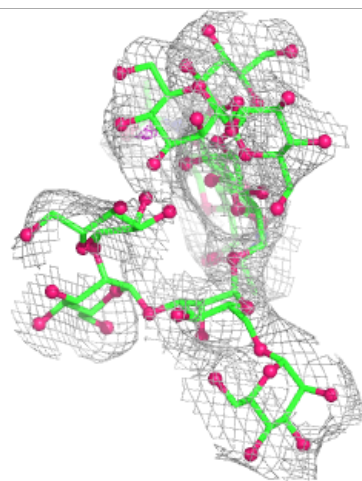
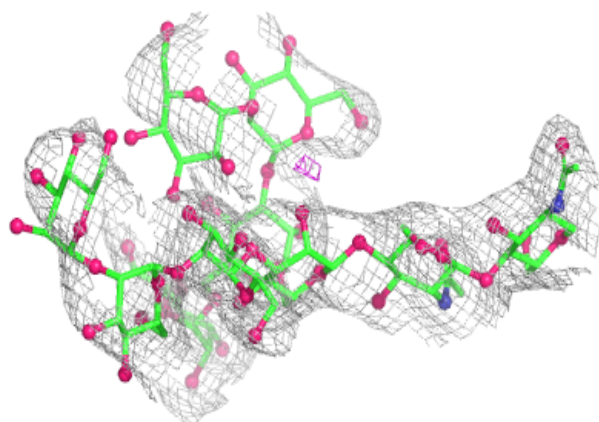
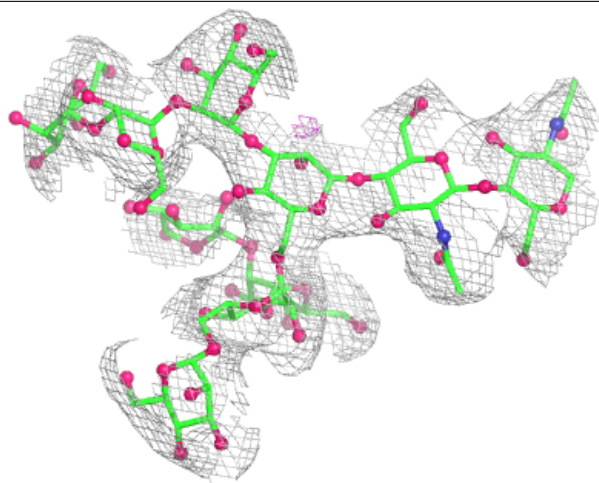
Electron density around Chain M:

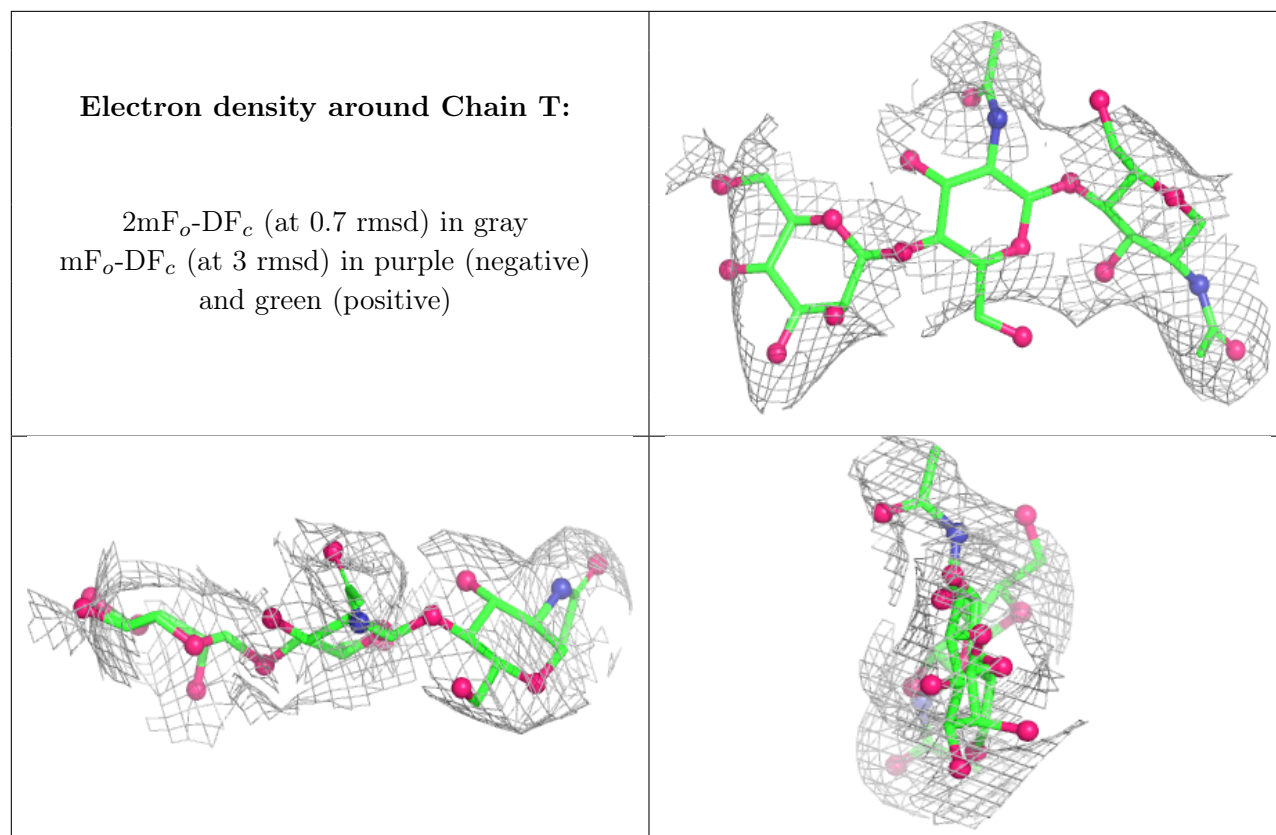
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain P:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



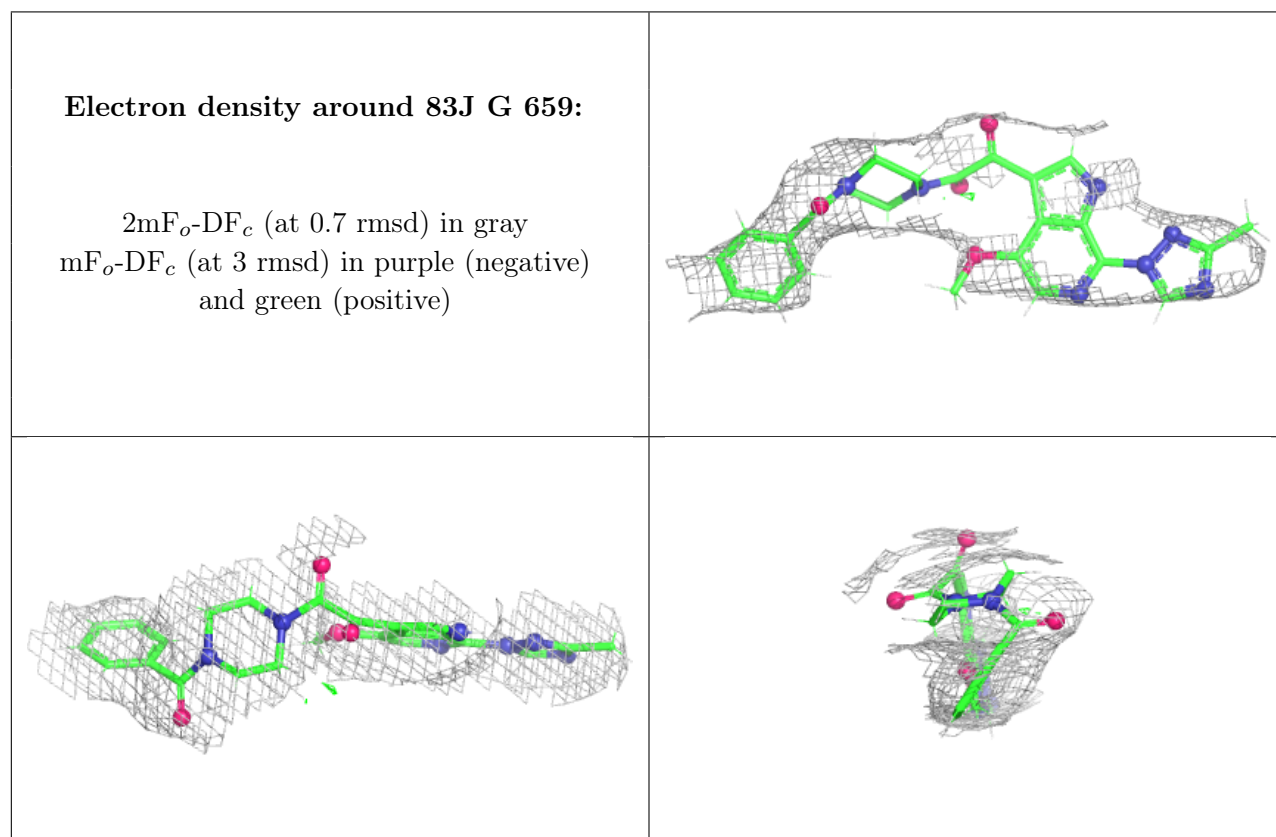


6.4 Ligands [i](#)

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, 95th 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 ²)	Q<0.9
15	NAG	G	648	14/15	0.97	0.04	107,150,178,185	0
14	SO4	G	603	5/5	0.98	0.07	249,250,250,255	5
15	NAG	B	703	14/15	0.98	0.04	152,180,214,227	0
15	NAG	G	633	14/15	0.98	0.03	92,109,131,132	0
14	SO4	G	601	5/5	0.98	0.03	127,154,158,172	0
15	NAG	G	658	14/15	0.98	0.04	46,129,151,151	0
15	NAG	H	301	14/15	0.98	0.03	107,120,132,139	0
15	NAG	G	611	14/15	0.99	0.03	72,100,115,133	0
14	SO4	L	301	5/5	0.99	0.06	106,107,107,109	5
15	NAG	B	702	14/15	0.99	0.04	147,185,195,199	0
14	SO4	G	602	5/5	0.99	0.04	149,163,168,169	0
15	NAG	B	704	14/15	0.99	0.02	113,143,156,160	0
14	SO4	B	701	5/5	1.00	0.02	113,121,127,134	0
16	83J	G	659	35/35	1.00	0.03	14,62,114,138	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.