



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:33 AM UTC

PDB ID : 6OM2 / pdb_00006om2
Title : Crystal structure of atypical integrin alphaV beta8 with proTGF-beta1 ligand peptide
Authors : Wang, J.C.; Springer, T.A.
Deposited on : 2019-04-17
Resolution : 2.77 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:

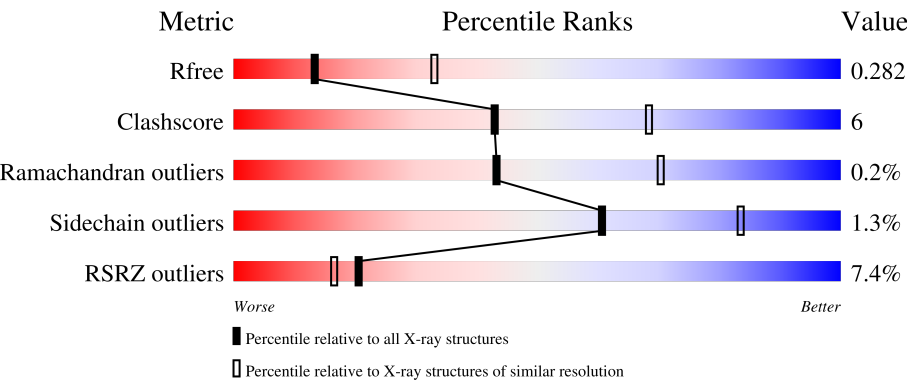
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	A	598	5% 92% 8%
1	C	598	5% 87% 12%
2	B	421	9% 63% 10% 26%
2	D	421	7% 66% 12% 22%
3	E	11	45% 55% 36% 9%

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Mol	Chain	Length	Quality of chain
3	F	11	
4	G	3	
4	K	3	
4	S	3	
5	H	7	
5	L	7	
5	O	7	
6	I	5	
7	J	4	
8	M	2	
8	P	2	
8	Q	2	
8	R	2	
9	N	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	M	1	-	-	X	-
8	NAG	M	2	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 28790 atoms, of which 13455 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	598	Total	C	H	N	O	S	0	0	0
			8991	2927	4371	785	887	21			
1	C	596	Total	C	H	N	O	S	0	0	0
			8981	2923	4369	783	885	21			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	GLY	-	insertion	UNP P06756
A	401	CYS	MET	engineered mutation	UNP P06756
A	596	THR	-	expression tag	UNP P06756
A	597	GLY	-	expression tag	UNP P06756
A	598	GLY	-	expression tag	UNP P06756
C	400	GLY	-	insertion	UNP P06756
C	401	CYS	MET	engineered mutation	UNP P06756
C	596	THR	-	expression tag	UNP P06756
C	597	GLY	-	expression tag	UNP P06756
C	598	GLY	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	310	Total	C	H	N	O	S	0	0	0
			4747	1551	2301	419	460	16			
2	D	330	Total	C	H	N	O	S	0	0	0
			5003	1638	2414	446	489	16			

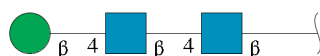
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	259	CYS	VAL	engineered mutation	UNP P26012
D	259	CYS	VAL	engineered mutation	UNP P26012

- Molecule 3 is a protein called proTGF-beta1 RGD peptide.

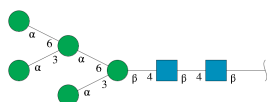
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	10	Total	C	N	O	0	0	1
			68	40	16	12			
3	F	9	Total	C	N	O	0	0	1
			64	38	15	11			

- Molecule 4 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.



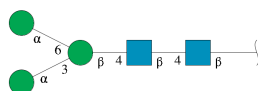
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	S	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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
5	H	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	L	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 6 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
6	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 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.



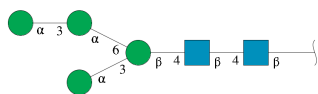
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 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
8	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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.

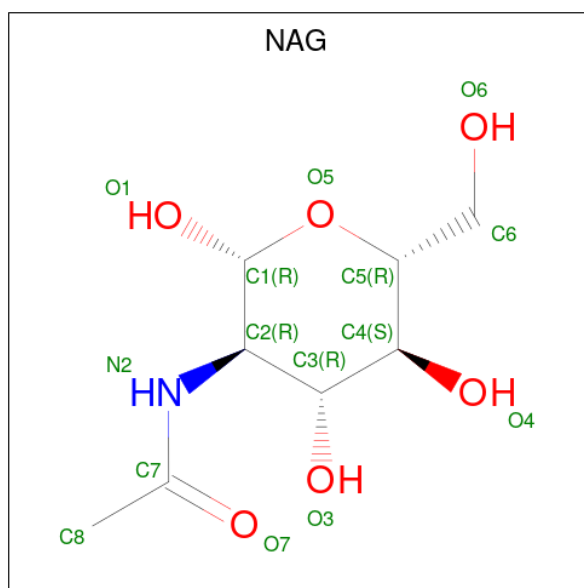


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	N	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	Ca	0	0
			4	4		
10	B	1	Total	Ca	0	0
			1	1		
10	C	4	Total	Ca	0	0
			4	4		
10	D	1	Total	Ca	0	0
			1	1		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



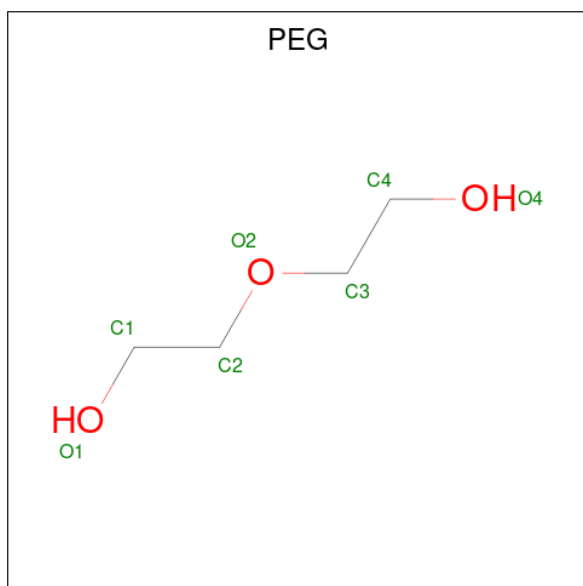
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

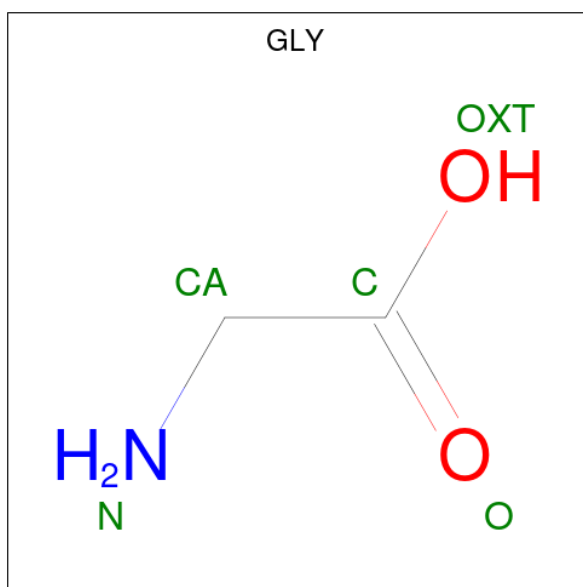


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	Mg	0	0
			1	1		
13	D	1	Total	Mg	0	0
			1	1		

- Molecule 14 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	N	O	0	0
			4	2	1	1		

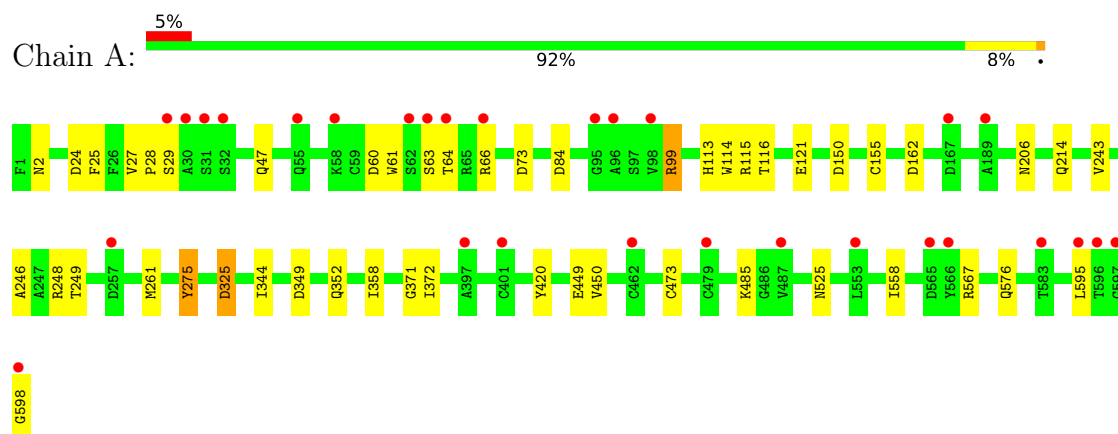
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	75	Total	O	0	0
			75	75		
15	B	11	Total	O	0	0
			11	11		
15	C	97	Total	O	0	0
			97	97		
15	D	19	Total	O	0	0
			19	19		
15	E	1	Total	O	0	0
			1	1		

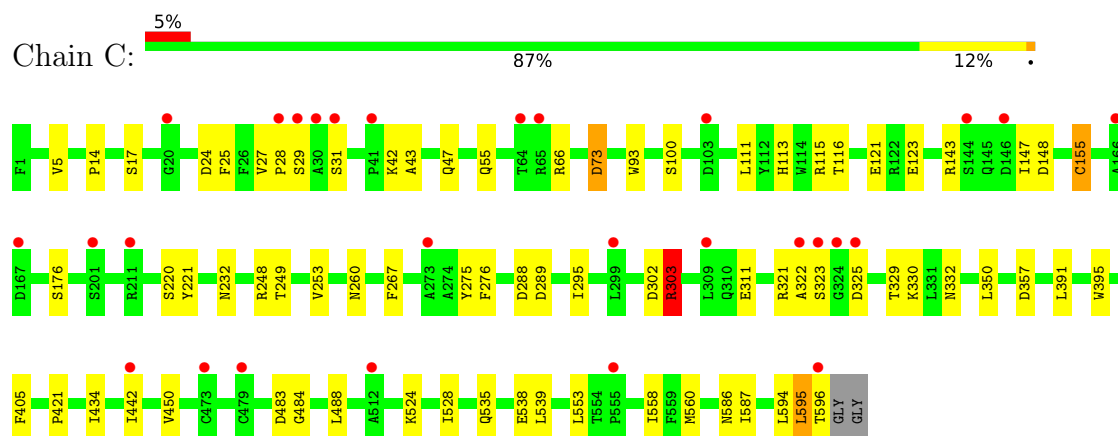
3 Residue-property plots [i](#)

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.

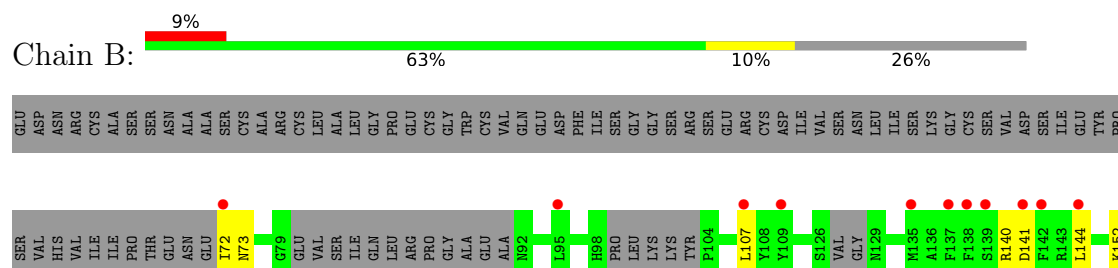
• Molecule 1: Integrin alpha-V

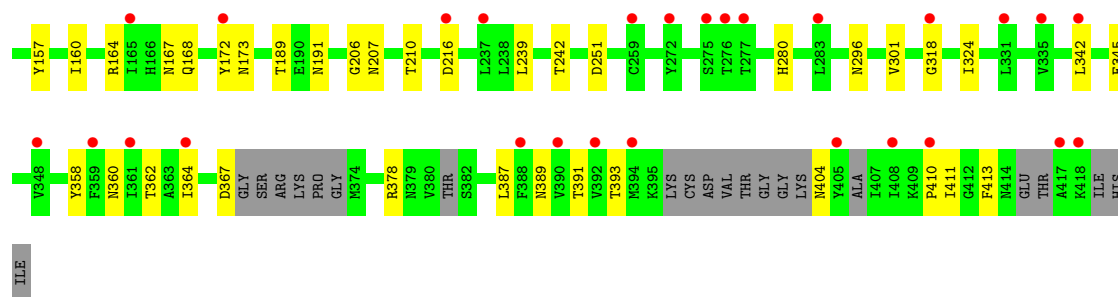


• Molecule 1: Integrin alpha-V

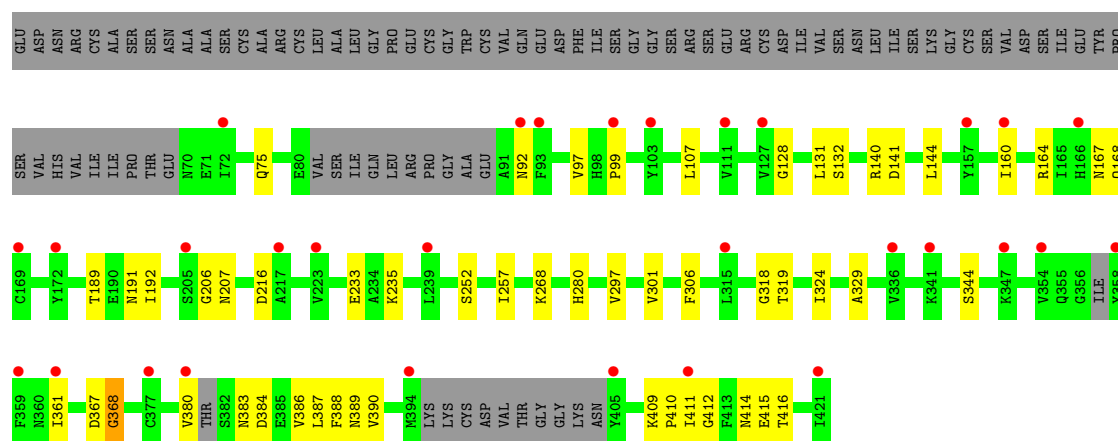


• Molecule 2: Integrin beta-8

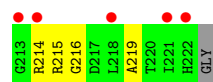




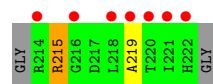
• Molecule 2: Integrin beta-8



• Molecule 3: proTGF-beta1 RGD peptide



• Molecule 3: proTGF-beta1 RGD peptide



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

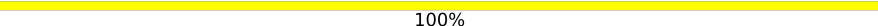


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67% 33%

MAG1
MAG2
BMA3

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

Chain S:  100%

MAG1
MAG2
BMA3

- Molecule 5: 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 H:  14% 86%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 5: 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 L:  14% 57% 29%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 5: 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 O:  29% 71%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 6: 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 I:  40% 40% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 7: 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 J:  25% 25% 50%

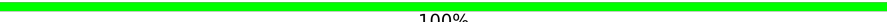
 NAG1
NAG2
BMA3
MAN4

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

Chain M:  50% 50%

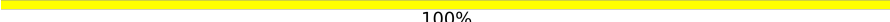
 NAG1
NAG2

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

Chain P:  100%

 NAG1
NAG2

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

Chain Q:  100%

 NAG1
NAG2

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

Chain R:  50% 50%

 NAG1
NAG2

- Molecule 9: alpha-D-mannopyranose-(1-3)-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 N:  50% 50%

 NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	161.19Å 53.85Å 176.62Å 90.00° 111.47° 90.00°	Depositor
Resolution (Å)	47.43 – 2.77 47.43 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.43-2.77) 98.6 (47.43-2.77)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.251 , 0.282 0.253 , 0.282	Depositor DCC
R_{free} test set	2000 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28790	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: NAG, BMA, MAN, PEG, CA, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/4724	0.30	0/6395
1	C	0.14	0/4716	0.33	0/6385
2	B	0.12	0/2489	0.34	0/3361
2	D	0.12	0/2639	0.32	0/3571
3	E	0.11	0/67	0.37	0/88
3	F	0.13	0/63	0.37	0/83
All	All	0.13	0/14698	0.32	0/19883

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	A	4620	4371	4468	35	0
1	C	4612	4369	4462	52	0
2	B	2446	2301	2412	30	0
2	D	2589	2414	2554	37	0
3	E	68	0	70	3	0
3	F	64	0	67	1	0
4	G	39	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	39	0	34	0	0
4	S	39	0	34	5	0
5	H	83	0	70	1	0
5	L	83	0	70	3	0
5	O	83	0	70	7	0
6	I	61	0	52	4	0
7	J	50	0	43	4	0
8	M	28	0	25	11	0
8	P	28	0	25	0	0
8	Q	28	0	25	2	0
8	R	28	0	25	5	0
9	N	72	0	61	0	0
10	A	4	0	0	0	0
10	B	1	0	0	0	0
10	C	4	0	0	0	0
10	D	1	0	0	0	0
11	A	28	0	26	0	0
11	D	14	0	13	1	0
12	A	7	0	10	0	0
12	C	7	0	10	1	0
13	B	1	0	0	0	0
13	D	1	0	0	0	0
14	C	4	0	2	1	0
15	A	75	0	0	6	0
15	B	11	0	0	0	0
15	C	97	0	0	3	0
15	D	19	0	0	2	0
15	E	1	0	0	0	0
All	All	15335	13455	14662	184	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 6.

All (184) 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)
2:D:233:GLU:OE1	8:R:2:NAG:O4	1.88	0.89
1:A:121:GLU:OE1	2:B:164:ARG:NH2	2.12	0.82
1:C:289:ASP:OD2	5:H:2:NAG:H5	1.80	0.81
8:M:1:NAG:H62	8:M:2:NAG:N2	1.96	0.80
5:O:3:BMA:H2	5:O:7:MAN:H2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:2:NAG:H61	4:S:3:BMA:H2	1.64	0.78
2:D:268:LYS:O	15:D:3301:HOH:O	2.05	0.75
1:C:596:THR:HG1	14:C:601:GLY:N	1.85	0.73
2:D:318:GLY:CA	2:D:411:ILE:HD11	2.19	0.72
15:C:702:HOH:O	5:O:7:MAN:O4	2.09	0.71
2:B:164:ARG:HA	2:B:167:ASN:O	1.93	0.69
2:D:318:GLY:HA2	2:D:411:ILE:HD11	1.73	0.69
1:C:595:LEU:HD12	1:C:595:LEU:H	1.58	0.69
1:A:63:SER:OG	1:A:64:THR:N	2.27	0.69
1:A:449:GLU:OE1	7:J:4:MAN:O4	2.10	0.68
5:O:3:BMA:C2	5:O:7:MAN:H2	2.24	0.68
5:O:4:MAN:O4	5:O:5:MAN:H5	1.93	0.68
1:C:302:ASP:OD2	1:C:332:ASN:ND2	2.27	0.68
1:C:232:ASN:HD22	8:M:2:NAG:H81	1.59	0.68
2:D:414:ASN:ND2	8:R:1:NAG:O7	2.26	0.68
5:O:4:MAN:H3	5:O:5:MAN:H3	1.76	0.68
8:Q:1:NAG:H62	8:Q:2:NAG:N2	2.09	0.67
1:A:28:PRO:O	1:A:29:SER:OG	2.13	0.66
2:D:318:GLY:N	2:D:411:ILE:HD11	2.12	0.65
8:R:1:NAG:H61	8:R:2:NAG:HN2	1.61	0.65
2:D:329:ALA:O	15:D:3302:HOH:O	2.15	0.65
8:Q:1:NAG:H62	8:Q:2:NAG:HN2	1.62	0.64
2:D:233:GLU:CD	8:R:1:NAG:H4	2.23	0.64
2:B:152:LYS:NZ	2:B:216:ASP:OD2	2.24	0.63
8:M:1:NAG:H4	8:M:2:NAG:HN2	1.64	0.62
2:B:189:THR:HG22	2:B:191:ASN:H	1.65	0.61
2:B:404:ASN:O	2:B:404:ASN:ND2	2.33	0.61
15:C:741:HOH:O	8:M:1:NAG:H81	2.01	0.61
1:A:567:ARG:HA	1:A:576:GLN:NE2	2.15	0.61
1:A:325:ASP:N	1:A:325:ASP:OD1	2.34	0.61
2:B:210:THR:OG1	3:E:216:GLY:HA2	2.00	0.60
7:J:3:BMA:O2	7:J:4:MAN:O5	2.18	0.60
2:D:164:ARG:HA	2:D:167:ASN:O	2.01	0.60
1:C:47:GLN:NE2	1:C:73:ASP:OD2	2.35	0.59
11:D:3201:NAG:O7	11:D:3201:NAG:O3	2.19	0.59
1:C:303:ARG:HH21	1:C:303:ARG:HG3	1.68	0.58
1:A:60:ASP:OD1	1:A:61:TRP:N	2.36	0.58
8:M:1:NAG:H62	8:M:2:NAG:C7	2.33	0.58
2:D:189:THR:HG22	2:D:191:ASN:H	1.67	0.58
1:C:24:ASP:OD1	1:C:25:PHE:N	2.36	0.58
8:M:2:NAG:O7	8:M:2:NAG:O3	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:TRP:CZ3	1:C:434:ILE:HD11	2.39	0.57
2:D:132:SER:HB3	2:D:192:ILE:HD12	1.87	0.57
2:B:410:PRO:HB2	2:B:413:PHE:HB2	1.87	0.57
1:C:395:TRP:HZ3	1:C:434:ILE:HD11	1.69	0.57
1:A:248:ARG:O	1:A:249:THR:OG1	2.20	0.56
3:F:215:ARG:HA	3:F:219:ALA:HB2	1.86	0.56
2:D:99:PRO:HG3	2:D:384:ASP:O	2.06	0.56
15:A:2129:HOH:O	6:I:3:BMA:H5	2.05	0.56
1:C:143:ARG:NH2	15:C:707:HOH:O	2.39	0.56
1:A:420:TYR:OH	1:A:485:LYS:O	2.09	0.55
2:B:72:ILE:HG22	2:B:72:ILE:O	2.07	0.55
1:C:28:PRO:HG2	1:C:31:SER:HB3	1.87	0.55
2:B:157:TYR:OH	2:B:251:ASP:O	2.25	0.55
1:A:275:TYR:OH	2:B:251:ASP:OD1	2.20	0.54
1:A:243:VAL:HG12	1:A:246:ALA:HB2	1.89	0.54
2:D:191:ASN:ND2	4:S:1:NAG:O7	2.40	0.53
2:B:345:GLU:OE1	2:B:378:ARG:NE	2.34	0.53
1:C:442:ILE:HD11	1:C:488:LEU:HD22	1.91	0.53
8:M:1:NAG:H62	8:M:2:NAG:C2	2.38	0.53
1:C:553:LEU:HD23	1:C:595:LEU:HD21	1.89	0.53
1:A:349:ASP:O	1:A:352:GLN:NE2	2.42	0.53
2:D:75:GLN:HB3	2:D:415:GLU:HG3	1.90	0.53
1:A:113:HIS:CD2	2:B:160:ILE:HD11	2.44	0.52
2:B:360:ASN:HB3	2:B:391:THR:HB	1.92	0.52
2:B:168:GLN:HG3	2:B:206:GLY:O	2.10	0.52
1:A:206:ASN:OD1	8:M:2:NAG:H3	2.10	0.51
1:C:350:LEU:N	1:C:357:ASP:OD2	2.41	0.51
15:A:2116:HOH:O	6:I:3:BMA:H61	2.09	0.51
1:C:321:ARG:HB2	1:C:325:ASP:O	2.11	0.51
2:D:92:ASN:HB2	2:D:389:ASN:HD21	1.76	0.50
2:D:140:ARG:O	2:D:141:ASP:HB2	2.10	0.50
4:G:2:NAG:O3	4:G:3:BMA:C1	2.59	0.50
1:A:27:VAL:O	1:A:27:VAL:HG13	2.12	0.50
2:D:107:LEU:O	2:D:144:LEU:HA	2.12	0.50
1:C:248:ARG:O	1:C:249:THR:OG1	2.25	0.49
2:D:301:VAL:O	2:D:324:ILE:N	2.32	0.49
5:O:1:NAG:H61	5:O:2:NAG:C1	2.43	0.49
1:C:27:VAL:HG13	1:C:27:VAL:O	2.13	0.48
1:C:115:ARG:O	1:C:116:THR:OG1	2.14	0.48
2:D:168:GLN:HG3	2:D:206:GLY:O	2.13	0.48
4:S:1:NAG:O4	4:S:2:NAG:O7	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLN:NE2	1:A:73:ASP:O	2.46	0.48
2:B:367:ASP:OD1	2:B:367:ASP:C	2.56	0.48
2:B:242:THR:O	2:B:301:VAL:HA	2.14	0.47
4:G:1:NAG:O3	4:G:2:NAG:O5	2.25	0.47
1:C:350:LEU:HA	1:C:421:PRO:HG2	1.96	0.47
5:L:4:MAN:H62	5:L:6:MAN:H3	1.96	0.47
8:M:1:NAG:H4	8:M:2:NAG:N2	2.27	0.47
1:C:113:HIS:CD2	2:D:160:ILE:HD11	2.49	0.47
1:C:405:PHE:HE2	1:C:434:ILE:HD13	1.77	0.47
2:B:172:TYR:HE1	3:E:214:ARG:NH1	2.12	0.47
2:B:301:VAL:O	2:B:324:ILE:N	2.38	0.47
1:C:14:PRO:O	1:C:17:SER:OG	2.28	0.47
8:M:2:NAG:C7	8:M:2:NAG:HO3	2.21	0.47
2:B:72:ILE:O	2:B:73:ASN:CG	2.57	0.47
4:S:1:NAG:C6	4:S:2:NAG:C1	2.93	0.47
1:C:303:ARG:HH21	1:C:303:ARG:CG	2.27	0.47
2:D:99:PRO:HG2	2:D:383:ASN:HA	1.96	0.47
2:B:358:TYR:HB2	2:B:393:THR:HG22	1.97	0.47
1:C:42:LYS:O	5:L:1:NAG:H82	2.15	0.46
1:C:288:ASP:O	1:C:289:ASP:HB3	2.14	0.46
1:C:5:VAL:HG12	1:C:5:VAL:O	2.15	0.46
15:A:2103:HOH:O	6:I:5:MAN:O6	2.21	0.46
1:C:560:MET:CE	1:C:587:ILE:HD11	2.45	0.46
1:A:243:VAL:CG1	1:A:246:ALA:HB2	2.46	0.46
1:C:528:ILE:HG22	1:C:535:GLN:HB2	1.96	0.46
2:B:140:ARG:O	2:B:141:ASP:HB2	2.15	0.46
3:E:215:ARG:HA	3:E:219:ALA:HB2	1.96	0.46
2:B:107:LEU:HD11	2:B:239:LEU:HB2	1.98	0.45
1:C:442:ILE:HD11	1:C:488:LEU:CD2	2.46	0.45
2:D:414:ASN:OD1	2:D:415:GLU:HG2	2.16	0.45
1:A:598:GLY:HA2	15:A:2132:HOH:O	2.15	0.45
2:D:387:LEU:HD23	2:D:387:LEU:N	2.31	0.45
1:C:28:PRO:O	1:C:29:SER:OG	2.26	0.45
1:C:121:GLU:OE1	2:D:164:ARG:NH2	2.50	0.44
2:D:361:ILE:HG12	2:D:390:VAL:HG23	1.99	0.44
5:O:4:MAN:H62	5:O:6:MAN:H2	1.85	0.44
1:A:28:PRO:O	1:A:29:SER:CB	2.65	0.44
4:S:2:NAG:H61	4:S:3:BMA:C2	2.42	0.44
1:C:538:GLU:C	1:C:539:LEU:HD12	2.43	0.44
1:A:150:ASP:OD1	1:A:150:ASP:N	2.50	0.44
1:C:595:LEU:HD12	1:C:595:LEU:N	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:SER:HB2	1:C:43:ALA:HB2	1.99	0.44
1:A:84:ASP:OD2	1:A:115:ARG:NE	2.51	0.43
1:C:483:ASP:OD1	1:C:484:GLY:N	2.49	0.43
1:A:214:GLN:OE1	1:A:214:GLN:N	2.43	0.43
2:D:409:LYS:HG2	2:D:416:THR:HG22	1.99	0.43
1:A:344:ILE:CG2	1:A:358:ILE:HD11	2.49	0.43
2:B:364:ILE:CG2	2:B:387:LEU:HD11	2.48	0.43
1:C:594:LEU:C	1:C:594:LEU:HD23	2.43	0.43
2:B:172:TYR:O	2:B:173:ASN:OD1	2.36	0.43
2:D:216:ASP:OD1	2:D:280:HIS:ND1	2.51	0.43
2:B:107:LEU:O	2:B:144:LEU:HA	2.19	0.43
2:B:362:THR:N	2:B:389:ASN:O	2.49	0.43
1:A:114:TRP:CZ2	1:A:116:THR:HA	2.53	0.43
2:D:97:VAL:HG22	2:D:386:VAL:HG21	2.00	0.43
1:C:276:PHE:CZ	1:C:295:ILE:HG21	2.54	0.42
2:B:411:ILE:O	2:B:411:ILE:HG23	2.19	0.42
7:J:3:BMA:C2	7:J:4:MAN:O5	2.68	0.42
1:A:63:SER:HG	1:A:64:THR:H	1.61	0.42
15:A:2166:HOH:O	6:I:5:MAN:H62	2.19	0.42
1:C:450:VAL:HG21	1:C:558:ILE:HD12	2.02	0.42
1:C:329:THR:HG22	1:C:330:LYS:N	2.33	0.42
2:D:367:ASP:OD1	2:D:368:GLY:N	2.53	0.42
1:C:253:VAL:HB	1:C:267:PHE:HB2	2.02	0.42
2:B:318:GLY:HA2	2:B:411:ILE:HD11	2.01	0.42
1:A:115:ARG:O	1:A:116:THR:OG1	2.25	0.42
1:C:43:ALA:HB3	1:C:55:GLN:HG3	2.01	0.42
2:D:235:LYS:NZ	2:D:412:GLY:O	2.46	0.42
1:A:115:ARG:HA	1:A:121:GLU:O	2.20	0.41
1:C:220:SER:O	1:C:221:TYR:HB2	2.20	0.41
1:A:99:ARG:HG2	1:A:162:ASP:HA	2.01	0.41
1:A:371:GLY:O	1:A:372:ILE:HD13	2.20	0.41
2:D:301:VAL:HG21	2:D:306:PHE:HA	2.01	0.41
1:C:322:ALA:H	12:C:632:PEG:H22	1.85	0.41
1:C:391:LEU:N	1:C:391:LEU:HD12	2.35	0.41
1:C:260:ASN:HD22	8:M:1:NAG:C7	2.32	0.41
1:A:261:MET:O	1:A:261:MET:HG3	2.21	0.41
1:A:473:CYS:O	7:J:1:NAG:O6	2.35	0.41
1:C:155:CYS:HB2	1:C:176:SER:OG	2.20	0.41
2:B:296:ASN:CB	2:B:342:LEU:HD21	2.50	0.41
2:D:297:VAL:HB	2:D:319:THR:HG22	2.02	0.41
1:A:2:ASN:OD1	1:A:2:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:VAL:HG21	1:A:558:ILE:HD12	2.03	0.41
1:A:525:ASN:O	15:A:2104:HOH:O	2.22	0.41
2:D:344:SER:HA	2:D:380:VAL:HG12	2.03	0.41
1:A:24:ASP:OD1	1:A:25:PHE:N	2.50	0.40
2:B:216:ASP:OD1	2:B:280:HIS:HA	2.21	0.40
1:C:115:ARG:O	1:C:116:THR:CB	2.68	0.40
1:C:115:ARG:HA	1:C:121:GLU:O	2.20	0.40
1:C:147:ILE:O	1:C:148:ASP:HB2	2.20	0.40
2:D:410:PRO:HD2	2:D:415:GLU:O	2.21	0.40
2:D:128:GLY:O	2:D:131:LEU:N	2.54	0.40
5:L:4:MAN:H61	5:L:6:MAN:H2	1.24	0.40
1:C:93:TRP:CD1	1:C:111:LEU:HD12	2.56	0.40
1:C:121:GLU:HG3	1:C:123:GLU:HG3	2.04	0.40
2:D:252:SER:HB3	2:D:257:ILE:HB	2.03	0.40
2:D:414:ASN:ND2	8:R:1:NAG:C7	2.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	596/598 (100%)	551 (92%)	45 (8%)	0	100	100
1	C	594/598 (99%)	562 (95%)	31 (5%)	1 (0%)	43	70
2	B	292/421 (69%)	264 (90%)	28 (10%)	0	100	100
2	D	320/421 (76%)	295 (92%)	23 (7%)	2 (1%)	21	47
3	E	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
3	F	7/11 (64%)	7 (100%)	0	0	100	100
All	All	1817/2060 (88%)	1686 (93%)	128 (7%)	3 (0%)	43	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	388	PHE
1	C	303	ARG
2	D	368	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	488/488 (100%)	482 (99%)	6 (1%)	63	84
1	C	488/488 (100%)	477 (98%)	11 (2%)	44	75
2	B	277/369 (75%)	276 (100%)	1 (0%)	84	93
2	D	291/369 (79%)	290 (100%)	1 (0%)	86	94
3	E	6/7 (86%)	6 (100%)	0	100	100
3	F	6/7 (86%)	5 (83%)	1 (17%)	2	7
All	All	1556/1728 (90%)	1536 (99%)	20 (1%)	61	83

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	99	ARG
1	A	155	CYS
1	A	275	TYR
1	A	325	ASP
1	A	595	LEU
2	B	207	ASN
1	C	66	ARG
1	C	73	ASP
1	C	100	SER
1	C	155	CYS
1	C	275	TYR
1	C	303	ARG
1	C	311	GLU
1	C	323	SER
1	C	524	LYS

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Mol	Chain	Res	Type
1	C	586	ASN
1	C	595	LEU
2	D	207	ASN
3	F	215	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	ASN
1	A	590	GLN
1	A	592	HIS
2	B	73	ASN
2	B	118	HIS
2	B	120	ASN
2	B	227	HIS
2	B	296	ASN
2	B	302	GLN
1	C	92	GLN
1	C	206	ASN
1	C	475	ASN
1	C	590	GLN
1	C	592	HIS
2	D	120	ASN
2	D	302	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 ⓘ

53 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
4	NAG	G	1	4,1	14,14,15	0.35	0	17,19,21	0.48	0
4	NAG	G	2	4	14,14,15	0.41	0	17,19,21	0.51	0
4	BMA	G	3	4	11,11,12	0.70	0	15,15,17	0.78	0
5	NAG	H	1	5,1	14,14,15	0.19	0	17,19,21	0.50	0
5	NAG	H	2	5	14,14,15	0.52	0	17,19,21	0.47	0
5	BMA	H	3	5	11,11,12	0.79	0	15,15,17	0.98	1 (6%)
5	MAN	H	4	5	11,11,12	1.13	1 (9%)	15,15,17	0.88	0
5	MAN	H	5	5	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
5	MAN	H	6	5	11,11,12	1.30	1 (9%)	15,15,17	1.07	1 (6%)
5	MAN	H	7	5	11,11,12	0.90	1 (9%)	15,15,17	0.82	1 (6%)
6	NAG	I	1	6,1	14,14,15	0.45	0	17,19,21	0.51	0
6	NAG	I	2	6	14,14,15	0.18	0	17,19,21	0.51	0
6	BMA	I	3	6	11,11,12	0.71	0	15,15,17	0.81	0
6	MAN	I	4	6	11,11,12	0.68	0	15,15,17	0.94	2 (13%)
6	MAN	I	5	6	11,11,12	0.66	0	15,15,17	0.95	2 (13%)
7	NAG	J	1	7,1	14,14,15	0.18	0	17,19,21	0.44	0
7	NAG	J	2	7	14,14,15	0.25	0	17,19,21	0.41	0
7	BMA	J	3	7	11,11,12	1.00	1 (9%)	15,15,17	1.36	1 (6%)
7	MAN	J	4	7	11,11,12	0.78	1 (9%)	15,15,17	1.27	2 (13%)
4	NAG	K	1	4,2	14,14,15	0.77	1 (7%)	17,19,21	1.12	2 (11%)
4	NAG	K	2	4	14,14,15	0.29	0	17,19,21	0.37	0
4	BMA	K	3	4	11,11,12	0.54	0	15,15,17	0.87	0
5	NAG	L	1	5,1	14,14,15	0.43	0	17,19,21	0.45	0
5	NAG	L	2	5	14,14,15	0.34	0	17,19,21	0.41	0
5	BMA	L	3	5	11,11,12	0.68	0	15,15,17	0.86	1 (6%)
5	MAN	L	4	5	11,11,12	0.91	1 (9%)	15,15,17	1.41	2 (13%)
5	MAN	L	5	5	11,11,12	0.86	1 (9%)	15,15,17	1.48	4 (26%)
5	MAN	L	6	5	11,11,12	0.81	0	15,15,17	1.14	2 (13%)
5	MAN	L	7	5	11,11,12	0.61	0	15,15,17	1.06	2 (13%)
8	NAG	M	1	8,1	14,14,15	0.42	0	17,19,21	0.43	0
8	NAG	M	2	8	14,14,15	0.53	0	17,19,21	0.65	1 (5%)
9	NAG	N	1	9,1	14,14,15	0.30	0	17,19,21	0.44	0
9	NAG	N	2	9	14,14,15	0.19	0	17,19,21	0.48	0
9	BMA	N	3	9	11,11,12	0.65	0	15,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	N	4	9	11,11,12	0.83	1 (9%)	15,15,17	0.87	1 (6%)
9	MAN	N	5	9	11,11,12	0.70	0	15,15,17	1.00	2 (13%)
9	MAN	N	6	9	11,11,12	0.72	0	15,15,17	0.90	2 (13%)
5	NAG	O	1	5,1	14,14,15	0.18	0	17,19,21	0.49	0
5	NAG	O	2	5	14,14,15	0.29	0	17,19,21	0.53	0
5	BMA	O	3	5	11,11,12	1.07	0	15,15,17	1.15	1 (6%)
5	MAN	O	4	5	11,11,12	0.86	1 (9%)	15,15,17	1.28	2 (13%)
5	MAN	O	5	5	11,11,12	0.73	0	15,15,17	1.48	2 (13%)
5	MAN	O	6	5	11,11,12	0.73	1 (9%)	15,15,17	1.34	2 (13%)
5	MAN	O	7	5	11,11,12	0.76	0	15,15,17	1.05	2 (13%)
8	NAG	P	1	8,1	14,14,15	0.40	0	17,19,21	0.53	0
8	NAG	P	2	8	14,14,15	0.36	0	17,19,21	0.53	0
8	NAG	Q	1	8,1	14,14,15	0.46	0	17,19,21	0.46	0
8	NAG	Q	2	8	14,14,15	0.23	0	17,19,21	0.45	0
8	NAG	R	1	2,8	14,14,15	0.67	0	17,19,21	0.70	1 (5%)
8	NAG	R	2	8	14,14,15	0.25	0	17,19,21	0.67	0
4	NAG	S	1	4,2	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	S	2	4	14,14,15	0.25	0	17,19,21	0.37	0
4	BMA	S	3	4	11,11,12	0.58	0	15,15,17	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	MAN	H	4	5	-	2/2/19/22	0/1/1/1
5	MAN	H	5	5	-	2/2/19/22	0/1/1/1
5	MAN	H	6	5	-	0/2/19/22	0/1/1/1
5	MAN	H	7	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1
4	BMA	S	3	4	-	2/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	6	MAN	O5-C1	-3.56	1.37	1.43
5	H	4	MAN	O5-C1	-3.34	1.38	1.43
5	H	7	MAN	O5-C1	-2.47	1.39	1.43
5	L	5	MAN	C1-C2	2.34	1.57	1.52
7	J	3	BMA	O3-C3	2.31	1.48	1.43
4	K	1	NAG	C1-C2	2.26	1.55	1.52
9	N	4	MAN	O5-C1	-2.22	1.40	1.43
5	O	4	MAN	C1-C2	2.20	1.57	1.52
5	L	4	MAN	C1-C2	2.16	1.57	1.52
7	J	4	MAN	O5-C5	2.08	1.47	1.43
5	O	6	MAN	C1-C2	2.06	1.57	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	5	MAN	C1-O5-C5	4.23	117.86	112.19
7	J	3	BMA	O3-C3-C2	3.72	117.64	110.05
7	J	4	MAN	C1-O5-C5	3.69	117.13	112.19
5	L	5	MAN	C1-O5-C5	3.58	116.98	112.19
5	L	4	MAN	C1-O5-C5	3.49	116.86	112.19
4	K	1	NAG	C1-O5-C5	3.31	116.63	112.19
5	O	6	MAN	C1-O5-C5	3.31	116.62	112.19
5	O	4	MAN	C1-O5-C5	3.04	116.26	112.19
5	L	7	MAN	C1-O5-C5	2.71	115.82	112.19
5	H	5	MAN	C1-O5-C5	2.61	115.68	112.19
5	O	7	MAN	O2-C2-C3	-2.57	104.82	110.15
9	N	5	MAN	C1-O5-C5	2.49	115.53	112.19
5	O	3	BMA	C3-C4-C5	2.49	114.75	110.23
5	O	7	MAN	C1-O5-C5	2.47	115.50	112.19
5	O	5	MAN	O2-C2-C3	-2.45	105.07	110.15
5	H	6	MAN	O2-C2-C3	-2.38	105.23	110.15
5	O	4	MAN	O2-C2-C3	-2.37	105.25	110.15
8	R	1	NAG	C1-O5-C5	2.36	115.35	112.19
5	L	5	MAN	C1-C2-C3	2.35	113.07	109.64
5	L	6	MAN	C1-O5-C5	2.31	115.28	112.19
6	I	5	MAN	O2-C2-C3	-2.29	105.40	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	4	MAN	O2-C2-C3	-2.28	105.42	110.15
6	I	4	MAN	C1-O5-C5	2.23	115.17	112.19
5	L	4	MAN	O2-C2-C3	-2.20	105.59	110.15
9	N	5	MAN	O2-C2-C3	-2.20	105.60	110.15
5	H	7	MAN	O2-C2-C3	-2.20	105.60	110.15
5	O	6	MAN	O2-C2-C3	-2.17	105.65	110.15
9	N	4	MAN	O2-C2-C3	-2.16	105.67	110.15
8	M	2	NAG	C1-O5-C5	2.15	115.07	112.19
5	L	7	MAN	O2-C2-C3	-2.15	105.70	110.15
5	L	5	MAN	O2-C2-C3	-2.11	105.78	110.15
6	I	5	MAN	C1-O5-C5	2.11	115.01	112.19
9	N	6	MAN	O2-C2-C3	-2.10	105.80	110.15
4	K	1	NAG	O4-C4-C3	2.09	115.31	110.38
6	I	4	MAN	O2-C2-C3	-2.09	105.83	110.15
5	L	5	MAN	O5-C1-C2	2.08	115.75	110.79
9	N	6	MAN	C1-O5-C5	2.07	114.96	112.19
5	H	3	BMA	C1-O5-C5	2.07	114.96	112.19
5	H	5	MAN	O2-C2-C3	-2.06	105.88	110.15
5	L	6	MAN	O2-C2-C3	-2.06	105.89	110.15
5	L	3	BMA	C1-O5-C5	2.01	114.89	112.19

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	4	MAN	C4-C5-C6-O6
8	P	2	NAG	O5-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
8	R	1	NAG	O5-C5-C6-O6
8	R	2	NAG	O5-C5-C6-O6
9	N	1	NAG	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
9	N	1	NAG	C4-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
9	N	2	NAG	C4-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
8	M	1	NAG	O5-C5-C6-O6
4	S	3	BMA	O5-C5-C6-O6
8	Q	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	N	2	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
8	P	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
8	R	1	NAG	C4-C5-C6-O6
4	S	3	BMA	C4-C5-C6-O6
8	M	1	NAG	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
8	Q	2	NAG	C4-C5-C6-O6
8	Q	1	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
5	O	3	BMA	C4-C5-C6-O6
8	R	2	NAG	C4-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
7	J	2	NAG	C4-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	L	7	MAN	C4-C5-C6-O6
5	L	7	MAN	O5-C5-C6-O6
8	M	2	NAG	C4-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6
5	H	5	MAN	C4-C5-C6-O6
8	P	1	NAG	C4-C5-C6-O6
7	J	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
8	M	2	NAG	O5-C5-C6-O6
8	Q	1	NAG	C4-C5-C6-O6
5	H	5	MAN	O5-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
8	M	2	NAG	C3-C2-N2-C7
8	R	2	NAG	C3-C2-N2-C7
4	G	2	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
8	P	1	NAG	O5-C5-C6-O6
6	I	5	MAN	C4-C5-C6-O6
4	S	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	S	2	NAG	C1-C2-N2-C7
5	H	2	NAG	C1-C2-N2-C7
8	M	2	NAG	C1-C2-N2-C7
8	R	1	NAG	C1-C2-N2-C7
8	R	2	NAG	C1-C2-N2-C7
6	I	4	MAN	C4-C5-C6-O6
5	L	6	MAN	C4-C5-C6-O6
5	O	5	MAN	C4-C5-C6-O6
4	K	3	BMA	C4-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	4	MAN	C1-C2-C3-C4-C5-O5
5	O	7	MAN	C1-C2-C3-C4-C5-O5

28 monomers are involved in 44 short contacts:

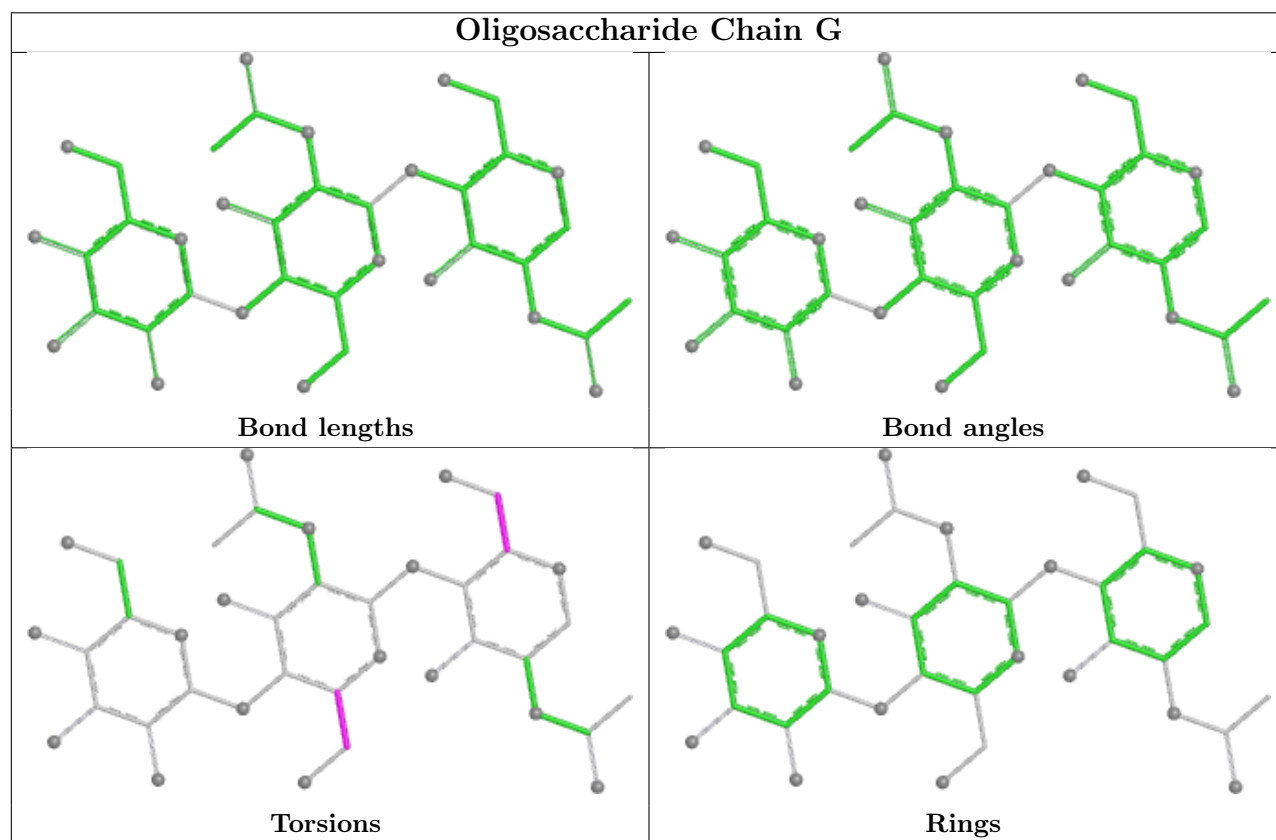
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3	BMA	1	0
8	M	2	NAG	9	0
7	J	3	BMA	2	0
4	G	1	NAG	1	0
5	O	6	MAN	1	0
7	J	1	NAG	1	0
4	S	1	NAG	3	0
8	R	2	NAG	2	0
5	O	7	MAN	3	0
8	Q	2	NAG	2	0
5	O	2	NAG	1	0
5	O	5	MAN	2	0
5	L	6	MAN	2	0
4	G	2	NAG	2	0
6	I	3	BMA	2	0
5	H	2	NAG	1	0
4	S	3	BMA	2	0
5	O	4	MAN	3	0
6	I	5	MAN	2	0
7	J	4	MAN	3	0
8	M	1	NAG	7	0
5	O	3	BMA	2	0
5	O	1	NAG	1	0

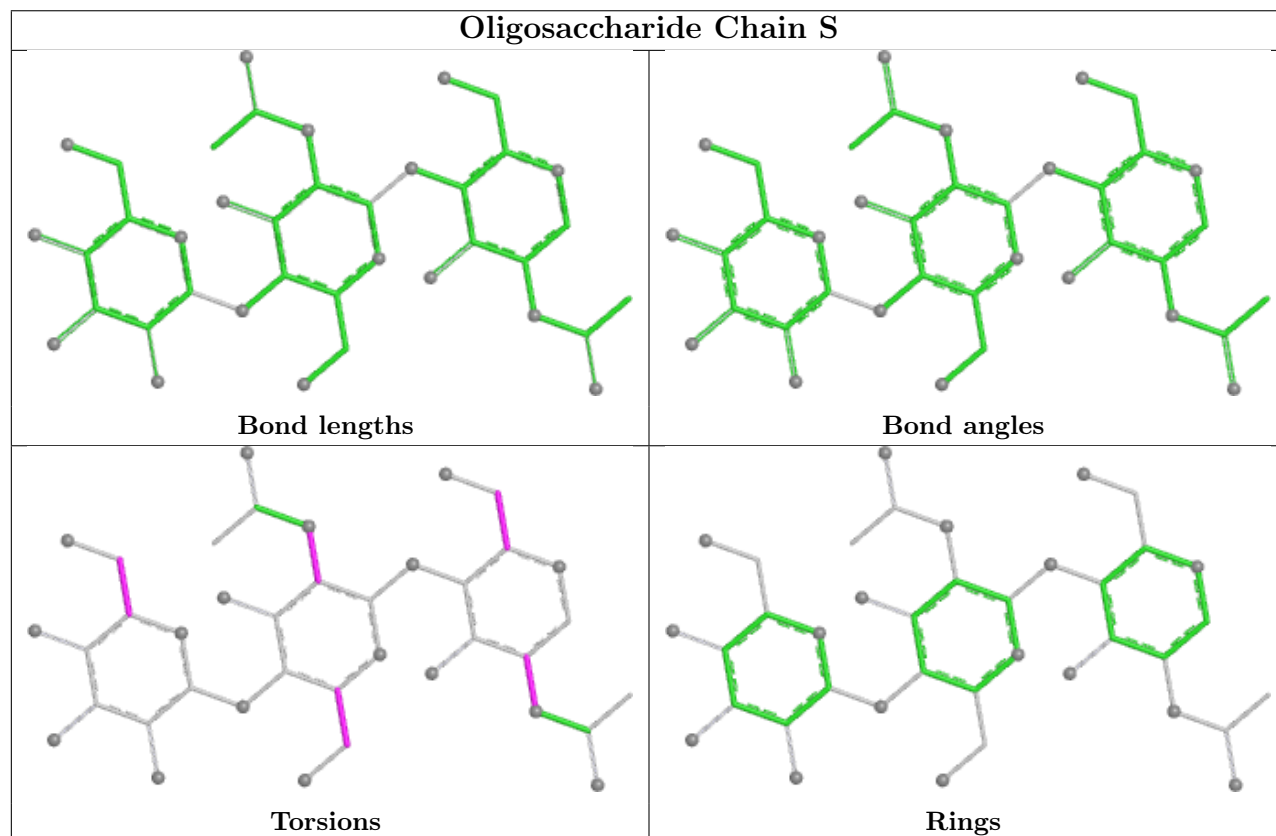
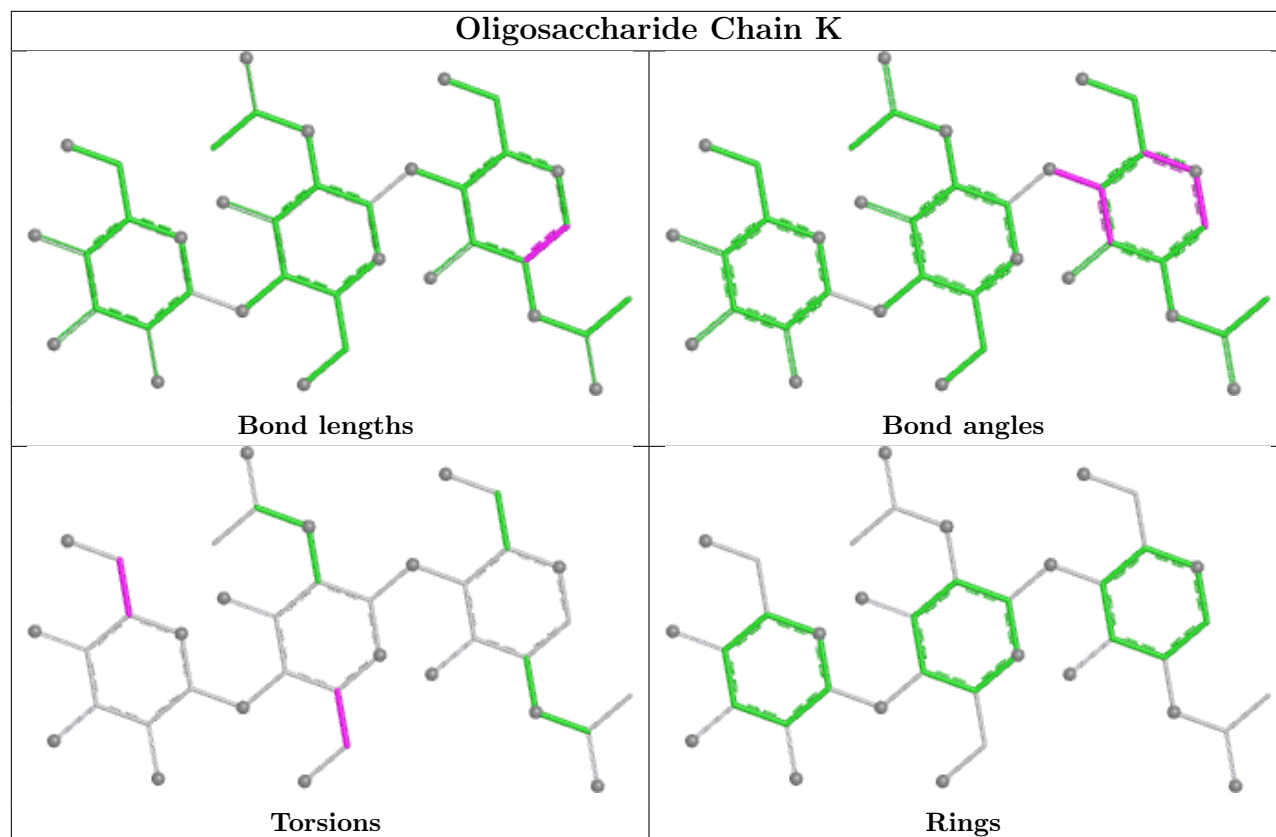
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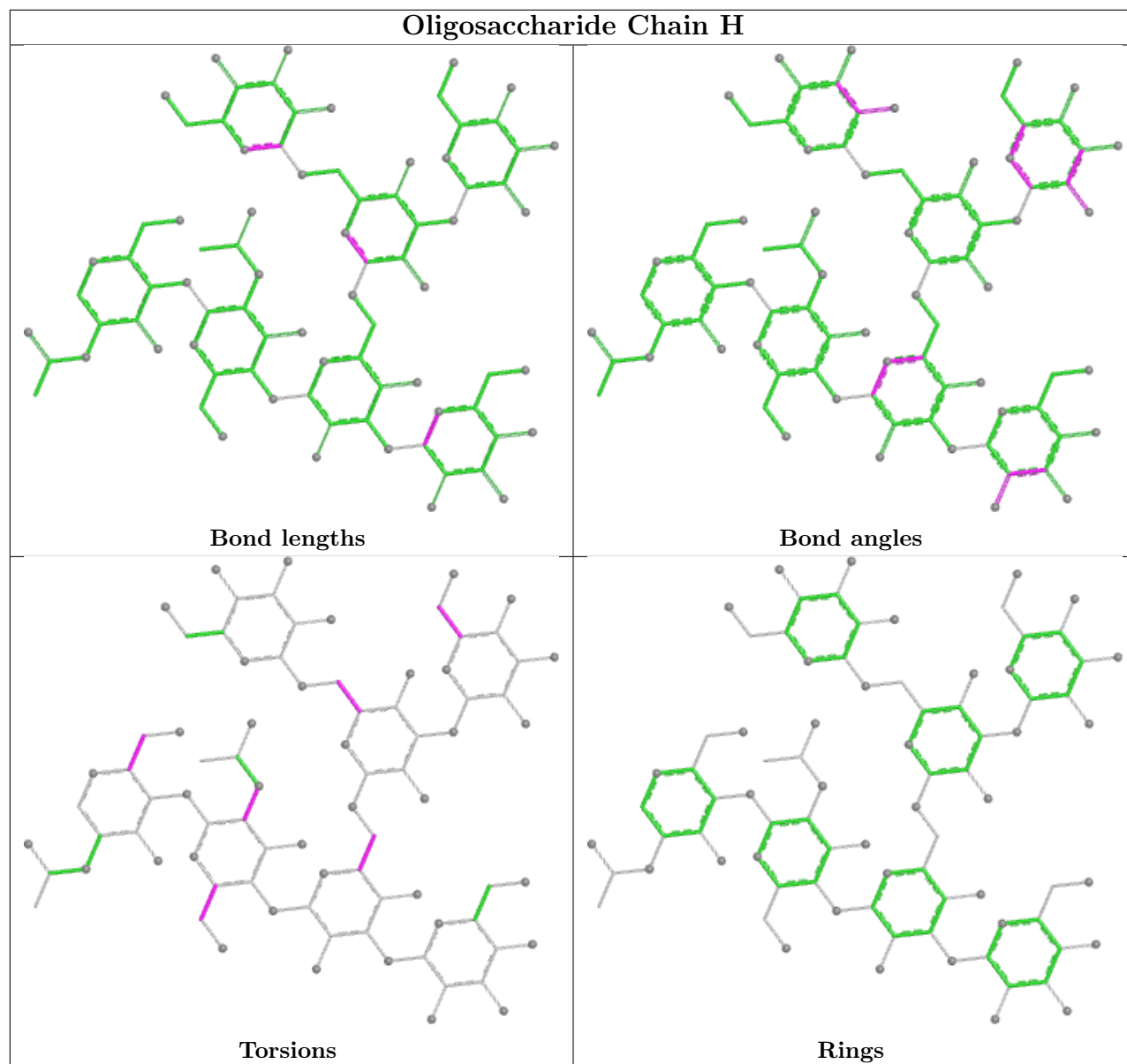
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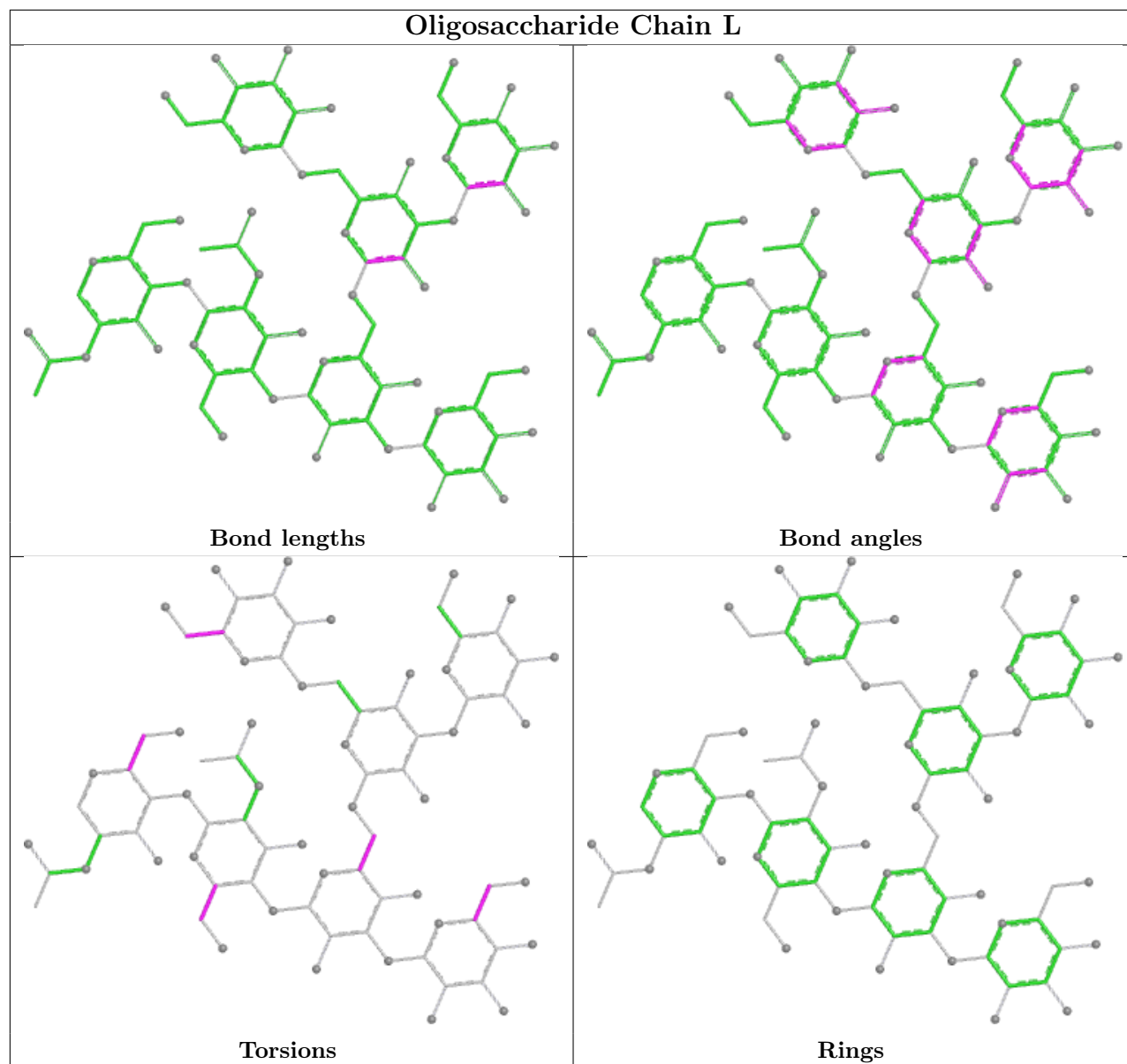
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	2	NAG	4	0
8	Q	1	NAG	2	0
8	R	1	NAG	4	0
5	L	1	NAG	1	0
5	L	4	MAN	2	0

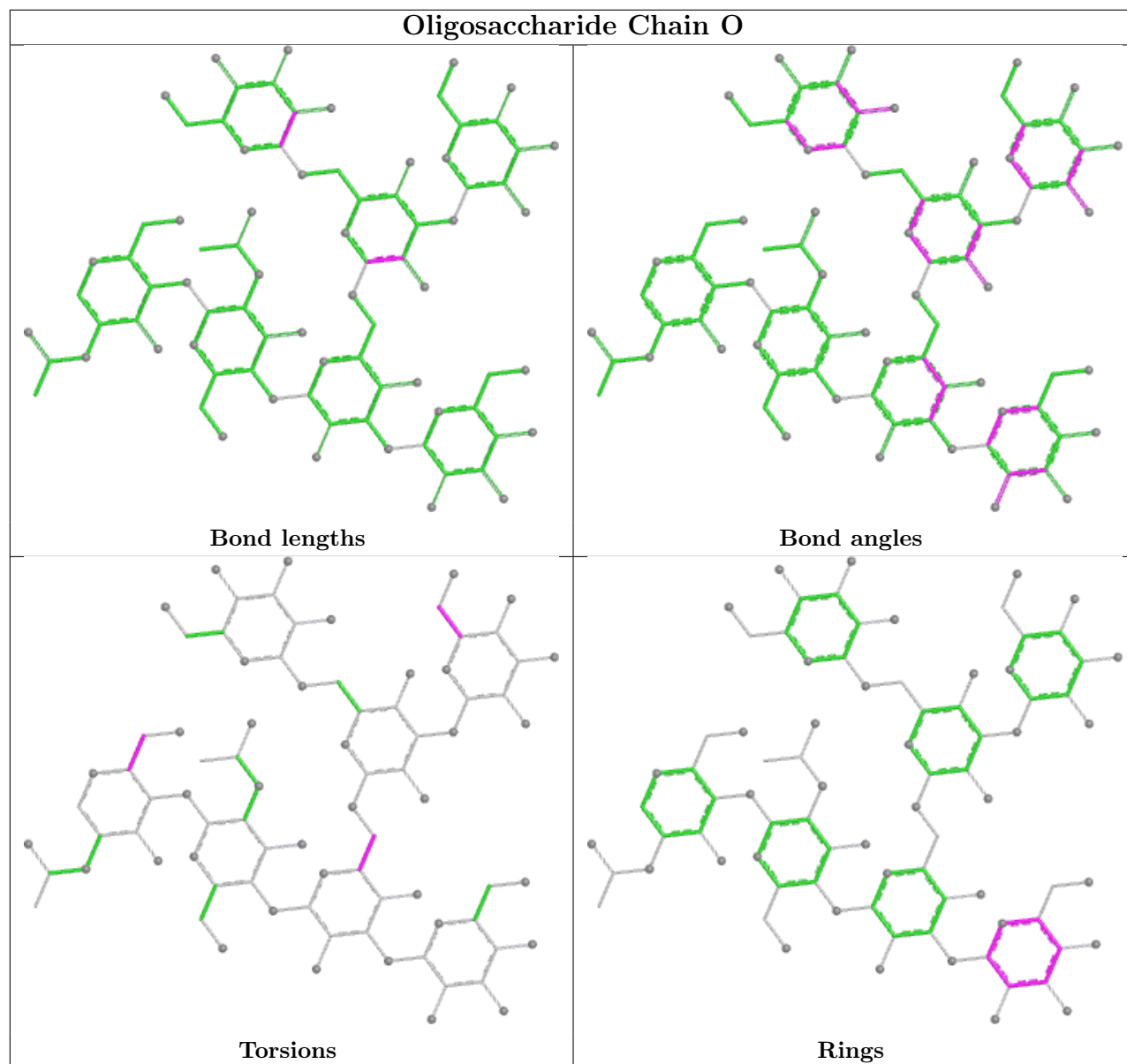
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

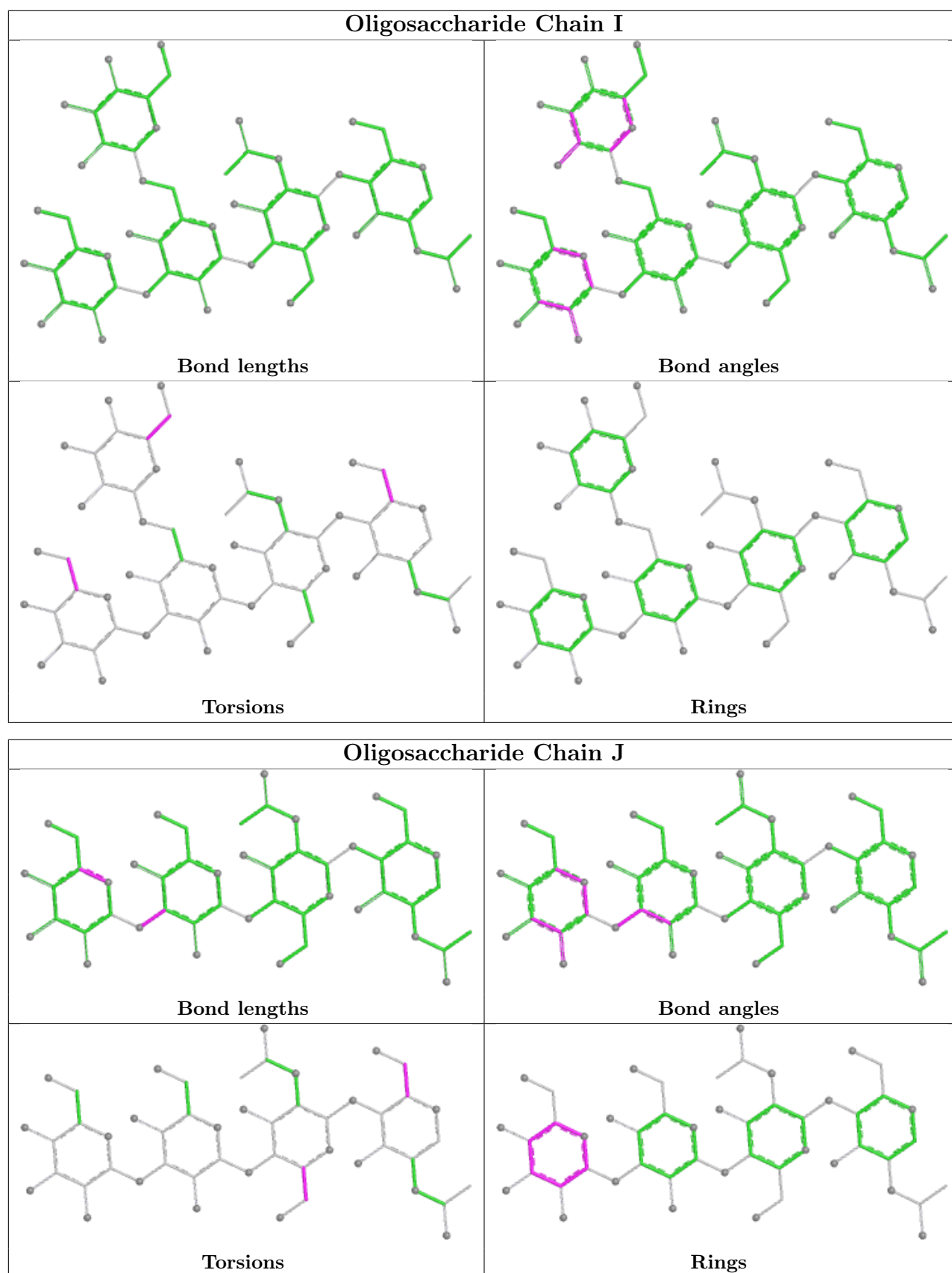


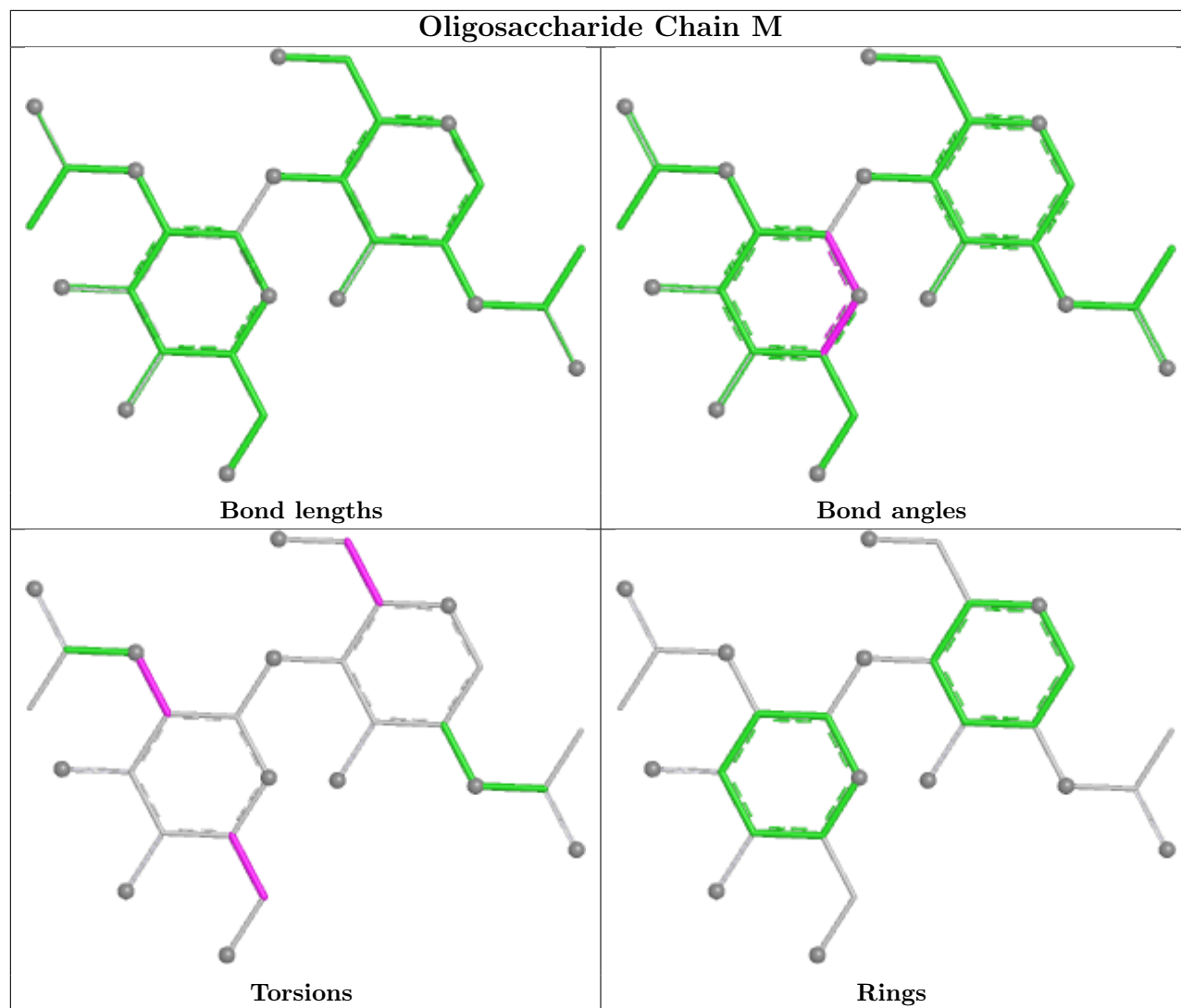


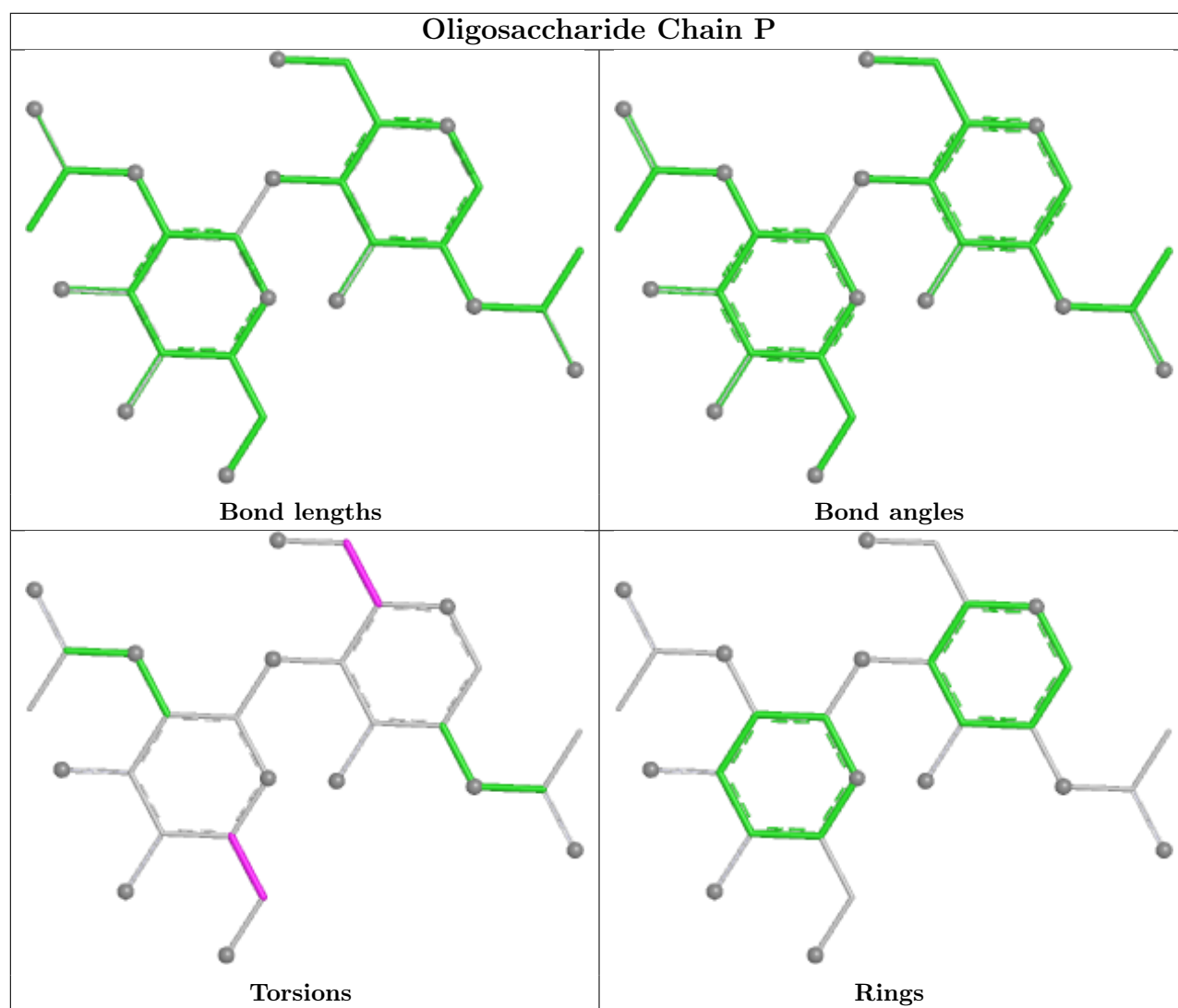


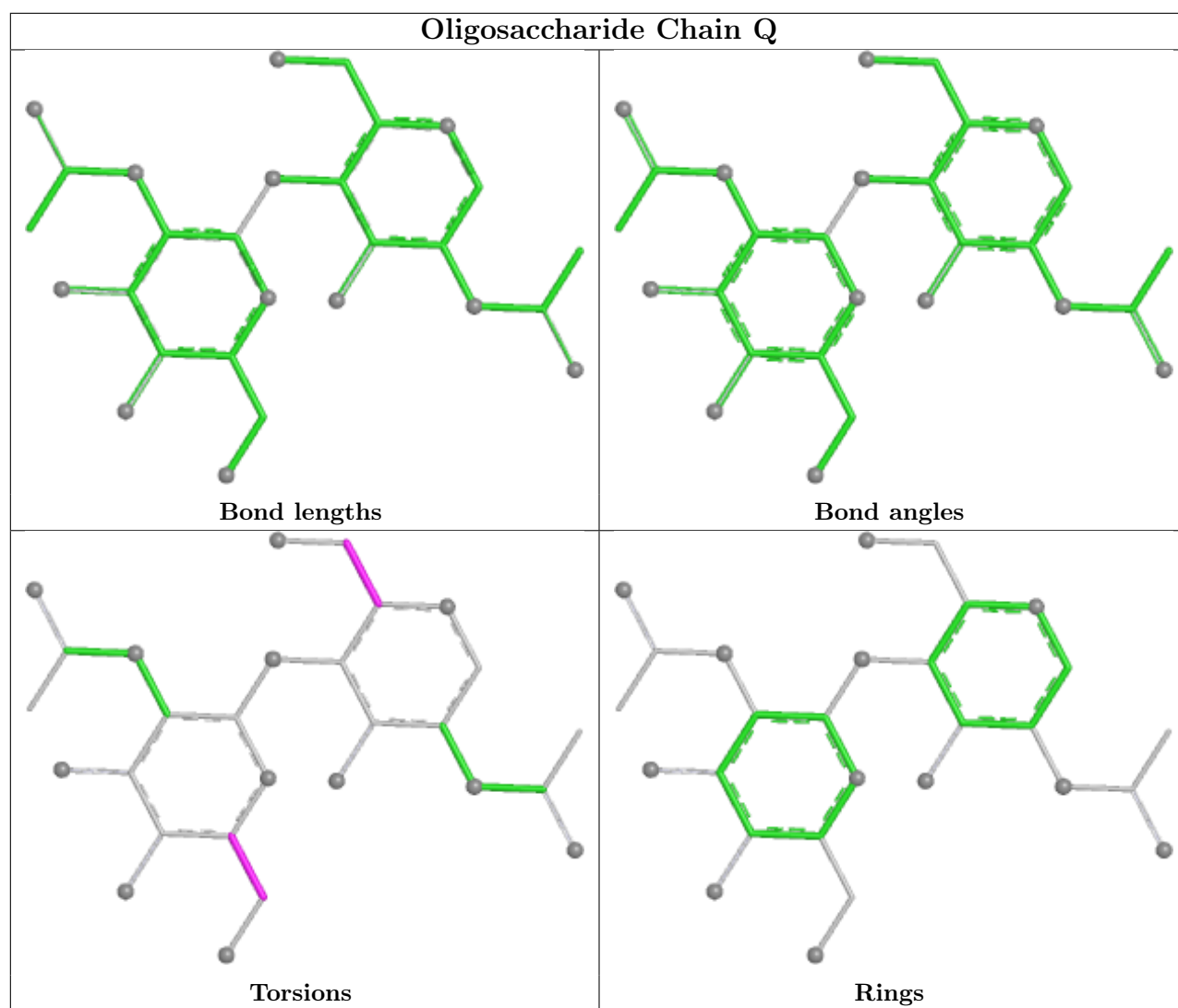


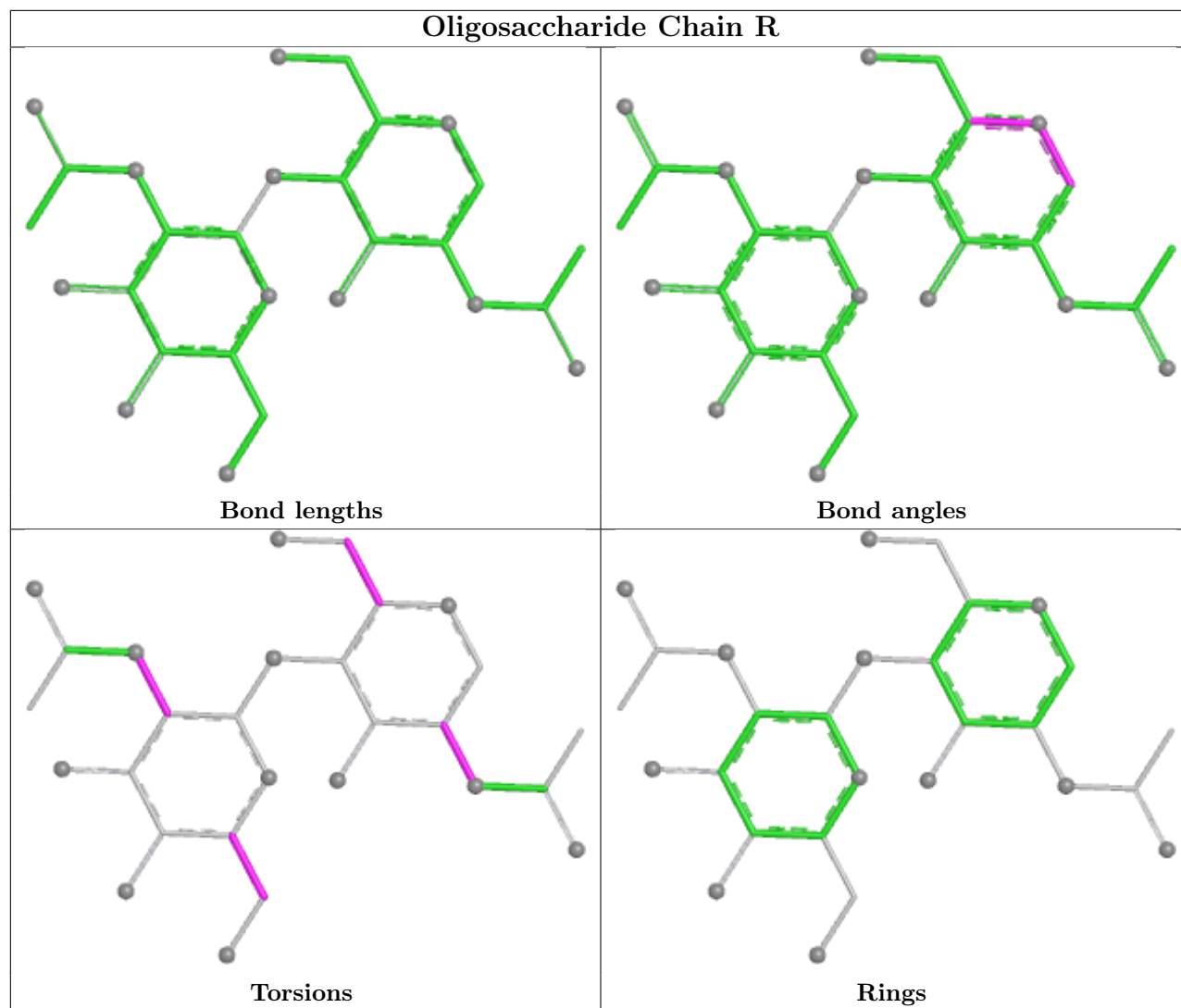


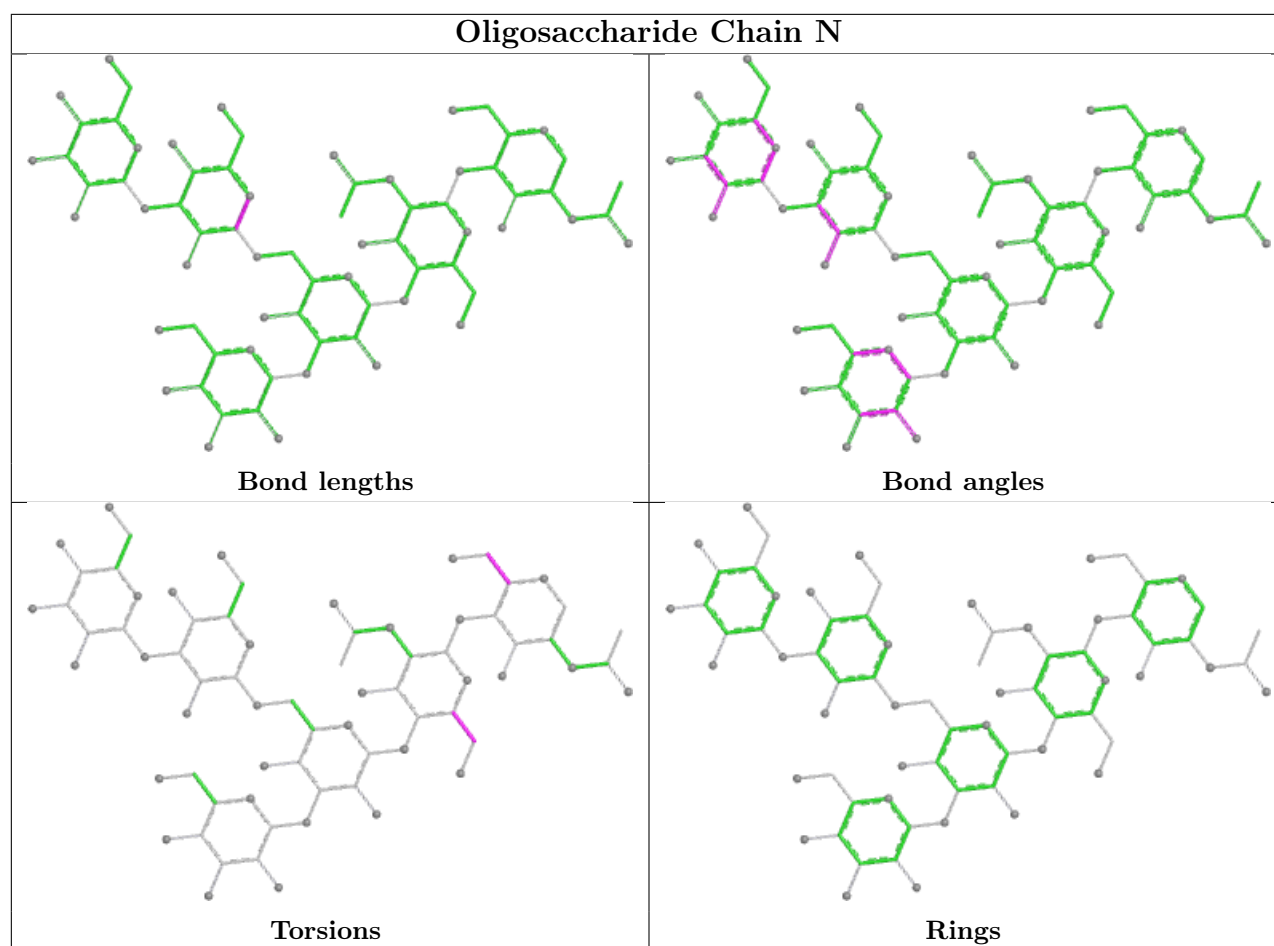












5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	NAG	A	2024	1	14,14,15	0.27	0	17,19,21	0.46	0
12	PEG	C	632	-	6,6,6	0.51	0	5,5,5	0.32	0
11	NAG	D	3201	2	14,14,15	0.24	0	17,19,21	0.34	0
12	PEG	A	2026	-	6,6,6	0.50	0	5,5,5	0.24	0
11	NAG	A	2025	1	14,14,15	0.25	0	17,19,21	0.45	0
14	GLY	C	601	-	3,3,4	0.60	0	1,2,4	0.33	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
11	NAG	A	2024	1	-	2/6/23/26	0/1/1/1
12	PEG	C	632	-	-	1/4/4/4	-
11	NAG	D	3201	2	-	4/6/23/26	0/1/1/1
12	PEG	A	2026	-	-	1/4/4/4	-
11	NAG	A	2025	1	-	2/6/23/26	0/1/1/1
14	GLY	C	601	-	-	0/0/1/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2024	NAG	O5-C5-C6-O6
11	A	2024	NAG	C4-C5-C6-O6
11	A	2025	NAG	C4-C5-C6-O6
11	A	2025	NAG	O5-C5-C6-O6
11	D	3201	NAG	O5-C5-C6-O6
12	A	2026	PEG	C1-C2-O2-C3
11	D	3201	NAG	C3-C2-N2-C7
12	C	632	PEG	C1-C2-O2-C3
11	D	3201	NAG	C1-C2-N2-C7
11	D	3201	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	632	PEG	1	0
11	D	3201	NAG	1	0
14	C	601	GLY	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	A	598/598 (100%)	0.56	29 (4%)	35 30	64, 102, 170, 252	0
1	C	596/598 (99%)	0.55	28 (4%)	36 31	63, 96, 144, 244	0
2	B	310/421 (73%)	1.10	38 (12%)	8 6	76, 173, 241, 303	0
2	D	330/421 (78%)	0.99	30 (9%)	15 12	75, 150, 220, 288	0
3	E	10/11 (90%)	2.30	5 (50%)	0 0	102, 118, 135, 135	0
3	F	9/11 (81%)	3.15	7 (77%)	0 0	102, 114, 151, 153	0
All	All	1853/2060 (89%)	0.74	137 (7%)	20 16	63, 112, 214, 303	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	222	HIS	6.5
3	E	222	HIS	5.7
2	B	95	LEU	5.5
1	A	487	VAL	5.2
1	C	596	THR	5.1
2	B	72	ILE	4.7
3	F	214	ARG	4.7
1	A	597	GLY	4.7
1	C	29	SER	4.6
1	A	596	THR	4.2
1	A	598	GLY	4.1
2	B	109	TYR	4.0
3	E	213	GLY	3.5
1	C	30	ALA	3.4
1	C	64	THR	3.3
2	D	354	VAL	3.3
3	F	220	THR	3.3
1	C	324	GLY	3.3
1	A	462	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	107	LEU	3.2
1	A	64	THR	3.2
1	A	32	SER	3.2
2	B	165	ILE	3.2
3	E	214	ARG	3.1
3	F	221	ILE	3.1
2	B	137	PHE	3.1
2	B	361	ILE	3.1
1	A	98	VAL	3.1
1	C	479	CYS	3.1
3	F	218	LEU	3.0
2	B	259	CYS	3.0
2	B	335	VAL	3.0
2	B	359	PHE	3.0
2	B	142	PHE	3.0
2	B	418	LYS	2.9
1	C	325	ASP	2.9
2	D	421	ILE	2.9
2	B	388	PHE	2.9
2	D	127	VAL	2.9
3	F	219	ALA	2.9
2	D	336	VAL	2.8
2	D	72	ILE	2.8
1	A	397	ALA	2.8
1	A	583	THR	2.8
2	B	348	VAL	2.8
2	D	103	TYR	2.8
1	A	479	CYS	2.8
1	A	29	SER	2.8
2	D	315	LEU	2.8
2	B	135	MET	2.8
2	D	217	ALA	2.8
2	B	138	PHE	2.8
1	A	66	ARG	2.8
2	B	408	ILE	2.7
1	C	309	LEU	2.7
1	A	189	ALA	2.7
1	A	63	SER	2.7
1	C	442	ILE	2.7
1	C	555	PRO	2.7
2	D	157	TYR	2.7
2	D	359	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	410	PRO	2.6
1	C	166	ALA	2.6
1	C	31	SER	2.6
2	D	411	ILE	2.6
1	C	211	ARG	2.5
2	D	394	MET	2.5
2	B	237	LEU	2.5
2	D	111	VAL	2.5
1	A	565	ASP	2.5
1	C	512	ALA	2.5
2	D	92	ASN	2.5
1	A	257	ASP	2.5
1	C	273	ALA	2.5
2	B	417	ALA	2.5
2	D	160	ILE	2.4
3	E	218	LEU	2.4
1	C	473	CYS	2.4
2	D	166	HIS	2.4
2	B	394	MET	2.4
1	A	30	ALA	2.4
1	A	62	SER	2.4
2	B	277	THR	2.4
1	A	31	SER	2.4
2	B	144	LEU	2.4
2	B	342	LEU	2.4
2	D	99	PRO	2.4
1	A	553	LEU	2.3
1	A	566	TYR	2.3
2	B	405	TYR	2.3
2	D	169	CYS	2.3
1	C	299	LEU	2.3
2	D	361	ILE	2.3
2	B	272	TYR	2.3
2	B	141	ASP	2.3
2	B	390	VAL	2.3
2	D	239	LEU	2.3
2	B	275	SER	2.3
1	C	28	PRO	2.3
1	A	595	LEU	2.3
2	D	377	CYS	2.3
2	D	93	PHE	2.3
2	D	405	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	103	ASP	2.3
1	C	322	ALA	2.2
3	E	221	ILE	2.2
2	D	172	TYR	2.2
1	C	167	ASP	2.2
2	B	139	SER	2.2
2	D	205	SER	2.2
2	B	392	VAL	2.2
1	C	144	SER	2.2
1	C	323	SER	2.2
2	B	283	LEU	2.2
2	D	380	VAL	2.2
1	A	401	CYS	2.2
1	C	65	ARG	2.2
1	C	20	GLY	2.2
1	C	201	SER	2.2
2	D	341	LYS	2.2
1	A	55	GLN	2.2
1	C	41	PRO	2.1
1	A	58	LYS	2.1
2	B	318	GLY	2.1
1	A	167	ASP	2.1
1	C	146	ASP	2.1
2	B	276	THR	2.1
2	D	223	VAL	2.1
1	A	96	ALA	2.1
2	D	347	LYS	2.1
1	A	95	GLY	2.1
2	B	216	ASP	2.0
2	B	364	ILE	2.0
3	F	216	GLY	2.0
2	D	358	TYR	2.0
2	B	331	LEU	2.0
2	B	172	TYR	2.0

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

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

6.3 Carbohydrates

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.

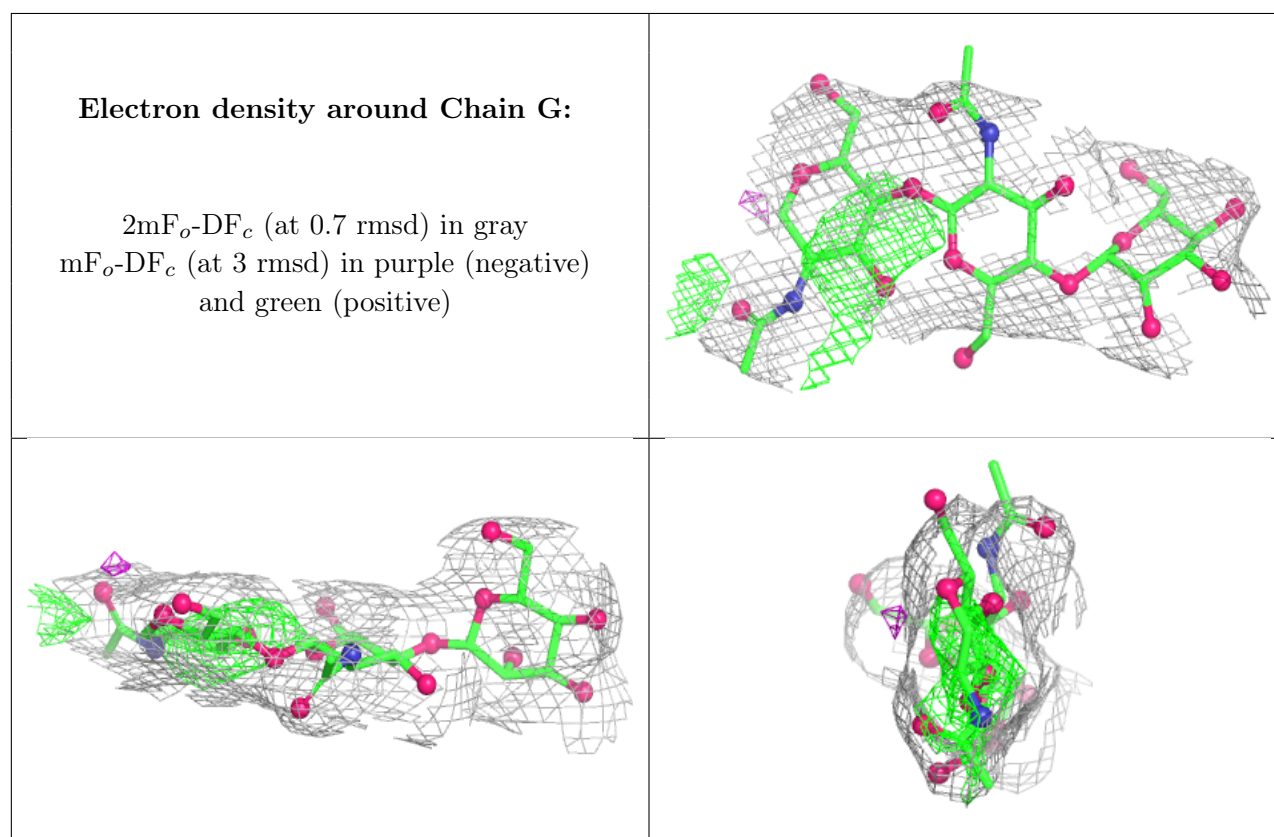
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	K	3	11/12	0.11	0.12	207,209,211,211	0
4	BMA	S	3	11/12	0.24	0.13	182,186,187,188	0
4	NAG	K	2	14/15	0.31	0.17	215,219,221,223	0
8	NAG	M	1	14/15	0.45	0.18	122,133,145,152	0
8	NAG	M	2	14/15	0.48	0.19	155,156,158,159	0
4	NAG	S	2	14/15	0.51	0.14	192,197,201,203	0
5	MAN	L	4	11/12	0.52	0.13	151,152,153,154	0
5	MAN	L	7	11/12	0.52	0.13	152,153,154,154	0
8	NAG	Q	1	14/15	0.54	0.19	136,157,164,171	0
5	MAN	L	5	11/12	0.55	0.13	143,151,154,154	0
8	NAG	R	2	14/15	0.55	0.17	199,201,204,206	0
4	NAG	K	1	14/15	0.62	0.16	215,227,231,231	0
5	MAN	O	5	11/12	0.62	0.17	123,124,125,125	0
4	NAG	S	1	14/15	0.63	0.15	184,201,212,214	0
5	MAN	O	7	11/12	0.63	0.20	117,123,125,126	0
8	NAG	Q	2	14/15	0.66	0.13	175,178,180,180	0
4	BMA	G	3	11/12	0.66	0.10	135,136,138,139	0
8	NAG	R	1	14/15	0.68	0.19	206,211,213,214	0
9	MAN	N	5	11/12	0.71	0.15	121,124,126,127	0
7	BMA	J	3	11/12	0.72	0.14	115,116,118,118	0
5	MAN	L	6	11/12	0.75	0.19	151,152,153,155	0
7	MAN	J	4	11/12	0.75	0.17	113,116,120,120	0
5	MAN	H	6	11/12	0.75	0.18	83,90,94,95	0
5	MAN	O	6	11/12	0.76	0.23	132,138,140,141	0
9	MAN	N	6	11/12	0.76	0.12	108,109,111,111	0
8	NAG	P	1	14/15	0.77	0.18	99,105,110,111	0
4	NAG	G	2	14/15	0.78	0.14	133,135,137,137	0
8	NAG	P	2	14/15	0.79	0.16	109,110,111,113	0
5	BMA	L	3	11/12	0.81	0.08	143,145,150,151	0
5	BMA	O	3	11/12	0.81	0.14	109,112,120,120	0
5	MAN	O	4	11/12	0.81	0.15	121,122,124,127	0
6	MAN	I	4	11/12	0.81	0.22	112,114,115,117	0
5	NAG	O	2	14/15	0.82	0.17	109,114,117,118	0
9	NAG	N	2	14/15	0.82	0.16	82,90,94,95	0
5	NAG	L	2	14/15	0.83	0.16	126,129,135,139	0
5	MAN	H	5	11/12	0.83	0.17	88,90,94,96	0
6	BMA	I	3	11/12	0.84	0.11	100,102,105,109	0

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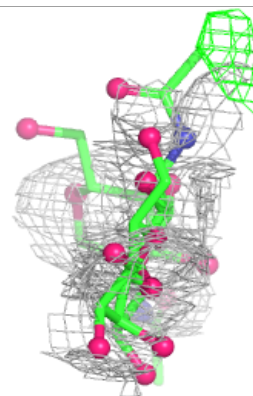
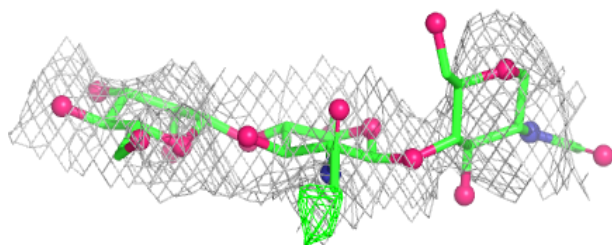
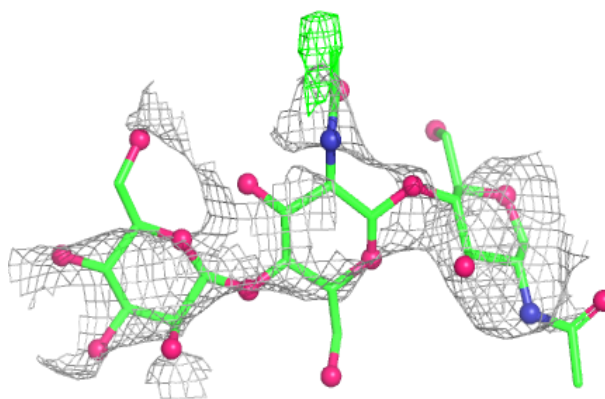
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MAN	N	4	11/12	0.84	0.11	107,111,115,118	0
5	BMA	H	3	11/12	0.85	0.10	85,87,91,93	0
7	NAG	J	1	14/15	0.85	0.15	101,111,115,119	0
5	MAN	H	7	11/12	0.85	0.14	95,96,97,97	0
4	NAG	G	1	14/15	0.85	0.18	122,127,127,132	0
6	MAN	I	5	11/12	0.87	0.12	94,97,100,100	0
5	NAG	O	1	14/15	0.88	0.15	83,99,107,108	0
5	MAN	H	4	11/12	0.89	0.15	80,84,87,88	0
5	NAG	H	2	14/15	0.90	0.11	85,88,90,91	0
9	BMA	N	3	11/12	0.90	0.09	97,103,107,108	0
6	NAG	I	2	14/15	0.90	0.14	91,95,97,99	0
5	NAG	H	1	14/15	0.90	0.12	82,91,96,99	0
5	NAG	L	1	14/15	0.90	0.14	110,116,119,122	0
7	NAG	J	2	14/15	0.91	0.12	111,113,114,115	0
6	NAG	I	1	14/15	0.92	0.16	76,84,90,97	0
9	NAG	N	1	14/15	0.93	0.11	75,80,83,88	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.

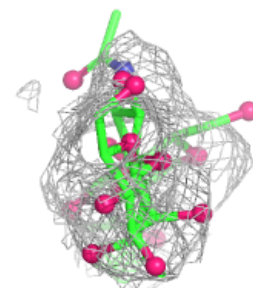
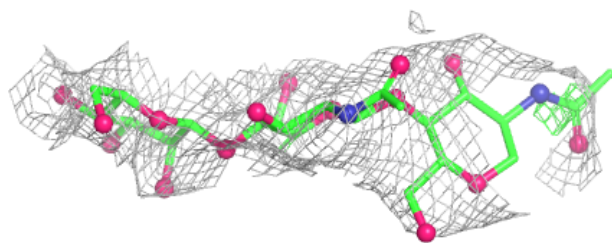
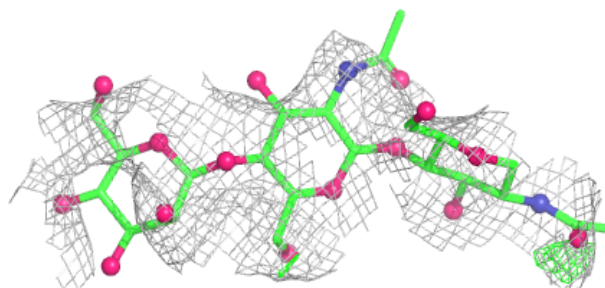


Electron density around Chain K:

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

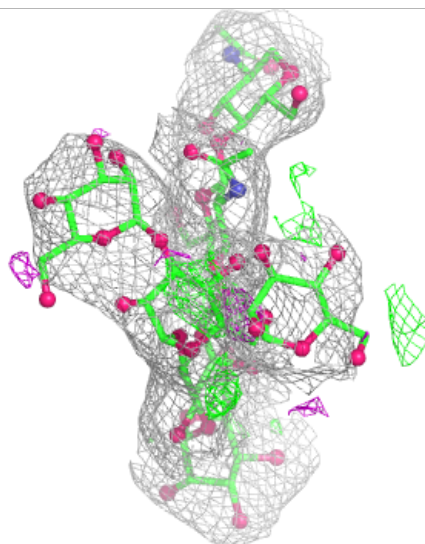
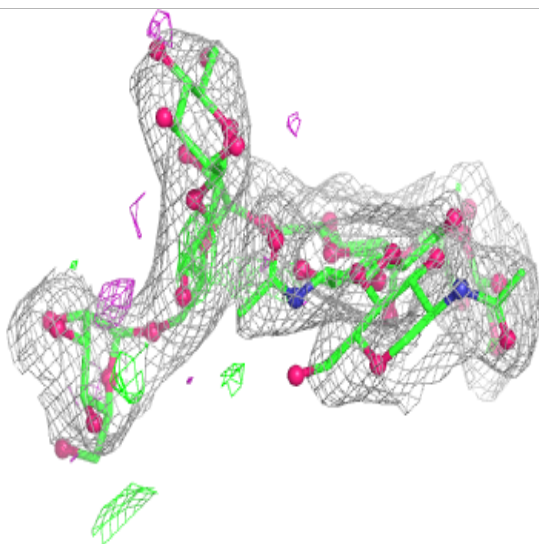
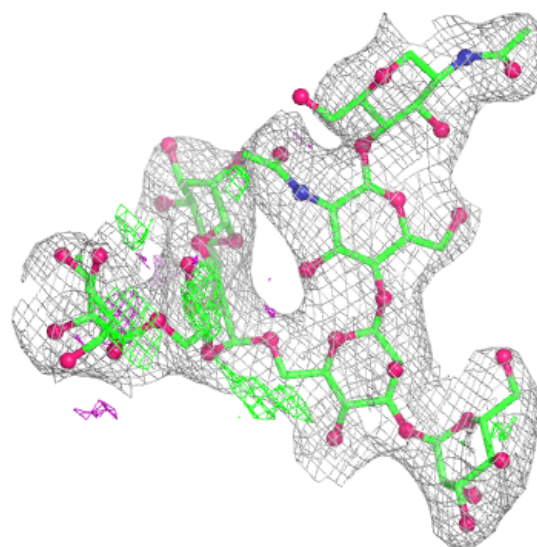
**Electron density around Chain S:**

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



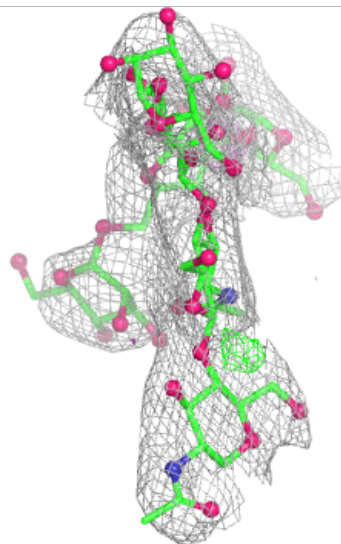
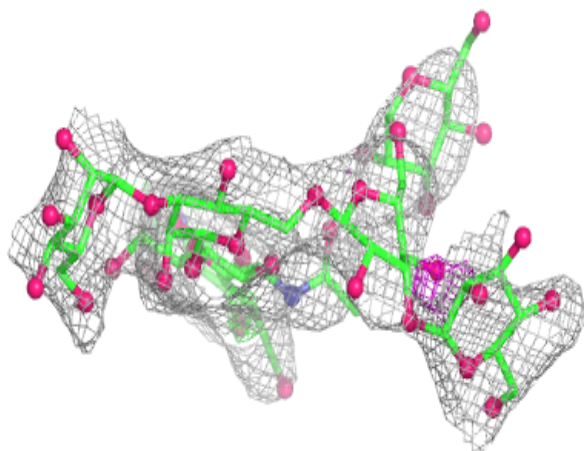
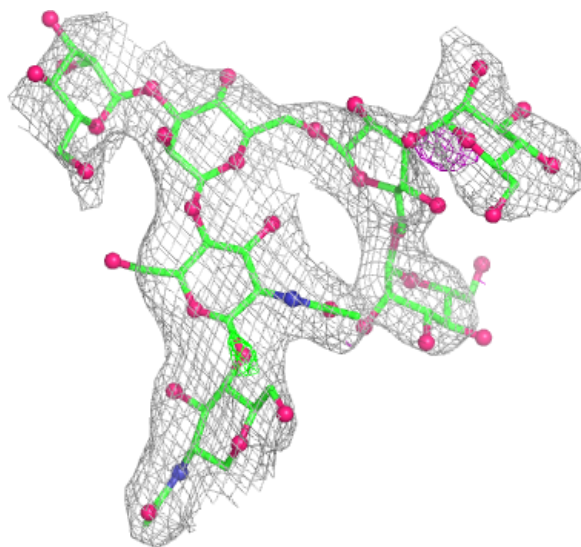
Electron density around Chain H:

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



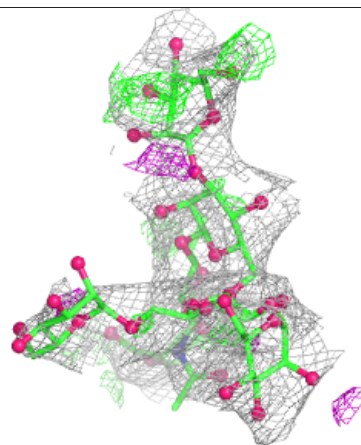
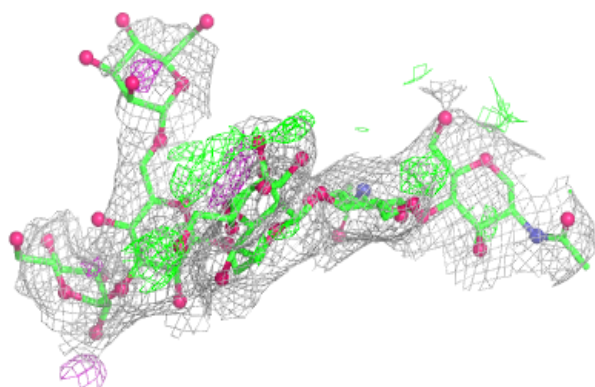
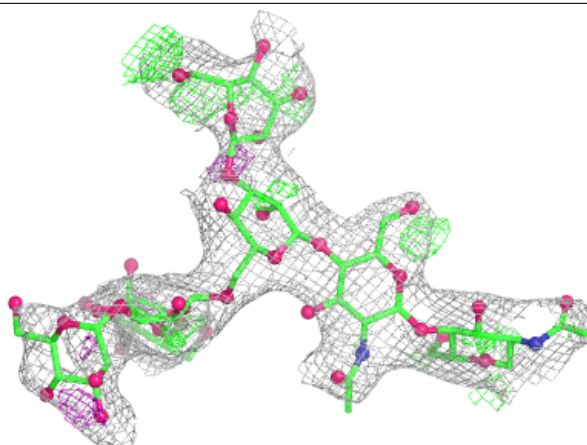
Electron density around Chain L:

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

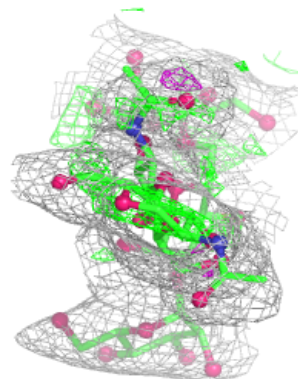
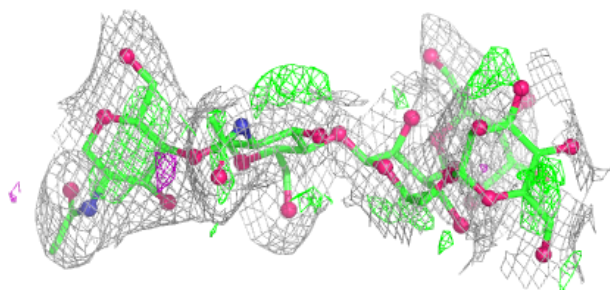
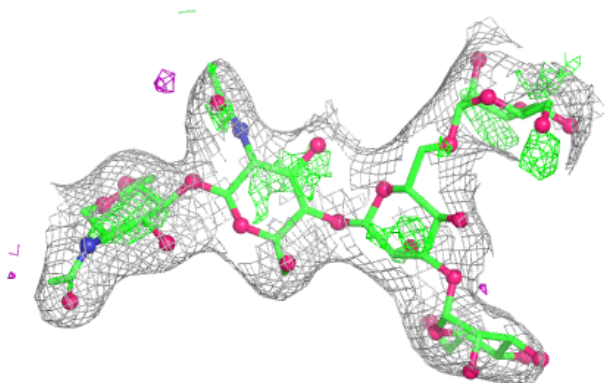


Electron density around Chain O:

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

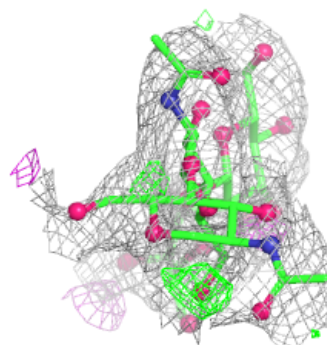
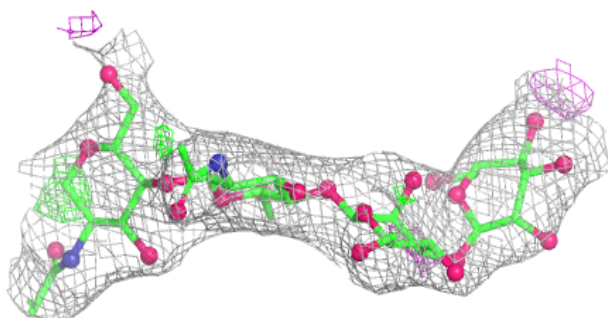
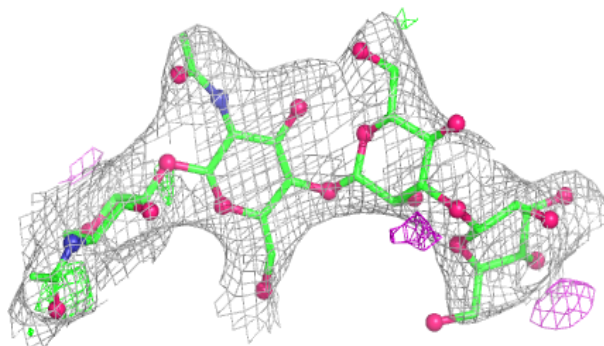
**Electron density around Chain I:**

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

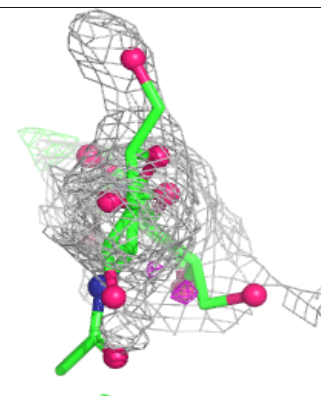
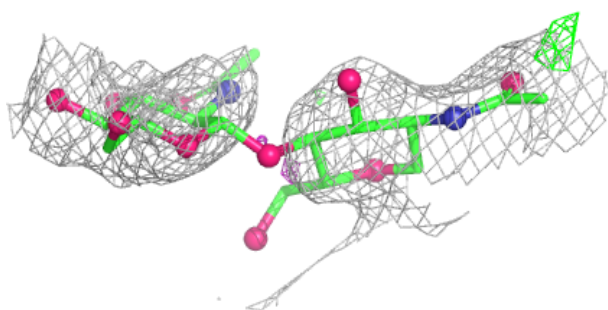
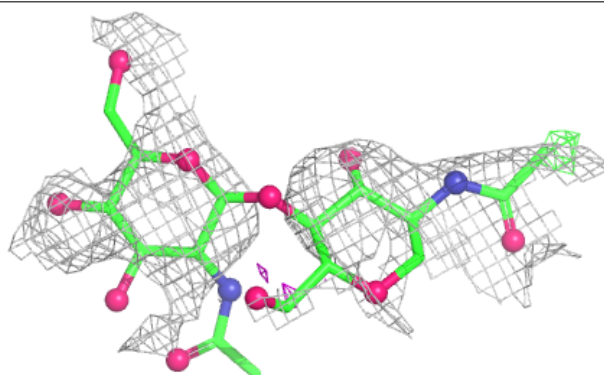


Electron density around Chain J:

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

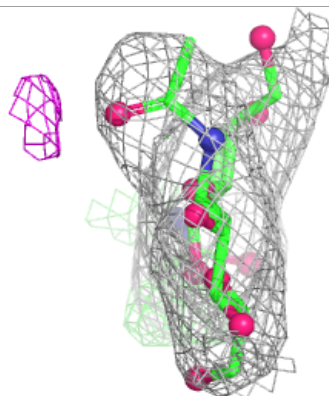
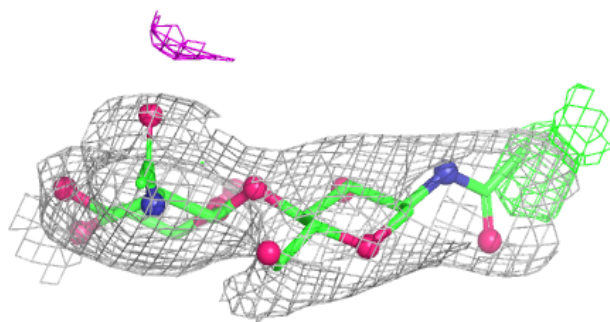
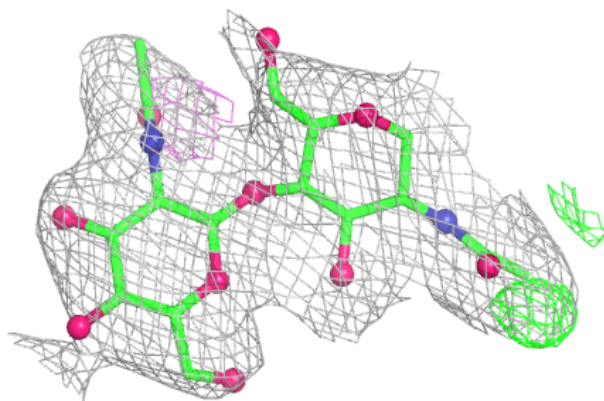
**Electron density around Chain M:**

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

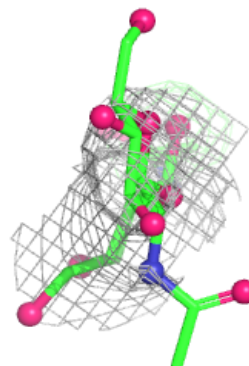
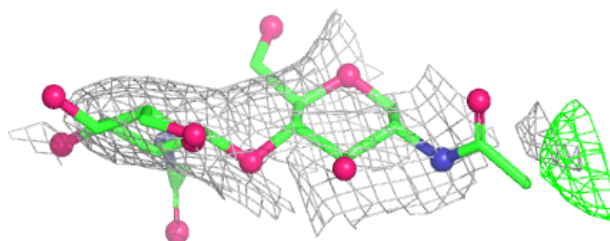
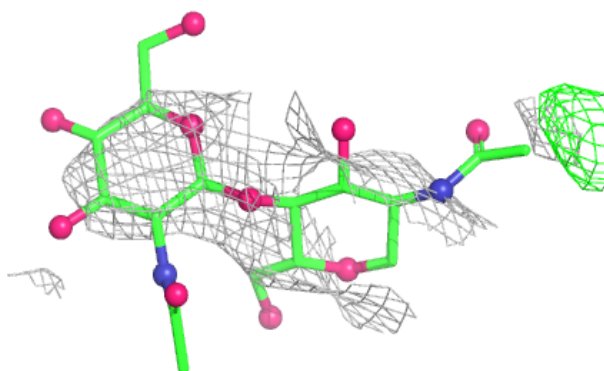


Electron density around Chain P:

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

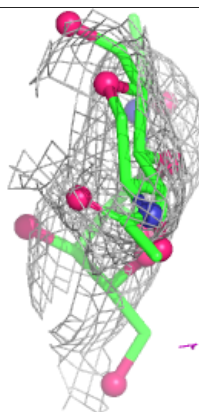
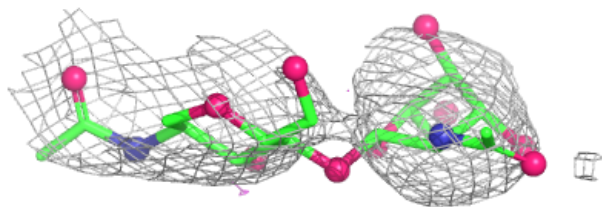
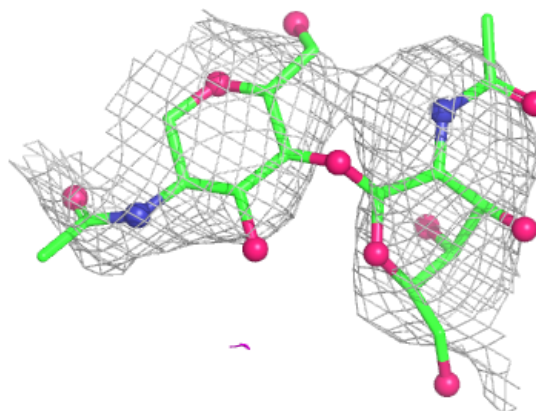
**Electron density around Chain Q:**

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

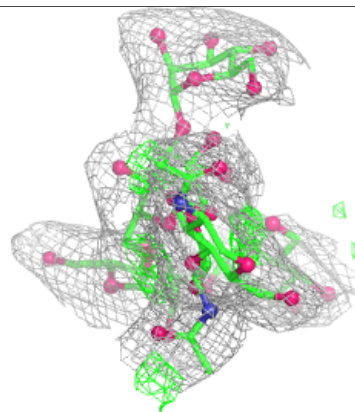
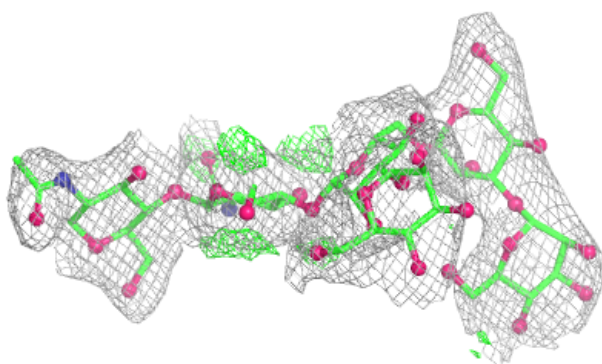
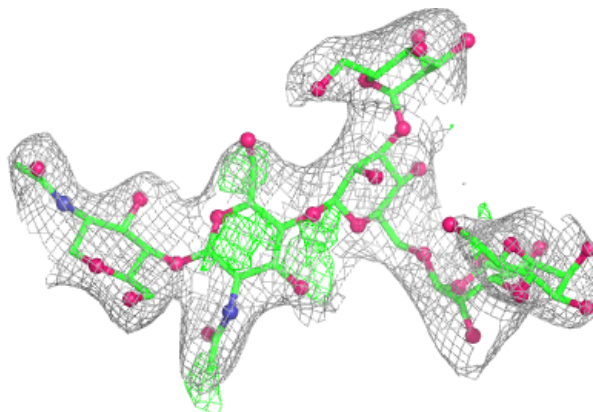


Electron density around Chain R:

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

**Electron density around Chain N:**

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
11	NAG	D	3201	14/15	0.46	0.16	189,202,212,212	0
14	GLY	C	601	4/5	0.58	0.29	102,102,103,104	0
11	NAG	A	2024	14/15	0.64	0.20	125,132,136,137	0
11	NAG	A	2025	14/15	0.70	0.14	104,122,126,128	0
12	PEG	C	632	7/7	0.82	0.24	75,77,78,79	0
12	PEG	A	2026	7/7	0.86	0.19	84,87,87,88	0
13	MG	D	3208	1/1	0.95	0.07	106,106,106,106	0
10	CA	B	2002	1/1	0.96	0.05	94,94,94,94	0
10	CA	D	3204	1/1	0.97	0.05	92,92,92,92	0
13	MG	B	2001	1/1	0.98	0.04	103,103,103,103	0
10	CA	A	2004	1/1	0.98	0.05	78,78,78,78	0
10	CA	C	604	1/1	0.98	0.04	66,66,66,66	0
10	CA	C	603	1/1	0.99	0.04	61,61,61,61	0
10	CA	A	2003	1/1	0.99	0.05	73,73,73,73	0
10	CA	C	605	1/1	0.99	0.06	82,82,82,82	0
10	CA	A	2001	1/1	0.99	0.02	69,69,69,69	0
10	CA	A	2002	1/1	0.99	0.04	70,70,70,70	0
10	CA	C	602	1/1	0.99	0.03	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.