



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:52 PM UTC

PDB ID : 6P7Y / pdb_00006p7y
Title : Crystal Structure of the Cedar henipavirus Attachment G Glycoprotein globular domain in complex with the receptor ephrin-B2
Authors : Xu, K.; Nikolov, D.B.; Xu, Y.
Deposited on : 2019-06-06
Resolution : 2.84 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

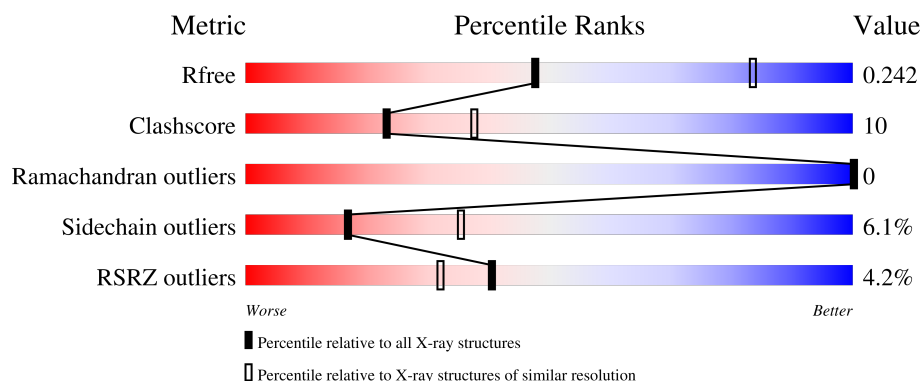
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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.



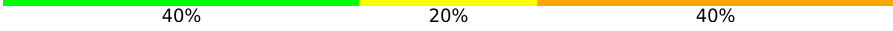
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	430	
1	C	430	
2	B	144	
2	D	144	
3	E	3	

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Mol	Chain	Length	Quality of chain
3	M	3	
4	F	3	
4	L	3	
5	G	7	
6	H	5	
6	I	5	
6	J	5	
6	K	5	
6	O	5	
7	N	4	

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
4	FUC	F	3	X	-	-	-
4	FUC	L	3	X	-	-	-
5	FUC	G	6	X	-	-	-
5	FUC	G	7	X	-	-	-
8	NAG	A	719	X	-	-	-
8	NAG	C	709	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 9852 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Attachment glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3441	2185	566	665	25			
1	C	430	Total	C	N	O	S	0	0	0
			3441	2185	566	665	25			

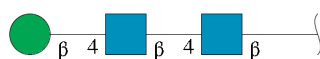
- Molecule 2 is a protein called Ephrin-B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	137	Total	C	N	O	S	0	0	0
			1098	704	177	210	7			
2	D	136	Total	C	N	O	S	0	0	0
			1093	701	176	209	7			

There are 2 discrepancies between the modelled and reference sequences:

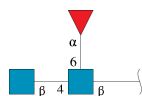
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	GLN	ASN	conflict	UNP P52799
D	36	GLN	ASN	conflict	UNP P52799

- Molecule 3 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.



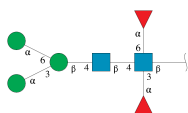
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O		0	0	0
			39	22	2	15				
3	M	3	Total	C	N	O		0	0	0
			39	22	2	15				

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



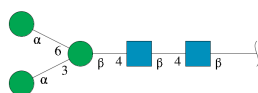
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	L	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 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)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	7	Total	C	N	O	0	0	0
			81	46	2	33			

- 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.



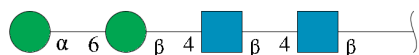
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	K	5	Total	C	N	O	0	0	0
			61	34	2	25			

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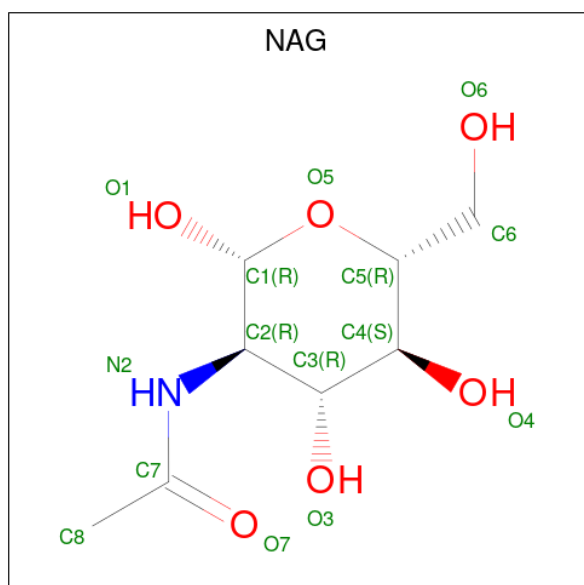
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	O	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is an oligosaccharide called 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
7	N	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

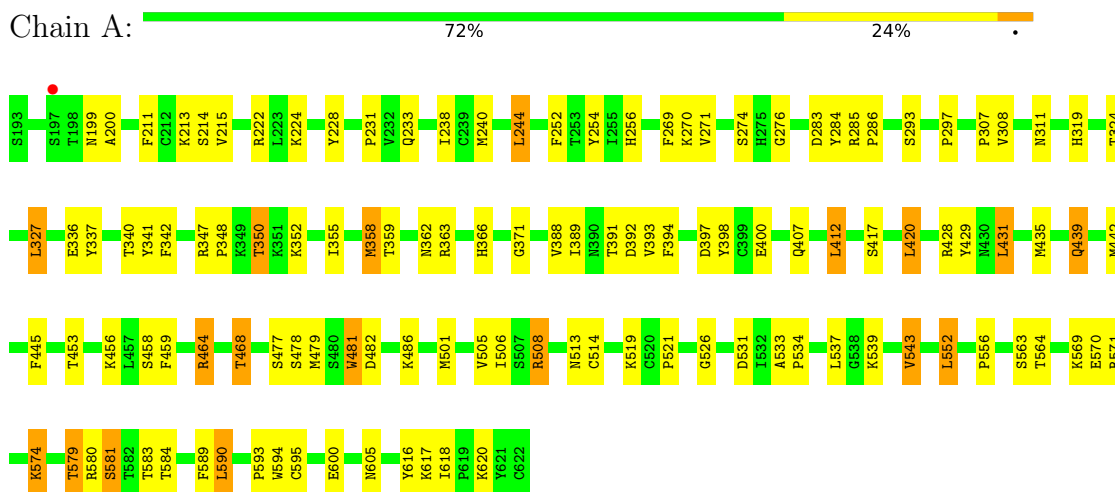
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	90	Total 90	O 90	0	0
9	B	11	Total 11	O 11	0	0
9	C	60	Total 60	O 60	0	0

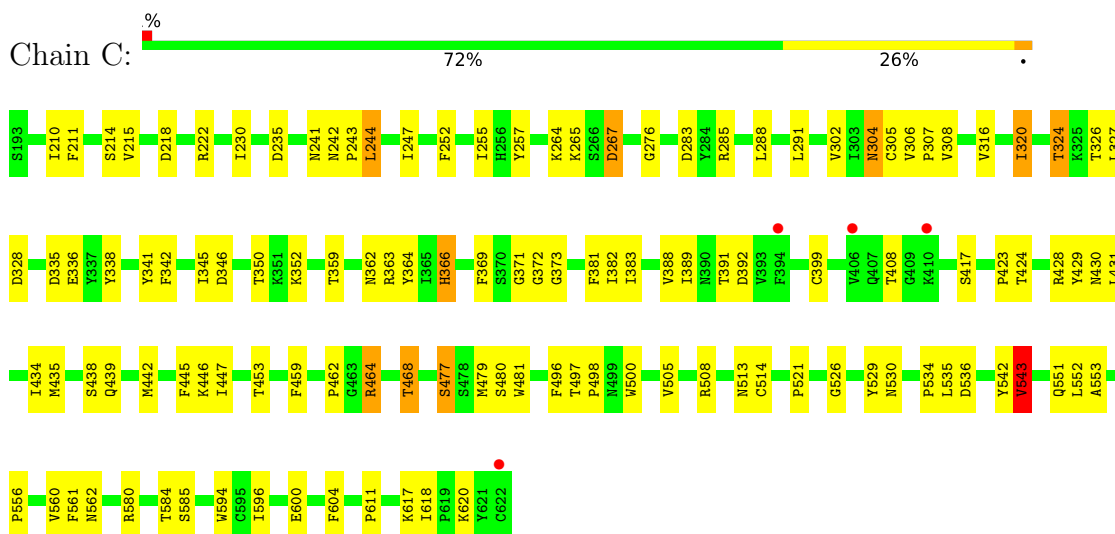
3 Residue-property plots

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: Attachment glycoprotein

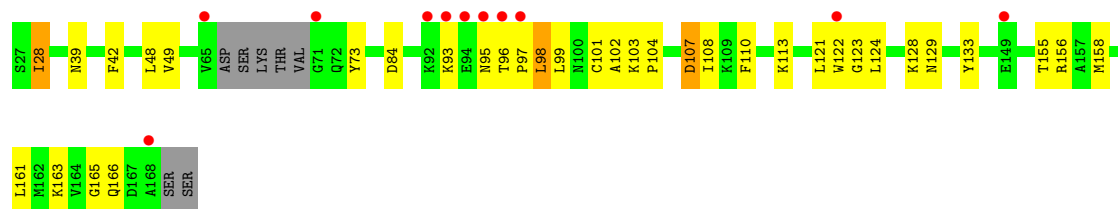


• Molecule 1: Attachment glycoprotein

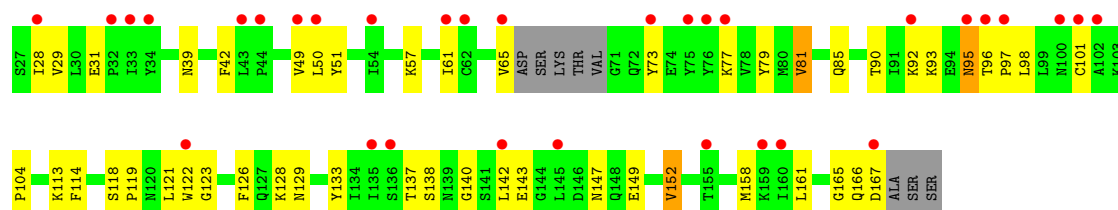


• Molecule 2: Ephrin-B2





• Molecule 2: Ephrin-B2



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



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



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

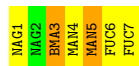


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

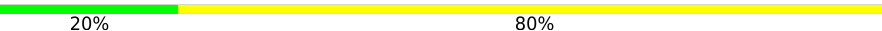


- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  14% 57% 29%

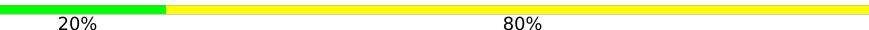


- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  20% 80%

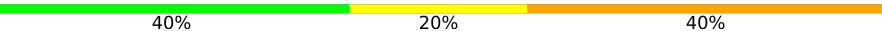


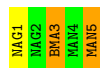
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  20% 80%

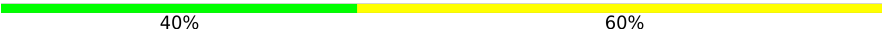


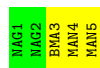
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  40% 20% 40%

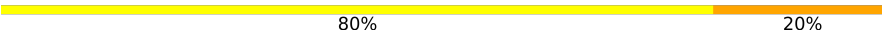


- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  40% 60%



- 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 O:  80% 20%



- Molecule 7: 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 N:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	207.02Å 207.02Å 120.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.97 – 2.84 45.97 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.97-2.84) 93.7 (45.97-2.84)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.207 , 0.240 0.208 , 0.242	Depositor DCC
R_{free} test set	1998 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9852	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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, FUC, MAN, 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	A	0.67	0/3528	1.01	7/4789 (0.1%)
1	C	0.61	0/3528	0.97	9/4789 (0.2%)
2	B	0.55	0/1120	0.99	3/1510 (0.2%)
2	D	0.41	0/1115	0.96	6/1503 (0.4%)
All	All	0.60	0/9291	0.99	25/12591 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	543	VAL	CB-CA-C	-7.52	99.96	111.31
1	C	604	PHE	N-CA-C	6.38	120.00	112.72
1	A	543	VAL	CB-CA-C	-6.37	101.69	111.31
1	C	618	ILE	CA-C-N	6.27	126.64	119.93
1	C	618	ILE	C-N-CA	6.27	126.64	119.93
1	C	291	LEU	N-CA-C	5.93	118.63	111.40
2	D	140	GLY	N-CA-C	-5.72	107.16	114.37
2	D	118	SER	CA-C-N	5.59	125.68	119.87
2	D	118	SER	C-N-CA	5.59	125.68	119.87
2	B	28	ILE	N-CA-C	5.58	115.63	108.82
1	C	371	GLY	N-CA-C	5.53	118.08	110.56
2	B	103	LYS	CA-C-N	5.41	125.02	119.56
2	B	103	LYS	C-N-CA	5.41	125.02	119.56
1	A	506	ILE	N-CA-C	5.40	116.05	109.30
1	A	552	LEU	N-CA-C	5.29	117.54	110.35
1	A	513	ASN	N-CA-C	5.19	117.68	111.71
1	C	513	ASN	N-CA-C	5.16	117.64	111.71
1	A	564	THR	N-CA-C	5.16	118.03	111.69
1	A	371	GLY	N-CA-C	5.14	117.56	110.56
1	C	304	ASN	N-CA-C	5.11	116.61	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	61	ILE	N-CA-C	5.09	115.23	108.11
2	D	123	GLY	N-CA-C	-5.05	107.64	115.67
1	C	342	PHE	N-CA-C	5.03	114.97	107.88
1	A	481	TRP	N-CA-C	5.02	117.48	111.71
2	D	98	LEU	N-CA-C	-5.01	105.73	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3441	0	3309	75	0
1	C	3441	0	3311	72	0
2	B	1098	0	1088	20	0
2	D	1093	0	1083	28	0
3	E	39	0	34	1	0
3	M	39	0	34	0	0
4	F	38	0	34	1	0
4	L	38	0	34	3	0
5	G	81	0	70	1	0
6	H	61	0	52	0	0
6	I	61	0	52	0	0
6	J	61	0	52	1	0
6	K	61	0	52	0	0
6	O	61	0	52	2	0
7	N	50	0	43	0	0
8	A	14	0	13	0	0
8	C	14	0	13	0	0
9	A	90	0	0	15	0
9	B	11	0	0	2	0
9	C	60	0	0	12	0
All	All	9852	0	9326	195	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 (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:MET:HE3	9:A:813:HOH:O	1.66	0.95
2:B:39:ASN:O	9:B:201:HOH:O	1.94	0.86
9:C:801:HOH:O	6:O:1:NAG:H2	1.79	0.82
1:A:284:TYR:O	9:A:801:HOH:O	1.99	0.80
1:A:569:LYS:NZ	9:A:808:HOH:O	2.13	0.77
1:A:228:TYR:OH	9:A:802:HOH:O	2.02	0.76
2:D:128:LYS:HG3	2:D:165:GLY:HA3	1.69	0.74
1:C:468:THR:HG21	1:C:534:PRO:HD2	1.70	0.73
9:C:801:HOH:O	6:O:1:NAG:O7	2.06	0.73
1:A:458:SER:O	9:A:803:HOH:O	2.07	0.71
1:A:589:PHE:O	9:A:805:HOH:O	2.09	0.71
1:A:286:PRO:O	9:A:804:HOH:O	2.08	0.70
1:A:400:GLU:OE1	9:A:806:HOH:O	2.10	0.69
1:C:462:PRO:O	1:C:477:SER:OG	2.11	0.69
1:A:199:ASN:ND2	9:A:809:HOH:O	2.21	0.68
1:A:293:SER:OG	9:A:807:HOH:O	2.11	0.68
2:D:49:VAL:HG22	2:D:161:LEU:HB3	1.75	0.67
1:A:283:ASP:HB3	1:A:285:ARG:HG2	1.77	0.67
1:C:214:SER:OG	1:C:215:VAL:N	2.27	0.66
1:A:297:PRO:HG3	1:A:350:THR:HG21	1.77	0.65
1:C:556:PRO:O	9:C:802:HOH:O	2.14	0.65
2:B:96:THR:HB	2:B:122:TRP:CH2	2.31	0.65
2:B:128:LYS:HG3	2:B:165:GLY:HA3	1.79	0.64
1:C:341:TYR:CZ	1:C:442:MET:HG3	2.33	0.64
1:A:341:TYR:CZ	1:A:442:MET:HG3	2.33	0.64
1:C:222:ARG:NH2	9:C:803:HOH:O	2.14	0.64
1:C:283:ASP:HB3	1:C:285:ARG:HG2	1.80	0.63
1:C:392:ASP:OD2	1:C:417:SER:OG	2.17	0.62
1:C:480:SER:CB	9:C:809:HOH:O	2.48	0.62
1:A:347:ARG:NH1	9:A:810:HOH:O	2.24	0.61
1:A:392:ASP:OD2	1:A:417:SER:OG	2.19	0.61
1:C:267:ASP:OD1	1:C:267:ASP:N	2.27	0.61
1:A:531:ASP:OD2	1:A:583:THR:HG23	1.99	0.60
1:A:458:SER:HB2	1:A:486:LYS:HE2	1.82	0.60
2:D:65:VAL:N	2:D:104:PRO:O	2.35	0.59
2:B:42:PHE:CD1	2:B:158:MET:HA	2.38	0.59
1:C:535:LEU:HD11	1:C:543:VAL:HG22	1.84	0.59
2:B:129:ASN:HA	2:B:166:GLN:HE21	1.67	0.58
1:C:230:ILE:HD13	1:C:611:PRO:HG2	1.85	0.58
1:A:231:PRO:HB2	1:A:240:MET:HE1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:GLU:HG2	1:C:352:LYS:HE3	1.87	0.57
1:C:445:PHE:HB3	1:C:447:ILE:HD11	1.86	0.57
1:C:399:CYS:HB2	9:C:818:HOH:O	2.02	0.57
1:C:498:PRO:HG2	1:C:500:TRP:CZ2	2.40	0.57
1:C:536:ASP:HA	9:C:812:HOH:O	2.04	0.56
2:B:73:TYR:CG	2:B:104:PRO:HB3	2.41	0.56
1:C:430:ASN:HB2	1:C:459:PHE:CE1	2.40	0.56
1:A:389:ILE:HG22	1:A:429:TYR:HB2	1.88	0.54
1:C:438:SER:HB2	1:C:446:LYS:HB3	1.89	0.54
1:C:399:CYS:CB	9:C:818:HOH:O	2.54	0.54
2:D:147:ASN:ND2	2:D:149:GLU:O	2.41	0.54
1:A:244:LEU:HD23	1:A:307:PRO:HD3	1.88	0.54
1:A:580:ARG:HD2	1:A:600:GLU:OE1	2.08	0.54
1:C:326:THR:OG1	1:C:335:ASP:OD2	2.18	0.54
1:C:580:ARG:HD2	1:C:600:GLU:OE1	2.08	0.54
2:B:155:THR:OG1	2:B:156:ARG:N	2.40	0.54
1:A:269:PHE:HE2	1:A:270:LYS:HD2	1.73	0.53
1:A:347:ARG:HA	1:A:347:ARG:HE	1.74	0.53
1:C:530:ASN:ND2	9:C:817:HOH:O	2.42	0.53
1:A:311:ASN:HD22	3:E:1:NAG:H83	1.72	0.53
1:A:481:TRP:CD2	1:A:521:PRO:HA	2.43	0.53
1:C:542:TYR:HB2	1:C:561:PHE:CE1	2.44	0.53
1:C:257:TYR:OH	1:C:305:CYS:HB2	2.08	0.53
1:A:479:MET:HA	1:A:526:GLY:O	2.09	0.52
1:A:254:TYR:HB3	1:A:274:SER:HB2	1.92	0.52
1:A:478:SER:O	1:A:508:ARG:NH1	2.39	0.52
1:C:372:GLY:HA3	1:C:529:TYR:OH	2.10	0.51
1:A:327:LEU:HB2	9:A:836:HOH:O	2.10	0.51
2:B:133:TYR:CE2	2:B:161:LEU:HD13	2.46	0.51
1:C:244:LEU:HD23	1:C:307:PRO:HD3	1.92	0.51
2:D:114:PHE:HA	2:D:126:PHE:HD2	1.76	0.51
2:D:77:LYS:HB3	2:D:79:TYR:HE1	1.76	0.50
1:A:222:ARG:NH1	9:A:801:HOH:O	2.41	0.50
2:B:96:THR:HG23	2:B:97:PRO:HD2	1.93	0.50
1:A:358:MET:HE1	1:A:435:MET:HE2	1.94	0.50
1:A:252:PHE:CE2	1:A:276:GLY:HA3	2.47	0.49
1:C:235:ASP:OD2	9:C:804:HOH:O	2.19	0.49
1:A:342:PHE:HB3	1:A:348:PRO:HA	1.94	0.49
1:C:243:PRO:HD2	1:C:600:GLU:HB2	1.94	0.49
1:C:302:VAL:HA	1:C:320:ILE:HG22	1.94	0.49
2:D:129:ASN:HA	2:D:166:GLN:HE21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ASN:OD1	1:C:363:ARG:N	2.40	0.49
2:D:81:VAL:O	2:D:133:TYR:HB2	2.13	0.49
1:C:241:ASN:OD1	1:C:257:TYR:HB2	2.13	0.48
1:A:508:ARG:NH2	1:A:514:CYS:O	2.47	0.48
1:C:362:ASN:HB3	1:C:364:TYR:CZ	2.49	0.48
2:D:137:THR:OG1	2:D:147:ASN:O	2.27	0.48
4:L:1:NAG:O3	4:L:2:NAG:O5	2.32	0.48
1:A:388:VAL:HG11	1:A:428:ARG:HD3	1.95	0.48
1:A:224:LYS:NZ	9:A:828:HOH:O	2.47	0.48
1:C:542:TYR:HB2	1:C:561:PHE:CZ	2.49	0.48
1:A:269:PHE:CE2	1:A:270:LYS:HD2	2.49	0.47
1:A:394:PHE:CE1	1:A:431:LEU:HD13	2.50	0.47
1:C:327:LEU:HA	1:C:366:HIS:HD2	1.79	0.47
1:A:481:TRP:CG	1:A:521:PRO:HA	2.48	0.47
1:C:252:PHE:CE2	1:C:276:GLY:HA3	2.49	0.47
2:D:138:SER:O	2:D:152:VAL:N	2.46	0.47
1:A:552:LEU:HD13	2:B:113:LYS:HD2	1.96	0.47
1:C:324:THR:HG22	9:C:813:HOH:O	2.14	0.47
1:A:211:PHE:HA	1:A:620:LYS:HA	1.96	0.47
1:A:407:GLN:HG3	2:B:102:ALA:CB	2.44	0.47
1:A:593:PRO:HG2	1:A:618:ILE:HB	1.96	0.47
1:C:392:ASP:HB2	1:C:429:TYR:CZ	2.50	0.46
2:D:96:THR:HG23	2:D:97:PRO:HD2	1.97	0.46
1:A:439:GLN:HB2	1:A:445:PHE:CE1	2.49	0.46
1:C:242:ASN:N	1:C:600:GLU:OE2	2.33	0.46
1:C:328:ASP:OD2	1:C:424:THR:HG21	2.15	0.46
1:A:319:HIS:CD2	1:A:337:TYR:CE2	3.03	0.46
1:A:594:TRP:CH2	1:A:617:LYS:HB2	2.51	0.46
1:C:327:LEU:HA	1:C:366:HIS:CD2	2.51	0.46
1:A:574:LYS:HB2	1:A:574:LYS:HE2	1.67	0.46
1:A:595:CYS:HB2	1:A:616:TYR:CE2	2.50	0.46
1:A:340:THR:OG1	1:A:350:THR:HB	2.15	0.46
1:C:453:THR:OG1	1:C:497:THR:HA	2.16	0.46
1:A:213:LYS:HD3	1:A:539:LYS:HG3	1.98	0.45
1:C:423:PRO:HB2	2:D:96:THR:OG1	2.16	0.45
1:C:288:LEU:HD21	1:C:596:ILE:HD13	1.98	0.45
1:C:247:ILE:HD12	1:C:585:SER:HB2	1.98	0.45
1:A:397:ASP:N	9:A:815:HOH:O	2.30	0.45
1:A:589:PHE:HB3	1:A:594:TRP:CD1	2.52	0.45
1:C:211:PHE:HA	1:C:620:LYS:HA	1.98	0.45
1:A:570:GLU:HG2	1:A:571:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:MET:HA	1:C:526:GLY:O	2.17	0.45
6:J:3:BMA:H5	6:J:5:MAN:H2	1.99	0.45
1:A:482:ASP:OD1	1:A:519:LYS:NZ	2.49	0.44
2:B:98:LEU:HB3	2:B:110:PHE:CE2	2.52	0.44
1:C:255:ILE:HD11	1:C:316:VAL:HG22	1.98	0.44
1:C:320:ILE:HD11	1:C:338:TYR:HE2	1.81	0.44
1:C:464:ARG:NH2	1:C:584:THR:O	2.50	0.44
1:A:233:GLN:HG2	1:A:238:ILE:HB	2.00	0.44
1:C:594:TRP:CZ2	1:C:617:LYS:HD2	2.53	0.44
2:D:79:TYR:CD2	2:D:95:ASN:HB3	2.53	0.44
1:A:400:GLU:HA	1:A:412:LEU:HD13	2.00	0.44
2:D:73:TYR:CG	2:D:104:PRO:HB3	2.53	0.44
2:D:133:TYR:HE2	2:D:161:LEU:HD12	1.83	0.44
1:A:362:ASN:OD1	1:A:363:ARG:N	2.46	0.43
1:C:543:VAL:HG13	1:C:560:VAL:HG22	2.01	0.43
1:C:594:TRP:CH2	1:C:617:LYS:HB2	2.54	0.43
2:D:49:VAL:HG13	2:D:161:LEU:HD22	2.00	0.43
2:D:50:LEU:HD23	2:D:50:LEU:HA	1.87	0.43
2:B:99:LEU:HD22	2:B:108:ILE:HG22	2.00	0.43
2:D:152:VAL:HG13	2:D:158:MET:HG3	2.00	0.43
5:G:3:BMA:H62	5:G:5:MAN:H2	1.69	0.43
1:A:393:VAL:O	1:A:393:VAL:HG12	2.18	0.43
1:A:581:SER:HB2	1:A:600:GLU:OE1	2.19	0.43
2:B:96:THR:HB	2:B:122:TRP:CZ2	2.53	0.43
1:C:336:GLU:OE2	4:L:1:NAG:H83	2.19	0.43
1:C:383:ILE:HD12	1:C:383:ILE:N	2.33	0.43
1:C:434:ILE:HD13	1:C:496:PHE:CD1	2.54	0.43
1:C:562:ASN:ND2	9:C:814:HOH:O	2.38	0.43
1:C:345:ILE:HG13	1:C:346:ASP:N	2.33	0.43
1:A:355:ILE:HD13	1:A:355:ILE:HA	1.82	0.43
2:D:39:ASN:HB3	2:D:42:PHE:CD2	2.54	0.43
1:A:556:PRO:HD3	1:A:579:THR:HG23	2.00	0.43
1:C:388:VAL:HG11	1:C:428:ARG:HD3	2.00	0.43
1:A:398:TYR:CG	1:A:456:LYS:HG2	2.54	0.42
1:C:304:ASN:HB3	1:C:369:PHE:O	2.19	0.42
2:D:85:GLN:NE2	2:D:90:THR:O	2.52	0.42
1:C:265:LYS:HE3	1:C:265:LYS:HB2	1.66	0.42
1:C:553:ALA:HB2	2:D:119:PRO:HD3	2.00	0.42
1:A:214:SER:OG	1:A:215:VAL:N	2.53	0.42
1:C:435:MET:HE3	1:C:435:MET:HB2	1.96	0.42
1:A:336:GLU:OE1	4:F:1:NAG:H83	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ILE:HG22	1:C:429:TYR:HB2	2.01	0.42
1:C:382:ILE:C	1:C:383:ILE:HD12	2.45	0.42
1:C:481:TRP:HA	1:C:514:CYS:SG	2.60	0.42
1:C:551:GLN:O	2:D:119:PRO:HG3	2.19	0.42
2:D:79:TYR:HD2	2:D:95:ASN:HD22	1.68	0.41
2:D:142:LEU:O	2:D:143:GLU:HB3	2.20	0.41
1:A:533:ALA:HA	1:A:534:PRO:HD3	1.89	0.41
2:B:163:LYS:HB3	2:B:166:GLN:OE1	2.20	0.41
1:A:605:ASN:OD1	1:A:605:ASN:N	2.53	0.41
2:B:48:LEU:HD12	2:B:49:VAL:N	2.36	0.41
2:B:123:GLY:O	2:B:124:LEU:C	2.63	0.41
1:C:306:VAL:HG13	1:C:373:GLY:HA2	2.03	0.41
1:C:481:TRP:CD2	1:C:521:PRO:HA	2.56	0.41
1:A:464:ARG:NH2	1:A:584:THR:O	2.54	0.41
4:L:1:NAG:H62	4:L:3:FUC:H2	1.51	0.41
1:A:580:ARG:NH2	1:A:600:GLU:OE2	2.53	0.41
1:A:391:THR:O	1:A:393:VAL:HG23	2.20	0.41
1:A:468:THR:HG21	1:A:534:PRO:HD2	2.02	0.41
1:A:200:ALA:HB1	1:A:590:LEU:HD13	2.02	0.41
1:A:420:LEU:HD22	1:A:459:PHE:HA	2.03	0.41
2:B:73:TYR:CD2	2:B:104:PRO:HB3	2.56	0.41
1:C:381:PHE:HB3	1:C:383:ILE:HD11	2.03	0.41
1:A:336:GLU:HG2	1:A:352:LYS:HE3	2.03	0.41
1:C:210:ILE:HD13	1:C:210:ILE:HA	1.92	0.41
1:A:594:TRP:CZ2	1:A:617:LYS:HD2	2.55	0.40
1:C:552:LEU:HD13	2:D:113:LYS:HD2	2.03	0.40
2:D:77:LYS:HB3	2:D:79:TYR:CE1	2.56	0.40
2:B:107:ASP:OD1	2:B:107:ASP:N	2.50	0.40
1:A:537:LEU:HD23	1:A:537:LEU:HA	1.82	0.40
2:B:156:ARG:NH2	9:B:206:HOH:O	2.55	0.40
2:D:51:TYR:CD1	2:D:167:ASP:HA	2.56	0.40
2:D:29:VAL:HG22	2:D:57:LYS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/430 (100%)	412 (96%)	16 (4%)	0	100	100
1	C	428/430 (100%)	413 (96%)	15 (4%)	0	100	100
2	B	133/144 (92%)	129 (97%)	4 (3%)	0	100	100
2	D	132/144 (92%)	128 (97%)	4 (3%)	0	100	100
All	All	1121/1148 (98%)	1082 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/399 (100%)	373 (94%)	26 (6%)	15	32
1	C	399/399 (100%)	379 (95%)	20 (5%)	22	44
2	B	123/130 (95%)	115 (94%)	8 (6%)	15	32
2	D	123/130 (95%)	113 (92%)	10 (8%)	11	24
All	All	1044/1058 (99%)	980 (94%)	64 (6%)	17	35

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	LEU
1	A	256	HIS
1	A	271	VAL
1	A	308	VAL
1	A	324	THR
1	A	327	LEU
1	A	350	THR
1	A	358	MET

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Mol	Chain	Res	Type
1	A	359	THR
1	A	366	HIS
1	A	412	LEU
1	A	420	LEU
1	A	431	LEU
1	A	439	GLN
1	A	453	THR
1	A	464	ARG
1	A	468	THR
1	A	477	SER
1	A	505	VAL
1	A	508	ARG
1	A	543	VAL
1	A	563	SER
1	A	574	LYS
1	A	579	THR
1	A	581	SER
1	A	590	LEU
2	B	28	ILE
2	B	84	ASP
2	B	93	LYS
2	B	95	ASN
2	B	98	LEU
2	B	101	CYS
2	B	107	ASP
2	B	121	LEU
1	C	218	ASP
1	C	244	LEU
1	C	264	LYS
1	C	267	ASP
1	C	308	VAL
1	C	320	ILE
1	C	324	THR
1	C	350	THR
1	C	359	THR
1	C	366	HIS
1	C	391	THR
1	C	408	THR
1	C	431	LEU
1	C	439	GLN
1	C	464	ARG
1	C	468	THR

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Mol	Chain	Res	Type
1	C	477	SER
1	C	505	VAL
1	C	508	ARG
1	C	543	VAL
2	D	28	ILE
2	D	31	GLU
2	D	81	VAL
2	D	92	LYS
2	D	93	LYS
2	D	95	ASN
2	D	101	CYS
2	D	121	LEU
2	D	122	TRP
2	D	152	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	HIS
1	A	301	GLN
1	A	356	ASN
1	A	511	GLN
2	B	115	GLN
1	C	356	ASN
1	C	471	GLN
1	C	476	GLN
2	D	85	GLN
2	D	106	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 ⓘ

48 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$
3	NAG	E	1	1,3	14,14,15	0.32	0	17,19,21	0.48	0
3	NAG	E	2	3	14,14,15	0.57	0	17,19,21	0.50	0
3	BMA	E	3	3	11,11,12	1.04	1 (9%)	15,15,17	1.13	1 (6%)
4	NAG	F	1	4,1	14,14,15	0.47	0	17,19,21	0.64	0
4	NAG	F	2	4	14,14,15	0.59	0	17,19,21	0.43	0
4	FUC	F	3	4	10,10,11	1.19	1 (10%)	14,14,16	1.20	2 (14%)
5	NAG	G	1	5,1	14,14,15	0.86	1 (7%)	17,19,21	0.76	0
5	NAG	G	2	5	14,14,15	0.29	0	17,19,21	0.56	0
5	BMA	G	3	5	11,11,12	1.52	1 (9%)	15,15,17	1.48	3 (20%)
5	MAN	G	4	5	11,11,12	1.82	3 (27%)	15,15,17	1.28	1 (6%)
5	MAN	G	5	5	11,11,12	1.49	2 (18%)	15,15,17	1.11	1 (6%)
5	FUC	G	6	5	10,10,11	2.08	3 (30%)	14,14,16	1.55	3 (21%)
5	FUC	G	7	5	10,10,11	1.56	2 (20%)	14,14,16	1.08	1 (7%)
6	NAG	H	1	1,6	14,14,15	0.66	1 (7%)	17,19,21	0.60	0
6	NAG	H	2	6	14,14,15	0.45	0	17,19,21	0.56	0
6	BMA	H	3	6	11,11,12	1.32	2 (18%)	15,15,17	0.84	0
6	MAN	H	4	6	11,11,12	1.22	0	15,15,17	0.94	1 (6%)
6	MAN	H	5	6	11,11,12	1.71	3 (27%)	15,15,17	1.20	1 (6%)
6	NAG	I	1	1,6	14,14,15	0.42	0	17,19,21	0.61	0
6	NAG	I	2	6	14,14,15	0.83	1 (7%)	17,19,21	0.64	0
6	BMA	I	3	6	11,11,12	1.00	0	15,15,17	1.18	1 (6%)
6	MAN	I	4	6	11,11,12	1.01	0	15,15,17	1.22	2 (13%)
6	MAN	I	5	6	11,11,12	1.78	3 (27%)	15,15,17	1.92	3 (20%)
6	NAG	J	1	1,6	14,14,15	1.09	1 (7%)	17,19,21	0.78	0
6	NAG	J	2	6	14,14,15	0.22	0	17,19,21	0.42	0
6	BMA	J	3	6	11,11,12	1.27	2 (18%)	15,15,17	0.77	0
6	MAN	J	4	6	11,11,12	0.95	0	15,15,17	1.07	0
6	MAN	J	5	6	11,11,12	1.70	2 (18%)	15,15,17	1.10	0
6	NAG	K	1	1,6	14,14,15	0.36	0	17,19,21	0.53	0
6	NAG	K	2	6	14,14,15	0.25	0	17,19,21	0.50	0
6	BMA	K	3	6	11,11,12	1.37	3 (27%)	15,15,17	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	K	4	6	11,11,12	1.11	2 (18%)	15,15,17	1.61	2 (13%)
6	MAN	K	5	6	11,11,12	0.99	0	15,15,17	1.09	1 (6%)
4	NAG	L	1	4,1	14,14,15	0.45	0	17,19,21	0.59	0
4	NAG	L	2	4	14,14,15	0.32	0	17,19,21	0.62	0
4	FUC	L	3	4	10,10,11	1.19	1 (10%)	14,14,16	1.08	1 (7%)
3	NAG	M	1	1,3	14,14,15	0.44	0	17,19,21	0.88	0
3	NAG	M	2	3	14,14,15	0.55	0	17,19,21	0.68	0
3	BMA	M	3	3	11,11,12	1.07	1 (9%)	15,15,17	1.28	1 (6%)
7	NAG	N	1	7,1	14,14,15	0.52	0	17,19,21	0.50	0
7	NAG	N	2	7	14,14,15	0.63	0	17,19,21	0.72	0
7	BMA	N	3	7	11,11,12	1.51	2 (18%)	15,15,17	0.88	0
7	MAN	N	4	7	11,11,12	1.90	4 (36%)	15,15,17	1.18	1 (6%)
6	NAG	O	1	1,6	14,14,15	0.75	1 (7%)	17,19,21	0.74	0
6	NAG	O	2	6	14,14,15	0.80	1 (7%)	17,19,21	0.91	0
6	BMA	O	3	6	11,11,12	1.39	2 (18%)	15,15,17	1.39	1 (6%)
6	MAN	O	4	6	11,11,12	1.17	1 (9%)	15,15,17	1.30	2 (13%)
6	MAN	O	5	6	11,11,12	1.65	3 (27%)	15,15,17	1.67	3 (20%)

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

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

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

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	5	MAN	C2-C3	4.00	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	6	FUC	C4-C3	4.00	1.62	1.52
5	G	4	MAN	C2-C3	3.95	1.58	1.52
5	G	3	BMA	C2-C3	3.92	1.58	1.52
6	J	1	NAG	O5-C1	-3.82	1.37	1.43
6	O	5	MAN	C1-C2	3.36	1.60	1.52
6	H	5	MAN	O5-C5	3.28	1.49	1.43
7	N	4	MAN	C2-C3	3.26	1.57	1.52
6	I	5	MAN	C2-C3	3.23	1.57	1.52
5	G	6	FUC	O5-C5	3.20	1.49	1.43
7	N	4	MAN	O5-C5	3.15	1.49	1.43
6	H	5	MAN	C2-C3	3.12	1.57	1.52
5	G	6	FUC	C4-C5	3.08	1.59	1.52
5	G	7	FUC	C1-C2	3.04	1.59	1.52
6	I	5	MAN	C1-C2	2.96	1.59	1.52
6	J	5	MAN	C1-C2	2.92	1.59	1.52
6	I	2	NAG	O5-C1	-2.91	1.38	1.43
5	G	1	NAG	O5-C1	-2.90	1.38	1.43
7	N	4	MAN	C1-C2	2.75	1.58	1.52
4	F	3	FUC	O5-C5	2.74	1.49	1.43
3	E	3	BMA	C1-C2	2.71	1.58	1.52
6	O	1	NAG	O5-C1	-2.68	1.39	1.43
6	O	5	MAN	O5-C5	2.67	1.48	1.43
6	O	5	MAN	C2-C3	2.63	1.56	1.52
7	N	3	BMA	C4-C3	2.63	1.59	1.52
6	J	3	BMA	C1-C2	2.62	1.58	1.52
6	J	3	BMA	C2-C3	2.55	1.56	1.52
5	G	5	MAN	C2-C3	2.55	1.56	1.52
6	O	3	BMA	C2-C3	2.52	1.56	1.52
7	N	4	MAN	C4-C3	2.45	1.58	1.52
6	I	5	MAN	O5-C5	2.43	1.48	1.43
6	H	3	BMA	C2-C3	2.42	1.56	1.52
5	G	4	MAN	C1-C2	2.39	1.57	1.52
6	O	2	NAG	C1-C2	2.39	1.55	1.52
3	M	3	BMA	C1-C2	2.36	1.57	1.52
6	K	3	BMA	C4-C5	2.33	1.58	1.53
5	G	7	FUC	O5-C5	2.33	1.48	1.43
7	N	3	BMA	C4-C5	2.33	1.58	1.53
6	H	1	NAG	O5-C1	-2.30	1.39	1.43
5	G	5	MAN	C4-C3	2.22	1.58	1.52
6	H	5	MAN	C4-C5	2.21	1.57	1.53
4	L	3	FUC	C1-C2	2.19	1.57	1.52
6	K	3	BMA	C2-C3	2.16	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	4	MAN	C4-C3	2.13	1.57	1.52
6	O	4	MAN	O5-C5	2.10	1.47	1.43
6	K	4	MAN	C2-C3	2.09	1.55	1.52
6	K	3	BMA	C4-C3	2.08	1.57	1.52
6	H	3	BMA	C4-C3	2.07	1.57	1.52
6	O	3	BMA	C1-C2	2.04	1.57	1.52
6	K	4	MAN	C1-C2	2.03	1.57	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	5	MAN	C1-O5-C5	5.49	119.55	112.19
6	K	4	MAN	C1-O5-C5	4.93	118.80	112.19
6	O	3	BMA	C1-O5-C5	3.85	117.35	112.19
6	O	5	MAN	C1-O5-C5	3.79	117.27	112.19
3	M	3	BMA	C1-O5-C5	3.66	117.09	112.19
6	O	4	MAN	C1-O5-C5	3.59	117.00	112.19
5	G	5	MAN	C1-O5-C5	3.28	116.58	112.19
6	H	5	MAN	C1-O5-C5	3.27	116.57	112.19
5	G	3	BMA	C2-C3-C4	3.19	116.48	110.86
6	I	4	MAN	C1-O5-C5	3.09	116.33	112.19
6	K	5	MAN	C1-O5-C5	3.07	116.30	112.19
5	G	4	MAN	C1-O5-C5	3.02	116.23	112.19
5	G	3	BMA	C1-C2-C3	2.92	113.89	109.64
5	G	6	FUC	O5-C5-C4	2.89	114.75	109.55
4	F	3	FUC	C1-O5-C5	2.71	119.37	112.97
5	G	6	FUC	O2-C2-C1	2.71	115.43	109.22
6	I	3	BMA	C1-O5-C5	2.64	115.72	112.19
6	K	4	MAN	O5-C1-C2	2.61	117.02	110.79
5	G	7	FUC	O2-C2-C1	2.50	114.95	109.22
6	O	5	MAN	C3-C4-C5	-2.49	105.72	110.23
6	I	5	MAN	O5-C1-C2	2.43	116.58	110.79
6	I	5	MAN	C1-C2-C3	2.28	112.96	109.64
6	I	4	MAN	O2-C2-C3	-2.25	105.50	110.15
6	O	5	MAN	C1-C2-C3	2.20	112.85	109.64
4	L	3	FUC	C1-C2-C3	2.20	112.85	109.64
5	G	6	FUC	C3-C4-C5	2.17	113.11	109.81
6	H	4	MAN	C1-O5-C5	2.09	114.99	112.19
6	O	4	MAN	C1-C2-C3	-2.07	106.63	109.64
3	E	3	BMA	C1-O5-C5	2.06	114.95	112.19
5	G	3	BMA	C1-O5-C5	2.04	114.93	112.19
4	F	3	FUC	O2-C2-C1	2.04	113.90	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	4	MAN	C1-O5-C5	2.02	114.89	112.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	3	FUC	C1
4	L	3	FUC	C1
5	G	6	FUC	C1
5	G	7	FUC	C1

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	2	NAG	O5-C5-C6-O6
6	I	5	MAN	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
6	I	5	MAN	C4-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
6	O	5	MAN	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
6	I	4	MAN	O5-C5-C6-O6
6	O	4	MAN	C4-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
6	O	3	BMA	O5-C5-C6-O6
6	O	4	MAN	O5-C5-C6-O6
7	N	4	MAN	O5-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6
6	J	5	MAN	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
6	O	3	BMA	C4-C5-C6-O6
6	J	5	MAN	O5-C5-C6-O6
7	N	2	NAG	O5-C5-C6-O6
6	I	4	MAN	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	M	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
6	H	2	NAG	C8-C7-N2-C2
6	H	2	NAG	O7-C7-N2-C2
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
6	O	2	NAG	C8-C7-N2-C2
6	O	2	NAG	O7-C7-N2-C2
7	N	2	NAG	C8-C7-N2-C2
7	N	2	NAG	O7-C7-N2-C2
6	H	5	MAN	O5-C5-C6-O6
7	N	2	NAG	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	H	3	BMA	C4-C5-C6-O6
6	O	5	MAN	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	M	3	BMA	O5-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
7	N	4	MAN	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	H	5	MAN	C4-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	N	4	MAN	C1-C2-C3-C4-C5-O5

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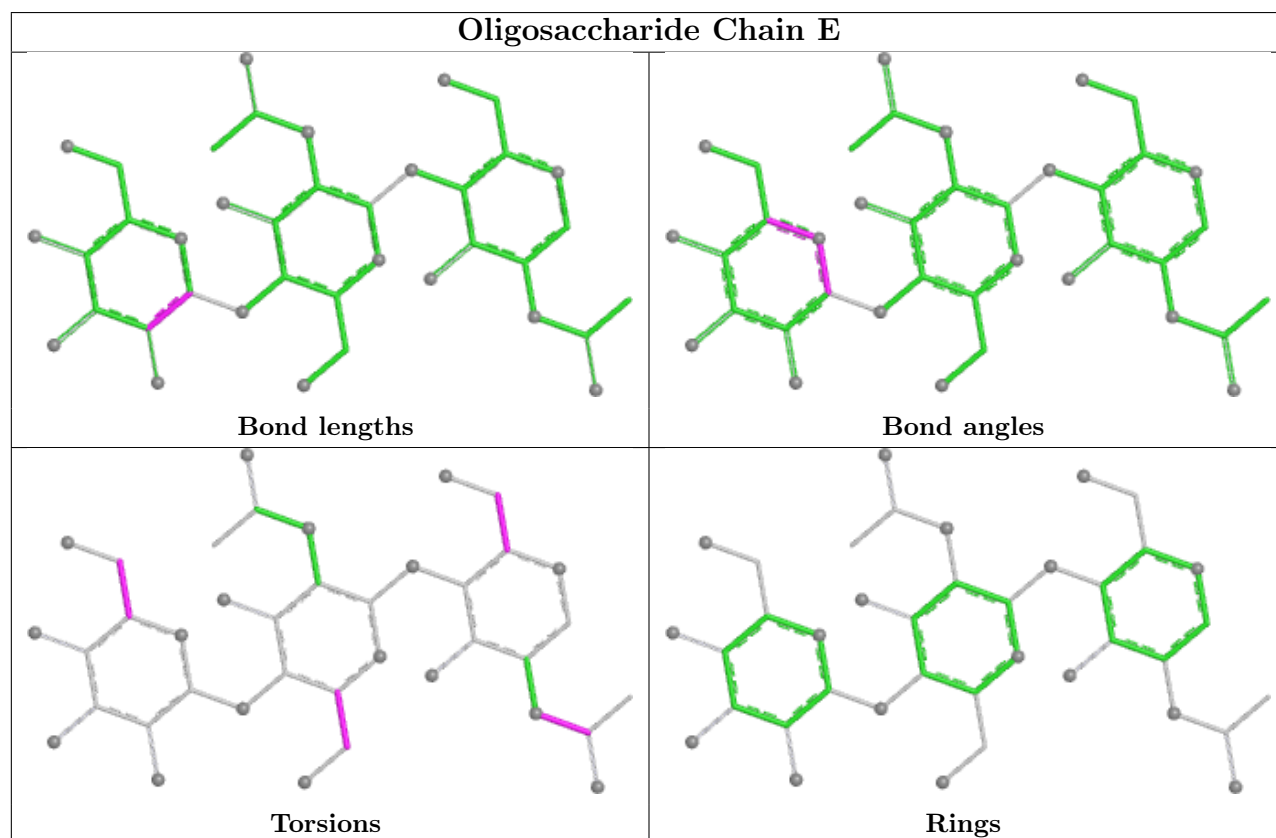
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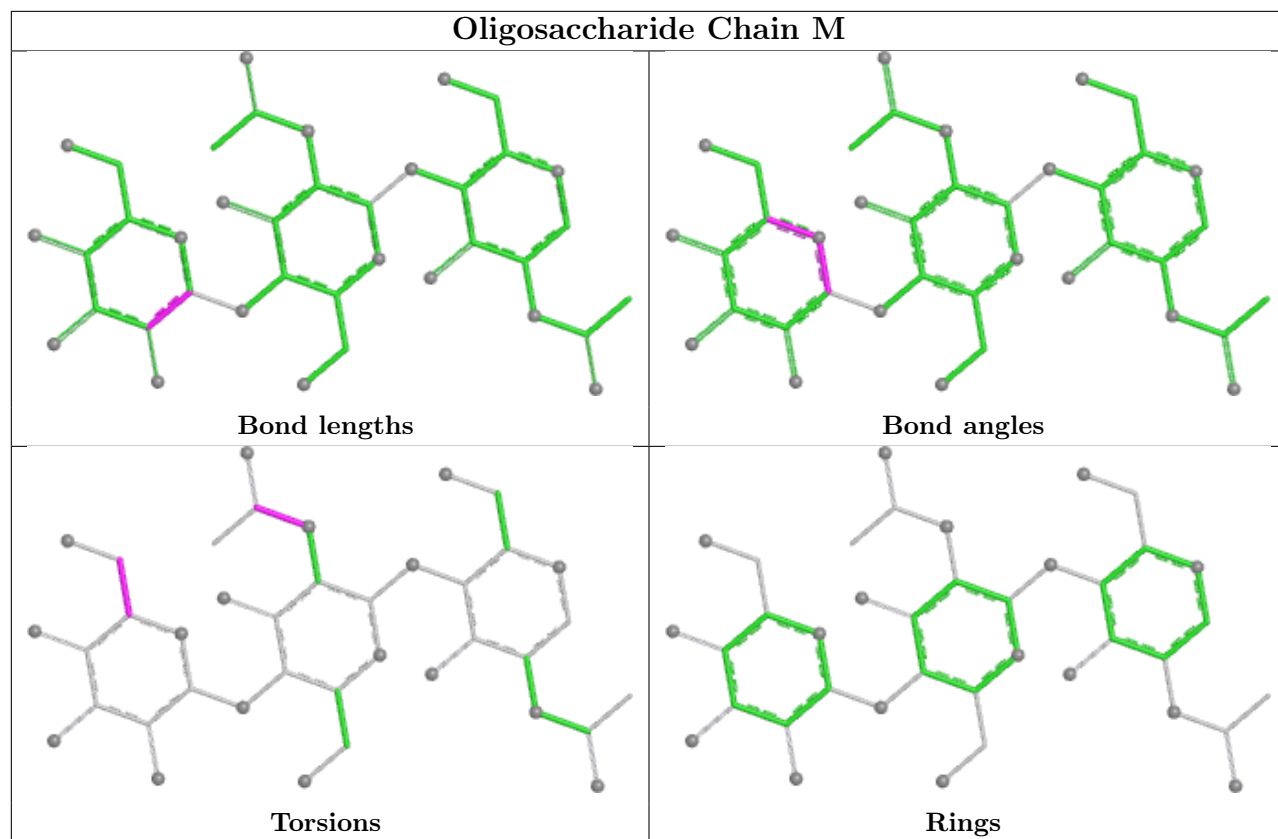
Mol	Chain	Res	Type	Atoms
6	H	5	MAN	C1-C2-C3-C4-C5-O5

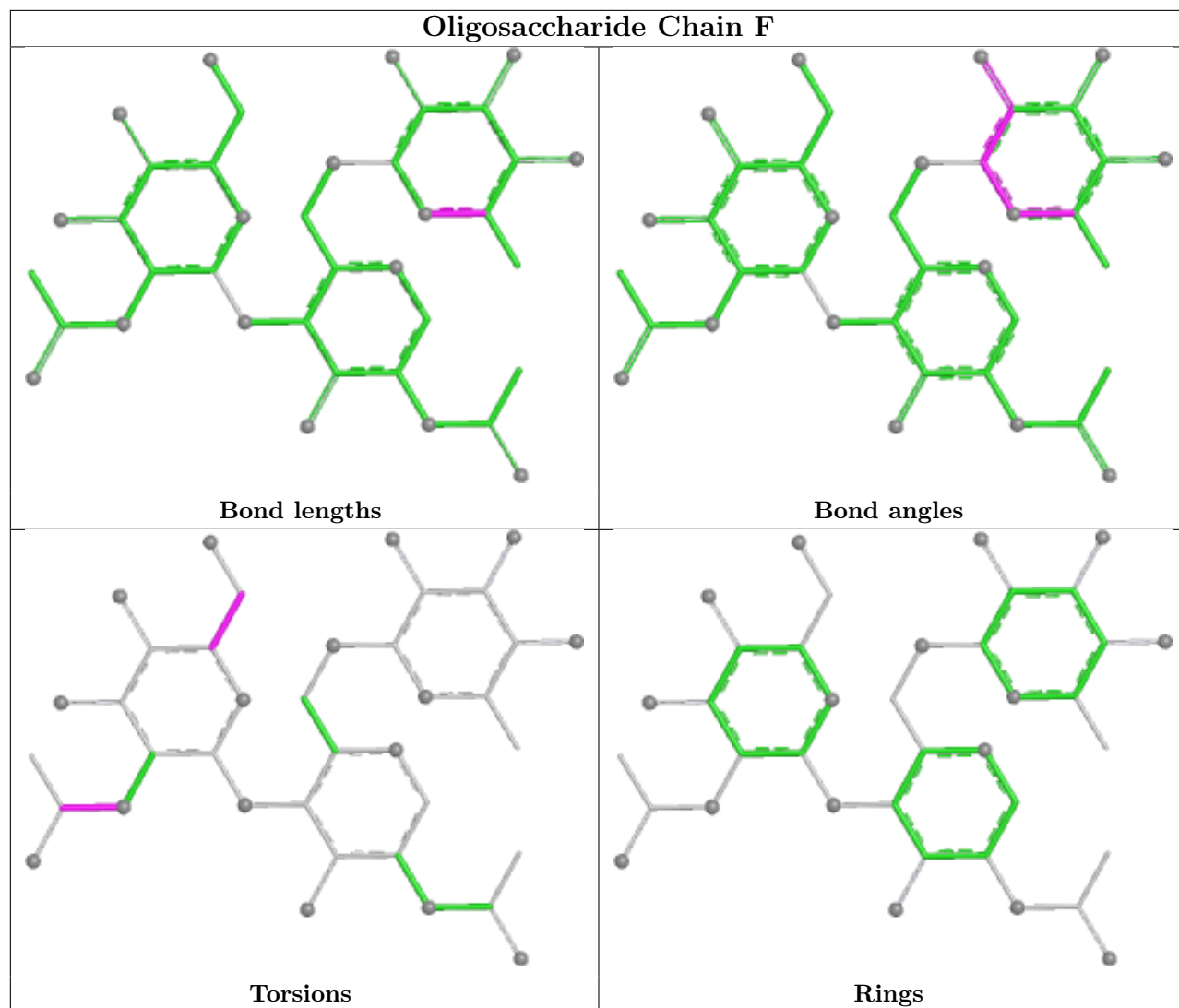
10 monomers are involved in 9 short contacts:

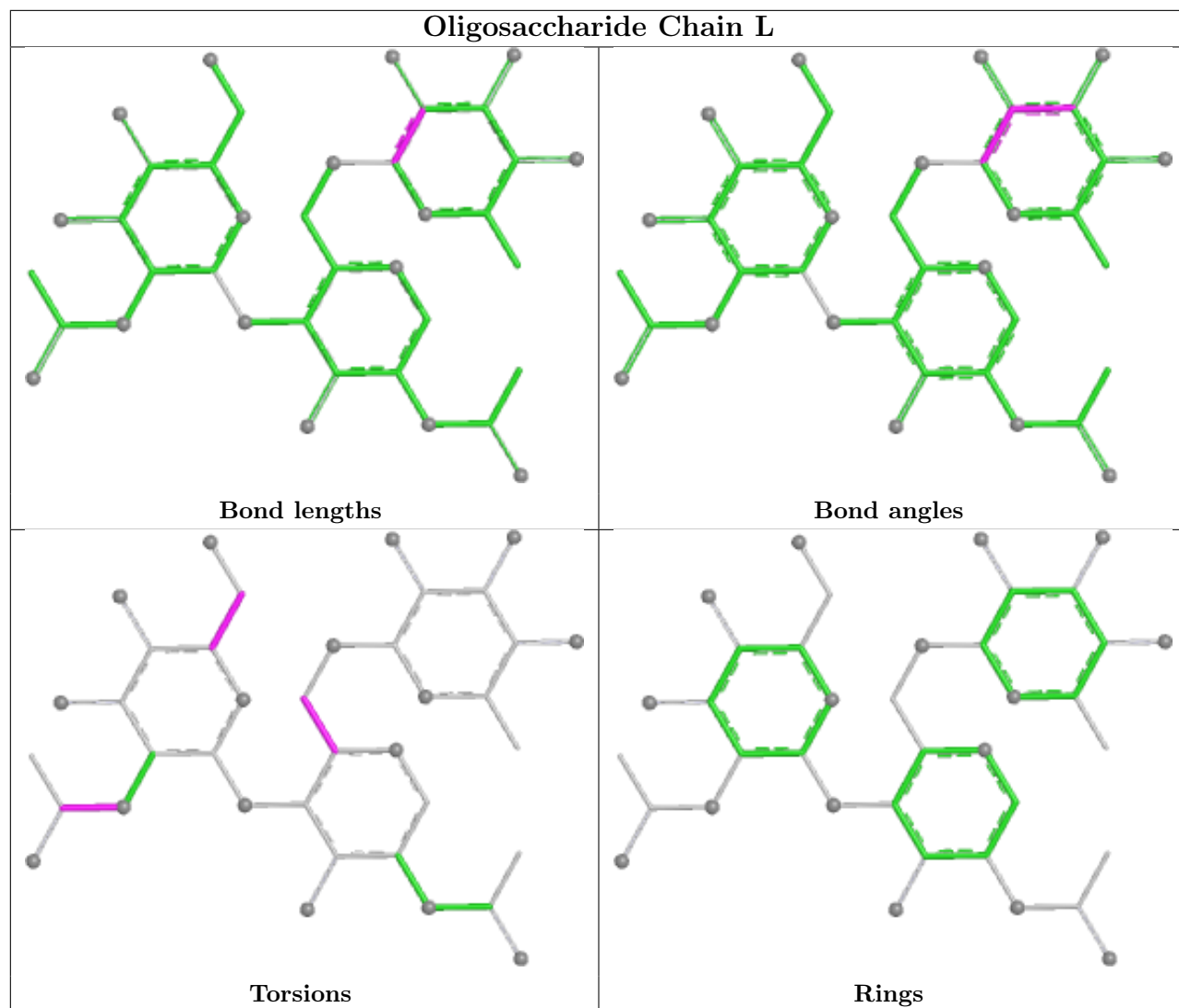
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0
5	G	3	BMA	1	0
6	O	1	NAG	2	0
6	J	3	BMA	1	0
4	L	1	NAG	3	0
4	L	3	FUC	1	0
4	F	1	NAG	1	0
5	G	5	MAN	1	0
4	L	2	NAG	1	0
6	J	5	MAN	1	0

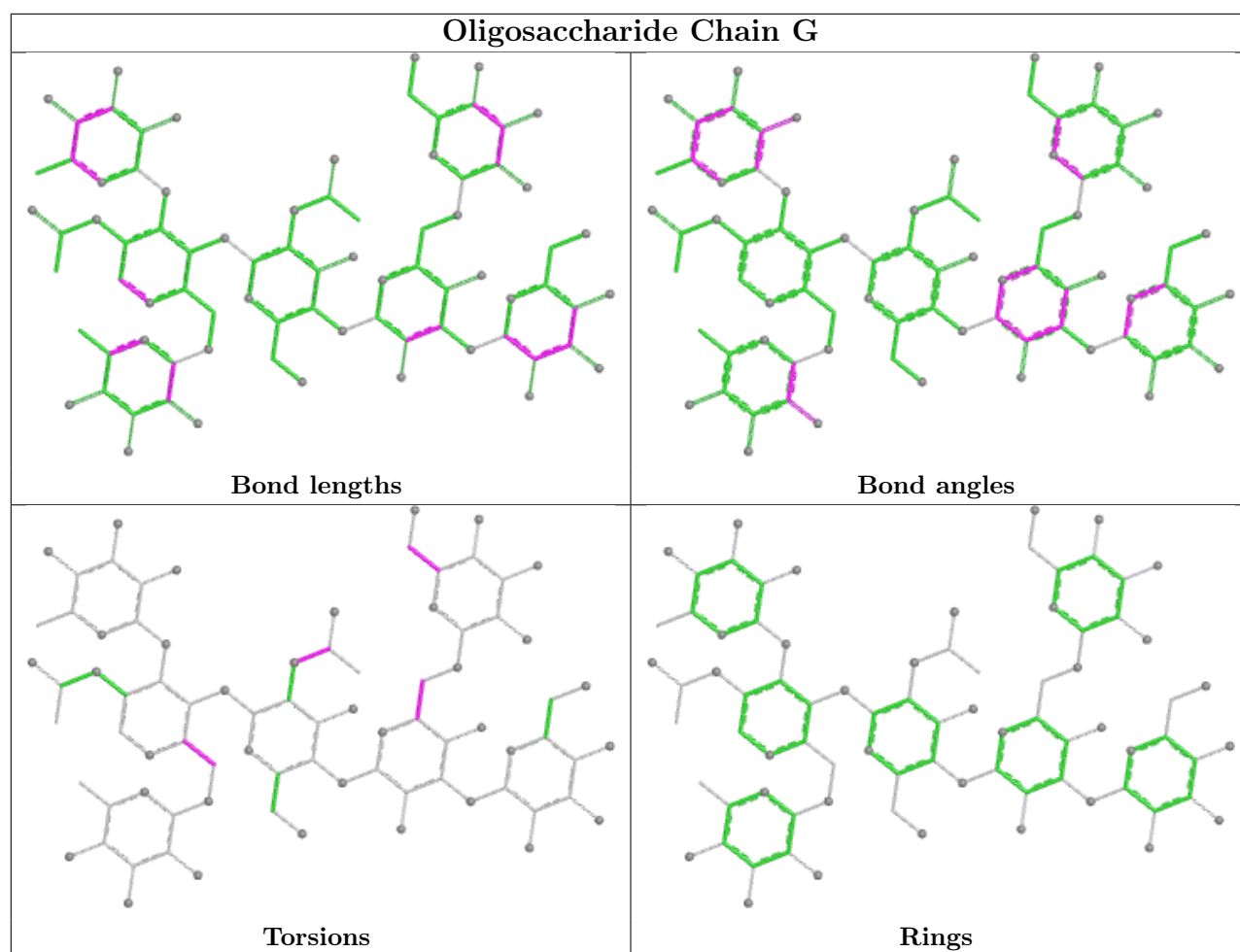
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

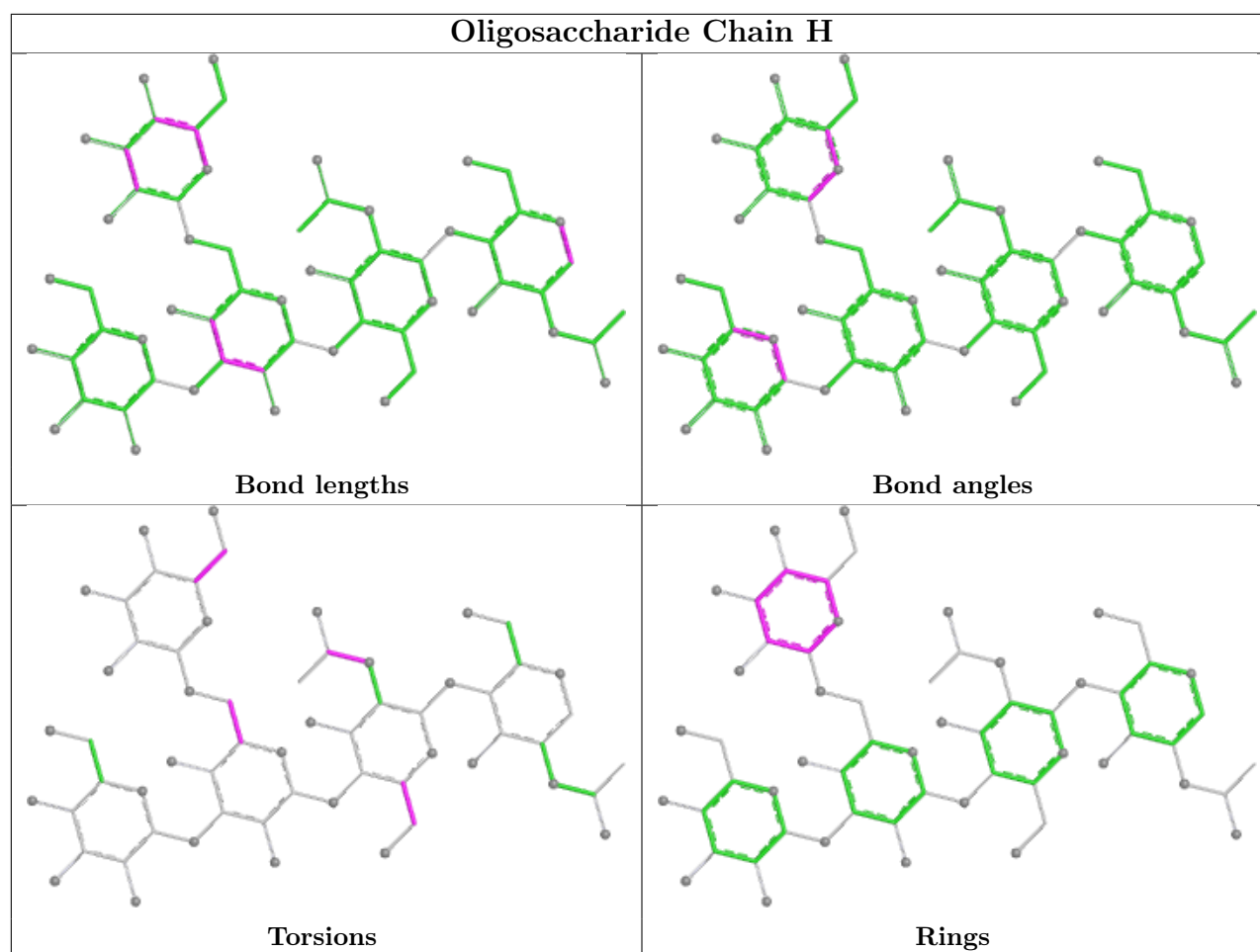


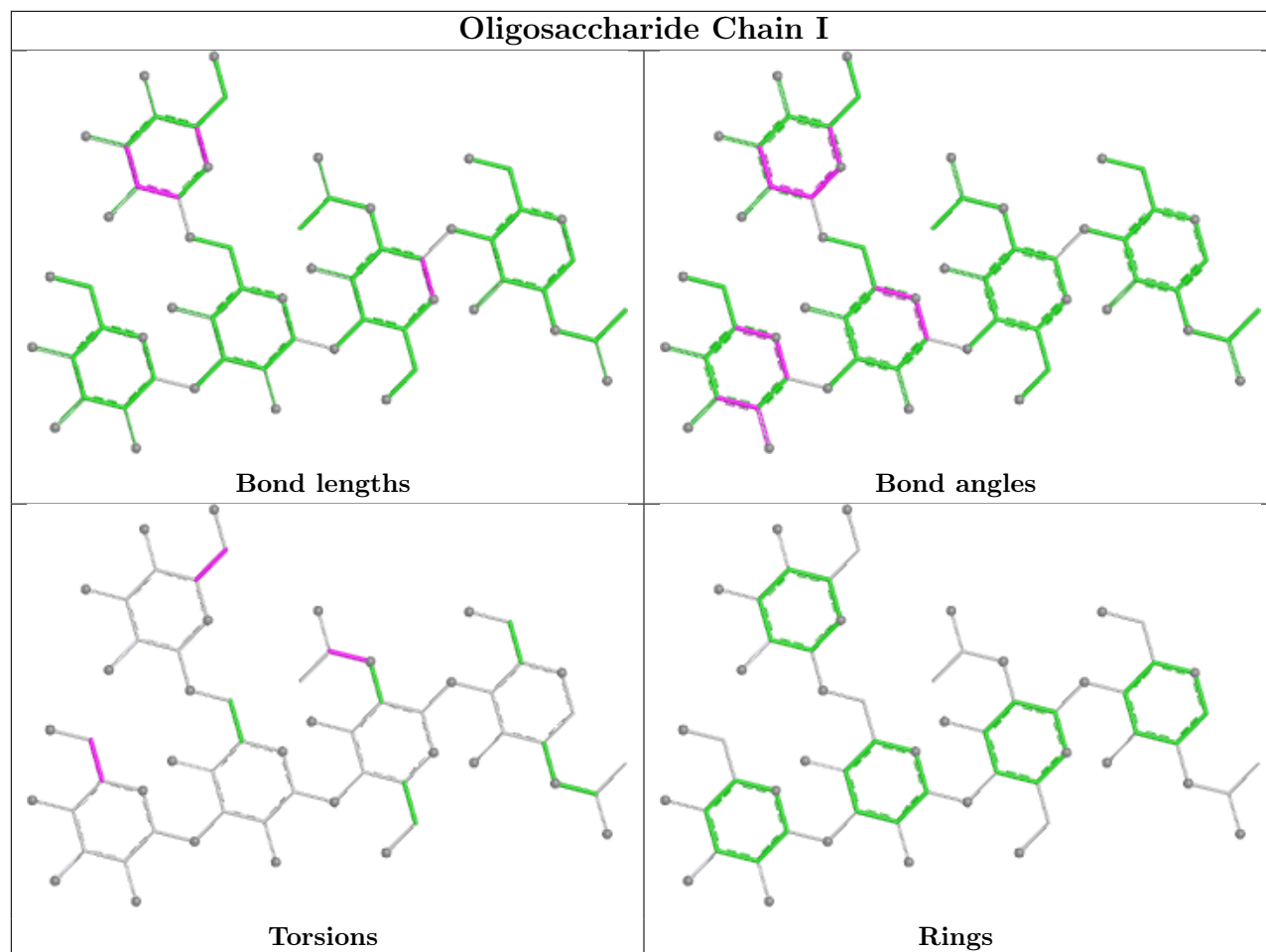


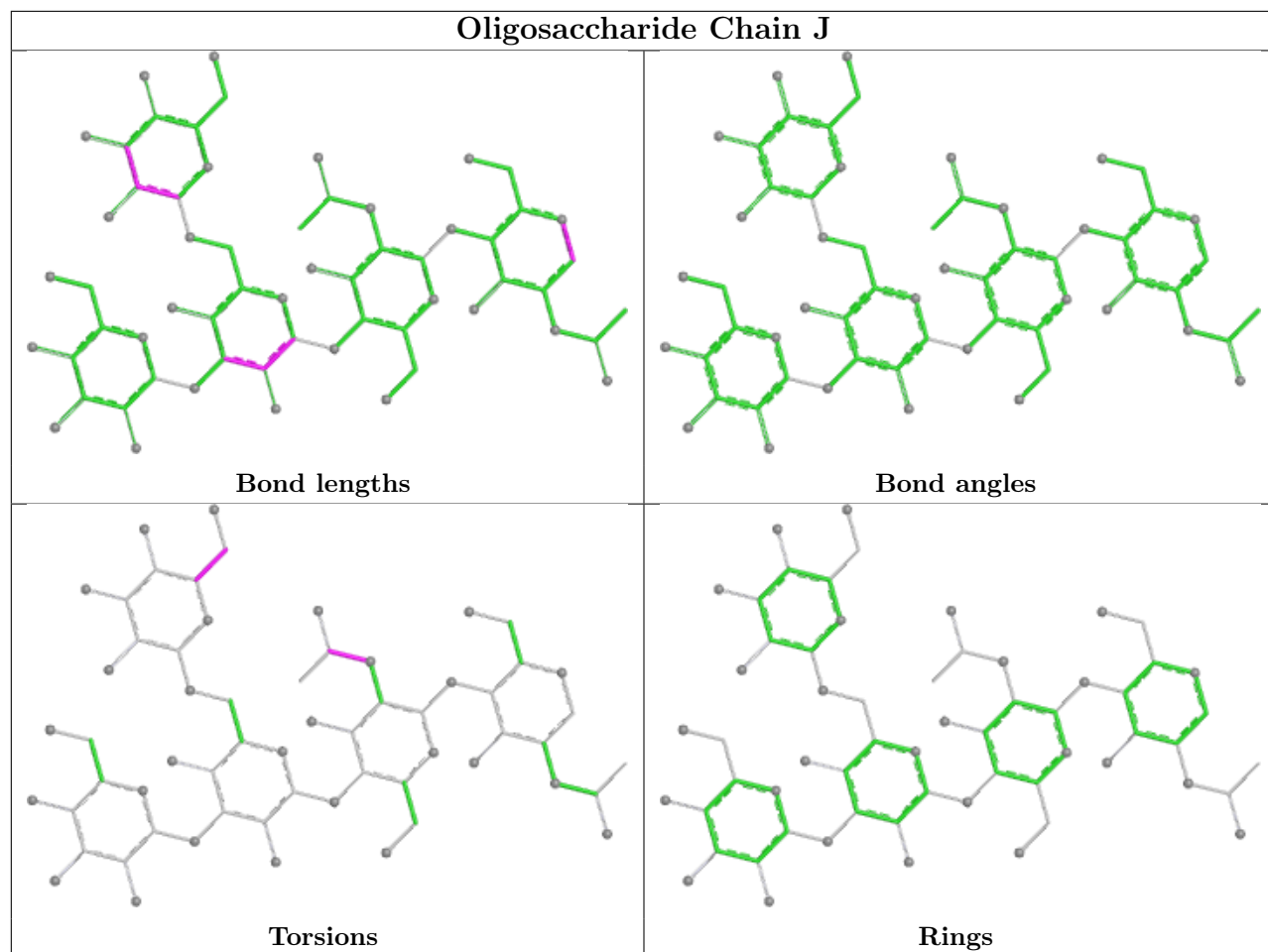


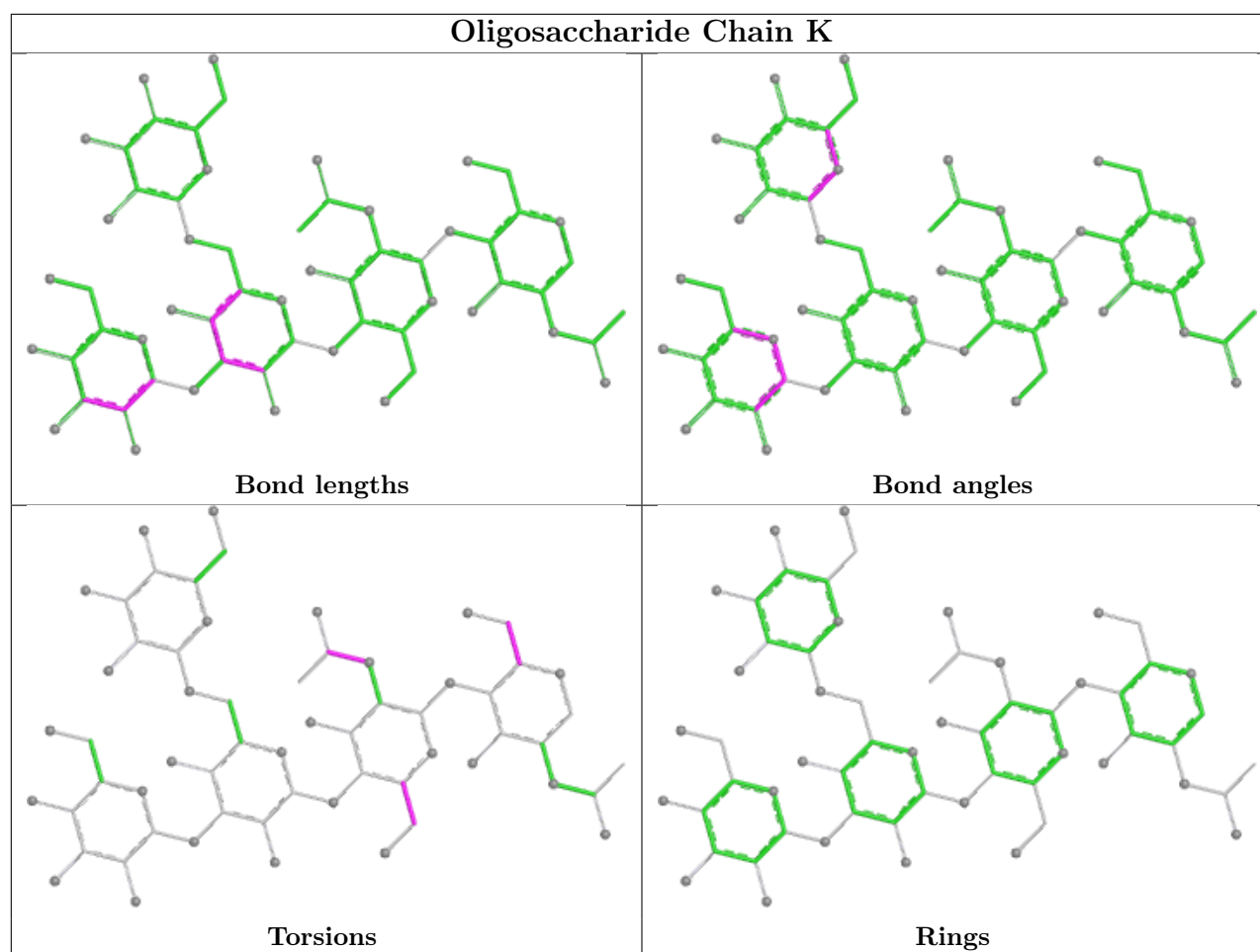


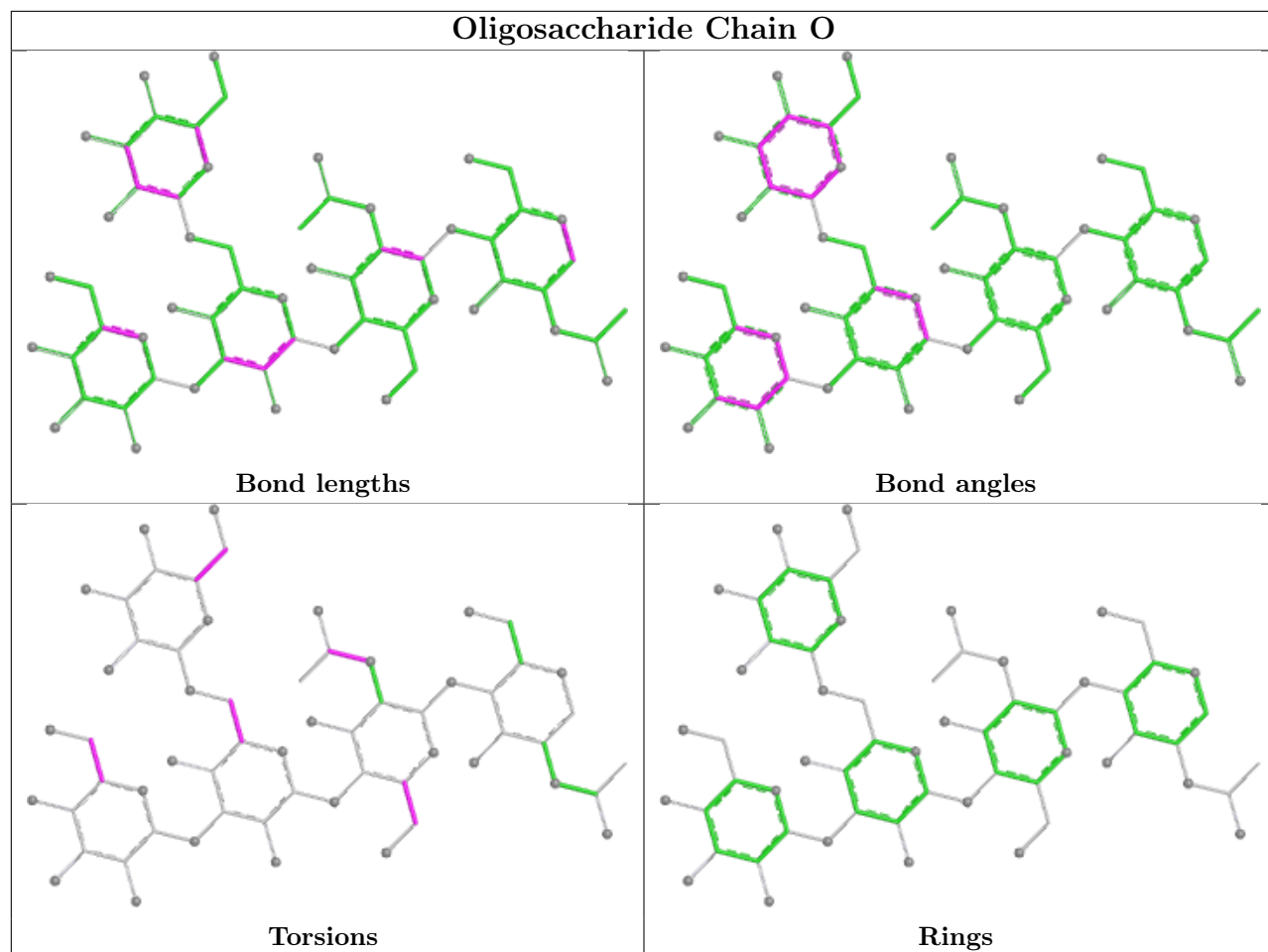


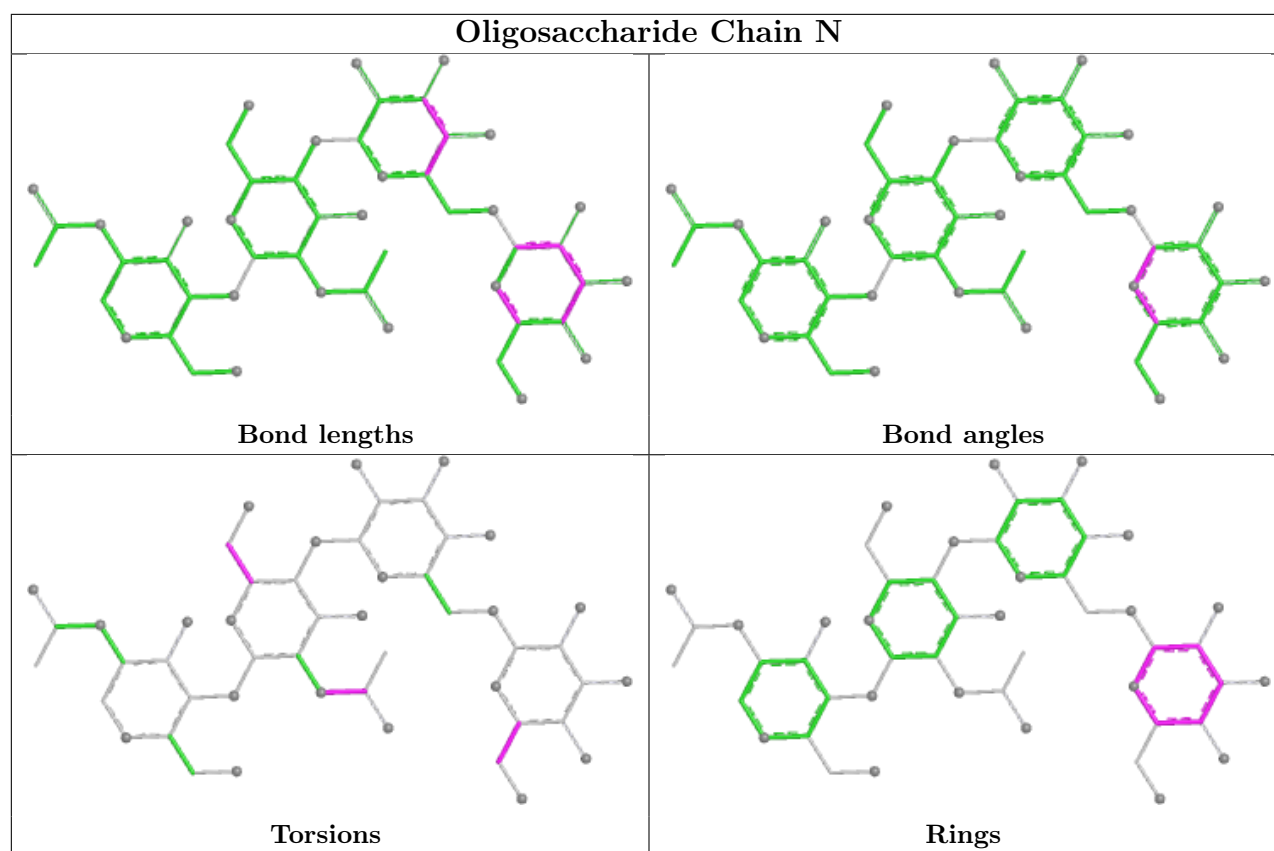












5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
8	NAG	A	719	1	14,14,15	0.50	0	17,19,21	0.43	0
8	NAG	C	709	1	14,14,15	0.56	0	17,19,21	0.60	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	719	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	C	709	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	709	NAG	C1-O5-C5	2.07	114.96	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	719	NAG	C1
8	C	709	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	719	NAG	O5-C5-C6-O6
8	A	719	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	430/430 (100%)	-0.29	1 (0%) 91 91	22, 45, 78, 114	0
1	C	430/430 (100%)	0.00	4 (0%) 81 76	29, 56, 93, 113	0
2	B	137/144 (95%)	0.35	11 (8%) 18 14	39, 71, 93, 108	0
2	D	136/144 (94%)	1.31	32 (23%) 2 1	59, 123, 140, 145	0
All	All	1133/1148 (98%)	0.09	48 (4%) 40 32	22, 56, 126, 145	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	65	VAL	4.9
2	B	65	VAL	4.6
2	B	94	GLU	4.5
2	D	102	ALA	4.4
2	B	93	LYS	4.3
2	D	75	TYR	4.1
2	D	101	CYS	3.7
1	A	197	SER	3.6
2	B	168	ALA	3.5
2	D	61	ILE	3.4
2	D	77	LYS	3.4
2	D	142	LEU	3.4
2	D	159	LYS	3.4
2	B	149	GLU	3.1
2	D	97	PRO	3.1
2	B	95	ASN	3.0
2	D	136	SER	3.0
2	D	96	THR	3.0
2	D	76	TYR	2.9
2	D	43	LEU	2.9
2	B	96	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	71	GLY	2.7
2	D	122	TRP	2.7
2	D	32	PRO	2.7
2	D	54	ILE	2.6
2	D	34	TYR	2.6
2	B	97	PRO	2.6
2	D	62	CYS	2.5
2	D	73	TYR	2.4
2	D	33	ILE	2.4
2	D	100	ASN	2.4
1	C	406	VAL	2.3
2	B	92	LYS	2.3
2	D	160	ILE	2.3
2	D	50	LEU	2.3
2	D	28	ILE	2.3
2	D	95	ASN	2.3
1	C	410	LYS	2.3
2	D	145	LEU	2.3
2	D	135	ILE	2.3
2	D	155	THR	2.2
2	D	49	VAL	2.2
2	D	44	PRO	2.1
2	B	122	TRP	2.1
2	D	92	LYS	2.1
2	D	167	ASP	2.1
1	C	622	CYS	2.0
1	C	394	PHE	2.0

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($\text{\AA}^2$)	Q<0.9
6	MAN	K	5	11/12	0.32	0.13	127,147,151,152	0

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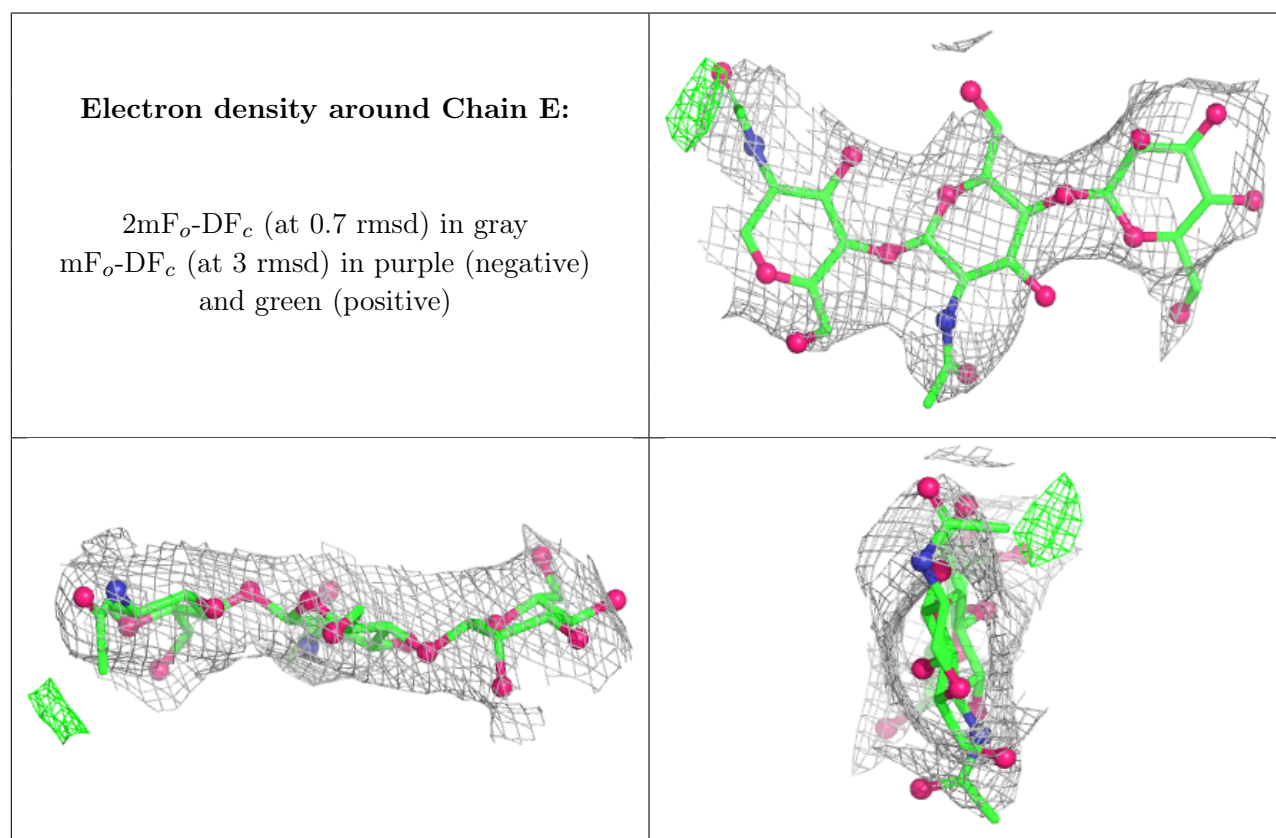
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	M	3	11/12	0.33	0.14	126,135,142,144	0
6	MAN	K	4	11/12	0.34	0.14	121,133,139,139	0
4	NAG	F	2	14/15	0.36	0.17	111,121,126,129	0
6	MAN	O	5	11/12	0.37	0.17	95,106,114,116	0
6	MAN	H	5	11/12	0.38	0.17	109,120,124,126	0
6	BMA	K	3	11/12	0.40	0.13	137,141,147,147	0
4	FUC	L	3	10/11	0.42	0.16	121,128,133,133	0
7	BMA	N	3	11/12	0.44	0.16	107,115,121,122	0
5	NAG	G	2	14/15	0.46	0.17	105,112,118,119	0
6	MAN	I	5	11/12	0.51	0.18	93,109,114,114	0
3	BMA	E	3	11/12	0.52	0.12	111,120,126,129	0
6	MAN	O	4	11/12	0.52	0.17	96,119,130,131	0
4	NAG	L	2	14/15	0.53	0.14	102,128,133,134	0
6	MAN	J	4	11/12	0.53	0.12	113,133,137,139	0
6	BMA	H	3	11/12	0.56	0.12	108,112,119,122	0
5	FUC	G	7	10/11	0.56	0.24	104,113,120,122	0
6	MAN	J	5	11/12	0.62	0.13	111,123,124,125	0
6	NAG	K	2	14/15	0.62	0.14	109,117,128,131	0
5	FUC	G	6	10/11	0.64	0.17	85,100,104,104	0
7	NAG	N	2	14/15	0.64	0.13	82,98,115,119	0
5	BMA	G	3	11/12	0.64	0.15	100,105,108,116	0
7	MAN	N	4	11/12	0.65	0.14	90,102,112,112	0
3	NAG	M	2	14/15	0.66	0.15	98,113,124,129	0
4	FUC	F	3	10/11	0.66	0.19	84,96,100,103	0
5	NAG	G	1	14/15	0.68	0.14	79,100,108,109	0
5	MAN	G	5	11/12	0.68	0.18	88,104,113,114	0
6	NAG	O	2	14/15	0.69	0.16	89,100,112,118	0
5	MAN	G	4	11/12	0.69	0.17	79,96,100,102	0
6	BMA	O	3	11/12	0.70	0.12	103,120,128,129	0
6	MAN	H	4	11/12	0.71	0.12	117,125,135,135	0
3	NAG	E	2	14/15	0.73	0.14	97,109,119,122	0
6	MAN	I	4	11/12	0.73	0.11	92,104,108,108	0
6	BMA	J	3	11/12	0.75	0.12	107,116,123,126	0
6	NAG	J	2	14/15	0.79	0.12	77,83,94,102	0
3	NAG	M	1	14/15	0.82	0.12	71,78,87,96	0
6	NAG	H	2	14/15	0.82	0.12	65,75,89,96	0
6	BMA	I	3	11/12	0.83	0.09	83,90,102,102	0
4	NAG	L	1	14/15	0.84	0.10	79,102,120,126	0
6	NAG	I	2	14/15	0.88	0.10	52,61,77,78	0
4	NAG	F	1	14/15	0.89	0.09	56,82,97,107	0
3	NAG	E	1	14/15	0.89	0.11	74,82,88,90	0
6	NAG	J	1	14/15	0.93	0.10	55,61,73,76	0

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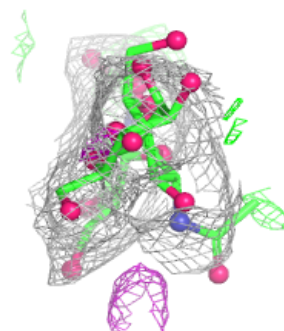
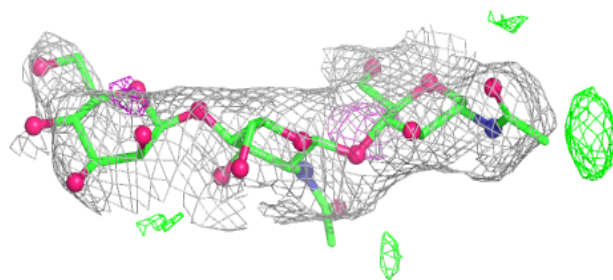
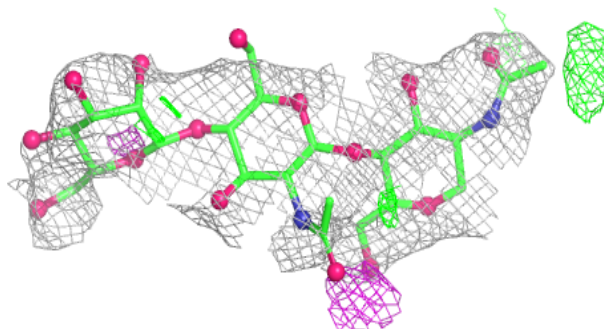
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	O	1	14/15	0.94	0.08	58,68,82,88	0
6	NAG	K	1	14/15	0.94	0.08	78,94,105,108	0
7	NAG	N	1	14/15	0.95	0.07	53,68,85,87	0
6	NAG	I	1	14/15	0.96	0.08	34,42,56,71	0
6	NAG	H	1	14/15	0.98	0.07	43,49,59,60	0

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.



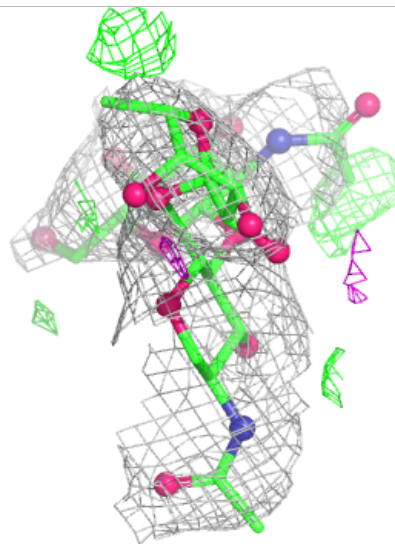
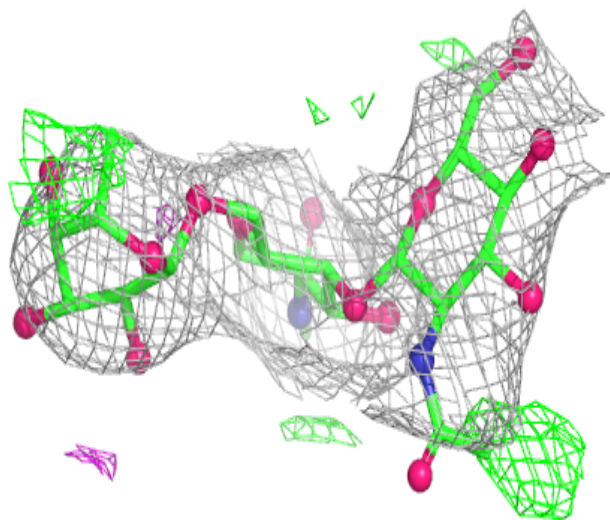
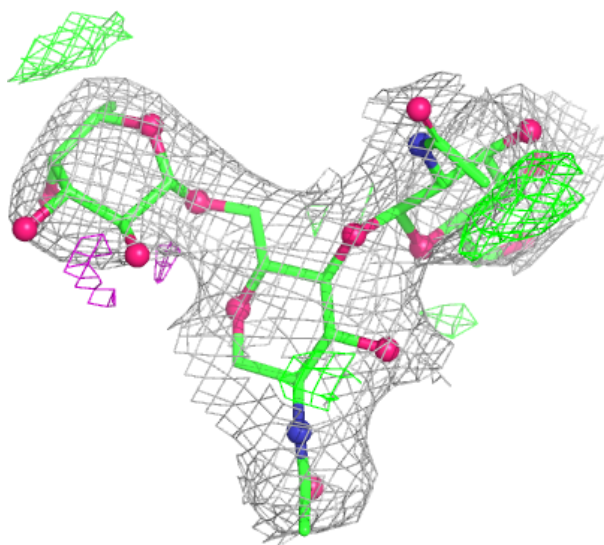
Electron density around Chain M:

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



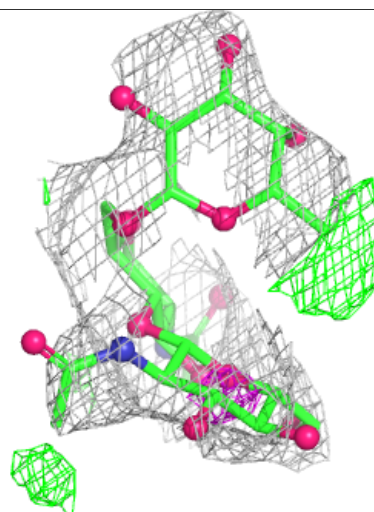
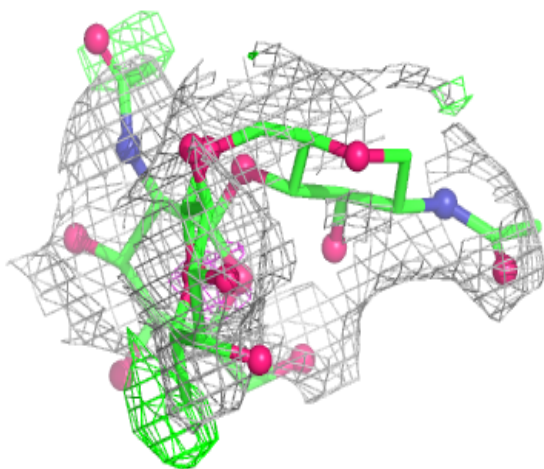
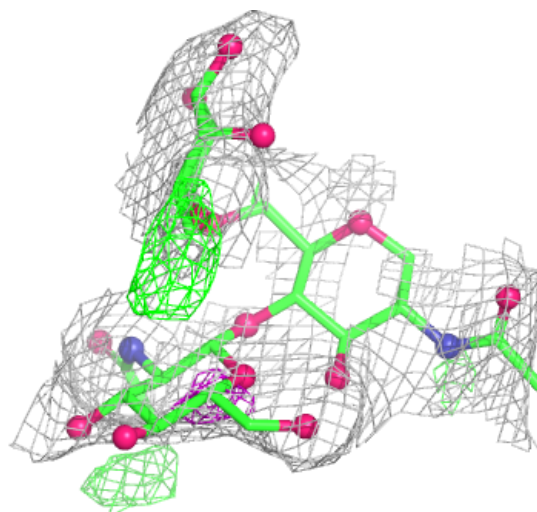
Electron density around Chain F:

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



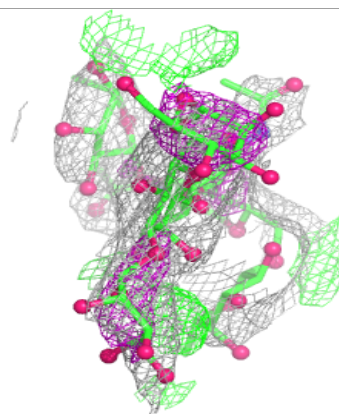
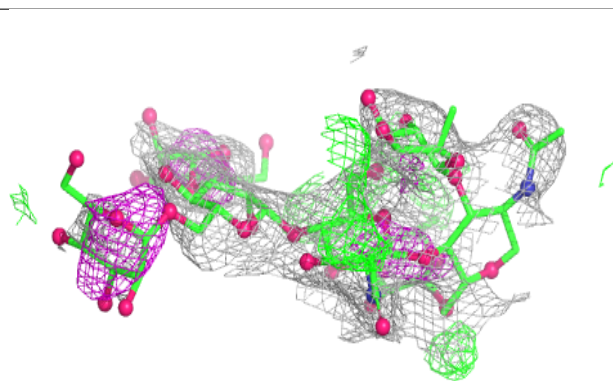
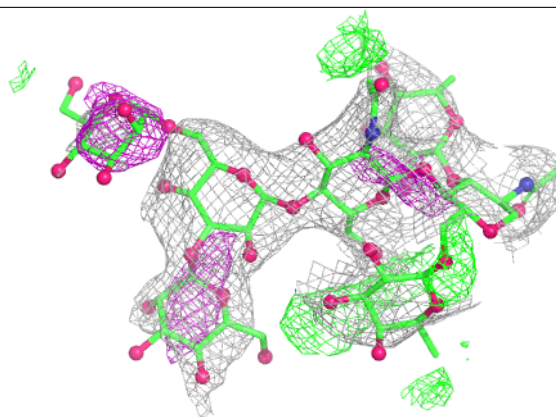
Electron density around Chain L:

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



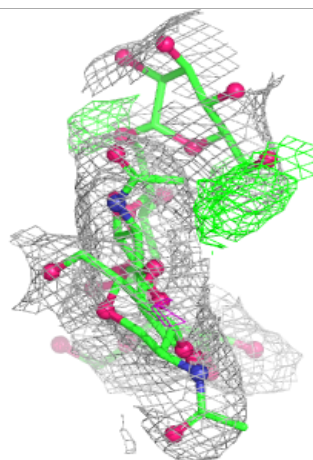
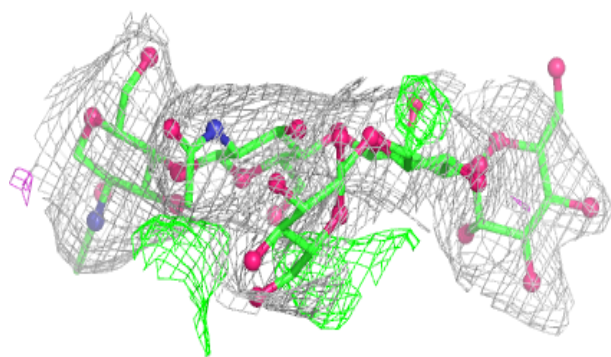
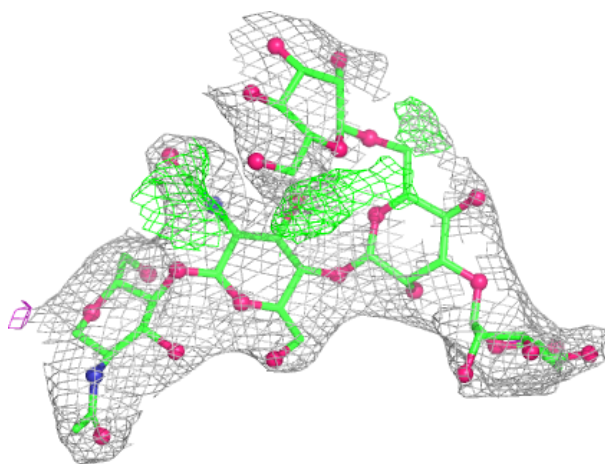
Electron density around Chain G:

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



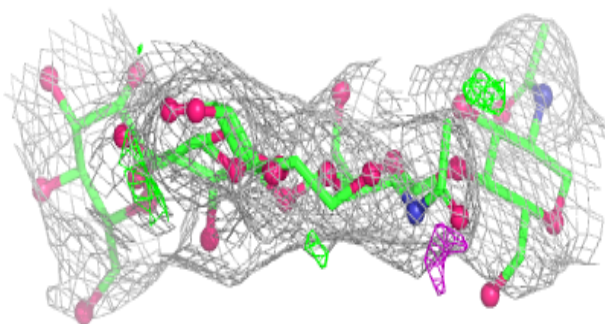
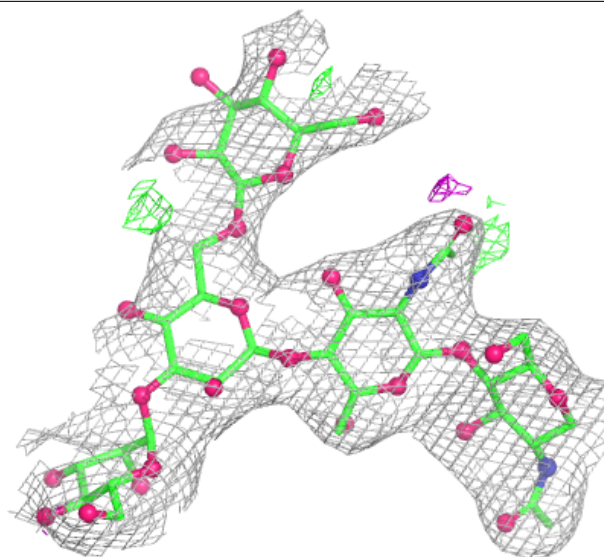
Electron density around Chain H:

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



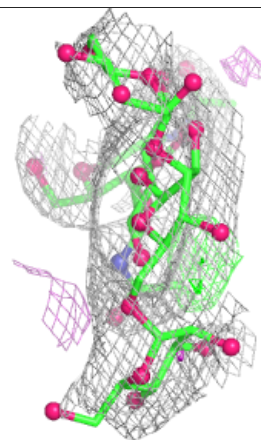
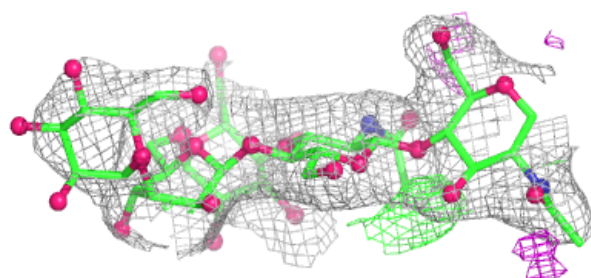
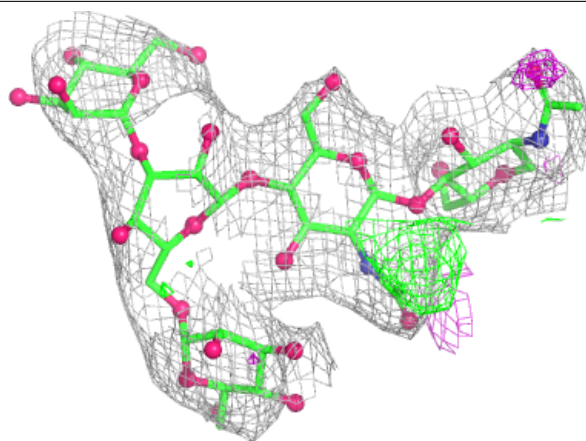
Electron density around Chain I:

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



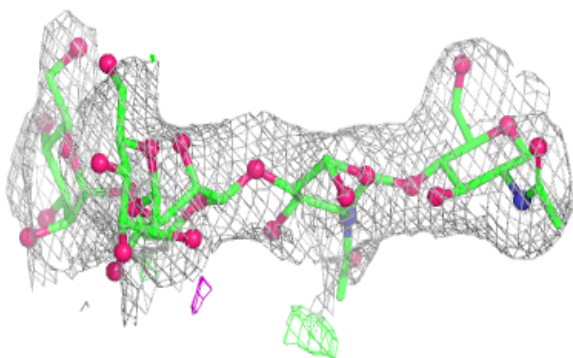
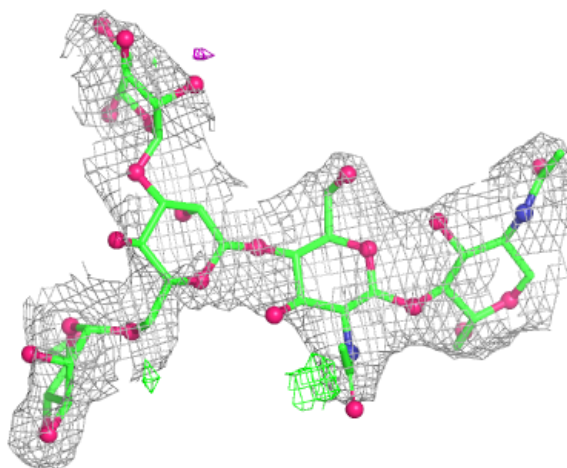
Electron density around Chain J:

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



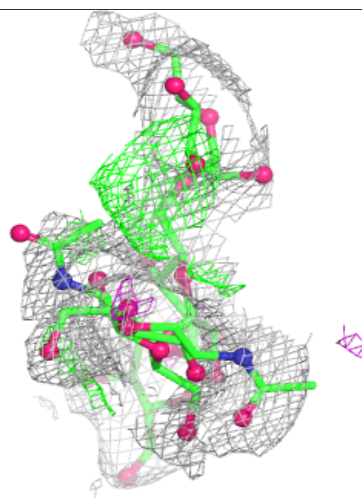
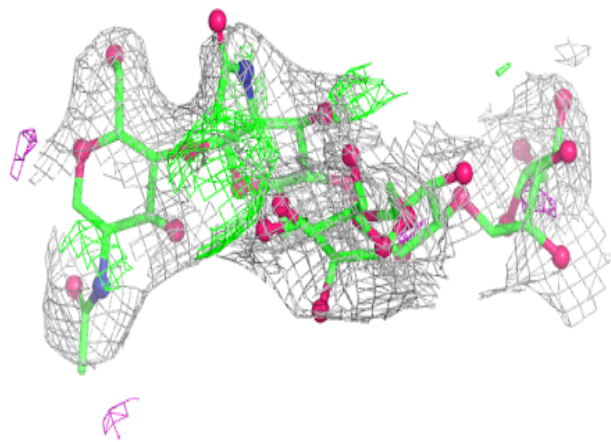
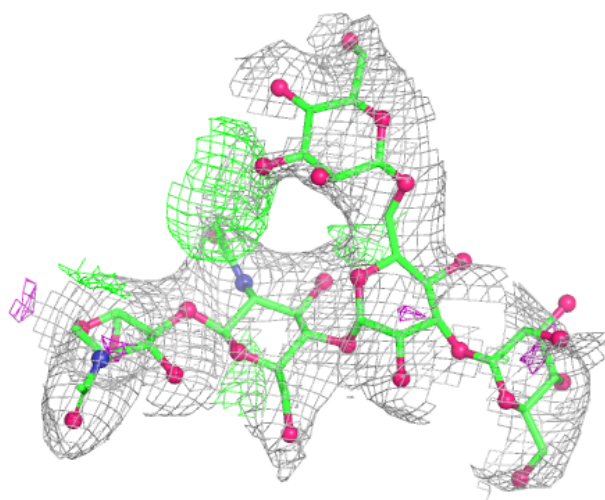
Electron density around Chain K:

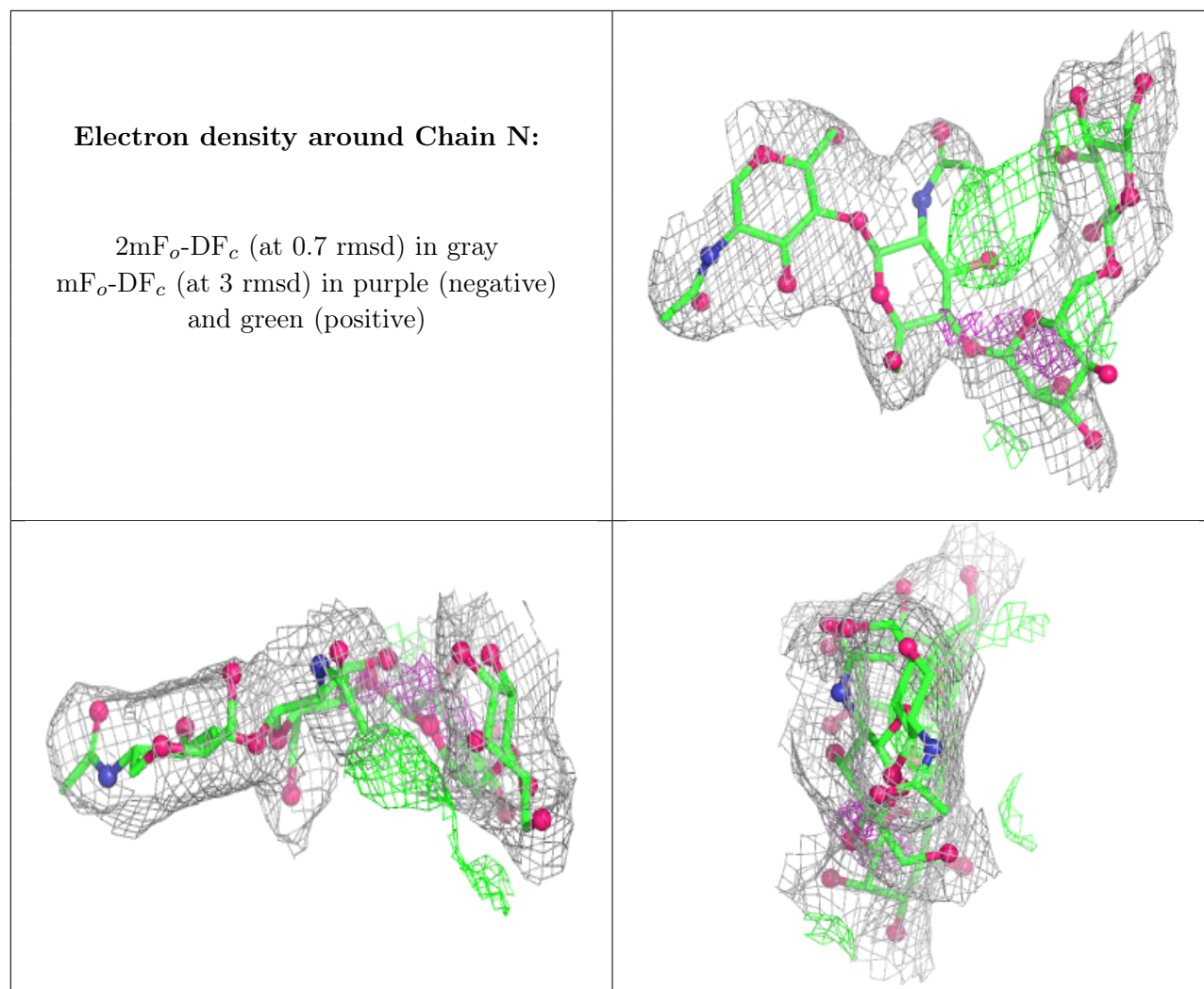
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
8	NAG	C	709	14/15	0.21	0.17	103,122,131,132	0
8	NAG	A	719	14/15	0.51	0.15	111,127,131,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.