



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:19 PM UTC

PDB ID : 7UYI / pdb_00007uyi
Title : Crystal structure of the computationally optimized broadly reactive H1 influenza hemagglutinin P1
Authors : Dzimianski, J.V.; DuBois, R.M.
Deposited on : 2022-05-06
Resolution : 3.00 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

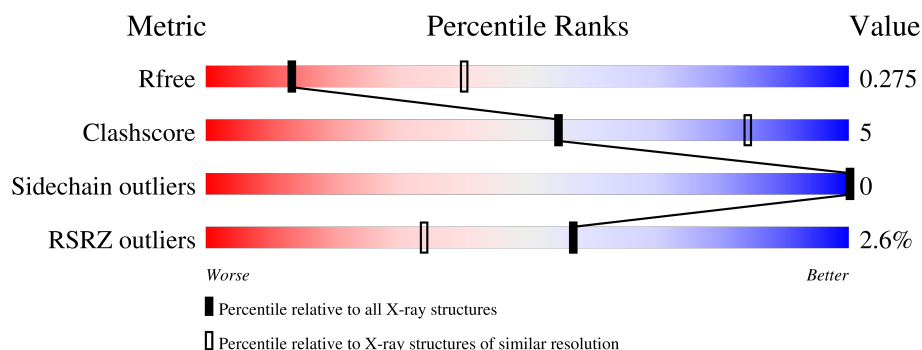
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	513	2% 80%14%6%
1	B	513	3% 81%13%6%
1	C	513	2% 81%13%6%
1	D	513	2% 81%9%10%
1	E	513	2% 81%11%8%
1	F	513	4% 83%9%8%

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Mol	Chain	Length	Quality of chain
2	G	4	
2	P	4	
3	H	2	
3	I	2	
3	K	2	
3	O	2	
3	Q	2	
4	J	3	
4	L	3	
4	M	3	
5	N	5	
5	R	5	

2 Entry composition [i](#)

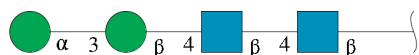
There are 7 unique types of molecules in this entry. The entry contains 23338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 COBRA P1 HA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3818	2394	659	746	19			
1	B	481	Total	C	N	O	S	0	1	0
			3804	2384	657	744	19			
1	C	481	Total	C	N	O	S	0	1	0
			3806	2383	658	746	19			
1	E	474	Total	C	N	O	S	0	0	0
			3753	2358	647	729	19			
1	F	473	Total	C	N	O	S	0	0	0
			3746	2350	647	730	19			
1	D	460	Total	C	N	O	S	0	0	0
			3643	2290	627	707	19			

- Molecule 2 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.



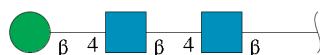
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



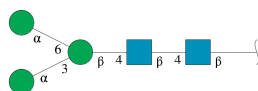
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	M	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)]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	N	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

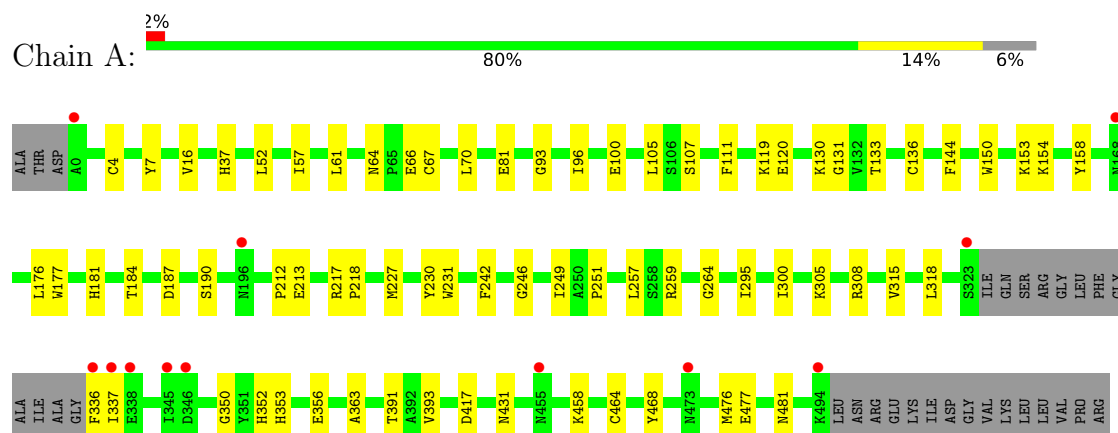
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	O	0	0
			4	4		
7	B	4	Total	O	0	0
			4	4		
7	C	5	Total	O	0	0
			5	5		
7	E	6	Total	O	0	0
			6	6		
7	F	1	Total	O	0	0
			1	1		
7	D	3	Total	O	0	0
			3	3		

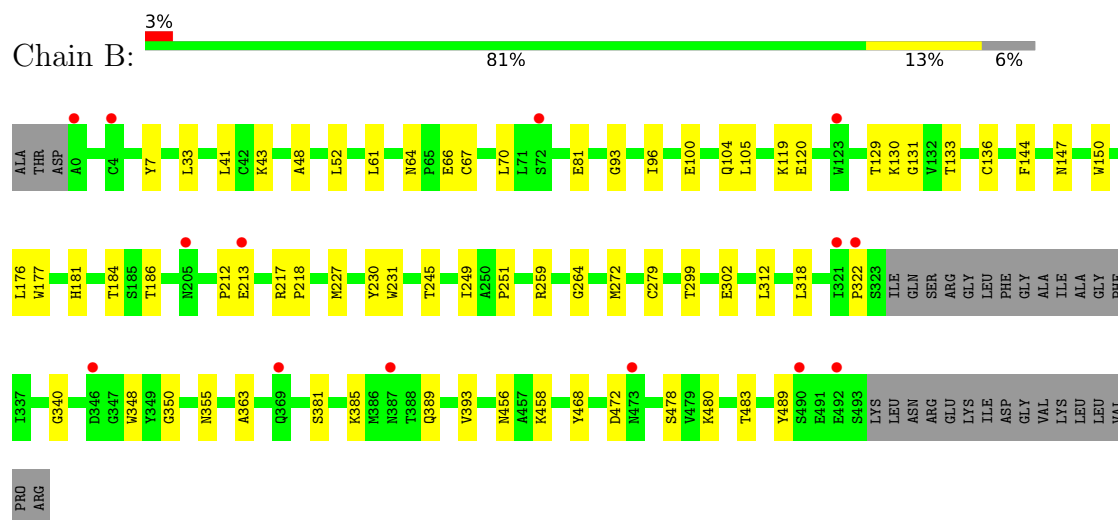
3 Residue-property plots [i](#)

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.

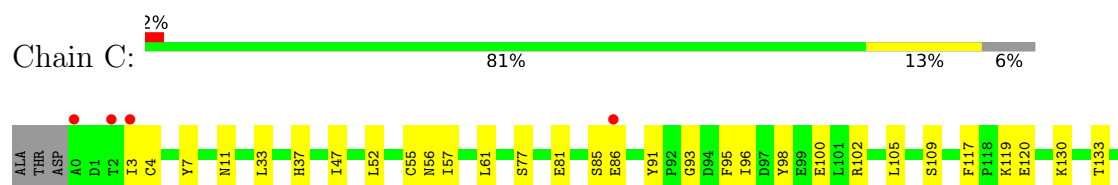
• Molecule 1: COBRA P1 HA

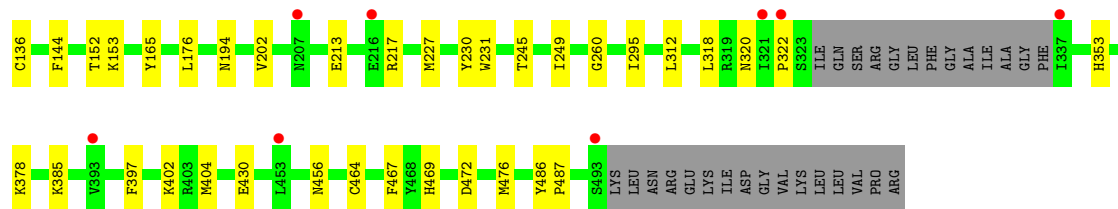


• Molecule 1: COBRA P1 HA

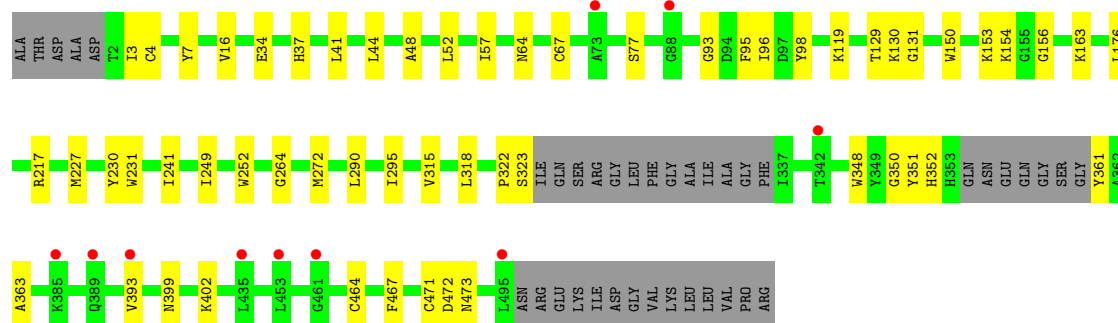
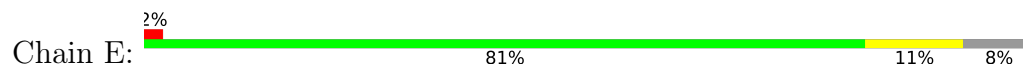


• Molecule 1: COBRA P1 HA

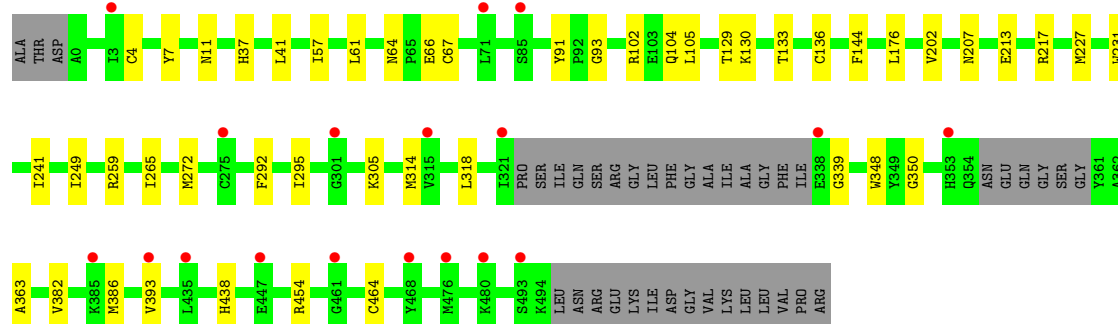
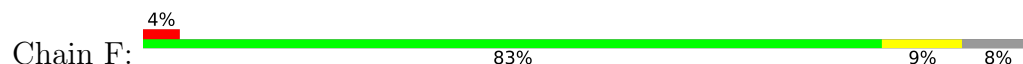




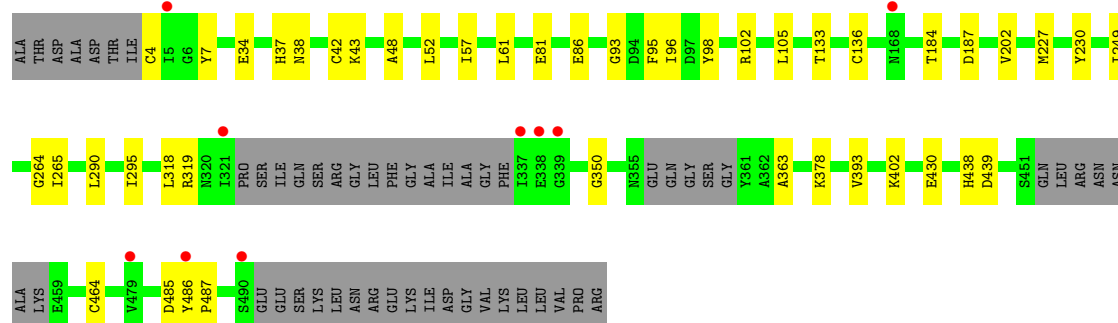
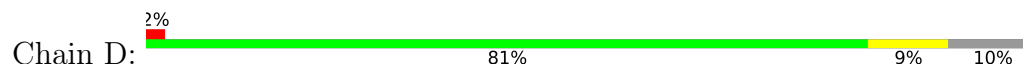
• Molecule 1: COBRA P1 HA



• Molecule 1: COBRA P1 HA



• Molecule 1: COBRA P1 HA



- Molecule 2: 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 G: 

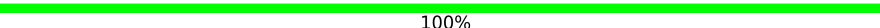


- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 



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

Chain H: 



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

Chain I: 



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

Chain K: 

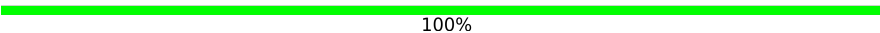


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 



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

Chain Q: 



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

Chain J: 67% 33%



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

Chain L: 100%



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

Chain M: 33% 67%



- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 40% 60%



- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 40% 60%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.85Å 77.56Å 222.52Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	47.75 – 3.00 47.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.75-3.00) 99.8 (47.75-3.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.226 , 0.270 (Not available) , 0.275	Depositor DCC
R_{free} test set	4570 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23338	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.09	0/3906	0.27	0/5292
1	B	0.09	0/3894	0.28	0/5276
1	C	0.10	0/3893	0.29	0/5276
1	D	0.09	0/3727	0.26	0/5049
1	E	0.09	0/3839	0.27	0/5201
1	F	0.08	0/3831	0.27	0/5189
All	All	0.09	0/23090	0.27	0/31283

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 [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	3818	0	3657	44	0
1	B	3804	0	3648	43	0
1	C	3806	0	3642	44	0
1	D	3643	0	3489	27	0
1	E	3753	0	3611	36	0
1	F	3746	0	3596	36	0
2	G	50	0	43	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	50	0	43	1	0
3	H	28	0	25	0	0
3	I	28	0	25	1	0
3	K	28	0	25	0	0
3	O	28	0	25	1	0
3	Q	28	0	25	0	0
4	J	39	0	34	1	0
4	L	39	0	34	0	0
4	M	39	0	34	1	0
5	N	61	0	52	0	0
5	R	61	0	52	1	0
6	A	56	0	52	2	0
6	B	56	0	52	0	0
6	C	56	0	52	2	0
6	D	56	0	52	0	0
6	E	14	0	13	0	0
6	F	28	0	26	0	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
7	C	5	0	0	0	0
7	D	3	0	0	0	0
7	E	6	0	0	0	0
7	F	1	0	0	0	0
All	All	23338	0	22307	220	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 5.

All (220) 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:F:61:LEU:HD11	1:F:105:LEU:HD11	1.57	0.86
1:C:61:LEU:HD11	1:C:105:LEU:HD11	1.63	0.79
1:A:264:GLY:HA3	1:A:393:VAL:HG11	1.65	0.79
1:B:129:THR:HG22	1:B:130:LYS:H	1.51	0.76
1:C:227:MET:HE3	1:C:249:ILE:HG13	1.67	0.76
1:B:227:MET:HE3	1:B:249:ILE:HG13	1.68	0.74
1:D:61:LEU:HD11	1:D:105:LEU:HD11	1.67	0.74
1:D:227:MET:HE3	1:D:249:ILE:HG13	1.67	0.74
1:A:227:MET:HE3	1:A:249:ILE:HG13	1.70	0.73
1:A:61:LEU:HD11	1:A:105:LEU:HD11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HD11	1:B:105:LEU:HD11	1.70	0.72
1:E:4:CYS:HB2	1:E:352:HIS:HB3	1.71	0.72
1:A:154:LYS:HE3	6:A:601:NAG:H81	1.72	0.72
1:B:264:GLY:HA3	1:B:393:VAL:HG11	1.72	0.72
1:F:7:TYR:HB2	1:F:318:LEU:HD13	1.72	0.71
1:E:322:PRO:HG2	1:F:11:ASN:HB2	1.72	0.71
1:E:227:MET:HE3	1:E:249:ILE:HG13	1.73	0.69
1:D:7:TYR:HB2	1:D:318:LEU:HD13	1.75	0.68
1:A:7:TYR:HB2	1:A:318:LEU:HD13	1.75	0.68
1:B:458:LYS:HE3	1:F:454:ARG:HH22	1.58	0.66
1:C:56:ASN:OD1	1:C:57:ILE:N	2.26	0.66
1:F:227:MET:HE3	1:F:249:ILE:HG13	1.78	0.66
1:C:130:LYS:HB3	1:C:152:THR:HG21	1.78	0.65
1:A:100:GLU:OE2	1:C:402:LYS:N	2.30	0.65
1:D:318:LEU:HD21	1:D:438:HIS:HB3	1.80	0.64
1:B:100:GLU:OE2	1:D:402:LYS:N	2.30	0.64
1:A:308:ARG:NH1	1:A:417:ASP:OD1	2.32	0.63
1:E:264:GLY:HA3	1:E:393:VAL:HG21	1.80	0.63
1:E:154:LYS:HE3	3:O:1:NAG:H81	1.82	0.61
1:E:129:THR:HG22	1:E:130:LYS:H	1.65	0.61
1:A:130:LYS:HD3	6:A:601:NAG:H62	1.84	0.60
1:B:131:GLY:HA3	1:B:150:TRP:HB3	1.83	0.60
1:A:218:PRO:HD3	1:E:241:ILE:HD13	1.84	0.59
1:F:129:THR:HG22	1:F:130:LYS:H	1.66	0.59
1:C:119:LYS:NZ	1:C:120:GLU:OE2	2.33	0.59
1:A:4:CYS:HB2	1:A:352:HIS:HB3	1.82	0.59
1:A:52:LEU:HD12	1:A:81:GLU:HG2	1.83	0.59
1:C:100:GLU:OE2	1:E:402:LYS:N	2.33	0.59
1:A:131:GLY:HA3	1:A:150:TRP:HB3	1.85	0.58
1:C:37:HIS:HB3	1:C:295:ILE:HD13	1.85	0.58
1:A:66:GLU:HG2	2:G:1:NAG:H82	1.86	0.57
1:E:323:SER:HB3	1:F:11:ASN:HB3	1.85	0.57
1:E:48:ALA:HB1	1:E:272:MET:HE1	1.85	0.57
1:A:133:THR:HG23	1:A:136:CYS:H	1.69	0.57
1:C:86:GLU:HG3	4:M:1:NAG:H61	1.88	0.56
1:B:130:LYS:HG3	1:B:131:GLY:H	1.71	0.56
1:E:37:HIS:HD2	1:E:295:ILE:HD12	1.71	0.55
1:B:61:LEU:O	1:B:147:ASN:ND2	2.34	0.55
1:F:314:MET:HE1	1:F:382:VAL:HG21	1.87	0.55
1:C:4:CYS:HA	1:C:464:CYS:HA	1.90	0.54
1:A:242:PHE:HE2	1:A:251:PRO:HG2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:THR:HG23	1:D:187:ASP:H	1.71	0.54
1:B:218:PRO:HD3	1:F:241:ILE:HD13	1.90	0.54
1:B:299:THR:OG1	1:B:389:GLN:NE2	2.41	0.54
1:C:486:TYR:CD2	1:C:487:PRO:HD3	2.43	0.54
1:F:57:ILE:HD11	1:F:265:ILE:HG21	1.90	0.53
1:C:353:HIS:NE2	1:C:476:MET:HG3	2.23	0.53
1:F:7:TYR:H	1:F:339:GLY:HA2	1.73	0.53
1:C:486:TYR:CG	1:C:487:PRO:HD3	2.43	0.53
1:D:264:GLY:HA3	1:D:393:VAL:HG11	1.90	0.52
1:B:133:THR:HG23	1:B:136:CYS:H	1.74	0.52
1:B:322:PRO:HG3	1:B:340:GLY:H	1.74	0.52
1:D:37:HIS:HB3	1:D:295:ILE:HD13	1.90	0.52
1:B:177:TRP:HB3	1:B:251:PRO:HG3	1.92	0.51
1:A:107:SER:OG	1:A:259:ARG:NH1	2.43	0.51
1:A:184:THR:HG23	1:A:187:ASP:H	1.75	0.51
1:D:133:THR:HG23	1:D:136:CYS:H	1.75	0.51
1:A:67:CYS:HB3	1:A:70:LEU:HD12	1.92	0.51
1:A:144:PHE:HZ	1:A:227:MET:HE1	1.76	0.51
1:D:350:GLY:HA3	1:D:363:ALA:HA	1.92	0.51
1:F:7:TYR:CZ	1:F:339:GLY:HA3	2.47	0.50
1:C:11:ASN:HD22	6:C:601:NAG:C7	2.24	0.50
1:E:4:CYS:HA	1:E:464:CYS:HA	1.93	0.50
1:D:378:LYS:NZ	1:D:430:GLU:OE1	2.44	0.50
1:B:64:ASN:HB3	1:B:67:CYS:SG	2.52	0.49
1:B:318:LEU:HD11	1:B:348:TRP:HB3	1.94	0.49
1:A:336:PHE:HD2	1:A:337:ILE:HG22	1.78	0.49
1:C:3:ILE:HD11	1:C:476:MET:SD	2.52	0.49
1:F:37:HIS:HD2	1:F:295:ILE:HD12	1.77	0.49
1:C:52:LEU:HD12	1:C:81:GLU:HG3	1.94	0.49
3:I:1:NAG:H62	3:I:2:NAG:H82	1.94	0.49
1:B:129:THR:HG22	1:B:130:LYS:N	2.25	0.49
1:E:52:LEU:HD11	1:E:57:ILE:HD13	1.95	0.49
1:A:350:GLY:HA3	1:A:363:ALA:HA	1.95	0.48
1:E:318:LEU:HD11	1:E:348:TRP:HB3	1.94	0.48
1:C:93:GLY:HA3	1:C:227:MET:O	2.13	0.48
1:B:119:LYS:NZ	1:B:120:GLU:OE2	2.46	0.48
1:D:319:ARG:HH12	1:D:439:ASP:CG	2.21	0.48
1:C:176:LEU:HD23	1:C:231:TRP:HB3	1.95	0.48
1:B:52:LEU:HD12	1:B:81:GLU:HG2	1.96	0.48
1:B:93:GLY:HA3	1:B:227:MET:O	2.14	0.48
1:B:355:ASN:HD21	1:B:472:ASP:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ASN:ND2	1:B:489:TYR:O	2.47	0.48
1:F:213:GLU:O	1:F:217:ARG:NH2	2.35	0.48
1:E:96:ILE:HG13	1:E:230:TYR:CE2	2.49	0.48
1:D:93:GLY:HA3	1:D:227:MET:O	2.13	0.48
1:C:47:ILE:HB	1:C:77:SER:HB3	1.96	0.47
1:E:176:LEU:HD23	1:E:231:TRP:HB3	1.96	0.47
1:E:472:ASP:OD1	1:E:473:ASN:N	2.44	0.47
1:C:91:TYR:HD2	1:C:133:THR:HG21	1.79	0.47
1:C:213:GLU:HG3	1:C:217:ARG:HH21	1.79	0.47
1:B:217:ARG:HG2	1:F:202:VAL:HG11	1.96	0.47
1:E:95:PHE:HB3	1:E:98:TYR:HB2	1.97	0.47
1:F:176:LEU:HD23	1:F:231:TRP:HB3	1.96	0.47
1:A:477:GLU:O	1:A:481:ASN:HB2	2.15	0.47
1:E:350:GLY:HA3	1:E:363:ALA:HA	1.94	0.47
1:A:64:ASN:HB3	1:A:67:CYS:SG	2.55	0.47
1:C:133:THR:HG23	1:C:136:CYS:H	1.79	0.47
1:C:202:VAL:HG11	1:E:217:ARG:HG2	1.95	0.47
1:D:57:ILE:HD11	1:D:265:ILE:HD13	1.97	0.47
1:A:37:HIS:HB3	1:A:295:ILE:HD13	1.97	0.47
1:B:144:PHE:HZ	1:B:227:MET:HE1	1.79	0.47
1:B:350:GLY:HA3	1:B:363:ALA:HA	1.96	0.47
1:A:242:PHE:CE2	1:A:251:PRO:HG2	2.49	0.46
1:A:300:ILE:HD13	1:A:391:THR:HG23	1.97	0.46
1:C:320:ASN:O	1:C:322:PRO:HD3	2.14	0.46
1:D:86:GLU:HG3	5:R:1:NAG:H61	1.96	0.46
1:B:478:SER:HB3	1:B:483:THR:O	2.15	0.46
1:A:16:VAL:HG21	1:A:315:VAL:HG22	1.96	0.46
1:A:119:LYS:NZ	1:A:120:GLU:OE2	2.39	0.46
1:C:95:PHE:HB3	1:C:98:TYR:HB2	1.98	0.46
1:A:93:GLY:HA3	1:A:227:MET:O	2.15	0.46
1:C:57:ILE:HD12	1:C:102:ARG:NE	2.30	0.46
1:C:11:ASN:ND2	6:C:601:NAG:O7	2.49	0.46
1:E:41:LEU:HB2	1:E:272:MET:HA	1.99	0.45
1:B:104:GLN:OE1	1:B:259:ARG:NH2	2.50	0.45
1:C:55:CYS:O	1:C:85:SER:HB2	2.16	0.45
1:C:378:LYS:NZ	1:C:430:GLU:OE1	2.34	0.45
1:C:467:PHE:HB3	1:C:469:HIS:O	2.16	0.45
1:F:7:TYR:CE2	1:F:339:GLY:HA3	2.51	0.45
1:A:52:LEU:HD11	1:A:57:ILE:HD13	1.99	0.45
1:E:16:VAL:HG21	1:E:315:VAL:HG22	1.98	0.45
1:E:34:GLU:HB2	1:E:290:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:LEU:HB2	1:F:272:MET:HA	1.99	0.45
1:E:467:PHE:HD2	1:E:471:CYS:HB2	1.81	0.45
1:A:153:LYS:HE2	1:A:190:SER:O	2.16	0.45
1:A:177:TRP:HB3	1:A:251:PRO:HG3	1.98	0.45
1:C:472:ASP:O	1:C:476:MET:HG2	2.16	0.45
1:A:353:HIS:HB2	1:A:476:MET:SD	2.57	0.44
1:C:456:ASN:HB3	1:C:469:HIS:CD2	2.52	0.44
1:F:57:ILE:HD12	1:F:102:ARG:NE	2.31	0.44
1:F:91:TYR:HD2	1:F:133:THR:HG21	1.83	0.44
1:F:133:THR:HG23	1:F:136:CYS:H	1.82	0.44
1:C:144:PHE:HZ	1:C:227:MET:HE1	1.82	0.44
1:D:38:ASN:ND2	1:D:42:CYS:SG	2.89	0.44
1:A:356:GLU:CD	1:A:356:GLU:H	2.25	0.44
1:C:117:PHE:CE1	1:C:165:TYR:HB2	2.51	0.44
1:B:33:LEU:HB2	1:B:312:LEU:HB2	2.00	0.44
1:E:129:THR:HG22	1:E:130:LYS:N	2.30	0.44
1:B:176:LEU:HD23	1:B:231:TRP:HB3	1.98	0.44
1:C:7:TYR:HB2	1:C:318:LEU:HD22	2.00	0.44
1:C:397:PHE:HE1	1:C:404:MET:HE3	1.83	0.44
1:F:217:ARG:HG2	1:D:202:VAL:HG11	2.00	0.44
1:A:305:LYS:HE3	1:A:305:LYS:HB2	1.76	0.44
1:E:3:ILE:HD11	1:E:351:TYR:HB3	2.00	0.44
1:F:305:LYS:HE3	1:F:305:LYS:HB2	1.85	0.44
1:D:485:ASP:OD1	1:D:487:PRO:HD2	2.18	0.44
1:C:194:ASN:HD22	1:C:245:THR:HB	1.83	0.43
1:B:66:GLU:HG2	4:J:1:NAG:H82	1.99	0.43
1:F:144:PHE:HZ	1:F:227:MET:HE1	1.82	0.43
1:B:279:CYS:HB2	1:B:302:GLU:O	2.19	0.43
1:A:4:CYS:HA	1:A:464:CYS:HA	2.01	0.43
1:B:181:HIS:ND1	1:B:212:PRO:HA	2.34	0.43
1:E:64:ASN:HB3	1:E:67:CYS:SG	2.59	0.43
1:F:265:ILE:H	1:F:393:VAL:HG21	1.84	0.43
1:D:52:LEU:HD12	1:D:81:GLU:HB3	2.00	0.43
1:B:381:SER:O	1:B:385:LYS:HG2	2.19	0.43
1:E:399:ASN:OD1	1:E:399:ASN:N	2.52	0.43
1:F:202:VAL:HG13	1:F:207:ASN:HB3	2.01	0.43
1:D:95:PHE:HB3	1:D:98:TYR:HB2	2.01	0.43
1:B:96:ILE:HG13	1:B:230:TYR:CE1	2.54	0.43
1:F:104:GLN:O	1:F:259:ARG:NH1	2.52	0.42
1:D:57:ILE:HD12	1:D:102:ARG:NE	2.34	0.42
1:E:131:GLY:HA3	1:E:150:TRP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:GLU:HG2	2:P:1:NAG:H82	2.01	0.42
1:F:64:ASN:HB3	1:F:67:CYS:SG	2.59	0.42
1:B:67:CYS:HB3	1:B:70:LEU:HD12	2.01	0.42
1:C:96:ILE:HG13	1:C:230:TYR:CE2	2.55	0.42
1:D:4:CYS:HA	1:D:464:CYS:HA	2.00	0.42
1:B:7:TYR:HB2	1:B:318:LEU:HD22	2.01	0.42
1:F:292:PHE:HZ	1:F:386:MET:HE3	1.84	0.42
1:C:385:LYS:HD3	1:C:385:LYS:HA	1.76	0.42
1:E:44:LEU:HB3	1:E:77:SER:HB2	2.01	0.42
1:D:43:LYS:HE3	1:D:48:ALA:HB2	2.02	0.42
1:D:486:TYR:HB3	1:D:487:PRO:HD3	2.00	0.42
1:A:96:ILE:HG13	1:A:230:TYR:CE1	2.55	0.42
1:D:318:LEU:CD2	1:D:438:HIS:HB3	2.50	0.42
1:B:43:LYS:HG2	1:B:48:ALA:HA	2.02	0.41
1:C:213:GLU:HG3	1:C:217:ARG:NH2	2.35	0.41
1:C:130:LYS:HG2	1:C:130:LYS:O	2.20	0.41
1:A:181:HIS:CE1	1:A:212:PRO:HA	2.55	0.41
1:B:245:THR:HG22	1:B:245:THR:O	2.20	0.41
1:F:93:GLY:HA3	1:F:227:MET:O	2.20	0.41
1:F:350:GLY:HA3	1:F:363:ALA:HA	2.02	0.41
1:C:152:THR:OG1	1:C:153:LYS:N	2.53	0.41
1:F:4:CYS:HA	1:F:464:CYS:HA	2.02	0.41
1:F:318:LEU:HD23	1:F:438:HIS:CG	2.56	0.41
1:B:184:THR:HG22	1:B:186:THR:H	1.86	0.41
1:C:109:SER:HB3	1:C:260:GLY:HA3	2.01	0.41
1:E:163:LYS:HD2	1:E:163:LYS:HA	1.90	0.41
1:B:41:LEU:HB2	1:B:272:MET:HA	2.02	0.41
1:B:213:GLU:O	1:B:217:ARG:NH2	2.44	0.41
1:E:7:TYR:HB2	1:E:318:LEU:HD22	2.02	0.41
1:D:34:GLU:HB2	1:D:290:LEU:HD12	2.03	0.41
1:A:111:PHE:HB3	1:A:257:LEU:HD23	2.02	0.41
1:F:318:LEU:HD11	1:F:348:TRP:HB3	2.03	0.41
1:D:96:ILE:HG13	1:D:230:TYR:CE2	2.56	0.41
1:A:213:GLU:O	1:A:217:ARG:NH2	2.44	0.41
1:B:480:LYS:HB3	1:B:480:LYS:HE2	1.82	0.41
1:E:119:LYS:HD2	1:E:252:TRP:CZ2	2.56	0.41
1:E:153:LYS:HE3	1:E:156:GLY:HA2	2.03	0.41
1:F:57:ILE:HD11	1:F:265:ILE:HD13	2.03	0.41
1:B:458:LYS:HB2	1:B:468:TYR:CZ	2.56	0.40
1:E:352:HIS:HA	1:E:361:TYR:HA	2.03	0.40
1:A:158:TYR:CZ	1:A:246:GLY:HA2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LEU:HD23	1:A:231:TRP:HB3	2.03	0.40
1:A:315:VAL:HG23	1:A:431:ASN:CG	2.47	0.40
1:A:458:LYS:HB2	1:A:468:TYR:CZ	2.56	0.40
1:C:33:LEU:HB2	1:C:312:LEU:HB2	2.03	0.40
1:E:93:GLY:HA3	1:E:227:MET:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/446 (95%)	423 (100%)	0	100	100
1	B	422/446 (95%)	422 (100%)	0	100	100
1	C	422/446 (95%)	422 (100%)	0	100	100
1	D	404/446 (91%)	404 (100%)	0	100	100
1	E	417/446 (94%)	417 (100%)	0	100	100
1	F	415/446 (93%)	415 (100%)	0	100	100
All	All	2503/2676 (94%)	2503 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	B	193	GLN

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Mol	Chain	Res	Type
1	B	354	GLN
1	C	126	HIS
1	C	180	HIS
1	C	194	ASN
1	C	456	ASN
1	E	37	HIS
1	E	283	GLN
1	E	444	ASN
1	E	455	ASN
1	E	469	HIS
1	F	37	HIS
1	F	189	GLN
1	D	353	HIS
1	D	389	GLN
1	D	444	ASN

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 ⓘ

37 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	G	1	1,2	14,14,15	0.30	0	17,19,21	0.70	1 (5%)
2	NAG	G	2	2	14,14,15	0.21	0	17,19,21	0.44	0
2	BMA	G	3	2	11,11,12	0.53	0	15,15,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	G	4	2	11,11,12	0.62	0	15,15,17	1.08	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.36	0	17,19,21	0.46	0
3	NAG	H	2	3	14,14,15	0.21	0	17,19,21	0.37	0
3	NAG	I	1	1,3	14,14,15	0.29	0	17,19,21	0.52	0
3	NAG	I	2	3	14,14,15	0.54	0	17,19,21	1.62	3 (17%)
4	NAG	J	1	4,1	14,14,15	0.28	0	17,19,21	0.67	1 (5%)
4	NAG	J	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	BMA	J	3	4	11,11,12	0.62	0	15,15,17	0.69	0
3	NAG	K	1	1,3	14,14,15	0.40	0	17,19,21	0.42	0
3	NAG	K	2	3	14,14,15	0.43	0	17,19,21	0.63	1 (5%)
4	NAG	L	1	4,1	14,14,15	0.27	0	17,19,21	0.53	0
4	NAG	L	2	4	14,14,15	0.44	0	17,19,21	0.40	0
4	BMA	L	3	4	11,11,12	0.56	0	15,15,17	0.68	0
4	NAG	M	1	4,1	14,14,15	0.65	0	17,19,21	0.59	0
4	NAG	M	2	4	14,14,15	0.63	0	17,19,21	0.65	1 (5%)
4	BMA	M	3	4	11,11,12	0.69	0	15,15,17	0.75	0
5	NAG	N	1	1,5	14,14,15	0.35	0	17,19,21	0.75	1 (5%)
5	NAG	N	2	5	14,14,15	0.16	0	17,19,21	0.38	0
5	BMA	N	3	5	11,11,12	0.53	0	15,15,17	0.80	0
5	MAN	N	4	5	11,11,12	0.62	0	15,15,17	1.08	2 (13%)
5	MAN	N	5	5	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
3	NAG	O	1	1,3	14,14,15	0.62	0	17,19,21	0.63	1 (5%)
3	NAG	O	2	3	14,14,15	0.65	0	17,19,21	0.79	1 (5%)
2	NAG	P	1	1,2	14,14,15	0.32	0	17,19,21	0.55	0
2	NAG	P	2	2	14,14,15	0.31	0	17,19,21	0.57	0
2	BMA	P	3	2	11,11,12	0.76	0	15,15,17	0.72	0
2	MAN	P	4	2	11,11,12	0.64	0	15,15,17	1.20	2 (13%)
3	NAG	Q	1	1,3	14,14,15	0.35	0	17,19,21	0.40	0
3	NAG	Q	2	3	14,14,15	0.36	0	17,19,21	0.50	0
5	NAG	R	1	1,5	14,14,15	0.34	0	17,19,21	0.55	0
5	NAG	R	2	5	14,14,15	0.24	0	17,19,21	0.41	0
5	BMA	R	3	5	11,11,12	0.68	0	15,15,17	0.65	0
5	MAN	R	4	5	11,11,12	0.55	0	15,15,17	1.01	1 (6%)
5	MAN	R	5	5	11,11,12	0.66	0	15,15,17	1.05	2 (13%)

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

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

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	C2-N2-C7	5.39	130.13	122.90
2	P	4	MAN	C1-O5-C5	3.56	116.96	112.19
2	G	4	MAN	C1-O5-C5	3.04	116.26	112.19
5	N	4	MAN	C1-O5-C5	2.98	116.18	112.19
5	R	5	MAN	C1-O5-C5	2.89	116.06	112.19
5	N	5	MAN	C1-O5-C5	2.78	115.92	112.19
5	R	4	MAN	C1-O5-C5	2.69	115.79	112.19
5	N	1	NAG	C1-O5-C5	2.65	115.74	112.19
2	G	1	NAG	C1-O5-C5	2.50	115.53	112.19
4	J	1	NAG	C1-O5-C5	2.31	115.28	112.19
3	I	2	NAG	C1-C2-N2	2.29	114.05	110.43
5	N	4	MAN	O2-C2-C3	-2.27	105.45	110.15
3	O	2	NAG	C1-O5-C5	2.25	115.20	112.19
5	R	5	MAN	O2-C2-C3	-2.23	105.53	110.15
2	G	4	MAN	O2-C2-C3	-2.23	105.53	110.15
2	P	4	MAN	O2-C2-C3	-2.22	105.55	110.15
3	K	2	NAG	C1-O5-C5	2.18	115.10	112.19
4	M	2	NAG	C1-O5-C5	2.15	115.07	112.19
3	I	2	NAG	C1-O5-C5	2.10	115.00	112.19
5	N	5	MAN	O2-C2-C3	-2.09	105.83	110.15
3	O	1	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1	NAG	C4-C5-C6-O6
5	N	3	BMA	O5-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
4	M	1	NAG	O5-C5-C6-O6
5	N	5	MAN	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
5	N	3	BMA	C4-C5-C6-O6
4	L	3	BMA	O5-C5-C6-O6
5	R	4	MAN	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C1-C2-N2-C7

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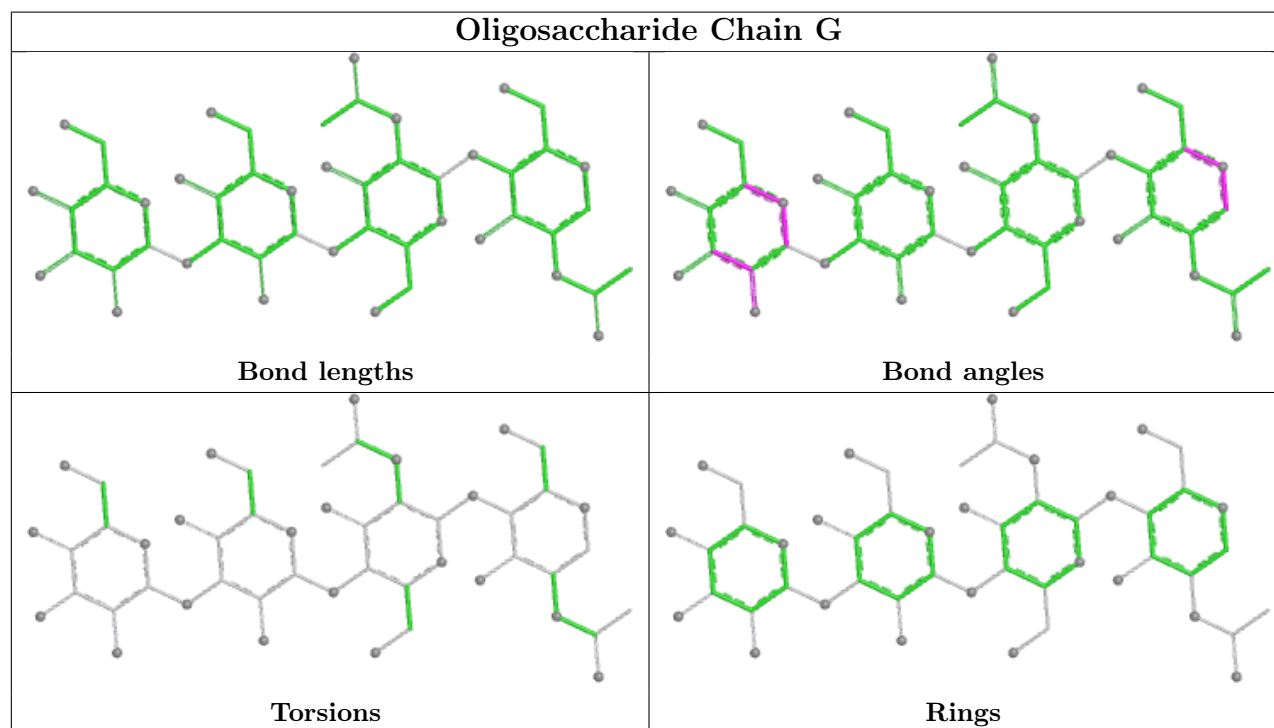
Mol	Chain	Res	Type	Atoms
5	N	2	NAG	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	C1-C2-N2-C7
3	Q	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C3-C2-N2-C7

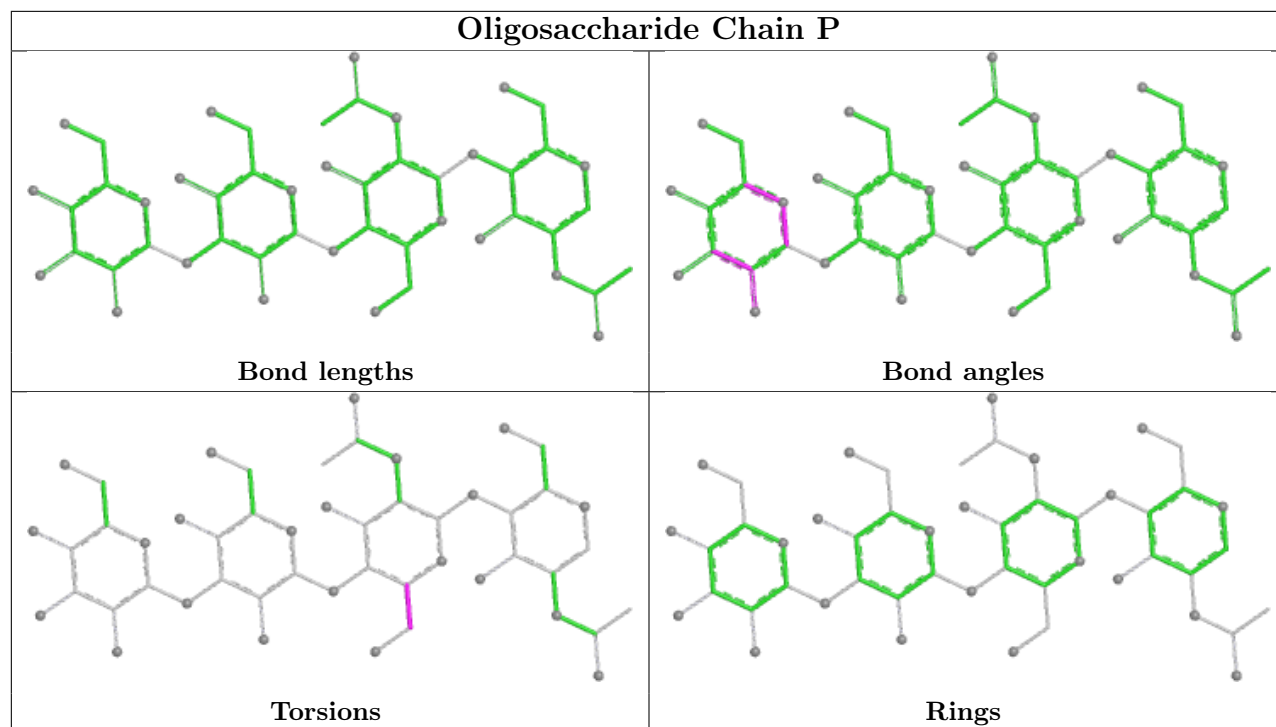
There are no ring outliers.

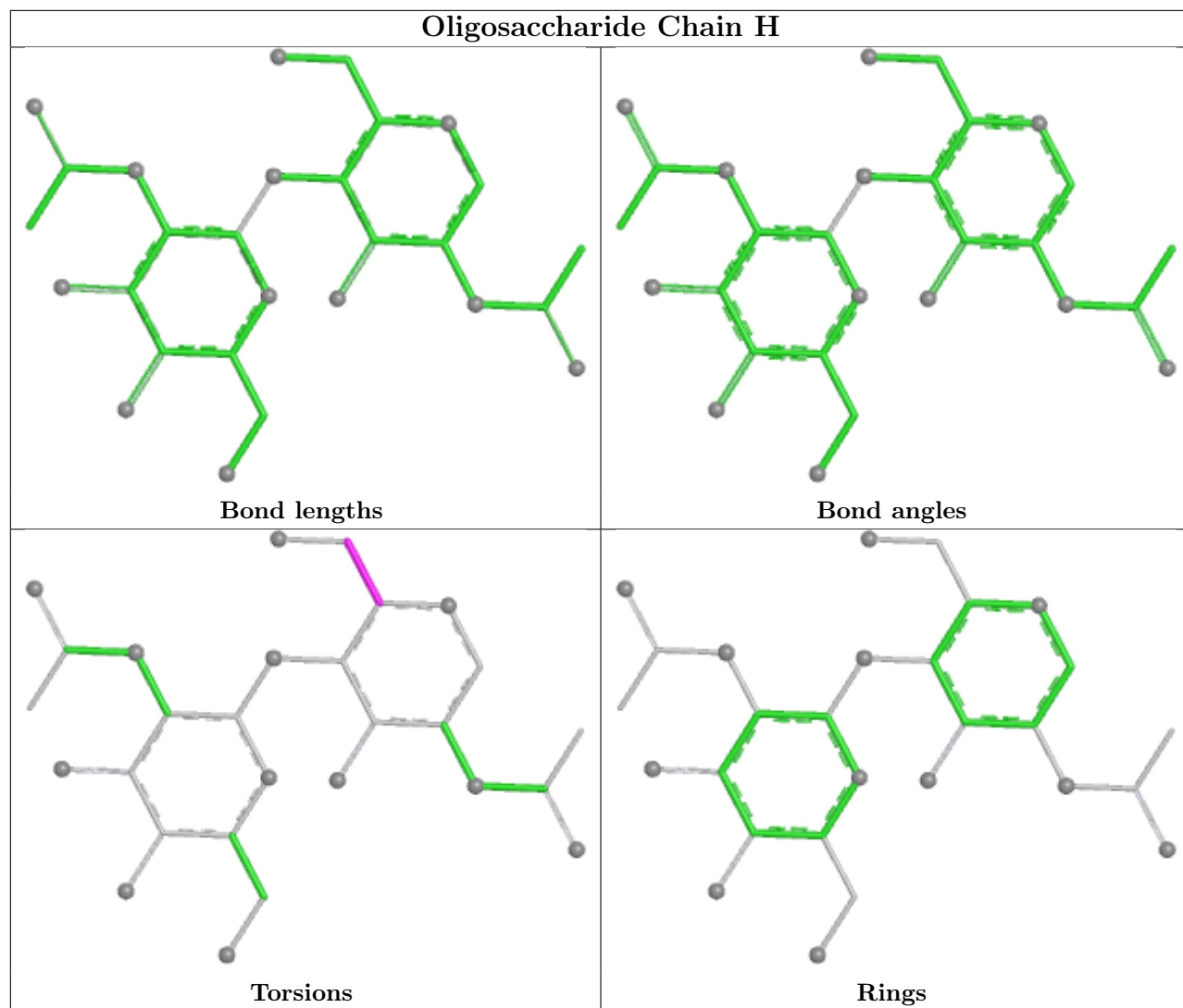
8 monomers are involved in 7 short contacts:

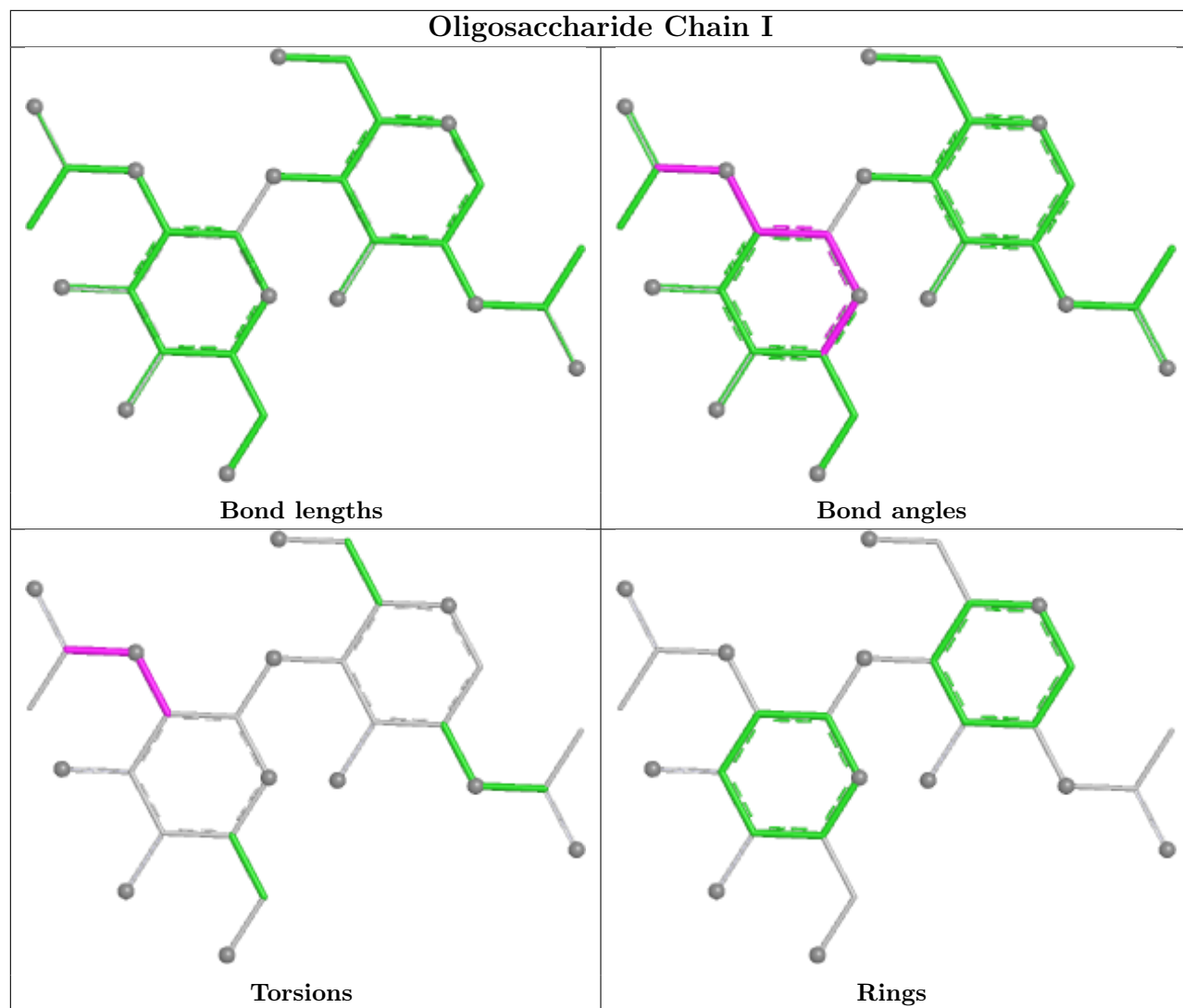
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	1	NAG	1	0
5	R	1	NAG	1	0
3	I	2	NAG	1	0
3	O	1	NAG	1	0
4	M	1	NAG	1	0
4	J	1	NAG	1	0
3	I	1	NAG	1	0
2	G	1	NAG	1	0

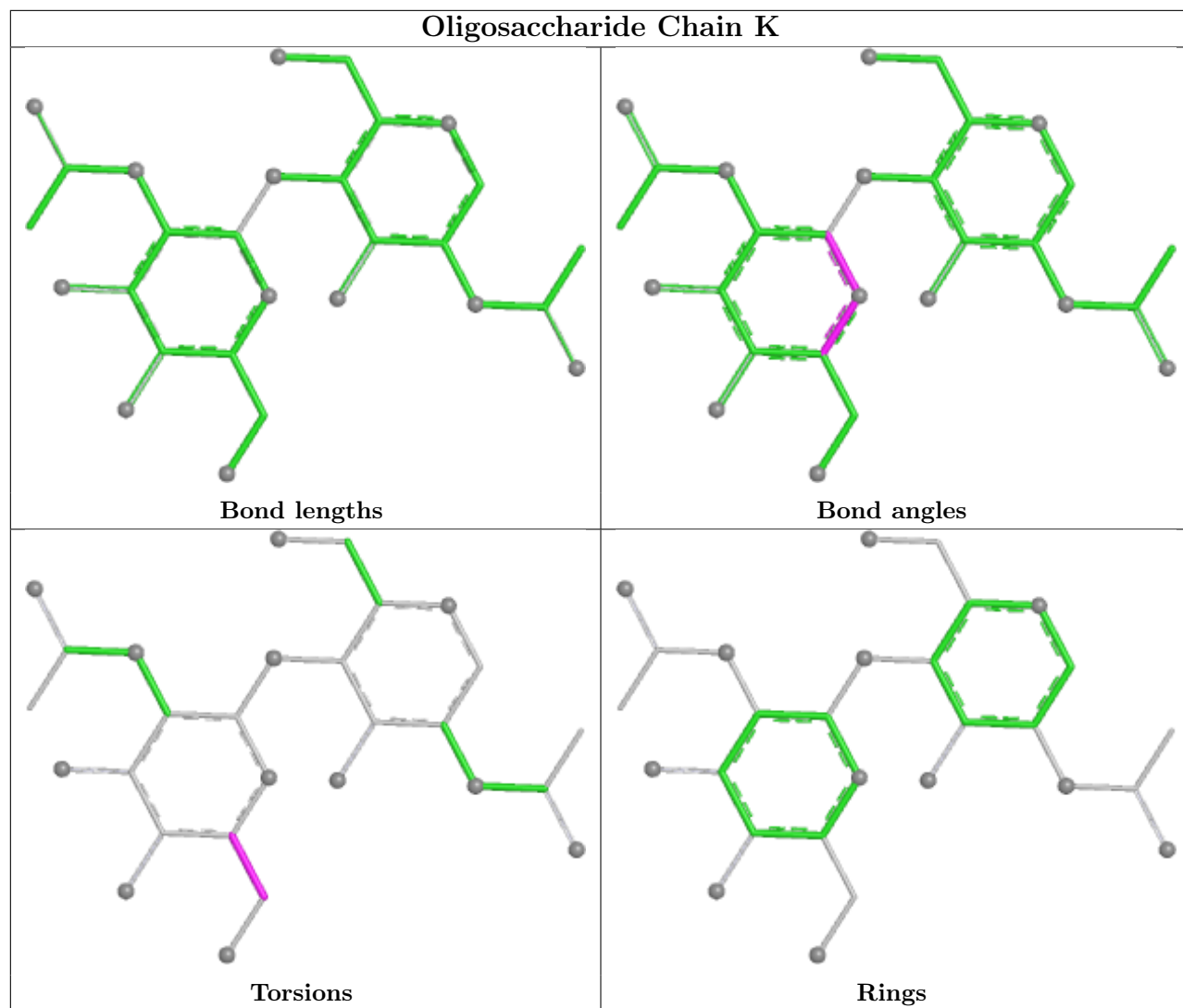
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

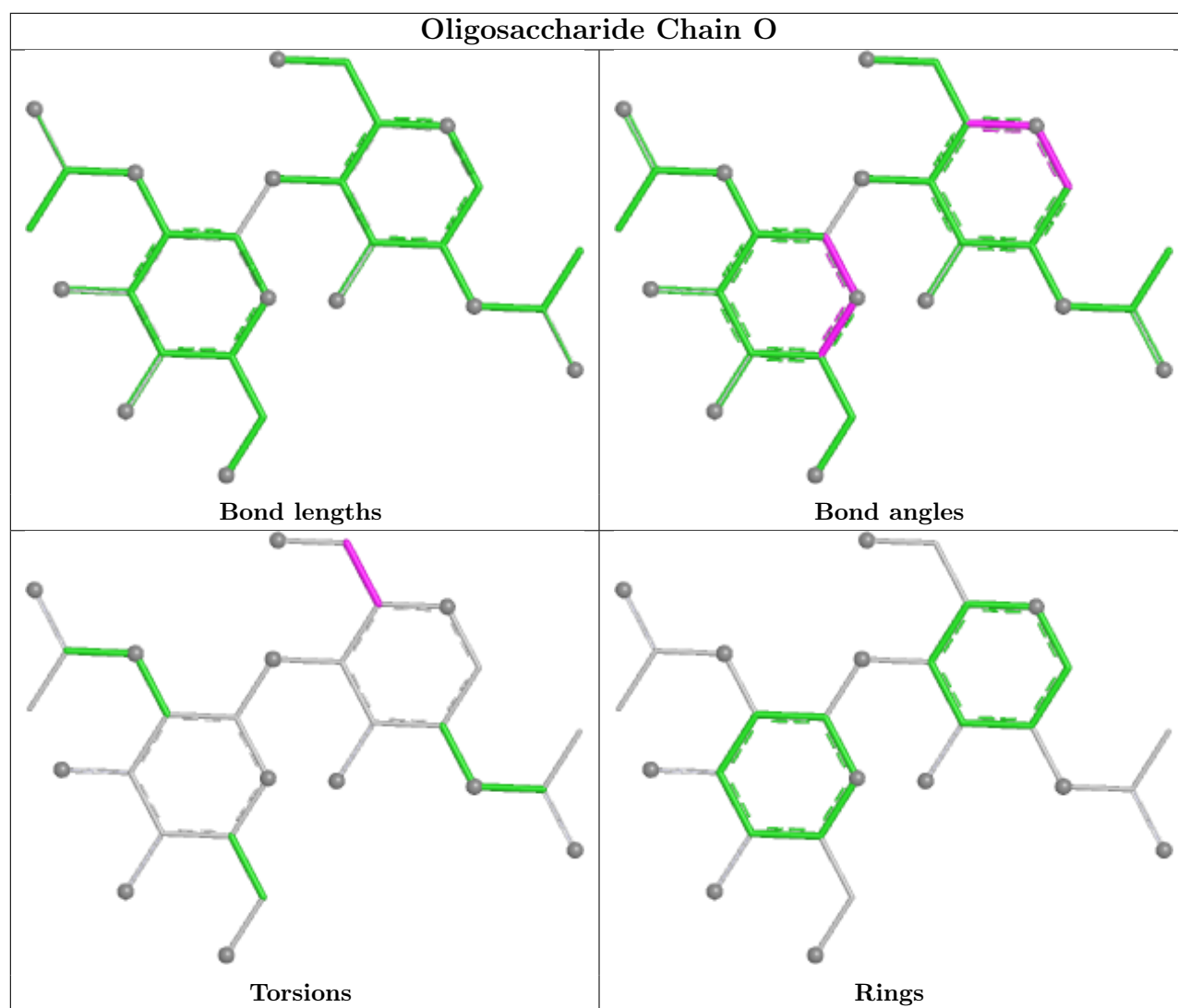


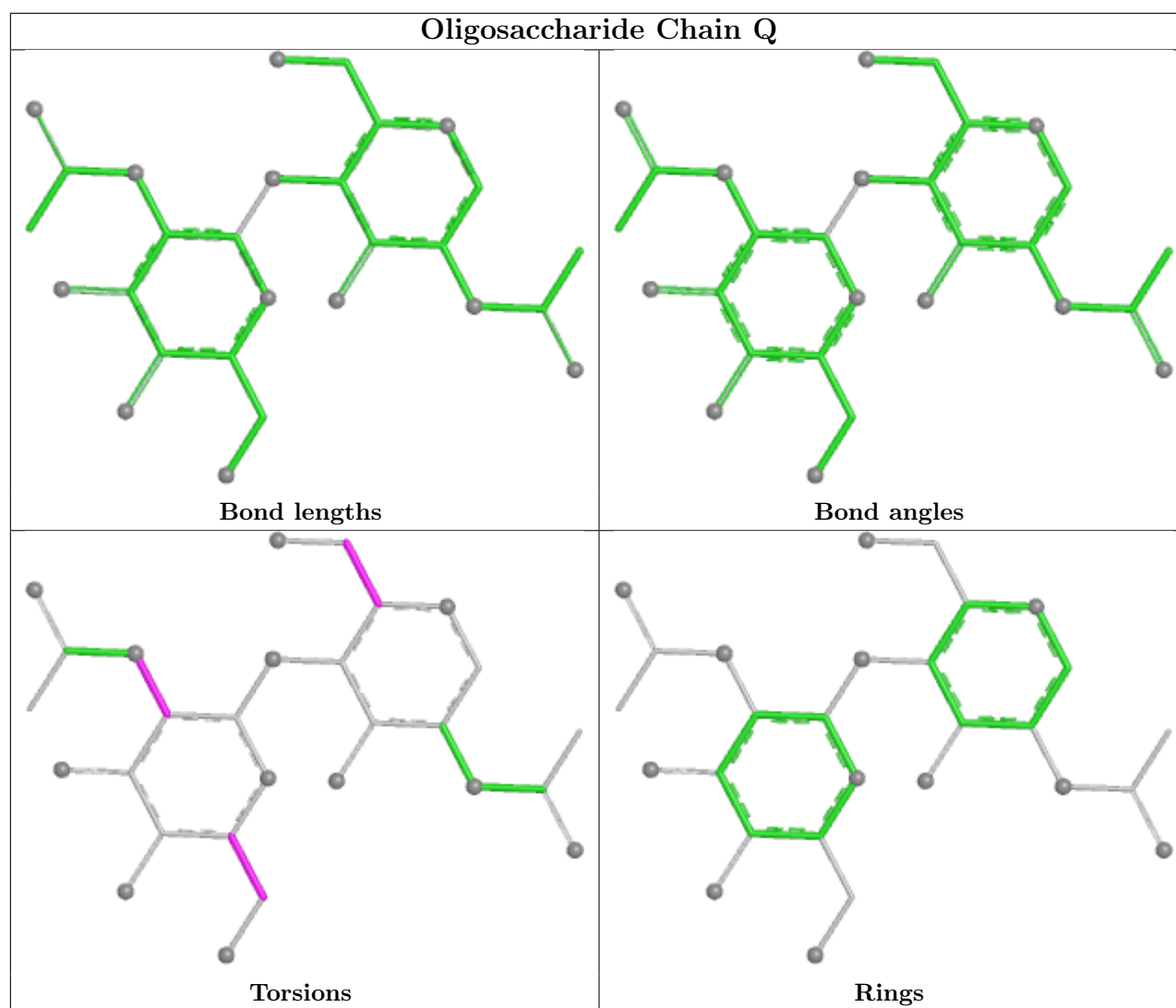


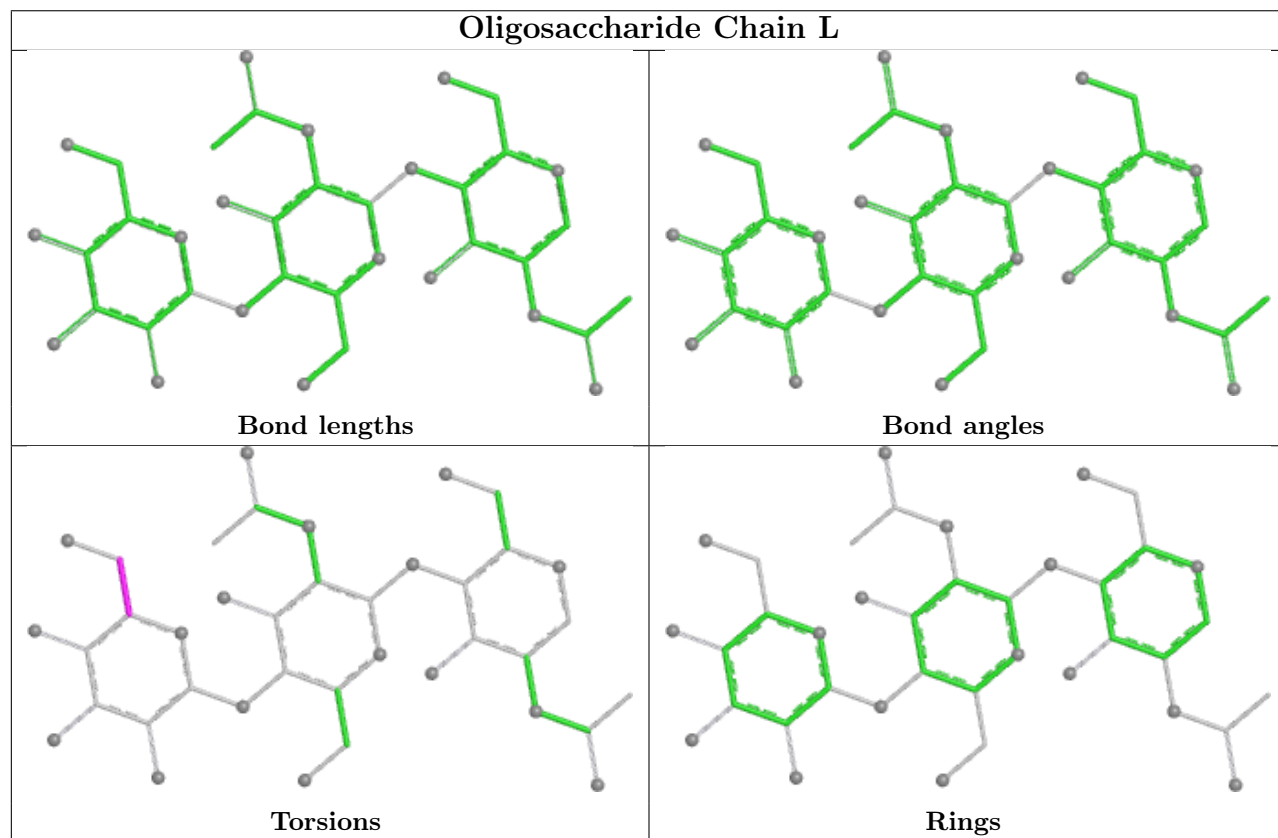
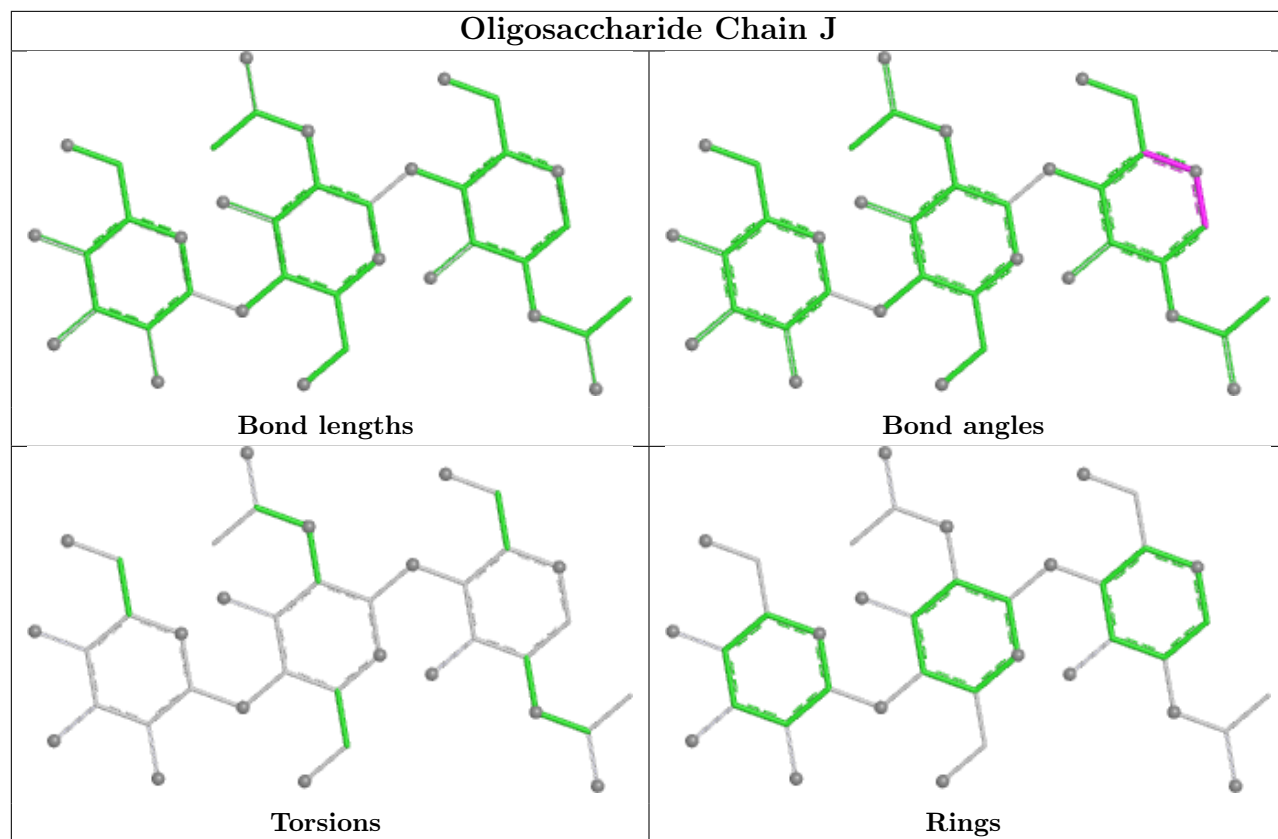


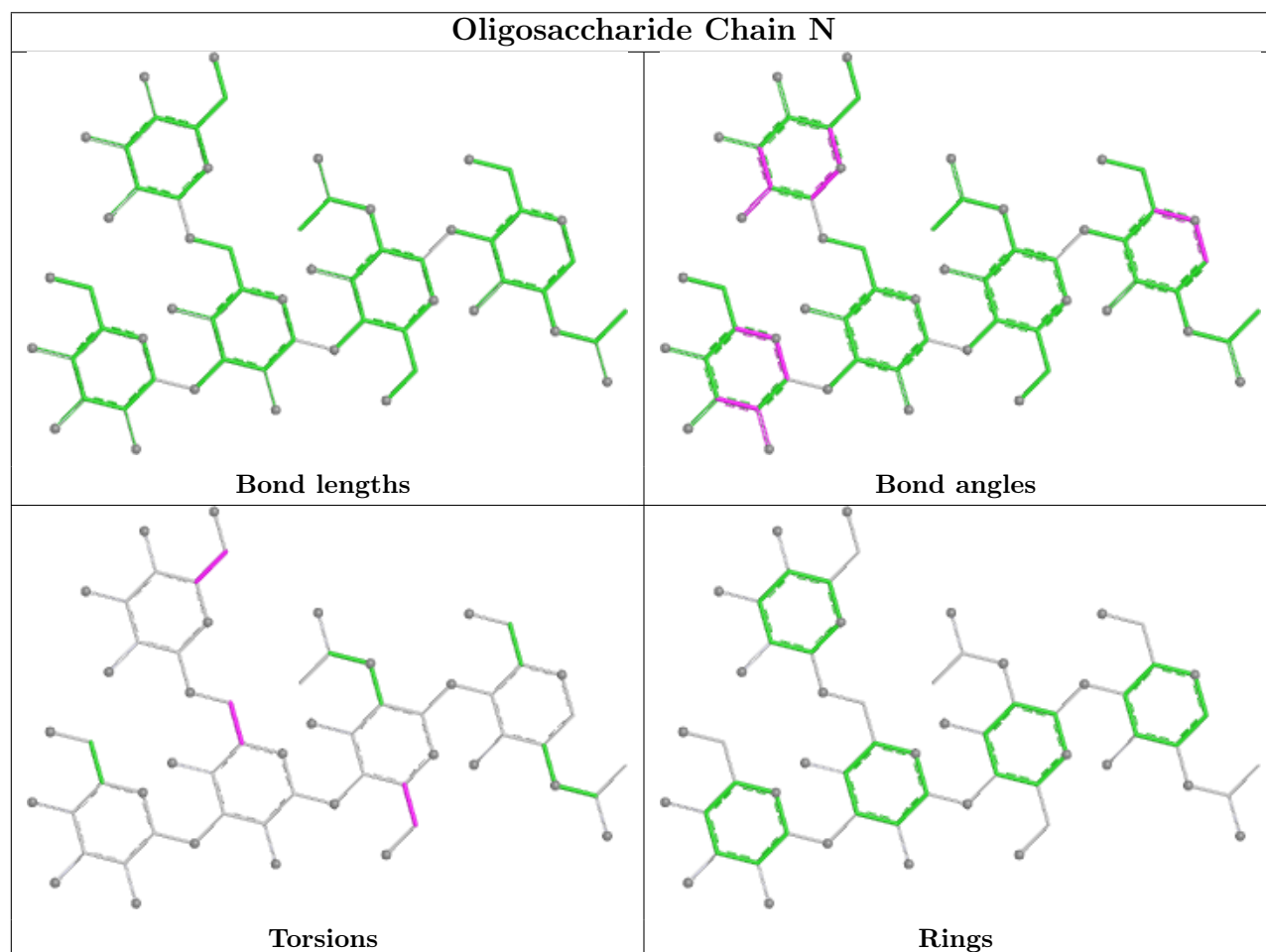
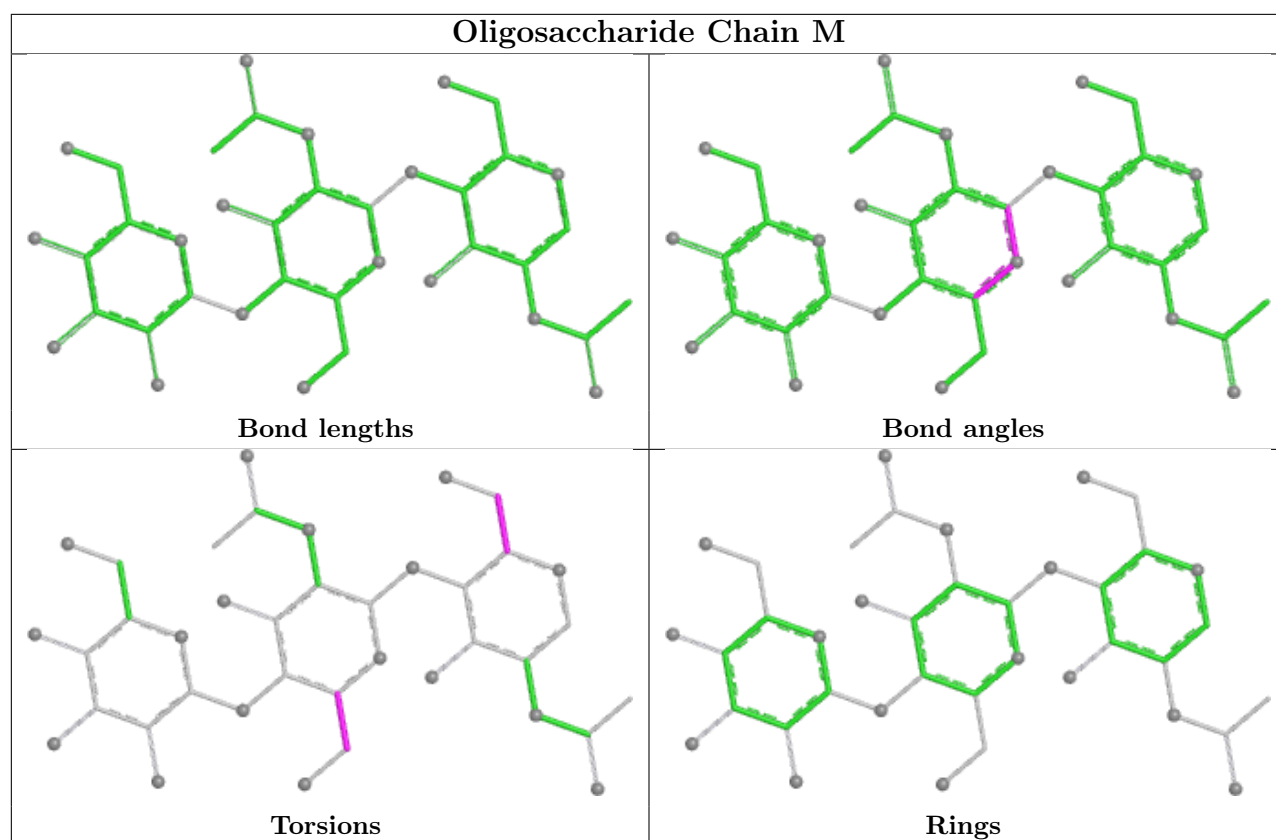


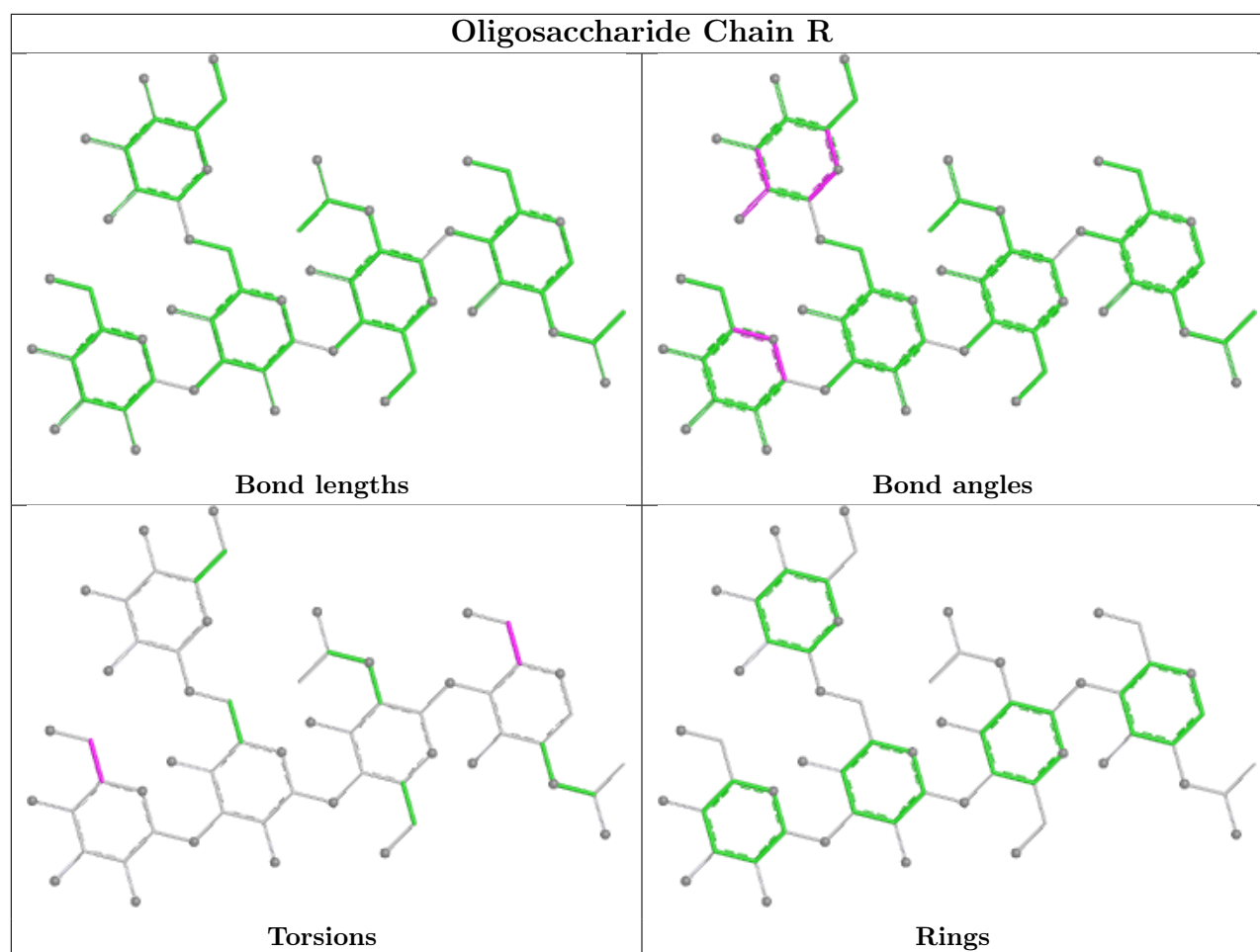












5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
6	NAG	A	601	1	14,14,15	0.28	0	17,19,21	0.52	0
6	NAG	B	603	1	14,14,15	0.58	0	17,19,21	0.65	1 (5%)
6	NAG	D	604	1	14,14,15	0.30	0	17,19,21	0.48	0
6	NAG	B	604	1	14,14,15	0.48	0	17,19,21	0.47	0
6	NAG	A	602	1	14,14,15	0.33	0	17,19,21	0.44	0
6	NAG	D	601	1	14,14,15	0.21	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	601	1	14,14,15	0.50	0	17,19,21	0.52	0
6	NAG	E	601	1	14,14,15	0.21	0	17,19,21	0.40	0
6	NAG	A	604	1	14,14,15	0.18	0	17,19,21	0.37	0
6	NAG	C	602	1	14,14,15	0.28	0	17,19,21	0.48	0
6	NAG	A	603	1	14,14,15	0.19	0	17,19,21	0.42	0
6	NAG	D	602	1	14,14,15	0.30	0	17,19,21	0.56	0
6	NAG	B	602	1	14,14,15	0.57	0	17,19,21	0.49	0
6	NAG	C	603	1	14,14,15	0.25	0	17,19,21	0.52	0
6	NAG	F	602	1	14,14,15	0.25	0	17,19,21	0.46	0
6	NAG	C	604	1	14,14,15	0.34	0	17,19,21	0.52	0
6	NAG	F	601	1	14,14,15	0.25	0	17,19,21	0.37	0
6	NAG	C	601	1	14,14,15	0.26	0	17,19,21	0.62	0
6	NAG	D	603	1	14,14,15	0.58	0	17,19,21	0.78	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
6	NAG	A	601	1	-	0/6/23/26	0/1/1/1
6	NAG	B	603	1	-	1/6/23/26	0/1/1/1
6	NAG	D	604	1	-	2/6/23/26	0/1/1/1
6	NAG	B	604	1	-	1/6/23/26	0/1/1/1
6	NAG	A	602	1	-	1/6/23/26	0/1/1/1
6	NAG	D	601	1	-	0/6/23/26	0/1/1/1
6	NAG	B	601	1	-	1/6/23/26	0/1/1/1
6	NAG	E	601	1	-	2/6/23/26	0/1/1/1
6	NAG	A	604	1	-	0/6/23/26	0/1/1/1
6	NAG	C	602	1	-	0/6/23/26	0/1/1/1
6	NAG	A	603	1	-	0/6/23/26	0/1/1/1
6	NAG	D	602	1	-	0/6/23/26	0/1/1/1
6	NAG	B	602	1	-	1/6/23/26	0/1/1/1
6	NAG	C	603	1	-	0/6/23/26	0/1/1/1
6	NAG	F	602	1	-	1/6/23/26	0/1/1/1
6	NAG	C	604	1	-	1/6/23/26	0/1/1/1
6	NAG	F	601	1	-	0/6/23/26	0/1/1/1
6	NAG	C	601	1	-	0/6/23/26	0/1/1/1
6	NAG	D	603	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	D	603	NAG	C1-O5-C5	2.45	115.47	112.19
6	B	603	NAG	C1-O5-C5	2.18	115.11	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	601	NAG	O5-C5-C6-O6
6	B	601	NAG	O5-C5-C6-O6
6	C	604	NAG	O5-C5-C6-O6
6	F	602	NAG	O5-C5-C6-O6
6	A	602	NAG	O5-C5-C6-O6
6	B	604	NAG	O5-C5-C6-O6
6	B	603	NAG	O5-C5-C6-O6
6	B	602	NAG	O5-C5-C6-O6
6	D	604	NAG	O5-C5-C6-O6
6	D	604	NAG	C4-C5-C6-O6
6	E	601	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	601	NAG	2	0
6	C	601	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	483/513 (94%)	0.17	12 (2%)	58 35	30, 64, 118, 179	0
1	B	481/513 (93%)	0.28	14 (2%)	53 31	29, 70, 124, 192	1 (0%)
1	C	481/513 (93%)	0.28	12 (2%)	58 35	27, 72, 165, 237	1 (0%)
1	D	460/513 (89%)	0.29	9 (1%)	65 41	30, 76, 156, 208	0
1	E	474/513 (92%)	0.30	10 (2%)	63 40	30, 75, 153, 189	0
1	F	473/513 (92%)	0.31	18 (3%)	44 24	30, 80, 154, 198	0
All	All	2852/3078 (92%)	0.27	75 (2%)	57 34	27, 73, 149, 237	2 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	207[A]	ASN	11.0
1	C	393	VAL	4.3
1	D	321	ILE	4.1
1	E	495	LEU	4.0
1	B	473	ASN	3.8
1	A	346	ASP	3.8
1	C	86	GLU	3.6
1	A	473	ASN	3.4
1	B	213	GLU	3.3
1	F	461	GLY	3.2
1	C	493	SER	3.0
1	A	345	ILE	3.0
1	F	85	SER	3.0
1	C	3	ILE	3.0
1	B	322	PRO	3.0
1	A	336	PHE	2.9
1	A	323	SER	2.9
1	B	0	ALA	2.8
1	B	321	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	88	GLY	2.8
1	C	0	ALA	2.7
1	E	461	GLY	2.7
1	E	453	LEU	2.7
1	F	321	ILE	2.7
1	A	338	GLU	2.6
1	F	3	ILE	2.6
1	F	476	MET	2.6
1	D	337	ILE	2.6
1	F	447	GLU	2.6
1	C	322	PRO	2.5
1	D	5	ILE	2.5
1	F	301	GLY	2.5
1	F	393	VAL	2.5
1	A	337	ILE	2.5
1	A	494	LYS	2.5
1	B	4	CYS	2.4
1	A	168	ASN	2.4
1	D	490	SER	2.4
1	B	387	ASN	2.4
1	E	389	GLN	2.4
1	F	275	CYS	2.4
1	C	337	ILE	2.3
1	D	168	ASN	2.3
1	F	435	LEU	2.3
1	D	479	VAL	2.3
1	E	342	THR	2.3
1	F	493	SER	2.3
1	B	205	ASN	2.3
1	B	492	GLU	2.3
1	C	216	GLU	2.3
1	C	2	THR	2.3
1	F	468	TYR	2.3
1	F	71	LEU	2.2
1	F	353	HIS	2.2
1	D	338	GLU	2.2
1	E	435	LEU	2.2
1	B	490	SER	2.2
1	B	369	GLN	2.2
1	A	196	ASN	2.2
1	F	338	GLU	2.2
1	B	346	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	385	LYS	2.2
1	A	455	ASN	2.2
1	E	393	VAL	2.1
1	E	73	ALA	2.1
1	C	321	ILE	2.1
1	D	486	TYR	2.1
1	B	72	SER	2.1
1	E	385	LYS	2.1
1	C	453	LEU	2.1
1	F	480	LYS	2.0
1	D	339	GLY	2.0
1	B	123	TRP	2.0
1	A	0	ALA	2.0
1	F	315	VAL	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(Å ²)	Q<0.9
5	MAN	N	5	11/12	0.29	0.17	102,116,132,133	0
3	NAG	H	2	14/15	0.33	0.14	86,114,128,130	0
2	MAN	P	4	11/12	0.37	0.17	106,129,140,141	0
3	NAG	K	2	14/15	0.38	0.16	93,124,138,143	0
3	NAG	Q	2	14/15	0.44	0.15	91,123,134,135	0
3	NAG	O	2	14/15	0.45	0.14	96,135,141,141	0
4	BMA	L	3	11/12	0.46	0.13	87,129,135,138	0
3	NAG	K	1	14/15	0.47	0.14	69,98,115,129	0
4	BMA	M	3	11/12	0.51	0.15	93,104,114,115	0
2	BMA	P	3	11/12	0.52	0.14	83,114,120,120	0
5	MAN	N	4	11/12	0.53	0.15	82,118,129,136	0
5	MAN	R	5	11/12	0.54	0.14	100,120,135,137	0
4	BMA	J	3	11/12	0.61	0.13	91,108,119,122	0
5	BMA	R	3	11/12	0.63	0.14	103,121,129,129	0

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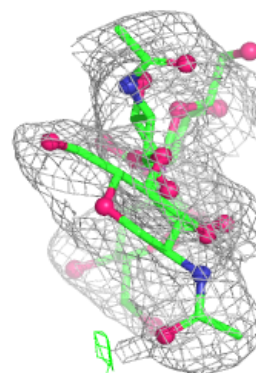
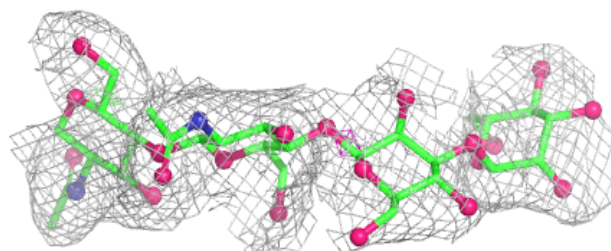
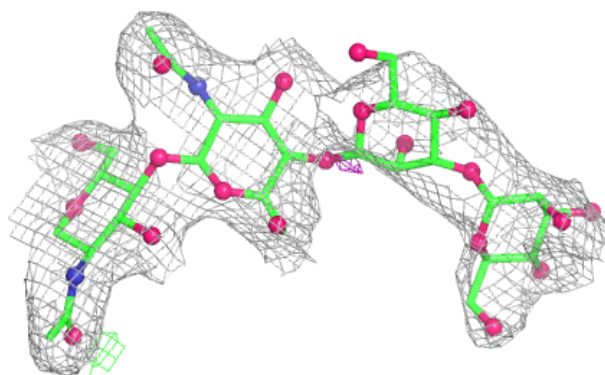
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	O	1	14/15	0.63	0.16	93,106,129,129	0
5	MAN	R	4	11/12	0.66	0.16	78,106,117,122	0
2	MAN	G	4	11/12	0.66	0.12	94,134,144,149	0
5	BMA	N	3	11/12	0.68	0.13	91,114,119,121	0
2	BMA	G	3	11/12	0.68	0.11	115,118,128,128	0
4	NAG	L	2	14/15	0.71	0.13	93,103,116,126	0
3	NAG	I	2	14/15	0.75	0.13	75,91,104,108	0
3	NAG	H	1	14/15	0.76	0.12	67,89,110,115	0
5	NAG	R	2	14/15	0.78	0.11	67,96,105,110	0
4	NAG	L	1	14/15	0.79	0.13	64,77,102,111	0
4	NAG	M	2	14/15	0.81	0.12	81,94,104,123	0
4	NAG	J	2	14/15	0.83	0.11	79,92,108,119	0
2	NAG	P	2	14/15	0.83	0.11	57,84,101,110	0
5	NAG	N	2	14/15	0.85	0.11	73,80,94,96	0
3	NAG	Q	1	14/15	0.85	0.11	92,111,122,131	0
2	NAG	G	2	14/15	0.87	0.10	77,84,107,127	0
3	NAG	I	1	14/15	0.87	0.11	56,65,84,84	0
4	NAG	M	1	14/15	0.87	0.11	61,71,86,100	0
5	NAG	R	1	14/15	0.87	0.12	67,73,85,91	0
4	NAG	J	1	14/15	0.89	0.10	62,75,91,91	0
2	NAG	G	1	14/15	0.90	0.09	52,65,76,77	0
5	NAG	N	1	14/15	0.91	0.10	52,69,85,95	0
2	NAG	P	1	14/15	0.92	0.10	57,62,85,91	0

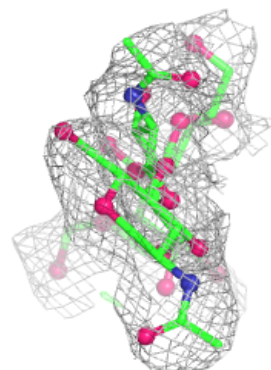
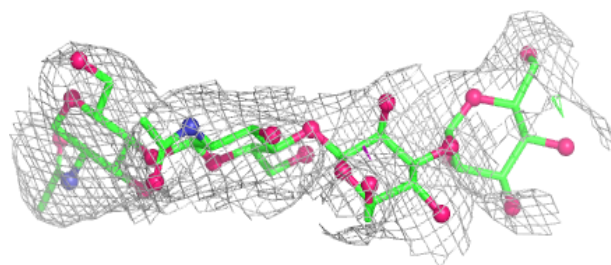
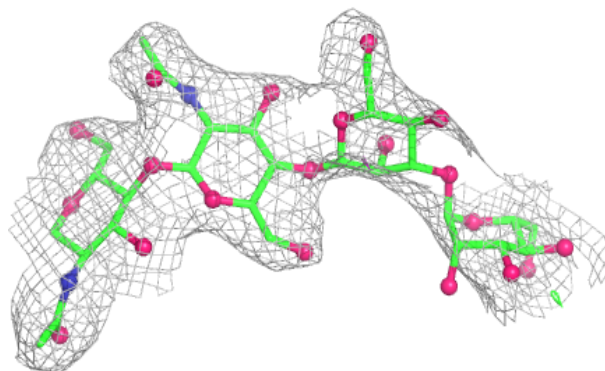
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

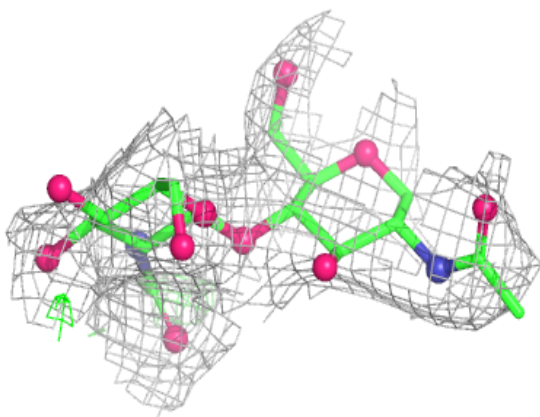
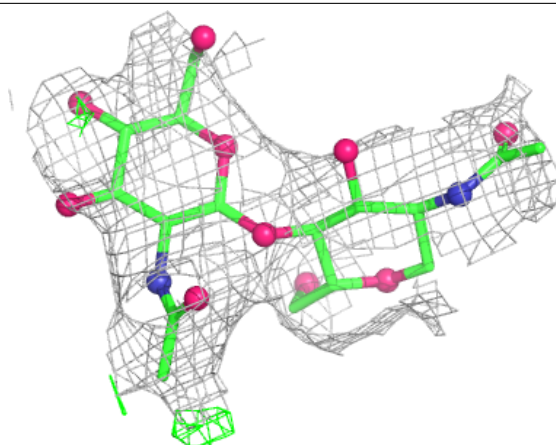
**Electron density around Chain P:**

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



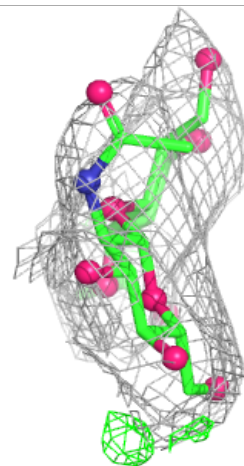
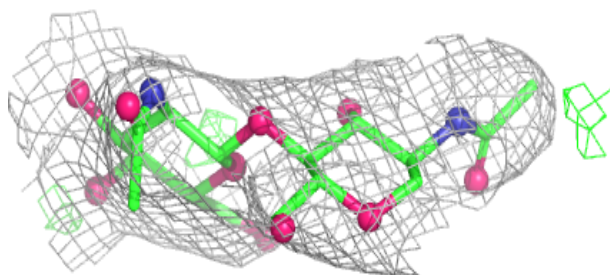
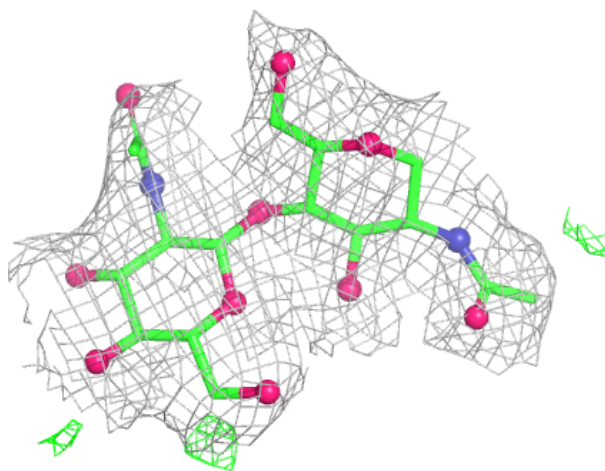
Electron density around Chain H:

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



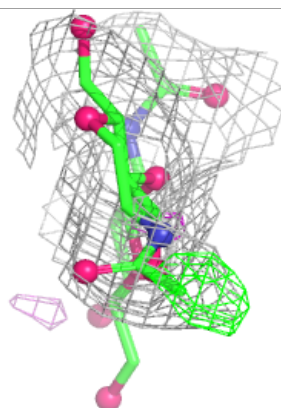
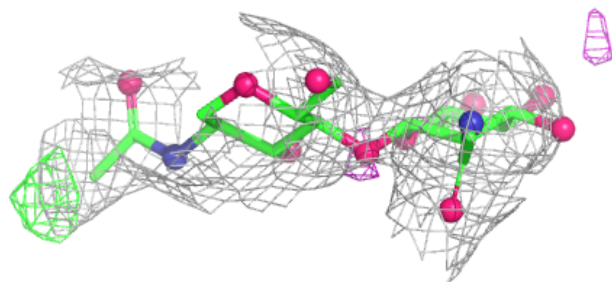
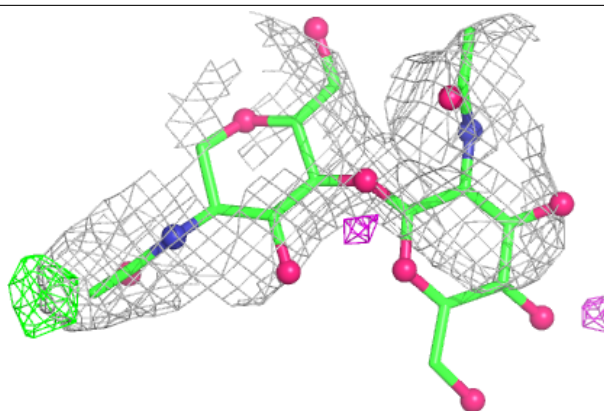
Electron density around Chain I:

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

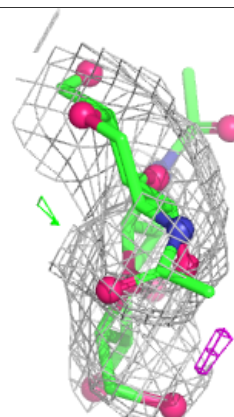
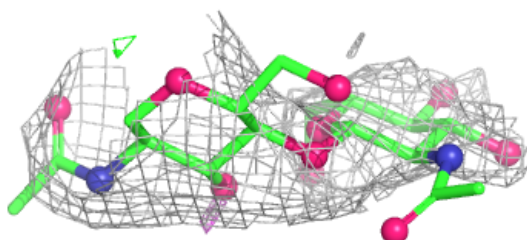
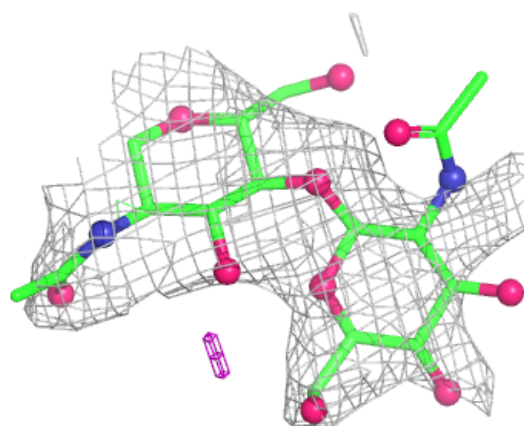


Electron density around Chain K:

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

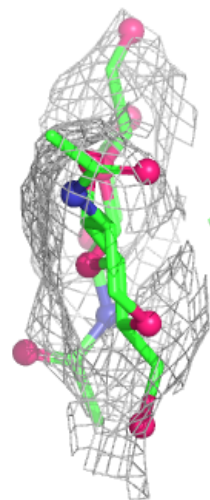
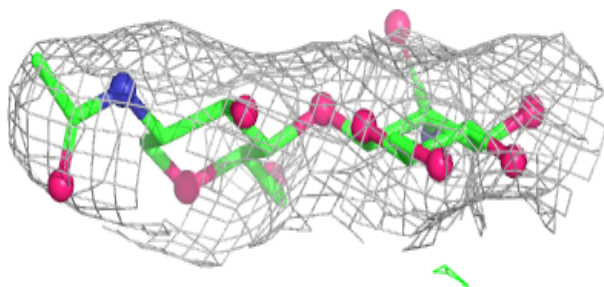
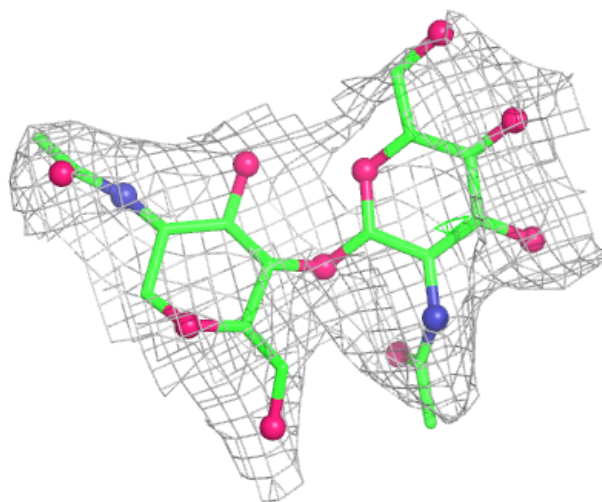
**Electron density around Chain O:**

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



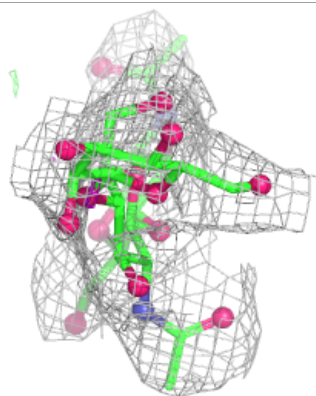
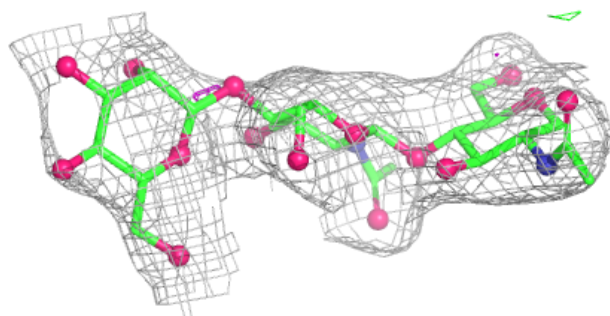
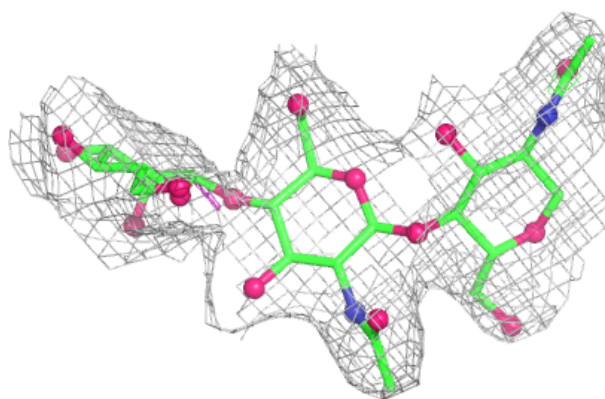
Electron density around Chain Q:

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

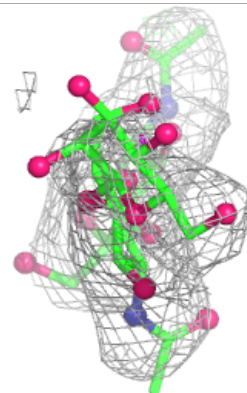
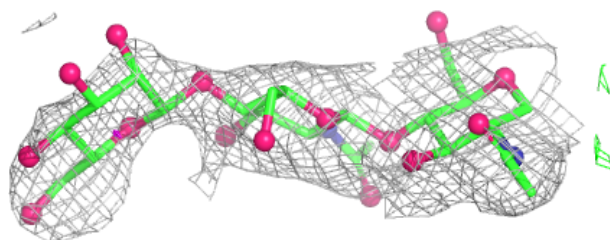
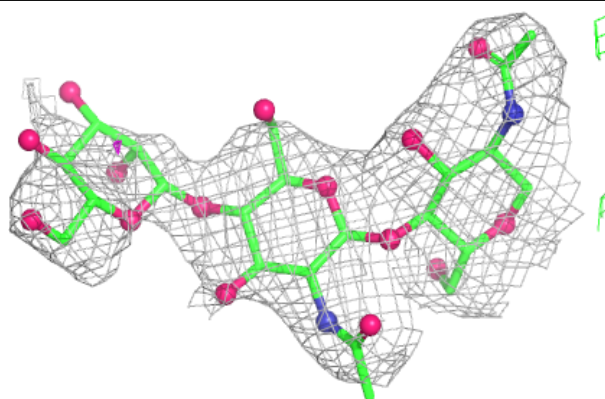


Electron density around Chain J:

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

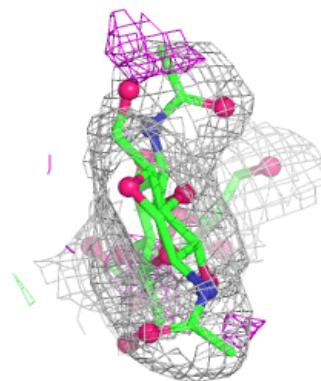
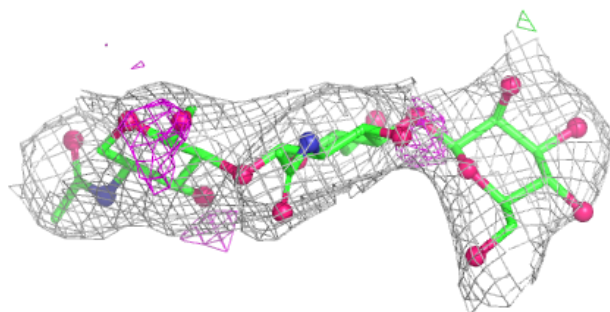
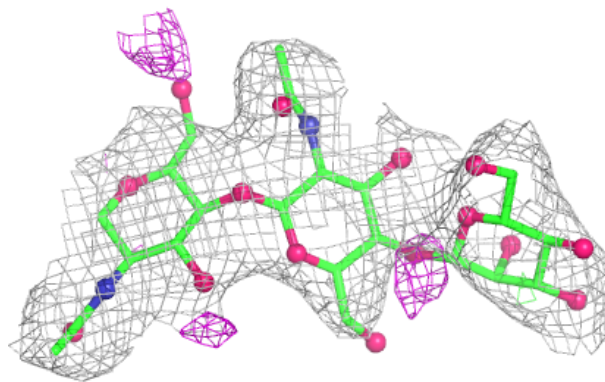
**Electron density around Chain L:**

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



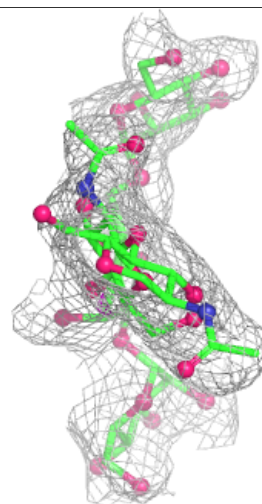
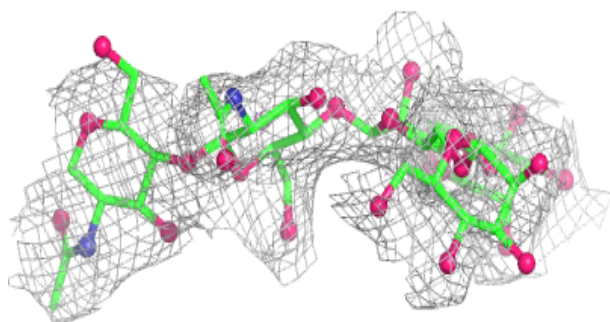
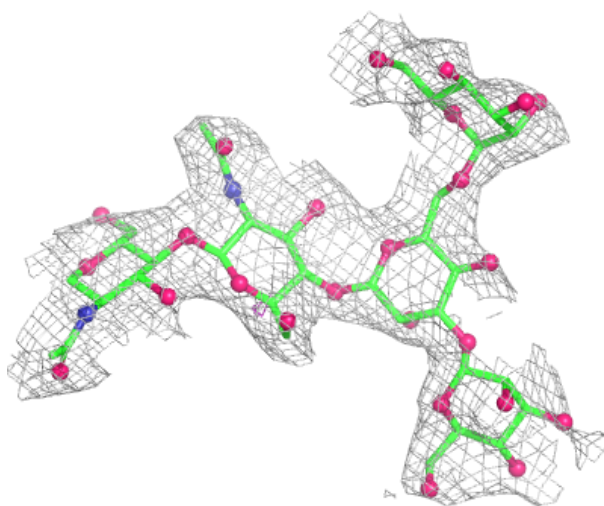
Electron density around Chain M:

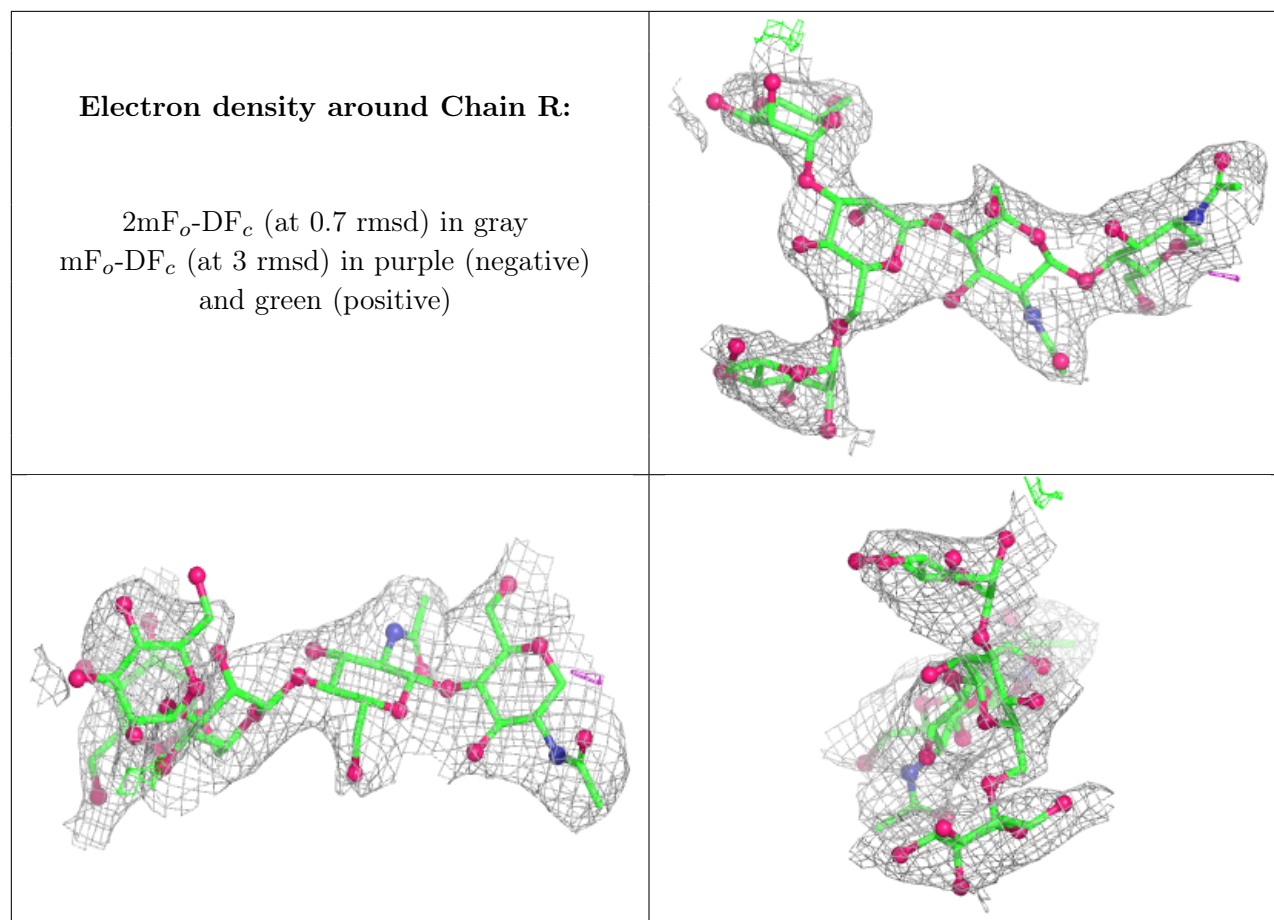
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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(Å ²)	Q<0.9
6	NAG	D	601	14/15	0.30	0.16	93,127,140,140	0
6	NAG	F	601	14/15	0.52	0.18	96,112,123,124	0
6	NAG	D	604	14/15	0.54	0.13	92,114,122,122	0
6	NAG	A	604	14/15	0.55	0.14	109,129,139,143	0
6	NAG	B	604	14/15	0.56	0.16	109,134,148,151	0
6	NAG	C	604	14/15	0.59	0.14	73,106,121,122	0
6	NAG	C	601	14/15	0.61	0.12	90,117,127,127	0
6	NAG	D	602	14/15	0.67	0.11	88,122,134,135	0
6	NAG	D	603	14/15	0.69	0.14	92,106,111,112	0
6	NAG	F	602	14/15	0.70	0.14	94,112,124,146	0
6	NAG	E	601	14/15	0.71	0.12	101,113,119,130	0
6	NAG	B	601	14/15	0.72	0.15	83,103,112,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	C	603	14/15	0.72	0.13	86,103,108,109	0
6	NAG	B	603	14/15	0.73	0.12	90,103,115,117	0
6	NAG	A	603	14/15	0.74	0.11	85,98,111,115	0
6	NAG	B	602	14/15	0.75	0.15	82,111,119,120	0
6	NAG	C	602	14/15	0.76	0.10	65,105,115,116	0
6	NAG	A	602	14/15	0.76	0.12	81,102,116,130	0
6	NAG	A	601	14/15	0.79	0.11	67,89,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.