



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:09 PM UTC

PDB ID : 6B0N / pdb_00006b0n
Title : Crystal structure of the cleavage-independent prefusion HIV Env glycoprotein trimer of the clade A BG505 isolate (NFL construct) in complex with Fabs PGT122 and PGV19 at 3.39 Å
Authors : Sarkar, A.; Irimia, A.; Wilson, I.A.
Deposited on : 2017-09-14
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

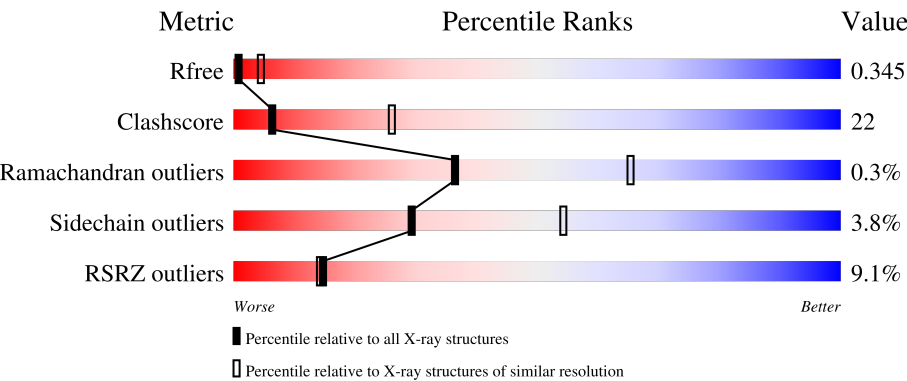
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 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.



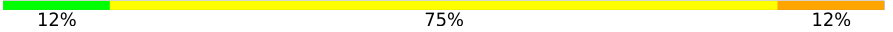
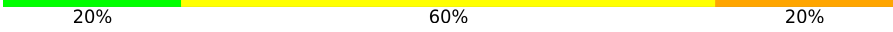
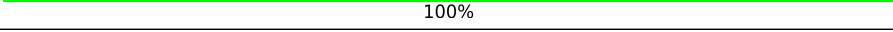
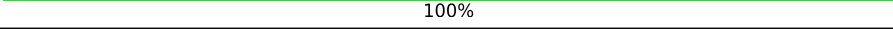
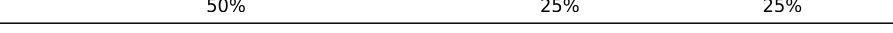
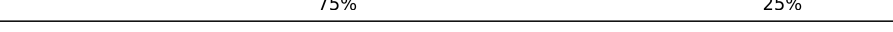
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	D	223	7% 52%22%23%
2	E	209	8% 72%14%13%
3	G	638	11% 63%28%
4	H	235	6% 74%22%
5	L	213	5% 70%27%

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Mol	Chain	Length	Quality of chain
6	A	7	
7	B	3	
7	C	3	
8	F	8	
9	I	5	
9	O	5	
10	J	2	
10	P	2	
10	R	2	
11	K	4	
12	M	8	
13	N	3	
14	Q	4	
15	S	8	

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
10	NAG	P	1	-	-	X	-
10	NAG	P	2	-	-	X	-
12	BMA	M	3	-	-	X	-
13	MAN	N	1	-	-	X	-
14	BMA	Q	1	-	-	X	-
16	NAG	G	1133	-	-	X	-
17	MAN	G	1266	-	-	X	-
8	MAN	F	7	-	-	X	-
9	NAG	O	1	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 11789 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 PGV19 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	171	Total	C	N	O	S	0	0	0
			1341	851	237	244	9			

- Molecule 2 is a protein called PGV19 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	182	Total	C	N	O	S	0	0	0
			1375	866	233	272	4			

- Molecule 3 is a protein called Envelope glycoprotein gp140.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	610	Total	C	N	O	S	0	0	0
			4754	2992	832	898	32			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	507	GLY	-	linker	UNP Q2N0S6
G	508	GLY	-	linker	UNP Q2N0S6
G	509	GLY	-	linker	UNP Q2N0S6
G	509A	GLY	-	linker	UNP Q2N0S6
G	509B	GLY	-	linker	UNP Q2N0S6
G	509C	SER	-	linker	UNP Q2N0S6
G	509D	GLY	-	linker	UNP Q2N0S6
G	509E	GLY	-	linker	UNP Q2N0S6
G	509F	GLY	-	linker	UNP Q2N0S6
G	509G	GLY	-	linker	UNP Q2N0S6
G	511	SER	-	linker	UNP Q2N0S6
G	559	PRO	ILE	engineered mutation	UNP Q2N0S9

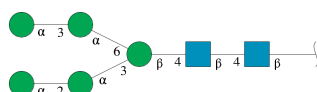
- Molecule 4 is a protein called PGT122 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	232	Total	C	N	O	S	0	0	0
			1767	1122	300	340	5			

- Molecule 5 is a protein called PGT122 light chain.

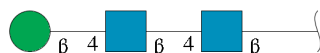
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	210	Total	C	N	O	S	0	0	0
			1586	997	266	319	4			

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



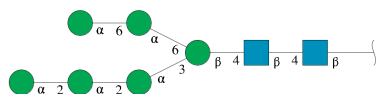
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	A	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 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.



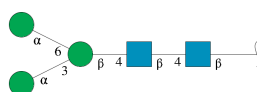
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	F	8	Total	C	N	O	0	0	0
			94	52	2	40			

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



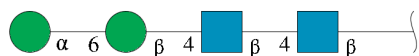
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
9	O	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



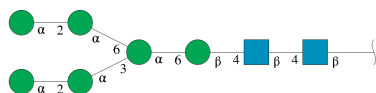
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 11 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
11	K	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



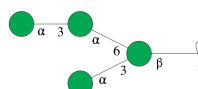
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	M	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



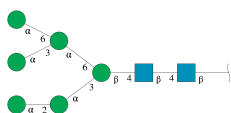
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
13	N	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose.



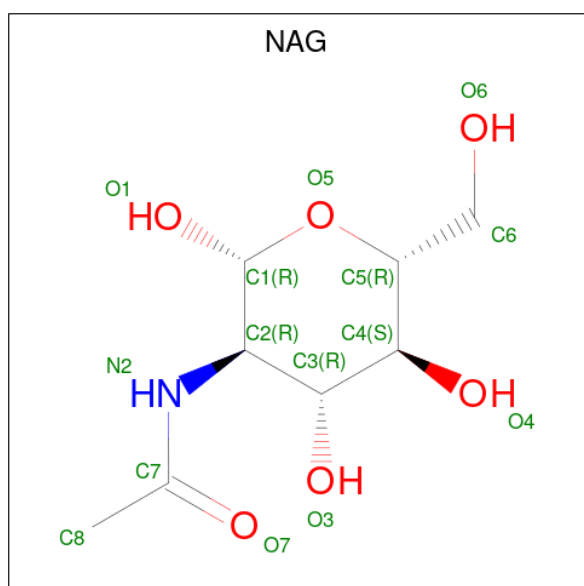
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
14	Q	4	Total	C	O	0	0	0
			44	24	20			

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	S	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



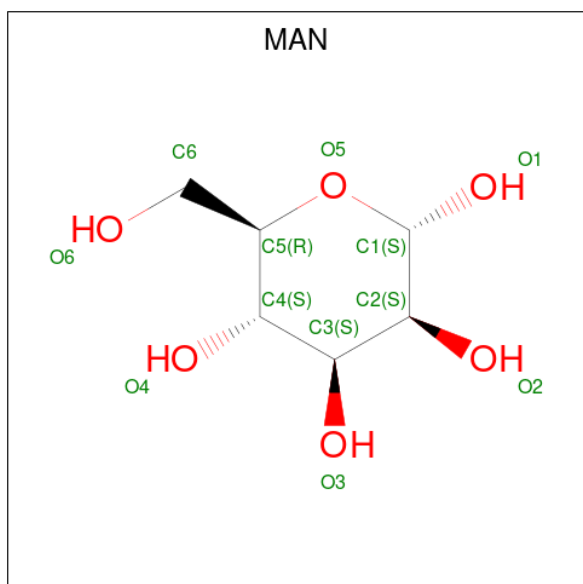
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		

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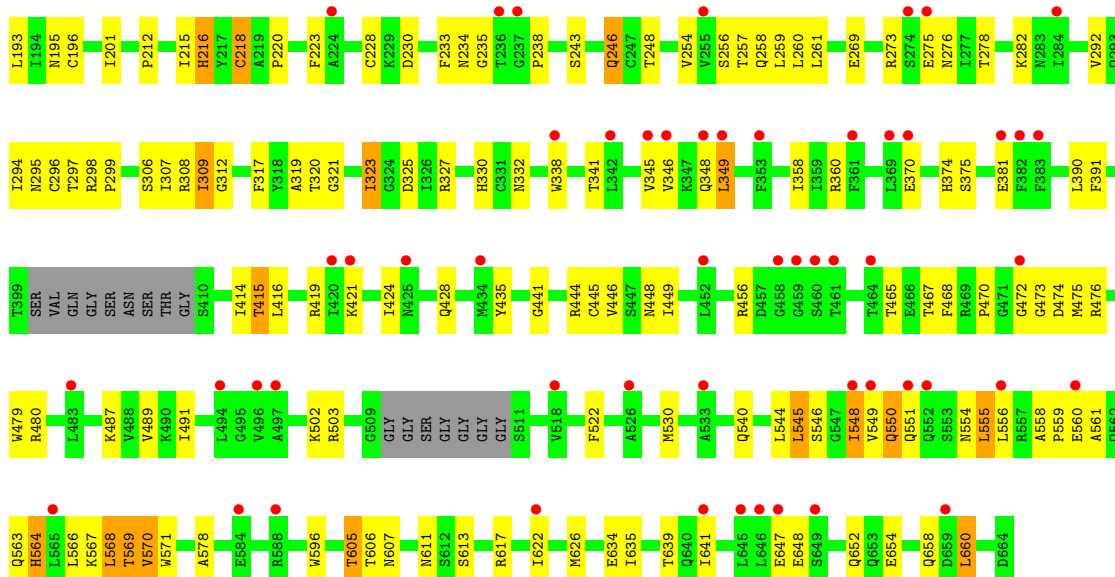
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		

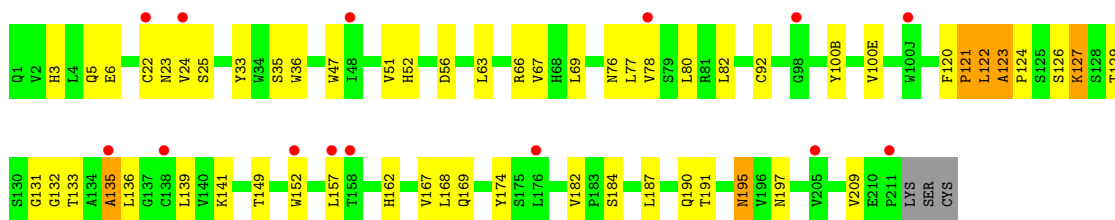
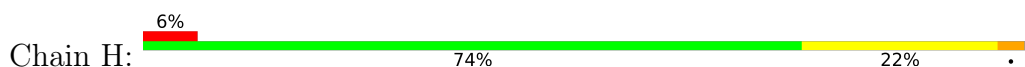
- Molecule 17 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



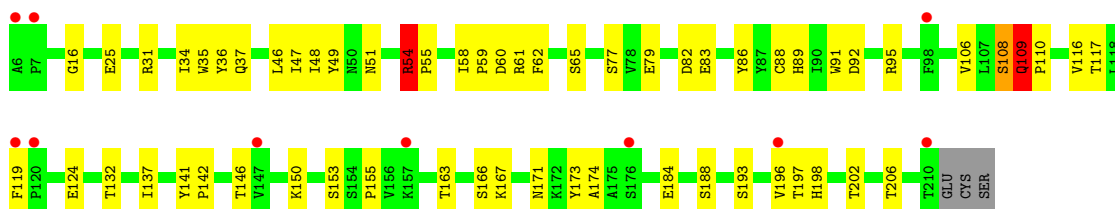
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	G	1	Total	C	O	0	0
			11	6	5		
17	G	1	Total	C	O	0	0
			11	6	5		



• Molecule 4: PGT122 Fab heavy chain



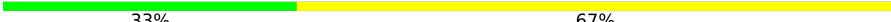
• Molecule 5: PGT122 light chain



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



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

Chain B:  33% 67%

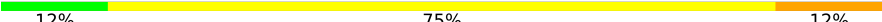


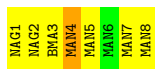
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  67% 33%

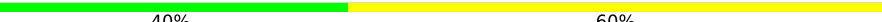


- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  12% 75% 12%

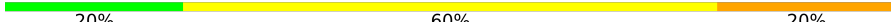


- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  40% 60%



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

Chain O:  20% 60% 20%



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

Chain J:  100%

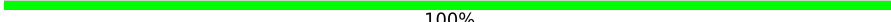


- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%

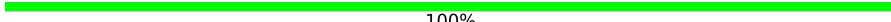
MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2

- Molecule 11: 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:  100%

MAG1
MAG2
MAN3
MAN4

- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain N:  67% 33%

MAN1
MAN2
MAN3

- Molecule 14: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose

Chain Q:  50% 25% 25%

MAN1
MAN2
MAN3
MAN4

- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



HA01
HA02
HA03
HA04
HA05
HA06
HA07
HA08

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	161.25Å 161.25Å 245.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.85 – 3.40 48.85 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.85-3.40) 98.6 (48.85-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.12_2829: 000)	Depositor
R, R_{free}	0.335 , 0.346 0.338 , 0.345	Depositor DCC
R_{free} test set	2458 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	91.9	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 22.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	11789	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: MAN, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	D	0.39	1/1375 (0.1%)	0.54	0/1861
2	E	0.23	0/1410	0.46	3/1914 (0.2%)
3	G	0.50	0/4847	0.80	11/6582 (0.2%)
4	H	0.37	1/1815 (0.1%)	0.54	5/2479 (0.2%)
5	L	0.39	0/1629	0.85	6/2232 (0.3%)
All	All	0.42	2/11076 (0.0%)	0.71	25/15068 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	ARG	C-N	6.22	1.41	1.33
4	H	135	ALA	CA-C	-5.63	1.46	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	109	GLN	CA-C-N	13.77	133.97	119.78
5	L	109	GLN	C-N-CA	13.77	133.97	119.78
5	L	54	ARG	CA-C-N	13.63	134.01	120.52
5	L	54	ARG	C-N-CA	13.63	134.01	120.52
3	G	75	VAL	CA-C-N	9.60	129.97	119.90
3	G	75	VAL	C-N-CA	9.60	129.97	119.90
4	H	123	ALA	CA-C-N	8.62	128.55	119.85
4	H	123	ALA	C-N-CA	8.62	128.55	119.85
2	E	81	GLU	N-CA-C	-8.01	102.53	111.82
4	H	131	GLY	N-CA-C	-7.98	102.02	111.36
2	E	79	GLN	N-CA-C	-6.84	99.02	109.41
4	H	120	PHE	CA-C-N	-6.56	111.64	119.84
4	H	120	PHE	C-N-CA	-6.56	111.64	119.84
2	E	81	GLU	N-CA-CB	5.85	119.34	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	153	SER	N-CA-C	5.76	117.64	111.36
3	G	71	THR	N-CA-C	-5.64	106.20	112.57
3	G	312	GLY	CA-C-N	-5.62	114.00	119.90
3	G	312	GLY	C-N-CA	-5.62	114.00	119.90
3	G	246	GLN	N-CA-C	5.56	117.14	111.14
3	G	550	GLN	CA-C-O	-5.55	115.83	122.27
5	L	108	SER	CA-C-O	-5.39	115.46	122.14
3	G	248	THR	CA-CB-OG1	-5.14	101.89	109.60
3	G	415	THR	CB-CA-C	5.12	118.59	109.38
3	G	660	LEU	N-CA-C	-5.11	105.71	111.28
3	G	65	LYS	O-C-N	5.04	127.26	122.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1341	0	1285	73	0
2	E	1375	0	1320	20	0
3	G	4754	0	4644	242	1
4	H	1767	0	1738	67	0
5	L	1586	0	1526	74	0
6	A	83	0	70	1	0
7	B	39	0	34	1	0
7	C	39	0	33	2	0
8	F	94	0	79	16	0
9	I	61	0	52	1	0
9	O	61	0	51	18	0
10	J	28	0	25	0	0
10	P	28	0	25	26	0
10	R	28	0	22	0	0
11	K	50	0	43	0	0
12	M	94	0	79	11	0
13	N	33	0	28	9	0
14	Q	44	0	34	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	S	94	0	79	1	0
16	G	168	0	156	12	0
17	G	22	0	20	16	0
All	All	11789	0	11343	512	1

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 22.

All (512) 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)
3:G:133:ASN:HD21	16:G:1133:NAG:C1	1.06	1.63
3:G:64:GLU:HB2	3:G:66:HIS:CE1	1.37	1.55
5:L:35:TRP:CD1	5:L:48:ILE:HD11	1.45	1.52
3:G:64:GLU:CB	3:G:66:HIS:CE1	1.89	1.51
3:G:325:ASP:OD2	4:H:100(B):TYR:CD1	1.70	1.44
17:G:1201:MAN:C1	7:C:3:BMA:O3	1.63	1.43
5:L:54:ARG:NH2	5:L:60:ASP:HA	1.10	1.43
3:G:133:ASN:ND2	16:G:1133:NAG:C1	1.81	1.41
17:G:1266:MAN:C1	8:F:7:MAN:O3	1.70	1.38
5:L:109:GLN:HE22	5:L:171:ASN:CB	1.36	1.37
1:D:36:TRP:CZ3	1:D:92:CYS:HB3	1.60	1.35
5:L:35:TRP:HD1	5:L:48:ILE:CD1	1.38	1.33
5:L:54:ARG:NH2	5:L:60:ASP:CA	1.90	1.31
5:L:109:GLN:NE2	5:L:171:ASN:CB	1.93	1.31
10:P:2:NAG:O4	14:Q:1:BMA:C1	1.85	1.25
17:G:1266:MAN:C1	8:F:7:MAN:C3	2.16	1.24
9:O:1:NAG:C5	10:P:1:NAG:HN2	1.50	1.23
9:O:1:NAG:C6	10:P:1:NAG:HN2	1.50	1.22
17:G:1266:MAN:C2	8:F:7:MAN:H4	1.70	1.22
3:G:75:VAL:CG2	3:G:76:PRO:HD2	1.71	1.21
17:G:1266:MAN:C1	8:F:7:MAN:H4	1.70	1.21
12:M:3:BMA:C3	13:N:1:MAN:C1	2.18	1.21
12:M:3:BMA:H3	13:N:1:MAN:C1	1.69	1.21
3:G:64:GLU:CB	3:G:66:HIS:HE1	1.37	1.20
17:G:1266:MAN:H2	8:F:7:MAN:O4	1.42	1.19
17:G:1266:MAN:C1	8:F:7:MAN:C4	2.19	1.19
5:L:54:ARG:NH2	5:L:59:PRO:O	1.76	1.18
17:G:1266:MAN:H2	8:F:7:MAN:C4	1.72	1.17
1:D:51:VAL:HG23	1:D:57:VAL:CG1	1.73	1.16
3:G:164:GLU:OE2	3:G:308:ARG:NH2	1.79	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:184:SER:CA	4:H:187:LEU:HD23	1.77	1.12
9:O:1:NAG:H5	10:P:1:NAG:H3	1.31	1.12
4:H:184:SER:O	4:H:187:LEU:HG	1.48	1.12
9:O:1:NAG:H62	10:P:1:NAG:N2	1.64	1.12
9:O:1:NAG:H62	10:P:1:NAG:C8	1.77	1.12
16:G:1235:NAG:C1	16:G:1234:NAG:O4	1.98	1.11
17:G:1266:MAN:C2	8:F:7:MAN:C4	2.28	1.11
1:D:51:VAL:HG23	1:D:57:VAL:HG13	1.12	1.10
3:G:346:VAL:HA	3:G:349:LEU:HD13	1.22	1.09
3:G:325:ASP:OD2	4:H:100(B):TYR:CE1	2.05	1.08
3:G:570:VAL:HG13	3:G:571:TRP:H	0.93	1.08
1:D:36:TRP:HD1	1:D:69:MET:SD	1.77	1.07
3:G:64:GLU:CA	3:G:66:HIS:HE1	1.51	1.07
9:O:1:NAG:H5	10:P:1:NAG:C3	1.83	1.07
3:G:64:GLU:HB2	3:G:66:HIS:NE2	1.68	1.06
3:G:346:VAL:CA	3:G:349:LEU:HD13	1.86	1.05
3:G:349:LEU:HD12	3:G:349:LEU:H	1.20	1.04
3:G:75:VAL:HG22	3:G:76:PRO:HD2	1.39	1.04
4:H:122:LEU:HD12	5:L:119:PHE:HD2	1.17	1.04
1:D:51:VAL:CG2	1:D:57:VAL:CG1	2.34	1.03
9:O:1:NAG:H62	10:P:1:NAG:C7	1.86	1.03
9:O:1:NAG:C6	10:P:1:NAG:N2	2.21	1.01
1:D:51:VAL:CB	1:D:57:VAL:HG12	1.90	1.00
1:D:51:VAL:HB	1:D:57:VAL:HG12	1.43	0.99
4:H:184:SER:HA	4:H:187:LEU:HD23	1.01	0.99
3:G:325:ASP:OD2	4:H:100(B):TYR:CG	2.15	0.99
5:L:35:TRP:HB2	5:L:48:ILE:HG13	1.45	0.99
3:G:332:ASN:OD1	3:G:415:THR:OG1	1.79	0.98
3:G:81:PRO:C	3:G:82:GLN:OE1	2.07	0.97
5:L:54:ARG:NH1	5:L:62:PHE:O	1.97	0.97
3:G:570:VAL:HG13	3:G:571:TRP:N	1.66	0.97
5:L:54:ARG:HH22	5:L:60:ASP:HA	1.24	0.96
3:G:55:ALA:N	3:G:74:CYS:SG	2.35	0.96
4:H:122:LEU:HD21	4:H:139:LEU:HB2	1.49	0.95
3:G:75:VAL:HG23	3:G:76:PRO:HD2	1.47	0.95
12:M:3:BMA:O3	13:N:1:MAN:C1	2.17	0.93
5:L:54:ARG:NH2	5:L:59:PRO:C	2.26	0.93
9:O:1:NAG:C5	10:P:1:NAG:N2	2.31	0.92
3:G:64:GLU:CB	3:G:66:HIS:NE2	2.29	0.92
1:D:71:ARG:NE	1:D:73:PHE:HE1	1.66	0.92
1:D:36:TRP:CD1	1:D:69:MET:SD	2.63	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:54:ARG:HH21	5:L:60:ASP:HA	1.18	0.92
3:G:133:ASN:ND2	16:G:1133:NAG:C2	2.34	0.90
3:G:275:GLU:OE1	3:G:282:LYS:NZ	2.03	0.90
1:D:36:TRP:CZ3	1:D:92:CYS:CB	2.52	0.90
4:H:122:LEU:HD12	5:L:119:PHE:CD2	2.05	0.90
3:G:568:LEU:HD12	3:G:568:LEU:H	1.34	0.90
10:P:2:NAG:HO4	14:Q:1:BMA:C1	1.80	0.89
3:G:64:GLU:HB3	3:G:66:HIS:CE1	2.06	0.88
3:G:259:LEU:HD23	3:G:449:ILE:HD13	1.55	0.88
4:H:122:LEU:CD1	5:L:119:PHE:HD2	1.86	0.88
5:L:54:ARG:HH22	5:L:60:ASP:CA	1.72	0.88
1:D:59:TYR:OH	1:D:69:MET:N	2.07	0.87
3:G:82:GLN:OE1	3:G:82:GLN:N	2.07	0.87
3:G:64:GLU:CA	3:G:66:HIS:CE1	2.26	0.87
9:O:1:NAG:H5	10:P:1:NAG:HN2	1.39	0.87
3:G:570:VAL:CG1	3:G:571:TRP:H	1.71	0.87
1:D:51:VAL:CB	1:D:57:VAL:CG1	2.53	0.87
3:G:133:ASN:HD21	16:G:1133:NAG:C2	1.88	0.86
3:G:607:ASN:O	3:G:607:ASN:ND2	2.07	0.86
3:G:67:ASN:O	3:G:70:ALA:O	1.91	0.86
4:H:63:LEU:CD1	4:H:67:VAL:HB	2.06	0.86
4:H:63:LEU:HD13	4:H:67:VAL:HB	1.57	0.85
5:L:35:TRP:CD1	5:L:48:ILE:CD1	2.28	0.85
1:D:22:CYS:HB2	1:D:36:TRP:HH2	1.42	0.85
1:D:36:TRP:HZ3	1:D:92:CYS:HB3	1.40	0.85
9:O:1:NAG:H62	10:P:1:NAG:H83	1.56	0.85
1:D:36:TRP:CE3	1:D:92:CYS:HB3	2.12	0.85
4:H:184:SER:O	4:H:187:LEU:CG	2.23	0.85
5:L:150:LYS:HZ2	5:L:155:PRO:HD3	1.42	0.85
5:L:54:ARG:HH21	5:L:59:PRO:C	1.85	0.84
1:D:48:MET:HG2	1:D:63:PHE:HE2	1.41	0.84
1:D:51:VAL:HB	1:D:57:VAL:CG1	2.07	0.84
3:G:80:ASN:OD1	3:G:81:PRO:HD2	1.78	0.83
3:G:60:ALA:HB3	3:G:65:LYS:HE3	1.58	0.83
1:D:35:HIS:HD2	1:D:47:TRP:HE1	1.26	0.83
17:G:1266:MAN:C1	8:F:7:MAN:O2	2.27	0.83
3:G:360:ARG:HB3	3:G:467:THR:HG22	1.61	0.83
5:L:35:TRP:HB2	5:L:48:ILE:CG1	2.09	0.82
1:D:51:VAL:CG2	1:D:57:VAL:HG13	2.00	0.82
4:H:184:SER:HA	4:H:187:LEU:CD2	1.98	0.82
9:O:1:NAG:H62	10:P:1:NAG:HN2	1.21	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:234:ASN:OD1	3:G:235:GLY:N	2.13	0.81
1:D:71:ARG:CZ	1:D:73:PHE:HE1	1.94	0.81
3:G:92:GLU:HB3	3:G:238:PRO:HA	1.64	0.80
1:D:22:CYS:HB2	1:D:36:TRP:CH2	2.16	0.80
3:G:78:ASP:OD1	3:G:550:GLN:CB	2.31	0.79
9:O:1:NAG:H5	10:P:1:NAG:N2	1.94	0.79
3:G:569:THR:O	3:G:570:VAL:HG12	1.83	0.79
3:G:37:THR:HG22	3:G:605:THR:HG22	1.64	0.79
3:G:275:GLU:OE1	3:G:282:LYS:CE	2.31	0.79
3:G:474:ASP:OD1	3:G:475:MET:N	2.16	0.79
3:G:561:ALA:H	3:G:564:HIS:CE1	1.99	0.79
4:H:141:LYS:NZ	5:L:132:THR:OG1	2.17	0.77
1:D:35:HIS:CD2	1:D:50:TRP:HB3	2.19	0.77
3:G:570:VAL:CG1	3:G:571:TRP:N	2.40	0.77
3:G:275:GLU:OE1	3:G:282:LYS:HD2	1.85	0.77
3:G:246:GLN:NE2	3:G:548:ILE:HG22	2.00	0.76
17:G:1266:MAN:C1	8:F:7:MAN:HO3	1.95	0.76
3:G:555:LEU:N	3:G:555:LEU:HD23	2.01	0.75
3:G:133:ASN:ND2	16:G:1133:NAG:O7	2.19	0.75
1:D:59:TYR:CE1	1:D:69:MET:HE2	2.21	0.75
3:G:556:LEU:O	3:G:559:PRO:HD2	1.86	0.74
4:H:122:LEU:N	4:H:122:LEU:HD23	2.01	0.74
3:G:133:ASN:CG	16:G:1133:NAG:C1	2.59	0.74
3:G:456:ARG:HD2	3:G:468:PHE:HE1	1.52	0.74
5:L:54:ARG:NH2	5:L:60:ASP:N	2.34	0.74
3:G:75:VAL:HG21	3:G:556:LEU:HB3	1.69	0.74
10:P:2:NAG:O4	14:Q:1:BMA:C2	2.36	0.74
3:G:67:ASN:HD21	3:G:69:TRP:HD1	1.35	0.73
3:G:78:ASP:OD2	3:G:79:PRO:HD2	1.87	0.73
1:D:53:LEU:C	1:D:53:LEU:HD23	2.13	0.73
5:L:54:ARG:HH21	5:L:60:ASP:N	1.86	0.72
3:G:102:GLU:O	3:G:106:THR:HG23	1.89	0.72
1:D:40:ALA:HB3	1:D:43:ARG:HB2	1.72	0.72
1:D:50:TRP:NE1	1:D:58:SER:HB3	2.05	0.72
12:M:3:BMA:O3	13:N:1:MAN:C2	2.37	0.72
1:D:48:MET:HG2	1:D:63:PHE:CE2	2.25	0.71
3:G:491:ILE:HD11	3:G:544:LEU:HD23	1.70	0.71
5:L:109:GLN:HB2	5:L:110:PRO:CD	2.20	0.71
1:D:142:VAL:HG11	1:D:178:LEU:H	1.55	0.71
17:G:1201:MAN:C1	7:C:3:BMA:C3	2.68	0.71
5:L:54:ARG:CZ	5:L:60:ASP:HA	2.11	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:635:ILE:O	3:G:639:THR:OG1	2.08	0.70
4:H:3:HIS:HB3	4:H:25:SER:HB2	1.71	0.70
3:G:309:ILE:HG21	3:G:317:PHE:HB3	1.74	0.70
17:G:1266:MAN:C1	8:F:7:MAN:C2	2.69	0.70
4:H:184:SER:O	4:H:187:LEU:CD2	2.39	0.70
3:G:346:VAL:CA	3:G:349:LEU:CD1	2.64	0.70
5:L:54:ARG:HH21	5:L:60:ASP:CA	1.79	0.69
2:E:52:ASN:OD1	2:E:52:ASN:N	2.26	0.69
5:L:54:ARG:HH22	5:L:60:ASP:C	2.00	0.69
1:D:59:TYR:HH	1:D:69:MET:H	1.41	0.69
4:H:126:SER:OG	4:H:127:LYS:HD3	1.93	0.69
3:G:259:LEU:CD2	3:G:449:ILE:HD13	2.23	0.69
3:G:275:GLU:OE1	3:G:282:LYS:CD	2.41	0.69
5:L:35:TRP:HD1	5:L:48:ILE:HD11	0.56	0.69
1:D:71:ARG:CZ	1:D:73:PHE:CE1	2.76	0.68
1:D:47:TRP:HZ2	1:D:50:TRP:HD1	1.42	0.68
2:E:29:GLY:HA3	3:G:278:THR:HG21	1.75	0.68
4:H:22:CYS:HB2	4:H:36:TRP:CH2	2.28	0.68
9:O:1:NAG:H5	10:P:1:NAG:C2	2.23	0.68
1:D:66:ARG:NH1	1:D:86:ASP:OD2	2.27	0.68
3:G:349:LEU:HD12	3:G:349:LEU:N	2.03	0.68
4:H:22:CYS:HB3	4:H:78:VAL:HB	1.74	0.68
3:G:246:GLN:HE21	3:G:548:ILE:HG22	1.58	0.67
3:G:75:VAL:CG2	3:G:76:PRO:CD	2.62	0.67
4:H:121:PRO:CB	4:H:209:VAL:HG22	2.25	0.67
9:O:1:NAG:C6	10:P:1:NAG:H83	2.25	0.66
5:L:109:GLN:CB	5:L:110:PRO:CD	2.73	0.66
4:H:63:LEU:HD12	4:H:63:LEU:O	1.96	0.65
3:G:346:VAL:HA	3:G:349:LEU:CD1	2.13	0.65
3:G:568:LEU:H	3:G:568:LEU:CD1	2.02	0.65
17:G:1266:MAN:C2	8:F:7:MAN:O4	2.30	0.65
4:H:121:PRO:HB2	4:H:209:VAL:HG22	1.79	0.65
1:D:51:VAL:CA	1:D:57:VAL:HG12	2.27	0.64
3:G:568:LEU:HD12	3:G:568:LEU:N	2.07	0.64
3:G:64:GLU:HB3	3:G:66:HIS:NE2	2.10	0.64
3:G:246:GLN:NE2	3:G:548:ILE:CG2	2.62	0.63
4:H:184:SER:CA	4:H:187:LEU:CD2	2.66	0.63
5:L:47:ILE:HG22	5:L:48:ILE:HG23	1.79	0.63
5:L:37:GLN:HB2	5:L:47:ILE:HD11	1.81	0.63
3:G:561:ALA:N	3:G:564:HIS:CE1	2.66	0.63
12:M:3:BMA:O4	13:N:1:MAN:C1	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:298:ARG:NH2	3:G:441:GLY:O	2.31	0.62
4:H:167:VAL:HG22	5:L:163:THR:HB	1.82	0.62
3:G:258:GLN:HG3	3:G:374:HIS:HA	1.81	0.62
5:L:54:ARG:HB3	5:L:55:PRO:HD2	1.80	0.62
4:H:5:GLN:HB3	4:H:23:ASN:HB2	1.81	0.62
5:L:117:THR:HG22	5:L:119:PHE:CE1	2.34	0.62
3:G:101:VAL:HG11	3:G:480:ARG:HG2	1.81	0.62
3:G:201:ILE:HD11	3:G:435:TYR:HB2	1.81	0.61
5:L:49:TYR:HE1	5:L:54:ARG:C	2.07	0.61
3:G:259:LEU:HD23	3:G:449:ILE:CD1	2.27	0.61
3:G:349:LEU:H	3:G:349:LEU:CD1	1.98	0.61
1:D:71:ARG:NE	1:D:73:PHE:CE1	2.58	0.61
4:H:66:ARG:NH1	4:H:82:LEU:HD11	2.16	0.61
3:G:75:VAL:HG22	3:G:76:PRO:CD	2.25	0.61
1:D:39:GLN:HB2	1:D:45:LEU:HD23	1.82	0.60
3:G:491:ILE:HD11	3:G:544:LEU:CD2	2.30	0.60
3:G:67:ASN:HD21	3:G:69:TRP:CD1	2.19	0.60
5:L:35:TRP:CD1	5:L:48:ILE:CG1	2.85	0.60
3:G:215:ILE:O	3:G:215:ILE:HG13	2.01	0.60
2:E:46:LEU:HD21	2:E:49:PHE:HB3	1.84	0.59
5:L:82:ASP:O	5:L:86:TYR:OH	2.14	0.59
3:G:654:GLU:O	3:G:658:GLN:HB2	2.03	0.59
3:G:294:ILE:O	3:G:446:VAL:HA	2.03	0.59
5:L:109:GLN:HB2	5:L:110:PRO:HD3	1.84	0.59
4:H:124:PRO:HG3	4:H:136:LEU:HA	1.84	0.58
4:H:24:VAL:O	4:H:76:ASN:ND2	2.36	0.58
3:G:456:ARG:HD2	3:G:468:PHE:CE1	2.36	0.58
3:G:65:LYS:C	3:G:66:HIS:ND1	2.62	0.58
4:H:195:ASN:N	4:H:195:ASN:OD1	2.34	0.58
3:G:78:ASP:OD2	3:G:79:PRO:CD	2.52	0.58
17:G:1266:MAN:C3	8:F:7:MAN:H4	2.33	0.58
5:L:146:THR:OG1	5:L:197:THR:O	2.18	0.58
12:M:3:BMA:C4	13:N:1:MAN:C1	2.82	0.58
3:G:73:ALA:CB	3:G:571:TRP:HD1	2.16	0.57
3:G:78:ASP:CG	3:G:550:GLN:CB	2.78	0.57
3:G:102:GLU:O	3:G:102:GLU:HG3	2.04	0.57
3:G:95:MET:HE1	3:G:273:ARG:HB3	1.87	0.57
4:H:35:SER:HB3	4:H:47:TRP:HE1	1.70	0.57
4:H:51:VAL:HB	4:H:69:LEU:HD13	1.85	0.57
2:E:50:SER:OG	9:I:2:NAG:H82	2.04	0.57
3:G:254:VAL:HG11	3:G:261:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:295:ASN:OD1	3:G:446:VAL:HG12	2.05	0.57
3:G:346:VAL:C	3:G:349:LEU:HD13	2.28	0.57
3:G:73:ALA:HB2	3:G:566:LEU:HD13	1.87	0.57
3:G:68:VAL:O	3:G:111:LEU:HD22	2.05	0.57
3:G:491:ILE:CD1	3:G:544:LEU:CD2	2.83	0.57
3:G:548:ILE:HG12	3:G:549:VAL:HG13	1.87	0.57
3:G:60:ALA:HB3	3:G:65:LYS:CE	2.31	0.56
3:G:108:ILE:N	3:G:108:ILE:HD13	2.19	0.56
5:L:109:GLN:HB2	5:L:110:PRO:HD2	1.87	0.56
2:E:34:SER:OG	2:E:89:ASN:OD1	2.23	0.56
3:G:138:ILE:HA	3:G:150:MET:N	2.20	0.56
1:D:1:GLU:O	1:D:1:GLU:HG2	2.05	0.56
3:G:134:VAL:HG13	6:A:1:NAG:H81	1.87	0.56
3:G:309:ILE:CG2	3:G:317:PHE:HB3	2.36	0.56
1:D:53:LEU:HD23	1:D:53:LEU:O	2.05	0.56
3:G:93:PHE:CZ	3:G:228:CYS:HB2	2.41	0.56
4:H:126:SER:O	4:H:127:LYS:HD3	2.05	0.56
4:H:135:ALA:O	4:H:136:LEU:HB2	2.06	0.55
1:D:35:HIS:CD2	1:D:47:TRP:HE1	2.15	0.55
5:L:92:ASP:HB3	5:L:95:ARG:HB2	1.87	0.55
3:G:47:ASP:HB3	3:G:487:LYS:HE2	1.89	0.55
3:G:296:CYS:HB2	3:G:445:CYS:HB2	1.88	0.55
1:D:35:HIS:NE2	1:D:50:TRP:HB3	2.21	0.55
3:G:551:GLN:O	3:G:556:LEU:HG	2.07	0.55
3:G:596:TRP:CD1	3:G:647:GLU:HA	2.41	0.55
3:G:86:LEU:HB3	3:G:89:VAL:HG21	1.89	0.54
4:H:126:SER:C	4:H:127:LYS:HD3	2.32	0.54
4:H:133:THR:HA	4:H:182:VAL:O	2.07	0.54
1:D:61:ARG:HH12	3:G:467:THR:CG2	2.21	0.54
1:D:73:PHE:N	1:D:73:PHE:CD1	2.73	0.54
3:G:184:ILE:O	3:G:184:ILE:HG23	2.07	0.54
3:G:566:LEU:HD11	3:G:570:VAL:HG12	1.88	0.54
3:G:256:SER:HB3	3:G:259:LEU:O	2.07	0.54
1:D:39:GLN:OE1	2:E:38:GLN:NE2	2.40	0.54
3:G:47:ASP:HA	3:G:489:VAL:HA	1.90	0.54
3:G:133:ASN:ND2	16:G:1133:NAG:H2	2.22	0.54
3:G:175:LEU:HD13	3:G:321:GLY:O	2.07	0.53
4:H:132:GLY:O	4:H:133:THR:OG1	2.19	0.53
4:H:168:LEU:HD12	4:H:174:TYR:CZ	2.44	0.53
9:O:1:NAG:C5	10:P:1:NAG:H3	2.21	0.53
1:D:61:ARG:HH12	3:G:467:THR:HG23	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:45:TRP:CD1	3:G:45:TRP:C	2.86	0.53
3:G:78:ASP:CG	3:G:79:PRO:HD2	2.34	0.53
3:G:545:LEU:HD22	3:G:546:SER:H	1.74	0.53
2:E:106(A):LEU:HD12	2:E:106(A):LEU:N	2.23	0.53
1:D:87:THR:HB	1:D:111:VAL:HG22	1.89	0.53
5:L:117:THR:CG2	5:L:119:PHE:CE1	2.91	0.53
16:G:1235:NAG:C1	16:G:1234:NAG:C4	2.86	0.53
1:D:51:VAL:HA	1:D:57:VAL:HG12	1.90	0.53
3:G:55:ALA:HB3	3:G:216:HIS:HB2	1.90	0.53
3:G:295:ASN:HB3	12:M:1:NAG:H81	1.89	0.53
9:O:1:NAG:C6	10:P:1:NAG:C8	2.68	0.53
4:H:133:THR:H	4:H:184:SER:H	1.57	0.52
1:D:59:TYR:HE1	1:D:69:MET:HG3	1.73	0.52
3:G:596:TRP:HD1	3:G:647:GLU:HA	1.74	0.52
3:G:75:VAL:HG23	3:G:76:PRO:CD	2.31	0.52
5:L:55:PRO:HG2	5:L:58:ILE:HG13	1.92	0.52
3:G:269:GLU:CD	3:G:348:GLN:HE22	2.17	0.52
3:G:84:ILE:O	3:G:243:SER:HB2	2.10	0.52
5:L:150:LYS:NZ	5:L:155:PRO:HD3	2.20	0.52
3:G:276:ASN:OD1	3:G:278:THR:OG1	2.25	0.52
3:G:161:MET:HE2	3:G:162:THR:HG22	1.92	0.52
3:G:323:ILE:N	3:G:323:ILE:CD1	2.73	0.52
4:H:184:SER:C	4:H:187:LEU:HD23	2.35	0.52
3:G:73:ALA:HB3	3:G:571:TRP:CD1	2.46	0.51
3:G:104:MET:O	3:G:107:ASP:HB2	2.10	0.51
4:H:121:PRO:HB3	4:H:209:VAL:HG22	1.91	0.51
4:H:122:LEU:CD1	5:L:119:PHE:CD2	2.79	0.51
3:G:269:GLU:HB3	3:G:348:GLN:NE2	2.24	0.51
4:H:5:GLN:O	4:H:23:ASN:N	2.43	0.51
4:H:36:TRP:CZ3	4:H:92:CYS:HB2	2.46	0.51
3:G:80:ASN:OD1	3:G:81:PRO:CD	2.56	0.51
5:L:79:GLU:HG2	5:L:82:ASP:OD2	2.10	0.51
3:G:212:PRO:HG2	3:G:254:VAL:HG22	1.93	0.51
12:M:3:BMA:O3	13:N:1:MAN:H3	2.11	0.51
3:G:391:PHE:CD2	3:G:470:PRO:HG2	2.45	0.51
3:G:476:ARG:HA	3:G:479:TRP:CD1	2.46	0.51
3:G:257:THR:HG21	3:G:370:GLU:O	2.10	0.51
10:P:1:NAG:O3	10:P:2:NAG:C1	2.59	0.51
1:D:140:CYS:N	1:D:180:SER:O	2.44	0.50
3:G:108:ILE:N	3:G:108:ILE:CD1	2.73	0.50
4:H:127:LYS:O	4:H:127:LYS:HG2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:159:PHE:CE1	3:G:172:VAL:HG23	2.47	0.50
3:G:567:LYS:HB2	3:G:568:LEU:HD12	1.93	0.50
3:G:66:HIS:ND1	3:G:66:HIS:N	2.59	0.50
3:G:73:ALA:HB3	3:G:571:TRP:HD1	1.75	0.50
1:D:30:THR:HA	1:D:52(A):PRO:HB2	1.93	0.50
3:G:230:ASP:HB3	3:G:233:PHE:HB2	1.94	0.50
3:G:64:GLU:CB	3:G:66:HIS:HE2	2.20	0.49
3:G:164:GLU:OE2	3:G:308:ARG:HD2	2.12	0.49
3:G:220:PRO:HG2	3:G:223:PHE:CD1	2.46	0.49
3:G:617:ARG:NH1	3:G:634:GLU:OE2	2.45	0.49
3:G:73:ALA:HB2	3:G:566:LEU:CD1	2.42	0.49
3:G:338:TRP:CE2	3:G:390:LEU:HD12	2.47	0.49
1:D:51:VAL:O	1:D:51:VAL:HG13	2.13	0.49
17:G:1266:MAN:H2	8:F:7:MAN:H4	1.45	0.49
3:G:648:GLU:HG2	3:G:652:GLN:HB3	1.94	0.49
10:P:2:NAG:C4	14:Q:1:BMA:C1	2.88	0.49
1:D:55:GLY:O	1:D:56:GLY:C	2.55	0.49
1:D:51:VAL:CG2	1:D:57:VAL:HG11	2.38	0.49
3:G:257:THR:OG1	3:G:375:SER:HB3	2.13	0.49
3:G:93:PHE:HB3	3:G:487:LYS:HD2	1.94	0.48
5:L:83:GLU:OE1	5:L:106:VAL:HG22	2.13	0.48
3:G:47:ASP:N	3:G:47:ASP:OD1	2.45	0.48
3:G:133:ASN:ND2	16:G:1133:NAG:C7	2.77	0.48
3:G:323:ILE:N	3:G:323:ILE:HD12	2.28	0.48
3:G:195:ASN:C	3:G:195:ASN:ND2	2.72	0.48
5:L:34:ILE:HB	5:L:89:HIS:HB3	1.94	0.48
5:L:54:ARG:HB3	5:L:55:PRO:CD	2.44	0.48
3:G:530:MET:N	3:G:626:MET:O	2.46	0.48
1:D:13:LYS:HG2	1:D:14:PRO:HD2	1.94	0.48
3:G:555:LEU:N	3:G:555:LEU:CD2	2.73	0.48
4:H:190:GLN:OE1	4:H:191:THR:N	2.37	0.48
3:G:175:LEU:HB2	3:G:320:THR:HB	1.96	0.48
3:G:491:ILE:HD12	3:G:544:LEU:HD21	1.96	0.48
3:G:569:THR:O	3:G:570:VAL:CG1	2.59	0.47
10:P:2:NAG:O4	14:Q:1:BMA:H2	2.13	0.47
3:G:292:VAL:HB	3:G:449:ILE:HB	1.96	0.47
3:G:563:GLN:HA	3:G:566:LEU:HB3	1.96	0.47
3:G:64:GLU:HB2	3:G:66:HIS:HE2	1.66	0.47
1:D:53:LEU:C	1:D:53:LEU:CD2	2.85	0.47
3:G:53:PHE:CE1	3:G:218:CYS:HB2	2.50	0.47
3:G:216:HIS:N	3:G:216:HIS:CD2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:184:GLU:O	5:L:188:SER:OG	2.31	0.47
8:F:1:NAG:H61	8:F:2:NAG:HN2	1.80	0.47
3:G:71:THR:O	3:G:71:THR:OG1	2.30	0.47
3:G:611:ASN:OD1	3:G:613:SER:OG	2.26	0.47
16:G:1137:NAG:H83	5:L:91:TRP:HE3	1.80	0.47
5:L:36:TYR:HD1	5:L:46:LEU:HA	1.79	0.47
3:G:88:ASN:OD1	16:G:1088:NAG:O5	2.31	0.47
3:G:558:ALA:N	3:G:559:PRO:HD2	2.29	0.47
5:L:61:ARG:NH1	5:L:82:ASP:OD2	2.47	0.47
3:G:136:ASN:OD1	3:G:150:MET:HE3	2.15	0.47
3:G:153:GLU:HB3	3:G:178:ARG:H	1.80	0.47
3:G:358:ILE:HB	3:G:465:THR:HA	1.97	0.47
1:D:166:PHE:CE2	2:E:137:SER:HB2	2.51	0.46
3:G:306:SER:O	3:G:306:SER:OG	2.29	0.46
3:G:330:HIS:HA	3:G:416:LEU:O	2.15	0.46
5:L:54:ARG:CB	5:L:55:PRO:CD	2.93	0.46
5:L:141:TYR:C	5:L:198:HIS:HE2	2.23	0.46
1:D:53:LEU:CD2	3:G:473:GLY:O	2.63	0.46
2:E:34:SER:HB3	2:E:49:PHE:O	2.15	0.46
3:G:45:TRP:HA	3:G:491:ILE:HA	1.98	0.46
3:G:51:THR:O	3:G:51:THR:OG1	2.24	0.46
9:O:1:NAG:H61	9:O:2:NAG:N2	2.31	0.46
3:G:53:PHE:H	3:G:53:PHE:HD1	1.64	0.46
3:G:296:CYS:O	3:G:445:CYS:N	2.41	0.46
4:H:132:GLY:C	4:H:133:THR:HG1	2.18	0.46
4:H:33:TYR:HE2	4:H:56:ASP:OD2	1.98	0.46
1:D:39:GLN:O	1:D:88:ALA:HB1	2.16	0.46
3:G:561:ALA:N	3:G:564:HIS:ND1	2.64	0.46
3:G:45:TRP:CD1	3:G:45:TRP:O	2.69	0.46
5:L:197:THR:HA	5:L:202:THR:HA	1.97	0.46
12:M:3:BMA:O3	13:N:1:MAN:C3	2.64	0.46
2:E:42:ARG:HD3	2:E:42:ARG:HA	1.73	0.45
3:G:338:TRP:CD2	3:G:390:LEU:HD12	2.51	0.45
3:G:325:ASP:CG	4:H:100(B):TYR:CD1	2.77	0.45
5:L:51:ASN:ND2	5:L:65:SER:O	2.36	0.45
5:L:109:GLN:HE21	5:L:171:ASN:CB	2.14	0.45
4:H:122:LEU:CD2	4:H:139:LEU:HB2	2.32	0.45
2:E:106(A):LEU:HA	2:E:107:GLY:HA2	1.58	0.45
10:P:1:NAG:HO3	10:P:2:NAG:C1	2.29	0.45
3:G:67:ASN:ND2	3:G:69:TRP:HD1	2.11	0.45
3:G:82:GLN:HB2	3:G:549:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:101:VAL:HG11	3:G:480:ARG:CG	2.46	0.45
3:G:84:ILE:HG22	3:G:86:LEU:HD12	1.99	0.45
3:G:551:GLN:HA	3:G:555:LEU:HG	1.99	0.45
12:M:3:BMA:O3	13:N:1:MAN:H2	2.17	0.45
3:G:309:ILE:HG13	3:G:309:ILE:O	2.16	0.44
4:H:36:TRP:CG	4:H:80:LEU:HD12	2.51	0.44
3:G:161:MET:HE3	3:G:161:MET:HA	1.99	0.44
4:H:123:ALA:HA	4:H:124:PRO:HD3	1.63	0.44
2:E:110:LYS:HG2	2:E:198:GLU:HG3	1.99	0.44
3:G:345:VAL:HG12	3:G:349:LEU:HD21	2.00	0.44
3:G:136:ASN:HD21	3:G:150:MET:HE3	1.80	0.44
2:E:149:LYS:HA	2:E:150:ALA:HA	1.57	0.44
3:G:540:GLN:O	3:G:544:LEU:HG	2.18	0.44
3:G:551:GLN:HA	3:G:555:LEU:HD12	1.98	0.44
2:E:25:ALA:HB3	2:E:69:ASN:HB3	2.00	0.44
3:G:502:LYS:HD3	3:G:503:ARG:N	2.32	0.44
4:H:184:SER:C	4:H:187:LEU:CD2	2.89	0.44
1:D:17:SER:HA	1:D:82:PHE:O	2.18	0.44
3:G:183:GLN:HA	3:G:191:TYR:HD1	1.81	0.44
1:D:66:ARG:O	1:D:82(A):ARG:N	2.50	0.44
1:D:100(C):PHE:N	2:E:36:TYR:OH	2.49	0.44
3:G:136:ASN:OD1	3:G:150:MET:CE	2.65	0.44
5:L:49:TYR:CE1	5:L:54:ARG:C	2.94	0.44
5:L:108:SER:O	5:L:108:SER:OG	2.31	0.44
3:G:298:ARG:NH1	3:G:381:GLU:OE2	2.51	0.43
3:G:62:GLU:HB2	3:G:65:LYS:HE2	2.00	0.43
3:G:192:ARG:HH11	3:G:196:CYS:HB2	1.84	0.43
3:G:193:LEU:HD23	3:G:193:LEU:HA	1.76	0.43
1:D:152:VAL:HA	1:D:198:VAL:HG22	2.00	0.43
1:D:59:TYR:CD1	1:D:69:MET:HE2	2.53	0.43
3:G:86:LEU:HB3	3:G:89:VAL:CG2	2.48	0.43
4:H:152:TRP:HB3	4:H:157:LEU:HD23	2.01	0.43
4:H:168:LEU:HD12	4:H:174:TYR:CE2	2.54	0.43
1:D:148:GLU:N	1:D:149:PRO:HD2	2.34	0.43
1:D:53:LEU:HG	3:G:428:GLN:HG3	2.01	0.43
4:H:132:GLY:HA3	4:H:184:SER:OG	2.19	0.43
3:G:220:PRO:HB3	3:G:578:ALA:HB1	2.00	0.43
3:G:257:THR:HG22	3:G:472:GLY:HA3	2.00	0.43
4:H:6:GLU:HG3	4:H:92:CYS:HB3	2.01	0.43
5:L:141:TYR:CD1	5:L:142:PRO:HA	2.54	0.43
1:D:59:TYR:HE1	1:D:69:MET:HE2	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:63:LEU:CD1	4:H:63:LEU:O	2.65	0.43
2:E:124:GLU:OE2	2:E:131:THR:OG1	2.34	0.42
3:G:174:SER:OG	3:G:175:LEU:N	2.52	0.42
3:G:95:MET:HE3	3:G:96:TRP:CE2	2.54	0.42
5:L:35:TRP:CB	5:L:48:ILE:CG1	2.92	0.42
5:L:166:SER:O	5:L:174:ALA:N	2.51	0.42
8:F:3:BMA:H2	8:F:4:MAN:H5	2.01	0.42
5:L:137:ILE:HG12	5:L:196:VAL:HG21	2.00	0.42
1:D:75:ILE:O	1:D:76:ASP:C	2.62	0.42
1:D:200:HIS:HB2	1:D:203:SER:OG	2.19	0.42
3:G:325:ASP:OD2	4:H:100(B):TYR:CZ	2.67	0.42
5:L:54:ARG:CB	5:L:55:PRO:HD2	2.45	0.42
3:G:567:LYS:HB2	3:G:568:LEU:H	1.59	0.42
5:L:167:LYS:HA	5:L:173:TYR:HA	2.02	0.42
3:G:136:ASN:ND2	3:G:150:MET:HE3	2.34	0.42
3:G:551:GLN:HA	3:G:555:LEU:CG	2.49	0.42
4:H:52:HIS:HB3	4:H:56:ASP:HB3	2.02	0.42
3:G:78:ASP:OD2	3:G:79:PRO:N	2.52	0.42
3:G:151:ARG:C	3:G:151:ARG:HD2	2.43	0.42
1:D:50:TRP:HE1	1:D:58:SER:HB3	1.79	0.42
3:G:55:ALA:HA	3:G:75:VAL:O	2.20	0.42
5:L:16:GLY:C	5:L:77:SER:HA	2.44	0.42
3:G:73:ALA:CB	3:G:566:LEU:HD13	2.50	0.42
3:G:360:ARG:O	3:G:467:THR:HA	2.20	0.42
3:G:555:LEU:HD23	3:G:555:LEU:H	1.84	0.42
2:E:82:ASP:O	2:E:86:TYR:OH	2.27	0.42
3:G:75:VAL:CG2	3:G:556:LEU:HB3	2.46	0.42
3:G:330:HIS:NE2	12:M:1:NAG:H3	2.34	0.42
3:G:346:VAL:C	3:G:349:LEU:CD1	2.91	0.42
5:L:116:VAL:HG12	5:L:137:ILE:HG13	2.02	0.42
1:D:83:LYS:O	1:D:111:VAL:HG21	2.20	0.41
3:G:153:GLU:OE2	3:G:419:ARG:NE	2.46	0.41
5:L:55:PRO:HG2	5:L:58:ILE:CG1	2.50	0.41
1:D:53:LEU:HD22	3:G:473:GLY:O	2.20	0.41
2:E:139:PHE:HE2	2:E:143:ALA:H	1.68	0.41
3:G:544:LEU:HD23	3:G:544:LEU:HA	1.66	0.41
4:H:122:LEU:HD23	4:H:122:LEU:H	1.81	0.41
3:G:93:PHE:HD2	3:G:487:LYS:HD2	1.84	0.41
3:G:448:ASN:HD22	15:S:1:NAG:H83	1.84	0.41
4:H:168:LEU:HD23	4:H:169:GLN:O	2.20	0.41
5:L:141:TYR:CG	5:L:142:PRO:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:150:LYS:HD3	5:L:155:PRO:HB3	2.02	0.41
2:E:164:PRO:HB2	2:E:172:TYR:HB3	2.02	0.41
3:G:160:ASN:HD22	7:B:1:NAG:H83	1.84	0.41
3:G:491:ILE:HD13	3:G:522:PHE:HZ	1.85	0.41
4:H:149:THR:OG1	4:H:197:ASN:HB3	2.21	0.41
2:E:35:TRP:CG	2:E:73:LEU:HD12	2.56	0.41
3:G:530:MET:HG3	3:G:626:MET:O	2.21	0.41
10:P:1:NAG:O3	10:P:2:NAG:O5	2.35	0.41
1:D:75:ILE:H	1:D:75:ILE:HG12	1.73	0.41
3:G:317:PHE:CE2	3:G:319:ALA:HB2	2.56	0.41
5:L:25:GLU:HG3	5:L:31:ARG:NH2	2.36	0.41
5:L:193:SER:HB2	5:L:206:THR:HG22	2.02	0.41
10:P:2:NAG:C3	14:Q:1:BMA:C1	2.99	0.41
1:D:7:SER:OG	1:D:20:VAL:HG13	2.21	0.41
3:G:309:ILE:HD13	3:G:317:PHE:HB2	2.03	0.41
3:G:421:LYS:HE3	3:G:424:ILE:HG22	2.02	0.41
4:H:126:SER:O	4:H:127:LYS:HG2	2.21	0.41
5:L:34:ILE:O	5:L:88:CYS:HA	2.21	0.41
1:D:83:LYS:HB2	1:D:83:LYS:HE3	1.83	0.40
3:G:84:ILE:HG22	3:G:86:LEU:CD1	2.51	0.40
3:G:104:MET:HA	3:G:107:ASP:HB2	2.02	0.40
3:G:297:THR:HG22	3:G:444:ARG:HG2	2.02	0.40
3:G:299:PRO:HB2	3:G:327:ARG:HB2	2.03	0.40
3:G:622:ILE:O	3:G:626:MET:HB2	2.21	0.40
3:G:654:GLU:O	3:G:658:GLN:N	2.36	0.40
3:G:158:SER:HA	3:G:173:TYR:HA	2.02	0.40
4:H:63:LEU:CD1	4:H:67:VAL:CB	2.91	0.40
3:G:195:ASN:C	3:G:195:ASN:HD22	2.29	0.40
4:H:63:LEU:HD12	4:H:67:VAL:HB	1.98	0.40
1:D:50:TRP:CZ3	1:D:52:ARG:NH1	2.90	0.40
3:G:260:LEU:N	3:G:260:LEU:CD1	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:103:GLN:NE2	3:G:560:GLU:OE2[3_685]	1.96	0.24

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	D	163/223 (73%)	157 (96%)	6 (4%)	0	100	100
2	E	176/209 (84%)	171 (97%)	5 (3%)	0	100	100
3	G	598/638 (94%)	572 (96%)	25 (4%)	1 (0%)	43	71
4	H	230/235 (98%)	222 (96%)	6 (3%)	2 (1%)	14	42
5	L	208/213 (98%)	201 (97%)	6 (3%)	1 (0%)	24	54
All	All	1375/1518 (91%)	1323 (96%)	48 (4%)	4 (0%)	36	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	100(E)	VAL
5	L	109	GLN
3	G	570	VAL
4	H	121	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	142/185 (77%)	138 (97%)	4 (3%)	38	60
2	E	153/176 (87%)	150 (98%)	3 (2%)	48	65
3	G	527/552 (96%)	496 (94%)	31 (6%)	18	44
4	H	201/205 (98%)	195 (97%)	6 (3%)	36	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	L	177/181 (98%)	175 (99%)	2 (1%)	65	74
All	All	1200/1299 (92%)	1154 (96%)	46 (4%)	29	54

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	52	ARG
1	D	52(A)	PRO
1	D	73	PHE
1	D	75	ILE
2	E	50	SER
2	E	51	VAL
2	E	52	ASN
3	G	53	PHE
3	G	62	GLU
3	G	66	HIS
3	G	68	VAL
3	G	71	THR
3	G	77	THR
3	G	82	GLN
3	G	93	PHE
3	G	102	GLU
3	G	108	ILE
3	G	110	SER
3	G	111	LEU
3	G	216	HIS
3	G	218	CYS
3	G	307	ILE
3	G	309	ILE
3	G	323	ILE
3	G	341	THR
3	G	349	LEU
3	G	414	ILE
3	G	545	LEU
3	G	548	ILE
3	G	554	ASN
3	G	555	LEU
3	G	564	HIS
3	G	568	LEU
3	G	569	THR
3	G	605	THR
3	G	606	THR

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Mol	Chain	Res	Type
3	G	641	ILE
3	G	660	LEU
4	H	77	LEU
4	H	122	LEU
4	H	127	LYS
4	H	129	THR
4	H	162	HIS
4	H	195	ASN
5	L	54	ARG
5	L	124	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	35	HIS
1	D	64	GLN
3	G	99	ASN
3	G	133	ASN
3	G	216	HIS
3	G	246	GLN
3	G	249	HIS
3	G	348	GLN
3	G	374	HIS
4	H	169	GLN
5	L	109	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

64 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	$\# Z > 2$
6	NAG	A	1	3,6	14,14,15	0.54	0	17,19,21	0.79	0
6	NAG	A	2	6	14,14,15	0.52	0	17,19,21	0.77	0
6	BMA	A	3	6	11,11,12	0.36	0	15,15,17	0.68	0
6	MAN	A	4	6	11,11,12	0.49	0	15,15,17	0.70	0
6	MAN	A	5	6	11,11,12	0.47	0	15,15,17	0.71	0
6	MAN	A	6	6	11,11,12	0.40	0	15,15,17	0.73	0
6	MAN	A	7	6	11,11,12	0.40	0	15,15,17	1.10	1 (6%)
7	NAG	B	1	3,7	14,14,15	0.61	0	17,19,21	0.74	0
7	NAG	B	2	7	14,14,15	0.89	0	17,19,21	1.88	3 (17%)
7	BMA	B	3	7	11,11,12	0.44	0	15,15,17	0.59	0
7	NAG	C	1	3,7	14,14,15	0.26	0	17,19,21	0.51	0
7	NAG	C	2	7	14,14,15	0.33	0	17,19,21	0.67	0
7	BMA	C	3	7	11,11,12	1.05	1 (9%)	15,15,17	1.19	2 (13%)
8	NAG	F	1	3,8	14,14,15	0.49	0	17,19,21	0.82	0
8	NAG	F	2	8	14,14,15	0.54	0	17,19,21	0.83	0
8	BMA	F	3	8	11,11,12	0.48	0	15,15,17	0.71	0
8	MAN	F	4	8	11,11,12	0.43	0	15,15,17	1.09	1 (6%)
8	MAN	F	5	8	11,11,12	0.46	0	15,15,17	1.70	4 (26%)
8	MAN	F	6	8	11,11,12	0.44	0	15,15,17	1.08	0
8	MAN	F	7	8	11,11,12	0.40	0	15,15,17	0.72	0
8	MAN	F	8	8	11,11,12	0.40	0	15,15,17	1.10	1 (6%)
9	NAG	I	1	3,9	14,14,15	0.85	0	17,19,21	1.86	3 (17%)
9	NAG	I	2	9	14,14,15	0.69	0	17,19,21	0.99	0
9	BMA	I	3	9	11,11,12	0.79	0	15,15,17	0.80	1 (6%)
9	MAN	I	4	9	11,11,12	0.45	0	15,15,17	0.60	0
9	MAN	I	5	9	11,11,12	0.62	0	15,15,17	0.73	0
10	NAG	J	1	3,10	14,14,15	0.49	0	17,19,21	0.74	0
10	NAG	J	2	10	14,14,15	0.58	0	17,19,21	0.81	0
11	NAG	K	1	3,11	14,14,15	0.57	0	17,19,21	0.86	0
11	NAG	K	2	11	14,14,15	0.58	0	17,19,21	0.78	0
11	BMA	K	3	11	11,11,12	0.51	0	15,15,17	0.63	0
11	MAN	K	4	11	11,11,12	0.54	0	15,15,17	0.68	0
12	NAG	M	1	3,12	14,14,15	0.32	0	17,19,21	0.47	0
12	NAG	M	2	12	14,14,15	0.37	0	17,19,21	0.67	0
12	BMA	M	3	12	11,11,12	0.62	0	15,15,17	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	M	4	12	11,11,12	0.77	0	15,15,17	1.57	1 (6%)
12	MAN	M	5	12	11,11,12	0.38	0	15,15,17	0.98	0
12	MAN	M	6	12	11,11,12	0.53	0	15,15,17	1.00	2 (13%)
12	MAN	M	7	12	11,11,12	0.45	0	15,15,17	0.71	0
12	MAN	M	8	12	11,11,12	0.44	0	15,15,17	0.65	0
13	MAN	N	1	13	11,11,12	0.40	0	15,15,17	0.67	0
13	MAN	N	2	13	11,11,12	0.41	0	15,15,17	0.71	0
13	MAN	N	3	13	11,11,12	0.41	0	15,15,17	0.67	0
9	NAG	O	1	3,9	14,14,15	0.65	0	17,19,21	0.93	0
9	NAG	O	2	9	14,14,15	0.61	0	17,19,21	2.68	5 (29%)
9	BMA	O	3	9	11,11,12	0.77	1 (9%)	15,15,17	1.44	3 (20%)
9	MAN	O	4	9	11,11,12	0.47	0	15,15,17	1.15	1 (6%)
9	MAN	O	5	9	11,11,12	0.61	0	15,15,17	0.99	0
10	NAG	P	1	3,10	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
10	NAG	P	2	10	14,14,15	0.79	0	17,19,21	0.78	0
14	BMA	Q	1	14	11,11,12	0.59	0	15,15,17	1.06	1 (6%)
14	MAN	Q	2	14	11,11,12	0.44	0	15,15,17	0.70	0
14	MAN	Q	3	14	11,11,12	0.46	0	15,15,17	0.69	0
14	MAN	Q	4	14	11,11,12	0.56	0	15,15,17	2.64	4 (26%)
10	NAG	R	1	3,10	14,14,15	0.64	0	17,19,21	0.85	0
10	NAG	R	2	10	14,14,15	0.72	0	17,19,21	0.76	0
15	NAG	S	1	3,15	14,14,15	0.55	0	17,19,21	0.81	0
15	NAG	S	2	15	14,14,15	0.61	0	17,19,21	0.82	0
15	BMA	S	3	15	11,11,12	0.34	0	15,15,17	1.35	2 (13%)
15	MAN	S	4	15	11,11,12	0.44	0	15,15,17	0.61	0
15	MAN	S	5	15	11,11,12	0.44	0	15,15,17	0.61	0
15	MAN	S	6	15	11,11,12	0.41	0	15,15,17	0.98	0
15	MAN	S	7	15	11,11,12	0.29	0	15,15,17	0.76	0
15	MAN	S	8	15	11,11,12	0.42	0	15,15,17	0.92	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	6	6	-	1/2/19/22	0/1/1/1
6	MAN	A	7	6	-	0/2/19/22	0/1/1/1
7	NAG	B	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	B	2	7	-	4/6/23/26	0/1/1/1
7	BMA	B	3	7	-	0/2/19/22	0/1/1/1
7	NAG	C	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	2	7	-	0/6/23/26	0/1/1/1
7	BMA	C	3	7	-	1/2/19/22	0/1/1/1
8	NAG	F	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	0/6/23/26	0/1/1/1
8	BMA	F	3	8	-	0/2/19/22	0/1/1/1
8	MAN	F	4	8	-	0/2/19/22	0/1/1/1
8	MAN	F	5	8	-	1/2/19/22	0/1/1/1
8	MAN	F	6	8	-	2/2/19/22	0/1/1/1
8	MAN	F	7	8	-	2/2/19/22	0/1/1/1
8	MAN	F	8	8	-	0/2/19/22	0/1/1/1
9	NAG	I	1	3,9	-	6/6/23/26	0/1/1/1
9	NAG	I	2	9	-	2/6/23/26	0/1/1/1
9	BMA	I	3	9	-	0/2/19/22	0/1/1/1
9	MAN	I	4	9	-	1/2/19/22	0/1/1/1
9	MAN	I	5	9	-	0/2/19/22	0/1/1/1
10	NAG	J	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	J	2	10	-	0/6/23/26	0/1/1/1
11	NAG	K	1	3,11	-	0/6/23/26	0/1/1/1
11	NAG	K	2	11	-	0/6/23/26	0/1/1/1
11	BMA	K	3	11	-	2/2/19/22	0/1/1/1
11	MAN	K	4	11	-	0/2/19/22	0/1/1/1
12	NAG	M	1	3,12	-	2/6/23/26	0/1/1/1
12	NAG	M	2	12	-	4/6/23/26	0/1/1/1
12	BMA	M	3	12	-	0/2/19/22	0/1/1/1
12	MAN	M	4	12	-	0/2/19/22	0/1/1/1
12	MAN	M	5	12	-	1/2/19/22	0/1/1/1
12	MAN	M	6	12	-	0/2/19/22	0/1/1/1
12	MAN	M	7	12	-	0/2/19/22	0/1/1/1
12	MAN	M	8	12	-	0/2/19/22	0/1/1/1
13	MAN	N	1	13	-	0/2/19/22	0/1/1/1
13	MAN	N	2	13	-	0/2/19/22	0/1/1/1
13	MAN	N	3	13	-	1/2/19/22	0/1/1/1
9	NAG	O	1	3,9	-	2/6/23/26	0/1/1/1
9	NAG	O	2	9	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	O	3	9	-	2/2/19/22	0/1/1/1
9	MAN	O	4	9	-	0/2/19/22	0/1/1/1
9	MAN	O	5	9	-	0/2/19/22	0/1/1/1
10	NAG	P	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	P	2	10	-	2/6/23/26	0/1/1/1
14	BMA	Q	1	14	-	0/2/19/22	0/1/1/1
14	MAN	Q	2	14	-	0/2/19/22	0/1/1/1
14	MAN	Q	3	14	-	0/2/19/22	0/1/1/1
14	MAN	Q	4	14	-	2/2/19/22	0/1/1/1
10	NAG	R	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	R	2	10	-	0/6/23/26	0/1/1/1
15	NAG	S	1	3,15	-	2/6/23/26	0/1/1/1
15	NAG	S	2	15	-	0/6/23/26	0/1/1/1
15	BMA	S	3	15	-	1/2/19/22	0/1/1/1
15	MAN	S	4	15	-	0/2/19/22	0/1/1/1
15	MAN	S	5	15	-	0/2/19/22	0/1/1/1
15	MAN	S	6	15	-	2/2/19/22	0/1/1/1
15	MAN	S	7	15	-	0/2/19/22	0/1/1/1
15	MAN	S	8	15	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	3	BMA	C2-C3	2.10	1.55	1.52
9	O	3	BMA	O5-C1	-2.05	1.40	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	O	2	NAG	O3-C3-C2	-6.66	95.57	109.40
7	B	2	NAG	C2-N2-C7	6.10	131.07	122.90
9	I	1	NAG	C2-N2-C7	5.99	130.92	122.90
9	O	2	NAG	C1-O5-C5	5.85	120.03	112.19
14	Q	4	MAN	O3-C3-C4	-5.85	96.59	110.38
14	Q	4	MAN	O4-C4-C5	-5.80	95.03	109.32
14	Q	4	MAN	O5-C5-C6	-4.31	99.28	107.66
9	O	2	NAG	O5-C1-C2	-4.11	104.93	111.29
8	F	5	MAN	O5-C5-C6	4.07	115.59	107.66
7	C	3	BMA	C1-O5-C5	3.78	117.26	112.19
9	O	3	BMA	O5-C5-C6	3.46	114.39	107.66
6	A	7	MAN	C1-O5-C5	-3.44	107.58	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	8	MAN	C1-O5-C5	-3.43	107.59	112.19
12	M	4	MAN	C6-C5-C4	-3.40	104.67	113.02
14	Q	4	MAN	O2-C2-C3	3.39	117.17	110.15
15	S	3	BMA	C2-C3-C4	-3.34	104.98	110.86
9	O	2	NAG	O4-C4-C3	3.32	118.20	110.38
9	O	2	NAG	C1-C2-N2	-2.72	106.15	110.43
9	I	1	NAG	C1-C2-N2	2.56	114.47	110.43
14	Q	1	BMA	C2-C3-C4	2.38	115.04	110.86
8	F	4	MAN	C2-C3-C4	-2.37	106.69	110.86
10	P	1	NAG	C8-C7-N2	2.35	120.02	116.12
8	F	5	MAN	O2-C2-C3	2.34	115.01	110.15
7	C	3	BMA	O3-C3-C2	2.34	114.83	110.05
9	O	3	BMA	O3-C3-C2	2.30	114.75	110.05
7	B	2	NAG	C8-C7-N2	2.28	119.90	116.12
9	I	1	NAG	C8-C7-N2	2.27	119.89	116.12
9	O	4	MAN	C2-C3-C4	-2.27	106.87	110.86
8	F	5	MAN	O2-C2-C1	2.23	114.33	109.22
9	O	3	BMA	C3-C4-C5	-2.22	106.21	110.23
10	P	1	NAG	C2-N2-C7	-2.17	120.00	122.90
12	M	6	MAN	O4-C4-C3	-2.14	105.34	110.38
9	I	3	BMA	C6-C5-C4	-2.12	107.80	113.02
7	B	2	NAG	C1-C2-N2	2.12	113.78	110.43
12	M	6	MAN	C2-C3-C4	-2.06	107.23	110.86
8	F	5	MAN	O3-C3-C4	-2.02	105.62	110.38
15	S	3	BMA	O3-C3-C4	-2.01	105.64	110.38

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	O	2	NAG	C1-C2-N2-C7
9	O	2	NAG	C8-C7-N2-C2
9	O	2	NAG	O7-C7-N2-C2
12	M	2	NAG	O5-C5-C6-O6
14	Q	4	MAN	O5-C5-C6-O6
14	Q	4	MAN	C4-C5-C6-O6
8	F	5	MAN	O5-C5-C6-O6
9	O	3	BMA	O5-C5-C6-O6
12	M	2	NAG	C4-C5-C6-O6
9	O	3	BMA	C4-C5-C6-O6
8	F	6	MAN	C4-C5-C6-O6
7	B	1	NAG	C8-C7-N2-C2

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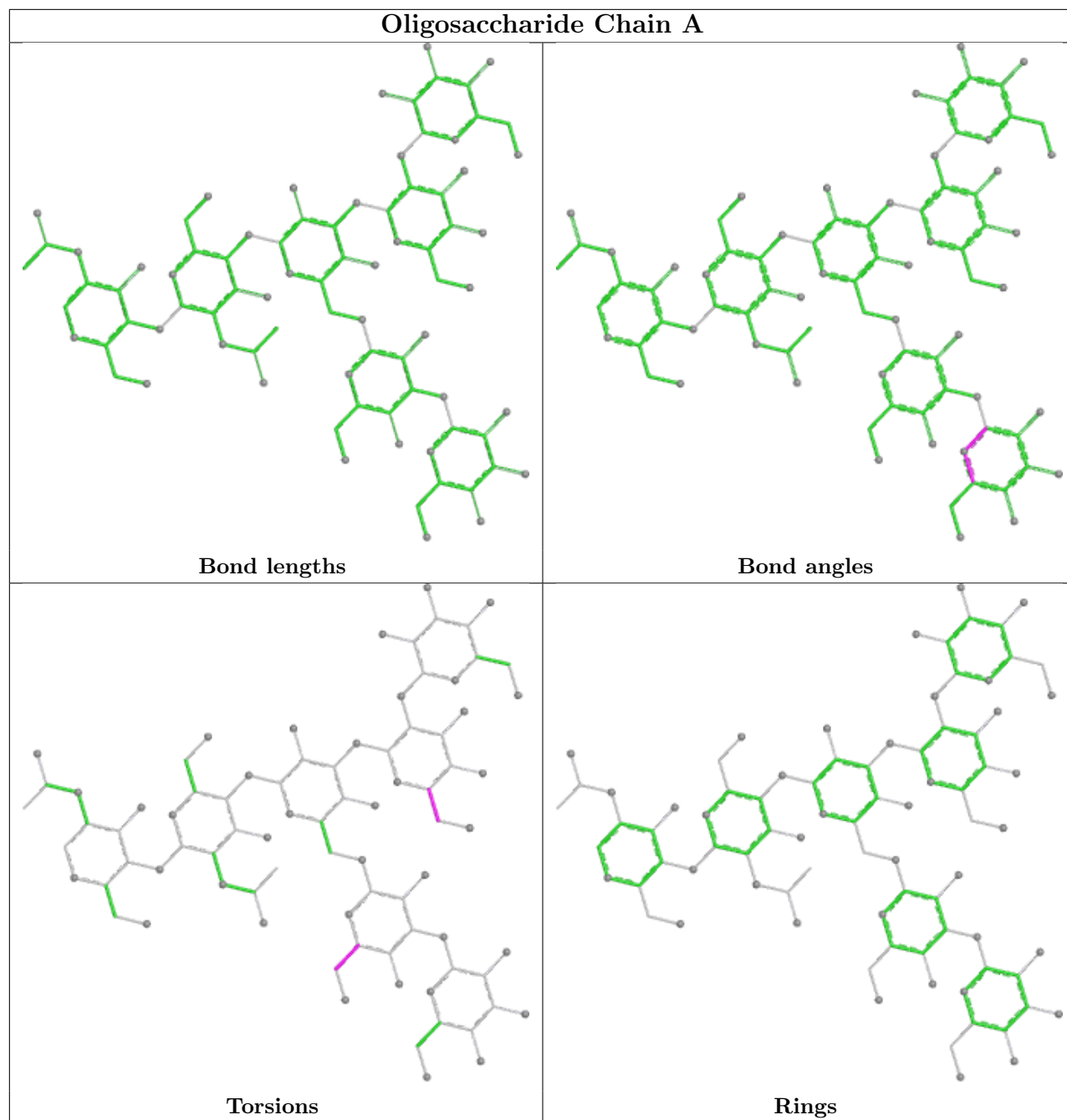
Mol	Chain	Res	Type	Atoms
7	B	1	NAG	O7-C7-N2-C2
7	B	2	NAG	C8-C7-N2-C2
7	B	2	NAG	O7-C7-N2-C2
9	I	1	NAG	C8-C7-N2-C2
9	I	1	NAG	O7-C7-N2-C2
15	S	1	NAG	C8-C7-N2-C2
15	S	1	NAG	O7-C7-N2-C2
8	F	7	MAN	O5-C5-C6-O6
8	F	7	MAN	C4-C5-C6-O6
10	P	2	NAG	C4-C5-C6-O6
8	F	6	MAN	O5-C5-C6-O6
9	I	1	NAG	O5-C5-C6-O6
12	M	5	MAN	O5-C5-C6-O6
10	P	2	NAG	O5-C5-C6-O6
9	I	4	MAN	O5-C5-C6-O6
6	A	4	MAN	O5-C5-C6-O6
13	N	3	MAN	O5-C5-C6-O6
9	O	1	NAG	C1-C2-N2-C7
15	S	3	BMA	C4-C5-C6-O6
7	B	2	NAG	C3-C2-N2-C7
9	I	1	NAG	C3-C2-N2-C7
9	I	2	NAG	C3-C2-N2-C7
9	O	1	NAG	C3-C2-N2-C7
12	M	2	NAG	C3-C2-N2-C7
11	K	3	BMA	C4-C5-C6-O6
11	K	3	BMA	O5-C5-C6-O6
9	I	1	NAG	C4-C5-C6-O6
12	M	1	NAG	C4-C5-C6-O6
7	B	2	NAG	C1-C2-N2-C7
9	I	1	NAG	C1-C2-N2-C7
9	I	2	NAG	C1-C2-N2-C7
12	M	2	NAG	C1-C2-N2-C7
15	S	6	MAN	O5-C5-C6-O6
12	M	1	NAG	O5-C5-C6-O6
6	A	6	MAN	O5-C5-C6-O6
15	S	6	MAN	C4-C5-C6-O6
7	C	3	BMA	C4-C5-C6-O6

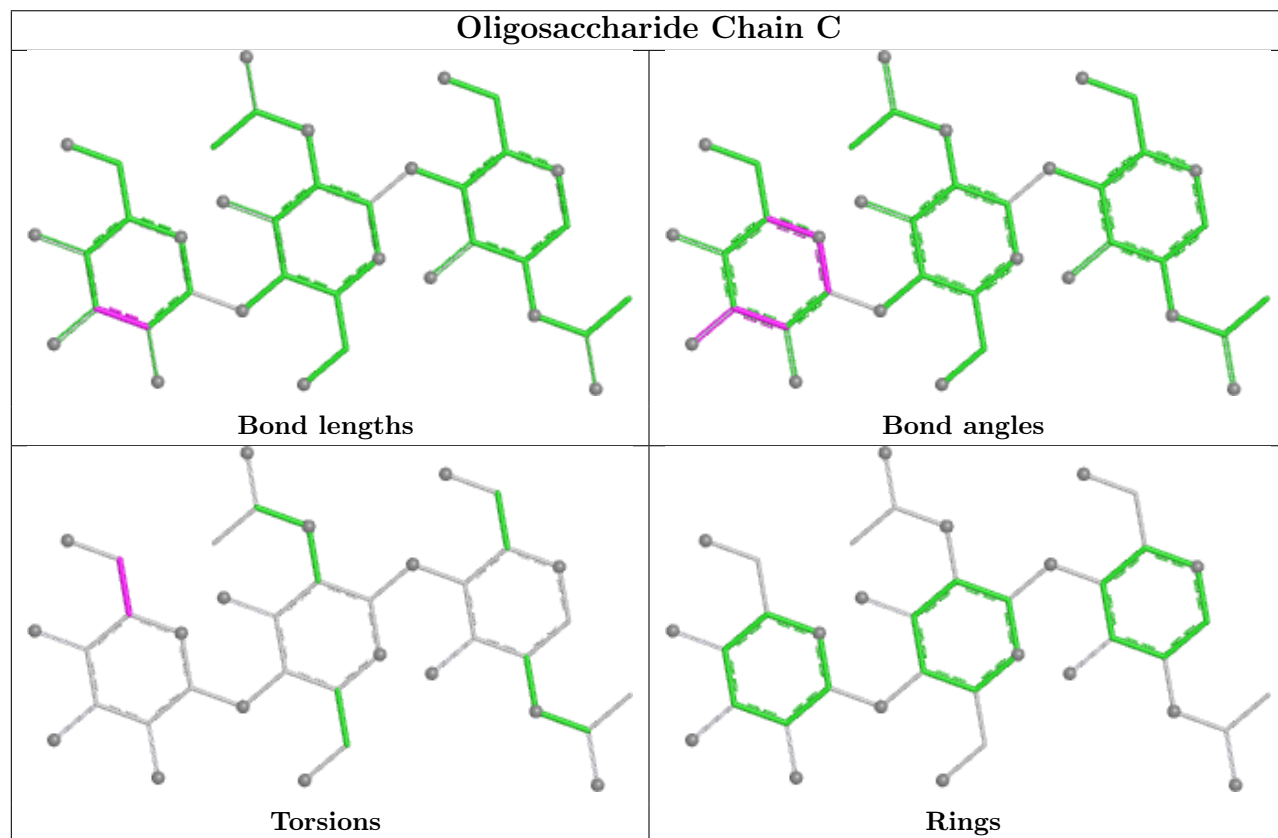
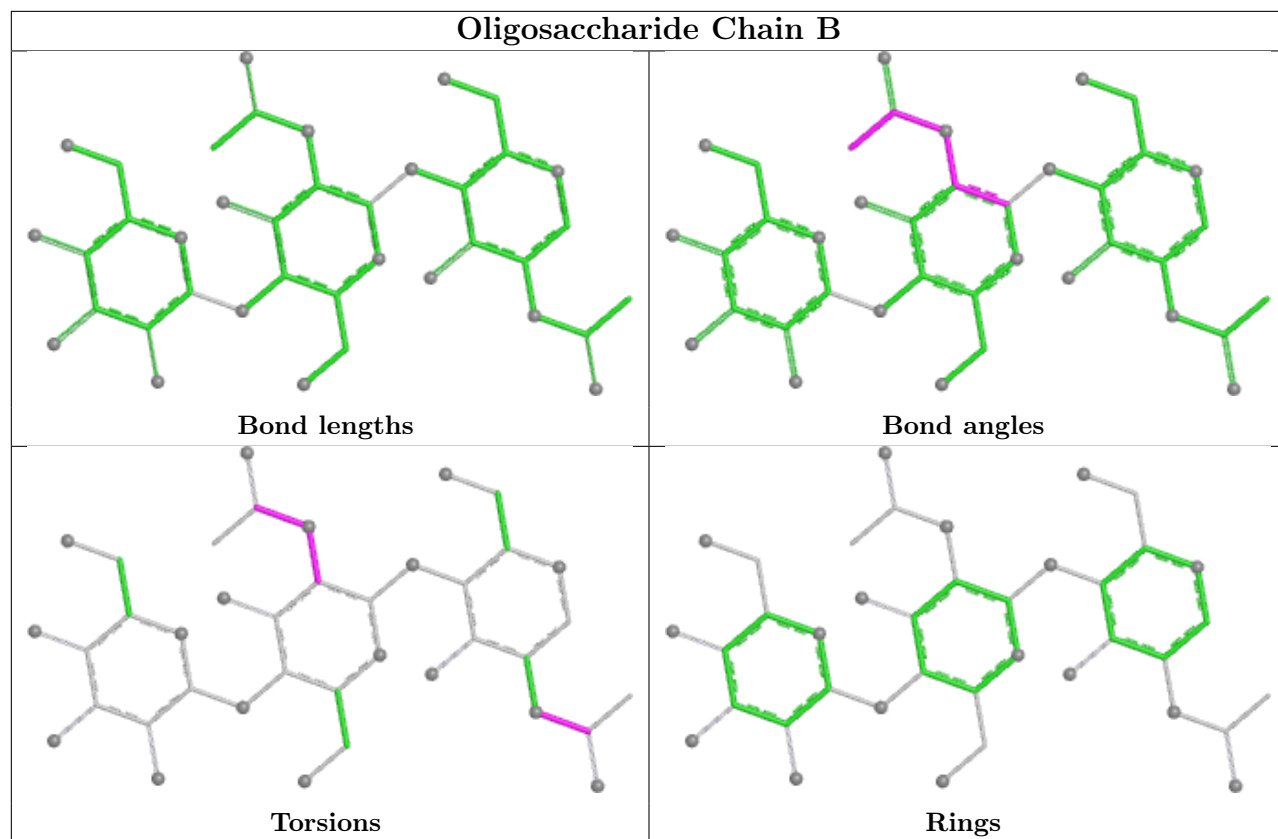
There are no ring outliers.

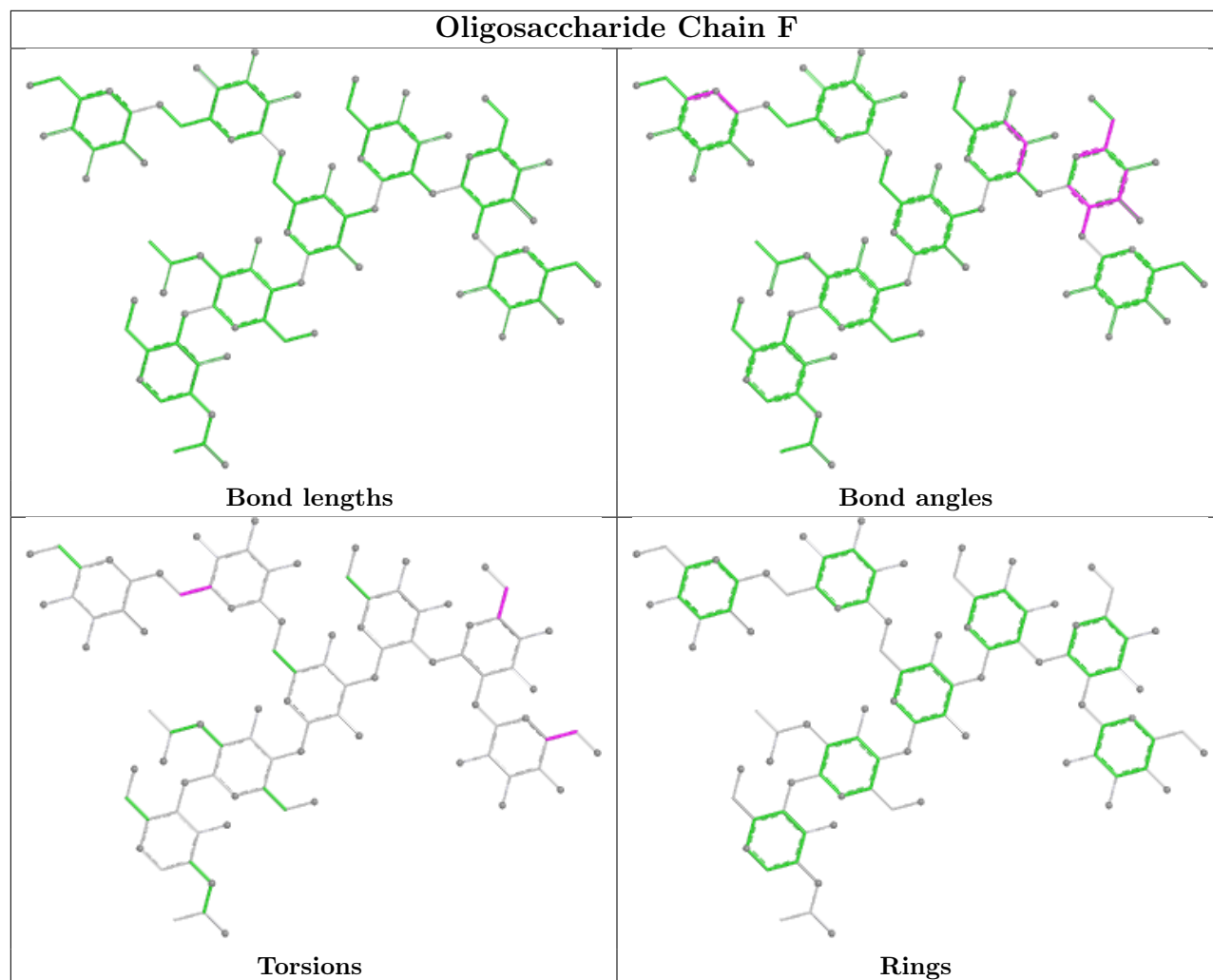
18 monomers are involved in 60 short contacts:

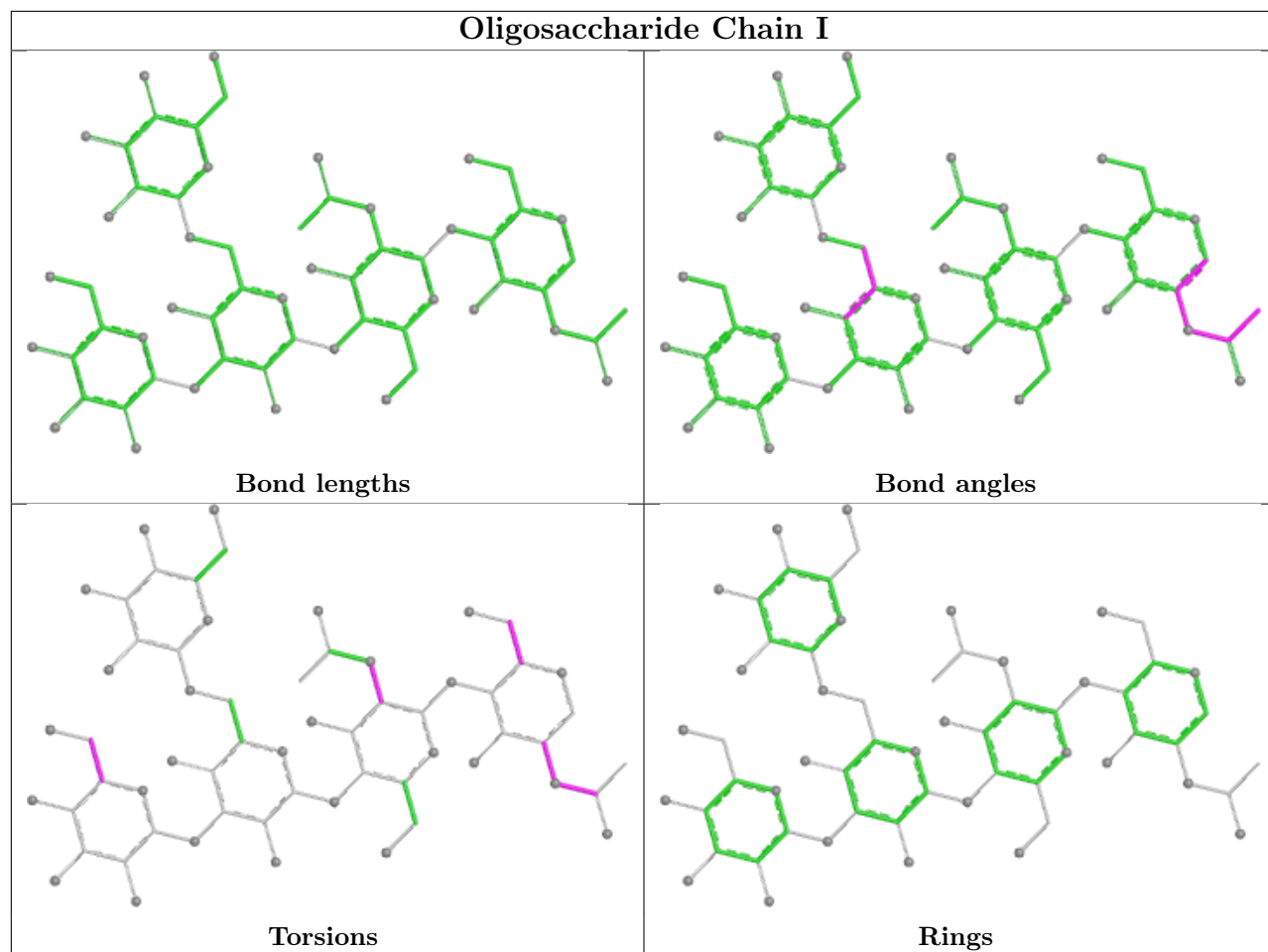
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	3	BMA	2	0
12	M	1	NAG	2	0
12	M	3	BMA	9	0
8	F	2	NAG	1	0
7	B	1	NAG	1	0
9	O	1	NAG	18	0
8	F	1	NAG	1	0
8	F	4	MAN	1	0
10	P	1	NAG	20	0
8	F	3	BMA	1	0
14	Q	1	BMA	6	0
6	A	1	NAG	1	0
15	S	1	NAG	1	0
9	O	2	NAG	1	0
10	P	2	NAG	9	0
13	N	1	MAN	9	0
8	F	7	MAN	14	0
9	I	2	NAG	1	0

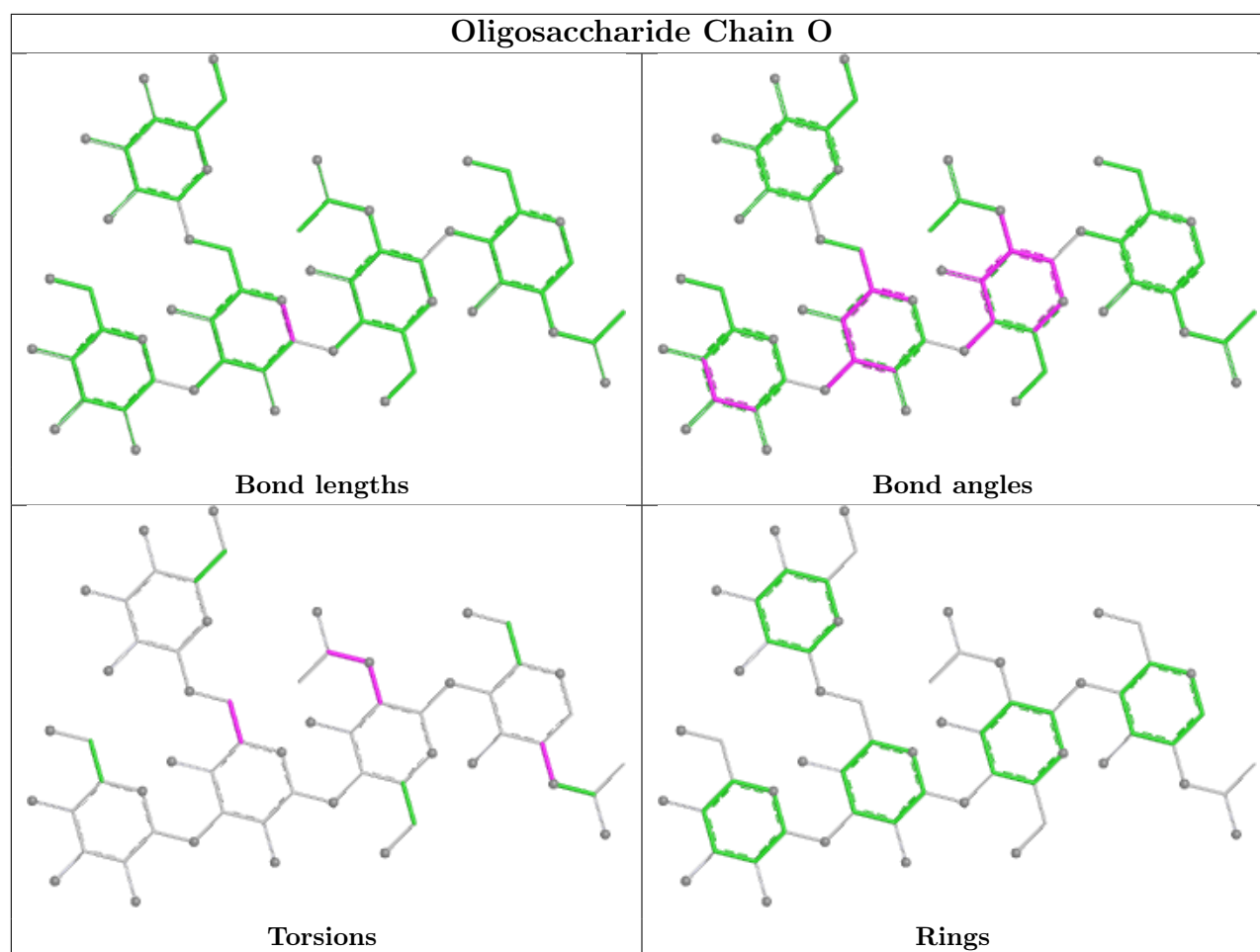
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

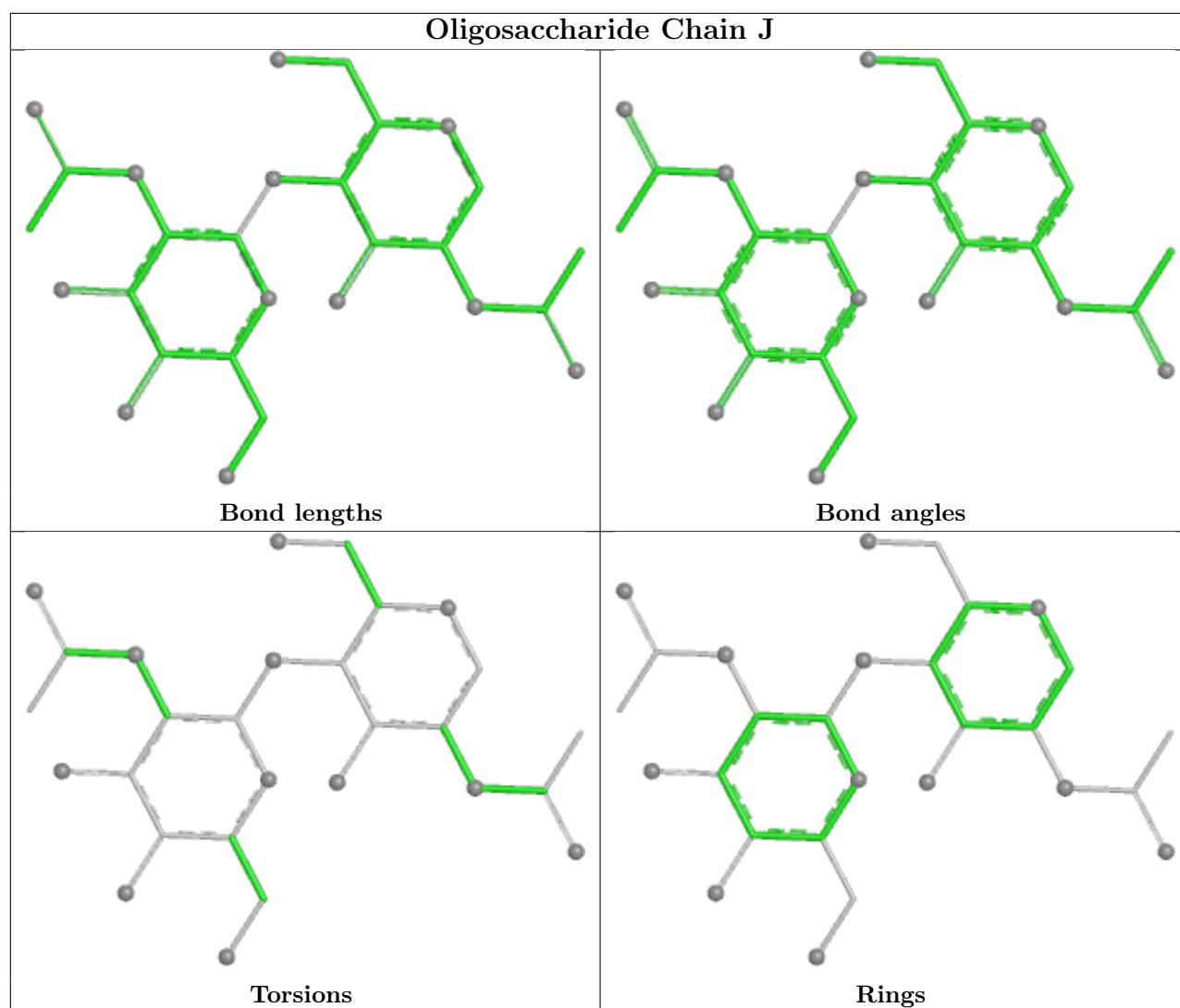


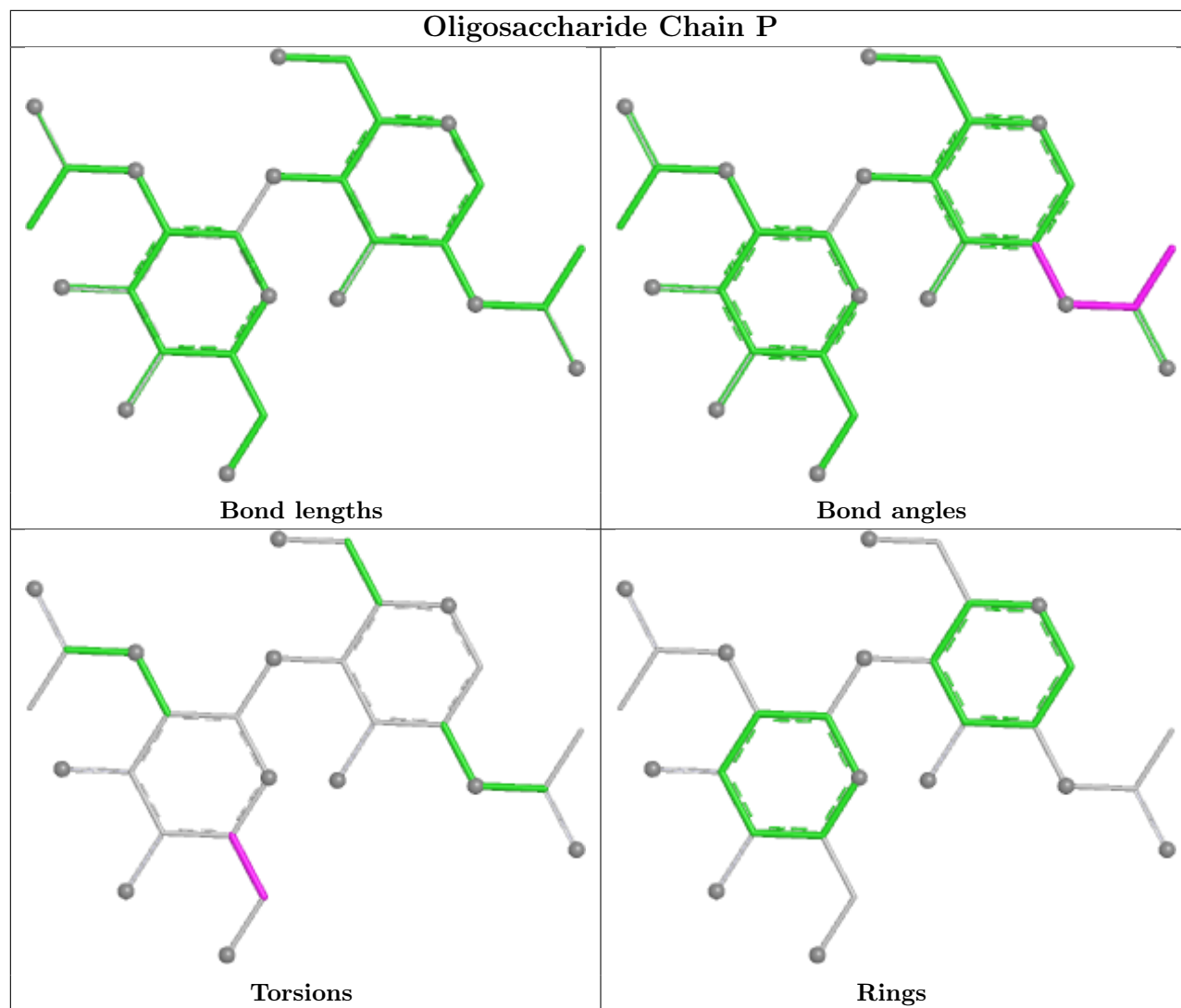


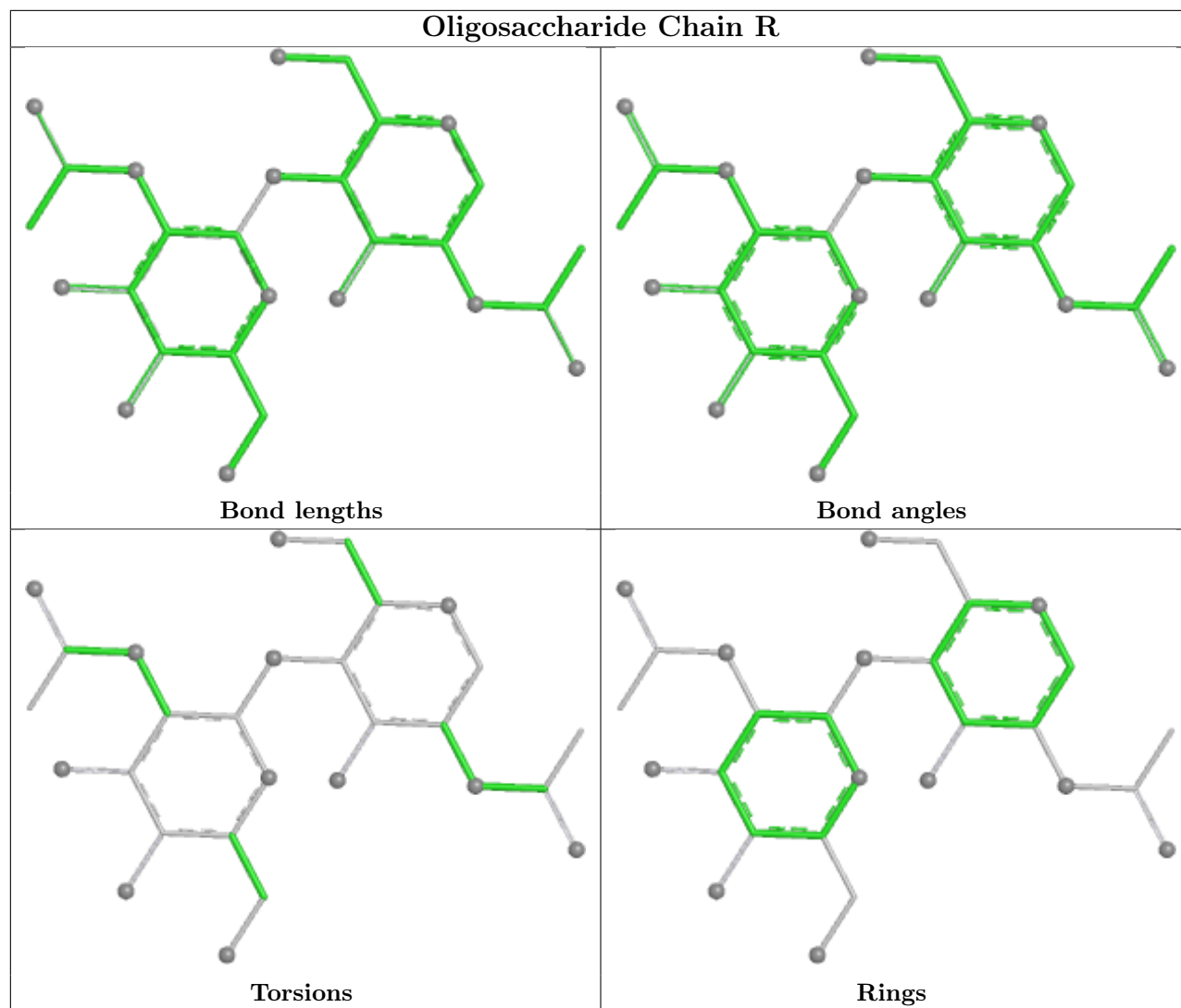


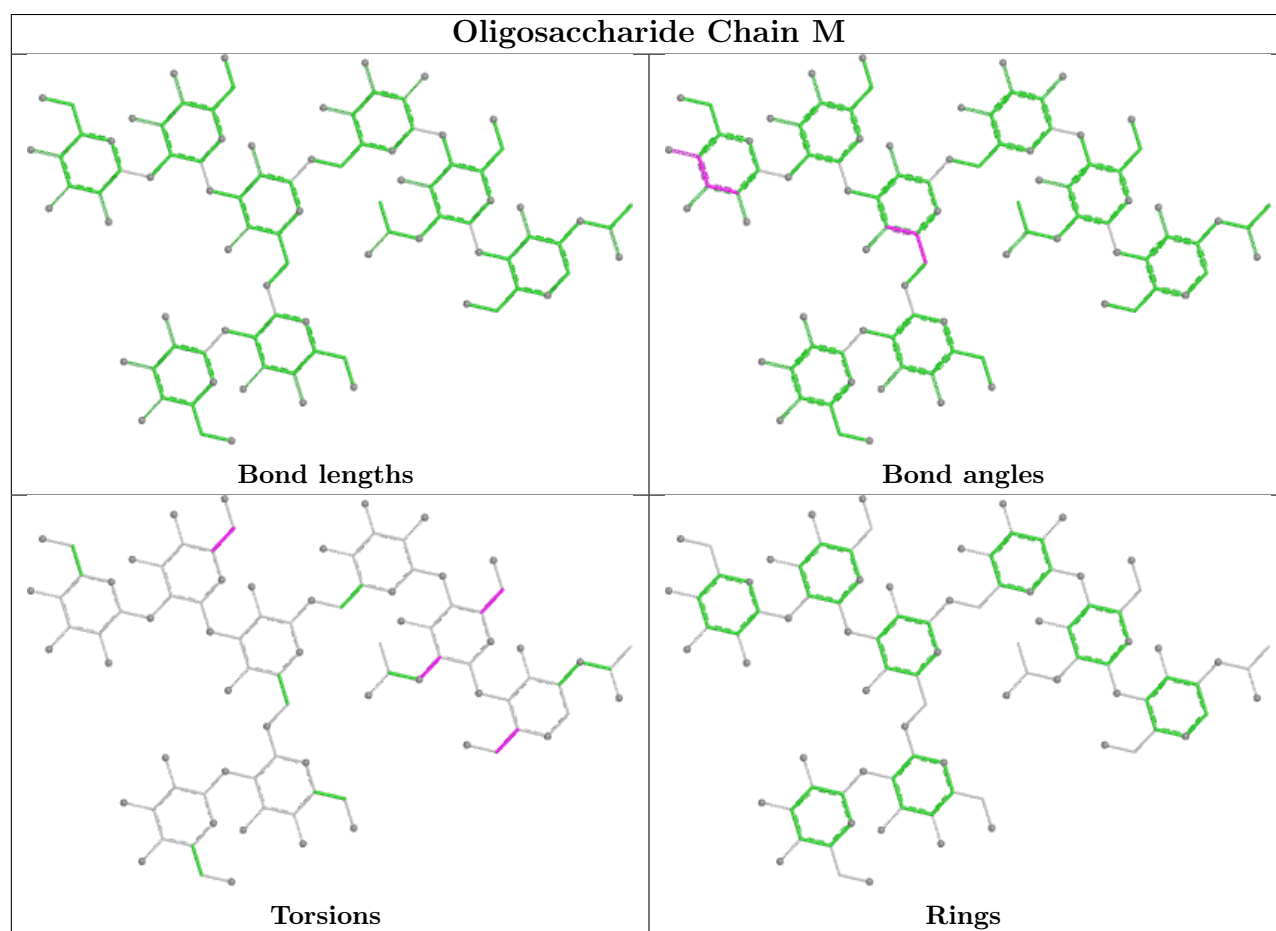
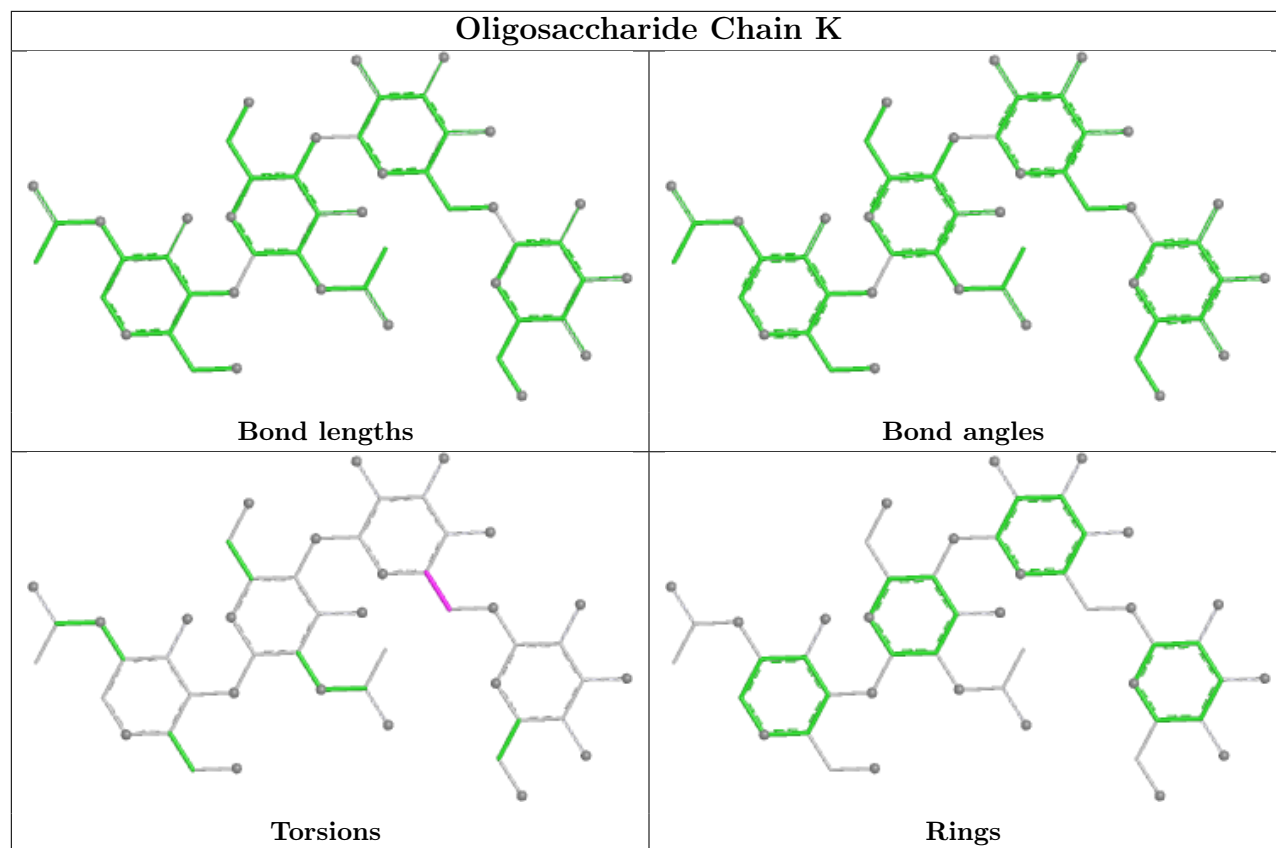


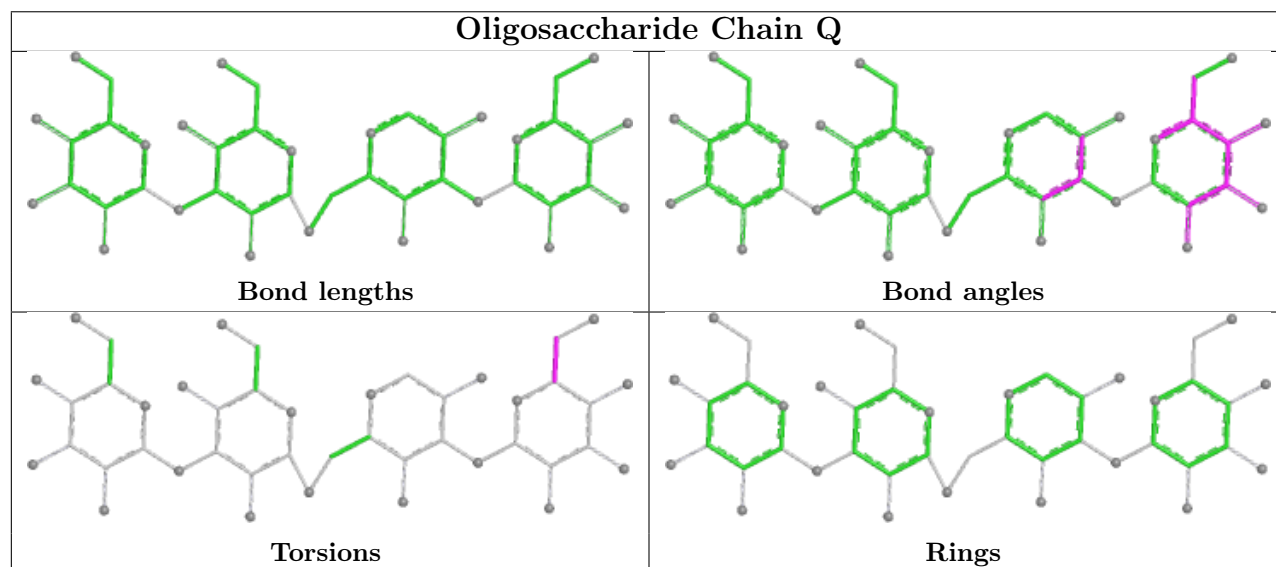
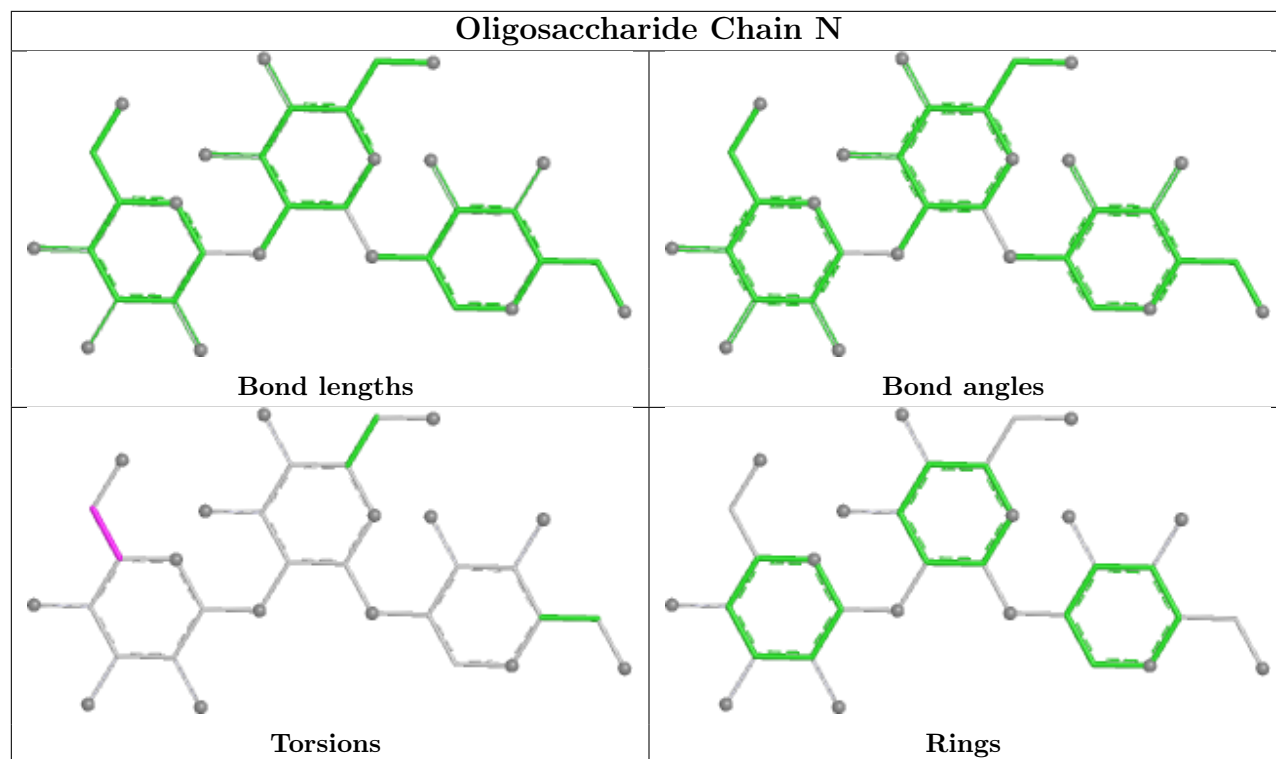


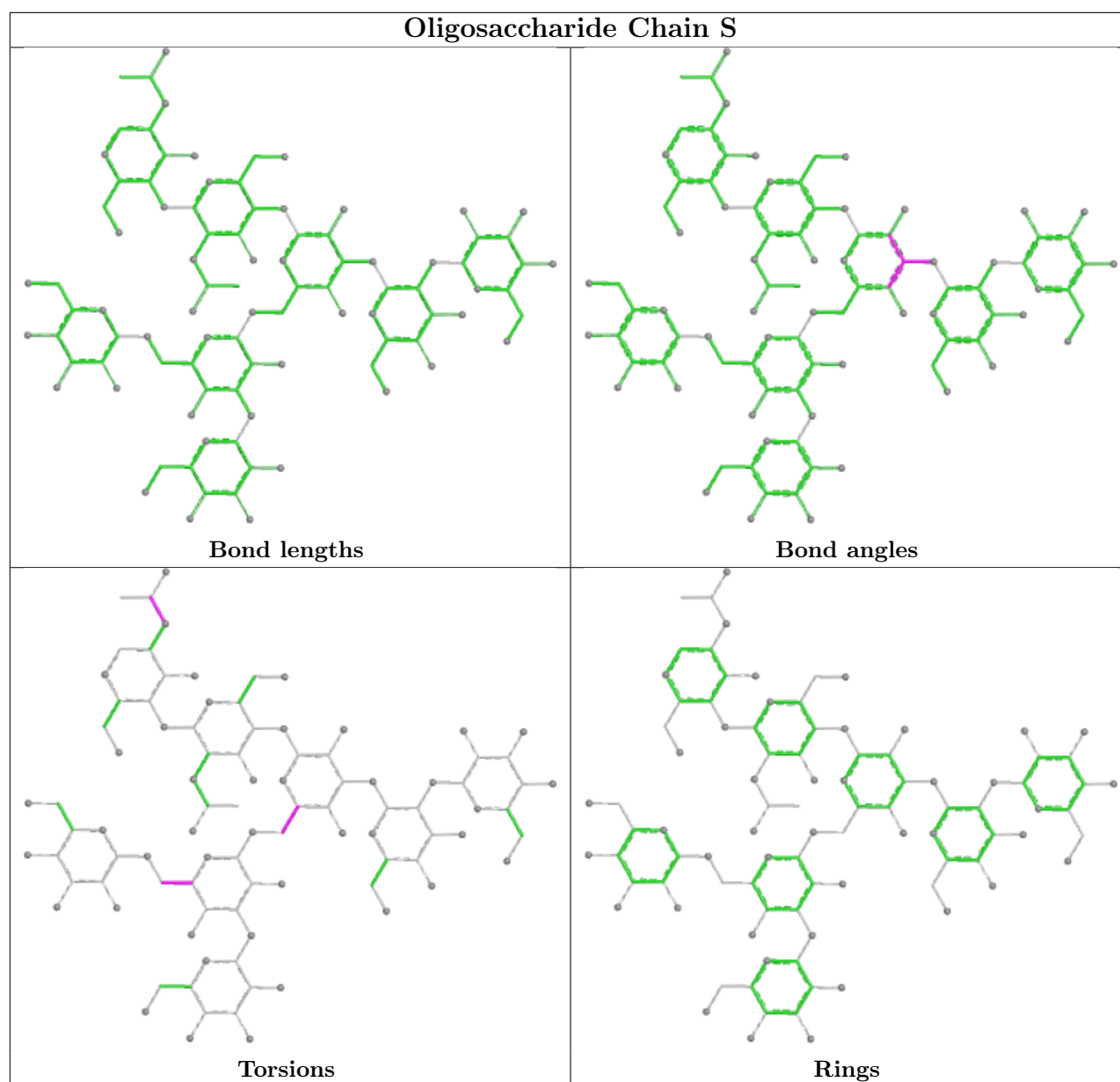












5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	NAG	G	1839	3	14,14,15	0.60	0	17,19,21	0.77	0
17	MAN	G	1266	-	11,11,12	0.36	0	15,15,17	0.70	0
16	NAG	G	1133	-	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
16	NAG	G	1137	3	14,14,15	0.61	0	17,19,21	0.75	0
16	NAG	G	1611	3	14,14,15	0.61	0	17,19,21	1.01	0
16	NAG	G	1235	-	14,14,15	0.57	0	17,19,21	0.79	0
16	NAG	G	1637	3	14,14,15	0.55	0	17,19,21	0.83	0
16	NAG	G	1355	3	14,14,15	0.42	0	17,19,21	0.76	0
17	MAN	G	1201	-	11,11,12	0.57	0	15,15,17	3.22	4 (26%)
16	NAG	G	1088	3	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
16	NAG	G	1618	3	14,14,15	0.63	0	17,19,21	0.72	0
16	NAG	G	1625	3	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
16	NAG	G	1840	3	14,14,15	0.99	0	17,19,21	1.77	4 (23%)
16	NAG	G	1234	-	14,14,15	0.43	0	17,19,21	1.17	2 (11%)

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
16	NAG	G	1839	3	-	0/6/23/26	0/1/1/1
17	MAN	G	1266	-	-	1/2/19/22	0/1/1/1
16	NAG	G	1133	-	-	0/6/23/26	0/1/1/1
16	NAG	G	1137	3	-	1/6/23/26	0/1/1/1
16	NAG	G	1611	3	-	2/6/23/26	0/1/1/1
16	NAG	G	1235	-	-	1/6/23/26	0/1/1/1
16	NAG	G	1637	3	-	0/6/23/26	0/1/1/1
16	NAG	G	1355	3	-	1/6/23/26	0/1/1/1
17	MAN	G	1201	-	-	0/2/19/22	0/1/1/1
16	NAG	G	1088	3	-	0/6/23/26	0/1/1/1
16	NAG	G	1618	3	-	0/6/23/26	0/1/1/1
16	NAG	G	1625	3	-	0/6/23/26	0/1/1/1
16	NAG	G	1840	3	-	4/6/23/26	0/1/1/1
16	NAG	G	1234	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	1201	MAN	O2-C2-C3	7.91	126.53	110.15
17	G	1201	MAN	O3-C3-C4	-5.83	96.63	110.38
17	G	1201	MAN	O4-C4-C5	-5.81	95.01	109.32
16	G	1840	NAG	C2-N2-C7	5.74	130.60	122.90
17	G	1201	MAN	O5-C5-C6	-4.31	99.27	107.66
16	G	1234	NAG	C8-C7-N2	2.38	120.07	116.12
16	G	1840	NAG	C8-C7-N2	2.36	120.03	116.12
16	G	1088	NAG	C8-C7-N2	2.35	120.02	116.12
16	G	1625	NAG	C8-C7-N2	2.34	120.00	116.12
16	G	1133	NAG	C8-C7-N2	2.32	119.97	116.12
16	G	1840	NAG	C1-C2-N2	2.19	113.89	110.43
16	G	1133	NAG	C2-N2-C7	-2.19	119.97	122.90
16	G	1088	NAG	C2-N2-C7	-2.14	120.03	122.90
16	G	1234	NAG	C2-N2-C7	-2.13	120.04	122.90
16	G	1625	NAG	C2-N2-C7	-2.13	120.05	122.90
16	G	1840	NAG	O7-C7-C8	-2.03	118.44	122.05

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	G	1840	NAG	C8-C7-N2-C2
16	G	1840	NAG	O7-C7-N2-C2
17	G	1266	MAN	O5-C5-C6-O6
16	G	1137	NAG	O5-C5-C6-O6
16	G	1611	NAG	C3-C2-N2-C7
16	G	1235	NAG	C1-C2-N2-C7
16	G	1611	NAG	C1-C2-N2-C7
16	G	1840	NAG	C1-C2-N2-C7
16	G	1355	NAG	C1-C2-N2-C7
16	G	1840	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	G	1266	MAN	14	0
16	G	1133	NAG	8	0
16	G	1137	NAG	1	0
16	G	1235	NAG	2	0
17	G	1201	MAN	2	0
16	G	1088	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	1234	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	D	171/223 (76%)	0.53	15 (8%)	15 14	81, 125, 206, 214	0
2	E	182/209 (87%)	0.50	17 (9%)	14 14	130, 168, 244, 255	0
3	G	610/638 (95%)	0.69	72 (11%)	9 10	51, 91, 145, 196	2 (0%)
4	H	232/235 (98%)	0.35	14 (6%)	27 21	96, 123, 149, 161	0
5	L	210/213 (98%)	0.28	10 (4%)	35 26	90, 119, 177, 199	0
All	All	1405/1518 (92%)	0.53	128 (9%)	15 14	51, 115, 211, 255	2 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	496	VAL	5.2
5	L	7	PRO	4.5
3	G	459	GLY	4.5
3	G	369	LEU	4.2
3	G	180	ASP	4.0
2	E	41	GLY	4.0
3	G	150	MET	3.9
4	H	157	LEU	3.9
3	G	36	VAL	3.8
3	G	179	LEU	3.8
5	L	119	PHE	3.8
1	D	118	GLY	3.5
2	E	186	LYS	3.5
1	D	150	VAL	3.5
2	E	6	GLN	3.5
1	D	156	SER	3.4
3	G	55	ALA	3.3
3	G	526	ALA	3.3
1	D	175	LEU	3.3
3	G	275	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	141	LEU	3.2
3	G	483	LEU	3.2
3	G	659	ASP	3.2
2	E	99	GLY	3.2
3	G	421	LYS	3.2
3	G	346	VAL	3.2
4	H	22	CYS	3.1
3	G	236	THR	3.1
1	D	144	ASP	3.1
3	G	458	GLY	3.1
4	H	138	CYS	3.1
3	G	349	LEU	3.1
4	H	135	ALA	3.0
1	D	143	LYS	3.0
3	G	497	ALA	3.0
2	E	37	GLN	3.0
3	G	353	PHE	3.0
3	G	464	THR	3.0
3	G	255	VAL	3.0
3	G	136	ASN	3.0
2	E	30	PHE	3.0
3	G	565	LEU	3.0
4	H	211	PRO	3.0
3	G	494	LEU	2.9
3	G	274	SER	2.9
3	G	460	SER	2.9
3	G	345	VAL	2.9
2	E	91	TYR	2.9
3	G	647	GLU	2.9
4	H	78	VAL	2.8
3	G	342	LEU	2.8
3	G	370	GLU	2.8
3	G	645	LEU	2.8
3	G	153	GLU	2.8
2	E	106	VAL	2.7
2	E	98	PHE	2.7
3	G	548	ILE	2.6
3	G	646	LEU	2.6
3	G	128	THR	2.6
2	E	120	PRO	2.6
3	G	107	ASP	2.6
3	G	518	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	G	622	ILE	2.6
1	D	91	PHE	2.5
3	G	284	ILE	2.5
3	G	461	THR	2.5
3	G	188	ASN	2.5
4	H	100(J)	TRP	2.5
4	H	158	THR	2.5
4	H	176	LEU	2.5
3	G	348	GLN	2.5
3	G	425	ASN	2.4
3	G	338	TRP	2.4
3	G	649	SER	2.4
3	G	361	PHE	2.4
3	G	139	THR	2.4
5	L	98	PHE	2.4
2	E	31	SER	2.4
3	G	556	LEU	2.4
3	G	552	GLN	2.4
1	D	1	GLU	2.4
3	G	69	TRP	2.4
4	H	152	TRP	2.4
1	D	155	ASN	2.4
3	G	472	GLY	2.4
5	L	6	ALA	2.4
2	E	96	GLU	2.4
3	G	237	GLY	2.3
3	G	100	MET	2.3
3	G	383	PHE	2.3
4	H	205	VAL	2.3
4	H	48	ILE	2.3
5	L	176	SER	2.3
3	G	560	GLU	2.3
5	L	157	LYS	2.3
3	G	381	GLU	2.3
4	H	98	GLY	2.2
3	G	549	VAL	2.2
3	G	551	GLN	2.2
3	G	434	MET	2.2
1	D	100(A)	TRP	2.2
2	E	150	ALA	2.2
3	G	533	ALA	2.2
5	L	120	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	382	PHE	2.2
5	L	196	VAL	2.2
3	G	641	ILE	2.2
2	E	128	ASN	2.2
1	D	198	VAL	2.1
4	H	24	VAL	2.1
3	G	420	ILE	2.1
1	D	89	LEU	2.1
3	G	224	ALA	2.1
3	G	43	PRO	2.1
2	E	46	LEU	2.1
3	G	52	LEU	2.1
3	G	101	VAL	2.1
5	L	147	VAL	2.1
3	G	588	ARG	2.1
3	G	584	GLU	2.1
2	E	121	SER	2.1
3	G	64	GLU	2.1
3	G	452	LEU	2.0
1	D	151	THR	2.0
1	D	204	ASN	2.0
5	L	210	THR	2.0
3	G	167	ASP	2.0
2	E	101	GLY	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
6	NAG	A	1	14/15	-	-	128,129,130,130	0
6	NAG	A	2	14/15	-	-	130,131,132,132	0
6	BMA	A	3	11/12	-	-	132,134,135,135	0
6	MAN	A	4	11/12	-	-	133,134,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MAN	A	5	11/12	-	-	133,134,135,137	11
6	MAN	A	6	11/12	-	-	136,136,139,139	0
6	MAN	A	7	11/12	-	-	53,53,53,53	0
7	NAG	B	1	14/15	-	-	133,134,135,135	0
7	NAG	B	2	14/15	-	-	136,136,138,139	0
7	BMA	B	3	11/12	-	-	138,140,141,141	0
7	NAG	C	1	14/15	-	-	123,140,152,157	0
7	NAG	C	2	14/15	-	-	136,151,158,165	0
7	BMA	C	3	11/12	-	-	171,177,190,195	0
14	MAN	Q	2	11/12	0.16	0.17	152,155,159,159	11
15	MAN	S	5	11/12	0.28	0.16	161,162,163,163	11
15	MAN	S	4	11/12	0.38	0.11	157,158,159,160	11
12	MAN	M	5	11/12	0.40	0.31	150,152,158,158	11
14	MAN	Q	3	11/12	0.44	0.15	144,152,155,158	0
9	MAN	I	5	11/12	0.49	0.34	161,163,165,166	0
12	BMA	M	3	11/12	0.51	0.16	84,102,116,128	0
8	MAN	F	8	11/12	-	-	53,53,53,53	0
10	NAG	P	2	14/15	0.57	0.16	141,142,143,143	0
15	MAN	S	7	11/12	0.58	0.08	157,158,159,159	0
13	MAN	N	3	11/12	0.60	0.23	142,143,147,150	0
8	MAN	F	5	11/12	0.60	0.13	126,128,129,129	11
15	BMA	S	3	11/12	0.61	0.09	157,159,160,160	0
15	NAG	S	1	14/15	0.61	0.14	149,150,153,153	0
9	MAN	O	4	11/12	0.62	0.16	141,146,148,149	0
12	MAN	M	7	11/12	0.63	0.15	155,159,162,164	0
9	BMA	I	3	11/12	0.64	0.28	157,158,162,162	0
15	NAG	S	2	14/15	0.64	0.12	154,155,157,157	0
12	MAN	M	6	11/12	0.66	0.21	39,39,39,39	11
10	NAG	R	2	14/15	0.67	0.10	157,159,161,162	0
8	MAN	F	6	11/12	0.70	0.08	39,39,39,39	0
15	MAN	S	6	11/12	0.71	0.10	159,160,162,163	0
14	MAN	Q	4	11/12	0.71	0.19	39,39,39,39	0
12	NAG	M	2	14/15	0.72	0.19	61,89,109,117	0
9	NAG	O	1	14/15	0.74	0.12	142,144,145,146	0
10	NAG	J	1	14/15	0.74	0.14	138,142,145,146	0
11	BMA	K	3	11/12	-	-	148,150,153,154	0
11	MAN	K	4	11/12	-	-	145,147,150,150	0
12	MAN	M	4	11/12	0.75	0.14	147,149,152,154	0
10	NAG	J	2	14/15	0.75	0.21	146,148,151,152	0
12	NAG	M	1	14/15	0.75	0.14	87,106,110,121	0
8	BMA	F	3	11/12	0.76	0.07	143,144,147,149	11
8	MAN	F	4	11/12	0.77	0.10	136,140,142,142	11

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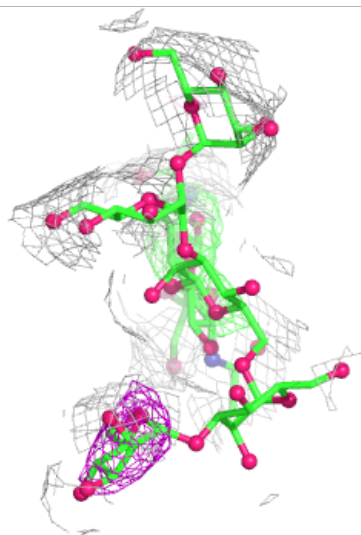
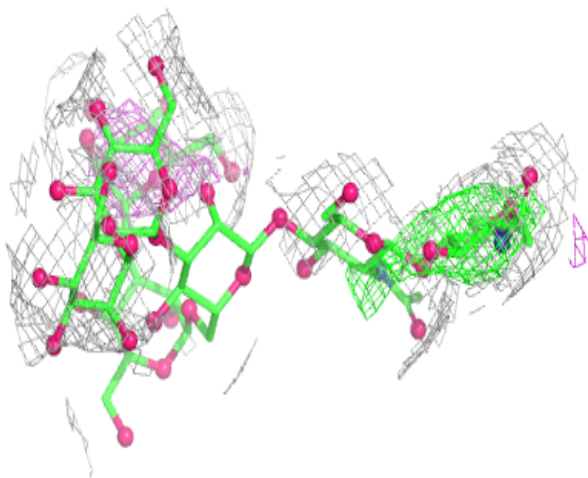
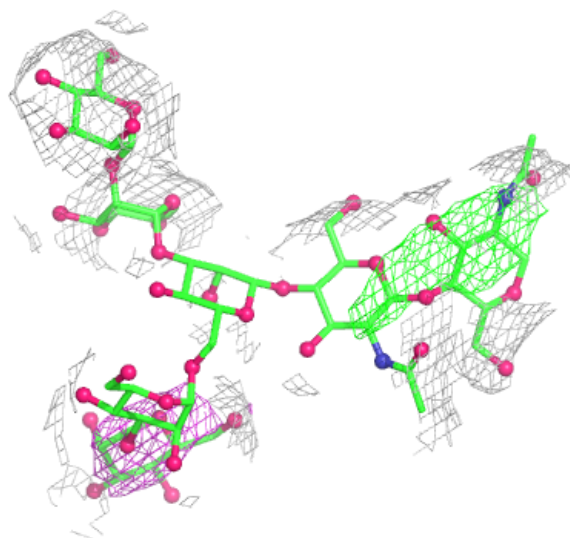
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MAN	O	5	11/12	0.78	0.13	39,39,39,39	0
11	NAG	K	1	14/15	0.78	0.11	136,137,140,140	0
13	MAN	N	2	11/12	0.79	0.14	139,140,143,145	0
8	NAG	F	2	14/15	0.80	0.12	138,144,151,153	0
10	NAG	P	1	14/15	0.80	0.14	53,53,53,53	0
15	MAN	S	8	11/12	0.80	0.23	39,39,39,39	0
14	BMA	Q	1	11/12	0.82	0.17	39,39,39,39	0
9	NAG	I	2	14/15	0.82	0.22	156,159,161,163	14
13	MAN	N	1	11/12	0.82	0.14	134,136,138,138	0
9	BMA	O	3	11/12	0.83	0.08	53,53,53,53	0
11	NAG	K	2	14/15	0.83	0.09	140,143,146,146	0
10	NAG	R	1	14/15	0.83	0.10	142,150,157,158	0
8	MAN	F	7	11/12	0.83	0.17	151,153,155,156	11
12	MAN	M	8	11/12	0.85	0.16	155,160,166,168	11
8	NAG	F	1	14/15	0.87	0.17	136,142,148,149	0
9	MAN	I	4	11/12	0.88	0.19	153,155,157,157	11
9	NAG	O	2	14/15	0.89	0.10	39,39,39,39	0
9	NAG	I	1	14/15	0.90	0.19	154,157,161,162	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.

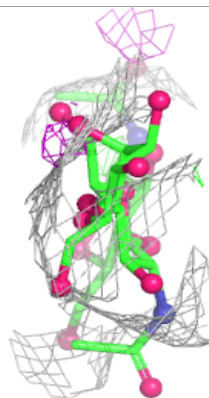
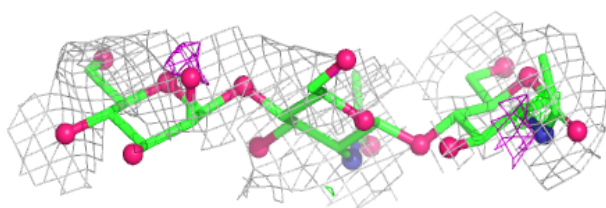
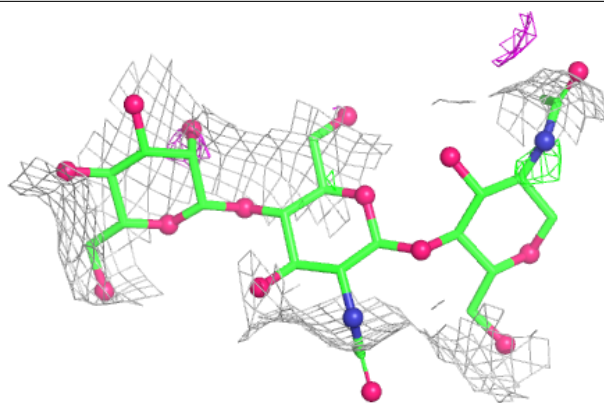
Electron density around Chain A:

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

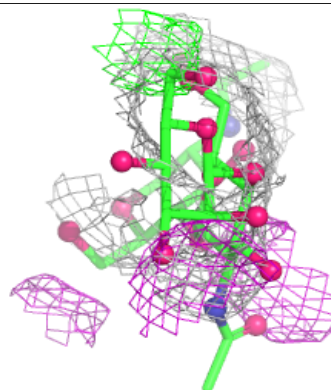
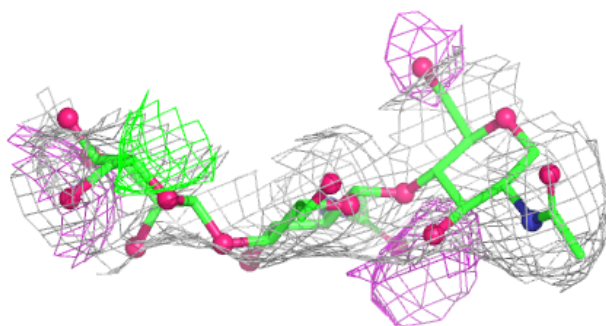
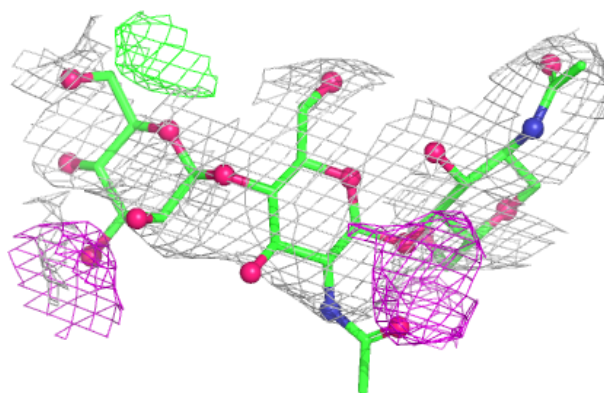


Electron density around Chain B:

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

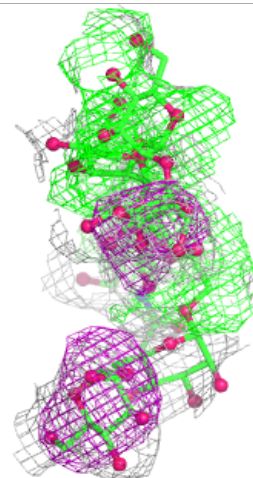
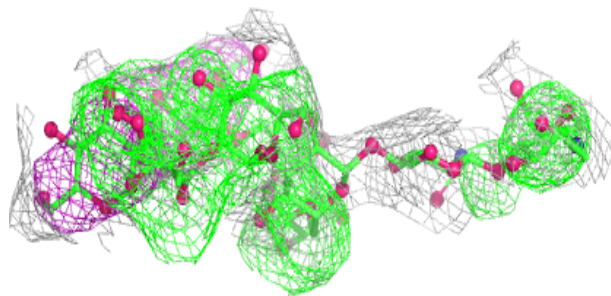
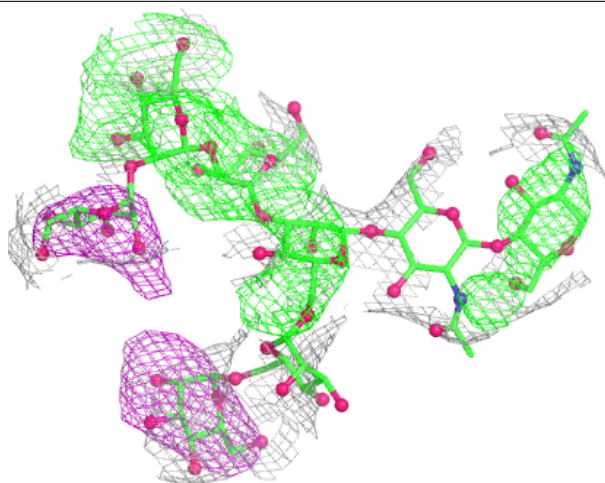
**Electron density around Chain C:**

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



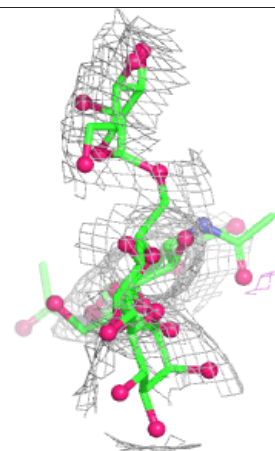
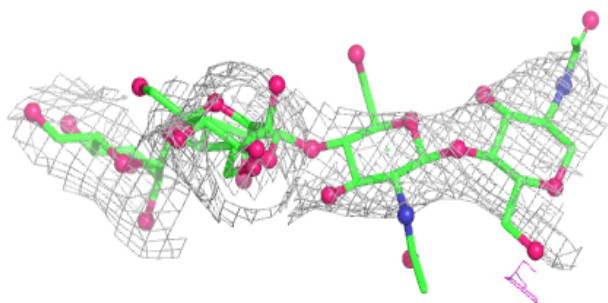
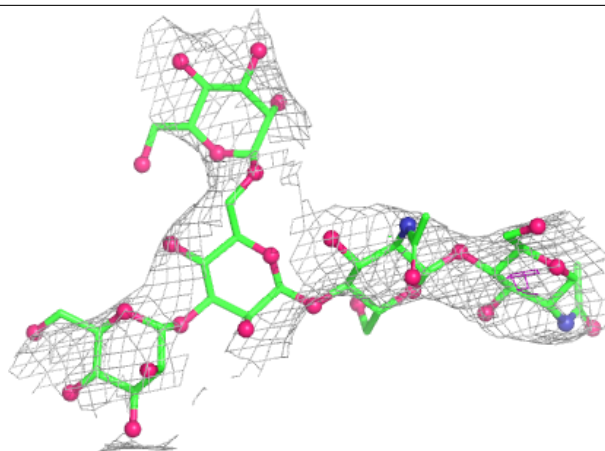
Electron density around Chain F:

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



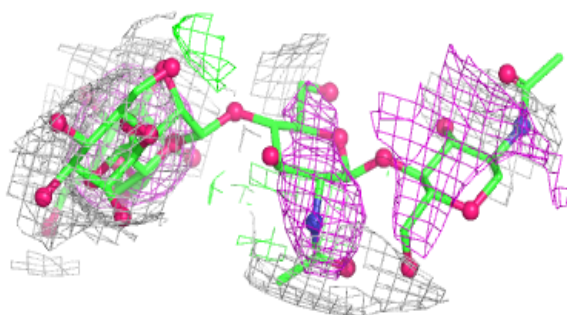
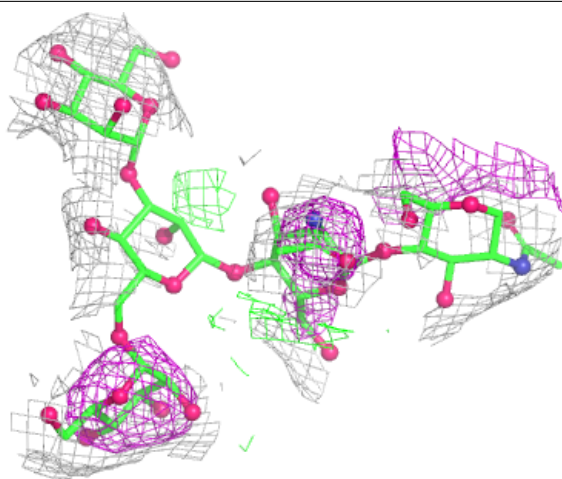
Electron density around Chain I:

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



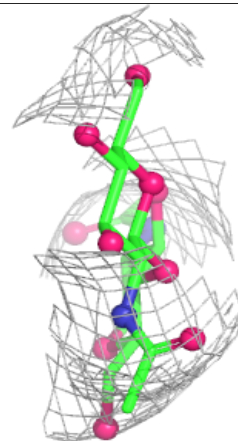
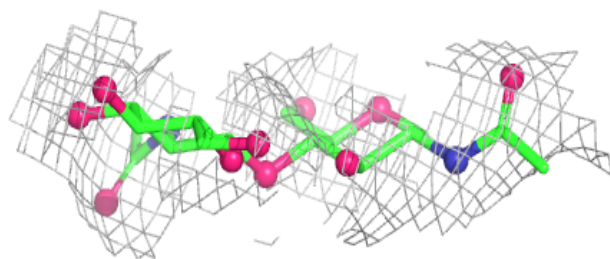
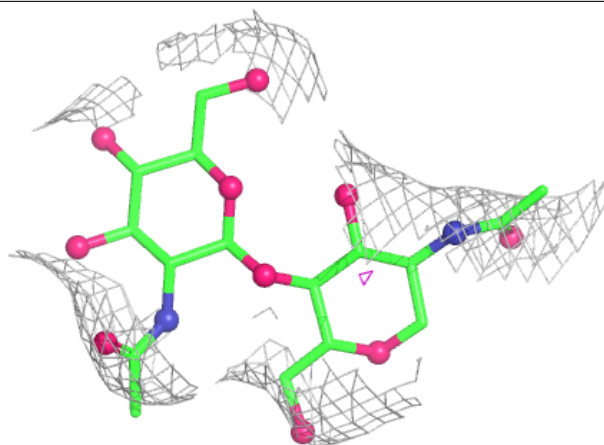
Electron density around Chain O:

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



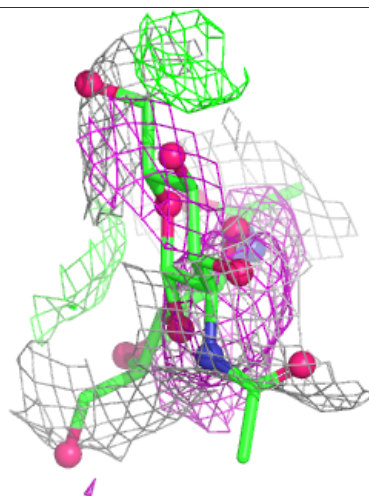
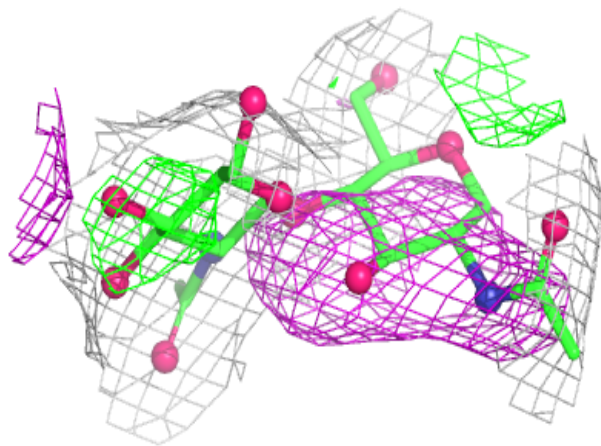
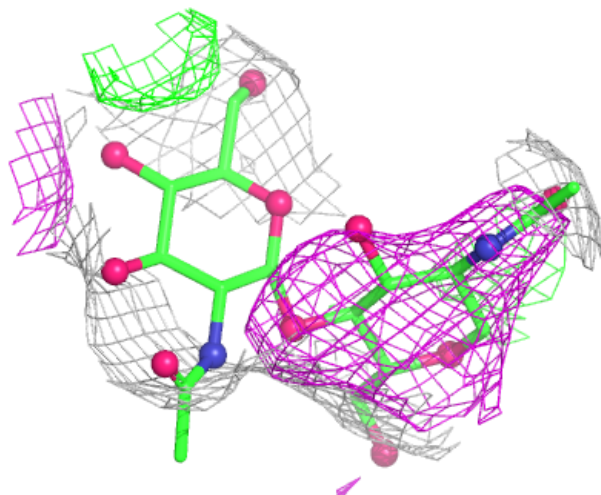
Electron density around Chain J:

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



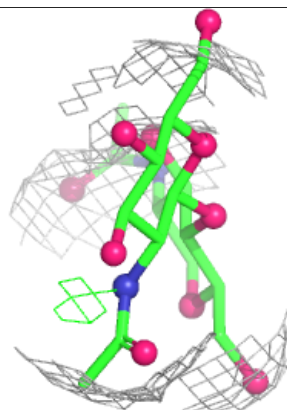
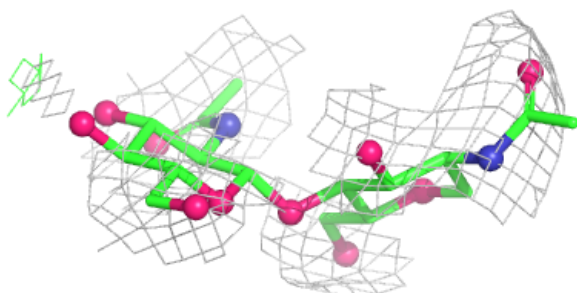
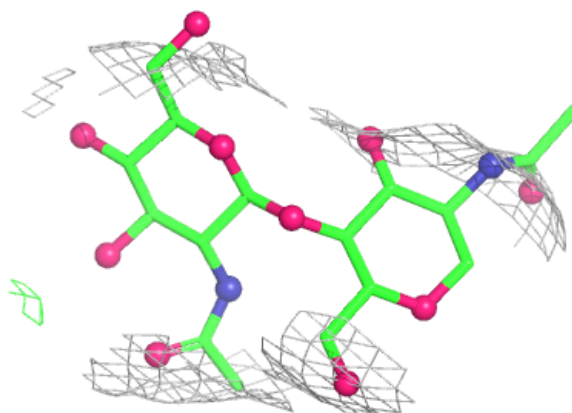
Electron density around Chain P:

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

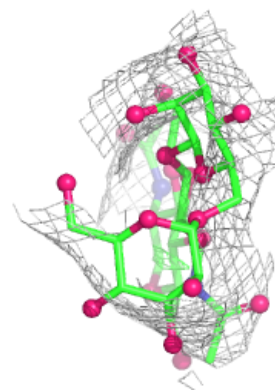
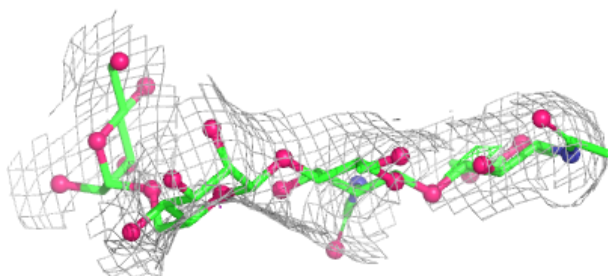
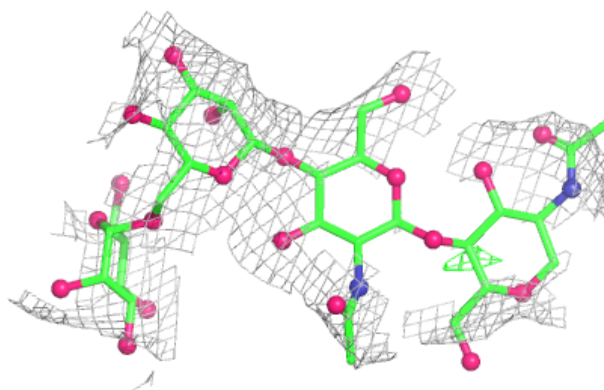


Electron density around Chain R:

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

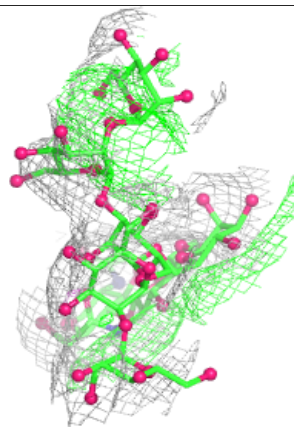
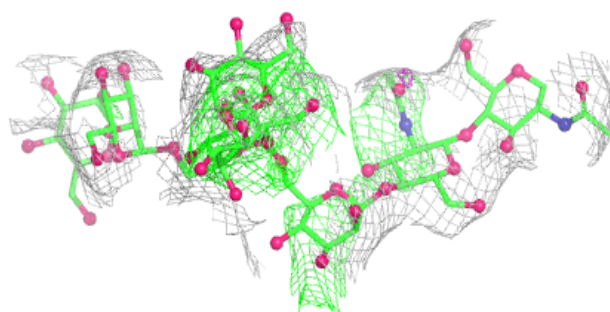
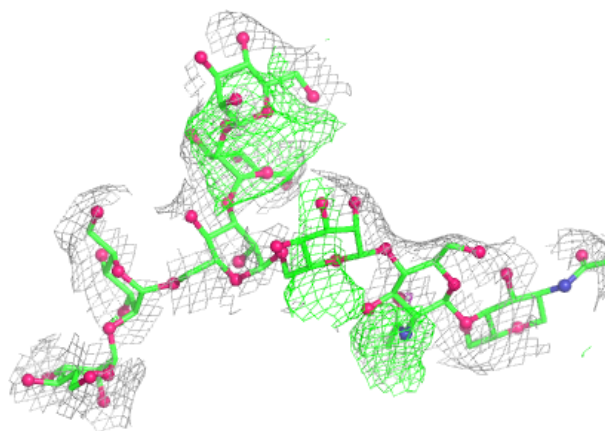
**Electron density around Chain K:**

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



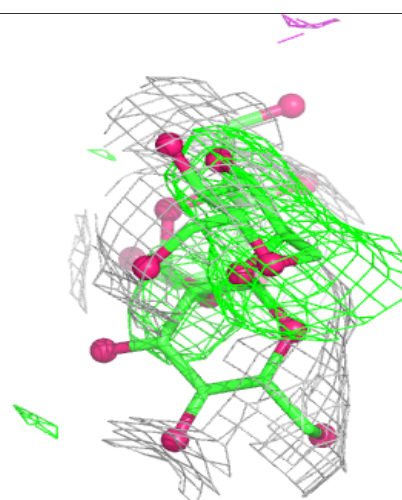
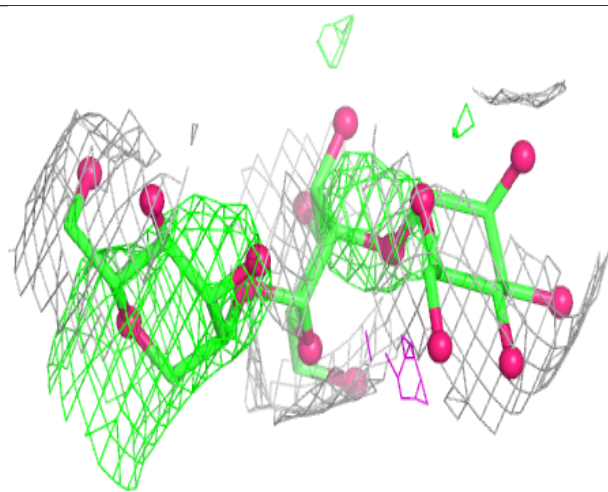
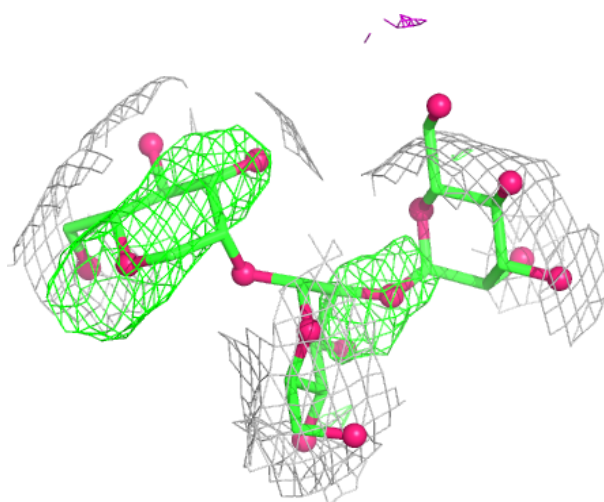
Electron density around Chain M:

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



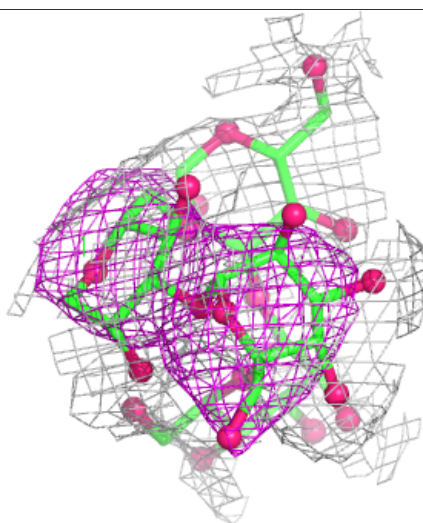
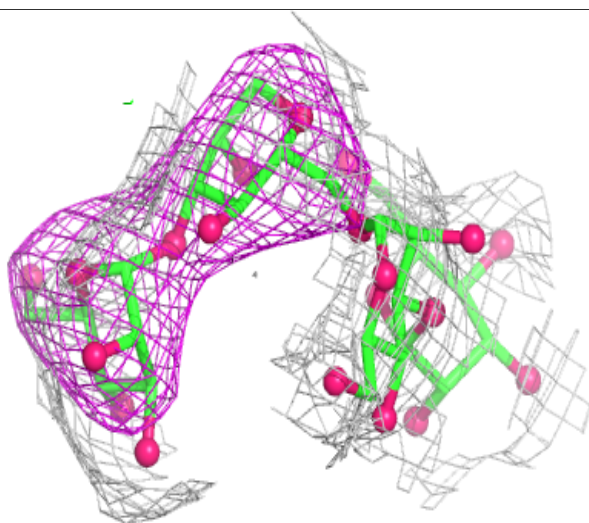
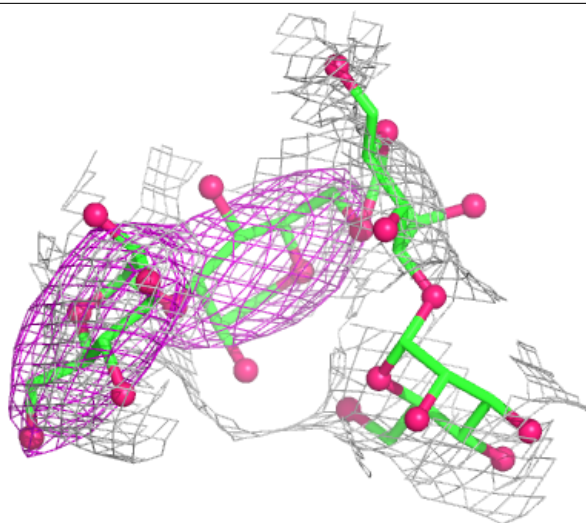
Electron density around Chain N:

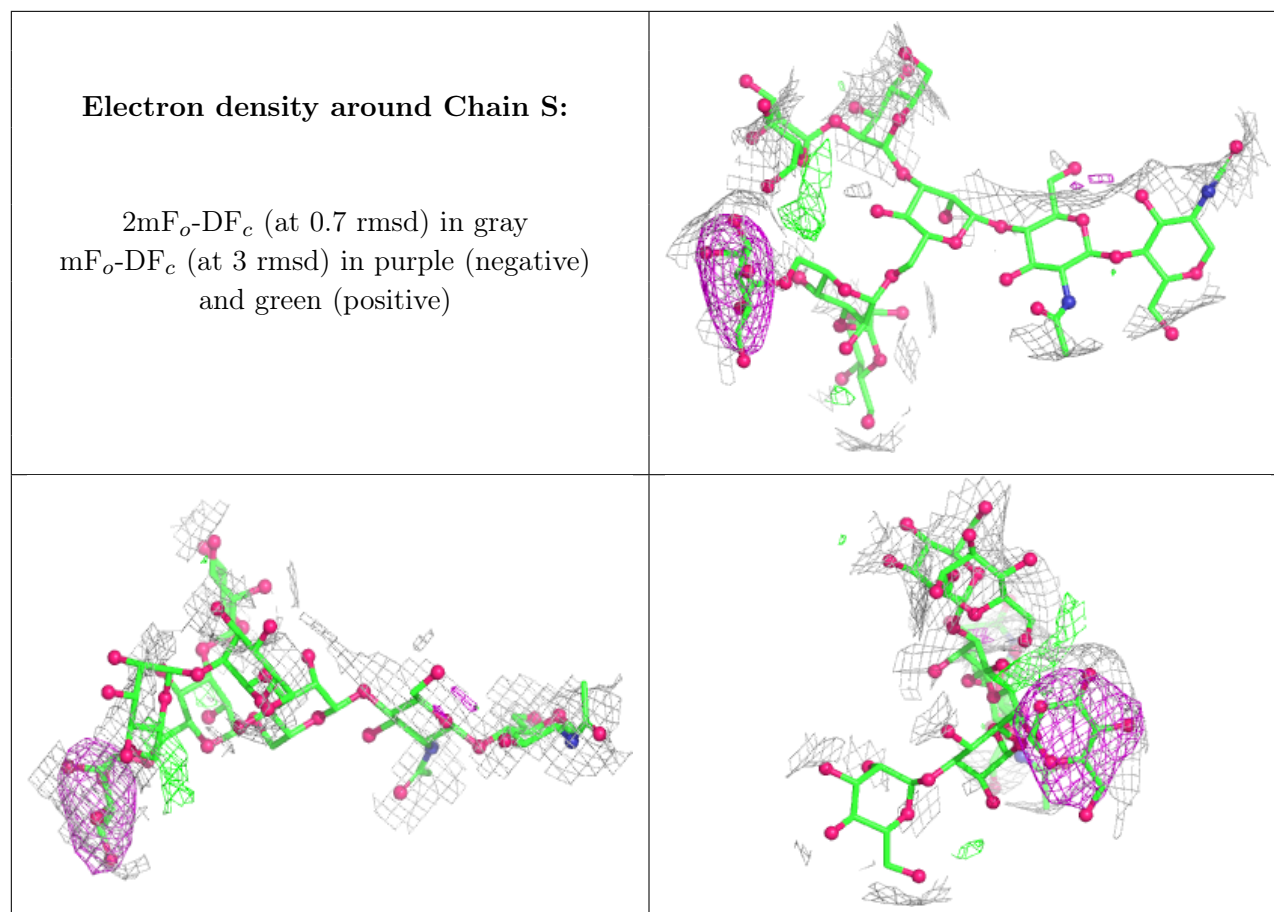
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
16	NAG	G	1840	14/15	0.35	0.14	130,132,133,133	0
16	NAG	G	1839	14/15	0.40	0.13	159,165,169,170	0
17	MAN	G	1201	11/12	0.58	0.29	39,39,39,39	0
16	NAG	G	1133	14/15	0.62	0.19	53,53,53,53	0
16	NAG	G	1235	14/15	0.64	0.21	152,153,156,158	14
17	MAN	G	1266	11/12	0.65	0.16	126,128,129,129	11
16	NAG	G	1088	14/15	0.65	0.17	53,53,53,53	0
16	NAG	G	1618	14/15	0.68	0.10	170,176,181,184	0
16	NAG	G	1355	14/15	0.73	0.26	63,63,63,63	14
16	NAG	G	1625	14/15	0.79	0.18	53,53,53,53	0
16	NAG	G	1637	14/15	0.79	0.18	155,156,158,159	0
16	NAG	G	1137	14/15	0.84	0.16	132,135,138,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	NAG	G	1611	14/15	0.84	0.18	157,160,162,162	0
16	NAG	G	1234	14/15	0.85	0.14	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.