



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 03:28 PM UTC

PDB ID : 3RG1 / pdb_00003rg1
Title : Crystal structure of the RP105/MD-1 complex
Authors : Yoon, S.I.; Hong, M.; Wilson, I.A.
Deposited on : 2011-04-07
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

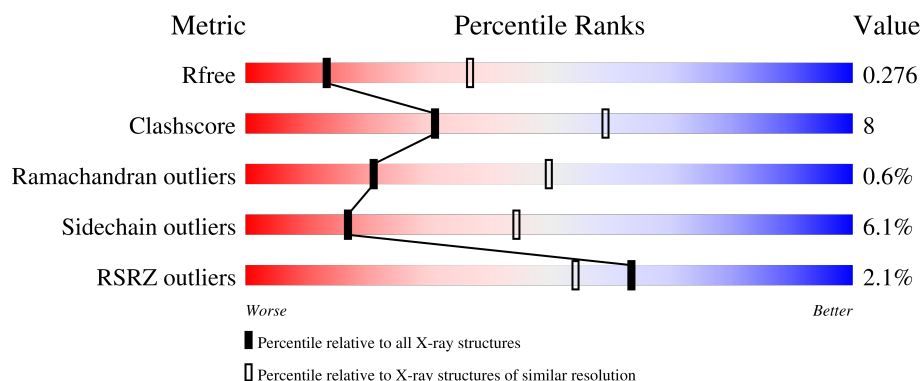
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	612	79% 16% ..
1	B	612	79% 17% ..
1	E	612	4% 76% 19% ..
1	F	612	77% 19% ..
1	I	612	3% 55% 9% 35%

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Mol	Chain	Length	Quality of chain
1	J	612	
1	M	612	
1	N	612	
2	C	147	
2	D	147	
2	G	147	
2	H	147	
2	K	147	
2	L	147	
2	O	147	
2	P	147	
3	Q	3	
3	S	3	
3	U	3	
3	W	3	
3	Y	3	
3	a	3	
3	c	3	
3	e	3	
4	R	8	
4	T	8	
4	V	8	
4	X	8	
4	Z	8	
4	b	8	

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Mol	Chain	Length	Quality of chain
4	d	8	 62% 38%
4	f	8	 88% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 43795 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 CD180 molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4450	2805	766	860	19			
1	E	592	Total	C	N	O	S	0	0	0
			4381	2763	750	849	19			
1	I	397	Total	C	N	O	S	0	0	0
			2931	1862	489	570	10			
1	M	593	Total	C	N	O	S	0	0	0
			4447	2806	763	859	19			
1	B	599	Total	C	N	O	S	0	0	0
			4616	2921	788	885	22			
1	F	599	Total	C	N	O	S	0	0	0
			4493	2833	768	870	22			
1	J	599	Total	C	N	O	S	0	0	0
			4458	2816	756	865	21			
1	N	599	Total	C	N	O	S	0	0	0
			4591	2909	783	877	22			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP A6QNK7
A	23	GLY	-	expression tag	UNP A6QNK7
A	627	THR	-	expression tag	UNP A6QNK7
A	628	HIS	-	expression tag	UNP A6QNK7
A	629	MET	-	expression tag	UNP A6QNK7
A	630	LEU	-	expression tag	UNP A6QNK7
A	631	VAL	-	expression tag	UNP A6QNK7
A	632	PRO	-	expression tag	UNP A6QNK7
A	633	ARG	-	expression tag	UNP A6QNK7
E	22	ALA	-	expression tag	UNP A6QNK7
E	23	GLY	-	expression tag	UNP A6QNK7
E	627	THR	-	expression tag	UNP A6QNK7
E	628	HIS	-	expression tag	UNP A6QNK7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	629	MET	-	expression tag	UNP A6QNK7
E	630	LEU	-	expression tag	UNP A6QNK7
E	631	VAL	-	expression tag	UNP A6QNK7
E	632	PRO	-	expression tag	UNP A6QNK7
E	633	ARG	-	expression tag	UNP A6QNK7
I	22	ALA	-	expression tag	UNP A6QNK7
I	23	GLY	-	expression tag	UNP A6QNK7
I	627	THR	-	expression tag	UNP A6QNK7
I	628	HIS	-	expression tag	UNP A6QNK7
I	629	MET	-	expression tag	UNP A6QNK7
I	630	LEU	-	expression tag	UNP A6QNK7
I	631	VAL	-	expression tag	UNP A6QNK7
I	632	PRO	-	expression tag	UNP A6QNK7
I	633	ARG	-	expression tag	UNP A6QNK7
M	22	ALA	-	expression tag	UNP A6QNK7
M	23	GLY	-	expression tag	UNP A6QNK7
M	627	THR	-	expression tag	UNP A6QNK7
M	628	HIS	-	expression tag	UNP A6QNK7
M	629	MET	-	expression tag	UNP A6QNK7
M	630	LEU	-	expression tag	UNP A6QNK7
M	631	VAL	-	expression tag	UNP A6QNK7
M	632	PRO	-	expression tag	UNP A6QNK7
M	633	ARG	-	expression tag	UNP A6QNK7
B	22	ALA	-	expression tag	UNP A6QNK7
B	23	GLY	-	expression tag	UNP A6QNK7
B	627	THR	-	expression tag	UNP A6QNK7
B	628	HIS	-	expression tag	UNP A6QNK7
B	629	MET	-	expression tag	UNP A6QNK7
B	630	LEU	-	expression tag	UNP A6QNK7
B	631	VAL	-	expression tag	UNP A6QNK7
B	632	PRO	-	expression tag	UNP A6QNK7
B	633	ARG	-	expression tag	UNP A6QNK7
F	22	ALA	-	expression tag	UNP A6QNK7
F	23	GLY	-	expression tag	UNP A6QNK7
F	627	THR	-	expression tag	UNP A6QNK7
F	628	HIS	-	expression tag	UNP A6QNK7
F	629	MET	-	expression tag	UNP A6QNK7
F	630	LEU	-	expression tag	UNP A6QNK7
F	631	VAL	-	expression tag	UNP A6QNK7
F	632	PRO	-	expression tag	UNP A6QNK7
F	633	ARG	-	expression tag	UNP A6QNK7
J	22	ALA	-	expression tag	UNP A6QNK7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	23	GLY	-	expression tag	UNP A6QNK7
J	627	THR	-	expression tag	UNP A6QNK7
J	628	HIS	-	expression tag	UNP A6QNK7
J	629	MET	-	expression tag	UNP A6QNK7
J	630	LEU	-	expression tag	UNP A6QNK7
J	631	VAL	-	expression tag	UNP A6QNK7
J	632	PRO	-	expression tag	UNP A6QNK7
J	633	ARG	-	expression tag	UNP A6QNK7
N	22	ALA	-	expression tag	UNP A6QNK7
N	23	GLY	-	expression tag	UNP A6QNK7
N	627	THR	-	expression tag	UNP A6QNK7
N	628	HIS	-	expression tag	UNP A6QNK7
N	629	MET	-	expression tag	UNP A6QNK7
N	630	LEU	-	expression tag	UNP A6QNK7
N	631	VAL	-	expression tag	UNP A6QNK7
N	632	PRO	-	expression tag	UNP A6QNK7
N	633	ARG	-	expression tag	UNP A6QNK7

- Molecule 2 is a protein called LY86 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	138	Total	C	N	O	S	0	0	0
			1026	656	170	193	7			
2	D	136	Total	C	N	O	S	0	0	0
			1022	656	167	192	7			
2	G	138	Total	C	N	O	S	0	0	0
			1031	664	170	190	7			
2	H	138	Total	C	N	O	S	0	0	0
			1046	667	176	196	7			
2	K	136	Total	C	N	O	S	0	0	0
			1003	640	167	189	7			
2	L	138	Total	C	N	O	S	0	0	0
			1046	667	172	200	7			
2	O	138	Total	C	N	O	S	0	0	0
			1028	658	169	194	7			
2	P	135	Total	C	N	O	S	0	0	0
			1001	640	166	188	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ALA	-	expression tag	UNP A4IFT3

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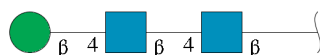
Chain	Residue	Modelled	Actual	Comment	Reference
C	160	ALA	-	expression tag	UNP A4IFT3
C	161	ARG	-	expression tag	UNP A4IFT3
C	162	GLY	-	expression tag	UNP A4IFT3
C	163	LEU	-	expression tag	UNP A4IFT3
C	164	VAL	-	expression tag	UNP A4IFT3
C	165	PRO	-	expression tag	UNP A4IFT3
C	166	ARG	-	expression tag	UNP A4IFT3
D	20	ALA	-	expression tag	UNP A4IFT3
D	160	ALA	-	expression tag	UNP A4IFT3
D	161	ARG	-	expression tag	UNP A4IFT3
D	162	GLY	-	expression tag	UNP A4IFT3
D	163	LEU	-	expression tag	UNP A4IFT3
D	164	VAL	-	expression tag	UNP A4IFT3
D	165	PRO	-	expression tag	UNP A4IFT3
D	166	ARG	-	expression tag	UNP A4IFT3
G	20	ALA	-	expression tag	UNP A4IFT3
G	160	ALA	-	expression tag	UNP A4IFT3
G	161	ARG	-	expression tag	UNP A4IFT3
G	162	GLY	-	expression tag	UNP A4IFT3
G	163	LEU	-	expression tag	UNP A4IFT3
G	164	VAL	-	expression tag	UNP A4IFT3
G	165	PRO	-	expression tag	UNP A4IFT3
G	166	ARG	-	expression tag	UNP A4IFT3
H	20	ALA	-	expression tag	UNP A4IFT3
H	160	ALA	-	expression tag	UNP A4IFT3
H	161	ARG	-	expression tag	UNP A4IFT3
H	162	GLY	-	expression tag	UNP A4IFT3
H	163	LEU	-	expression tag	UNP A4IFT3
H	164	VAL	-	expression tag	UNP A4IFT3
H	165	PRO	-	expression tag	UNP A4IFT3
H	166	ARG	-	expression tag	UNP A4IFT3
K	20	ALA	-	expression tag	UNP A4IFT3
K	160	ALA	-	expression tag	UNP A4IFT3
K	161	ARG	-	expression tag	UNP A4IFT3
K	162	GLY	-	expression tag	UNP A4IFT3
K	163	LEU	-	expression tag	UNP A4IFT3
K	164	VAL	-	expression tag	UNP A4IFT3
K	165	PRO	-	expression tag	UNP A4IFT3
K	166	ARG	-	expression tag	UNP A4IFT3
L	20	ALA	-	expression tag	UNP A4IFT3
L	160	ALA	-	expression tag	UNP A4IFT3
L	161	ARG	-	expression tag	UNP A4IFT3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	162	GLY	-	expression tag	UNP A4IFT3
L	163	LEU	-	expression tag	UNP A4IFT3
L	164	VAL	-	expression tag	UNP A4IFT3
L	165	PRO	-	expression tag	UNP A4IFT3
L	166	ARG	-	expression tag	UNP A4IFT3
O	20	ALA	-	expression tag	UNP A4IFT3
O	160	ALA	-	expression tag	UNP A4IFT3
O	161	ARG	-	expression tag	UNP A4IFT3
O	162	GLY	-	expression tag	UNP A4IFT3
O	163	LEU	-	expression tag	UNP A4IFT3
O	164	VAL	-	expression tag	UNP A4IFT3
O	165	PRO	-	expression tag	UNP A4IFT3
O	166	ARG	-	expression tag	UNP A4IFT3
P	20	ALA	-	expression tag	UNP A4IFT3
P	160	ALA	-	expression tag	UNP A4IFT3
P	161	ARG	-	expression tag	UNP A4IFT3
P	162	GLY	-	expression tag	UNP A4IFT3
P	163	LEU	-	expression tag	UNP A4IFT3
P	164	VAL	-	expression tag	UNP A4IFT3
P	165	PRO	-	expression tag	UNP A4IFT3
P	166	ARG	-	expression tag	UNP A4IFT3

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



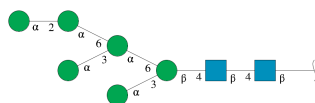
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	S	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	U	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	a	3	Total	C	N	O	0	0	0
			39	22	2	15			

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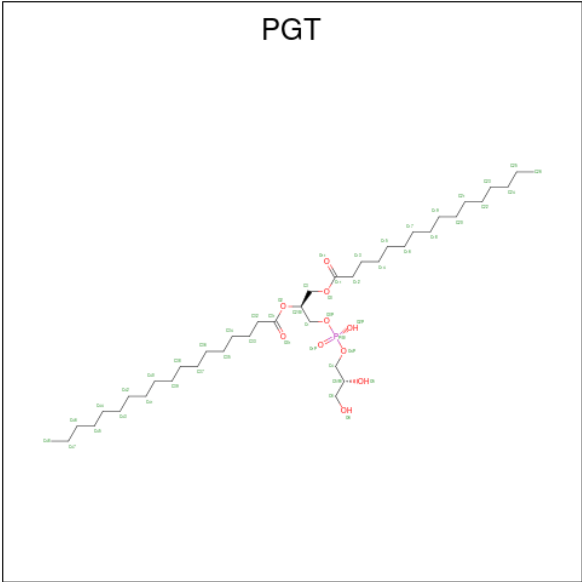
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	c	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	e	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	R	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	T	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	V	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	X	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	Z	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	b	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	d	8	Total	C	N	O	0	0	0
			94	52	2	40			
4	f	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 5 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			31	27	4		
5	H	1	Total	C	O	0	0
			31	27	4		
5	L	1	Total	C	O	0	0
			31	27	4		
5	P	1	Total	C	O	0	0
			31	27	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	E	2	Total	O	0	0
			2	2		
6	I	1	Total	O	0	0
			1	1		
6	M	5	Total	O	0	0
			5	5		
6	B	9	Total	O	0	0
			9	9		
6	F	1	Total	O	0	0
			1	1		
6	J	1	Total	O	0	0
			1	1		
6	N	6	Total	O	0	0
			6	6		

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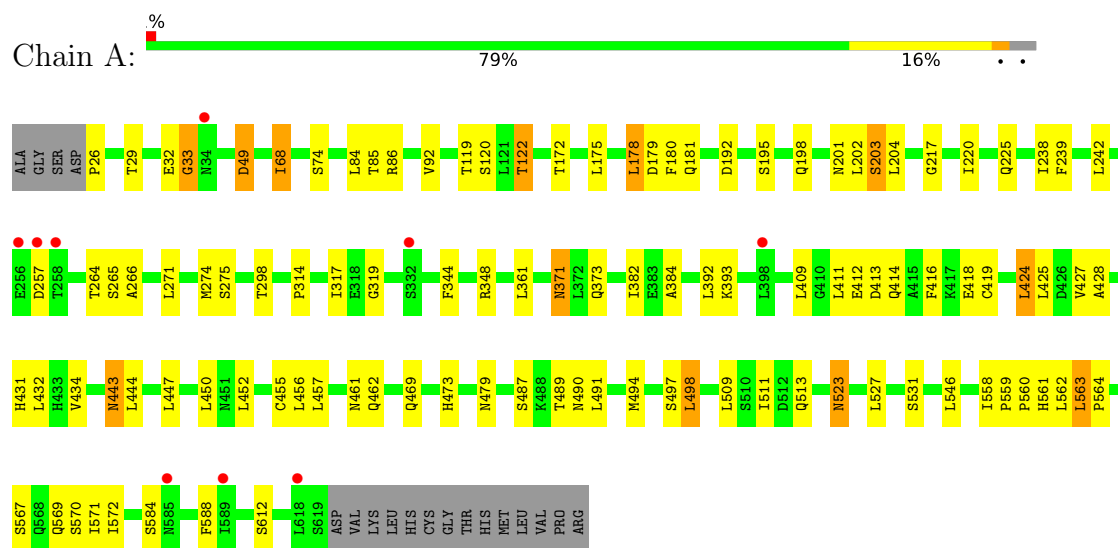
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total 1	O 1	0	0
6	D	3	Total 3	O 3	0	0
6	G	1	Total 1	O 1	0	0
6	L	1	Total 1	O 1	0	0

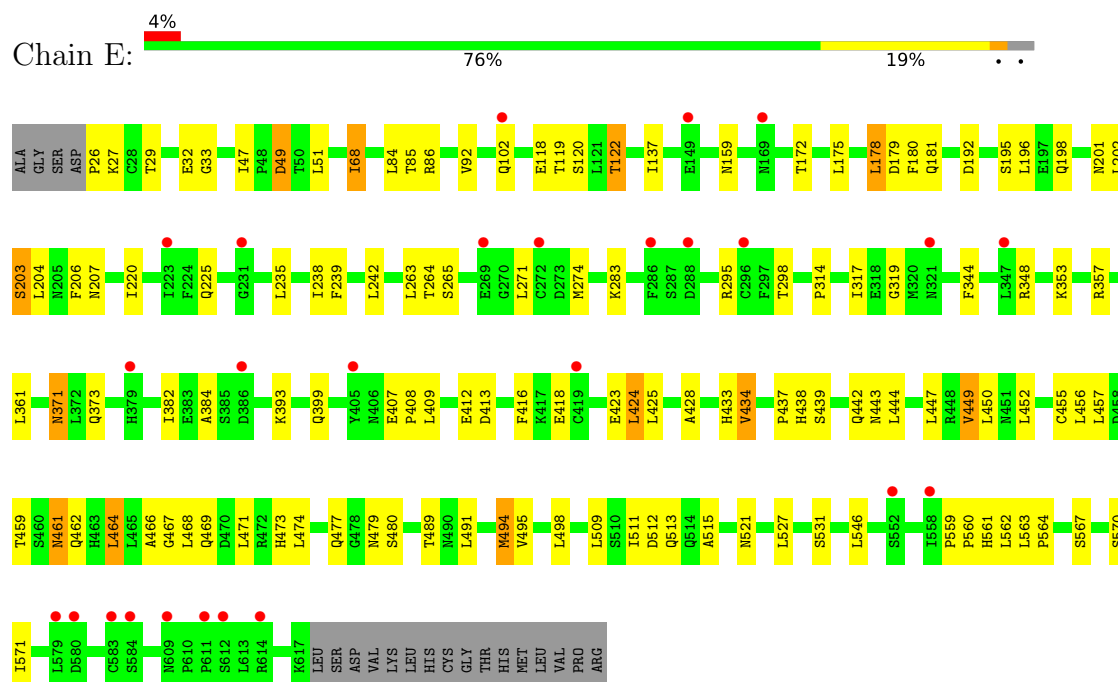
3 Residue-property plots [i](#)

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: CD180 molecule



• Molecule 1: CD180 molecule



Chain I:

3% 55% 9% 35%

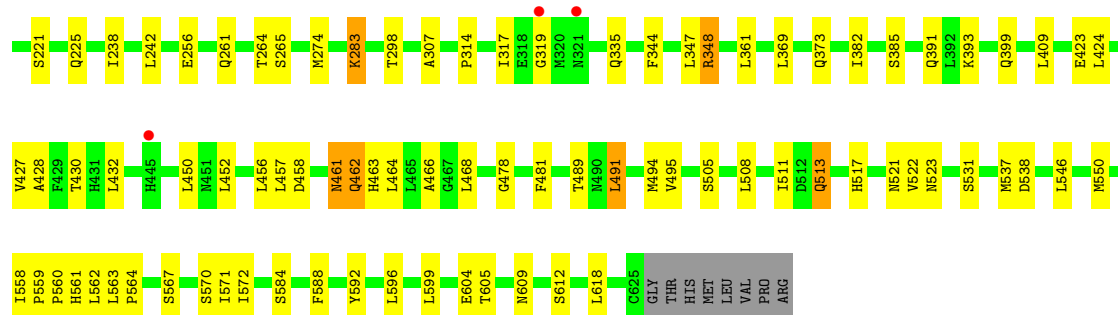
Position	Amino Acid	Category
1	ALA	Green
2	GLY	Green
3	SER	Green
4	ASP	Green
5	P26	Green
6	G33	Green
7	N34	Green
8	E46	Green
9	I47	Green
10	P48	Green
11	D49	Green
12	T50	Green
13	L51	Green
14	I68	Green
15	L84	Green
16	T85	Green
17	R86	Green
18	V92	Green
19	Q102	Green
20	T119	Green
21	S120	Green
22	I121	Green
23	T122	Green
24	I137	Green
25	E149	Green
26	S158	Green
27	N159	Green
28	E168	Green
29	T172	Green
30	L175	Green
31	L178	Green
32	D179	Green
33	F180	Green
34	Q181	Green
35	D192	Green
36	S195	Green
37	L196	Green
38	E197	Green
39	Q198	Green
40	N201	Green
41	L202	Green
42	S203	Green
43	L204	Green
44	N205	Green
45	G206	Green
46	G207	Green
47	G208	Green
48	Q225	Green
49	L235	Green
50	I238	Green
51	F239	Green
52	Q243	Green
53	D260	Green
54	L263	Green
55	T264	Green
56	S265	Green
57	A266	Green
58	L271	Green
59	K283	Green
60	S290	Green
61	S291	Green
62	S292	Green
63	T298	Green
64	L310	Green
65	N311	Green
66	G312	Green
67	L313	Green
68	P314	Green
69	A428	Green
70	F429	Green
71	T430	Green
72	E431	Green
73	G432	Green
74	M433	Green
75	N434	Green
76	F344	Green
77	R348	Green
78	L366	Green
79	Q373	Green
80	L377	Green
81	I382	Green
82	GLU	Green
83	ALA	Green
84	ARG	Green
85	V449	Green
86	L450	Green
87	N451	Green
88	L452	Green
89	CYS	Green
90	CYS	Green
91	ALA	Green
92	GLY	Green
93	SER	Green
94	ASP	Green
95	GLN	Green
96	ASP	Green
97	GLY	Green
98	ASP	Green
99	GLY	Green
100	ASP	Green
101	THR	Green
102	ASP	Green
103	GLN	Green
104	HIS	Green
105	CYS	Green
106	GLY	Green
107	LEU	Green
108	LEU	Green
109	LEU	Green
110	LEU	Green
111	LEU	Green
112	LEU	Green
113	LEU	Green
114	LEU	Green
115	LEU	Green
116	LEU	Green
117	LEU	Green
118	LEU	Green
119	LEU	Green
120	LEU	Green
121	LEU	Green
122	LEU	Green
123	LEU	Green
124	LEU	Green
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126	LEU	Green
127	LEU	Green
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137	LEU	Green
138	LEU	Green
139	LEU	Green
140	LEU	Green
141	LEU	Green
142	LEU	Green
143	LEU	Green
144	LEU	Green
145	LEU	Green
146	LEU	Green
147	LEU	Green
148	LEU	Green
149	LEU	Green
150	LEU	Green
151	LEU	Green
152	LEU	Green
153	LEU	Green
154	LEU	Green
155	LEU	Green
156	LEU	Green
157	LEU	Green
158	LEU	Green
159	LEU	Green
160	LEU	Green
161		

Chain M:

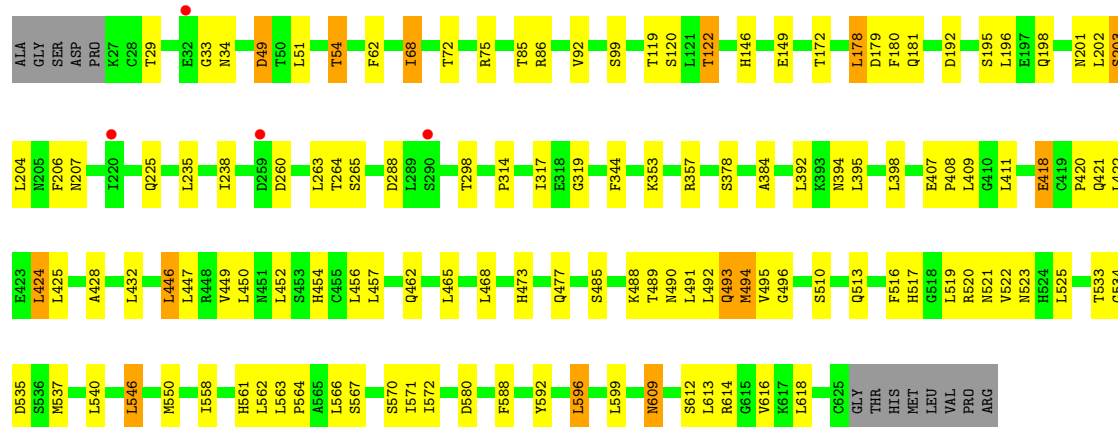
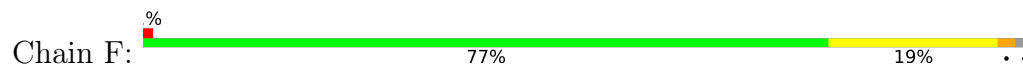
Category	Value	Color
L491	1	Yellow
L494	1	Yellow
M494	1	Yellow
V495	1	Yellow
L500	1	Yellow
L501	1	Yellow
T502	1	Yellow
L503	1	Yellow
L507	1	Yellow
L508	1	Yellow
L509	1	Yellow
S510	1	Yellow
L511	1	Yellow
L512	1	Yellow
L513	1	Yellow
L514	1	Yellow
A515	1	Yellow
L518	1	Yellow
L519	1	Yellow
S520	1	Yellow
L521	1	Yellow
L522	1	Yellow
L523	1	Yellow
S531	1	Yellow
L532	1	Yellow
L536	1	Yellow
L546	1	Yellow
L555	1	Yellow
H561	1	Yellow
L562	1	Yellow
L563	1	Yellow
P564	1	Yellow
S567	1	Yellow
Q568	1	Yellow
S570	1	Yellow
L571	1	Yellow
L572	1	Yellow
D580	1	Yellow
C583	1	Yellow
N609	1	Yellow
S612	1	Yellow
L618	1	Yellow
SER	1	Yellow
ASP	1	Yellow
V491	1	Yellow
S378	1	Yellow
E383	1	Yellow
C388	1	Yellow
R389	1	Yellow
L390	1	Yellow
Q391	1	Yellow
L392	1	Yellow
K393	1	Yellow
N394	1	Yellow
L395	1	Yellow
L403	1	Yellow
E407	1	Yellow
P408	1	Yellow
L409	1	Yellow
G410	1	Yellow
L411	1	Yellow
Q414	1	Yellow
A415	1	Yellow
F416	1	Yellow
K417	1	Yellow
E418	1	Yellow
L424	1	Yellow
L425	1	Yellow
D426	1	Yellow
V427	1	Yellow
A428	1	Yellow
L432	1	Yellow
Q442	1	Yellow
M443	1	Yellow
L444	1	Yellow
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V449	1	Yellow
L450	1	Yellow
M451	1	Yellow
L452	1	Yellow
C455	1	Yellow
L456	1	Yellow
T459	1	Yellow
S460	1	Yellow
M461	1	Yellow
Q469	1	Yellow
H473	1	Yellow
I486	1	Yellow
T489	1	Yellow
M490	1	Yellow
L204	1	Yellow
M205	1	Yellow
F206	1	Yellow
T220	1	Yellow
T223	1	Yellow
F224	1	Yellow
Q225	1	Yellow
G23	1	Yellow
L235	1	Yellow
T238	1	Yellow
F239	1	Yellow
K240	1	Yellow
G241	1	Yellow
L242	1	Yellow
D257	1	Yellow
T258	1	Yellow
L263	1	Yellow
T264	1	Yellow
S265	1	Yellow
L271	1	Yellow
M274	1	Yellow
T286	1	Yellow
R299	1	Yellow
N311	1	Yellow
P314	1	Yellow
T317	1	Yellow
E318	1	Yellow
G319	1	Yellow
A341	1	Yellow
F344	1	Yellow
P345	1	Yellow
S346	1	Yellow
L347	1	Yellow
R348	1	Yellow
R357	1	Yellow
T363	1	Yellow
R364	1	Yellow
C365	1	Yellow
L366	1	Yellow
E367	1	Yellow
K368	1	Yellow
S195	1	Yellow
Q198	1	Yellow
N201	1	Yellow
L202	1	Yellow
S203	1	Yellow
L184	1	Yellow
T85	1	Yellow
R86	1	Yellow
V92	1	Yellow
T119	1	Yellow
S120	1	Yellow
L121	1	Yellow
T122	1	Yellow
I137	1	Yellow
E149	1	Yellow
M159	1	Yellow
H160	1	Yellow
T164	1	Yellow
M165	1	Yellow
L166	1	Yellow
T172	1	Yellow
L178	1	Yellow
D179	1	Yellow
F180	1	Yellow
Q181	1	Yellow
I185	1	Yellow
D		

Chain B:

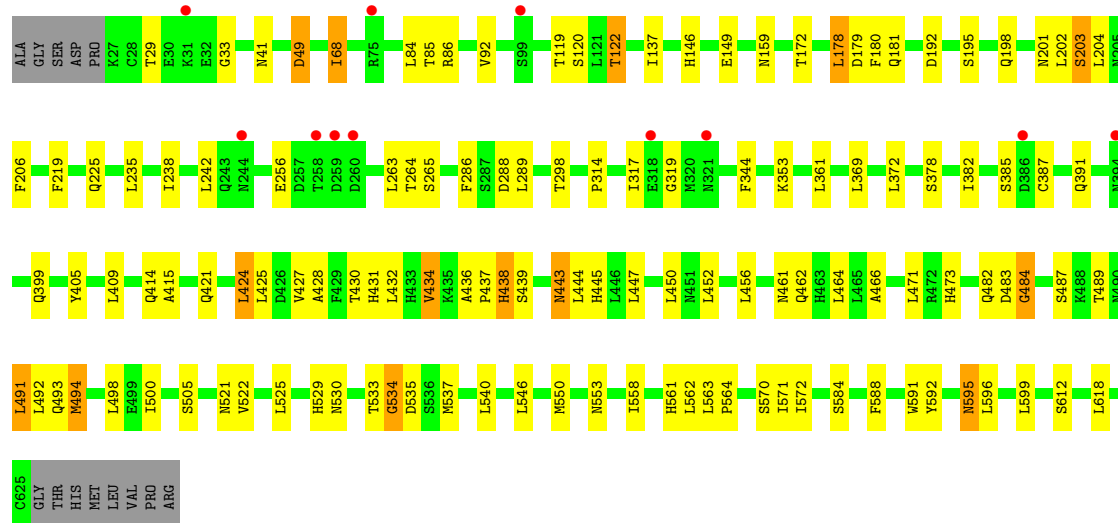
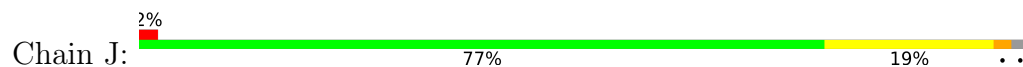
Residue	Category
ALA	Green
GLY	Green
SER	Green
ASP	Green
P80	Green
K27	Green
C28	Green
T29	Green
E32	Green
G33	Green
M41	Green
D49	Green
I68	Green
Q89	Green
I70	Green
T71	Green
T85	Green
R86	Green
W91	Green
V92	Green
E118	Green
T119	Green
S120	Green
L121	Green
T122	Green
H146	Green
E149	Green
I164	Green
T172	Green
L175	Green
L178	Green
D179	Green
F180	Green
Q181	Green
D192	Green
S196	Green
Q198	Green
N201	Green
L202	Green
S203	Green
L204	Green
W205	Green



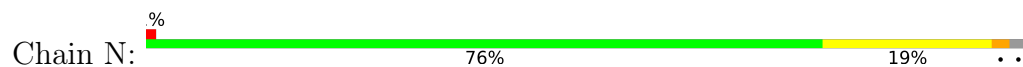
• Molecule 1: CD180 molecule

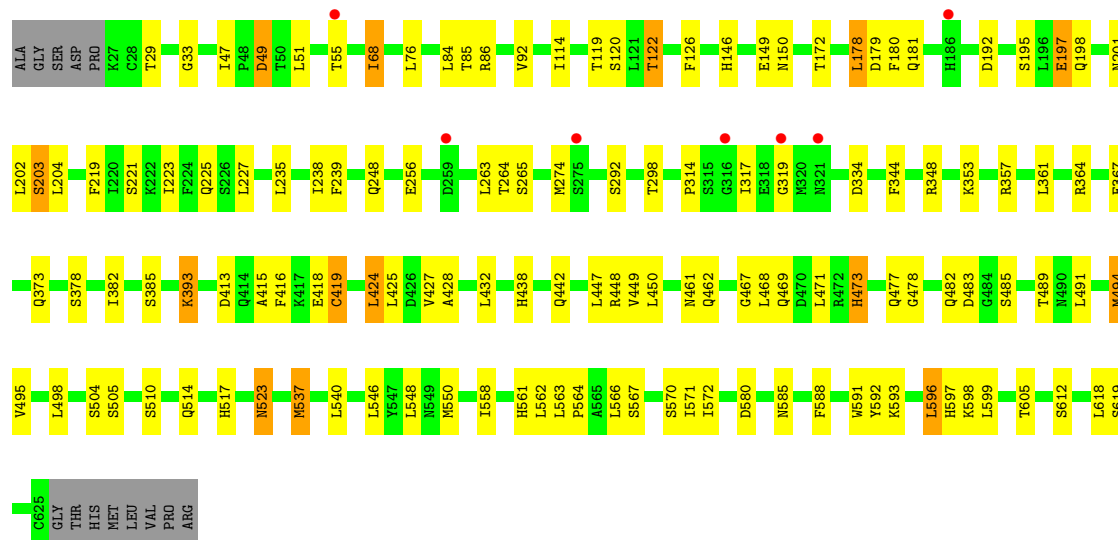


• Molecule 1: CD180 molecule

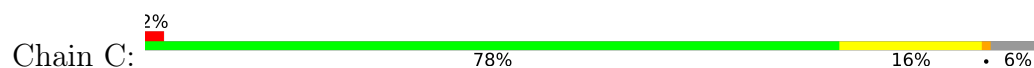


• Molecule 1: CD180 molecule

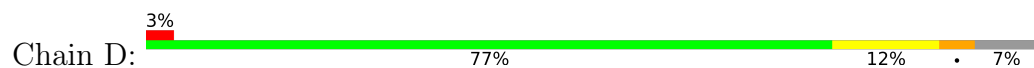




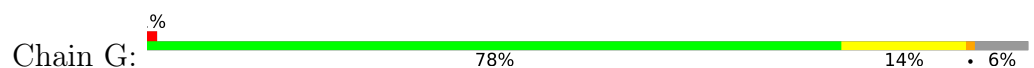
• Molecule 2: LY86 protein



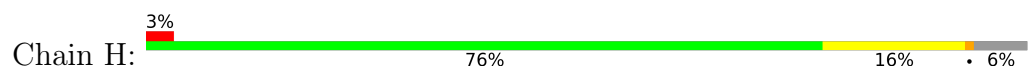
• Molecule 2: LY86 protein



• Molecule 2: LY86 protein



• Molecule 2: LY86 protein



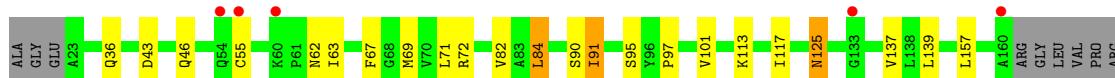
• Molecule 2: LY86 protein

Chain K: 

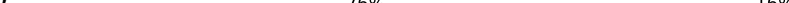


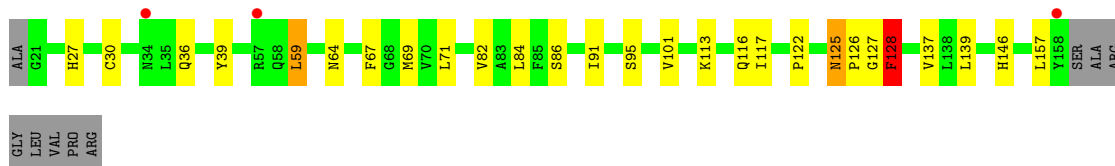
- Molecule 2: LY86 protein

Chain L:



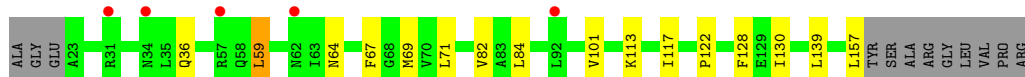
- Molecule 2: LY86 protein

Chain O:  2% 76% 16% 6%



- Molecule 2: LY86 protein

Chain P: 

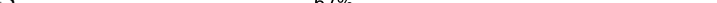


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  67% 33%



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

Chain S:  67% 33%



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

Chain U: 67% 33%



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



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



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



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



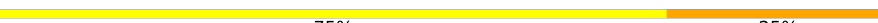
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain T:  75% 25%

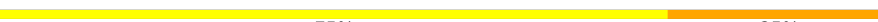
NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

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

Chain V:  62% 38%

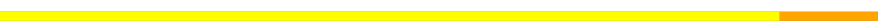
NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

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

Chain X:  75% 25%

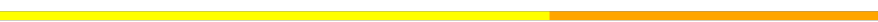
NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

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

Chain Z:  88% 12%

NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

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

Chain b:  62% 38%

NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

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

-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  62% 38%

MAG1	MAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

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

Chain f:  88% 12%

MAG1	MAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	101.51Å 141.58Å 141.95Å 94.00° 91.66° 91.37°	Depositor
Resolution (Å)	20.00 – 2.91 20.00 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.5 (20.00-2.91) 92.6 (20.00-2.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.238 , 0.276 0.240 , 0.276	Depositor DCC
R_{free} test set	8030 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l 0.013 for -h,l,k 0.022 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	43795	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.83	0/4537	0.90	0/6190
1	B	0.91	0/4708	0.94	2/6409 (0.0%)
1	E	0.68	0/4467	0.82	1/6104 (0.0%)
1	F	0.67	0/4581	0.81	3/6256 (0.0%)
1	I	0.65	0/2980	0.79	0/4064
1	J	0.69	0/4546	0.82	1/6213 (0.0%)
1	M	0.84	0/4534	0.89	0/6189
1	N	0.84	0/4682	0.90	2/6377 (0.0%)
2	C	0.86	0/1051	0.91	0/1436
2	D	0.88	0/1048	0.90	0/1432
2	G	0.76	0/1057	0.87	0/1443
2	H	0.83	0/1072	0.92	2/1463 (0.1%)
2	K	0.64	0/1026	0.80	0/1401
2	L	0.78	0/1072	0.86	4/1464 (0.3%)
2	O	0.88	0/1054	0.87	1/1440 (0.1%)
2	P	0.90	0/1026	0.85	0/1402
All	All	0.78	0/43441	0.86	16/59283 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	521	ASN	N-CA-C	6.85	120.60	112.93
1	B	517	HIS	N-CA-C	-6.36	102.10	110.43
2	H	91	ILE	CB-CA-C	-5.89	105.14	110.91
1	N	419	CYS	CA-C-N	5.76	126.26	120.04
1	N	419	CYS	C-N-CA	5.76	126.26	120.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4450	0	4175	64	0
1	B	4616	0	4440	76	0
1	E	4381	0	4045	90	0
1	F	4493	0	4211	78	0
1	I	2931	0	2684	39	0
1	J	4458	0	4137	79	0
1	M	4447	0	4175	75	0
1	N	4591	0	4415	84	0
2	C	1026	0	929	16	0
2	D	1022	0	927	17	0
2	G	1031	0	946	14	0
2	H	1046	0	953	16	0
2	K	1003	0	895	11	0
2	L	1046	0	947	12	0
2	O	1028	0	923	16	0
2	P	1001	0	898	9	0
3	Q	39	0	34	1	0
3	S	39	0	34	1	0
3	U	39	0	34	3	0
3	W	39	0	34	1	0
3	Y	39	0	34	2	0
3	a	39	0	34	2	0
3	c	39	0	34	2	0
3	e	39	0	34	1	0
4	R	94	0	79	0	0
4	T	94	0	79	1	0
4	V	94	0	79	2	0
4	X	94	0	79	2	0
4	Z	94	0	79	1	0
4	b	94	0	79	4	0
4	d	94	0	79	4	0
4	f	94	0	79	1	0
5	D	31	0	44	1	0
5	H	31	0	44	1	0
5	L	31	0	44	1	0
5	P	31	0	44	1	0
6	A	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	9	0	0	0	0
6	C	1	0	0	0	0
6	D	3	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	L	1	0	0	0	0
6	M	5	0	0	0	0
6	N	6	0	0	0	0
All	All	43795	0	40780	697	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 8.

The worst 5 of 697 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:J:450:LEU:HD11	1:J:452:LEU:HD21	1.48	0.95
1:N:523:ASN:HD22	1:N:523:ASN:C	1.75	0.94
1:N:537:MET:HE3	1:N:550:MET:HE3	1.49	0.94
2:H:82:VAL:HG22	2:H:139:LEU:HD23	1.49	0.93
1:M:242:LEU:HB2	1:M:274:MET:HE1	1.50	0.93

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	592/612 (97%)	552 (93%)	36 (6%)	4 (1%)	18 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	597/612 (98%)	556 (93%)	38 (6%)	3 (0%)	24	53
1	E	590/612 (96%)	544 (92%)	43 (7%)	3 (0%)	24	53
1	F	597/612 (98%)	557 (93%)	37 (6%)	3 (0%)	24	53
1	I	383/612 (63%)	361 (94%)	21 (6%)	1 (0%)	36	64
1	J	597/612 (98%)	553 (93%)	39 (6%)	5 (1%)	16	43
1	M	591/612 (97%)	546 (92%)	43 (7%)	2 (0%)	36	64
1	N	597/612 (98%)	560 (94%)	35 (6%)	2 (0%)	36	64
2	C	136/147 (92%)	125 (92%)	8 (6%)	3 (2%)	5	19
2	D	134/147 (91%)	125 (93%)	8 (6%)	1 (1%)	18	46
2	G	136/147 (92%)	127 (93%)	6 (4%)	3 (2%)	5	19
2	H	136/147 (92%)	126 (93%)	9 (7%)	1 (1%)	18	46
2	K	132/147 (90%)	125 (95%)	6 (4%)	1 (1%)	16	43
2	L	136/147 (92%)	127 (93%)	8 (6%)	1 (1%)	18	46
2	O	136/147 (92%)	129 (95%)	6 (4%)	1 (1%)	18	46
2	P	133/147 (90%)	123 (92%)	9 (7%)	1 (1%)	16	43
All	All	5623/6072 (93%)	5236 (93%)	352 (6%)	35 (1%)	21	50

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	494	MET
1	J	438	HIS
1	J	534	GLY
1	N	494	MET
2	C	128	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	481/561 (86%)	454 (94%)	27 (6%)	19	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	516/561 (92%)	483 (94%)	33 (6%)	16	43
1	E	463/561 (82%)	436 (94%)	27 (6%)	18	47
1	F	488/561 (87%)	456 (93%)	32 (7%)	15	41
1	I	304/561 (54%)	287 (94%)	17 (6%)	19	48
1	J	478/561 (85%)	449 (94%)	29 (6%)	17	44
1	M	481/561 (86%)	444 (92%)	37 (8%)	12	34
1	N	511/561 (91%)	481 (94%)	30 (6%)	18	46
2	C	102/125 (82%)	97 (95%)	5 (5%)	22	52
2	D	103/125 (82%)	95 (92%)	8 (8%)	11	33
2	G	103/125 (82%)	98 (95%)	5 (5%)	22	52
2	H	105/125 (84%)	98 (93%)	7 (7%)	15	41
2	K	98/125 (78%)	94 (96%)	4 (4%)	27	60
2	L	106/125 (85%)	100 (94%)	6 (6%)	18	48
2	O	102/125 (82%)	96 (94%)	6 (6%)	18	46
2	P	99/125 (79%)	95 (96%)	4 (4%)	28	61
All	All	4540/5488 (83%)	4263 (94%)	277 (6%)	17	44

5 of 277 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	612	SER
2	D	62	ASN
2	K	134	ASP
1	M	456	LEU
1	M	442	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 191 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	523	ASN
1	N	311	ASN
1	J	104	ASN
1	J	477	GLN
1	N	576	HIS

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 ⓘ

88 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	Q	1	3,1	14,14,15	0.79	0	17,19,21	1.20	2 (11%)
3	NAG	Q	2	3	14,14,15	0.77	0	17,19,21	1.71	4 (23%)
3	BMA	Q	3	3	11,11,12	1.03	0	15,15,17	1.16	1 (6%)
4	NAG	R	1	4,1	14,14,15	0.52	0	17,19,21	1.47	3 (17%)
4	NAG	R	2	4	14,14,15	0.67	0	17,19,21	1.13	1 (5%)
4	BMA	R	3	4	11,11,12	0.76	0	15,15,17	1.39	2 (13%)
4	MAN	R	4	4	11,11,12	0.73	0	15,15,17	1.14	3 (20%)
4	MAN	R	5	4	11,11,12	0.67	0	15,15,17	2.01	4 (26%)
4	MAN	R	6	4	11,11,12	0.79	0	15,15,17	2.76	5 (33%)
4	MAN	R	7	4	11,11,12	0.76	0	15,15,17	0.93	0
4	MAN	R	8	4	11,11,12	0.84	0	15,15,17	2.18	6 (40%)
3	NAG	S	1	3,1	14,14,15	0.81	0	17,19,21	1.13	2 (11%)
3	NAG	S	2	3	14,14,15	0.76	0	17,19,21	1.69	5 (29%)
3	BMA	S	3	3	11,11,12	1.34	0	15,15,17	1.17	1 (6%)
4	NAG	T	1	4,1	14,14,15	0.58	0	17,19,21	1.20	2 (11%)
4	NAG	T	2	4	14,14,15	0.90	0	17,19,21	1.35	2 (11%)
4	BMA	T	3	4	11,11,12	1.20	2 (18%)	15,15,17	1.10	1 (6%)
4	MAN	T	4	4	11,11,12	0.56	0	15,15,17	0.96	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	T	5	4	11,11,12	0.67	0	15,15,17	2.34	4 (26%)
4	MAN	T	6	4	11,11,12	0.65	0	15,15,17	2.52	7 (46%)
4	MAN	T	7	4	11,11,12	0.89	0	15,15,17	1.20	1 (6%)
4	MAN	T	8	4	11,11,12	0.86	0	15,15,17	2.22	7 (46%)
3	NAG	U	1	3	14,14,15	0.77	0	17,19,21	1.59	3 (17%)
3	NAG	U	2	3	14,14,15	0.45	0	17,19,21	1.89	4 (23%)
3	BMA	U	3	3	11,11,12	1.25	0	15,15,17	0.92	1 (6%)
4	NAG	V	1	4,1	14,14,15	0.72	0	17,19,21	1.19	3 (17%)
4	NAG	V	2	4	14,14,15	0.68	0	17,19,21	1.39	1 (5%)
4	BMA	V	3	4	11,11,12	1.16	1 (9%)	15,15,17	1.19	2 (13%)
4	MAN	V	4	4	11,11,12	0.63	0	15,15,17	1.32	1 (6%)
4	MAN	V	5	4	11,11,12	0.86	1 (9%)	15,15,17	2.43	6 (40%)
4	MAN	V	6	4	11,11,12	0.75	0	15,15,17	2.49	4 (26%)
4	MAN	V	7	4	11,11,12	0.82	0	15,15,17	1.15	1 (6%)
4	MAN	V	8	4	11,11,12	0.64	0	15,15,17	2.01	5 (33%)
3	NAG	W	1	3,1	14,14,15	0.86	1 (7%)	17,19,21	1.32	3 (17%)
3	NAG	W	2	3	14,14,15	0.82	1 (7%)	17,19,21	1.54	4 (23%)
3	BMA	W	3	3	11,11,12	1.02	0	15,15,17	1.07	1 (6%)
4	NAG	X	1	4,1	14,14,15	0.54	0	17,19,21	1.53	3 (17%)
4	NAG	X	2	4	14,14,15	0.79	0	17,19,21	1.38	4 (23%)
4	BMA	X	3	4	11,11,12	0.79	0	15,15,17	1.09	1 (6%)
4	MAN	X	4	4	11,11,12	0.88	0	15,15,17	1.03	1 (6%)
4	MAN	X	5	4	11,11,12	0.63	0	15,15,17	1.94	3 (20%)
4	MAN	X	6	4	11,11,12	0.77	0	15,15,17	2.51	5 (33%)
4	MAN	X	7	4	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
4	MAN	X	8	4	11,11,12	0.83	0	15,15,17	1.96	6 (40%)
3	NAG	Y	1	3,1	14,14,15	1.15	2 (14%)	17,19,21	1.72	3 (17%)
3	NAG	Y	2	3	14,14,15	0.86	0	17,19,21	1.47	3 (17%)
3	BMA	Y	3	3	11,11,12	0.90	0	15,15,17	1.16	1 (6%)
4	NAG	Z	1	4,1	14,14,15	0.96	1 (7%)	17,19,21	1.44	3 (17%)
4	NAG	Z	2	4	14,14,15	1.08	1 (7%)	17,19,21	1.50	4 (23%)
4	BMA	Z	3	4	11,11,12	0.63	0	15,15,17	1.42	3 (20%)
4	MAN	Z	4	4	11,11,12	1.08	1 (9%)	15,15,17	1.42	2 (13%)
4	MAN	Z	5	4	11,11,12	1.21	1 (9%)	15,15,17	2.21	5 (33%)
4	MAN	Z	6	4	11,11,12	1.11	2 (18%)	15,15,17	2.41	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	Z	7	4	11,11,12	1.25	1 (9%)	15,15,17	1.44	4 (26%)
4	MAN	Z	8	4	11,11,12	0.77	0	15,15,17	1.99	7 (46%)
3	NAG	a	1	3,1	14,14,15	0.60	0	17,19,21	1.65	2 (11%)
3	NAG	a	2	3	14,14,15	0.61	0	17,19,21	2.06	3 (17%)
3	BMA	a	3	3	11,11,12	1.13	0	15,15,17	1.07	1 (6%)
4	NAG	b	1	4,1	14,14,15	0.53	0	17,19,21	1.03	2 (11%)
4	NAG	b	2	4	14,14,15	0.66	0	17,19,21	1.11	1 (5%)
4	BMA	b	3	4	11,11,12	0.81	0	15,15,17	1.12	2 (13%)
4	MAN	b	4	4	11,11,12	0.53	0	15,15,17	1.07	1 (6%)
4	MAN	b	5	4	11,11,12	0.89	0	15,15,17	2.15	5 (33%)
4	MAN	b	6	4	11,11,12	0.82	0	15,15,17	2.56	6 (40%)
4	MAN	b	7	4	11,11,12	0.82	0	15,15,17	1.09	1 (6%)
4	MAN	b	8	4	11,11,12	0.93	0	15,15,17	2.20	6 (40%)
3	NAG	c	1	3,1	14,14,15	0.75	0	17,19,21	1.67	2 (11%)
3	NAG	c	2	3	14,14,15	0.59	0	17,19,21	1.98	4 (23%)
3	BMA	c	3	3	11,11,12	1.11	0	15,15,17	1.10	1 (6%)
4	NAG	d	1	4,1	14,14,15	0.35	0	17,19,21	1.21	2 (11%)
4	NAG	d	2	4	14,14,15	0.83	0	17,19,21	1.20	2 (11%)
4	BMA	d	3	4	11,11,12	0.84	0	15,15,17	1.24	2 (13%)
4	MAN	d	4	4	11,11,12	0.65	0	15,15,17	0.92	1 (6%)
4	MAN	d	5	4	11,11,12	0.94	0	15,15,17	2.19	5 (33%)
4	MAN	d	6	4	11,11,12	0.66	0	15,15,17	2.55	5 (33%)
4	MAN	d	7	4	11,11,12	0.89	1 (9%)	15,15,17	1.12	0
4	MAN	d	8	4	11,11,12	0.86	0	15,15,17	1.83	4 (26%)
3	NAG	e	1	3,1	14,14,15	0.85	1 (7%)	17,19,21	1.64	3 (17%)
3	NAG	e	2	3	14,14,15	0.75	0	17,19,21	1.44	5 (29%)
3	BMA	e	3	3	11,11,12	1.07	0	15,15,17	1.04	1 (6%)
4	NAG	f	1	4,1	14,14,15	0.69	0	17,19,21	1.52	4 (23%)
4	NAG	f	2	4	14,14,15	0.86	1 (7%)	17,19,21	1.49	3 (17%)
4	BMA	f	3	4	11,11,12	0.71	0	15,15,17	1.29	2 (13%)
4	MAN	f	4	4	11,11,12	0.77	0	15,15,17	1.19	1 (6%)
4	MAN	f	5	4	11,11,12	0.95	0	15,15,17	2.04	2 (13%)
4	MAN	f	6	4	11,11,12	0.98	0	15,15,17	2.63	5 (33%)
4	MAN	f	7	4	11,11,12	1.14	1 (9%)	15,15,17	1.29	1 (6%)
4	MAN	f	8	4	11,11,12	0.67	0	15,15,17	2.03	6 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	BMA	R	3	4	-	0/2/19/22	0/1/1/1
4	MAN	R	4	4	-	0/2/19/22	0/1/1/1
4	MAN	R	5	4	-	0/2/19/22	0/1/1/1
4	MAN	R	6	4	-	2/2/19/22	1/1/1/1
4	MAN	R	7	4	-	2/2/19/22	0/1/1/1
4	MAN	R	8	4	-	2/2/19/22	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	BMA	S	3	3	-	0/2/19/22	0/1/1/1
4	NAG	T	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
4	MAN	T	4	4	-	0/2/19/22	0/1/1/1
4	MAN	T	5	4	-	0/2/19/22	0/1/1/1
4	MAN	T	6	4	-	2/2/19/22	1/1/1/1
4	MAN	T	7	4	-	2/2/19/22	0/1/1/1
4	MAN	T	8	4	-	2/2/19/22	0/1/1/1
3	NAG	U	1	3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	BMA	V	3	4	-	0/2/19/22	0/1/1/1
4	MAN	V	4	4	-	0/2/19/22	0/1/1/1
4	MAN	V	5	4	-	0/2/19/22	0/1/1/1
4	MAN	V	6	4	-	2/2/19/22	1/1/1/1
4	MAN	V	7	4	-	2/2/19/22	0/1/1/1
4	MAN	V	8	4	-	2/2/19/22	0/1/1/1
3	NAG	W	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	W	3	3	-	0/2/19/22	0/1/1/1
4	NAG	X	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	BMA	X	3	4	-	0/2/19/22	0/1/1/1
4	MAN	X	4	4	-	0/2/19/22	0/1/1/1
4	MAN	X	5	4	-	0/2/19/22	0/1/1/1
4	MAN	X	6	4	-	2/2/19/22	1/1/1/1
4	MAN	X	7	4	-	2/2/19/22	0/1/1/1
4	MAN	X	8	4	-	2/2/19/22	0/1/1/1
3	NAG	Y	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Y	3	3	-	0/2/19/22	0/1/1/1
4	NAG	Z	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	0/2/19/22	0/1/1/1
4	MAN	Z	4	4	-	0/2/19/22	0/1/1/1
4	MAN	Z	5	4	-	0/2/19/22	0/1/1/1
4	MAN	Z	6	4	-	2/2/19/22	1/1/1/1
4	MAN	Z	7	4	-	2/2/19/22	0/1/1/1
4	MAN	Z	8	4	-	2/2/19/22	0/1/1/1
3	NAG	a	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	BMA	a	3	3	-	0/2/19/22	0/1/1/1
4	NAG	b	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	BMA	b	3	4	-	0/2/19/22	0/1/1/1
4	MAN	b	4	4	-	0/2/19/22	0/1/1/1
4	MAN	b	5	4	-	0/2/19/22	0/1/1/1
4	MAN	b	6	4	-	2/2/19/22	1/1/1/1
4	MAN	b	7	4	-	2/2/19/22	0/1/1/1
4	MAN	b	8	4	-	2/2/19/22	0/1/1/1
3	NAG	c	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	BMA	c	3	3	-	0/2/19/22	0/1/1/1
4	NAG	d	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1
4	BMA	d	3	4	-	0/2/19/22	0/1/1/1
4	MAN	d	4	4	-	0/2/19/22	0/1/1/1
4	MAN	d	5	4	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	d	6	4	-	2/2/19/22	1/1/1/1
4	MAN	d	7	4	-	2/2/19/22	0/1/1/1
4	MAN	d	8	4	-	2/2/19/22	0/1/1/1
3	NAG	e	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1
3	BMA	e	3	3	-	0/2/19/22	0/1/1/1
4	NAG	f	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	f	2	4	-	0/6/23/26	0/1/1/1
4	BMA	f	3	4	-	0/2/19/22	0/1/1/1
4	MAN	f	4	4	-	0/2/19/22	0/1/1/1
4	MAN	f	5	4	-	0/2/19/22	0/1/1/1
4	MAN	f	6	4	-	2/2/19/22	1/1/1/1
4	MAN	f	7	4	-	2/2/19/22	0/1/1/1
4	MAN	f	8	4	-	2/2/19/22	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	f	7	MAN	O5-C5	-3.13	1.37	1.43
3	Y	1	NAG	O5-C5	-2.90	1.37	1.43
4	Z	2	NAG	O5-C1	-2.65	1.39	1.43
4	Z	7	MAN	O5-C5	-2.64	1.38	1.43
3	Y	1	NAG	O5-C1	-2.55	1.39	1.43

The worst 5 of 260 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	5	MAN	O2-C2-C1	6.60	124.34	109.22
4	T	5	MAN	O2-C2-C1	6.47	124.04	109.22
3	a	2	NAG	C1-O5-C5	-6.41	103.59	112.19
4	Z	5	MAN	O2-C2-C1	5.91	122.75	109.22
4	X	6	MAN	C1-O5-C5	-5.90	104.28	112.19

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	c	2	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	a	2	NAG	O5-C5-C6-O6
4	X	7	MAN	O5-C5-C6-O6

5 of 8 ring outliers are listed below:

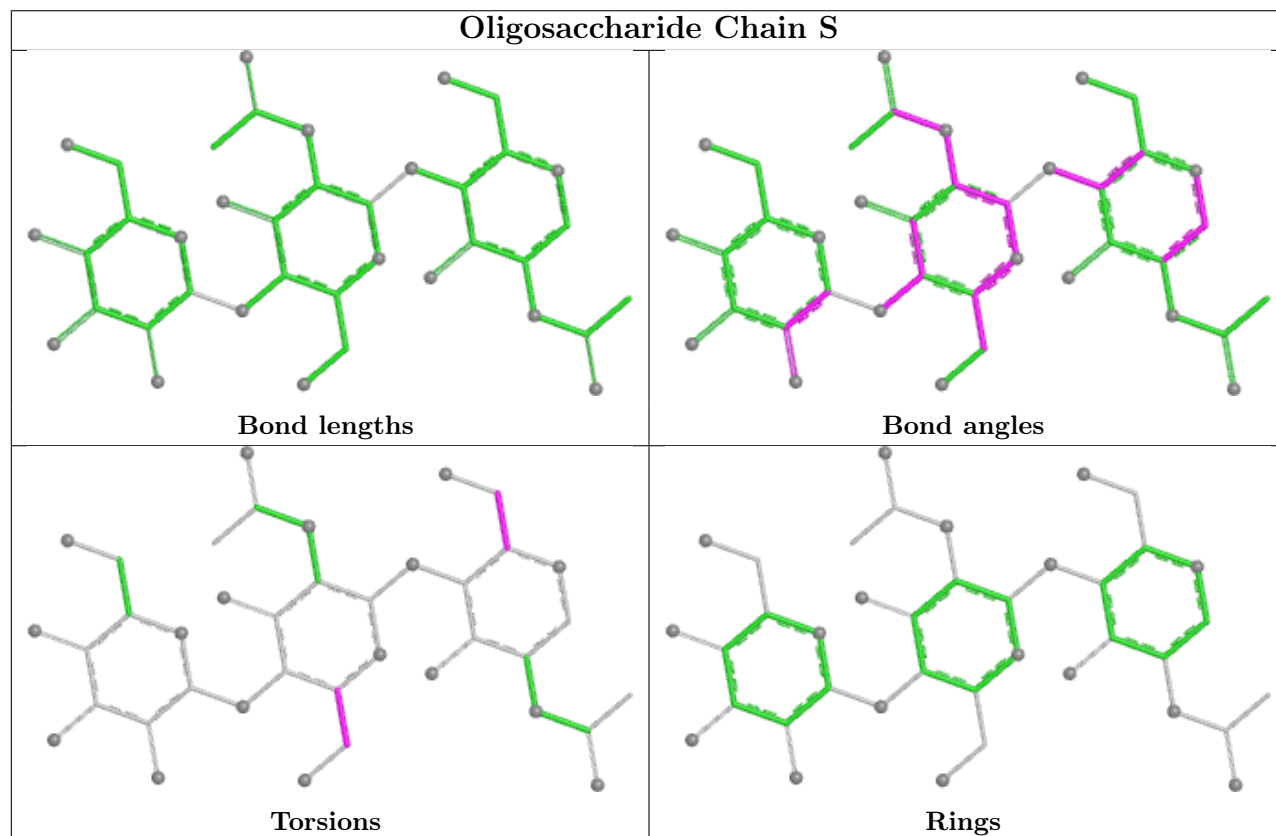
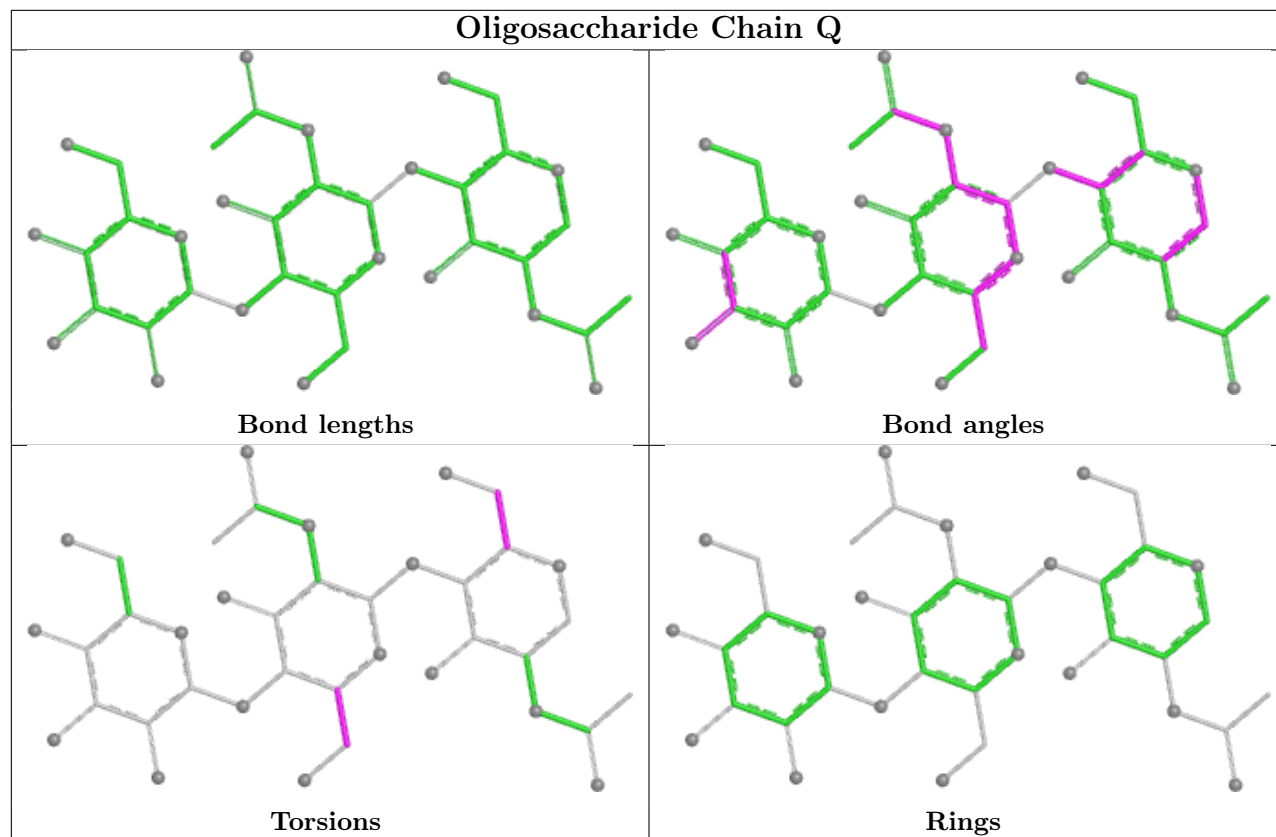
Mol	Chain	Res	Type	Atoms
4	X	6	MAN	C1-C2-C3-C4-C5-O5
4	d	6	MAN	C1-C2-C3-C4-C5-O5
4	R	6	MAN	C1-C2-C3-C4-C5-O5
4	f	6	MAN	C1-C2-C3-C4-C5-O5
4	b	6	MAN	C1-C2-C3-C4-C5-O5

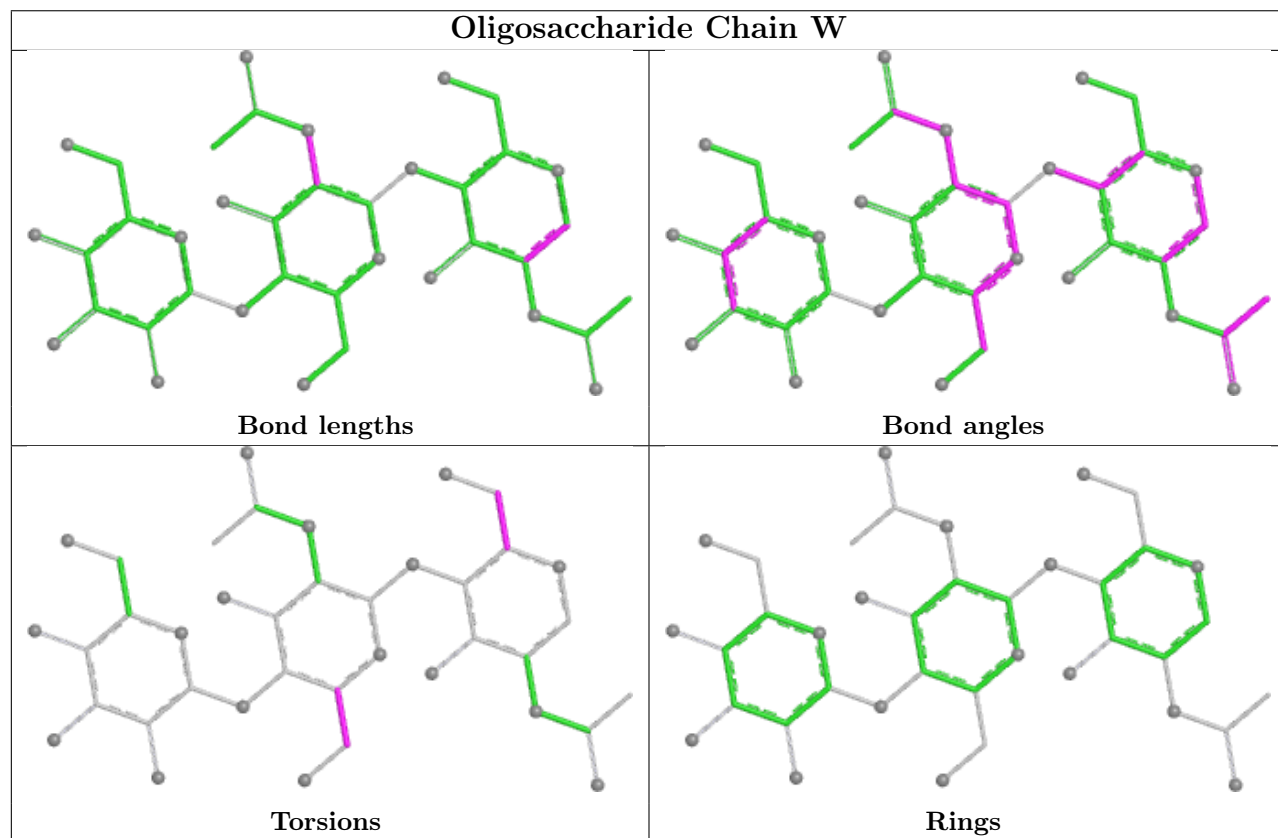
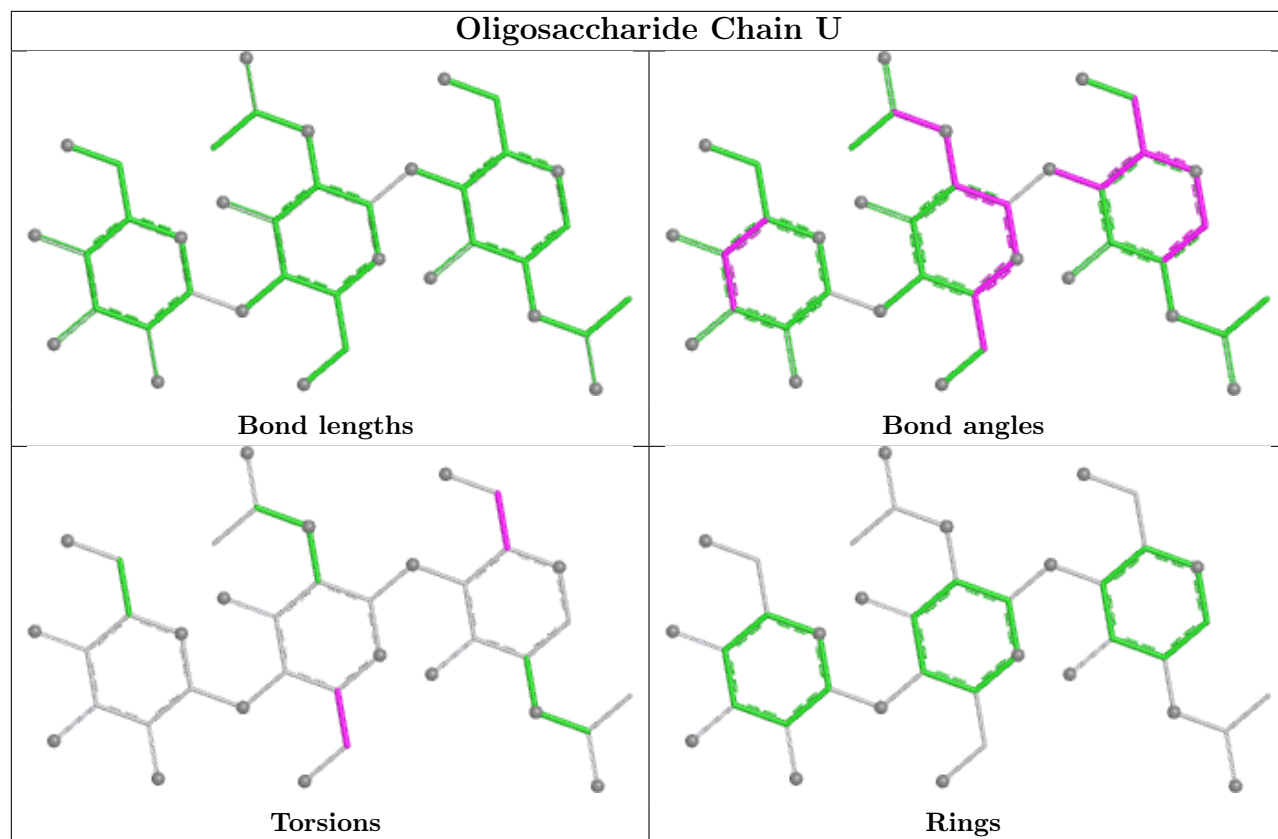
25 monomers are involved in 25 short contacts:

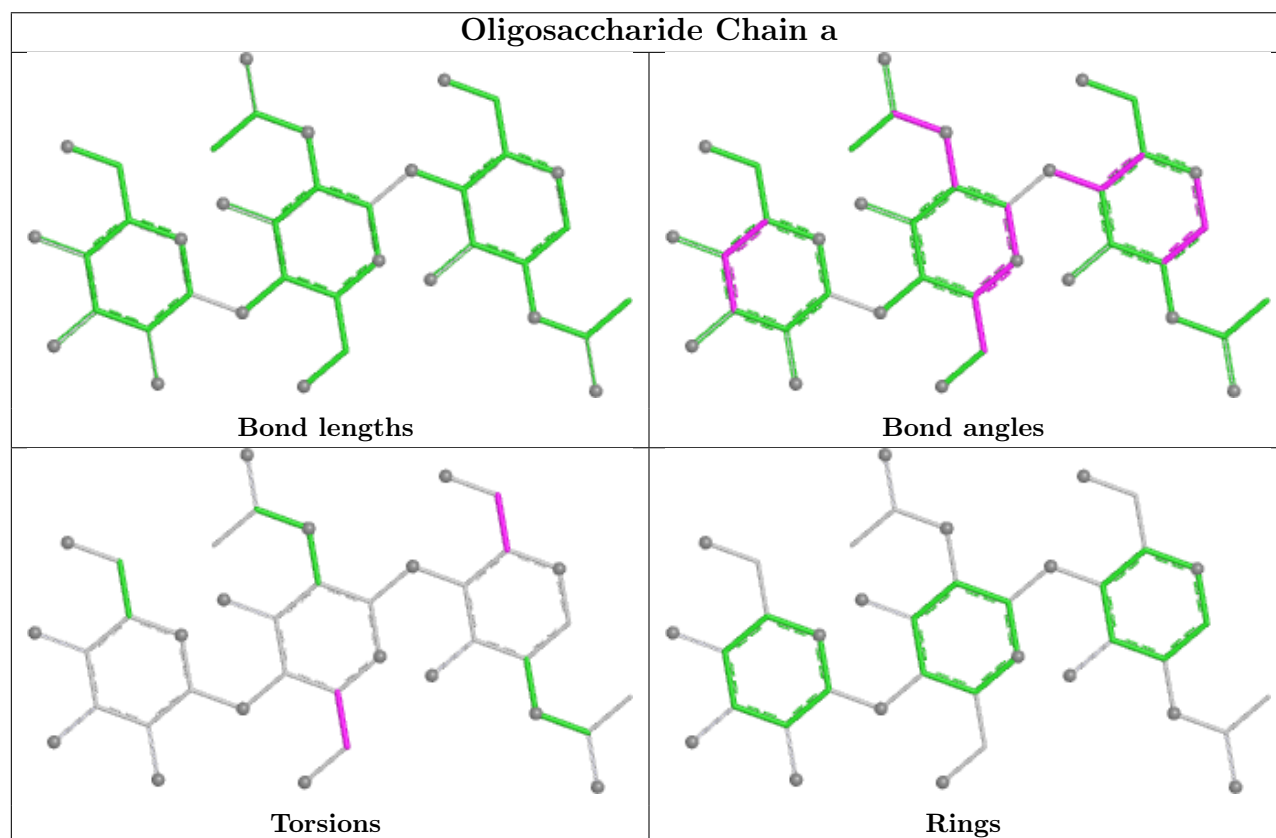
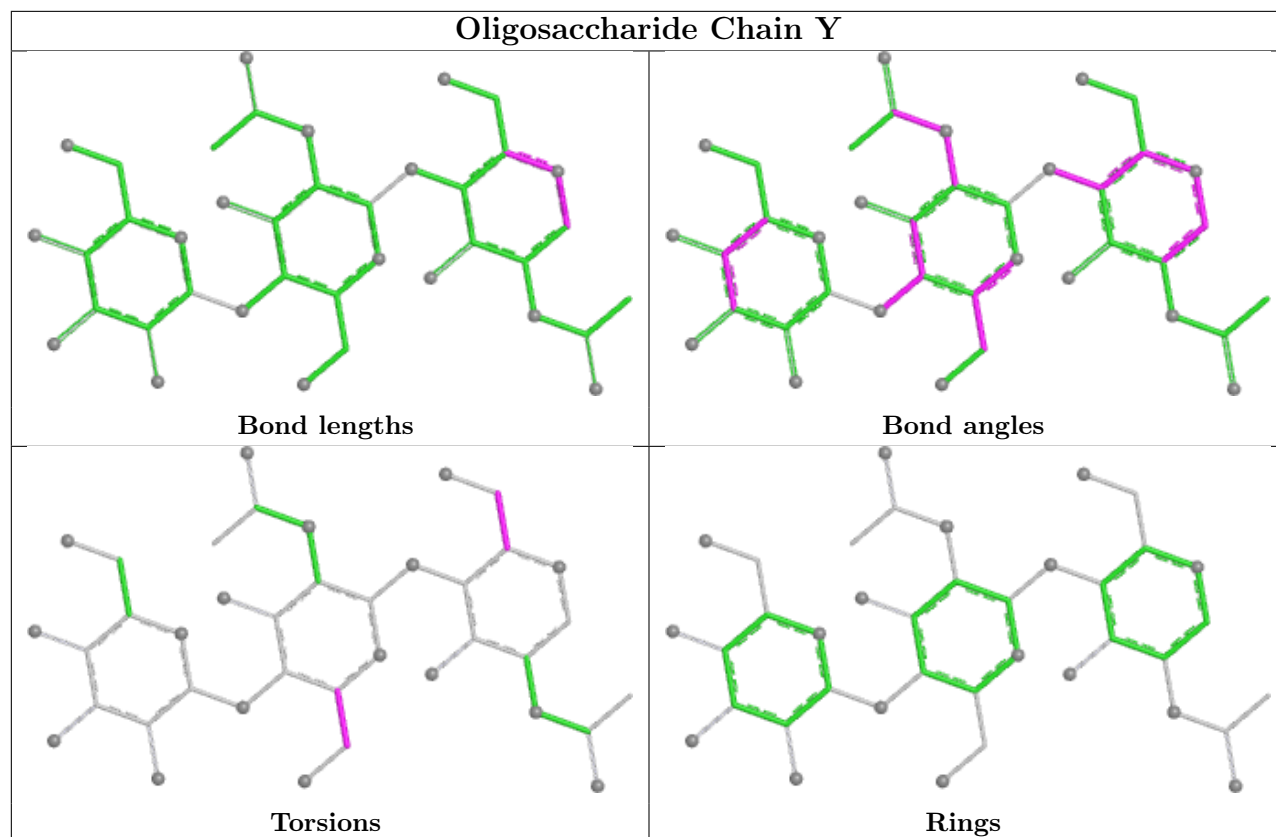
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	a	1	NAG	1	0
3	Y	1	NAG	1	0
3	Y	2	NAG	1	0
3	S	1	NAG	1	0
4	d	6	MAN	2	0
4	b	5	MAN	1	0
3	a	2	NAG	1	0
4	b	6	MAN	1	0
4	T	5	MAN	1	0
4	b	1	NAG	2	0
4	Z	1	NAG	1	0
4	T	6	MAN	1	0
4	d	1	NAG	1	0
3	c	1	NAG	2	0
4	f	1	NAG	1	0
4	V	5	MAN	1	0
4	V	1	NAG	1	0
3	Q	1	NAG	1	0
3	U	1	NAG	3	0
4	V	6	MAN	1	0
4	d	5	MAN	2	0
4	X	5	MAN	1	0
4	X	1	NAG	1	0
3	W	1	NAG	1	0
3	e	1	NAG	1	0

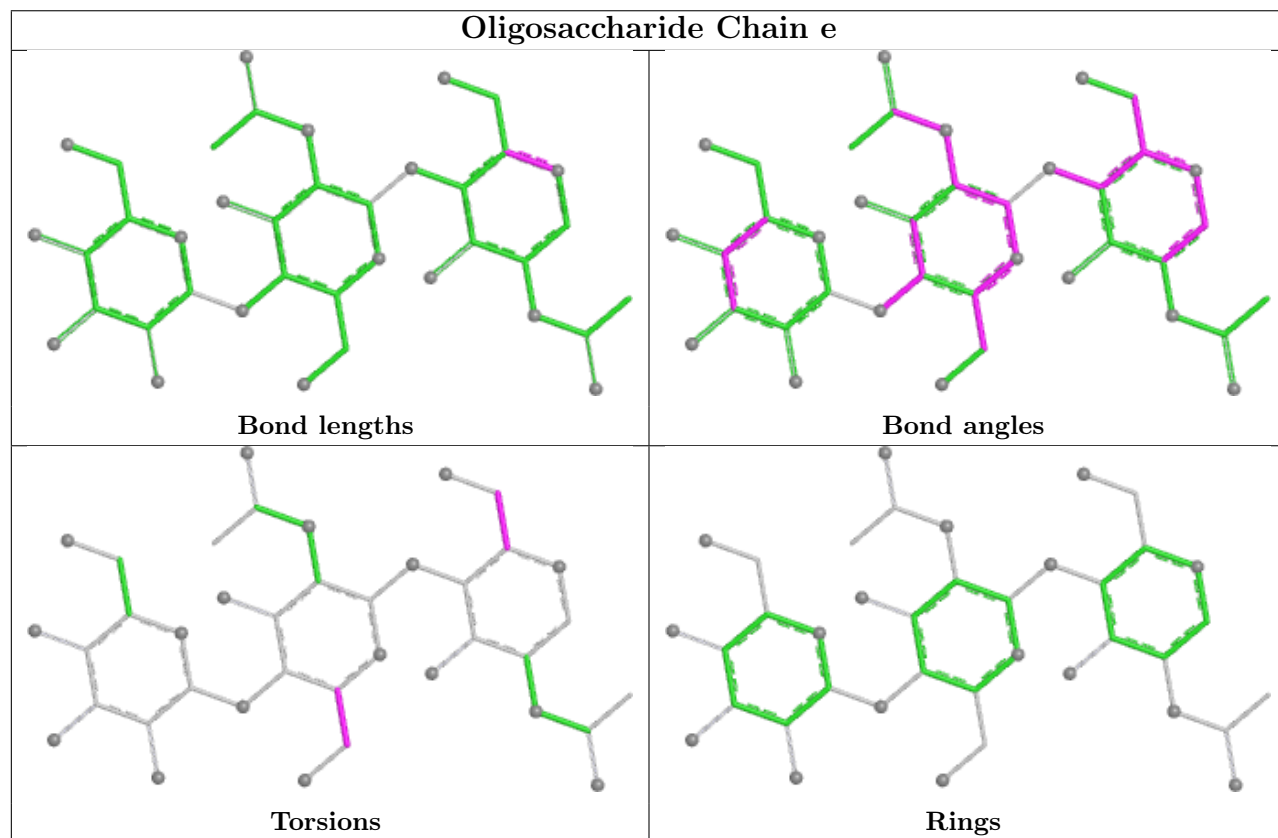
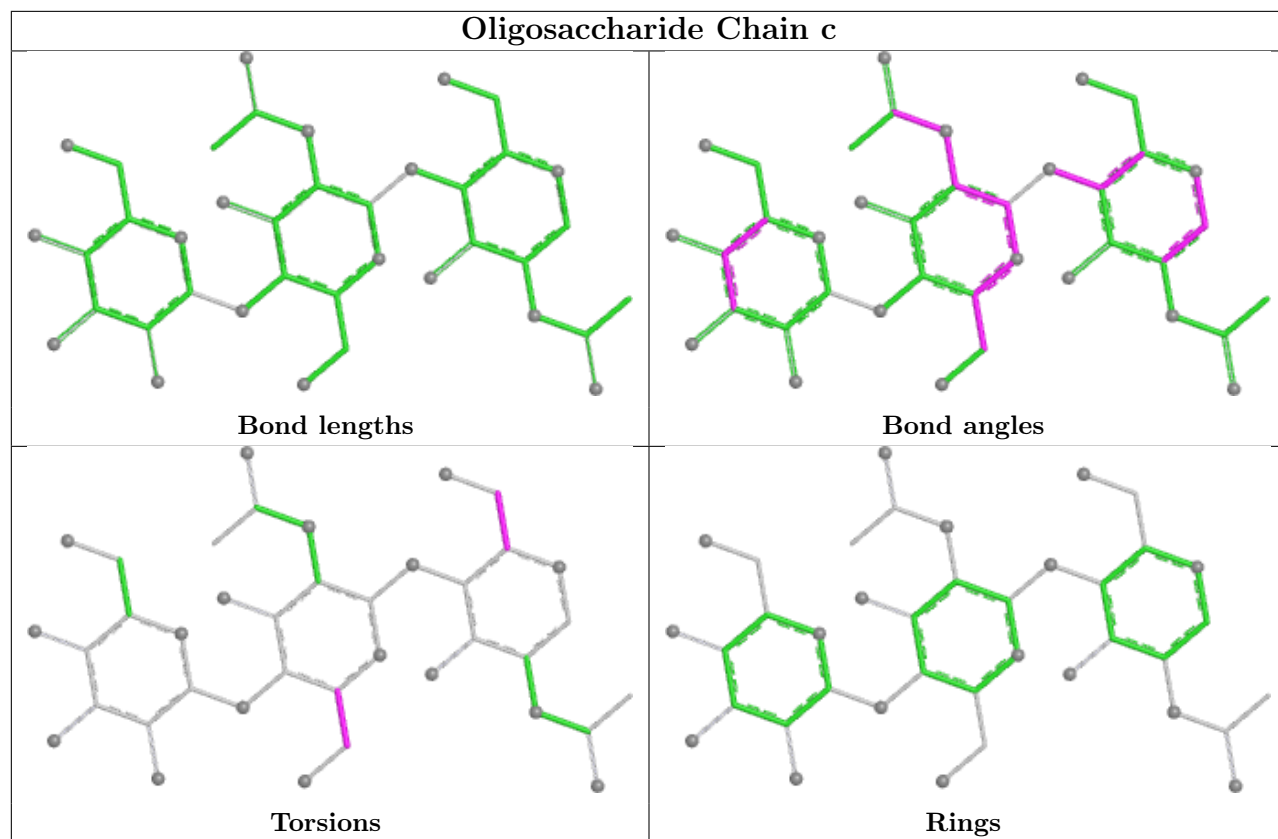
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

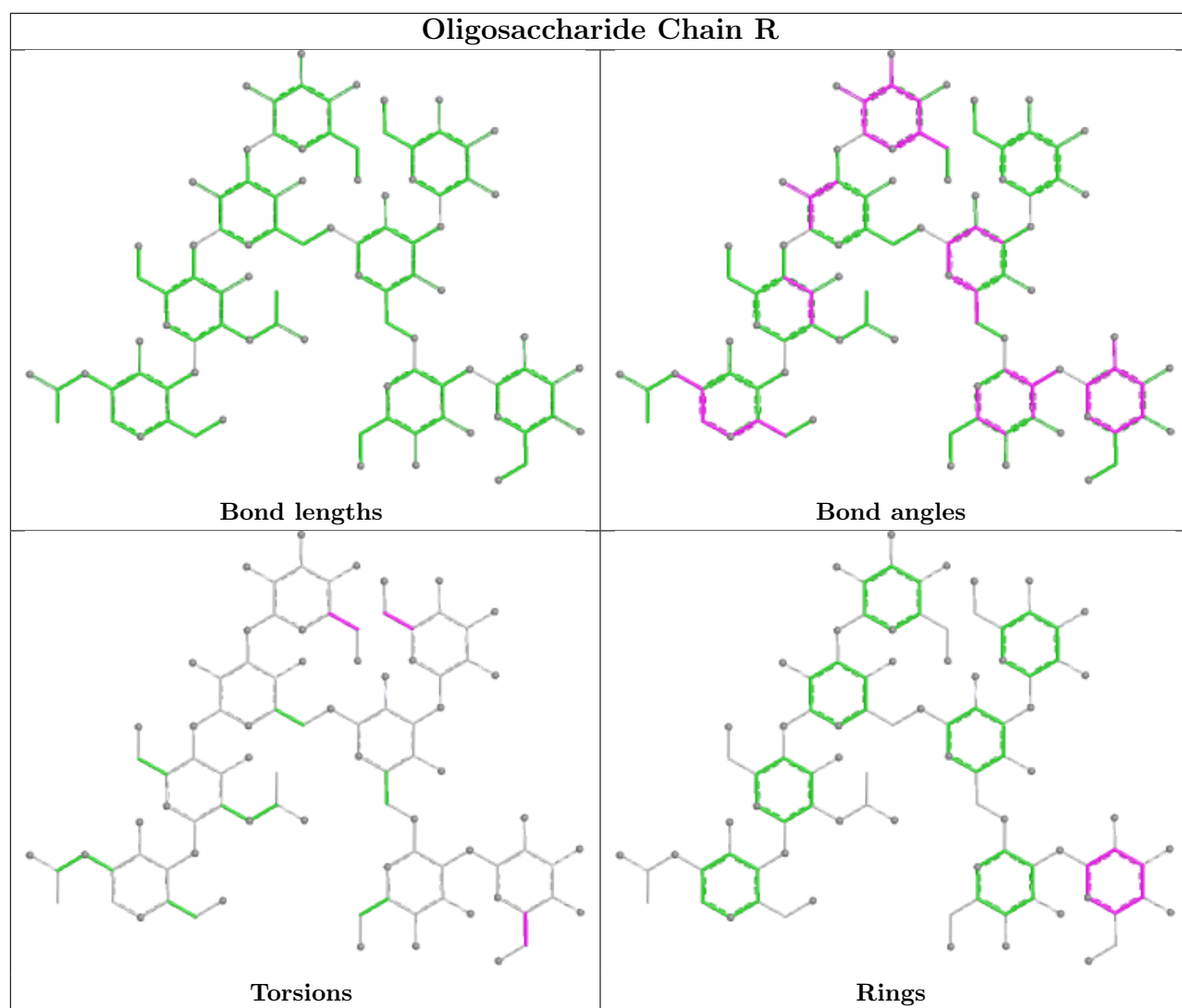
bond angles, torsion angles, and ring geometry for oligosaccharide.

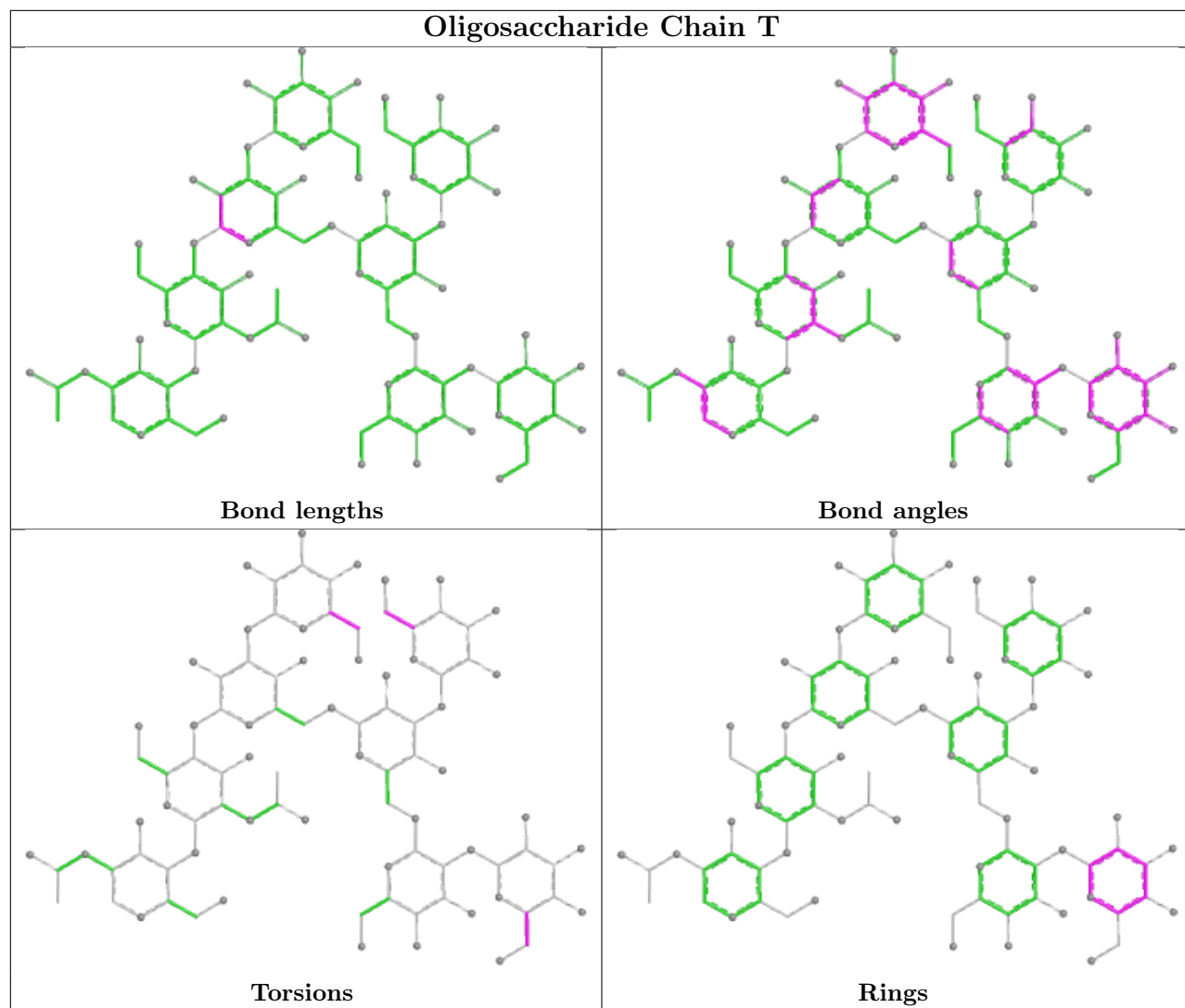




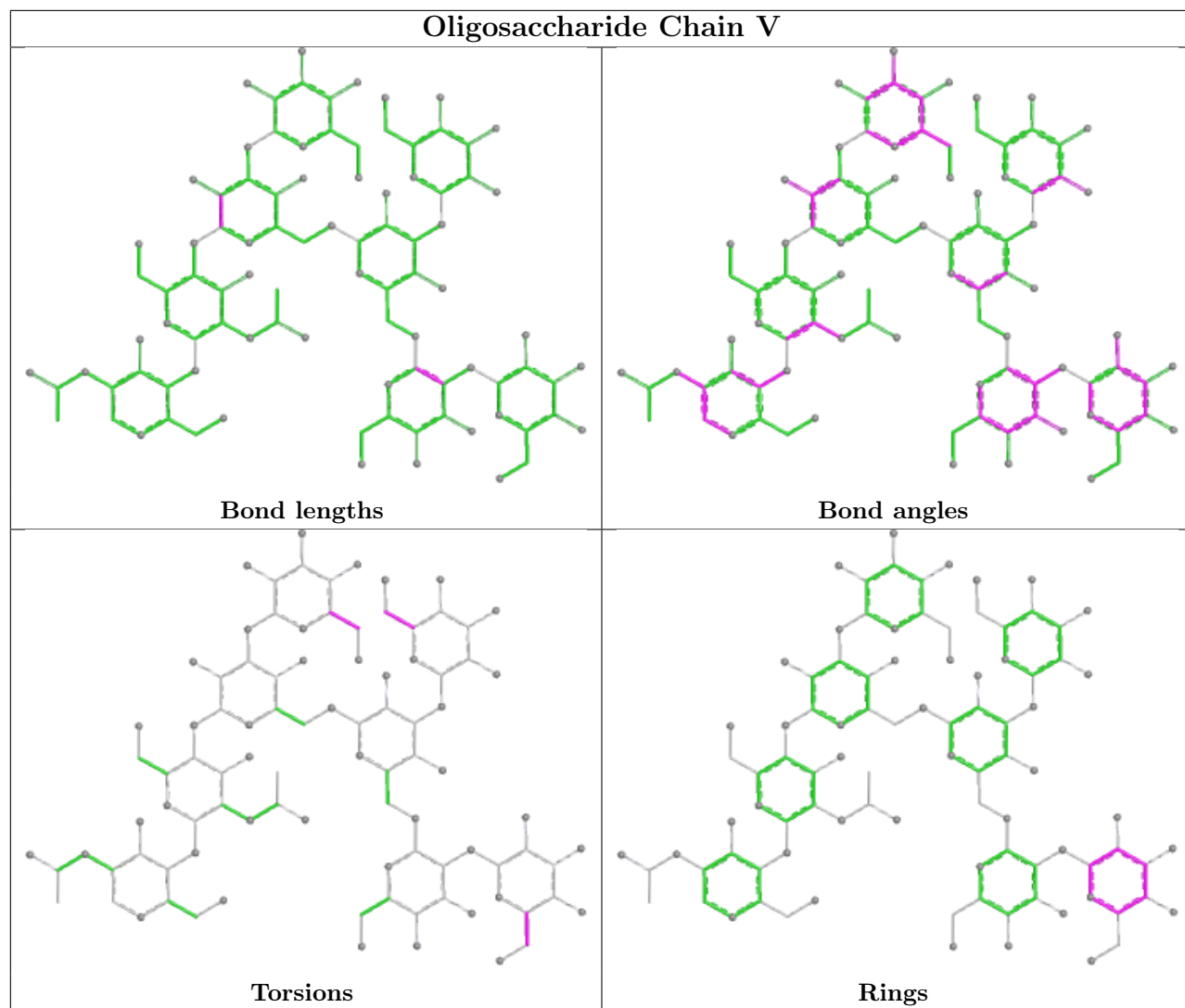


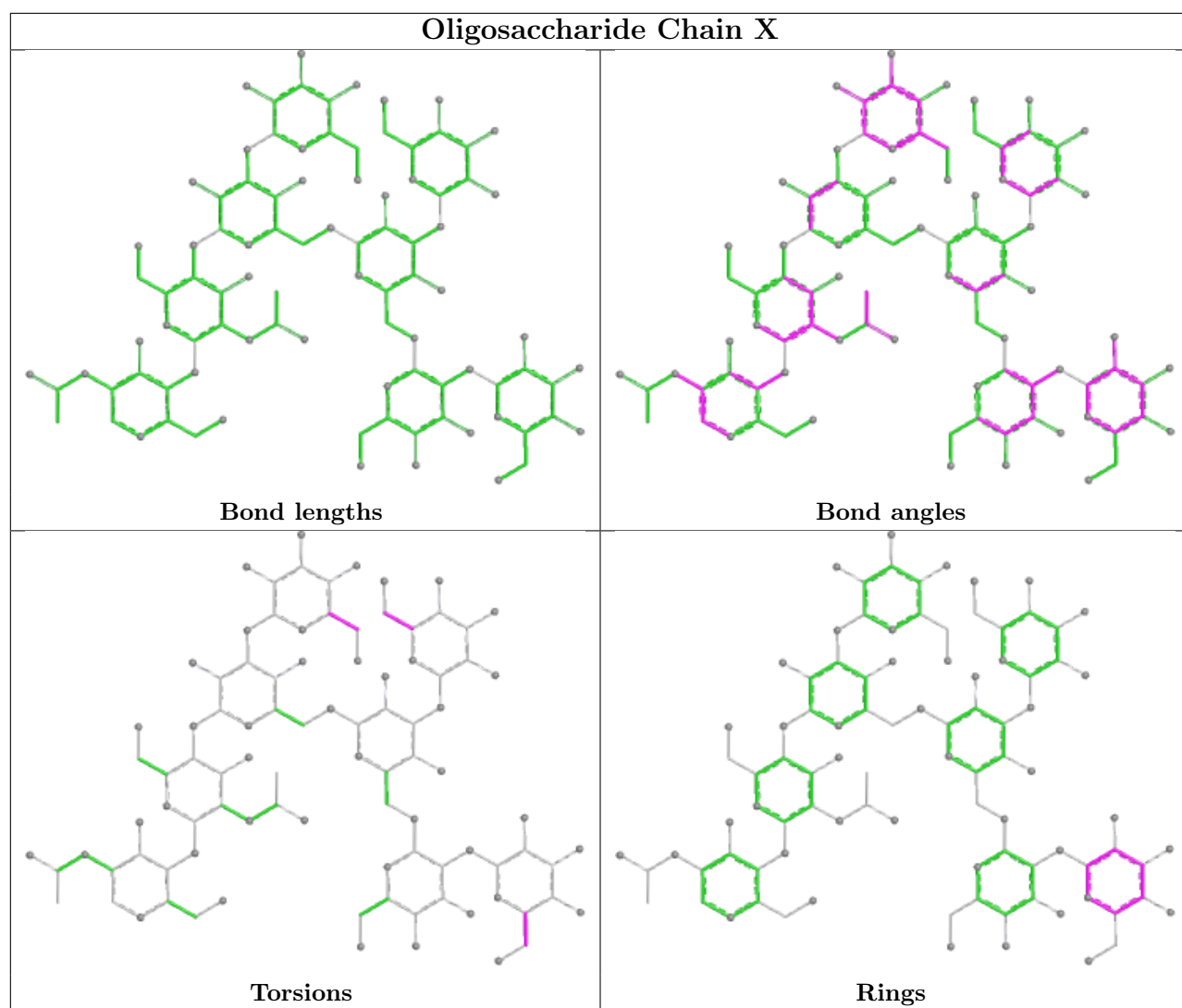


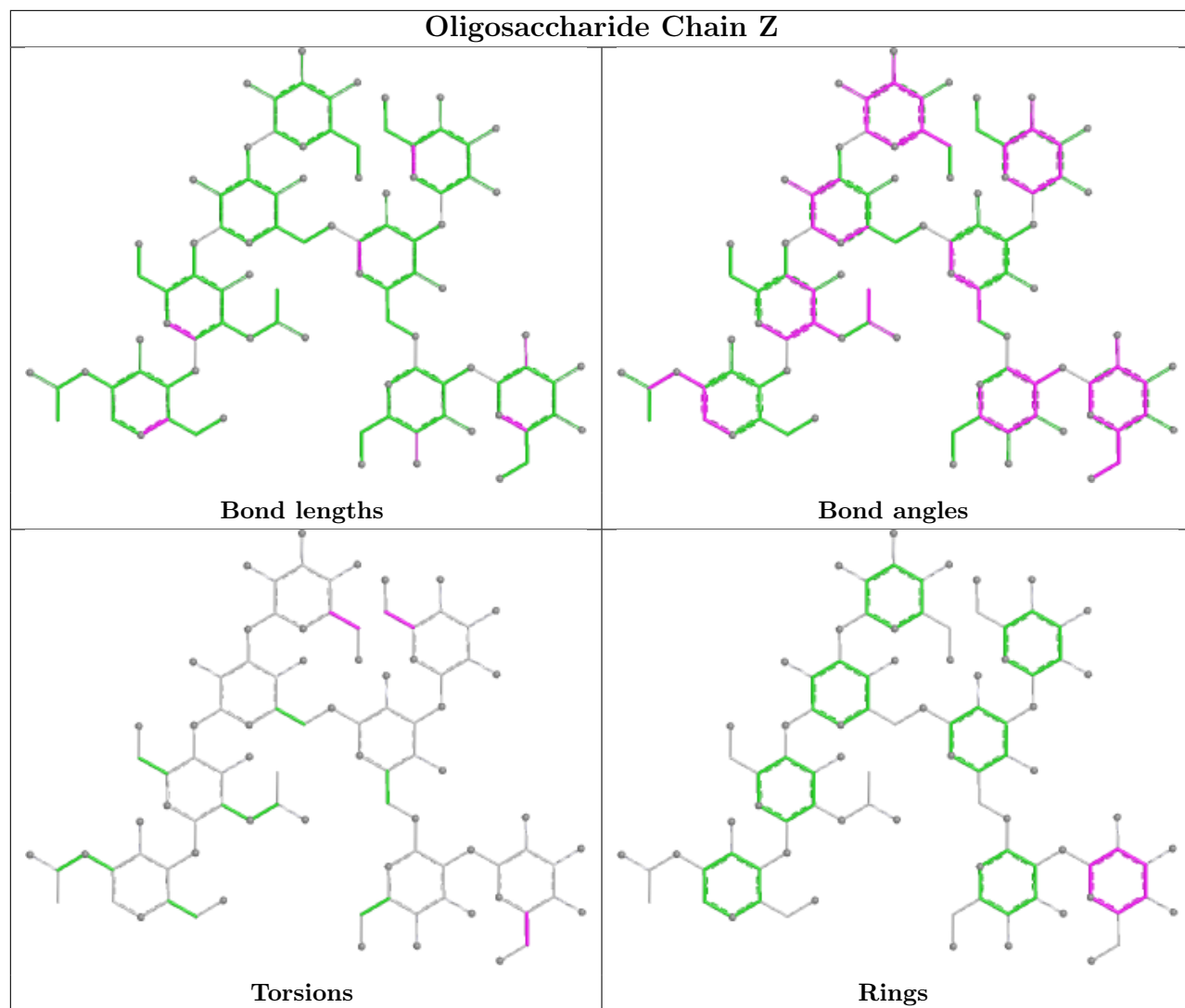


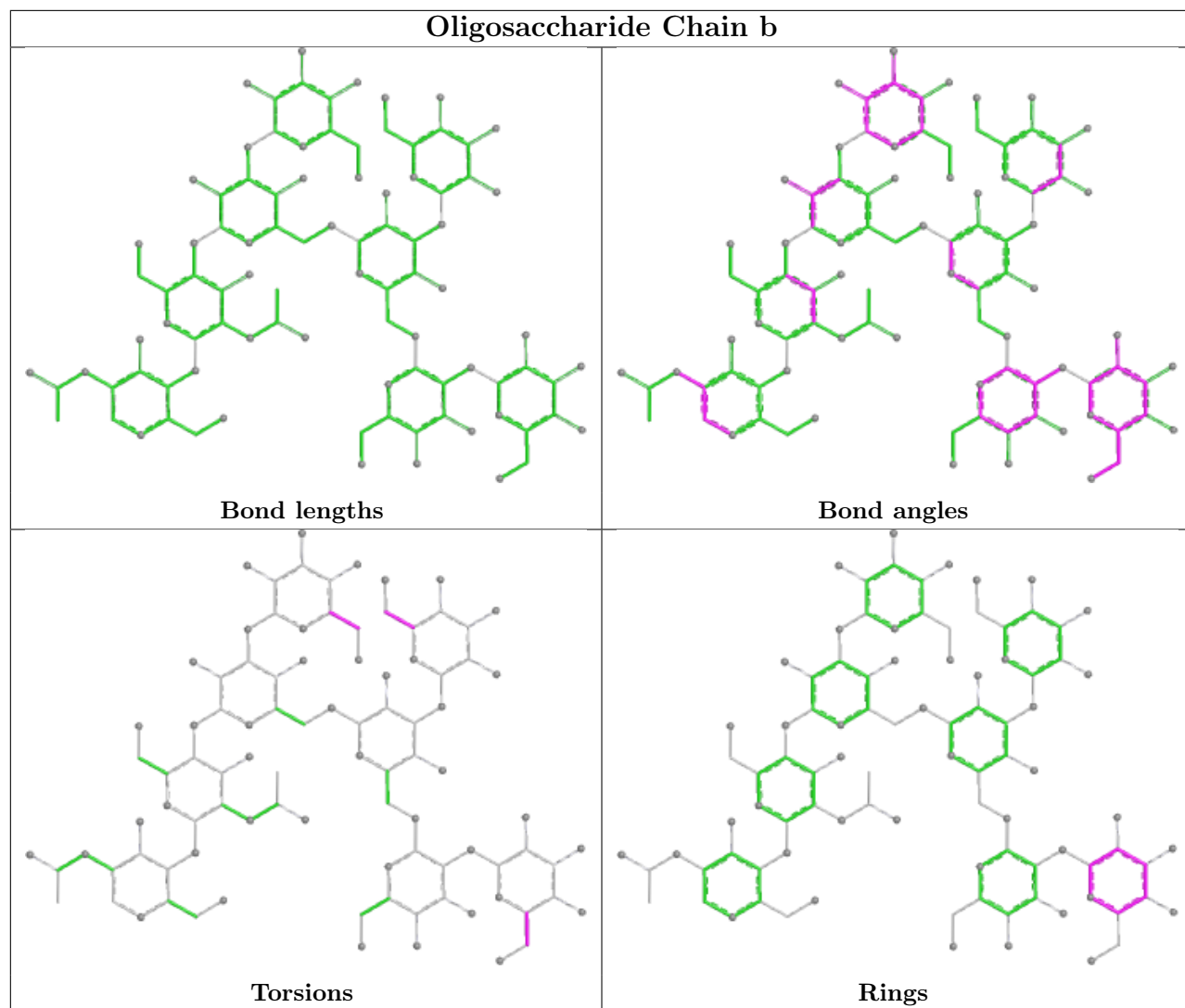


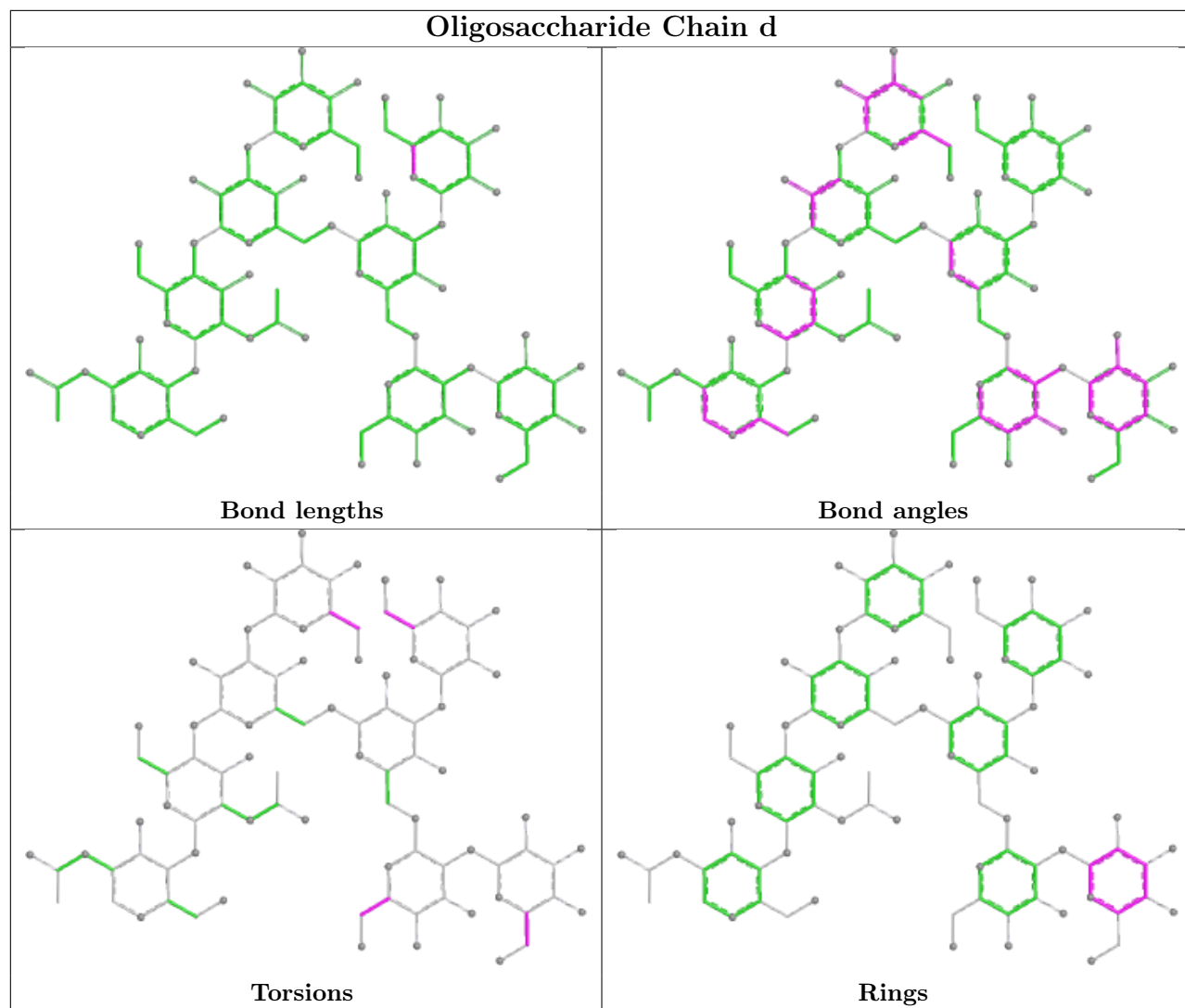
Oligosaccharide Chain V

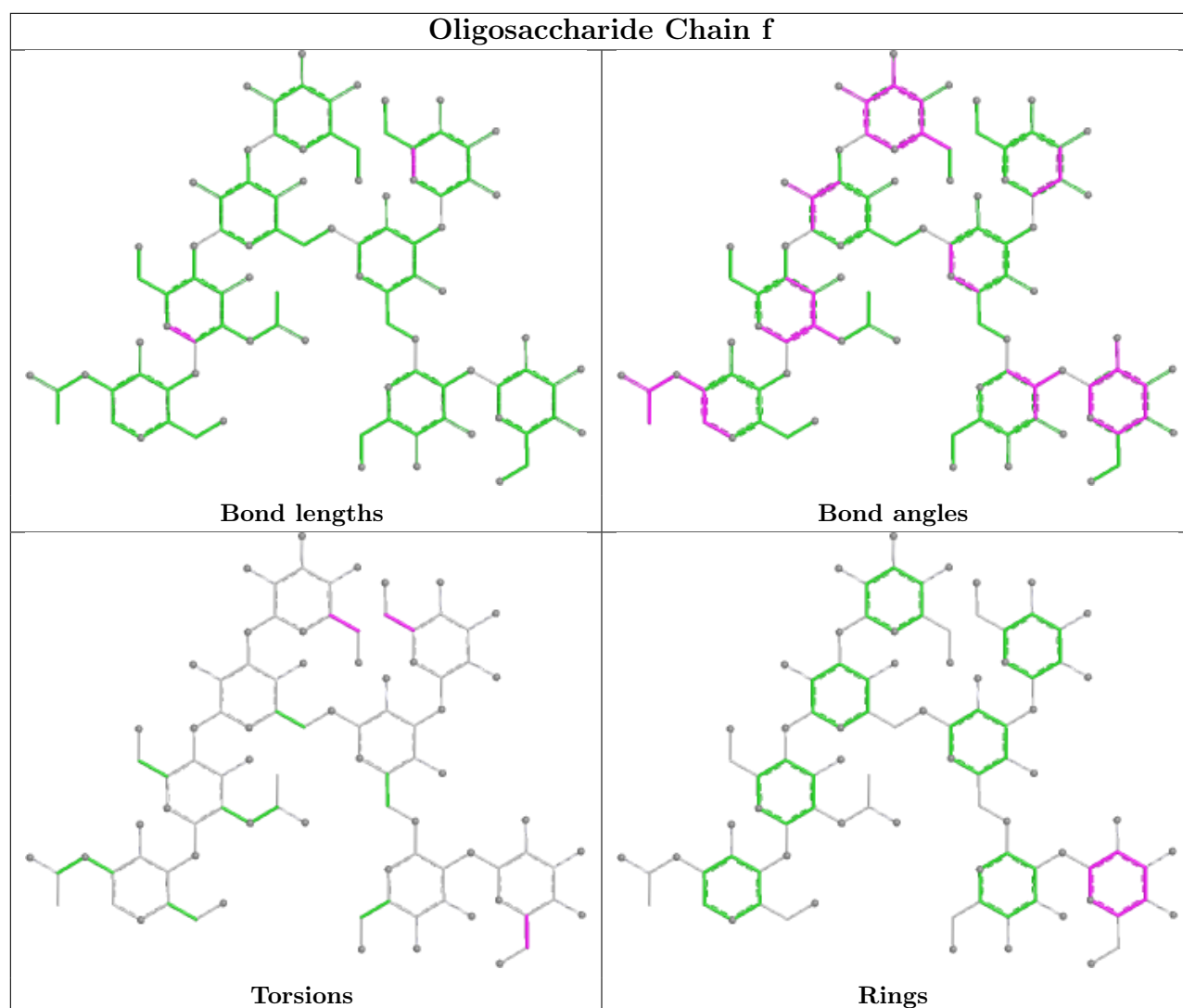












5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
5	PGT	D	201	-	30,30,50	1.03	3 (10%)	31,31,56	1.12	4 (12%)
5	PGT	P	201	-	30,30,50	1.08	3 (10%)	31,31,56	1.17	4 (12%)
5	PGT	L	201	-	30,30,50	1.11	3 (10%)	31,31,56	1.05	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PGT	H	201	-	30,30,50	1.13	2 (6%)	31,31,56	1.17	3 (9%)

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
5	PGT	D	201	-	-	17/30/30/55	-
5	PGT	P	201	-	-	17/30/30/55	-
5	PGT	L	201	-	-	16/30/30/55	-
5	PGT	H	201	-	-	17/30/30/55	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	201	PGT	C32-C31	2.29	1.57	1.50
5	H	201	PGT	O3-C11	2.28	1.40	1.33
5	P	201	PGT	O3-C11	2.26	1.39	1.33
5	H	201	PGT	C32-C31	2.24	1.57	1.50
5	P	201	PGT	C32-C31	2.20	1.57	1.50

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	201	PGT	O3-C11-C12	3.27	121.79	111.83
5	D	201	PGT	O2-C31-C32	3.12	121.36	111.83
5	P	201	PGT	O2-C31-C32	3.09	121.25	111.83
5	H	201	PGT	O2-C31-C32	3.02	121.06	111.83
5	P	201	PGT	O3-C11-C12	2.98	120.93	111.83

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

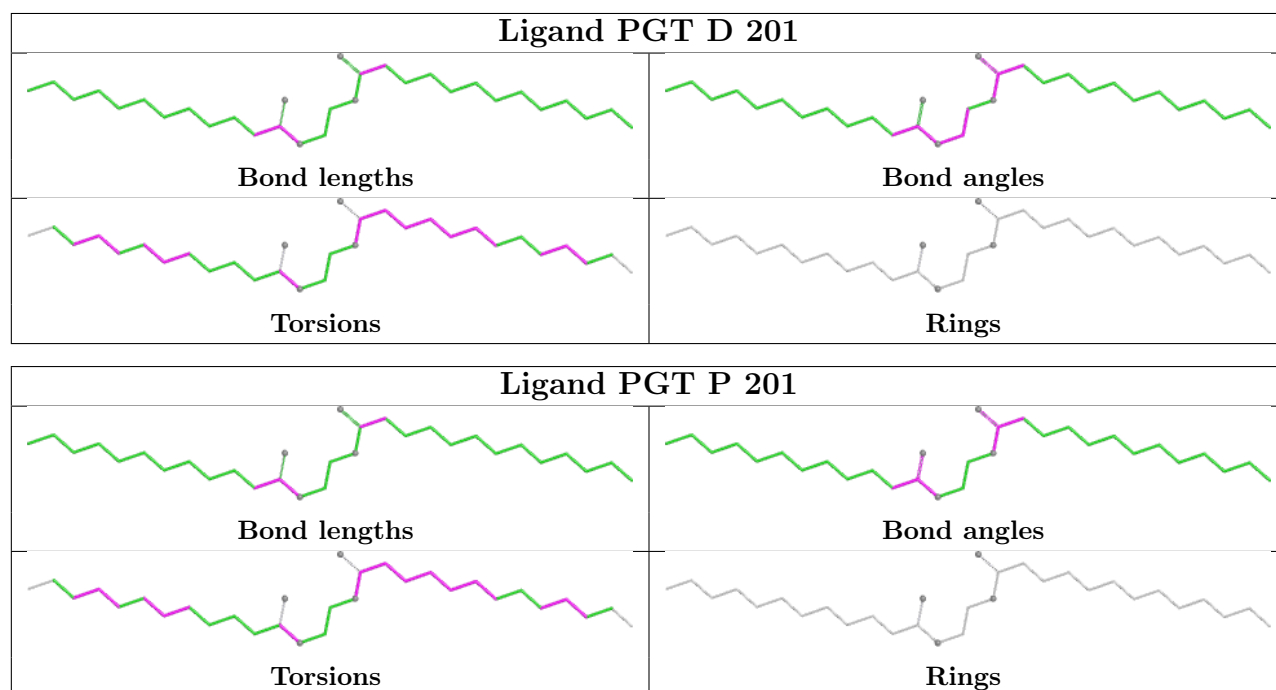
Mol	Chain	Res	Type	Atoms
5	D	201	PGT	C12-C11-O3-C3
5	H	201	PGT	C12-C11-O3-C3
5	H	201	PGT	O11-C11-O3-C3
5	P	201	PGT	O11-C11-O3-C3
5	D	201	PGT	O11-C11-O3-C3

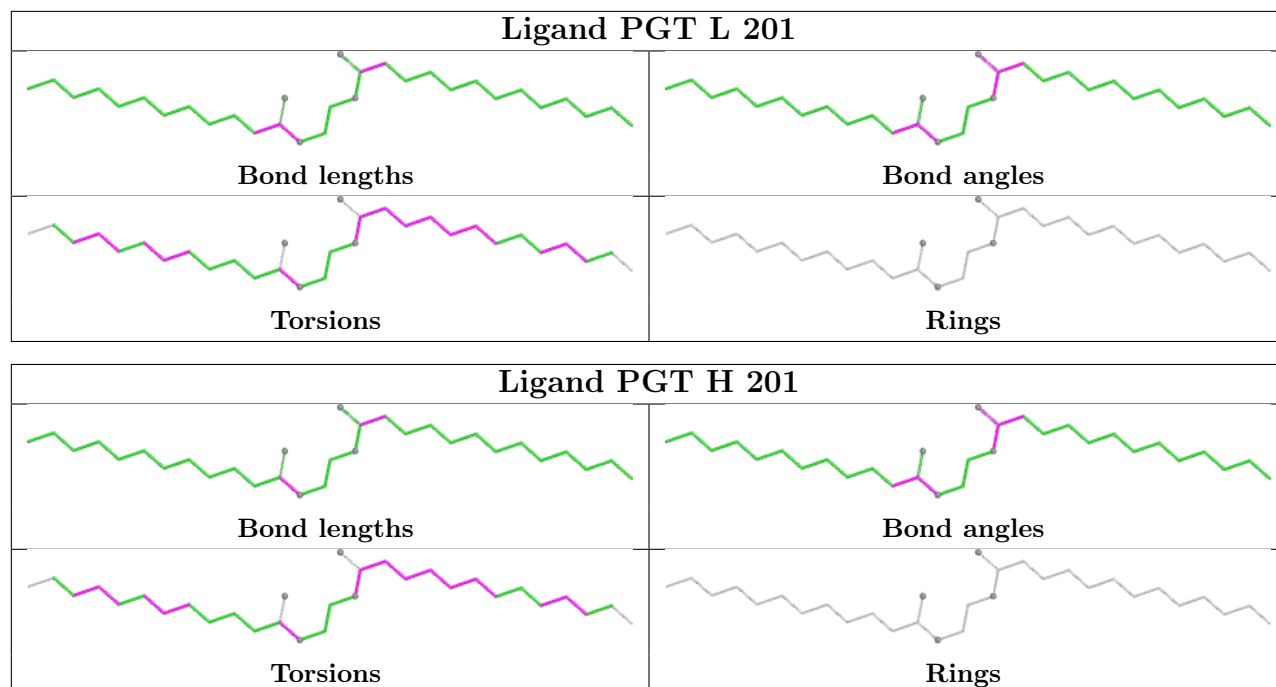
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	201	PGT	1	0
5	P	201	PGT	1	0
5	L	201	PGT	1	0
5	H	201	PGT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	594/612 (97%)	0.09	9 (1%) 72 64	47, 67, 96, 120	0
1	B	599/612 (97%)	-0.09	4 (0%) 84 79	41, 59, 76, 85	0
1	E	592/612 (96%)	0.39	26 (4%) 39 30	55, 94, 128, 161	0
1	F	599/612 (97%)	0.17	4 (0%) 84 79	57, 85, 118, 134	0
1	I	397/612 (64%)	0.46	20 (5%) 34 27	55, 94, 136, 151	0
1	J	599/612 (97%)	0.28	11 (1%) 67 59	65, 89, 114, 127	0
1	M	593/612 (96%)	0.10	9 (1%) 72 64	47, 71, 98, 124	0
1	N	599/612 (97%)	-0.05	7 (1%) 76 69	46, 63, 88, 104	0
2	C	138/147 (93%)	-0.02	3 (2%) 62 53	46, 61, 98, 108	0
2	D	136/147 (92%)	-0.01	5 (3%) 45 36	43, 59, 108, 125	0
2	G	138/147 (93%)	0.04	2 (1%) 73 65	54, 72, 104, 112	0
2	H	138/147 (93%)	-0.07	4 (2%) 53 44	54, 65, 82, 86	0
2	K	136/147 (92%)	0.32	4 (2%) 53 44	59, 84, 139, 159	0
2	L	138/147 (93%)	0.04	5 (3%) 46 37	57, 68, 85, 93	0
2	O	138/147 (93%)	-0.07	3 (2%) 62 53	45, 59, 100, 117	0
2	P	135/147 (91%)	0.06	5 (3%) 45 36	45, 64, 112, 131	0
All	All	5669/6072 (93%)	0.13	121 (2%) 63 54	41, 74, 116, 161	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	453	SER	6.2
1	B	319	GLY	5.9
2	G	34	ASN	4.5
2	L	54	GLN	4.3
2	G	158	TYR	4.1

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	U	3	11/12	0.59	0.12	51,54,56,58	0
3	BMA	S	3	11/12	0.72	0.13	51,54,56,58	0
4	MAN	R	8	11/12	0.75	0.09	51,51,54,55	0
4	BMA	T	3	11/12	0.75	0.12	46,47,48,49	0
4	MAN	V	8	11/12	0.75	0.10	51,51,54,55	0
4	MAN	T	8	11/12	0.76	0.10	51,51,54,55	0
4	MAN	V	6	11/12	0.77	0.11	47,48,53,56	0
3	BMA	W	3	11/12	0.77	0.10	52,54,56,58	0
3	BMA	Q	3	11/12	0.78	0.09	51,54,56,58	0
4	NAG	T	2	14/15	0.78	0.14	47,48,50,51	0
4	MAN	R	7	11/12	0.79	0.10	47,49,50,52	0
4	BMA	V	3	11/12	0.79	0.11	46,47,48,49	0
4	MAN	X	8	11/12	0.79	0.09	51,51,54,55	0
3	NAG	U	1	14/15	0.80	0.12	44,46,50,51	0
3	BMA	Y	3	11/12	0.80	0.10	51,54,56,58	0
3	NAG	a	1	14/15	-	-	44,46,50,51	0
3	NAG	a	2	14/15	-	-	47,50,52,56	0
3	BMA	a	3	11/12	-	-	51,54,56,58	0
3	NAG	c	1	14/15	-	-	43,46,49,51	0
3	NAG	c	2	14/15	-	-	47,50,52,56	0
3	BMA	c	3	11/12	-	-	51,54,56,58	0
3	NAG	e	1	14/15	-	-	43,46,49,51	0
3	NAG	e	2	14/15	-	-	47,49,52,56	0
3	BMA	e	3	11/12	-	-	51,54,56,57	0
4	MAN	V	7	11/12	0.80	0.09	47,49,50,52	0
4	NAG	T	1	14/15	0.80	0.12	45,48,51,52	0
4	NAG	V	2	14/15	0.80	0.13	46,48,50,50	0
3	NAG	S	2	14/15	0.81	0.11	47,50,53,56	0
4	MAN	Z	7	11/12	0.81	0.11	47,49,49,52	0
3	NAG	U	2	14/15	0.82	0.10	48,50,52,56	0
4	MAN	X	6	11/12	0.83	0.12	47,48,53,56	0
4	MAN	T	6	11/12	0.83	0.12	47,48,53,56	0

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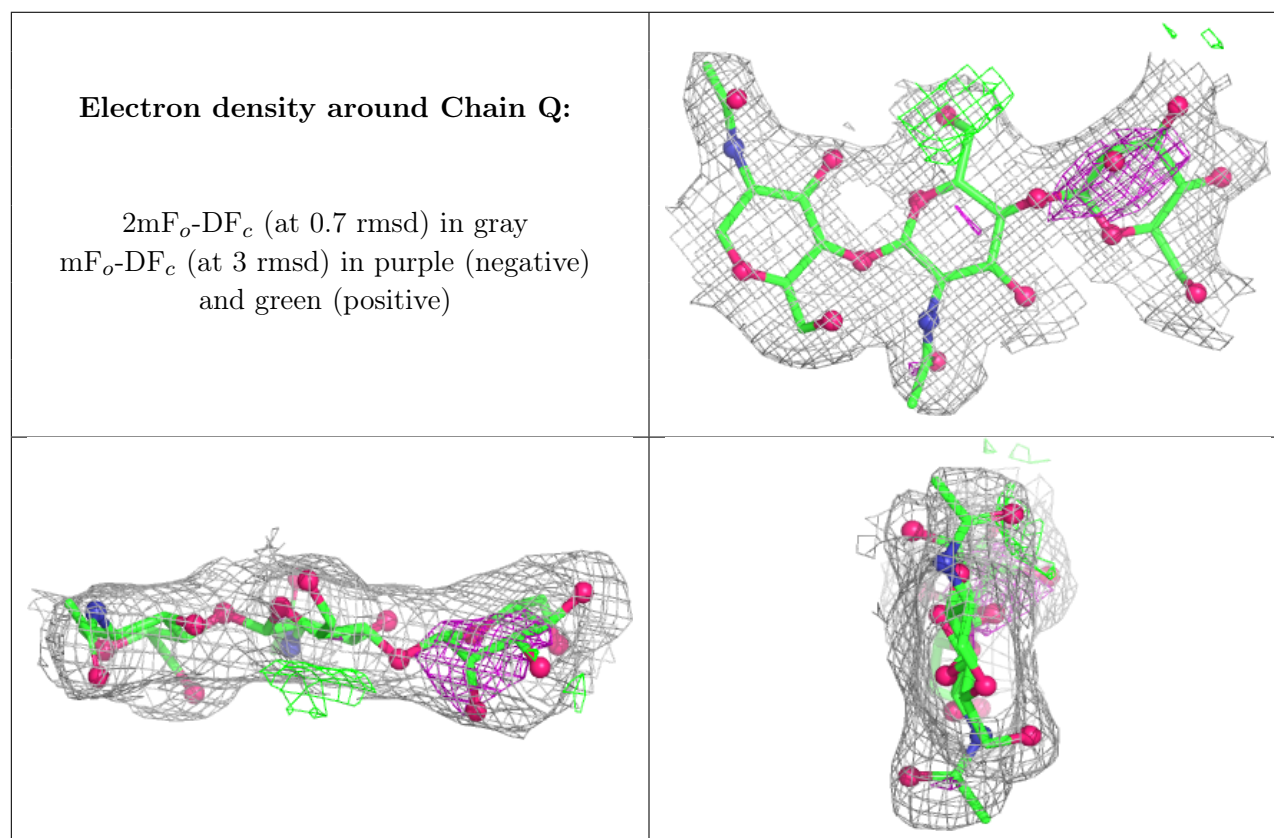
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	X	2	14/15	0.83	0.11	46,48,50,51	0
4	MAN	Z	8	11/12	0.83	0.12	51,51,54,55	0
4	MAN	X	7	11/12	0.84	0.09	47,49,49,52	0
4	NAG	V	1	14/15	0.84	0.12	45,48,51,52	0
4	MAN	R	6	11/12	0.85	0.12	47,48,53,56	0
4	MAN	T	4	11/12	0.86	0.09	46,47,48,49	0
3	NAG	S	1	14/15	0.86	0.10	44,46,50,51	0
4	MAN	T	7	11/12	0.86	0.08	47,49,50,52	0
3	NAG	Q	2	14/15	0.86	0.08	47,50,52,56	0
4	MAN	T	5	11/12	0.87	0.10	47,47,48,50	0
3	NAG	Y	2	14/15	0.89	0.09	47,49,52,56	0
4	NAG	Z	2	14/15	0.89	0.14	46,48,50,50	0
3	NAG	W	2	14/15	0.89	0.08	47,50,52,56	0
4	MAN	V	4	11/12	0.89	0.09	46,47,48,49	0
4	MAN	Z	6	11/12	0.90	0.12	46,48,53,56	0
4	NAG	R	2	14/15	0.90	0.08	47,48,50,50	0
4	MAN	V	5	11/12	0.90	0.10	46,47,49,50	0
4	MAN	R	4	11/12	0.91	0.08	46,47,48,49	0
4	NAG	X	1	14/15	0.91	0.08	45,48,51,52	0
4	BMA	Z	3	11/12	0.91	0.10	46,46,47,49	0
4	MAN	Z	4	11/12	0.91	0.09	46,46,48,48	0
4	MAN	R	5	11/12	0.91	0.07	46,47,48,49	0
3	NAG	W	1	14/15	0.91	0.10	44,46,49,51	0
3	NAG	Q	1	14/15	0.91	0.09	44,46,50,51	0
4	BMA	X	3	11/12	0.92	0.06	46,47,47,49	0
4	NAG	R	1	14/15	0.92	0.09	45,47,51,52	0
4	MAN	X	4	11/12	0.93	0.07	46,47,48,49	0
4	BMA	R	3	11/12	0.93	0.07	46,47,48,49	0
3	NAG	Y	1	14/15	0.94	0.08	43,46,49,51	0
4	MAN	X	5	11/12	0.94	0.06	46,47,48,49	0
4	MAN	Z	5	11/12	0.94	0.09	46,47,48,49	0
4	NAG	Z	1	14/15	0.95	0.09	45,47,51,52	0
4	NAG	b	1	14/15	-	-	45,48,51,52	0
4	NAG	b	2	14/15	-	-	47,48,50,50	0
4	BMA	b	3	11/12	-	-	46,47,48,49	0
4	MAN	b	4	11/12	-	-	46,47,48,49	0
4	MAN	b	5	11/12	-	-	46,47,48,49	0
4	MAN	b	6	11/12	-	-	47,48,53,56	0
4	MAN	b	7	11/12	-	-	47,49,49,52	0
4	MAN	b	8	11/12	-	-	51,51,54,55	0
4	NAG	d	1	14/15	-	-	45,48,51,52	0
4	NAG	d	2	14/15	-	-	47,48,50,50	0

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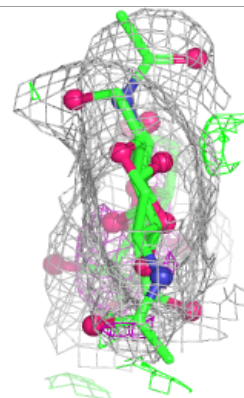
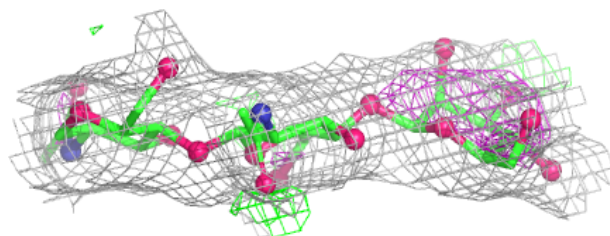
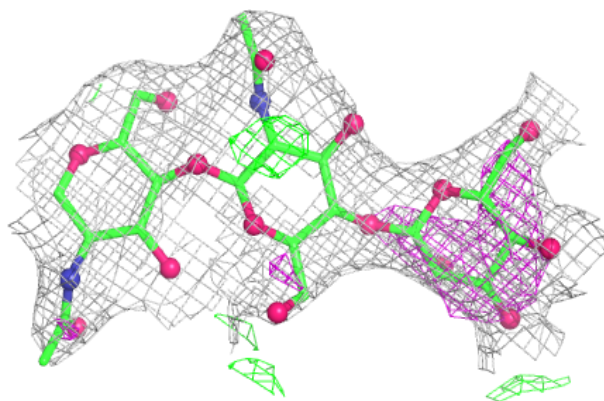
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	d	3	11/12	-	-	46,47,48,49	0
4	MAN	d	4	11/12	-	-	46,47,48,48	0
4	MAN	d	5	11/12	-	-	46,47,49,49	0
4	MAN	d	6	11/12	-	-	47,48,53,56	0
4	MAN	d	7	11/12	-	-	47,49,49,53	0
4	MAN	d	8	11/12	-	-	51,51,54,55	0
4	NAG	f	1	14/15	-	-	45,47,51,52	0
4	NAG	f	2	14/15	-	-	46,47,50,50	0
4	BMA	f	3	11/12	-	-	46,46,47,49	0
4	MAN	f	4	11/12	-	-	46,47,48,48	0
4	MAN	f	5	11/12	-	-	46,47,48,49	0
4	MAN	f	6	11/12	-	-	47,48,53,56	0
4	MAN	f	7	11/12	-	-	47,49,49,52	0
4	MAN	f	8	11/12	-	-	51,51,54,55	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.

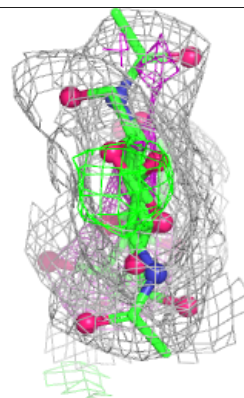
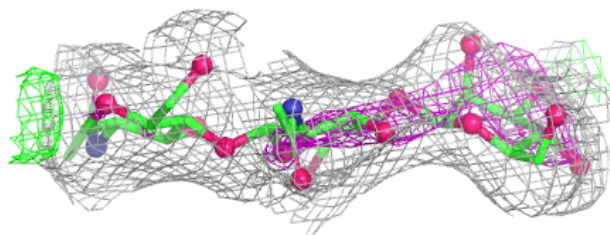
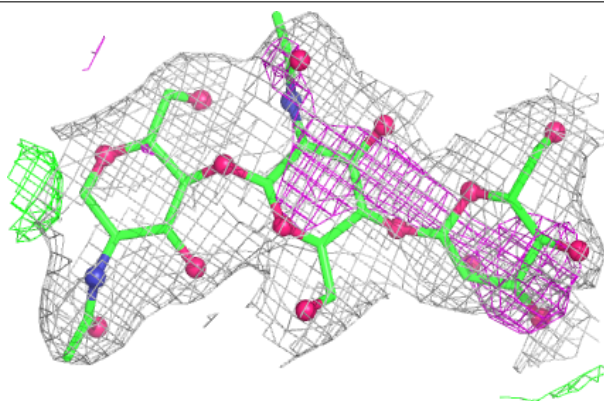


Electron density around Chain S:

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

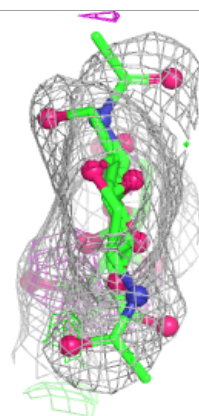
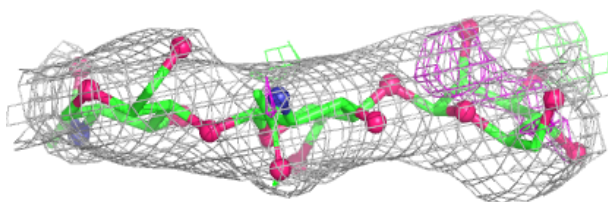
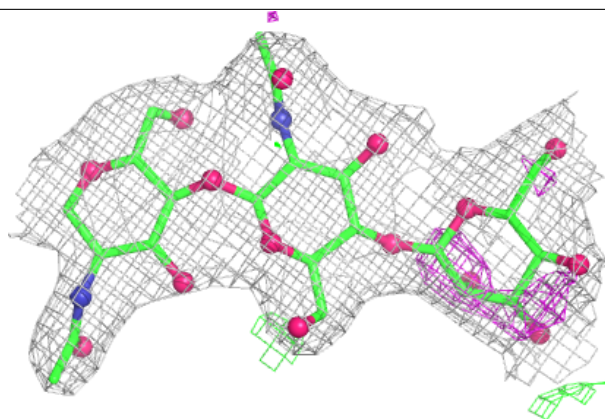
**Electron density around Chain U:**

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

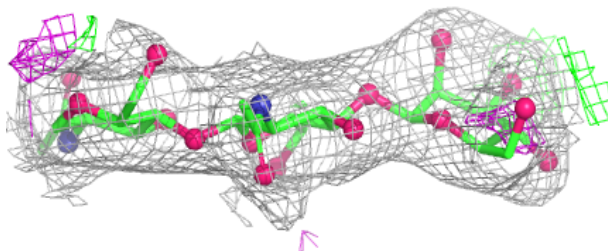
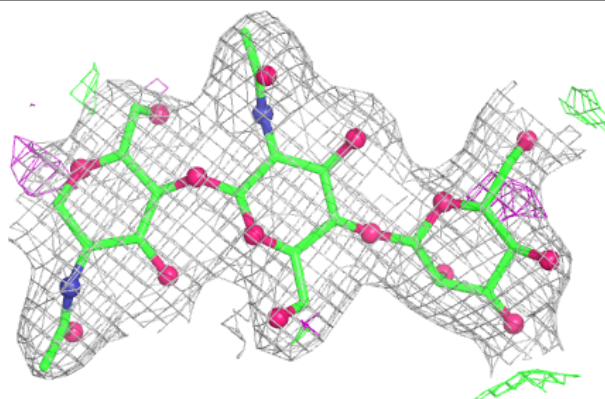


Electron density around Chain W:

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

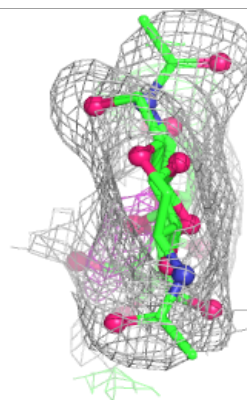
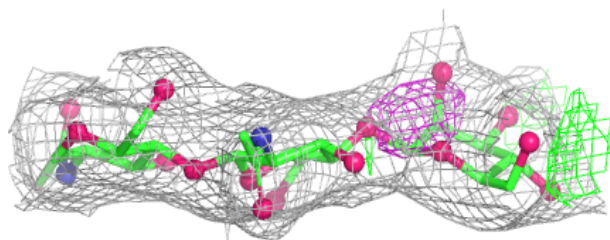
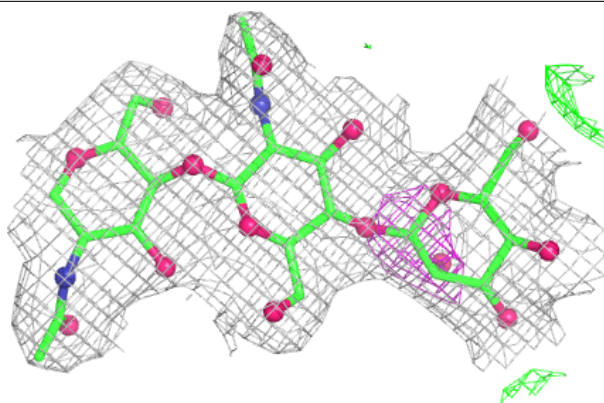
**Electron density around Chain Y:**

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

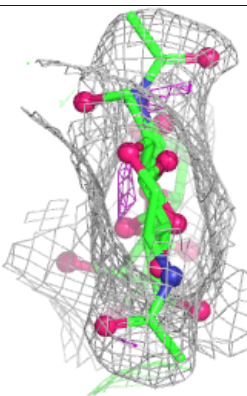
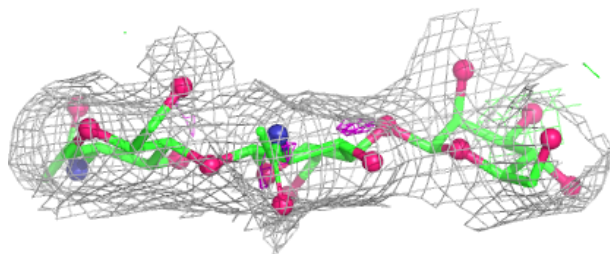
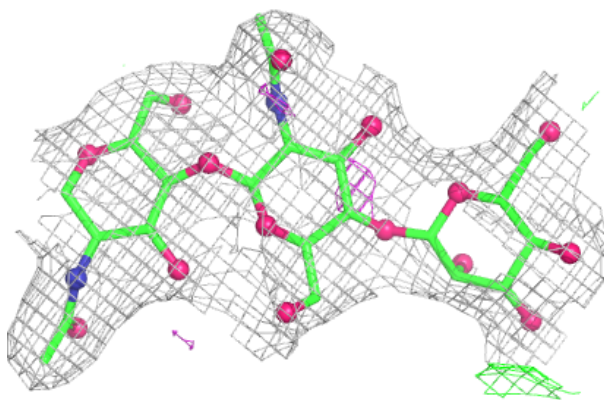


Electron density around Chain a:

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

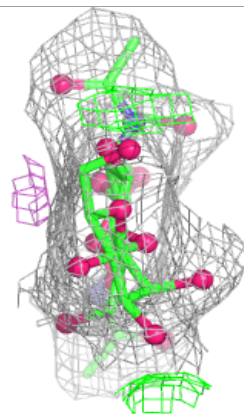
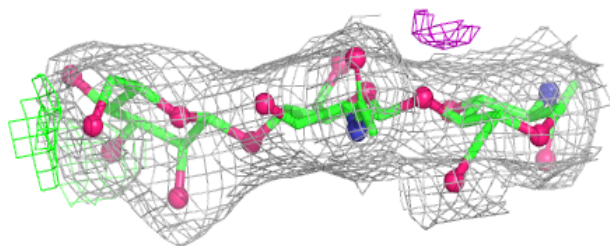
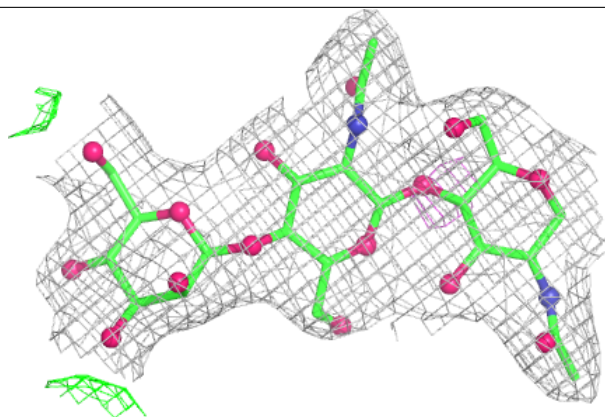
**Electron density around Chain c:**

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



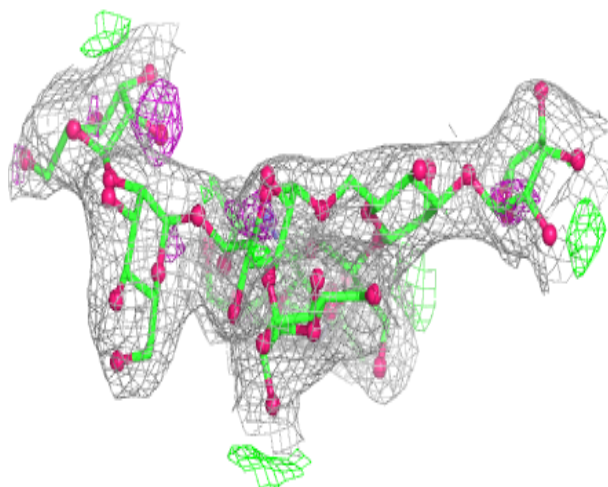
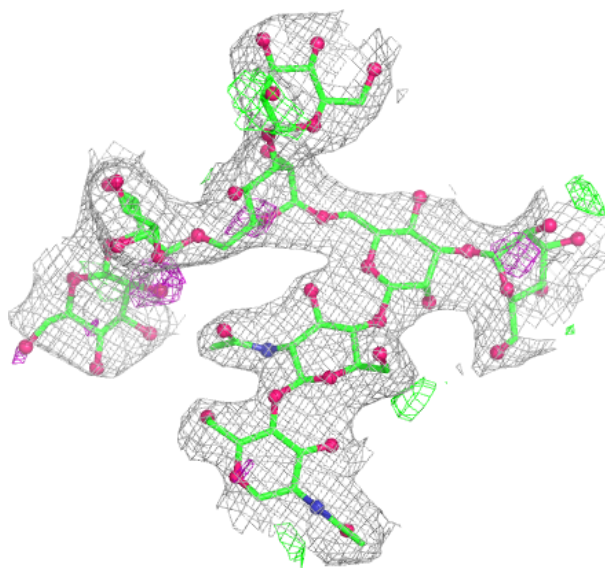
Electron density around Chain e:

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



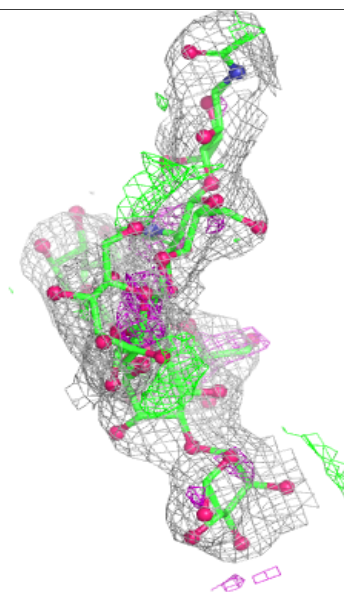
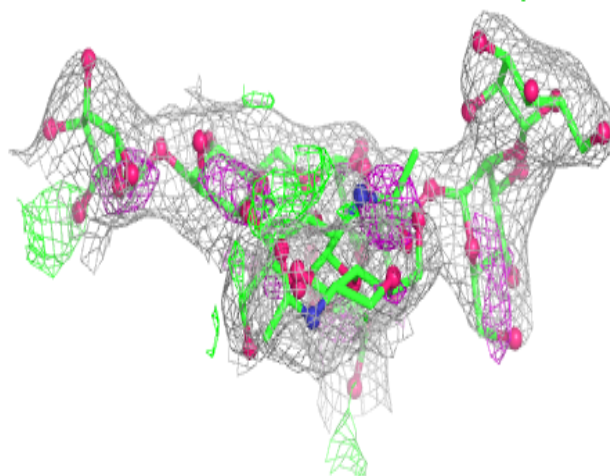
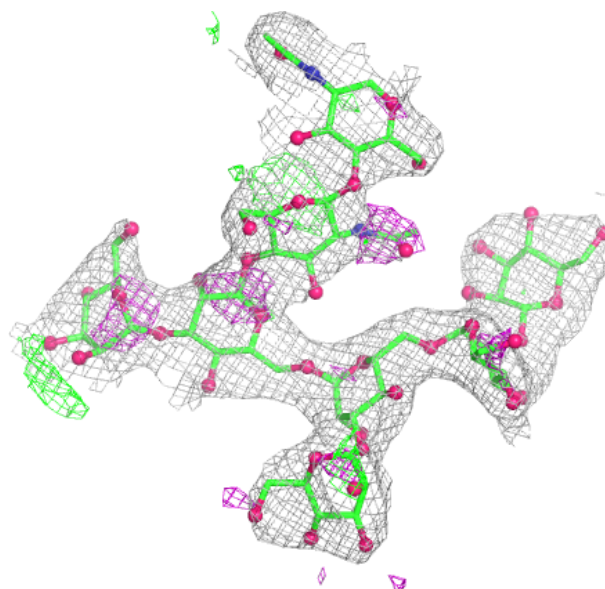
Electron density around Chain R:

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



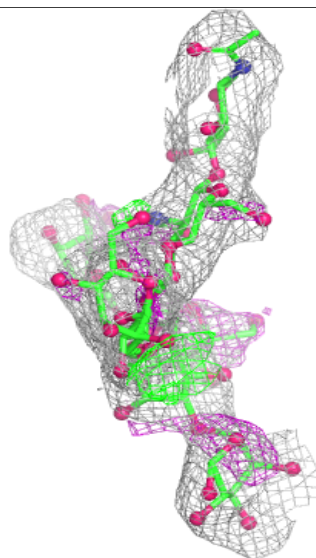
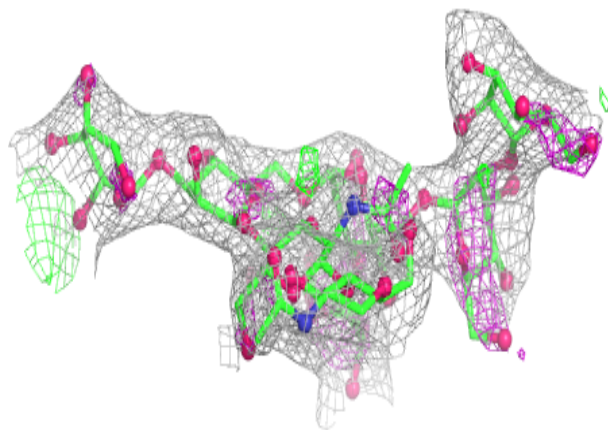
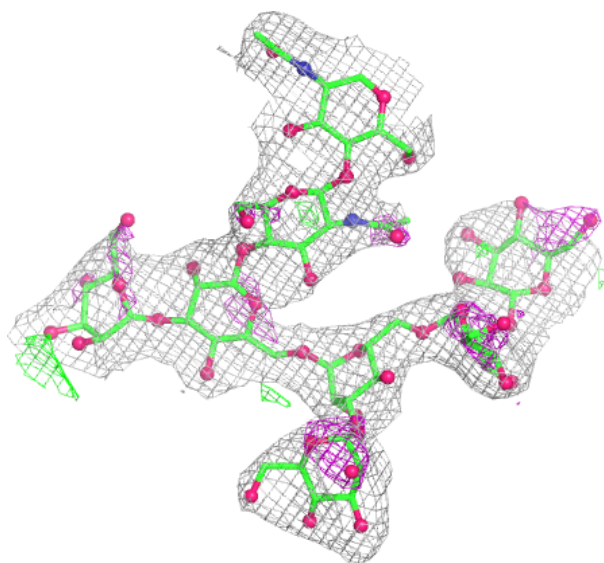
Electron density around Chain T:

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



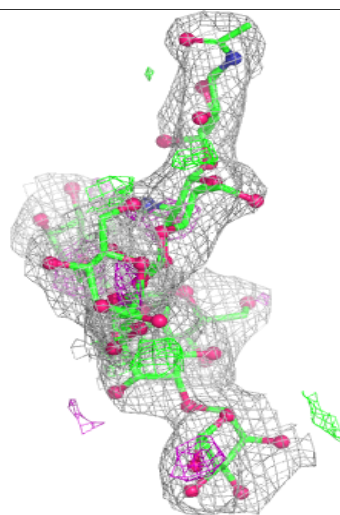
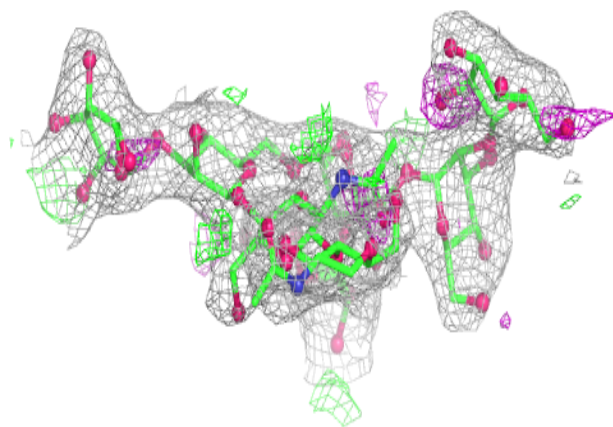
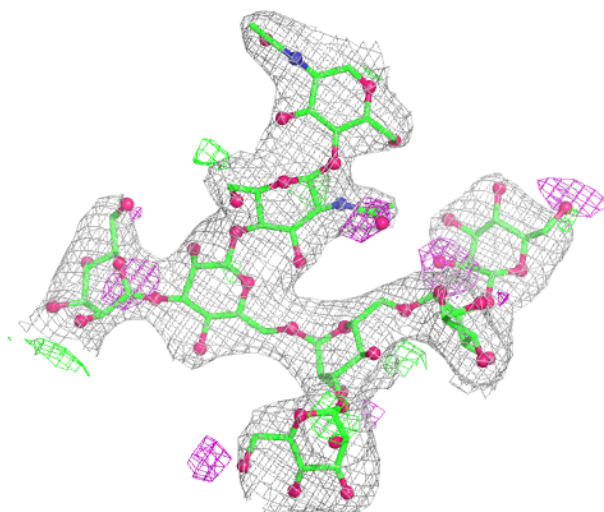
Electron density around Chain V:

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



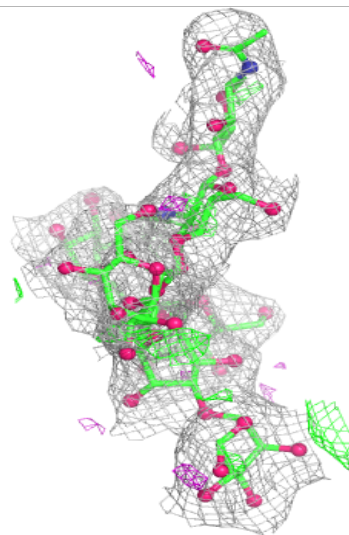
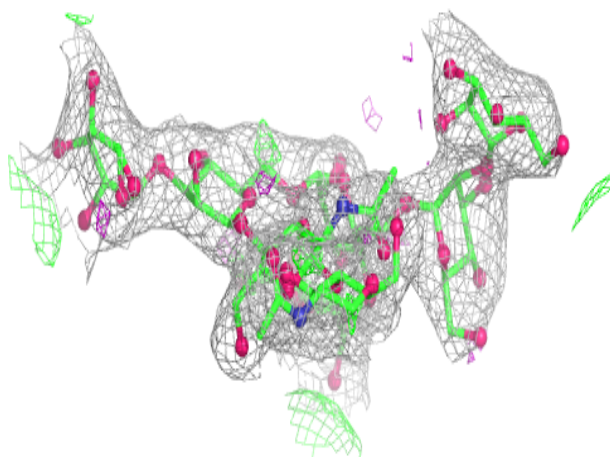
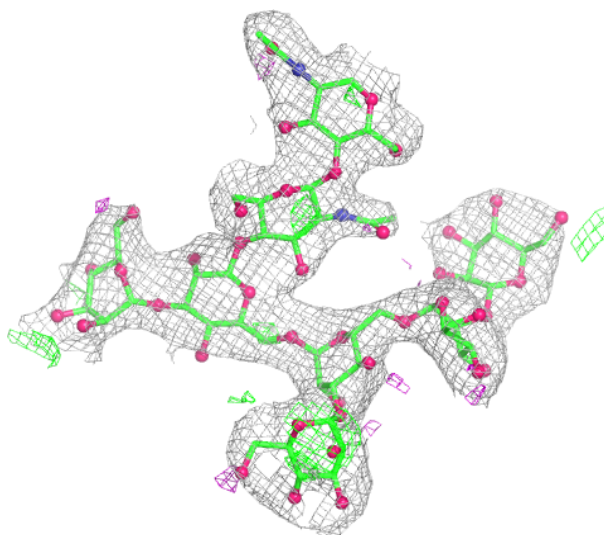
Electron density around Chain X:

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



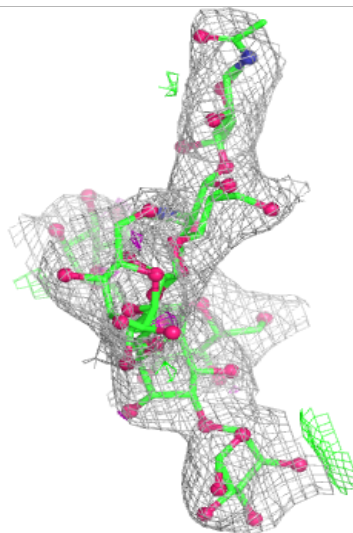
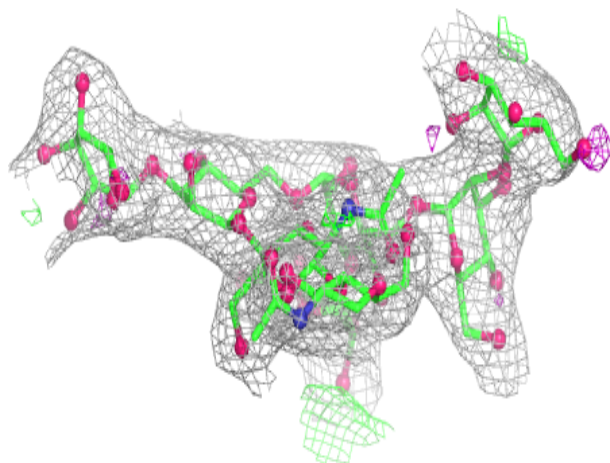
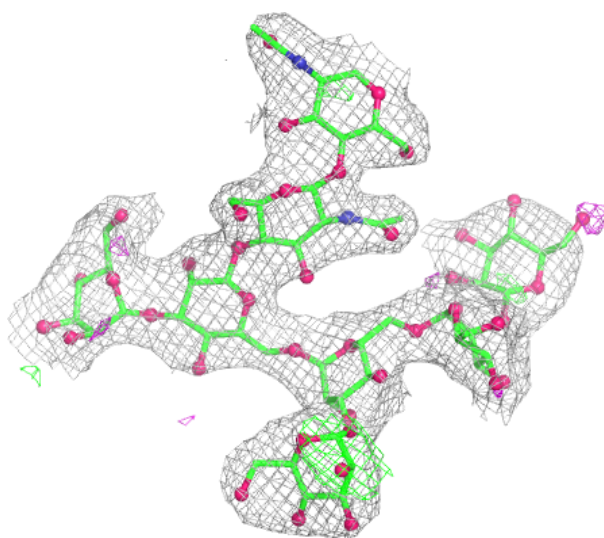
Electron density around Chain Z:

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



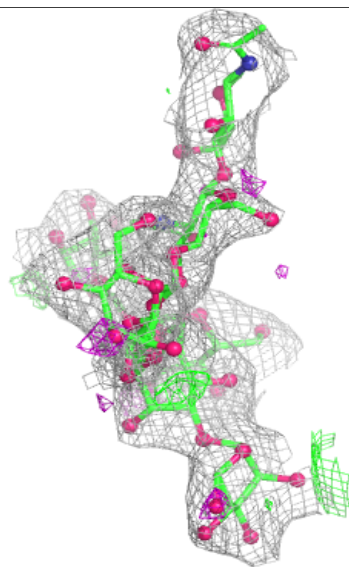
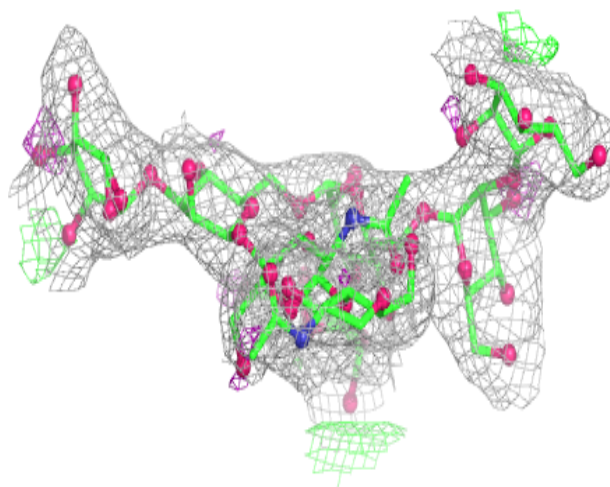
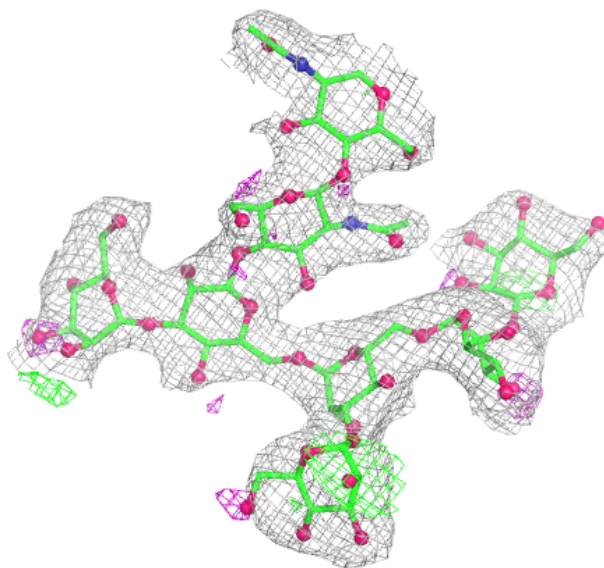
Electron density around Chain b:

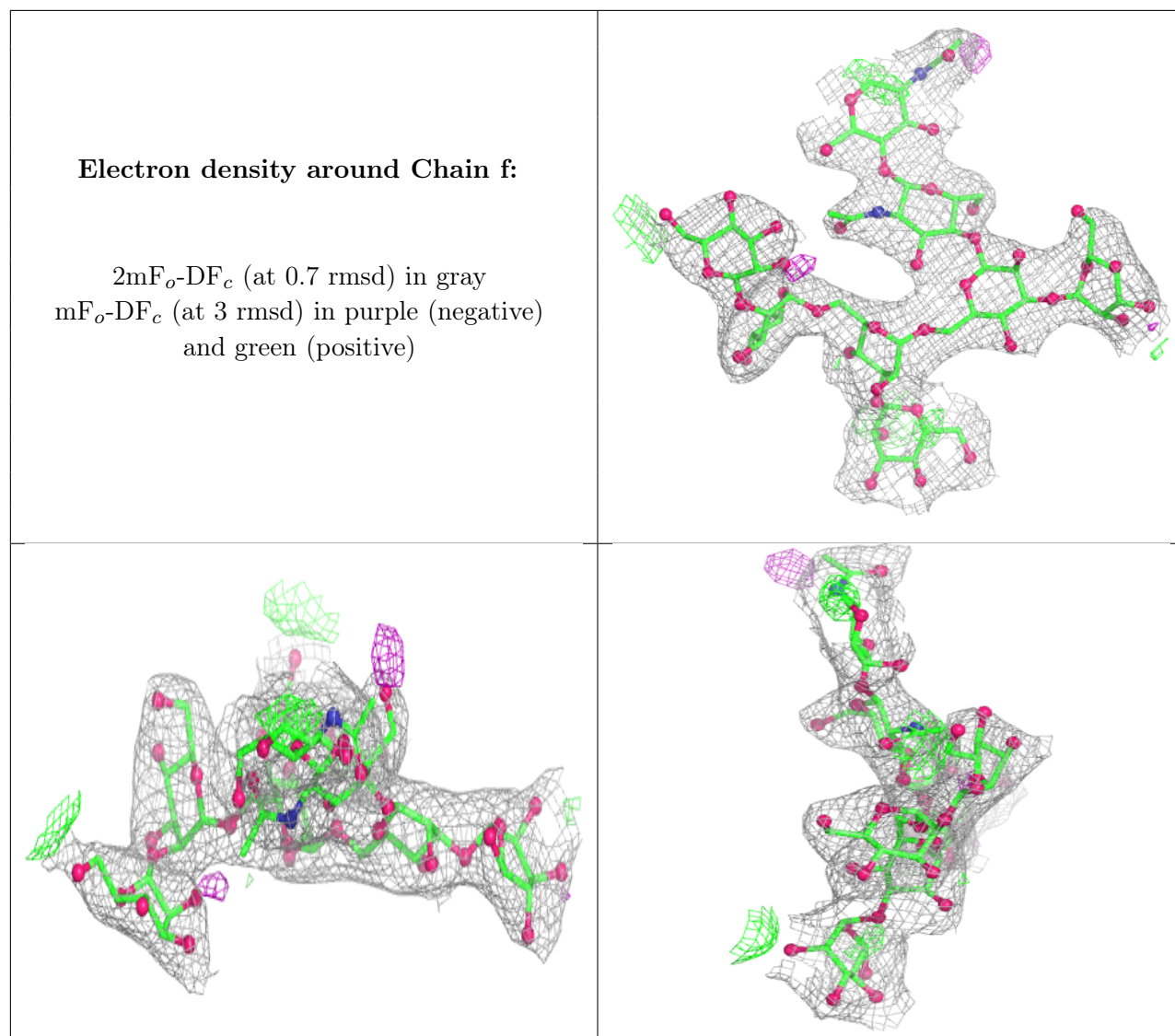
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain d:

$2mF_o-DF_c$ (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.

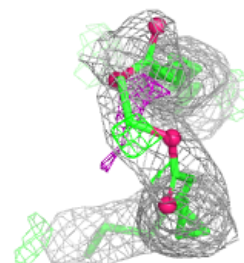
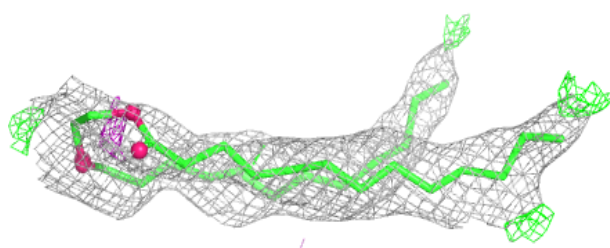
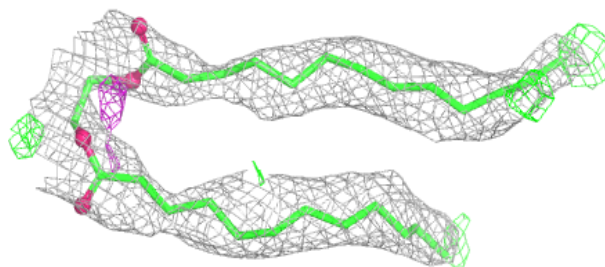
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PGT	H	201	31/51	0.71	0.20	71,79,92,93	0
5	PGT	L	201	31/51	0.72	0.23	71,78,92,93	0
5	PGT	P	201	31/51	0.77	0.16	71,78,92,93	0
5	PGT	D	201	31/51	0.79	0.18	71,78,92,93	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

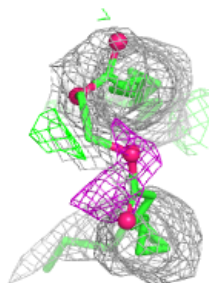
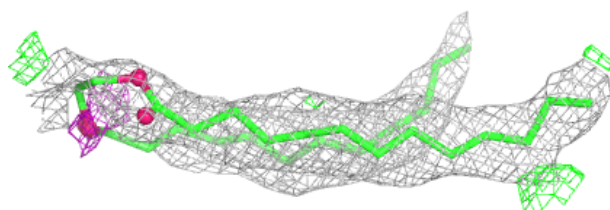
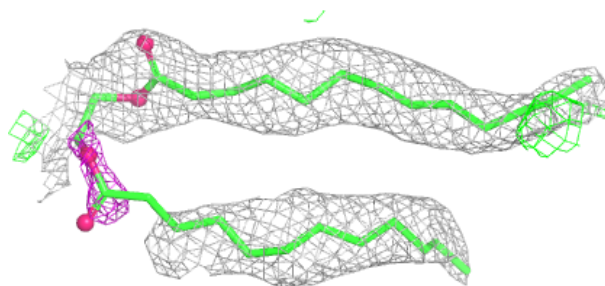
Electron density around PGT H 201:

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



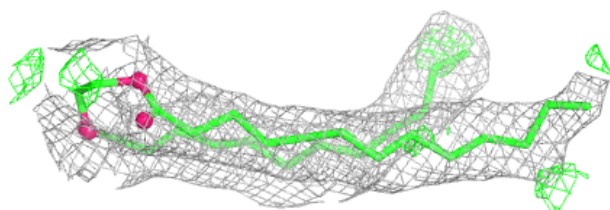
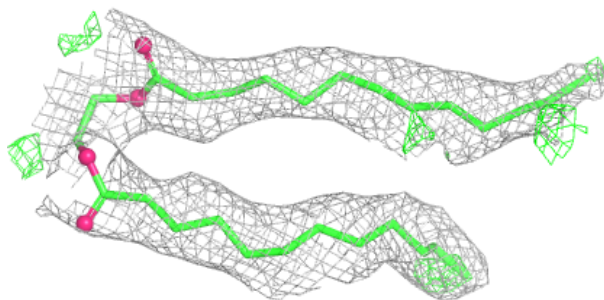
Electron density around PGT L 201:

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

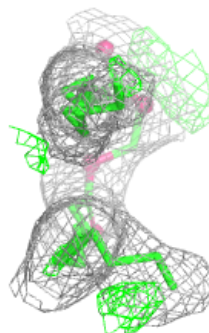
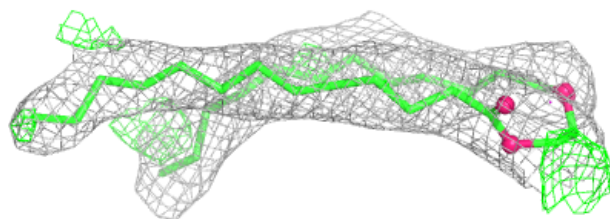
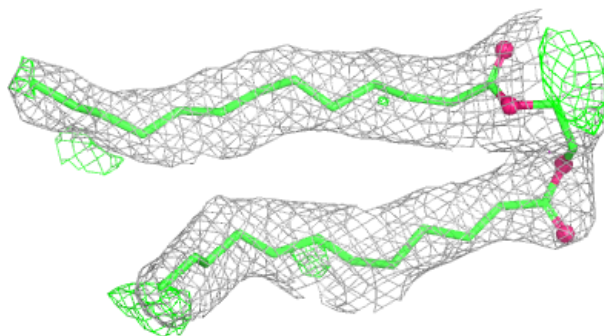


Electron density around PGT P 201:

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

**Electron density around PGT D 201:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.