wwPDB X-ray Structure Validation Summary Report (i)

Nov 12, 2024 – 04:50 PM EST

PDB ID	:	3RG1
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 (i) 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 (i)) were used in the production of this report:

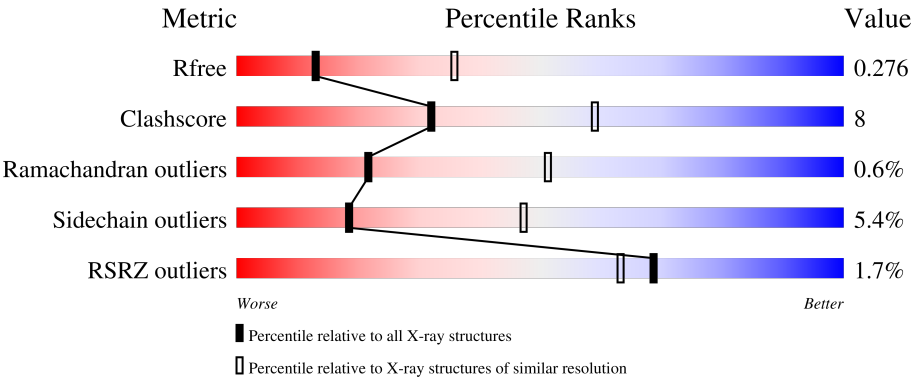
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.91 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}	164625	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (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 <=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	3% 78% 17%
1	F	612	79% 17%
1	I	612	2% 55% 9% 35%

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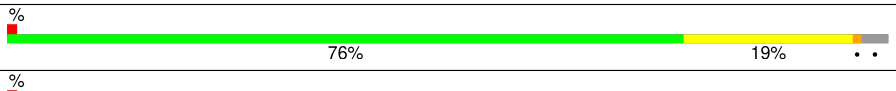
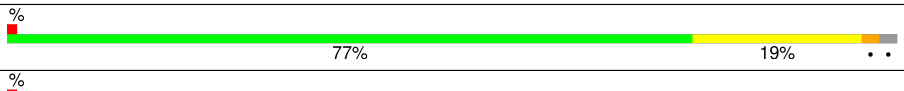
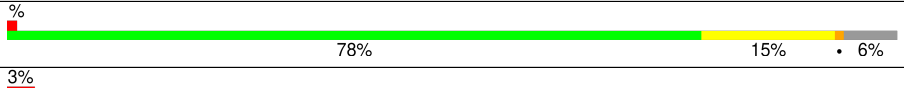
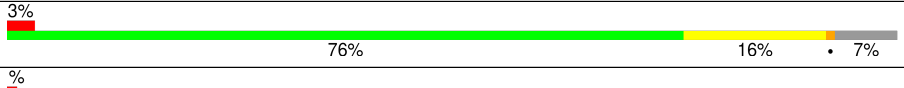
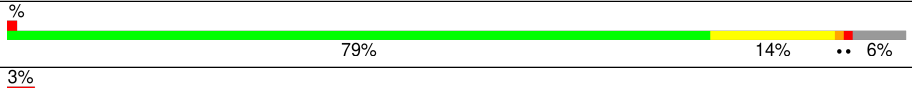
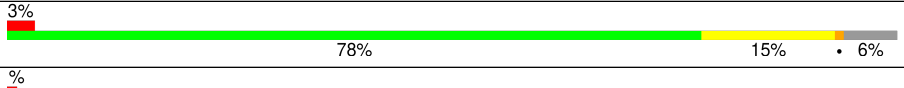
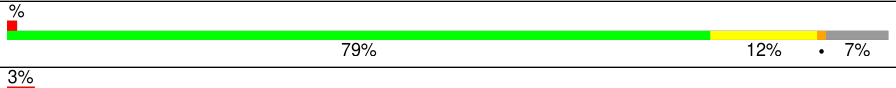
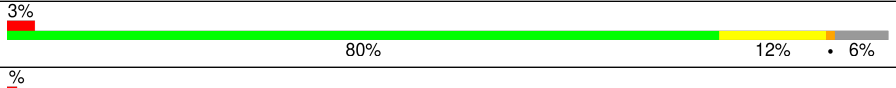
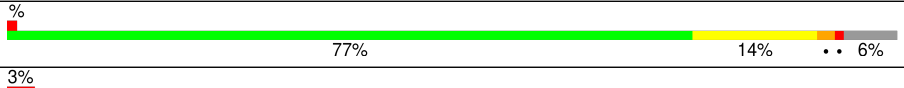
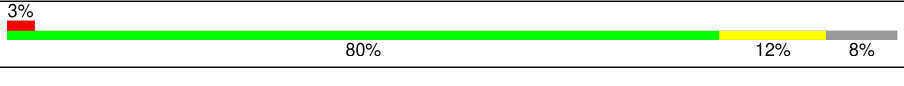
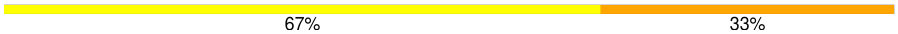
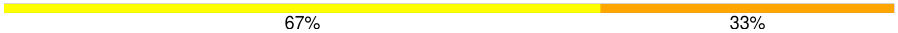
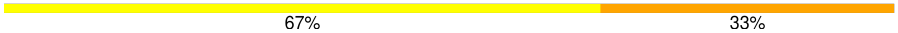
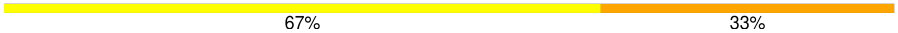
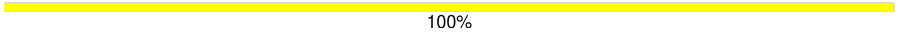
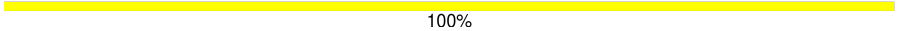
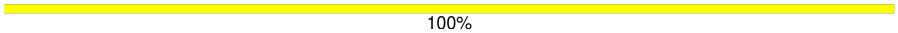
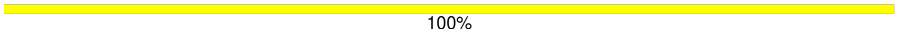
Mol	Chain	Length	Quality of chain
1	J	612	
1	M	612	
1	N	612	
2	C	147	
2	D	147	
2	G	147	
2	H	147	
2	K	147	
2	L	147	
2	O	147	
2	P	147	
3	Q	3	
3	S	3	
3	U	3	
3	W	3	
3	Y	3	
3	a	3	
3	c	3	
3	e	3	
4	R	8	
4	T	8	
4	V	8	
4	X	8	
4	Z	8	
4	b	8	

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Mol	Chain	Length	Quality of chain
4	d	8	100%
4	f	8	100%

2 Entry composition (i)

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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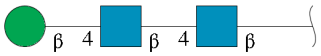
Chain	Residue	Modelled	Actual	Comment	Reference
L	162	GLY	-	expression tag	UNP A4IFT3
L	163	LEU	-	expression tag	UNP A4IFT3
L	164	VAL	-	expression tag	UNP A4IFT3
L	165	PRO	-	expression tag	UNP A4IFT3
L	166	ARG	-	expression tag	UNP A4IFT3
O	20	ALA	-	expression tag	UNP A4IFT3
O	160	ALA	-	expression tag	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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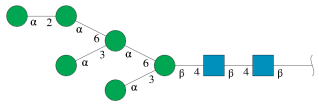
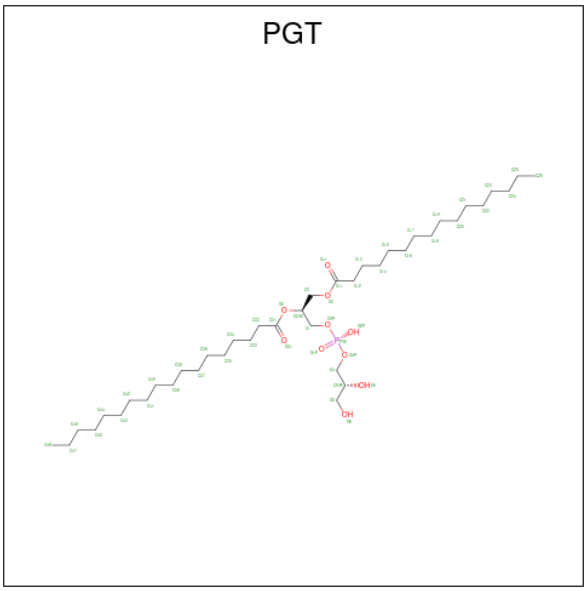
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	c	3	Total C N O 39 22 2 15	0	0	0
3	e	3	Total C N O 39 22 2 15	0	0	0

- 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 94 52 2 40	0	0	0
4	T	8	Total C N O 94 52 2 40	0	0	0
4	V	8	Total C N O 94 52 2 40	0	0	0
4	X	8	Total C N O 94 52 2 40	0	0	0
4	Z	8	Total C N O 94 52 2 40	0	0	0
4	b	8	Total C N O 94 52 2 40	0	0	0
4	d	8	Total C N O 94 52 2 40	0	0	0
4	f	8	Total C N O 94 52 2 40	0	0	0

- Molecule 5 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$).



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

- Molecule 6 is water.

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

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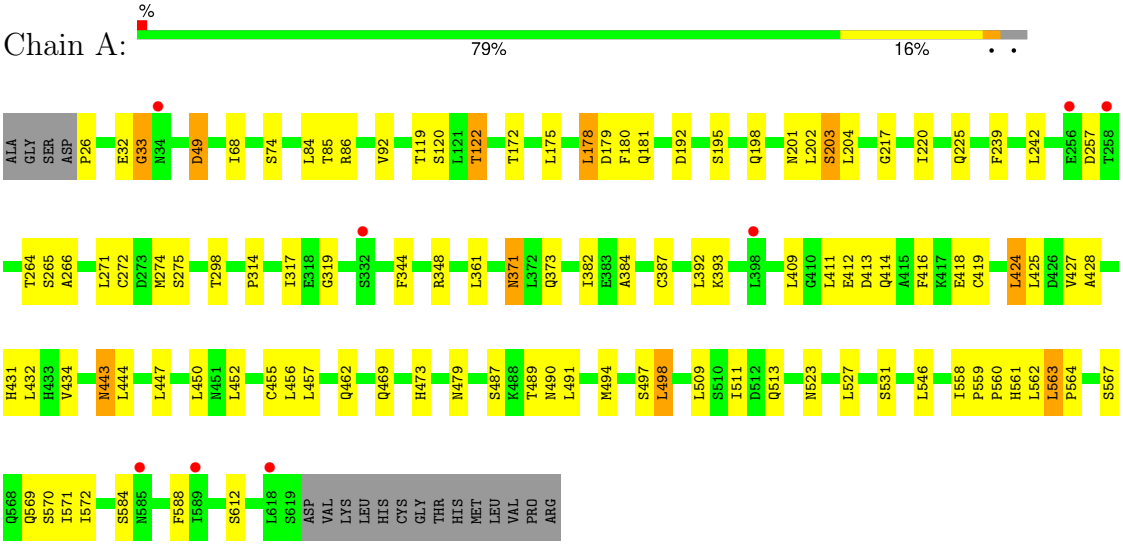
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O 1 1	0	0
6	D	3	Total O 3 3	0	0
6	G	1	Total O 1 1	0	0
6	L	1	Total O 1 1	0	0

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.

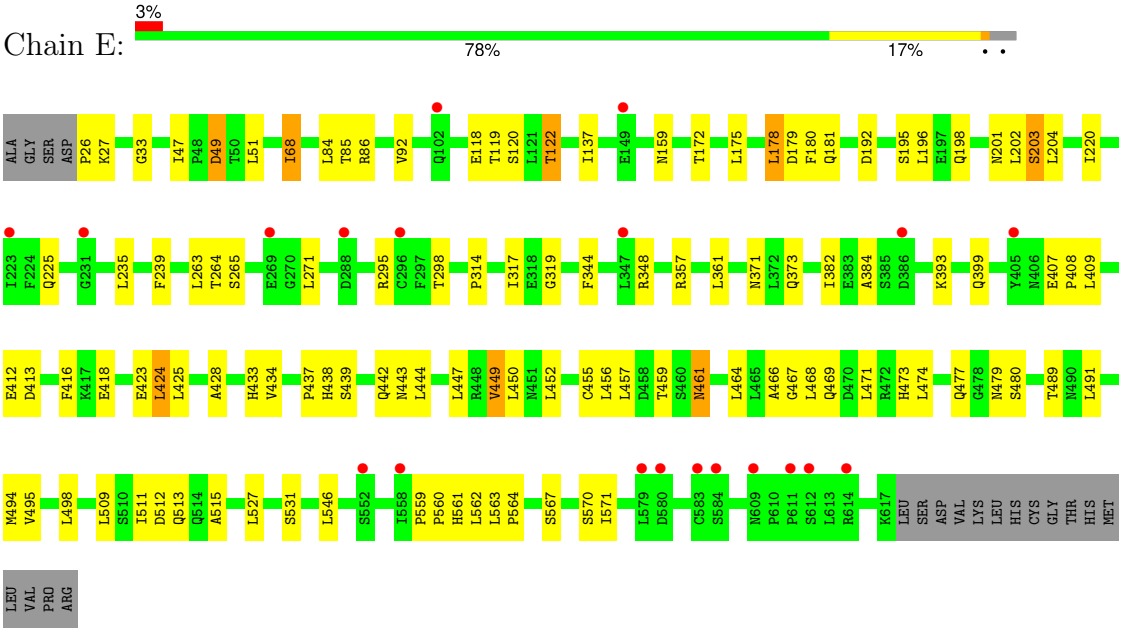
• Molecule 1: CD180 molecule

Chain A:



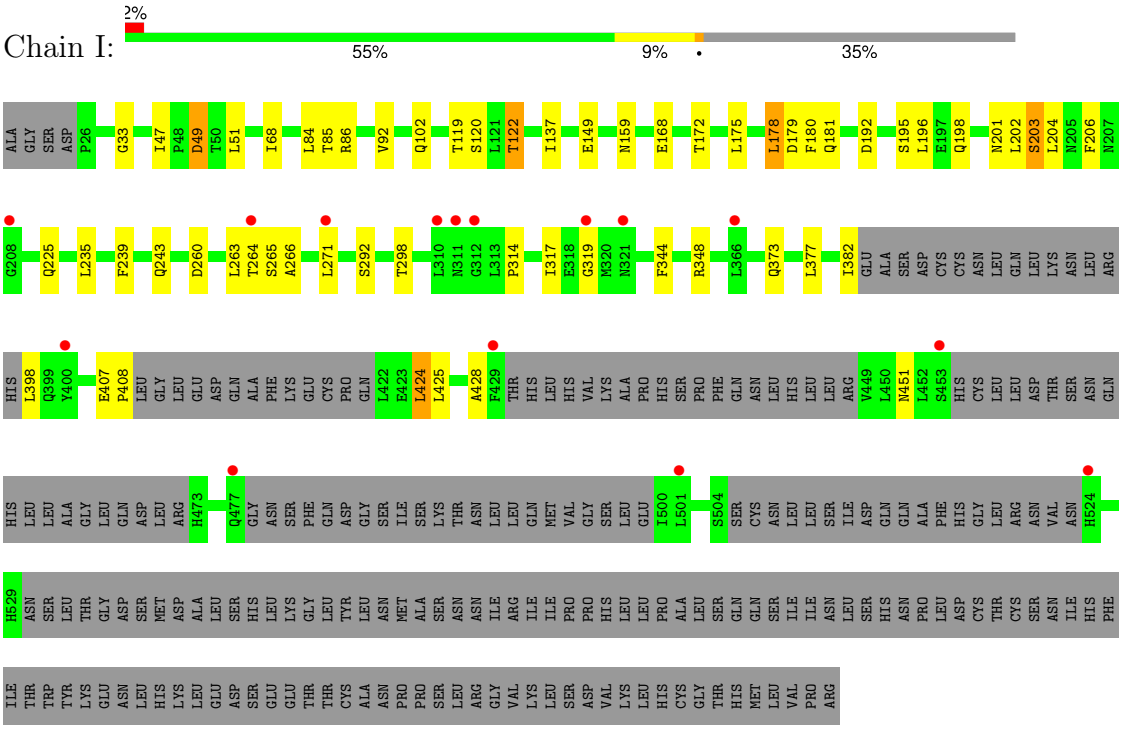
• Molecule 1: CD180 molecule

Chain E:



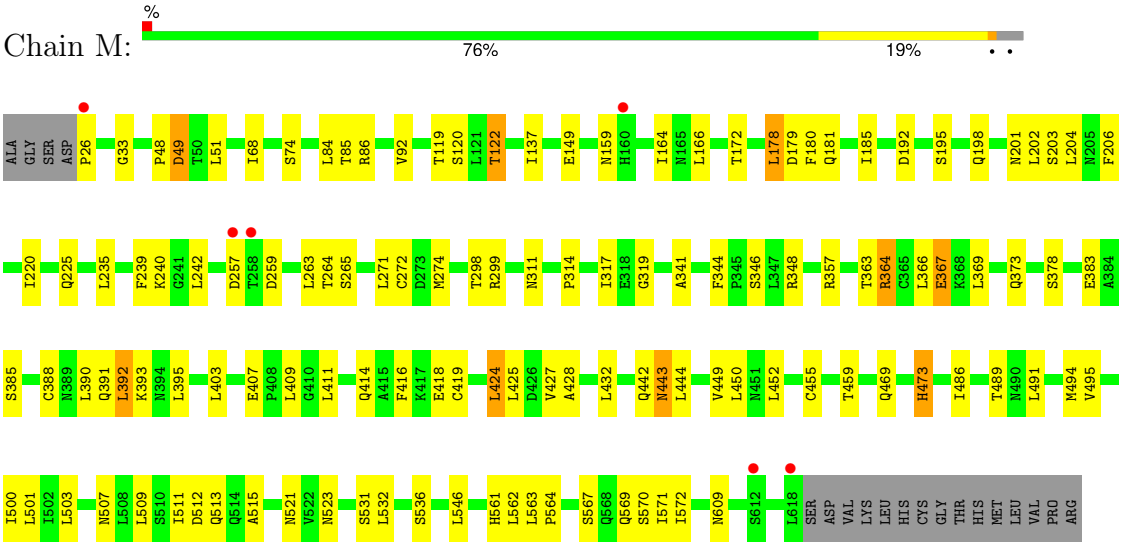
• Molecule 1: CD180 molecule

Chain I:



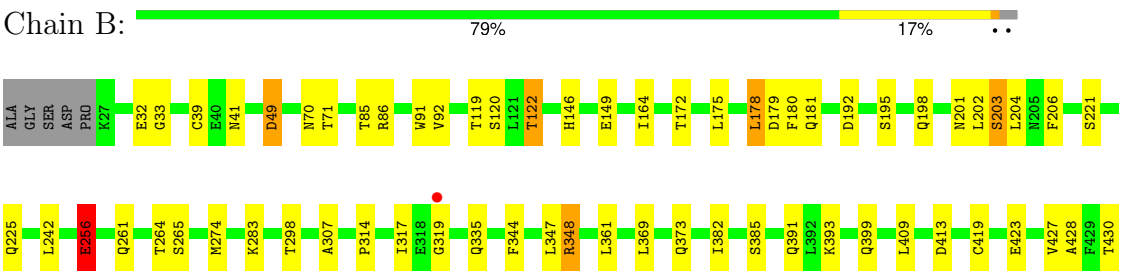
• Molecule 1: CD180 molecule

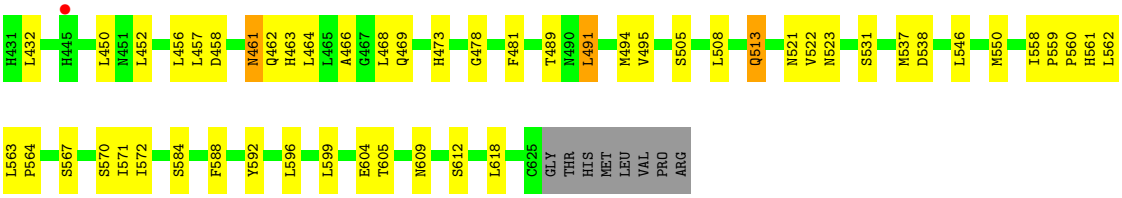
Chain M:



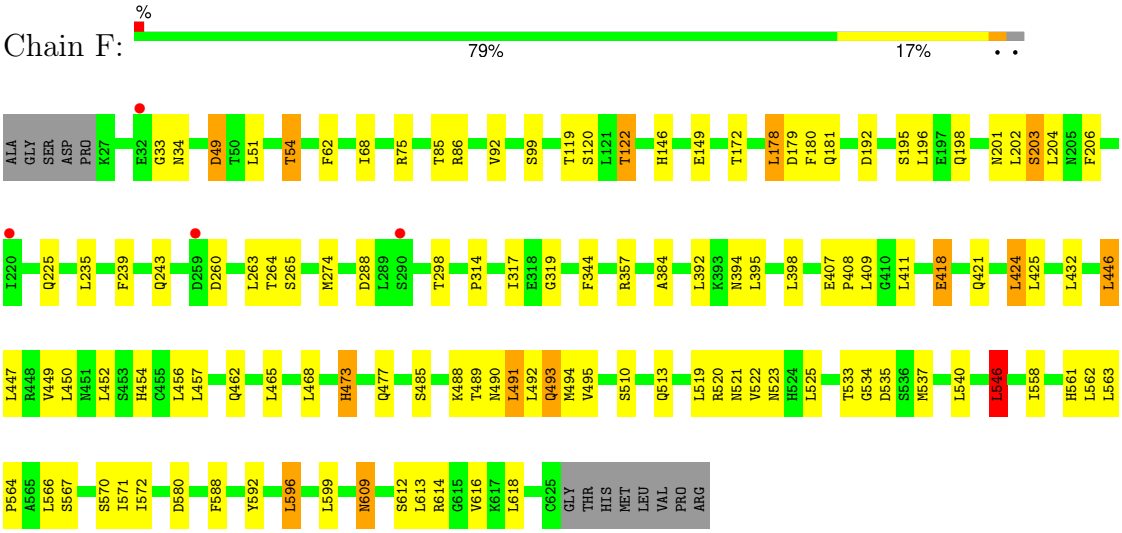
• Molecule 1: CD180 molecule

Chain B:

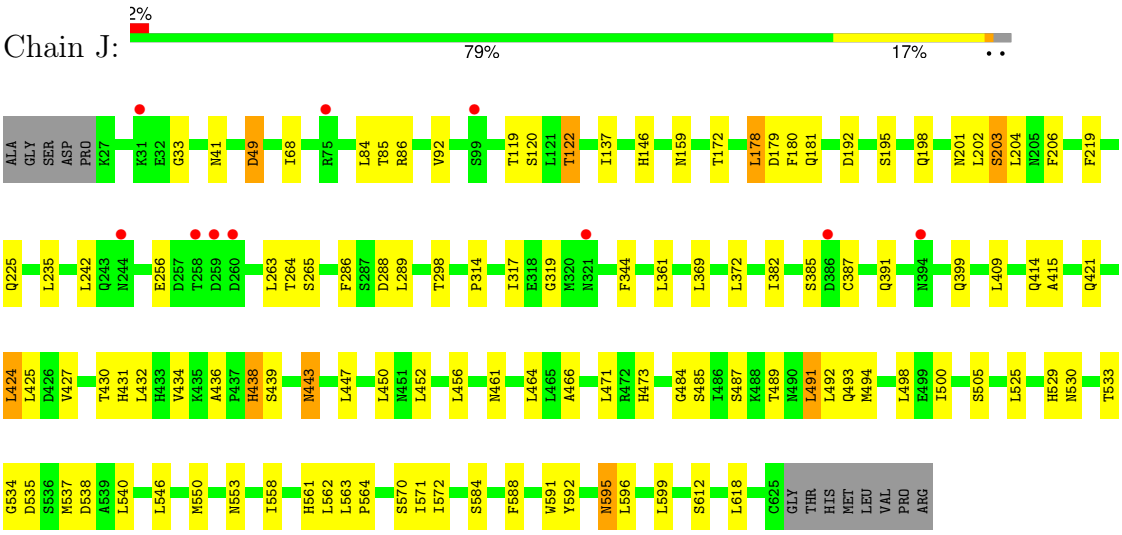




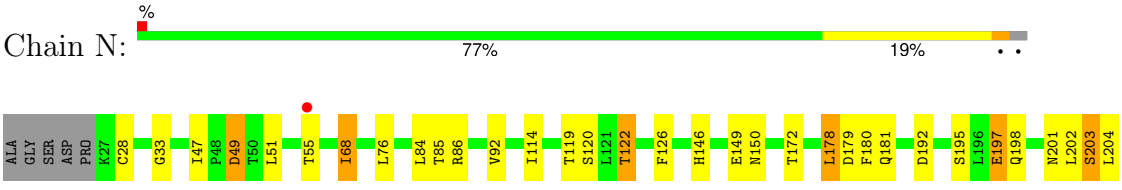
• Molecule 1: CD180 molecule

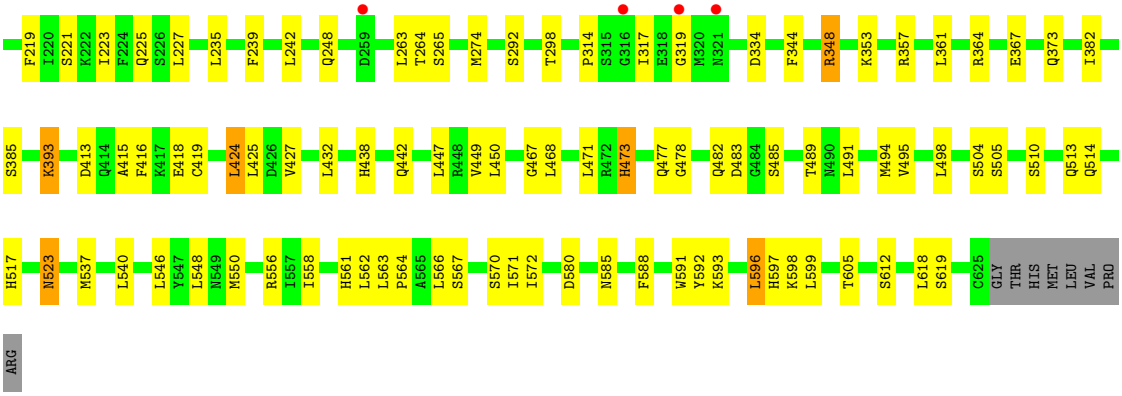


• Molecule 1: CD180 molecule

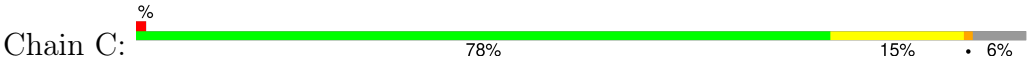


• Molecule 1: CD180 molecule

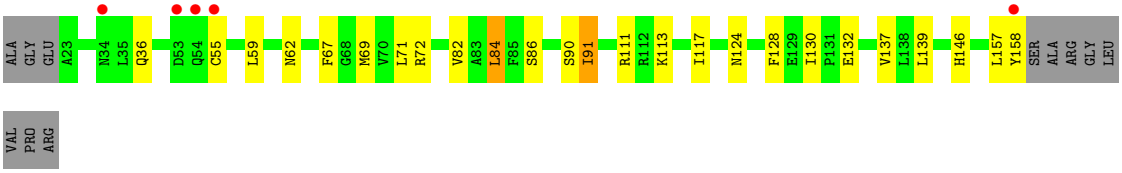




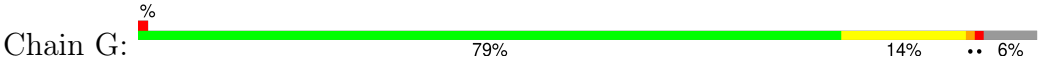
• Molecule 2: LY86 protein



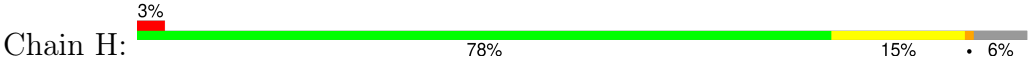
• Molecule 2: LY86 protein

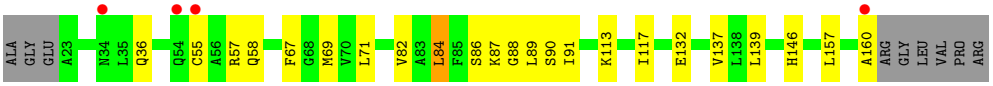


• Molecule 2: LY86 protein

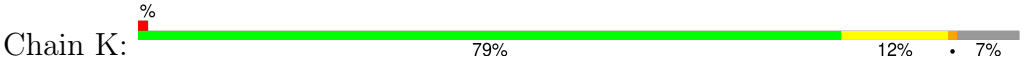


• Molecule 2: LY86 protein



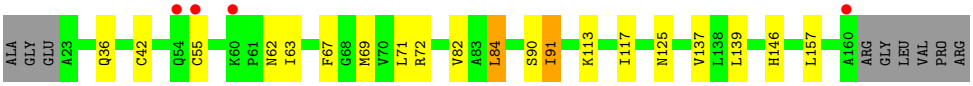


• Molecule 2: LY86 protein



• Molecule 2: LY86 protein

Chain L:

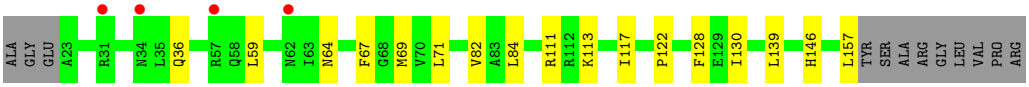


• Molecule 2: LY86 protein

Chain O:

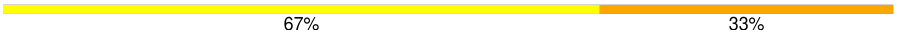
• Molecule 2: LY86 protein

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:



• 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:

• 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:

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

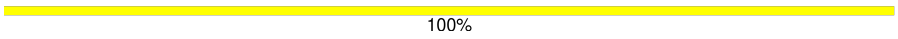
Chain W:

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

Chain Y:

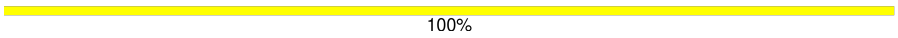
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



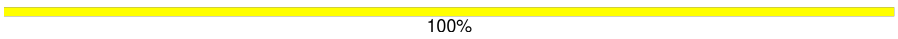
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



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

Chain e:



• 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 R:

• 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-glucopyranos
e

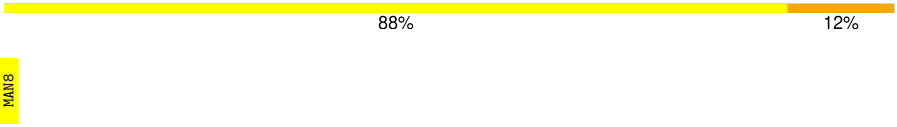
Chain T:

• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyran
ose-(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-glucopyranos
e

Chain V:

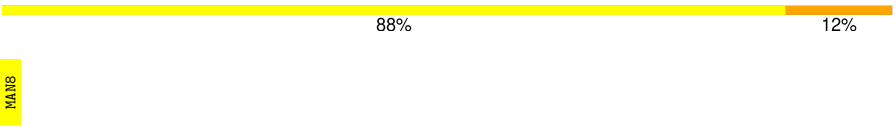
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyran
ose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1
-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos
e

Chain X:



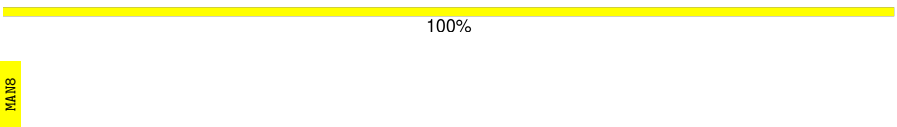
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyran
ose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1
-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos
e

Chain Z:



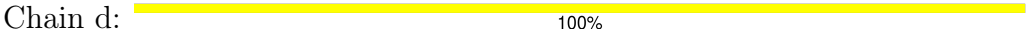
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyran
ose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1
-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos
e

Chain b:



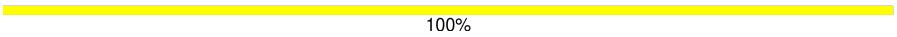
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyran
ose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1
-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos
e

Chain d:



• 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:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	8028 reflections (5.02%)	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 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PGT, NAG, BMA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.63	0/4537	0.67	0/6190
1	B	0.70	3/4708 (0.1%)	0.74	0/6409
1	E	0.50	0/4467	0.60	0/6104
1	F	0.50	0/4581	0.62	1/6256 (0.0%)
1	I	0.49	0/2980	0.58	0/4064
1	J	0.50	0/4546	0.62	0/6213
1	M	0.63	1/4534 (0.0%)	0.68	0/6189
1	N	0.65	1/4682 (0.0%)	0.69	1/6377 (0.0%)
2	C	0.70	1/1051 (0.1%)	0.69	1/1436 (0.1%)
2	D	0.73	0/1048	0.73	2/1432 (0.1%)
2	G	0.61	0/1057	0.69	1/1443 (0.1%)
2	H	0.68	0/1072	0.71	0/1463
2	K	0.52	0/1026	0.63	1/1401 (0.1%)
2	L	0.63	0/1072	0.67	0/1464
2	O	0.71	0/1054	0.70	1/1440 (0.1%)
2	P	0.70	0/1026	0.71	1/1402 (0.1%)
All	All	0.60	6/43441 (0.0%)	0.66	9/59283 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	28	CYS	CB-SG	5.89	1.92	1.82
1	B	256	GLU	CG-CD	5.68	1.60	1.51
1	B	39	CYS	CB-SG	-5.64	1.72	1.81
1	M	419	CYS	CB-SG	-5.39	1.73	1.81
2	C	30	CYS	CB-SG	-5.21	1.73	1.81

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	111	ARG	NE-CZ-NH2	-6.15	117.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	92	LEU	CA-CB-CG	6.03	129.17	115.30
2	K	59	LEU	CA-CB-CG	5.48	127.91	115.30
2	D	111	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	C	55	CYS	CA-CB-SG	-5.29	104.48	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4450	0	4175	61	0
1	B	4616	0	4440	75	0
1	E	4381	0	4045	84	0
1	F	4493	0	4211	73	0
1	I	2931	0	2684	37	0
1	J	4458	0	4137	70	0
1	M	4447	0	4175	73	0
1	N	4591	0	4415	82	0
2	C	1026	0	929	17	0
2	D	1022	0	927	16	0
2	G	1031	0	946	13	0
2	H	1046	0	953	13	0
2	K	1003	0	895	9	0
2	L	1046	0	947	11	0
2	O	1028	0	923	15	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	0	0
3	c	39	0	34	0	0
3	e	39	0	34	0	0
4	R	94	0	79	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	94	0	79	1	0
4	V	94	0	79	2	0
4	X	94	0	79	1	0
4	Z	94	0	79	1	0
4	b	94	0	79	0	0
4	d	94	0	79	0	0
4	f	94	0	79	0	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
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	658	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 658 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
2:H:82:VAL:HG22	2:H:139:LEU:HD23	1.49	0.93
1:M:242:LEU:HB2	1:M:274:MET:HE1	1.52	0.92
1:N:523:ASN:HD22	1:N:523:ASN:C	1.75	0.90
2:D:62:ASN:HD22	2:D:124:ASN:HA	1.38	0.89

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	592/612 (97%)	552 (93%)	36 (6%)	4 (1%)	19	47
1	B	597/612 (98%)	556 (93%)	38 (6%)	3 (0%)	25	55
1	E	590/612 (96%)	544 (92%)	43 (7%)	3 (0%)	25	55
1	F	597/612 (98%)	557 (93%)	37 (6%)	3 (0%)	25	55
1	I	383/612 (63%)	361 (94%)	21 (6%)	1 (0%)	37	65
1	J	597/612 (98%)	553 (93%)	39 (6%)	5 (1%)	16	44
1	M	591/612 (97%)	546 (92%)	43 (7%)	2 (0%)	37	65
1	N	597/612 (98%)	560 (94%)	35 (6%)	2 (0%)	37	65
2	C	136/147 (92%)	125 (92%)	8 (6%)	3 (2%)	5	20
2	D	134/147 (91%)	125 (93%)	8 (6%)	1 (1%)	19	47
2	G	136/147 (92%)	127 (93%)	6 (4%)	3 (2%)	5	20
2	H	136/147 (92%)	126 (93%)	9 (7%)	1 (1%)	19	47
2	K	132/147 (90%)	125 (95%)	6 (4%)	1 (1%)	16	44
2	L	136/147 (92%)	127 (93%)	8 (6%)	1 (1%)	19	47
2	O	136/147 (92%)	129 (95%)	6 (4%)	1 (1%)	19	47
2	P	133/147 (90%)	123 (92%)	9 (7%)	1 (1%)	16	44
All	All	5623/6072 (93%)	5236 (93%)	352 (6%)	35 (1%)	22	51

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	481/561 (86%)	455 (95%)	26 (5%)	18	47
1	B	516/561 (92%)	484 (94%)	32 (6%)	15	41
1	E	463/561 (82%)	445 (96%)	18 (4%)	27	60
1	F	488/561 (87%)	457 (94%)	31 (6%)	14	40
1	I	304/561 (54%)	291 (96%)	13 (4%)	25	56
1	J	478/561 (85%)	454 (95%)	24 (5%)	20	50
1	M	481/561 (86%)	449 (93%)	32 (7%)	13	37
1	N	511/561 (91%)	484 (95%)	27 (5%)	19	48
2	C	102/125 (82%)	98 (96%)	4 (4%)	27	60
2	D	103/125 (82%)	98 (95%)	5 (5%)	21	51
2	G	103/125 (82%)	98 (95%)	5 (5%)	21	51
2	H	105/125 (84%)	98 (93%)	7 (7%)	13	37
2	K	98/125 (78%)	92 (94%)	6 (6%)	15	42
2	L	106/125 (85%)	99 (93%)	7 (7%)	14	38
2	O	102/125 (82%)	96 (94%)	6 (6%)	16	43
2	P	99/125 (79%)	96 (97%)	3 (3%)	36	69
All	All	4540/5488 (83%)	4294 (95%)	246 (5%)	18	47

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	546	LEU
2	H	90	SER
1	F	510	SER
2	H	84	LEU
2	L	146	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	261	GLN
2	G	62	ASN
1	F	225	GLN
2	G	36	GLN
2	L	62	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	1,3	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	1,4	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	1,3	14,14,15	0.81	0	17,19,21	1.13	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	1,4	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%)
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	1,4	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	1,3	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	1,4	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	1,3	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	Z	1	1,4	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%)
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	1,3	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	1,4	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	1,3	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	1,4	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	1,3	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	1,4	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	1,3	-	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	1,4	-	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	1,3	-	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	1,4	-	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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,3	-	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	1,4	-	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
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	1,3	-	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	1,4	-	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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
3	a	2	NAG	O5-C5-C6-O6
4	X	7	MAN	O5-C5-C6-O6

5 of 8 ring outliers are listed below:

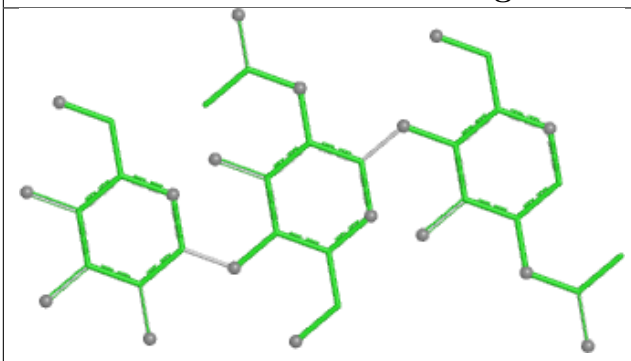
Mol	Chain	Res	Type	Atoms
4	X	6	MAN	C1-C2-C3-C4-C5-O5
4	d	6	MAN	C1-C2-C3-C4-C5-O5
4	R	6	MAN	C1-C2-C3-C4-C5-O5
4	f	6	MAN	C1-C2-C3-C4-C5-O5
4	b	6	MAN	C1-C2-C3-C4-C5-O5

13 monomers are involved in 11 short contacts:

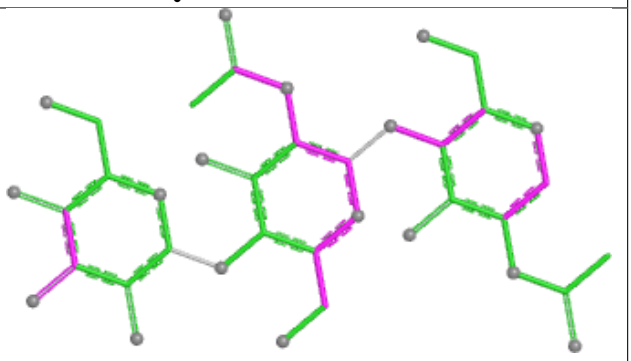
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	1	NAG	1	0
3	Q	1	NAG	1	0
3	Y	1	NAG	1	0
3	S	1	NAG	1	0
4	T	5	MAN	1	0
3	Y	2	NAG	1	0
4	V	6	MAN	1	0
4	V	1	NAG	1	0
4	X	1	NAG	1	0
4	T	6	MAN	1	0
3	W	1	NAG	1	0
4	V	5	MAN	1	0
3	U	1	NAG	3	0

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

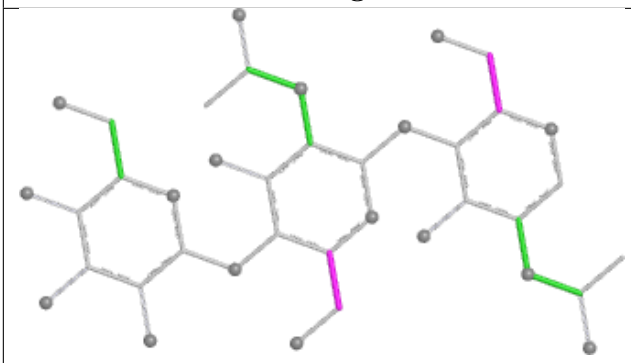
Oligosaccharide Chain Q



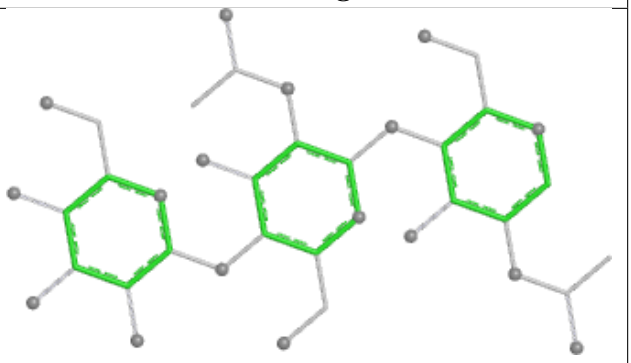
Bond lengths



Bond angles

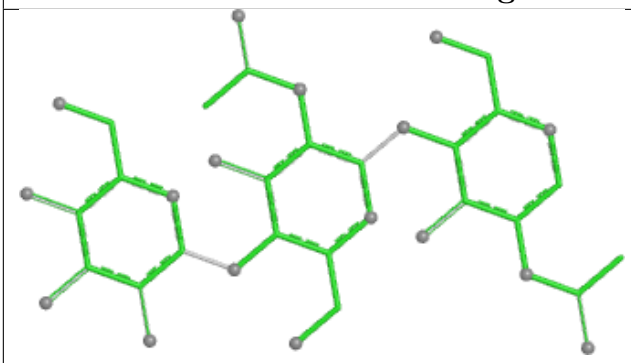


Torsions

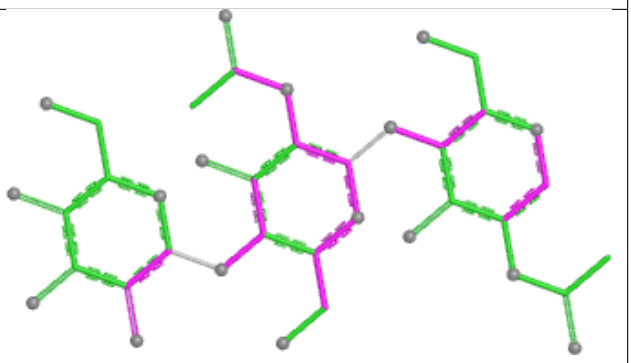


Rings

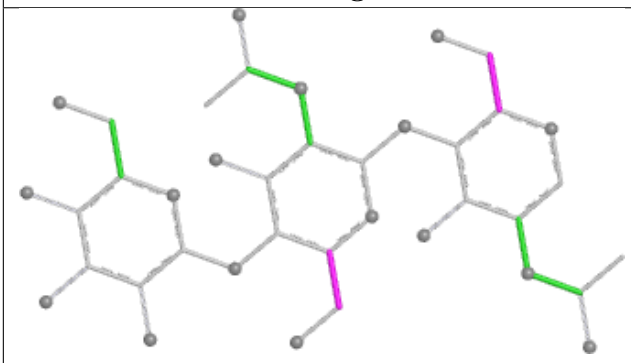
Oligosaccharide Chain S



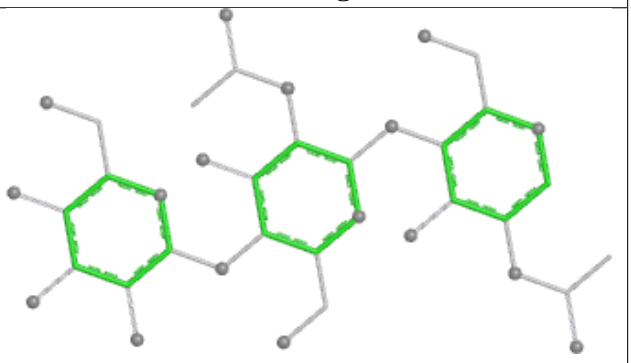
Bond lengths



Bond angles

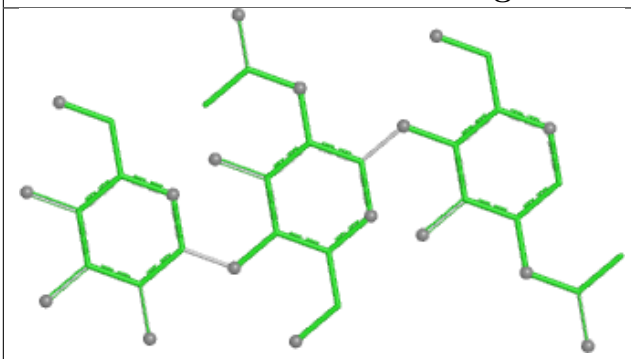


Torsions

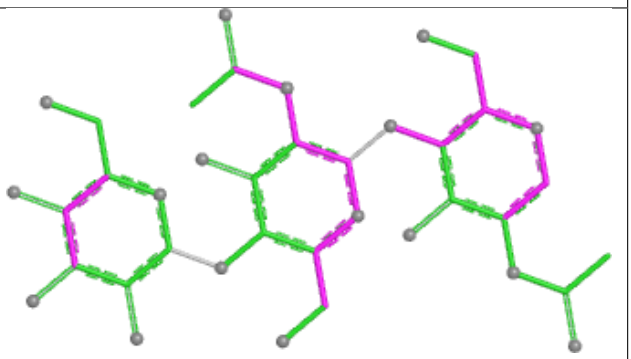


Rings

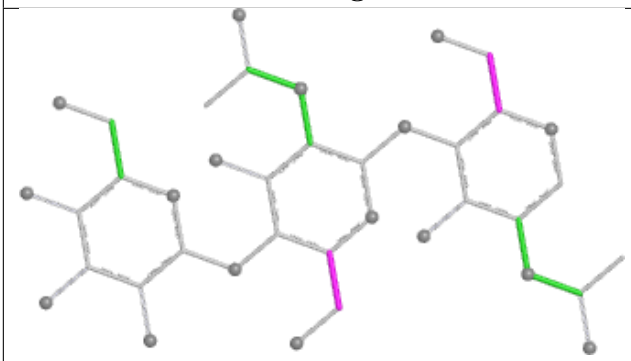
Oligosaccharide Chain U



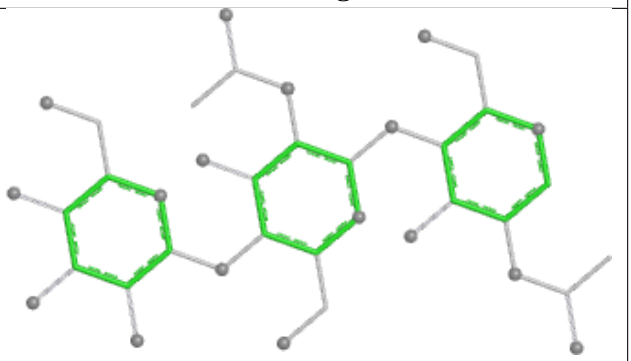
Bond lengths



Bond angles

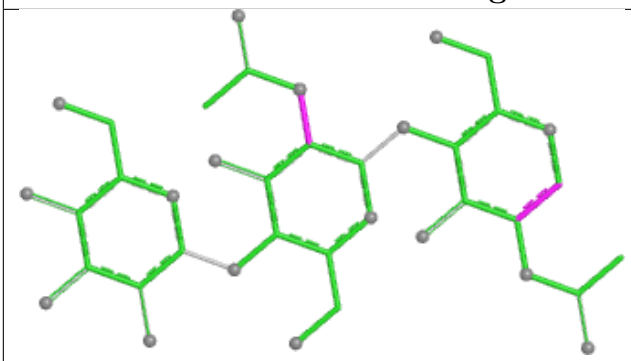


Torsions

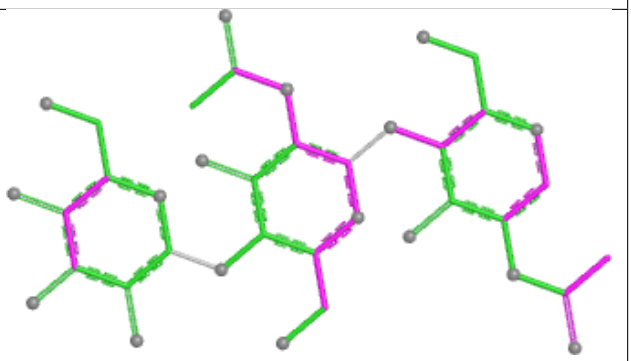


Rings

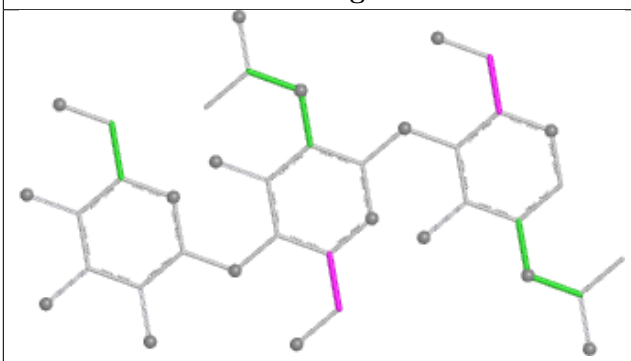
Oligosaccharide Chain W



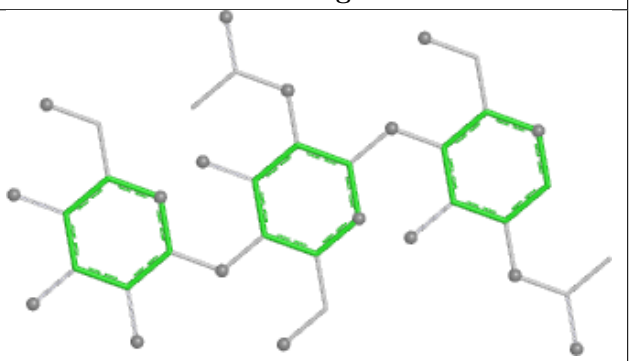
Bond lengths



Bond angles

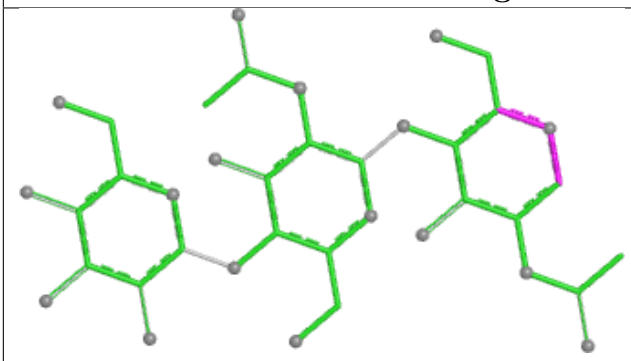


Torsions

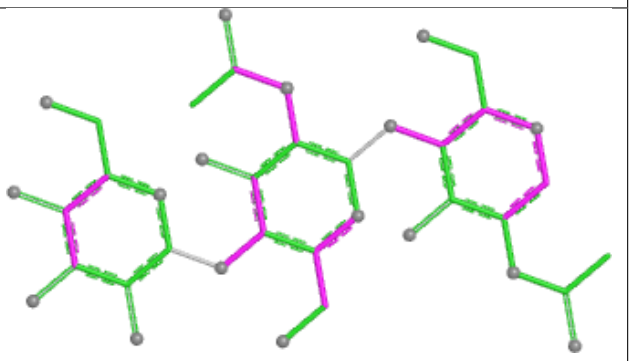


Rings

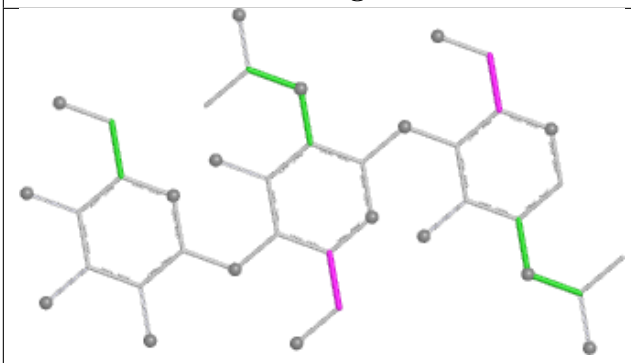
Oligosaccharide Chain Y



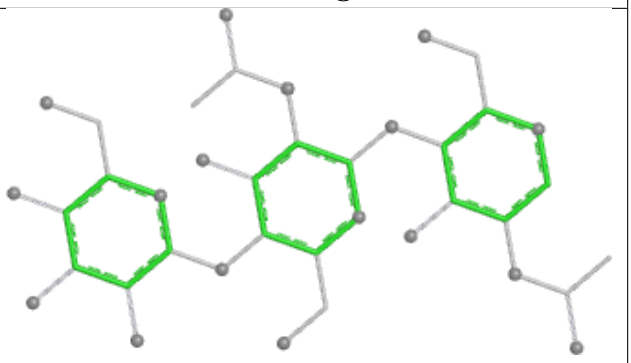
Bond lengths



Bond angles

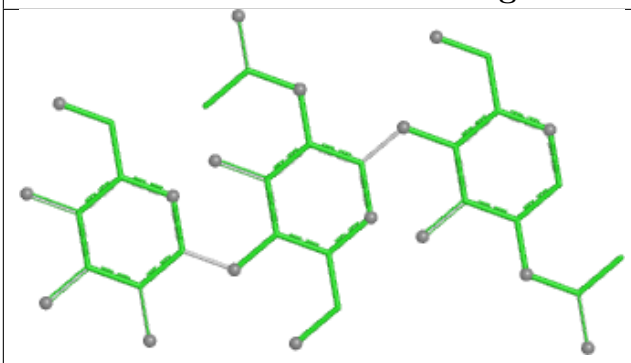


Torsions

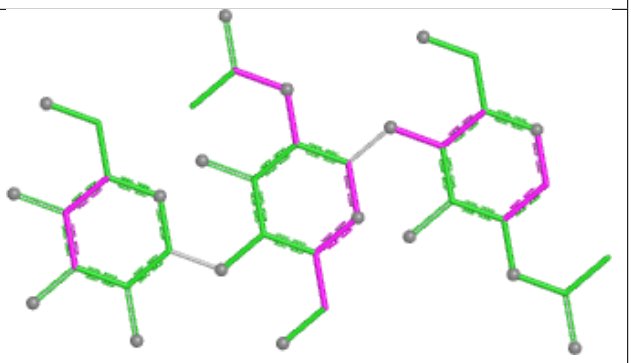


Rings

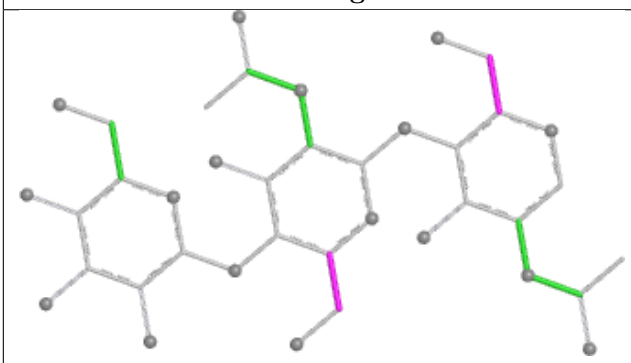
Oligosaccharide Chain a



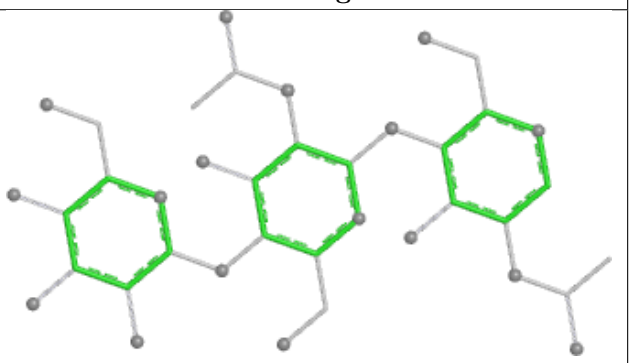
Bond lengths



Bond angles

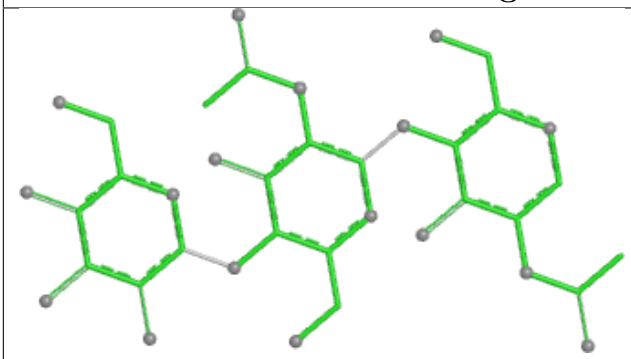


Torsions

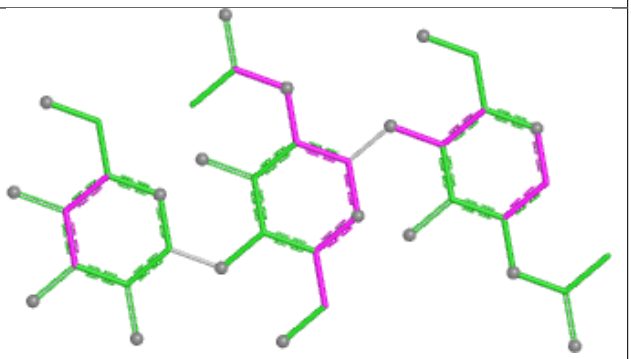


Rings

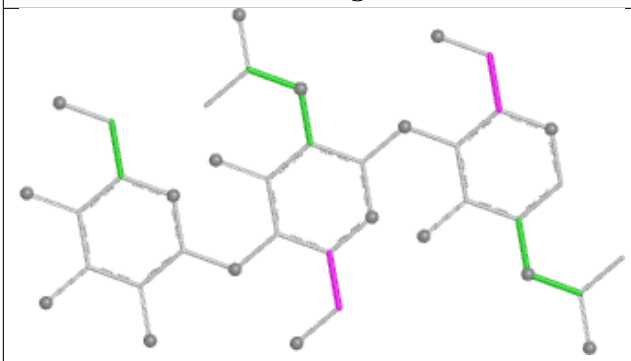
Oligosaccharide Chain c



Bond lengths



Bond angles



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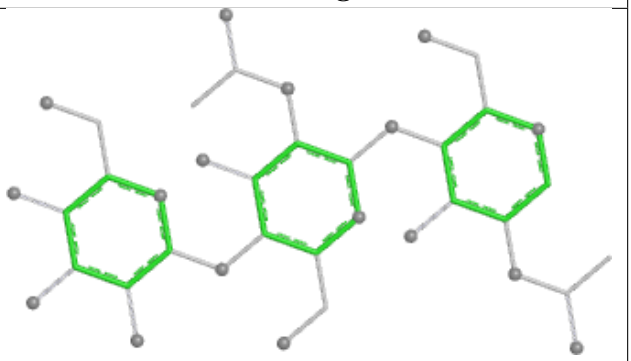
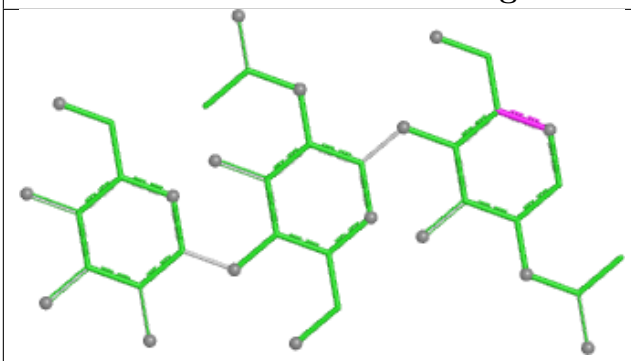
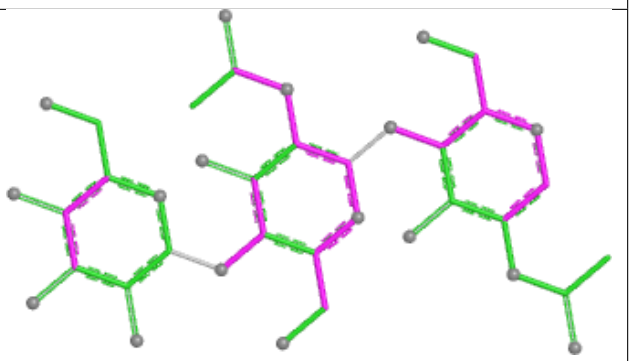


Rings

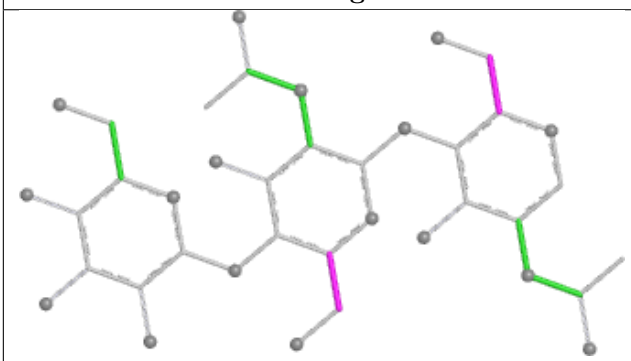
Oligosaccharide Chain e



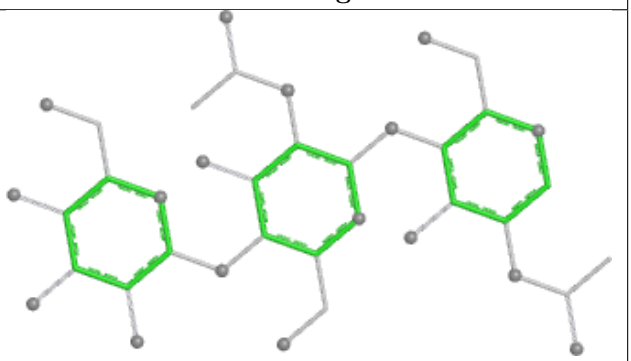
Bond lengths



Bond angles

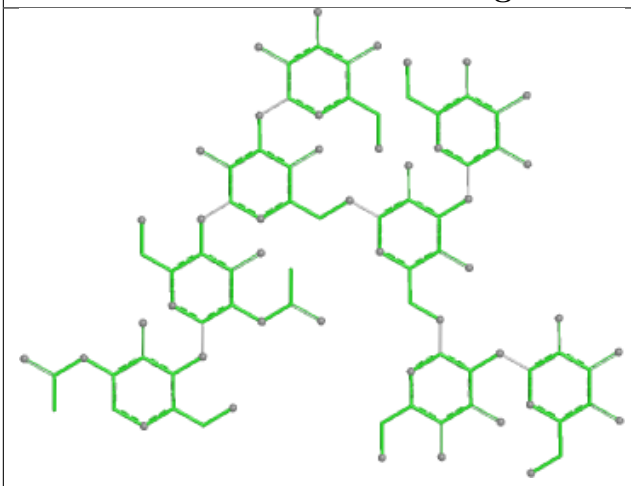


Torsions



Rings

Oligosaccharide Chain R



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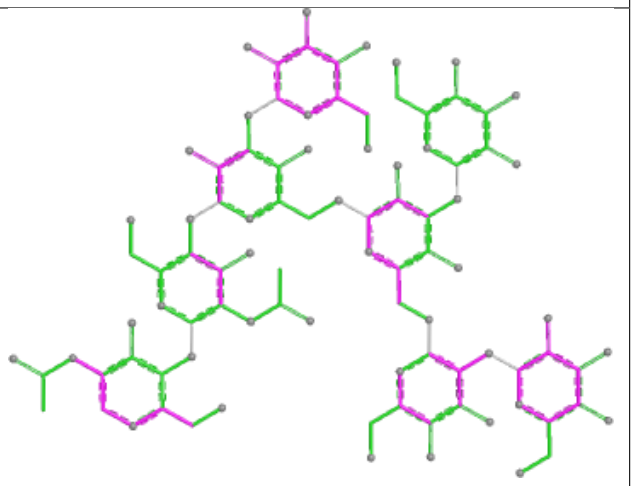
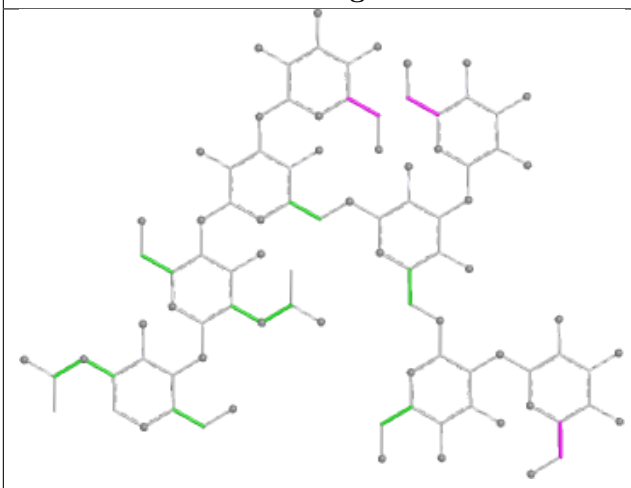


Bond angles



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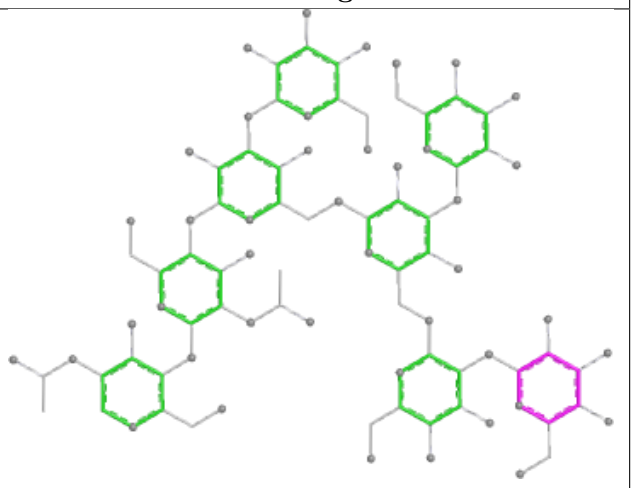
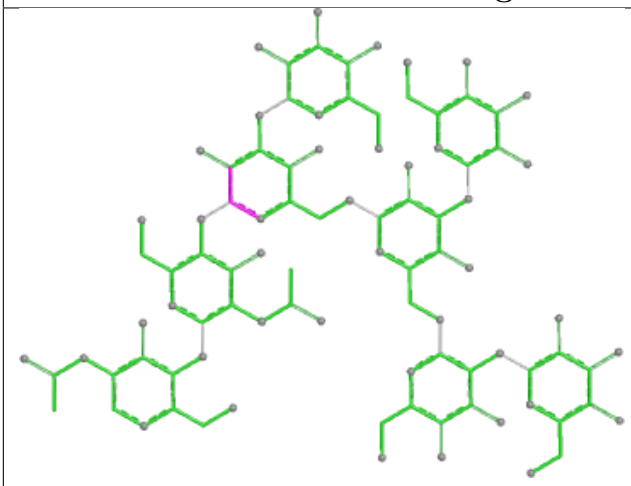
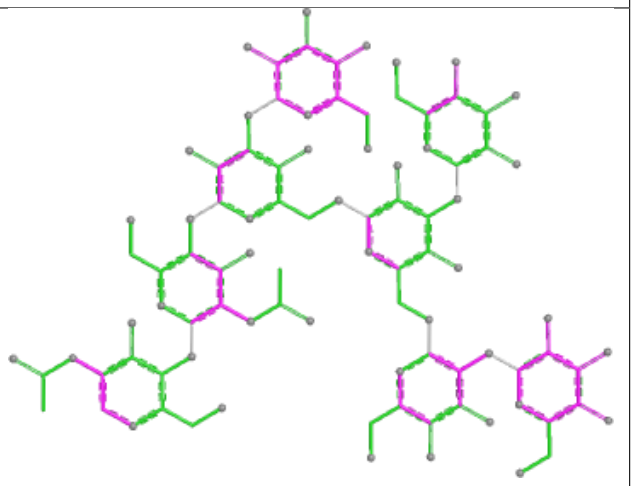


Rings

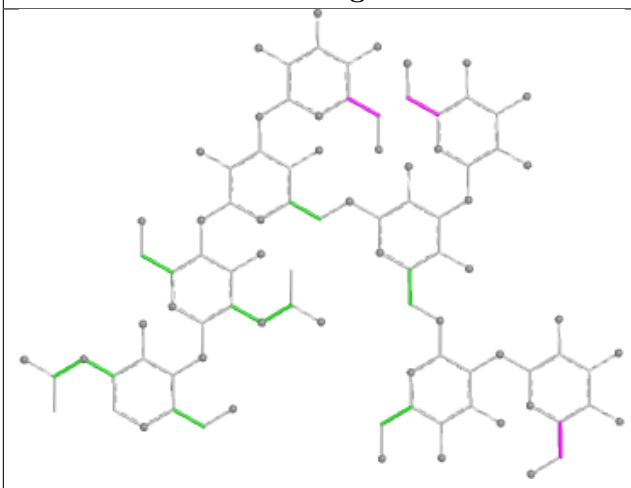
Oligosaccharide Chain T



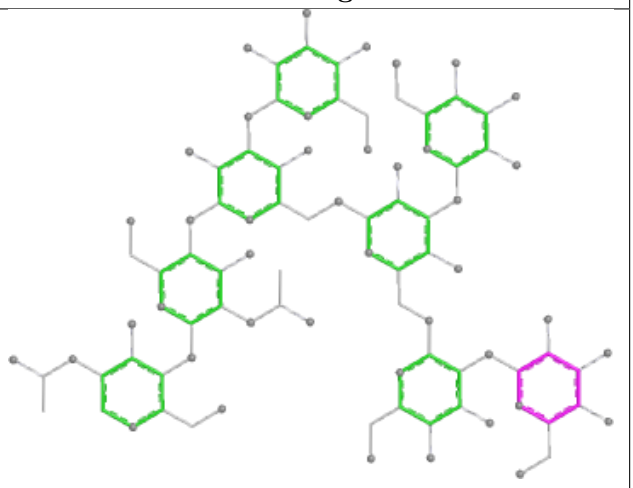
Bond lengths



Bond angles

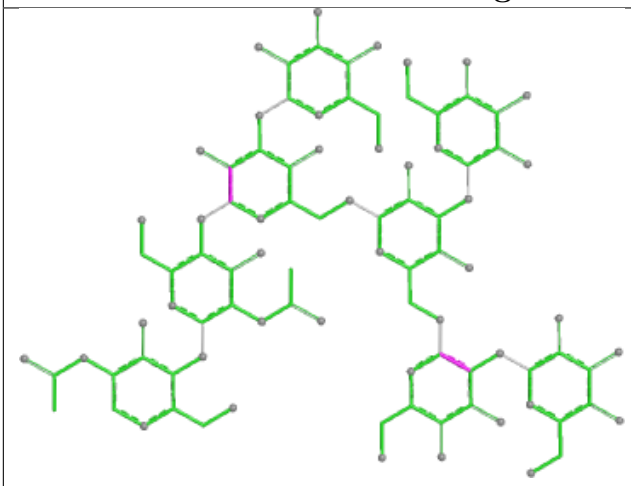


Torsions

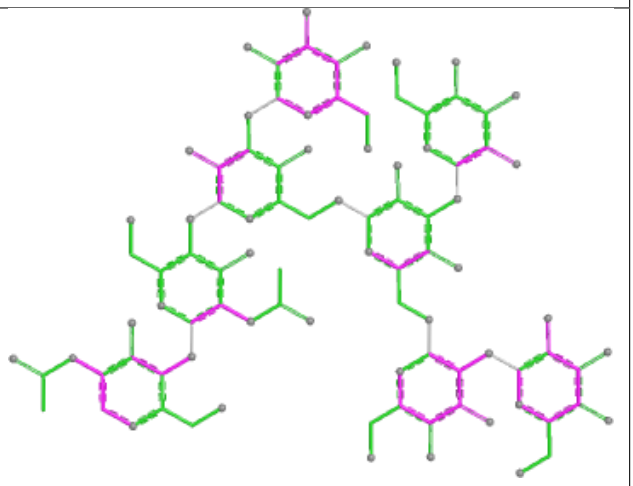


Rings

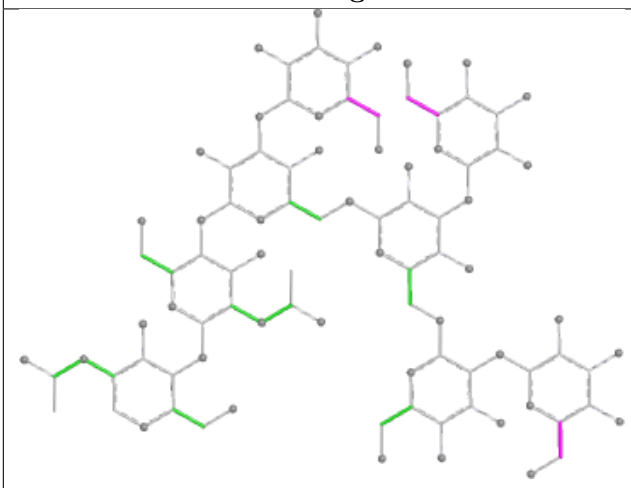
Oligosaccharide Chain V



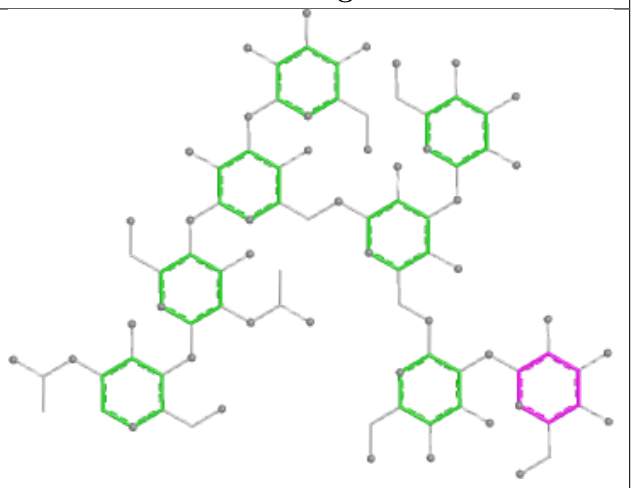
Bond lengths



Bond angles

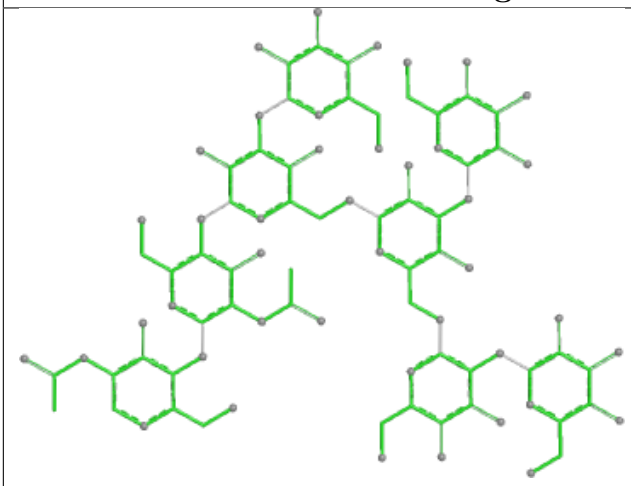


Torsions

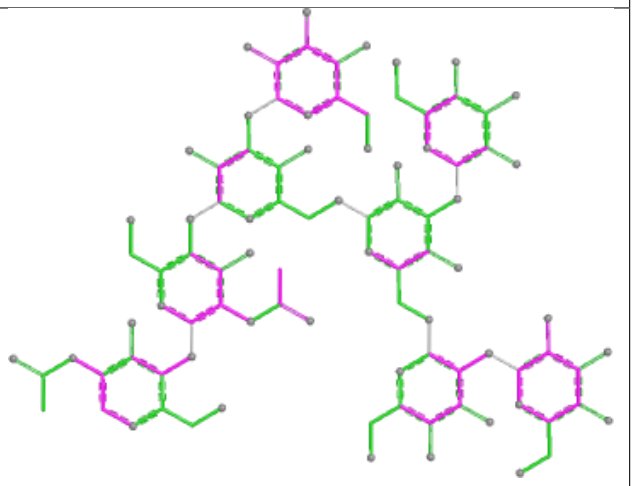


Rings

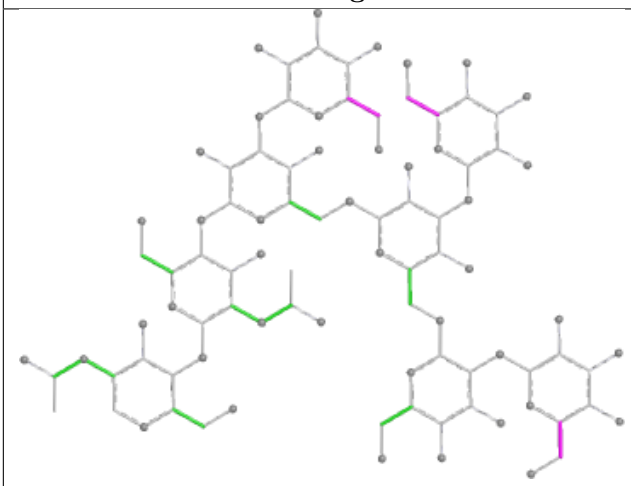
Oligosaccharide Chain X



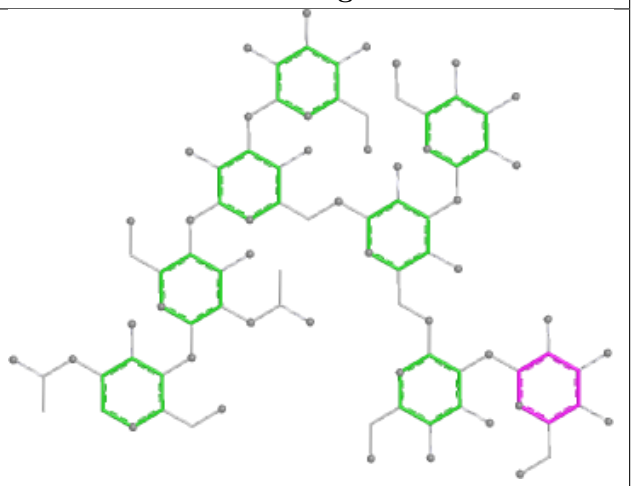
Bond lengths



Bond angles

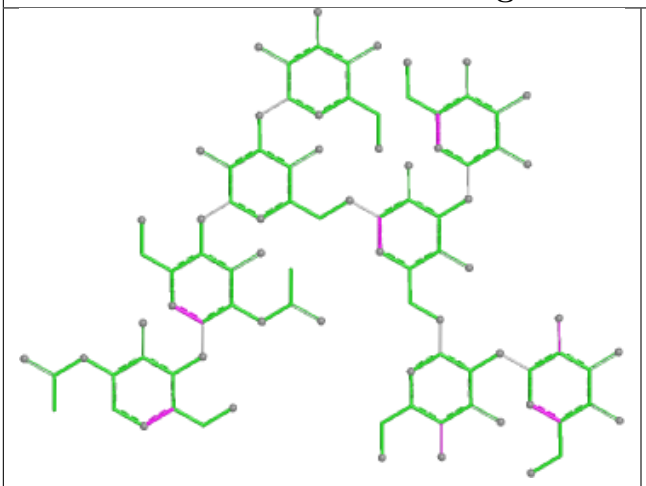


Torsions

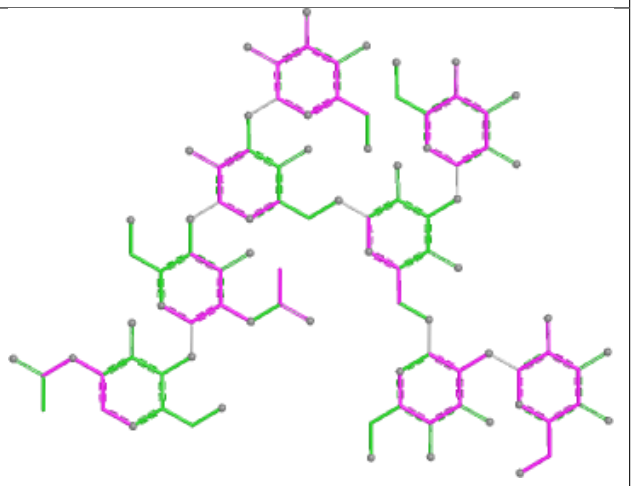


Rings

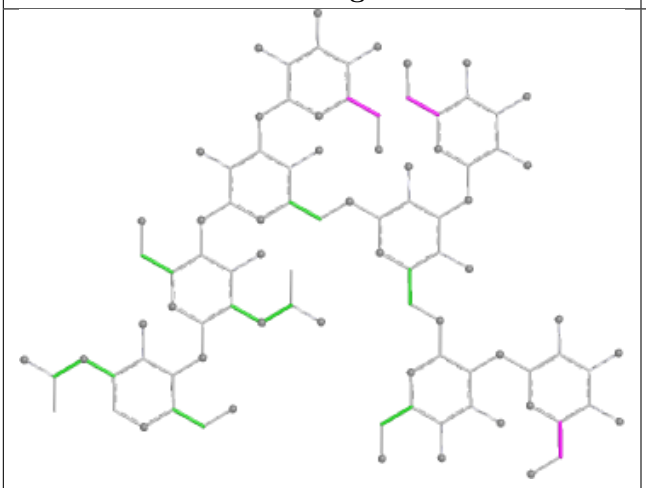
Oligosaccharide Chain Z



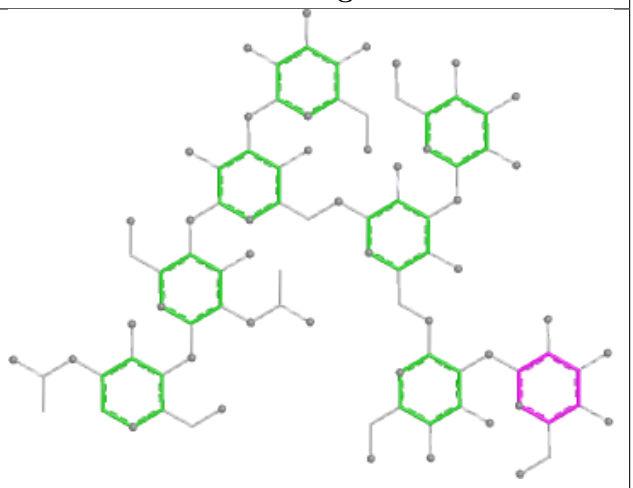
Bond lengths



Bond angles

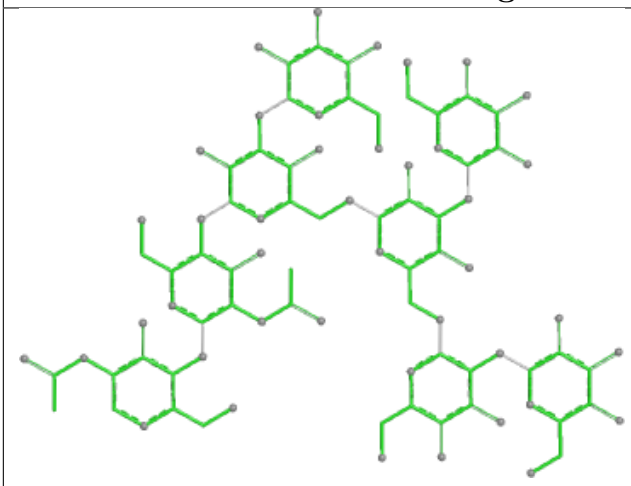


Torsions

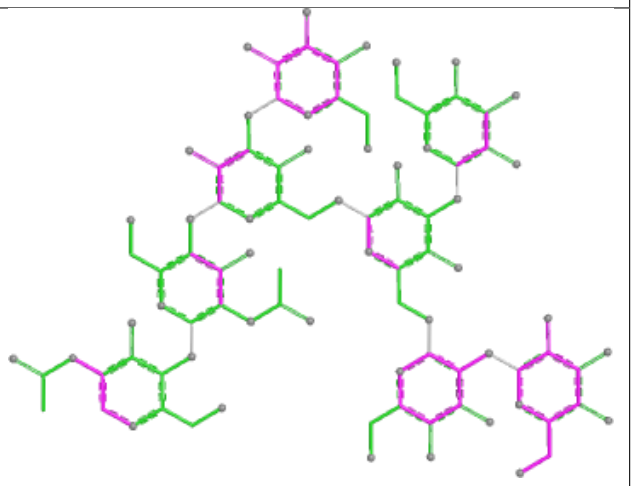


Rings

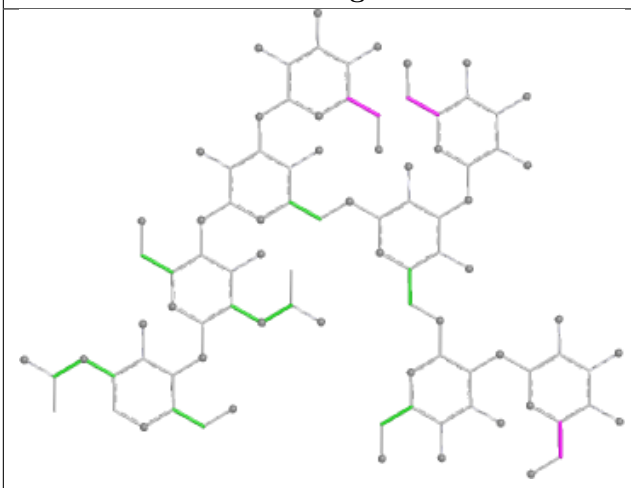
Oligosaccharide Chain b



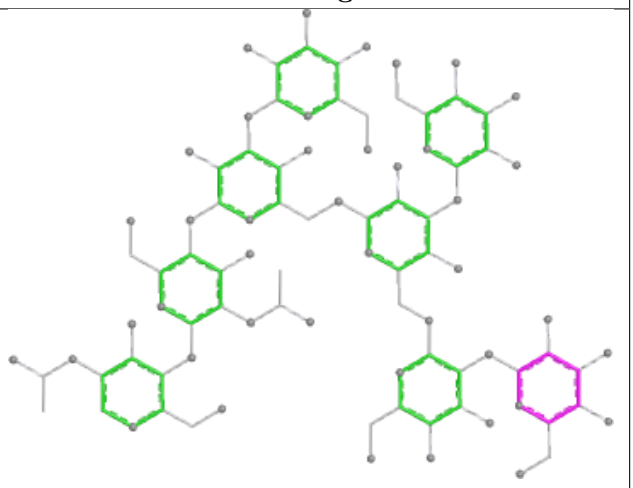
Bond lengths



Bond angles

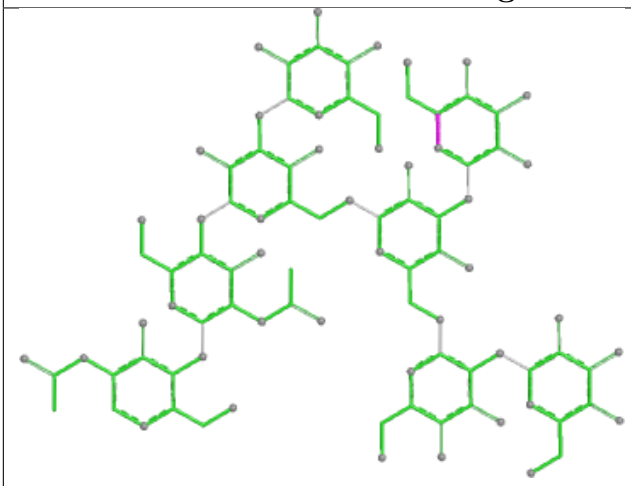


Torsions

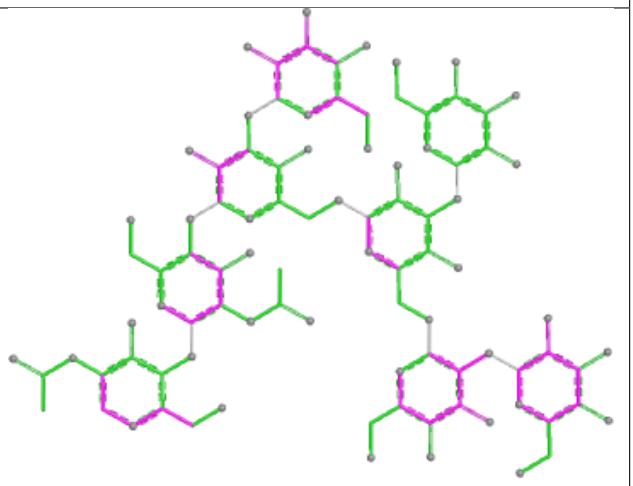


Rings

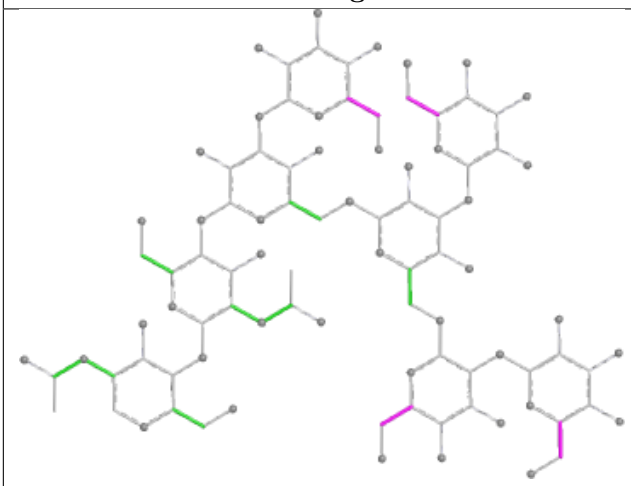
Oligosaccharide Chain d



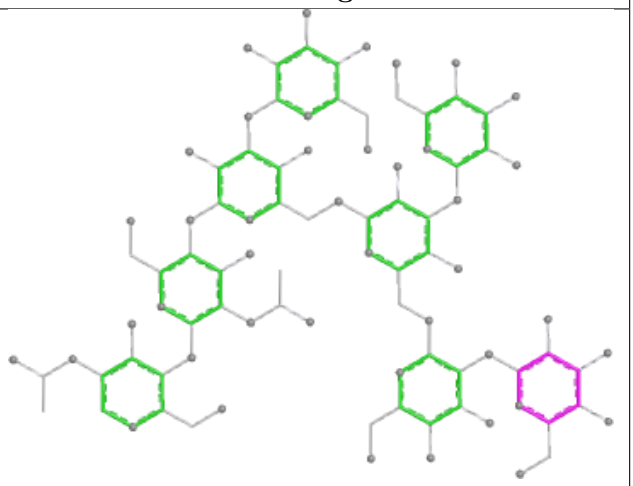
Bond lengths



Bond angles

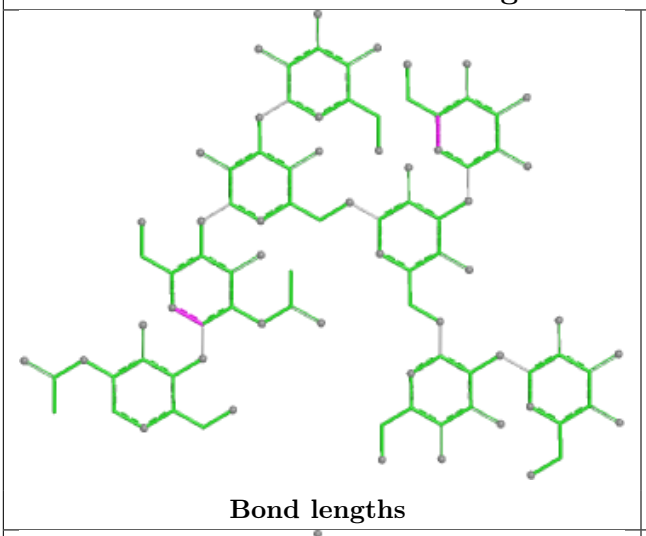


Torsions

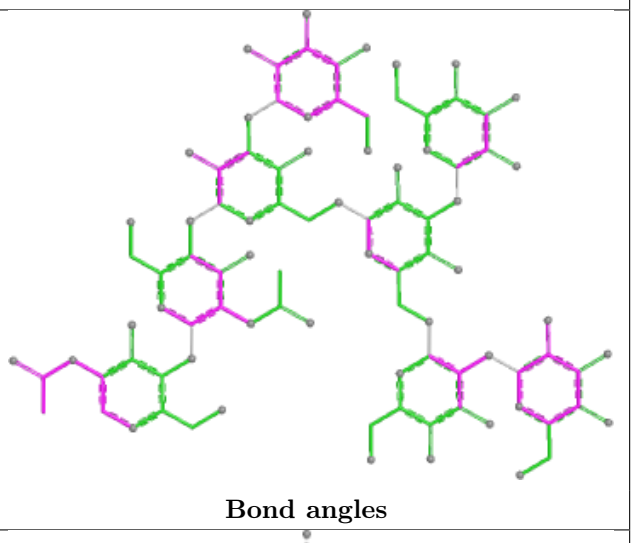


Rings

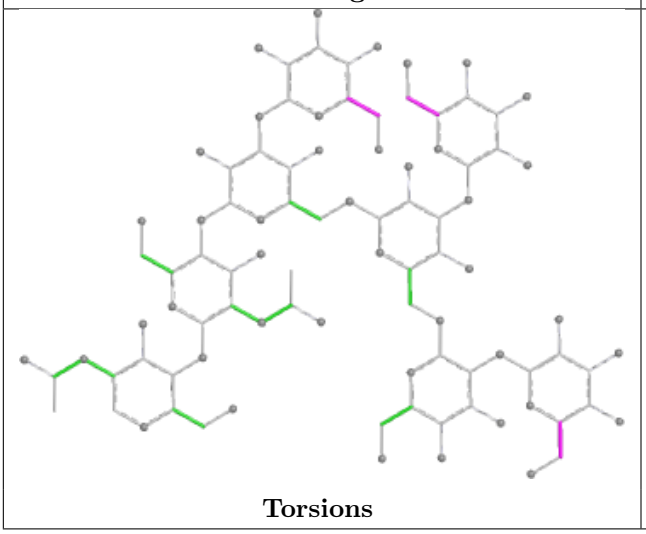
Oligosaccharide Chain f



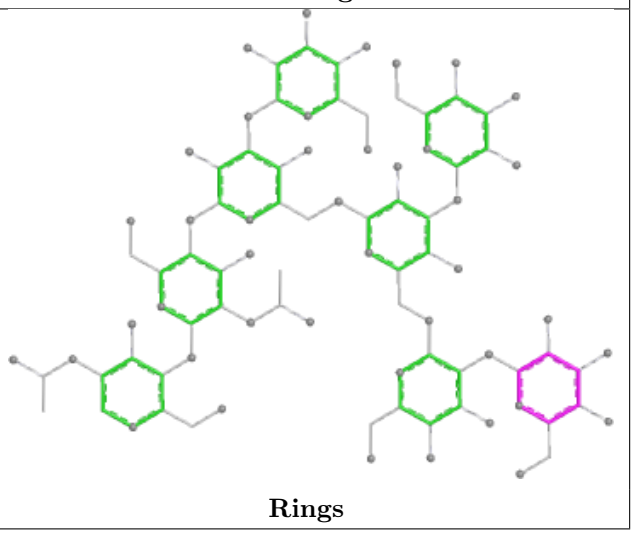
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

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	H	201	-	30,30,50	1.13	2 (6%)	31,31,56	1.17	3 (9%)
5	PGT	L	201	-	30,30,50	1.11	3 (10%)	31,31,56	1.05	3 (9%)
5	PGT	P	201	-	30,30,50	1.08	3 (10%)	31,31,56	1.17	4 (12%)

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%)

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	H	201	-	-	17/30/30/55	-
5	PGT	L	201	-	-	16/30/30/55	-
5	PGT	P	201	-	-	17/30/30/55	-
5	PGT	D	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(^{o})	Ideal(^{o})
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:

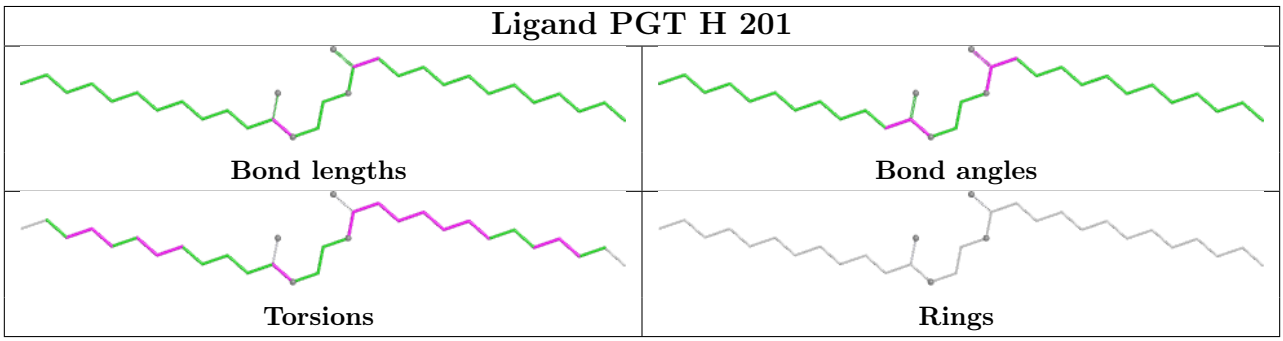
Mol	Chain	Res	Type	Atoms
5	D	201	PGT	C12-C11-O3-C3
5	H	201	PGT	C12-C11-O3-C3
5	H	201	PGT	O11-C11-O3-C3
5	P	201	PGT	O11-C11-O3-C3
5	D	201	PGT	O11-C11-O3-C3

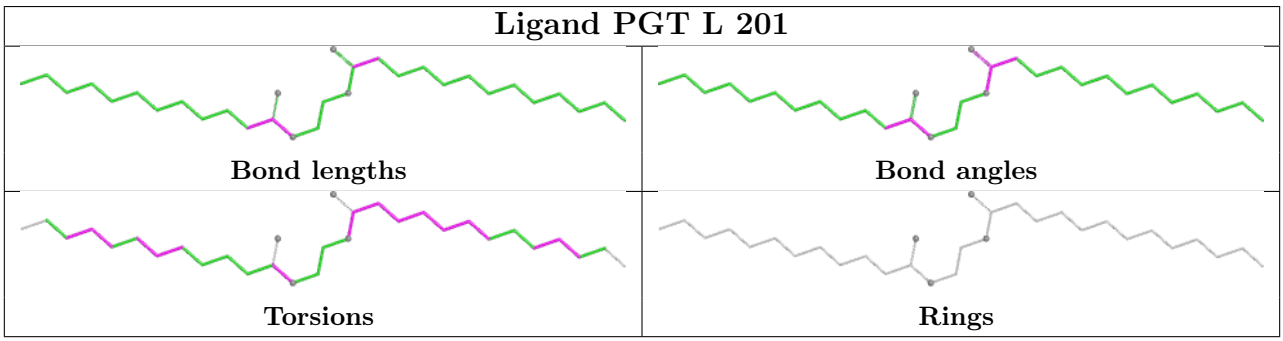
There are no ring outliers.

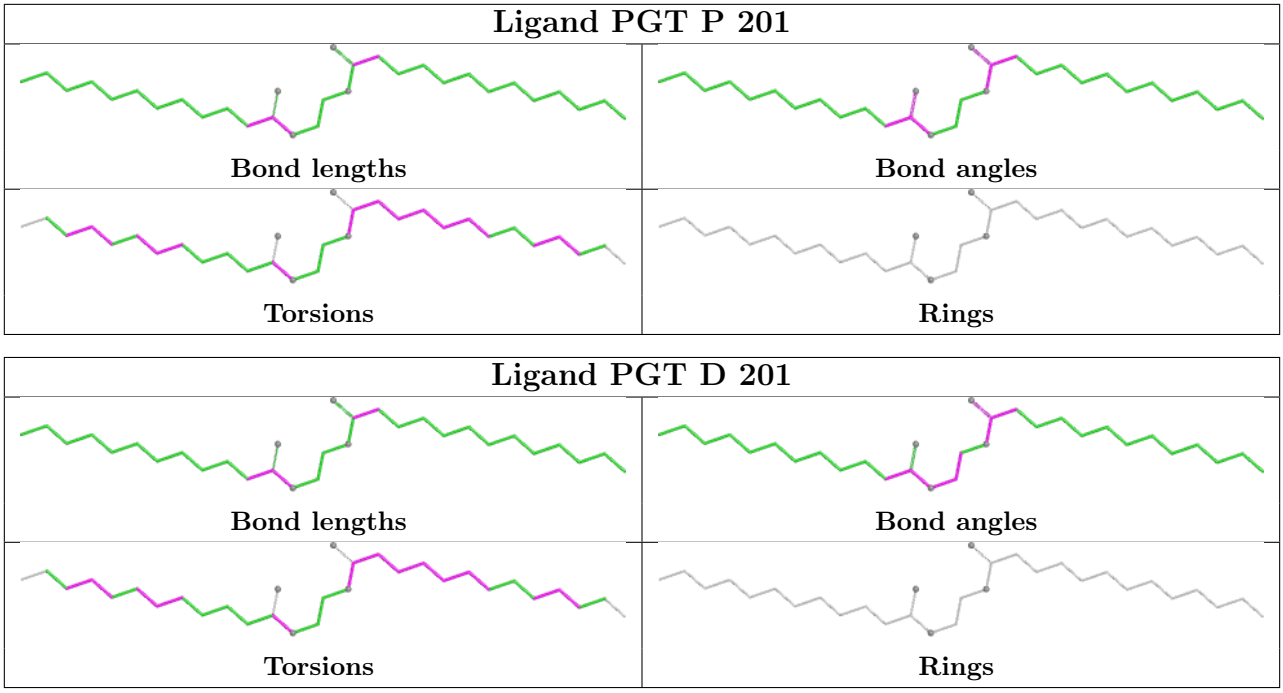
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	201	PGT	1	0
5	L	201	PGT	1	0
5	P	201	PGT	1	0
5	D	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 then 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, 95^{th} 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%)	-0.06	8 (1%)	74	69	47, 67, 96, 120	0
1	B	599/612 (97%)	-0.24	2 (0%)	90	88	41, 59, 76, 85	0
1	E	592/612 (96%)	0.24	20 (3%)	48	42	55, 94, 128, 161	0
1	F	599/612 (97%)	0.02	4 (0%)	84	81	57, 85, 118, 134	0
1	I	397/612 (64%)	0.31	15 (3%)	44	38	55, 94, 136, 151	0
1	J	599/612 (97%)	0.13	10 (1%)	69	63	65, 89, 114, 127	0
1	M	593/612 (96%)	-0.05	6 (1%)	79	74	47, 71, 98, 124	0
1	N	599/612 (97%)	-0.20	5 (0%)	82	78	46, 63, 88, 104	0
2	C	138/147 (93%)	-0.17	1 (0%)	84	81	46, 61, 98, 108	0
2	D	136/147 (92%)	-0.16	5 (3%)	45	39	43, 59, 108, 125	0
2	G	138/147 (93%)	-0.11	2 (1%)	73	68	54, 72, 104, 112	0
2	H	138/147 (93%)	-0.22	4 (2%)	54	48	54, 65, 82, 86	0
2	K	136/147 (92%)	0.17	2 (1%)	71	66	59, 84, 139, 159	0
2	L	138/147 (93%)	-0.11	4 (2%)	54	48	57, 68, 85, 93	0
2	O	138/147 (93%)	-0.22	2 (1%)	73	68	45, 59, 100, 117	0
2	P	135/147 (91%)	-0.08	4 (2%)	52	47	45, 64, 112, 131	0
All	All	5669/6072 (93%)	-0.02	94 (1%)	69	63	41, 74, 116, 161	0

The worst 5 of 94 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	4.4
2	L	54	GLN	4.3
2	G	158	TYR	4.1

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)

SUGAR-RSR INFOmissingINFO

6.4 Ligands (i)

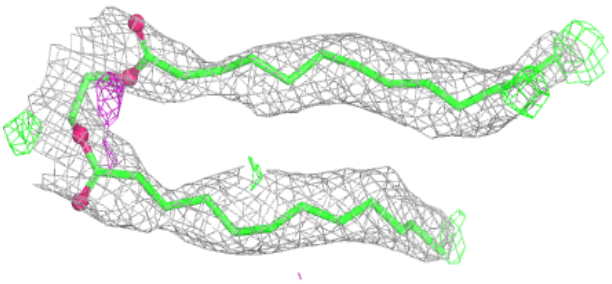
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

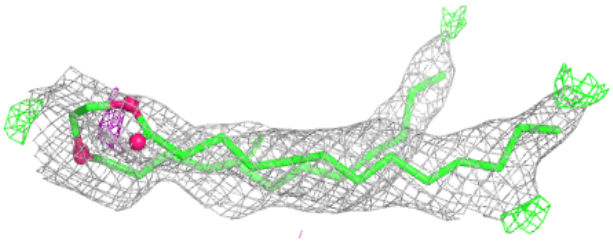
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGT	H	201	31/51	0.71	0.20	71,79,92,93	0
5	PGT	L	201	31/51	0.72	0.23	71,78,92,93	0
5	PGT	P	201	31/51	0.77	0.16	71,78,92,93	0
5	PGT	D	201	31/51	0.79	0.18	71,78,92,93	0

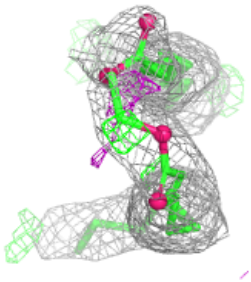
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

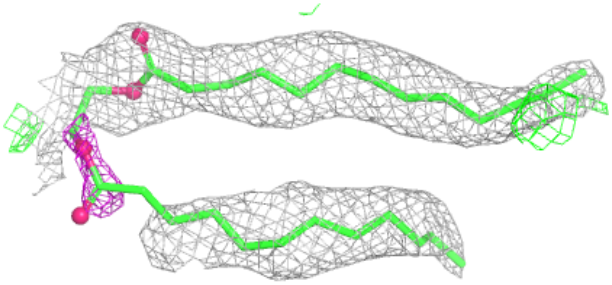


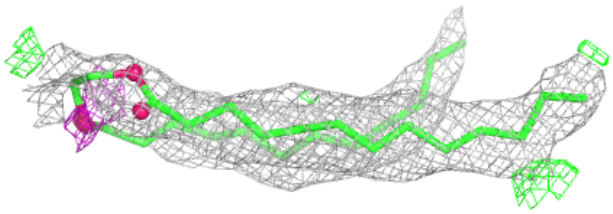


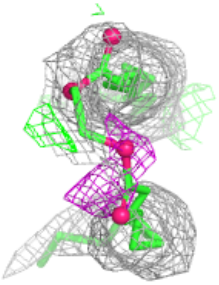


Electron density around PGT L 201:

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

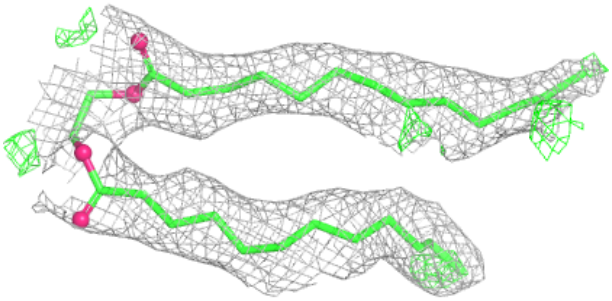


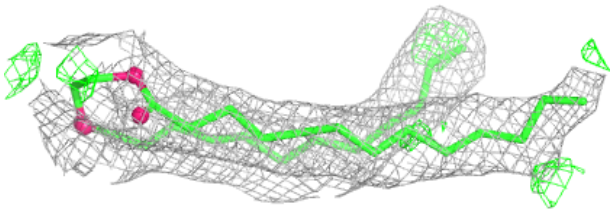


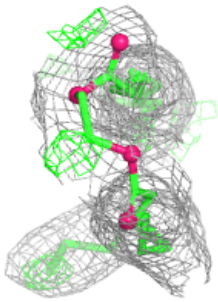


Electron density around PGT P 201:

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

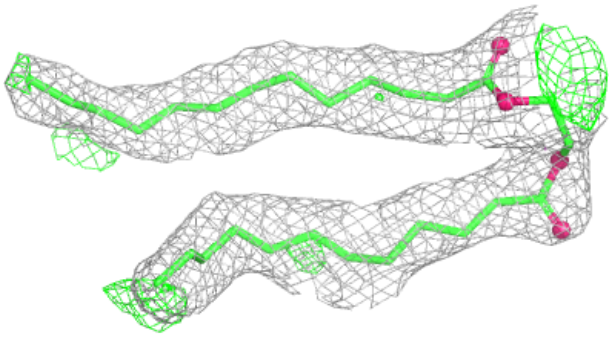


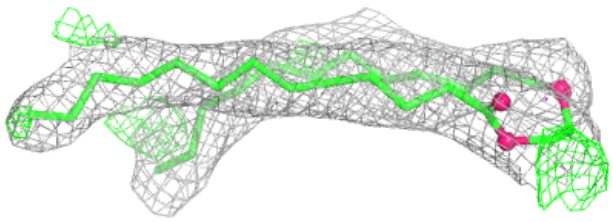


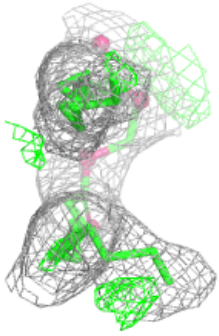


Electron density around PGT D 201:

$2mF_o$-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.