Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 09:40 AM EDT

PDB ID	:	6OPO
EMDB ID	:	EMD-20151
Title	:	Symmetric model of CD4- and 17-bound B41 HIV-1 Env SOSIP in complex with DDM
Authors	:	Ozorowski, G.; Torres, J.L.; Ward, A.B.
Deposited on	:	2019-04-25
Resolution	:	3.50 Å(reported)
Based on initial model	:	5VN3

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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 (1)) were used in the production of this report:

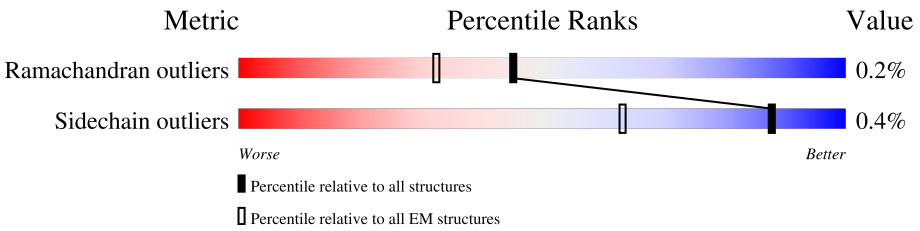
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	524	70% • 27%
1	D	524	70% • 27%
1	J	524	70% • 27%
2	E	214	50% • 49%
2	K	214	49% • 49%
2	L	214	50% • 49%
3	B	153	86% • 10%
3	F	153	86% • 10%
3	M	153	86% • 10%

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Mol	Chain	Length	Quality of chain
4	C	208	46% 53%
4	G	208	46% 53%
4	N	208	46% 53%
5	H	229	52% • 45%
5	I	229	52% • 45%
5	O	229	52% • 45%
6	P	2	100%
6	Q	2	100%
6	S	2	100%
6	T	2	100%
6	U	2	100%
6	V	2	100%
6	W	2	100%
6	X	2	100%
6	Z	2	100%
6	a	2	100%
6	c	2	100%
6	d	2	100%
6	e	2	100%
6	f	2	100%
6	g	2	100%
6	h	2	100%
6	j	2	100%
6	k	2	100%
6	m	2	100%

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Mol	Chain	Length	Quality of chain
6	n	2	100%
6	o	2	100%
6	p	2	100%
6	q	2	100%
6	r	2	100%
7	R	5	100%
7	b	5	100%
7	l	5	100%
8	Y	3	100%
8	i	3	100%
8	s	3	100%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 21441 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	384	3004	1882	532	567	23	0	0
1	D	384	3004	1882	532	567	23	0	0
1	J	384	3004	1882	532	567	23	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP B3UES2
A	-3	ASP	-	expression tag	UNP B3UES2
A	-2	ALA	-	expression tag	UNP B3UES2
A	-1	MET	-	expression tag	UNP B3UES2
A	0	LYS	-	expression tag	UNP B3UES2
A	1	ARG	-	expression tag	UNP B3UES2
A	2	GLY	-	expression tag	UNP B3UES2
A	3	LEU	-	expression tag	UNP B3UES2
A	4	CYS	-	expression tag	UNP B3UES2
A	5	CYS	-	expression tag	UNP B3UES2
A	6	VAL	-	expression tag	UNP B3UES2
A	7	LEU	-	expression tag	UNP B3UES2
A	8	LEU	-	expression tag	UNP B3UES2
A	9	LEU	-	expression tag	UNP B3UES2
A	10	CYS	-	expression tag	UNP B3UES2
A	11	GLY	-	expression tag	UNP B3UES2
A	12	ALA	-	expression tag	UNP B3UES2
A	13	VAL	-	expression tag	UNP B3UES2
A	14	PHE	-	expression tag	UNP B3UES2
A	15	VAL	-	expression tag	UNP B3UES2
A	16	SER	-	expression tag	UNP B3UES2
A	17	PRO	-	expression tag	UNP B3UES2
A	18	SER	-	expression tag	UNP B3UES2
A	19	GLN	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLU	-	expression tag	UNP B3UES2
A	21	ILE	-	expression tag	UNP B3UES2
A	22	HIS	-	expression tag	UNP B3UES2
A	23	ALA	-	expression tag	UNP B3UES2
A	24	ARG	-	expression tag	UNP B3UES2
A	25	PHE	-	expression tag	UNP B3UES2
A	26	ARG	-	expression tag	UNP B3UES2
A	27	ARG	-	expression tag	UNP B3UES2
A	28	GLY	-	expression tag	UNP B3UES2
A	29	ALA	-	expression tag	UNP B3UES2
A	30	ARG	-	expression tag	UNP B3UES2
A	501	CYS	ALA	engineered mutation	UNP B3UES2
A	509	ARG	GLU	engineered mutation	UNP B3UES2
A	510	ARG	LYS	engineered mutation	UNP B3UES2
A	512	ARG	ALA	engineered mutation	UNP B3UES2
A	513	ARG	VAL	engineered mutation	UNP B3UES2
D	-4	MET	-	initiating methionine	UNP B3UES2
D	-3	ASP	-	expression tag	UNP B3UES2
D	-2	ALA	-	expression tag	UNP B3UES2
D	-1	MET	-	expression tag	UNP B3UES2
D	0	LYS	-	expression tag	UNP B3UES2
D	1	ARG	-	expression tag	UNP B3UES2
D	2	GLY	-	expression tag	UNP B3UES2
D	3	LEU	-	expression tag	UNP B3UES2
D	4	CYS	-	expression tag	UNP B3UES2
D	5	CYS	-	expression tag	UNP B3UES2
D	6	VAL	-	expression tag	UNP B3UES2
D	7	LEU	-	expression tag	UNP B3UES2
D	8	LEU	-	expression tag	UNP B3UES2
D	9	LEU	-	expression tag	UNP B3UES2
D	10	CYS	-	expression tag	UNP B3UES2
D	11	GLY	-	expression tag	UNP B3UES2
D	12	ALA	-	expression tag	UNP B3UES2
D	13	VAL	-	expression tag	UNP B3UES2
D	14	PHE	-	expression tag	UNP B3UES2
D	15	VAL	-	expression tag	UNP B3UES2
D	16	SER	-	expression tag	UNP B3UES2
D	17	PRO	-	expression tag	UNP B3UES2
D	18	SER	-	expression tag	UNP B3UES2
D	19	GLN	-	expression tag	UNP B3UES2
D	20	GLU	-	expression tag	UNP B3UES2
D	21	ILE	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	22	HIS	-	expression tag	UNP B3UES2
D	23	ALA	-	expression tag	UNP B3UES2
D	24	ARG	-	expression tag	UNP B3UES2
D	25	PHE	-	expression tag	UNP B3UES2
D	26	ARG	-	expression tag	UNP B3UES2
D	27	ARG	-	expression tag	UNP B3UES2
D	28	GLY	-	expression tag	UNP B3UES2
D	29	ALA	-	expression tag	UNP B3UES2
D	30	ARG	-	expression tag	UNP B3UES2
D	501	CYS	ALA	engineered mutation	UNP B3UES2
D	509	ARG	GLU	engineered mutation	UNP B3UES2
D	510	ARG	LYS	engineered mutation	UNP B3UES2
D	512	ARG	ALA	engineered mutation	UNP B3UES2
D	513	ARG	VAL	engineered mutation	UNP B3UES2
J	-4	MET	-	initiating methionine	UNP B3UES2
J	-3	ASP	-	expression tag	UNP B3UES2
J	-2	ALA	-	expression tag	UNP B3UES2
J	-1	MET	-	expression tag	UNP B3UES2
J	0	LYS	-	expression tag	UNP B3UES2
J	1	ARG	-	expression tag	UNP B3UES2
J	2	GLY	-	expression tag	UNP B3UES2
J	3	LEU	-	expression tag	UNP B3UES2
J	4	CYS	-	expression tag	UNP B3UES2
J	5	CYS	-	expression tag	UNP B3UES2
J	6	VAL	-	expression tag	UNP B3UES2
J	7	LEU	-	expression tag	UNP B3UES2
J	8	LEU	-	expression tag	UNP B3UES2
J	9	LEU	-	expression tag	UNP B3UES2
J	10	CYS	-	expression tag	UNP B3UES2
J	11	GLY	-	expression tag	UNP B3UES2
J	12	ALA	-	expression tag	UNP B3UES2
J	13	VAL	-	expression tag	UNP B3UES2
J	14	PHE	-	expression tag	UNP B3UES2
J	15	VAL	-	expression tag	UNP B3UES2
J	16	SER	-	expression tag	UNP B3UES2
J	17	PRO	-	expression tag	UNP B3UES2
J	18	SER	-	expression tag	UNP B3UES2
J	19	GLN	-	expression tag	UNP B3UES2
J	20	GLU	-	expression tag	UNP B3UES2
J	21	ILE	-	expression tag	UNP B3UES2
J	22	HIS	-	expression tag	UNP B3UES2
J	23	ALA	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	24	ARG	-	expression tag	UNP B3UES2
J	25	PHE	-	expression tag	UNP B3UES2
J	26	ARG	-	expression tag	UNP B3UES2
J	27	ARG	-	expression tag	UNP B3UES2
J	28	GLY	-	expression tag	UNP B3UES2
J	29	ALA	-	expression tag	UNP B3UES2
J	30	ARG	-	expression tag	UNP B3UES2
J	501	CYS	ALA	engineered mutation	UNP B3UES2
J	509	ARG	GLU	engineered mutation	UNP B3UES2
J	510	ARG	LYS	engineered mutation	UNP B3UES2
J	512	ARG	ALA	engineered mutation	UNP B3UES2
J	513	ARG	VAL	engineered mutation	UNP B3UES2

- Molecule 2 is a protein called 17b Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	110	849	531	148	168	2	0	0
2	E	110	849	531	148	168	2	0	0
2	K	110	849	531	148	168	2	0	0

- Molecule 3 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	137	1089	695	185	201	8	0	0
3	F	137	1089	695	185	201	8	0	0
3	M	137	1089	695	185	201	8	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP B3UEZ6
B	605	CYS	THR	engineered mutation	UNP B3UEZ6
F	559	PRO	ILE	engineered mutation	UNP B3UEZ6
F	605	CYS	THR	engineered mutation	UNP B3UEZ6
M	559	PRO	ILE	engineered mutation	UNP B3UEZ6
M	605	CYS	THR	engineered mutation	UNP B3UEZ6

- Molecule 4 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	97	775	487	136	150	2	0	0
4	G	97	775	487	136	150	2	0	0
4	N	97	775	487	136	150	2	0	0

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP P01730
C	-18	GLU	-	expression tag	UNP P01730
C	-17	THR	-	expression tag	UNP P01730
C	-16	ASP	-	expression tag	UNP P01730
C	-15	THR	-	expression tag	UNP P01730
C	-14	LEU	-	expression tag	UNP P01730
C	-13	LEU	-	expression tag	UNP P01730
C	-12	LEU	-	expression tag	UNP P01730
C	-11	TRP	-	expression tag	UNP P01730
C	-10	VAL	-	expression tag	UNP P01730
C	-9	LEU	-	expression tag	UNP P01730
C	-8	LEU	-	expression tag	UNP P01730
C	-7	LEU	-	expression tag	UNP P01730
C	-6	TRP	-	expression tag	UNP P01730
C	-5	VAL	-	expression tag	UNP P01730
C	-4	PRO	-	expression tag	UNP P01730
C	-3	GLY	-	expression tag	UNP P01730
C	-2	SER	-	expression tag	UNP P01730
C	-1	THR	-	expression tag	UNP P01730
C	179	GLY	-	expression tag	UNP P01730
C	180	GLY	-	expression tag	UNP P01730
C	181	SER	-	expression tag	UNP P01730
C	182	GLY	-	expression tag	UNP P01730
C	183	HIS	-	expression tag	UNP P01730
C	184	HIS	-	expression tag	UNP P01730
C	185	HIS	-	expression tag	UNP P01730
C	186	HIS	-	expression tag	UNP P01730
C	187	HIS	-	expression tag	UNP P01730
C	188	HIS	-	expression tag	UNP P01730
G	-19	MET	-	initiating methionine	UNP P01730
G	-18	GLU	-	expression tag	UNP P01730
G	-17	THR	-	expression tag	UNP P01730

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	ASP	-	expression tag	UNP P01730
G	-15	THR	-	expression tag	UNP P01730
G	-14	LEU	-	expression tag	UNP P01730
G	-13	LEU	-	expression tag	UNP P01730
G	-12	LEU	-	expression tag	UNP P01730
G	-11	TRP	-	expression tag	UNP P01730
G	-10	VAL	-	expression tag	UNP P01730
G	-9	LEU	-	expression tag	UNP P01730
G	-8	LEU	-	expression tag	UNP P01730
G	-7	LEU	-	expression tag	UNP P01730
G	-6	TRP	-	expression tag	UNP P01730
G	-5	VAL	-	expression tag	UNP P01730
G	-4	PRO	-	expression tag	UNP P01730
G	-3	GLY	-	expression tag	UNP P01730
G	-2	SER	-	expression tag	UNP P01730
G	-1	THR	-	expression tag	UNP P01730
G	179	GLY	-	expression tag	UNP P01730
G	180	GLY	-	expression tag	UNP P01730
G	181	SER	-	expression tag	UNP P01730
G	182	GLY	-	expression tag	UNP P01730
G	183	HIS	-	expression tag	UNP P01730
G	184	HIS	-	expression tag	UNP P01730
G	185	HIS	-	expression tag	UNP P01730
G	186	HIS	-	expression tag	UNP P01730
G	187	HIS	-	expression tag	UNP P01730
G	188	HIS	-	expression tag	UNP P01730
N	-19	MET	-	initiating methionine	UNP P01730
N	-18	GLU	-	expression tag	UNP P01730
N	-17	THR	-	expression tag	UNP P01730
N	-16	ASP	-	expression tag	UNP P01730
N	-15	THR	-	expression tag	UNP P01730
N	-14	LEU	-	expression tag	UNP P01730
N	-13	LEU	-	expression tag	UNP P01730
N	-12	LEU	-	expression tag	UNP P01730
N	-11	TRP	-	expression tag	UNP P01730
N	-10	VAL	-	expression tag	UNP P01730
N	-9	LEU	-	expression tag	UNP P01730
N	-8	LEU	-	expression tag	UNP P01730
N	-7	LEU	-	expression tag	UNP P01730
N	-6	TRP	-	expression tag	UNP P01730
N	-5	VAL	-	expression tag	UNP P01730
N	-4	PRO	-	expression tag	UNP P01730

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-3	GLY	-	expression tag	UNP P01730
N	-2	SER	-	expression tag	UNP P01730
N	-1	THR	-	expression tag	UNP P01730
N	179	GLY	-	expression tag	UNP P01730
N	180	GLY	-	expression tag	UNP P01730
N	181	SER	-	expression tag	UNP P01730
N	182	GLY	-	expression tag	UNP P01730
N	183	HIS	-	expression tag	UNP P01730
N	184	HIS	-	expression tag	UNP P01730
N	185	HIS	-	expression tag	UNP P01730
N	186	HIS	-	expression tag	UNP P01730
N	187	HIS	-	expression tag	UNP P01730
N	188	HIS	-	expression tag	UNP P01730

- Molecule 5 is a protein called 17b Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	127	987	623	169	192	3	0	0
5	I	127	987	623	169	192	3	0	0
5	O	127	987	623	169	192	3	0	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	P	2	28	16	2	10	0	0
6	Q	2	28	16	2	10	0	0
6	S	2	28	16	2	10	0	0
6	T	2	28	16	2	10	0	0
6	U	2	28	16	2	10	0	0

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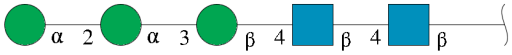
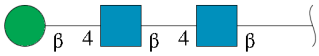
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	V	2	28	16	2	10	0	0
6	W	2	28	16	2	10	0	0
6	X	2	28	16	2	10	0	0
6	Z	2	28	16	2	10	0	0
6	a	2	28	16	2	10	0	0
6	c	2	28	16	2	10	0	0
6	d	2	28	16	2	10	0	0
6	e	2	28	16	2	10	0	0
6	f	2	28	16	2	10	0	0
6	g	2	28	16	2	10	0	0
6	h	2	28	16	2	10	0	0
6	j	2	28	16	2	10	0	0
6	k	2	28	16	2	10	0	0
6	m	2	28	16	2	10	0	0
6	n	2	28	16	2	10	0	0
6	o	2	28	16	2	10	0	0
6	p	2	28	16	2	10	0	0
6	q	2	28	16	2	10	0	0
6	r	2	28	16	2	10	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



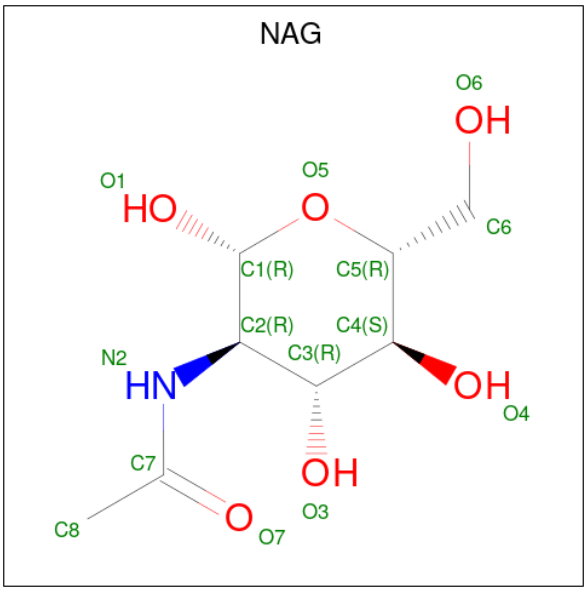
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	R	5	61	34	2	25	0	0
7	b	5	61	34	2	25	0	0
7	l	5	61	34	2	25	0	0

- Molecule 8 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				AltConf	Trace
			Total	C	N	O		
8	Y	3	39	22	2	15	0	0
8	i	3	39	22	2	15	0	0
8	s	3	39	22	2	15	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



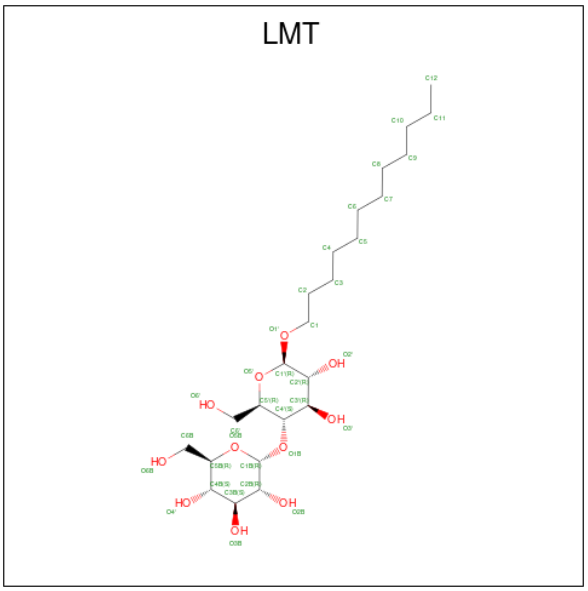
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	A	1	14	8	1	5	0
9	A	1	14	8	1	5	0
9	A	1	14	8	1	5	0
9	A	1	14	8	1	5	0
9	B	1	14	8	1	5	0
9	B	1	14	8	1	5	0
9	D	1	14	8	1	5	0
9	D	1	14	8	1	5	0
9	D	1	14	8	1	5	0
9	D	1	14	8	1	5	0
9	F	1	14	8	1	5	0
9	F	1	14	8	1	5	0
9	J	1	14	8	1	5	0
9	J	1	14	8	1	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	J	1	14	8	1	5	0
9	J	1	14	8	1	5	0
9	M	1	14	8	1	5	0
9	M	1	14	8	1	5	0

- Molecule 10 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



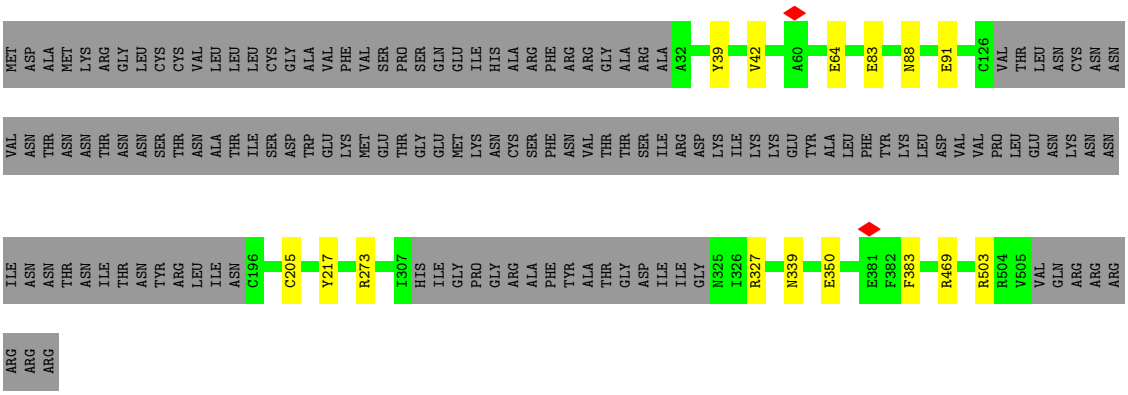
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	B	1	35	24	11	0
10	F	1	35	24	11	0
10	M	1	35	24	11	0

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

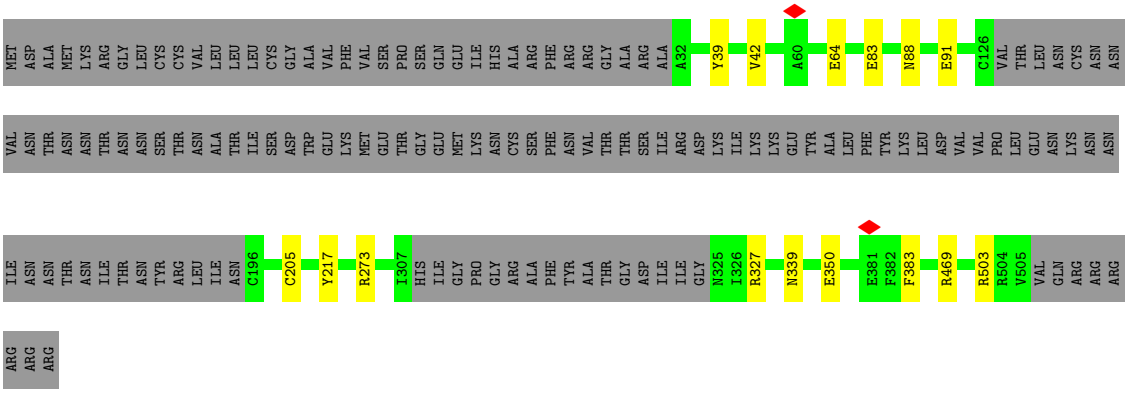
- Molecule 1: Envelope glycoprotein gp160

Chain A:



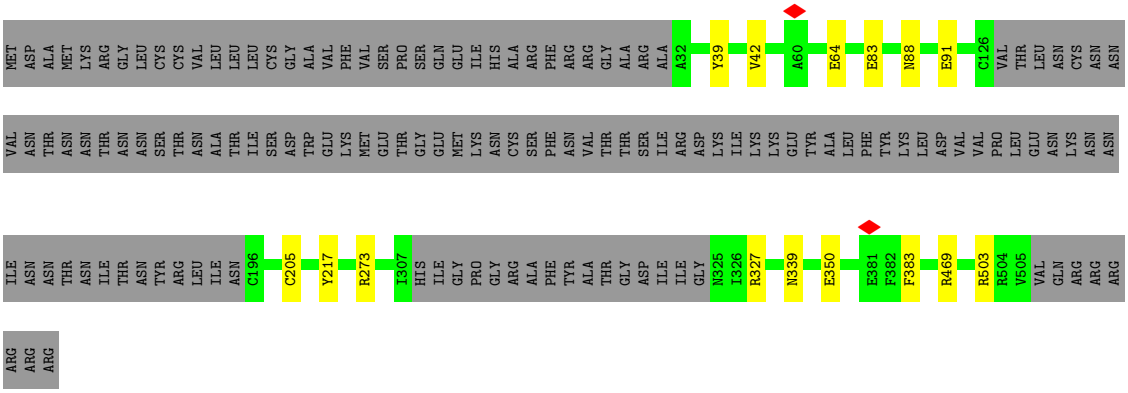
- Molecule 1: Envelope glycoprotein gp160

Chain D:



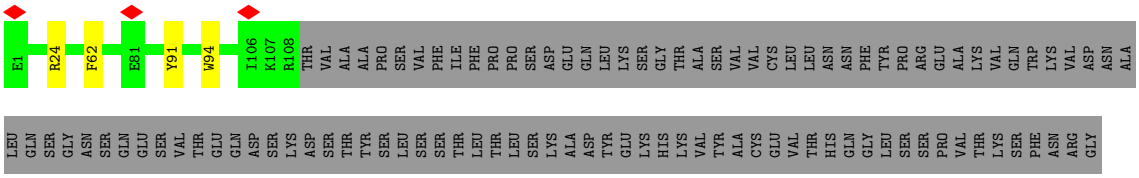
- Molecule 1: Envelope glycoprotein gp160

Chain J:



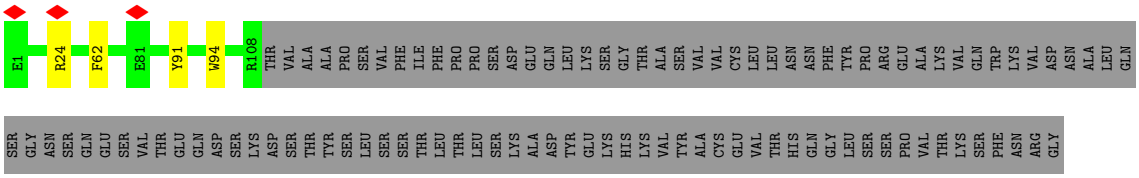
- Molecule 2: 17b Fab light chain

Chain L:



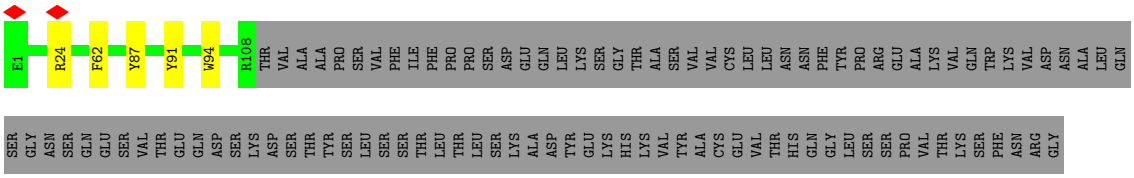
- Molecule 2: 17b Fab light chain

Chain E:



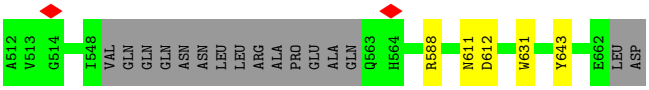
- Molecule 2: 17b Fab light chain

Chain K:



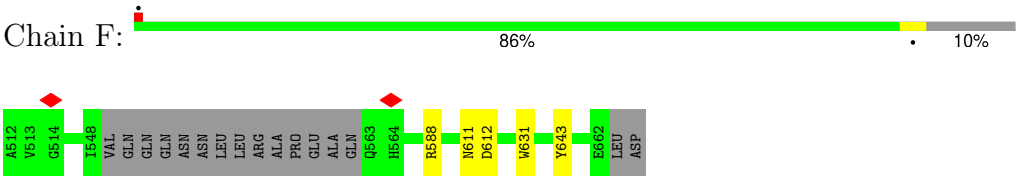
- Molecule 3: Envelope glycoprotein gp41

Chain B:



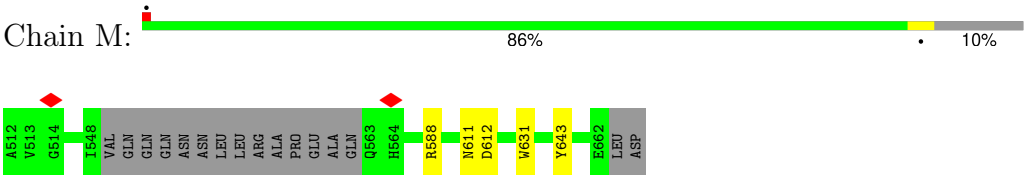
• Molecule 3: Envelope glycoprotein gp41

Chain F:



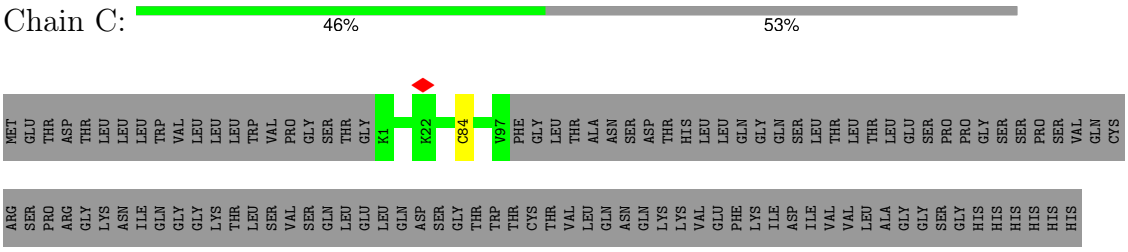
• Molecule 3: Envelope glycoprotein gp41

Chain M:



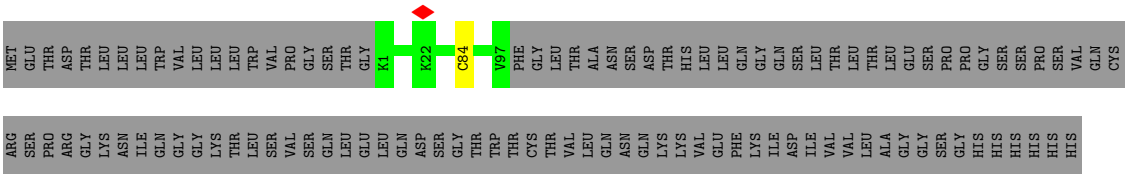
• Molecule 4: T-cell surface glycoprotein CD4

Chain C:



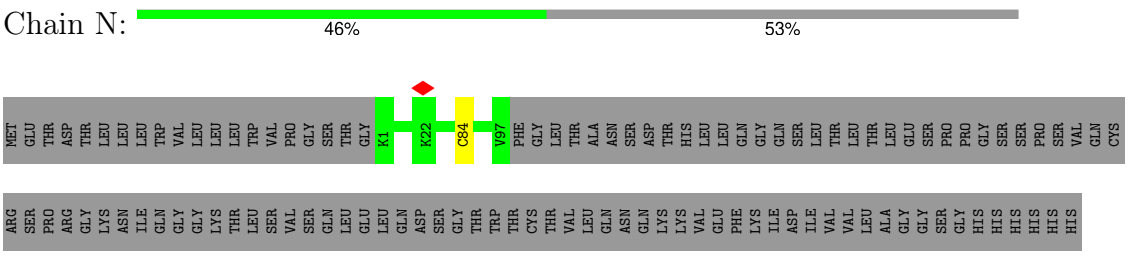
• Molecule 4: T-cell surface glycoprotein CD4

Chain G:



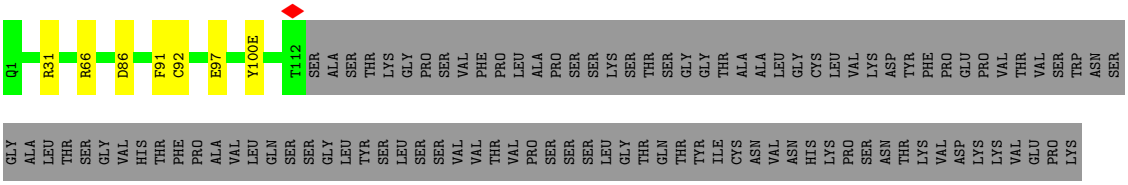
• Molecule 4: T-cell surface glycoprotein CD4

Chain N:



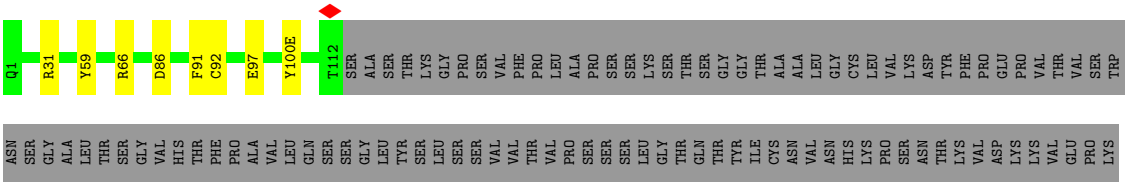
• Molecule 5: 17b Fab heavy chain

Chain H:



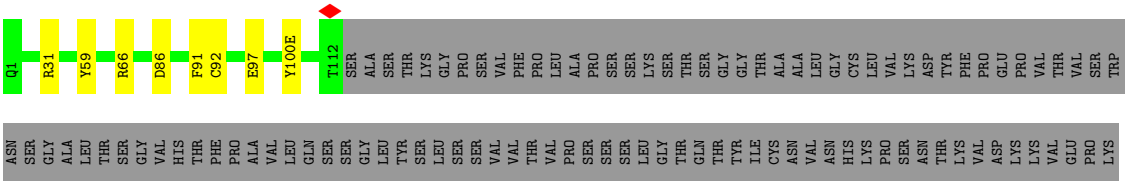
• Molecule 5: 17b Fab heavy chain

Chain I:



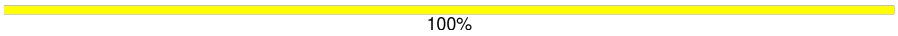
• Molecule 5: 17b Fab heavy chain

Chain O:



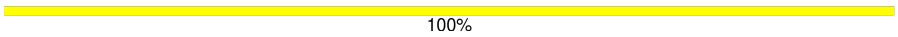
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



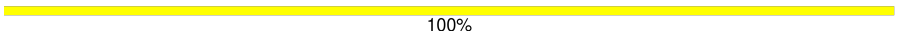
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r: 100%

NAG1
NAG2

• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 100%

NAG1
NAG2
BMA3
MAN4
MAN5

• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 100%

NAG1
NAG2
BMA3
MAN4
MAN5

• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l: 100%

NAG1
NAG2
BMA3
MAN4
MAN5

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 100%

NAG1
NAG2
BMA3

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i: 100%

NAG1
NAG2
BMA3

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s: 100%

NAG1
NAG2
BMA3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	183480	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.493	Depositor
Minimum map value	-2.680	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	377.27997, 377.27997, 377.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

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: NAG, BMA, LMT, 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	1.06	7/3070 (0.2%)	0.88	5/4177 (0.1%)
1	D	1.06	7/3070 (0.2%)	0.88	5/4177 (0.1%)
1	J	1.06	7/3070 (0.2%)	0.88	5/4177 (0.1%)
2	E	1.20	5/869 (0.6%)	1.04	2/1181 (0.2%)
2	K	1.20	6/869 (0.7%)	1.04	2/1181 (0.2%)
2	L	1.20	5/869 (0.6%)	1.04	2/1181 (0.2%)
3	B	1.14	2/1109 (0.2%)	0.86	2/1503 (0.1%)
3	F	1.14	2/1109 (0.2%)	0.86	2/1503 (0.1%)
3	M	1.15	2/1109 (0.2%)	0.86	2/1503 (0.1%)
4	C	1.06	1/785 (0.1%)	0.88	0/1053
4	G	1.06	1/785 (0.1%)	0.88	0/1053
4	N	1.06	1/785 (0.1%)	0.88	0/1053
5	H	1.14	4/1008 (0.4%)	1.04	6/1368 (0.4%)
5	I	1.15	4/1008 (0.4%)	1.04	7/1368 (0.5%)
5	O	1.14	4/1008 (0.4%)	1.04	7/1368 (0.5%)
All	All	1.11	58/20523 (0.3%)	0.92	47/27846 (0.2%)

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	91	TYR	CB-CG	-9.42	1.37	1.51
2	K	91	TYR	CB-CG	-9.40	1.37	1.51
2	E	91	TYR	CB-CG	-9.38	1.37	1.51
5	I	92	CYS	CB-SG	-7.35	1.69	1.82
5	O	92	CYS	CB-SG	-7.34	1.69	1.82
5	H	92	CYS	CB-SG	-7.33	1.69	1.82
4	C	84	CYS	CB-SG	-7.30	1.69	1.82
4	G	84	CYS	CB-SG	-7.25	1.70	1.82
4	N	84	CYS	CB-SG	-7.21	1.70	1.82
2	E	91	TYR	CD1-CE1	-6.37	1.29	1.39
2	K	91	TYR	CD1-CE1	-6.35	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	91	TYR	CD1-CE1	-6.34	1.29	1.39
1	D	205	CYS	CB-SG	-6.32	1.71	1.82
1	D	91	GLU	CD-OE1	-6.29	1.18	1.25
1	J	205	CYS	CB-SG	-6.28	1.71	1.82
1	A	205	CYS	CB-SG	-6.27	1.71	1.82
1	A	91	GLU	CD-OE1	-6.24	1.18	1.25
1	J	91	GLU	CD-OE1	-6.22	1.18	1.25
1	J	64	GLU	CG-CD	-6.11	1.42	1.51
1	A	64	GLU	CG-CD	-6.10	1.42	1.51
1	D	64	GLU	CG-CD	-6.10	1.42	1.51
1	D	42	VAL	CB-CG1	-6.05	1.40	1.52
1	J	42	VAL	CB-CG1	-6.05	1.40	1.52
2	K	94	TRP	CB-CG	-6.02	1.39	1.50
1	A	42	VAL	CB-CG1	-6.02	1.40	1.52
2	L	94	TRP	CB-CG	-6.02	1.39	1.50
2	E	94	TRP	CB-CG	-6.00	1.39	1.50
2	K	62	PHE	CB-CG	-5.76	1.41	1.51
5	O	100(E)	TYR	CB-CG	-5.76	1.43	1.51
2	E	62	PHE	CB-CG	-5.75	1.41	1.51
2	L	62	PHE	CB-CG	-5.73	1.41	1.51
5	I	100(E)	TYR	CB-CG	-5.71	1.43	1.51
5	H	100(E)	TYR	CB-CG	-5.69	1.43	1.51
3	M	631	TRP	CD2-CE2	-5.61	1.34	1.41
1	D	83	GLU	CD-OE2	-5.60	1.19	1.25
1	A	83	GLU	CD-OE2	-5.58	1.19	1.25
3	F	631	TRP	CD2-CE2	-5.58	1.34	1.41
1	J	83	GLU	CD-OE2	-5.56	1.19	1.25
3	B	631	TRP	CD2-CE2	-5.56	1.34	1.41
1	A	39	TYR	CB-CG	-5.52	1.43	1.51
1	D	39	TYR	CB-CG	-5.51	1.43	1.51
1	J	39	TYR	CB-CG	-5.51	1.43	1.51
5	I	97	GLU	CG-CD	-5.37	1.43	1.51
5	O	97	GLU	CG-CD	-5.36	1.44	1.51
5	H	97	GLU	CG-CD	-5.34	1.44	1.51
3	M	631	TRP	CB-CG	-5.34	1.40	1.50
3	F	631	TRP	CB-CG	-5.31	1.40	1.50
3	B	631	TRP	CB-CG	-5.31	1.40	1.50
2	E	91	TYR	CG-CD1	-5.17	1.32	1.39
1	A	350	GLU	CD-OE1	-5.16	1.20	1.25
1	J	350	GLU	CD-OE1	-5.15	1.20	1.25
2	K	91	TYR	CG-CD1	-5.15	1.32	1.39
5	H	97	GLU	CD-OE1	-5.15	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	350	GLU	CD-OE1	-5.14	1.20	1.25
2	L	91	TYR	CG-CD1	-5.14	1.32	1.39
5	I	97	GLU	CD-OE1	-5.09	1.20	1.25
5	O	97	GLU	CD-OE1	-5.07	1.20	1.25
2	K	87	TYR	CB-CG	-5.00	1.44	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	66	ARG	NE-CZ-NH2	-10.70	114.95	120.30
5	I	66	ARG	NE-CZ-NH2	-10.66	114.97	120.30
5	O	66	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	J	327	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	D	327	ARG	NE-CZ-NH2	-9.01	115.79	120.30
1	A	327	ARG	NE-CZ-NH2	-8.93	115.83	120.30
2	L	24	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	E	24	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	K	24	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	D	503	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	J	503	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	503	ARG	NE-CZ-NH1	8.33	124.47	120.30
5	H	66	ARG	NE-CZ-NH1	7.30	123.95	120.30
5	I	66	ARG	NE-CZ-NH1	7.29	123.95	120.30
5	O	66	ARG	NE-CZ-NH1	7.23	123.92	120.30
5	I	31	ARG	NE-CZ-NH2	-6.87	116.86	120.30
5	H	31	ARG	NE-CZ-NH2	-6.87	116.87	120.30
5	O	31	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	D	217	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	J	217	TYR	CB-CG-CD2	-6.66	117.00	121.00
1	A	217	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	J	273	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	273	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	D	273	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	K	91	TYR	CB-CG-CD1	-6.33	117.20	121.00
2	E	91	TYR	CB-CG-CD1	-6.33	117.20	121.00
2	L	91	TYR	CB-CG-CD1	-6.32	117.21	121.00
3	F	588	ARG	NE-CZ-NH2	-6.03	117.28	120.30
3	M	588	ARG	NE-CZ-NH2	-6.00	117.30	120.30
3	B	588	ARG	NE-CZ-NH2	-5.97	117.31	120.30
5	I	100(E)	TYR	CB-CG-CD2	-5.82	117.51	121.00
5	I	86	ASP	CB-CG-OD1	5.81	123.53	118.30
5	O	86	ASP	CB-CG-OD1	5.78	123.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	O	100(E)	TYR	CB-CG-CD2	-5.78	117.53	121.00
5	H	86	ASP	CB-CG-OD1	5.76	123.49	118.30
5	H	100(E)	TYR	CB-CG-CD2	-5.76	117.54	121.00
1	D	469	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	A	469	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	J	469	ARG	NE-CZ-NH2	5.28	122.94	120.30
3	M	643	TYR	CB-CG-CD1	-5.17	117.90	121.00
3	B	643	TYR	CB-CG-CD1	-5.16	117.90	121.00
3	F	643	TYR	CB-CG-CD1	-5.13	117.92	121.00
5	O	59	TYR	CB-CG-CD1	-5.13	117.92	121.00
5	I	59	TYR	CB-CG-CD1	-5.12	117.93	121.00
5	I	91	PHE	CB-CG-CD1	5.08	124.36	120.80
5	H	91	PHE	CB-CG-CD1	5.05	124.33	120.80
5	O	91	PHE	CB-CG-CD1	5.04	124.33	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 PDB entries followed by that with respect to all EM entries.

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	378/524 (72%)	367 (97%)	10 (3%)	1 (0%)	37	68
1	D	378/524 (72%)	367 (97%)	10 (3%)	1 (0%)	37	68
1	J	378/524 (72%)	367 (97%)	10 (3%)	1 (0%)	37	68
2	E	108/214 (50%)	106 (98%)	2 (2%)	0	100	100
2	K	108/214 (50%)	106 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	108/214 (50%)	106 (98%)	2 (2%)	0	100	100
3	B	133/153 (87%)	130 (98%)	2 (2%)	1 (1%)	16	51
3	F	133/153 (87%)	130 (98%)	2 (2%)	1 (1%)	16	51
3	M	133/153 (87%)	130 (98%)	2 (2%)	1 (1%)	16	51
4	C	95/208 (46%)	95 (100%)	0	0	100	100
4	G	95/208 (46%)	95 (100%)	0	0	100	100
4	N	95/208 (46%)	95 (100%)	0	0	100	100
5	H	125/229 (55%)	124 (99%)	1 (1%)	0	100	100
5	I	125/229 (55%)	124 (99%)	1 (1%)	0	100	100
5	O	125/229 (55%)	124 (99%)	1 (1%)	0	100	100
All	All	2517/3984 (63%)	2466 (98%)	45 (2%)	6 (0%)	45	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	612	ASP
3	F	612	ASP
3	M	612	ASP
1	A	383	PHE
1	D	383	PHE
1	J	383	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 PDB entries followed by that with respect to all EM entries.

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	338/461 (73%)	336 (99%)	2 (1%)	84	91
1	D	338/461 (73%)	336 (99%)	2 (1%)	84	91
1	J	338/461 (73%)	336 (99%)	2 (1%)	84	91
2	E	91/184 (50%)	91 (100%)	0	100	100
2	K	91/184 (50%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	91/184 (50%)	91 (100%)	0	100	100
3	B	116/130 (89%)	115 (99%)	1 (1%)	75	86
3	F	116/130 (89%)	115 (99%)	1 (1%)	75	86
3	M	116/130 (89%)	115 (99%)	1 (1%)	75	86
4	C	89/186 (48%)	89 (100%)	0	100	100
4	G	89/186 (48%)	89 (100%)	0	100	100
4	N	89/186 (48%)	89 (100%)	0	100	100
5	H	105/193 (54%)	105 (100%)	0	100	100
5	I	105/193 (54%)	105 (100%)	0	100	100
5	O	105/193 (54%)	105 (100%)	0	100	100
All	All	2217/3462 (64%)	2208 (100%)	9 (0%)	88	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	339	ASN
3	B	611	ASN
1	D	88	ASN
1	D	339	ASN
3	F	611	ASN
1	J	88	ASN
1	J	339	ASN
3	M	611	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	H	102	HIS
5	I	102	HIS
5	O	102	HIS

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)

72 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	P	1	1,6	14,14,15	1.95	3 (21%)	17,19,21	1.04	2 (11%)
6	NAG	P	2	6	14,14,15	2.11	2 (14%)	17,19,21	0.71	0
6	NAG	Q	1	1,6	14,14,15	1.99	3 (21%)	17,19,21	1.14	3 (17%)
6	NAG	Q	2	6	14,14,15	2.09	2 (14%)	17,19,21	0.69	0
7	NAG	R	1	1,7	14,14,15	2.00	1 (7%)	17,19,21	1.18	1 (5%)
7	NAG	R	2	7	14,14,15	2.07	4 (28%)	17,19,21	1.21	2 (11%)
7	BMA	R	3	7	11,11,12	1.88	2 (18%)	15,15,17	1.57	2 (13%)
7	MAN	R	4	7	11,11,12	1.53	2 (18%)	15,15,17	1.06	1 (6%)
7	MAN	R	5	7	11,11,12	1.80	2 (18%)	15,15,17	1.03	2 (13%)
6	NAG	S	1	1,6	14,14,15	2.08	4 (28%)	17,19,21	1.01	1 (5%)
6	NAG	S	2	6	14,14,15	2.12	2 (14%)	17,19,21	0.79	1 (5%)
6	NAG	T	1	1,6	14,14,15	2.07	3 (21%)	17,19,21	0.97	1 (5%)
6	NAG	T	2	6	14,14,15	2.12	2 (14%)	17,19,21	0.73	0
6	NAG	U	1	1,6	14,14,15	2.08	4 (28%)	17,19,21	0.80	1 (5%)
6	NAG	U	2	6	14,14,15	2.12	2 (14%)	17,19,21	0.74	0
6	NAG	V	1	1,6	14,14,15	1.96	3 (21%)	17,19,21	0.91	1 (5%)
6	NAG	V	2	6	14,14,15	2.10	2 (14%)	17,19,21	0.87	1 (5%)
6	NAG	W	1	1,6	14,14,15	1.92	2 (14%)	17,19,21	1.04	1 (5%)
6	NAG	W	2	6	14,14,15	2.12	2 (14%)	17,19,21	0.79	1 (5%)
6	NAG	X	1	1,6	14,14,15	1.95	3 (21%)	17,19,21	1.25	2 (11%)
6	NAG	X	2	6	14,14,15	2.08	2 (14%)	17,19,21	0.69	0
8	NAG	Y	1	8,1	14,14,15	2.12	5 (35%)	17,19,21	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	Y	2	8	14,14,15	2.15	4 (28%)	17,19,21	0.81	1 (5%)
8	BMA	Y	3	8	11,11,12	1.83	2 (18%)	15,15,17	0.85	1 (6%)
6	NAG	Z	1	1,6	14,14,15	1.94	3 (21%)	17,19,21	1.04	2 (11%)
6	NAG	Z	2	6	14,14,15	2.11	2 (14%)	17,19,21	0.70	0
6	NAG	a	1	1,6	14,14,15	2.00	3 (21%)	17,19,21	1.14	3 (17%)
6	NAG	a	2	6	14,14,15	2.08	2 (14%)	17,19,21	0.69	0
7	NAG	b	1	1,7	14,14,15	2.01	1 (7%)	17,19,21	1.18	1 (5%)
7	NAG	b	2	7	14,14,15	2.08	4 (28%)	17,19,21	1.20	2 (11%)
7	BMA	b	3	7	11,11,12	1.87	2 (18%)	15,15,17	1.58	2 (13%)
7	MAN	b	4	7	11,11,12	1.52	2 (18%)	15,15,17	1.07	1 (6%)
7	MAN	b	5	7	11,11,12	1.80	2 (18%)	15,15,17	1.03	2 (13%)
6	NAG	c	1	1,6	14,14,15	2.08	4 (28%)	17,19,21	1.01	1 (5%)
6	NAG	c	2	6	14,14,15	2.11	2 (14%)	17,19,21	0.79	1 (5%)
6	NAG	d	1	1,6	14,14,15	2.07	2 (14%)	17,19,21	0.97	1 (5%)
6	NAG	d	2	6	14,14,15	2.12	2 (14%)	17,19,21	0.73	0
6	NAG	e	1	1,6	14,14,15	2.08	4 (28%)	17,19,21	0.79	1 (5%)
6	NAG	e	2	6	14,14,15	2.12	2 (14%)	17,19,21	0.74	0
6	NAG	f	1	1,6	14,14,15	1.96	3 (21%)	17,19,21	0.91	1 (5%)
6	NAG	f	2	6	14,14,15	2.11	2 (14%)	17,19,21	0.88	1 (5%)
6	NAG	g	1	1,6	14,14,15	1.92	2 (14%)	17,19,21	1.04	1 (5%)
6	NAG	g	2	6	14,14,15	2.11	2 (14%)	17,19,21	0.79	1 (5%)
6	NAG	h	1	1,6	14,14,15	1.97	3 (21%)	17,19,21	1.25	2 (11%)
6	NAG	h	2	6	14,14,15	2.08	2 (14%)	17,19,21	0.70	0
8	NAG	i	1	8,1	14,14,15	2.13	5 (35%)	17,19,21	0.97	1 (5%)
8	NAG	i	2	8	14,14,15	2.15	4 (28%)	17,19,21	0.81	1 (5%)
8	BMA	i	3	8	11,11,12	1.84	2 (18%)	15,15,17	0.85	1 (6%)
6	NAG	j	1	1,6	14,14,15	1.95	3 (21%)	17,19,21	1.05	2 (11%)
6	NAG	j	2	6	14,14,15	2.11	2 (14%)	17,19,21	0.71	0
6	NAG	k	1	1,6	14,14,15	1.99	3 (21%)	17,19,21	1.14	3 (17%)
6	NAG	k	2	6	14,14,15	2.08	2 (14%)	17,19,21	0.69	0
7	NAG	l	1	1,7	14,14,15	2.00	1 (7%)	17,19,21	1.19	1 (5%)
7	NAG	l	2	7	14,14,15	2.08	4 (28%)	17,19,21	1.21	2 (11%)
7	BMA	l	3	7	11,11,12	1.87	2 (18%)	15,15,17	1.57	2 (13%)
7	MAN	l	4	7	11,11,12	1.53	2 (18%)	15,15,17	1.06	1 (6%)
7	MAN	l	5	7	11,11,12	1.81	2 (18%)	15,15,17	1.02	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	m	1	1,6	14,14,15	2.08	4 (28%)	17,19,21	1.01	1 (5%)
6	NAG	m	2	6	14,14,15	2.11	2 (14%)	17,19,21	0.80	1 (5%)
6	NAG	n	1	1,6	14,14,15	2.07	3 (21%)	17,19,21	0.98	1 (5%)
6	NAG	n	2	6	14,14,15	2.12	2 (14%)	17,19,21	0.73	0
6	NAG	o	1	1,6	14,14,15	2.09	4 (28%)	17,19,21	0.80	1 (5%)
6	NAG	o	2	6	14,14,15	2.13	2 (14%)	17,19,21	0.74	0
6	NAG	p	1	1,6	14,14,15	1.94	3 (21%)	17,19,21	0.90	1 (5%)
6	NAG	p	2	6	14,14,15	2.11	2 (14%)	17,19,21	0.88	1 (5%)
6	NAG	q	1	1,6	14,14,15	1.92	2 (14%)	17,19,21	1.03	1 (5%)
6	NAG	q	2	6	14,14,15	2.10	2 (14%)	17,19,21	0.79	1 (5%)
6	NAG	r	1	1,6	14,14,15	1.96	3 (21%)	17,19,21	1.24	2 (11%)
6	NAG	r	2	6	14,14,15	2.08	2 (14%)	17,19,21	0.69	0
8	NAG	s	1	8,1	14,14,15	2.13	5 (35%)	17,19,21	0.96	1 (5%)
8	NAG	s	2	8	14,14,15	2.14	4 (28%)	17,19,21	0.81	1 (5%)
8	BMA	s	3	8	11,11,12	1.83	2 (18%)	15,15,17	0.85	1 (6%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	NAG	W	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	NAG	X	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	X	2	6	-	1/6/23/26	0/1/1/1
8	NAG	Y	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	1/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	1/2/19/22	0/1/1/1
6	NAG	Z	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	NAG	a	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	a	2	6	-	1/6/23/26	0/1/1/1
7	NAG	b	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	2/6/23/26	0/1/1/1
7	BMA	b	3	7	-	2/2/19/22	0/1/1/1
7	MAN	b	4	7	-	1/2/19/22	0/1/1/1
7	MAN	b	5	7	-	1/2/19/22	0/1/1/1
6	NAG	c	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	c	2	6	-	1/6/23/26	0/1/1/1
6	NAG	d	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	d	2	6	-	2/6/23/26	0/1/1/1
6	NAG	e	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	e	2	6	-	2/6/23/26	0/1/1/1
6	NAG	f	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	NAG	g	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	g	2	6	-	2/6/23/26	0/1/1/1
6	NAG	h	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	h	2	6	-	1/6/23/26	0/1/1/1
8	NAG	i	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	i	2	8	-	1/6/23/26	0/1/1/1
8	BMA	i	3	8	-	1/2/19/22	0/1/1/1
6	NAG	j	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	j	2	6	-	2/6/23/26	0/1/1/1
6	NAG	k	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	k	2	6	-	1/6/23/26	0/1/1/1
7	NAG	l	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	l	2	7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	l	3	7	-	2/2/19/22	0/1/1/1
7	MAN	l	4	7	-	1/2/19/22	0/1/1/1
7	MAN	l	5	7	-	1/2/19/22	0/1/1/1
6	NAG	m	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	m	2	6	-	1/6/23/26	0/1/1/1
6	NAG	n	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	n	2	6	-	2/6/23/26	0/1/1/1
6	NAG	o	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	o	2	6	-	2/6/23/26	0/1/1/1
6	NAG	p	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	p	2	6	-	2/6/23/26	0/1/1/1
6	NAG	q	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	q	2	6	-	2/6/23/26	0/1/1/1
6	NAG	r	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	r	2	6	-	1/6/23/26	0/1/1/1
8	NAG	s	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	s	2	8	-	1/6/23/26	0/1/1/1
8	BMA	s	3	8	-	1/2/19/22	0/1/1/1

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	2	NAG	O5-C1	6.79	1.55	1.43
6	S	2	NAG	O5-C1	6.79	1.55	1.43
6	P	2	NAG	O5-C1	6.79	1.55	1.43
6	o	2	NAG	O5-C1	6.78	1.55	1.43
6	j	2	NAG	O5-C1	6.77	1.55	1.43
6	Q	2	NAG	O5-C1	6.77	1.55	1.43
6	c	2	NAG	O5-C1	6.76	1.55	1.43
6	U	2	NAG	O5-C1	6.76	1.55	1.43
6	e	2	NAG	O5-C1	6.76	1.55	1.43
6	m	2	NAG	O5-C1	6.76	1.55	1.43
6	a	2	NAG	O5-C1	6.75	1.55	1.43
6	W	2	NAG	O5-C1	6.74	1.55	1.43
6	k	2	NAG	O5-C1	6.73	1.55	1.43
6	r	2	NAG	O5-C1	6.70	1.54	1.43
6	X	2	NAG	O5-C1	6.68	1.54	1.43
6	h	2	NAG	O5-C1	6.68	1.54	1.43
6	g	2	NAG	O5-C1	6.67	1.54	1.43
6	d	2	NAG	O5-C1	6.66	1.54	1.43
6	q	2	NAG	O5-C1	6.66	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	n	2	NAG	O5-C1	6.65	1.54	1.43
6	T	2	NAG	O5-C1	6.65	1.54	1.43
6	p	2	NAG	O5-C1	6.64	1.54	1.43
6	f	2	NAG	O5-C1	6.64	1.54	1.43
8	Y	2	NAG	O5-C1	6.64	1.54	1.43
7	b	1	NAG	O5-C1	6.64	1.54	1.43
8	i	2	NAG	O5-C1	6.63	1.54	1.43
6	V	2	NAG	O5-C1	6.62	1.54	1.43
7	R	1	NAG	O5-C1	6.62	1.54	1.43
8	s	2	NAG	O5-C1	6.61	1.54	1.43
7	l	1	NAG	O5-C1	6.59	1.54	1.43
8	s	1	NAG	O5-C1	6.52	1.54	1.43
8	i	1	NAG	O5-C1	6.51	1.54	1.43
8	Y	1	NAG	O5-C1	6.49	1.54	1.43
6	T	1	NAG	O5-C1	6.37	1.54	1.43
6	S	1	NAG	O5-C1	6.34	1.54	1.43
6	n	1	NAG	O5-C1	6.33	1.54	1.43
6	c	1	NAG	O5-C1	6.33	1.54	1.43
6	m	1	NAG	O5-C1	6.33	1.54	1.43
6	o	1	NAG	O5-C1	6.33	1.54	1.43
6	d	1	NAG	O5-C1	6.33	1.54	1.43
7	b	2	NAG	O5-C1	6.31	1.54	1.43
6	e	1	NAG	O5-C1	6.31	1.54	1.43
6	U	1	NAG	O5-C1	6.31	1.54	1.43
7	l	2	NAG	O5-C1	6.30	1.54	1.43
7	R	2	NAG	O5-C1	6.29	1.54	1.43
6	j	1	NAG	O5-C1	6.10	1.53	1.43
6	P	1	NAG	O5-C1	6.07	1.53	1.43
6	Z	1	NAG	O5-C1	6.05	1.53	1.43
6	h	1	NAG	O5-C1	6.05	1.53	1.43
6	Q	1	NAG	O5-C1	6.04	1.53	1.43
6	a	1	NAG	O5-C1	6.04	1.53	1.43
6	k	1	NAG	O5-C1	6.03	1.53	1.43
6	r	1	NAG	O5-C1	6.02	1.53	1.43
6	X	1	NAG	O5-C1	6.01	1.53	1.43
6	g	1	NAG	O5-C1	5.88	1.53	1.43
6	W	1	NAG	O5-C1	5.88	1.53	1.43
6	q	1	NAG	O5-C1	5.87	1.53	1.43
6	f	1	NAG	O5-C1	5.86	1.53	1.43
6	V	1	NAG	O5-C1	5.85	1.53	1.43
6	p	1	NAG	O5-C1	5.77	1.53	1.43
7	b	5	MAN	O2-C2	-4.23	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	5	MAN	O2-C2	-4.21	1.34	1.43
7	l	5	MAN	O2-C2	-4.21	1.34	1.43
8	i	3	BMA	O2-C2	-4.19	1.34	1.43
8	Y	3	BMA	O2-C2	-4.17	1.34	1.43
8	s	3	BMA	O2-C2	-4.14	1.34	1.43
7	R	3	BMA	O2-C2	-4.11	1.34	1.43
7	l	3	BMA	O2-C2	-4.10	1.34	1.43
7	b	3	BMA	O2-C2	-4.10	1.34	1.43
7	b	4	MAN	O2-C2	-2.98	1.37	1.43
7	R	4	MAN	O2-C2	-2.98	1.37	1.43
7	l	4	MAN	O2-C2	-2.97	1.37	1.43
6	T	1	NAG	C3-C2	-2.51	1.47	1.52
6	d	1	NAG	C3-C2	-2.51	1.47	1.52
6	n	1	NAG	C3-C2	-2.48	1.47	1.52
8	i	1	NAG	C3-C2	-2.46	1.47	1.52
7	R	3	BMA	C2-C3	-2.46	1.48	1.52
7	b	3	BMA	C2-C3	-2.45	1.48	1.52
7	l	3	BMA	C2-C3	-2.45	1.48	1.52
8	s	1	NAG	C3-C2	-2.44	1.47	1.52
8	Y	1	NAG	C3-C2	-2.43	1.47	1.52
7	b	2	NAG	C3-C2	-2.41	1.47	1.52
7	R	2	NAG	C3-C2	-2.40	1.47	1.52
7	l	2	NAG	C3-C2	-2.40	1.47	1.52
6	e	1	NAG	C3-C2	-2.39	1.47	1.52
6	U	1	NAG	C3-C2	-2.39	1.47	1.52
6	o	1	NAG	C3-C2	-2.38	1.47	1.52
6	P	1	NAG	C3-C2	-2.37	1.47	1.52
6	j	1	NAG	C3-C2	-2.37	1.47	1.52
6	Z	1	NAG	C3-C2	-2.37	1.47	1.52
6	S	2	NAG	C3-C2	-2.36	1.47	1.52
6	c	2	NAG	C3-C2	-2.35	1.47	1.52
6	m	2	NAG	C3-C2	-2.35	1.47	1.52
8	s	3	BMA	C2-C3	-2.34	1.48	1.52
8	i	3	BMA	C2-C3	-2.33	1.48	1.52
6	f	2	NAG	C3-C2	-2.31	1.47	1.52
6	S	1	NAG	C1-C2	-2.31	1.49	1.52
6	c	1	NAG	C1-C2	-2.30	1.49	1.52
6	W	2	NAG	C3-C2	-2.30	1.47	1.52
7	R	5	MAN	C2-C3	-2.30	1.49	1.52
6	m	1	NAG	C1-C2	-2.30	1.49	1.52
6	V	2	NAG	C3-C2	-2.30	1.47	1.52
6	W	1	NAG	C3-C2	-2.29	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	1	NAG	C3-C2	-2.28	1.47	1.52
6	p	2	NAG	C3-C2	-2.28	1.47	1.52
8	Y	3	BMA	C2-C3	-2.28	1.49	1.52
6	a	1	NAG	C3-C2	-2.27	1.47	1.52
6	g	1	NAG	C3-C2	-2.27	1.47	1.52
6	q	1	NAG	C3-C2	-2.27	1.47	1.52
6	V	1	NAG	C3-C2	-2.27	1.47	1.52
6	g	2	NAG	C3-C2	-2.26	1.47	1.52
6	k	1	NAG	C3-C2	-2.26	1.47	1.52
6	p	1	NAG	C4-C3	2.26	1.58	1.52
6	f	1	NAG	C4-C3	2.26	1.58	1.52
6	Q	1	NAG	C3-C2	-2.26	1.47	1.52
6	q	2	NAG	C3-C2	-2.26	1.47	1.52
6	o	2	NAG	C3-C2	-2.25	1.47	1.52
7	l	5	MAN	C2-C3	-2.25	1.49	1.52
6	V	1	NAG	C4-C3	2.25	1.58	1.52
6	p	1	NAG	C3-C2	-2.25	1.47	1.52
6	U	2	NAG	C3-C2	-2.24	1.47	1.52
6	n	2	NAG	C3-C2	-2.24	1.47	1.52
6	e	2	NAG	C3-C2	-2.23	1.47	1.52
7	b	5	MAN	C2-C3	-2.22	1.49	1.52
6	Z	2	NAG	C3-C2	-2.22	1.47	1.52
6	d	2	NAG	C3-C2	-2.22	1.47	1.52
6	Q	2	NAG	C3-C2	-2.21	1.47	1.52
6	k	2	NAG	C3-C2	-2.21	1.47	1.52
6	T	2	NAG	C3-C2	-2.21	1.47	1.52
6	c	1	NAG	C3-C2	-2.21	1.47	1.52
6	S	1	NAG	C3-C2	-2.21	1.47	1.52
6	a	2	NAG	C3-C2	-2.20	1.47	1.52
8	Y	2	NAG	C1-C2	-2.20	1.49	1.52
6	j	2	NAG	C3-C2	-2.20	1.47	1.52
8	s	2	NAG	C1-C2	-2.19	1.49	1.52
6	m	1	NAG	C3-C2	-2.19	1.47	1.52
8	i	2	NAG	C3-C2	-2.19	1.47	1.52
8	i	2	NAG	C4-C3	2.19	1.58	1.52
6	P	2	NAG	C3-C2	-2.18	1.47	1.52
8	Y	2	NAG	C3-C2	-2.18	1.47	1.52
8	s	2	NAG	C4-C3	2.18	1.58	1.52
8	s	2	NAG	C3-C2	-2.16	1.48	1.52
6	o	1	NAG	C4-C3	2.16	1.57	1.52
6	e	1	NAG	C1-C2	-2.16	1.49	1.52
6	U	1	NAG	C1-C2	-2.15	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	2	NAG	C4-C3	2.15	1.57	1.52
6	h	2	NAG	C3-C2	-2.15	1.48	1.52
6	r	2	NAG	C3-C2	-2.15	1.48	1.52
6	o	1	NAG	C1-C2	-2.15	1.49	1.52
6	U	1	NAG	C4-C3	2.14	1.57	1.52
8	i	2	NAG	C1-C2	-2.14	1.49	1.52
6	e	1	NAG	C4-C3	2.14	1.57	1.52
6	X	2	NAG	C3-C2	-2.14	1.48	1.52
8	Y	1	NAG	C1-C2	-2.11	1.49	1.52
6	m	1	NAG	C4-C3	2.10	1.57	1.52
8	i	1	NAG	C4-C5	2.10	1.57	1.53
6	c	1	NAG	C4-C3	2.08	1.57	1.52
7	R	2	NAG	C4-C5	2.08	1.57	1.53
6	S	1	NAG	C4-C3	2.08	1.57	1.52
7	l	4	MAN	C2-C3	-2.08	1.49	1.52
7	b	2	NAG	C4-C5	2.08	1.57	1.53
7	l	2	NAG	C4-C3	2.08	1.57	1.52
8	s	1	NAG	C4-C5	2.08	1.57	1.53
8	Y	1	NAG	C4-C5	2.08	1.57	1.53
7	R	2	NAG	C4-C3	2.06	1.57	1.52
7	b	2	NAG	C4-C3	2.06	1.57	1.52
8	i	1	NAG	C1-C2	-2.06	1.49	1.52
7	R	4	MAN	C2-C3	-2.06	1.49	1.52
7	l	2	NAG	C4-C5	2.06	1.57	1.53
6	r	1	NAG	C4-C3	2.06	1.57	1.52
6	X	1	NAG	C3-C2	-2.05	1.48	1.52
6	r	1	NAG	C3-C2	-2.05	1.48	1.52
8	s	1	NAG	C1-C2	-2.05	1.49	1.52
6	h	1	NAG	C3-C2	-2.05	1.48	1.52
6	P	1	NAG	C4-C3	2.04	1.57	1.52
6	h	1	NAG	C4-C3	2.04	1.57	1.52
8	s	1	NAG	C4-C3	2.04	1.57	1.52
8	i	1	NAG	C4-C3	2.04	1.57	1.52
6	Q	1	NAG	C4-C3	2.04	1.57	1.52
6	X	1	NAG	C4-C3	2.03	1.57	1.52
7	b	4	MAN	C2-C3	-2.03	1.49	1.52
6	Z	1	NAG	C4-C3	2.03	1.57	1.52
6	k	1	NAG	C4-C3	2.03	1.57	1.52
6	j	1	NAG	C4-C3	2.02	1.57	1.52
6	T	1	NAG	C4-C3	2.02	1.57	1.52
6	n	1	NAG	C4-C3	2.02	1.57	1.52
6	a	1	NAG	C4-C3	2.02	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	1	NAG	C4-C3	2.01	1.57	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	l	1	NAG	C3-C4-C5	-3.59	103.73	110.23
7	b	3	BMA	C2-C3-C4	-3.59	104.55	110.86
7	R	3	BMA	C2-C3-C4	-3.57	104.58	110.86
7	l	3	BMA	C2-C3-C4	-3.56	104.60	110.86
7	b	1	NAG	C3-C4-C5	-3.56	103.78	110.23
7	R	1	NAG	C3-C4-C5	-3.55	103.79	110.23
6	X	1	NAG	C3-C4-C5	-3.33	104.19	110.23
6	h	1	NAG	C3-C4-C5	-3.33	104.20	110.23
6	r	1	NAG	C3-C4-C5	-3.32	104.21	110.23
6	X	1	NAG	C1-O5-C5	-3.02	108.14	112.19
6	h	1	NAG	C1-O5-C5	-3.01	108.15	112.19
6	r	1	NAG	C1-O5-C5	-2.98	108.19	112.19
7	b	3	BMA	C1-C2-C3	2.97	113.97	109.64
7	l	3	BMA	C1-C2-C3	2.95	113.94	109.64
7	R	3	BMA	C1-C2-C3	2.94	113.93	109.64
6	n	1	NAG	C1-O5-C5	-2.82	108.41	112.19
6	T	1	NAG	C1-O5-C5	-2.82	108.41	112.19
6	d	1	NAG	C1-O5-C5	-2.80	108.43	112.19
6	g	1	NAG	C3-C4-C5	-2.71	105.31	110.23
6	q	1	NAG	C3-C4-C5	-2.70	105.33	110.23
6	W	1	NAG	C3-C4-C5	-2.69	105.35	110.23
6	m	1	NAG	C3-C4-C5	-2.68	105.37	110.23
6	S	1	NAG	C3-C4-C5	-2.67	105.39	110.23
6	c	1	NAG	C3-C4-C5	-2.67	105.40	110.23
6	j	1	NAG	C3-C4-C5	-2.48	105.74	110.23
6	Q	1	NAG	O5-C5-C6	-2.48	102.84	107.66
6	k	1	NAG	O5-C5-C6	-2.47	102.85	107.66
6	p	2	NAG	C4-C3-C2	-2.47	107.40	111.02
6	Z	1	NAG	C3-C4-C5	-2.47	105.75	110.23
6	a	1	NAG	C3-C4-C5	-2.47	105.75	110.23
6	P	1	NAG	C3-C4-C5	-2.47	105.76	110.23
6	a	1	NAG	O5-C5-C6	-2.46	102.87	107.66
6	f	2	NAG	C4-C3-C2	-2.46	107.42	111.02
6	Q	1	NAG	C3-C4-C5	-2.45	105.78	110.23
6	k	1	NAG	C3-C4-C5	-2.45	105.80	110.23
6	V	2	NAG	C4-C3-C2	-2.43	107.46	111.02
7	b	5	MAN	C2-C3-C4	-2.37	106.69	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	R	5	MAN	C2-C3-C4	-2.36	106.72	110.86
7	l	5	MAN	C2-C3-C4	-2.32	106.78	110.86
7	b	4	MAN	C2-C3-C4	-2.30	106.81	110.86
7	R	4	MAN	C2-C3-C4	-2.29	106.84	110.86
7	l	4	MAN	C2-C3-C4	-2.29	106.84	110.86
6	p	1	NAG	C3-C4-C5	-2.28	106.09	110.23
6	f	1	NAG	C3-C4-C5	-2.28	106.09	110.23
6	k	1	NAG	O4-C4-C3	-2.28	105.00	110.38
7	l	2	NAG	C3-C4-C5	-2.27	106.11	110.23
6	V	1	NAG	C3-C4-C5	-2.27	106.11	110.23
7	l	2	NAG	O5-C5-C6	-2.27	103.25	107.66
7	b	2	NAG	C3-C4-C5	-2.26	106.13	110.23
6	Q	1	NAG	O4-C4-C3	-2.26	105.04	110.38
7	R	2	NAG	O5-C5-C6	-2.26	103.26	107.66
7	R	2	NAG	C3-C4-C5	-2.26	106.13	110.23
7	b	2	NAG	O5-C5-C6	-2.26	103.26	107.66
6	a	1	NAG	O4-C4-C3	-2.26	105.05	110.38
8	i	1	NAG	C3-C4-C5	-2.26	106.14	110.23
8	s	1	NAG	C3-C4-C5	-2.26	106.14	110.23
8	Y	1	NAG	C3-C4-C5	-2.25	106.15	110.23
6	j	1	NAG	C1-O5-C5	-2.16	109.29	112.19
6	P	1	NAG	C1-O5-C5	-2.14	109.32	112.19
6	Z	1	NAG	C1-O5-C5	-2.13	109.33	112.19
6	g	2	NAG	C4-C3-C2	-2.09	107.95	111.02
6	U	1	NAG	C3-C4-C5	-2.09	106.45	110.23
6	o	1	NAG	C3-C4-C5	-2.09	106.45	110.23
7	R	5	MAN	C1-C2-C3	2.08	112.68	109.64
6	e	1	NAG	C3-C4-C5	-2.08	106.47	110.23
6	q	2	NAG	C4-C3-C2	-2.08	107.98	111.02
8	i	3	BMA	C2-C3-C4	-2.07	107.22	110.86
7	b	5	MAN	C1-C2-C3	2.07	112.65	109.64
8	s	3	BMA	C2-C3-C4	-2.07	107.23	110.86
6	W	2	NAG	C4-C3-C2	-2.06	108.00	111.02
7	l	5	MAN	C1-C2-C3	2.06	112.64	109.64
8	Y	3	BMA	C2-C3-C4	-2.05	107.26	110.86
8	i	2	NAG	C3-C4-C5	-2.02	106.57	110.23
6	S	2	NAG	C4-C3-C2	-2.01	108.06	111.02
6	m	2	NAG	C4-C3-C2	-2.01	108.06	111.02
8	s	2	NAG	C3-C4-C5	-2.01	106.58	110.23
8	Y	2	NAG	C3-C4-C5	-2.01	106.59	110.23
6	c	2	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	2	NAG	C4-C5-C6-O6
7	b	2	NAG	C4-C5-C6-O6
7	l	2	NAG	C4-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
7	l	2	NAG	O5-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6
7	b	1	NAG	O5-C5-C6-O6
7	l	1	NAG	O5-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
6	e	2	NAG	C4-C5-C6-O6
6	o	2	NAG	C4-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6
6	q	2	NAG	O5-C5-C6-O6
6	g	2	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6
6	p	2	NAG	O5-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
6	d	2	NAG	O5-C5-C6-O6
6	j	2	NAG	O5-C5-C6-O6
6	n	2	NAG	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
6	e	2	NAG	O5-C5-C6-O6
6	o	2	NAG	O5-C5-C6-O6
7	R	3	BMA	O5-C5-C6-O6
7	b	3	BMA	O5-C5-C6-O6
7	l	3	BMA	O5-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
7	b	1	NAG	C4-C5-C6-O6
7	l	1	NAG	C4-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
8	i	1	NAG	C4-C5-C6-O6
8	s	1	NAG	C4-C5-C6-O6
7	R	3	BMA	C4-C5-C6-O6
7	b	3	BMA	C4-C5-C6-O6
7	l	3	BMA	C4-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
6	h	2	NAG	O5-C5-C6-O6
6	r	2	NAG	O5-C5-C6-O6

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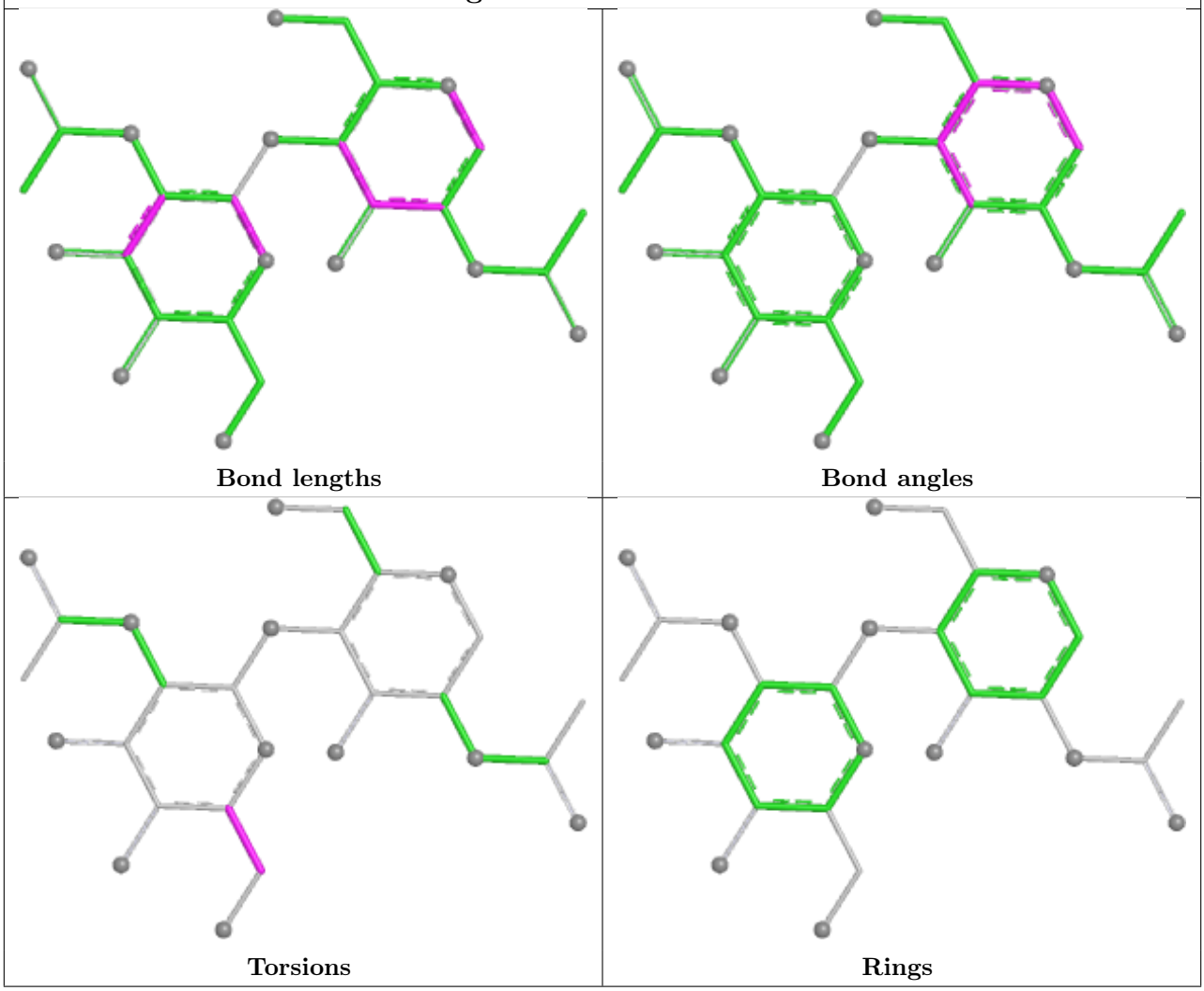
Mol	Chain	Res	Type	Atoms
6	S	2	NAG	O5-C5-C6-O6
6	c	2	NAG	O5-C5-C6-O6
6	m	2	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
6	k	2	NAG	O5-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
8	i	1	NAG	O5-C5-C6-O6
8	s	1	NAG	O5-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
8	Y	3	BMA	O5-C5-C6-O6
8	i	3	BMA	O5-C5-C6-O6
8	s	3	BMA	O5-C5-C6-O6
6	W	2	NAG	C4-C5-C6-O6
6	g	2	NAG	C4-C5-C6-O6
6	q	2	NAG	C4-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
6	h	1	NAG	O5-C5-C6-O6
6	r	1	NAG	O5-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6
8	i	2	NAG	O5-C5-C6-O6
8	s	2	NAG	O5-C5-C6-O6
7	R	4	MAN	O5-C5-C6-O6
7	R	5	MAN	O5-C5-C6-O6
7	b	4	MAN	O5-C5-C6-O6
7	b	5	MAN	O5-C5-C6-O6
7	l	4	MAN	O5-C5-C6-O6
7	l	5	MAN	O5-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	f	2	NAG	C4-C5-C6-O6
6	p	2	NAG	C4-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6
6	d	2	NAG	C4-C5-C6-O6
6	n	2	NAG	C4-C5-C6-O6
6	W	1	NAG	C4-C5-C6-O6
6	g	1	NAG	C4-C5-C6-O6
6	q	1	NAG	C4-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
6	P	2	NAG	C4-C5-C6-O6
6	j	2	NAG	C4-C5-C6-O6

There are no ring outliers.

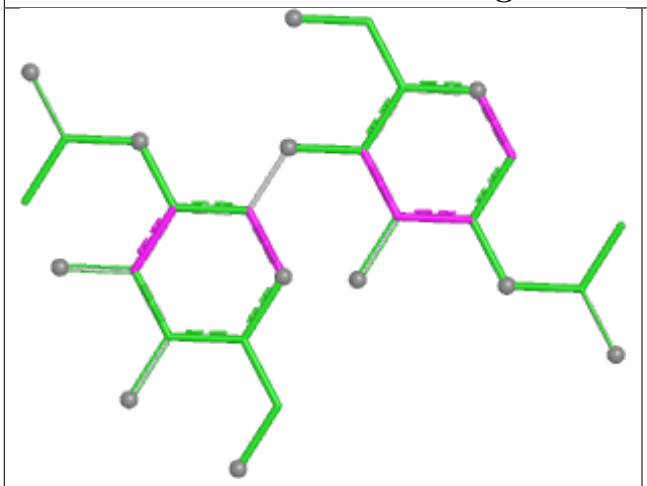
No monomer is involved in short contacts.

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

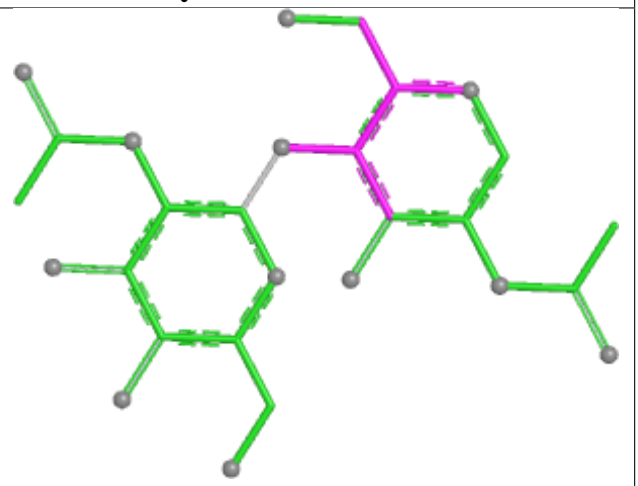
Oligosaccharide Chain P



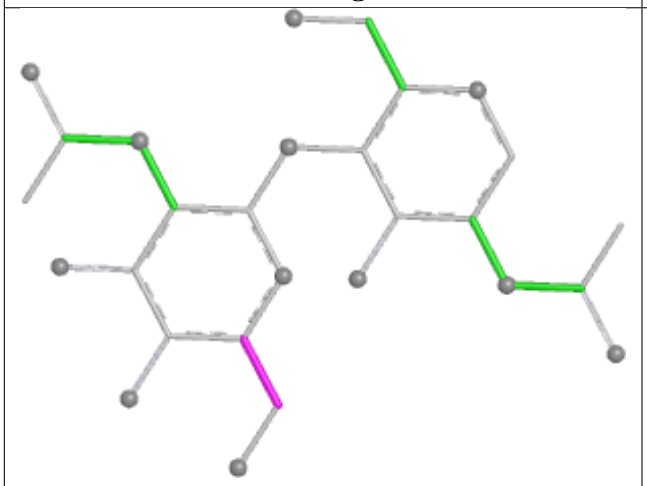
Oligosaccharide Chain Q



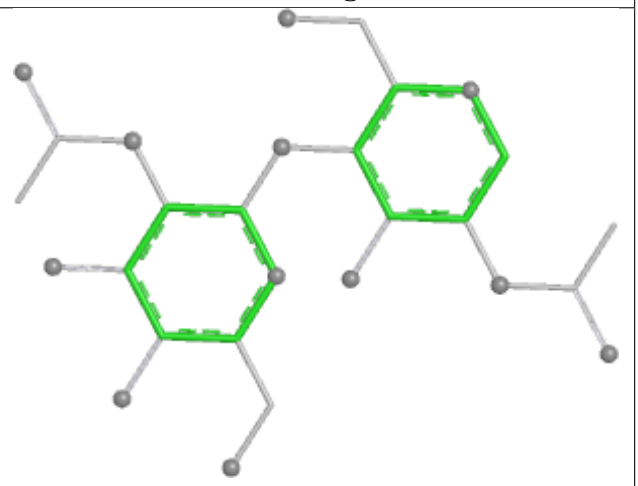
Bond lengths



Bond angles

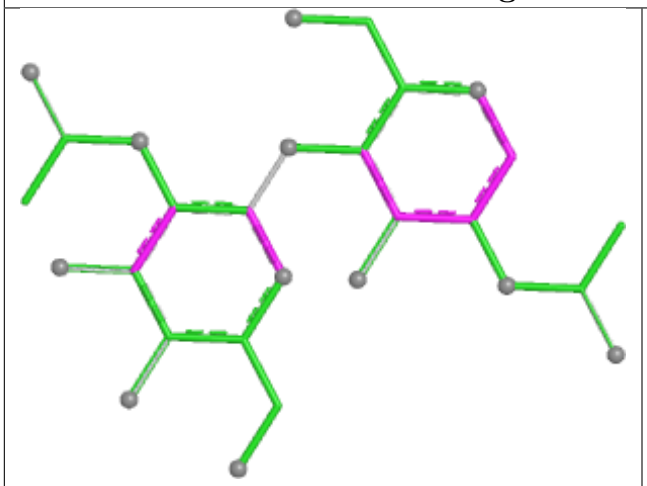


Torsions

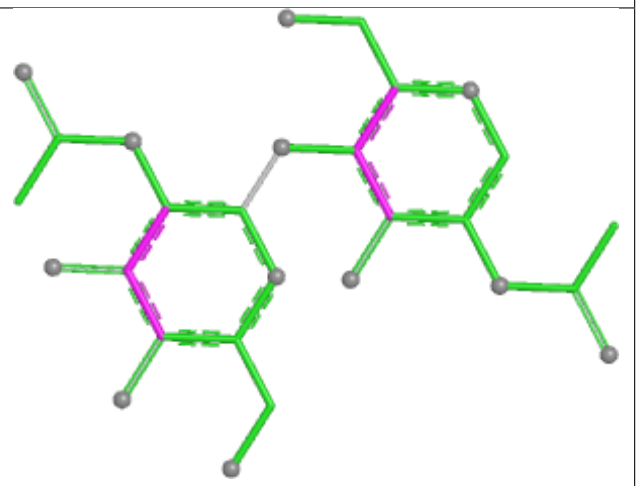


Rings

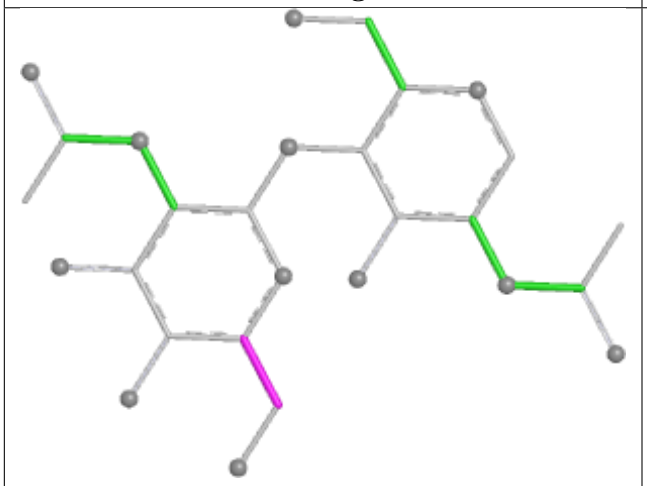
Oligosaccharide Chain S



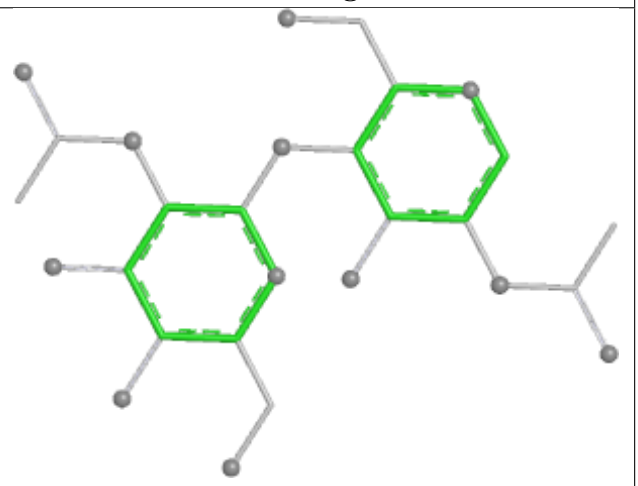
Bond lengths



Bond angles

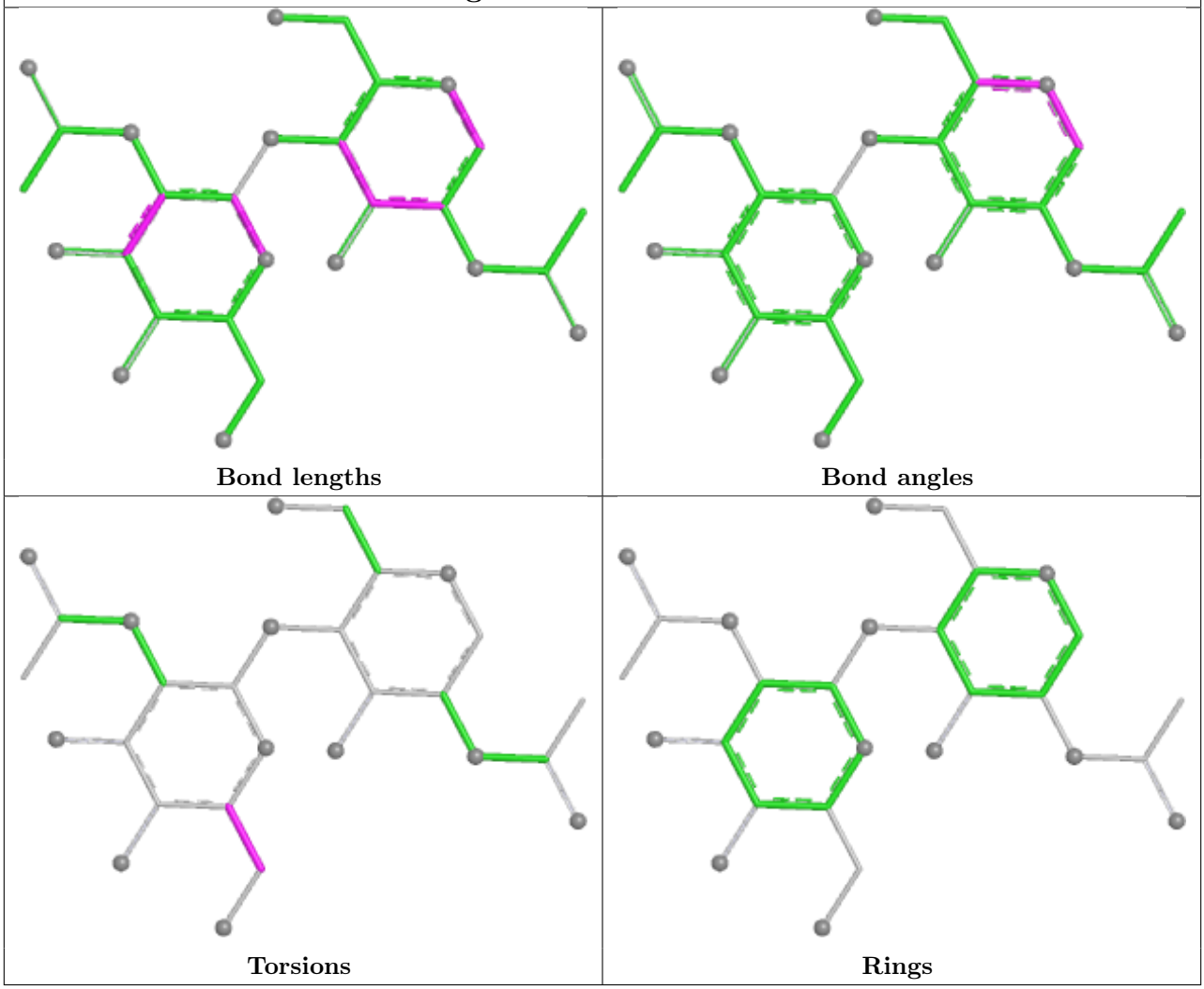


Torsions

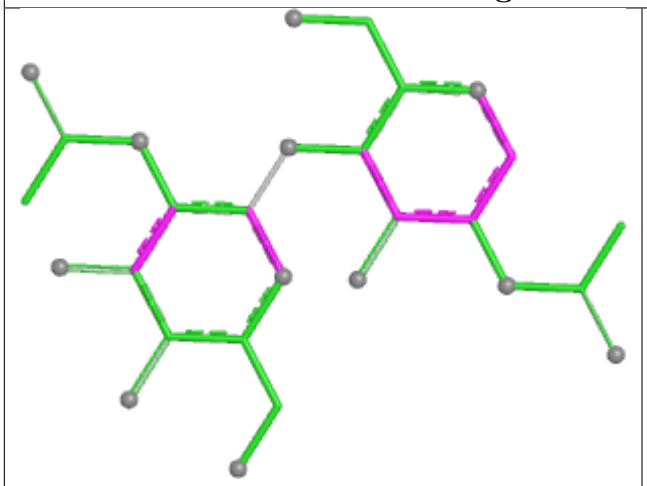


Rings

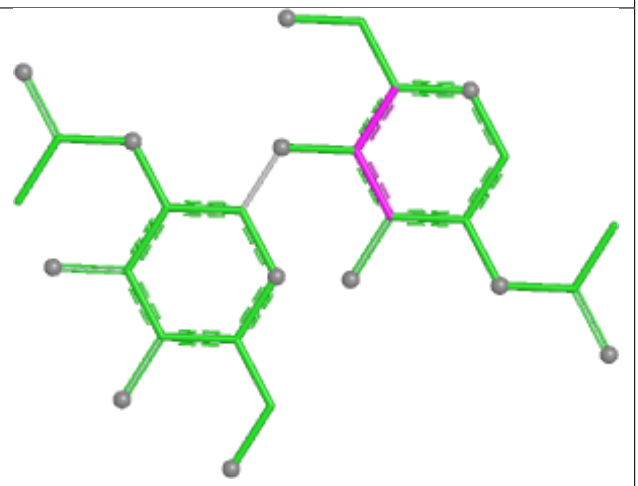
Oligosaccharide Chain T



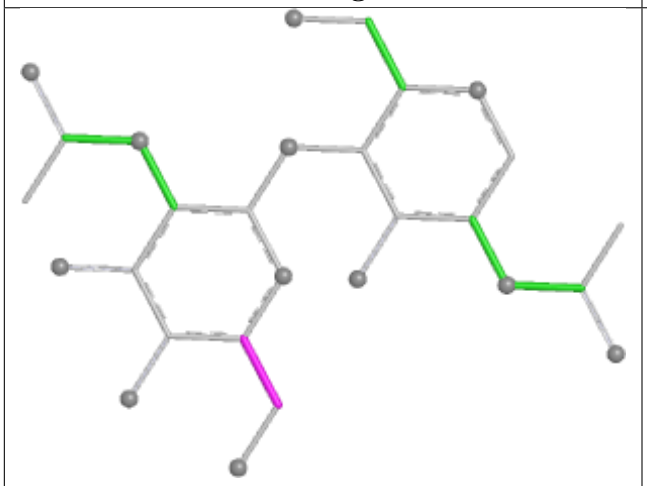
Oligosaccharide Chain U



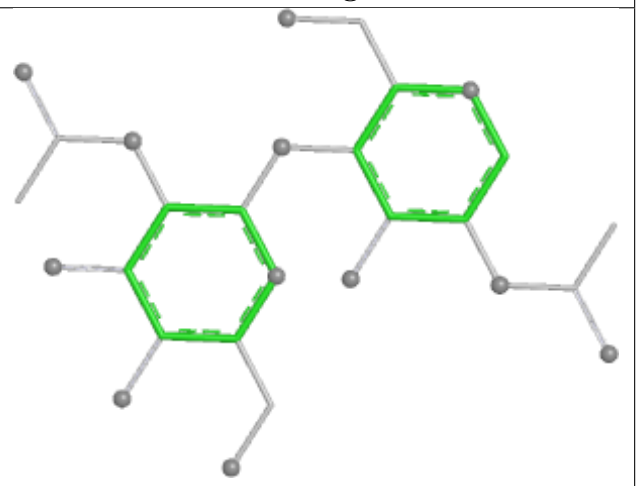
Bond lengths



Bond angles

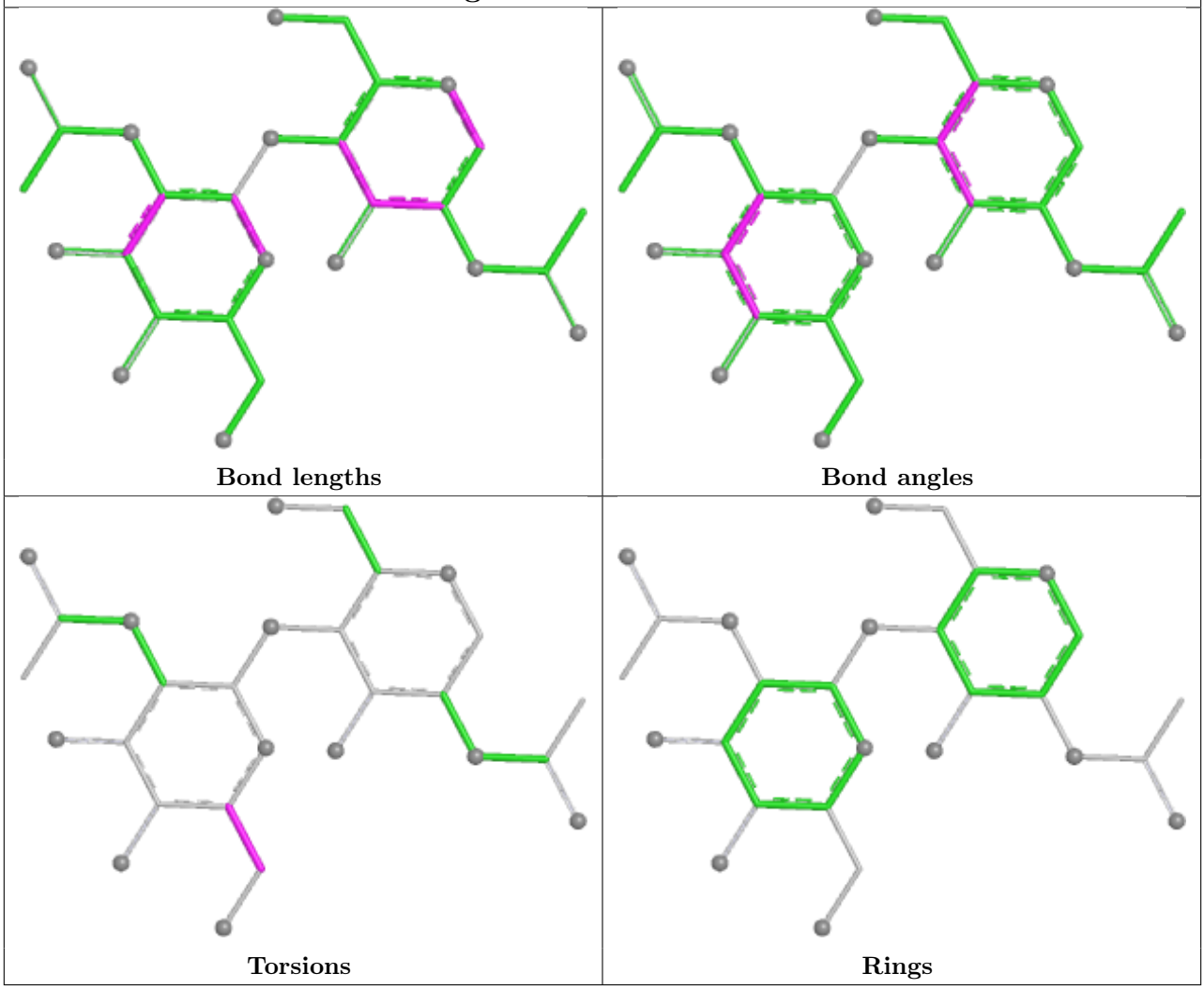


Torsions

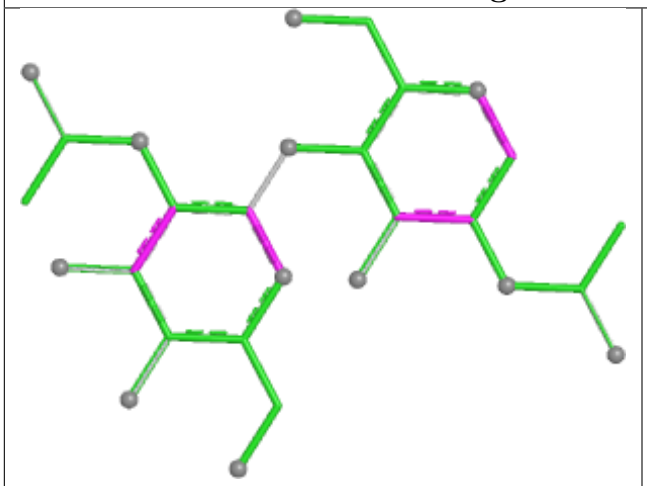


Rings

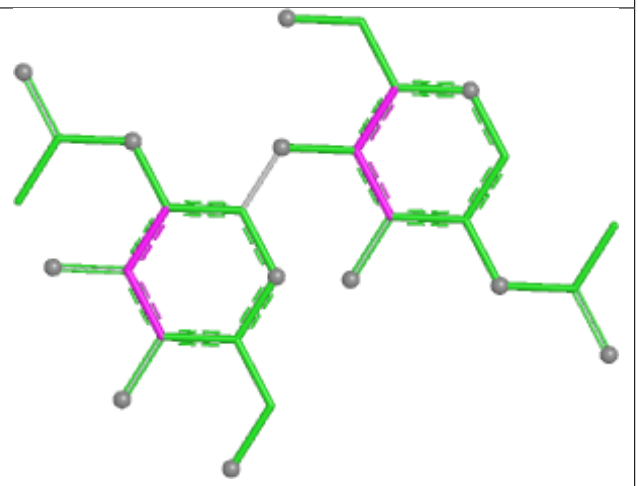
Oligosaccharide Chain V



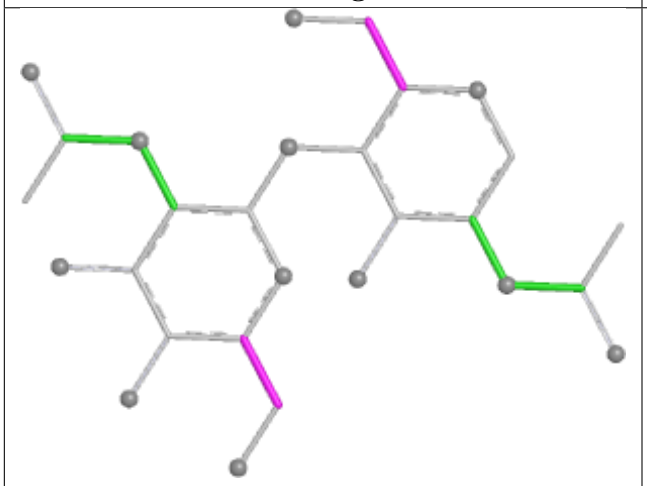
Oligosaccharide Chain W



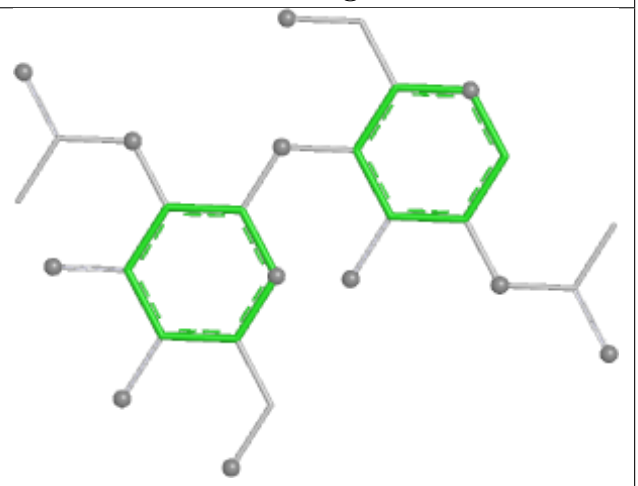
Bond lengths



Bond angles

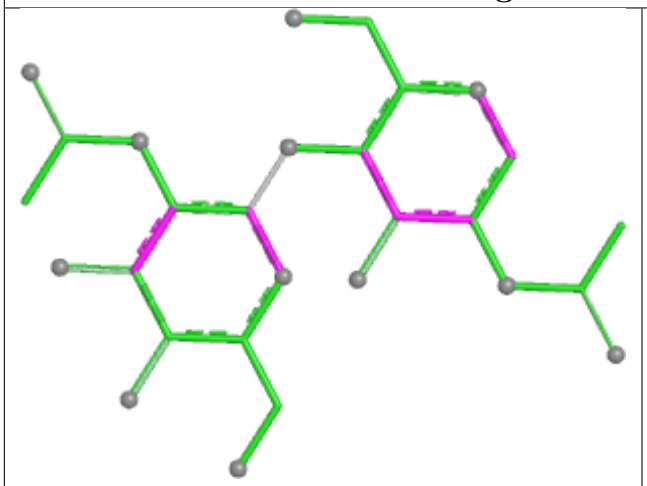


Torsions

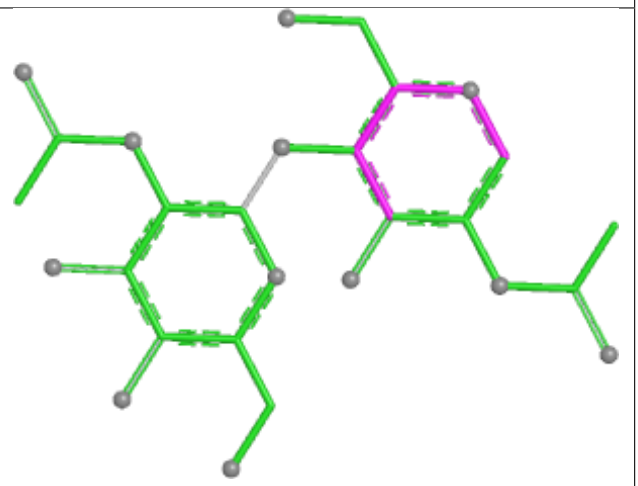


Rings

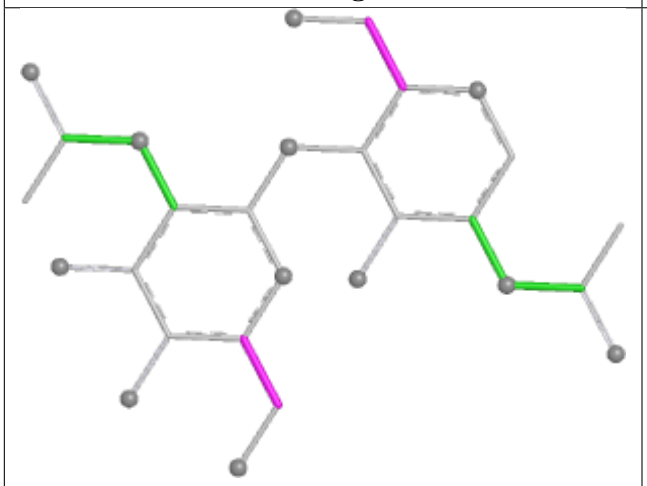
Oligosaccharide Chain X



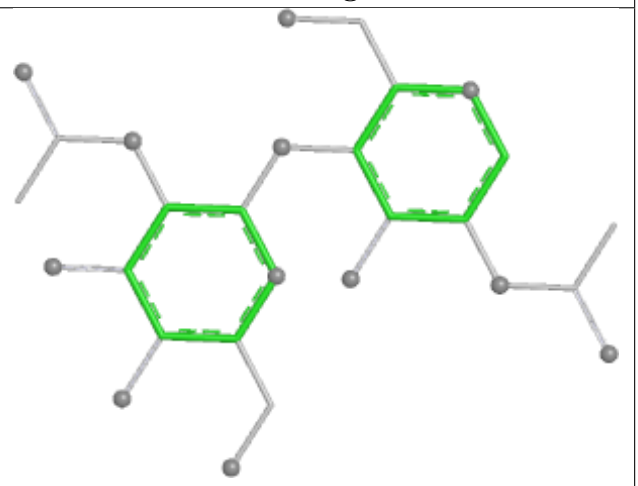
Bond lengths



Bond angles

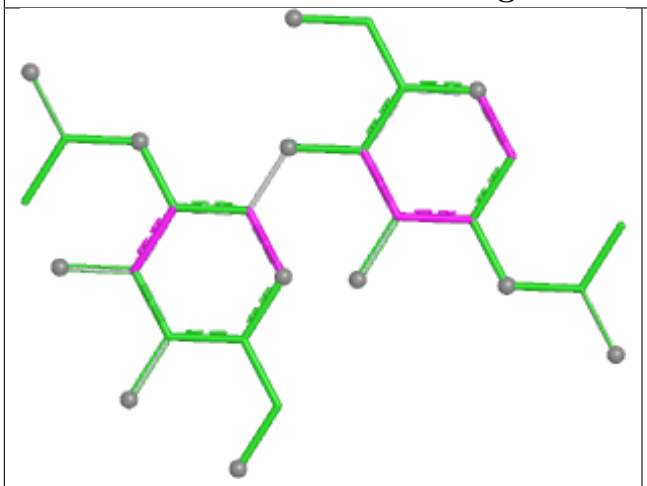


Torsions

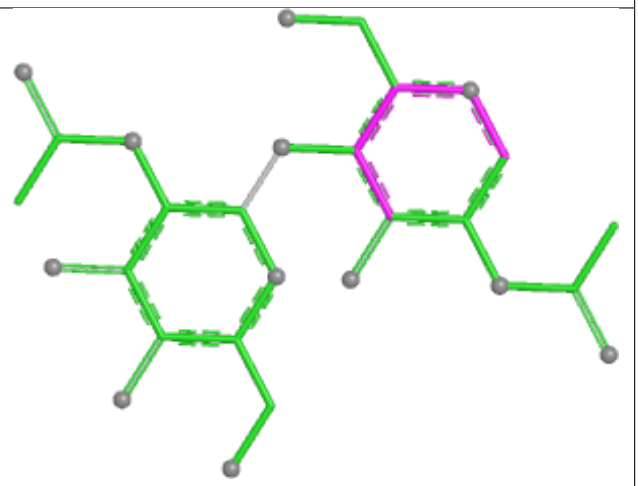


Rings

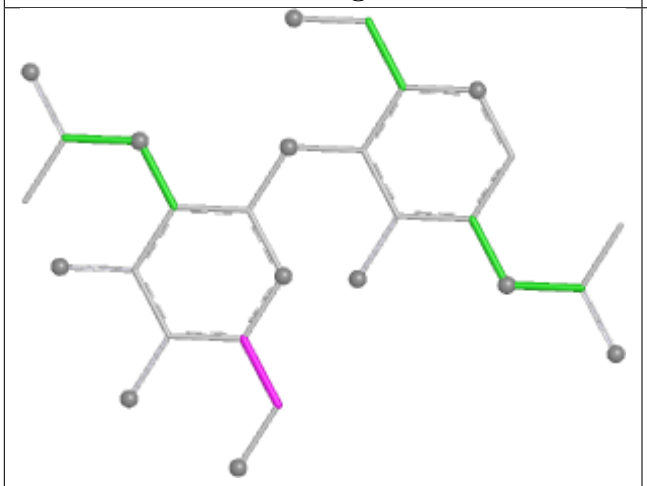
Oligosaccharide Chain Z



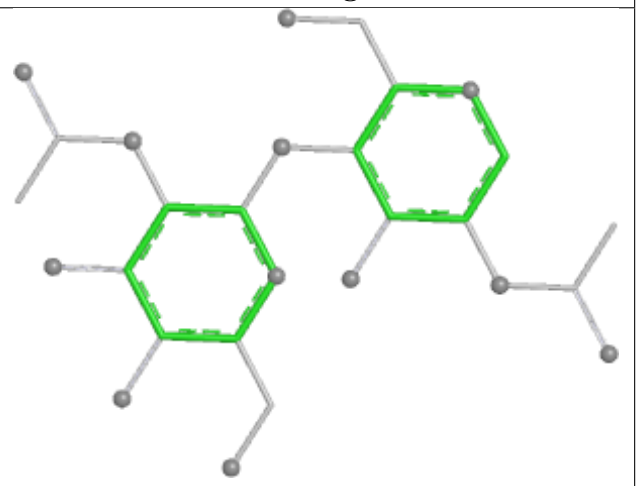
Bond lengths



Bond angles

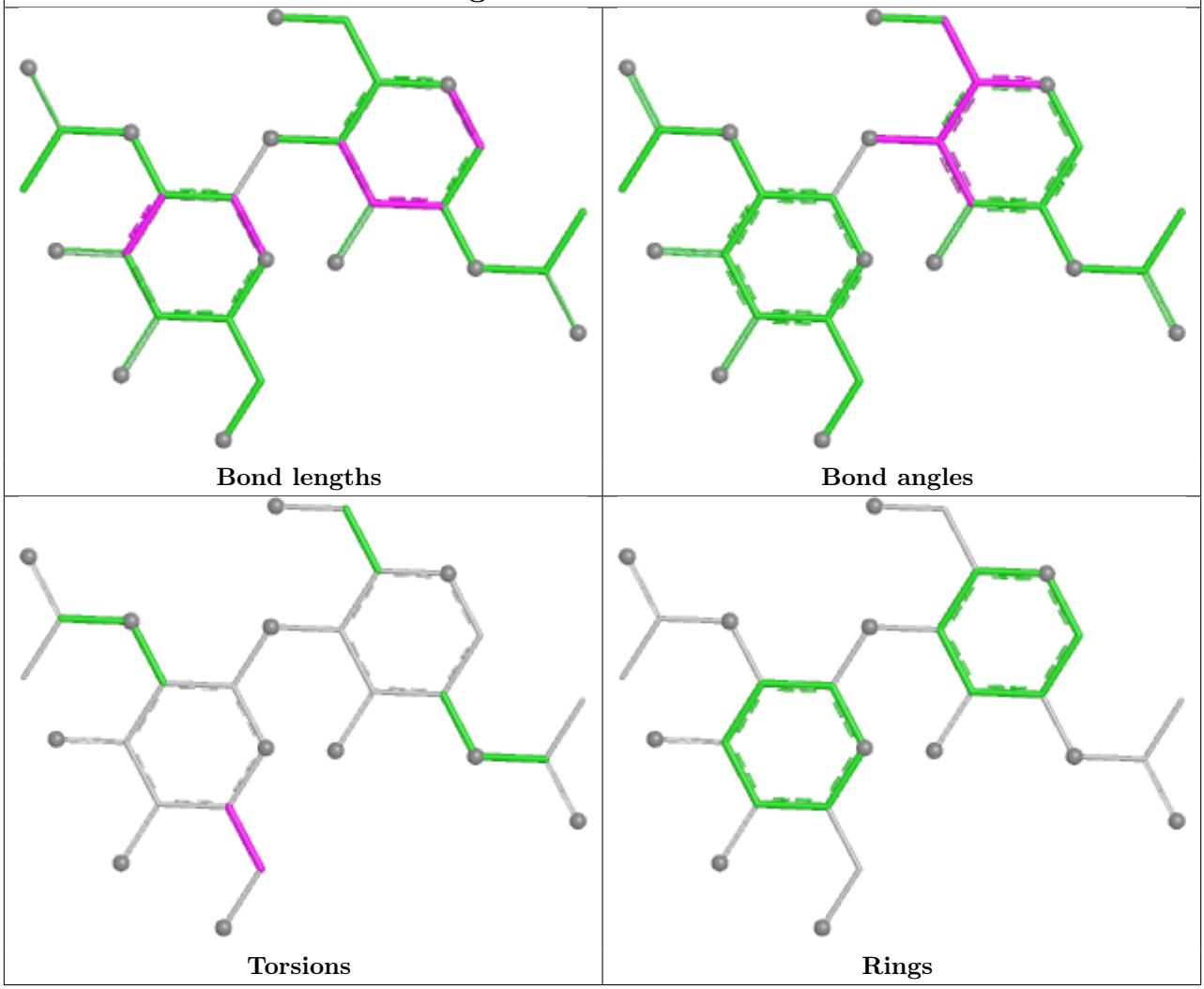


Torsions

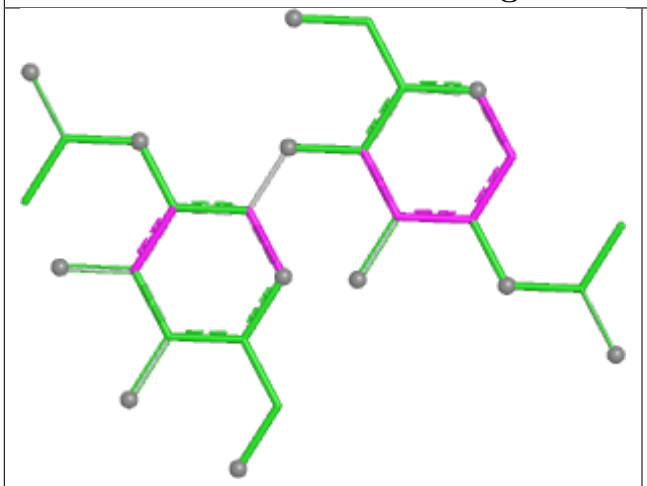


Rings

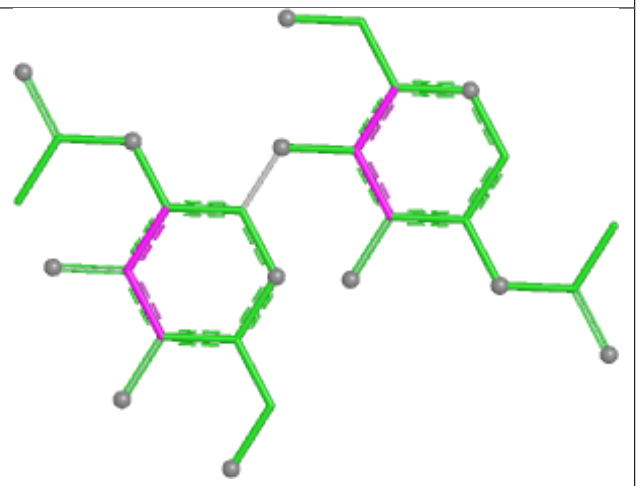
Oligosaccharide Chain a



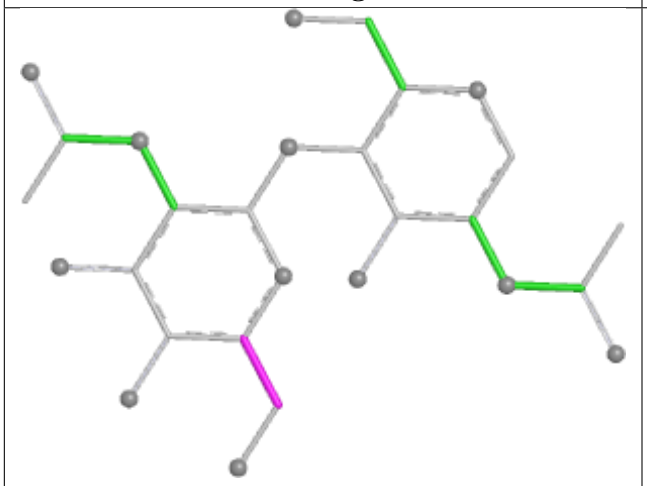
Oligosaccharide Chain c



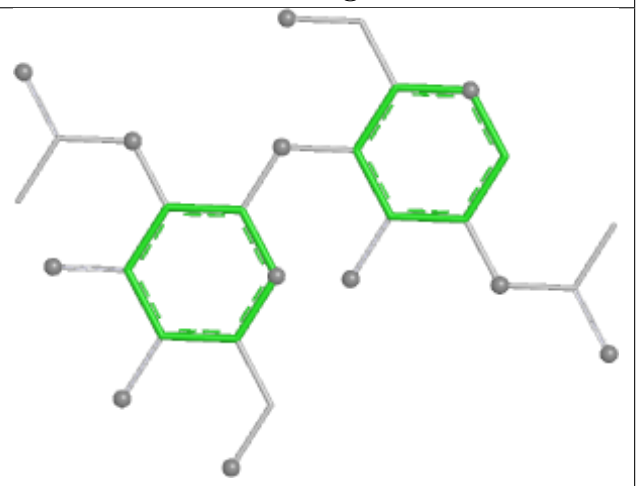
Bond lengths



Bond angles

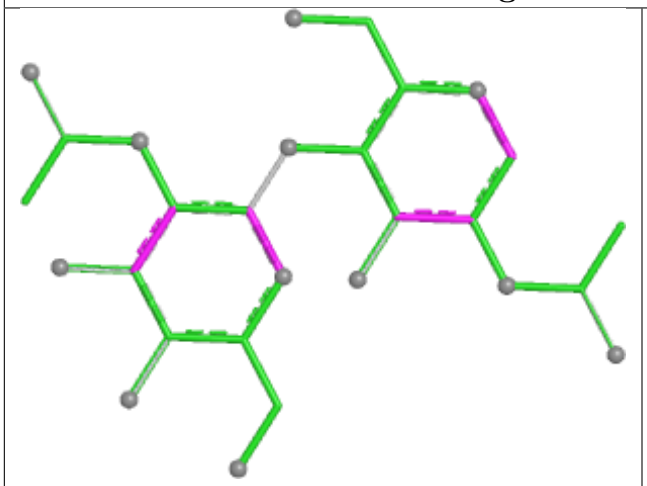


Torsions

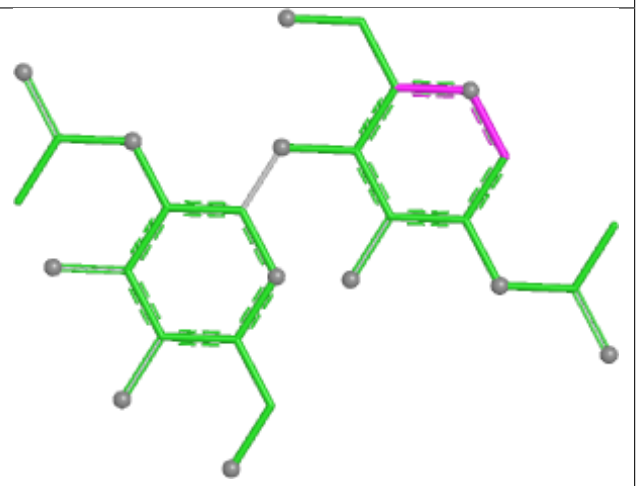


Rings

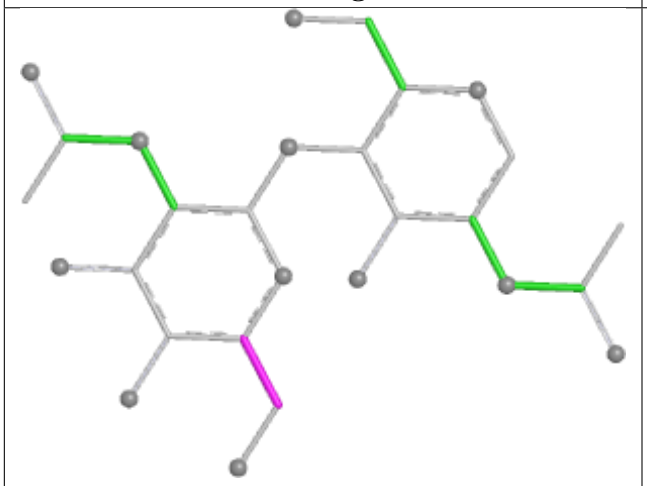
Oligosaccharide Chain d



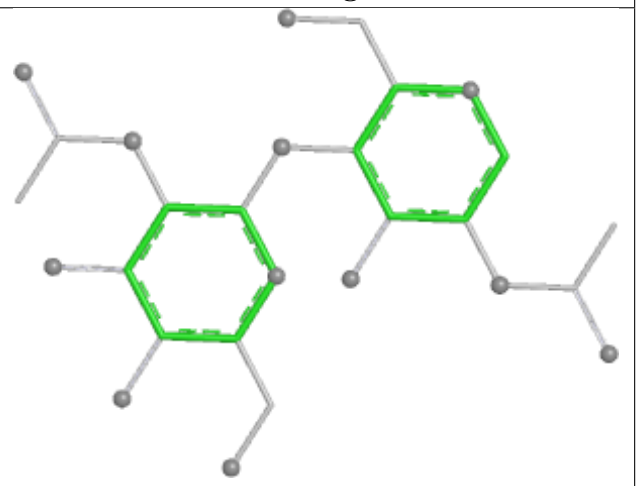
Bond lengths



Bond angles

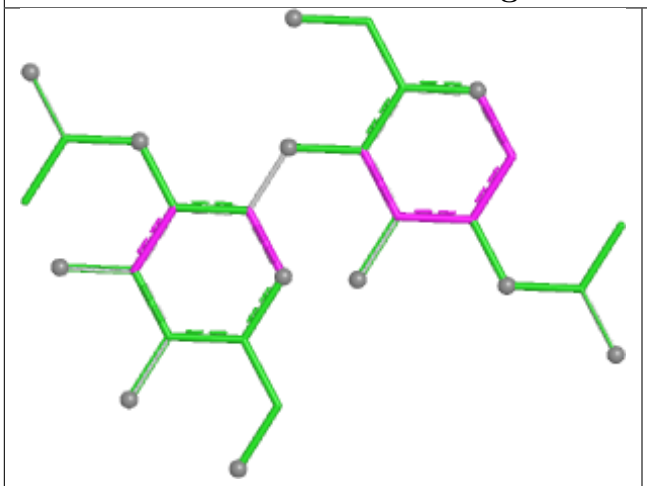


Torsions



Rings

Oligosaccharide Chain e



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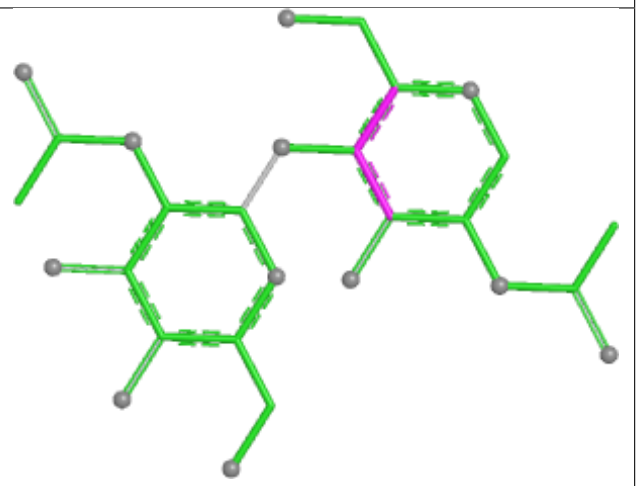

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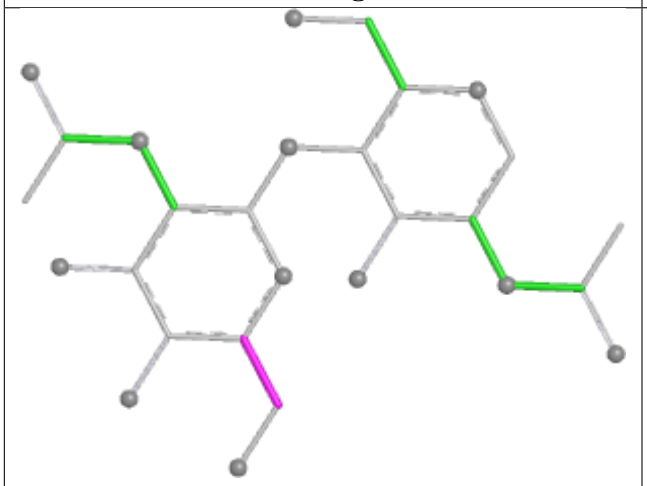

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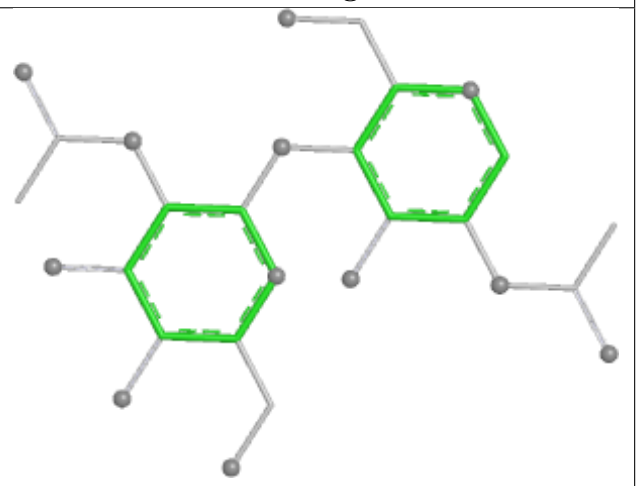
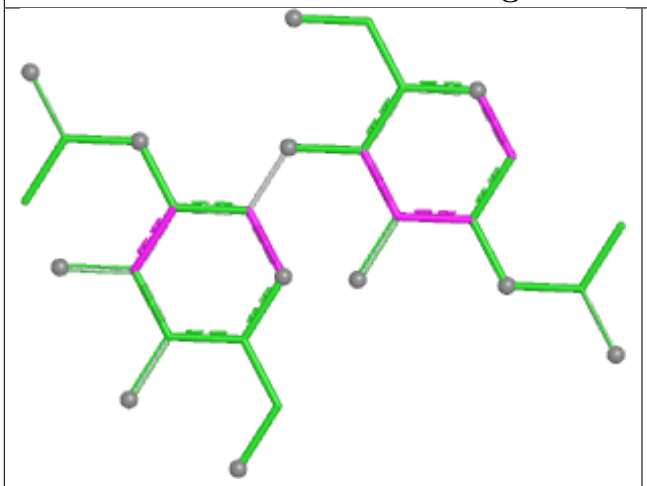


Rings

Oligosaccharide Chain f



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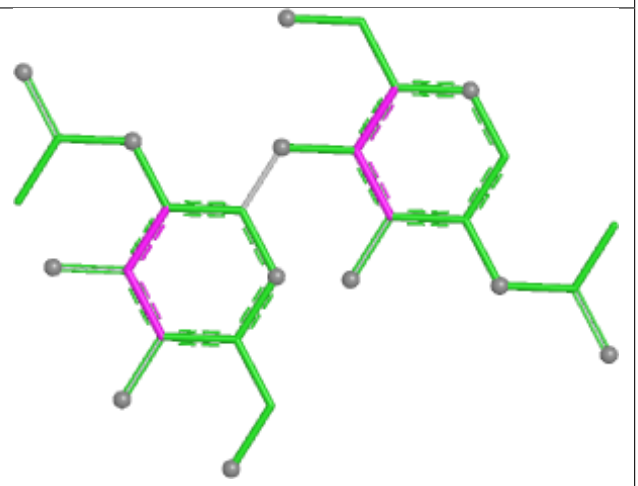
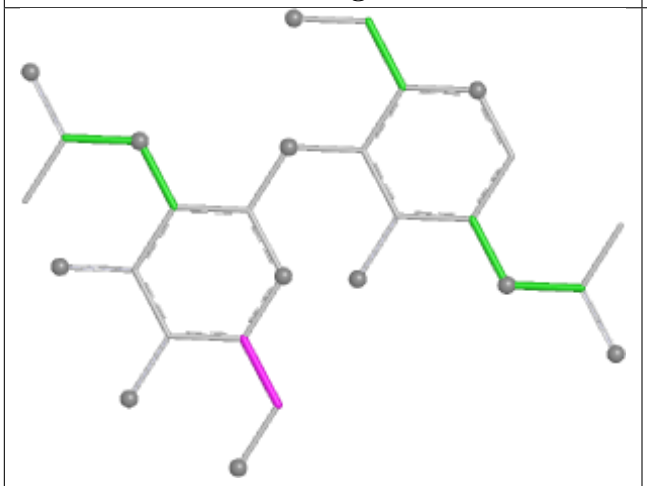


Bond angles



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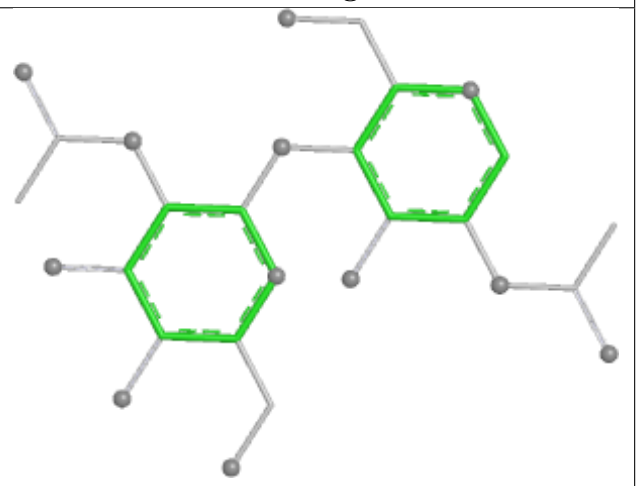
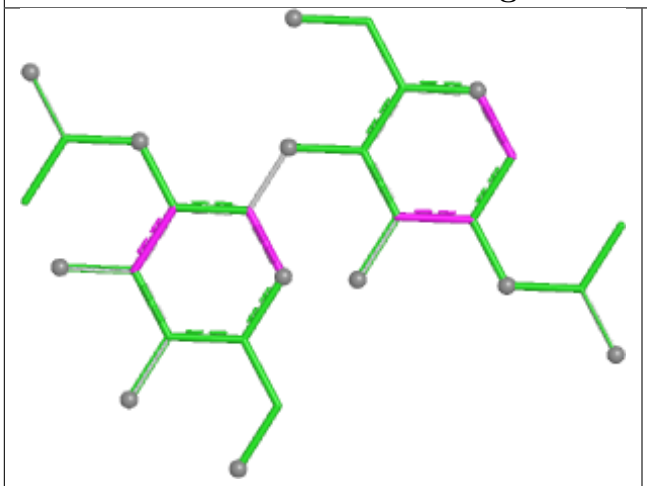


Rings

Oligosaccharide Chain g



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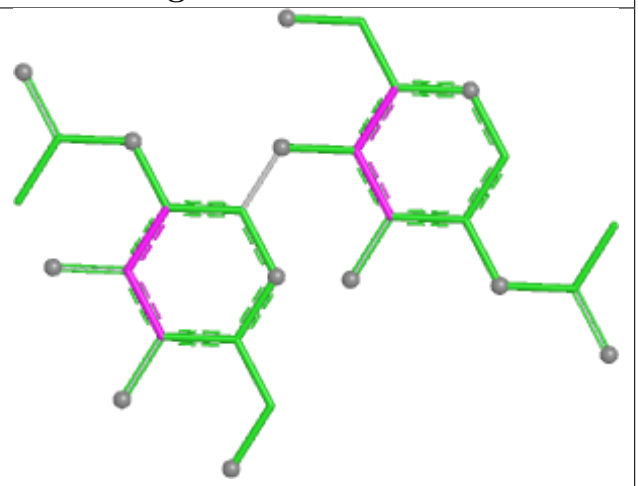

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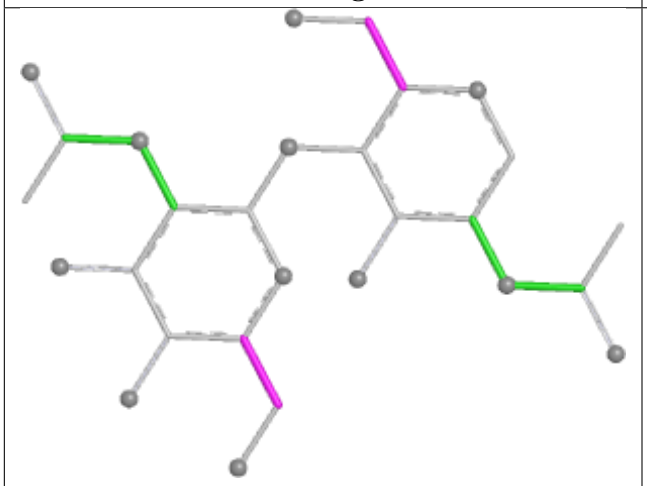

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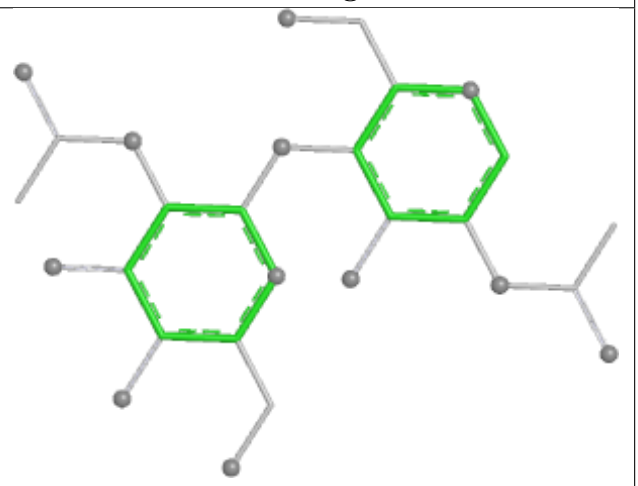
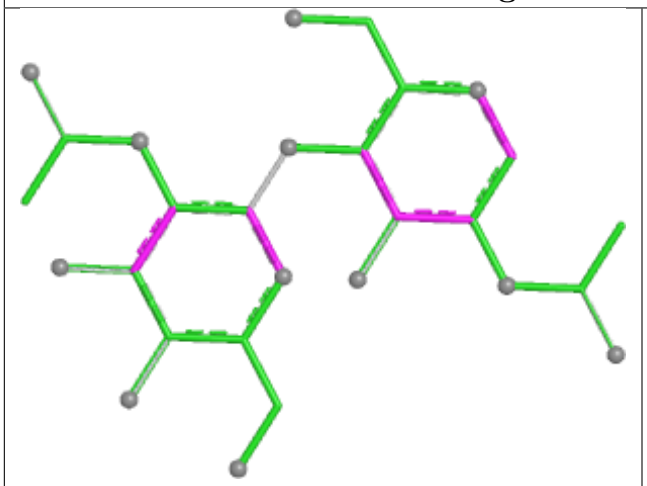


Rings

Oligosaccharide Chain h



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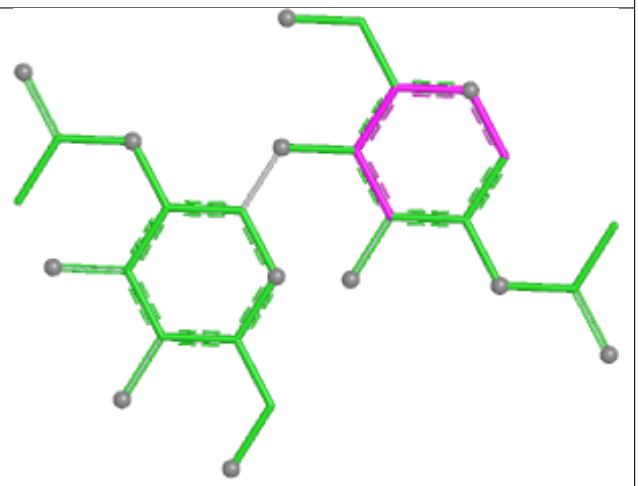

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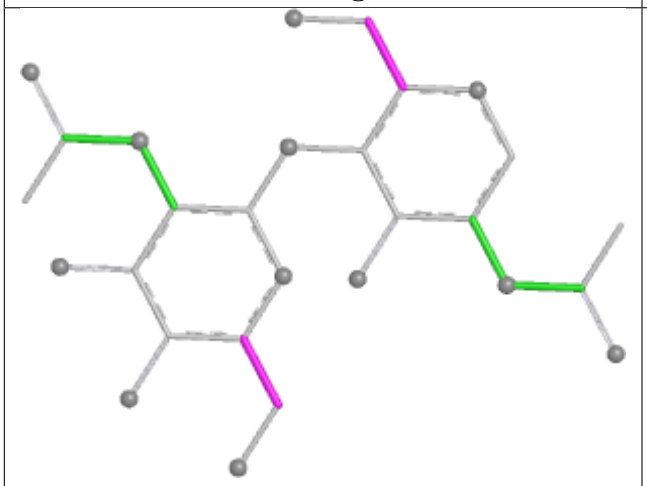

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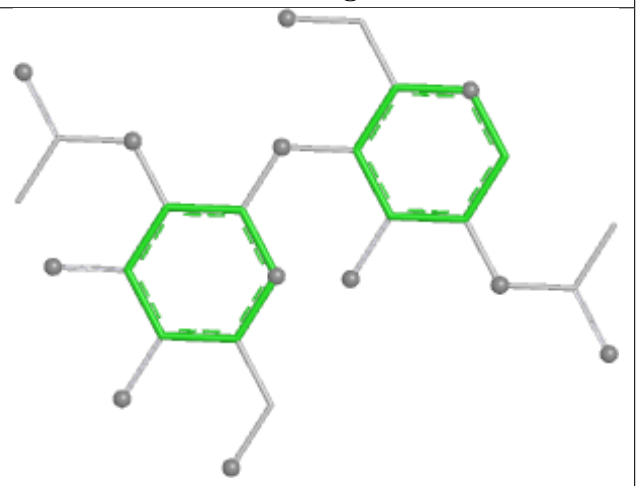
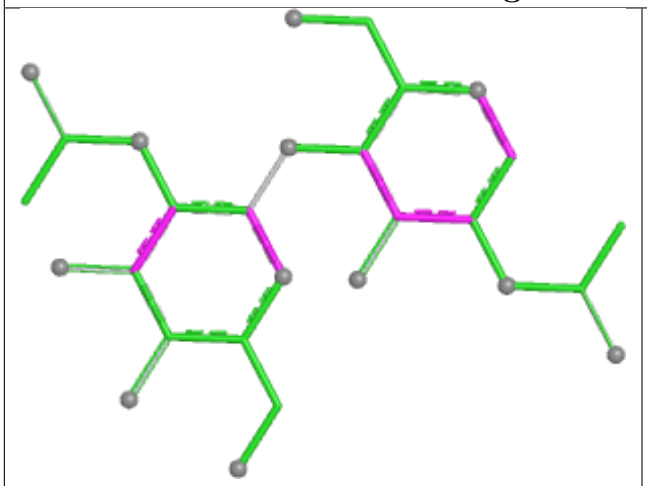


Rings

Oligosaccharide Chain j



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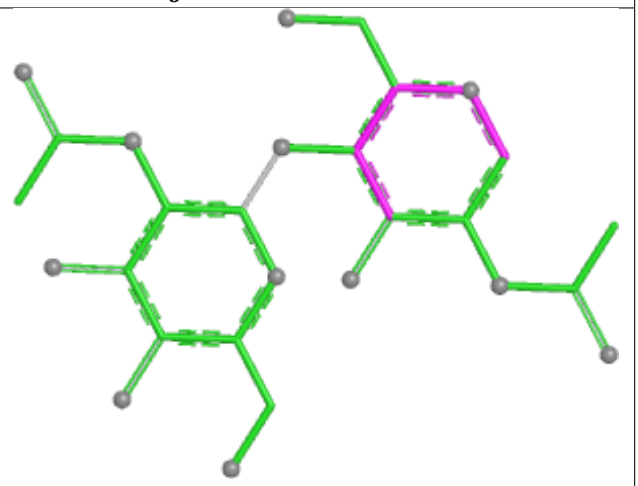
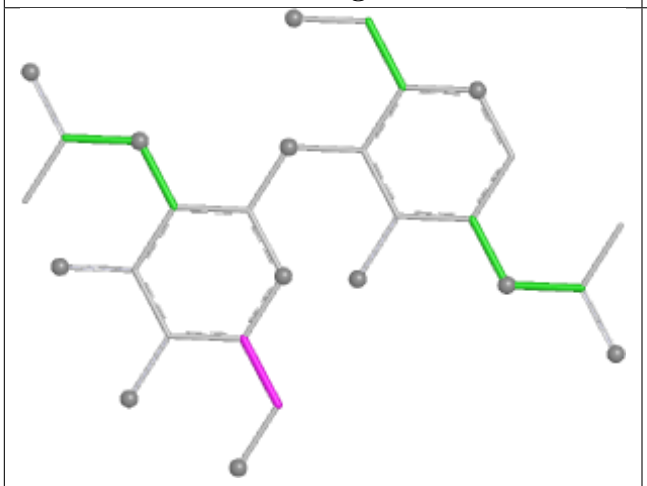


Bond angles



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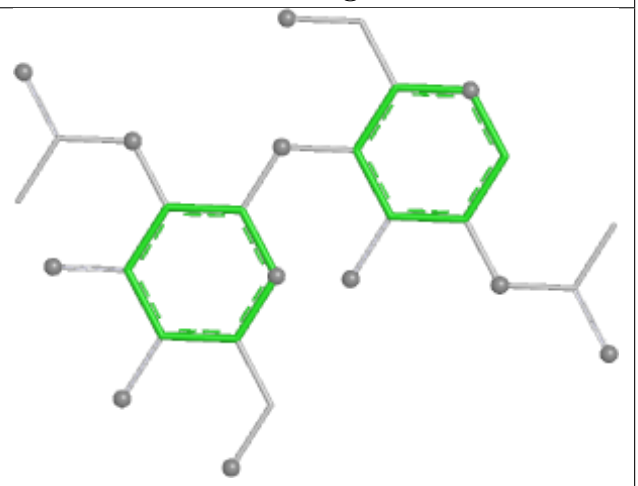
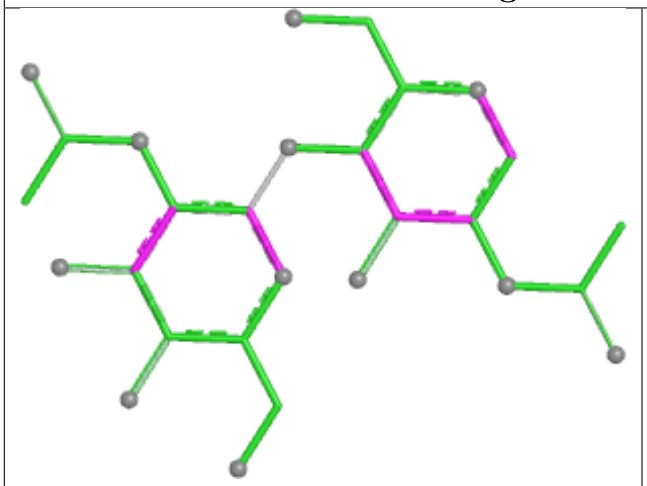


Rings

Oligosaccharide Chain k



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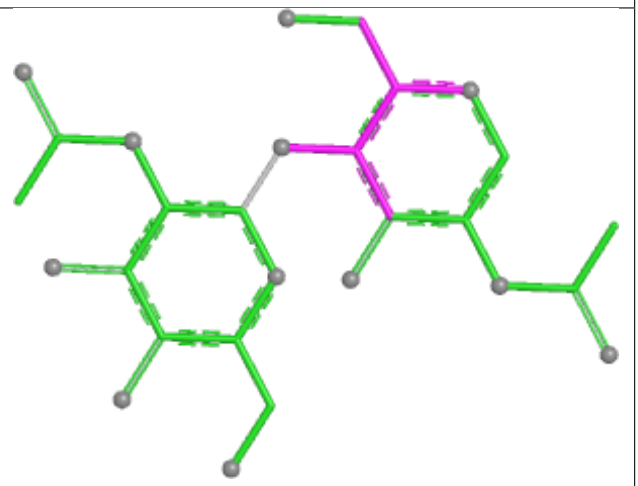
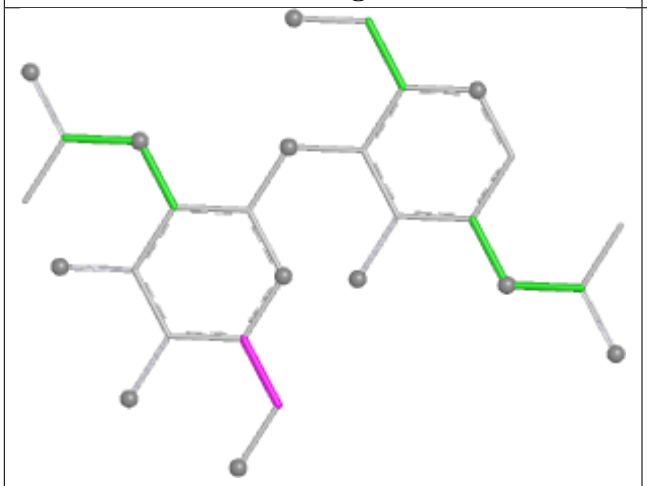


Bond angles



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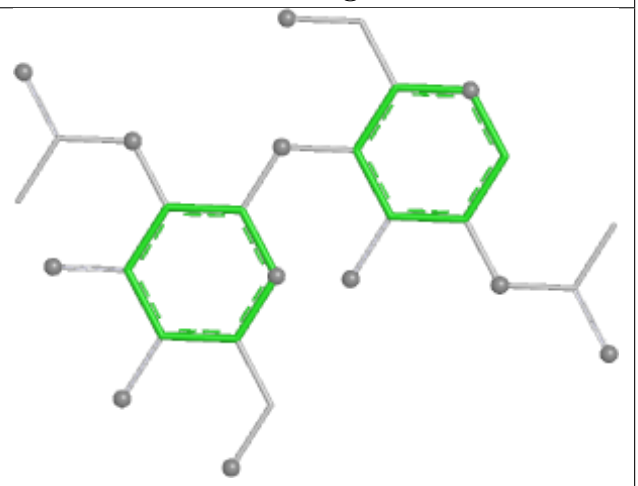
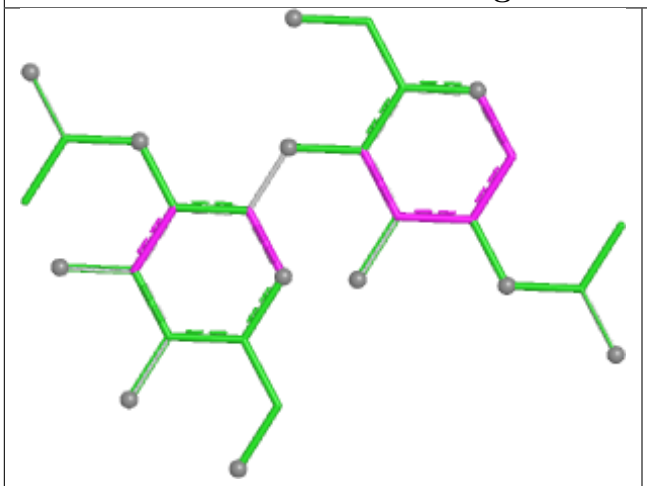


Rings

Oligosaccharide Chain m



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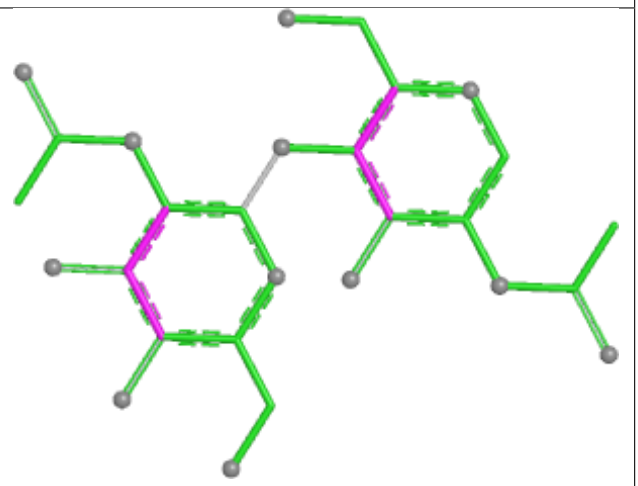

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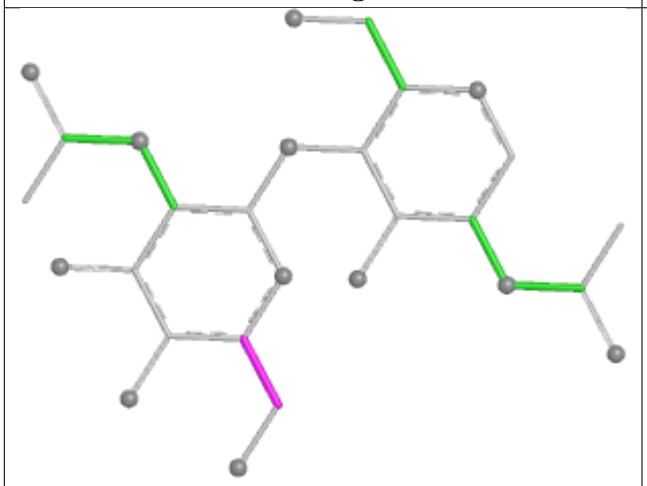

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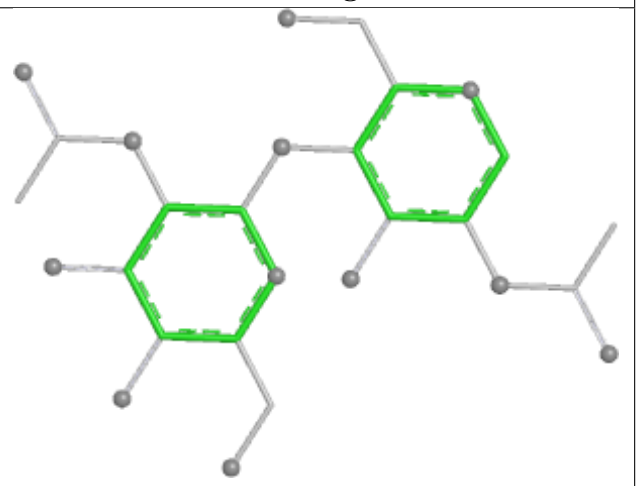
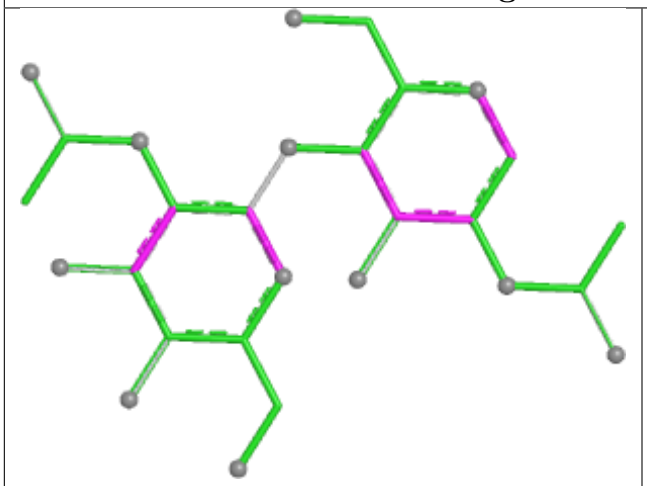


Rings

Oligosaccharide Chain n



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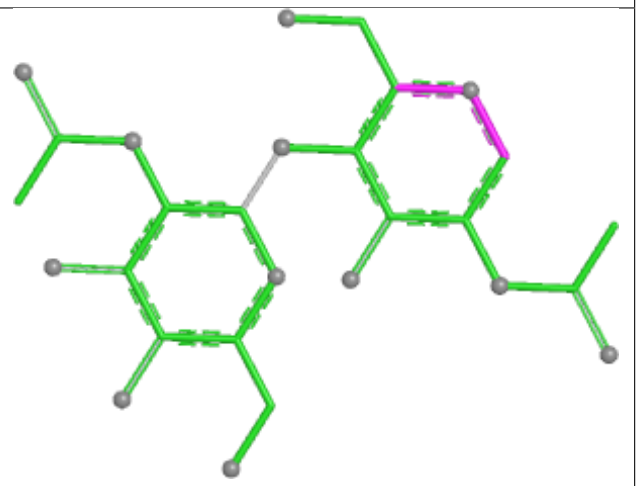
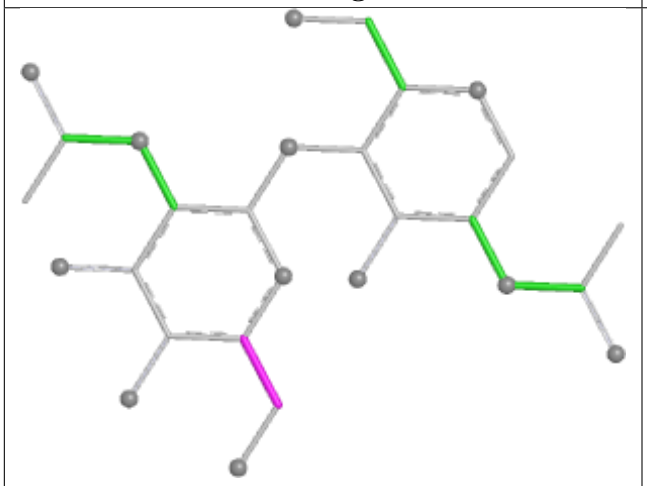


Bond angles



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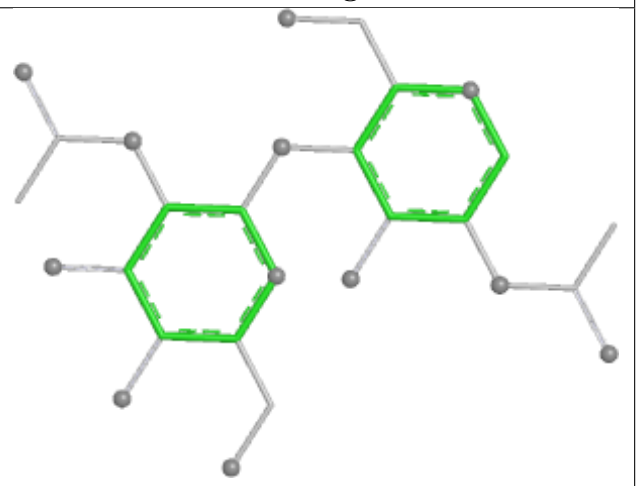
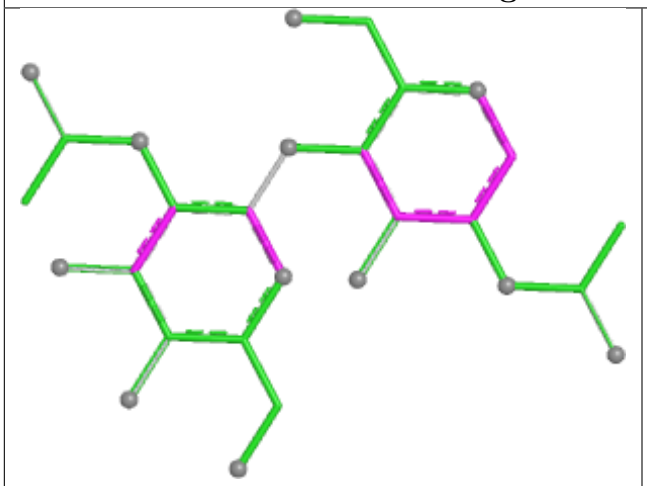


Rings

Oligosaccharide Chain o



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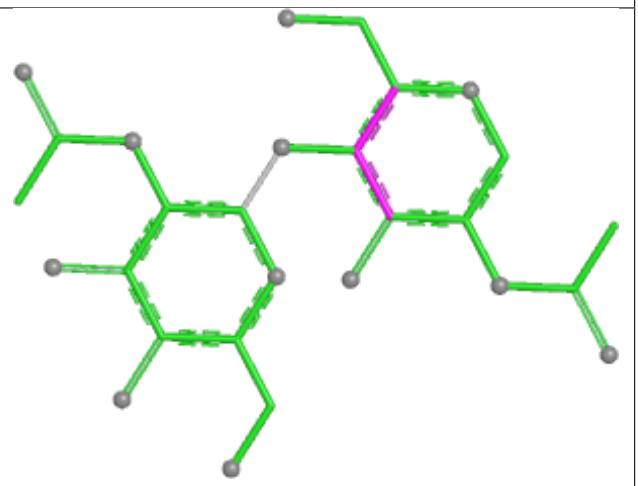

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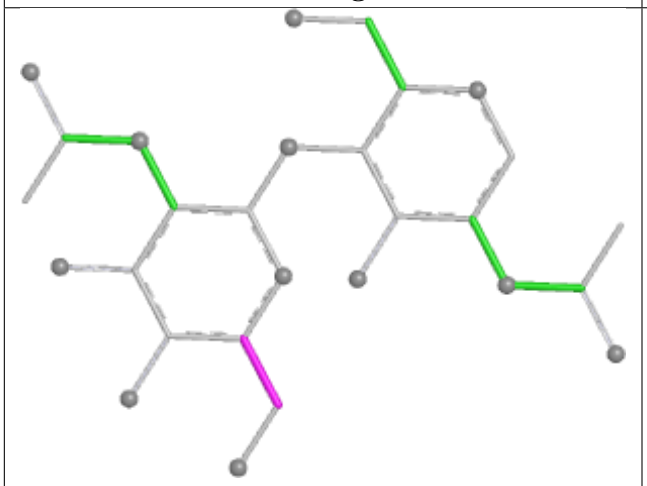

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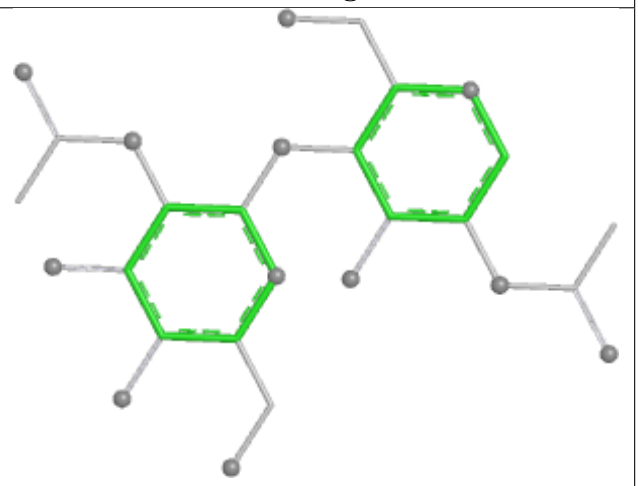
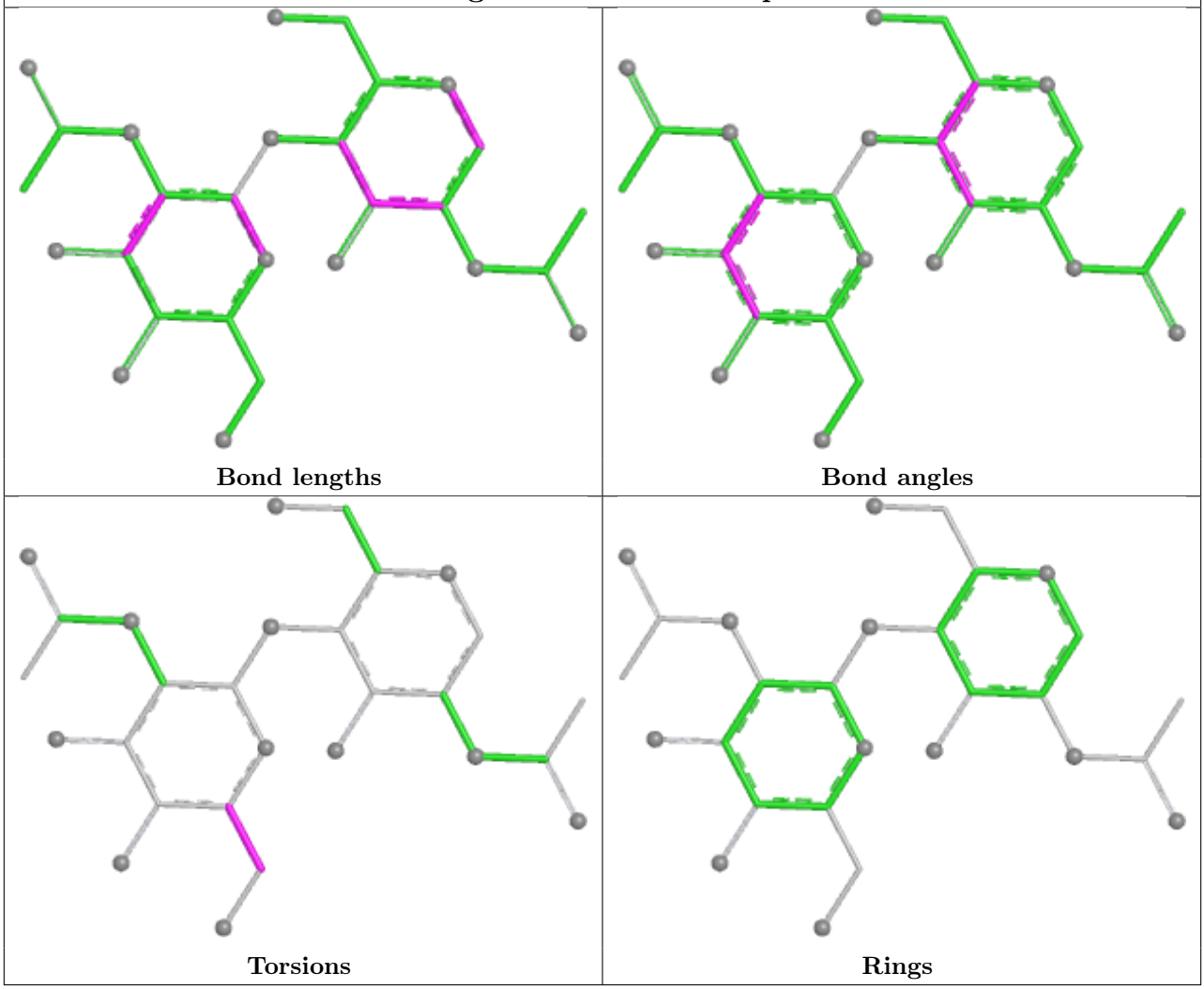
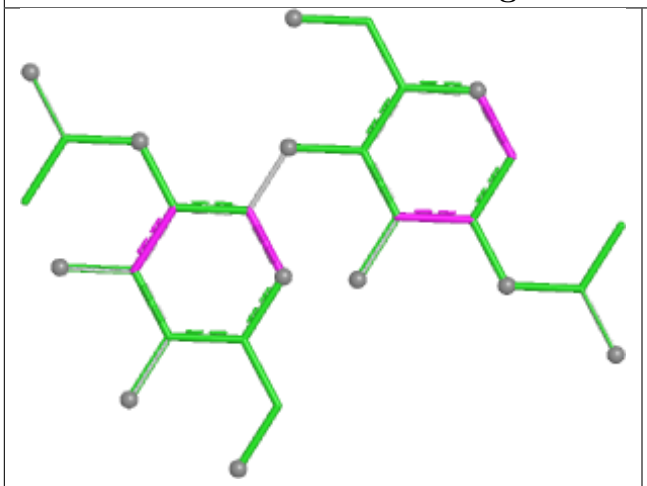


Rings

Oligosaccharide Chain p



Oligosaccharide Chain q



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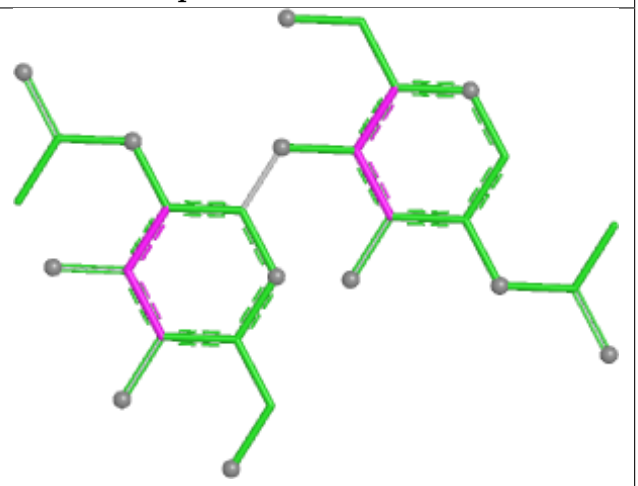
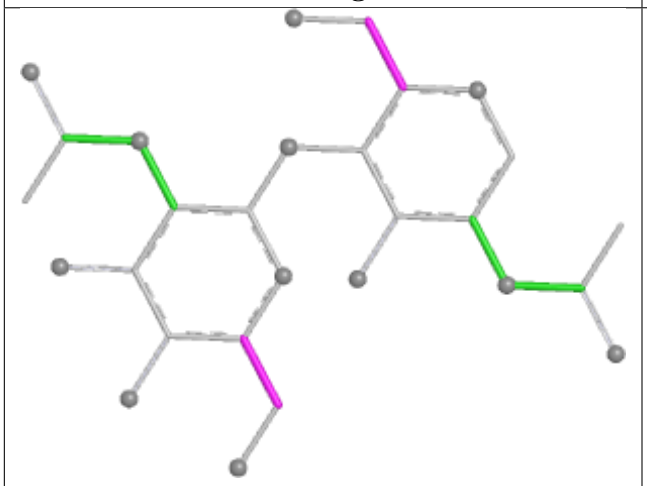


Bond angles



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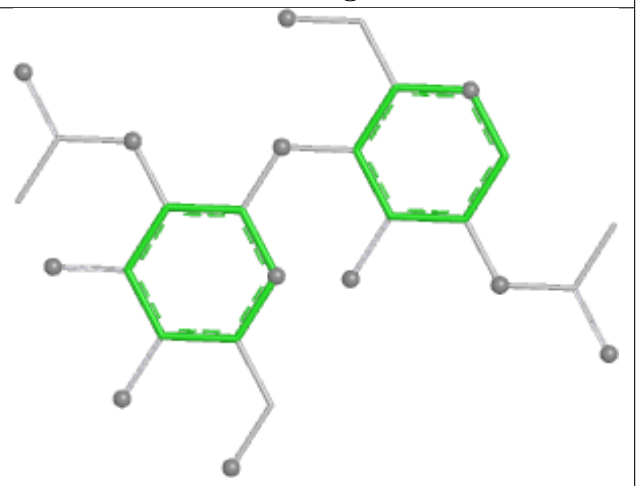
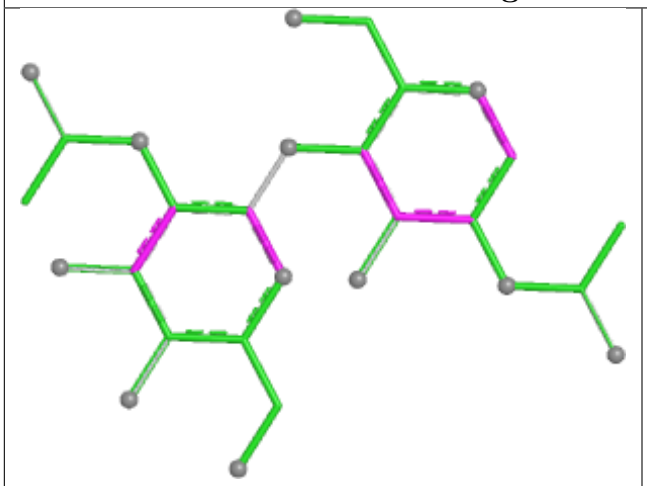


Rings

Oligosaccharide Chain r



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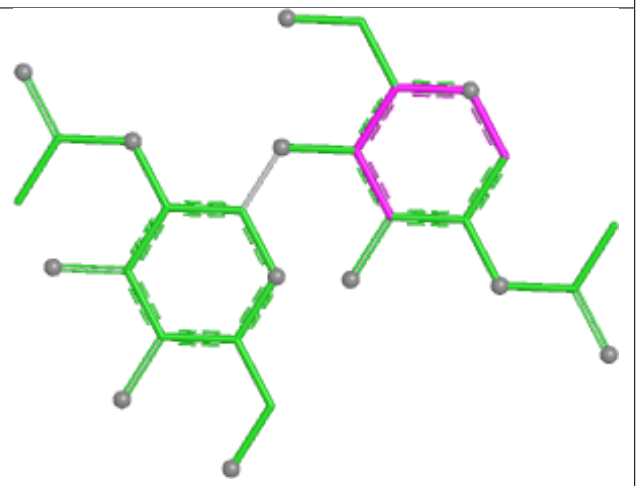

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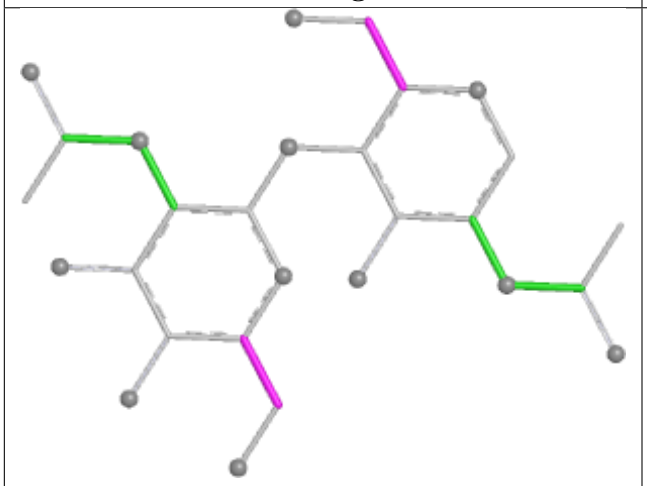

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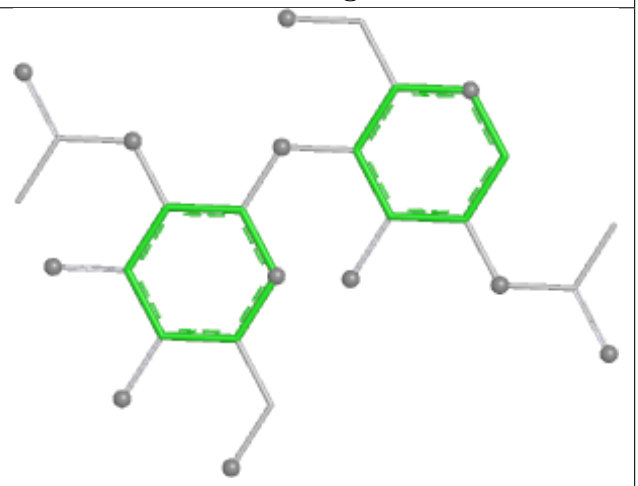
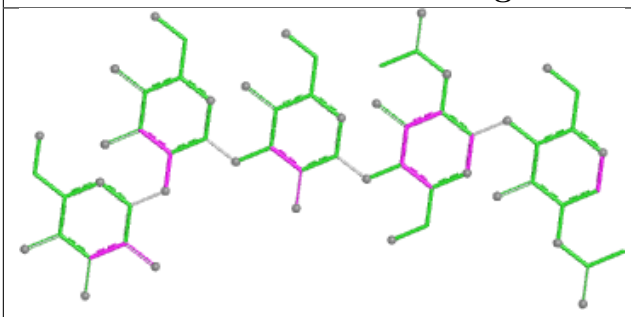


Rings

Oligosaccharide Chain R



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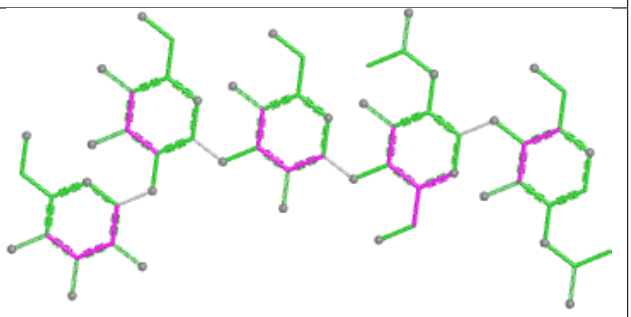
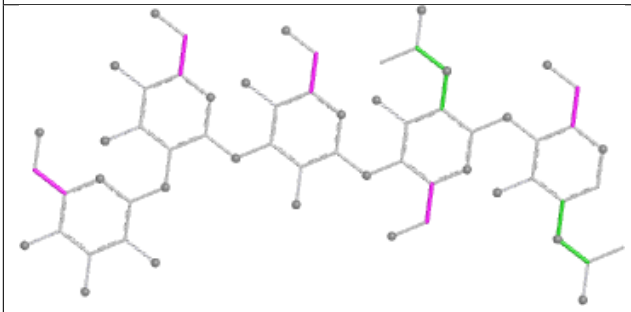


Bond angles



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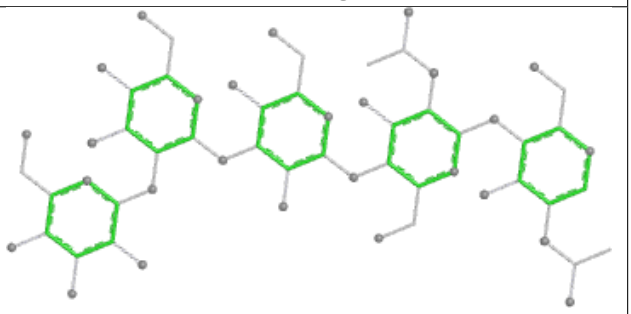
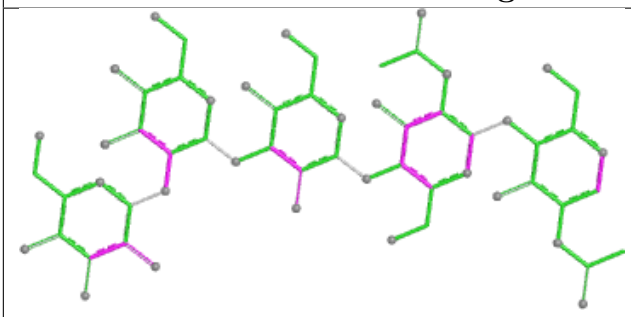


Rings

Oligosaccharide Chain b



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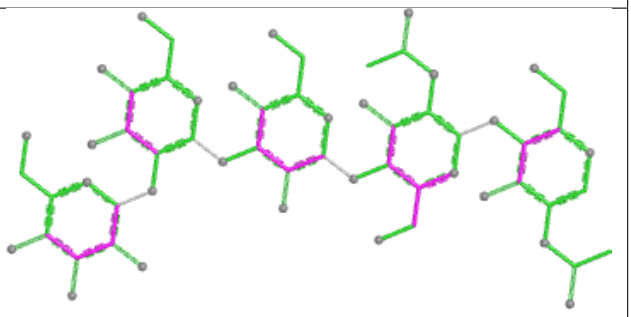
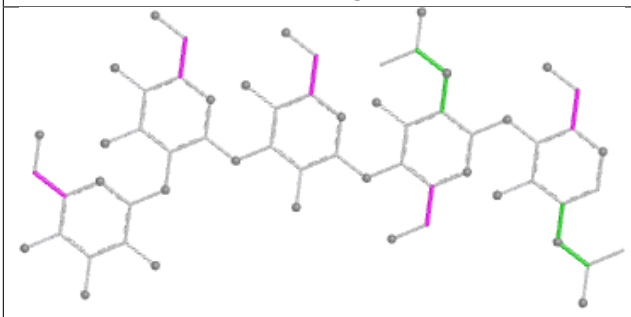
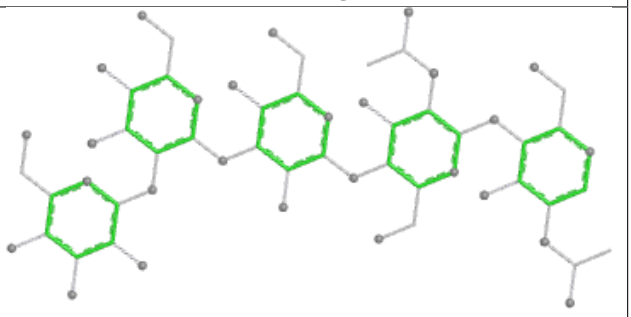


Bond angles

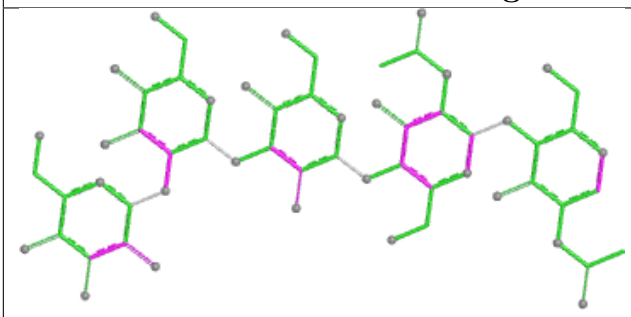


Torsions

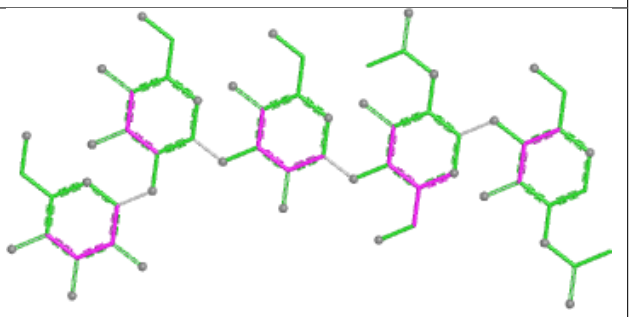


Rings

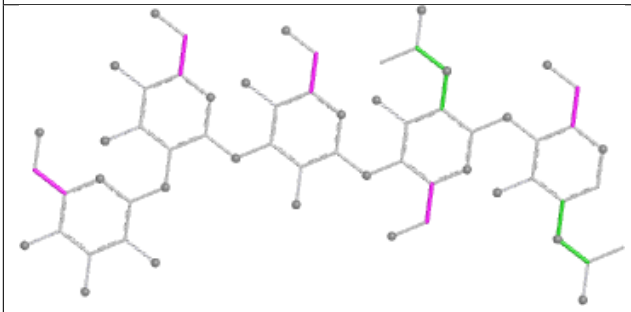
Oligosaccharide Chain l



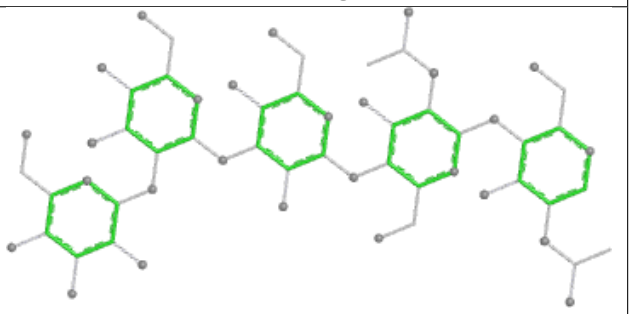
Bond lengths



Bond angles

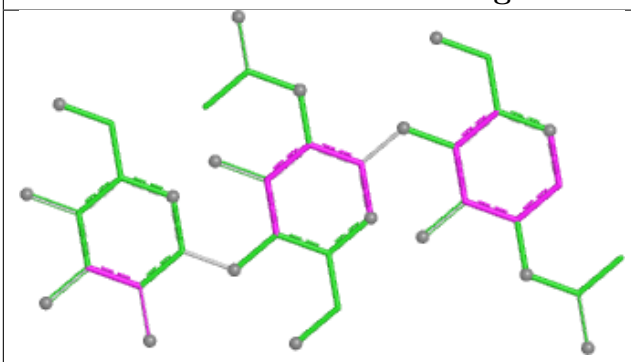


Torsions

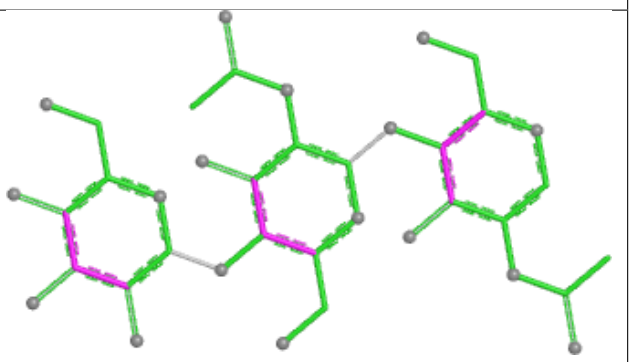


Rings

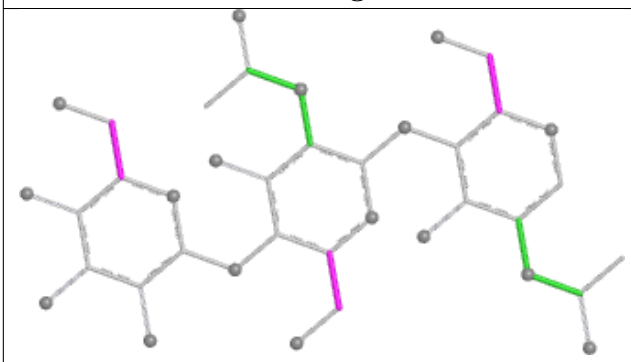
Oligosaccharide Chain Y



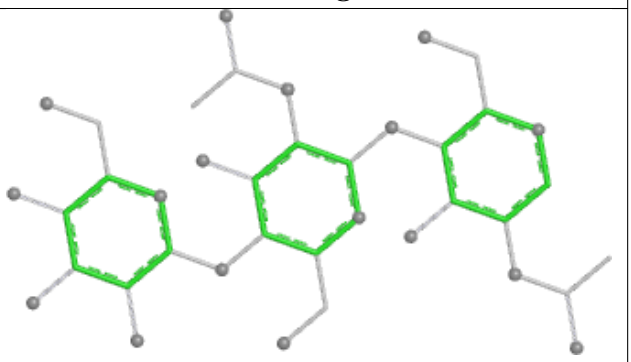
Bond lengths



Bond angles

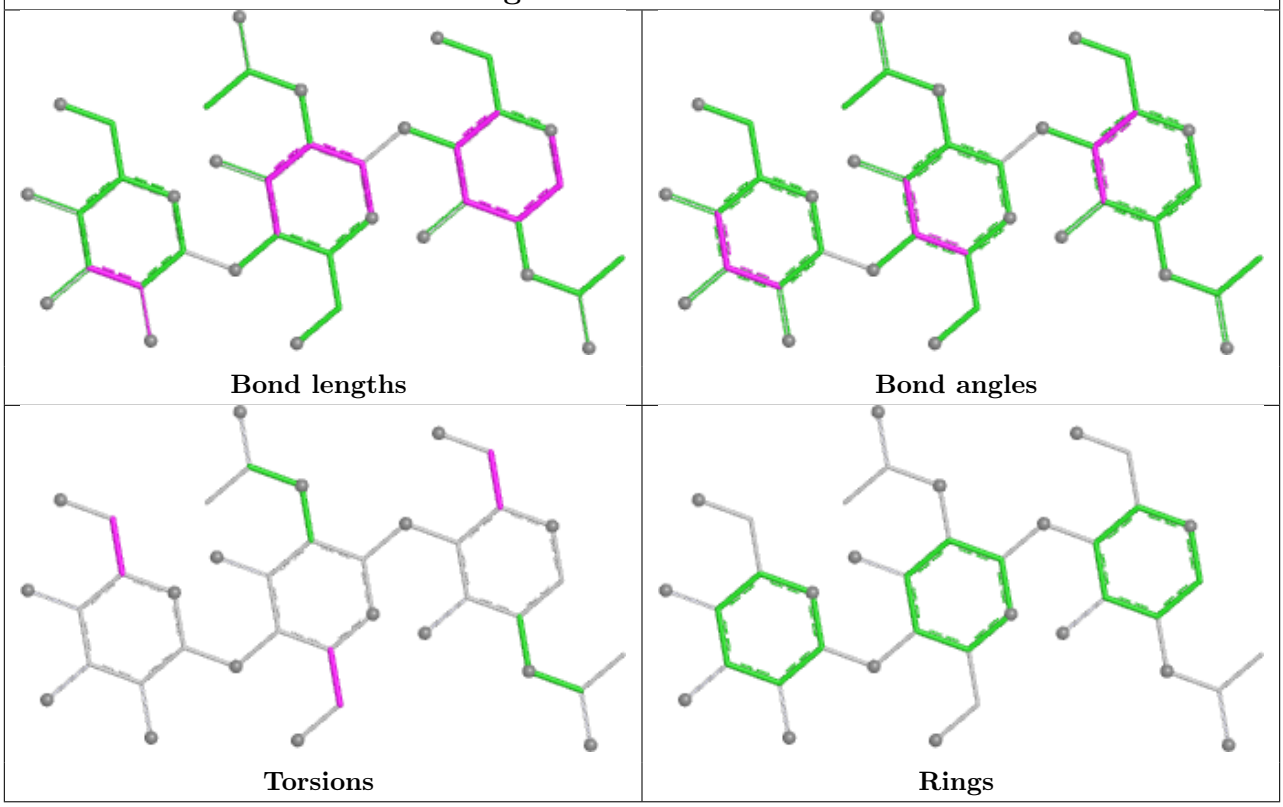


Torsions

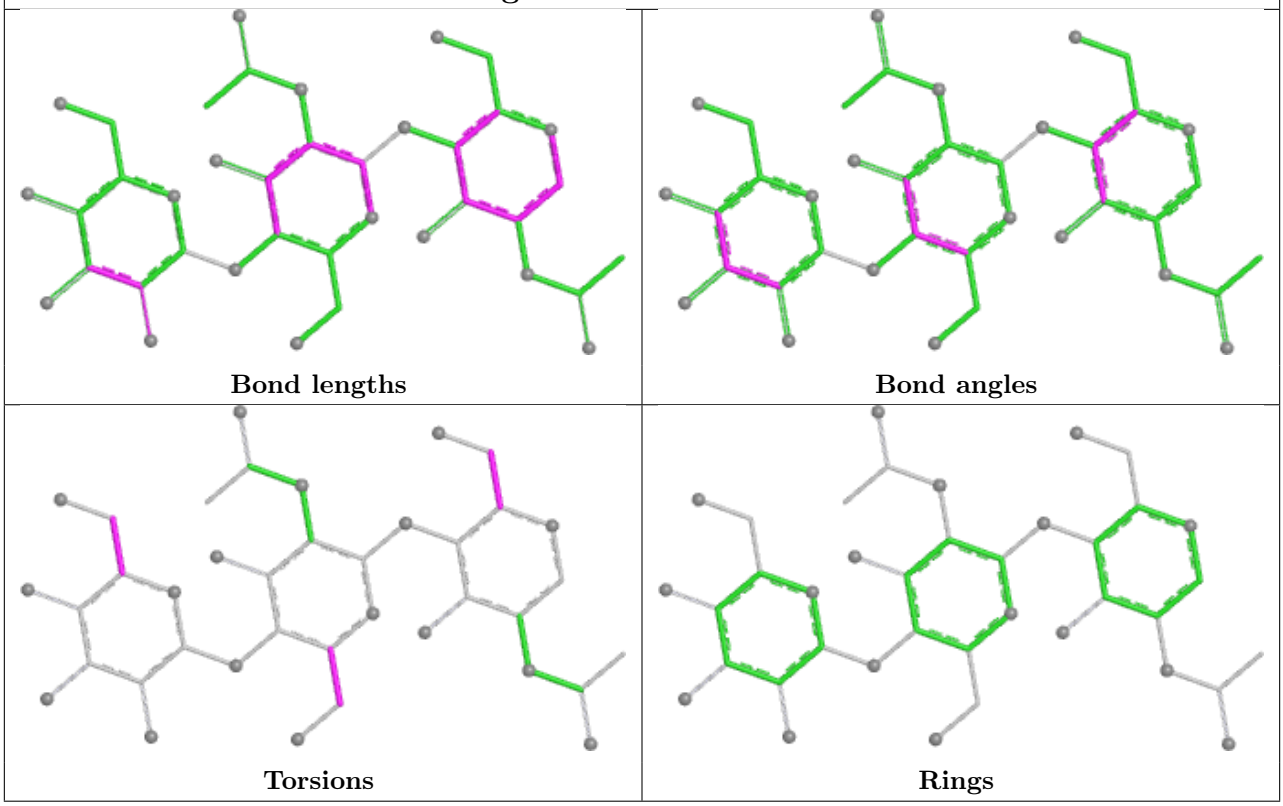


Rings

Oligosaccharide Chain i



Oligosaccharide Chain s



5.6 Ligand geometry (i)

21 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	$\#\|Z\| > 2$
9	NAG	D	628	1	14,14,15	2.08	2 (14%)	17,19,21	0.83	1 (5%)
9	NAG	D	617	1	14,14,15	2.02	2 (14%)	17,19,21	1.08	1 (5%)
10	LMT	B	701	-	36,36,36	1.33	2 (5%)	47,47,47	0.79	1 (2%)
9	NAG	B	703	3	14,14,15	2.07	2 (14%)	17,19,21	0.83	1 (5%)
9	NAG	D	601	1	14,14,15	2.06	3 (21%)	17,19,21	1.19	2 (11%)
9	NAG	B	702	3	14,14,15	2.02	2 (14%)	17,19,21	0.70	0
9	NAG	J	617	1	14,14,15	2.02	2 (14%)	17,19,21	1.08	1 (5%)
10	LMT	F	701	-	36,36,36	1.33	2 (5%)	47,47,47	0.79	1 (2%)
9	NAG	J	601	1	14,14,15	2.06	3 (21%)	17,19,21	1.19	2 (11%)
9	NAG	A	628	1	14,14,15	2.08	2 (14%)	17,19,21	0.83	1 (5%)
9	NAG	A	624	1	14,14,15	2.07	2 (14%)	17,19,21	0.88	0
9	NAG	F	703	3	14,14,15	2.07	2 (14%)	17,19,21	0.84	1 (5%)
10	LMT	M	701	-	36,36,36	1.33	2 (5%)	47,47,47	0.79	1 (2%)
9	NAG	M	703	3	14,14,15	2.07	2 (14%)	17,19,21	0.84	1 (5%)
9	NAG	D	624	1	14,14,15	2.07	2 (14%)	17,19,21	0.87	0
9	NAG	F	702	3	14,14,15	2.01	2 (14%)	17,19,21	0.70	0
9	NAG	M	702	3	14,14,15	2.02	2 (14%)	17,19,21	0.70	0
9	NAG	J	628	1	14,14,15	2.08	2 (14%)	17,19,21	0.83	1 (5%)
9	NAG	J	624	1	14,14,15	2.05	2 (14%)	17,19,21	0.88	0
9	NAG	A	601	1	14,14,15	2.07	3 (21%)	17,19,21	1.19	2 (11%)
9	NAG	A	617	1	14,14,15	2.03	2 (14%)	17,19,21	1.08	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	D	628	1	-	2/6/23/26	0/1/1/1
9	NAG	D	617	1	-	1/6/23/26	0/1/1/1
10	LMT	B	701	-	-	7/21/61/61	0/2/2/2
9	NAG	B	703	3	-	1/6/23/26	0/1/1/1
9	NAG	D	601	1	-	2/6/23/26	0/1/1/1
9	NAG	B	702	3	-	1/6/23/26	0/1/1/1
9	NAG	J	617	1	-	1/6/23/26	0/1/1/1
10	LMT	F	701	-	-	7/21/61/61	0/2/2/2
9	NAG	J	601	1	-	2/6/23/26	0/1/1/1
9	NAG	A	628	1	-	2/6/23/26	0/1/1/1
9	NAG	A	624	1	-	2/6/23/26	0/1/1/1
9	NAG	F	703	3	-	1/6/23/26	0/1/1/1
10	LMT	M	701	-	-	7/21/61/61	0/2/2/2
9	NAG	M	703	3	-	1/6/23/26	0/1/1/1
9	NAG	D	624	1	-	2/6/23/26	0/1/1/1
9	NAG	F	702	3	-	1/6/23/26	0/1/1/1
9	NAG	M	702	3	-	1/6/23/26	0/1/1/1
9	NAG	J	628	1	-	2/6/23/26	0/1/1/1
9	NAG	J	624	1	-	2/6/23/26	0/1/1/1
9	NAG	A	601	1	-	2/6/23/26	0/1/1/1
9	NAG	A	617	1	-	1/6/23/26	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	624	NAG	O5-C1	6.80	1.55	1.43
9	A	624	NAG	O5-C1	6.78	1.55	1.43
9	J	624	NAG	O5-C1	6.71	1.55	1.43
9	D	628	NAG	O5-C1	6.69	1.54	1.43
9	A	628	NAG	O5-C1	6.69	1.54	1.43
9	J	628	NAG	O5-C1	6.68	1.54	1.43
9	F	703	NAG	O5-C1	6.60	1.54	1.43
9	B	703	NAG	O5-C1	6.58	1.54	1.43
9	M	703	NAG	O5-C1	6.58	1.54	1.43
9	B	702	NAG	O5-C1	6.47	1.54	1.43
9	M	702	NAG	O5-C1	6.47	1.54	1.43
9	F	702	NAG	O5-C1	6.47	1.54	1.43
9	A	601	NAG	O5-C1	6.47	1.54	1.43
9	J	601	NAG	O5-C1	6.46	1.54	1.43
9	D	601	NAG	O5-C1	6.44	1.54	1.43
9	A	617	NAG	O5-C1	6.44	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	617	NAG	O5-C1	6.44	1.54	1.43
9	J	617	NAG	O5-C1	6.43	1.54	1.43
10	B	701	LMT	O1'-C1'	3.70	1.46	1.40
10	M	701	LMT	O1'-C1'	3.69	1.46	1.40
10	F	701	LMT	O1'-C1'	3.68	1.46	1.40
9	D	601	NAG	C3-C2	-2.40	1.47	1.52
9	A	617	NAG	C3-C2	-2.38	1.47	1.52
9	J	617	NAG	C3-C2	-2.37	1.47	1.52
9	J	601	NAG	C3-C2	-2.36	1.47	1.52
9	J	628	NAG	C3-C2	-2.36	1.47	1.52
9	A	601	NAG	C3-C2	-2.35	1.47	1.52
9	D	617	NAG	C3-C2	-2.35	1.47	1.52
9	D	628	NAG	C3-C2	-2.34	1.47	1.52
9	A	628	NAG	C3-C2	-2.33	1.47	1.52
9	M	703	NAG	C3-C2	-2.28	1.47	1.52
9	B	703	NAG	C3-C2	-2.27	1.47	1.52
9	F	703	NAG	C3-C2	-2.27	1.47	1.52
9	A	624	NAG	C3-C2	-2.22	1.47	1.52
9	D	624	NAG	C3-C2	-2.21	1.47	1.52
9	J	624	NAG	C3-C2	-2.17	1.48	1.52
10	B	701	LMT	C4B-C5B	2.07	1.57	1.53
10	M	701	LMT	C4B-C5B	2.05	1.57	1.53
9	J	601	NAG	C4-C3	2.04	1.57	1.52
9	D	601	NAG	C4-C3	2.04	1.57	1.52
10	F	701	LMT	C4B-C5B	2.03	1.57	1.53
9	B	702	NAG	C3-C2	-2.03	1.48	1.52
9	F	702	NAG	C3-C2	-2.01	1.48	1.52
9	M	702	NAG	C3-C2	-2.01	1.48	1.52
9	A	601	NAG	C4-C3	2.00	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	601	NAG	C4-C3-C2	-3.13	106.43	111.02
9	A	601	NAG	C4-C3-C2	-3.12	106.44	111.02
9	J	601	NAG	C4-C3-C2	-3.10	106.47	111.02
9	D	617	NAG	C4-C3-C2	-2.96	106.68	111.02
9	A	617	NAG	C4-C3-C2	-2.96	106.69	111.02
9	J	617	NAG	C4-C3-C2	-2.93	106.73	111.02
9	J	601	NAG	C1-O5-C5	-2.18	109.26	112.19
9	M	703	NAG	C4-C3-C2	-2.18	107.82	111.02
9	F	703	NAG	C4-C3-C2	-2.18	107.83	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	703	NAG	C4-C3-C2	-2.16	107.86	111.02
9	J	628	NAG	C4-C3-C2	-2.14	107.88	111.02
9	D	601	NAG	C1-O5-C5	-2.14	109.31	112.19
9	A	628	NAG	C4-C3-C2	-2.14	107.88	111.02
9	A	601	NAG	C1-O5-C5	-2.14	109.32	112.19
9	D	628	NAG	C4-C3-C2	-2.13	107.89	111.02
10	F	701	LMT	C1-O1'-C1'	2.08	117.24	113.68
10	M	701	LMT	C1-O1'-C1'	2.06	117.19	113.68
10	B	701	LMT	C1-O1'-C1'	2.05	117.18	113.68

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	701	LMT	O5'-C1'-O1'-C1
10	F	701	LMT	O5'-C1'-O1'-C1
10	M	701	LMT	O5'-C1'-O1'-C1
9	A	628	NAG	O5-C5-C6-O6
9	D	628	NAG	O5-C5-C6-O6
9	J	628	NAG	O5-C5-C6-O6
9	A	601	NAG	O5-C5-C6-O6
9	A	624	NAG	O5-C5-C6-O6
9	D	601	NAG	O5-C5-C6-O6
9	D	624	NAG	O5-C5-C6-O6
9	J	601	NAG	O5-C5-C6-O6
9	J	624	NAG	O5-C5-C6-O6
10	B	701	LMT	C4B-C5B-C6B-O6B
10	F	701	LMT	C4B-C5B-C6B-O6B
10	M	701	LMT	C4B-C5B-C6B-O6B
10	B	701	LMT	O5B-C5B-C6B-O6B
10	F	701	LMT	O5B-C5B-C6B-O6B
10	M	701	LMT	O5B-C5B-C6B-O6B
9	B	702	NAG	O5-C5-C6-O6
9	F	702	NAG	O5-C5-C6-O6
9	M	702	NAG	O5-C5-C6-O6
9	F	703	NAG	O5-C5-C6-O6
9	M	703	NAG	O5-C5-C6-O6
9	B	703	NAG	O5-C5-C6-O6
9	A	617	NAG	O5-C5-C6-O6
9	D	617	NAG	O5-C5-C6-O6
9	J	617	NAG	O5-C5-C6-O6
9	A	628	NAG	C4-C5-C6-O6

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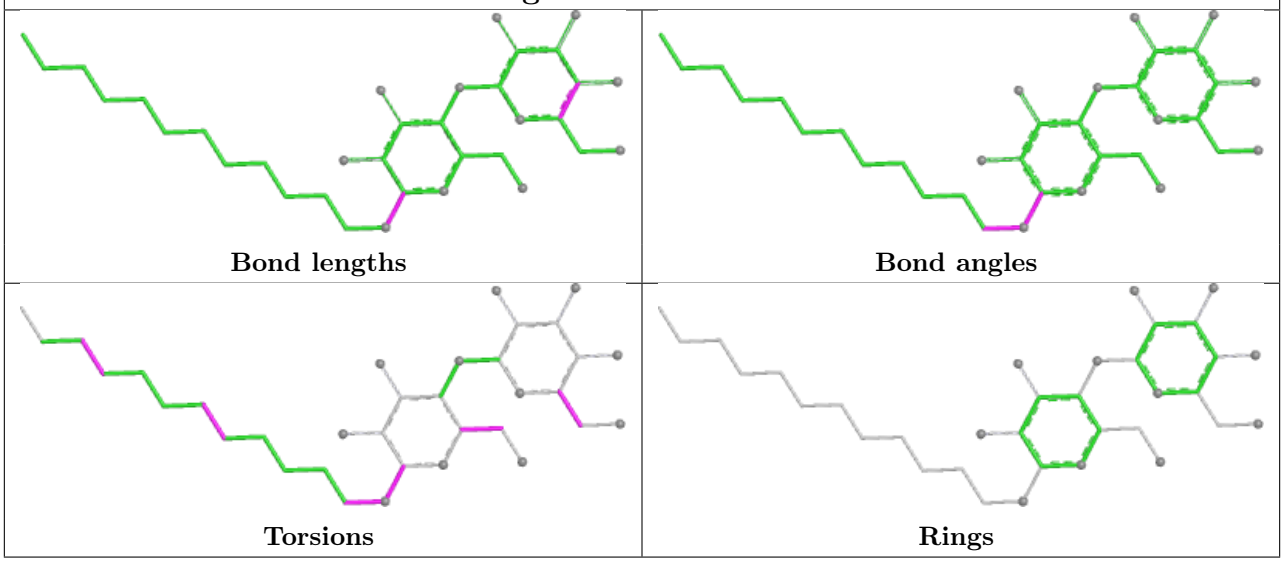
Mol	Chain	Res	Type	Atoms
9	D	628	NAG	C4-C5-C6-O6
9	J	628	NAG	C4-C5-C6-O6
10	B	701	LMT	O5'-C5'-C6'-O6'
10	F	701	LMT	O5'-C5'-C6'-O6'
10	M	701	LMT	O5'-C5'-C6'-O6'
10	B	701	LMT	C2-C1-O1'-C1'
10	F	701	LMT	C2-C1-O1'-C1'
10	M	701	LMT	C2-C1-O1'-C1'
10	B	701	LMT	C11-C10-C9-C8
10	F	701	LMT	C11-C10-C9-C8
10	M	701	LMT	C11-C10-C9-C8
10	F	701	LMT	C4-C5-C6-C7
10	M	701	LMT	C4-C5-C6-C7
10	B	701	LMT	C4-C5-C6-C7
9	J	601	NAG	C4-C5-C6-O6
9	A	601	NAG	C4-C5-C6-O6
9	D	601	NAG	C4-C5-C6-O6
9	D	624	NAG	C4-C5-C6-O6
9	J	624	NAG	C4-C5-C6-O6
9	A	624	NAG	C4-C5-C6-O6

There are no ring outliers.

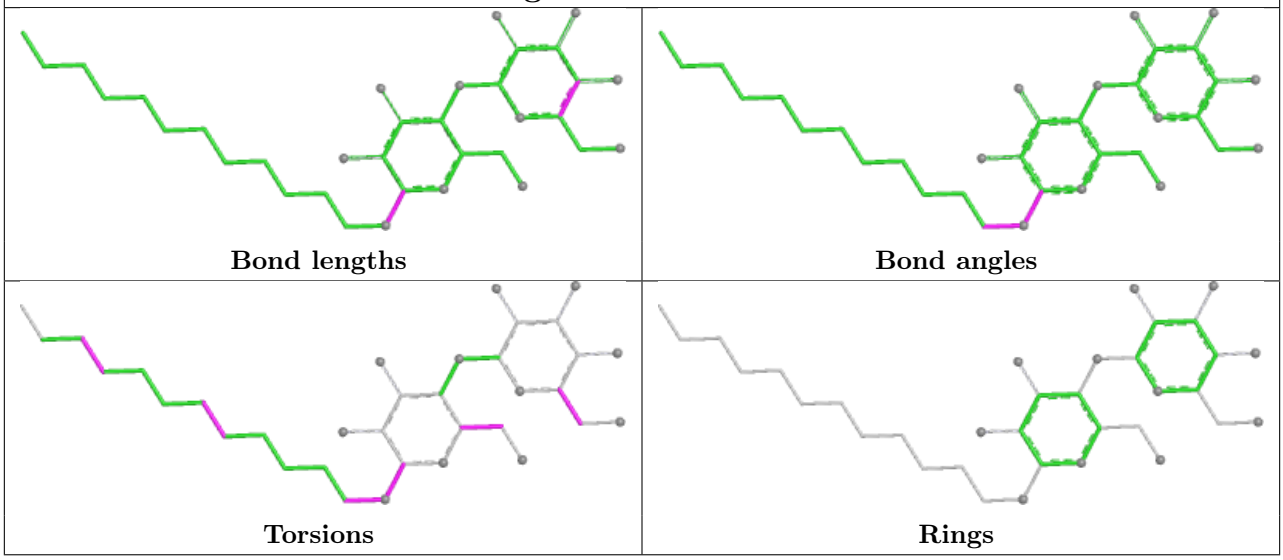
No monomer is involved in short contacts.

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.

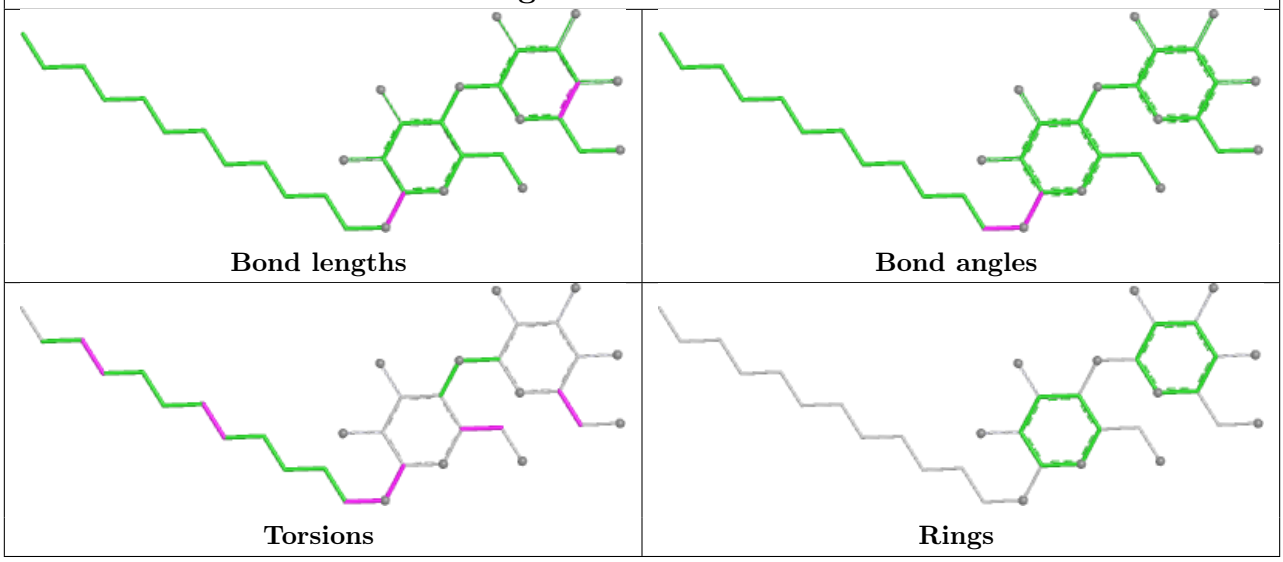
Ligand LMT B 701



Ligand LMT F 701



Ligand LMT M 701



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.

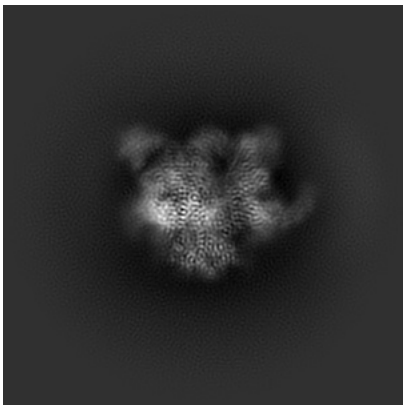
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20151. These allow visual inspection of the internal detail of the map and identification of artifacts.

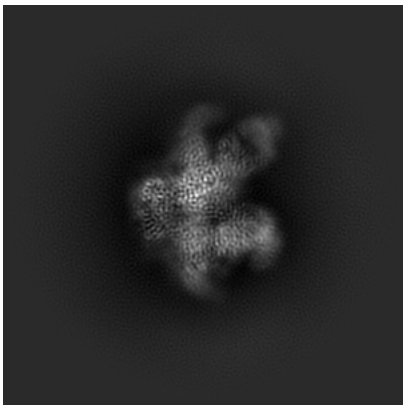
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

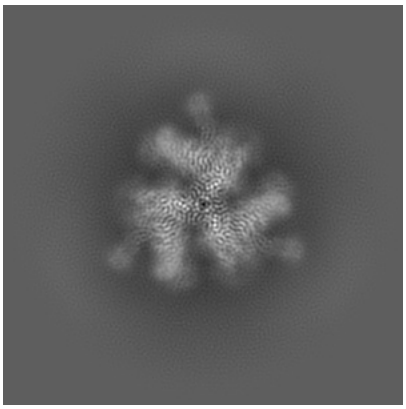
6.1.1 Primary map



X

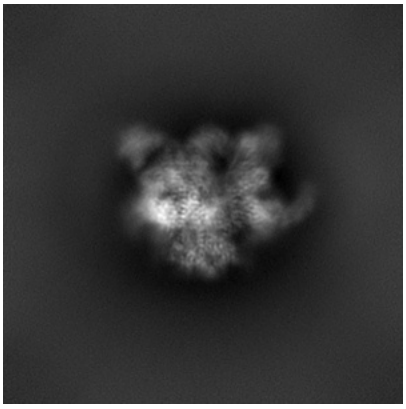


Y

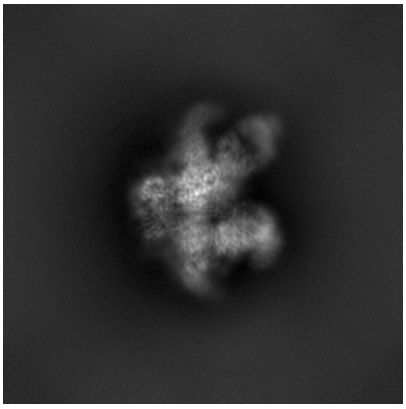


Z

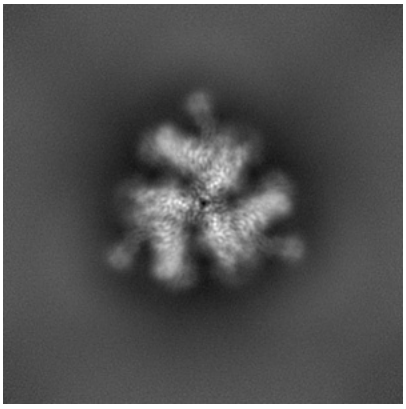
6.1.2 Raw map



X



Y

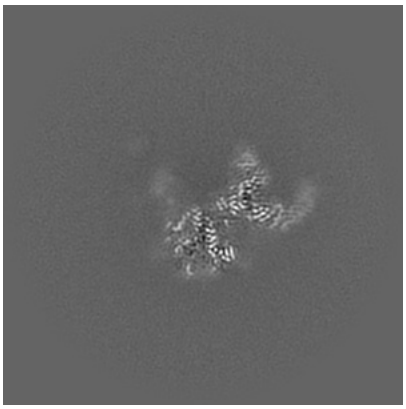


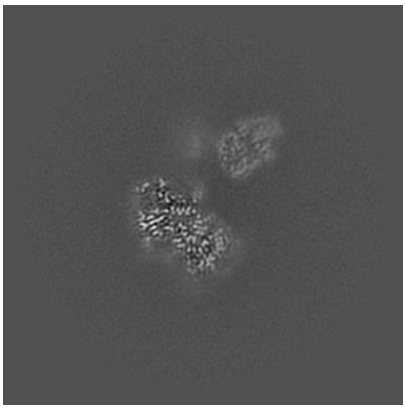
Z

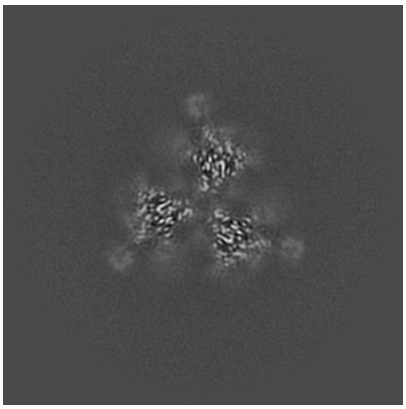
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

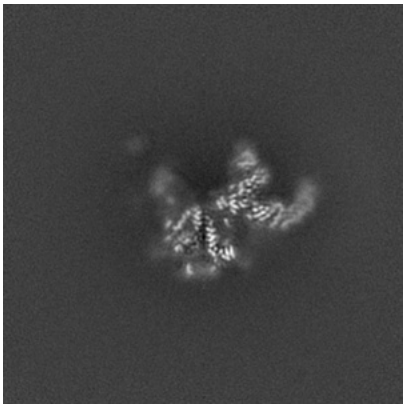
6.2.1 Primary map

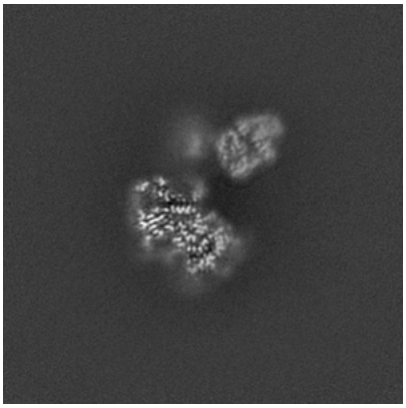

X Index: 144

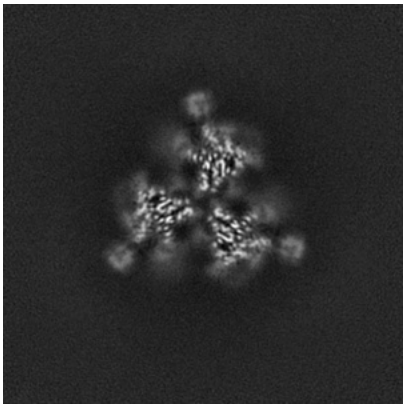

Y Index: 144


Z Index: 144

6.2.2 Raw map


X Index: 144

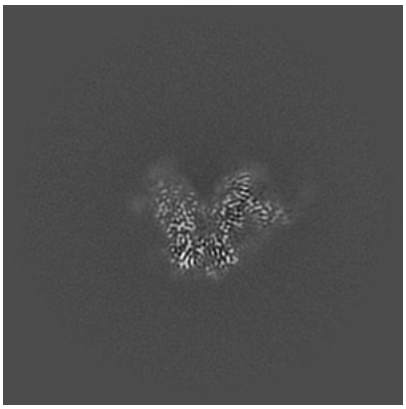

Y Index: 144

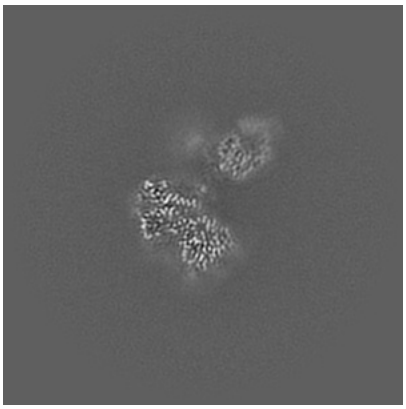

Z Index: 144

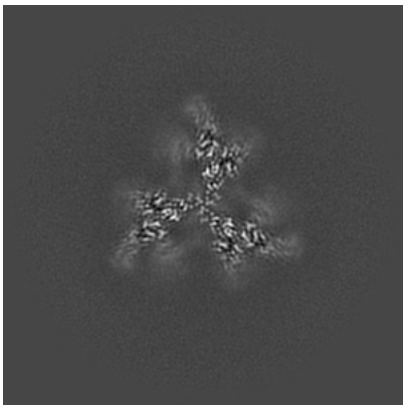
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

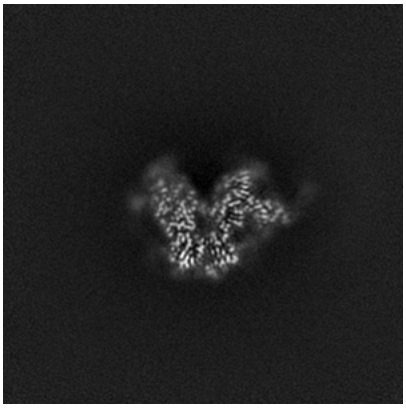
6.3.1 Primary map

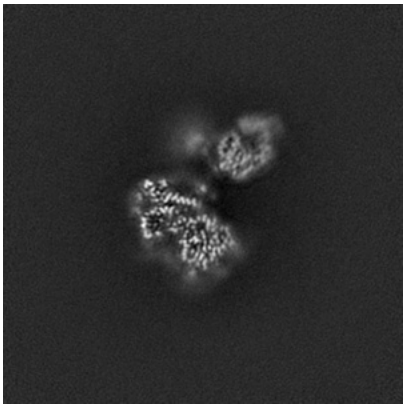

X Index: 152

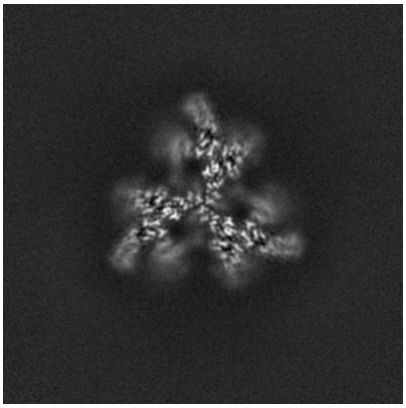

Y Index: 140


Z Index: 138

6.3.2 Raw map


X Index: 152

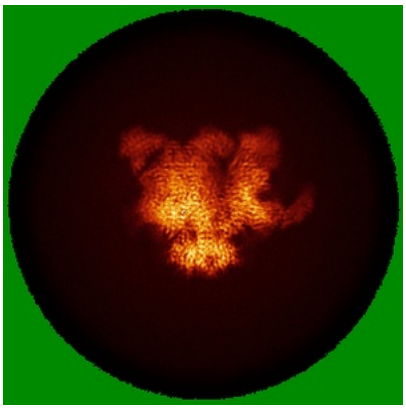

Y Index: 140

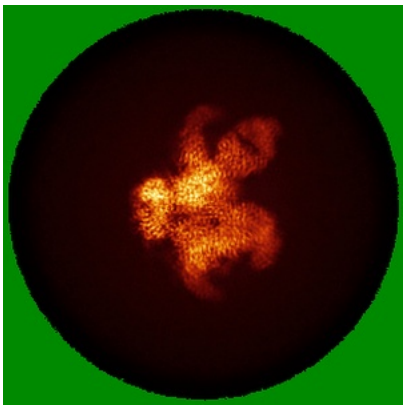

Z Index: 138

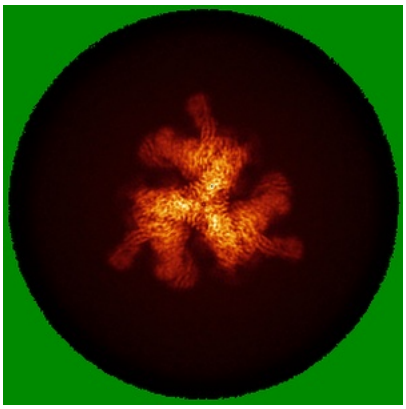
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

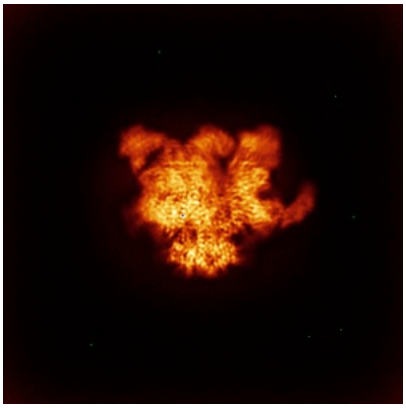
6.4.1 Primary map

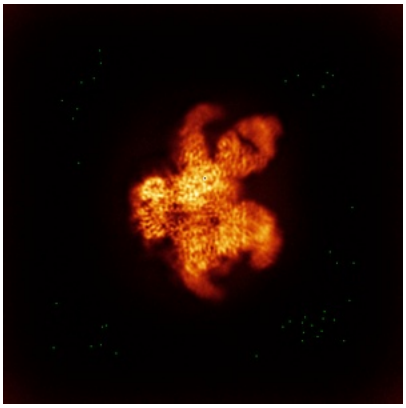

X

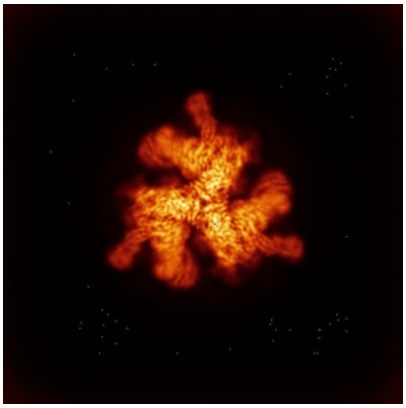

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

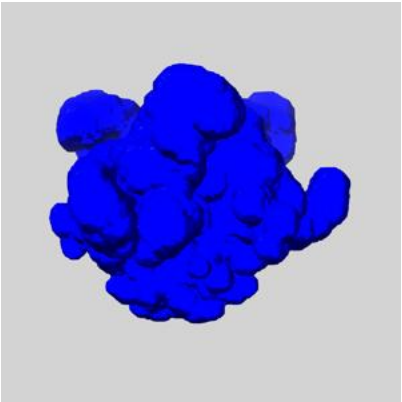
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

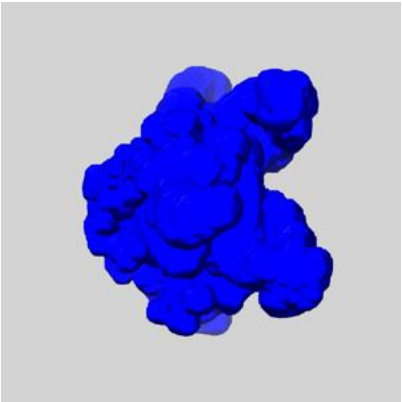
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

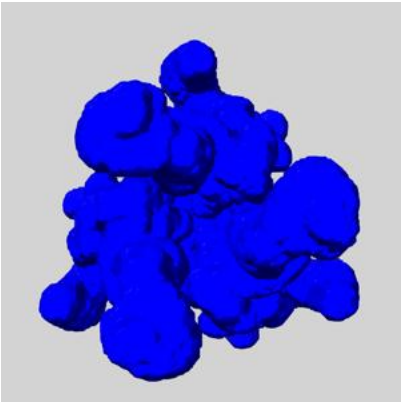
6.6.1 emd_20151_msk_1.map (i)



X



Y

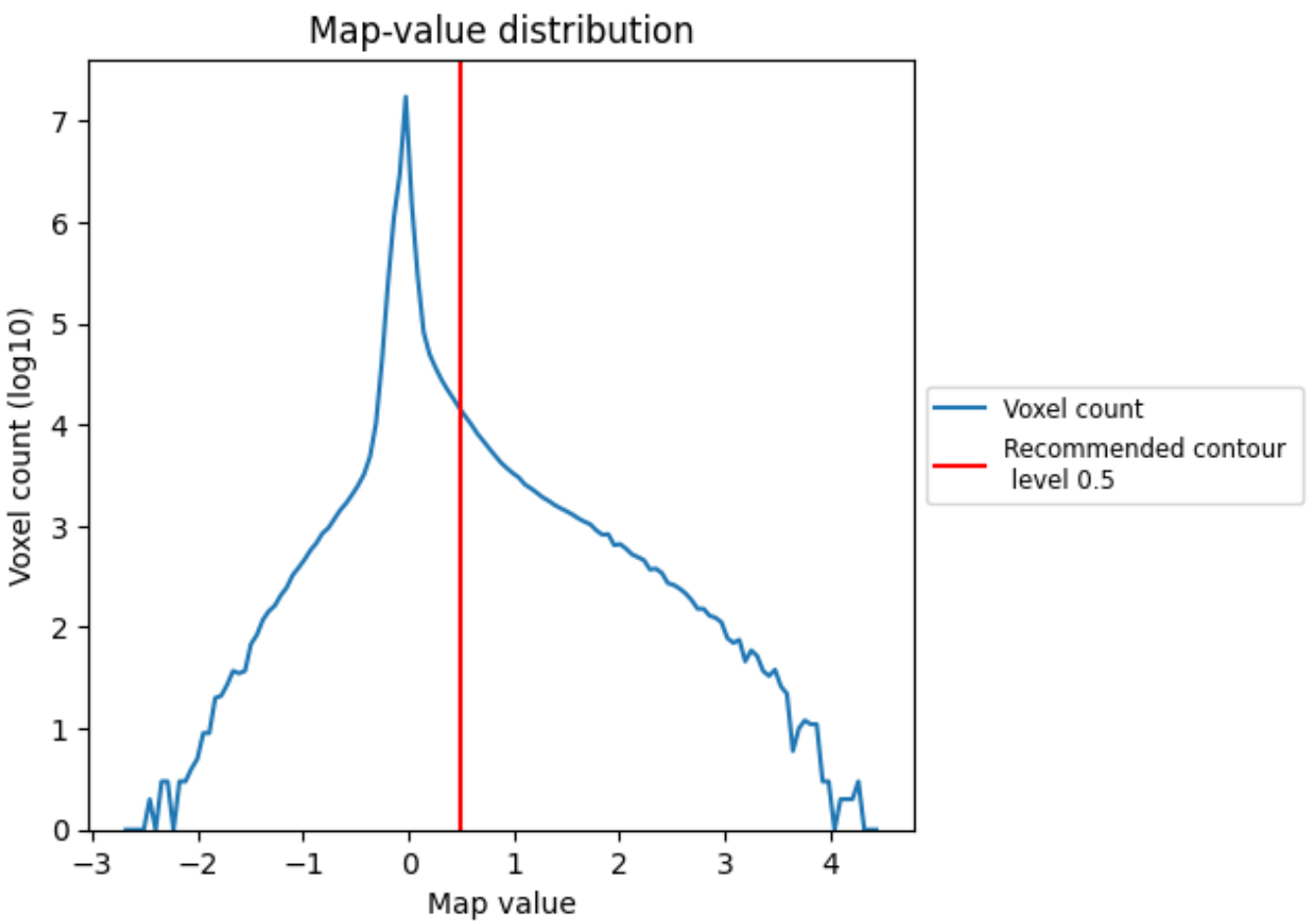


Z

7 Map analysis (i)

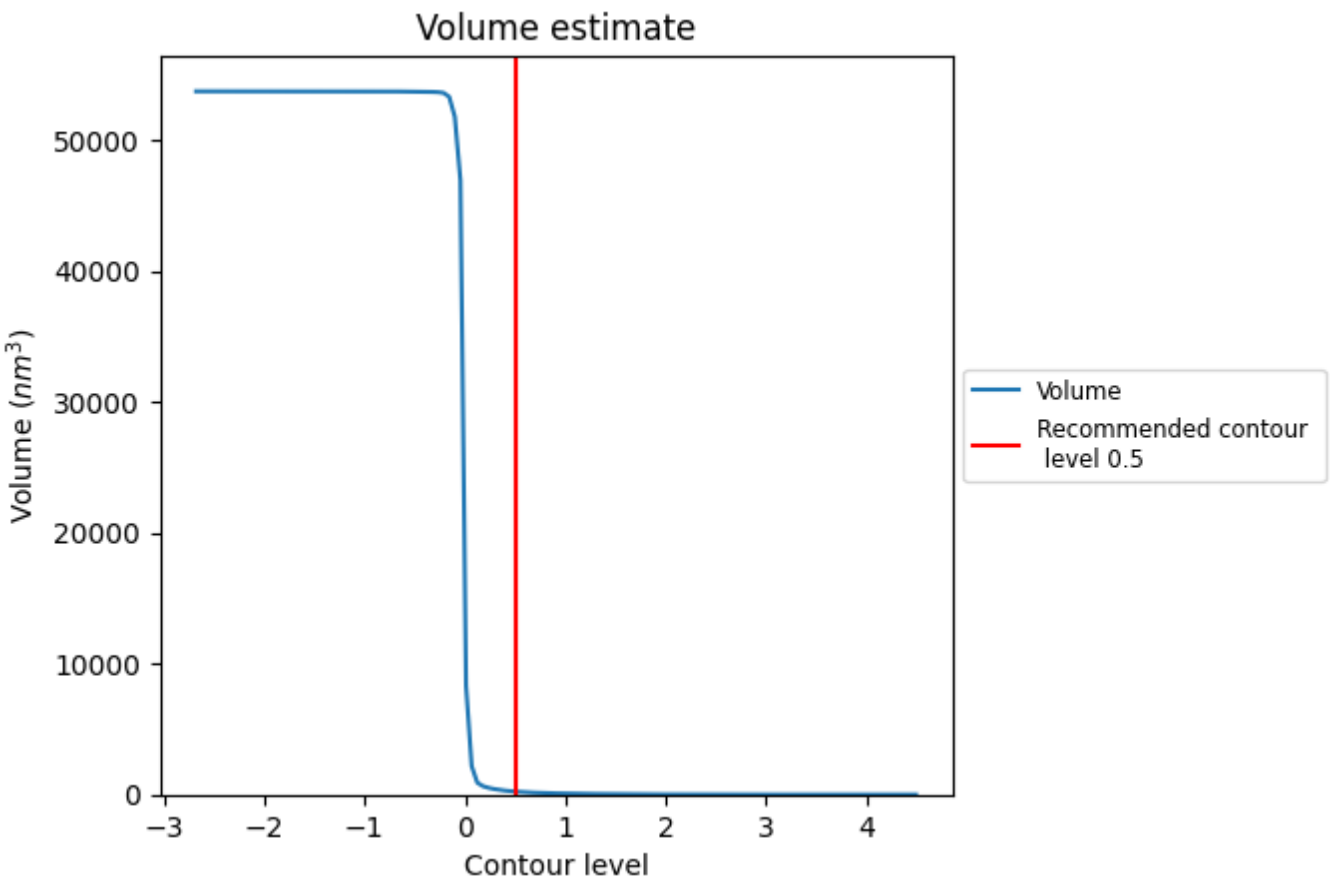
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

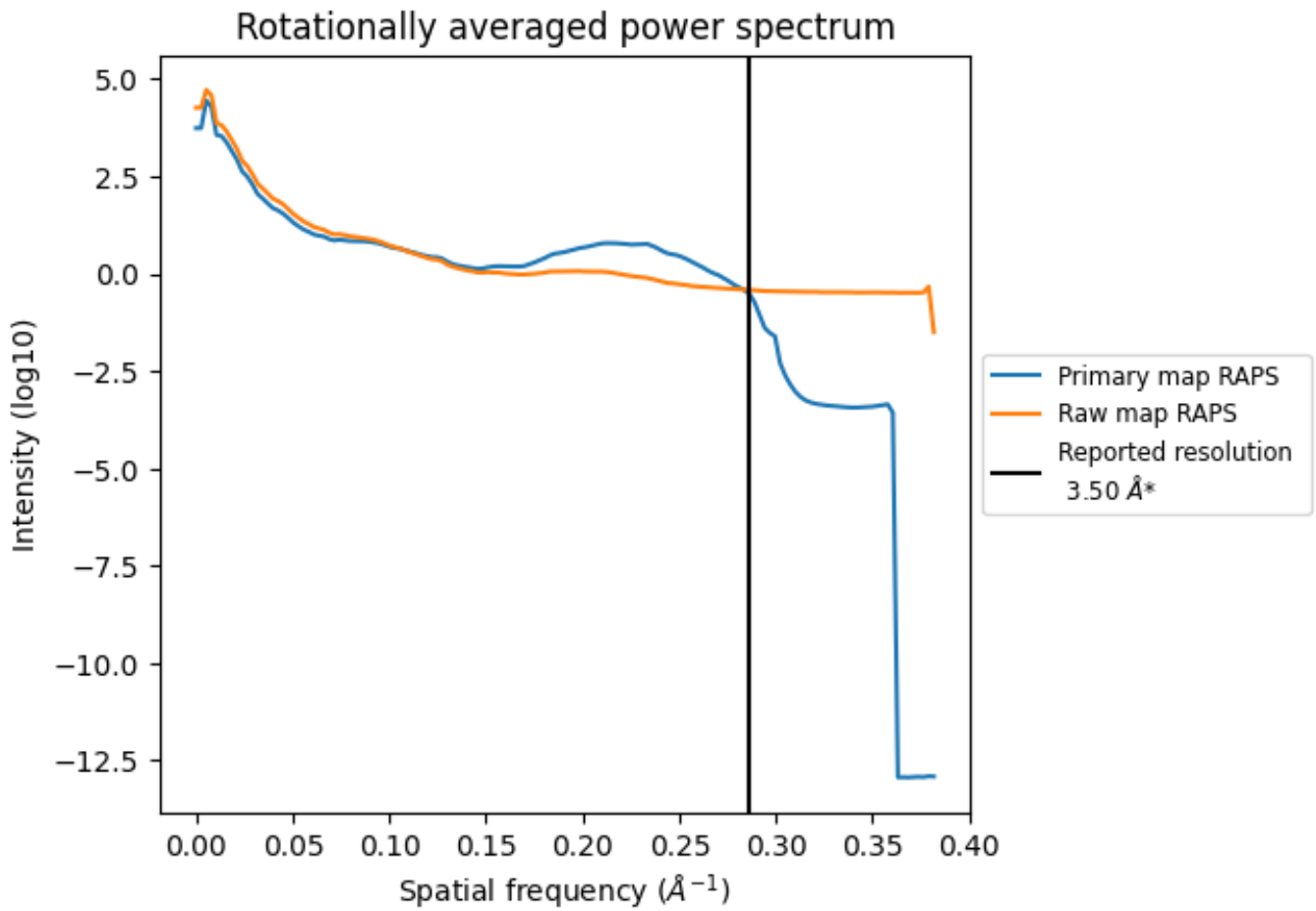
7.2 Volume estimate (i)



The volume at the recommended contour level is 228 nm^3; this corresponds to an approximate mass of 206 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

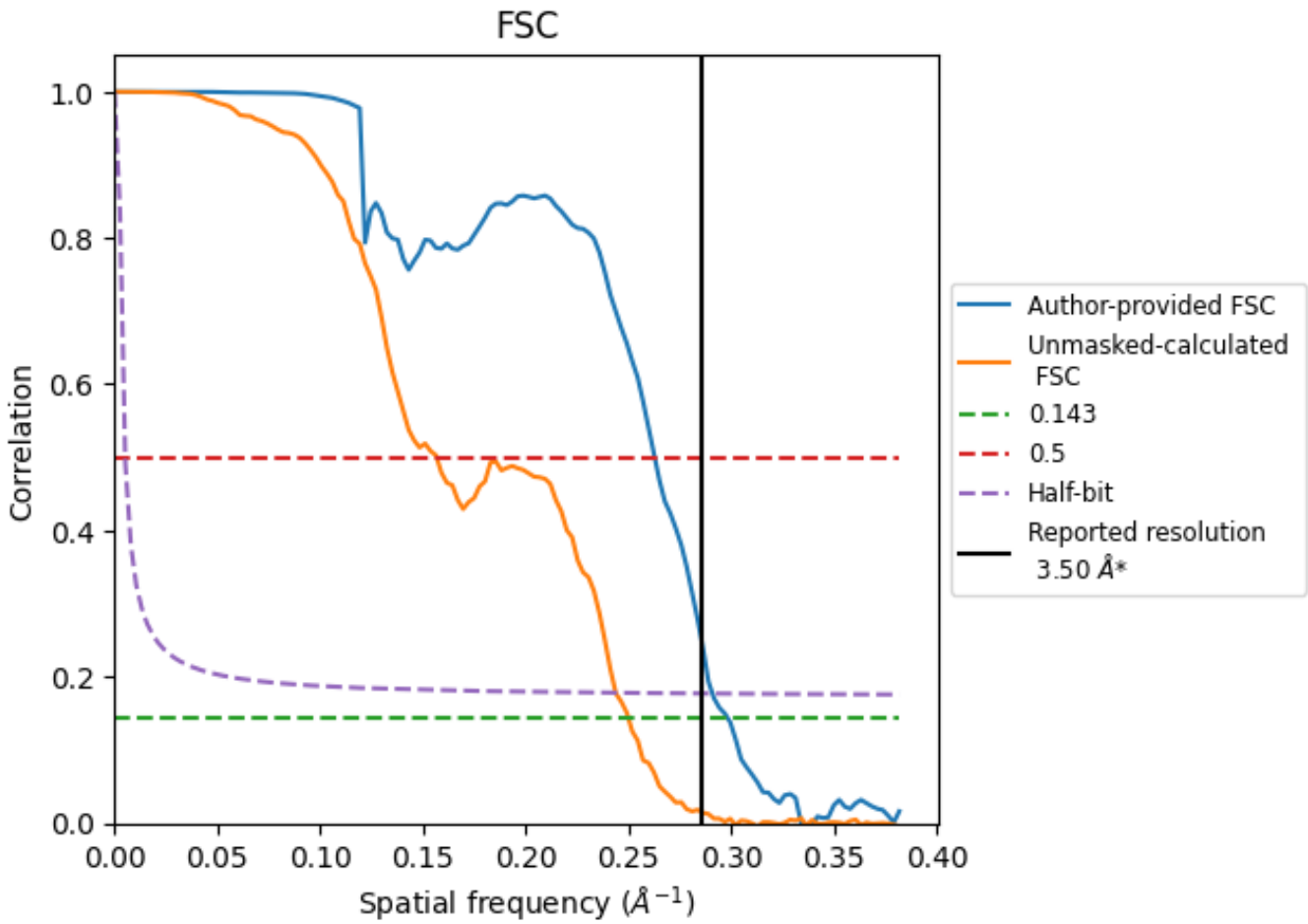


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

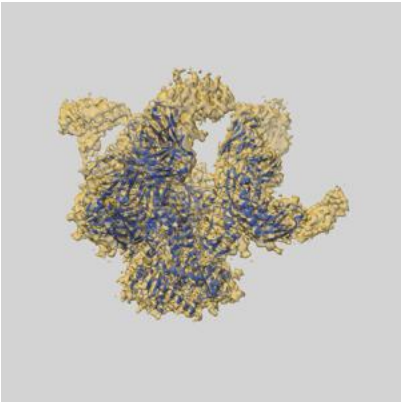
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.35	3.80	3.44
Unmasked-calculated*	4.00	6.38	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.00 differs from the reported value 3.5 by more than 10 %

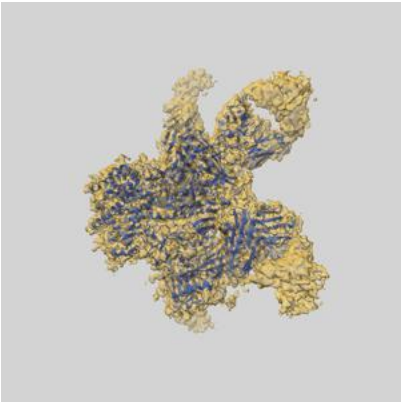
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20151 and PDB model 6OPO. Per-residue inclusion information can be found in section 3 on page 16.

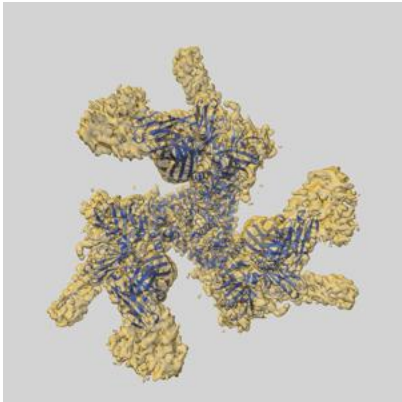
9.1 Map-model overlay (i)



X



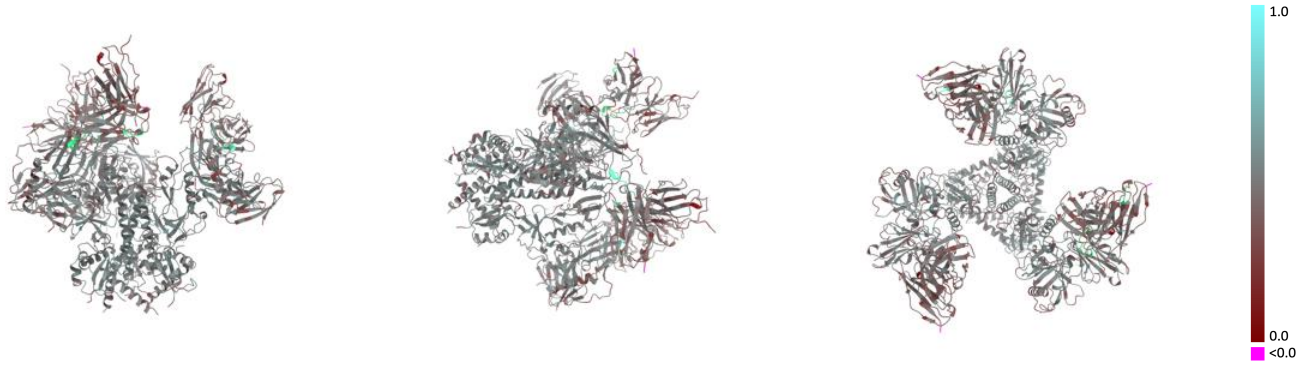
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

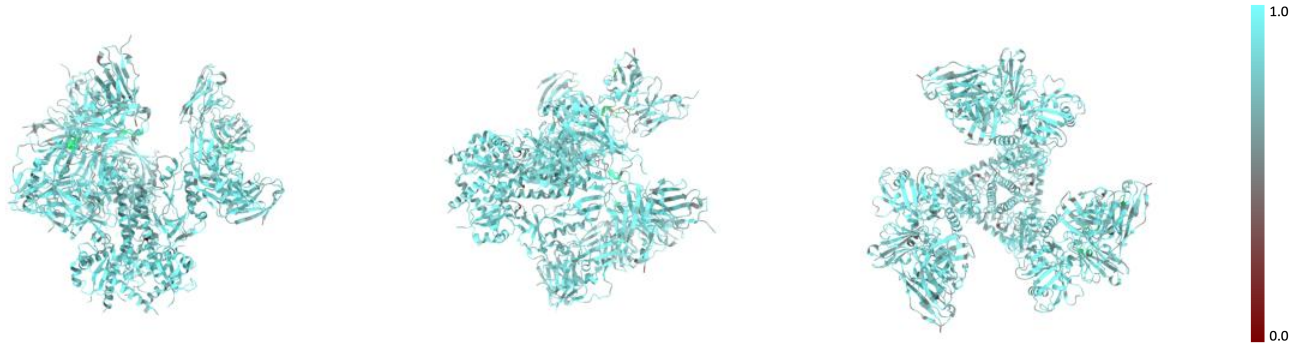
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

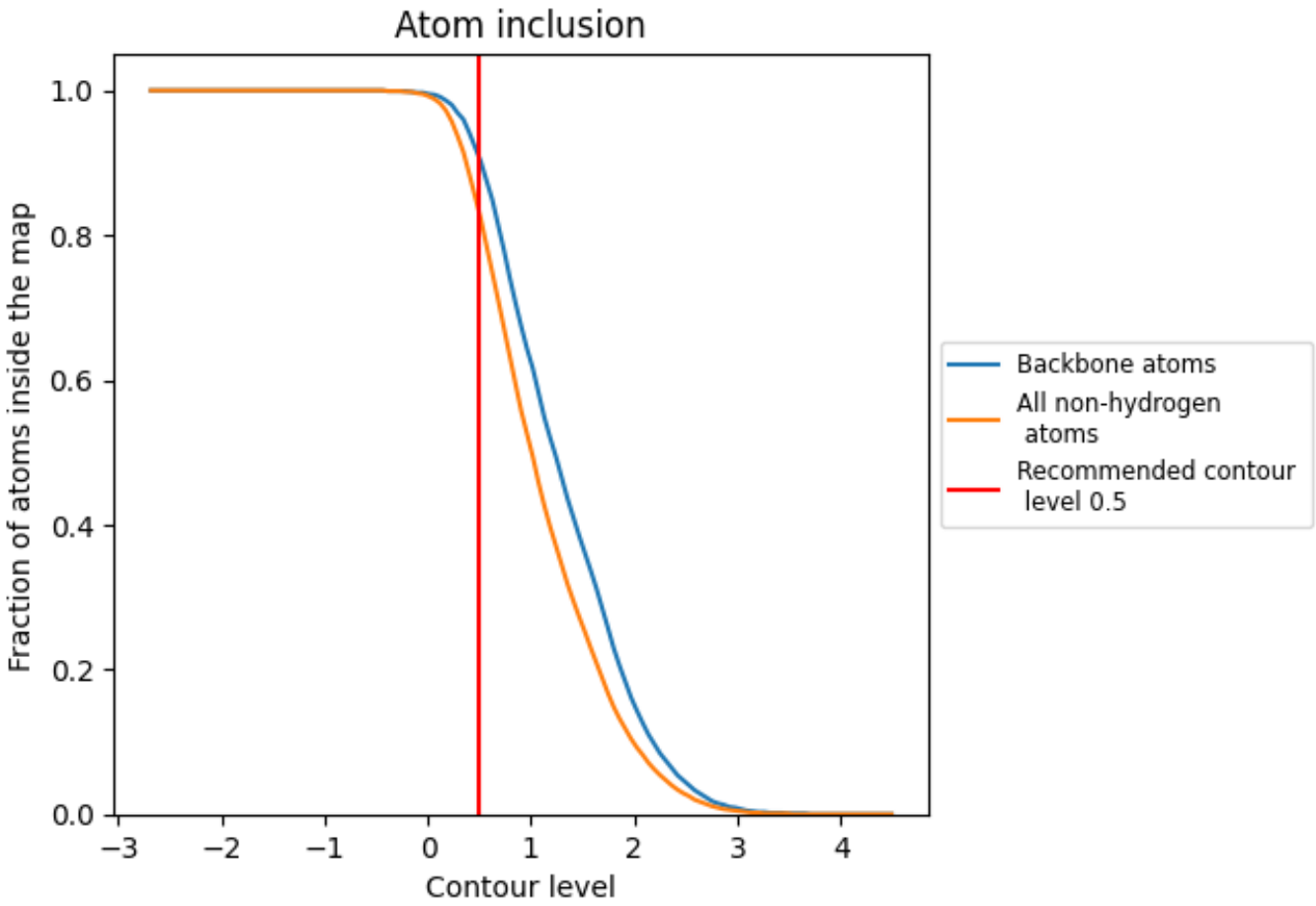
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.4480
A	0.8560	0.4730
B	0.8560	0.4820
C	0.7960	0.4440
D	0.8590	0.4740
E	0.7620	0.3730
F	0.8560	0.4790
G	0.7920	0.4430
H	0.8150	0.4060
I	0.8180	0.4050
J	0.8580	0.4730
K	0.7620	0.3720
L	0.7660	0.3780
M	0.8570	0.4800
N	0.7950	0.4420
O	0.8180	0.4030
P	0.6070	0.3090
Q	0.6790	0.4300
R	0.8850	0.4700
S	0.7860	0.3890
T	0.7140	0.4330
U	0.7860	0.3750
V	0.8210	0.4630
W	0.6790	0.4220
X	0.8570	0.4930
Y	0.7950	0.4020
Z	0.6070	0.3160
a	0.6790	0.4200
b	0.9020	0.4810
c	0.7860	0.4030
d	0.7500	0.4340
e	0.7860	0.3880
f	0.8210	0.4500
g	0.6790	0.4160
h	0.8570	0.4830

Continued on next page...

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Chain	Atom inclusion	Q-score
i	0.7440	0.4040
j	0.6070	0.3000
k	0.7140	0.4280
l	0.8850	0.4850
m	0.8210	0.3950
n	0.7500	0.4170
o	0.7860	0.3860
p	0.8210	0.4730
q	0.6790	0.4230
r	0.8570	0.4820
s	0.7690	0.3980