wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 30, 2023 – 10:40 PM JST

PDB ID : 4YD9
Title : Crystal structure of squid hemocyanin
Authors : Matsuno, A.; Gai, Z.; Kato, K.; Tanaka, Y.; Yao, M.
Deposited on : 2015-02-21
Resolution : 3.00 Å(reported)

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

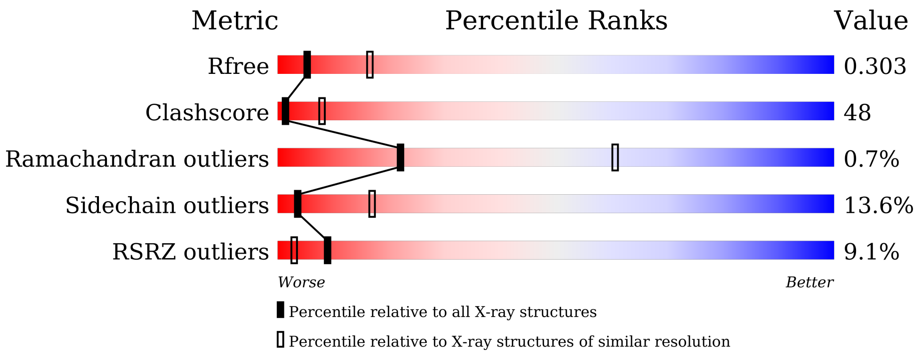
MolProbity	4.02b-467
Mogul	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	1.13
EDS	2.36
Percentile statistics	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	5.8.0158
CCP4	7.0.044 (Gargrove)
Ideal geometry (proteins)	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	2.36

1 Overall quality at a glance (i)

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

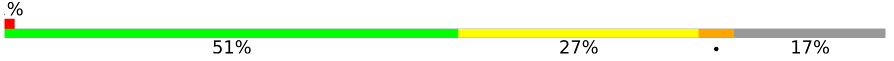
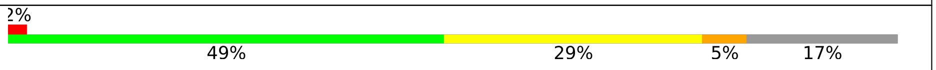
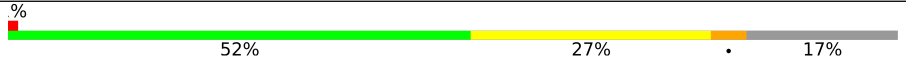
The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	2000	
1	D	2000	
1	G	2000	
1	J	2000	
1	M	2000	
1	P	2000	

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Mol	Chain	Length	Quality of chain
1	S	2000	2% 51% 27% • 17%
1	V	2000	% 50% 29% • 17%
1	Y	2000	% 50% 28% • 17%
1	b	2000	% 75% 8% 17%
2	B	920	59% 27% • 10%
2	E	920	% 54% 32% • 10%
2	H	920	% 55% 29% 6% 10%
2	K	920	% 54% 31% • 10%
2	N	920	% 57% 29% • 10%
2	Q	920	58% 27% 5% 10%
2	T	920	56% 29% • 10%
2	W	920	59% 27% • 10%
2	Z	920	% 57% 29% • 10%
2	c	920	% 81% 9% 10%
3	C	394	59% 15% 50% 26% • 7%
3	F	394	50% 16% 49% 25% • 7%
3	I	394	52% 13% 51% 26% • 7%
3	L	394	55% 15% 50% 26% • 7%
3	O	394	49% 16% 50% 25% • 7%
3	R	394	55% 14% 50% 26% • 7%
3	U	394	43% 17% 49% 24% • 7%
3	X	394	87% 16% 49% 26% • 7%
3	a	394	48% 62% 28% • 7%
3	d	394	84% 62% 28% • 7%
4	1	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	2	2	🟩 50% 🟧 50%
4	4	2	🟨 100%
4	6	2	🟨 50% 🟧 50%
4	7	2	🟧 100%
4	8	2	🟨 100%
4	9	2	🟧 100%
4	BA	2	🟧 100%
4	HA	2	🟨 50% 🟧 50%
4	IA	2	🟨 100%
4	JA	2	🟨 50% 🟧 50%
4	MA	2	🟧 100%
4	OA	2	🟧 100%
4	QA	2	🟩 50% 🟨 50%
4	RA	2	🟨 50% 🟧 50%
4	e	2	🟩 50% 🟨 50%
4	f	2	🟨 100%
4	i	2	🟩 50% 🟨 50%
4	j	2	🟨 100%
4	m	2	🟨 100%
4	n	2	🟨 100%
4	o	2	🟨 100%
4	p	2	🟩 50% 🟨 50%
4	q	2	🟨 100%
4	s	2	🟩 50% 🟨 50%
4	t	2	🟩 50% 🟨 50%

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Mol	Chain	Length	Quality of chain
4	u	2	🟨 100%
4	v	2	🟨 100%
4	x	2	🟩 50% 🟨 50%
5	AA	4	🟩 25% 🟨 50% 🟧 25%
5	FA	4	🟧 100%
5	KA	4	🟨 75% 🟧 25%
5	PA	4	🟨 50% 🟧 50%
5	g	4	🟩 50% 🟨 50%
5	l	4	🟩 50% 🟨 50%
6	3	3	🟩 33% 🟨 33% 🟧 33%
6	5	3	🟧 100%
6	CA	3	🟩 33% 🟧 67%
6	DA	3	🟨 33% 🟧 67%
6	EA	3	🟩 33% 🟨 33% 🟧 33%
6	GA	3	🟧 100%
6	LA	3	🟧 100%
6	NA	3	🟨 67% 🟧 33%
6	h	3	🟨 100%
6	k	3	🟩 33% 🟨 67%
6	r	3	🟩 67% 🟨 33%
6	w	3	🟨 100%
6	y	3	🟨 100%
7	z	5	🟩 20% 🟨 80%
8	0	4	🟨 25% 🟧 75%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	GA	1	-	-	X	-
6	NAG	GA	2	-	-	X	-
6	BMA	NA	3	-	-	-	X
7	MAN	z	4	-	-	-	X
8	NAG	0	2	-	-	X	-
9	CUO	A	5001	-	-	X	-
9	CUO	C	3401[A]	-	-	X	-
9	CUO	C	3401[B]	-	-	X	-
9	CUO	C	3402[A]	-	-	X	-
9	CUO	C	3402[B]	-	-	X	-
9	CUO	F	3401[B]	-	-	X	-
9	CUO	F	3402[A]	-	-	X	-
9	CUO	I	3401[A]	-	-	X	-
9	CUO	I	3402[A]	-	-	X	-
9	CUO	M	2105	-	-	X	-
9	CUO	O	3401[A]	-	-	X	-
9	CUO	O	3401[B]	-	-	X	-
9	CUO	P	5015[C]	-	-	-	X
9	CUO	P	5015[D]	-	-	-	X
9	CUO	S	2104	-	-	X	-
9	CUO	U	3401[A]	-	-	X	-
9	CUO	U	3401[B]	-	-	X	-
9	CUO	X	3401[A]	-	-	X	X
9	CUO	X	3401[B]	-	-	X	X
9	CUO	d	3401[A]	-	-	-	X
9	CUO	d	3401[B]	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 261470 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1656	Total 13318	C 8513	N 2259	O 2478	S 68	0	0	0
1	D	1656	Total 13318	C 8513	N 2259	O 2478	S 68	0	0	0
1	G	1656	Total 13318	C 8513	N 2259	O 2478	S 68	0	0	0
1	J	1656	Total 13318	C 8513	N 2259	O 2478	S 68	0	0	0
1	M	1656	Total 13318	C 8513	N 2259	O 2478	S 68	0	0	0
1	P	1656	Total 13318	C 8513	N 2259	O 2478	S 68	0	0	0
1	S	1656	Total 13318	C 8513	N 2259	O 2478	S 68	0	0	0
1	V	1656	Total 13318	C 8513	N 2259	O 2478	S 68	0	0	0
1	Y	1656	Total 13318	C 8513	N 2259	O 2478	S 68	0	0	0
1	b	1656	Total 13318	C 8513	N 2259	O 2478	S 68	0	0	0

- Molecule 2 is a protein called hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	825	Total 6704	C 4311	N 1128	O 1224	S 41	0	0	0
2	E	825	Total 6704	C 4311	N 1128	O 1224	S 41	0	0	0
2	H	825	Total 6704	C 4311	N 1128	O 1224	S 41	0	0	0
2	K	825	Total 6704	C 4311	N 1128	O 1224	S 41	0	0	0

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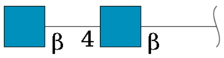
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	N	825	6704	4311	1128	1224	41	0	0	0
2	Q	825	6704	4311	1128	1224	41	0	0	0
2	T	825	6704	4311	1128	1224	41	0	0	0
2	W	825	6704	4311	1128	1224	41	0	0	0
2	Z	825	6704	4311	1128	1224	41	0	0	0
2	c	825	6704	4311	1128	1224	41	0	0	0

- Molecule 3 is a protein called hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	366	5912	3808	994	1076	34	0	366	0
3	F	366	5912	3808	994	1076	34	0	366	0
3	I	366	5912	3808	994	1076	34	0	366	0
3	L	366	5912	3808	994	1076	34	0	366	0
3	O	366	5912	3808	994	1076	34	0	366	0
3	R	366	5912	3808	994	1076	34	0	366	0
3	U	366	5912	3808	994	1076	34	0	366	0
3	X	366	5912	3808	994	1076	34	0	366	0
3	a	366	5912	3808	994	1076	34	0	366	0
3	d	366	5912	3808	994	1076	34	0	366	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	e	2	Total C N O 28 16 2 10	0	0	0
4	f	2	Total C N O 28 16 2 10	0	0	0
4	i	2	Total C N O 28 16 2 10	0	0	0
4	j	2	Total C N O 28 16 2 10	0	0	0
4	m	2	Total C N O 28 16 2 10	0	0	0
4	n	2	Total C N O 28 16 2 10	0	0	0
4	o	2	Total C N O 28 16 2 10	0	0	0
4	p	2	Total C N O 28 16 2 10	0	0	0
4	q	2	Total C N O 28 16 2 10	0	0	0
4	s	2	Total C N O 28 16 2 10	0	0	0
4	t	2	Total C N O 28 16 2 10	0	0	0
4	u	2	Total C N O 28 16 2 10	0	0	0
4	v	2	Total C N O 28 16 2 10	0	0	0
4	x	2	Total C N O 28 16 2 10	0	0	0
4	1	2	Total C N O 28 16 2 10	0	0	0
4	2	2	Total C N O 28 16 2 10	0	0	0
4	4	2	Total C N O 28 16 2 10	0	0	0
4	6	2	Total C N O 28 16 2 10	0	0	0
4	7	2	Total C N O 28 16 2 10	0	0	0
4	8	2	Total C N O 28 16 2 10	0	0	0
4	9	2	Total C N O 28 16 2 10	0	0	0
4	BA	2	Total C N O 28 16 2 10	0	0	0

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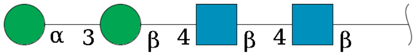
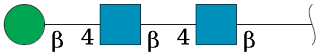
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	HA	2	Total C N O 28 16 2 10	0	0	0
4	IA	2	Total C N O 28 16 2 10	0	0	0
4	JA	2	Total C N O 28 16 2 10	0	0	0
4	MA	2	Total C N O 28 16 2 10	0	0	0
4	OA	2	Total C N O 28 16 2 10	0	0	0
4	QA	2	Total C N O 28 16 2 10	0	0	0
4	RA	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



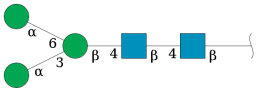
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	g	4	Total C N O 50 28 2 20	0	0	0
5	l	4	Total C N O 50 28 2 20	0	0	0
5	AA	4	Total C N O 50 28 2 20	0	0	0
5	FA	4	Total C N O 50 28 2 20	0	0	0
5	KA	4	Total C N O 50 28 2 20	0	0	0
5	PA	4	Total C N O 50 28 2 20	0	0	0

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



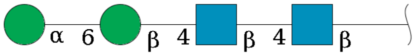
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	h	3	Total C N O 39 22 2 15	0	0	0
6	k	3	Total C N O 39 22 2 15	0	0	0
6	r	3	Total C N O 39 22 2 15	0	0	0
6	w	3	Total C N O 39 22 2 15	0	0	0
6	y	3	Total C N O 39 22 2 15	0	0	0
6	3	3	Total C N O 39 22 2 15	0	0	0
6	5	3	Total C N O 39 22 2 15	0	0	0
6	CA	3	Total C N O 39 22 2 15	0	0	0
6	DA	3	Total C N O 39 22 2 15	0	0	0
6	EA	3	Total C N O 39 22 2 15	0	0	0
6	GA	3	Total C N O 39 22 2 15	0	0	0
6	LA	3	Total C N O 39 22 2 15	0	0	0
6	NA	3	Total C N O 39 22 2 15	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



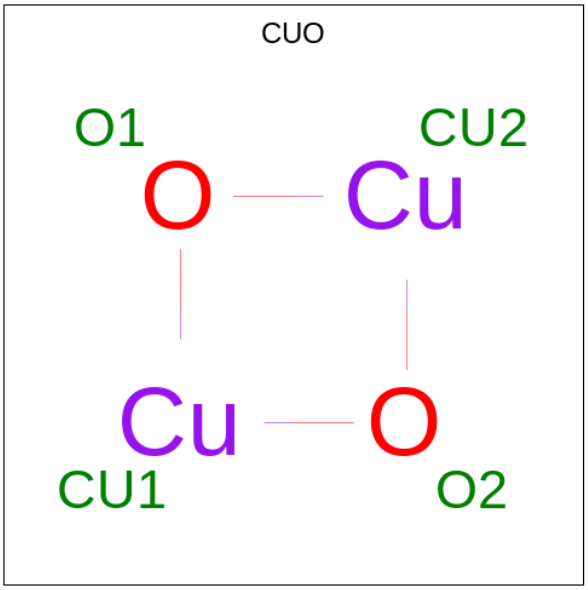
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	z	5	Total C N O 61 34 2 25	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	0	4	50	28	2	20	0	0	0

- Molecule 9 is CU2-O2 CLUSTER (three-letter code: CUO) (formula: Cu_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 4	Cu 2	O 2	0	0
9	A	1	Total 4	Cu 2	O 2	0	0
9	A	1	Total 4	Cu 2	O 2	0	0
9	A	1	Total 4	Cu 2	O 2	0	0
9	A	1	Total 8	Cu 4	O 4	0	1
9	B	1	Total 4	Cu 2	O 2	0	0
9	B	1	Total 4	Cu 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Cu O 8 4 4	0	1
9	C	1	Total Cu O 8 4 4	0	1
9	D	1	Total Cu O 4 2 2	0	0
9	D	1	Total Cu O 4 2 2	0	0
9	D	1	Total Cu O 4 2 2	0	0
9	D	1	Total Cu O 4 2 2	0	0
9	D	1	Total Cu O 8 4 4	0	1
9	E	1	Total Cu O 4 2 2	0	0
9	E	1	Total Cu O 4 2 2	0	0
9	F	1	Total Cu O 8 4 4	0	1
9	F	1	Total Cu O 8 4 4	0	1
9	G	1	Total Cu O 8 4 4	0	1
9	G	1	Total Cu O 4 2 2	0	0
9	G	1	Total Cu O 4 2 2	0	0
9	G	1	Total Cu O 4 2 2	0	0
9	G	1	Total Cu O 4 2 2	0	0
9	H	1	Total Cu O 4 2 2	0	0
9	H	1	Total Cu O 4 2 2	0	0
9	I	1	Total Cu O 8 4 4	0	1
9	I	1	Total Cu O 8 4 4	0	1
9	J	1	Total Cu O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	J	1	Total Cu O 4 2 2	0	0
9	J	1	Total Cu O 4 2 2	0	0
9	J	1	Total Cu O 4 2 2	0	0
9	J	1	Total Cu O 8 4 4	0	1
9	K	1	Total Cu O 4 2 2	0	0
9	K	1	Total Cu O 4 2 2	0	0
9	M	1	Total Cu O 8 4 4	0	1
9	M	1	Total Cu O 4 2 2	0	0
9	M	1	Total Cu O 4 2 2	0	0
9	M	1	Total Cu O 4 2 2	0	0
9	M	1	Total Cu O 4 2 2	0	0
9	N	1	Total Cu O 4 2 2	0	0
9	N	1	Total Cu O 4 2 2	0	0
9	O	1	Total Cu O 8 4 4	0	1
9	P	1	Total Cu O 4 2 2	0	0
9	P	1	Total Cu O 4 2 2	0	0
9	P	1	Total Cu O 4 2 2	0	0
9	P	1	Total Cu O 4 2 2	0	0
9	P	1	Total Cu O 8 4 4	0	1
9	Q	1	Total Cu O 4 2 2	0	0
9	Q	1	Total Cu O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	S	1	Total Cu O 8 4 4	0	1
9	S	1	Total Cu O 4 2 2	0	0
9	S	1	Total Cu O 4 2 2	0	0
9	S	1	Total Cu O 4 2 2	0	0
9	S	1	Total Cu O 4 2 2	0	0
9	T	1	Total Cu O 4 2 2	0	0
9	T	1	Total Cu O 4 2 2	0	0
9	U	1	Total Cu O 8 4 4	0	1
9	V	1	Total Cu O 4 2 2	0	0
9	V	1	Total Cu O 4 2 2	0	0
9	V	1	Total Cu O 4 2 2	0	0
9	V	1	Total Cu O 4 2 2	0	0
9	V	1	Total Cu O 8 4 4	0	1
9	W	1	Total Cu O 4 2 2	0	0
9	W	1	Total Cu O 4 2 2	0	0
9	X	1	Total Cu O 8 4 4	0	1
9	Y	1	Total Cu O 8 4 4	0	1
9	Y	1	Total Cu O 4 2 2	0	0
9	Y	1	Total Cu O 4 2 2	0	0
9	Y	1	Total Cu O 4 2 2	0	0
9	Y	1	Total Cu O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	Z	1	Total Cu O 4 2 2	0	0
9	Z	1	Total Cu O 4 2 2	0	0
9	b	1	Total Cu O 8 4 4	0	1
9	b	1	Total Cu O 4 2 2	0	0
9	b	1	Total Cu O 4 2 2	0	0
9	b	1	Total Cu O 4 2 2	0	0
9	b	1	Total Cu O 4 2 2	0	0
9	c	1	Total Cu O 4 2 2	0	0
9	c	1	Total Cu O 4 2 2	0	0
9	d	1	Total Cu O 8 4 4	0	1

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: hemocyanin

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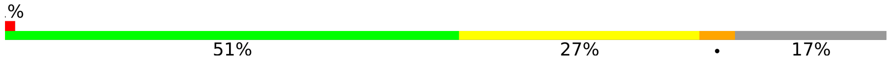

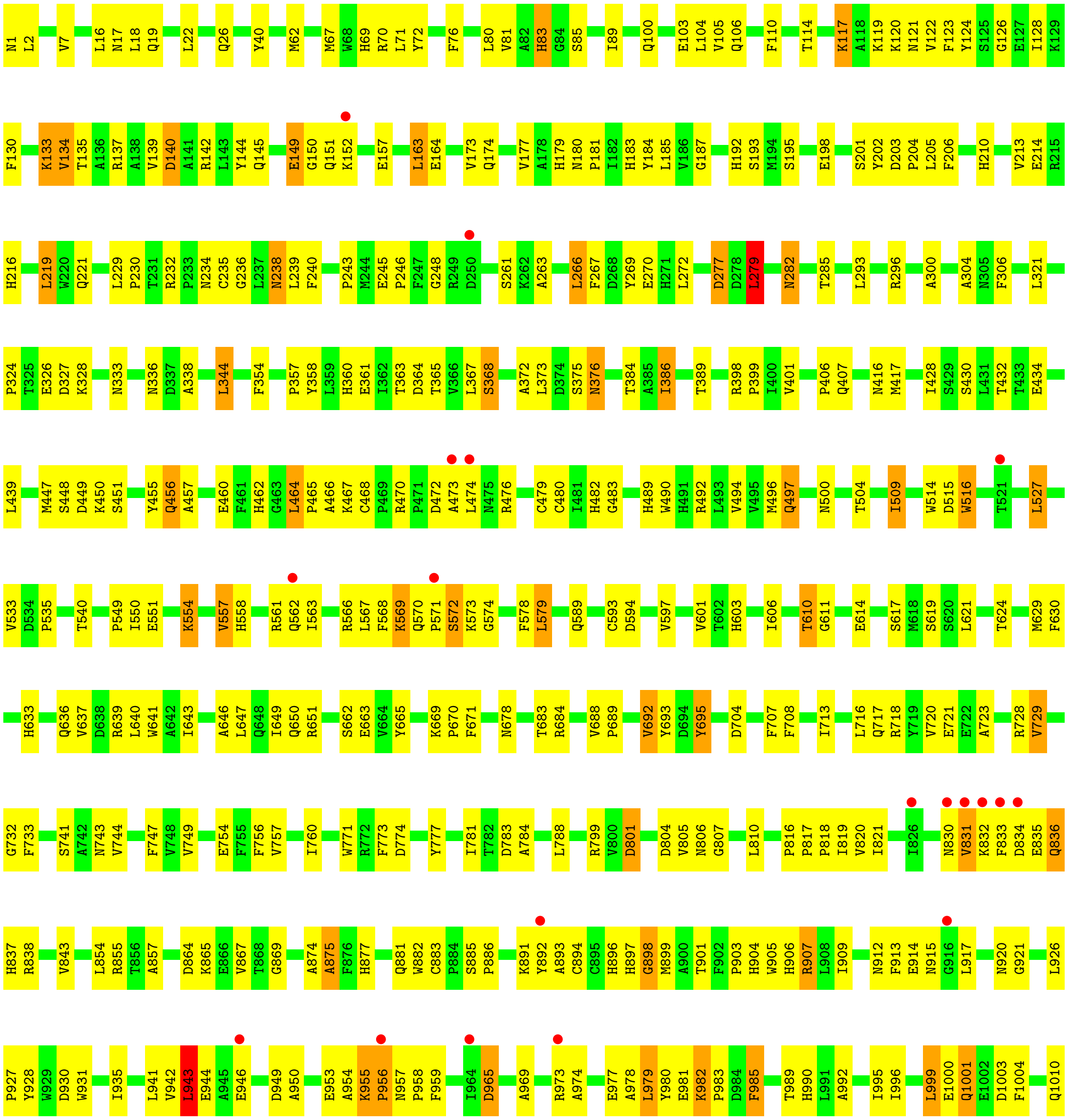

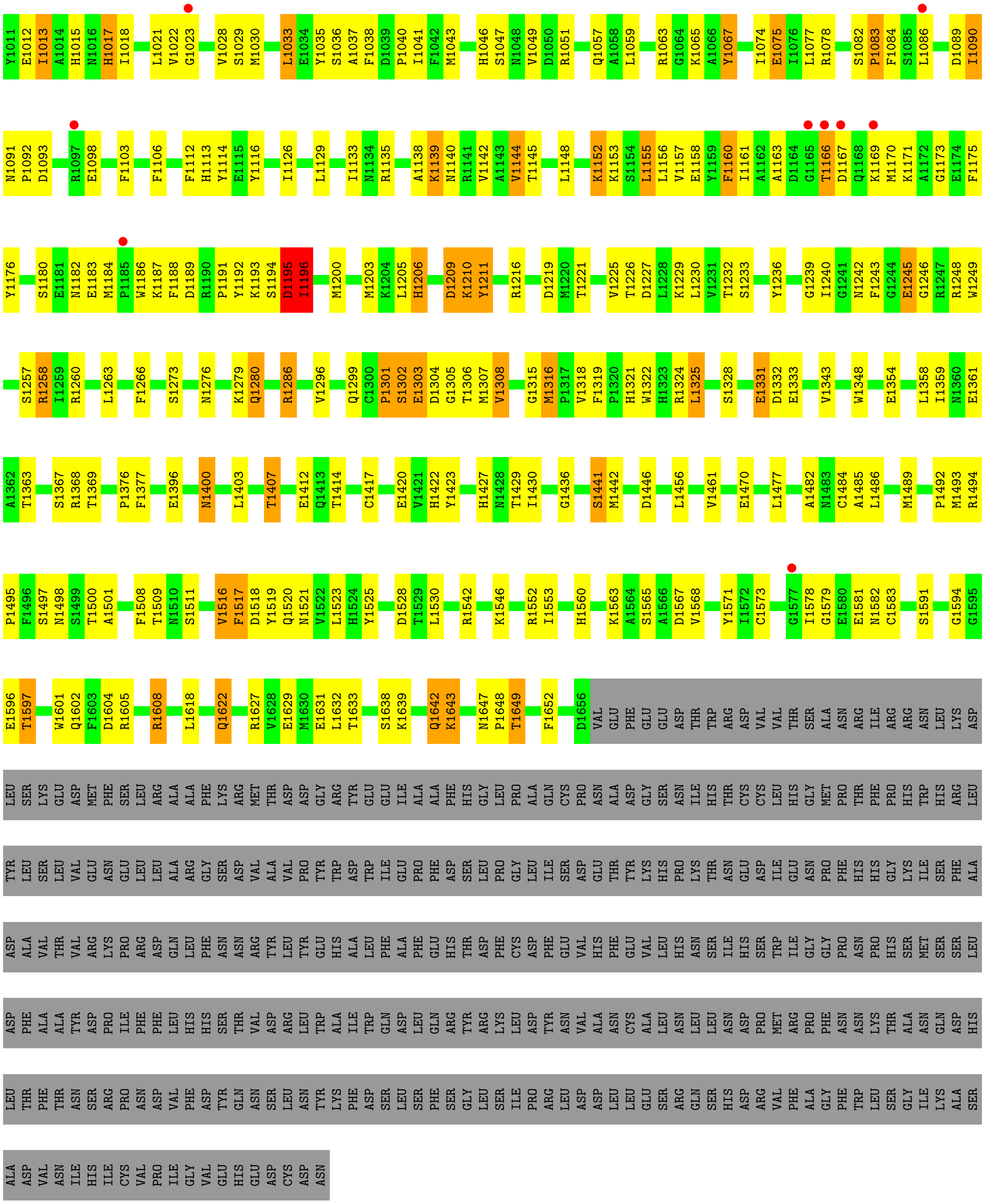

- Molecule 1: hemocyanin

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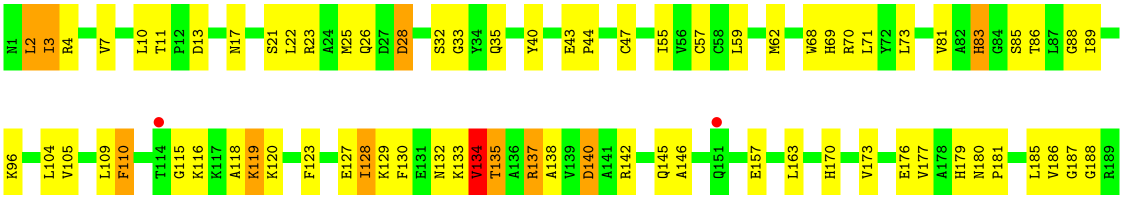

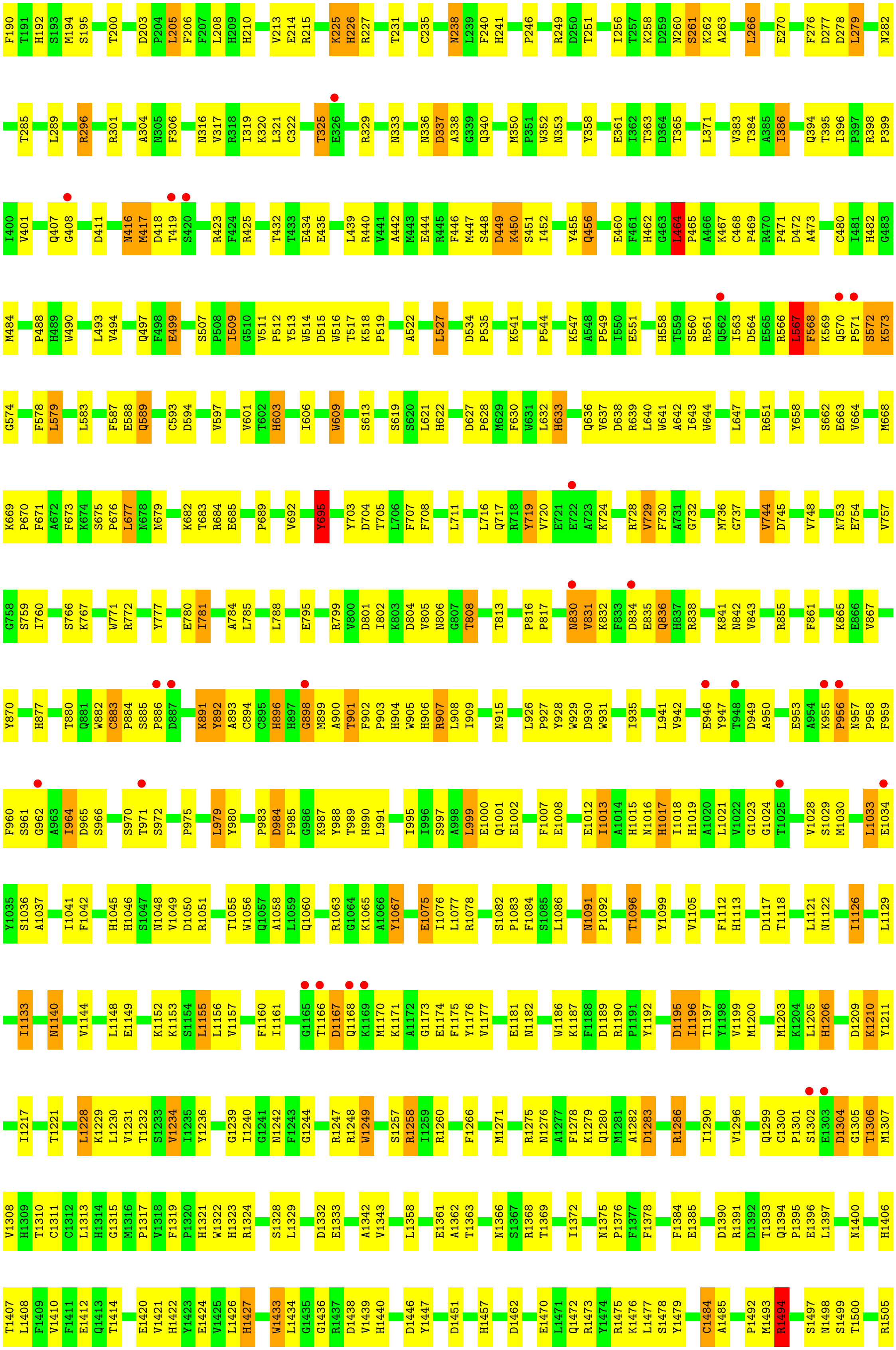
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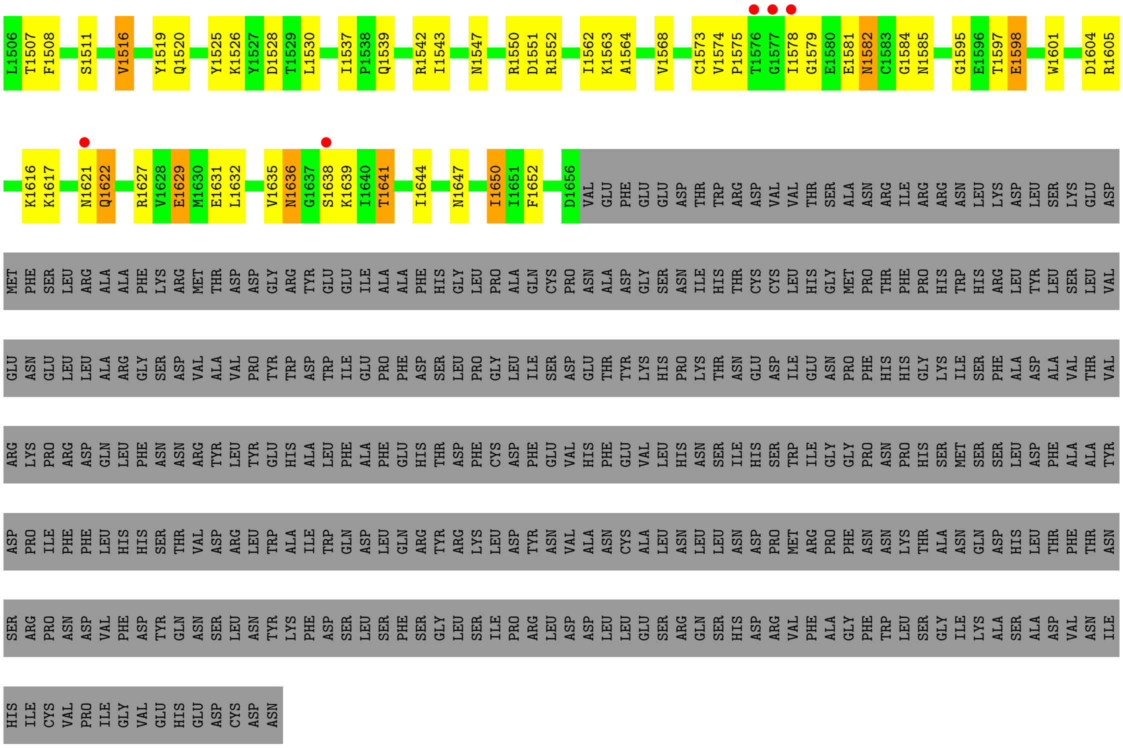
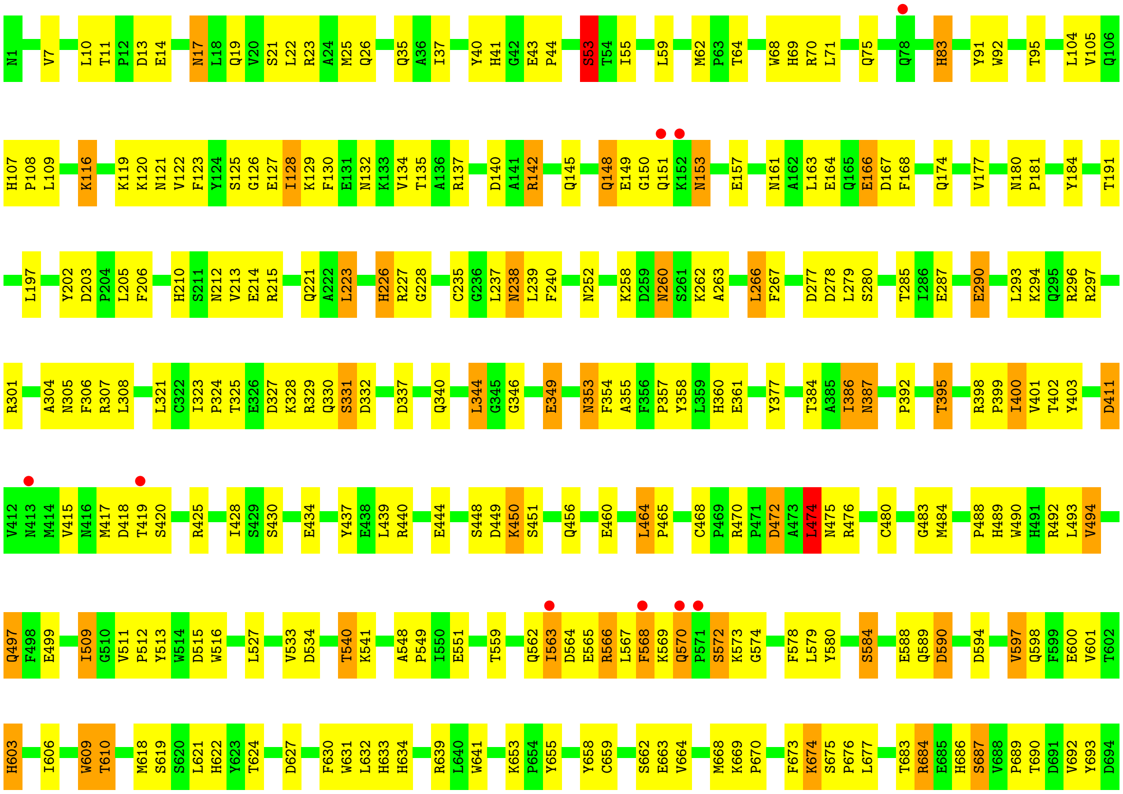
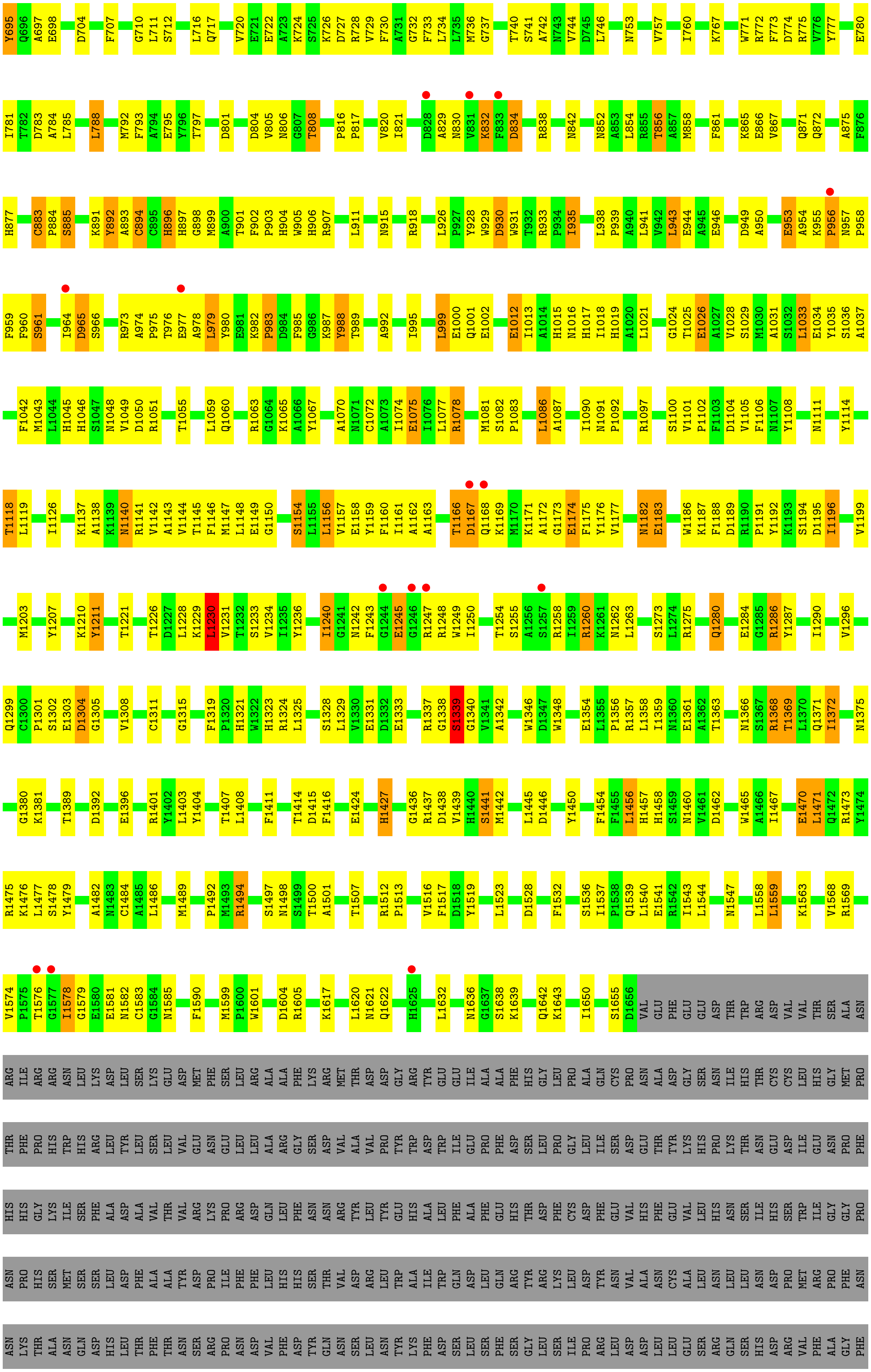


- Molecule 1: hemocyanin

Chain G:

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THR PHE PRO HIS TRP HIS ARG LEU TYR LEU SER LEU VAL GLU ASN GLU LEU LEU ALA ARG GLY SER ASP VAL ALA VAL PRO TYR TRP ASP TRP ILE GLU PRO PHE ASP SER LEU PRO GLY LEU ILE SER ASP GLU THR TYR LYS HIS PRO LYS THR ASN GLU ASP ILE GLU ASN PRO PHE
HIS HIS GLY LYS ILE SER PHE ALA ASP ALA VAL THR VAL ARG LYS PRO ARG ASP GLN LEU PHE ASN ASN ARG TYR LEU TYR GLU HIS ALA LEU PHE ALA PHE GLU HIS THR ASP PHE CYS ASP PHE GLU VAL HIS PHE GLU VAL LEU HIS ASN SER ILE HIS SER TRP ILE GLY GLY PRO
ASN PRO HIS SER MET SER SER LEU ASP PHE ALA ALA TYR ASP PRO ILE PHE PHE LEU HIS HIS SER THR VAL ASP ARG LEU TRP ALA ILE TRP GLN ASP LEU GLN ARG TYR ARG LYS LEU ASP TYR ASN VAL ALA ASN CYS ALA LEU LEU HIS ASN LEU LEU ASN ASP PRO MET ARG PRO PHE ASN
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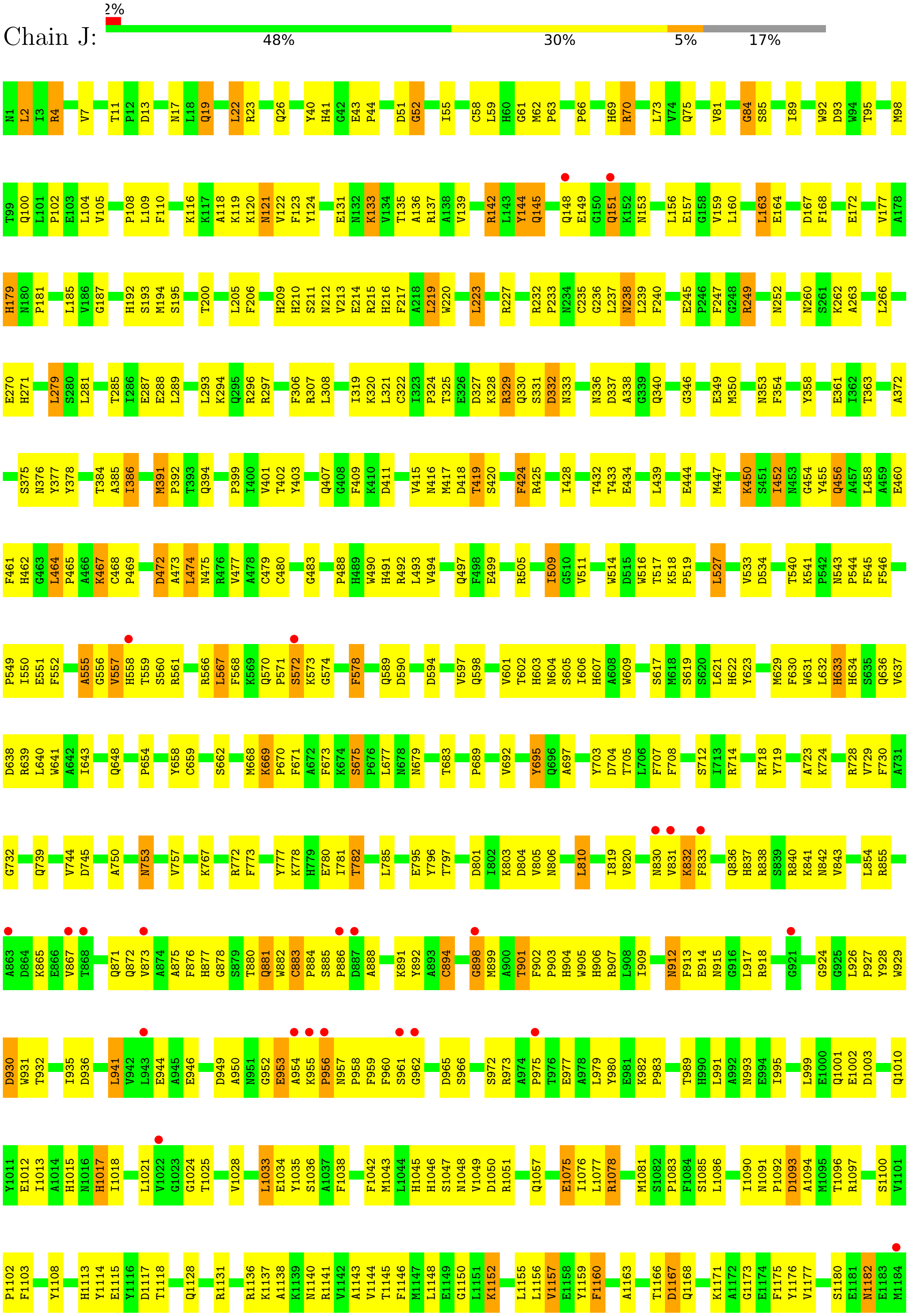
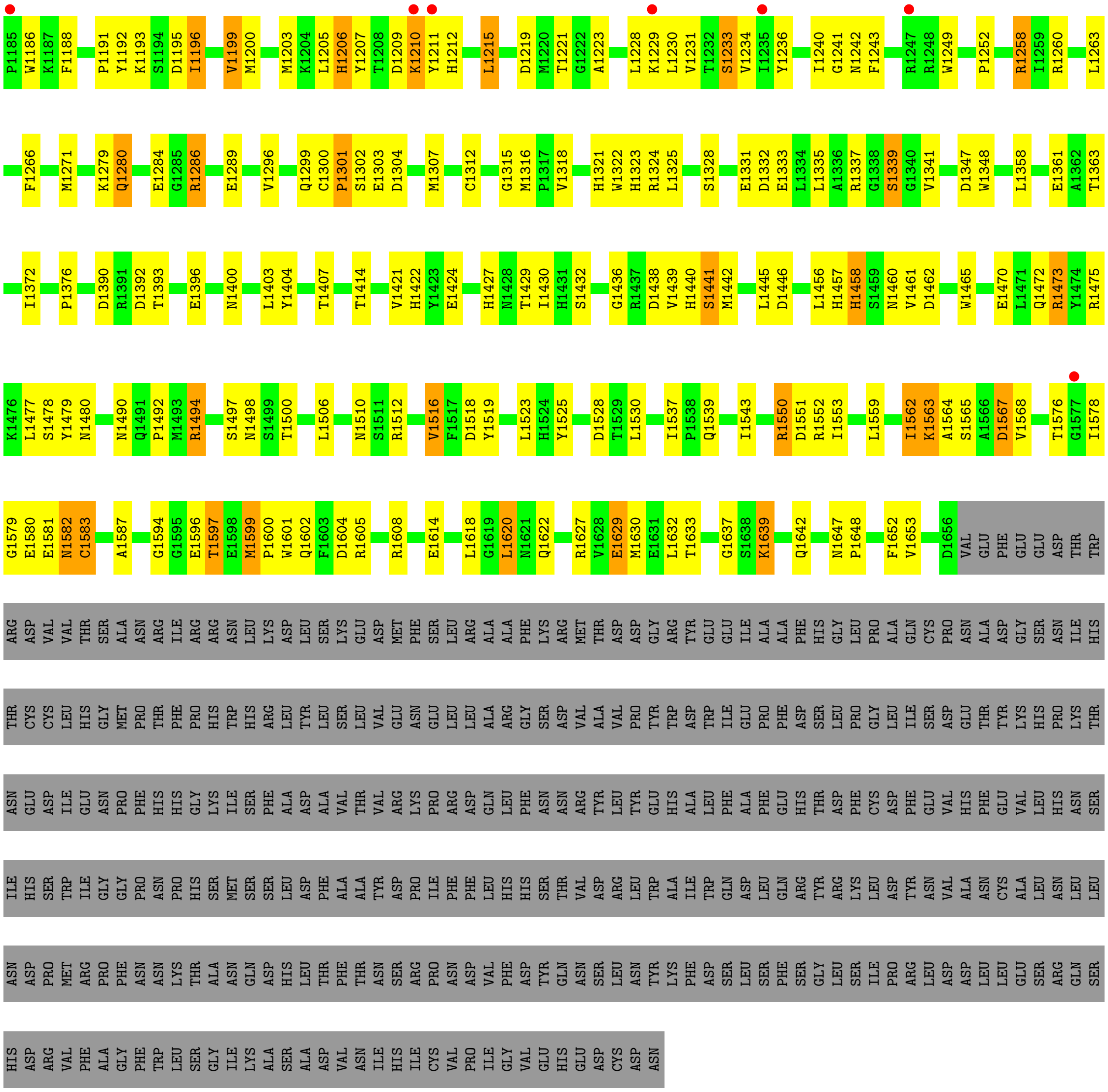
- Molecule 1: hemocyanin





- Molecule 1: hemocyanin

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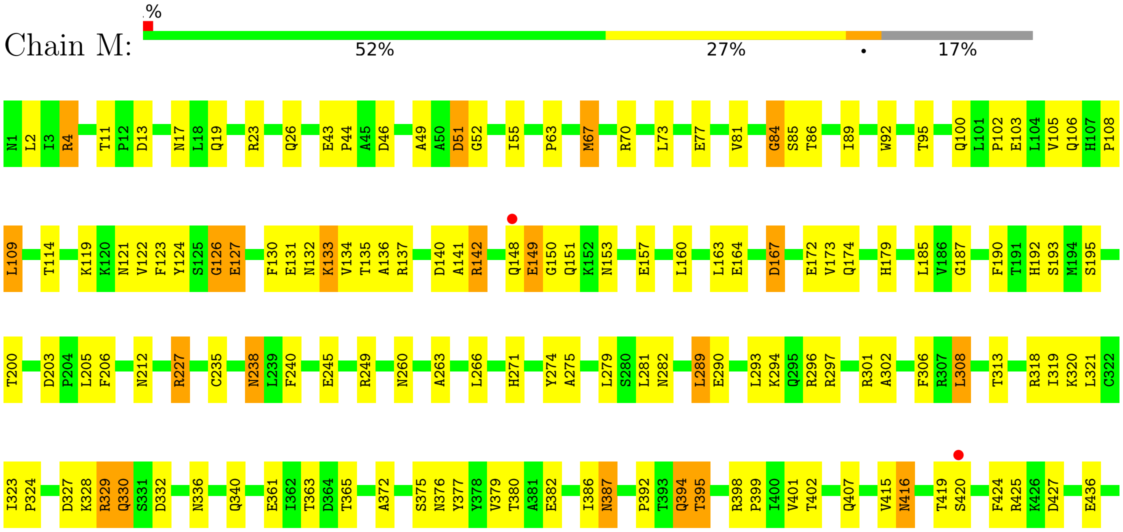

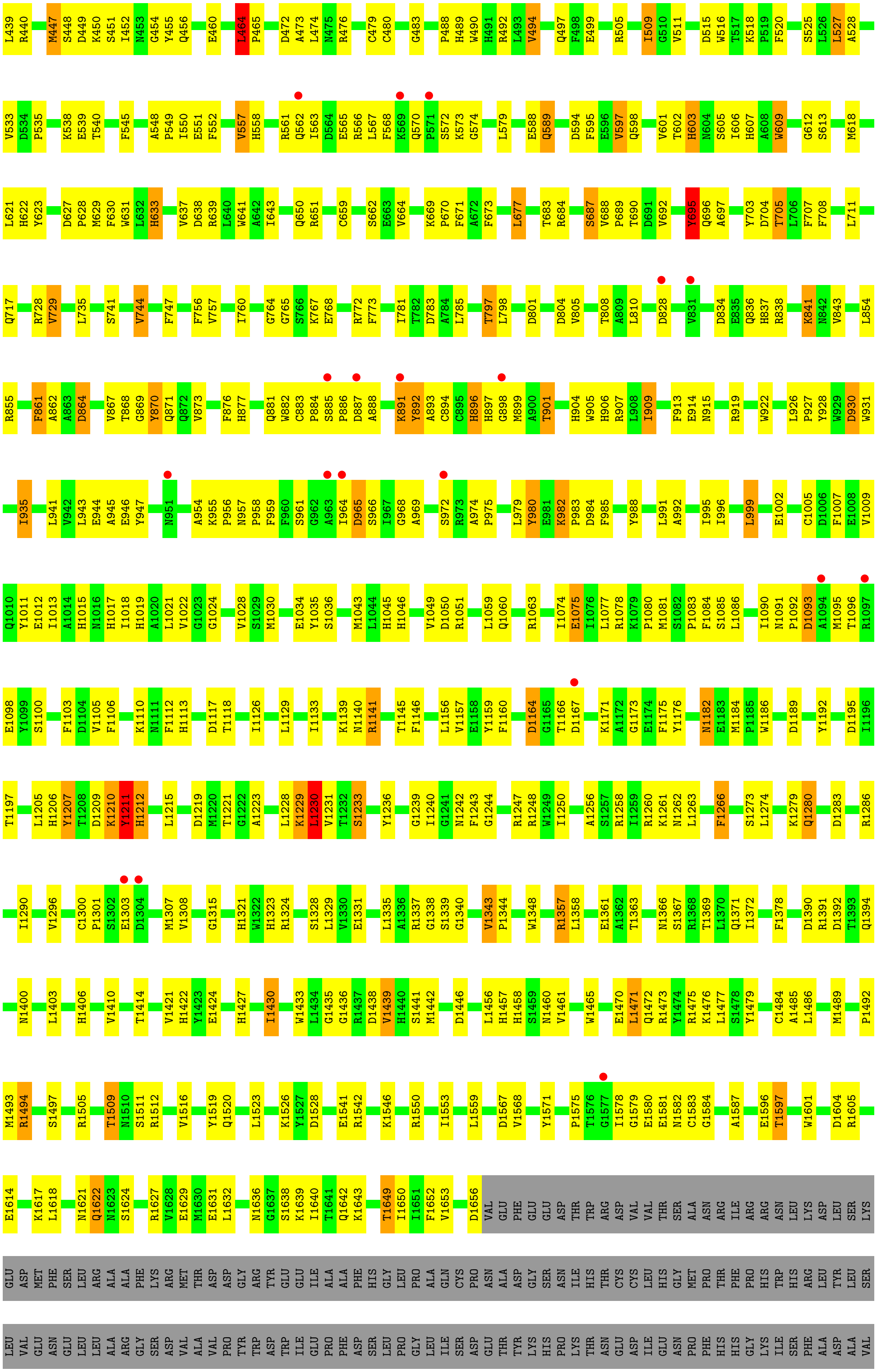
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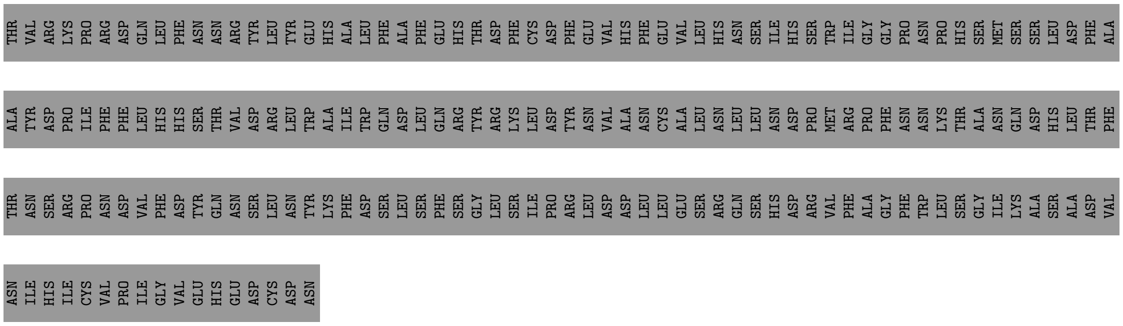
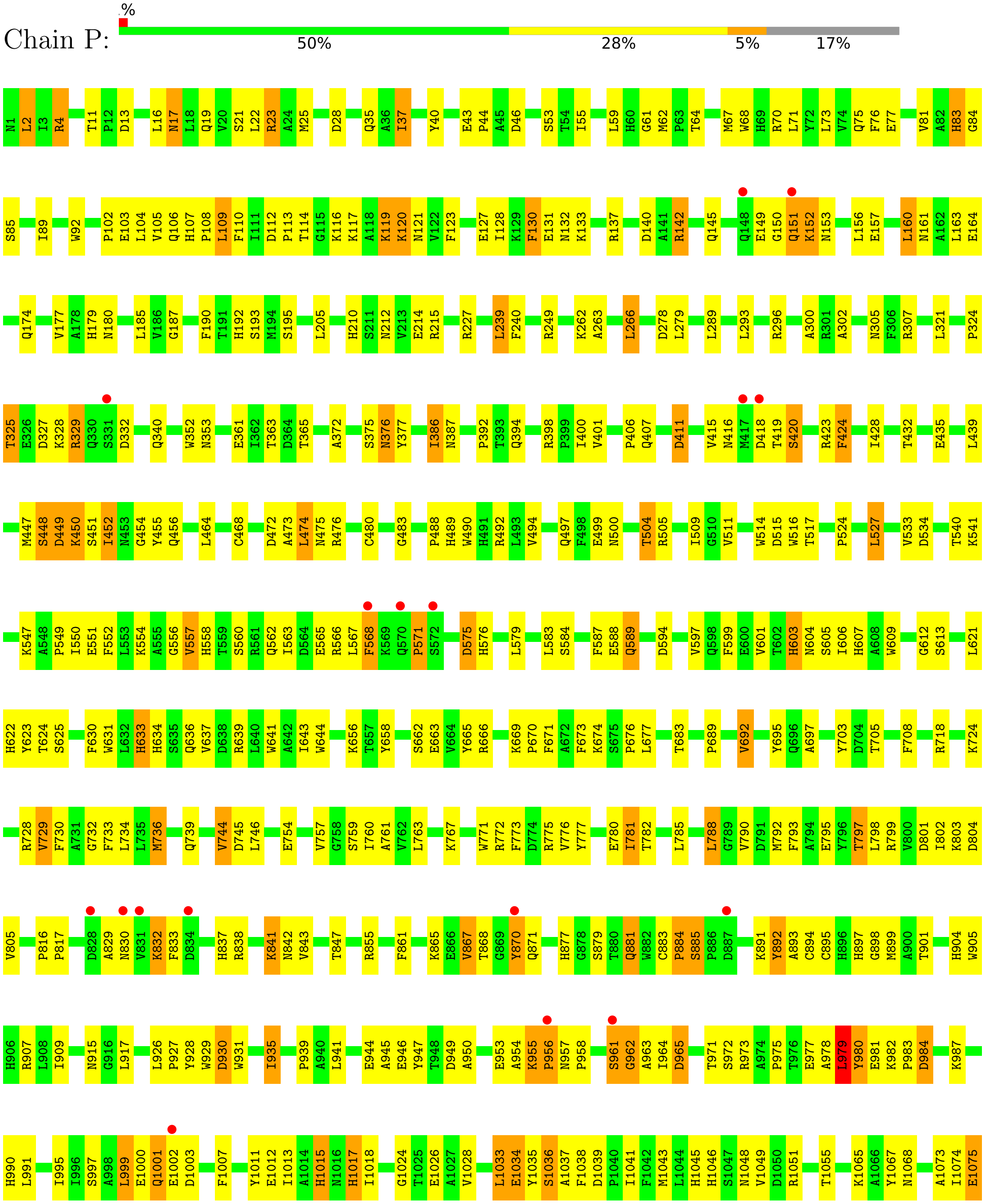
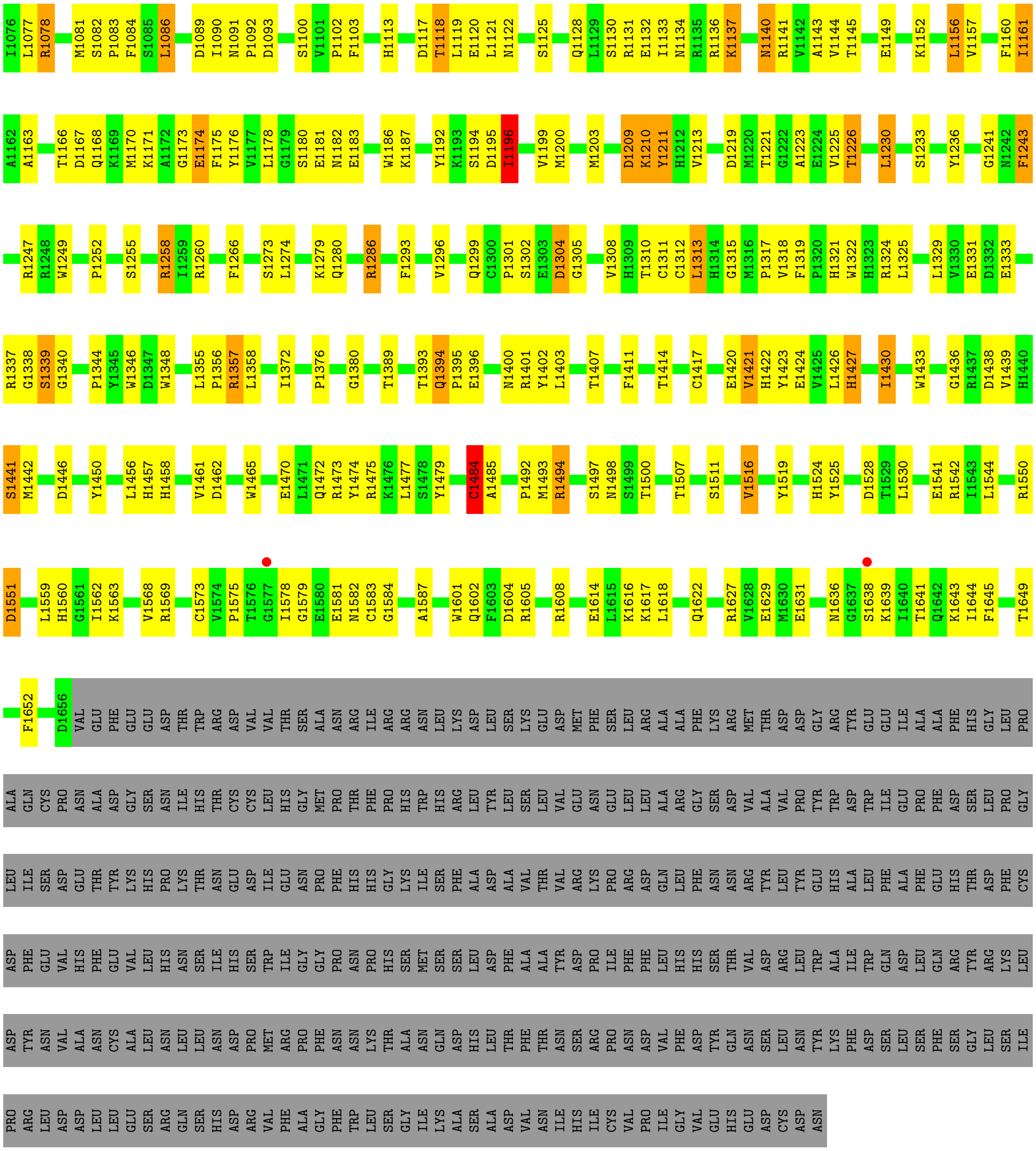


- Molecule 1: hemocyanin

Chain P:





- Molecule 1: hemocyanin

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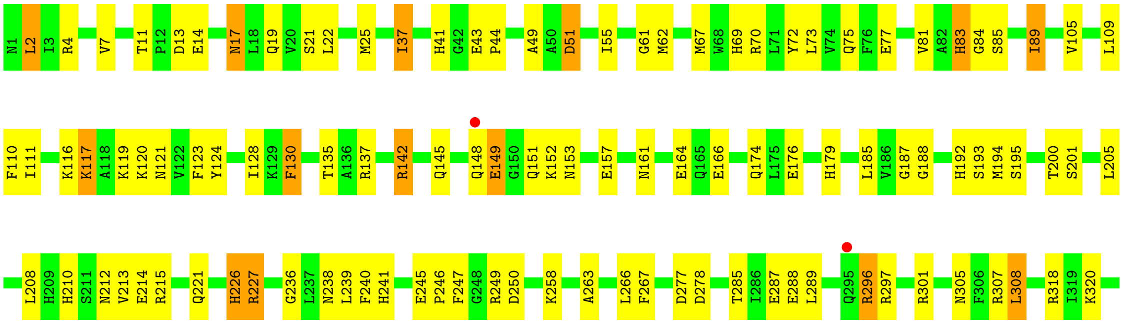

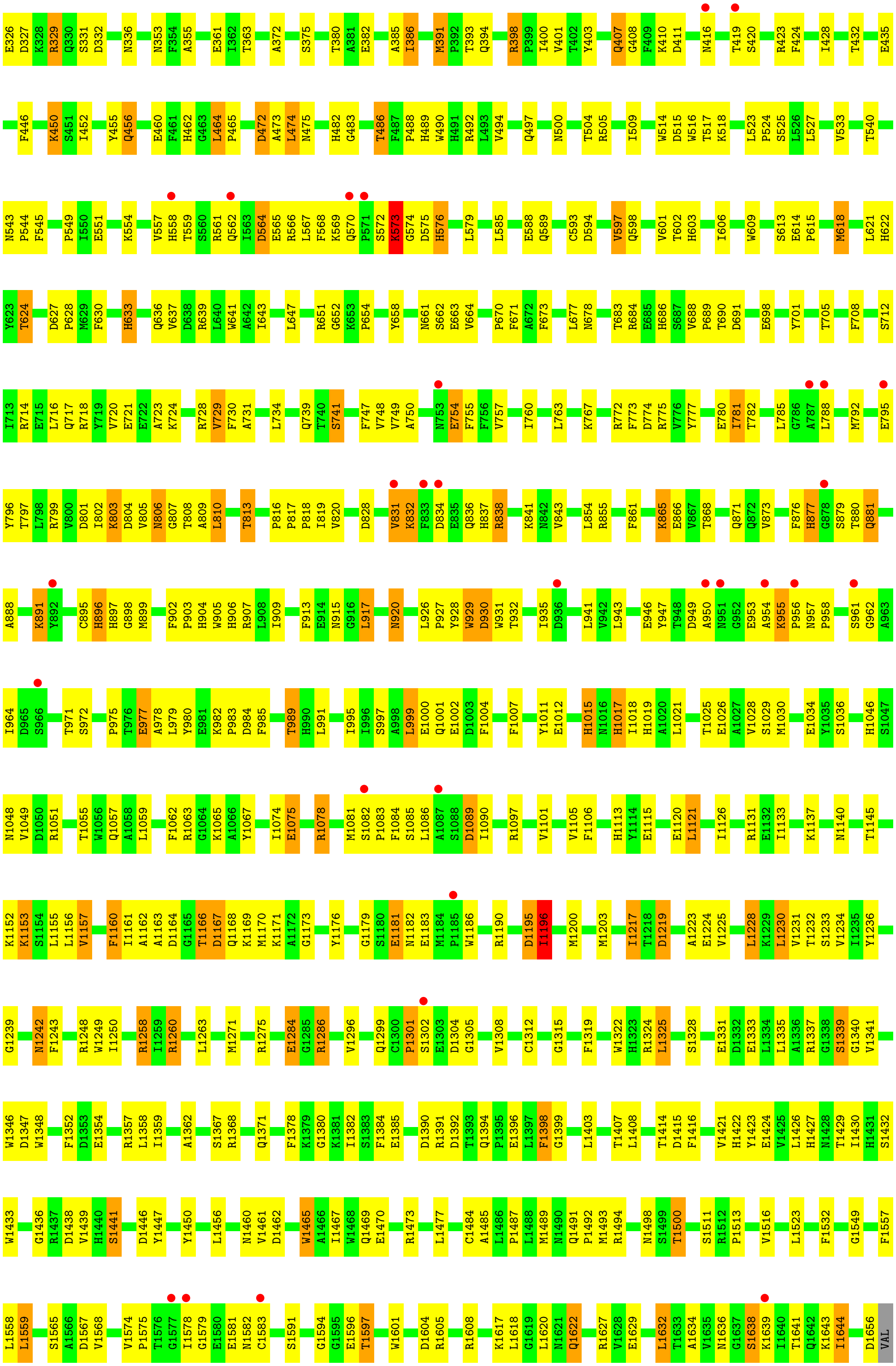
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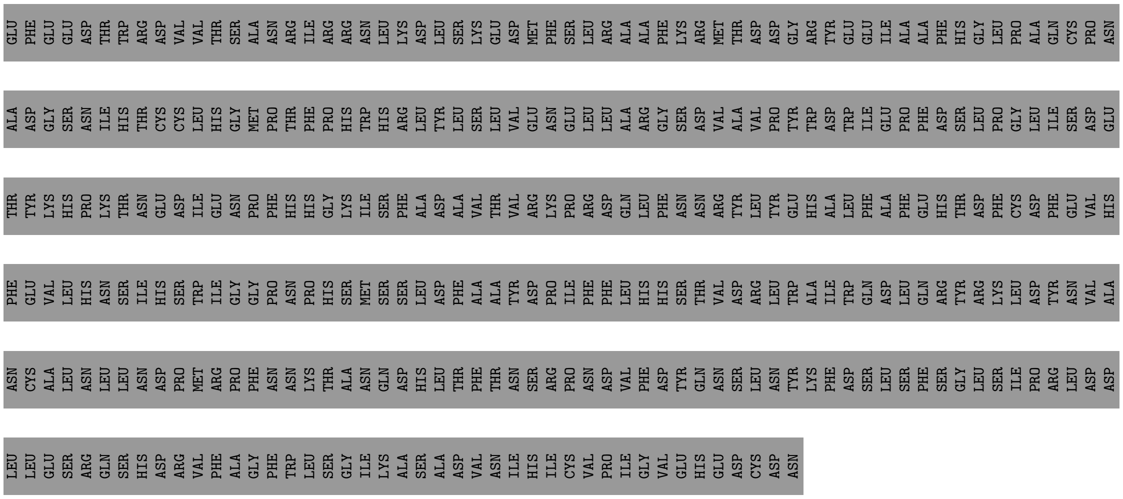
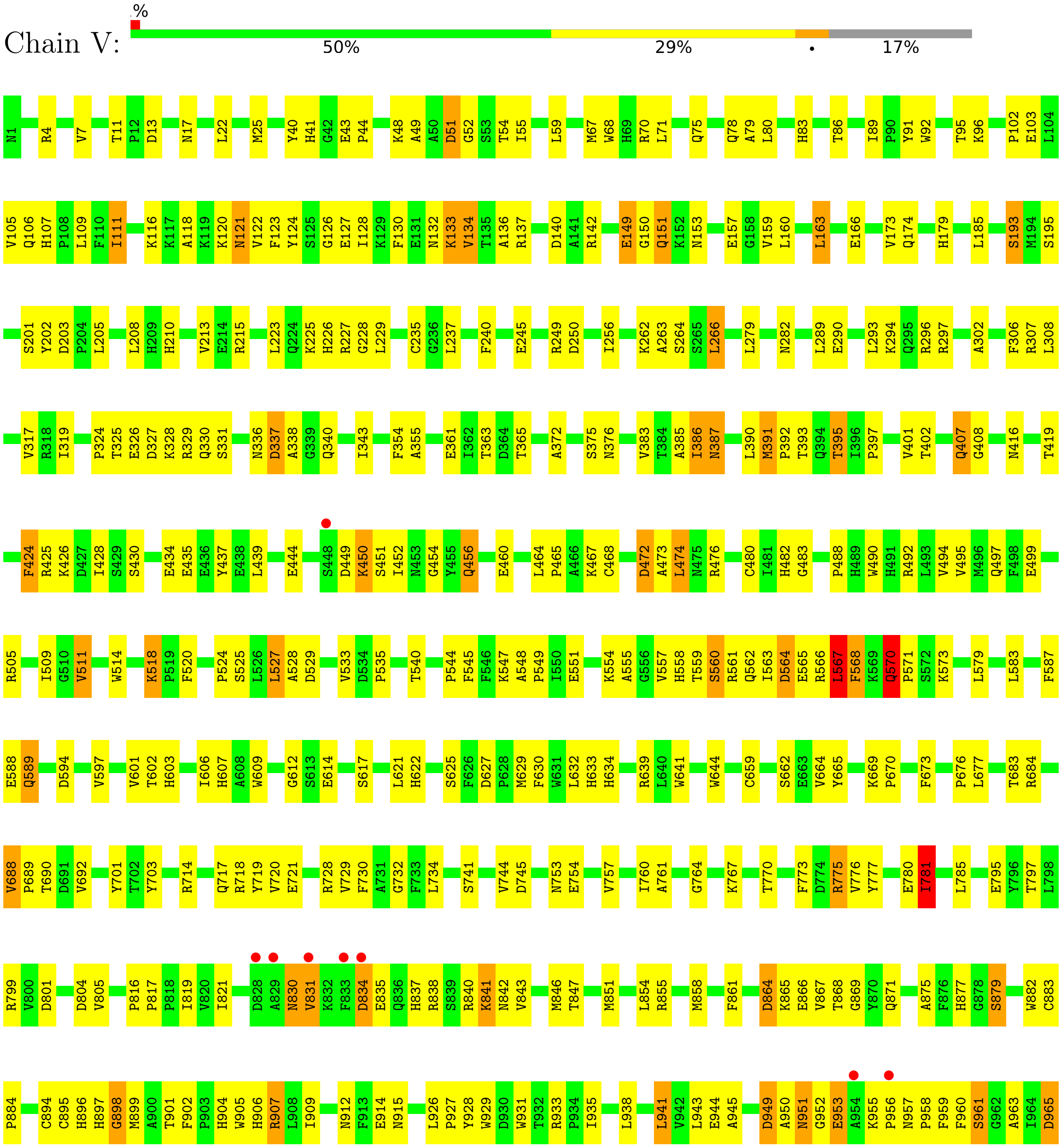
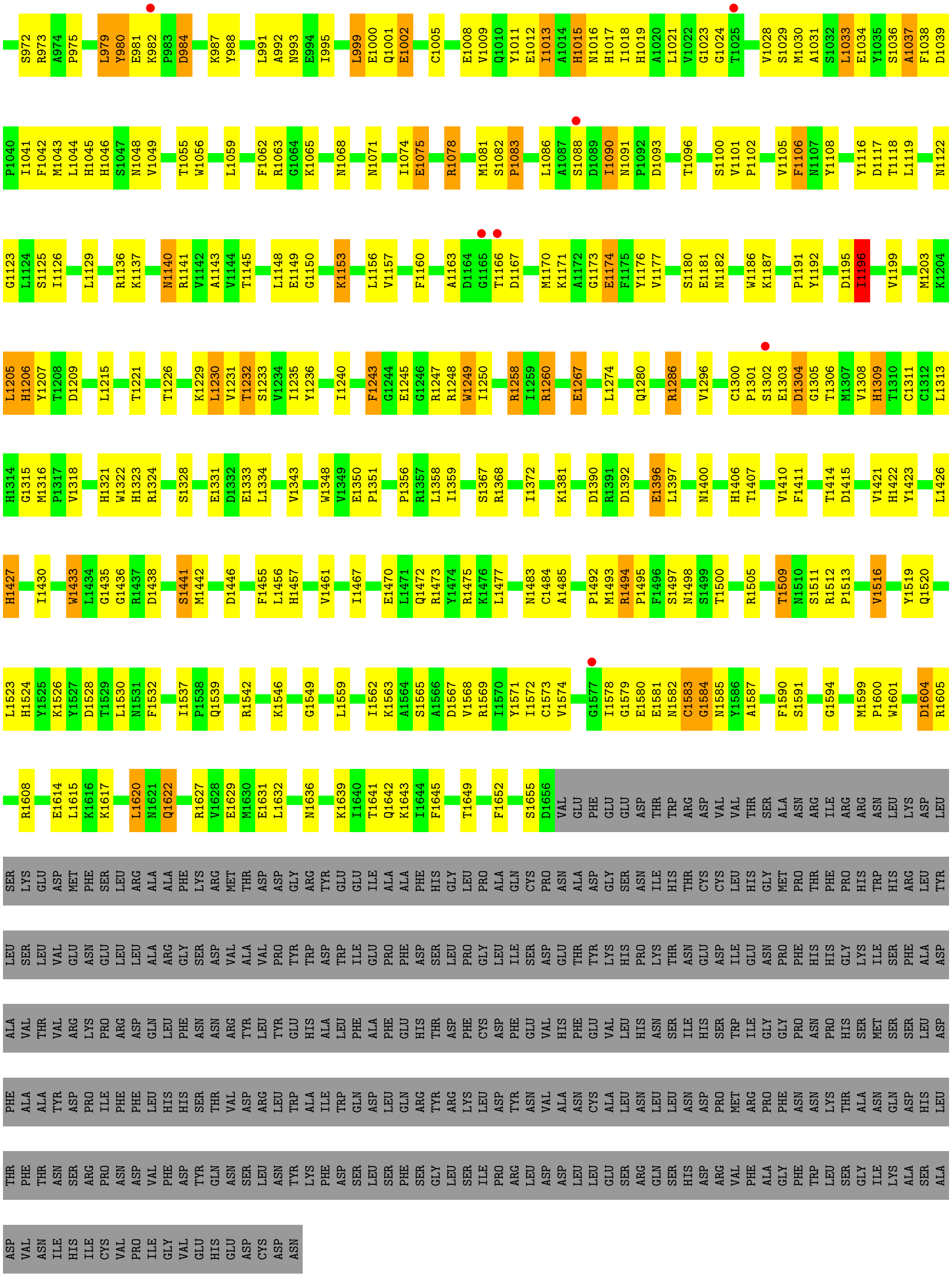
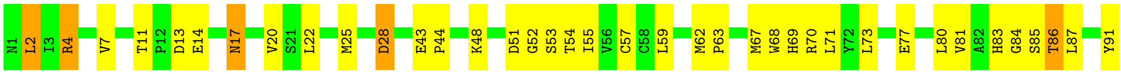


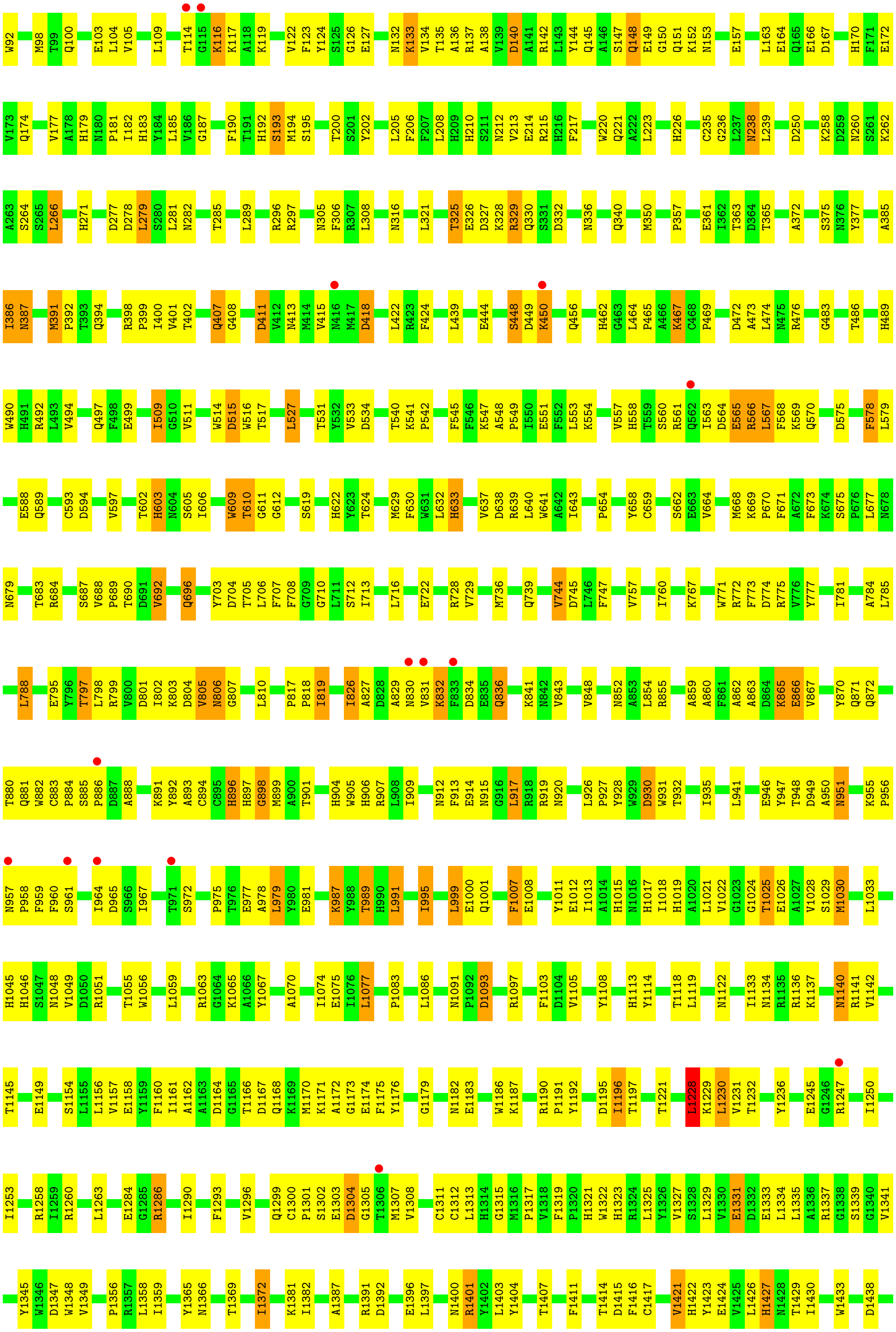
• Molecule 1: hemocyanin





- Molecule 1: hemocyanin

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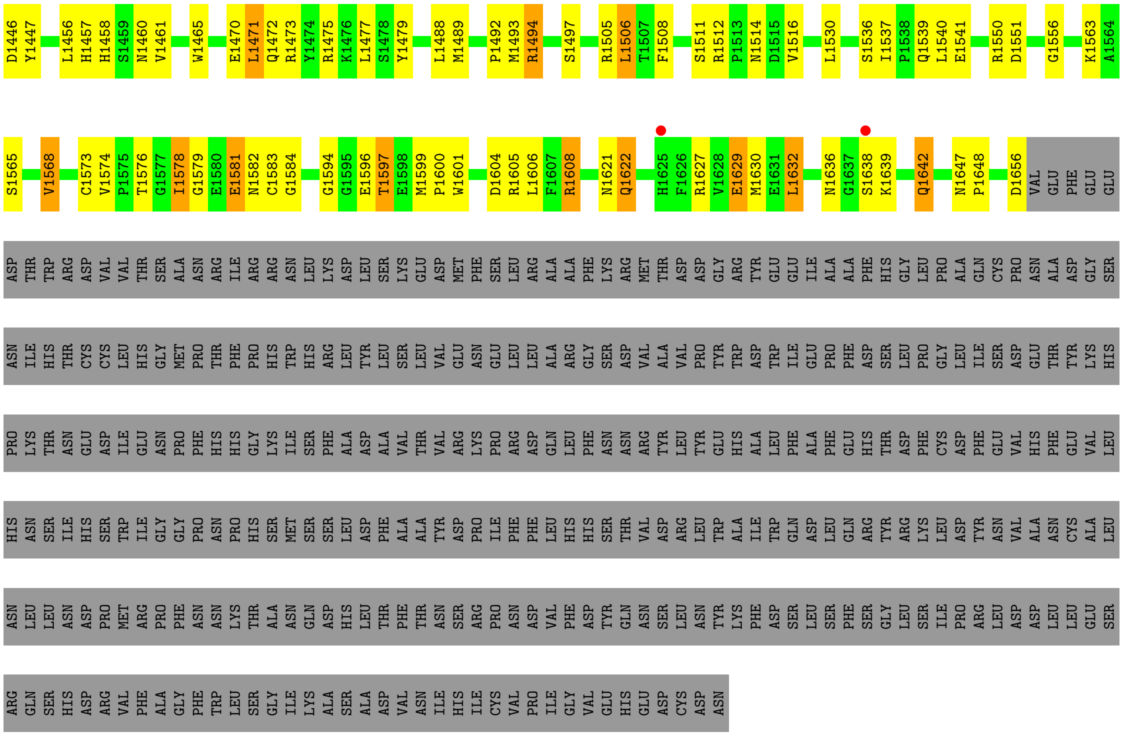
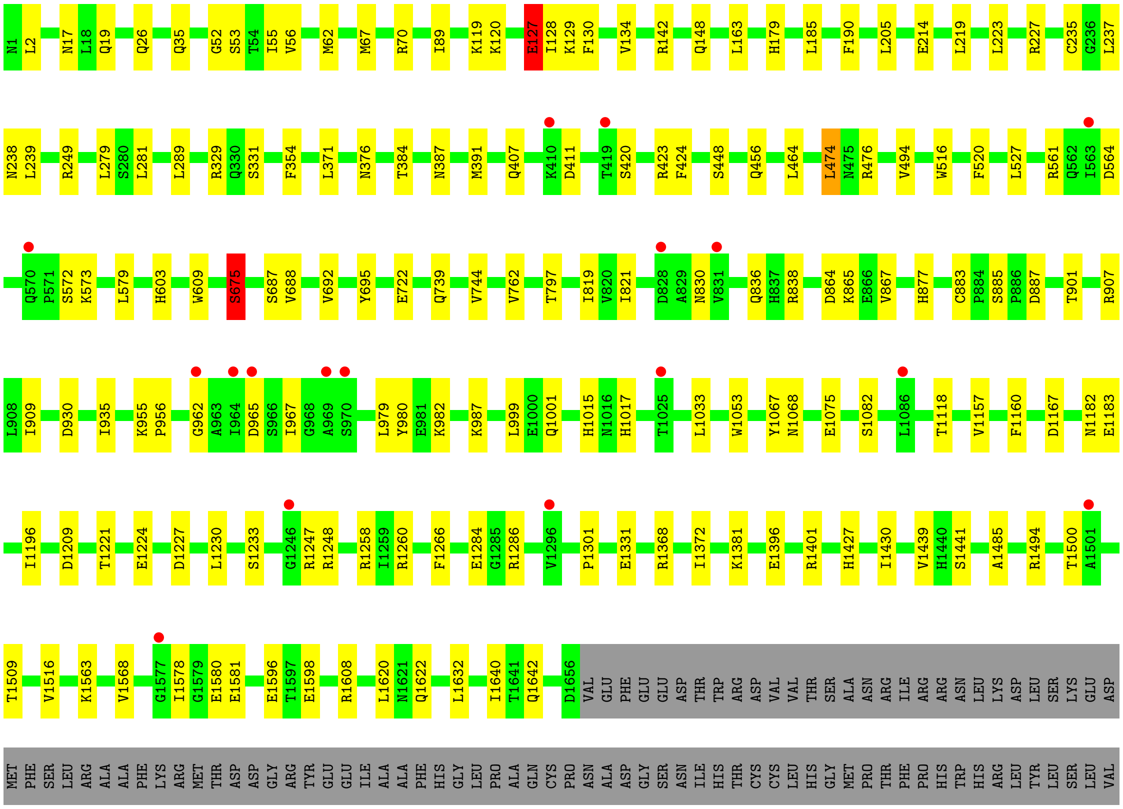
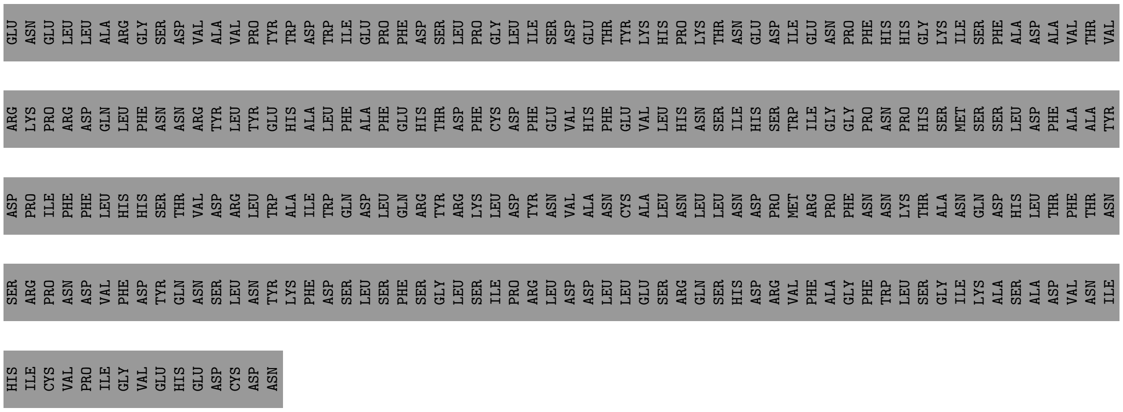


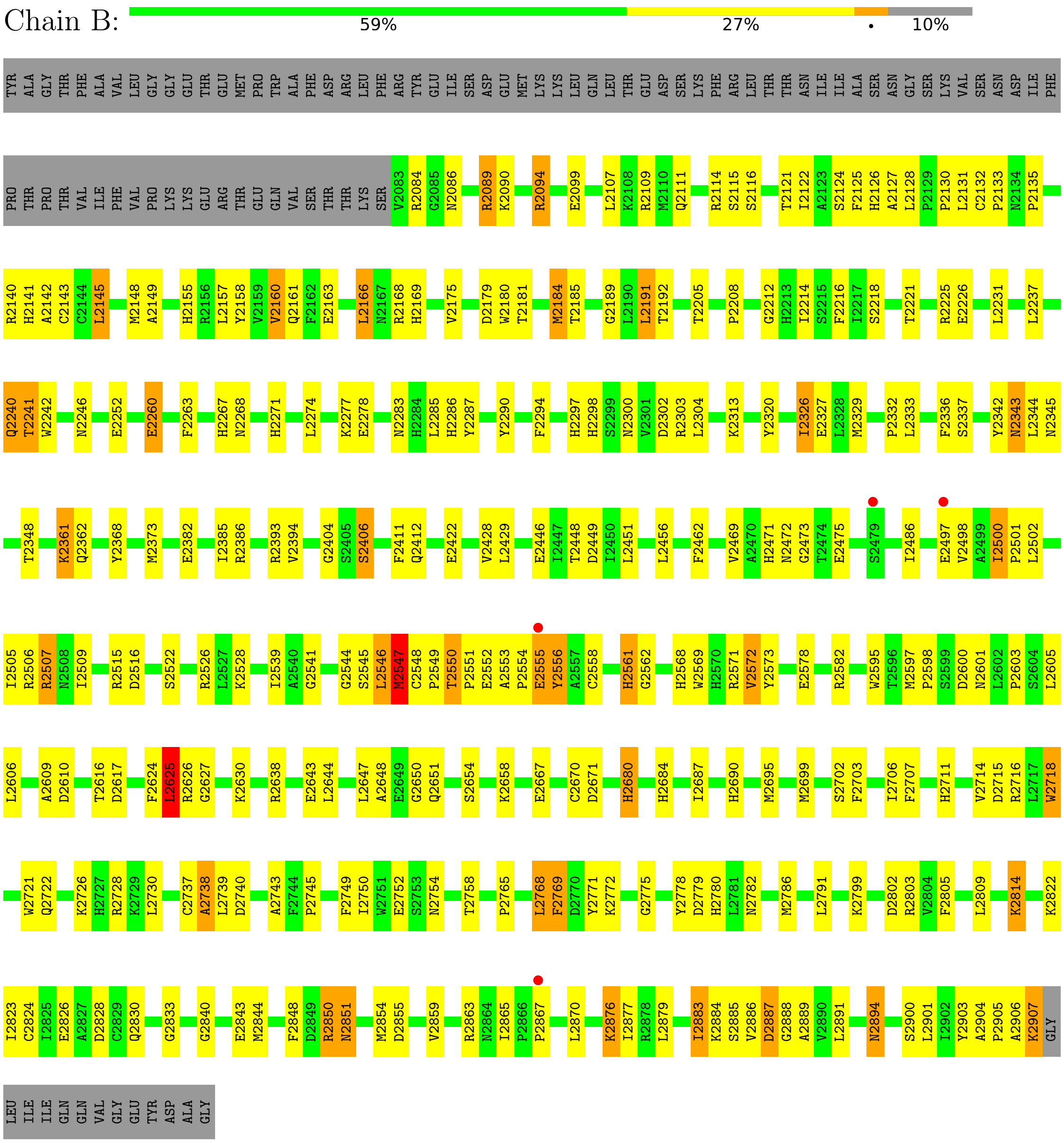
- Molecule 1: hemocyanin

Chain b:



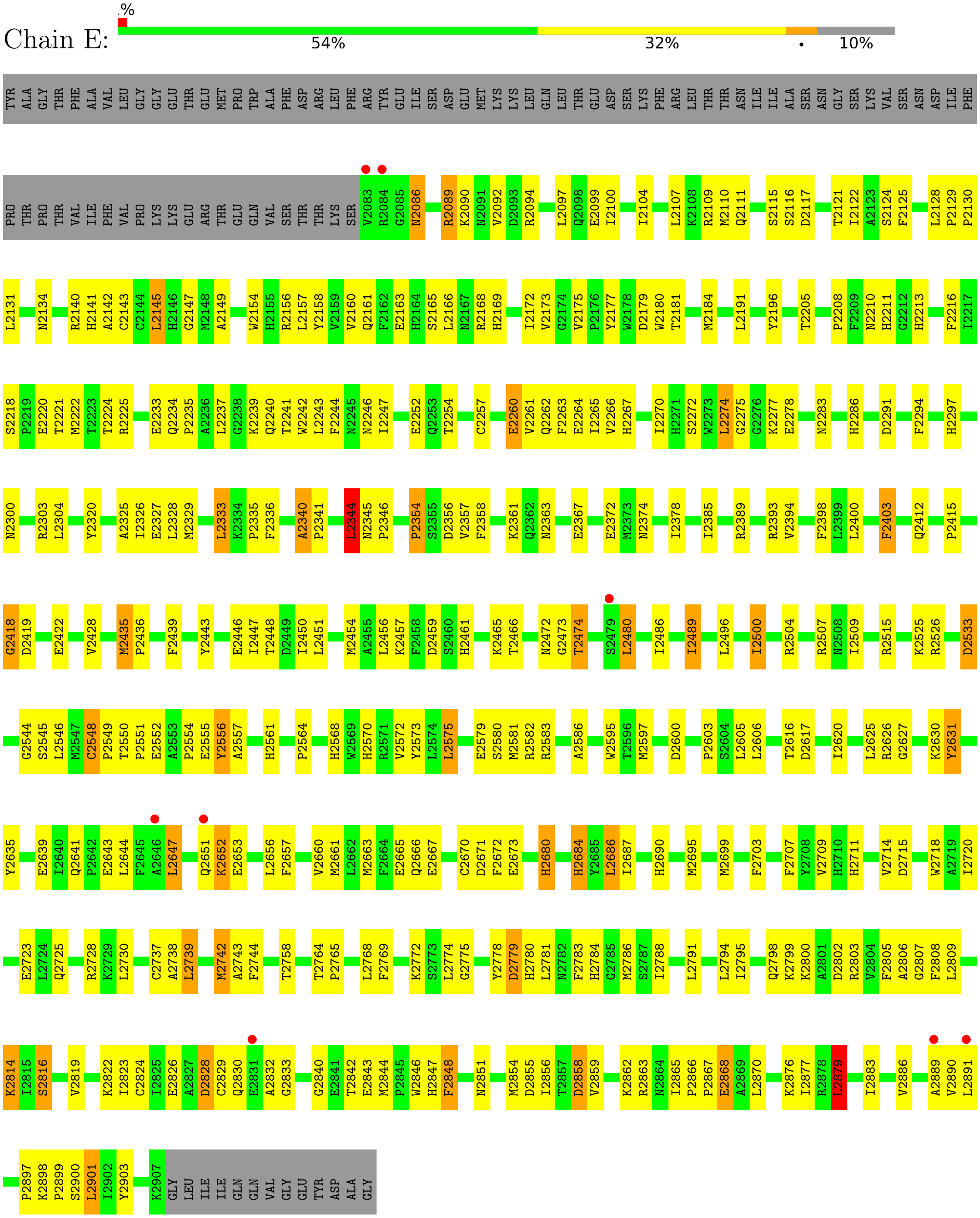


- Molecule 2: hemocyanin



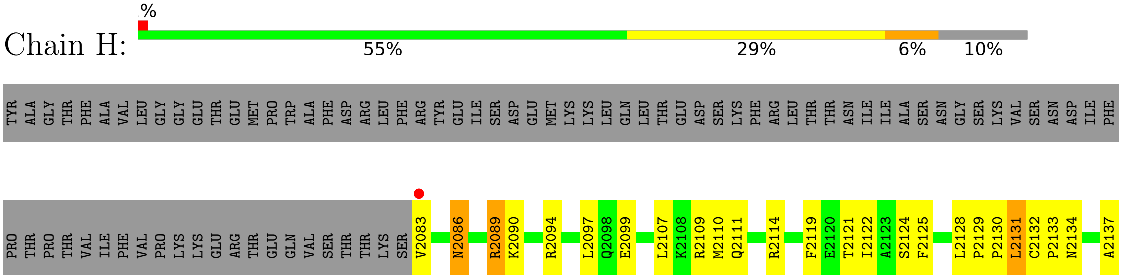
- Molecule 2: hemocyanin

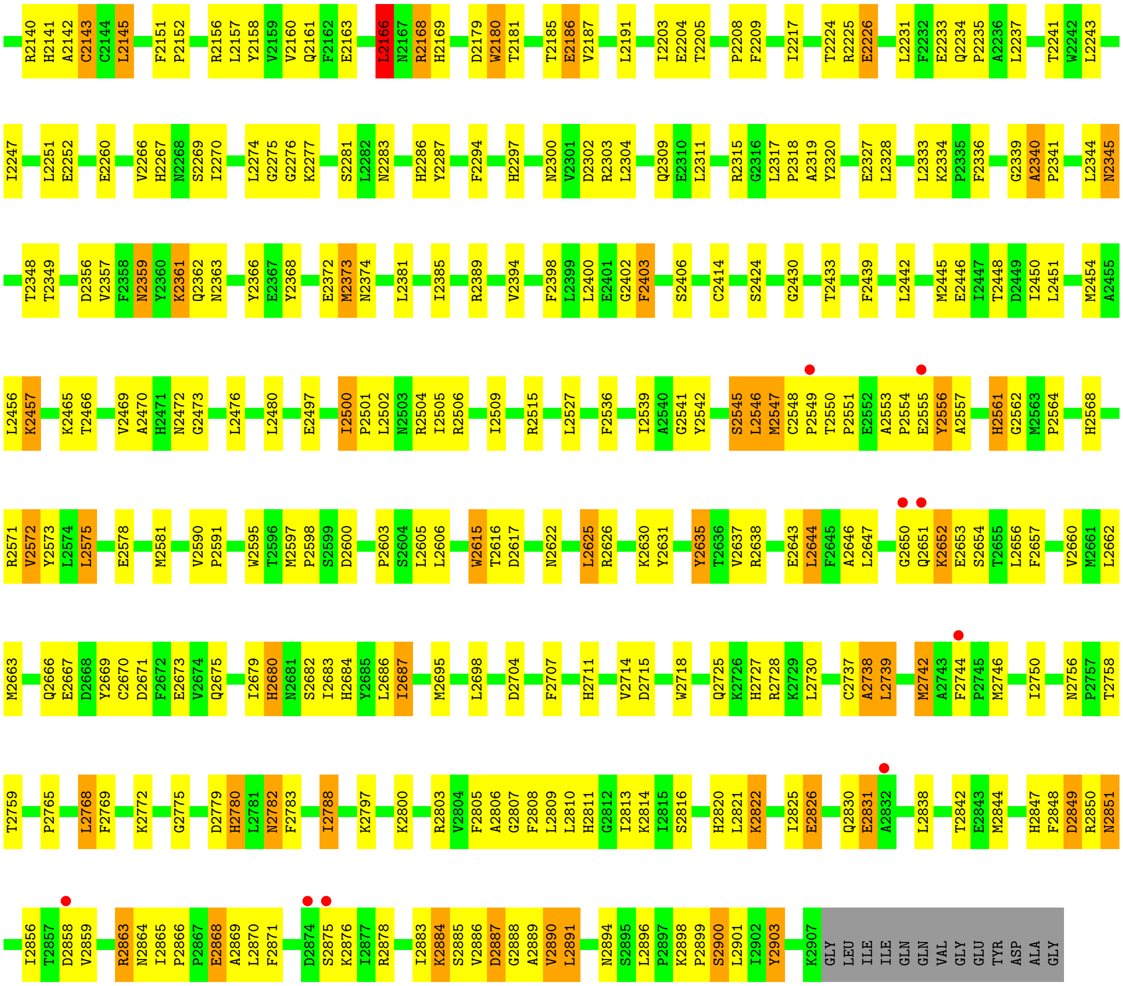
Chain E:



- Molecule 2: hemocyanin

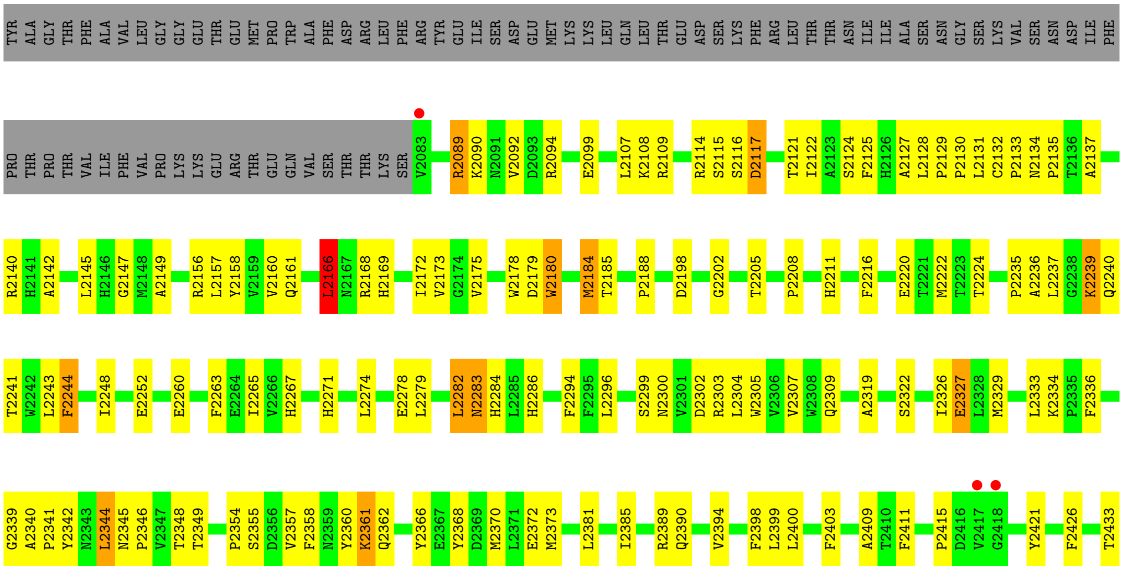
Chain H:

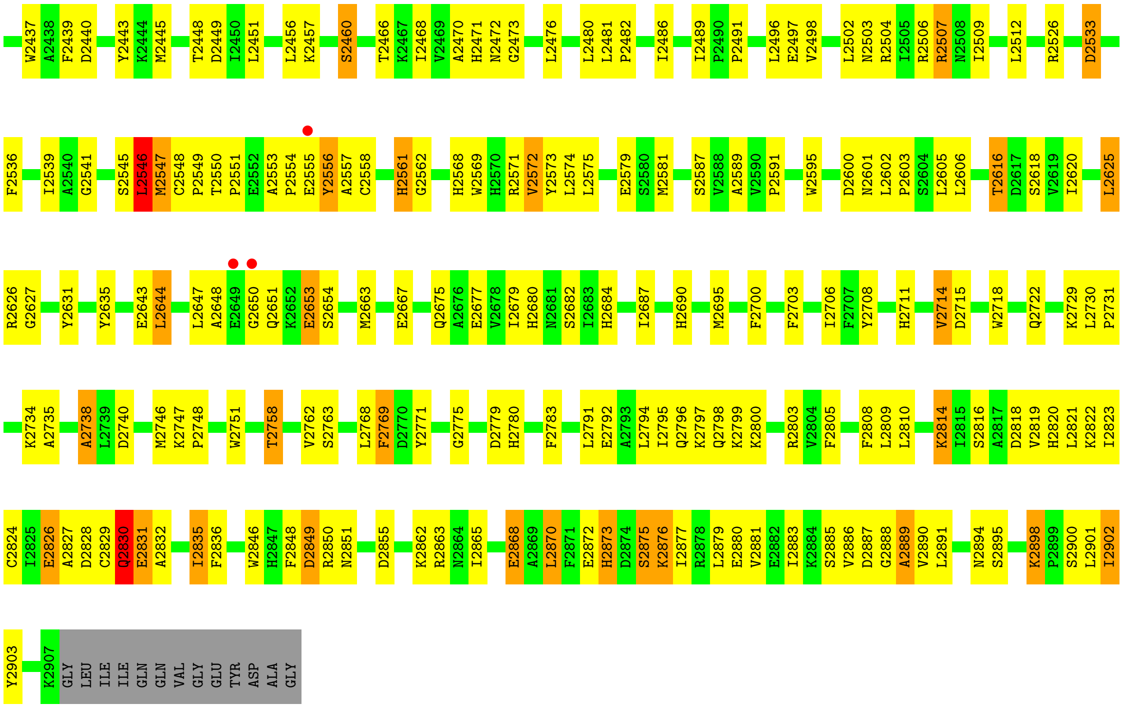




- Molecule 2: hemocyanin

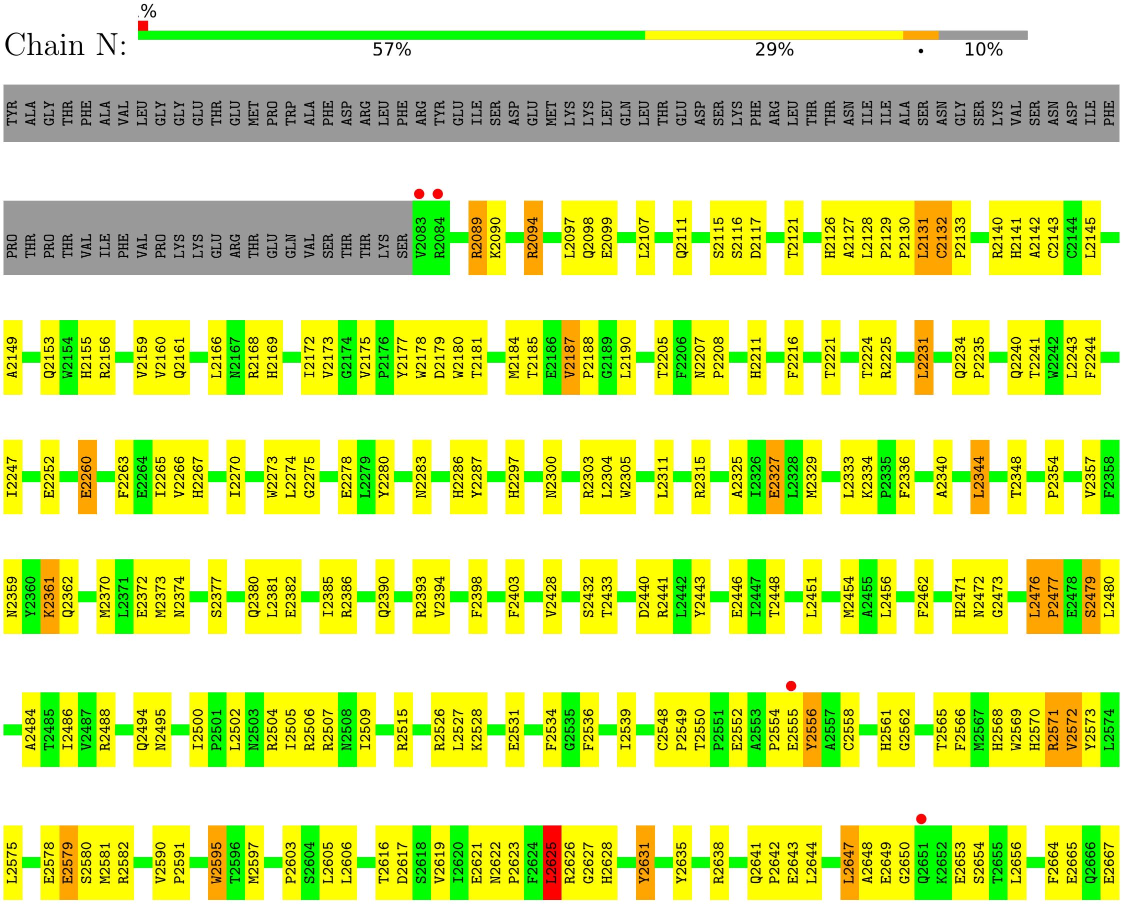
Chain K:

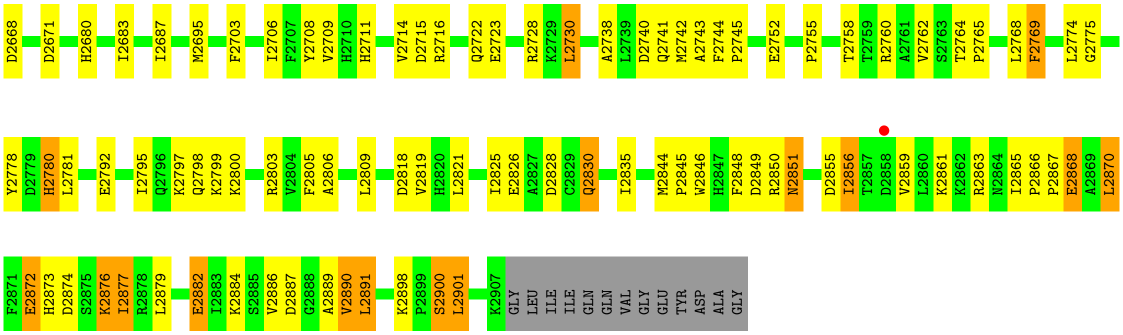




- Molecule 2: hemocyanin

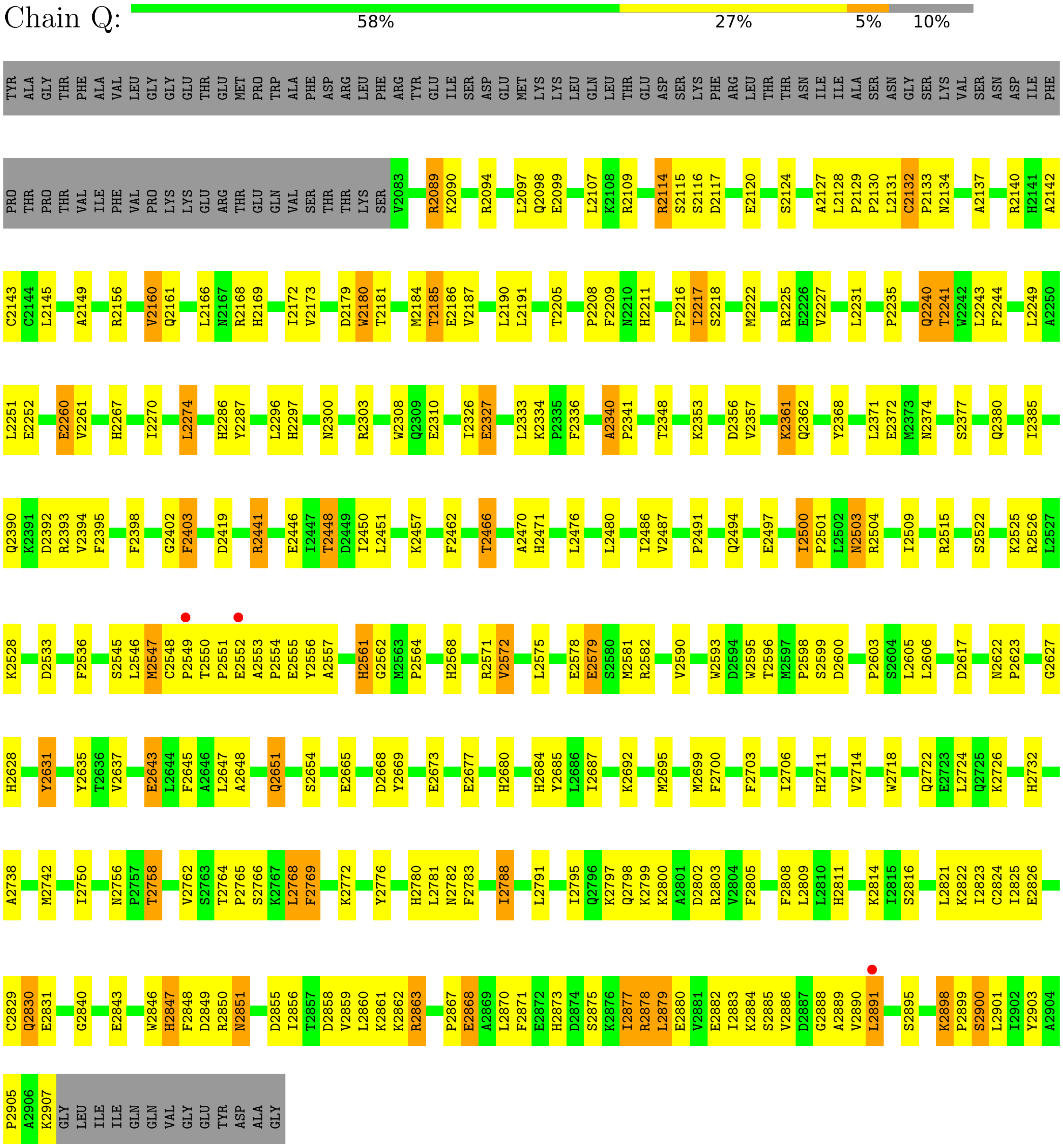
Chain N:



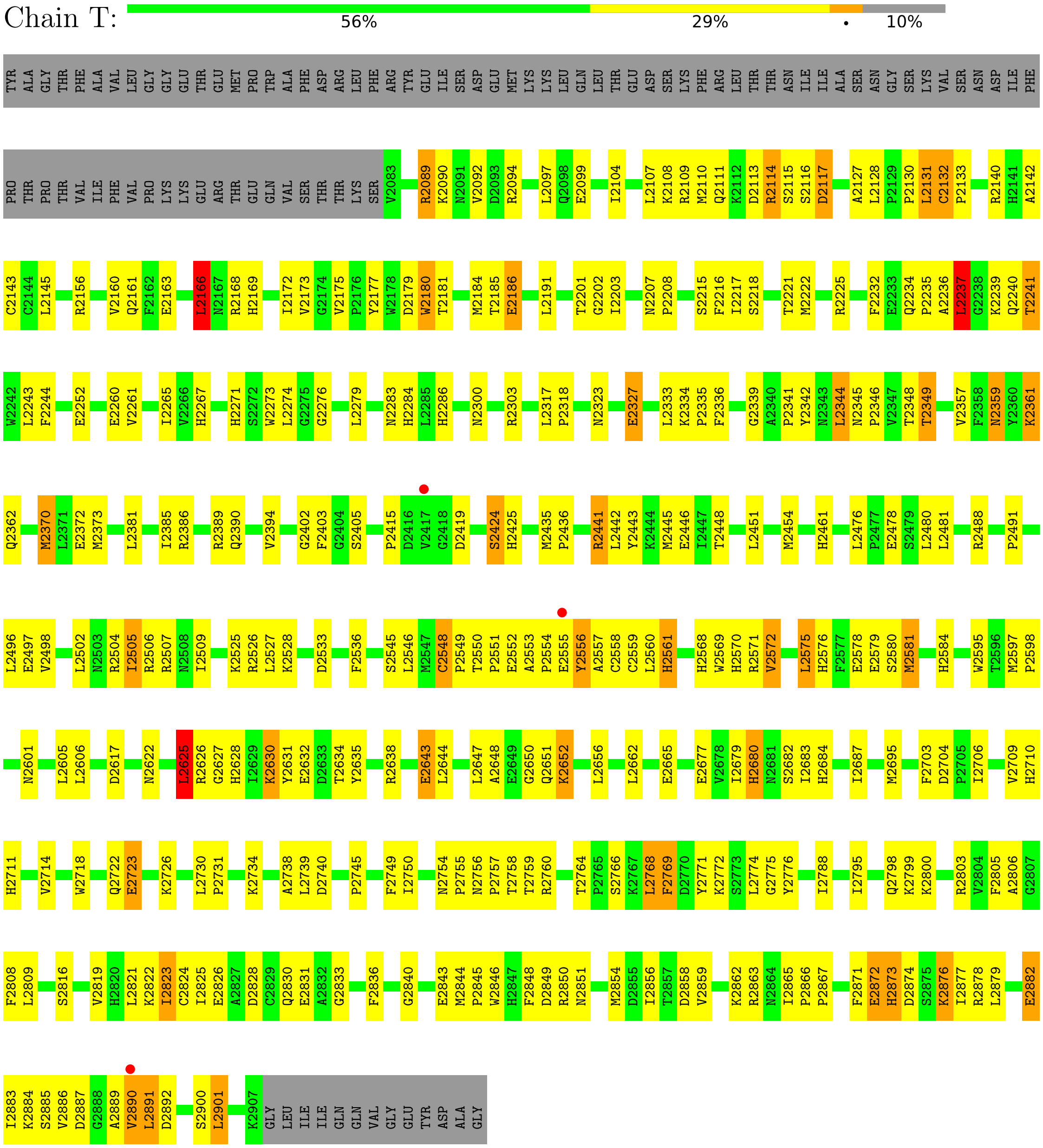


- Molecule 2: hemocyanin

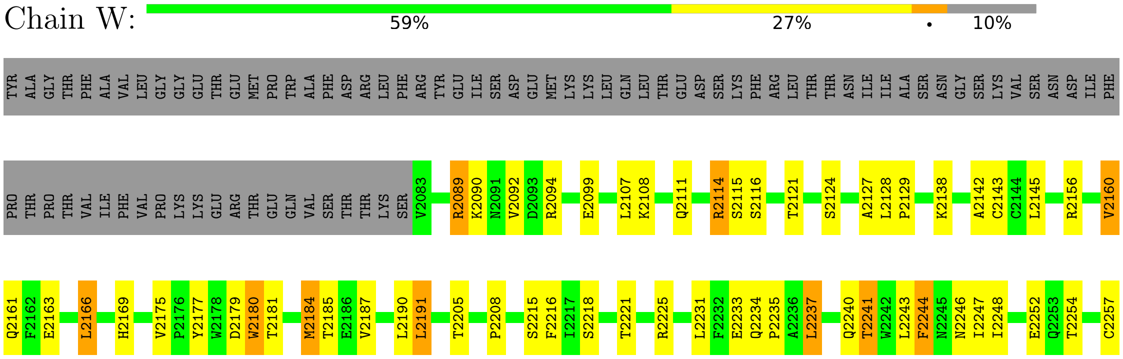
Chain Q:

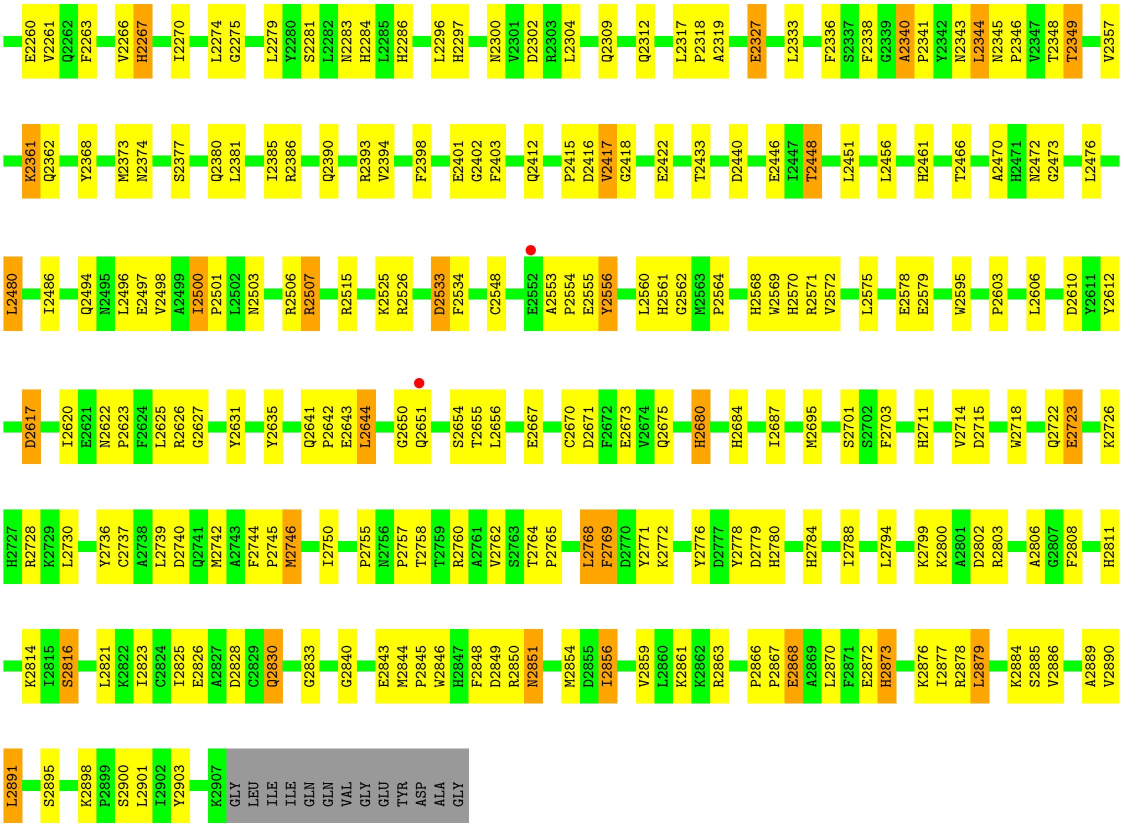


- Molecule 2: hemocyanin

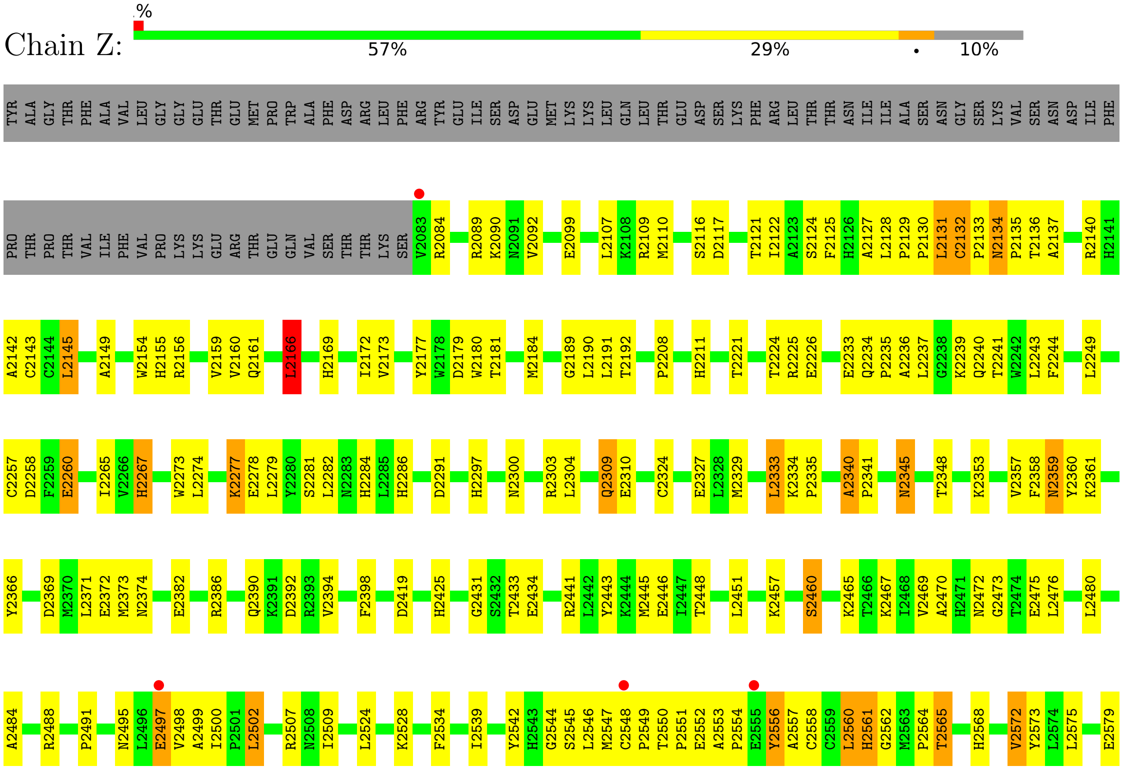


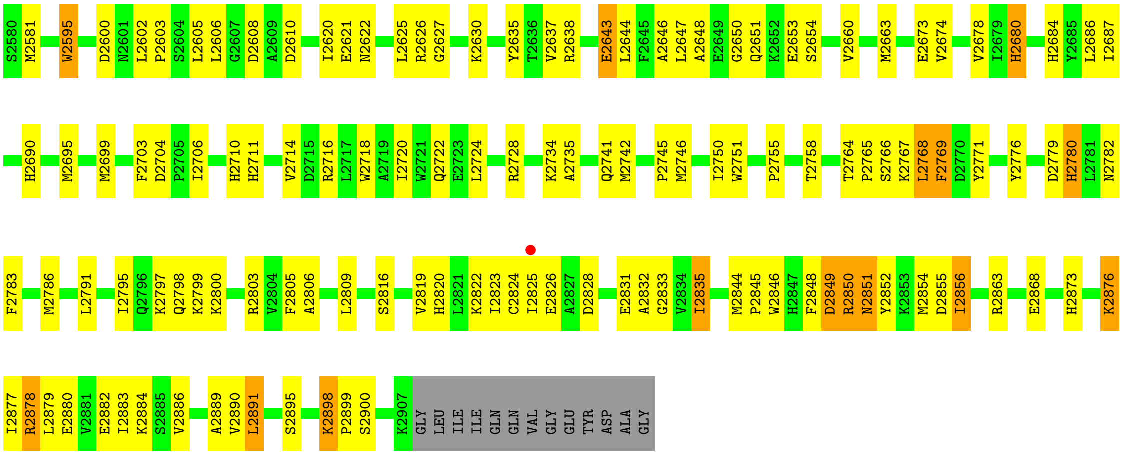
- Molecule 2: hemocyanin





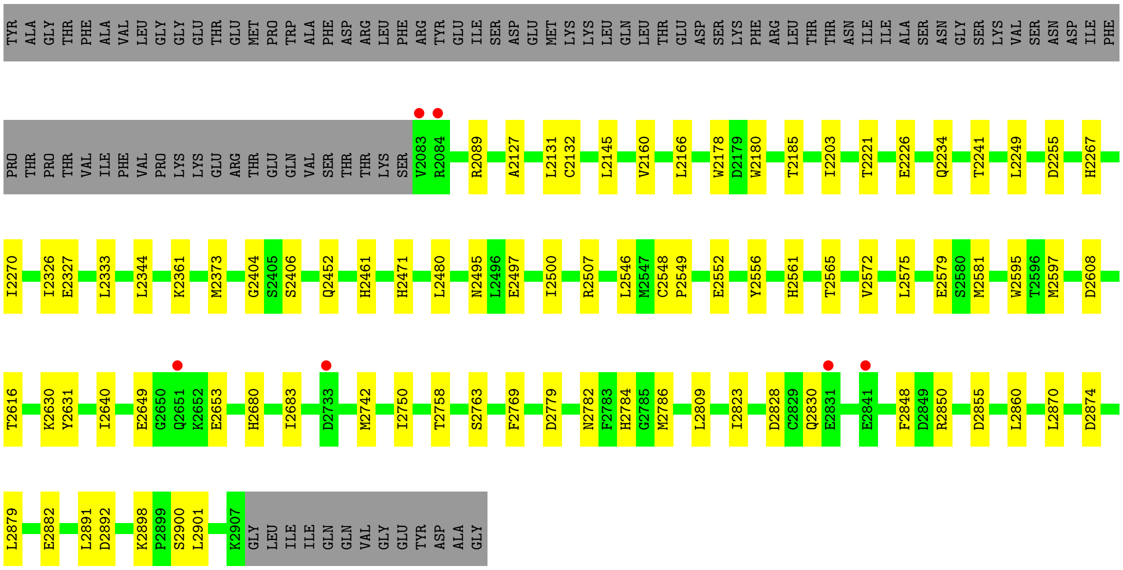
- Molecule 2: hemocyanin





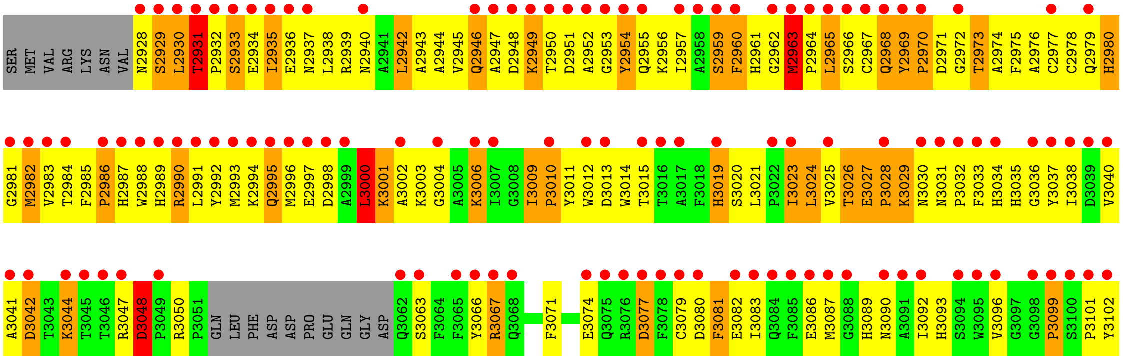
- Molecule 2: hemocyanin

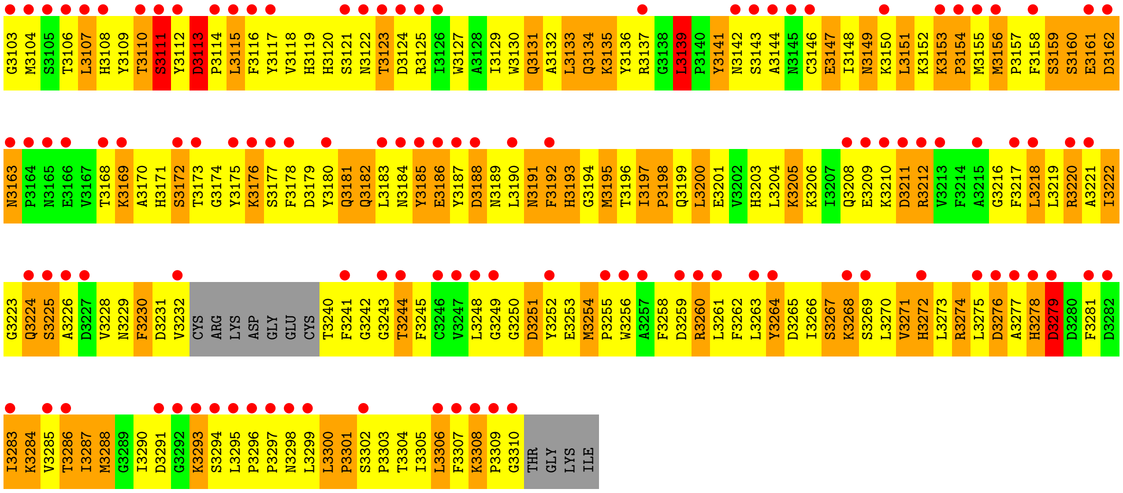
Chain c:



- Molecule 3: hemocyanin

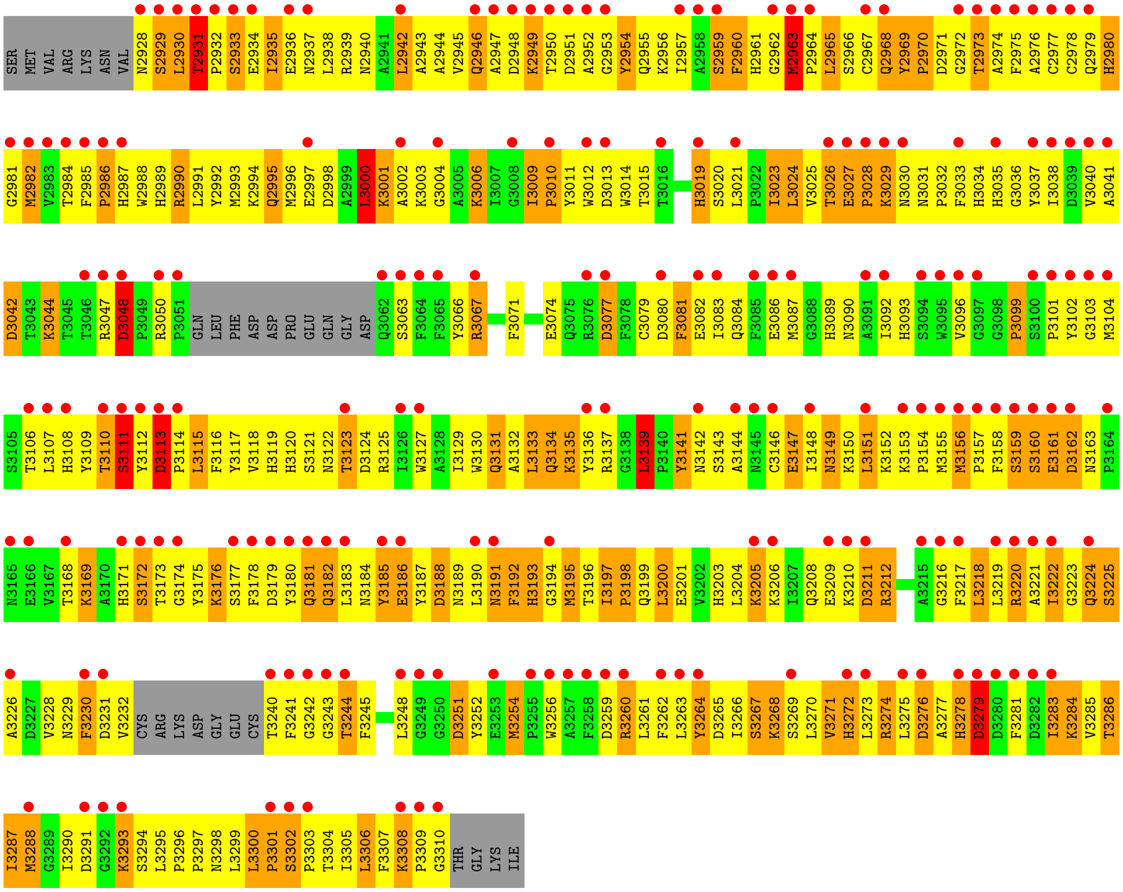
Chain C:





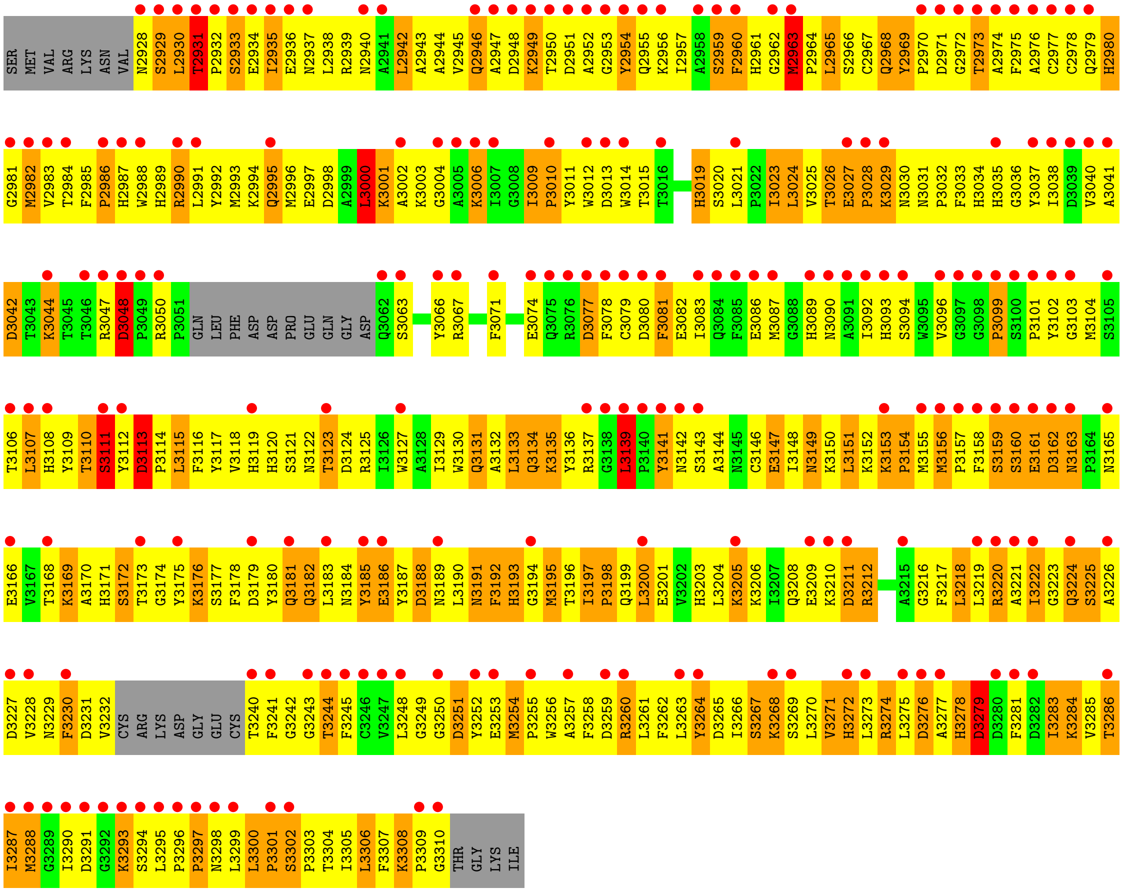
- Molecule 3: hemocyanin

Chain F:



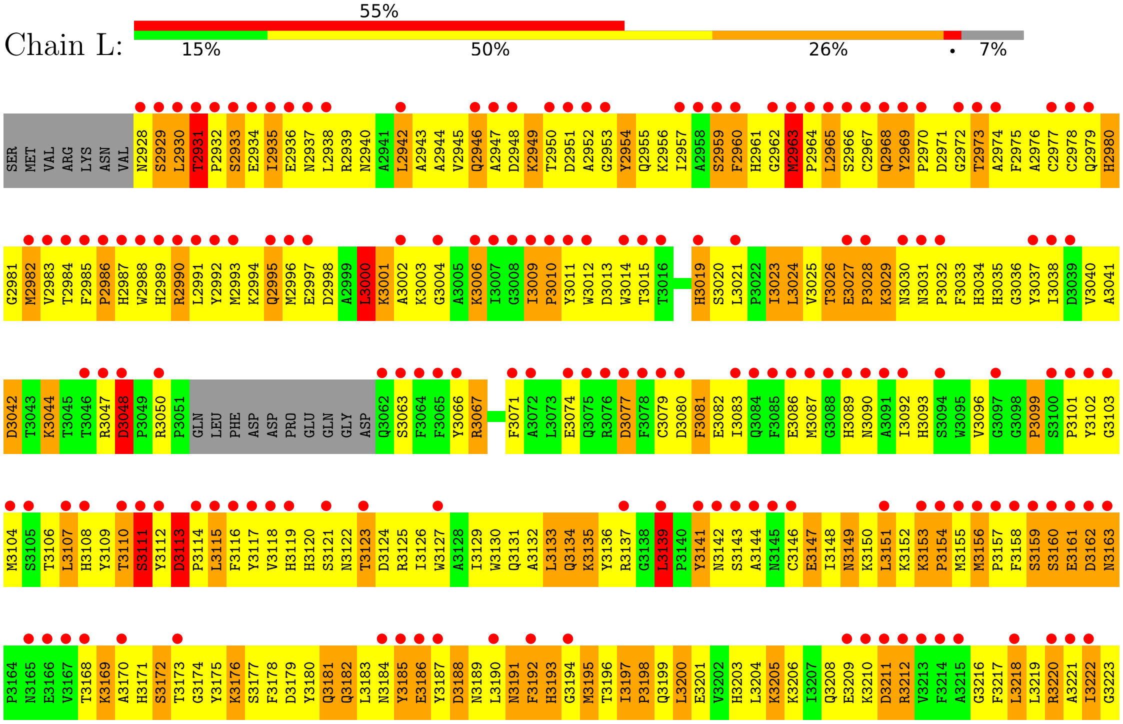
- Molecule 3: hemocyanin

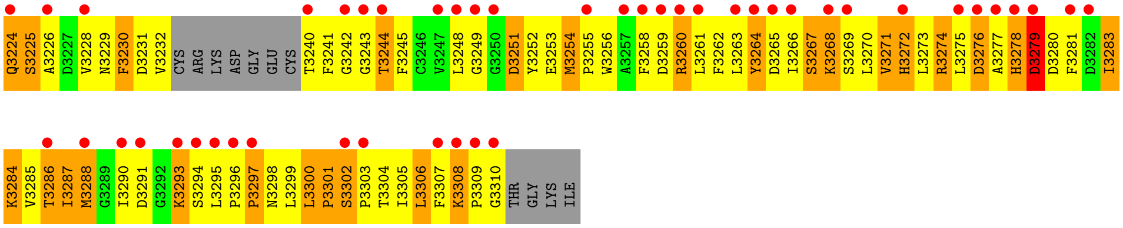
Chain I:



- Molecule 3: hemocyanin

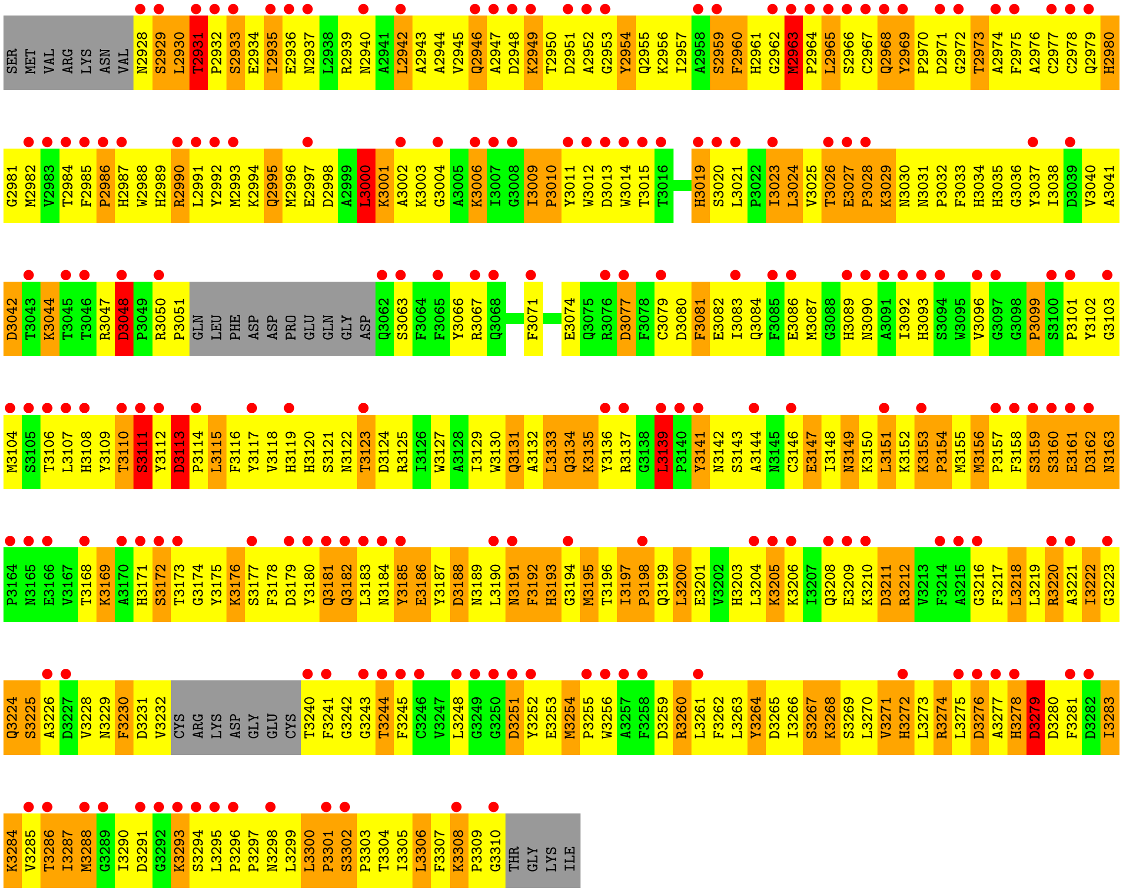
Chain L:





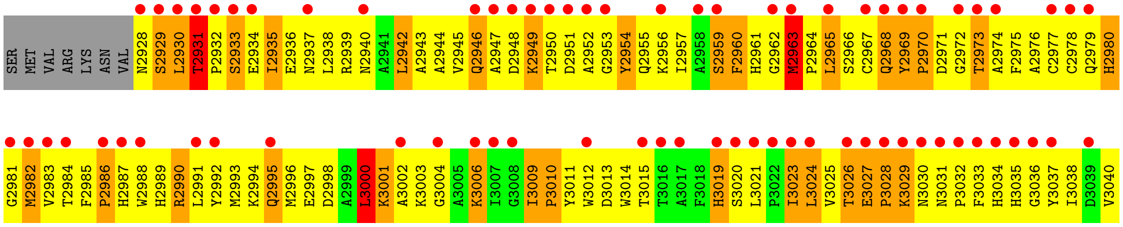
- Molecule 3: hemocyanin

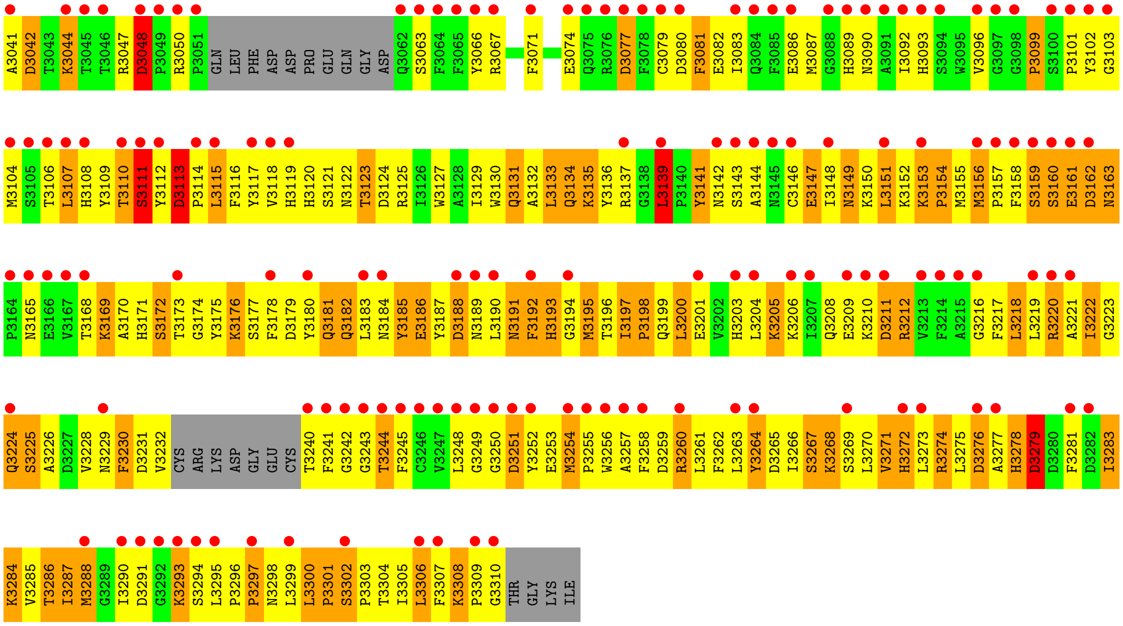
Chain O:



- Molecule 3: hemocyanin

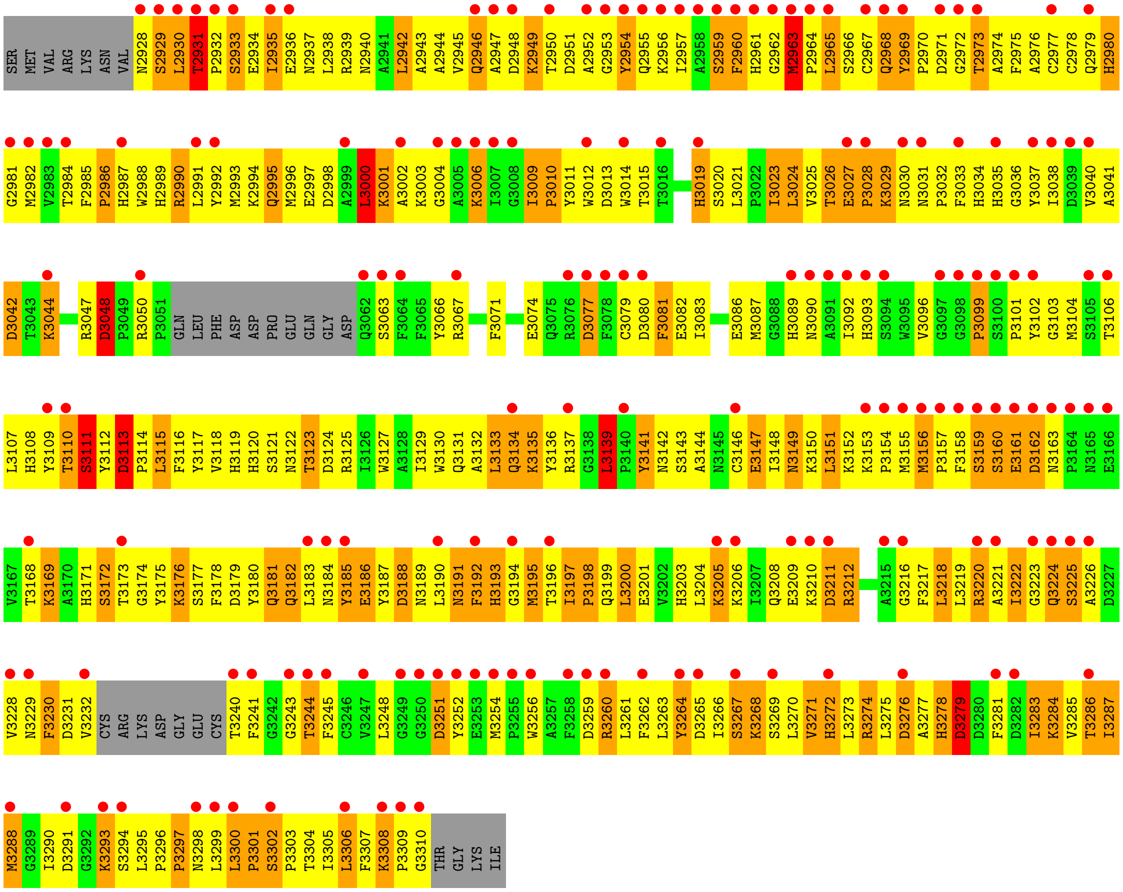
Chain R:





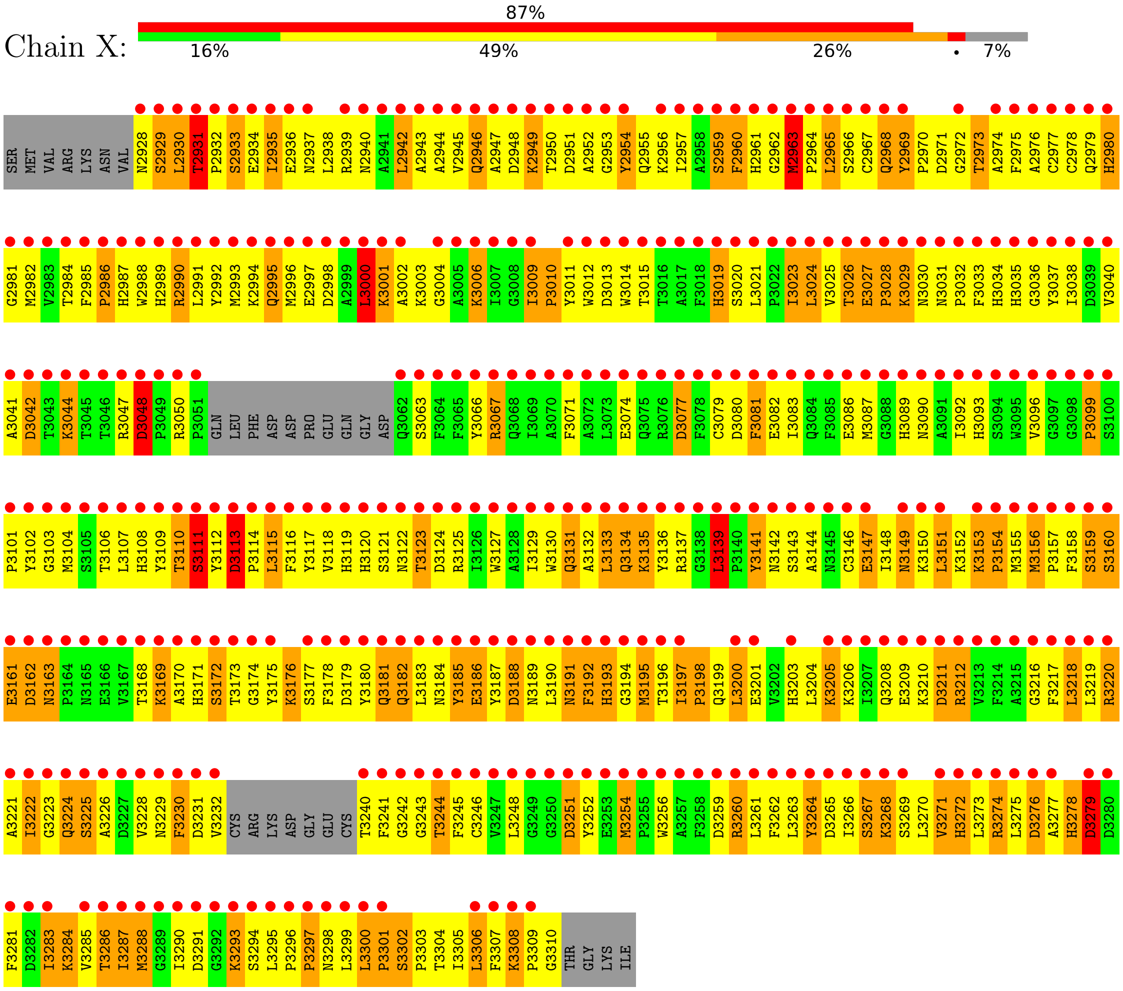
- Molecule 3: hemocyanin

Chain U:



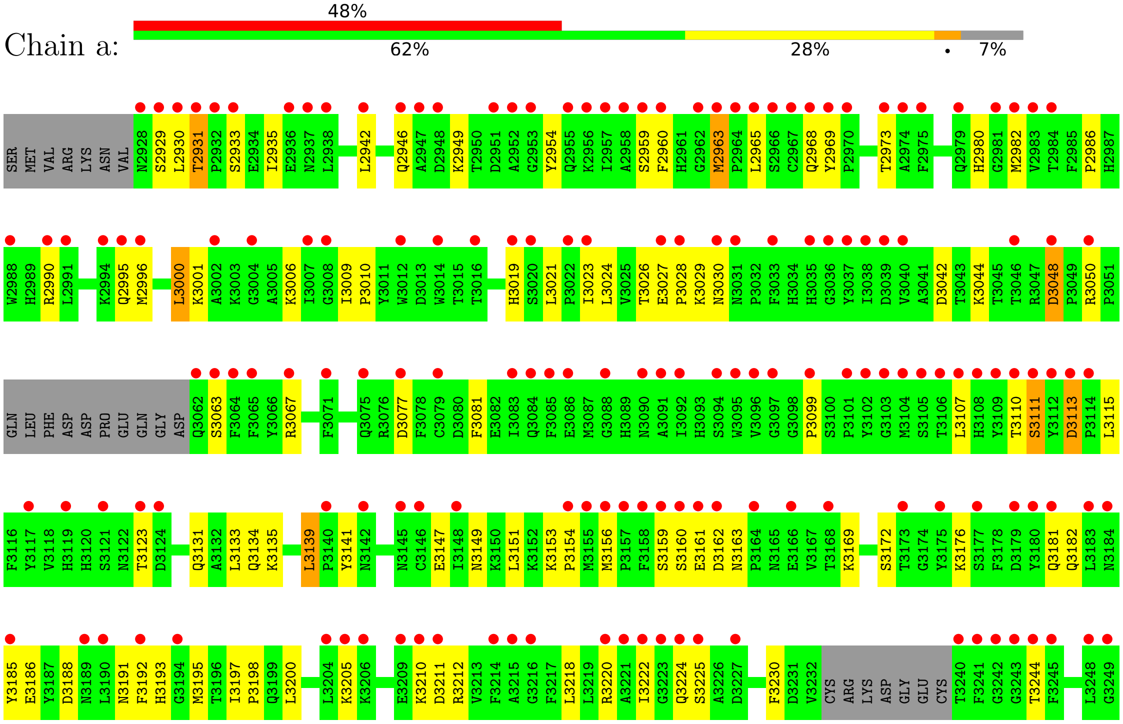
- Molecule 3: hemocyanin

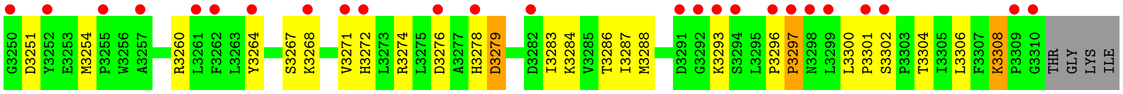
Chain X:



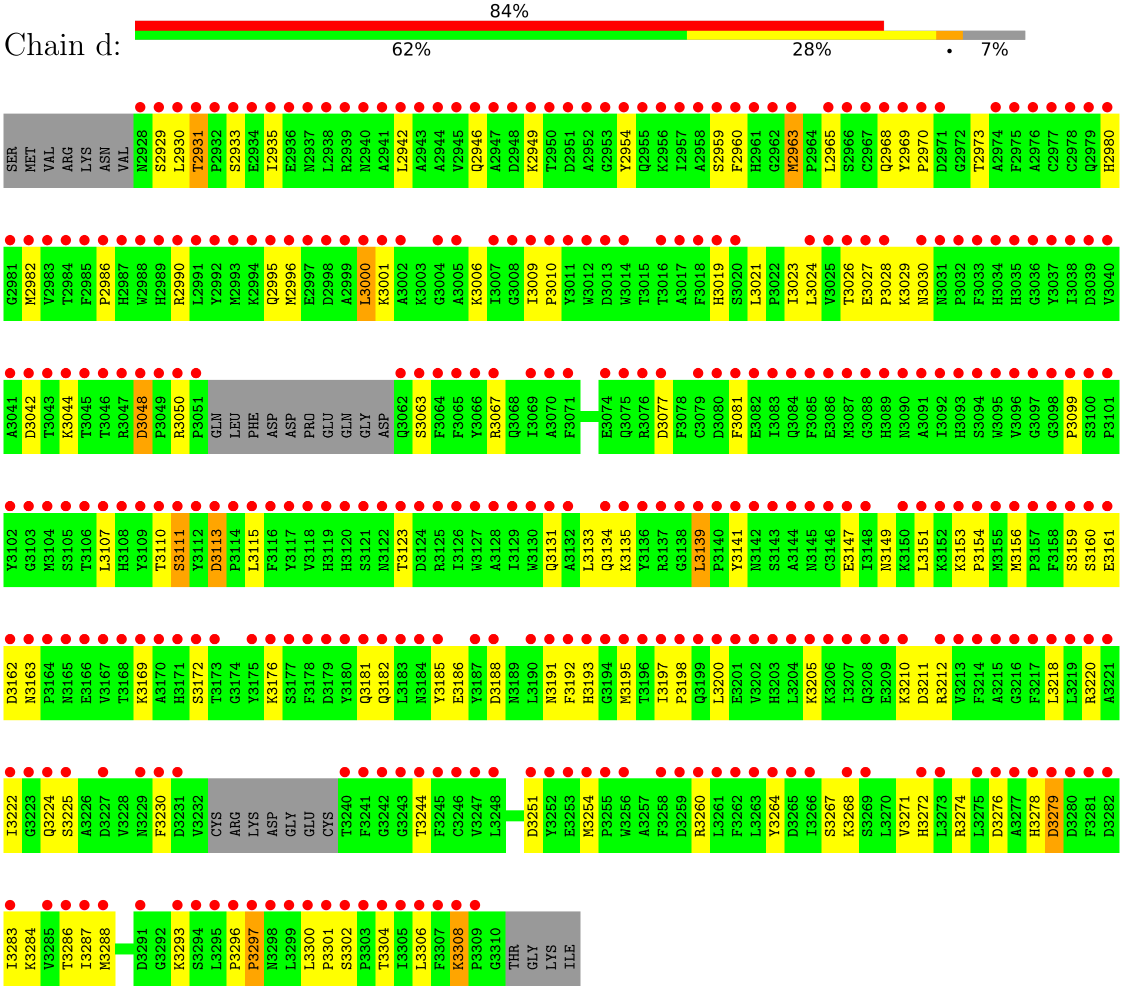
• Molecule 3: hemocyanin

Chain a:



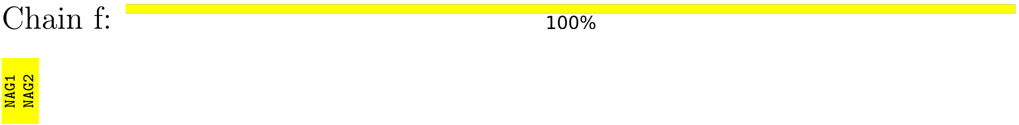


- Molecule 3: hemocyanin



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

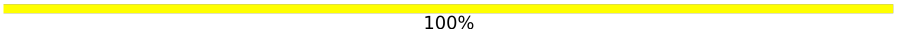
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



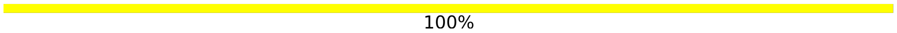
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

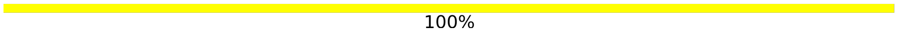

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:


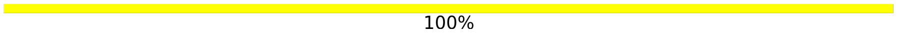
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:


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

Chain n:


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

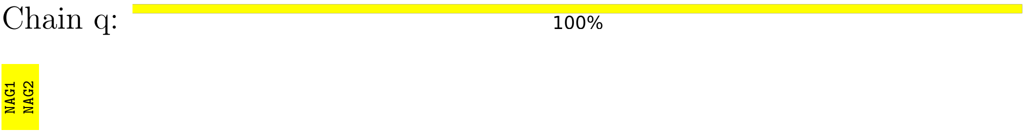
Chain o:


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

Chain p:

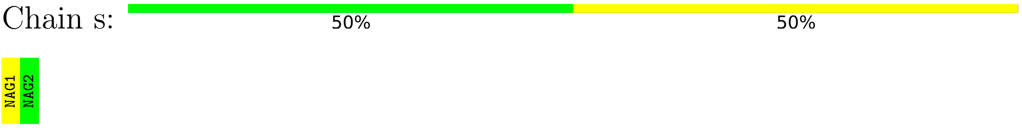

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:



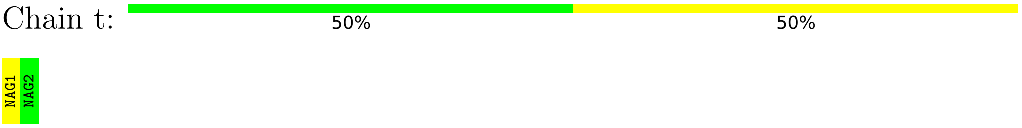
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:



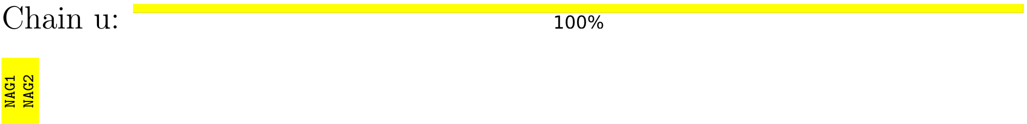
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:



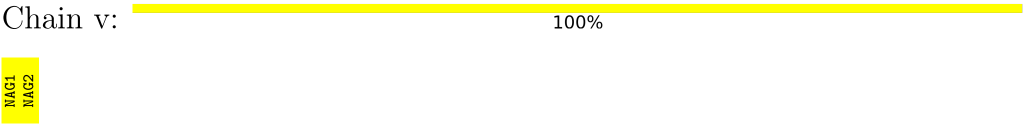
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



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

Chain v:

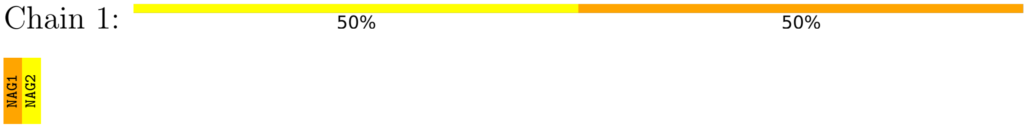


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:

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

Chain 1:

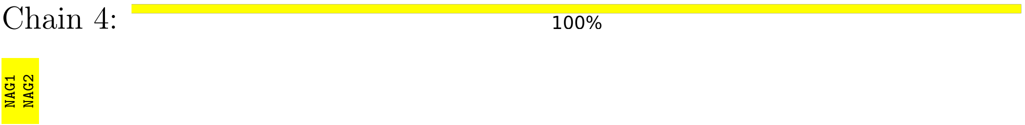


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:

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

Chain 4:

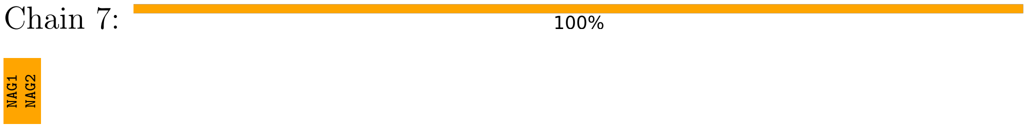


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:

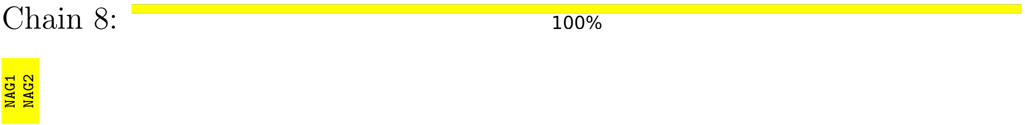
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:



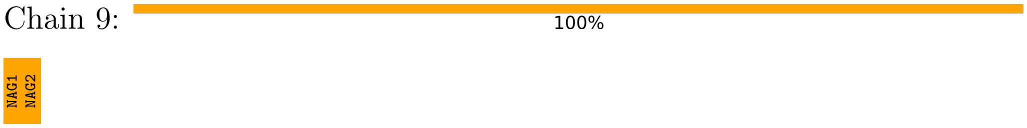
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8:



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

Chain 9:



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

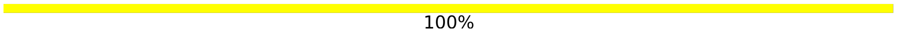
Chain BA:

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

Chain HA:

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

Chain IA:



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

Chain JA:

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

Chain MA:

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

Chain OA:

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

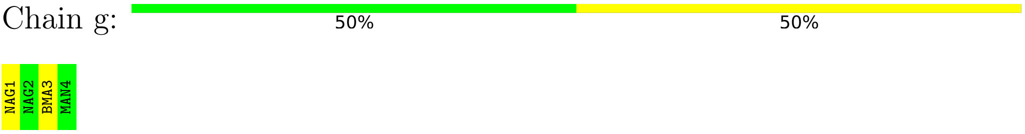
Chain QA:

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

Chain RA:

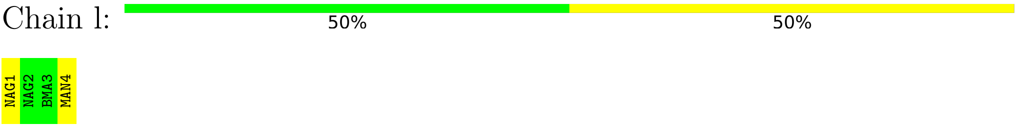
- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



- Molecule 5: 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:

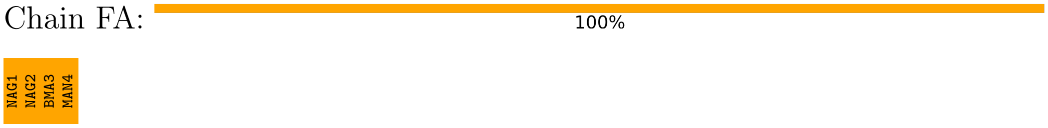


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:

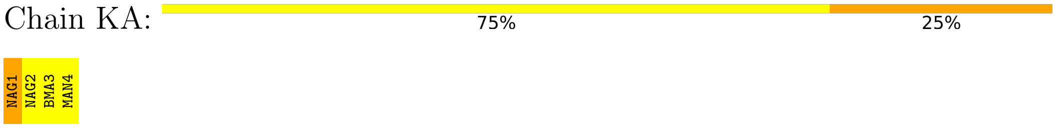
- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA:



- Molecule 5: 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 KA:

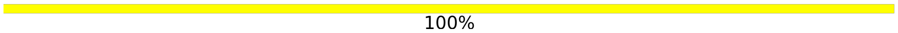


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain PA:

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

Chain h:

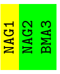


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:

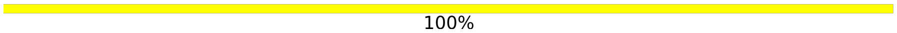
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



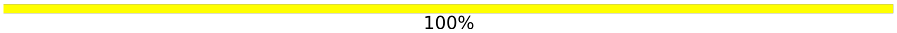
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:



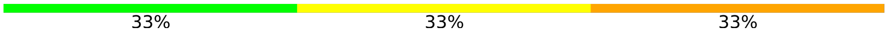
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:



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

Chain 3:



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

Chain 5:

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

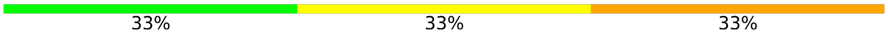
Chain CA:

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

Chain DA:

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

Chain EA:



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

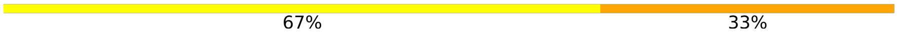
Chain GA:

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

Chain LA:

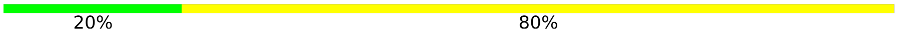
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain NA:



- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:



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

Chain 0:

4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	171.37Å 538.66Å 310.92Å 90.00° 104.09° 90.00°	Depositor
Resolution (Å)	49.10 – 3.00 49.10 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.10-3.00) 89.6 (49.10-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.274 , 0.303 0.275 , 0.303	Depositor DCC
R_{free} test set	53588 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	64.8	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 11.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	261470	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.29	0/13698	0.54	4/18607 (0.0%)
1	D	0.29	0/13698	0.54	4/18607 (0.0%)
1	G	0.28	0/13698	0.53	3/18607 (0.0%)
1	J	0.29	0/13698	0.53	2/18607 (0.0%)
1	M	0.28	0/13698	0.52	2/18607 (0.0%)
1	P	0.28	0/13698	0.53	3/18607 (0.0%)
1	S	0.27	0/13698	0.52	4/18607 (0.0%)
1	V	0.28	0/13698	0.52	4/18607 (0.0%)
1	Y	0.27	0/13698	0.51	3/18607 (0.0%)
1	b	0.27	0/13698	0.52	3/18607 (0.0%)
2	B	0.27	0/6909	0.51	2/9383 (0.0%)
2	E	0.28	0/6909	0.52	1/9383 (0.0%)
2	H	0.28	0/6909	0.51	2/9383 (0.0%)
2	K	0.28	0/6909	0.52	2/9383 (0.0%)
2	N	0.28	0/6909	0.50	1/9383 (0.0%)
2	Q	0.27	0/6909	0.50	0/9383
2	T	0.27	0/6909	0.50	2/9383 (0.0%)
2	W	0.26	0/6909	0.49	1/9383 (0.0%)
2	Z	0.27	0/6909	0.49	1/9383 (0.0%)
2	c	0.27	0/6909	0.49	0/9383
3	C	0.80	12/6100 (0.2%)	0.90	34/8282 (0.4%)
3	F	0.80	12/6100 (0.2%)	0.90	34/8282 (0.4%)
3	I	0.80	12/6100 (0.2%)	0.90	34/8282 (0.4%)
3	L	0.80	12/6100 (0.2%)	0.91	34/8282 (0.4%)
3	O	0.80	12/6100 (0.2%)	0.90	34/8282 (0.4%)
3	R	0.80	14/6100 (0.2%)	0.90	34/8282 (0.4%)
3	U	0.80	12/6100 (0.2%)	0.91	34/8282 (0.4%)
3	X	0.80	12/6100 (0.2%)	0.90	34/8282 (0.4%)
3	a	0.80	12/6100 (0.2%)	0.90	34/8282 (0.4%)
3	d	0.80	14/6100 (0.2%)	0.90	34/8282 (0.4%)
All	All	0.45	124/267070 (0.0%)	0.63	384/362720 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	3
1	G	0	1
1	J	0	2
1	M	0	1
1	S	0	3
1	Y	0	1
1	b	0	2
2	B	0	1
2	K	0	3
2	N	0	1
2	Q	0	1
2	T	0	2
2	W	0	1
2	Z	0	2
2	c	0	1
3	C	0	4
3	F	0	4
3	I	0	4
3	L	0	4
3	O	0	4
3	R	0	4
3	U	0	4
3	X	0	4
3	a	0	4
3	d	0	4
All	All	0	67

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3154[A]	PRO	N-CD	5.36	1.55	1.47
3	C	3154[B]	PRO	N-CD	5.36	1.55	1.47
3	X	3154[A]	PRO	N-CD	5.25	1.55	1.47
3	X	3154[B]	PRO	N-CD	5.25	1.55	1.47
3	O	3154[A]	PRO	N-CD	5.24	1.55	1.47

The worst 5 of 384 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	979	LEU	CA-CB-CG	7.97	133.62	115.30
1	V	567	LEU	CA-CB-CG	7.90	133.47	115.30
1	A	279	LEU	CA-CB-CG	7.27	132.02	115.30
2	K	2546	LEU	CA-CB-CG	6.93	131.25	115.30
1	M	1230	LEU	CA-CB-CG	6.68	130.67	115.30

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	464	LEU	Peptide
1	A	982	LYS	Peptide
2	B	2127	ALA	Peptide
3	C	3113[A]	ASP	Mainchain
3	C	3113[B]	ASP	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13318	0	12755	440	1
1	D	13318	0	12755	458	0
1	G	13318	0	12754	478	0
1	J	13318	0	12755	484	0
1	M	13318	0	12755	427	0
1	P	13318	0	12755	438	0
1	S	13318	0	12755	437	0
1	V	13318	0	12755	434	0
1	Y	13318	0	12744	397	0
1	b	13318	0	12754	0	1
2	B	6704	0	6445	197	0
2	E	6704	0	6445	232	0
2	H	6704	0	6445	230	0
2	K	6704	0	6445	209	0
2	N	6704	0	6445	192	0
2	Q	6704	0	6445	207	0
2	T	6704	0	6445	214	0
2	W	6704	0	6445	214	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	6704	0	6444	181	0
2	c	6704	0	6445	0	0
3	C	5912	0	5607	2272	0
3	F	5912	0	5599	1400	0
3	I	5912	0	5601	2391	0
3	L	5912	0	5604	2283	0
3	O	5912	0	5604	1994	0
3	R	5912	0	5597	2373	0
3	U	5912	0	5612	1410	0
3	X	5912	0	5598	1993	0
3	a	5912	0	5594	0	0
3	d	5912	0	5607	0	0
4	1	28	0	25	1	0
4	2	28	0	25	1	0
4	4	28	0	25	0	0
4	6	28	0	25	1	0
4	7	28	0	25	6	0
4	8	28	0	25	0	0
4	9	28	0	25	2	0
4	BA	28	0	25	5	0
4	HA	28	0	25	6	0
4	IA	28	0	25	0	0
4	JA	28	0	25	2	0
4	MA	28	0	25	8	0
4	OA	28	0	25	1	0
4	QA	28	0	25	0	0
4	RA	28	0	25	1	0
4	e	28	0	25	0	0
4	f	28	0	25	0	0
4	i	28	0	25	0	0
4	j	28	0	25	0	0
4	m	28	0	25	0	0
4	n	28	0	25	0	0
4	o	28	0	25	0	0
4	p	28	0	25	0	0
4	q	28	0	25	0	0
4	s	28	0	25	0	0
4	t	28	0	25	0	0
4	u	28	0	25	0	0
4	v	28	0	25	0	0
4	x	28	0	25	0	0
5	AA	50	0	43	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	FA	50	0	43	2	0
5	KA	50	0	43	1	0
5	PA	50	0	43	1	0
5	g	50	0	43	0	0
5	l	50	0	43	0	0
6	3	39	0	34	3	0
6	5	39	0	34	2	0
6	CA	39	0	34	3	0
6	DA	39	0	34	2	0
6	EA	39	0	34	1	0
6	GA	39	0	34	9	0
6	LA	39	0	34	5	0
6	NA	39	0	34	2	0
6	h	39	0	34	0	0
6	k	39	0	34	0	0
6	r	39	0	34	0	0
6	w	39	0	34	0	0
6	y	39	0	34	0	0
7	z	61	0	52	0	0
8	0	50	0	43	8	0
9	A	24	0	0	2	0
9	B	8	0	0	0	0
9	C	16	0	0	14	0
9	D	24	0	0	2	0
9	E	8	0	0	0	0
9	F	16	0	0	7	0
9	G	24	0	0	1	0
9	H	8	0	0	0	0
9	I	16	0	0	12	0
9	J	24	0	0	2	0
9	K	8	0	0	0	0
9	M	24	0	0	3	0
9	N	8	0	0	0	0
9	O	8	0	0	10	0
9	P	24	0	0	0	0
9	Q	8	0	0	0	0
9	S	24	0	0	3	0
9	T	8	0	0	1	0
9	U	8	0	0	10	0
9	V	24	0	0	2	0
9	W	8	0	0	1	0
9	X	8	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Y	24	0	0	3	0
9	Z	8	0	0	0	0
9	b	24	0	0	0	0
9	c	8	0	0	0	0
9	d	8	0	0	0	0
All	All	261470	0	249529	19298	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

The worst 5 of 19298 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3079[B]:CYS:CB	3:L:3161[B]:GLU:HG2	1.22	1.65
3:C:2982[B]:MET:SD	3:L:3156[B]:MET:HB2	1.37	1.64
3:C:2975[B]:PHE:CD1	3:L:3107[B]:LEU:HD11	1.28	1.63
3:I:3174[B]:GLY:CA	3:R:3154[B]:PRO:HB3	1.17	1.62
3:O:3153[B]:LYS:CD	3:X:3176[B]:LYS:HD3	1.31	1.60

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASN:N	1:b:887:ASP:OD1[1_455]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1654/2000 (83%)	1552 (94%)	89 (5%)	13 (1%)	19	57
1	D	1654/2000 (83%)	1541 (93%)	100 (6%)	13 (1%)	19	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	1654/2000 (83%)	1560 (94%)	78 (5%)	16 (1%)	15	53
1	J	1654/2000 (83%)	1537 (93%)	103 (6%)	14 (1%)	19	57
1	M	1654/2000 (83%)	1569 (95%)	73 (4%)	12 (1%)	22	60
1	P	1654/2000 (83%)	1562 (94%)	78 (5%)	14 (1%)	19	57
1	S	1654/2000 (83%)	1581 (96%)	64 (4%)	9 (0%)	29	68
1	V	1654/2000 (83%)	1570 (95%)	68 (4%)	16 (1%)	15	53
1	Y	1654/2000 (83%)	1580 (96%)	66 (4%)	8 (0%)	29	68
1	b	1654/2000 (83%)	1564 (95%)	80 (5%)	10 (1%)	25	64
2	B	823/920 (90%)	778 (94%)	40 (5%)	5 (1%)	25	64
2	E	823/920 (90%)	781 (95%)	34 (4%)	8 (1%)	15	53
2	H	823/920 (90%)	787 (96%)	33 (4%)	3 (0%)	34	72
2	K	823/920 (90%)	778 (94%)	37 (4%)	8 (1%)	15	53
2	N	823/920 (90%)	789 (96%)	32 (4%)	2 (0%)	47	82
2	Q	823/920 (90%)	787 (96%)	32 (4%)	4 (0%)	29	68
2	T	823/920 (90%)	794 (96%)	22 (3%)	7 (1%)	17	55
2	W	823/920 (90%)	791 (96%)	28 (3%)	4 (0%)	29	68
2	Z	823/920 (90%)	797 (97%)	23 (3%)	3 (0%)	34	72
2	c	823/920 (90%)	791 (96%)	29 (4%)	3 (0%)	34	72
3	C	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	19	57
3	F	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	19	57
3	I	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	19	57
3	L	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	19	57
3	O	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	19	57
3	R	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	19	57
3	U	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	19	57
3	X	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	19	57
3	a	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	19	57
3	d	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	19	57
All	All	31970/33140 (96%)	30149 (94%)	1589 (5%)	232 (1%)	22	60

5 of 232 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1196	ILE
1	D	695	TYR
1	D	1196	ILE
1	G	331	SER
1	G	1086	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1429/1738 (82%)	1278 (89%)	151 (11%)	6	26
1	D	1429/1738 (82%)	1267 (89%)	162 (11%)	6	24
1	G	1429/1738 (82%)	1264 (88%)	165 (12%)	5	24
1	J	1429/1738 (82%)	1266 (89%)	163 (11%)	5	24
1	M	1429/1738 (82%)	1284 (90%)	145 (10%)	7	29
1	P	1429/1738 (82%)	1264 (88%)	165 (12%)	5	24
1	S	1429/1738 (82%)	1269 (89%)	160 (11%)	6	24
1	V	1429/1738 (82%)	1270 (89%)	159 (11%)	6	25
1	Y	1429/1738 (82%)	1261 (88%)	168 (12%)	5	22
1	b	1429/1738 (82%)	1277 (89%)	152 (11%)	6	26
2	B	731/814 (90%)	666 (91%)	65 (9%)	9	35
2	E	731/814 (90%)	655 (90%)	76 (10%)	7	27
2	H	731/814 (90%)	634 (87%)	97 (13%)	4	17
2	K	731/814 (90%)	656 (90%)	75 (10%)	7	28
2	N	731/814 (90%)	652 (89%)	79 (11%)	6	26
2	Q	731/814 (90%)	654 (90%)	77 (10%)	7	27
2	T	731/814 (90%)	660 (90%)	71 (10%)	8	31
2	W	731/814 (90%)	659 (90%)	72 (10%)	8	30
2	Z	731/814 (90%)	655 (90%)	76 (10%)	7	27
2	c	731/814 (90%)	652 (89%)	79 (11%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	F	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	I	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	L	636/343 (185%)	430 (68%)	206 (32%)	0	1
3	O	636/343 (185%)	430 (68%)	206 (32%)	0	1
3	R	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	U	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	X	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	a	636/343 (185%)	432 (68%)	204 (32%)	0	1
3	d	636/343 (185%)	432 (68%)	204 (32%)	0	1
All	All	27960/28950 (97%)	23559 (84%)	4401 (16%)	3	13

5 of 4401 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Z	2260	GLU
3	a	3024[A]	LEU
2	Z	2233	GLU
2	c	2595	TRP
2	K	2873	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 300 such sidechains are listed below:

Mol	Chain	Res	Type
2	W	2741	GLN
2	c	2146	HIS
1	Y	679	ASN
2	Z	2134	ASN
1	J	161	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

130 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	$\#\|Z\| > 2$
8	NAG	0	1	8,1	14,14,15	0.72	1 (7%)	17,19,21	1.49	2 (11%)
8	NAG	0	2	8	14,14,15	0.52	0	17,19,21	1.50	4 (23%)
8	BMA	0	3	8	11,11,12	0.22	0	15,15,17	1.90	4 (26%)
8	MAN	0	4	8	11,11,12	0.32	0	15,15,17	0.89	1 (6%)
4	NAG	1	1	1,4	14,14,15	0.44	0	17,19,21	1.03	1 (5%)
4	NAG	1	2	4	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
4	NAG	2	1	2,4	14,14,15	1.05	1 (7%)	17,19,21	1.42	2 (11%)
4	NAG	2	2	4	14,14,15	0.31	0	17,19,21	0.73	0
6	NAG	3	1	1,6	14,14,15	0.96	1 (7%)	17,19,21	1.45	2 (11%)
6	NAG	3	2	6	14,14,15	0.40	0	17,19,21	0.77	0
6	BMA	3	3	6	11,11,12	0.26	0	15,15,17	0.62	0
4	NAG	4	1	1,4	14,14,15	0.72	1 (7%)	17,19,21	1.24	2 (11%)
4	NAG	4	2	4	14,14,15	0.41	0	17,19,21	1.19	2 (11%)
6	NAG	5	1	1,6	14,14,15	0.71	0	17,19,21	1.26	1 (5%)
6	NAG	5	2	6	14,14,15	0.31	0	17,19,21	1.00	1 (5%)
6	BMA	5	3	6	11,11,12	0.28	0	15,15,17	1.31	2 (13%)
4	NAG	6	1	1,4	14,14,15	0.90	1 (7%)	17,19,21	1.93	2 (11%)
4	NAG	6	2	4	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
4	NAG	7	1	2,4	14,14,15	0.81	1 (7%)	17,19,21	1.49	2 (11%)
4	NAG	7	2	4	14,14,15	0.43	0	17,19,21	1.07	2 (11%)
4	NAG	8	1	1,4	14,14,15	0.94	1 (7%)	17,19,21	1.85	2 (11%)
4	NAG	8	2	4	14,14,15	0.38	0	17,19,21	0.69	1 (5%)
4	NAG	9	1	1,4	14,14,15	0.89	1 (7%)	17,19,21	1.51	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	9	2	4	14,14,15	0.27	0	17,19,21	0.78	1 (5%)
5	NAG	AA	1	5,1	14,14,15	0.66	0	17,19,21	1.16	3 (17%)
5	NAG	AA	2	5	14,14,15	0.42	0	17,19,21	0.88	1 (5%)
5	BMA	AA	3	5	11,11,12	0.29	0	15,15,17	1.93	3 (20%)
5	MAN	AA	4	5	11,11,12	0.24	0	15,15,17	0.53	0
4	NAG	BA	1	1,4	14,14,15	0.71	0	17,19,21	1.37	3 (17%)
4	NAG	BA	2	4	14,14,15	0.57	0	17,19,21	1.10	1 (5%)
6	NAG	CA	1	2,6	14,14,15	1.04	1 (7%)	17,19,21	1.54	1 (5%)
6	NAG	CA	2	6	14,14,15	0.33	0	17,19,21	0.94	1 (5%)
6	BMA	CA	3	6	11,11,12	0.22	0	15,15,17	0.68	0
6	NAG	DA	1	1,6	14,14,15	0.76	1 (7%)	17,19,21	1.17	1 (5%)
6	NAG	DA	2	6	14,14,15	0.31	0	17,19,21	1.22	2 (11%)
6	BMA	DA	3	6	11,11,12	0.25	0	15,15,17	1.01	1 (6%)
6	NAG	EA	1	1,6	14,14,15	0.79	1 (7%)	17,19,21	1.35	2 (11%)
6	NAG	EA	2	6	14,14,15	0.37	0	17,19,21	2.26	4 (23%)
6	BMA	EA	3	6	11,11,12	0.23	0	15,15,17	0.78	0
5	NAG	FA	1	5,1	14,14,15	0.78	1 (7%)	17,19,21	1.36	2 (11%)
5	NAG	FA	2	5	14,14,15	0.48	0	17,19,21	0.90	1 (5%)
5	BMA	FA	3	5	11,11,12	0.61	0	15,15,17	1.41	2 (13%)
5	MAN	FA	4	5	11,11,12	0.21	0	15,15,17	1.29	2 (13%)
6	NAG	GA	1	1,6	14,14,15	0.71	0	17,19,21	1.32	1 (5%)
6	NAG	GA	2	6	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
6	BMA	GA	3	6	11,11,12	0.31	0	15,15,17	1.09	2 (13%)
4	NAG	HA	1	2,4	14,14,15	0.68	0	17,19,21	1.23	2 (11%)
4	NAG	HA	2	4	14,14,15	0.30	0	17,19,21	0.61	0
4	NAG	IA	1	1,4	14,14,15	0.80	1 (7%)	17,19,21	1.50	2 (11%)
4	NAG	IA	2	4	14,14,15	0.54	0	17,19,21	0.92	1 (5%)
4	NAG	JA	1	1,4	14,14,15	0.82	1 (7%)	17,19,21	1.23	1 (5%)
4	NAG	JA	2	4	14,14,15	0.35	0	17,19,21	0.75	0
5	NAG	KA	1	5,1	14,14,15	0.72	0	17,19,21	1.86	5 (29%)
5	NAG	KA	2	5	14,14,15	0.37	0	17,19,21	1.30	2 (11%)
5	BMA	KA	3	5	11,11,12	0.29	0	15,15,17	1.45	1 (6%)
5	MAN	KA	4	5	11,11,12	0.42	0	15,15,17	1.92	3 (20%)
6	NAG	LA	1	1,6	14,14,15	0.98	1 (7%)	17,19,21	2.35	4 (23%)
6	NAG	LA	2	6	14,14,15	0.46	0	17,19,21	1.16	2 (11%)
6	BMA	LA	3	6	11,11,12	0.22	0	15,15,17	0.79	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
4	NAG	MA	1	2,4	14,14,15	0.99	1 (7%)	17,19,21	2.38	3 (17%)
4	NAG	MA	2	4	14,14,15	0.32	0	17,19,21	1.69	3 (17%)
6	NAG	NA	1	1,6	14,14,15	0.72	1 (7%)	17,19,21	1.02	1 (5%)
6	NAG	NA	2	6	14,14,15	0.37	0	17,19,21	0.84	0
6	BMA	NA	3	6	11,11,12	0.25	0	15,15,17	0.95	1 (6%)
4	NAG	OA	1	1,4	14,14,15	1.17	1 (7%)	17,19,21	1.59	2 (11%)
4	NAG	OA	2	4	14,14,15	0.55	0	17,19,21	0.98	1 (5%)
5	NAG	PA	1	5,1	14,14,15	0.66	0	17,19,21	1.13	1 (5%)
5	NAG	PA	2	5	14,14,15	0.37	0	17,19,21	0.98	1 (5%)
5	BMA	PA	3	5	11,11,12	0.61	0	15,15,17	2.27	4 (26%)
5	MAN	PA	4	5	11,11,12	0.27	0	15,15,17	0.90	1 (6%)
4	NAG	QA	1	1,4	14,14,15	0.57	0	17,19,21	2.49	5 (29%)
4	NAG	QA	2	4	14,14,15	0.24	0	17,19,21	0.69	0
4	NAG	RA	1	2,4	14,14,15	1.13	1 (7%)	17,19,21	2.16	4 (23%)
4	NAG	RA	2	4	14,14,15	0.45	0	17,19,21	0.72	0
4	NAG	e	1	1,4	14,14,15	0.60	0	17,19,21	1.67	4 (23%)
4	NAG	e	2	4	14,14,15	0.34	0	17,19,21	0.52	0
4	NAG	f	1	1,4	14,14,15	0.90	1 (7%)	17,19,21	1.42	2 (11%)
4	NAG	f	2	4	14,14,15	0.24	0	17,19,21	1.01	1 (5%)
5	NAG	g	1	5,1	14,14,15	0.60	0	17,19,21	1.51	2 (11%)
5	NAG	g	2	5	14,14,15	0.50	0	17,19,21	1.05	0
5	BMA	g	3	5	11,11,12	0.49	0	15,15,17	2.19	4 (26%)
5	MAN	g	4	5	11,11,12	0.24	0	15,15,17	0.73	0
6	NAG	h	1	1,6	14,14,15	0.62	0	17,19,21	1.14	2 (11%)
6	NAG	h	2	6	14,14,15	0.57	0	17,19,21	1.09	1 (5%)
6	BMA	h	3	6	11,11,12	0.26	0	15,15,17	1.15	2 (13%)
4	NAG	i	1	2,4	14,14,15	1.06	1 (7%)	17,19,21	1.23	2 (11%)
4	NAG	i	2	4	14,14,15	0.42	0	17,19,21	0.86	0
4	NAG	j	1	1,4	14,14,15	1.00	1 (7%)	17,19,21	1.65	2 (11%)
4	NAG	j	2	4	14,14,15	0.49	0	17,19,21	1.36	3 (17%)
6	NAG	k	1	1,6	14,14,15	0.78	1 (7%)	17,19,21	1.10	1 (5%)
6	NAG	k	2	6	14,14,15	0.27	0	17,19,21	0.66	1 (5%)
6	BMA	k	3	6	11,11,12	0.25	0	15,15,17	0.53	0
5	NAG	l	1	5,1	14,14,15	0.69	0	17,19,21	1.21	1 (5%)
5	NAG	l	2	5	14,14,15	0.27	0	17,19,21	0.61	0
5	BMA	l	3	5	11,11,12	0.27	0	15,15,17	0.83	0
5	MAN	l	4	5	11,11,12	0.27	0	15,15,17	0.99	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	m	1	1,4	14,14,15	0.40	0	17,19,21	0.97	1 (5%)
4	NAG	m	2	4	14,14,15	0.36	0	17,19,21	0.91	1 (5%)
4	NAG	n	1	2,4	14,14,15	0.53	0	17,19,21	1.57	3 (17%)
4	NAG	n	2	4	14,14,15	0.38	0	17,19,21	0.99	1 (5%)
4	NAG	o	1	1,4	14,14,15	0.58	0	17,19,21	1.00	1 (5%)
4	NAG	o	2	4	14,14,15	0.43	0	17,19,21	1.13	2 (11%)
4	NAG	p	1	4	14,14,15	0.89	1 (7%)	17,19,21	1.94	4 (23%)
4	NAG	p	2	4	14,14,15	0.30	0	17,19,21	0.67	0
4	NAG	q	1	1,4	14,14,15	0.56	0	17,19,21	1.18	2 (11%)
4	NAG	q	2	4	14,14,15	0.51	0	17,19,21	0.87	1 (5%)
6	NAG	r	1	1,6	14,14,15	0.69	0	17,19,21	1.73	4 (23%)
6	NAG	r	2	6	14,14,15	0.58	0	17,19,21	1.02	0
6	BMA	r	3	6	11,11,12	0.23	0	15,15,17	0.63	0
4	NAG	s	1	2,4	14,14,15	0.80	1 (7%)	17,19,21	1.22	2 (11%)
4	NAG	s	2	4	14,14,15	0.34	0	17,19,21	0.77	0
4	NAG	t	1	1,4	14,14,15	0.64	0	17,19,21	1.50	3 (17%)
4	NAG	t	2	4	14,14,15	0.31	0	17,19,21	0.54	0
4	NAG	u	1	1,4	14,14,15	0.83	1 (7%)	17,19,21	1.64	3 (17%)
4	NAG	u	2	4	14,14,15	0.32	0	17,19,21	0.85	1 (5%)
4	NAG	v	1	1,4	14,14,15	0.58	0	17,19,21	1.11	1 (5%)
4	NAG	v	2	4	14,14,15	0.36	0	17,19,21	0.93	1 (5%)
6	NAG	w	1	1,6	14,14,15	0.71	1 (7%)	17,19,21	1.90	4 (23%)
6	NAG	w	2	6	14,14,15	0.42	0	17,19,21	1.17	1 (5%)
6	BMA	w	3	6	11,11,12	0.30	0	15,15,17	0.84	1 (6%)
4	NAG	x	1	2,4	14,14,15	0.50	0	17,19,21	0.91	0
4	NAG	x	2	4	14,14,15	0.48	0	17,19,21	1.03	1 (5%)
6	NAG	y	1	1,6	14,14,15	0.86	1 (7%)	17,19,21	1.18	1 (5%)
6	NAG	y	2	6	14,14,15	0.35	0	17,19,21	1.92	4 (23%)
6	BMA	y	3	6	11,11,12	0.22	0	15,15,17	1.24	2 (13%)
7	NAG	z	1	1,7	14,14,15	1.07	1 (7%)	17,19,21	2.10	3 (17%)
7	NAG	z	2	7	14,14,15	0.58	0	17,19,21	1.58	3 (17%)
7	BMA	z	3	7	11,11,12	0.45	0	15,15,17	2.58	5 (33%)
7	MAN	z	4	7	11,11,12	0.42	0	15,15,17	1.98	4 (26%)
7	MAN	z	5	7	11,11,12	0.22	0	15,15,17	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	0	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	0	2	8	-	2/6/23/26	0/1/1/1
8	BMA	0	3	8	-	0/2/19/22	0/1/1/1
8	MAN	0	4	8	-	0/2/19/22	0/1/1/1
4	NAG	1	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	1	2	4	-	0/6/23/26	0/1/1/1
4	NAG	2	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	2	2	4	-	0/6/23/26	0/1/1/1
6	NAG	3	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	3	2	6	-	0/6/23/26	0/1/1/1
6	BMA	3	3	6	-	2/2/19/22	0/1/1/1
4	NAG	4	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	4	2	4	-	4/6/23/26	0/1/1/1
6	NAG	5	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	5	2	6	-	2/6/23/26	0/1/1/1
6	BMA	5	3	6	-	2/2/19/22	0/1/1/1
4	NAG	6	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	6	2	4	-	0/6/23/26	0/1/1/1
4	NAG	7	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	7	2	4	-	4/6/23/26	0/1/1/1
4	NAG	8	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	8	2	4	-	0/6/23/26	0/1/1/1
4	NAG	9	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	9	2	4	-	0/6/23/26	0/1/1/1
5	NAG	AA	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	AA	2	5	-	4/6/23/26	0/1/1/1
5	BMA	AA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	AA	4	5	-	0/2/19/22	0/1/1/1
4	NAG	BA	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	BA	2	4	-	4/6/23/26	0/1/1/1
6	NAG	CA	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	CA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	CA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	DA	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	DA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	DA	3	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	EA	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	EA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	EA	3	6	-	0/2/19/22	0/1/1/1
5	NAG	FA	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	FA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	FA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	FA	4	5	-	0/2/19/22	0/1/1/1
6	NAG	GA	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	GA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	GA	3	6	-	0/2/19/22	0/1/1/1
4	NAG	HA	1	2,4	-	6/6/23/26	0/1/1/1
4	NAG	HA	2	4	-	0/6/23/26	0/1/1/1
4	NAG	IA	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	IA	2	4	-	4/6/23/26	0/1/1/1
4	NAG	JA	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	JA	2	4	-	4/6/23/26	0/1/1/1
5	NAG	KA	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	KA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	KA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	KA	4	5	-	0/2/19/22	0/1/1/1
6	NAG	LA	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	LA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	LA	3	6	-	0/2/19/22	0/1/1/1
4	NAG	MA	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	MA	2	4	-	1/6/23/26	0/1/1/1
6	NAG	NA	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	NA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	NA	3	6	-	0/2/19/22	0/1/1/1
4	NAG	OA	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	OA	2	4	-	3/6/23/26	0/1/1/1
5	NAG	PA	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	PA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	PA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	PA	4	5	-	0/2/19/22	0/1/1/1
4	NAG	QA	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	QA	2	4	-	0/6/23/26	0/1/1/1
4	NAG	RA	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	RA	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	e	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
4	NAG	f	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	f	2	4	-	0/6/23/26	0/1/1/1
5	NAG	g	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	g	2	5	-	3/6/23/26	0/1/1/1
5	BMA	g	3	5	-	2/2/19/22	0/1/1/1
5	MAN	g	4	5	-	0/2/19/22	0/1/1/1
6	NAG	h	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	h	2	6	-	0/6/23/26	0/1/1/1
6	BMA	h	3	6	-	0/2/19/22	0/1/1/1
4	NAG	i	1	2,4	-	6/6/23/26	0/1/1/1
4	NAG	i	2	4	-	0/6/23/26	0/1/1/1
4	NAG	j	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	j	2	4	-	6/6/23/26	0/1/1/1
6	NAG	k	1	1,6	-	6/6/23/26	0/1/1/1
6	NAG	k	2	6	-	0/6/23/26	0/1/1/1
6	BMA	k	3	6	-	0/2/19/22	0/1/1/1
5	NAG	l	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	l	2	5	-	0/6/23/26	0/1/1/1
5	BMA	l	3	5	-	0/2/19/22	0/1/1/1
5	MAN	l	4	5	-	0/2/19/22	0/1/1/1
4	NAG	m	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	m	2	4	-	6/6/23/26	0/1/1/1
4	NAG	n	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	n	2	4	-	0/6/23/26	0/1/1/1
4	NAG	o	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	o	2	4	-	1/6/23/26	0/1/1/1
4	NAG	p	1	4	-	2/6/23/26	0/1/1/1
4	NAG	p	2	4	-	0/6/23/26	0/1/1/1
4	NAG	q	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	q	2	4	-	4/6/23/26	0/1/1/1
6	NAG	r	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	r	2	6	-	4/6/23/26	0/1/1/1
6	BMA	r	3	6	-	0/2/19/22	0/1/1/1
4	NAG	s	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	s	2	4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	t	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	t	2	4	-	0/6/23/26	0/1/1/1
4	NAG	u	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	u	2	4	-	0/6/23/26	0/1/1/1
4	NAG	v	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	v	2	4	-	2/6/23/26	0/1/1/1
6	NAG	w	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	w	2	6	-	0/6/23/26	0/1/1/1
6	BMA	w	3	6	-	0/2/19/22	0/1/1/1
4	NAG	x	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	x	2	4	-	0/6/23/26	0/1/1/1
6	NAG	y	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	y	2	6	-	0/6/23/26	0/1/1/1
6	BMA	y	3	6	-	0/2/19/22	0/1/1/1
7	NAG	z	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	z	2	7	-	0/6/23/26	0/1/1/1
7	BMA	z	3	7	-	2/2/19/22	0/1/1/1
7	MAN	z	4	7	-	1/2/19/22	0/1/1/1
7	MAN	z	5	7	-	1/2/19/22	0/1/1/1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	OA	1	NAG	C1-C2	4.08	1.58	1.52
4	2	1	NAG	C1-C2	3.75	1.57	1.52
4	i	1	NAG	C1-C2	3.72	1.57	1.52
4	RA	1	NAG	C1-C2	3.70	1.57	1.52
7	z	1	NAG	C1-C2	3.65	1.57	1.52

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	LA	1	NAG	C1-O5-C5	8.01	123.04	112.19
4	MA	1	NAG	C1-O5-C5	7.93	122.94	112.19
4	RA	1	NAG	C1-O5-C5	7.38	122.19	112.19
4	QA	1	NAG	C2-N2-C7	-7.33	112.46	122.90
7	z	1	NAG	C1-O5-C5	7.09	121.79	112.19

There are no chirality outliers.

5 of 240 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	e	1	NAG	C8-C7-N2-C2
4	e	1	NAG	O7-C7-N2-C2
4	j	1	NAG	C3-C2-N2-C7
4	j	1	NAG	C8-C7-N2-C2
4	j	1	NAG	O7-C7-N2-C2

There are no ring outliers.

48 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	DA	2	NAG	2	0
5	FA	2	NAG	1	0
4	9	2	NAG	1	0
4	9	1	NAG	2	0
4	OA	1	NAG	1	0
6	5	2	NAG	2	0
6	LA	3	BMA	1	0
4	HA	2	NAG	2	0
6	LA	1	NAG	3	0
4	HA	1	NAG	4	0
4	1	1	NAG	1	0
4	MA	2	NAG	5	0
4	BA	1	NAG	3	0
6	3	1	NAG	3	0
6	NA	2	NAG	2	0
8	0	1	NAG	6	0
8	0	3	BMA	1	0
5	PA	2	NAG	1	0
8	0	2	NAG	8	0
5	KA	1	NAG	1	0
5	FA	1	NAG	1	0
6	GA	1	NAG	7	0
6	5	1	NAG	1	0
4	6	1	NAG	1	0
5	FA	3	BMA	1	0
4	RA	1	NAG	1	0
6	3	2	NAG	1	0
6	DA	1	NAG	2	0
6	NA	1	NAG	2	0
5	FA	4	MAN	1	0
6	CA	2	NAG	3	0
4	BA	2	NAG	3	0
6	LA	2	NAG	5	0

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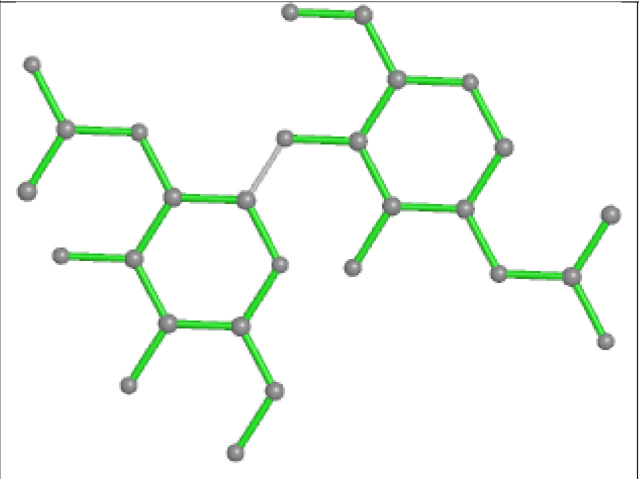
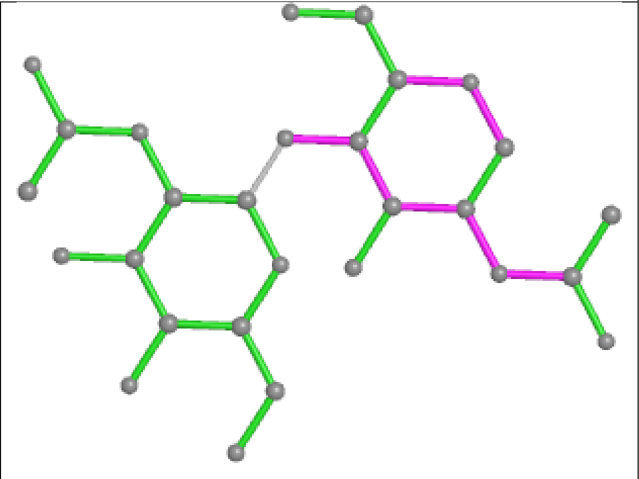
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	PA	1	NAG	1	0
4	MA	1	NAG	6	0
4	7	2	NAG	6	0
4	JA	2	NAG	1	0
6	5	3	BMA	1	0
6	GA	2	NAG	9	0
4	OA	2	NAG	1	0
4	RA	2	NAG	1	0
6	EA	1	NAG	1	0
6	CA	1	NAG	2	0
6	GA	3	BMA	2	0
5	AA	1	NAG	1	0
4	JA	1	NAG	2	0
4	2	1	NAG	1	0
4	7	1	NAG	6	0

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

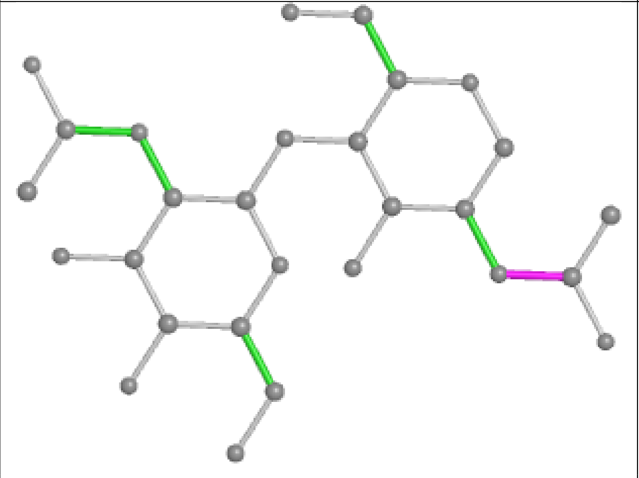
Oligosaccharide Chain e



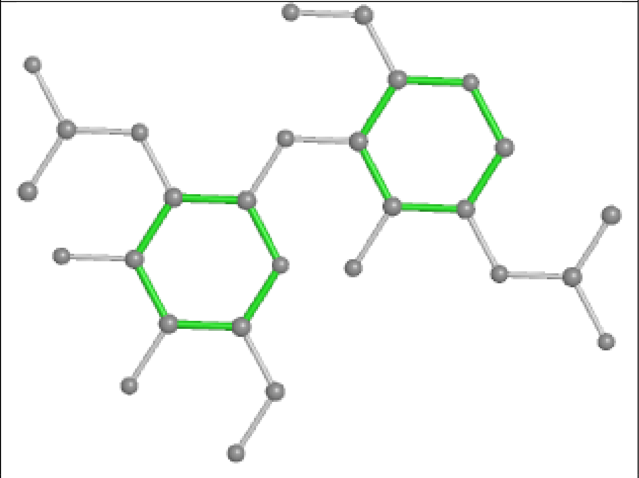
Bond lengths



Bond angles

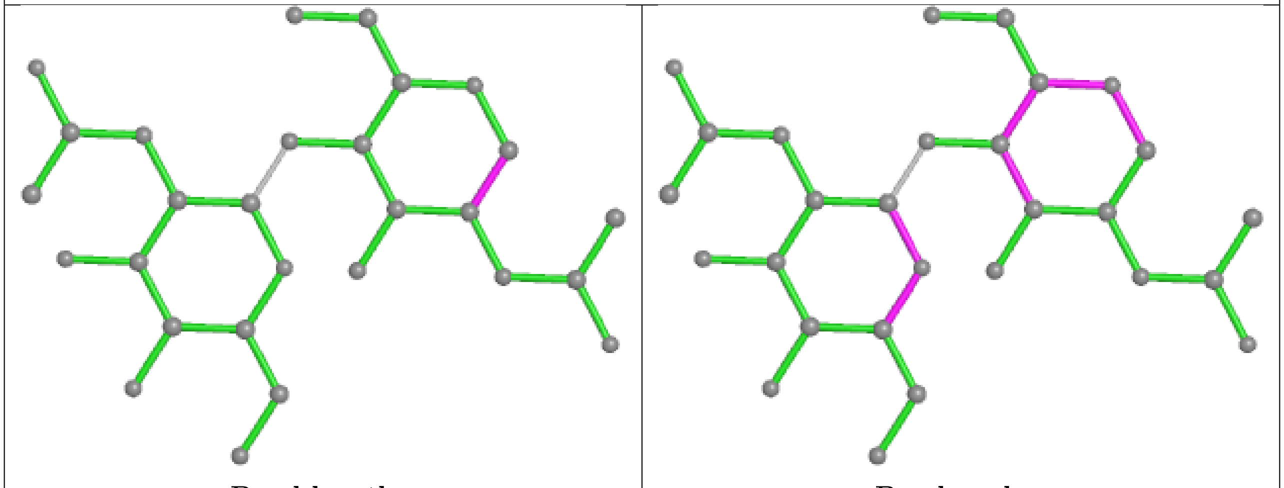


Torsions

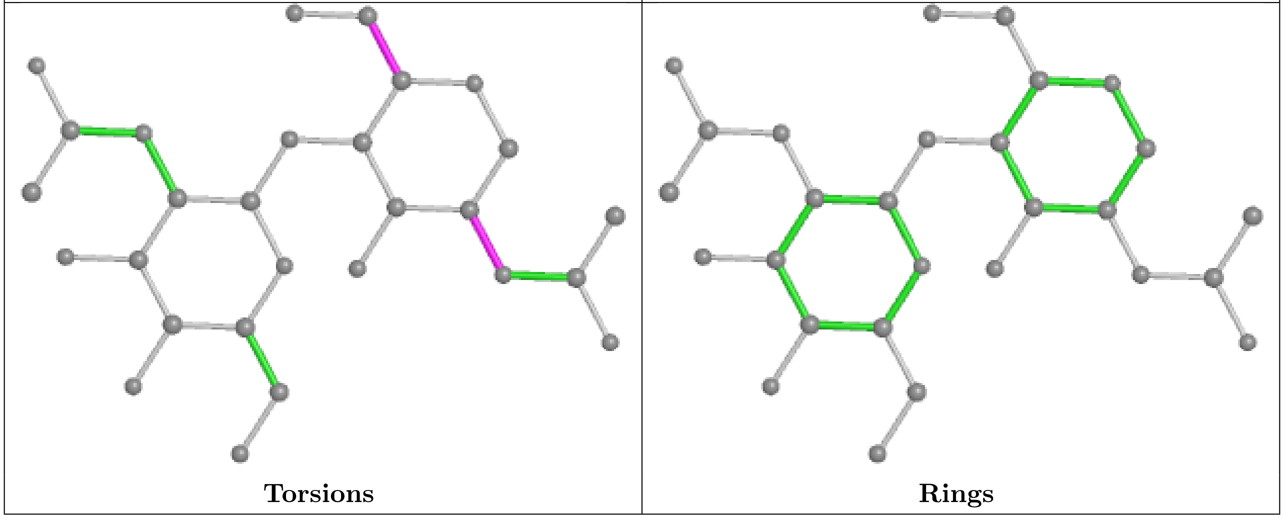


Rings

Oligosaccharide Chain f

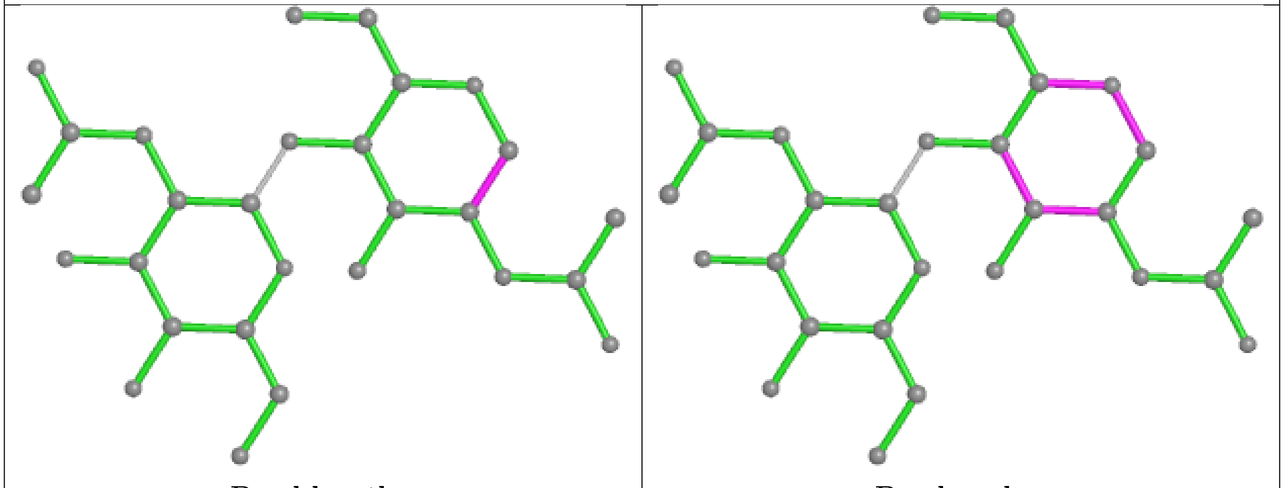


Bond lengths **Bond angles**

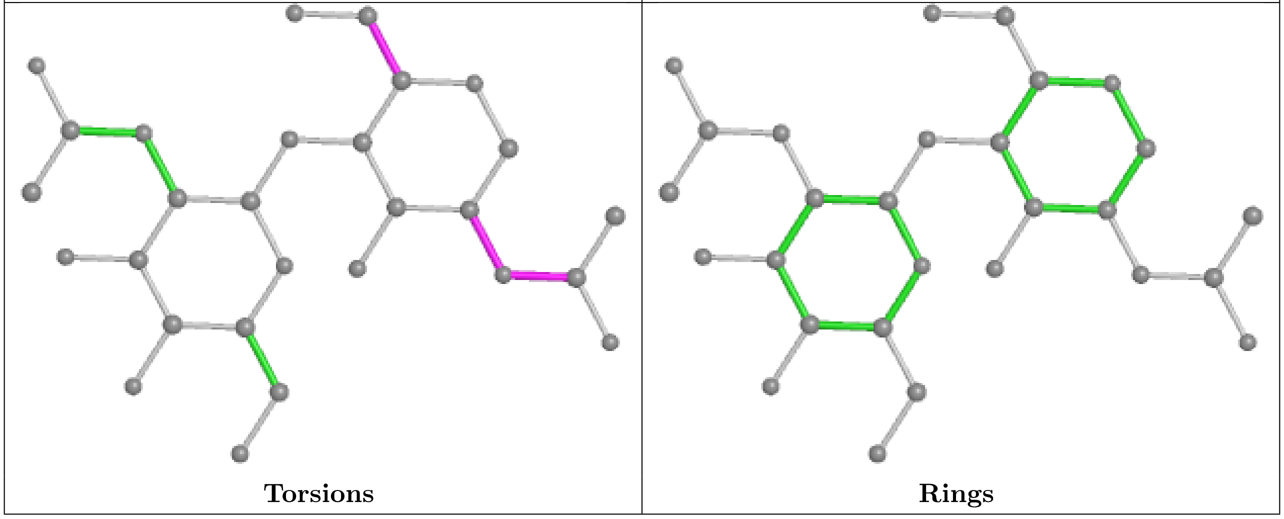


Torsions **Rings**

Oligosaccharide Chain i

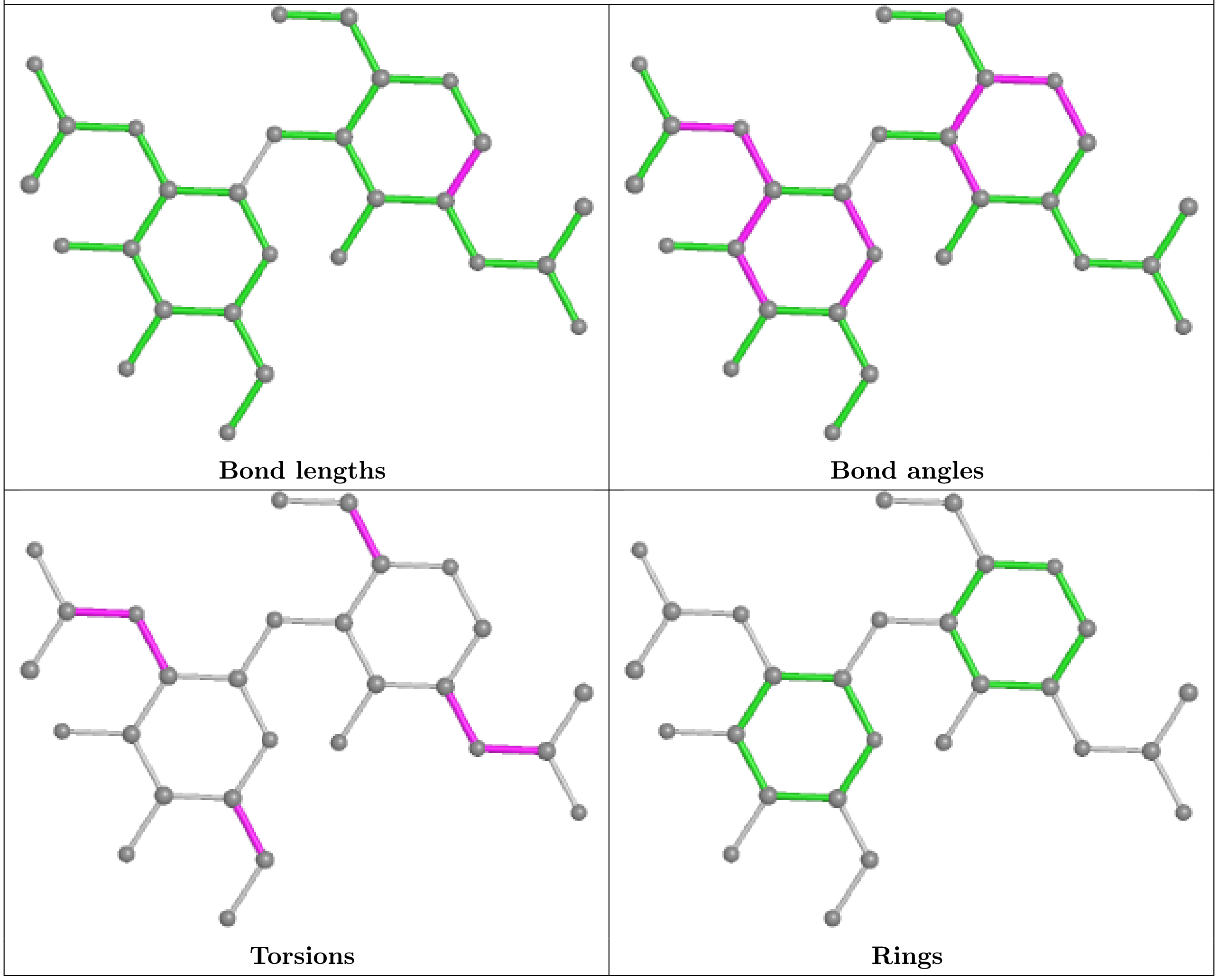


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain j



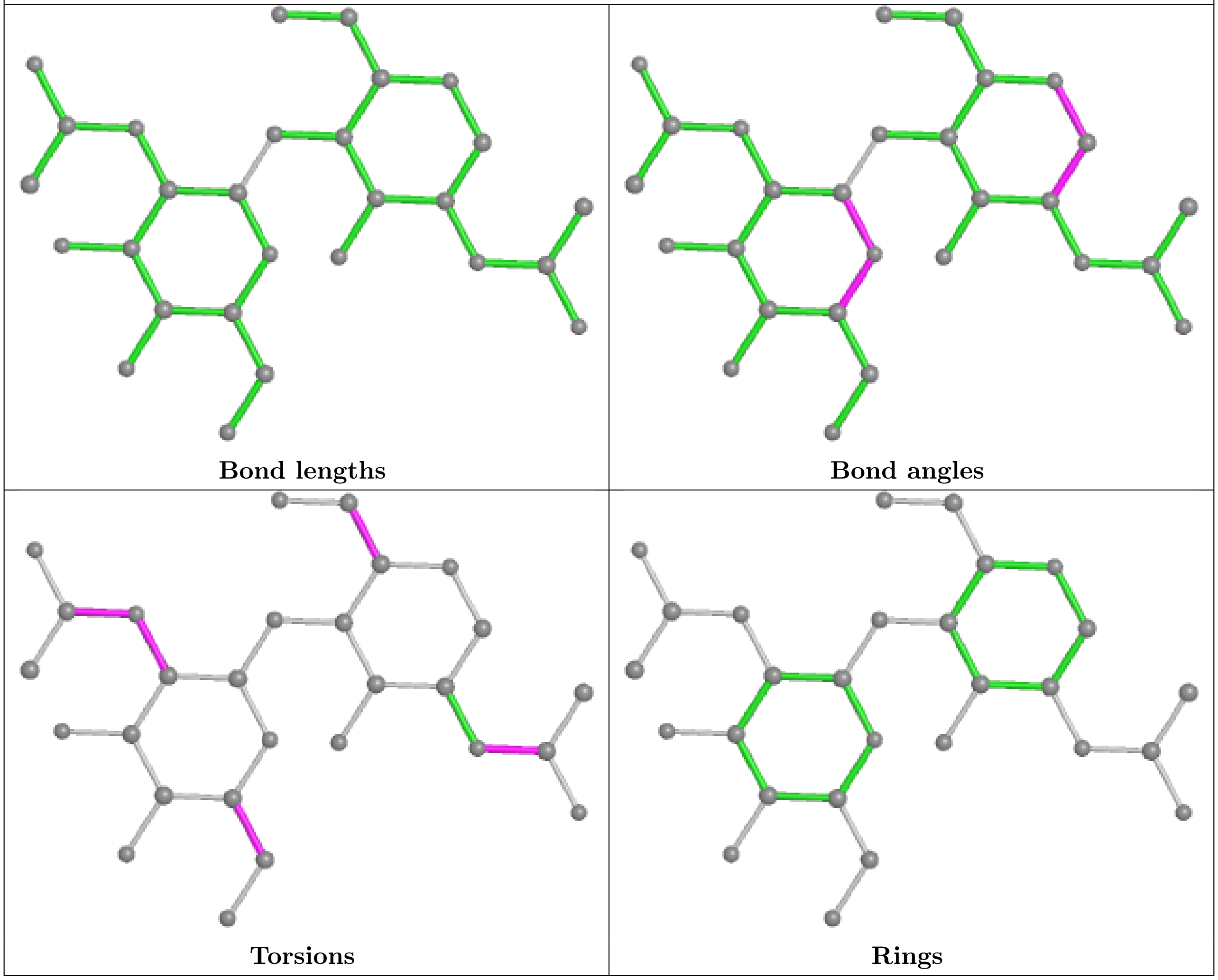
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain m



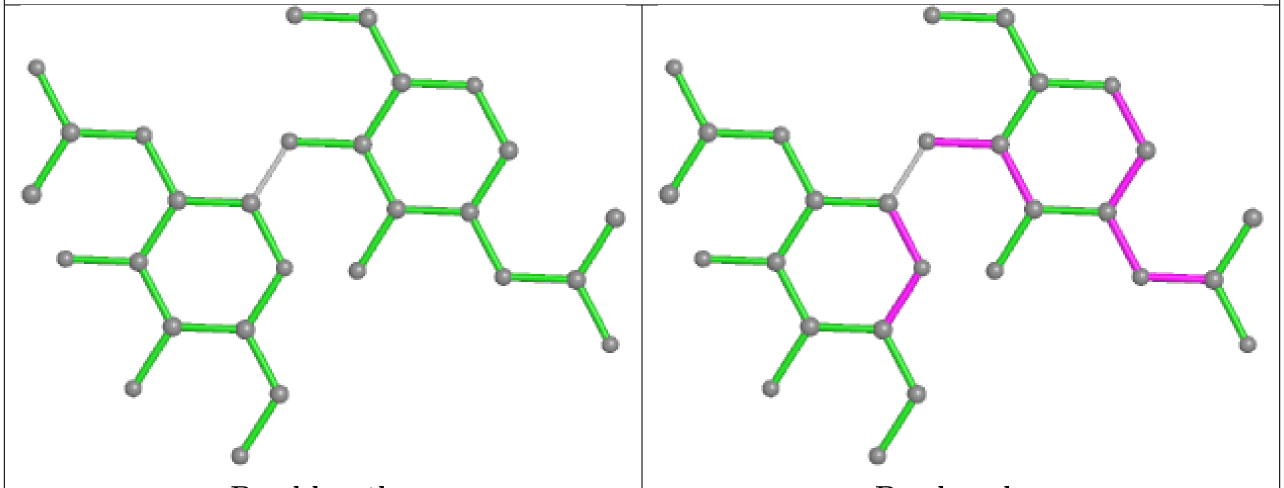
Bond lengths

Bond angles

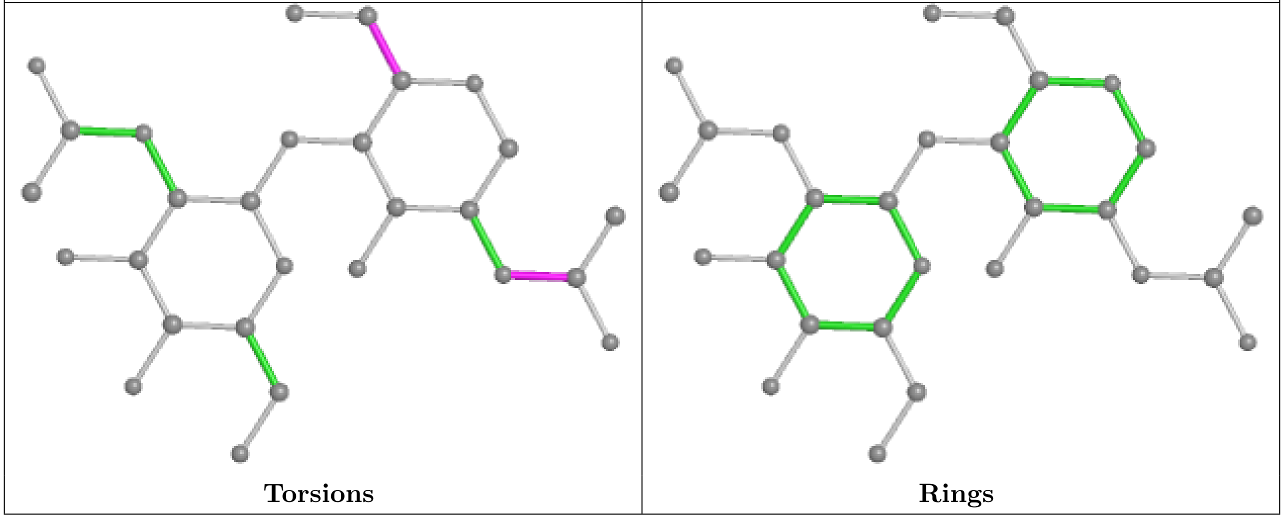
Torsions

Rings

Oligosaccharide Chain n

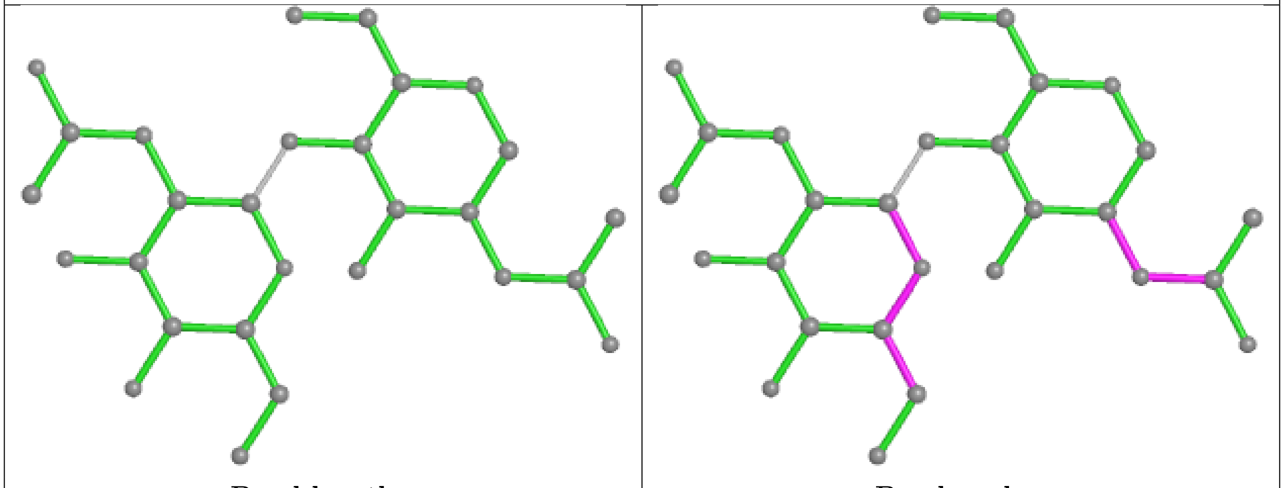


Bond lengths **Bond angles**

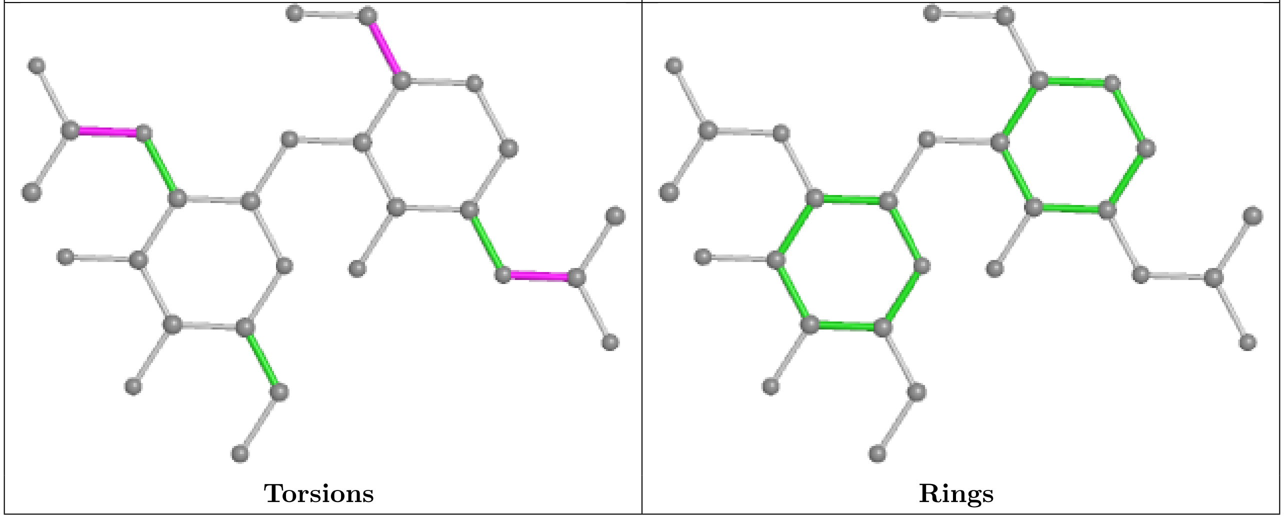


Torsions **Rings**

Oligosaccharide Chain o

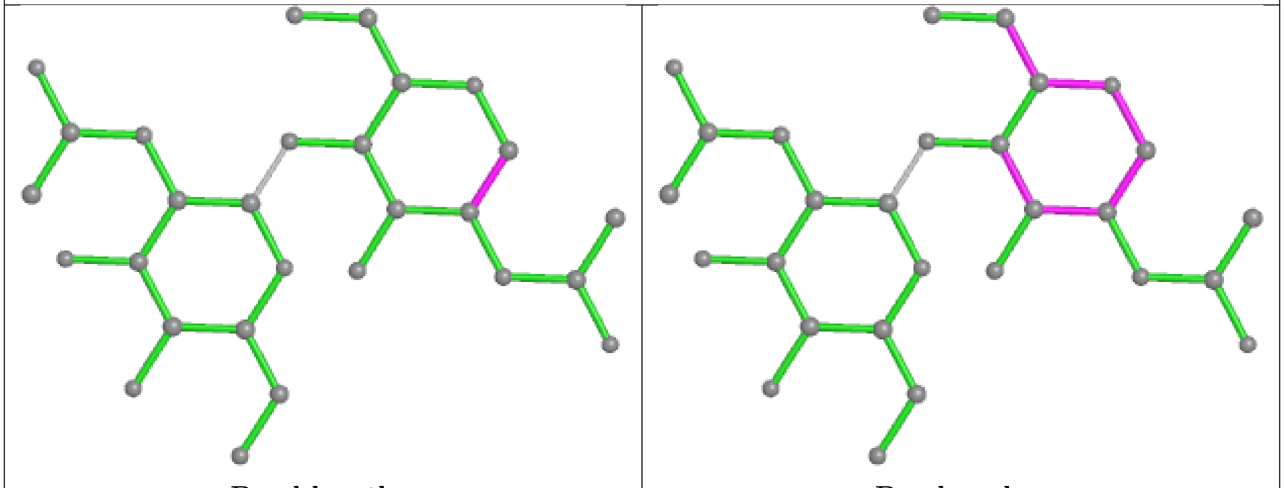


Bond lengths **Bond angles**



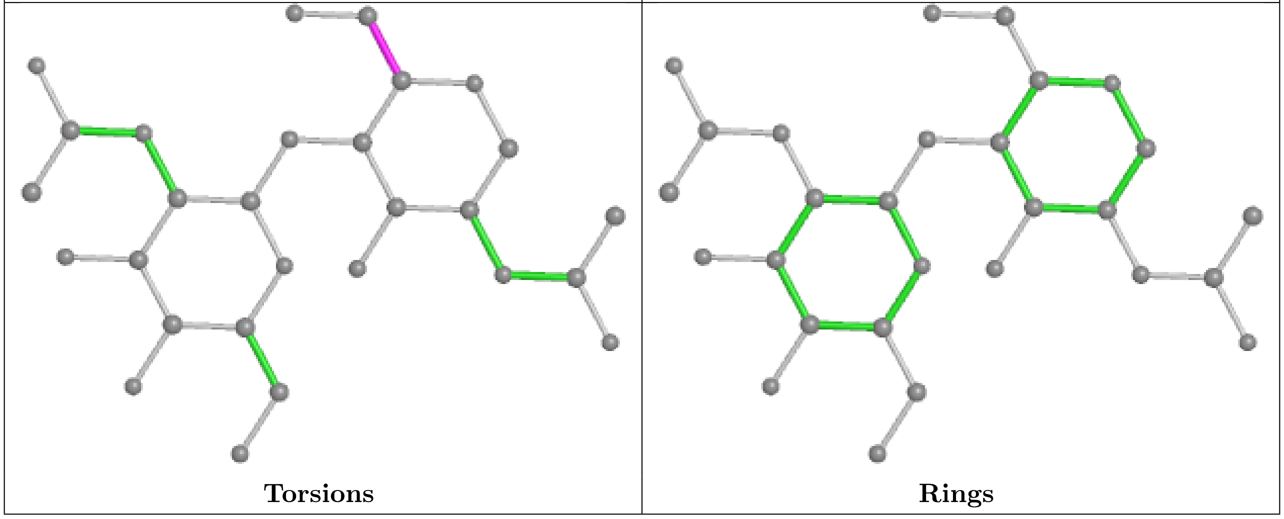
Torsions **Rings**

Oligosaccharide Chain p



Bond lengths

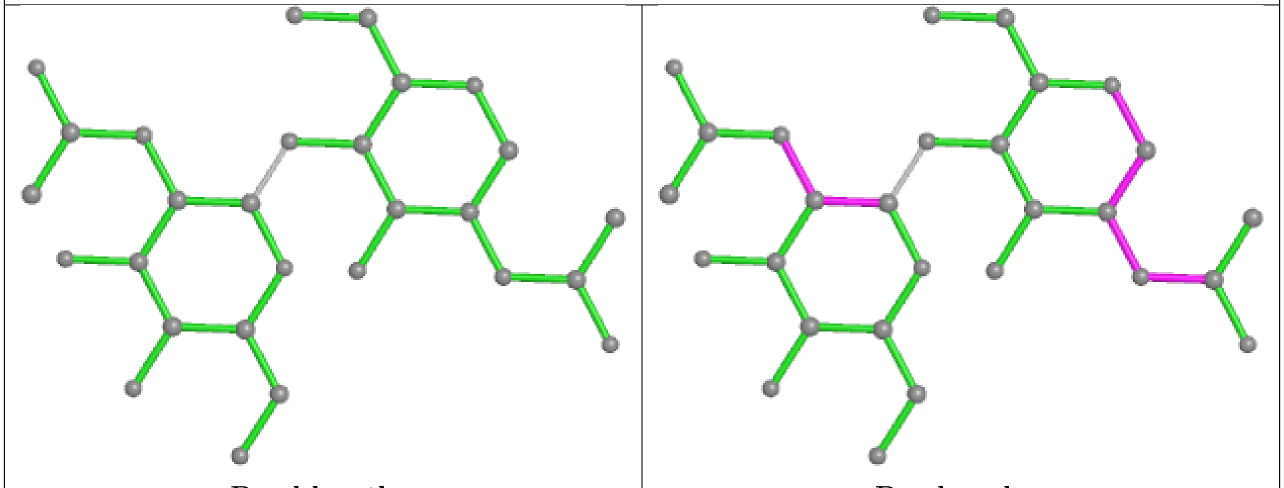
Bond angles



Torsions

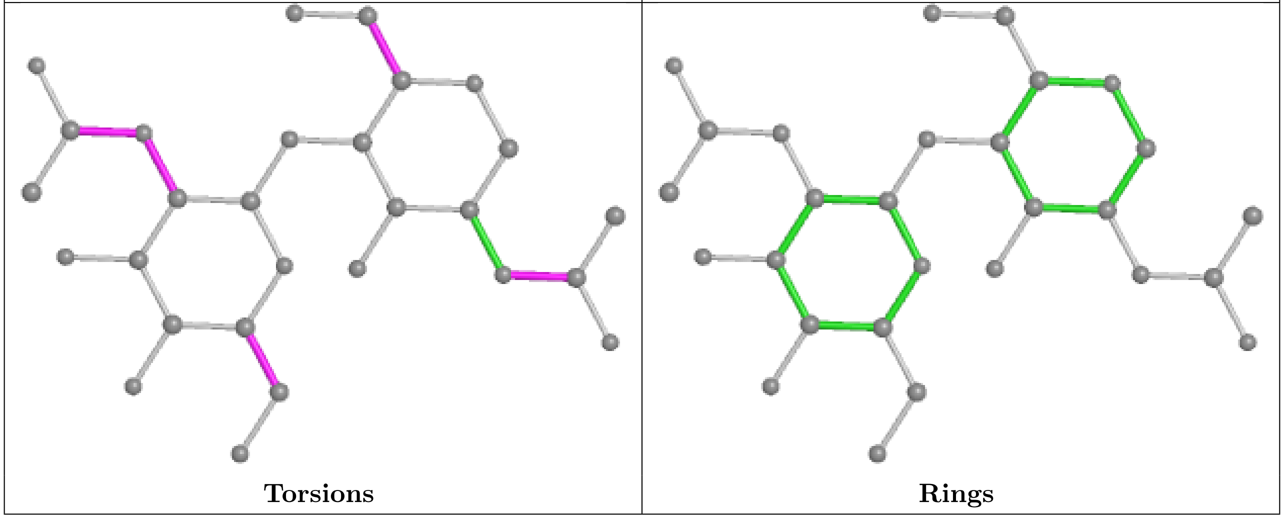
Rings

Oligosaccharide Chain q



Bond lengths

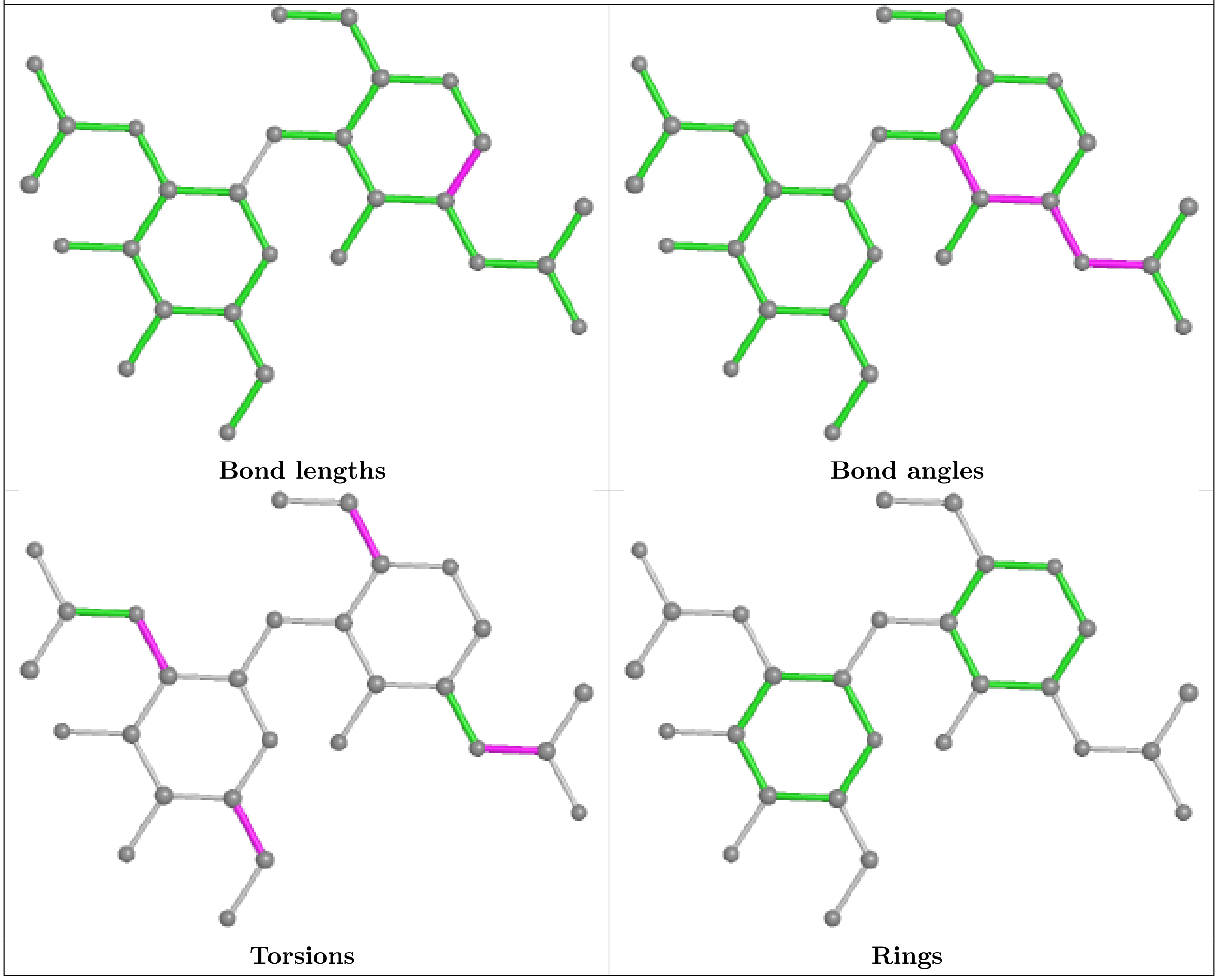
Bond angles



Torsions

Rings

Oligosaccharide Chain s



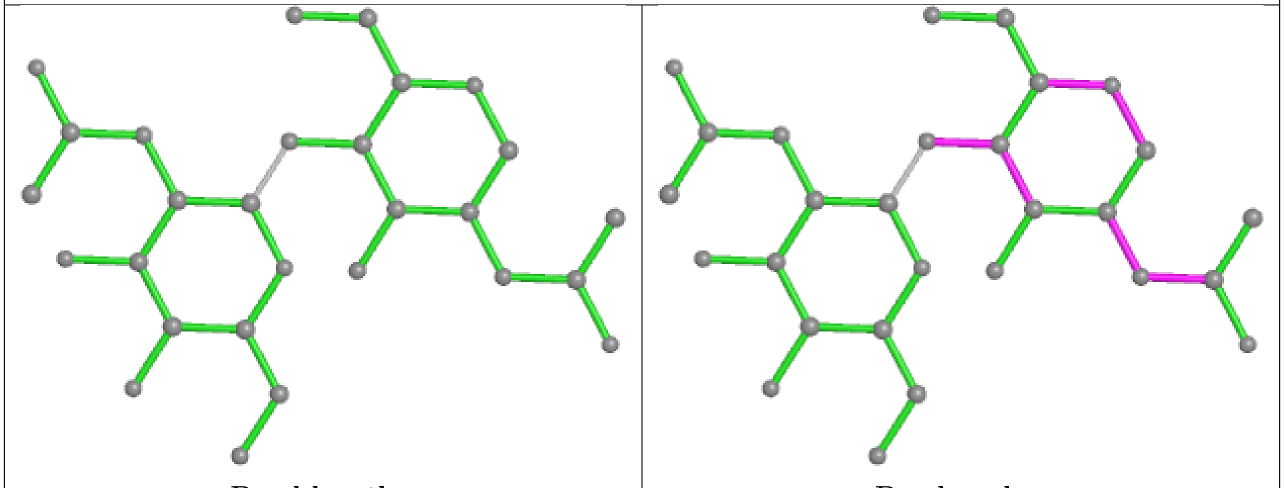
Bond lengths

Bond angles

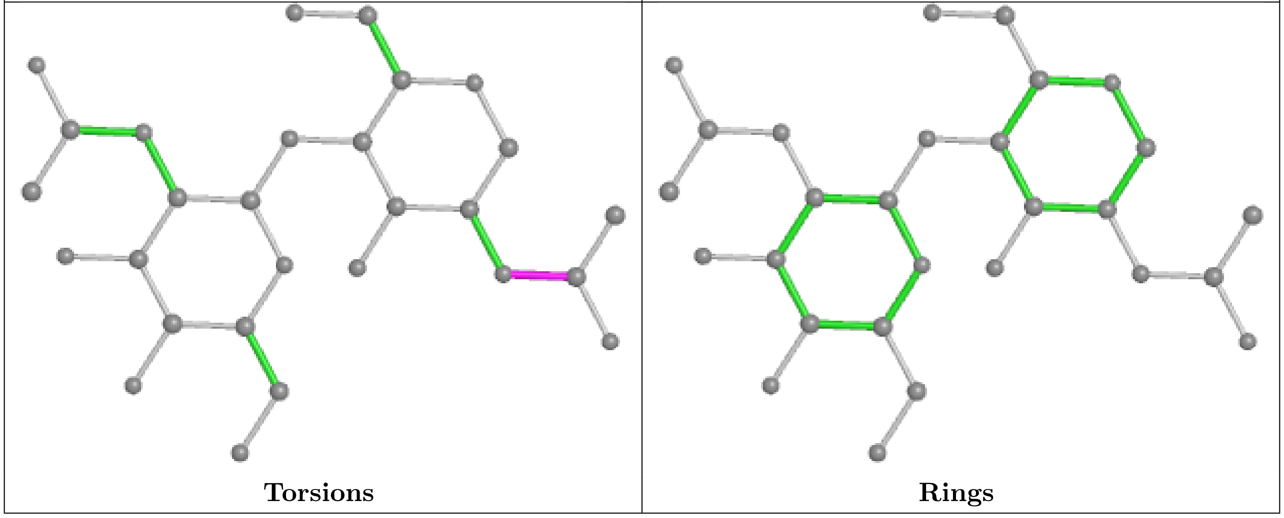
Torsions

Rings

Oligosaccharide Chain t

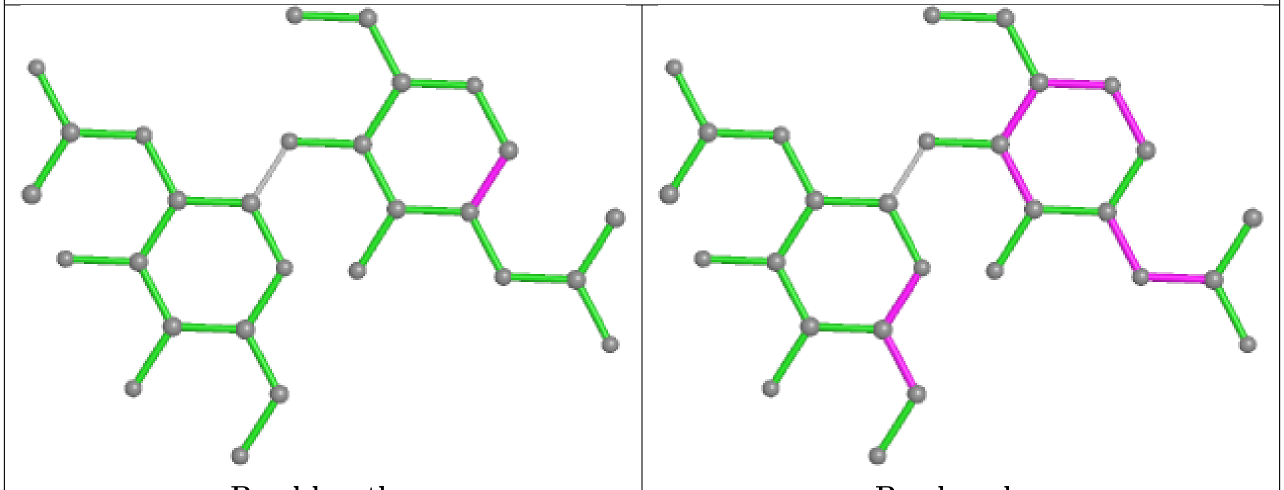


Bond lengths **Bond angles**

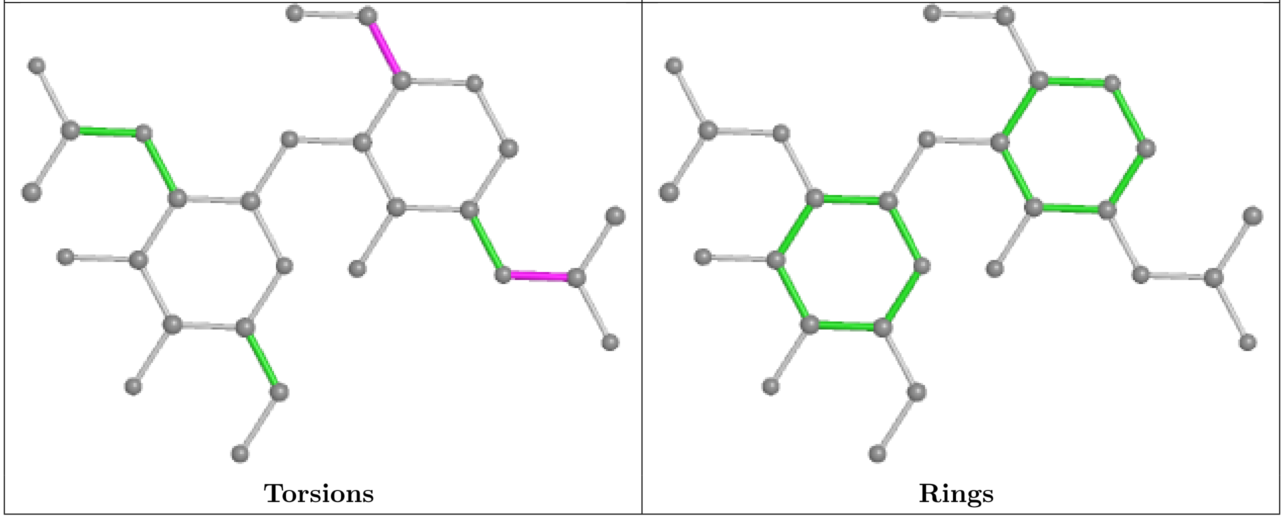


Torsions **Rings**

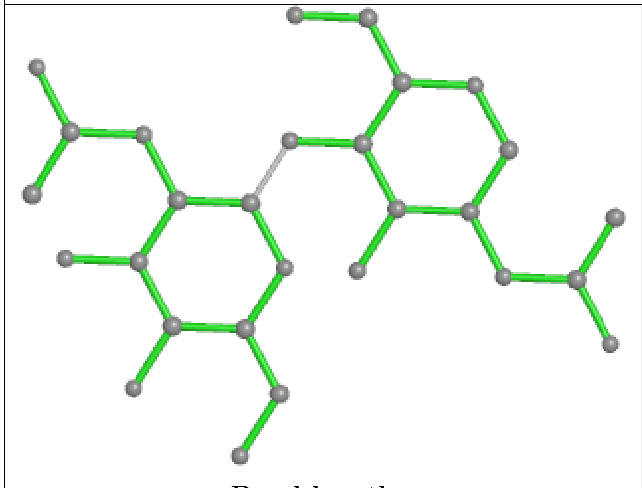
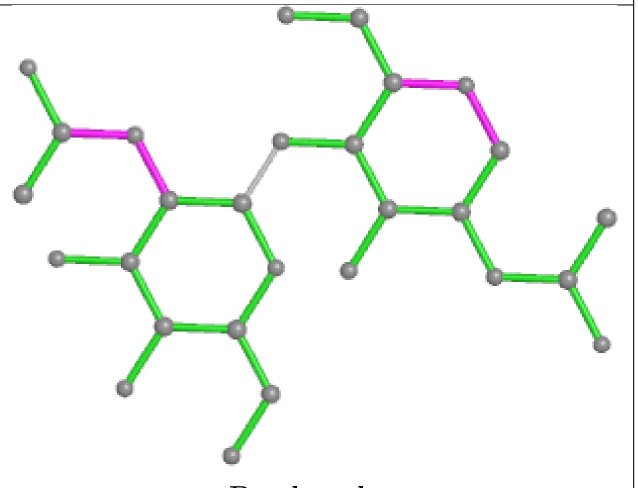
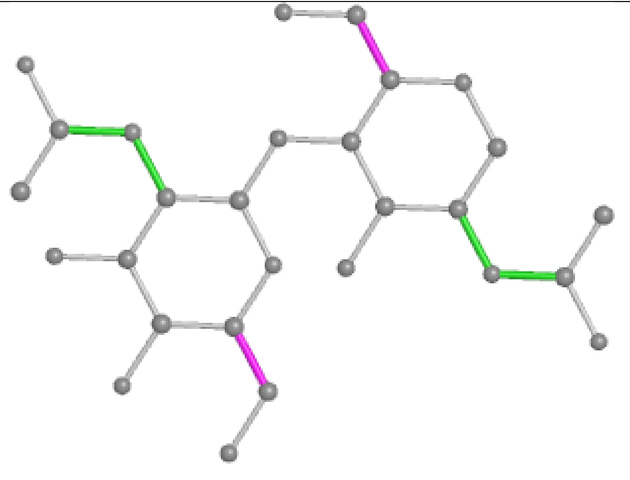
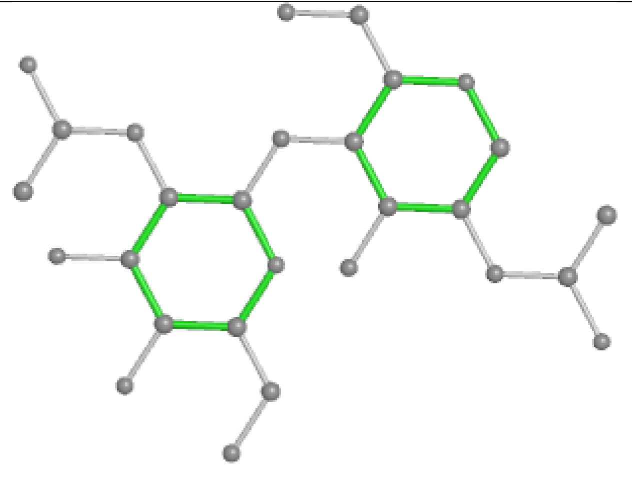
Oligosaccharide Chain u



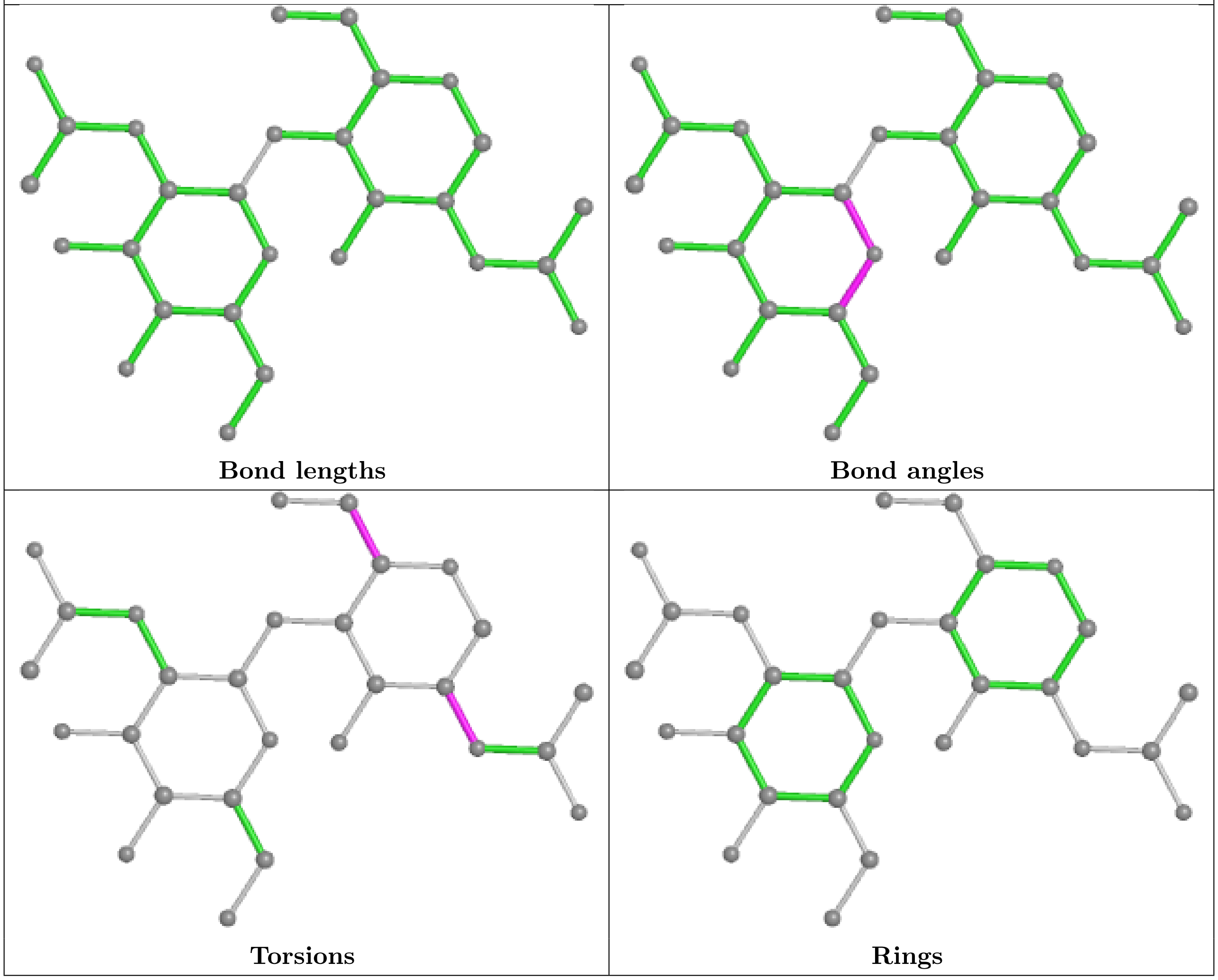
Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain v	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain x



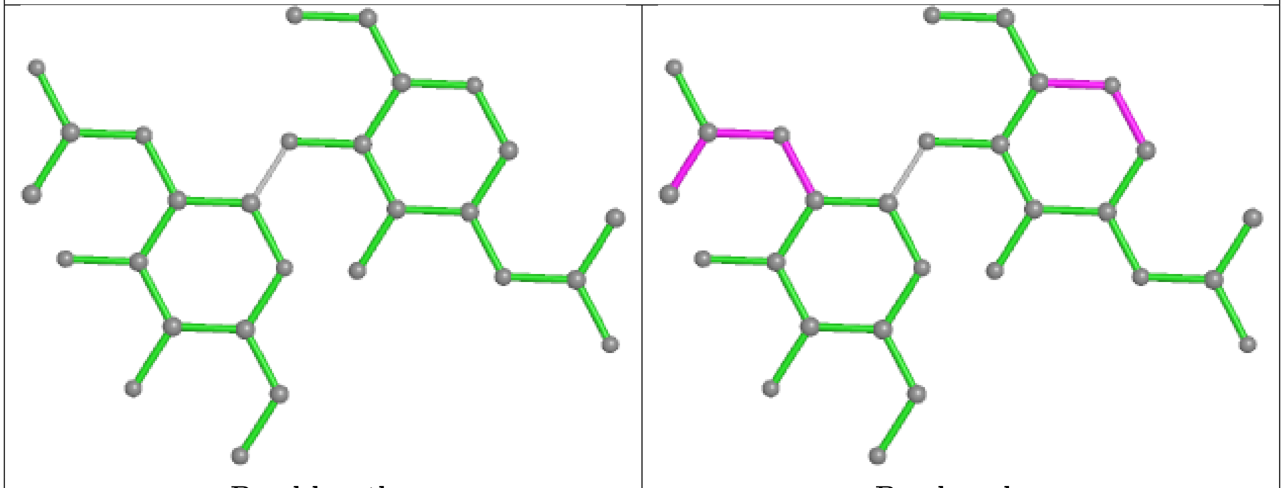
Bond lengths

Bond angles

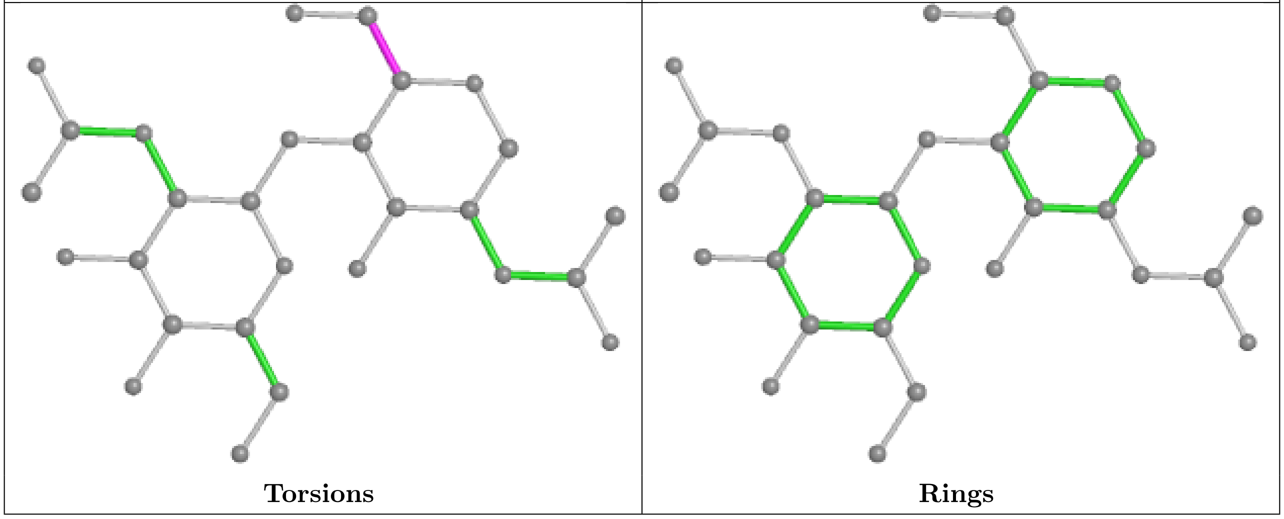
Torsions

Rings

Oligosaccharide Chain 1

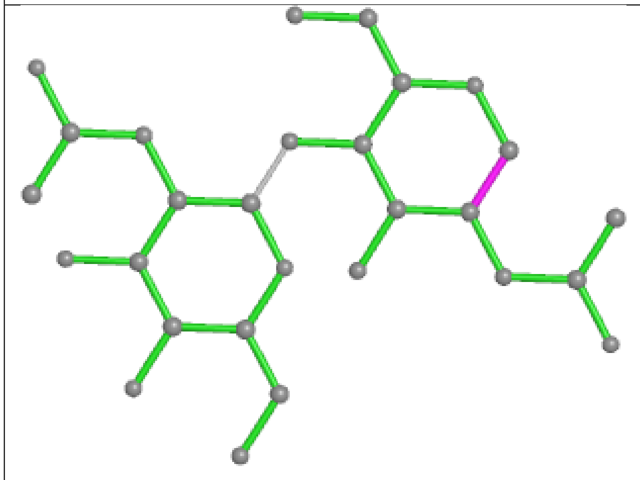


Bond lengths **Bond angles**

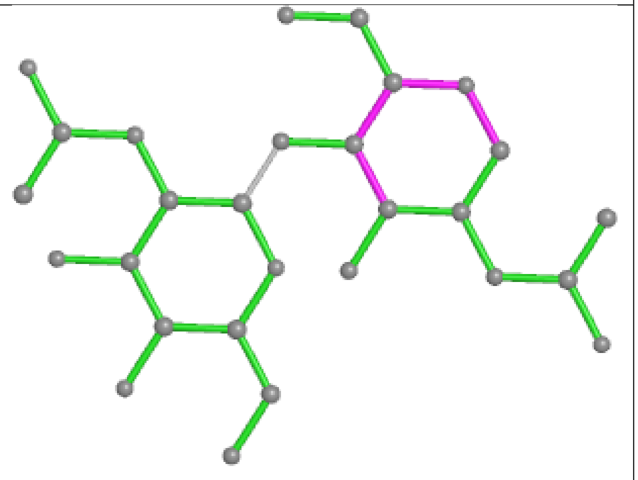


Torsions **Rings**

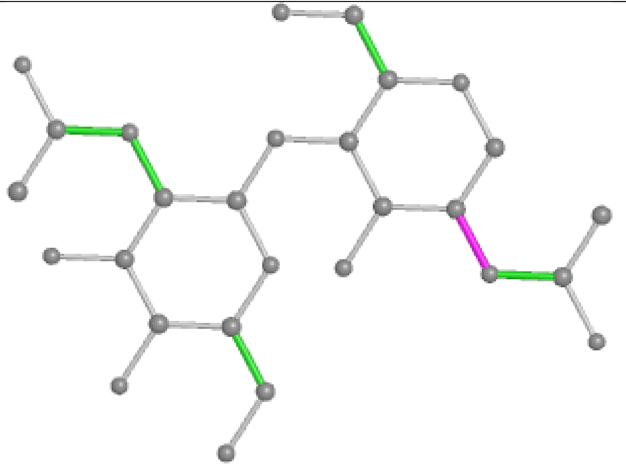
Oligosaccharide Chain 2



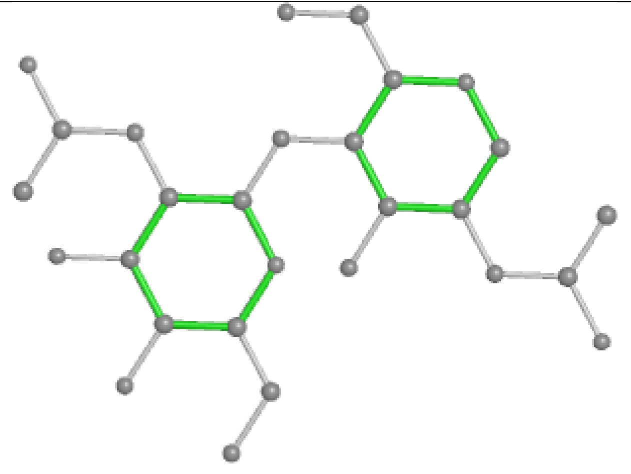
Bond lengths



Bond angles

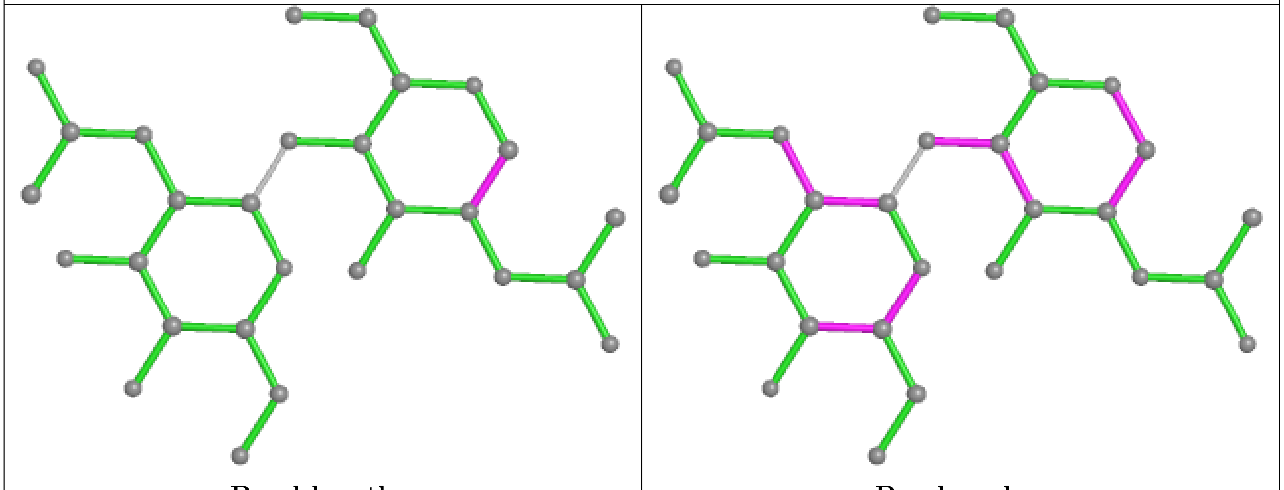


Torsions

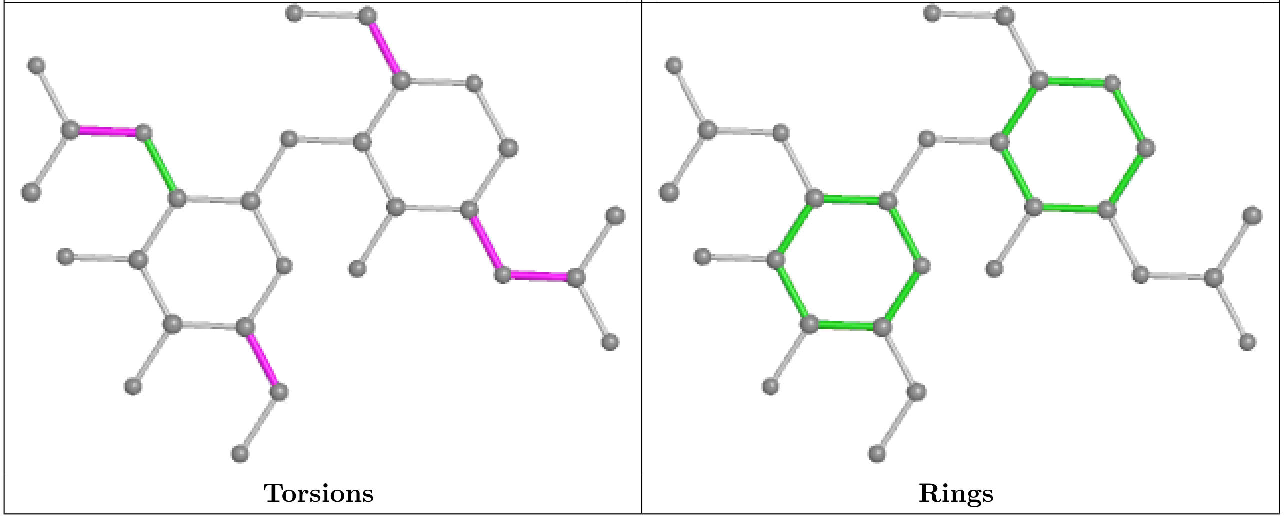


Rings

Oligosaccharide Chain 4

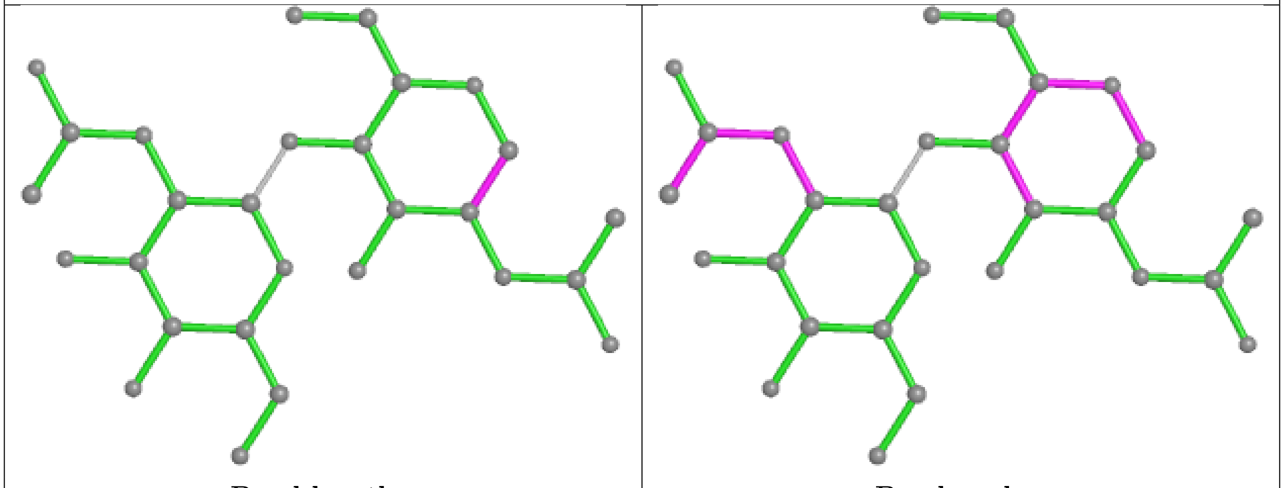


Bond lengths **Bond angles**



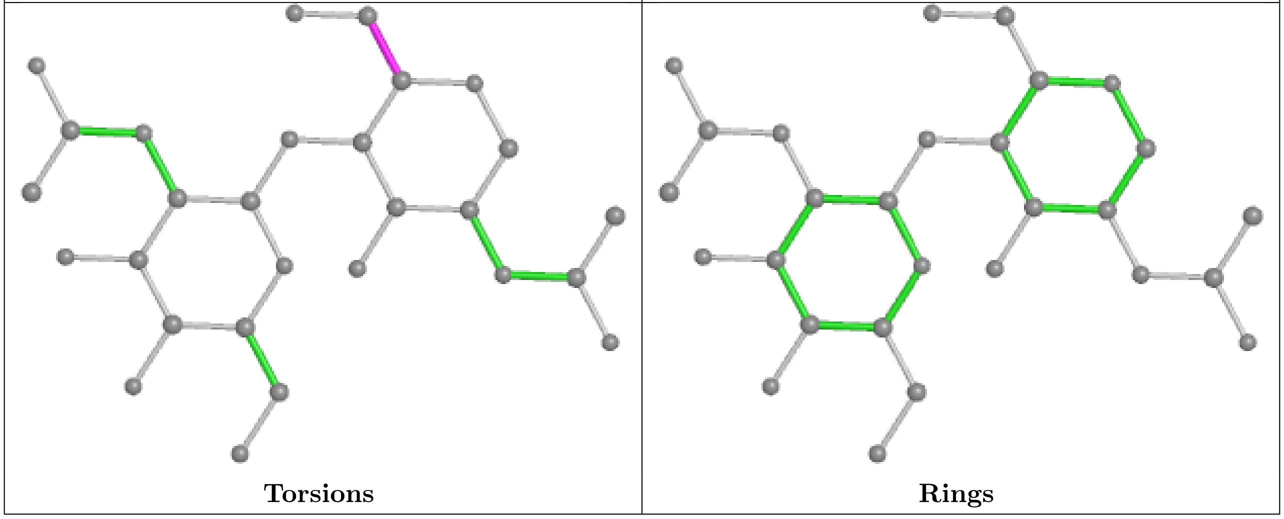
Torsions **Rings**

Oligosaccharide Chain 6



Bond lengths

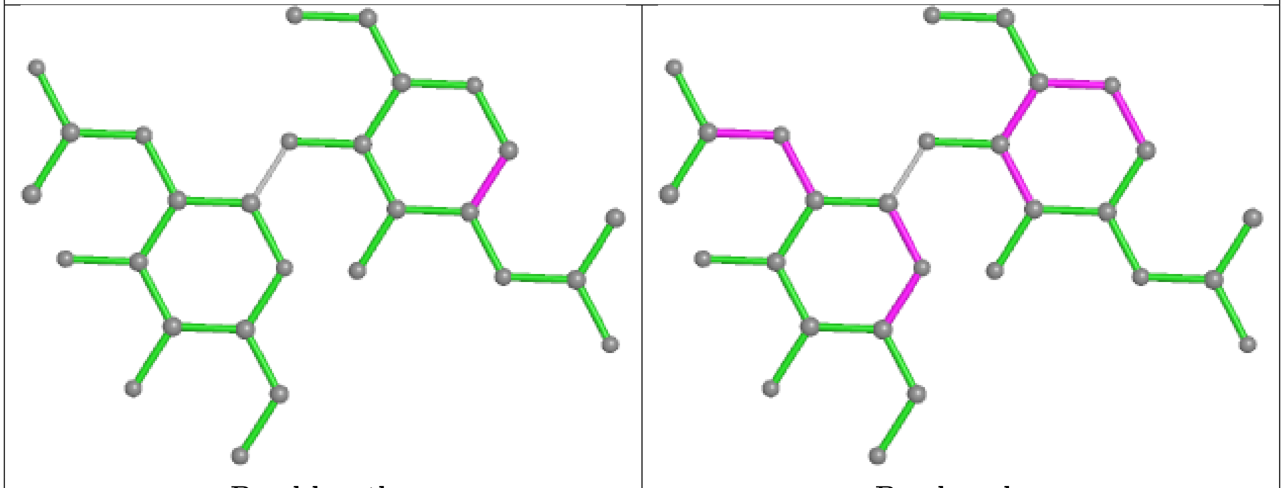
Bond angles



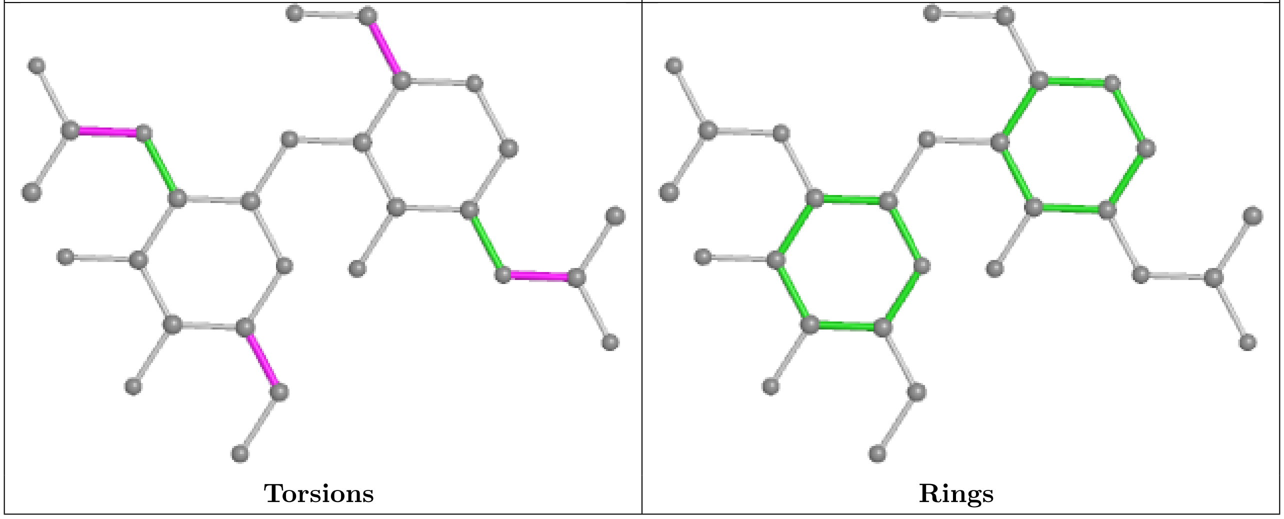
Torsions

Rings

Oligosaccharide Chain 7

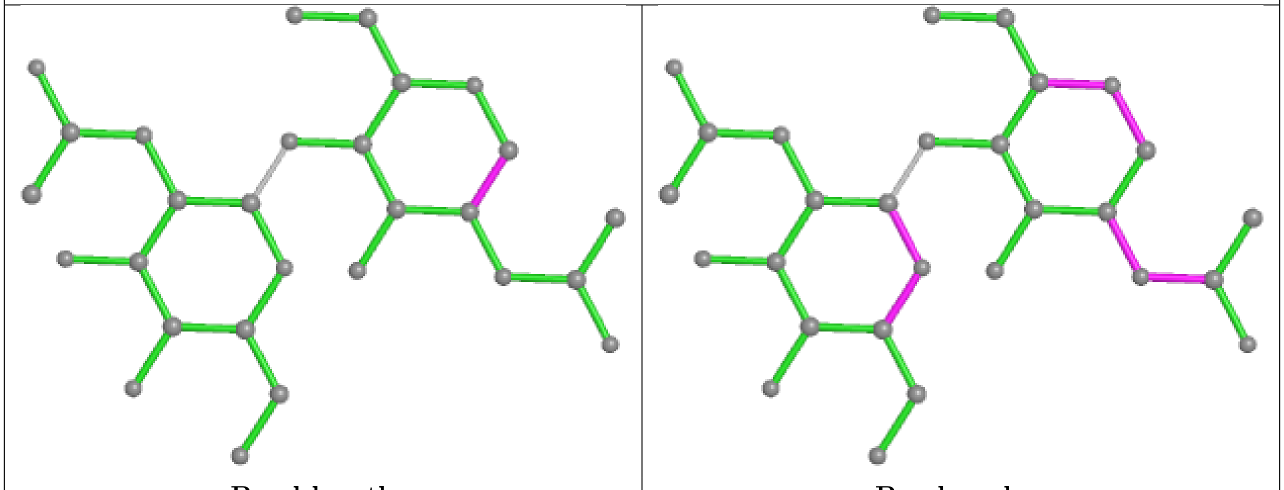


Bond lengths **Bond angles**



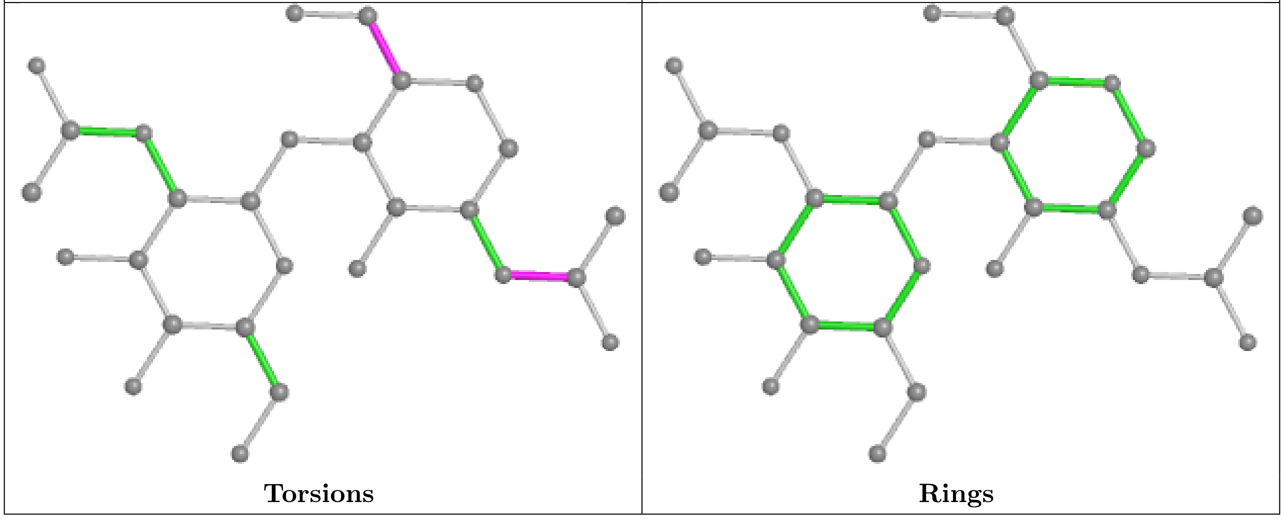
Torsions **Rings**

Oligosaccharide Chain 8



Bond lengths

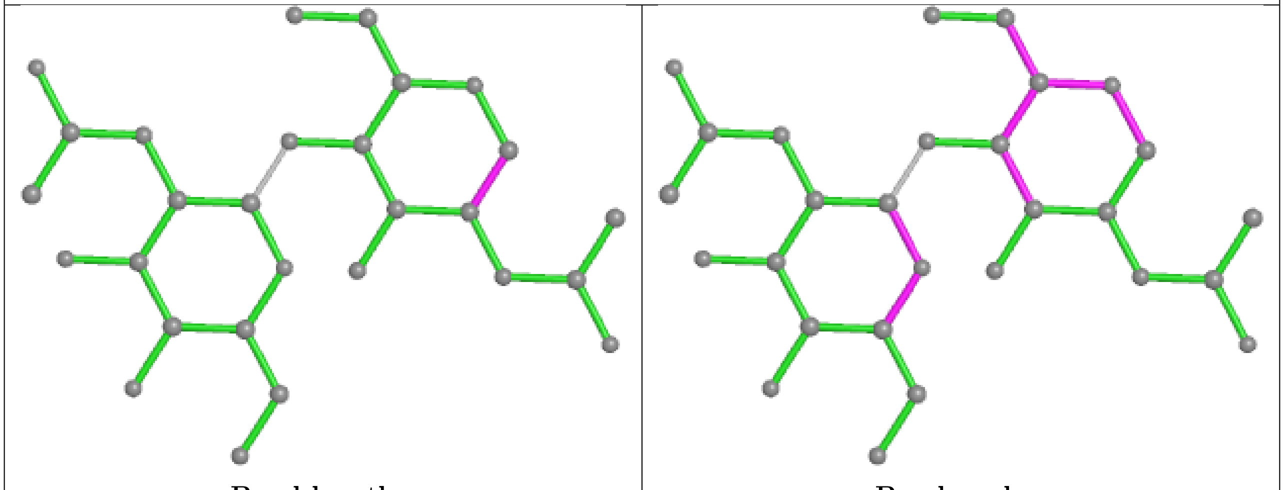
Bond angles



Torsions

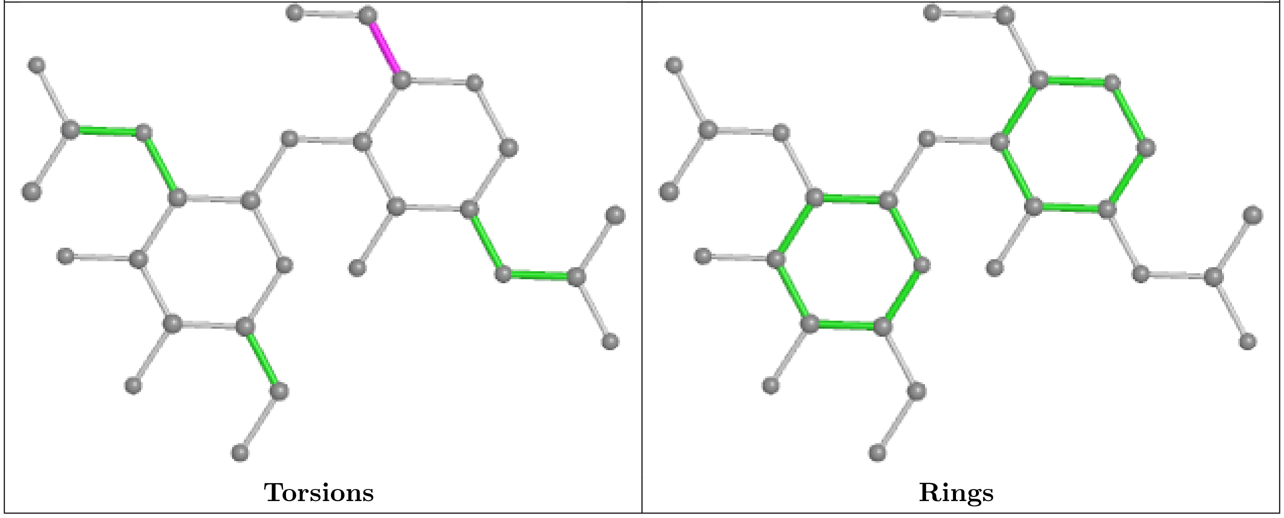
Rings

Oligosaccharide Chain 9



Bond lengths

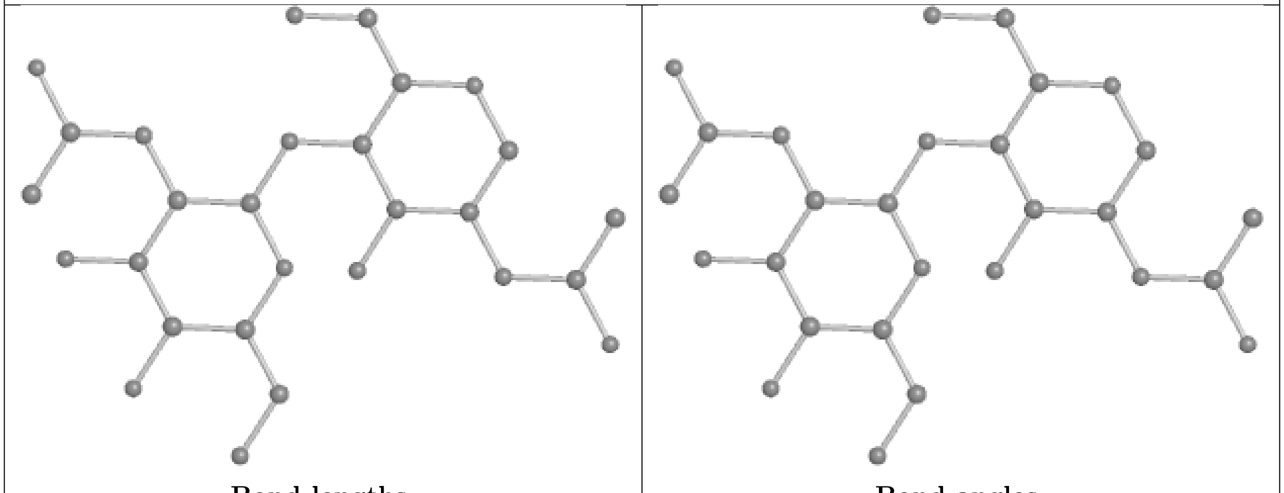
Bond angles



Torsions

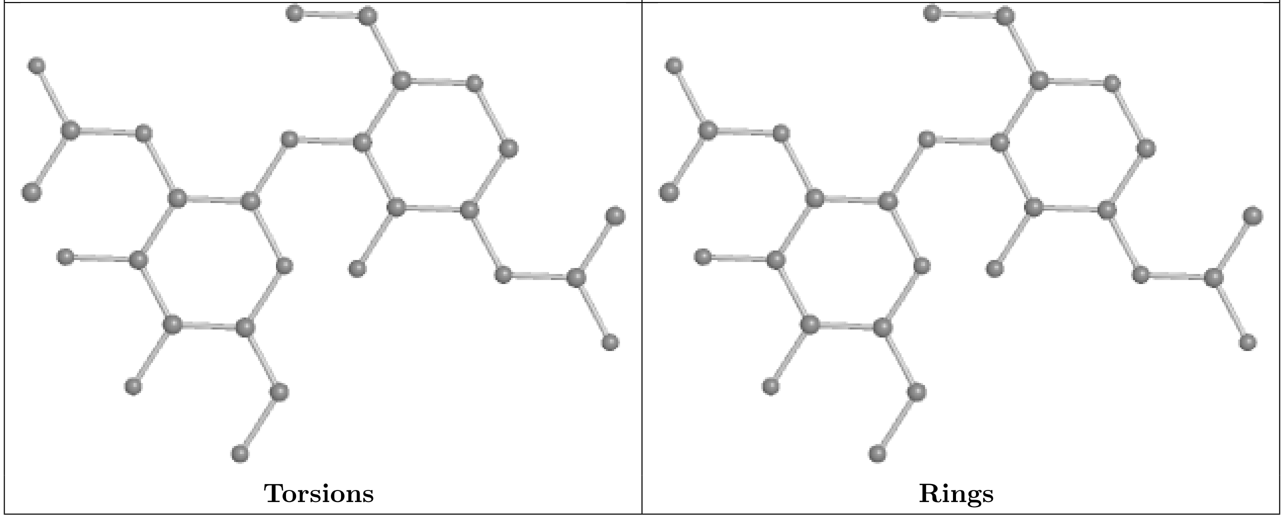
Rings

Oligosaccharide Chain BA



Bond lengths

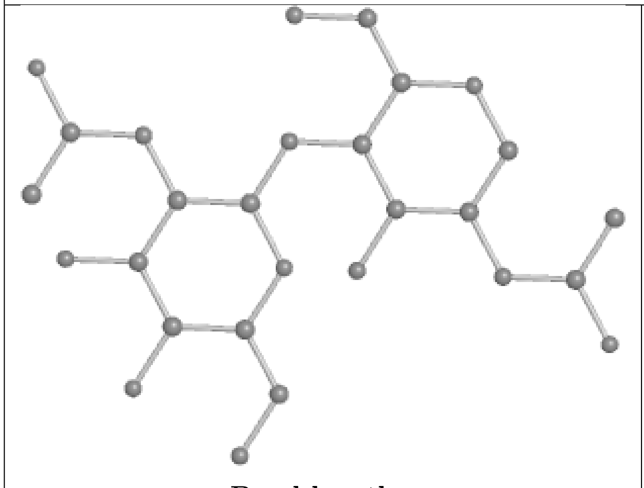
Bond angles



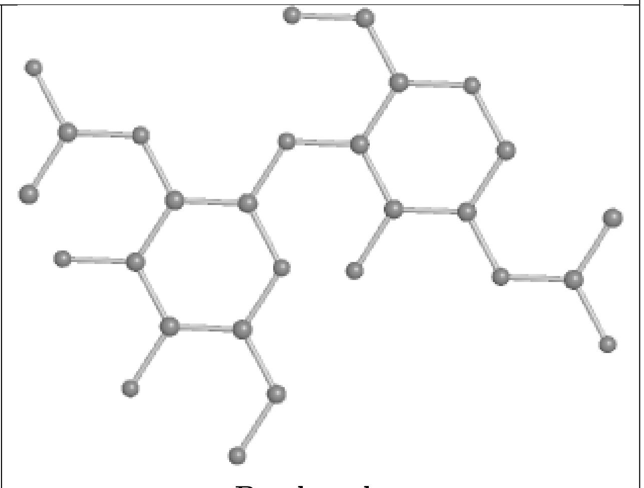
Torsions

Rings

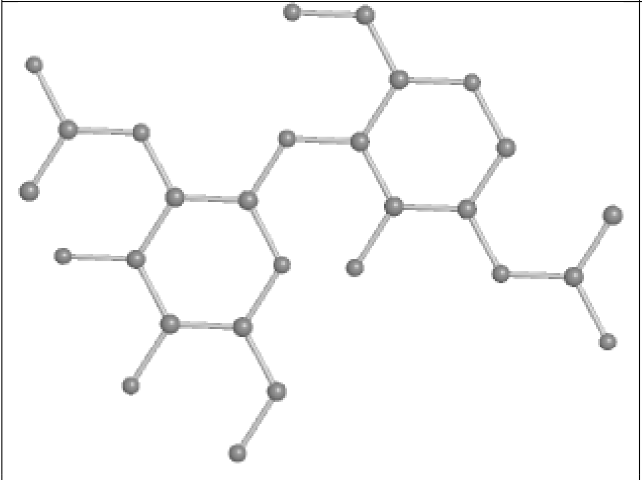
Oligosaccharide Chain HA



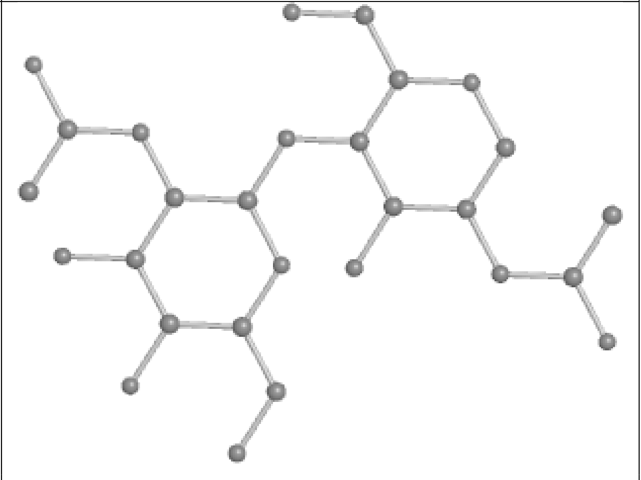
Bond lengths



Bond angles

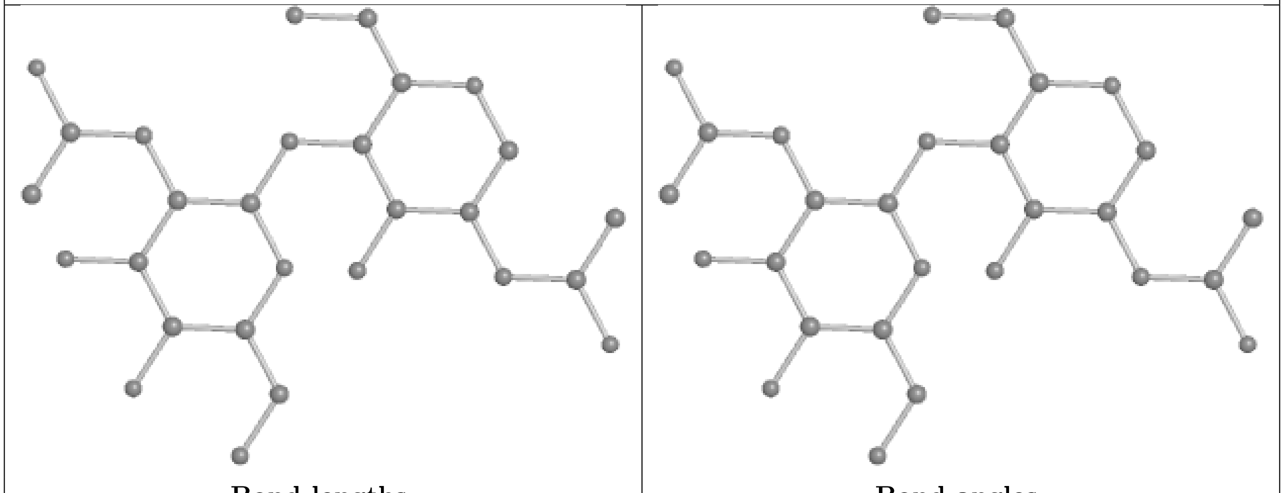


Torsions

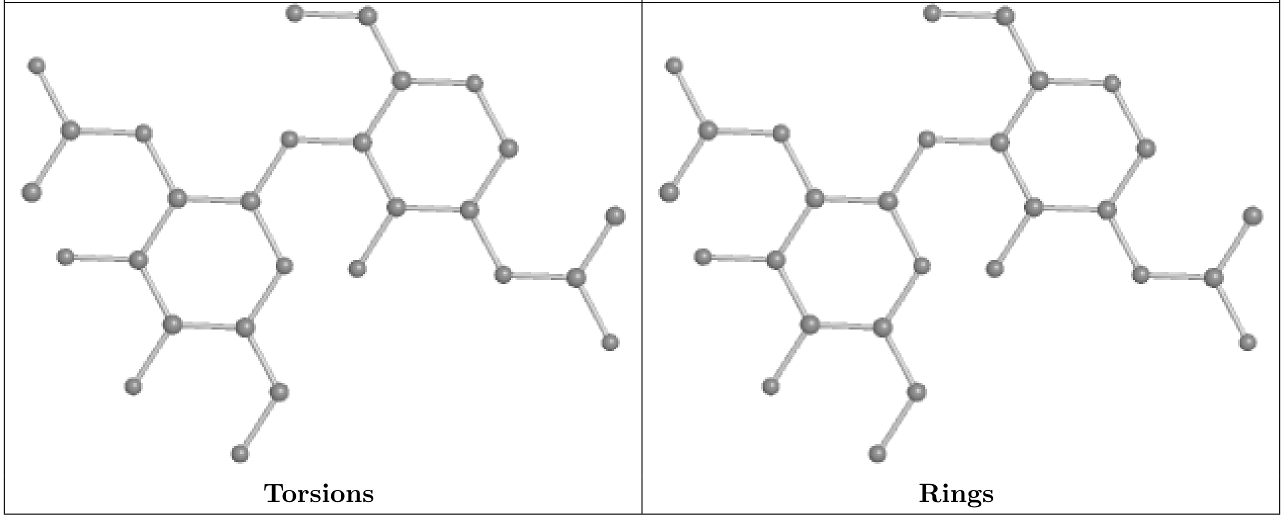


Rings

Oligosaccharide Chain IA

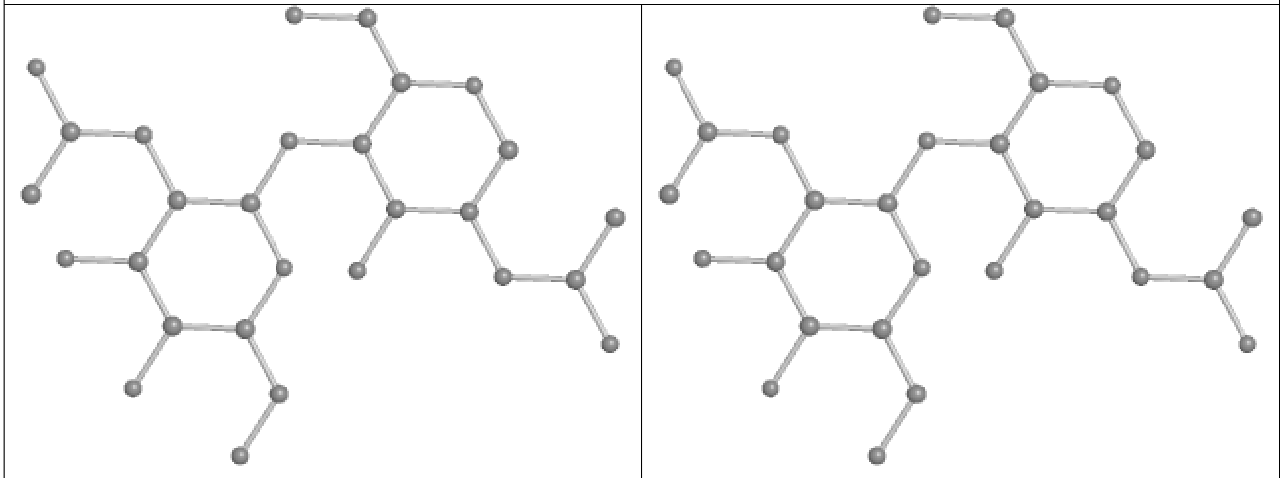


Bond lengths **Bond angles**



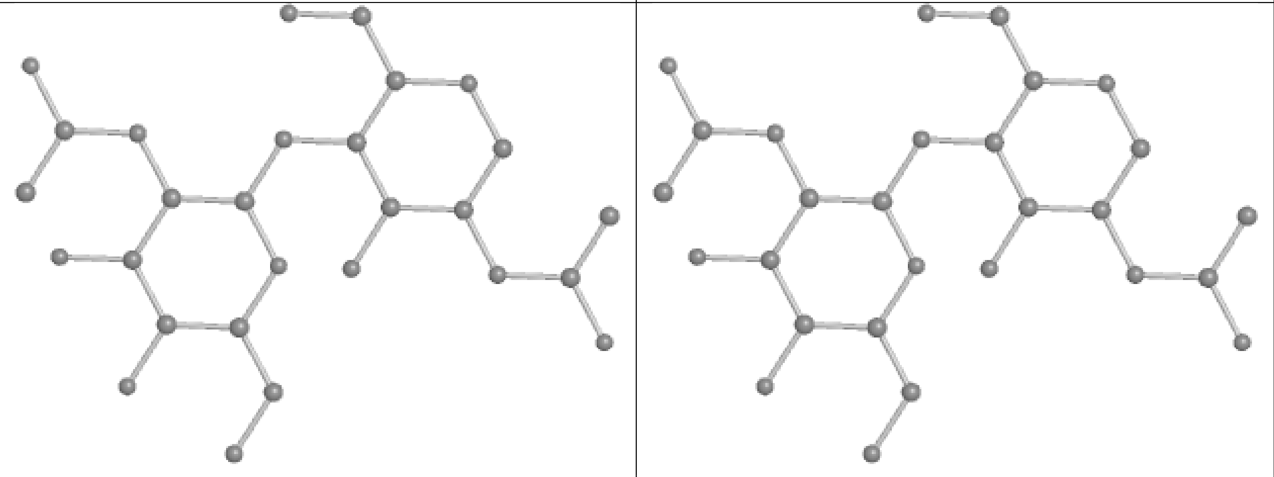
Torsions **Rings**

Oligosaccharide Chain JA



Bond lengths

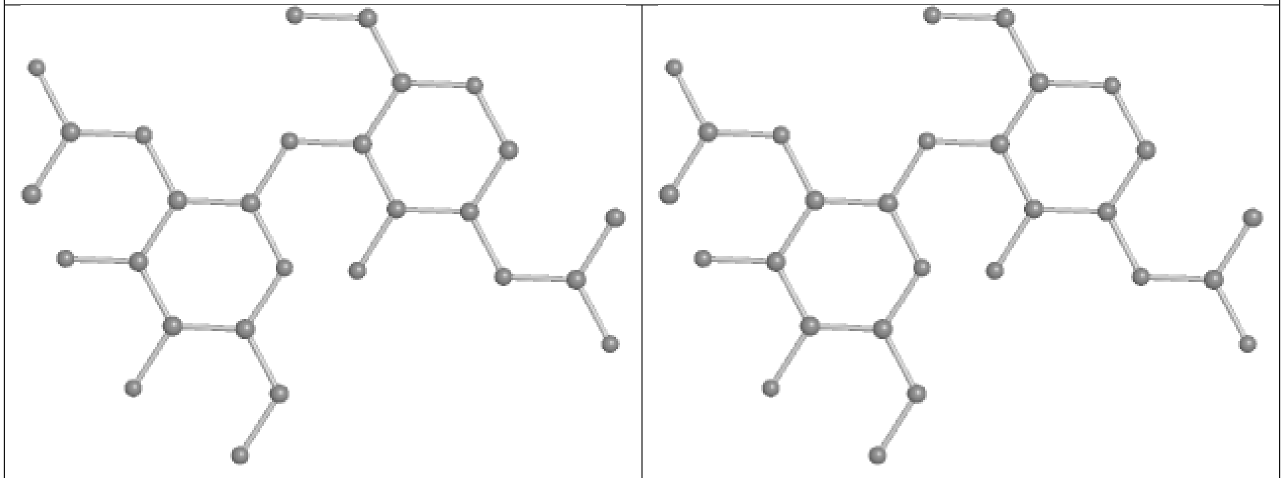
Bond angles



Torsions

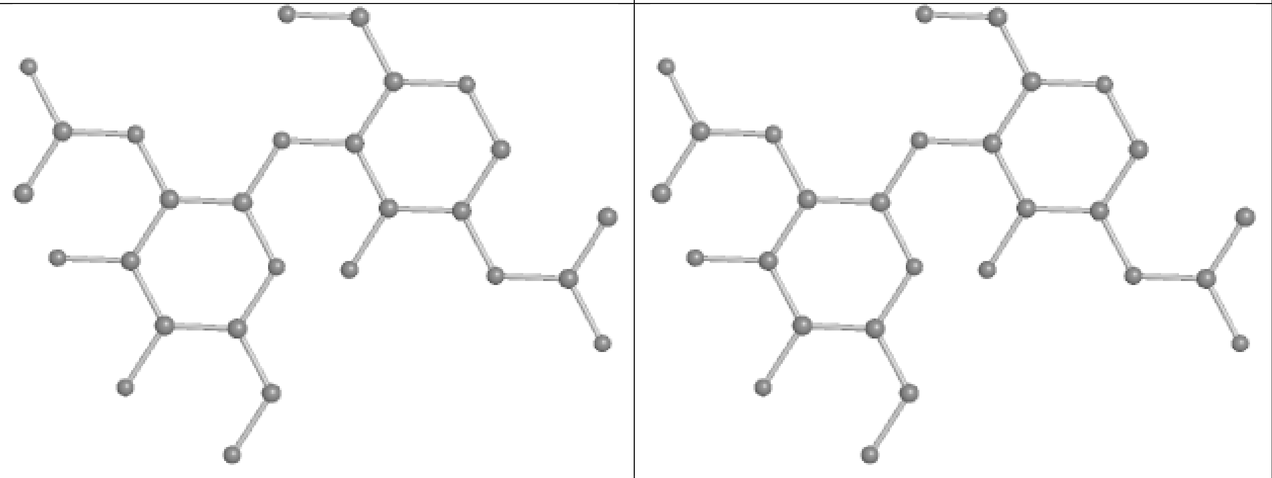
Rings

Oligosaccharide Chain MA



Bond lengths

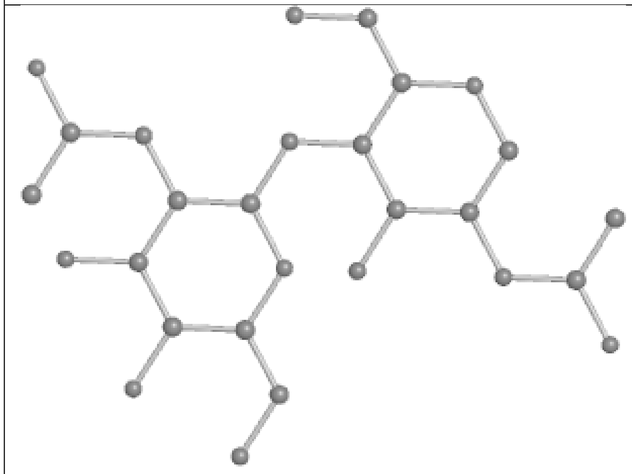
Bond angles

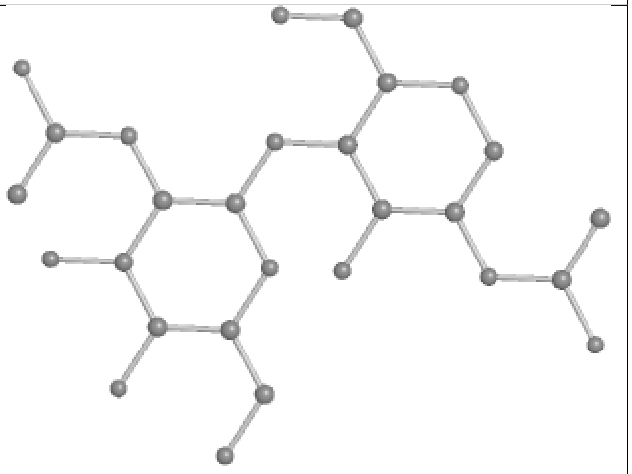


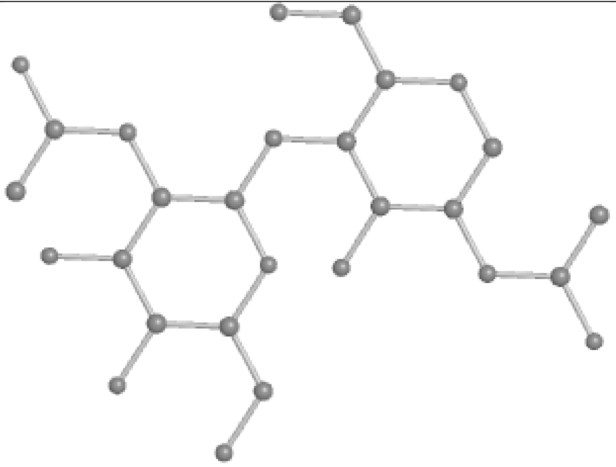
Torsions

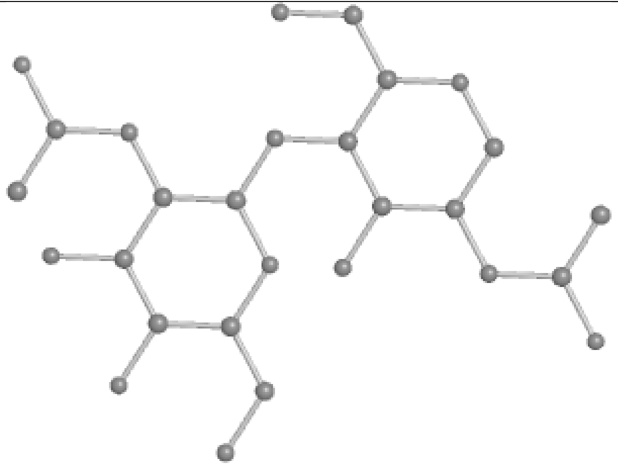
Rings

Oligosaccharide Chain OA

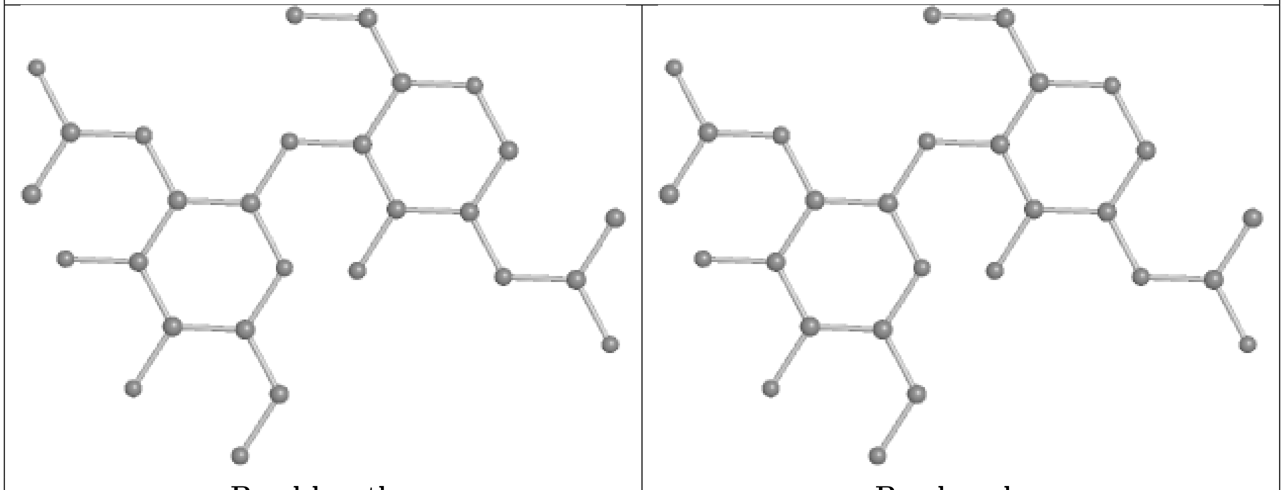

Bond lengths


Bond angles


Torsions

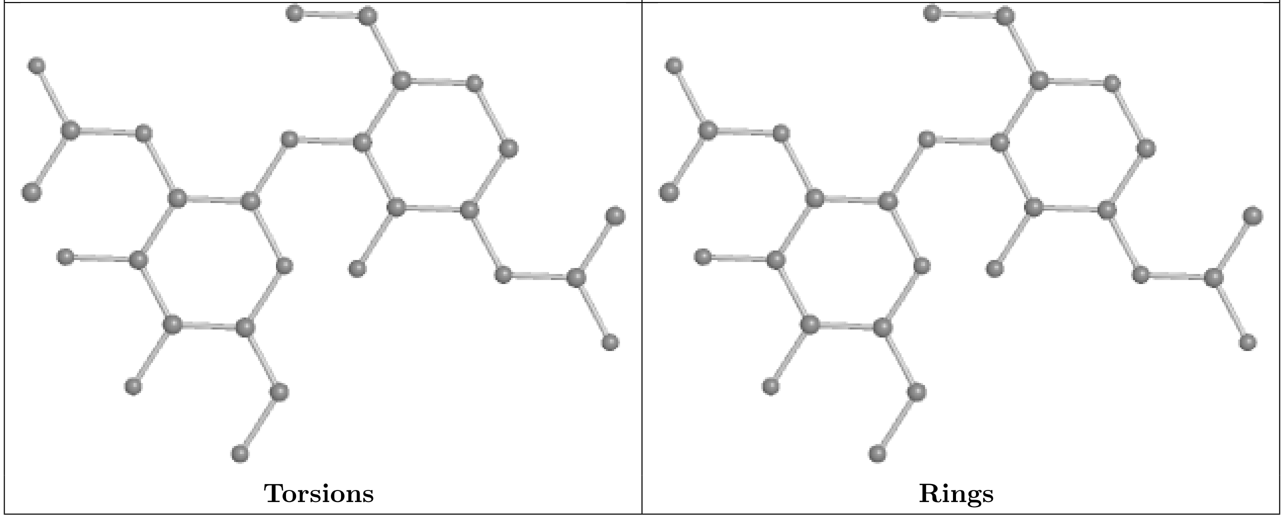

Rings

Oligosaccharide Chain QA



Bond lengths

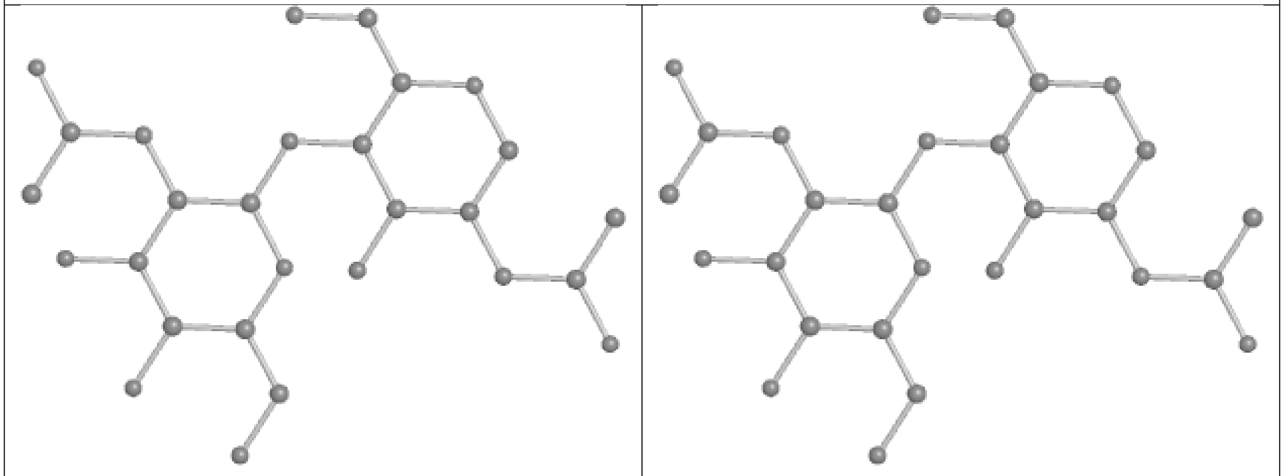
Bond angles



Torsions

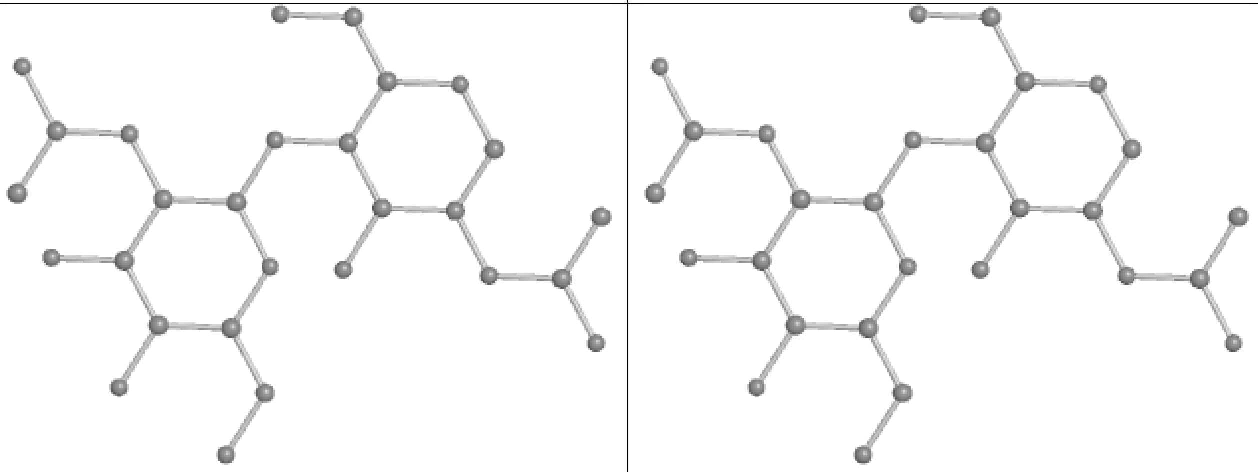
Rings

Oligosaccharide Chain RA



Bond lengths

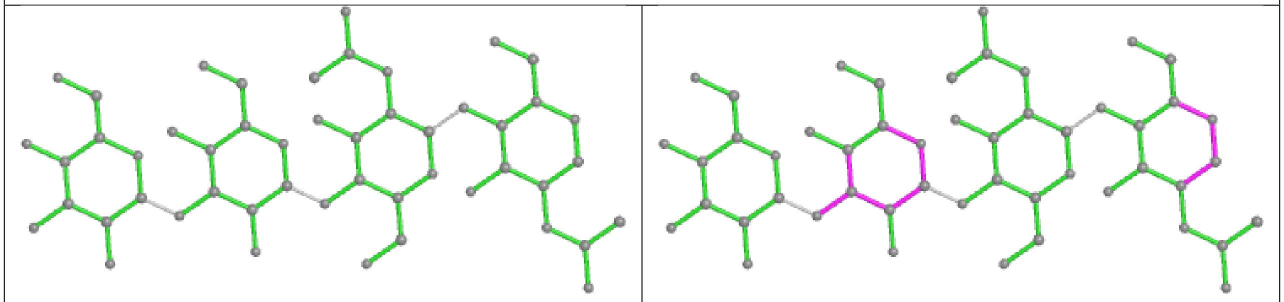
Bond angles



Torsions

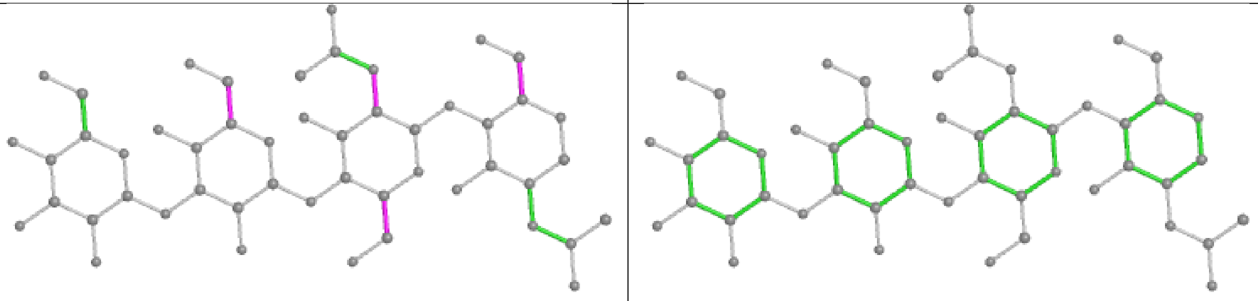
Rings

Oligosaccharide Chain g



Bond lengths

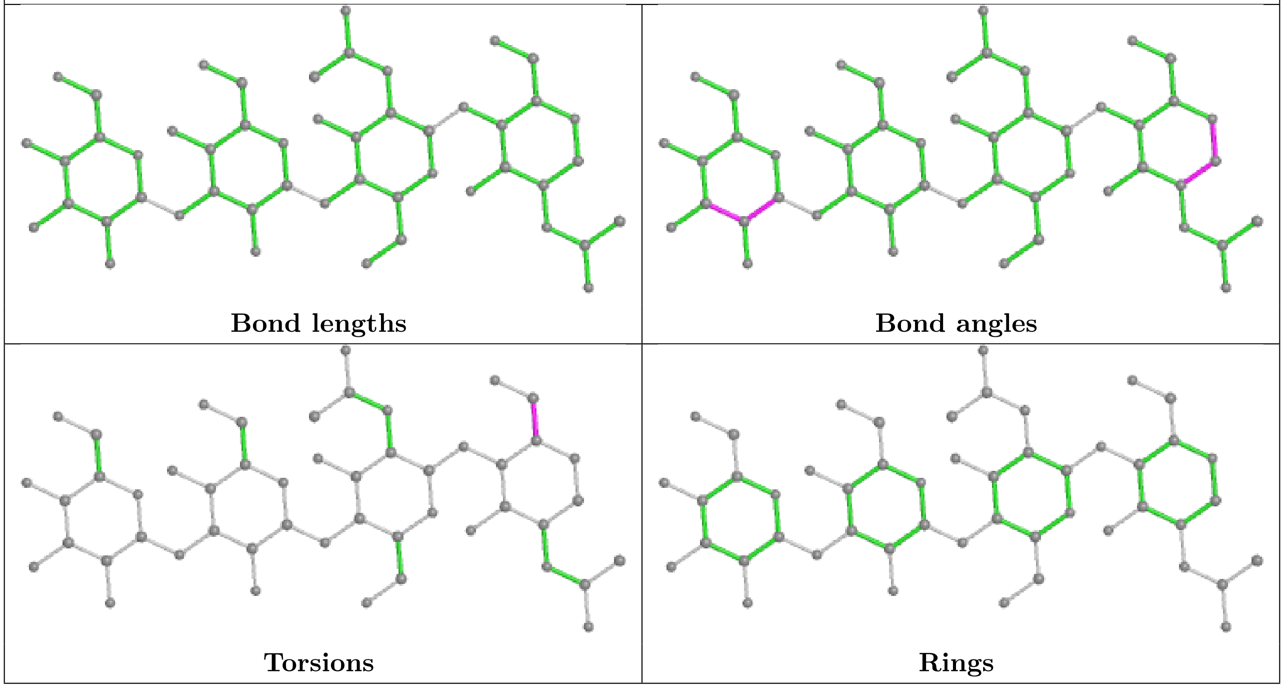
Bond angles



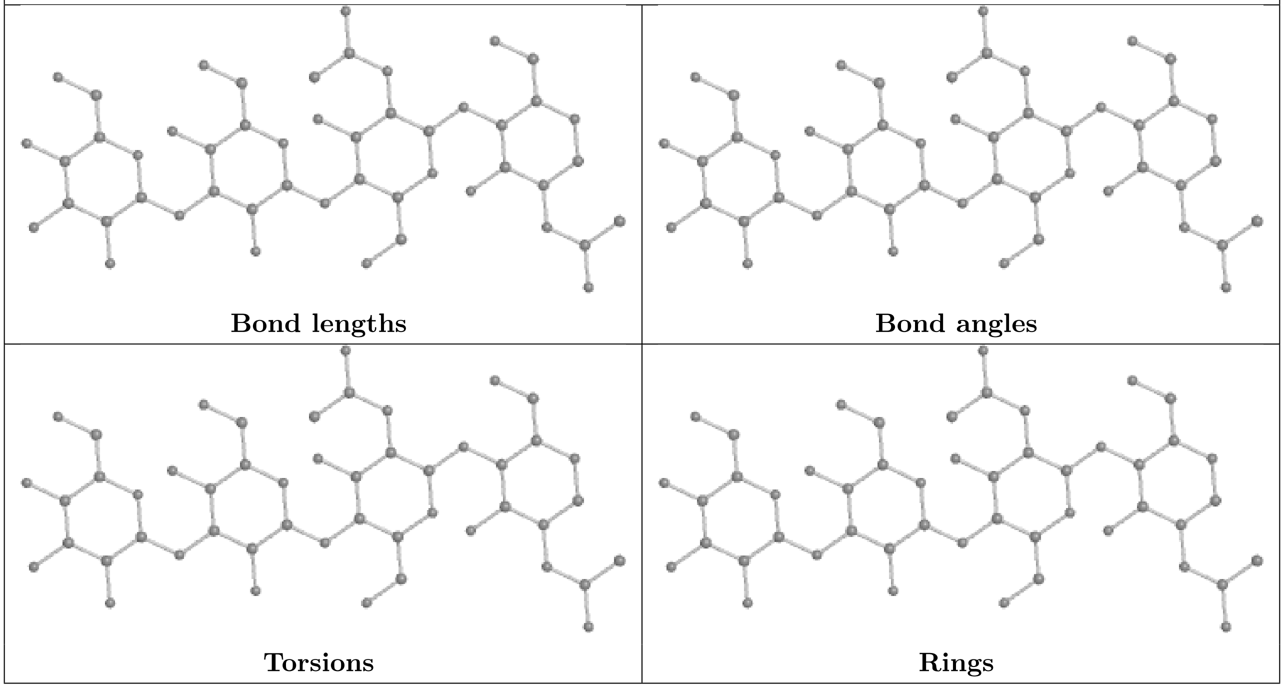
Torsions

Rings

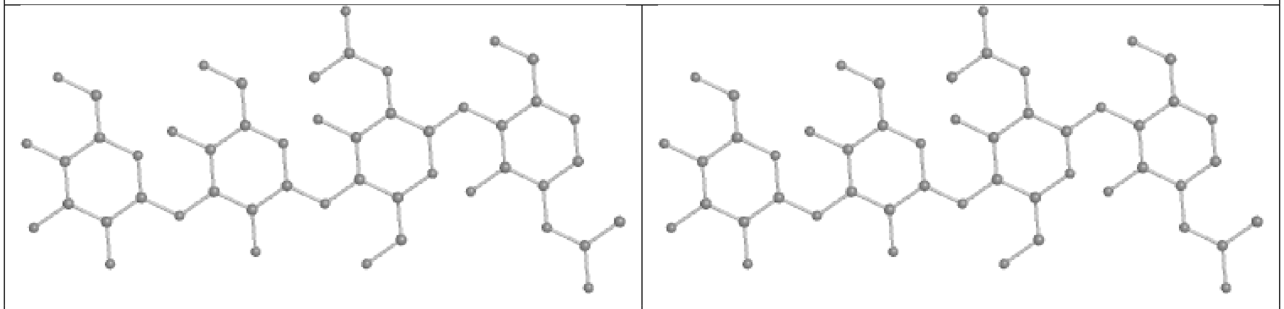
Oligosaccharide Chain l


Bond lengths
Bond angles
Torsions
Rings

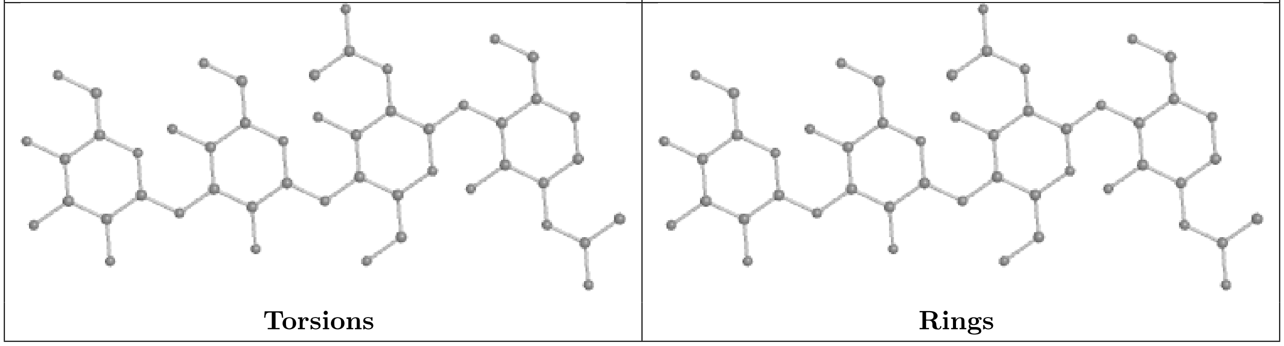
Oligosaccharide Chain AA


Bond lengths
Bond angles
Torsions
Rings

Oligosaccharide Chain FA

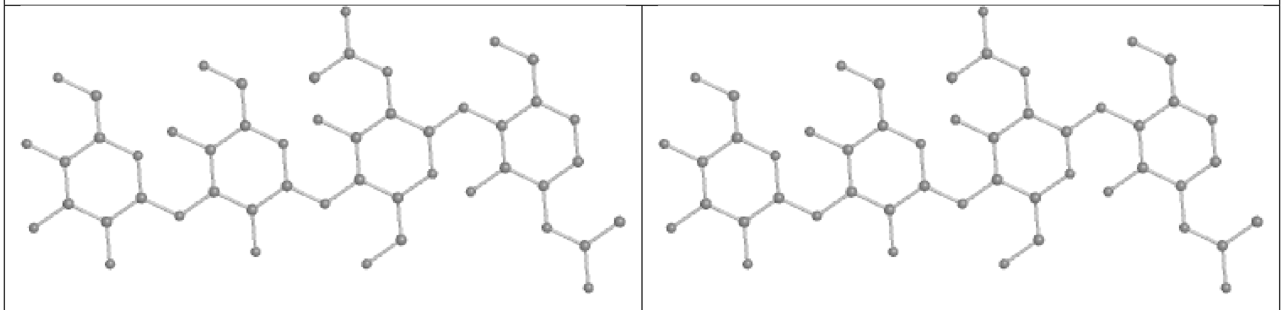


Bond lengths **Bond angles**

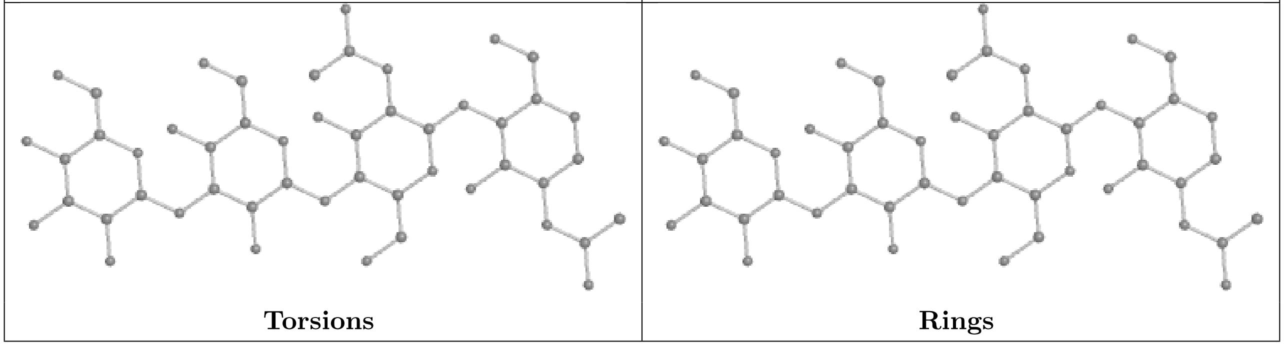


Torsions **Rings**

Oligosaccharide Chain KA

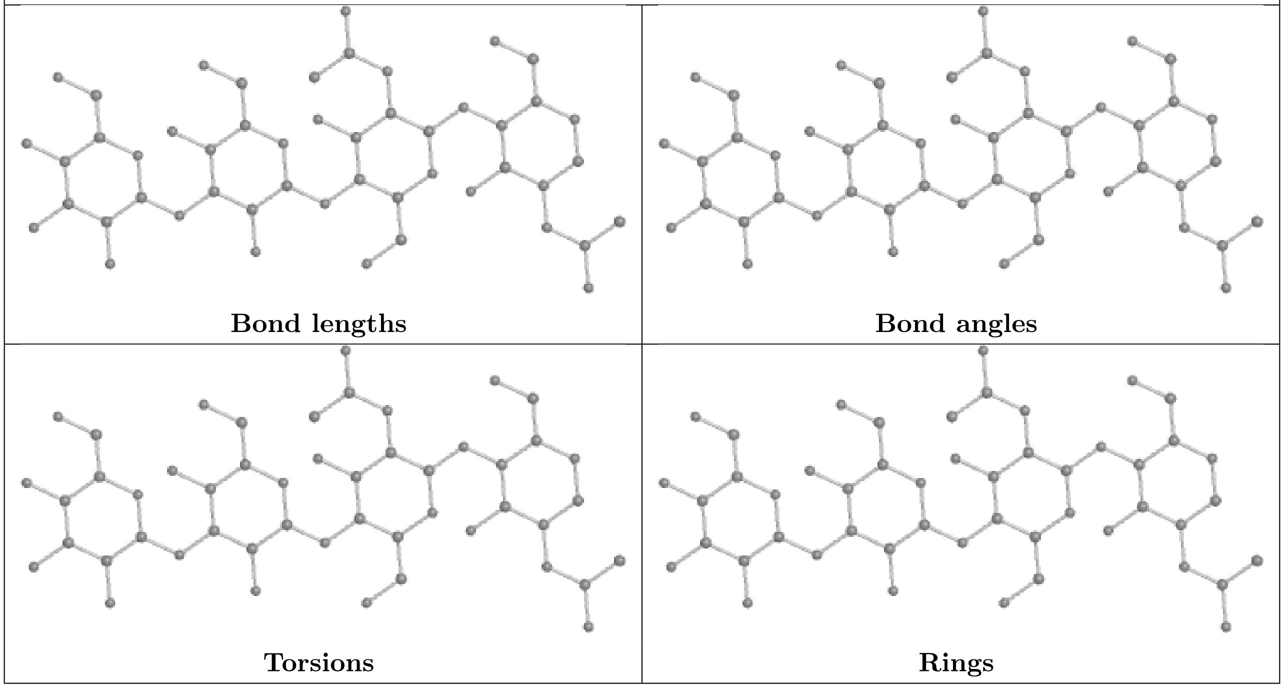


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain PA



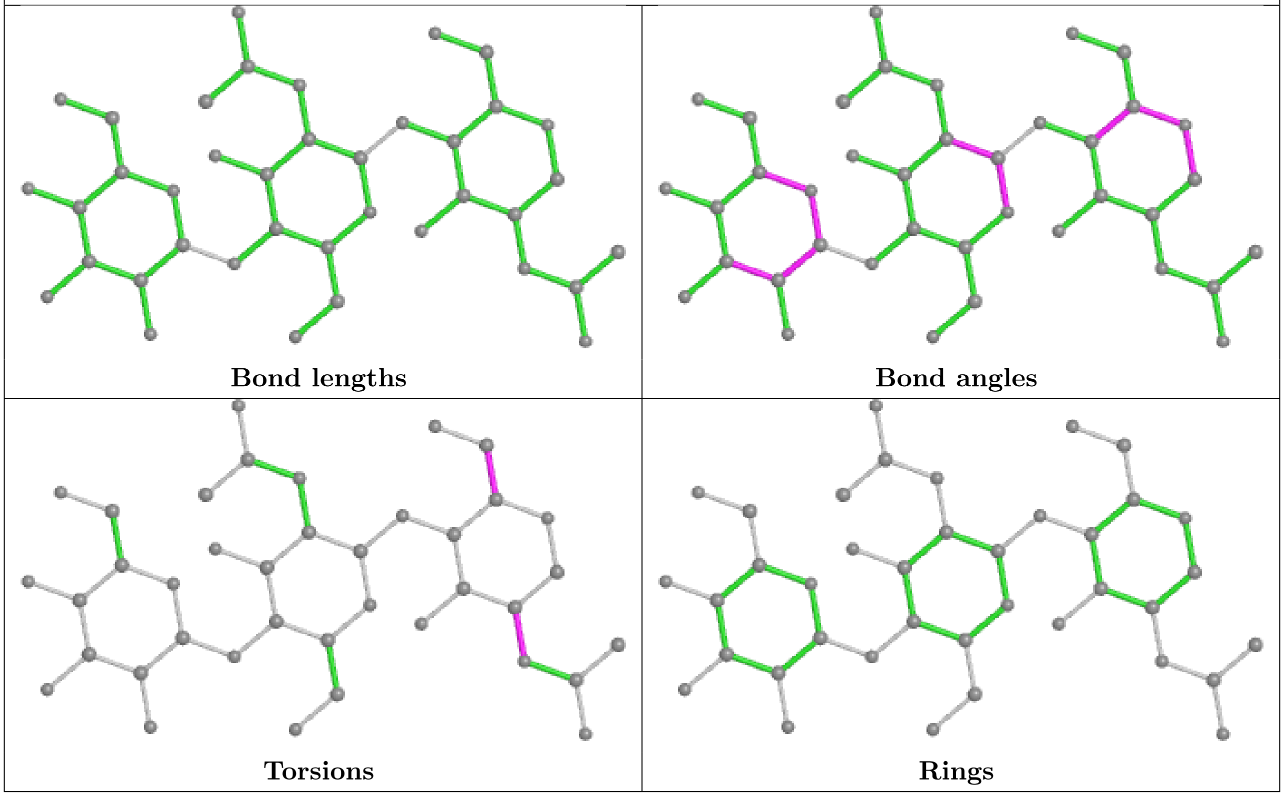
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain h



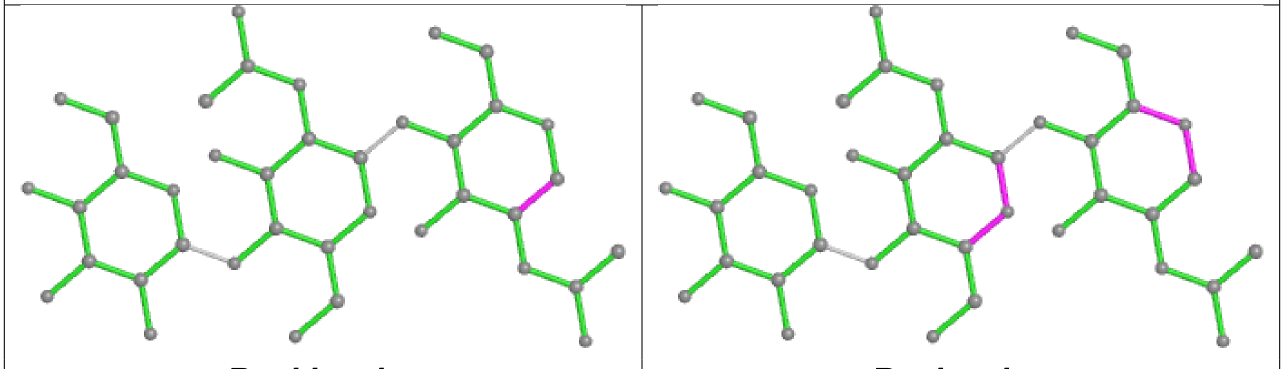
Bond lengths

Bond angles

Torsions

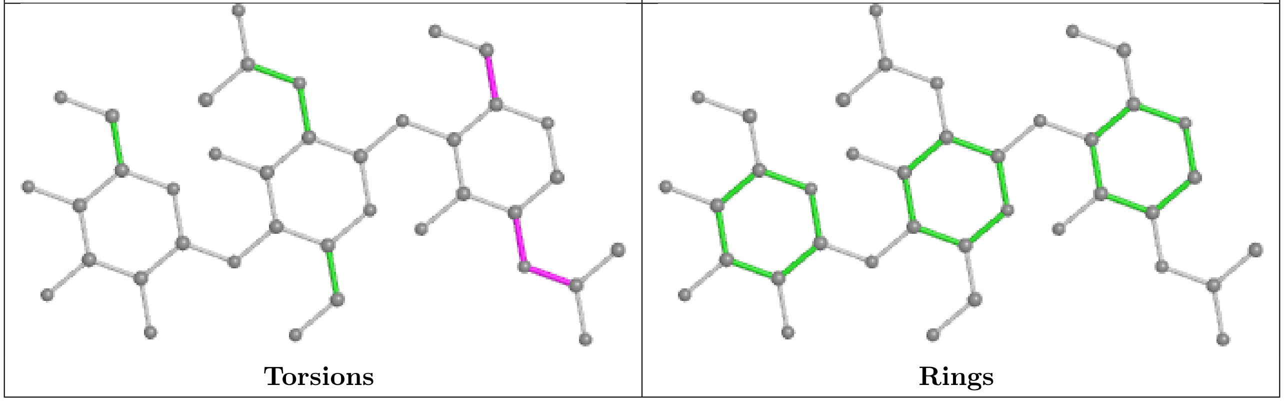
Rings

Oligosaccharide Chain k



Bond lengths

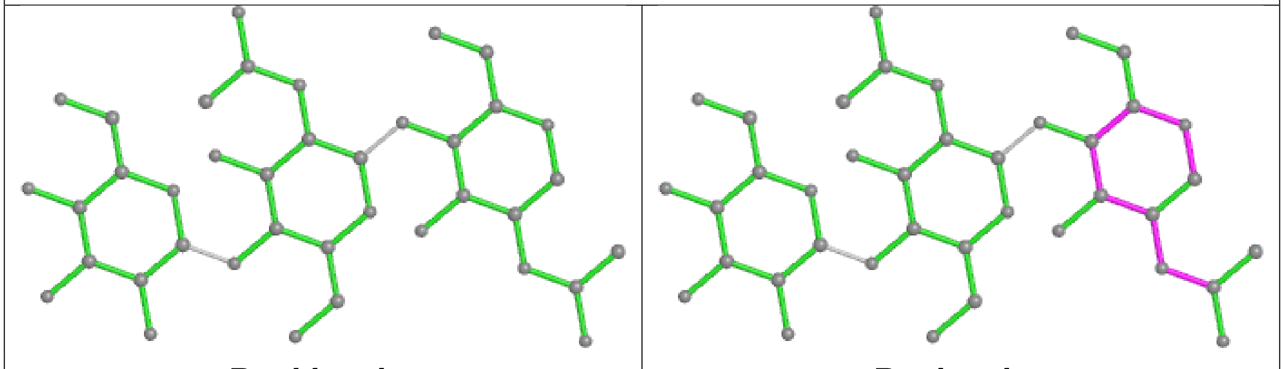
Bond angles



Torsions

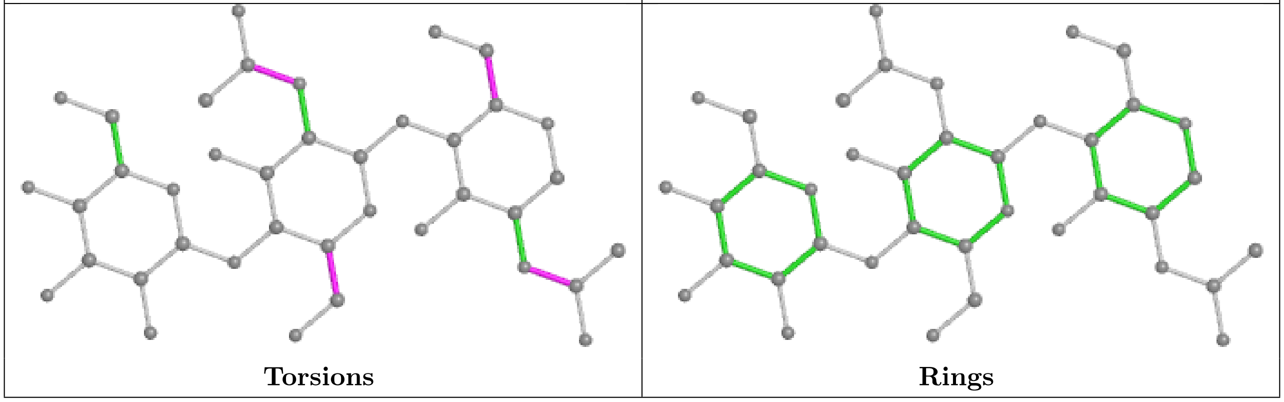
Rings

Oligosaccharide Chain r



Bond lengths

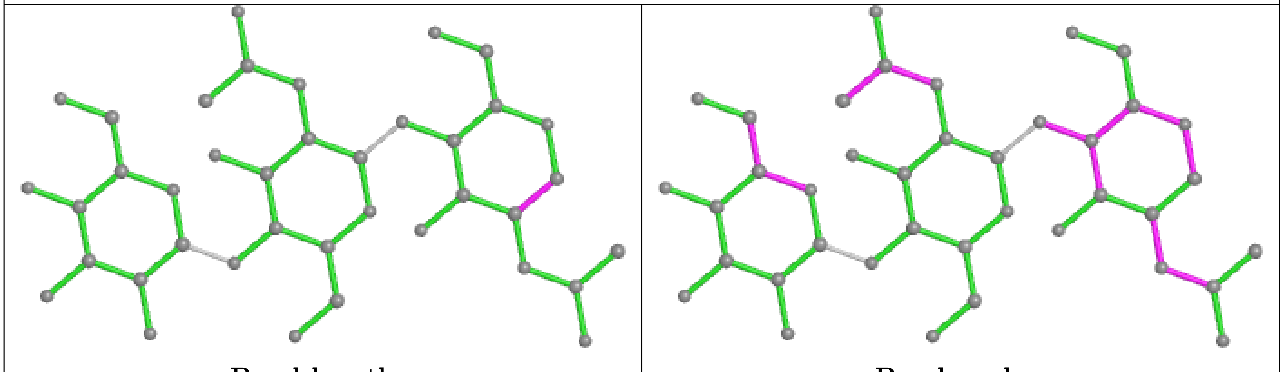
Bond angles



Torsions

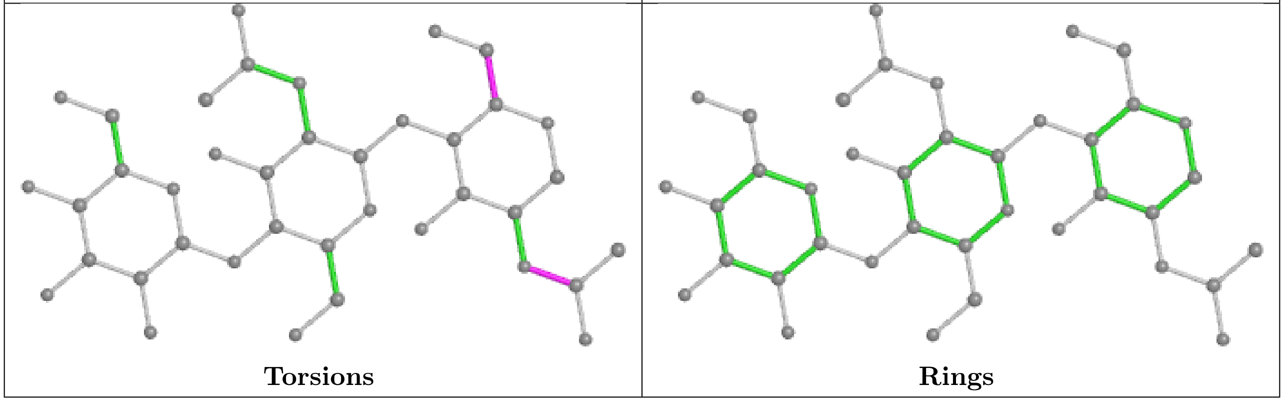
Rings

Oligosaccharide Chain w



Bond lengths

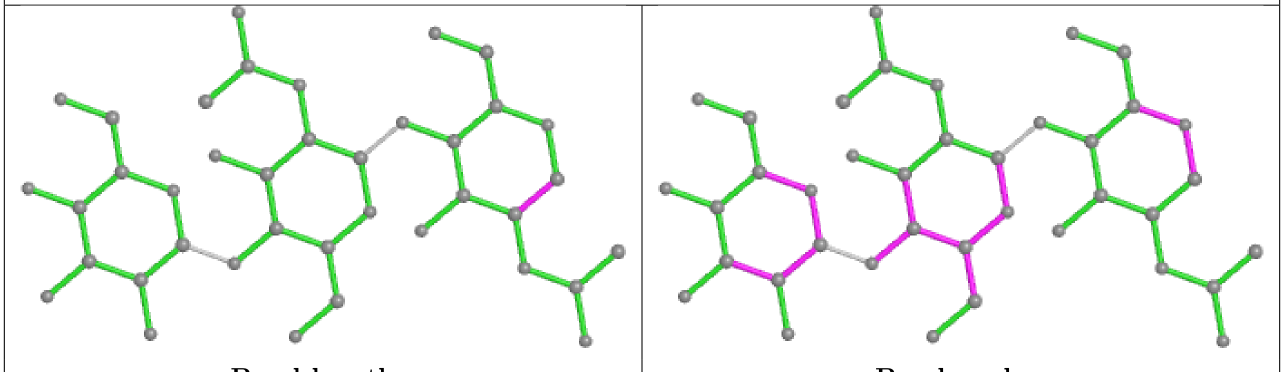
Bond angles



Torsions

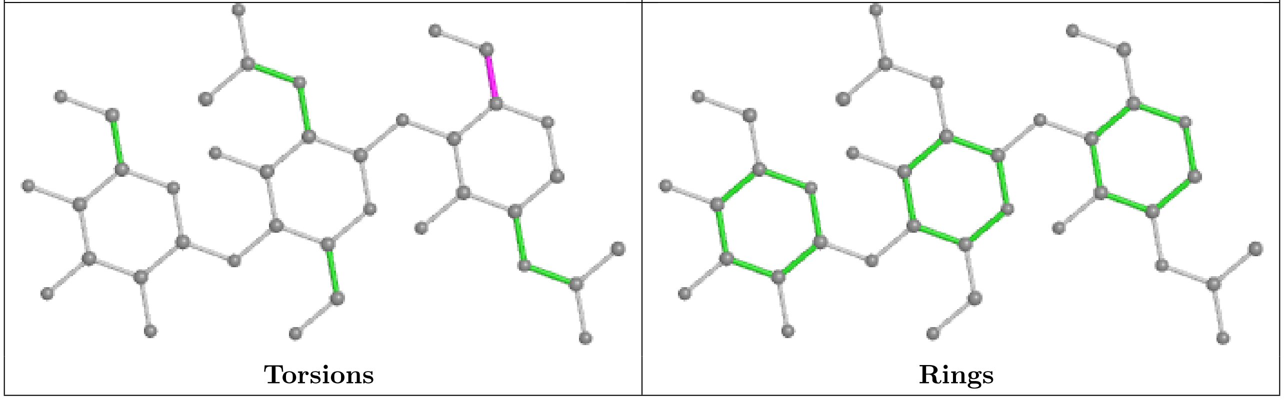
Rings

Oligosaccharide Chain y



Bond lengths

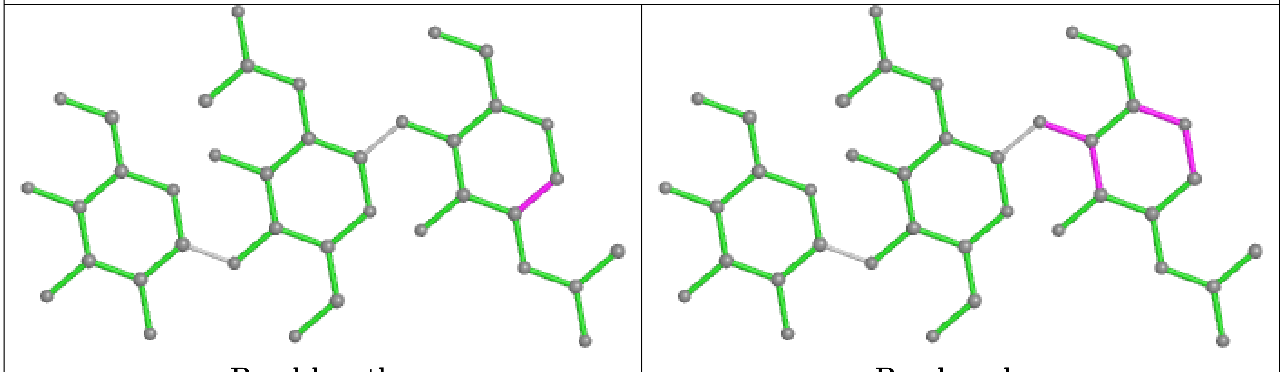
Bond angles



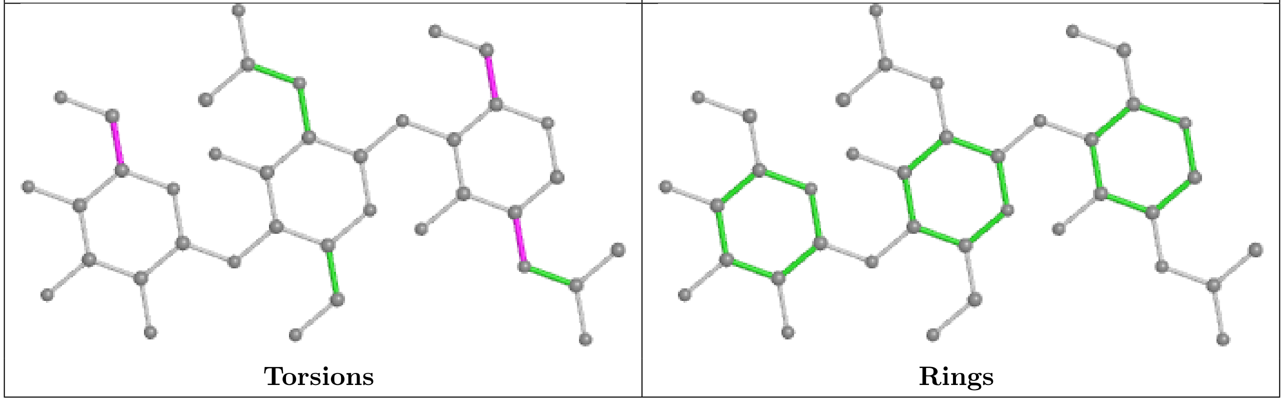
Torsions

Rings

Oligosaccharide Chain 3

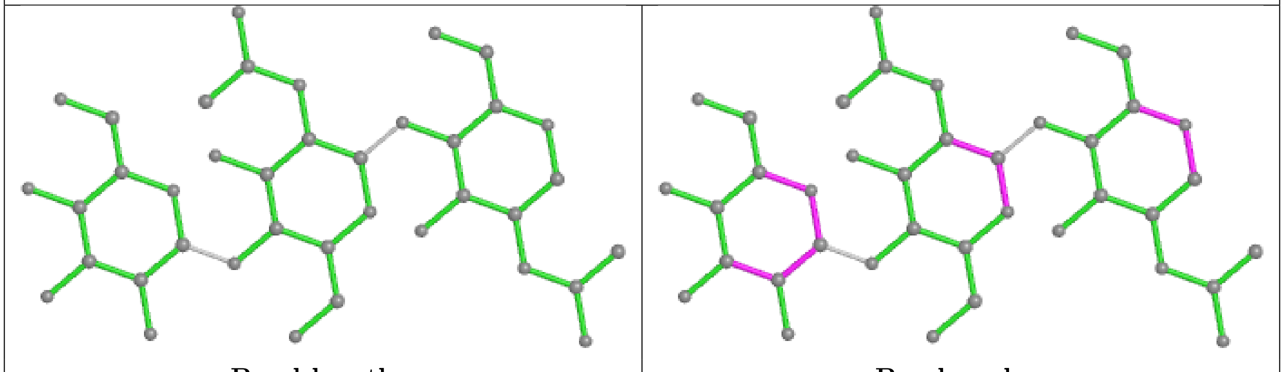


Bond lengths **Bond angles**

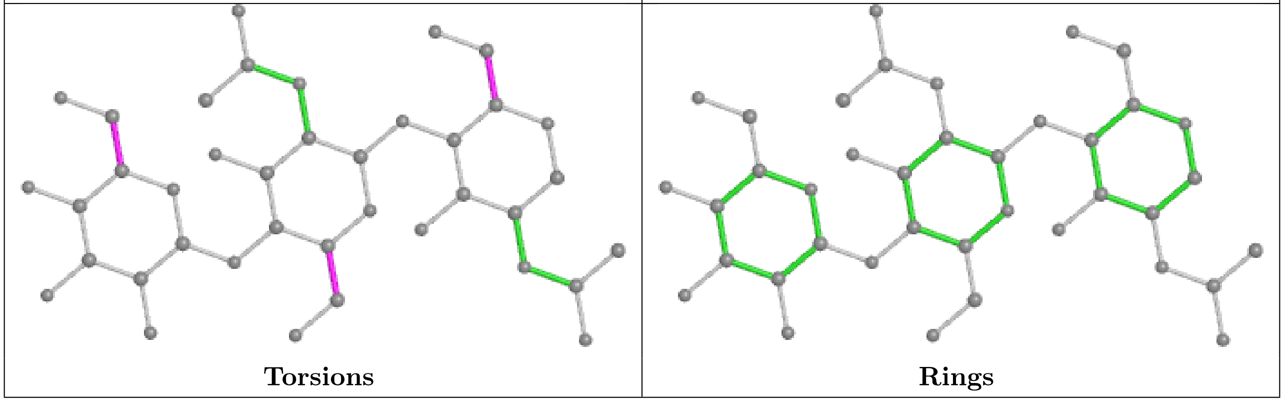


Torsions **Rings**

Oligosaccharide Chain 5

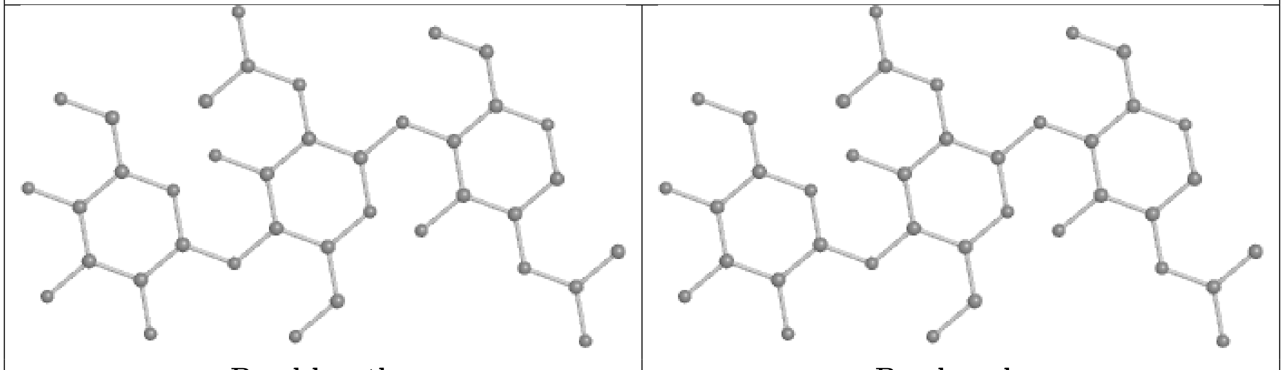


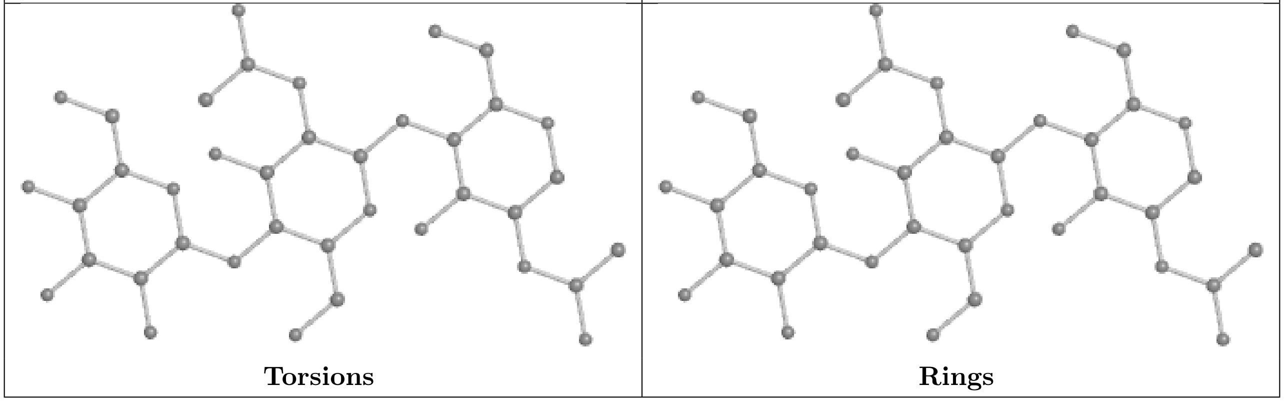
Bond lengths **Bond angles**



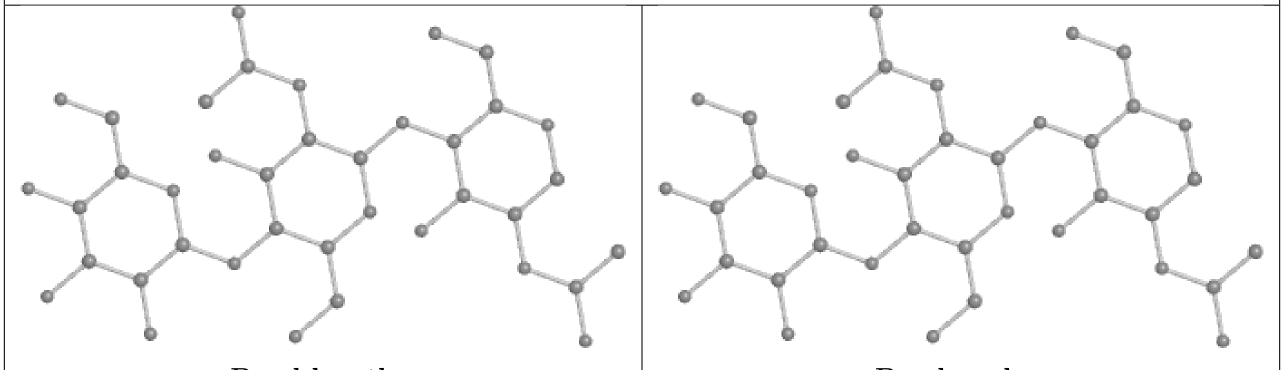
Torsions **Rings**

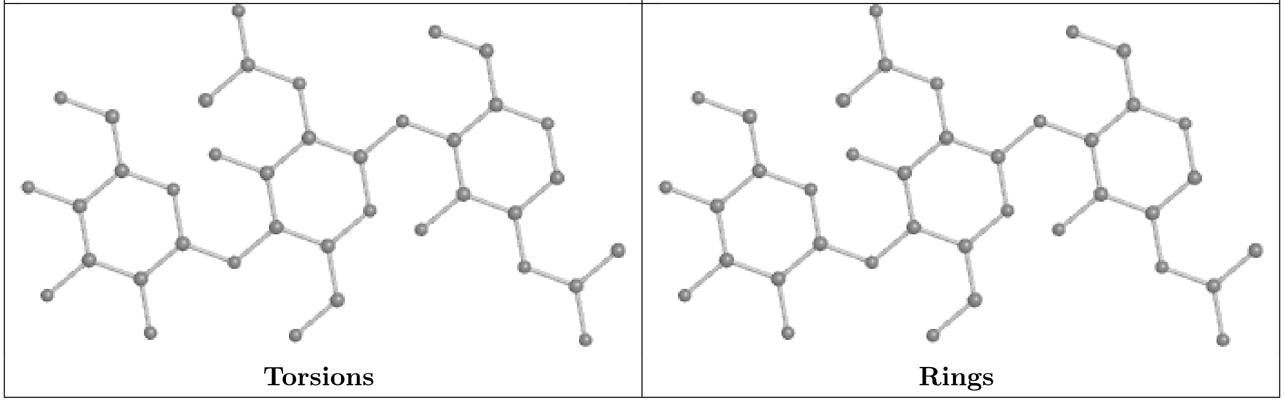
Oligosaccharide Chain CA


Bond lengths
Bond angles

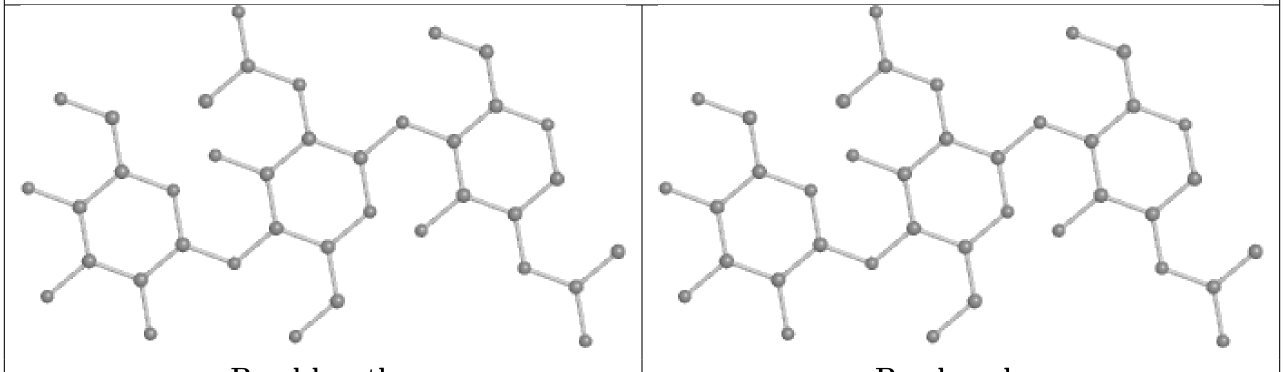

Torsions
Rings

Oligosaccharide Chain DA


Bond lengths
Bond angles

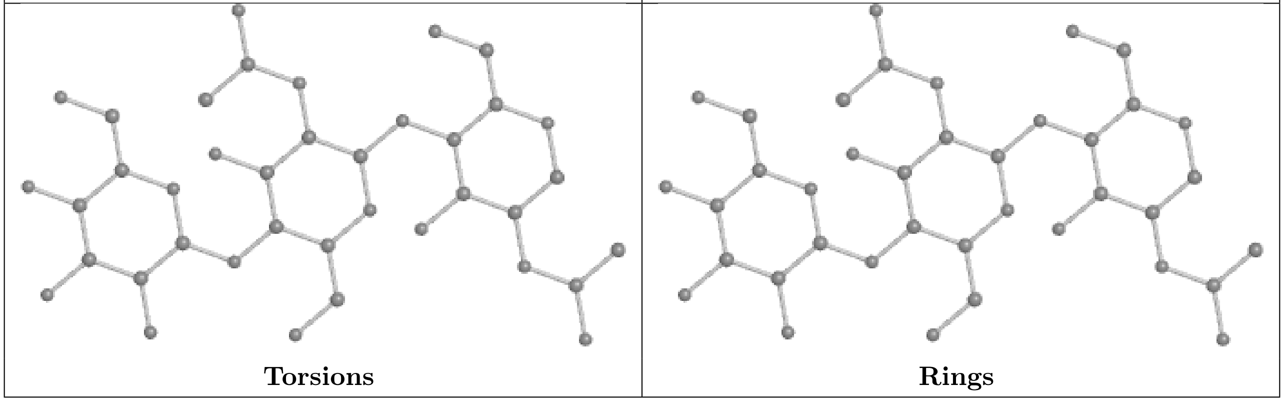

Torsions
Rings

Oligosaccharide Chain EA



Bond lengths

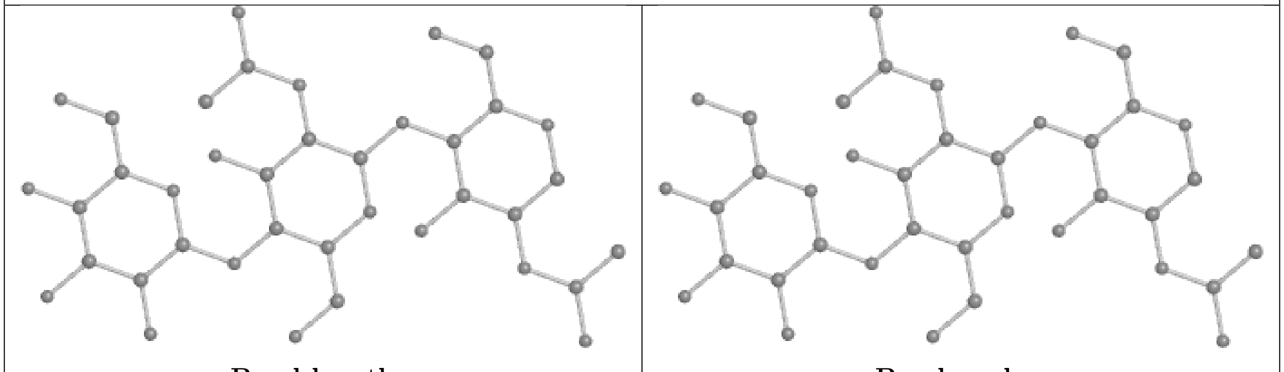
Bond angles



Torsions

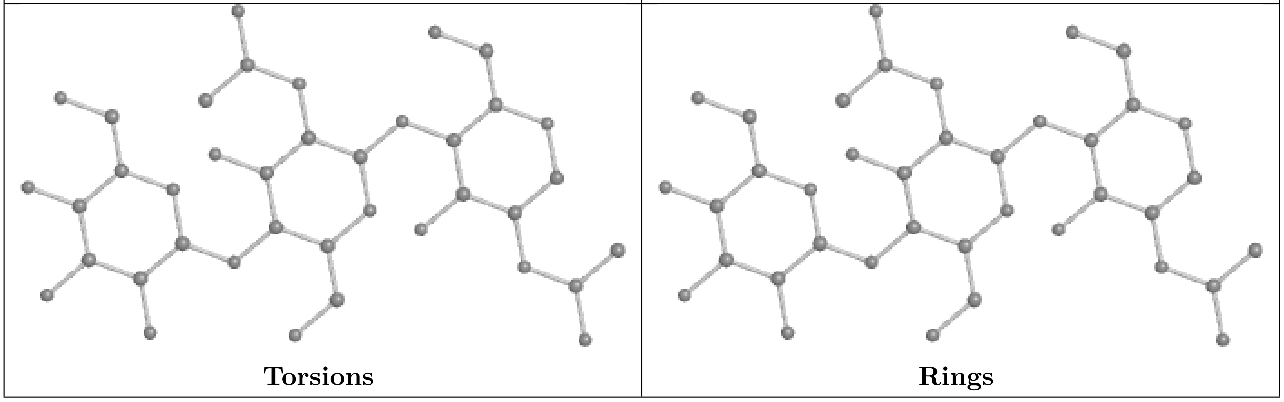
Rings

Oligosaccharide Chain GA



Bond lengths

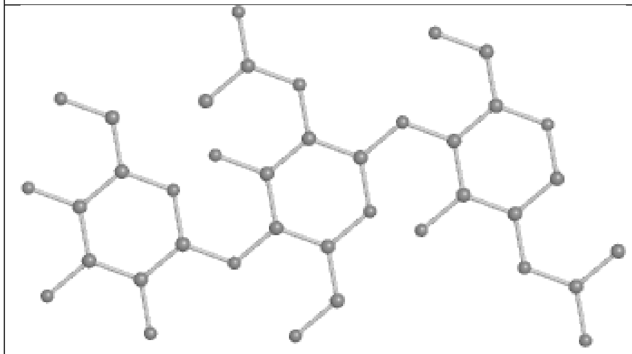
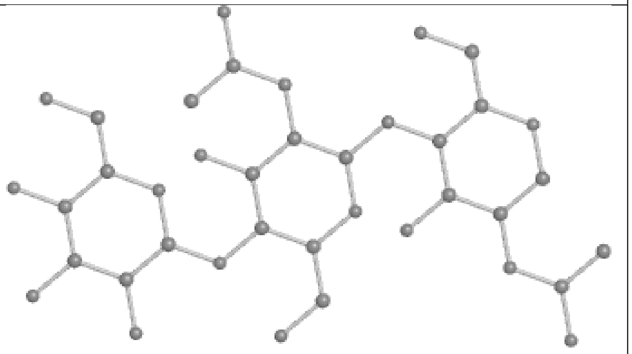
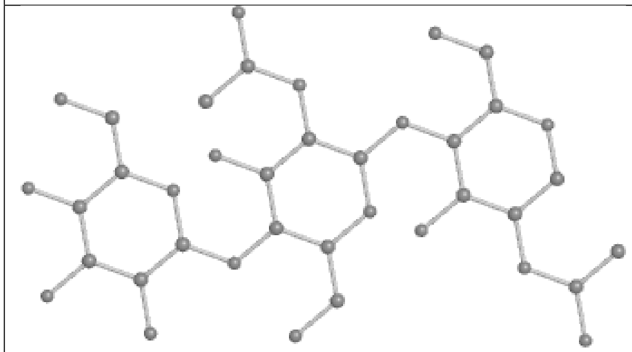
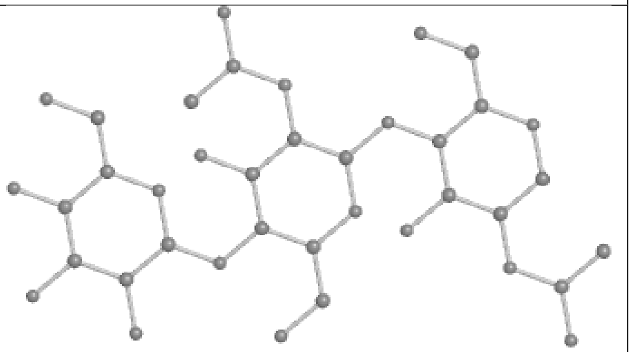
Bond angles



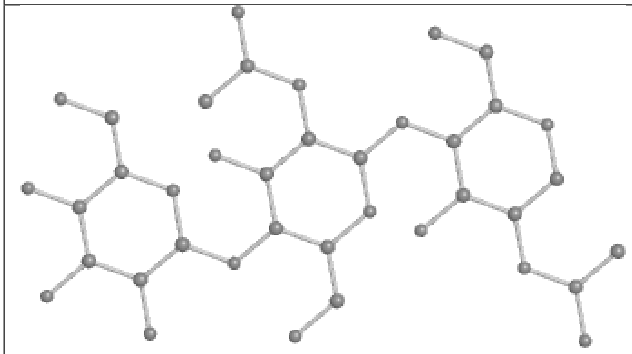
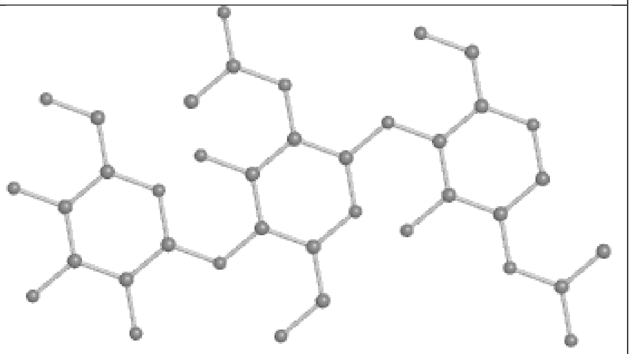
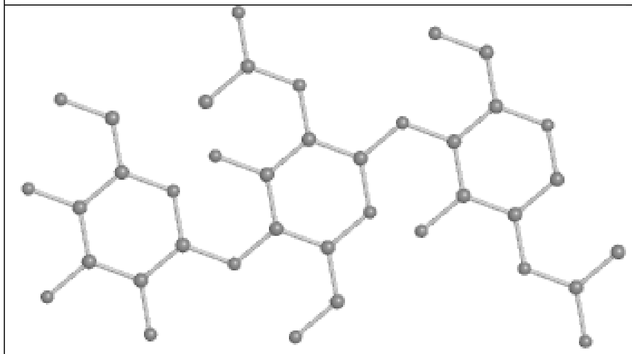
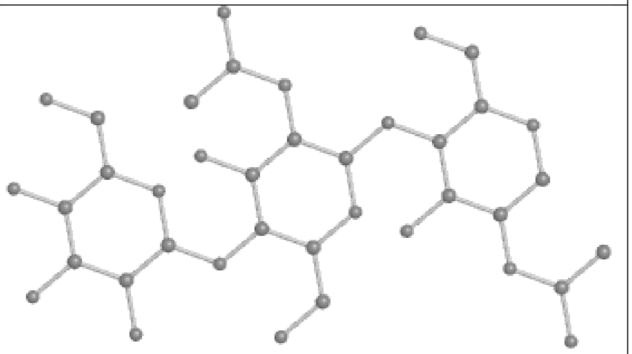
Torsions

Rings

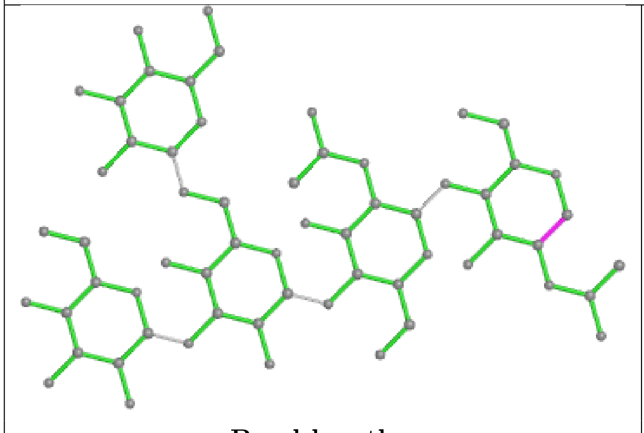
Oligosaccharide Chain LA

 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

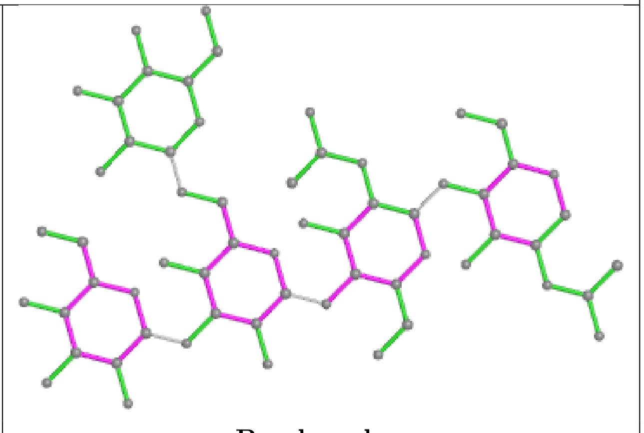
Oligosaccharide Chain NA

 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

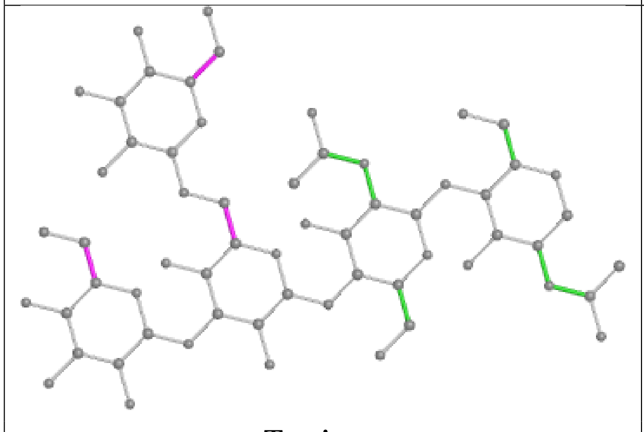
Oligosaccharide Chain z



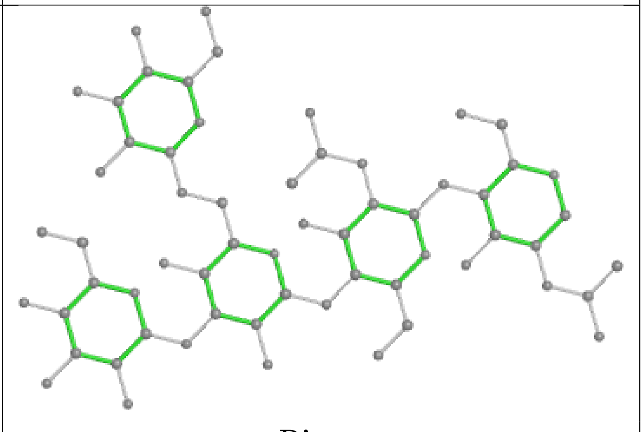
Bond lengths



Bond angles

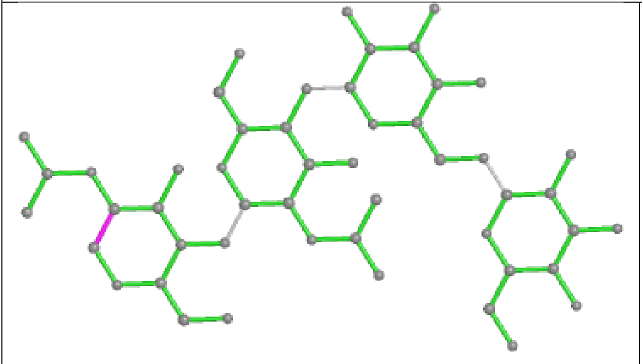


Torsions

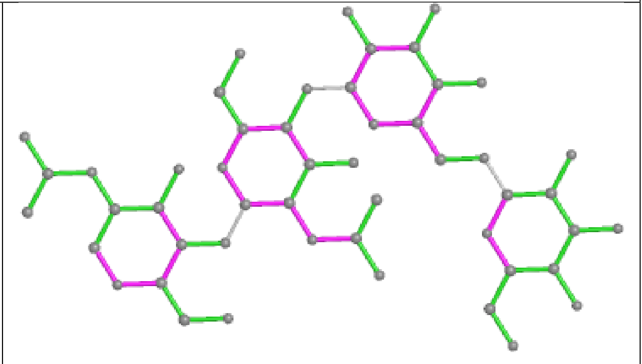


Rings

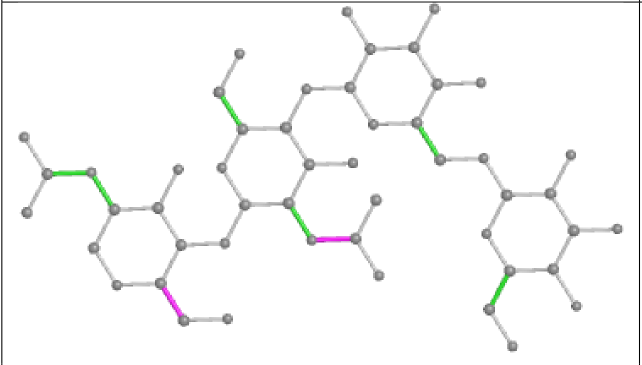
Oligosaccharide Chain 0



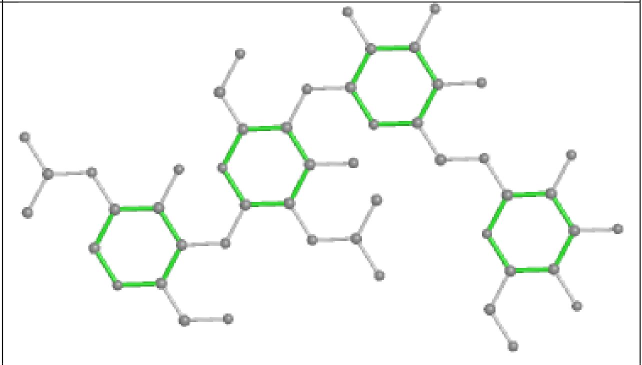
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry ⓘ

100 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	CUO	D	5016[C]	-	0,4,4	-	-	-		
9	CUO	I	3401[B]	3	0,4,4	-	-	-		
9	CUO	T	3001	2	0,4,4	-	-	-		
9	CUO	M	2105	1	0,4,4	-	-	-		
9	CUO	V	5004	1	0,4,4	-	-	-		
9	CUO	S	2102	1	0,4,4	-	-	-		
9	CUO	S	2104	1	0,4,4	-	-	-		
9	CUO	M	2103	1	0,4,4	-	-	-		
9	CUO	A	5016[D]	-	0,4,4	-	-	-		
9	CUO	S	2105	1	0,4,4	-	-	-		
9	CUO	V	5001	1	0,4,4	-	-	-		
9	CUO	G	2105	1	0,4,4	-	-	-		
9	CUO	N	3001	2	0,4,4	-	-	-		
9	CUO	V	5002	1	0,4,4	-	-	-		
9	CUO	b	2104	1	0,4,4	-	-	-		
9	CUO	C	3401[A]	3	0,4,4	-	-	-		
9	CUO	N	3002	2	0,4,4	-	-	-		
9	CUO	B	3001	2	0,4,4	-	-	-		
9	CUO	G	2104	1	0,4,4	-	-	-		
9	CUO	C	3401[B]	3	0,4,4	-	-	-		
9	CUO	Z	3001	2	0,4,4	-	-	-		
9	CUO	b	2102	1	0,4,4	-	-	-		
9	CUO	S	2103	1	0,4,4	-	-	-		
9	CUO	Y	2101[D]	-	0,4,4	-	-	-		
9	CUO	X	3401[A]	3	0,4,4	-	-	-		
9	CUO	W	3001	2	0,4,4	-	-	-		
9	CUO	X	3401[B]	3	0,4,4	-	-	-		
9	CUO	Y	2102	1	0,4,4	-	-	-		
9	CUO	B	3002	2	0,4,4	-	-	-		
9	CUO	H	3002	2	0,4,4	-	-	-		
9	CUO	Y	2105	1	0,4,4	-	-	-		
9	CUO	M	2101[D]	-	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	CUO	D	5002	1	0,4,4	-	-	-		
9	CUO	Y	2101[C]	-	0,4,4	-	-	-		
9	CUO	D	5001	1	0,4,4	-	-	-		
9	CUO	P	5015[D]	-	0,4,4	-	-	-		
9	CUO	G	2101[D]	-	0,4,4	-	-	-		
9	CUO	J	5004	1	0,4,4	-	-	-		
9	CUO	P	5002	1	0,4,4	-	-	-		
9	CUO	Q	3001	2	0,4,4	-	-	-		
9	CUO	S	2101[D]	-	0,4,4	-	-	-		
9	CUO	P	5003	1	0,4,4	-	-	-		
9	CUO	J	5014[D]	-	0,4,4	-	-	-		
9	CUO	F	3401[A]	3	0,4,4	-	-	-		
9	CUO	D	5004	1	0,4,4	-	-	-		
9	CUO	F	3401[B]	3	0,4,4	-	-	-		
9	CUO	C	3402[A]	3	0,4,4	-	-	-		
9	CUO	E	3002	2	0,4,4	-	-	-		
9	CUO	C	3402[B]	3	0,4,4	-	-	-		
9	CUO	M	2104	1	0,4,4	-	-	-		
9	CUO	A	5016[C]	-	0,4,4	-	-	-		
9	CUO	Y	2103	1	0,4,4	-	-	-		
9	CUO	E	3001	2	0,4,4	-	-	-		
9	CUO	G	2102	1	0,4,4	-	-	-		
9	CUO	b	2101[D]	-	0,4,4	-	-	-		
9	CUO	P	5004	1	0,4,4	-	-	-		
9	CUO	b	2105	1	0,4,4	-	-	-		
9	CUO	O	3401[A]	3	0,4,4	-	-	-		
9	CUO	Z	3002	2	0,4,4	-	-	-		
9	CUO	O	3401[B]	3	0,4,4	-	-	-		
9	CUO	A	5003	1	0,4,4	-	-	-		
9	CUO	P	5001	1	0,4,4	-	-	-		
9	CUO	U	3401[A]	3	0,4,4	-	-	-		
9	CUO	d	3401[A]	3	0,4,4	-	-	-		
9	CUO	U	3401[B]	3	0,4,4	-	-	-		
9	CUO	D	5016[D]	-	0,4,4	-	-	-		
9	CUO	F	3402[A]	3	0,4,4	-	-	-		
9	CUO	V	5003	1	0,4,4	-	-	-		
9	CUO	d	3401[B]	3	0,4,4	-	-	-		
9	CUO	F	3402[B]	3	0,4,4	-	-	-		
9	CUO	M	2101[C]	-	0,4,4	-	-	-		
9	CUO	c	3002	2	0,4,4	-	-	-		
9	CUO	P	5015[C]	-	0,4,4	-	-	-		
9	CUO	T	3002	2	0,4,4	-	-	-		
9	CUO	G	2101[C]	-	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
9	CUO	Q	3002	2	0,4,4	-	-	-		
9	CUO	S	2101[C]	-	0,4,4	-	-	-		
9	CUO	J	5001	1	0,4,4	-	-	-		
9	CUO	J	5014[C]	-	0,4,4	-	-	-		
9	CUO	J	5002	1	0,4,4	-	-	-		
9	CUO	V	5018[D]	-	0,4,4	-	-	-		
9	CUO	K	3002	2	0,4,4	-	-	-		
9	CUO	b	2103	1	0,4,4	-	-	-		
9	CUO	W	3002	2	0,4,4	-	-	-		
9	CUO	J	5003	1	0,4,4	-	-	-		
9	CUO	A	5002	1	0,4,4	-	-	-		
9	CUO	Y	2104	1	0,4,4	-	-	-		
9	CUO	b	2101[C]	-	0,4,4	-	-	-		
9	CUO	V	5018[C]	-	0,4,4	-	-	-		
9	CUO	K	3001	2	0,4,4	-	-	-		
9	CUO	D	5003	1	0,4,4	-	-	-		
9	CUO	A	5001	1	0,4,4	-	-	-		
9	CUO	M	2102	1	0,4,4	-	-	-		
9	CUO	A	5004	1	0,4,4	-	-	-		
9	CUO	G	2103	1	0,4,4	-	-	-		
9	CUO	I	3402[A]	3	0,4,4	-	-	-		
9	CUO	c	3001	2	0,4,4	-	-	-		
9	CUO	H	3001	2	0,4,4	-	-	-		
9	CUO	I	3402[B]	3	0,4,4	-	-	-		
9	CUO	I	3401[A]	3	0,4,4	-	-	-		

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	CUO	D	5016[C]	-	-	-	0/1/1/1
9	CUO	I	3401[B]	3	-	-	0/1/1/1
9	CUO	T	3001	2	-	-	0/1/1/1
9	CUO	M	2105	1	-	-	0/1/1/1
9	CUO	V	5004	1	-	-	0/1/1/1
9	CUO	S	2102	1	-	-	0/1/1/1
9	CUO	S	2104	1	-	-	0/1/1/1
9	CUO	M	2103	1	-	-	0/1/1/1
9	CUO	A	5016[D]	-	-	-	0/1/1/1
9	CUO	S	2105	1	-	-	0/1/1/1
9	CUO	V	5001	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CUO	G	2105	1	-	-	0/1/1/1
9	CUO	N	3001	2	-	-	0/1/1/1
9	CUO	V	5002	1	-	-	0/1/1/1
9	CUO	b	2104	1	-	-	0/1/1/1
9	CUO	C	3401[A]	3	-	-	0/1/1/1
9	CUO	N	3002	2	-	-	0/1/1/1
9	CUO	B	3001	2	-	-	0/1/1/1
9	CUO	G	2104	1	-	-	0/1/1/1
9	CUO	C	3401[B]	3	-	-	0/1/1/1
9	CUO	Z	3001	2	-	-	0/1/1/1
9	CUO	b	2102	1	-	-	0/1/1/1
9	CUO	S	2103	1	-	-	0/1/1/1
9	CUO	Y	2101[D]	-	-	-	0/1/1/1
9	CUO	X	3401[A]	3	-	-	0/1/1/1
9	CUO	W	3001	2	-	-	0/1/1/1
9	CUO	X	3401[B]	3	-	-	0/1/1/1
9	CUO	Y	2102	1	-	-	0/1/1/1
9	CUO	B	3002	2	-	-	0/1/1/1
9	CUO	H	3002	2	-	-	0/1/1/1
9	CUO	Y	2105	1	-	-	0/1/1/1
9	CUO	M	2101[D]	-	-	-	0/1/1/1
9	CUO	D	5002	1	-	-	0/1/1/1
9	CUO	Y	2101[C]	-	-	-	0/1/1/1
9	CUO	D	5001	1	-	-	0/1/1/1
9	CUO	P	5015[D]	-	-	-	0/1/1/1
9	CUO	G	2101[D]	-	-	-	0/1/1/1
9	CUO	J	5004	1	-	-	0/1/1/1
9	CUO	P	5002	1	-	-	0/1/1/1
9	CUO	Q	3001	2	-	-	0/1/1/1
9	CUO	S	2101[D]	-	-	-	0/1/1/1
9	CUO	P	5003	1	-	-	0/1/1/1
9	CUO	J	5014[D]	-	-	-	0/1/1/1
9	CUO	F	3401[A]	3	-	-	0/1/1/1
9	CUO	D	5004	1	-	-	0/1/1/1
9	CUO	F	3401[B]	3	-	-	0/1/1/1
9	CUO	C	3402[A]	3	-	-	0/1/1/1
9	CUO	E	3002	2	-	-	0/1/1/1
9	CUO	C	3402[B]	3	-	-	0/1/1/1
9	CUO	M	2104	1	-	-	0/1/1/1
9	CUO	A	5016[C]	-	-	-	0/1/1/1
9	CUO	Y	2103	1	-	-	0/1/1/1
9	CUO	E	3001	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CUO	G	2102	1	-	-	0/1/1/1
9	CUO	b	2101[D]	-	-	-	0/1/1/1
9	CUO	P	5004	1	-	-	0/1/1/1
9	CUO	b	2105	1	-	-	0/1/1/1
9	CUO	O	3401[A]	3	-	-	0/1/1/1
9	CUO	Z	3002	2	-	-	0/1/1/1
9	CUO	O	3401[B]	3	-	-	0/1/1/1
9	CUO	A	5003	1	-	-	0/1/1/1
9	CUO	P	5001	1	-	-	0/1/1/1
9	CUO	U	3401[A]	3	-	-	0/1/1/1
9	CUO	d	3401[A]	3	-	-	0/1/1/1
9	CUO	U	3401[B]	3	-	-	0/1/1/1
9	CUO	D	5016[D]	-	-	-	0/1/1/1
9	CUO	F	3402[A]	3	-	-	0/1/1/1
9	CUO	V	5003	1	-	-	0/1/1/1
9	CUO	d	3401[B]	3	-	-	0/1/1/1
9	CUO	F	3402[B]	3	-	-	0/1/1/1
9	CUO	M	2101[C]	-	-	-	0/1/1/1
9	CUO	c	3002	2	-	-	0/1/1/1
9	CUO	P	5015[C]	-	-	-	0/1/1/1
9	CUO	T	3002	2	-	-	0/1/1/1
9	CUO	G	2101[C]	-	-	-	0/1/1/1
9	CUO	Q	3002	2	-	-	0/1/1/1
9	CUO	S	2101[C]	-	-	-	0/1/1/1
9	CUO	J	5001	1	-	-	0/1/1/1
9	CUO	J	5014[C]	-	-	-	0/1/1/1
9	CUO	J	5002	1	-	-	0/1/1/1
9	CUO	V	5018[D]	-	-	-	0/1/1/1
9	CUO	K	3002	2	-	-	0/1/1/1
9	CUO	b	2103	1	-	-	0/1/1/1
9	CUO	W	3002	2	-	-	0/1/1/1
9	CUO	J	5003	1	-	-	0/1/1/1
9	CUO	A	5002	1	-	-	0/1/1/1
9	CUO	Y	2104	1	-	-	0/1/1/1
9	CUO	b	2101[C]	-	-	-	0/1/1/1
9	CUO	V	5018[C]	-	-	-	0/1/1/1
9	CUO	K	3001	2	-	-	0/1/1/1
9	CUO	D	5003	1	-	-	0/1/1/1
9	CUO	A	5001	1	-	-	0/1/1/1
9	CUO	M	2102	1	-	-	0/1/1/1
9	CUO	A	5004	1	-	-	0/1/1/1
9	CUO	G	2103	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CUO	I	3402[A]	3	-	-	0/1/1/1
9	CUO	c	3001	2	-	-	0/1/1/1
9	CUO	H	3001	2	-	-	0/1/1/1
9	CUO	I	3402[B]	3	-	-	0/1/1/1
9	CUO	I	3401[A]	3	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	3401[B]	CUO	1	0
9	M	2105	CUO	2	0
9	V	5004	CUO	1	0
9	S	2102	CUO	1	0
9	S	2104	CUO	2	0
9	C	3401[A]	CUO	5	0
9	G	2104	CUO	1	0
9	C	3401[B]	CUO	2	0
9	X	3401[A]	CUO	5	0
9	X	3401[B]	CUO	5	0
9	Y	2102	CUO	1	0
9	Y	2105	CUO	1	0
9	D	5001	CUO	1	0
9	D	5004	CUO	1	0
9	F	3401[B]	CUO	2	0
9	C	3402[A]	CUO	5	0
9	C	3402[B]	CUO	2	0
9	M	2104	CUO	1	0
9	O	3401[A]	CUO	5	0
9	O	3401[B]	CUO	5	0
9	U	3401[A]	CUO	5	0
9	U	3401[B]	CUO	5	0
9	F	3402[A]	CUO	5	0
9	V	5003	CUO	1	0
9	T	3002	CUO	1	0
9	J	5001	CUO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	5002	CUO	1	0
9	W	3002	CUO	1	0
9	Y	2104	CUO	1	0
9	A	5001	CUO	2	0
9	I	3402[A]	CUO	5	0
9	I	3402[B]	CUO	1	0
9	I	3401[A]	CUO	5	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1656/2000 (82%)	-0.30	28 (1%)	70	41	36, 70, 118, 164	0
1	D	1656/2000 (82%)	-0.30	34 (2%)	63	34	37, 67, 114, 176	0
1	G	1656/2000 (82%)	-0.33	24 (1%)	75	49	31, 68, 109, 152	0
1	J	1656/2000 (82%)	-0.30	31 (1%)	66	37	30, 64, 119, 162	0
1	M	1656/2000 (82%)	-0.40	21 (1%)	77	51	29, 56, 109, 157	0
1	P	1656/2000 (82%)	-0.44	19 (1%)	80	56	27, 53, 97, 176	0
1	S	1656/2000 (82%)	-0.40	32 (1%)	66	37	31, 60, 108, 164	0
1	V	1656/2000 (82%)	-0.46	15 (0%)	84	63	26, 55, 105, 154	0
1	Y	1656/2000 (82%)	-0.36	17 (1%)	82	59	31, 66, 112, 160	0
1	b	1656/2000 (82%)	-0.41	17 (1%)	82	59	30, 60, 105, 161	0
2	B	825/920 (89%)	-0.52	4 (0%)	91	75	32, 57, 101, 140	0
2	E	825/920 (89%)	-0.48	8 (0%)	82	59	30, 59, 106, 137	0
2	H	825/920 (89%)	-0.42	10 (1%)	79	54	31, 63, 112, 147	0
2	K	825/920 (89%)	-0.43	6 (0%)	87	69	34, 60, 101, 158	0
2	N	825/920 (89%)	-0.54	5 (0%)	89	72	21, 46, 92, 135	0
2	Q	825/920 (89%)	-0.54	3 (0%)	92	79	26, 49, 100, 134	0
2	T	825/920 (89%)	-0.51	3 (0%)	92	79	30, 53, 93, 137	0
2	W	825/920 (89%)	-0.54	2 (0%)	95	87	25, 53, 99, 129	0
2	Z	825/920 (89%)	-0.51	5 (0%)	89	72	25, 52, 95, 130	0
2	c	825/920 (89%)	-0.52	6 (0%)	87	69	26, 55, 103, 135	0
3	C	366/394 (92%)	2.76	232 (63%)	0	0	68, 90, 99, 110	0
3	F	366/394 (92%)	2.44	196 (53%)	0	0	56, 78, 88, 107	0
3	I	366/394 (92%)	2.52	204 (55%)	0	0	57, 78, 91, 111	0
3	L	366/394 (92%)	2.61	215 (58%)	0	0	64, 89, 99, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
3	O	366/394 (92%)	2.37	192 (52%)	0	0	52, 75, 95, 106	0
3	R	366/394 (92%)	2.52	215 (58%)	0	0	59, 79, 90, 109	0
3	U	366/394 (92%)	2.28	171 (46%)	0	0	52, 74, 93, 103	0
3	X	366/394 (92%)	4.89	344 (93%)	0	0	79, 102, 111, 116	0
3	a	366/394 (92%)	2.40	190 (51%)	0	0	54, 76, 88, 96	0
3	d	366/394 (92%)	4.59	331 (90%)	0	0	81, 99, 107, 111	0
All	All	28470/33140 (85%)	0.02	2580 (9%)	9	3	21, 63, 107, 176	0

The worst 5 of 2580 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	d	2977[A]	CYS	16.0
3	d	3101[A]	PRO	15.1
3	X	2979[A]	GLN	14.3
3	a	3062[A]	GLN	13.4
3	O	3062[A]	GLN	12.9

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	CA	3	11/12	0.39	0.29	96,123,130,130	0
5	BMA	FA	3	11/12	0.58	0.23	85,101,110,113	0
7	BMA	z	3	11/12	0.59	0.40	124,134,140,150	0
7	MAN	z	4	11/12	0.60	0.44	135,140,150,154	0
4	NAG	x	2	14/15	0.62	0.23	104,115,125,125	0
7	MAN	z	5	11/12	0.63	0.36	121,135,151,154	0
6	BMA	GA	3	11/12	0.64	0.29	130,136,142,143	0
4	NAG	4	2	14/15	0.66	0.32	78,96,107,116	0
6	BMA	5	3	11/12	0.68	0.19	98,114,124,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	KA	4	11/12	0.70	0.32	87,103,122,135	0
5	MAN	g	4	11/12	0.70	0.20	103,117,133,133	0
6	BMA	LA	3	11/12	0.70	0.25	101,110,119,119	0
8	BMA	0	3	11/12	0.71	0.25	97,112,128,130	0
6	BMA	h	3	11/12	0.72	0.31	108,114,120,126	0
5	MAN	FA	4	11/12	0.72	0.31	94,107,126,132	0
5	MAN	l	4	11/12	0.72	0.21	114,118,122,128	0
4	NAG	s	2	14/15	0.73	0.36	89,102,108,116	0
6	BMA	EA	3	11/12	0.74	0.35	104,115,132,134	0
6	BMA	NA	3	11/12	0.74	0.49	102,117,134,138	0
4	NAG	7	2	14/15	0.74	0.32	69,83,101,104	0
5	BMA	l	3	11/12	0.75	0.26	98,113,119,128	0
6	BMA	y	3	11/12	0.76	0.30	102,116,123,123	0
6	BMA	3	3	11/12	0.76	0.18	114,119,149,149	0
4	NAG	1	2	14/15	0.76	0.26	91,104,121,126	0
4	NAG	t	2	14/15	0.76	0.25	50,90,102,103	0
6	BMA	r	3	11/12	0.77	0.28	111,120,128,129	0
8	MAN	0	4	11/12	0.78	0.20	94,114,123,126	0
4	NAG	BA	2	14/15	0.79	0.19	62,82,95,101	0
6	NAG	w	2	14/15	0.80	0.19	88,104,108,111	0
5	NAG	g	2	14/15	0.80	0.29	99,105,109,109	0
4	NAG	m	1	14/15	0.81	0.19	77,91,99,104	0
7	NAG	z	2	14/15	0.81	0.29	92,105,121,128	0
6	NAG	DA	2	14/15	0.81	0.26	78,91,95,98	0
4	NAG	f	2	14/15	0.81	0.27	106,116,123,129	0
6	BMA	k	3	11/12	0.81	0.23	110,119,126,133	0
6	NAG	LA	1	14/15	0.81	0.21	78,87,93,98	0
4	NAG	QA	2	14/15	0.81	0.16	97,115,121,125	0
5	NAG	FA	2	14/15	0.82	0.20	74,88,101,105	0
6	NAG	CA	2	14/15	0.82	0.30	88,97,115,124	0
5	MAN	PA	4	11/12	0.82	0.15	107,112,125,133	0
4	NAG	n	2	14/15	0.82	0.28	72,91,105,110	0
5	NAG	l	2	14/15	0.82	0.21	69,84,96,97	0
5	MAN	AA	4	11/12	0.83	0.18	114,125,132,145	0
4	NAG	9	2	14/15	0.83	0.25	73,97,113,113	0
6	BMA	w	3	11/12	0.83	0.30	107,110,117,128	0
4	NAG	e	2	14/15	0.83	0.23	69,83,96,102	0
4	NAG	QA	1	14/15	0.83	0.22	97,107,114,118	0
6	NAG	5	2	14/15	0.84	0.17	61,77,95,103	0
4	NAG	MA	2	14/15	0.84	0.19	84,93,116,127	0
6	NAG	w	1	14/15	0.84	0.21	78,100,106,118	0
4	NAG	i	2	14/15	0.84	0.26	84,92,107,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	h	2	14/15	0.84	0.15	84,94,107,114	0
6	NAG	EA	2	14/15	0.84	0.20	70,82,98,108	0
4	NAG	u	2	14/15	0.84	0.22	86,100,114,132	0
6	NAG	GA	2	14/15	0.84	0.17	88,108,127,131	0
4	NAG	x	1	14/15	0.84	0.15	80,94,105,105	0
4	NAG	v	2	14/15	0.85	0.19	82,97,104,106	0
5	NAG	KA	2	14/15	0.85	0.19	67,81,92,93	0
5	BMA	KA	3	11/12	0.85	0.26	79,99,114,127	0
4	NAG	8	2	14/15	0.85	0.19	64,84,98,101	0
6	BMA	DA	3	11/12	0.85	0.24	82,103,108,108	0
4	NAG	1	1	14/15	0.85	0.19	88,96,102,103	0
7	NAG	z	1	14/15	0.86	0.16	79,85,93,96	0
4	NAG	m	2	14/15	0.86	0.23	80,95,108,108	0
4	NAG	JA	2	14/15	0.86	0.21	82,92,100,100	0
5	NAG	PA	2	14/15	0.86	0.15	72,80,89,91	0
6	NAG	3	1	14/15	0.86	0.19	46,67,81,90	0
8	NAG	0	2	14/15	0.86	0.16	58,78,82,90	0
5	BMA	PA	3	11/12	0.86	0.17	96,97,104,125	0
4	NAG	o	1	14/15	0.86	0.22	61,73,85,88	0
4	NAG	p	2	14/15	0.87	0.14	54,72,84,88	0
6	NAG	r	1	14/15	0.87	0.25	79,88,107,112	0
5	BMA	AA	3	11/12	0.87	0.14	112,120,124,127	0
5	BMA	g	3	11/12	0.88	0.17	110,124,133,139	0
4	NAG	HA	2	14/15	0.88	0.20	71,82,95,107	0
4	NAG	IA	2	14/15	0.88	0.15	75,89,96,100	0
4	NAG	JA	1	14/15	0.88	0.19	70,80,88,90	0
6	NAG	CA	1	14/15	0.88	0.17	59,71,83,91	0
5	NAG	g	1	14/15	0.88	0.18	57,79,95,97	0
4	NAG	6	2	14/15	0.88	0.21	49,73,85,91	0
6	NAG	k	1	14/15	0.88	0.15	71,83,92,99	0
4	NAG	i	1	14/15	0.89	0.19	59,68,91,95	0
4	NAG	t	1	14/15	0.89	0.15	53,69,82,85	0
4	NAG	6	1	14/15	0.89	0.19	74,81,89,91	0
6	NAG	3	2	14/15	0.89	0.17	61,82,96,102	0
6	NAG	GA	1	14/15	0.89	0.28	79,97,106,109	0
6	NAG	h	1	14/15	0.89	0.14	85,93,112,115	0
6	NAG	LA	2	14/15	0.90	0.14	76,89,100,104	0
4	NAG	e	1	14/15	0.90	0.11	62,79,86,94	0
5	NAG	AA	2	14/15	0.90	0.17	87,92,98,104	0
4	NAG	u	1	14/15	0.90	0.22	73,78,87,92	0
4	NAG	RA	1	14/15	0.90	0.21	75,83,99,108	0
4	NAG	HA	1	14/15	0.90	0.15	56,63,83,93	0

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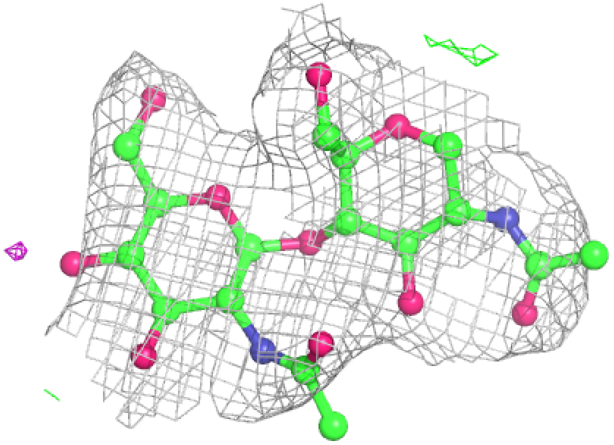
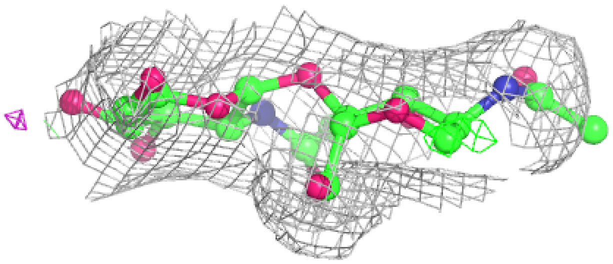
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	o	2	14/15	0.90	0.20	43,67,86,87	0
4	NAG	p	1	14/15	0.90	0.14	47,61,75,75	0
4	NAG	8	1	14/15	0.90	0.16	57,62,72,81	0
4	NAG	2	1	14/15	0.90	0.14	41,56,75,80	0
4	NAG	9	1	14/15	0.90	0.15	87,95,100,108	0
6	NAG	r	2	14/15	0.91	0.13	84,91,98,102	0
4	NAG	BA	1	14/15	0.91	0.16	80,84,96,97	0
4	NAG	IA	1	14/15	0.91	0.15	51,66,83,92	0
5	NAG	PA	1	14/15	0.91	0.19	62,72,77,78	0
4	NAG	OA	2	14/15	0.91	0.16	55,73,85,91	0
6	NAG	k	2	14/15	0.91	0.14	88,104,119,123	0
8	NAG	0	1	14/15	0.91	0.19	60,67,72,81	0
4	NAG	f	1	14/15	0.91	0.13	88,95,105,109	0
4	NAG	v	1	14/15	0.91	0.19	64,80,91,91	0
6	NAG	NA	2	14/15	0.91	0.23	61,80,101,112	0
4	NAG	n	1	14/15	0.92	0.17	67,77,90,98	0
4	NAG	q	2	14/15	0.92	0.16	80,88,92,93	0
6	NAG	DA	1	14/15	0.92	0.17	50,66,77,82	0
4	NAG	2	2	14/15	0.92	0.20	53,71,87,100	0
4	NAG	RA	2	14/15	0.92	0.24	83,92,102,114	0
5	NAG	l	1	14/15	0.92	0.15	52,57,72,76	0
4	NAG	s	1	14/15	0.93	0.18	71,77,85,90	0
6	NAG	y	1	14/15	0.93	0.13	52,67,74,75	0
4	NAG	q	1	14/15	0.93	0.15	56,67,78,80	0
5	NAG	FA	1	14/15	0.93	0.16	49,68,77,78	0
6	NAG	EA	1	14/15	0.93	0.15	46,58,71,75	0
4	NAG	j	1	14/15	0.93	0.16	59,67,76,76	0
4	NAG	j	2	14/15	0.94	0.19	49,57,73,79	0
6	NAG	y	2	14/15	0.94	0.22	65,83,94,109	0
4	NAG	7	1	14/15	0.94	0.14	57,70,83,84	0
6	NAG	NA	1	14/15	0.94	0.13	56,62,71,72	0
4	NAG	OA	1	14/15	0.94	0.11	57,70,80,85	0
4	NAG	MA	1	14/15	0.95	0.10	69,77,85,86	0
4	NAG	4	1	14/15	0.95	0.08	57,70,74,80	0
6	NAG	5	1	14/15	0.95	0.16	52,60,70,76	0
5	NAG	AA	1	14/15	0.95	0.14	61,71,75,75	0
5	NAG	KA	1	14/15	0.96	0.13	60,66,76,78	0

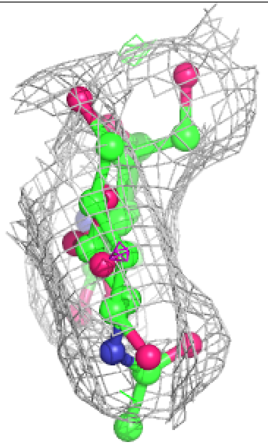
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain e:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

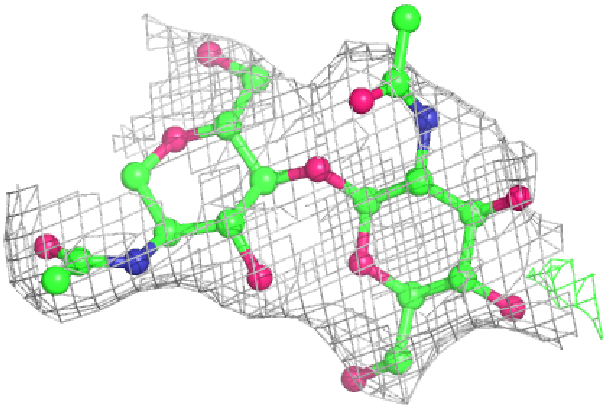


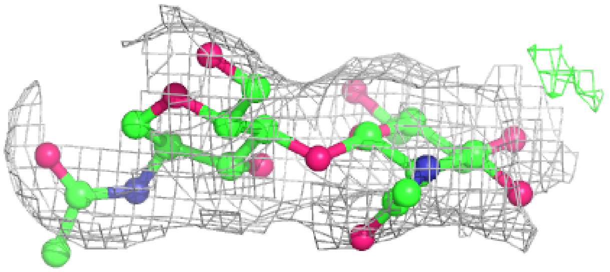


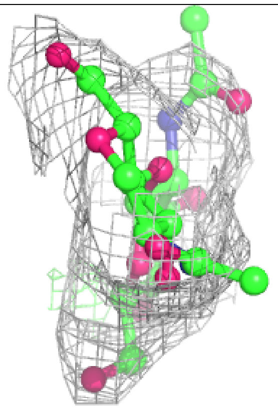


Electron density around Chain f:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

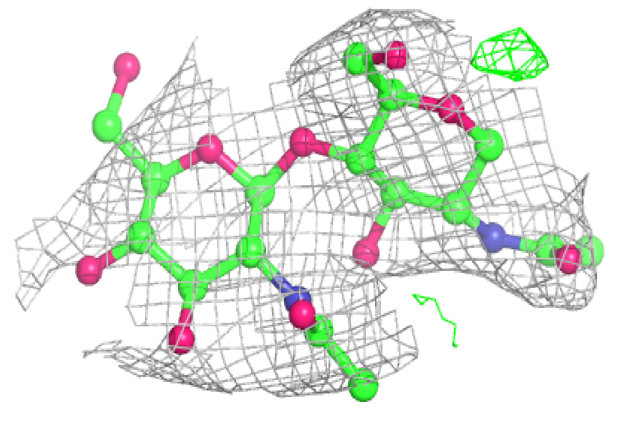


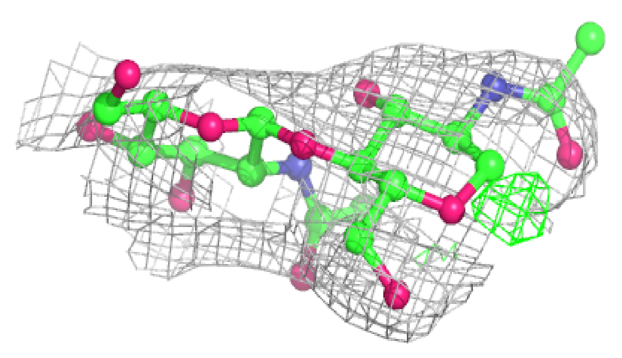


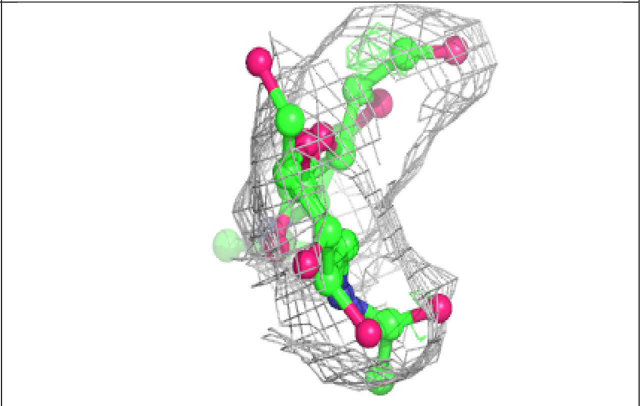


Electron density around Chain i:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

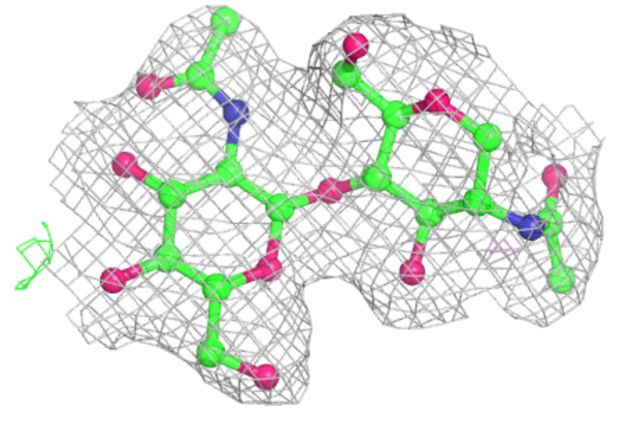


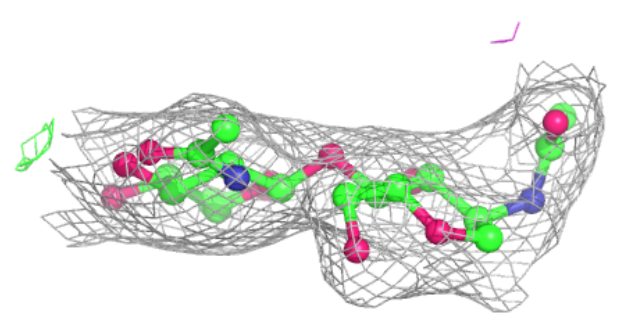


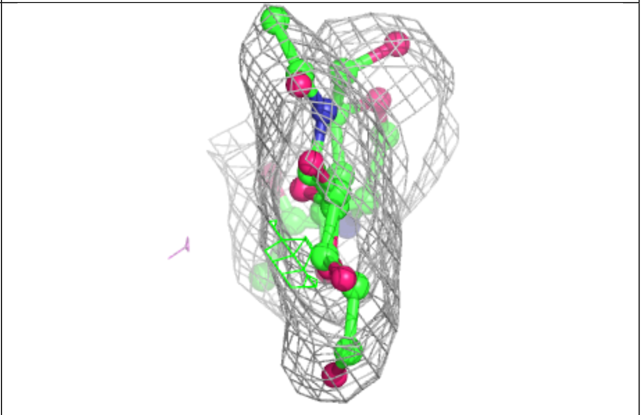


Electron density around Chain j:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

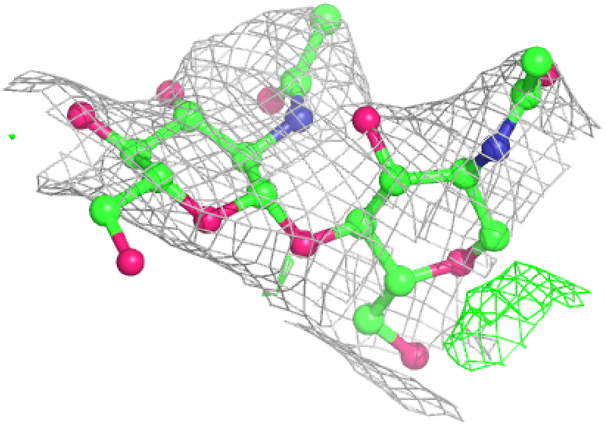


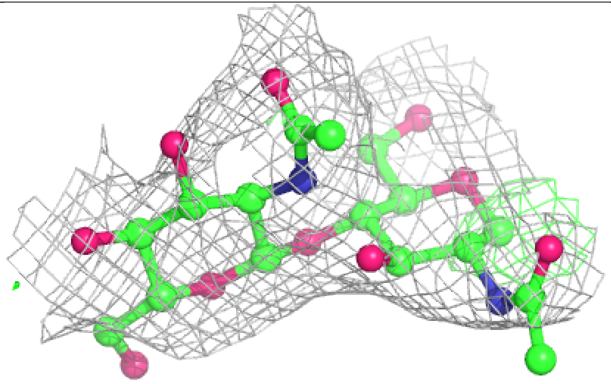


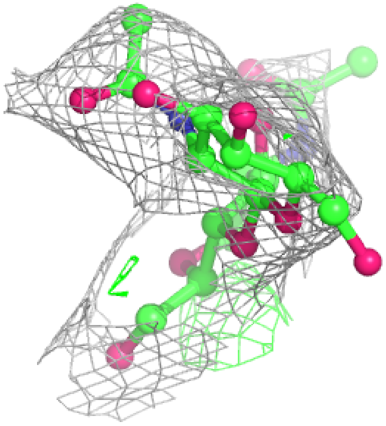


Electron density around Chain m:

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

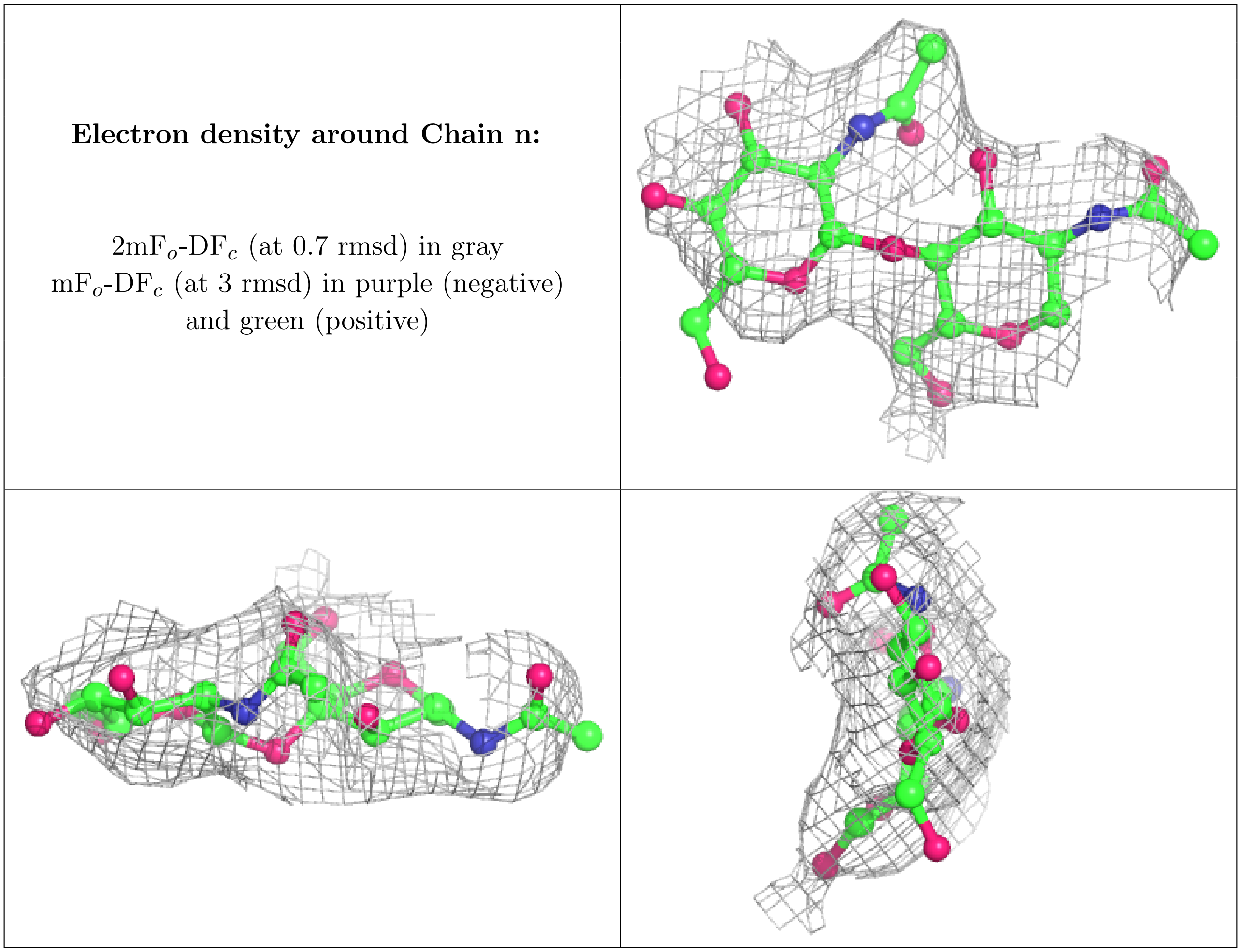






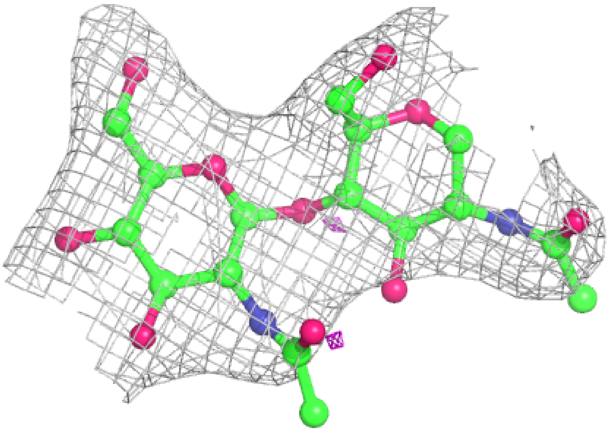
Electron density around Chain n:

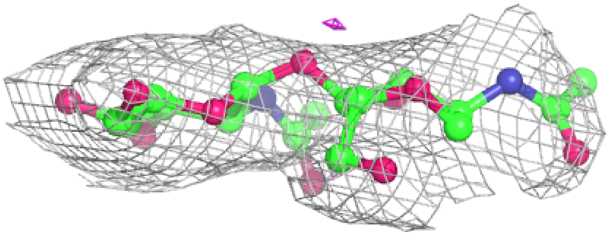
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

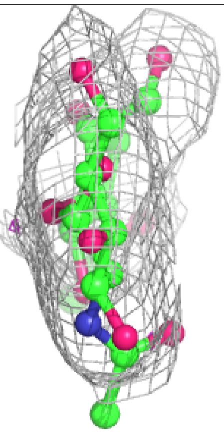


Electron density around Chain o:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

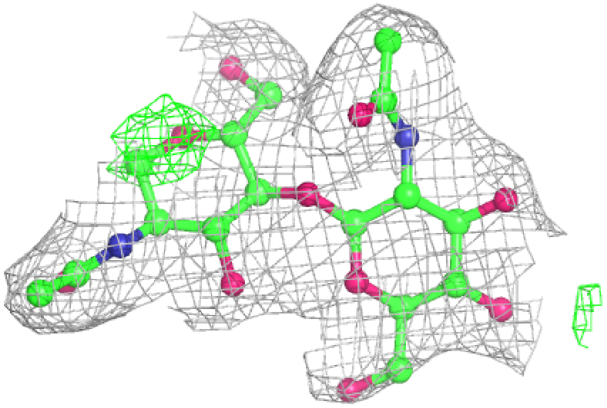


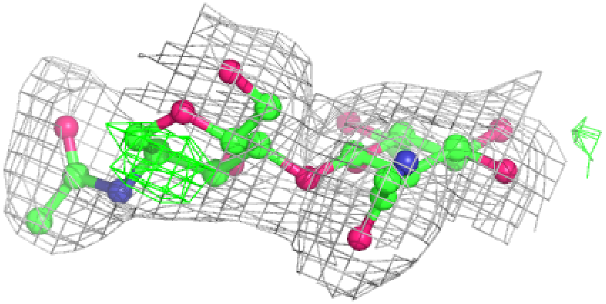


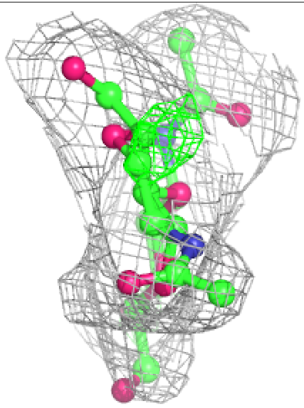


Electron density around Chain p:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

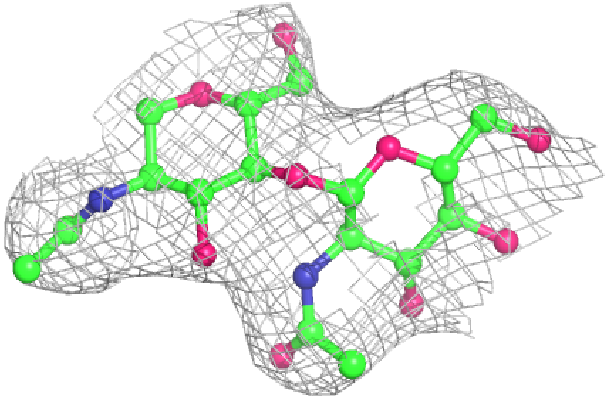


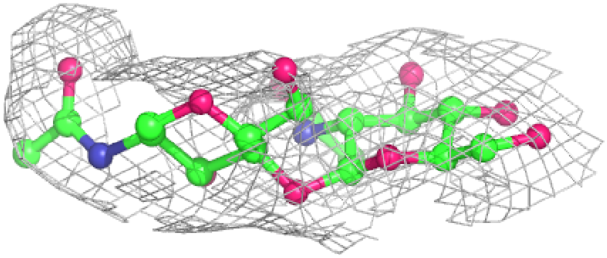


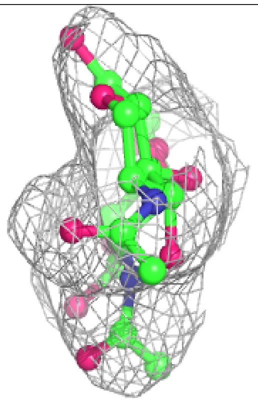


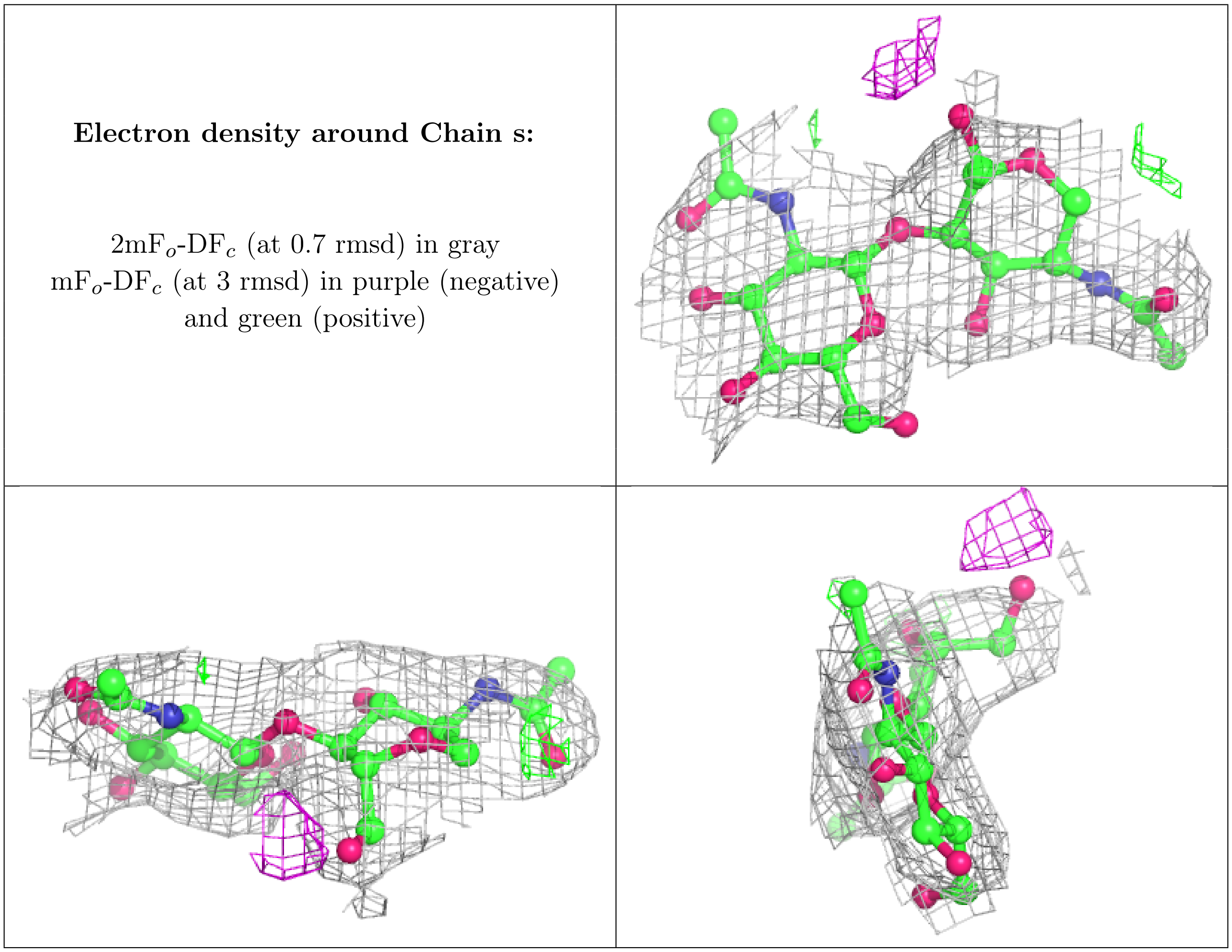
Electron density around Chain q:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







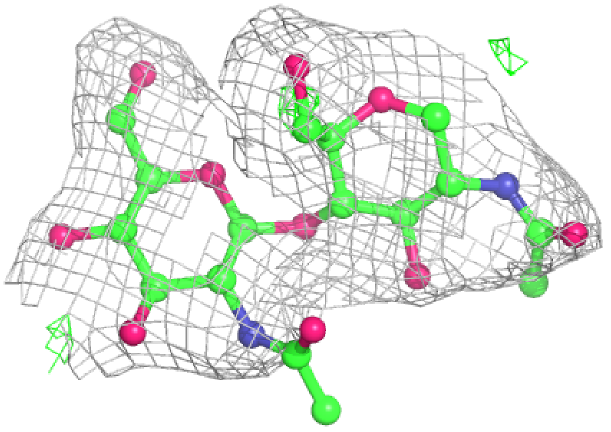


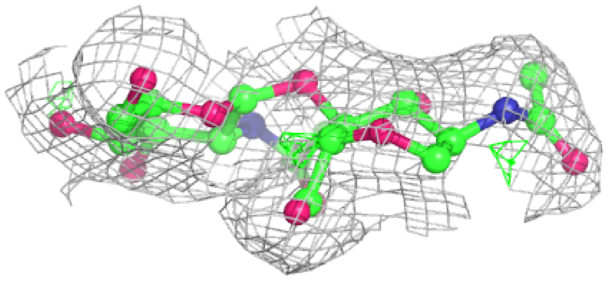
Electron density around Chain s:

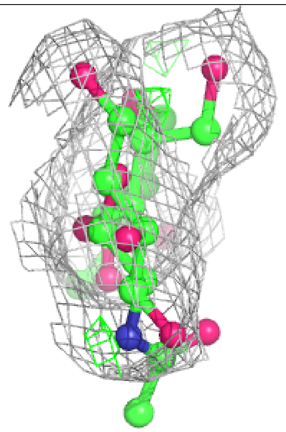
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain t:

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

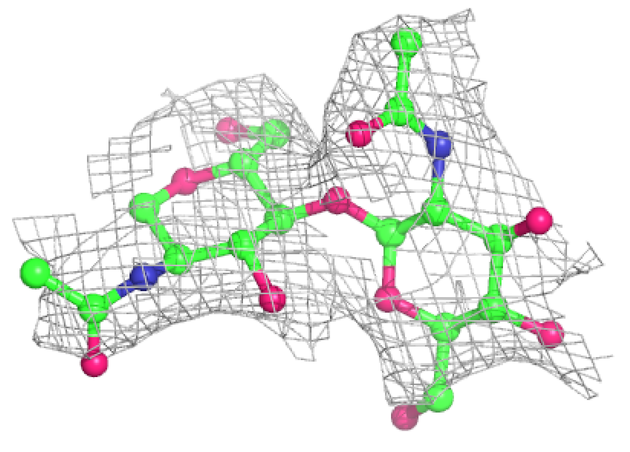


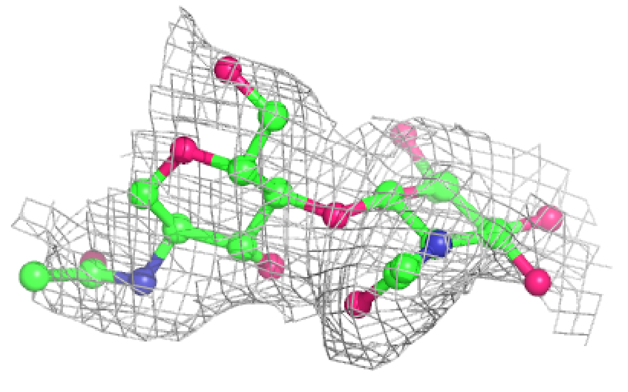


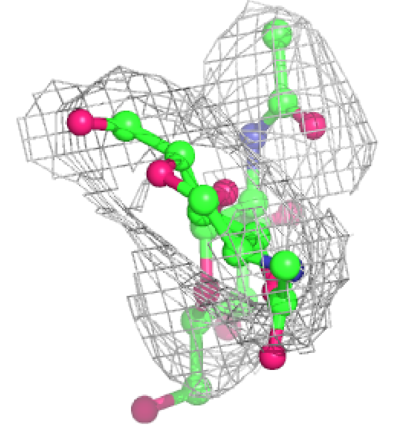


Electron density around Chain u:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

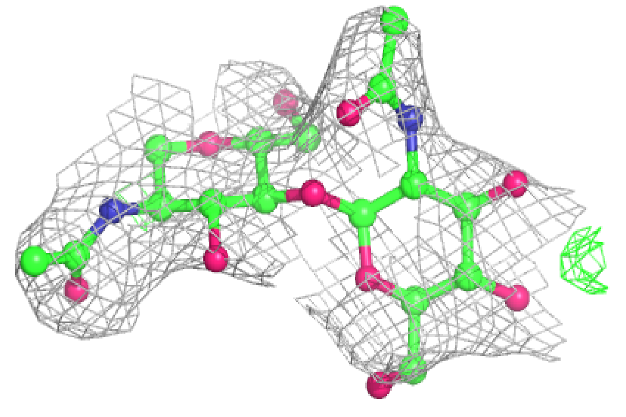


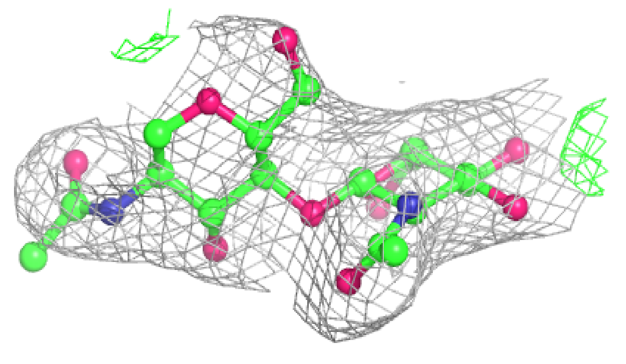


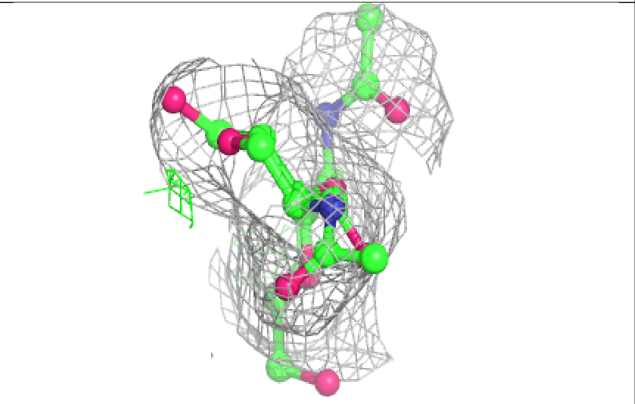


Electron density around Chain v:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

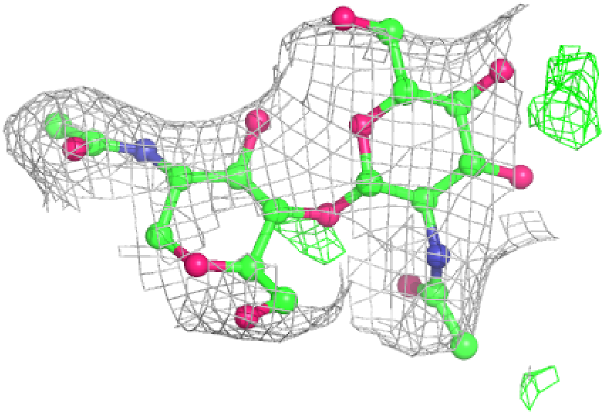


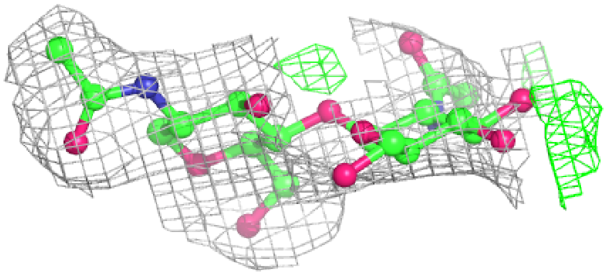


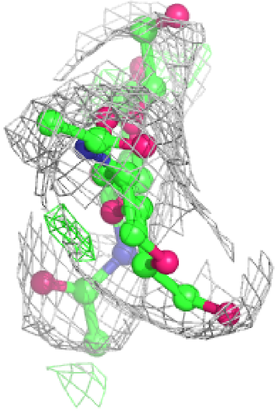


Electron density around Chain x:

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

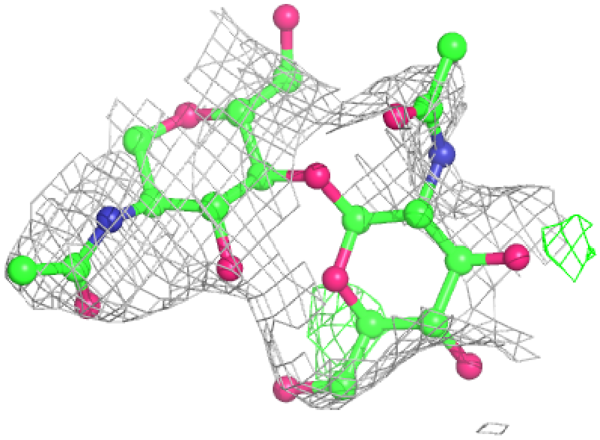


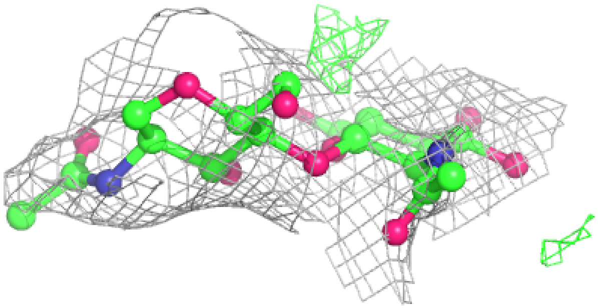




Electron density around Chain 1:

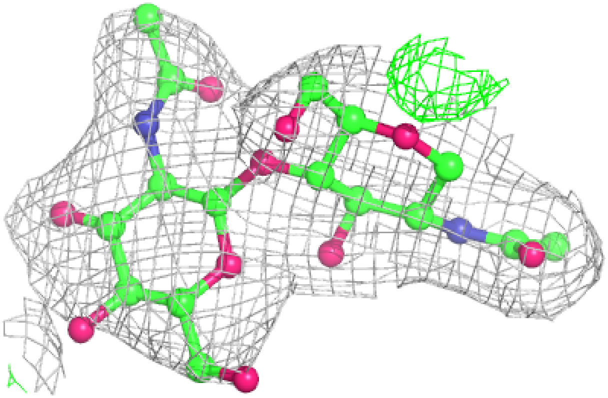
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

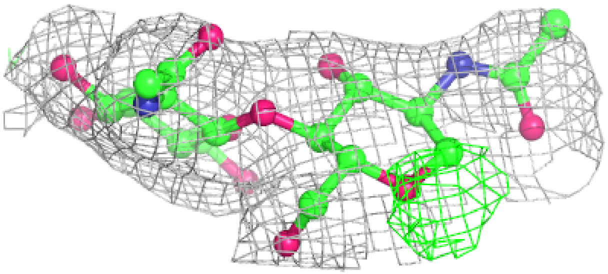


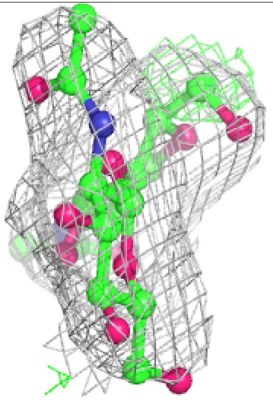


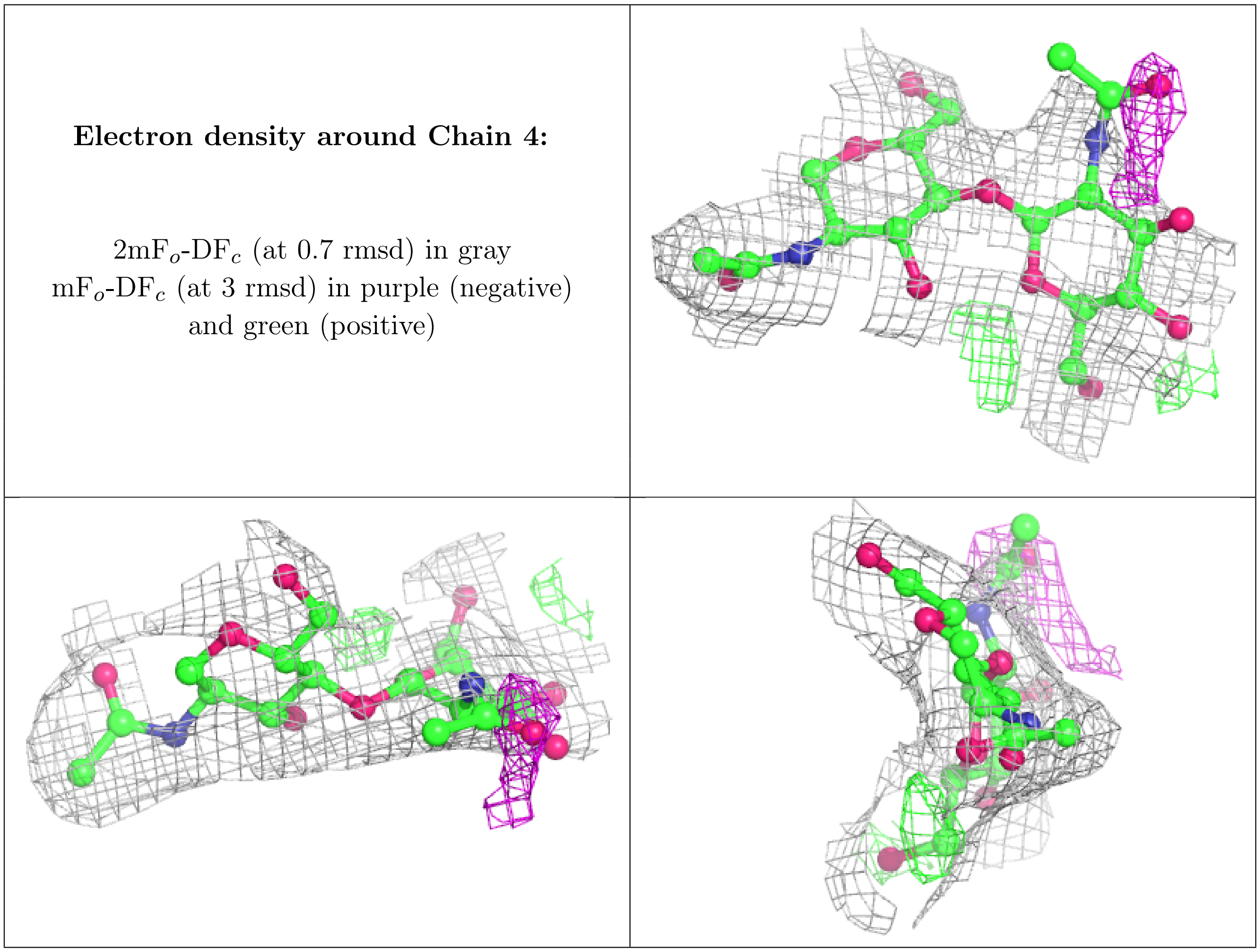
Electron density around Chain 2:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







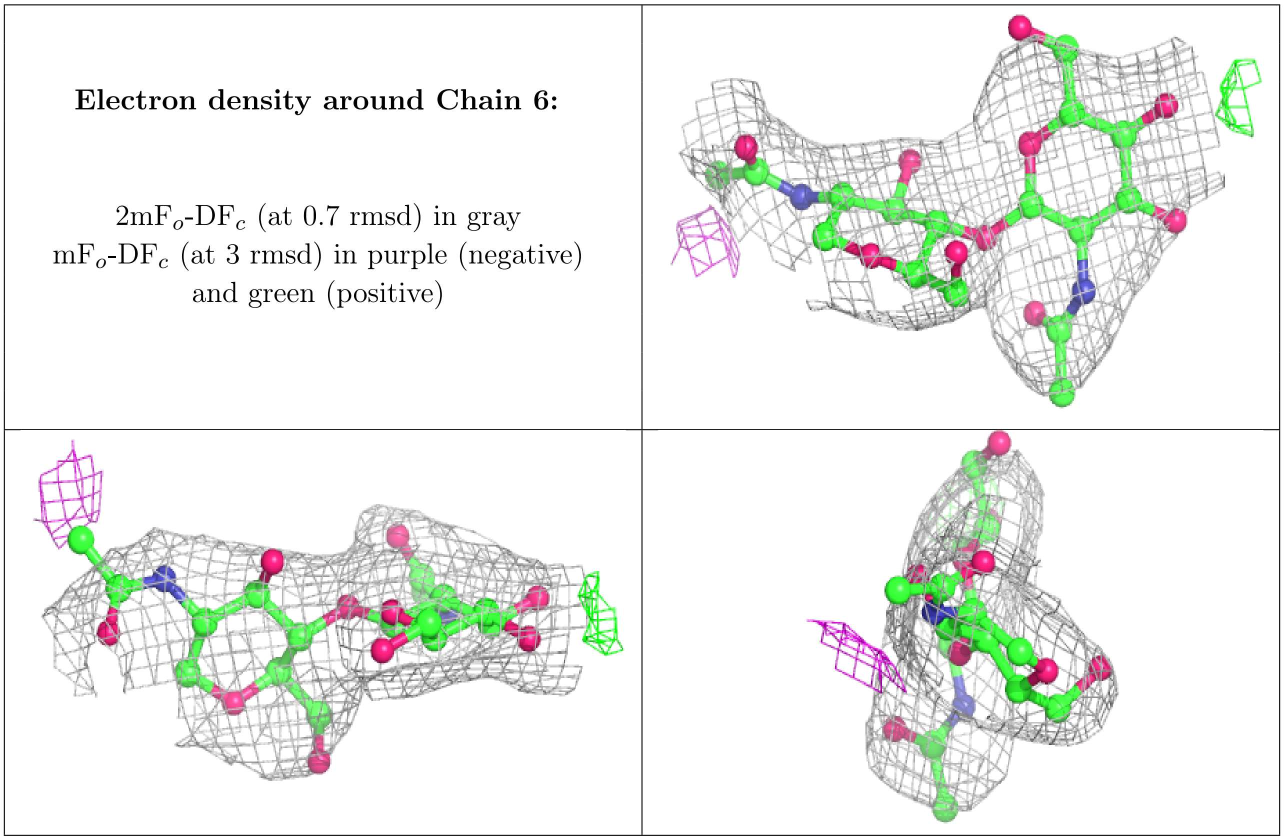


Electron density around Chain 4:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

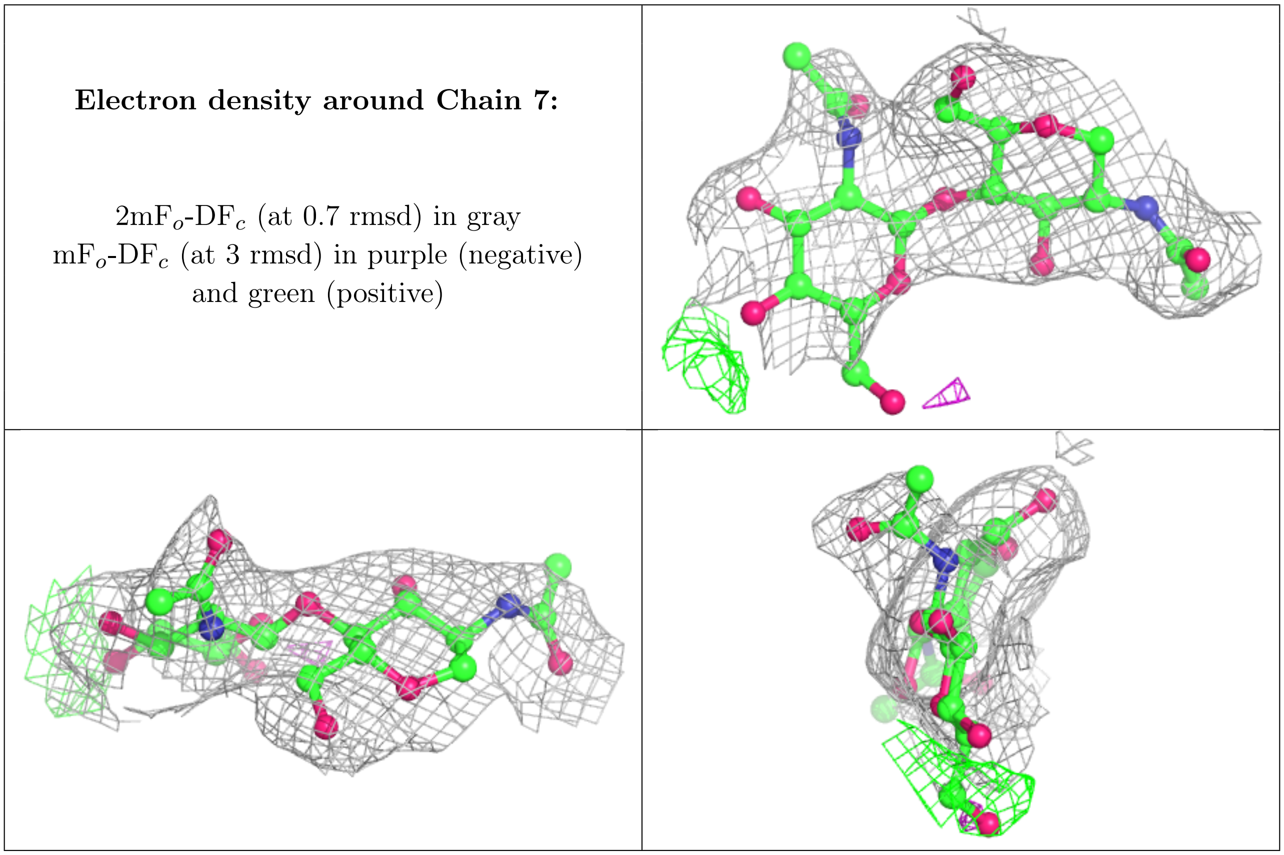
Electron density around Chain 6:

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



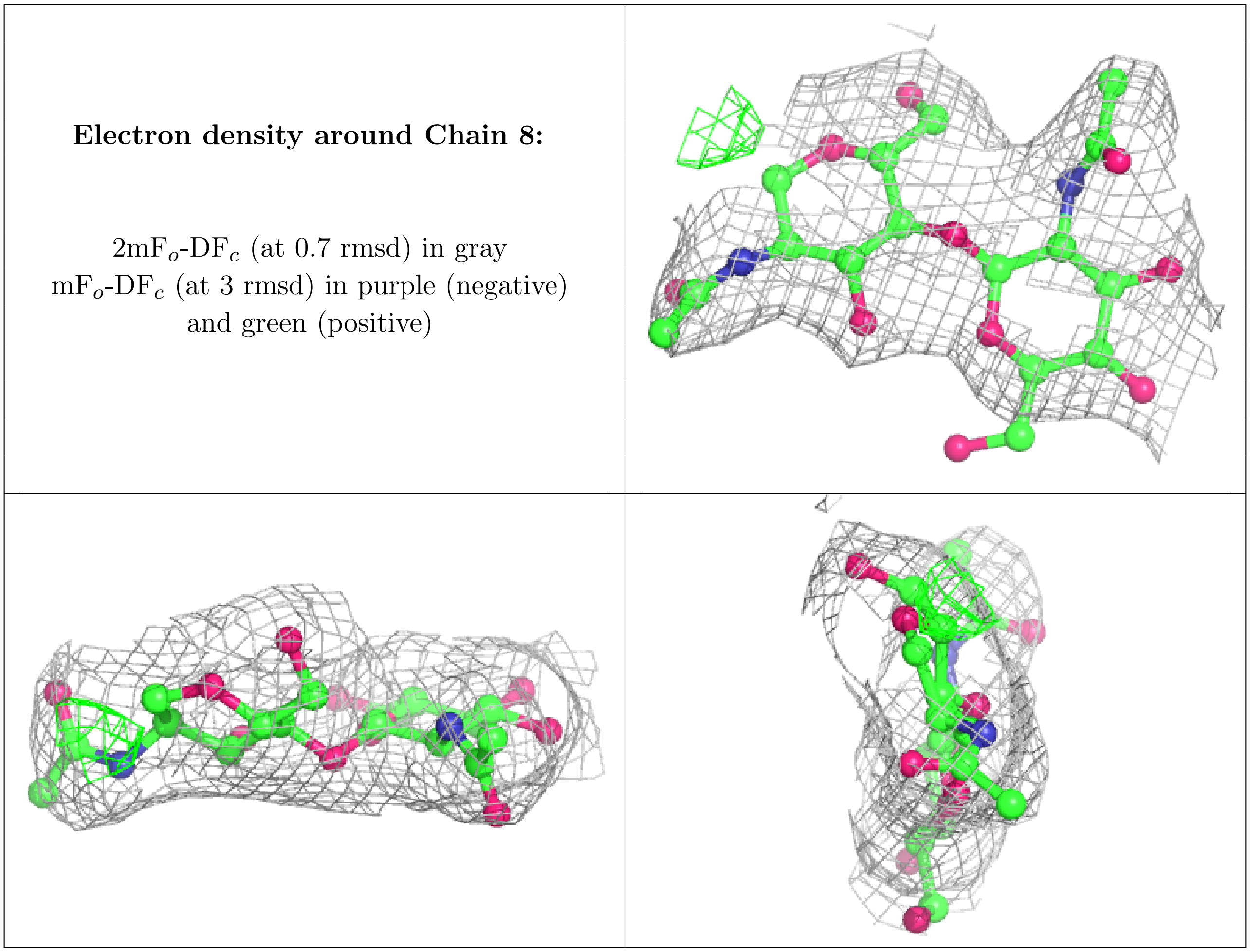
Electron density around Chain 7:

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



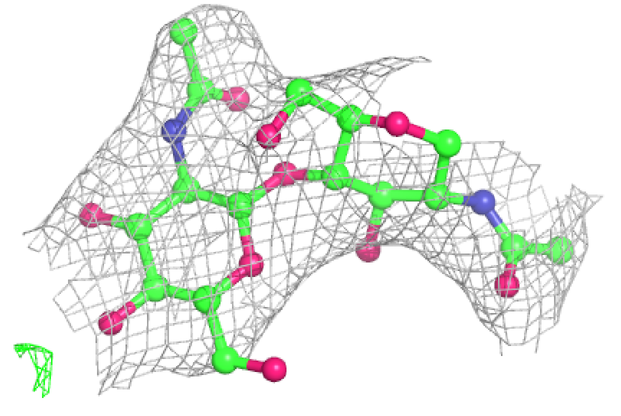
Electron density around Chain 8:

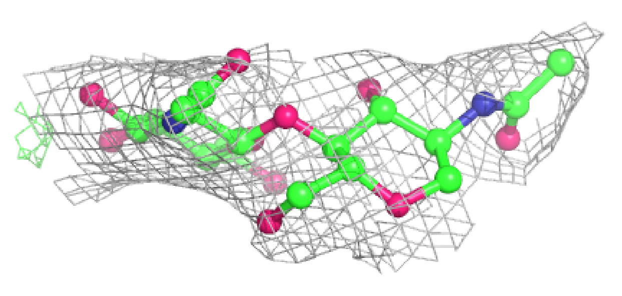
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

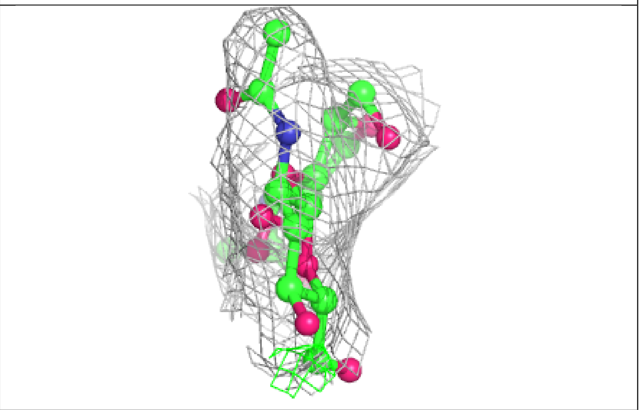


Electron density around Chain 9:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

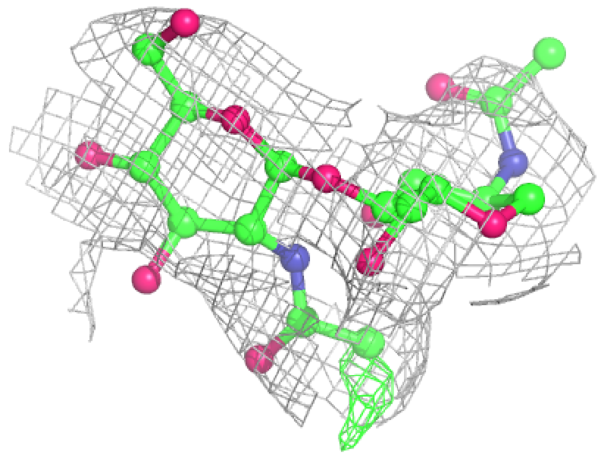


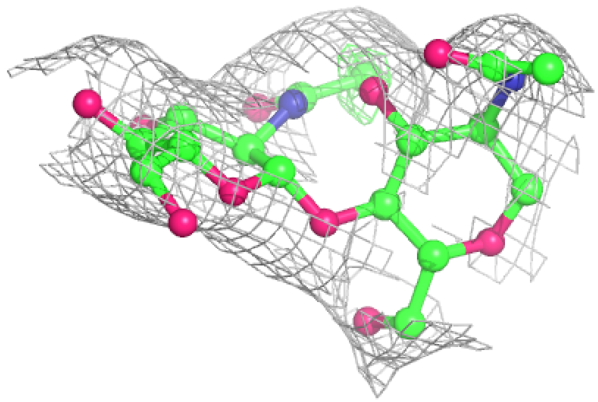


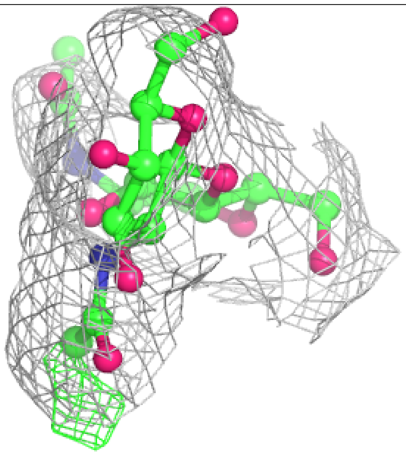


Electron density around Chain BA:

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

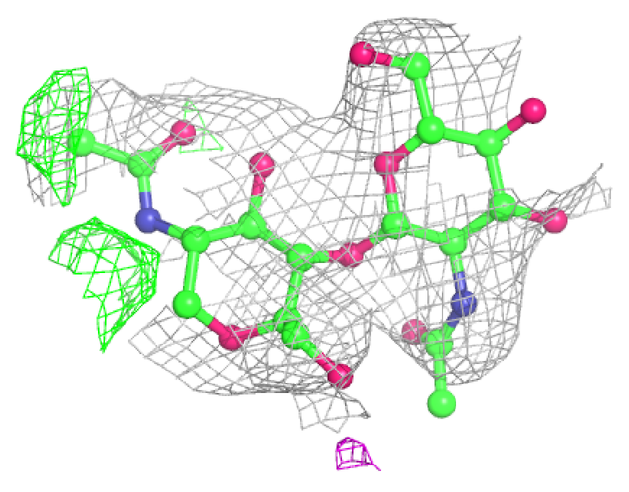


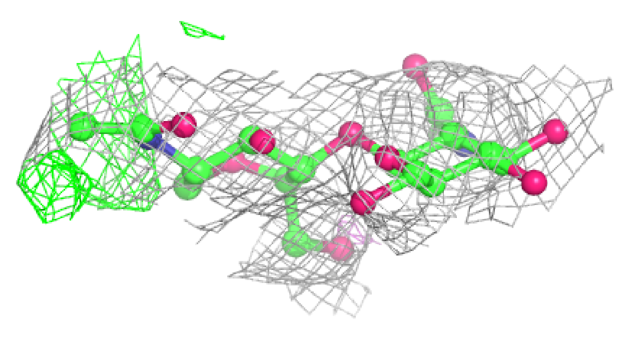


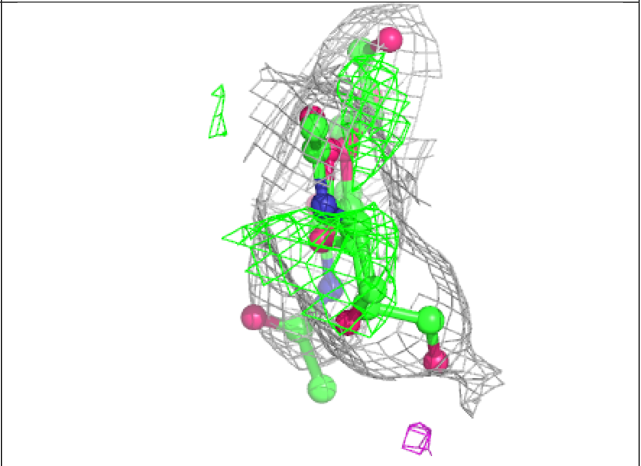


Electron density around Chain HA:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

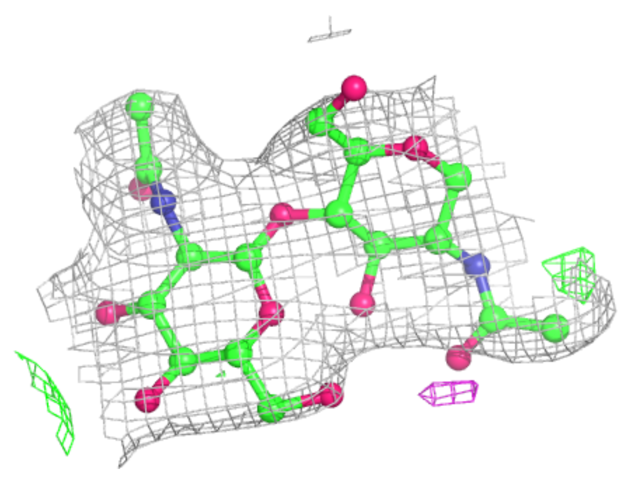


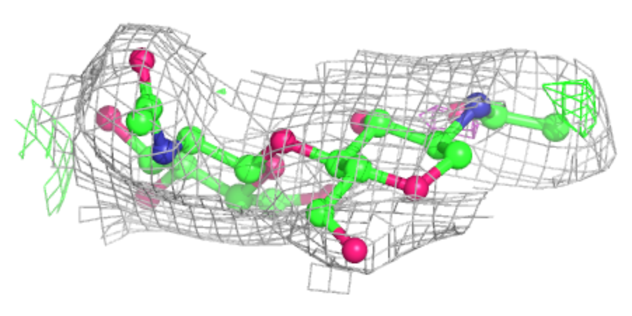


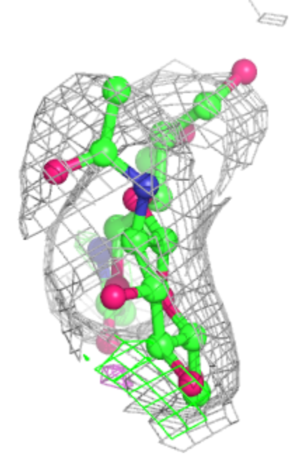


Electron density around Chain IA:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

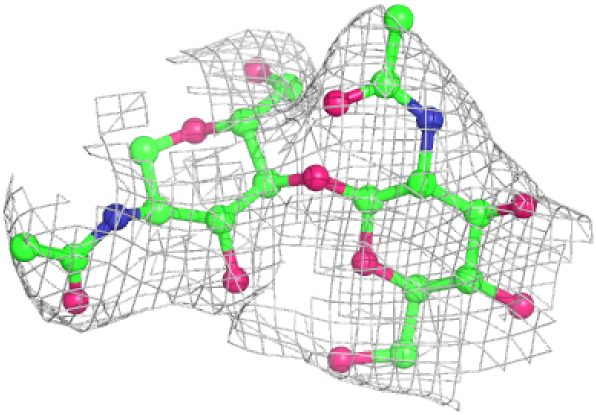


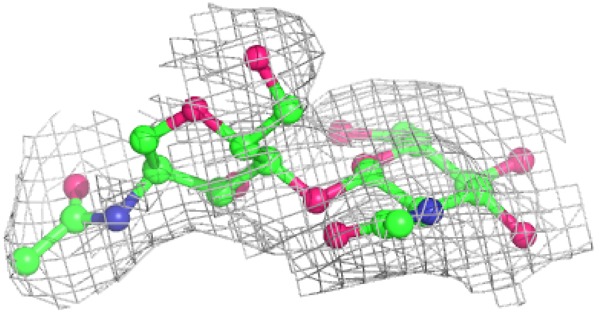


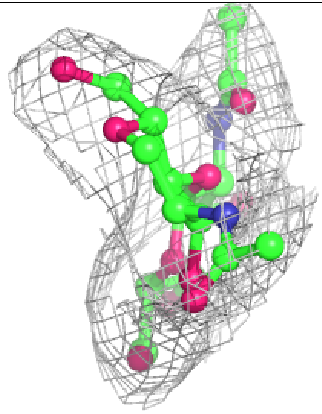


Electron density around Chain JA:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

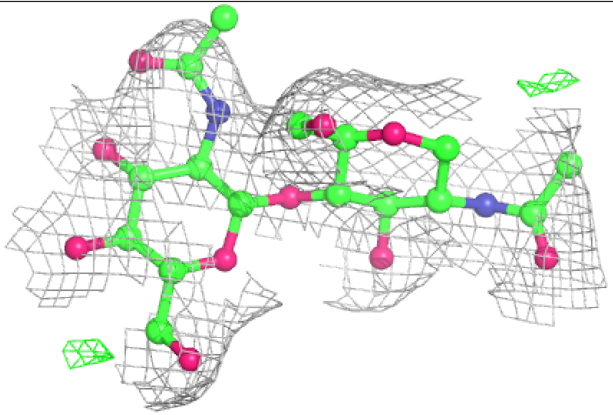


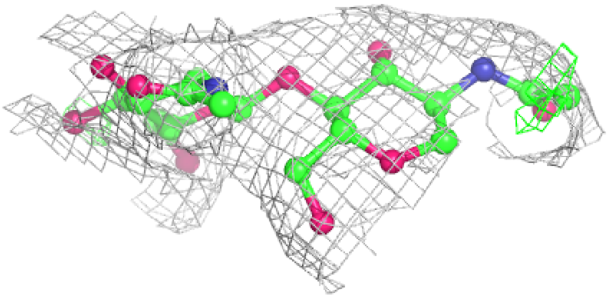


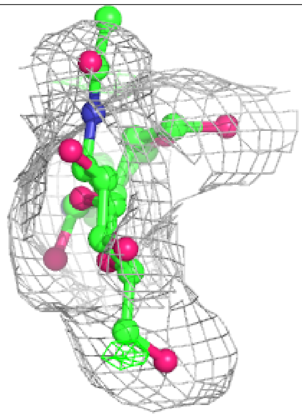


Electron density around Chain MA:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

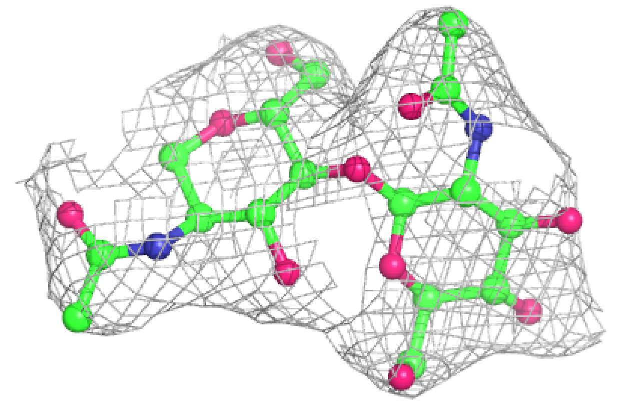


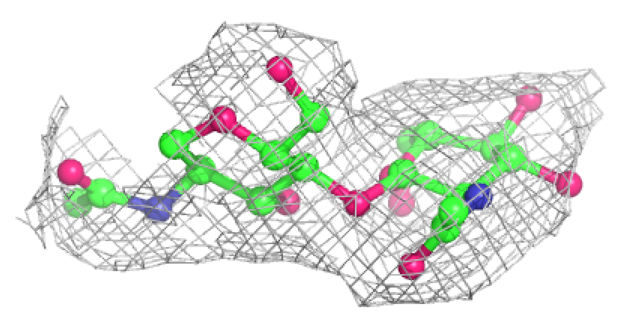


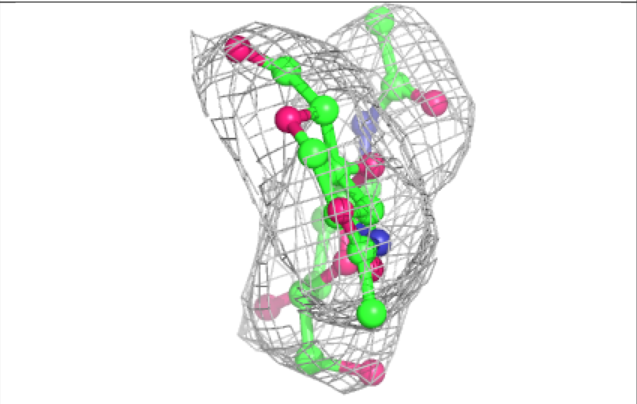


Electron density around Chain OA:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

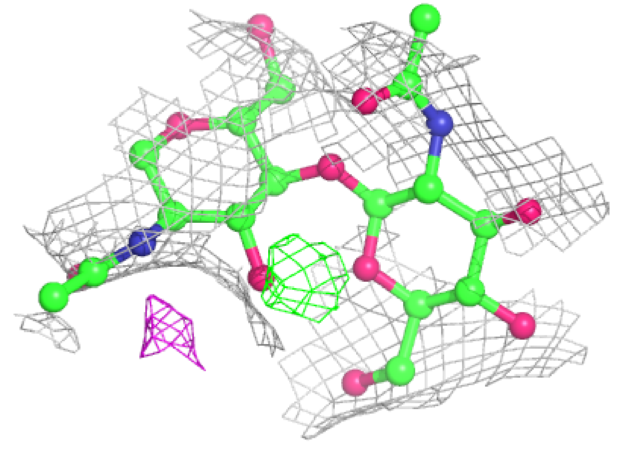


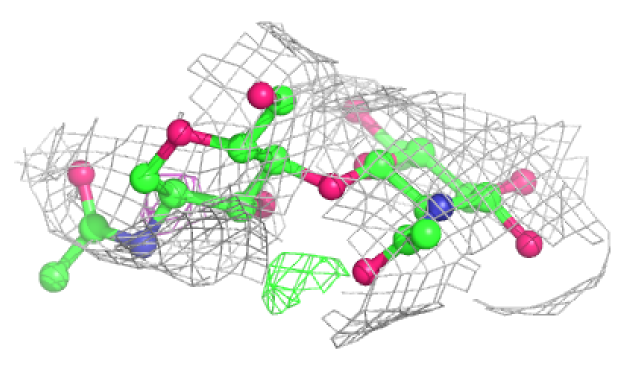


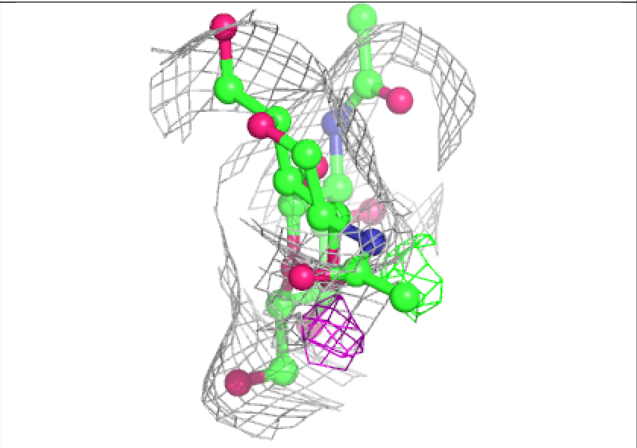


Electron density around Chain QA:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

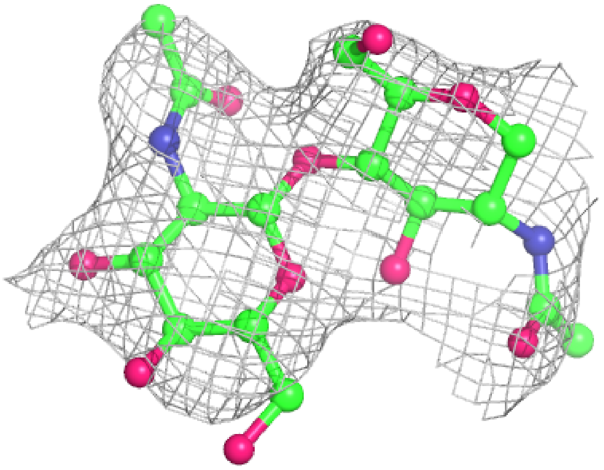


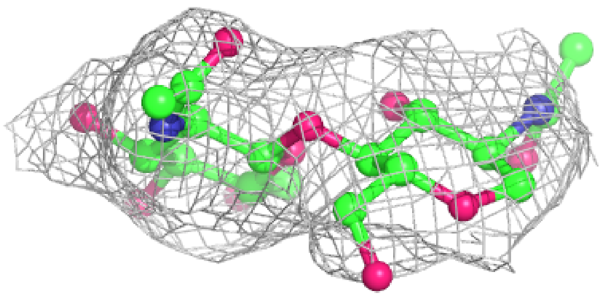


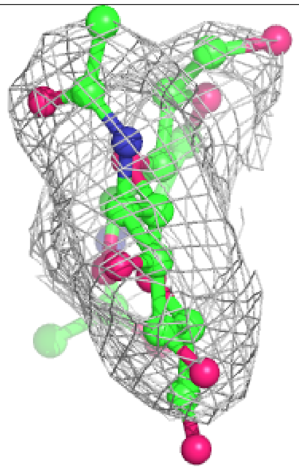


Electron density around Chain RA:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

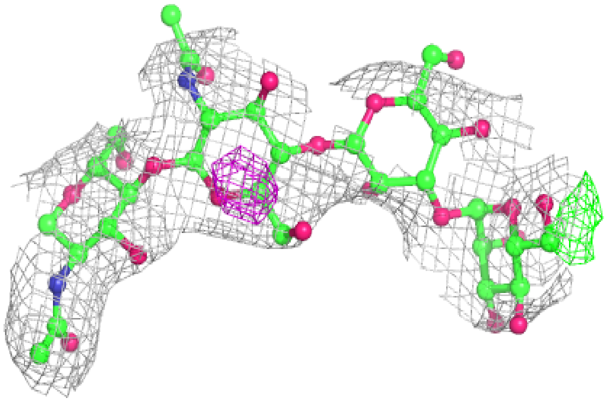


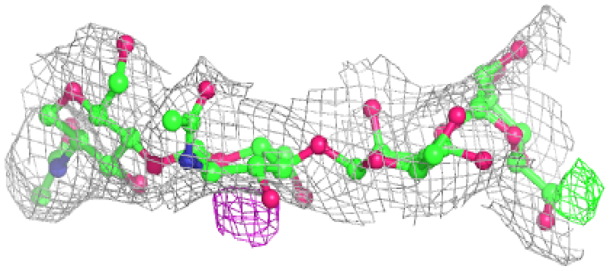


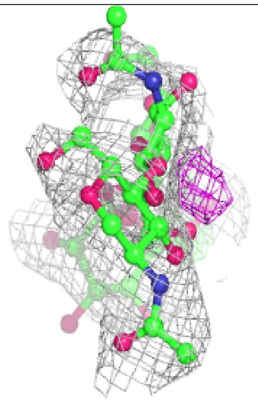


Electron density around Chain g:

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

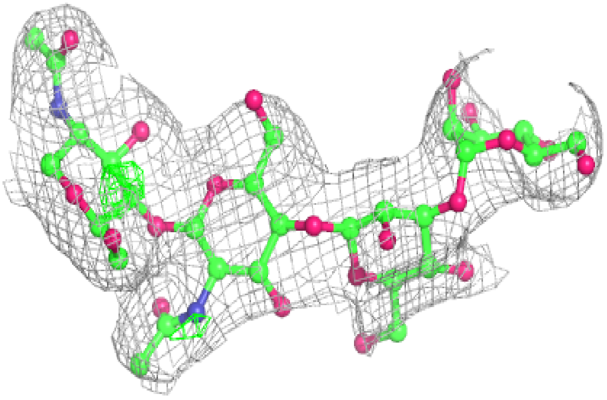


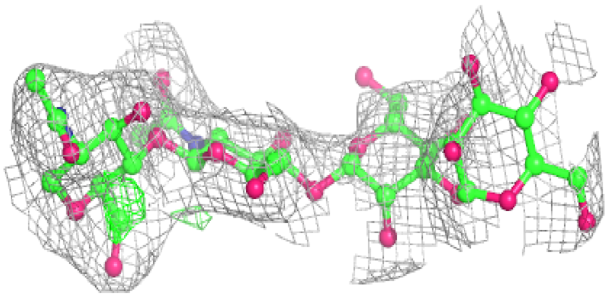


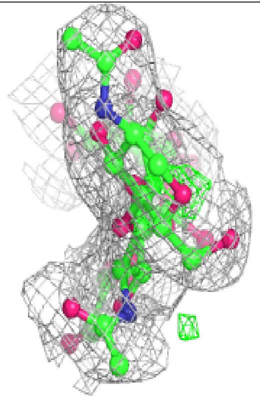


Electron density around Chain l:

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

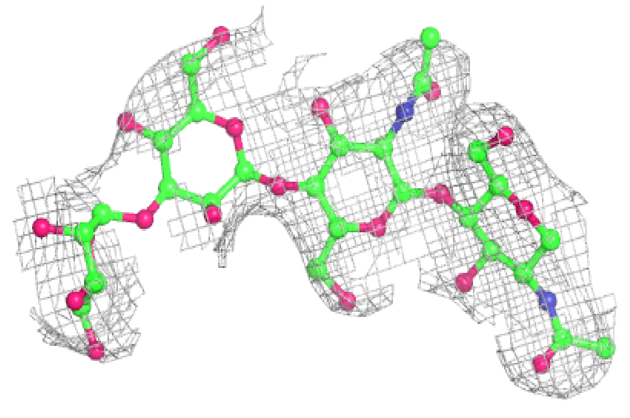


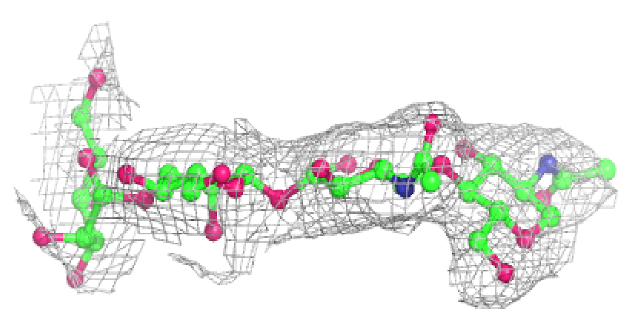


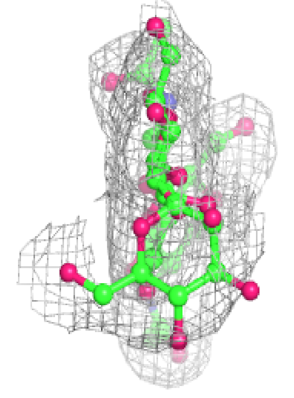


Electron density around Chain AA:

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

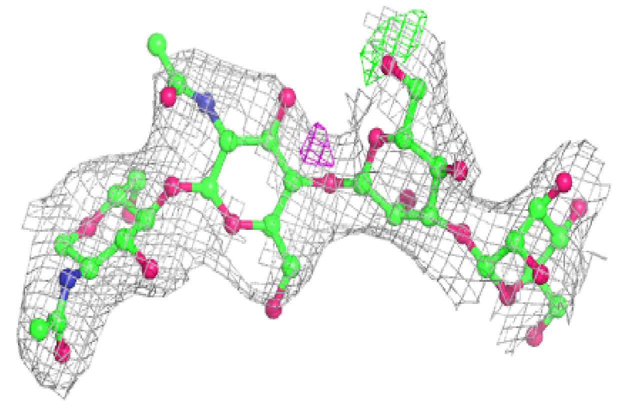


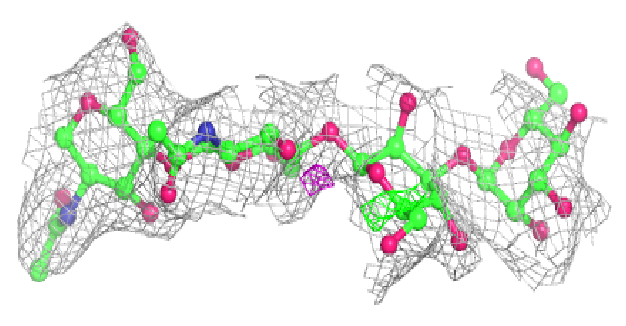


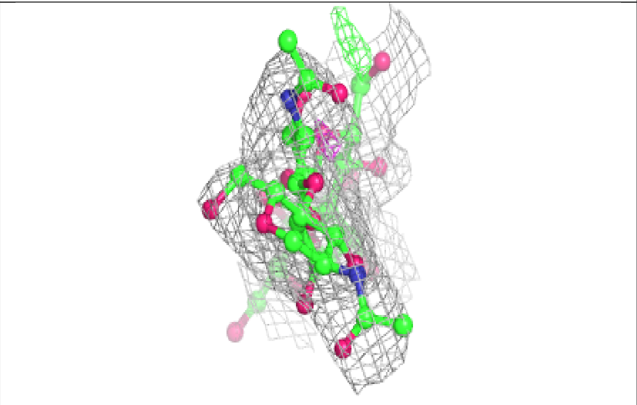


Electron density around Chain FA:

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

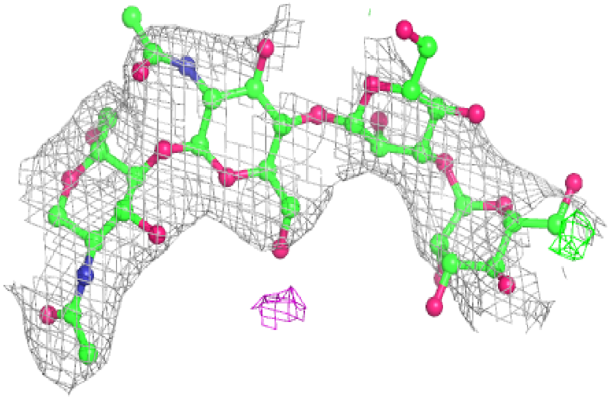


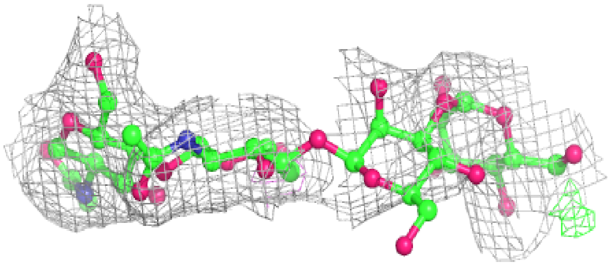


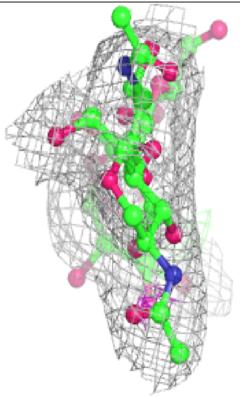


Electron density around Chain KA:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

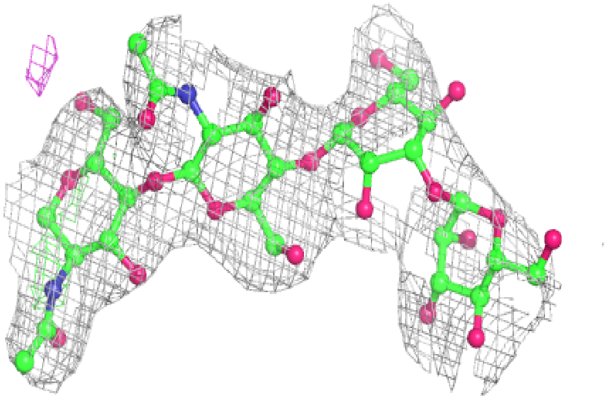


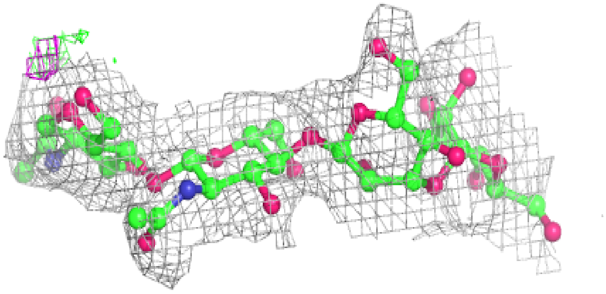


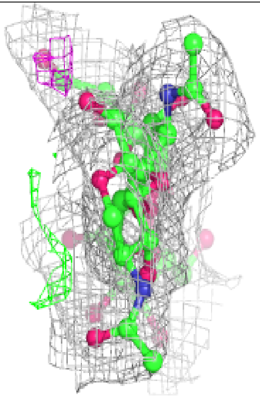


Electron density around Chain PA:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

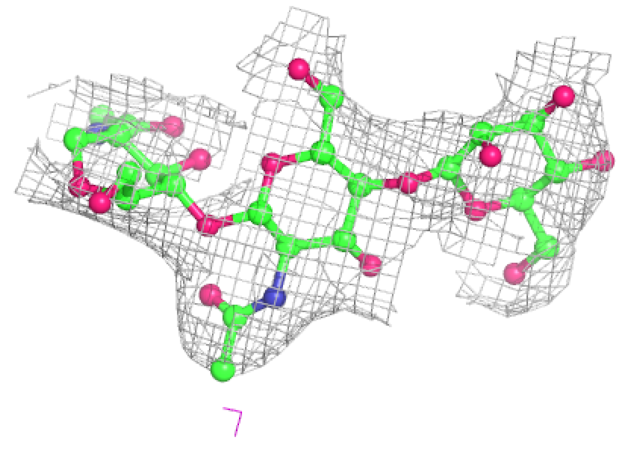


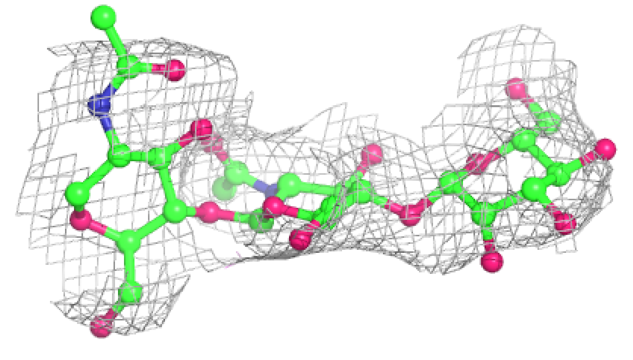


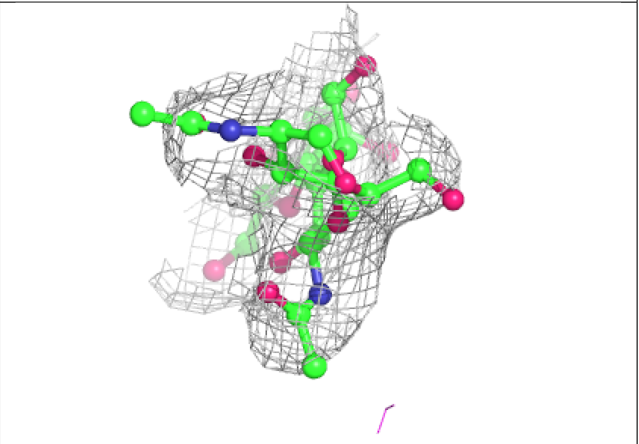


Electron density around Chain h:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

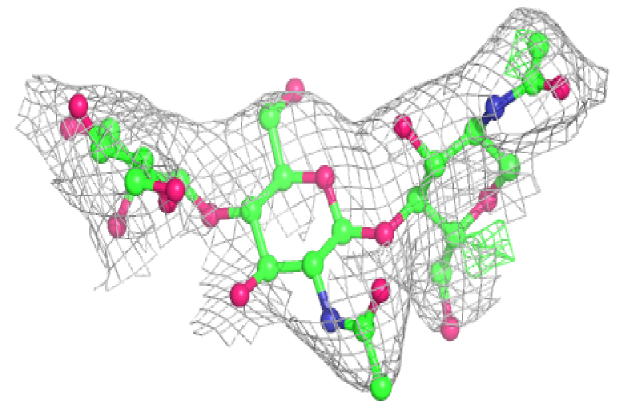


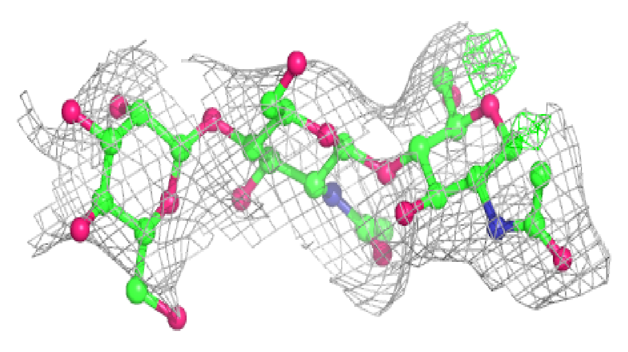


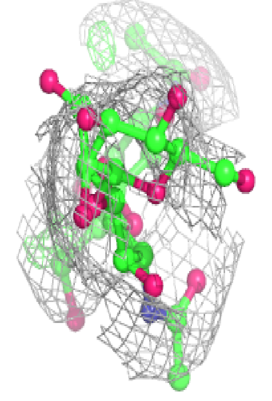


Electron density around Chain k:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

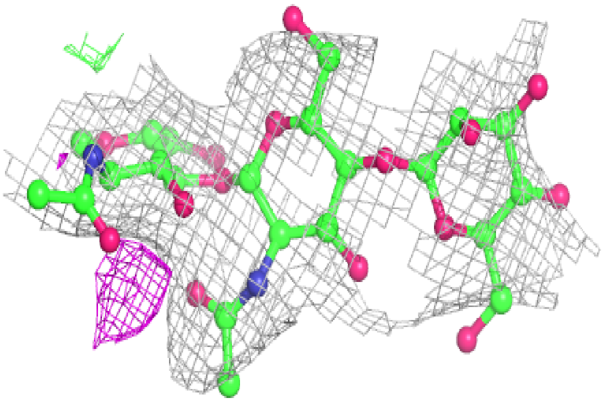


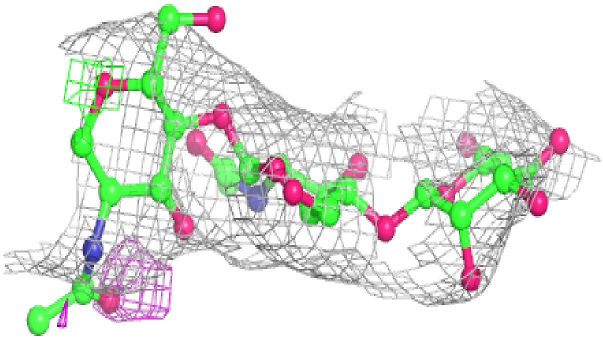


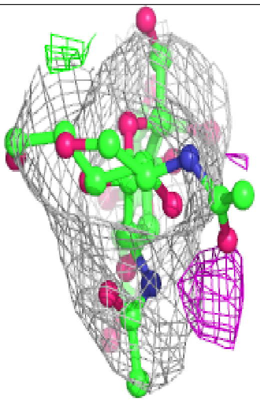


Electron density around Chain r:

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

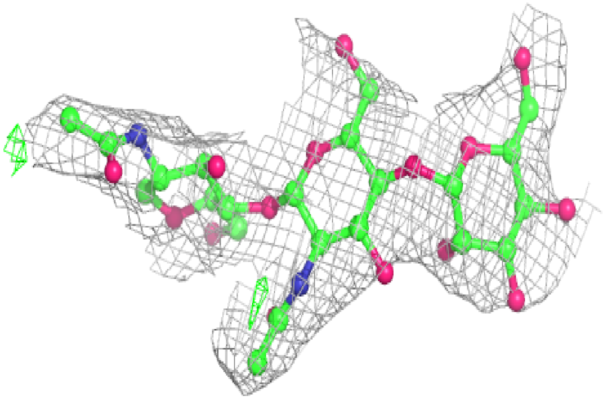


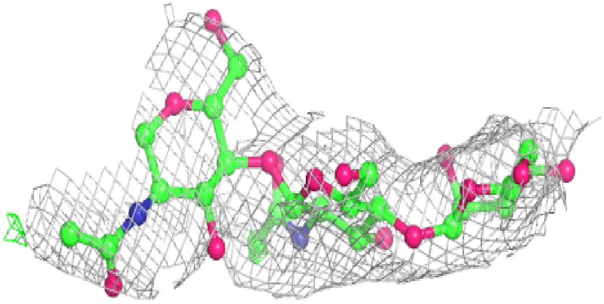


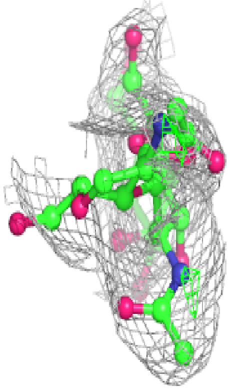


Electron density around Chain w:

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

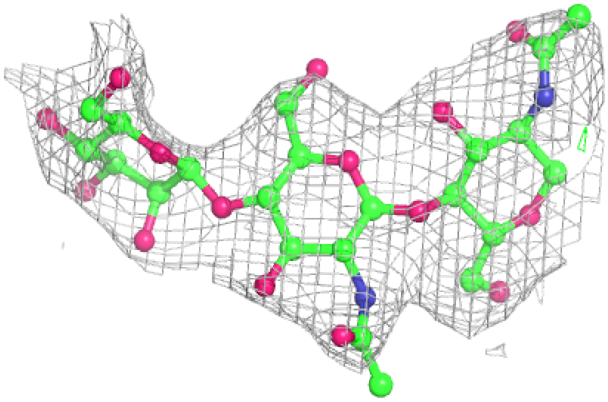


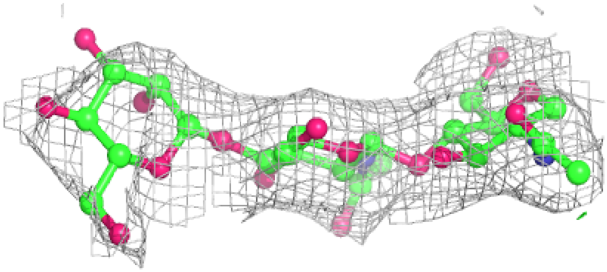


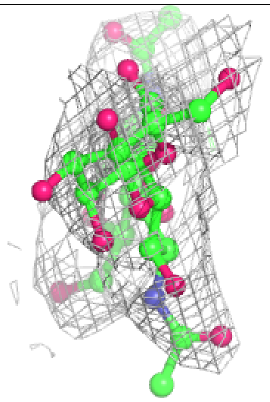


Electron density around Chain y:

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

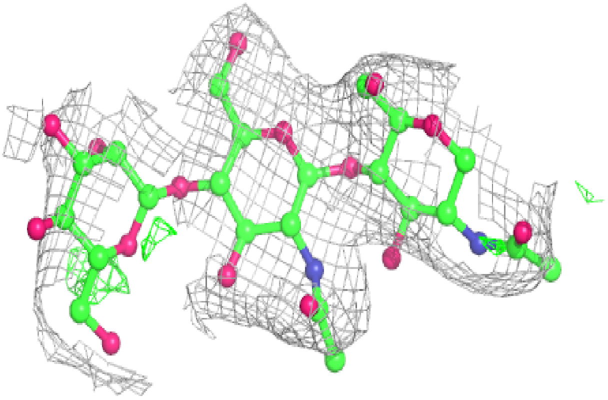


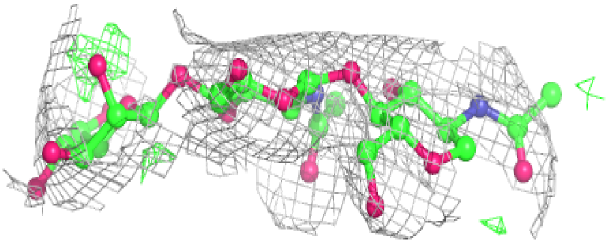


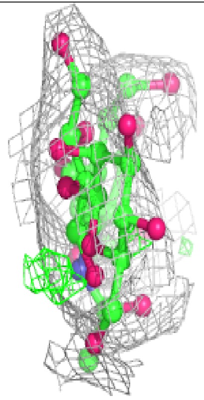


Electron density around Chain 3:

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

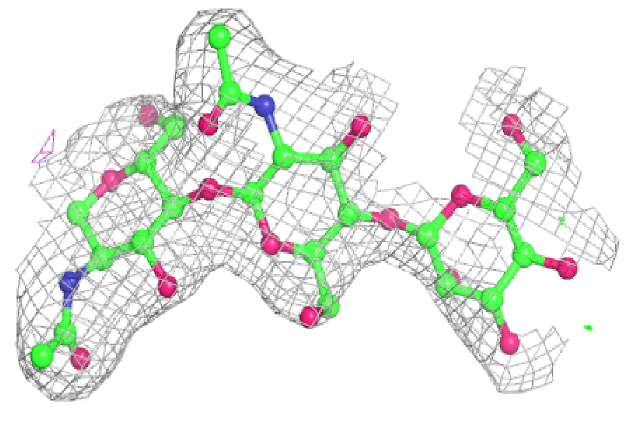


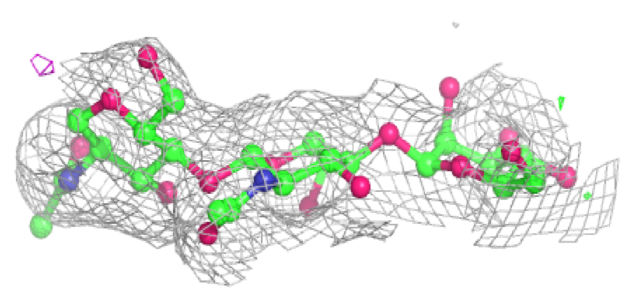


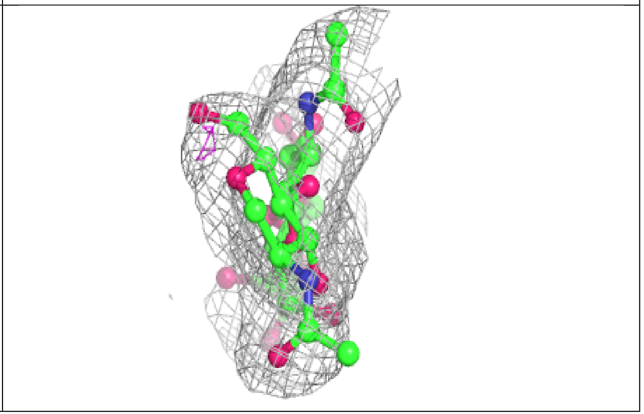


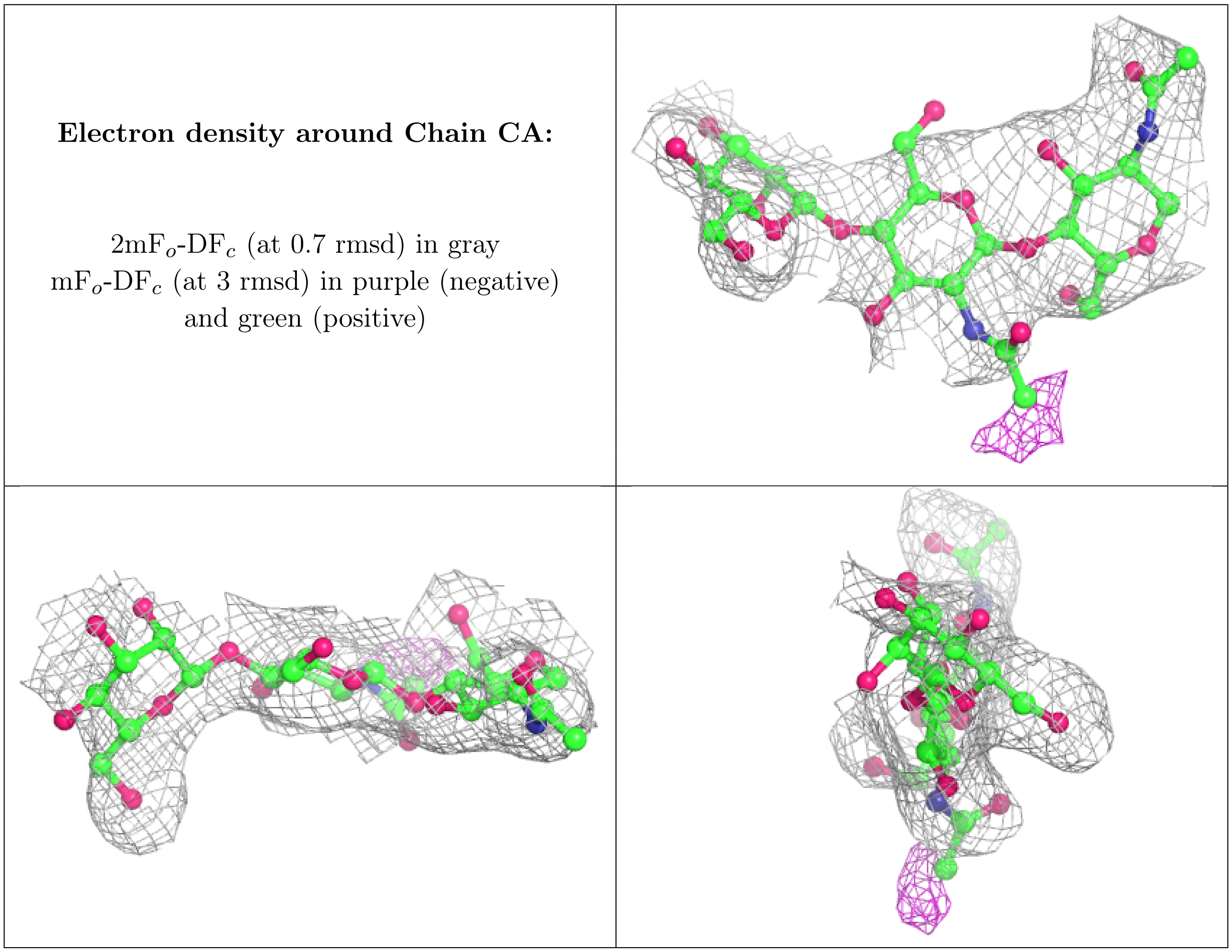
Electron density around Chain 5:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







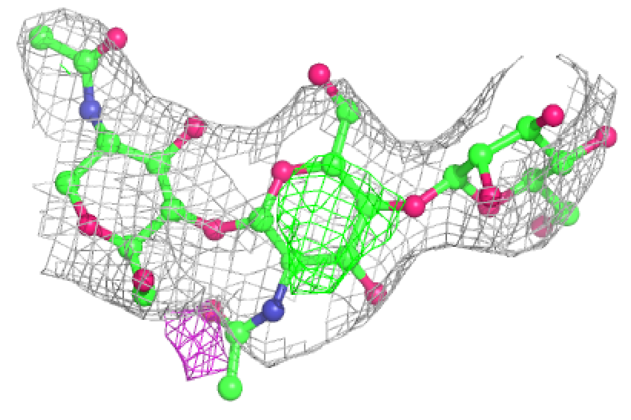


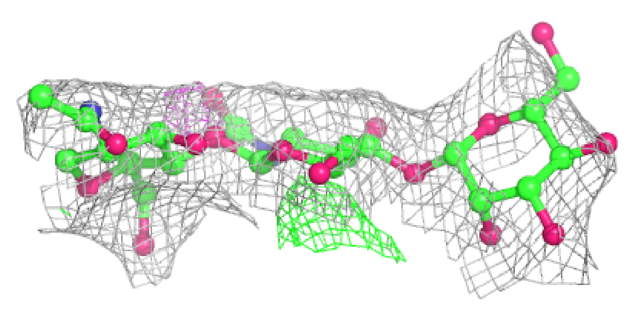
Electron density around Chain CA:

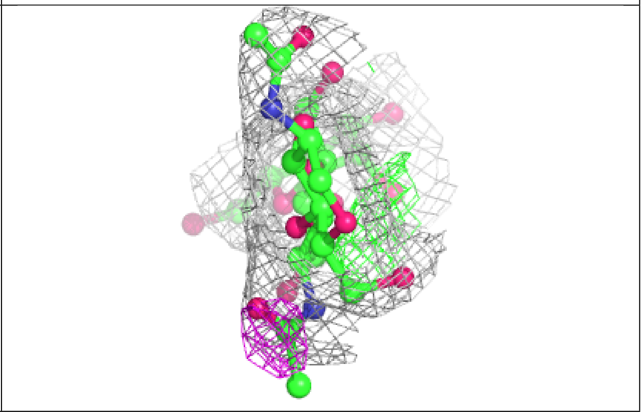
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

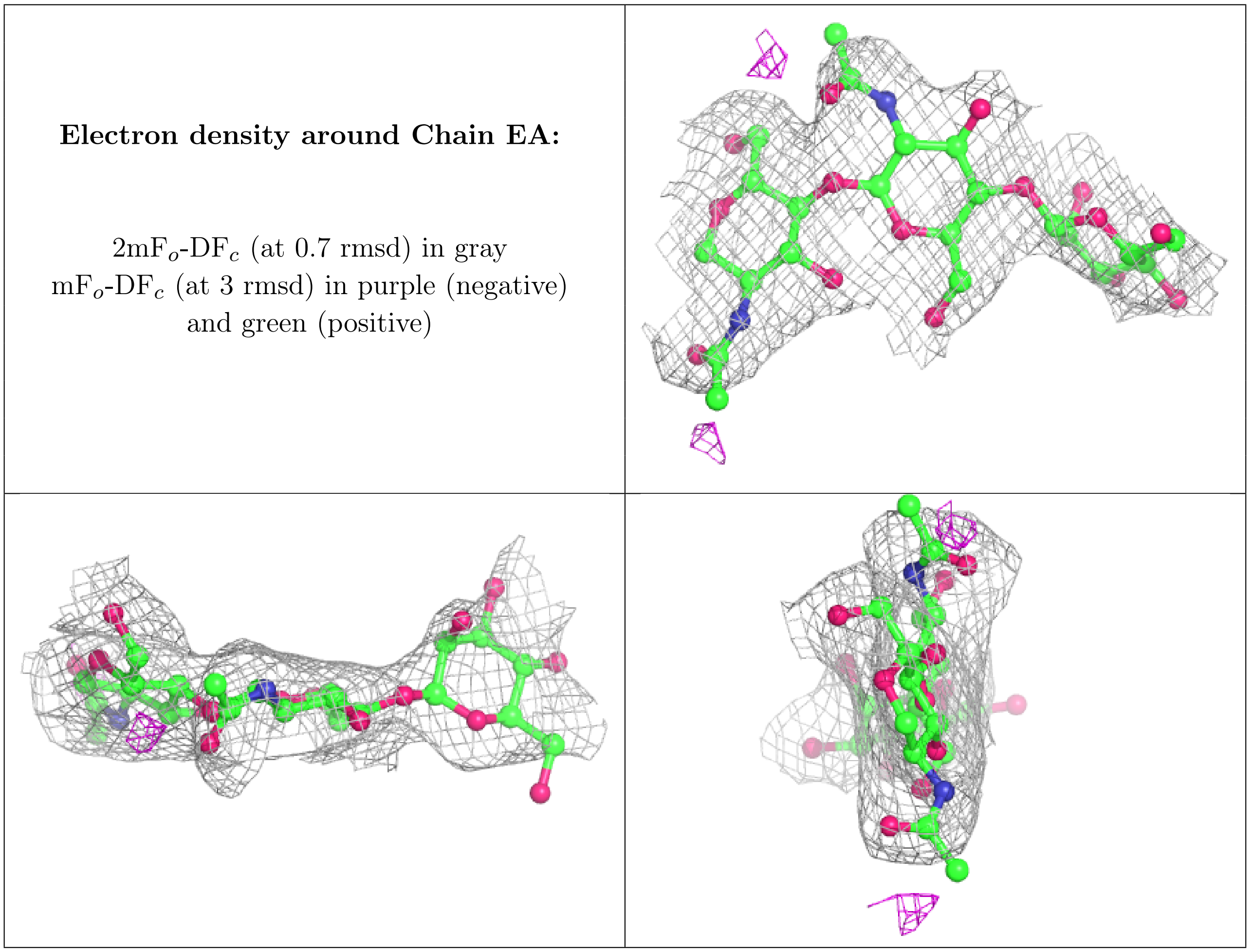
Electron density around Chain DA:

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







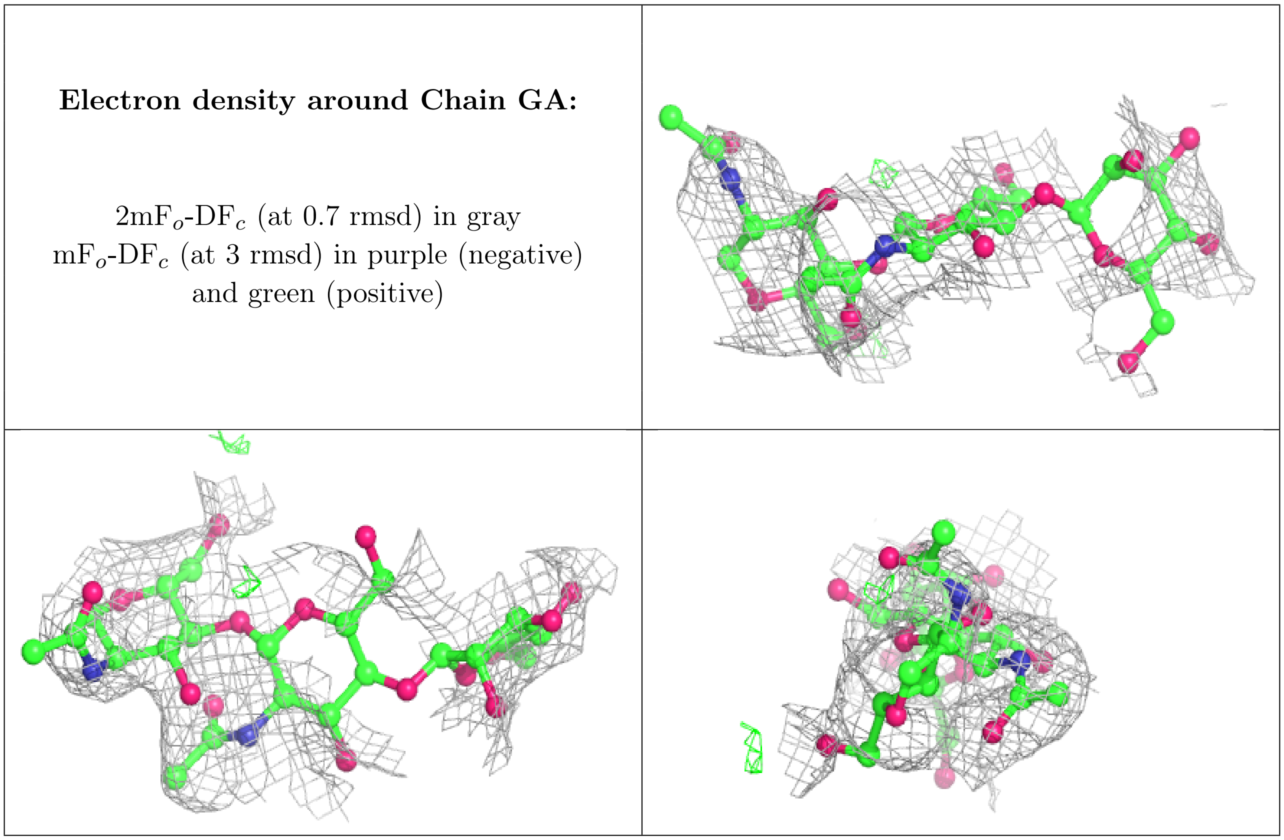


Electron density around Chain EA:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

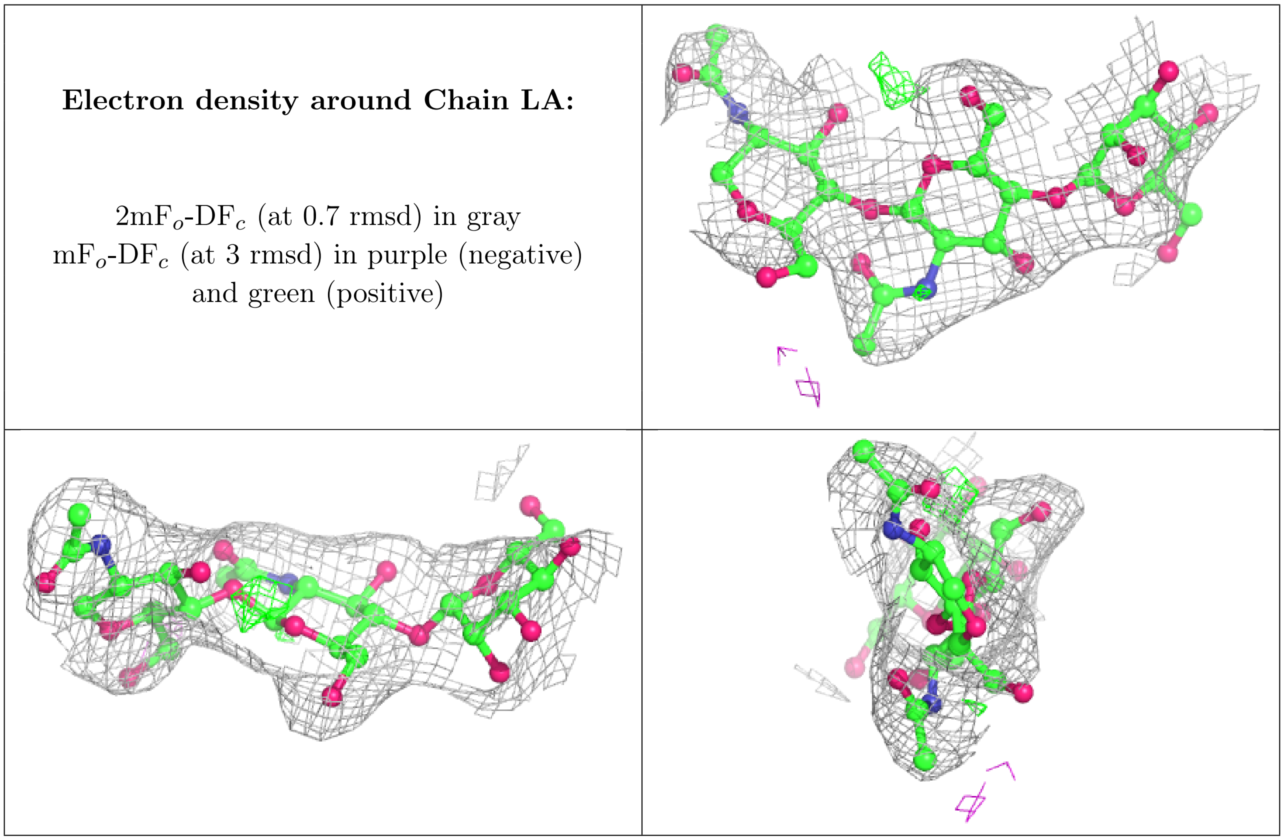
Electron density around Chain GA:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



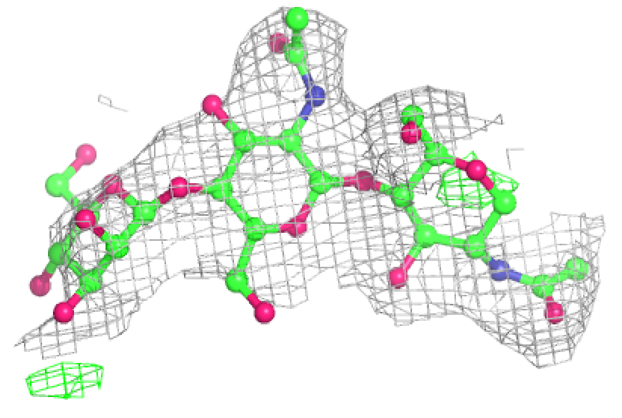
Electron density around Chain LA:

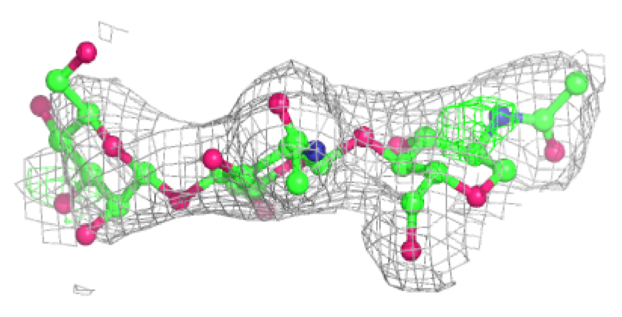
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

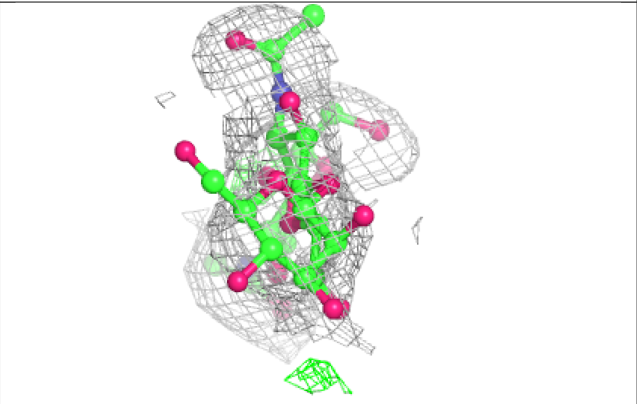


Electron density around Chain NA:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

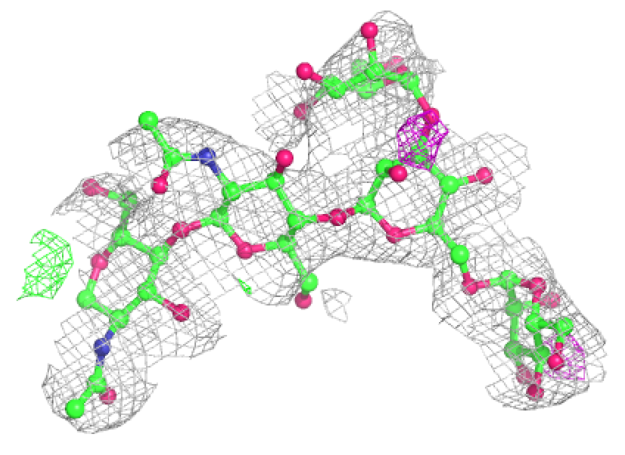


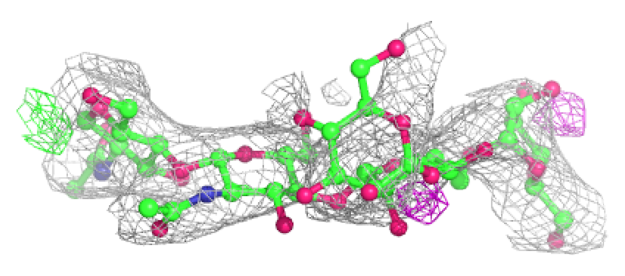


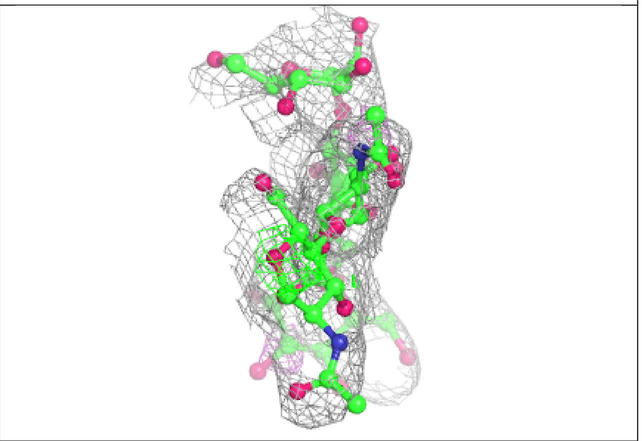


Electron density around Chain z:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

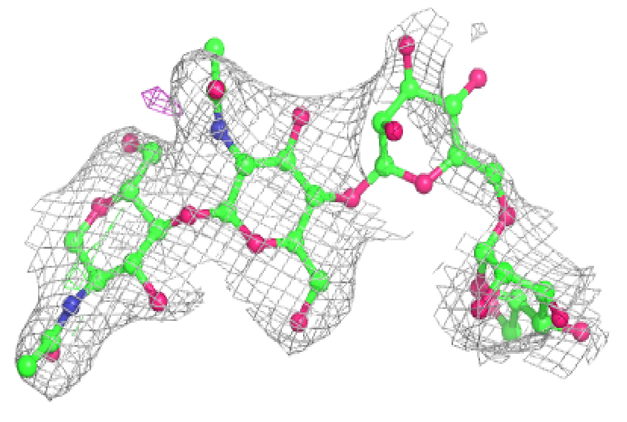


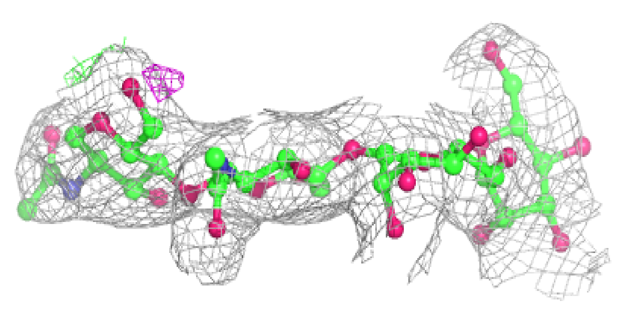


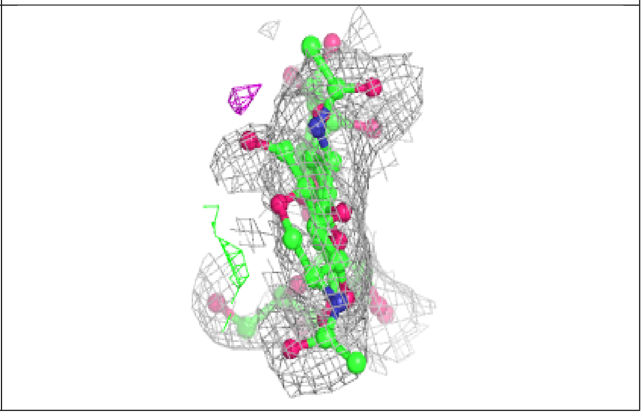


Electron density around Chain 0:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	CUO	X	3401[A]	4/4	0.39	0.56	121,121,121,121	4
9	CUO	X	3401[B]	4/4	0.39	0.56	121,121,121,121	4
9	CUO	I	3402[A]	4/4	0.49	0.23	84,84,84,84	4
9	CUO	I	3402[B]	4/4	0.49	0.23	84,84,84,84	4
9	CUO	V	5018[C]	4/4	0.52	0.36	113,113,113,113	4
9	CUO	V	5018[D]	4/4	0.52	0.36	113,113,113,113	4
9	CUO	P	5015[C]	4/4	0.52	0.42	114,114,114,114	4
9	CUO	P	5015[D]	4/4	0.52	0.42	114,114,114,114	4
9	CUO	J	5014[C]	4/4	0.59	0.31	98,98,98,98	4
9	CUO	J	5014[D]	4/4	0.59	0.31	98,98,98,98	4
9	CUO	D	5016[C]	4/4	0.59	0.30	109,109,109,109	4
9	CUO	D	5016[D]	4/4	0.59	0.30	109,109,109,109	4
9	CUO	d	3401[A]	4/4	0.60	0.43	111,111,111,111	4
9	CUO	d	3401[B]	4/4	0.60	0.43	111,111,111,111	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
9	CUO	A	5016[C]	4/4	0.62	0.20	95,95,95,95	4
9	CUO	A	5016[D]	4/4	0.62	0.20	95,95,95,95	4
9	CUO	S	2101[C]	4/4	0.65	0.27	94,94,94,94	4
9	CUO	S	2101[D]	4/4	0.65	0.27	94,94,94,94	4
9	CUO	O	3401[A]	4/4	0.67	0.32	85,85,85,85	4
9	CUO	O	3401[B]	4/4	0.67	0.32	85,85,85,85	4
9	CUO	b	2101[C]	4/4	0.68	0.31	106,106,106,106	4
9	CUO	b	2101[D]	4/4	0.68	0.31	106,106,106,106	4
9	CUO	G	2101[C]	4/4	0.69	0.28	104,104,104,104	4
9	CUO	G	2101[D]	4/4	0.69	0.28	104,104,104,104	4
9	CUO	U	3401[A]	4/4	0.69	0.36	81,81,81,81	4
9	CUO	U	3401[B]	4/4	0.69	0.36	81,81,81,81	4
9	CUO	F	3401[A]	4/4	0.70	0.23	86,86,86,86	4
9	CUO	F	3401[B]	4/4	0.70	0.23	86,86,86,86	4
9	CUO	C	3401[A]	4/4	0.71	0.28	99,99,99,99	4
9	CUO	C	3401[B]	4/4	0.71	0.28	99,99,99,99	4
9	CUO	M	2101[C]	4/4	0.71	0.27	103,103,103,103	4
9	CUO	M	2101[D]	4/4	0.71	0.27	103,103,103,103	4
9	CUO	Y	2101[C]	4/4	0.72	0.28	99,99,99,99	4
9	CUO	Y	2101[D]	4/4	0.72	0.28	99,99,99,99	4
9	CUO	C	3402[A]	4/4	0.73	0.31	100,100,100,100	4
9	CUO	C	3402[B]	4/4	0.73	0.31	100,100,100,100	4
9	CUO	F	3402[A]	4/4	0.74	0.28	85,85,85,85	4
9	CUO	F	3402[B]	4/4	0.74	0.28	85,85,85,85	4
9	CUO	I	3401[A]	4/4	0.76	0.21	84,84,84,84	4
9	CUO	I	3401[B]	4/4	0.76	0.21	84,84,84,84	4
9	CUO	E	3001	4/4	0.89	0.13	55,55,80,85	0
9	CUO	Y	2104	4/4	0.90	0.13	69,75,80,100	0
9	CUO	G	2104	4/4	0.90	0.17	58,85,92,97	0
9	CUO	V	5003	4/4	0.90	0.11	66,79,89,90	0
9	CUO	c	3001	4/4	0.90	0.16	48,56,77,80	0
9	CUO	M	2104	4/4	0.90	0.10	58,70,74,76	0
9	CUO	A	5001	4/4	0.90	0.12	70,73,87,92	0
9	CUO	B	3001	4/4	0.91	0.15	49,55,75,88	0
9	CUO	A	5002	4/4	0.91	0.17	55,75,89,91	0
9	CUO	b	2104	4/4	0.91	0.13	60,75,83,94	0
9	CUO	V	5002	4/4	0.92	0.14	50,61,67,72	0
9	CUO	D	5001	4/4	0.92	0.14	64,68,95,98	0
9	CUO	b	2105	4/4	0.92	0.11	54,57,68,74	0
9	CUO	T	3002	4/4	0.93	0.13	52,69,74,84	0
9	CUO	N	3001	4/4	0.93	0.14	36,39,74,80	0
9	CUO	J	5001	4/4	0.93	0.12	49,52,60,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	CUO	G	2103	4/4	0.93	0.14	49,58,62,73	0
9	CUO	P	5003	4/4	0.93	0.14	45,54,76,83	0
9	CUO	Y	2103	4/4	0.93	0.18	58,65,82,85	0
9	CUO	S	2104	4/4	0.93	0.11	74,79,82,87	0
9	CUO	S	2105	4/4	0.94	0.13	45,45,62,71	0
9	CUO	P	5002	4/4	0.94	0.12	56,59,75,82	0
9	CUO	D	5002	4/4	0.94	0.14	51,60,82,85	0
9	CUO	D	5003	4/4	0.94	0.08	60,62,67,79	0
9	CUO	Z	3002	4/4	0.94	0.11	48,68,69,72	0
9	CUO	J	5002	4/4	0.94	0.13	53,56,80,83	0
9	CUO	Q	3002	4/4	0.94	0.10	53,62,64,73	0
9	CUO	b	2103	4/4	0.94	0.13	55,59,71,73	0
9	CUO	J	5003	4/4	0.94	0.09	89,96,96,103	0
9	CUO	B	3002	4/4	0.94	0.14	57,58,80,91	0
9	CUO	W	3002	4/4	0.94	0.12	58,62,70,77	0
9	CUO	S	2102	4/4	0.94	0.13	54,65,85,90	0
9	CUO	A	5003	4/4	0.94	0.07	79,87,89,89	0
9	CUO	H	3001	4/4	0.95	0.11	58,60,72,78	0
9	CUO	P	5004	4/4	0.95	0.13	40,48,67,68	0
9	CUO	W	3001	4/4	0.95	0.13	37,41,72,78	0
9	CUO	N	3002	4/4	0.95	0.12	48,51,70,74	0
9	CUO	b	2102	4/4	0.95	0.10	60,63,73,78	0
9	CUO	J	5004	4/4	0.95	0.11	49,58,62,63	0
9	CUO	Q	3001	4/4	0.95	0.12	37,43,64,70	0
9	CUO	K	3002	4/4	0.95	0.11	52,69,75,79	0
9	CUO	P	5001	4/4	0.95	0.13	36,38,56,71	0
9	CUO	c	3002	4/4	0.95	0.08	70,71,79,80	0
9	CUO	Y	2102	4/4	0.95	0.10	59,67,69,83	0
9	CUO	M	2105	4/4	0.95	0.12	48,60,61,62	0
9	CUO	V	5004	4/4	0.96	0.12	44,50,62,65	0
9	CUO	A	5004	4/4	0.96	0.11	51,60,67,70	0
9	CUO	S	2103	4/4	0.96	0.13	49,52,72,80	0
9	CUO	K	3001	4/4	0.96	0.08	57,73,73,80	0
9	CUO	V	5001	4/4	0.96	0.15	39,39,64,66	0
9	CUO	Y	2105	4/4	0.96	0.10	47,59,61,62	0
9	CUO	Z	3001	4/4	0.96	0.12	46,54,67,69	0
9	CUO	G	2105	4/4	0.96	0.08	58,60,66,69	0
9	CUO	T	3001	4/4	0.96	0.13	44,59,84,85	0
9	CUO	G	2102	4/4	0.97	0.10	57,62,65,70	0
9	CUO	H	3002	4/4	0.97	0.08	67,79,83,84	0
9	CUO	M	2102	4/4	0.97	0.11	41,52,59,63	0
9	CUO	M	2103	4/4	0.97	0.11	50,59,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
9	CUO	D	5004	4/4	0.98	0.07	52,54,59,62	0
9	CUO	E	3002	4/4	0.98	0.06	57,61,67,68	0

6.5 Other polymers ⓘ

There are no such residues in this entry.