Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 01:02 PM BST

PDB ID	:	5LHD
Title	:	Structure of glycosylated human aminopeptidase N
Authors	:	Recacha, R.; Mudgal, G.; Santiago, C.; Casasnovas, J.M.
Deposited on	:	2016-07-11
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

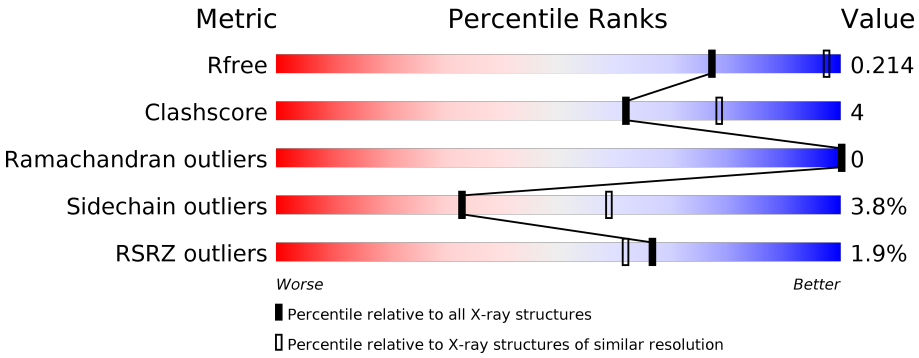
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	950	2% 84% 10% • 5%
1	B	950	2% 83% 12% • 5%
1	C	950	2% 81% 13% • 5%
1	D	950	2% 84% 11% • 5%
2	E	4	75% 25%
2	J	4	25% 75%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	4	50% 50%
2	R	4	75% 25%
3	F	5	80% 20%
3	L	5	20% 60% 20%
3	S	5	100%
4	G	2	50% 50%
4	I	2	100%
4	M	2	100%
4	N	2	100%
4	P	2	50% 50%
4	Q	2	100%
4	V	2	50% 50%
4	X	2	50% 50%
4	d	2	100%
4	e	2	50% 50%
4	f	2	100%
4	g	2	50% 50%
5	H	3	100%
5	O	3	67% 33%
5	U	3	67% 33%
5	Z	3	100%
5	b	3	67% 33%
5	c	3	100%
6	T	4	25% 75%
7	W	6	17% 50% 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	a	6	67% 33%
8	Y	6	50% 50%

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
11	EDO	A	1031	-	-	-	X
11	EDO	B	1030	-	-	-	X
11	EDO	B	1034	-	-	-	X
2	BMA	E	3	-	-	-	X
2	NAG	J	1	X	-	-	-
2	BMA	J	3	-	-	-	X
2	BMA	J	4	-	-	-	X
2	BMA	K	3	-	-	-	X
2	BMA	K	4	-	-	-	X
2	NAG	R	2	-	-	-	X
2	BMA	R	3	-	-	-	X
2	BMA	R	4	-	-	-	X
3	BMA	F	5	-	-	-	X
3	BMA	L	4	-	-	-	X
3	BMA	S	5	-	-	-	X
4	NAG	G	2	-	-	-	X
4	NAG	N	2	-	-	-	X
4	NAG	Q	1	X	-	-	-
4	NAG	Q	2	-	-	-	X
4	NAG	V	1	X	-	-	X
4	NAG	V	2	-	-	-	X
4	NAG	X	1	X	-	-	-
4	NAG	X	2	-	-	-	X
4	NAG	d	1	X	-	-	X
4	NAG	d	2	-	-	-	X
4	NAG	f	1	X	-	-	-
4	NAG	f	2	-	-	-	X
4	NAG	g	1	X	-	-	-
4	NAG	g	2	-	-	-	X
5	BMA	H	3	-	-	-	X
5	BMA	O	3	-	-	-	X
5	BMA	U	3	-	-	-	X
5	NAG	Z	2	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BMA	Z	3	-	-	-	X
5	BMA	b	3	-	-	-	X
5	NAG	c	2	-	-	-	X
5	BMA	c	3	-	-	-	X
6	BMA	T	4	-	-	-	X
7	BMA	W	3	-	-	-	X
7	BMA	W	4	-	-	-	X
7	BMA	W	5	-	-	-	X
7	BMA	W	6	-	-	-	X
7	BMA	a	5	-	-	-	X
7	BMA	a	6	-	-	-	X
8	NAG	Y	1	X	-	-	-
8	BMA	Y	5	-	-	-	X
8	BMA	Y	6	-	-	-	X
9	NAG	A	1015	X	-	-	-
9	NAG	A	1022	-	-	-	X
9	NAG	C	1117	X	-	-	-
9	NAG	D	1025	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 31338 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	0	0
			7285	4647	1226	1388	24			
1	B	904	Total	C	N	O	S	0	1	0
			7302	4656	1232	1390	24			
1	C	905	Total	C	N	O	S	0	0	0
			7300	4654	1231	1391	24			
1	D	904	Total	C	N	O	S	0	0	0
			7295	4651	1230	1390	24			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	TYR	-	expression tag	UNP P15144
A	19	PRO	-	expression tag	UNP P15144
A	20	TYR	-	expression tag	UNP P15144
A	21	ASP	-	expression tag	UNP P15144
A	22	VAL	-	expression tag	UNP P15144
A	23	PRO	-	expression tag	UNP P15144
A	24	ASP	-	expression tag	UNP P15144
A	25	TYR	-	expression tag	UNP P15144
A	26	ALA	-	expression tag	UNP P15144
A	27	GLY	-	expression tag	UNP P15144
A	28	ALA	-	expression tag	UNP P15144
A	29	GLN	-	expression tag	UNP P15144
A	30	PRO	-	expression tag	UNP P15144
A	31	ALA	-	expression tag	UNP P15144
A	32	ARG	-	expression tag	UNP P15144
A	33	SER	-	expression tag	UNP P15144
A	34	PRO	-	expression tag	UNP P15144
A	35	GLY	-	expression tag	UNP P15144
B	18	TYR	-	expression tag	UNP P15144
B	19	PRO	-	expression tag	UNP P15144
B	20	TYR	-	expression tag	UNP P15144

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ASP	-	expression tag	UNP P15144
B	22	VAL	-	expression tag	UNP P15144
B	23	PRO	-	expression tag	UNP P15144
B	24	ASP	-	expression tag	UNP P15144
B	25	TYR	-	expression tag	UNP P15144
B	26	ALA	-	expression tag	UNP P15144
B	27	GLY	-	expression tag	UNP P15144
B	28	ALA	-	expression tag	UNP P15144
B	29	GLN	-	expression tag	UNP P15144
B	30	PRO	-	expression tag	UNP P15144
B	31	ALA	-	expression tag	UNP P15144
B	32	ARG	-	expression tag	UNP P15144
B	33	SER	-	expression tag	UNP P15144
B	34	PRO	-	expression tag	UNP P15144
B	35	GLY	-	expression tag	UNP P15144
C	18	TYR	-	expression tag	UNP P15144
C	19	PRO	-	expression tag	UNP P15144
C	20	TYR	-	expression tag	UNP P15144
C	21	ASP	-	expression tag	UNP P15144
C	22	VAL	-	expression tag	UNP P15144
C	23	PRO	-	expression tag	UNP P15144
C	24	ASP	-	expression tag	UNP P15144
C	25	TYR	-	expression tag	UNP P15144
C	26	ALA	-	expression tag	UNP P15144
C	27	GLY	-	expression tag	UNP P15144
C	28	ALA	-	expression tag	UNP P15144
C	29	GLN	-	expression tag	UNP P15144
C	30	PRO	-	expression tag	UNP P15144
C	31	ALA	-	expression tag	UNP P15144
C	32	ARG	-	expression tag	UNP P15144
C	33	SER	-	expression tag	UNP P15144
C	34	PRO	-	expression tag	UNP P15144
C	35	GLY	-	expression tag	UNP P15144
D	18	TYR	-	expression tag	UNP P15144
D	19	PRO	-	expression tag	UNP P15144
D	20	TYR	-	expression tag	UNP P15144
D	21	ASP	-	expression tag	UNP P15144
D	22	VAL	-	expression tag	UNP P15144
D	23	PRO	-	expression tag	UNP P15144
D	24	ASP	-	expression tag	UNP P15144
D	25	TYR	-	expression tag	UNP P15144
D	26	ALA	-	expression tag	UNP P15144

Continued on next page...

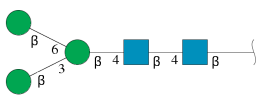
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	27	GLY	-	expression tag	UNP P15144
D	28	ALA	-	expression tag	UNP P15144
D	29	GLN	-	expression tag	UNP P15144
D	30	PRO	-	expression tag	UNP P15144
D	31	ALA	-	expression tag	UNP P15144
D	32	ARG	-	expression tag	UNP P15144
D	33	SER	-	expression tag	UNP P15144
D	34	PRO	-	expression tag	UNP P15144
D	35	GLY	-	expression tag	UNP P15144

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	J	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	L	5	Total	C	N	O	0	0	0
			61	34	2	25			

Continued on next page...

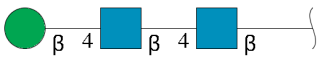
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	S	5	Total C N O 61 34 2 25	0	0	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	G	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	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	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	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	d	2	Total C N O 28 16 2 10	0	0	0
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	g	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 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.

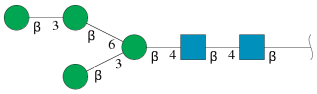


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	H	3	Total C N O 39 22 2 15	0	0	0
5	O	3	Total C N O 39 22 2 15	0	0	0
5	U	3	Total C N O 39 22 2 15	0	0	0
5	Z	3	Total C N O 39 22 2 15	0	0	0
5	b	3	Total C N O 39 22 2 15	0	0	0
5	c	3	Total C N O 39 22 2 15	0	0	0

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

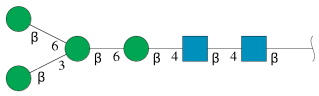
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	T	4	Total C N O 50 28 2 20	0	0	0

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose -(1-6)-[beta-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.



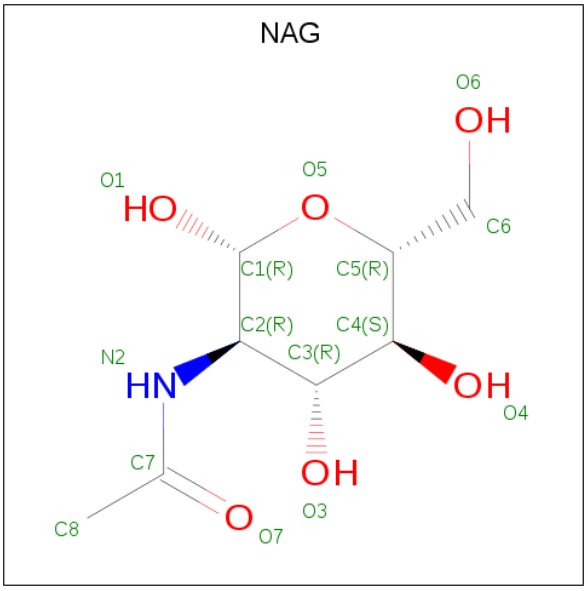
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	W	6	Total C N O 72 40 2 30	0	0	0
7	a	6	Total C N O 72 40 2 30	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	Y	6	Total C N O 72 40 2 30	0	0	0

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

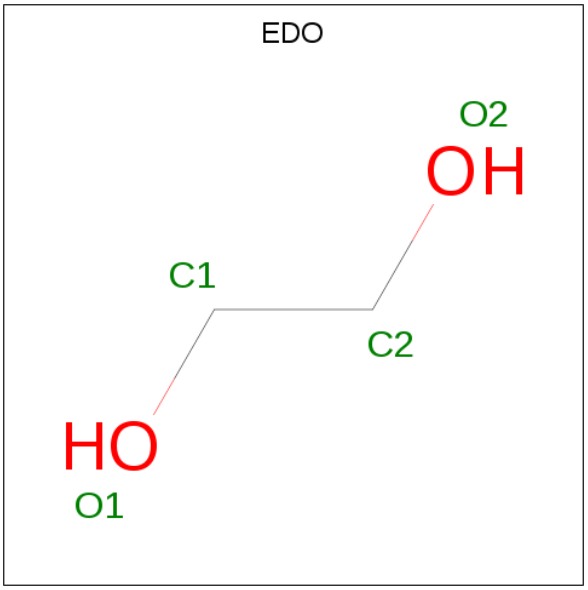


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 14 8 1 5	0	0
9	A	1	Total C N O 14 8 1 5	0	0
9	B	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	D	1	Total C N O 14 8 1 5	0	0
9	D	1	Total C N O 14 8 1 5	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Zn 1 1	0	0
10	A	1	Total Zn 1 1	0	0
10	D	1	Total Zn 1 1	0	0
10	C	1	Total Zn 1 1	0	0

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	A	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	157	Total O 157 157	0	0
12	B	186	Total O 186 186	0	0

Continued on next page...

Continued from previous page...

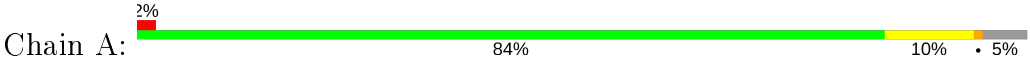
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	154	Total O 154 154	0	0
12	D	168	Total O 168 168	0	0

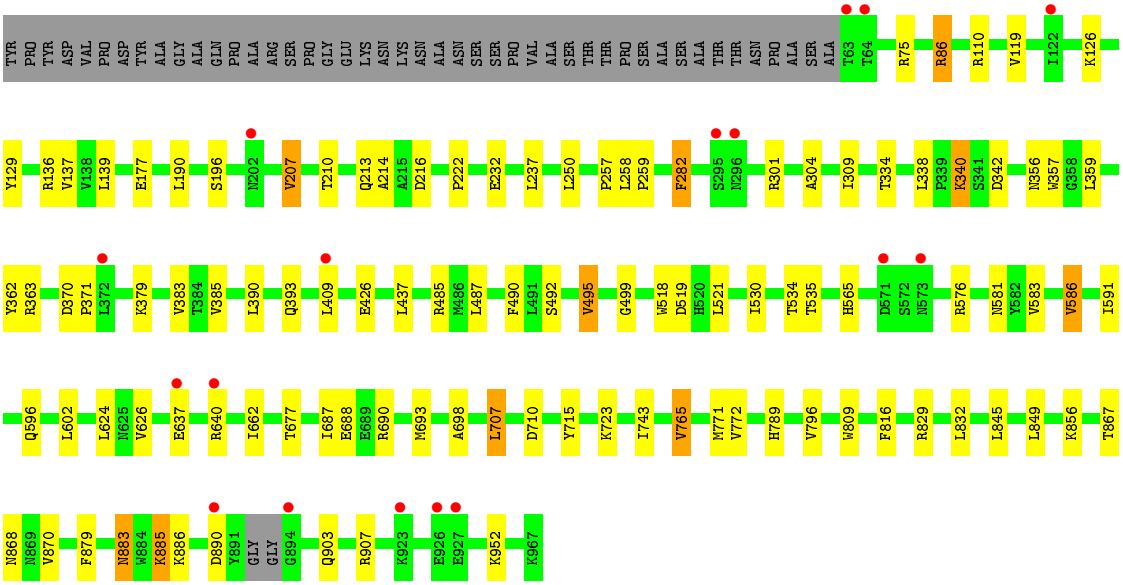
3 Residue-property plots (i)

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

- Molecule 1: Aminopeptidase N

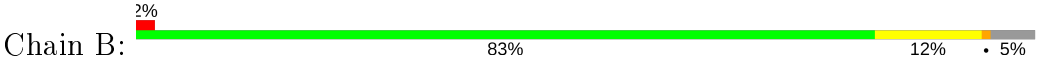
Chain A:

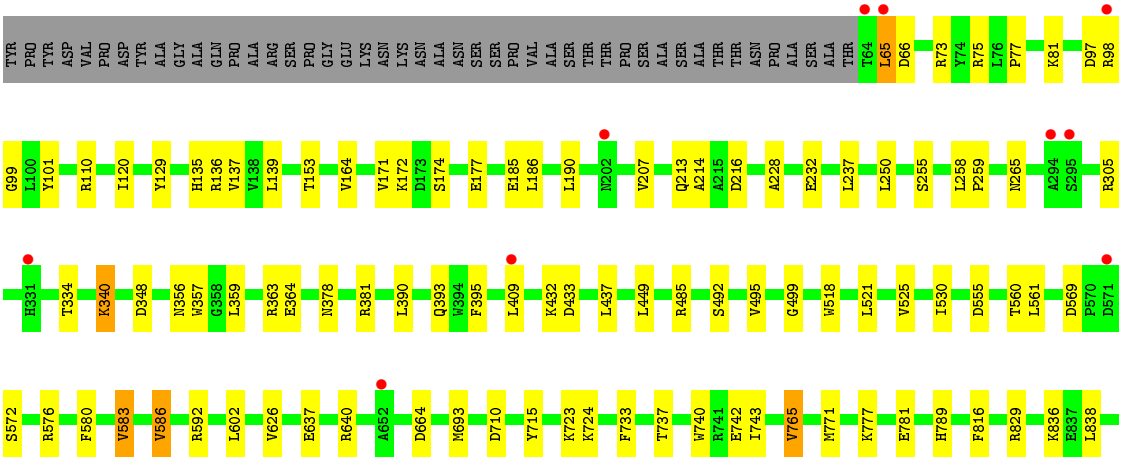


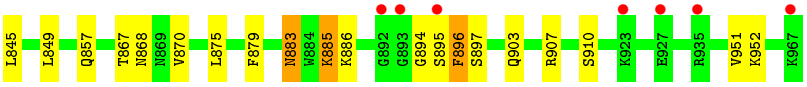


- Molecule 1: Aminopeptidase N

Chain B:

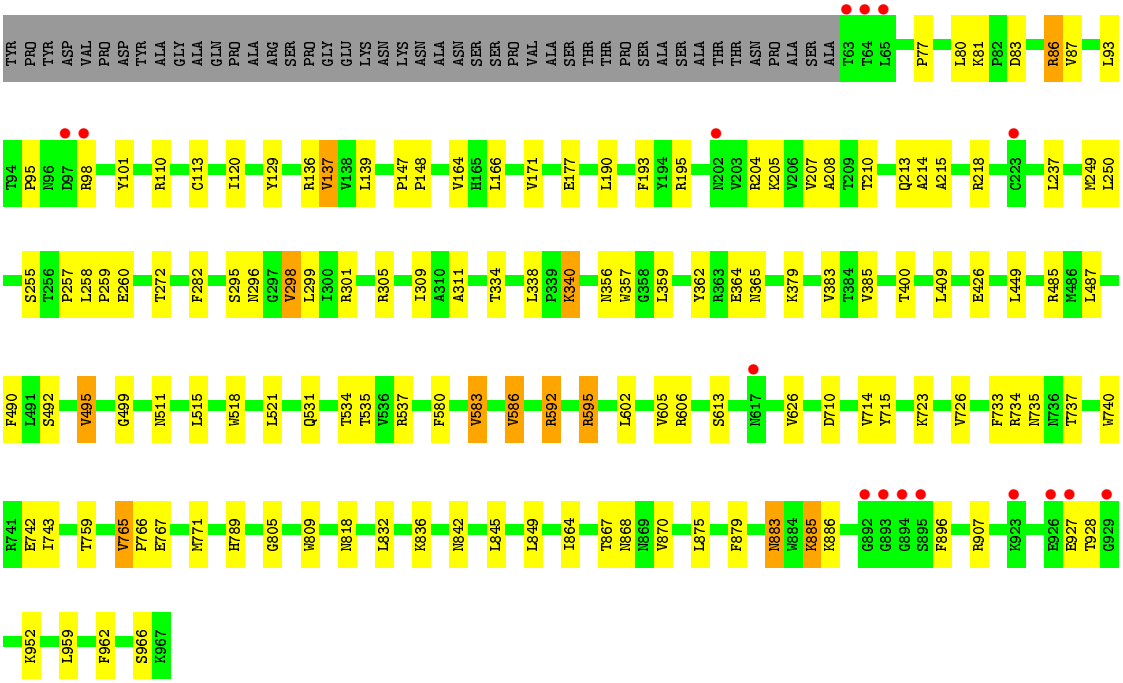






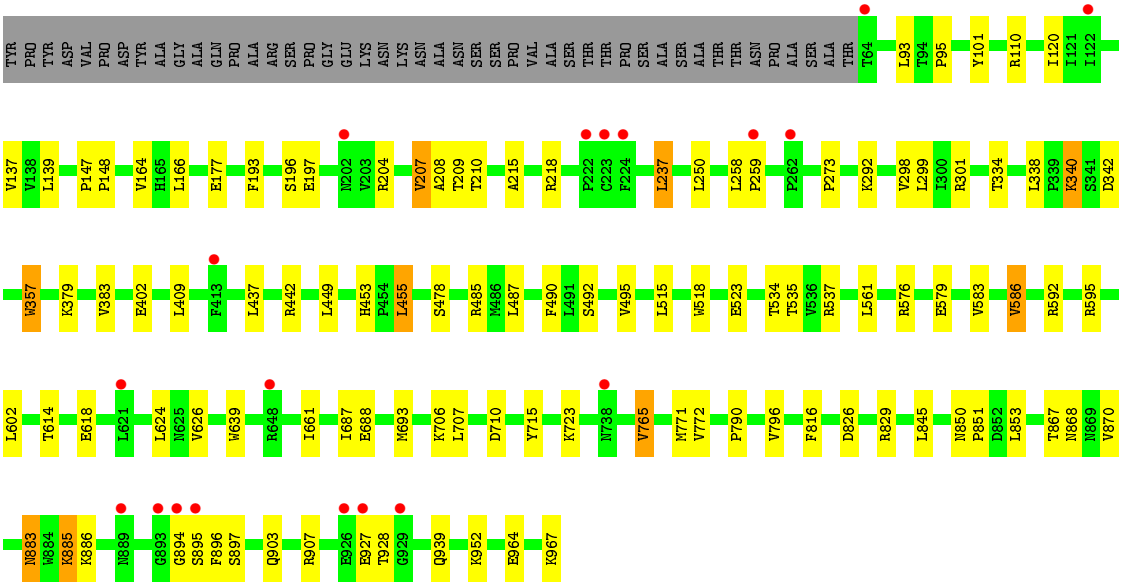
• Molecule 1: Aminopeptidase N

Chain C:



• Molecule 1: Aminopeptidase N

Chain D:

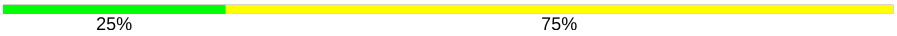


• Molecule 2: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 2: beta-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 J:



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

Chain K:

• Molecule 2: beta-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

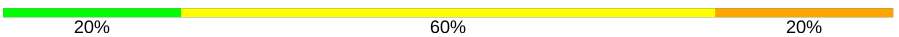
Chain R:

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

Chain F:

• Molecule 3: beta-D-mannopyranose-(1-3)-[beta-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 L:



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

se

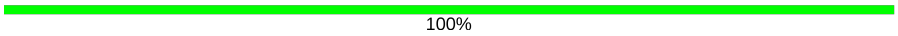
Chain S:

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

Chain G:

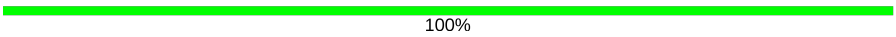
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



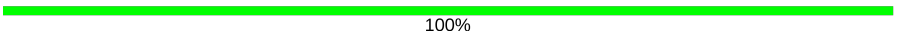
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain N:

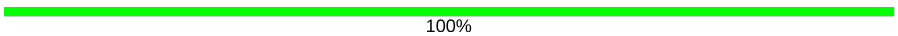


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 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

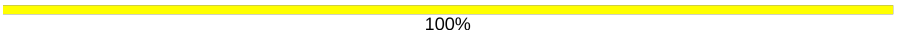
Chain V:

• 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 d:

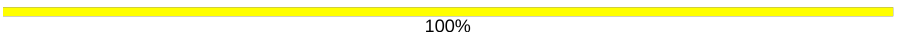


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

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

Chain f:

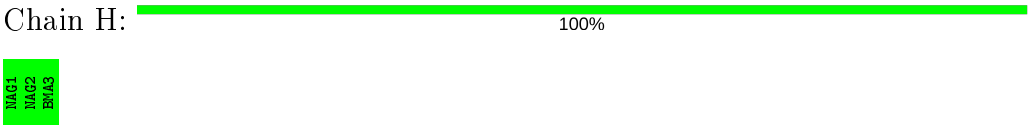


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

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

Chain H:



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

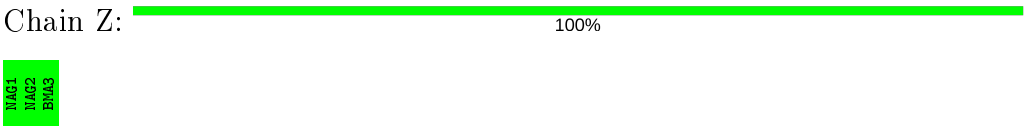
Chain O:

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

Chain U:

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

Chain Z:



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

Chain b:

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

Chain c:

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

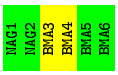
Chain T:

• Molecule 7: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-[beta-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 W:

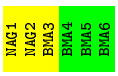
• Molecule 7: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose -(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido -2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 8: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-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 Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.09Å 168.86Å 244.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.60 24.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.97-2.60) 99.8 (24.96-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.60Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.181 , 0.214 0.182 , 0.214	Depositor DCC
R_{free} test set	8073 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	31338	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0639e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: ZN, BMA, NAG, EDO

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	0.23	0/7472	0.40	0/10179
1	B	0.24	0/7494	0.42	0/10208
1	C	0.23	0/7488	0.41	0/10200
1	D	0.23	0/7483	0.41	0/10193
All	All	0.23	0/29937	0.41	0/40780

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7285	0	7037	56	0
1	B	7302	0	7062	75	0
1	C	7300	0	7056	76	0
1	D	7295	0	7054	53	0
2	E	50	0	43	0	0
2	J	50	0	43	0	0
2	K	50	0	43	1	0
2	R	50	0	43	2	0
3	F	61	0	52	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	61	0	52	1	0
3	S	61	0	52	0	0
4	G	28	0	25	1	0
4	I	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	P	28	0	25	1	0
4	Q	28	0	25	0	0
4	V	28	0	25	0	0
4	X	28	0	25	0	0
4	d	28	0	25	0	0
4	e	28	0	25	0	0
4	f	28	0	25	0	0
4	g	28	0	25	0	0
5	H	39	0	34	0	0
5	O	39	0	34	0	0
5	U	39	0	34	0	0
5	Z	39	0	34	0	0
5	b	39	0	34	0	0
5	c	39	0	34	0	0
6	T	50	0	43	1	0
7	W	72	0	61	2	0
7	a	72	0	61	0	0
8	Y	72	0	61	0	0
9	A	28	0	26	0	0
9	B	14	0	13	0	0
9	C	14	0	13	0	0
9	D	28	0	26	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	A	68	0	102	6	0
11	B	48	0	72	8	0
11	C	48	0	72	2	0
11	D	20	0	30	0	0
12	A	157	0	0	8	1
12	B	186	0	0	15	0
12	C	154	0	0	11	1
12	D	168	0	0	6	0
All	All	31338	0	29621	261	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 4.

All (261) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLU:OE1	12:A:1101:HOH:O	1.81	0.96
1:C:77:PRO:O	12:C:1201:HOH:O	1.87	0.93
1:A:710:ASP:OD1	12:A:1102:HOH:O	1.95	0.84
1:A:530:ILE:O	12:A:1103:HOH:O	1.97	0.81
1:B:213:GLN:NE2	12:B:1105:HOH:O	2.13	0.81
1:C:426:GLU:O	12:C:1202:HOH:O	1.97	0.80
1:B:73:ARG:NH1	12:B:1106:HOH:O	2.15	0.80
1:A:222:PRO:HG2	11:A:1040:EDO:H11	1.62	0.79
1:B:737:THR:HG23	1:B:740:TRP:H	1.48	0.78
1:A:126:LYS:H	11:A:1032:EDO:H22	1.47	0.77
1:C:737:THR:HG23	1:C:740:TRP:H	1.49	0.77
1:A:581:ASN:ND2	1:B:65:LEU:O	2.18	0.76
1:A:119:VAL:HG13	11:A:1029:EDO:H12	1.69	0.75
1:C:137:VAL:O	12:C:1203:HOH:O	2.04	0.75
1:A:492:SER:HB3	1:A:495:VAL:HG13	1.70	0.73
1:B:77:PRO:O	12:B:1102:HOH:O	2.07	0.72
1:B:724:LYS:O	12:B:1103:HOH:O	2.08	0.71
1:B:432:LYS:NZ	12:B:1111:HOH:O	2.23	0.70
1:C:723:LYS:HG3	1:C:765:VAL:HG12	1.73	0.70
1:B:723:LYS:HG3	1:B:765:VAL:HG12	1.75	0.68
1:D:790:PRO:O	12:D:1101:HOH:O	2.11	0.68
1:C:485:ARG:NH2	1:C:626:VAL:O	2.26	0.68
1:A:426:GLU:O	12:A:1104:HOH:O	2.12	0.67
1:B:81:LYS:NZ	12:B:1114:HOH:O	2.27	0.67
1:C:492:SER:HB2	1:C:495:VAL:HG13	1.77	0.67
1:B:110:ARG:NH1	1:B:177:GLU:OE2	2.27	0.66
1:C:805:GLY:HA2	11:C:1146:EDO:H11	1.78	0.66
1:B:216:ASP:OD2	12:B:1104:HOH:O	2.12	0.66
1:A:110:ARG:NH1	1:A:177:GLU:OE2	2.28	0.66
1:C:531:GLN:NE2	12:C:1214:HOH:O	2.30	0.65
1:A:119:VAL:O	11:A:1029:EDO:O2	2.13	0.65
1:C:110:ARG:NH1	1:C:177:GLU:OE2	2.31	0.64
1:B:737:THR:OG1	1:B:742:GLU:O	2.15	0.64
1:B:185:GLU:OE2	12:B:1107:HOH:O	2.15	0.64
1:D:485:ARG:NH2	1:D:626:VAL:O	2.31	0.64
1:A:883:ASN:N	1:A:883:ASN:OD1	2.30	0.64
1:D:292:LYS:NZ	12:D:1104:HOH:O	2.29	0.63
1:A:723:LYS:HG3	1:A:765:VAL:HG12	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ARG:NH1	12:A:1108:HOH:O	2.22	0.62
1:B:98:ARG:NH1	12:B:1118:HOH:O	2.32	0.62
1:B:348:ASP:OD1	1:B:857:GLN:NE2	2.33	0.62
1:B:136:ARG:NH2	1:C:295:SER:O	2.34	0.61
1:C:733:PHE:O	1:C:737:THR:HG22	2.00	0.61
7:W:2:NAG:O3	7:W:4:BMA:O2	2.18	0.61
1:A:499:GLY:HA3	1:A:521:LEU:HD23	1.83	0.60
1:C:734:ARG:NH1	1:C:767:GLU:OE1	2.35	0.60
1:B:883:ASN:OD1	1:B:883:ASN:N	2.35	0.60
1:D:723:LYS:HG3	1:D:765:VAL:HG12	1.85	0.59
1:B:499:GLY:HA3	1:B:521:LEU:HD23	1.85	0.59
1:A:868:ASN:OD1	1:A:907:ARG:NH2	2.36	0.58
1:A:586:VAL:HG13	1:A:602:LEU:HB3	1.85	0.58
1:C:305:ARG:NH1	1:C:364:GLU:OE1	2.29	0.58
1:B:586:VAL:HG13	1:B:602:LEU:HB3	1.86	0.58
1:C:885:LYS:HD2	1:C:886:LYS:H	1.69	0.58
1:B:172:LYS:H	11:B:1034:EDO:H12	1.67	0.58
1:C:95:PRO:HG3	1:C:101:TYR:CZ	2.38	0.58
11:B:1027:EDO:H22	1:C:296:ASN:HB2	1.86	0.57
1:B:569:ASP:HB3	1:B:572:SER:HB3	1.86	0.57
1:D:196:SER:HB3	1:D:207:VAL:HG13	1.86	0.57
1:C:586:VAL:HG13	1:C:602:LEU:HB3	1.86	0.57
1:B:250:LEU:HG	1:B:340:LYS:HG2	1.87	0.57
1:C:311:ALA:O	12:C:1204:HOH:O	2.17	0.56
1:A:257:PRO:HG3	4:G:1:NAG:H62	1.87	0.56
1:A:485:ARG:NH2	1:A:626:VAL:O	2.38	0.56
1:D:868:ASN:OD1	1:D:907:ARG:NH2	2.39	0.56
1:D:885:LYS:HD2	1:D:886:LYS:H	1.71	0.56
1:C:737:THR:OG1	1:C:742:GLU:O	2.23	0.55
1:B:896:PHE:N	1:B:897:SER:HB3	2.21	0.55
1:A:196:SER:HB3	1:A:207:VAL:HG13	1.89	0.55
1:B:525:VAL:HG13	1:B:530:ILE:HB	1.89	0.54
1:B:75:ARG:NH2	12:B:1127:HOH:O	2.41	0.54
1:D:120:ILE:HG13	1:D:166:LEU:HD21	1.89	0.54
1:D:883:ASN:N	1:D:883:ASN:OD1	2.40	0.54
1:B:363:ARG:NH2	12:B:1123:HOH:O	2.35	0.54
1:D:437:LEU:HD11	1:D:693:MET:HG3	1.89	0.54
1:D:586:VAL:HG13	1:D:602:LEU:HB3	1.89	0.54
1:A:885:LYS:HD2	1:A:886:LYS:N	2.23	0.54
1:B:849:LEU:HD11	1:B:879:PHE:HZ	1.73	0.54
1:C:365:ASN:O	12:C:1206:HOH:O	2.18	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:818:ASN:OD1	12:C:1205:HOH:O	2.18	0.54
1:C:98:ARG:HH12	2:R:4:BMA:H62	1.72	0.54
1:C:250:LEU:HG	1:C:340:LYS:HG2	1.90	0.54
1:B:895:SER:HA	1:B:896:PHE:C	2.28	0.53
1:D:442:ARG:NH1	1:D:478:SER:OG	2.42	0.53
1:D:110:ARG:NH1	1:D:177:GLU:OE2	2.41	0.53
1:B:171:VAL:HA	11:B:1034:EDO:H12	1.91	0.53
1:B:305:ARG:NE	1:B:364:GLU:OE1	2.37	0.53
1:B:485:ARG:NH2	1:B:626:VAL:O	2.41	0.53
1:C:195:ARG:NH1	12:C:1228:HOH:O	2.42	0.53
1:C:120:ILE:HG13	1:C:166:LEU:HD21	1.92	0.52
1:D:93:LEU:HD21	1:D:208:ALA:HB2	1.92	0.52
1:D:258:LEU:HD12	1:D:259:PRO:HD2	1.91	0.52
1:A:86:ARG:NH1	12:A:1123:HOH:O	2.42	0.52
1:A:885:LYS:HD2	1:A:886:LYS:H	1.75	0.52
1:C:129:TYR:HB2	1:C:136:ARG:HG3	1.92	0.52
1:B:816:PHE:CE1	1:B:829:ARG:HG3	2.45	0.52
1:D:197:GLU:OE1	1:D:204:ARG:NH2	2.34	0.52
1:B:492:SER:HB2	1:B:495:VAL:HG13	1.92	0.51
1:C:842:ASN:HA	1:C:875:LEU:HD21	1.91	0.51
1:C:515:LEU:HD13	1:C:537:ARG:HH21	1.75	0.51
1:A:662:ILE:HD13	1:A:698:ALA:HB2	1.92	0.51
1:C:883:ASN:N	1:C:883:ASN:OD1	2.43	0.51
1:A:903:GLN:O	1:A:907:ARG:HG3	2.12	0.50
1:B:838:LEU:HD21	1:B:875:LEU:HD21	1.93	0.50
1:B:437:LEU:HD11	1:B:693:MET:HG3	1.94	0.50
1:B:885:LYS:HD2	1:B:886:LYS:N	2.26	0.50
1:C:499:GLY:HA3	1:C:521:LEU:HD23	1.93	0.50
1:A:849:LEU:HD11	1:A:879:PHE:HZ	1.77	0.49
1:B:433:ASP:HB3	1:B:693:MET:HE1	1.95	0.49
1:B:378:ASN:HD22	1:B:381:ARG:HH12	1.61	0.49
1:C:592:ARG:NH1	1:C:613:SER:O	2.45	0.49
1:D:455:LEU:HB2	12:D:1124:HOH:O	2.12	0.49
1:C:93:LEU:HD21	1:C:208:ALA:HB2	1.94	0.49
1:B:710:ASP:HA	1:B:715:TYR:CG	2.48	0.49
1:B:97:ASP:OD2	1:C:255:SER:N	2.33	0.49
1:D:579:GLU:HG3	12:D:1127:HOH:O	2.13	0.48
1:B:390:LEU:HA	1:B:393:GLN:HG2	1.95	0.48
1:B:733:PHE:O	1:B:737:THR:HG22	2.12	0.48
1:D:534:THR:OG1	1:D:535:THR:N	2.46	0.48
1:D:772:VAL:HG12	1:D:796:VAL:HG22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:NH2	11:A:1028:EDO:H22	2.29	0.48
1:D:639:TRP:HZ3	1:D:661:ILE:HG23	1.76	0.48
1:D:816:PHE:CE1	1:D:829:ARG:HG3	2.49	0.48
1:C:258:LEU:HD12	1:C:259:PRO:HD2	1.96	0.48
1:C:299:LEU:HD21	1:C:301:ARG:HD3	1.95	0.48
1:C:534:THR:OG1	1:C:535:THR:N	2.46	0.48
1:B:868:ASN:OD1	1:B:907:ARG:NH2	2.47	0.48
1:A:519:ASP:OD2	12:A:1106:HOH:O	2.20	0.48
1:D:927:GLU:HG2	1:D:928:THR:HG23	1.96	0.47
1:C:81:LYS:HG2	12:C:1280:HOH:O	2.14	0.47
1:C:962:PHE:O	1:C:966:SER:OG	2.17	0.47
1:A:772:VAL:HG12	1:A:796:VAL:HG22	1.97	0.47
1:C:362:TYR:HE2	1:C:385:VAL:HG12	1.79	0.47
1:C:868:ASN:OD1	1:C:907:ARG:NH2	2.47	0.47
1:B:356:ASN:HB2	1:B:359:LEU:O	2.14	0.47
1:A:258:LEU:HD12	1:A:259:PRO:HD2	1.96	0.47
1:C:592:ARG:O	1:C:595:ARG:HG3	2.15	0.47
1:C:849:LEU:HD11	1:C:879:PHE:HZ	1.79	0.47
1:A:213:GLN:HA	1:A:214:ALA:HA	1.56	0.47
1:B:120:ILE:HB	1:B:164:VAL:HB	1.95	0.47
1:A:304:ALA:HB3	1:A:309:ILE:HG13	1.97	0.47
1:D:453:HIS:O	12:D:1102:HOH:O	2.20	0.47
1:D:710:ASP:HA	1:D:715:TYR:CG	2.50	0.47
1:D:215:ALA:HB1	1:D:218:ARG:CZ	2.45	0.46
1:C:83:ASP:OD1	12:C:1207:HOH:O	2.21	0.46
1:A:687:ILE:HG23	1:A:688:GLU:HG3	1.98	0.46
1:A:816:PHE:CE1	1:A:829:ARG:HG3	2.51	0.46
1:C:885:LYS:HD2	1:C:886:LYS:N	2.30	0.46
1:A:250:LEU:HG	1:A:340:LYS:HG2	1.98	0.46
1:C:379:LYS:O	1:C:383:VAL:HG23	2.15	0.46
1:B:664:ASP:OD2	11:B:1031:EDO:O1	2.34	0.46
1:C:487:LEU:HA	1:C:490:PHE:CE2	2.51	0.46
1:B:395:PHE:CZ	11:B:1025:EDO:H21	2.51	0.46
1:B:153:THR:HG23	11:B:1027:EDO:H12	1.98	0.46
1:D:896:PHE:N	1:D:897:SER:HB3	2.31	0.46
1:B:883:ASN:HA	1:B:885:LYS:HE3	1.97	0.46
1:A:710:ASP:HA	1:A:715:TYR:CG	2.51	0.46
1:B:232:GLU:OE2	12:B:1108:HOH:O	2.21	0.45
1:D:120:ILE:HB	1:D:164:VAL:HB	1.98	0.45
1:D:250:LEU:HG	1:D:340:LYS:HG2	1.97	0.45
1:A:743:ILE:HD13	1:A:789:HIS:CE1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:PHE:O	1:C:583:VAL:HG13	2.17	0.45
7:W:3:BMA:H61	7:W:4:BMA:H2	1.61	0.45
1:C:726:VAL:HG21	1:C:759:THR:HB	1.99	0.45
1:D:402:GLU:HG2	3:L:5:BMA:H62	1.99	0.45
1:A:362:TYR:HE2	1:A:385:VAL:HG12	1.82	0.45
1:B:555:ASP:HB3	1:B:560:THR:HG22	1.99	0.45
1:C:864:ILE:HA	1:C:867:THR:HG22	1.99	0.45
1:C:356:ASN:HB2	1:C:359:LEU:O	2.17	0.44
1:D:273:PRO:HG2	1:D:357:TRP:CZ3	2.53	0.44
1:D:894:GLY:HA2	1:D:896:PHE:O	2.17	0.44
1:C:710:ASP:HA	1:C:715:TYR:CG	2.52	0.44
1:B:213:GLN:HA	1:B:214:ALA:HA	1.59	0.44
1:C:743:ILE:HD13	1:C:789:HIS:CE1	2.53	0.44
1:D:95:PRO:HG3	1:D:101:TYR:CZ	2.52	0.44
1:B:232:GLU:OE1	12:B:1109:HOH:O	2.21	0.44
1:B:99:GLY:O	12:B:1110:HOH:O	2.21	0.44
2:R:3:BMA:H61	2:R:4:BMA:H2	1.75	0.43
1:B:363:ARG:NE	12:B:1123:HOH:O	2.49	0.43
1:B:580:PHE:O	1:B:583:VAL:HG13	2.18	0.43
1:C:765:VAL:HA	1:C:766:PRO:HD3	1.89	0.43
1:C:886:LYS:HE2	1:C:886:LYS:HB3	1.84	0.43
1:A:591:ILE:HG22	1:A:596:GLN:HA	2.01	0.43
1:C:213:GLN:HA	1:C:214:ALA:HA	1.60	0.43
1:C:305:ARG:HD3	1:C:364:GLU:OE1	2.17	0.43
1:D:209:THR:OG1	1:D:210:THR:N	2.51	0.43
1:D:964:GLU:HA	1:D:967:LYS:HE3	2.00	0.43
1:A:129:TYR:CB	1:A:136:ARG:HG3	2.49	0.43
1:A:216:ASP:OD2	12:A:1107:HOH:O	2.21	0.43
1:C:296:ASN:OD1	1:C:298:VAL:HG12	2.18	0.43
1:D:895:SER:HA	1:D:896:PHE:C	2.39	0.43
1:B:885:LYS:HD2	1:B:886:LYS:H	1.83	0.43
1:B:637:GLU:OE1	1:B:640:ARG:NH1	2.51	0.43
1:A:809:TRP:CE2	1:A:832:LEU:HD22	2.53	0.43
1:B:174:SER:OG	1:D:523:GLU:OE2	2.26	0.43
1:A:390:LEU:HA	1:A:393:GLN:HG2	1.99	0.43
1:A:437:LEU:HD11	1:A:693:MET:HG3	2.01	0.43
1:B:258:LEU:HD12	1:B:259:PRO:HD2	2.01	0.43
1:C:400:THR:O	1:C:511:ASN:HA	2.19	0.42
1:D:903:GLN:O	1:D:907:ARG:HG3	2.18	0.42
1:C:927:GLU:HG2	1:C:928:THR:HG23	2.01	0.42
1:B:743:ILE:HD13	1:B:789:HIS:NE2	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:836:LYS:HE2	1:C:836:LYS:HB3	1.90	0.42
1:A:356:ASN:HB2	1:A:359:LEU:O	2.20	0.42
1:C:249:MET:HG2	1:C:272:THR:HG22	2.01	0.42
1:D:147:PRO:HA	1:D:148:PRO:HD3	1.94	0.42
1:D:237:LEU:HA	1:D:237:LEU:HD12	1.90	0.42
1:D:614:THR:HB	1:D:618:GLU:HG3	2.00	0.42
1:D:487:LEU:HA	1:D:490:PHE:CE2	2.55	0.42
1:A:379:LYS:O	1:A:383:VAL:HG23	2.20	0.42
1:C:215:ALA:HB1	1:C:218:ARG:CZ	2.49	0.42
1:A:301:ARG:HB2	1:A:342:ASP:OD1	2.19	0.42
1:B:228:ALA:HB3	11:B:1028:EDO:H21	2.01	0.42
1:B:737:THR:HG21	1:B:740:TRP:CE3	2.55	0.42
1:D:895:SER:HA	1:D:896:PHE:O	2.19	0.42
1:A:210:THR:HG21	1:A:282:PHE:CD1	2.55	0.42
1:A:707:LEU:HD12	1:A:707:LEU:HA	1.86	0.41
1:D:885:LYS:HD2	1:D:886:LYS:N	2.33	0.41
1:A:75:ARG:HH21	11:A:1028:EDO:H22	1.84	0.41
1:C:120:ILE:HB	1:C:164:VAL:HB	2.01	0.41
1:C:356:ASN:OD1	12:C:1208:HOH:O	2.22	0.41
1:C:362:TYR:CE2	1:C:385:VAL:HG12	2.55	0.41
1:D:299:LEU:HD21	1:D:301:ARG:HD3	2.02	0.41
4:P:1:NAG:H62	4:P:2:NAG:N2	2.35	0.41
1:A:487:LEU:HA	1:A:490:PHE:CE2	2.55	0.41
1:B:777:LYS:O	1:B:781:GLU:HG2	2.21	0.41
1:B:910:SER:HB2	1:B:951:VAL:HG21	2.03	0.41
1:C:809:TRP:CE2	1:C:832:LEU:HD22	2.55	0.41
1:D:515:LEU:HD13	1:D:537:ARG:NH2	2.36	0.41
1:D:826:ASP:OD1	1:D:829:ARG:NH2	2.48	0.41
1:D:687:ILE:HG23	1:D:688:GLU:HG3	2.02	0.41
1:B:723:LYS:HE3	1:B:765:VAL:HA	2.02	0.41
1:C:86:ARG:NH1	1:C:87:VAL:O	2.53	0.41
1:D:379:LYS:O	1:D:383:VAL:HG23	2.20	0.41
1:D:850:ASN:HA	1:D:851:PRO:HD3	1.94	0.41
1:B:101:TYR:HB3	1:B:186:LEU:HB3	2.02	0.41
1:B:65:LEU:HB3	1:B:66:ASP:H	1.71	0.41
1:C:147:PRO:HA	1:C:148:PRO:HD3	1.91	0.41
1:C:210:THR:HG21	1:C:282:PHE:CD1	2.55	0.41
1:C:714:VAL:HA	1:C:959:LEU:HD13	2.02	0.41
1:A:370:ASP:HA	1:A:371:PRO:HD2	1.94	0.41
1:B:894:GLY:HA2	1:B:896:PHE:O	2.20	0.41
1:B:129:TYR:CB	1:B:136:ARG:HG3	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:952:LYS:HB2	1:B:952:LYS:HE2	1.80	0.41
1:B:135:HIS:HA	11:B:1027:EDO:H21	2.03	0.40
1:C:605:VAL:HG12	1:C:606:ARG:HG3	2.03	0.40
1:A:637:GLU:OE1	1:A:640:ARG:NH2	2.52	0.40
1:A:849:LEU:HD11	1:A:879:PHE:CZ	2.56	0.40
1:C:129:TYR:CB	1:C:136:ARG:HG3	2.51	0.40
1:D:706:LYS:NZ	12:D:1110:HOH:O	2.39	0.40
1:A:362:TYR:CE2	1:A:385:VAL:HG12	2.55	0.40
1:A:534:THR:OG1	1:A:535:THR:N	2.54	0.40
1:B:836:LYS:HE2	1:B:836:LYS:HB3	1.92	0.40
1:B:903:GLN:O	1:B:907:ARG:HG3	2.21	0.40
1:C:80:LEU:HD23	1:C:113:CYS:HA	2.03	0.40
1:D:492:SER:OG	1:D:495:VAL:HG13	2.20	0.40
2:K:3:BMA:H61	2:K:4:BMA:O2	2.21	0.40
1:B:255:SER:OG	1:B:265:ASN:HB3	2.22	0.40
1:C:205:LYS:HA	11:C:1141:EDO:H22	2.03	0.40
1:C:257:PRO:HG3	6:T:1:NAG:H62	2.04	0.40
1:D:301:ARG:HB2	1:D:342:ASP:OD1	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1171:HOH:O	12:C:1310:HOH:O[3_555]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	899/950 (95%)	868 (97%)	31 (3%)	0	100	100
1	B	903/950 (95%)	870 (96%)	33 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	903/950 (95%)	874 (97%)	29 (3%)	0	100	100
1	D	902/950 (95%)	873 (97%)	29 (3%)	0	100	100
All	All	3607/3800 (95%)	3485 (97%)	122 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	800/837 (96%)	768 (96%)	32 (4%)	31	57
1	B	803/837 (96%)	778 (97%)	25 (3%)	40	66
1	C	802/837 (96%)	769 (96%)	33 (4%)	30	56
1	D	802/837 (96%)	770 (96%)	32 (4%)	31	57
All	All	3207/3348 (96%)	3085 (96%)	122 (4%)	33	59

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	137	VAL
1	A	139	LEU
1	A	190	LEU
1	A	207	VAL
1	A	237	LEU
1	A	282	PHE
1	A	334	THR
1	A	338	LEU
1	A	340	LYS
1	A	357	TRP
1	A	409	LEU
1	A	495	VAL
1	A	518	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	565	HIS
1	A	576	ARG
1	A	583	VAL
1	A	586	VAL
1	A	624	LEU
1	A	677	THR
1	A	690	ARG
1	A	707	LEU
1	A	765	VAL
1	A	771	MET
1	A	845	LEU
1	A	856	LYS
1	A	867	THR
1	A	870	VAL
1	A	883	ASN
1	A	885	LYS
1	A	890	ASP
1	A	952	LYS
1	B	65	LEU
1	B	137	VAL
1	B	139	LEU
1	B	190	LEU
1	B	207	VAL
1	B	237	LEU
1	B	334	THR
1	B	340	LYS
1	B	357	TRP
1	B	409	LEU
1	B	449	LEU
1	B	518	TRP
1	B	561	LEU
1	B	576	ARG
1	B	583	VAL
1	B	586	VAL
1	B	592	ARG
1	B	765	VAL
1	B	771	MET
1	B	845	LEU
1	B	867	THR
1	B	870	VAL
1	B	883	ASN
1	B	885	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	896	PHE
1	C	86	ARG
1	C	137	VAL
1	C	139	LEU
1	C	171	VAL
1	C	190	LEU
1	C	193	PHE
1	C	204	ARG
1	C	207	VAL
1	C	237	LEU
1	C	260	GLU
1	C	298	VAL
1	C	309	ILE
1	C	334	THR
1	C	338	LEU
1	C	340	LYS
1	C	357	TRP
1	C	409	LEU
1	C	449	LEU
1	C	495	VAL
1	C	518	TRP
1	C	583	VAL
1	C	586	VAL
1	C	592	ARG
1	C	595	ARG
1	C	735	ASN
1	C	765	VAL
1	C	771	MET
1	C	845	LEU
1	C	870	VAL
1	C	883	ASN
1	C	885	LYS
1	C	896	PHE
1	C	952	LYS
1	D	137	VAL
1	D	139	LEU
1	D	193	PHE
1	D	207	VAL
1	D	237	LEU
1	D	298	VAL
1	D	334	THR
1	D	338	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	340	LYS
1	D	357	TRP
1	D	409	LEU
1	D	449	LEU
1	D	455	LEU
1	D	518	TRP
1	D	561	LEU
1	D	576	ARG
1	D	583	VAL
1	D	586	VAL
1	D	592	ARG
1	D	595	ARG
1	D	624	LEU
1	D	707	LEU
1	D	765	VAL
1	D	771	MET
1	D	845	LEU
1	D	853	LEU
1	D	867	THR
1	D	870	VAL
1	D	883	ASN
1	D	885	LYS
1	D	939	GLN
1	D	952	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

95 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	$\#\|Z\| > 2$
2	NAG	E	1	1,2	14,14,15	0.54	0	17,19,21	0.68	0
2	NAG	E	2	2	14,14,15	0.54	0	17,19,21	0.82	0
2	BMA	E	3	2	11,11,12	0.58	0	15,15,17	1.21	2 (13%)
2	BMA	E	4	2	11,11,12	0.70	0	15,15,17	0.55	0
3	NAG	F	1	1,3	14,14,15	0.54	0	17,19,21	0.68	0
3	NAG	F	2	3	14,14,15	0.57	0	17,19,21	0.71	0
3	BMA	F	3	3	11,11,12	0.53	0	15,15,17	1.20	2 (13%)
3	BMA	F	4	3	11,11,12	0.60	0	15,15,17	0.64	0
3	BMA	F	5	3	11,11,12	0.59	0	15,15,17	0.90	0
4	NAG	G	1	1,4	14,14,15	0.50	0	17,19,21	0.80	0
4	NAG	G	2	4	14,14,15	0.57	0	17,19,21	0.77	0
5	NAG	H	1	1,5	14,14,15	0.60	0	17,19,21	0.74	0
5	NAG	H	2	5	14,14,15	0.60	0	17,19,21	0.91	0
5	BMA	H	3	5	11,11,12	0.64	0	15,15,17	0.76	0
4	NAG	I	1	1,4	14,14,15	0.58	0	17,19,21	0.78	0
4	NAG	I	2	4	14,14,15	0.51	0	17,19,21	0.67	0
2	NAG	J	1	1,2	14,14,15	0.54	0	17,19,21	0.82	1 (5%)
2	NAG	J	2	2	14,14,15	0.53	0	17,19,21	0.80	1 (5%)
2	BMA	J	3	2	11,11,12	0.54	0	15,15,17	0.93	1 (6%)
2	BMA	J	4	2	11,11,12	0.67	0	15,15,17	0.60	0
2	NAG	K	1	1,2	14,14,15	0.63	0	17,19,21	0.80	0
2	NAG	K	2	2	14,14,15	0.57	0	17,19,21	0.58	0
2	BMA	K	3	2	11,11,12	0.69	0	15,15,17	1.00	1 (6%)
2	BMA	K	4	2	11,11,12	0.87	1 (9%)	15,15,17	1.70	4 (26%)
3	NAG	L	1	1,3	14,14,15	0.57	0	17,19,21	0.73	0
3	NAG	L	2	3	14,14,15	0.44	0	17,19,21	1.42	2 (11%)
3	BMA	L	3	3	11,11,12	0.60	0	15,15,17	1.50	2 (13%)
3	BMA	L	4	3	11,11,12	0.55	0	15,15,17	1.38	2 (13%)
3	BMA	L	5	3	11,11,12	0.56	0	15,15,17	1.05	1 (6%)
4	NAG	M	1	1,4	14,14,15	0.60	0	17,19,21	0.83	0
4	NAG	M	2	4	14,14,15	0.56	0	17,19,21	0.65	0
4	NAG	N	1	1,4	14,14,15	0.59	0	17,19,21	0.73	0
4	NAG	N	2	4	14,14,15	0.50	0	17,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	O	1	1,5	14,14,15	0.47	0	17,19,21	1.03	1 (5%)
5	NAG	O	2	5	14,14,15	0.59	0	17,19,21	0.70	0
5	BMA	O	3	5	11,11,12	0.56	0	15,15,17	0.96	0
4	NAG	P	1	1,4	14,14,15	0.56	0	17,19,21	0.73	0
4	NAG	P	2	4	14,14,15	0.56	0	17,19,21	1.27	2 (11%)
4	NAG	Q	1	1,4	14,14,15	0.55	0	17,19,21	0.95	0
4	NAG	Q	2	4	14,14,15	0.50	0	17,19,21	0.81	0
2	NAG	R	1	1,2	14,14,15	0.68	0	17,19,21	1.56	3 (17%)
2	NAG	R	2	2	14,14,15	0.60	0	17,19,21	1.00	1 (5%)
2	BMA	R	3	2	11,11,12	0.63	0	15,15,17	0.89	1 (6%)
2	BMA	R	4	2	11,11,12	0.63	0	15,15,17	0.54	0
3	NAG	S	1	1,3	14,14,15	0.56	0	17,19,21	0.64	0
3	NAG	S	2	3	14,14,15	0.55	0	17,19,21	0.80	0
3	BMA	S	3	3	11,11,12	0.76	0	15,15,17	0.78	0
3	BMA	S	4	3	11,11,12	0.66	0	15,15,17	0.59	0
3	BMA	S	5	3	11,11,12	0.65	0	15,15,17	0.94	0
6	NAG	T	1	1,6	14,14,15	0.60	0	17,19,21	0.81	0
6	NAG	T	2	6	14,14,15	0.55	0	17,19,21	0.79	1 (5%)
6	BMA	T	3	6	11,11,12	0.61	0	15,15,17	0.76	0
6	BMA	T	4	6	11,11,12	0.62	0	15,15,17	1.02	1 (6%)
5	NAG	U	1	1,5	14,14,15	0.56	0	17,19,21	0.65	0
5	NAG	U	2	5	14,14,15	0.60	0	17,19,21	1.00	1 (5%)
5	BMA	U	3	5	11,11,12	0.65	0	15,15,17	0.77	0
4	NAG	V	1	1,4	14,14,15	0.59	0	17,19,21	0.99	1 (5%)
4	NAG	V	2	4	14,14,15	0.50	0	17,19,21	0.71	0
7	NAG	W	1	1,7	14,14,15	0.60	0	17,19,21	0.71	0
7	NAG	W	2	7	14,14,15	0.54	0	17,19,21	0.68	0
7	BMA	W	3	7	11,11,12	0.51	0	15,15,17	1.16	1 (6%)
7	BMA	W	4	7	11,11,12	0.62	0	15,15,17	1.83	4 (26%)
7	BMA	W	5	7	11,11,12	0.60	0	15,15,17	1.00	1 (6%)
7	BMA	W	6	7	11,11,12	0.62	0	15,15,17	1.10	1 (6%)
4	NAG	X	1	1,4	14,14,15	0.58	0	17,19,21	0.79	1 (5%)
4	NAG	X	2	4	14,14,15	0.54	0	17,19,21	0.65	0
8	NAG	Y	1	1,8	14,14,15	0.51	0	17,19,21	0.85	1 (5%)
8	NAG	Y	2	8	14,14,15	0.61	0	17,19,21	0.78	1 (5%)
8	BMA	Y	3	8	11,11,12	0.63	0	15,15,17	1.01	2 (13%)
8	BMA	Y	4	8	11,11,12	0.67	0	15,15,17	0.64	0
8	BMA	Y	5	8	11,11,12	0.65	0	15,15,17	0.66	0
8	BMA	Y	6	8	11,11,12	0.66	0	15,15,17	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	Z	1	1,5	14,14,15	0.55	0	17,19,21	0.64	0
5	NAG	Z	2	5	14,14,15	0.51	0	17,19,21	0.71	0
5	BMA	Z	3	5	11,11,12	0.64	0	15,15,17	1.06	0
7	NAG	a	1	1,7	14,14,15	0.59	0	17,19,21	0.60	0
7	NAG	a	2	7	14,14,15	0.54	0	17,19,21	0.72	0
7	BMA	a	3	7	11,11,12	0.63	0	15,15,17	1.31	1 (6%)
7	BMA	a	4	7	11,11,12	0.59	0	15,15,17	1.25	2 (13%)
7	BMA	a	5	7	11,11,12	0.59	0	15,15,17	1.12	0
7	BMA	a	6	7	11,11,12	0.84	0	15,15,17	0.75	0
5	NAG	b	1	1,5	14,14,15	0.50	0	17,19,21	0.92	0
5	NAG	b	2	5	14,14,15	0.59	0	17,19,21	0.71	0
5	BMA	b	3	5	11,11,12	0.57	0	15,15,17	1.09	2 (13%)
5	NAG	c	1	1,5	14,14,15	0.57	0	17,19,21	0.60	0
5	NAG	c	2	5	14,14,15	0.51	0	17,19,21	0.57	0
5	BMA	c	3	5	11,11,12	0.64	0	15,15,17	0.68	0
4	NAG	d	1	1,4	14,14,15	0.54	0	17,19,21	0.91	1 (5%)
4	NAG	d	2	4	14,14,15	0.51	0	17,19,21	1.20	1 (5%)
4	NAG	e	1	1,4	14,14,15	0.59	0	17,19,21	0.95	2 (11%)
4	NAG	e	2	4	14,14,15	0.46	0	17,19,21	0.80	0
4	NAG	f	1	1,4	14,14,15	0.62	0	17,19,21	1.30	2 (11%)
4	NAG	f	2	4	14,14,15	0.52	0	17,19,21	1.10	1 (5%)
4	NAG	g	1	1,4	14,14,15	0.49	0	17,19,21	0.68	0
4	NAG	g	2	4	14,14,15	0.53	0	17,19,21	1.00	1 (5%)

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
2	NAG	J	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	3/6/23/26	0/1/1/1
2	BMA	J	3	2	-	1/2/19/22	1/1/1/1
2	BMA	J	4	2	-	0/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	BMA	K	3	2	-	1/2/19/22	0/1/1/1
2	BMA	K	4	2	-	2/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
3	BMA	L	4	3	-	1/2/19/22	1/1/1/1
3	BMA	L	5	3	-	2/2/19/22	1/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	0/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	4/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	BMA	R	3	2	-	2/2/19/22	0/1/1/1
2	BMA	R	4	2	-	1/2/19/22	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	BMA	S	3	3	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	4	BMA	O5-C1	-2.13	1.40	1.43

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	4	BMA	O5-C1-C2	-4.47	103.87	110.77
3	L	4	BMA	C1-O5-C5	4.06	117.69	112.19
7	W	4	BMA	O3-C3-C2	-4.01	102.32	109.99
7	W	4	BMA	C1-C2-C3	3.87	114.43	109.67
2	R	1	NAG	C4-C3-C2	3.85	116.67	111.02
2	R	1	NAG	C3-C4-C5	3.72	116.88	110.24
7	W	3	BMA	O5-C5-C6	3.63	112.89	107.20
3	L	3	BMA	C1-O5-C5	3.60	117.07	112.19
3	L	5	BMA	C1-O5-C5	3.54	116.98	112.19
3	L	2	NAG	C1-O5-C5	3.53	116.97	112.19
7	a	3	BMA	C1-C2-C3	3.36	113.79	109.67
4	d	2	NAG	C1-O5-C5	3.36	116.74	112.19
2	K	4	BMA	O5-C5-C6	3.09	112.05	107.20
7	W	6	BMA	O5-C1-C2	3.06	115.49	110.77
2	J	3	BMA	O5-C5-C6	3.04	111.98	107.20
7	a	4	BMA	C1-O5-C5	3.03	116.30	112.19
7	W	5	BMA	O5-C1-C2	2.97	115.35	110.77
4	f	1	NAG	O5-C1-C2	2.96	115.96	111.29
3	F	3	BMA	O5-C5-C6	2.87	111.70	107.20
3	L	3	BMA	O5-C1-C2	-2.83	106.40	110.77
4	V	1	NAG	O5-C1-C2	-2.83	106.82	111.29
8	Y	3	BMA	O5-C5-C6	2.79	111.57	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	g	2	NAG	C1-O5-C5	2.77	115.94	112.19
3	F	3	BMA	O3-C3-C2	2.75	115.26	109.99
4	d	1	NAG	O5-C5-C6	2.65	111.36	107.20
2	E	3	BMA	O5-C1-C2	-2.59	106.77	110.77
4	P	2	NAG	C3-C4-C5	2.50	114.69	110.24
5	U	2	NAG	C4-C3-C2	2.45	114.61	111.02
8	Y	1	NAG	O5-C5-C6	2.45	111.04	107.20
2	R	3	BMA	O5-C5-C6	2.43	111.01	107.20
4	P	2	NAG	O5-C1-C2	-2.42	107.46	111.29
4	f	1	NAG	C1-O5-C5	2.39	115.42	112.19
7	W	4	BMA	C3-C4-C5	2.34	114.41	110.24
2	J	2	NAG	C1-O5-C5	2.28	115.28	112.19
4	e	1	NAG	O4-C4-C3	-2.28	105.08	110.35
7	a	4	BMA	C1-C2-C3	2.27	112.46	109.67
6	T	4	BMA	C1-C2-C3	-2.27	106.88	109.67
3	L	2	NAG	O4-C4-C5	2.25	114.87	109.30
2	R	1	NAG	O5-C1-C2	-2.22	107.78	111.29
5	b	3	BMA	O5-C1-C2	-2.22	107.35	110.77
4	f	2	NAG	C1-O5-C5	2.21	115.19	112.19
6	T	2	NAG	C1-O5-C5	2.17	115.14	112.19
2	K	4	BMA	C2-C3-C4	-2.16	107.16	110.89
3	L	4	BMA	C1-C2-C3	2.14	112.30	109.67
2	K	4	BMA	O2-C2-C1	2.13	113.51	109.15
2	R	2	NAG	C1-O5-C5	-2.11	109.33	112.19
5	O	1	NAG	O5-C1-C2	-2.11	107.96	111.29
2	E	3	BMA	C1-C2-C3	-2.08	107.10	109.67
8	Y	2	NAG	C4-C3-C2	2.08	114.06	111.02
4	e	1	NAG	C4-C3-C2	2.07	114.06	111.02
2	J	1	NAG	O5-C5-C6	2.07	110.45	107.20
2	K	3	BMA	O5-C5-C6	2.04	110.41	107.20
8	Y	3	BMA	C1-C2-C3	2.03	112.17	109.67
7	W	4	BMA	O6-C6-C5	-2.03	104.31	111.29
5	b	3	BMA	C1-C2-C3	-2.01	107.20	109.67
4	X	1	NAG	O5-C5-C6	2.00	110.35	107.20

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	X	1	NAG	C1
4	f	1	NAG	C1
2	J	1	NAG	C1
8	Y	1	NAG	C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
4	d	1	NAG	C1
4	Q	1	NAG	C1
4	g	1	NAG	C1
4	V	1	NAG	C1

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	1	NAG	C8-C7-N2-C2
4	X	1	NAG	O7-C7-N2-C2
7	W	1	NAG	C8-C7-N2-C2
7	W	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	f	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	g	1	NAG	C8-C7-N2-C2
4	g	1	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	V	2	NAG	O7-C7-N2-C2
8	Y	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	f	2	NAG	C8-C7-N2-C2
4	V	2	NAG	C8-C7-N2-C2
8	Y	2	NAG	C8-C7-N2-C2
2	R	3	BMA	O5-C5-C6-O6
7	W	4	BMA	C4-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
5	c	2	NAG	C8-C7-N2-C2
5	c	2	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
8	Y	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	Q	1	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
7	W	4	BMA	O5-C5-C6-O6
3	S	3	BMA	O5-C5-C6-O6
2	R	3	BMA	C4-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
5	Z	1	NAG	C8-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
8	Y	1	NAG	C8-C7-N2-C2
8	Y	1	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
5	b	1	NAG	C8-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
4	P	2	NAG	C8-C7-N2-C2
4	d	1	NAG	O5-C5-C6-O6
3	S	3	BMA	C4-C5-C6-O6
5	Z	1	NAG	O7-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
2	K	4	BMA	O5-C5-C6-O6
7	a	6	BMA	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
5	H	2	NAG	O7-C7-N2-C2
4	d	2	NAG	C8-C7-N2-C2
5	b	1	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	g	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	P	2	NAG	O7-C7-N2-C2
3	L	4	BMA	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
3	L	3	BMA	O5-C5-C6-O6
5	b	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
8	Y	3	BMA	C4-C5-C6-O6
3	F	4	BMA	O5-C5-C6-O6
3	L	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	c	3	BMA	O5-C5-C6-O6
4	d	2	NAG	O7-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	g	2	NAG	O7-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	X	1	NAG	O5-C5-C6-O6
2	R	4	BMA	O5-C5-C6-O6
4	d	2	NAG	O5-C5-C6-O6
5	b	1	NAG	O5-C5-C6-O6
7	a	4	BMA	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	K	3	BMA	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
8	Y	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
3	L	5	BMA	C4-C5-C6-O6
3	L	2	NAG	O7-C7-N2-C2
4	e	2	NAG	C8-C7-N2-C2
4	Q	1	NAG	C8-C7-N2-C2
4	e	1	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
4	d	1	NAG	C8-C7-N2-C2
8	Y	5	BMA	C4-C5-C6-O6
4	Q	1	NAG	O7-C7-N2-C2
8	Y	5	BMA	O5-C5-C6-O6
5	O	1	NAG	C1-C2-N2-C7
4	e	2	NAG	O7-C7-N2-C2
4	e	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C4-C5-C6-O6
2	K	4	BMA	C4-C5-C6-O6
7	a	6	BMA	C4-C5-C6-O6
3	L	5	BMA	O5-C5-C6-O6
4	d	1	NAG	O7-C7-N2-C2
4	X	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6
5	O	1	NAG	C3-C2-N2-C7
2	E	3	BMA	O5-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
4	X	2	NAG	O7-C7-N2-C2

All (3) ring outliers are listed below:

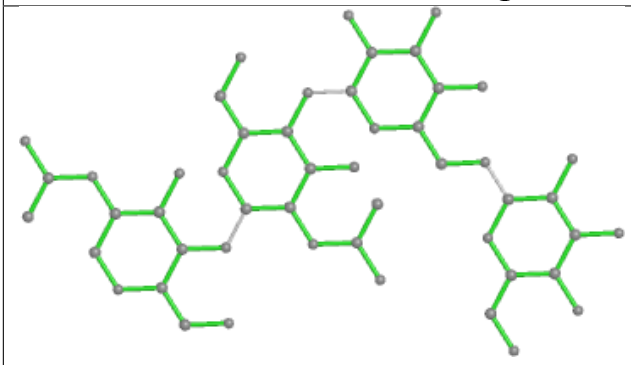
Mol	Chain	Res	Type	Atoms
3	L	5	BMA	C1-C2-C3-C4-C5-O5
2	J	3	BMA	C1-C2-C3-C4-C5-O5
3	L	4	BMA	C1-C2-C3-C4-C5-O5

12 monomers are involved in 9 short contacts:

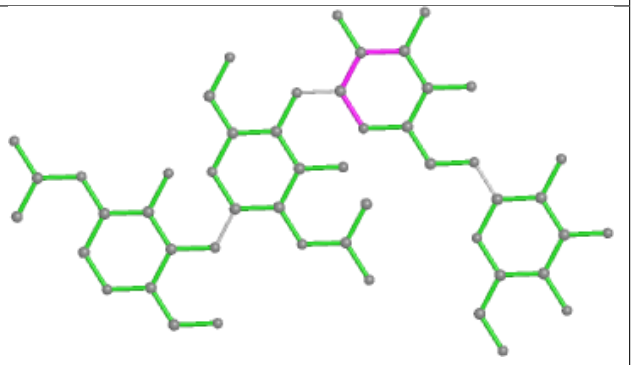
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	1	NAG	1	0
2	K	4	BMA	1	0
3	L	5	BMA	1	0
2	R	4	BMA	2	0
7	W	4	BMA	2	0
2	K	3	BMA	1	0
2	R	3	BMA	1	0
7	W	3	BMA	1	0
7	W	2	NAG	1	0
6	T	1	NAG	1	0
4	P	2	NAG	1	0
4	G	1	NAG	1	0

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

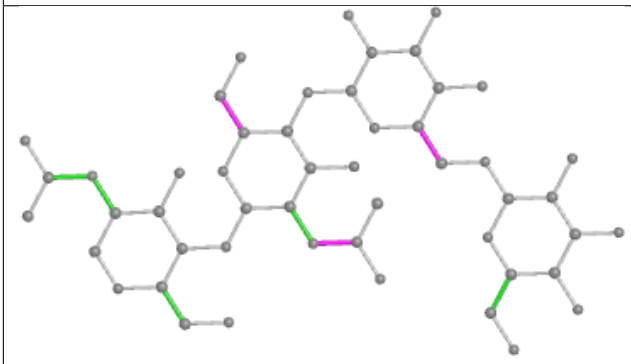
Oligosaccharide Chain E



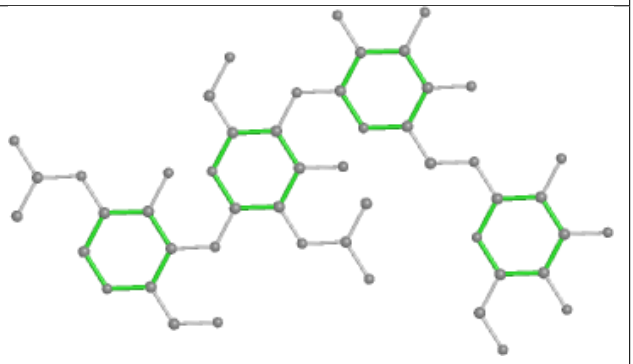
Bond lengths



Bond angles

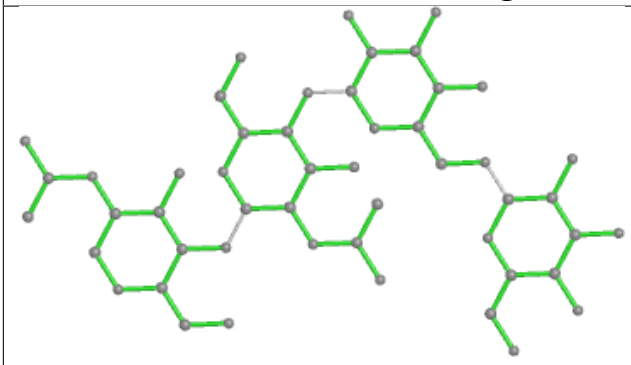


Torsions

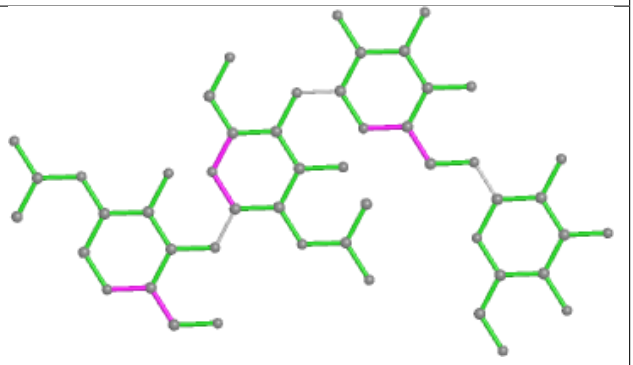


Rings

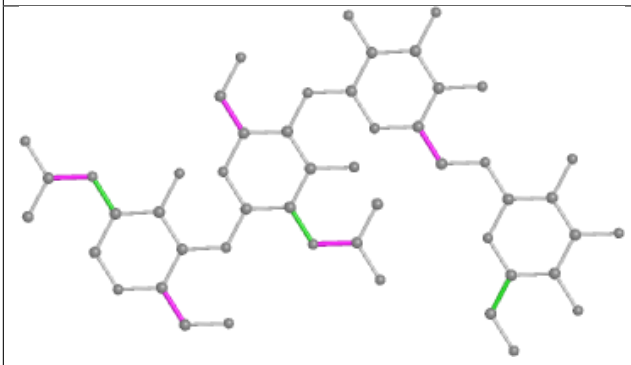
Oligosaccharide Chain J



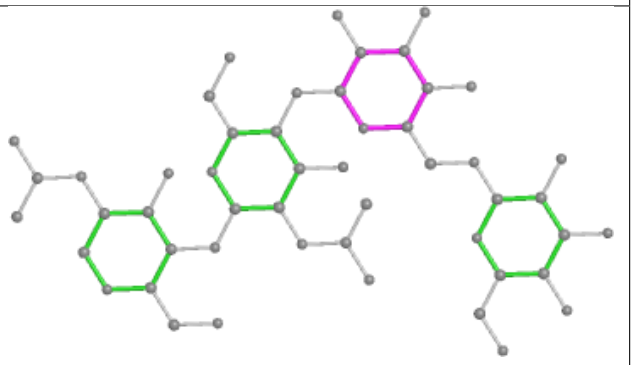
Bond lengths



Bond angles

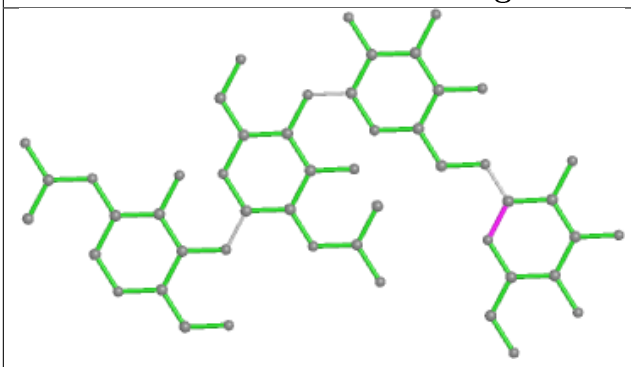


Torsions

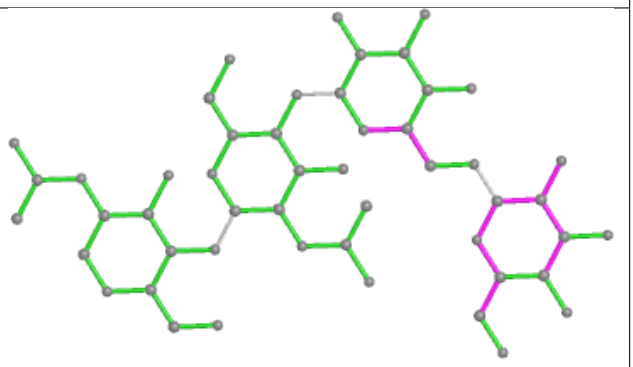


Rings

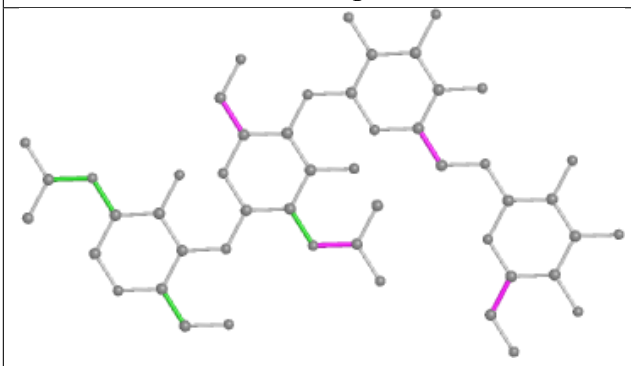
Oligosaccharide Chain K



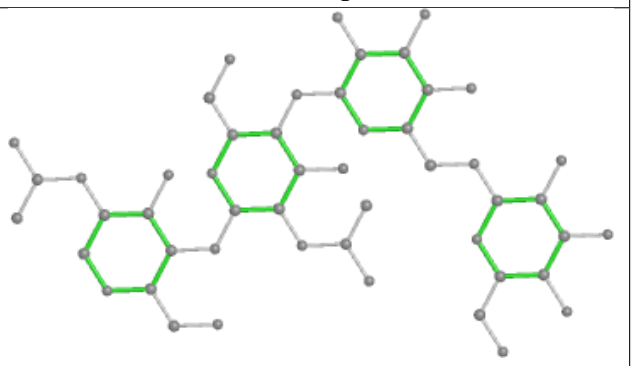
Bond lengths



Bond angles

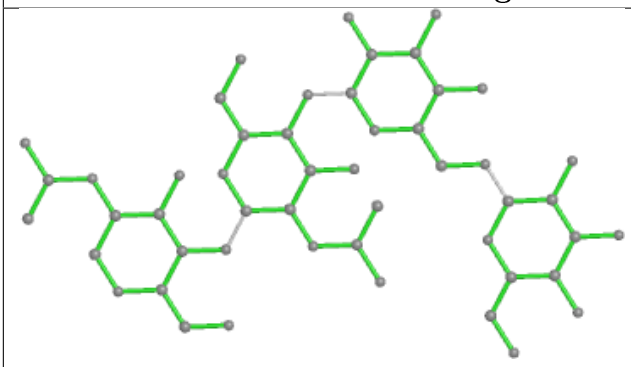


Torsions

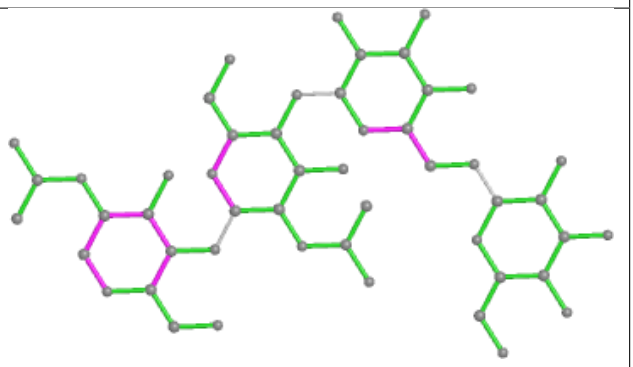


Rings

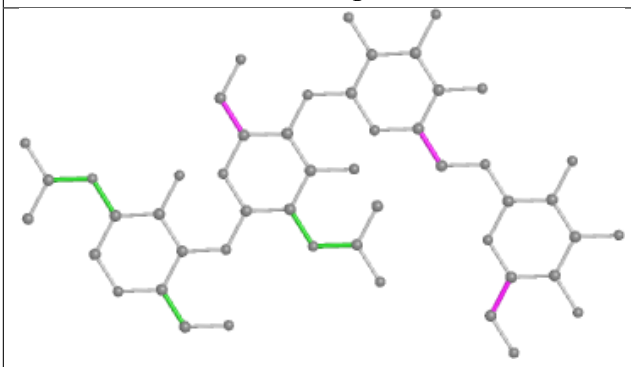
Oligosaccharide Chain R



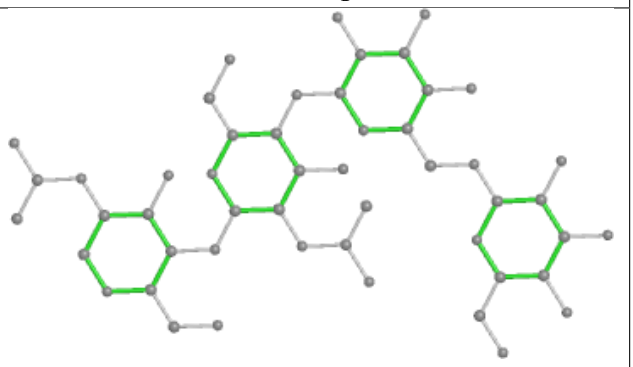
Bond lengths



Bond angles

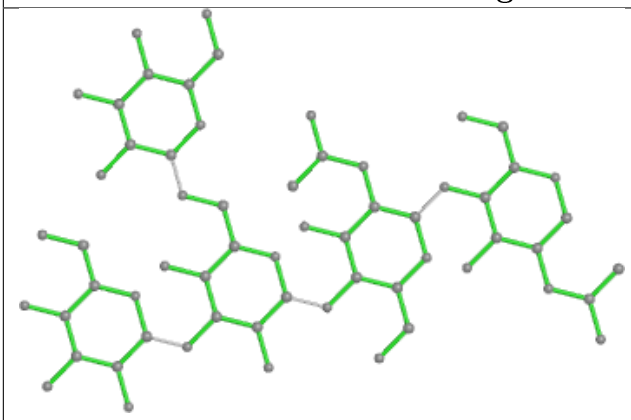


Torsions

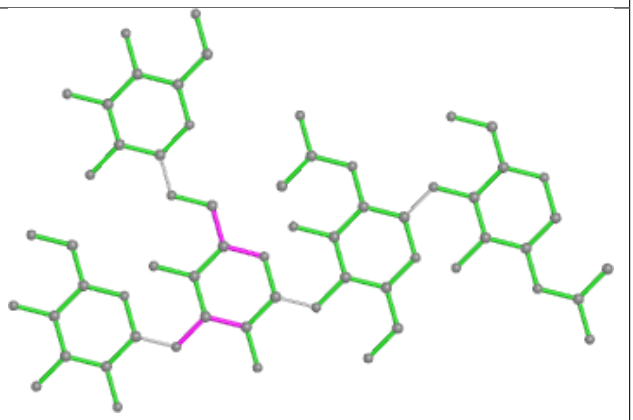


Rings

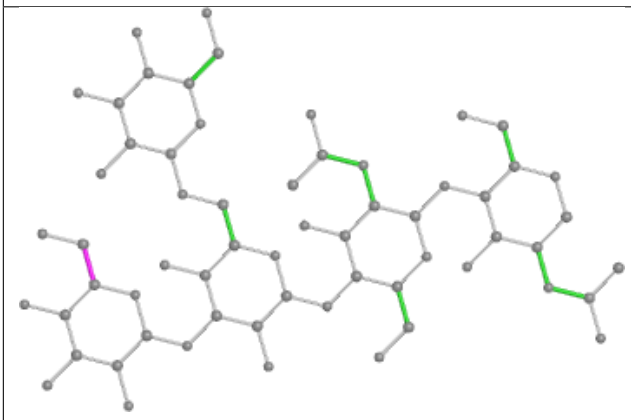
Oligosaccharide Chain F



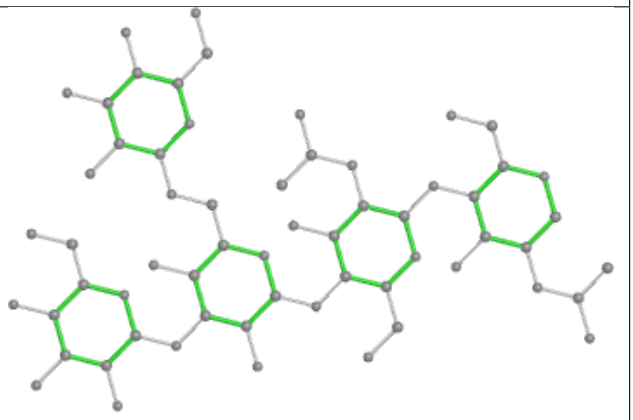
Bond lengths



Bond angles

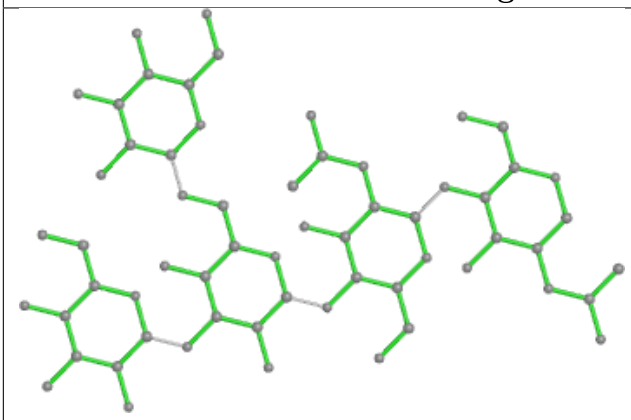


Torsions

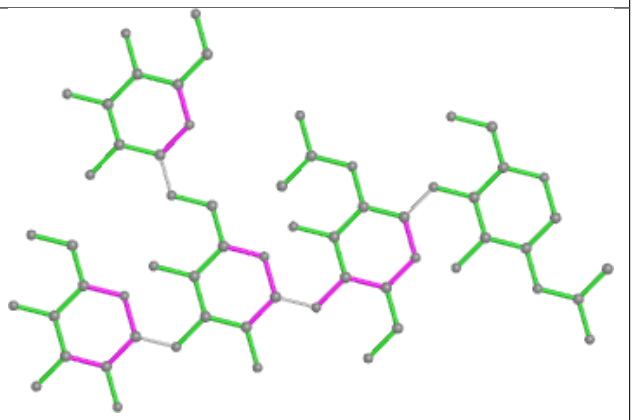


Rings

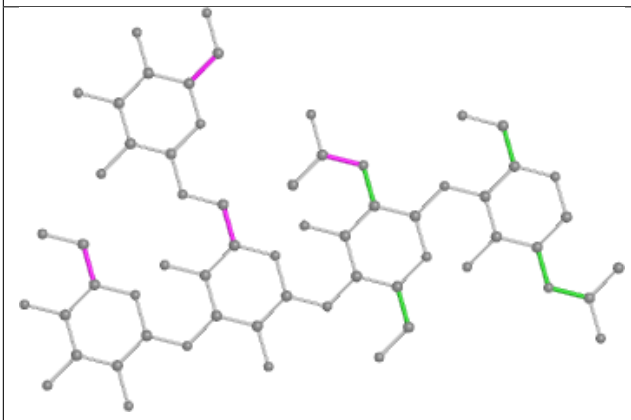
Oligosaccharide Chain L



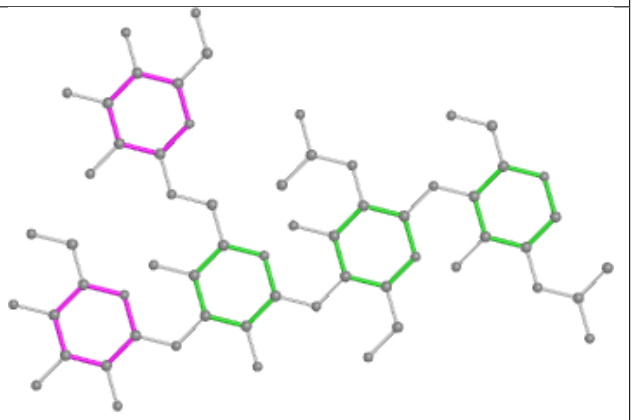
Bond lengths



Bond angles

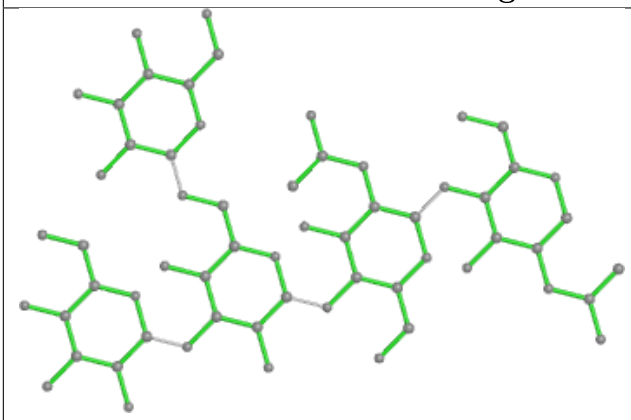


Torsions

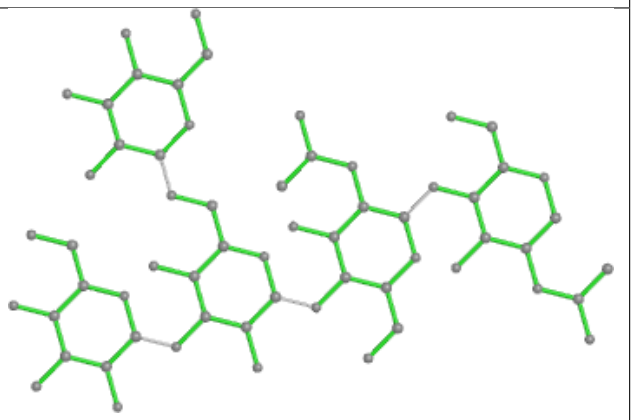


Rings

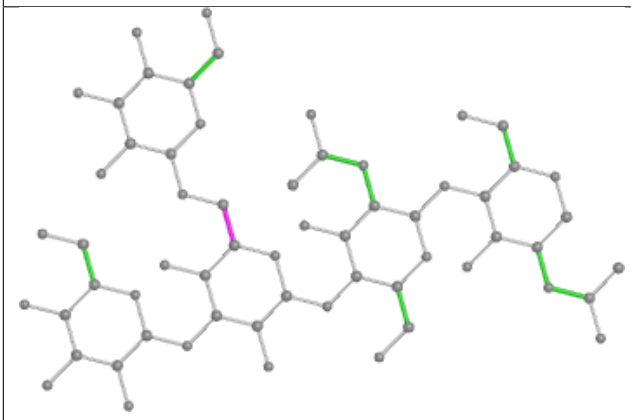
Oligosaccharide Chain S



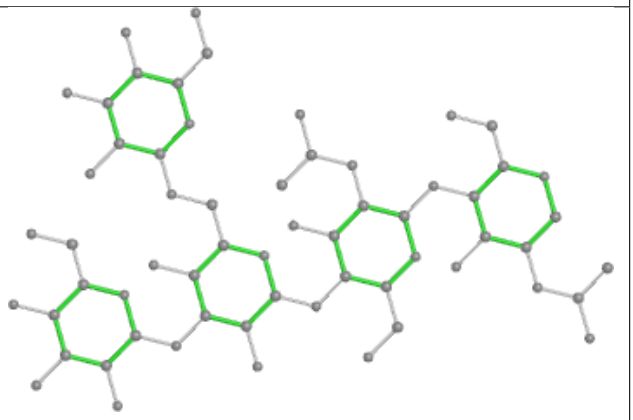
Bond lengths



Bond angles

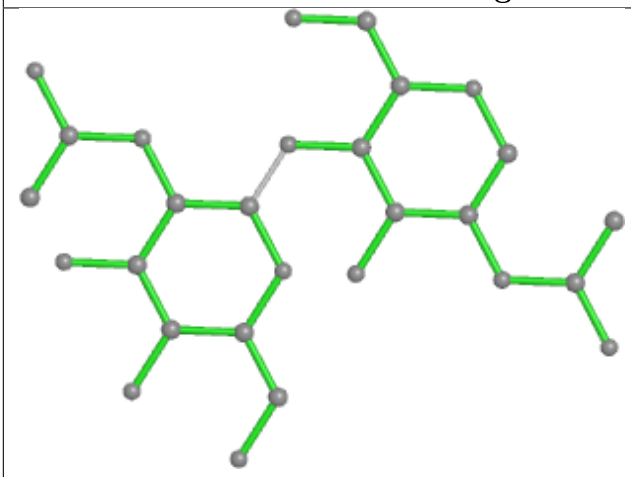


Torsions

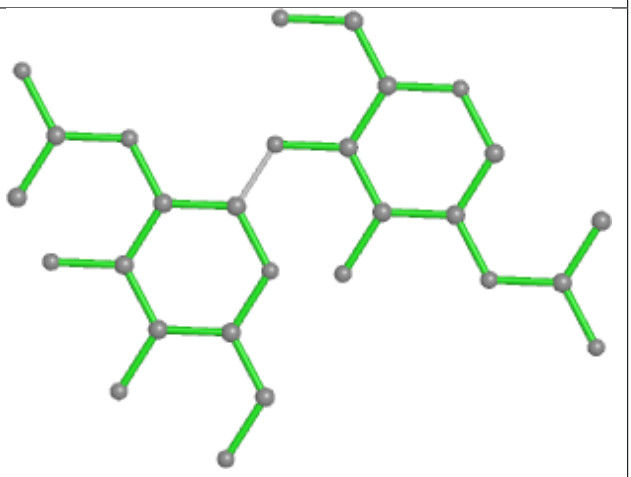


Rings

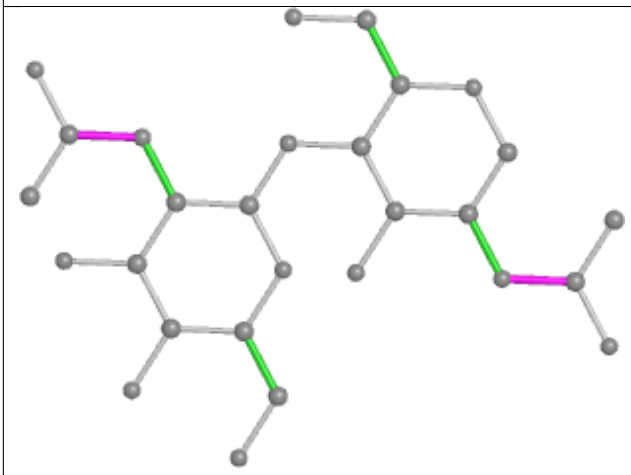
Oligosaccharide Chain G



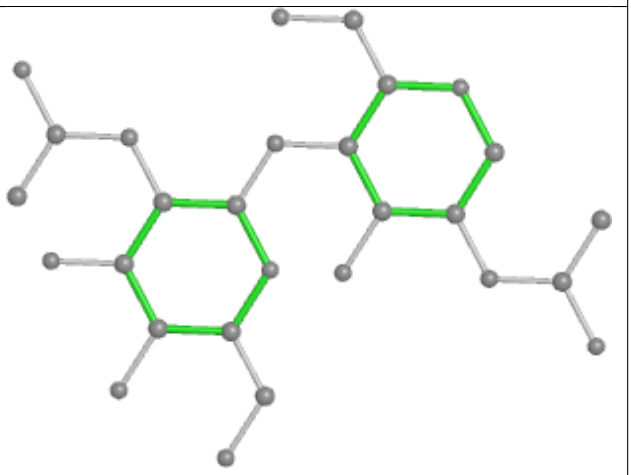
Bond lengths



Bond angles

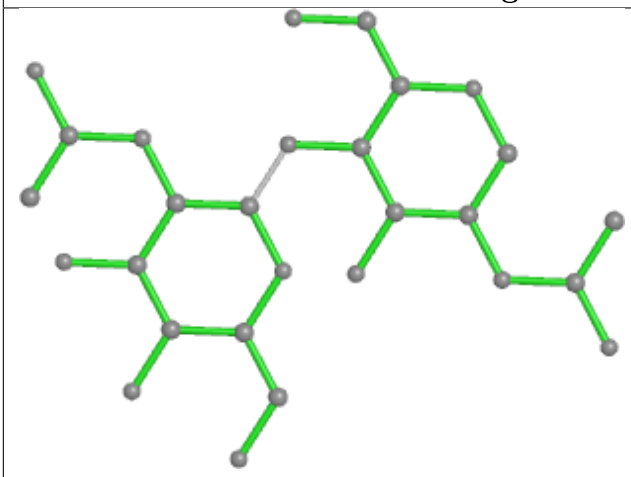


Torsions

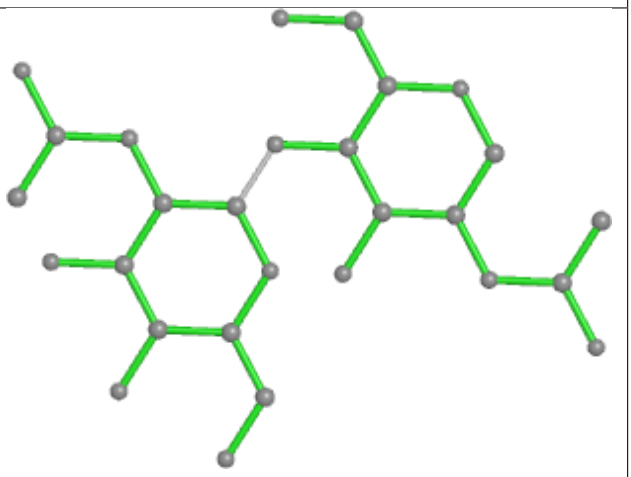


Rings

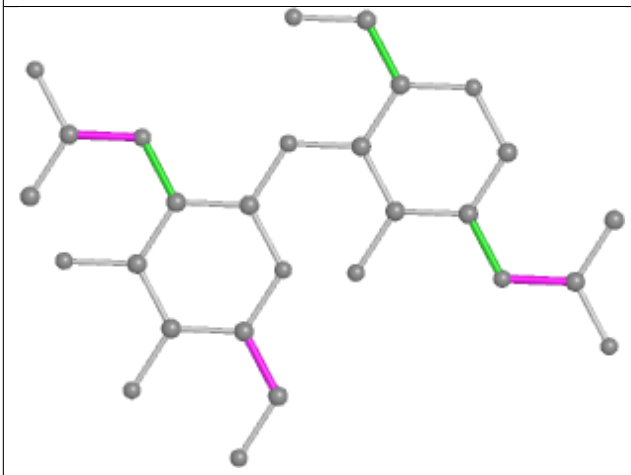
Oligosaccharide Chain I



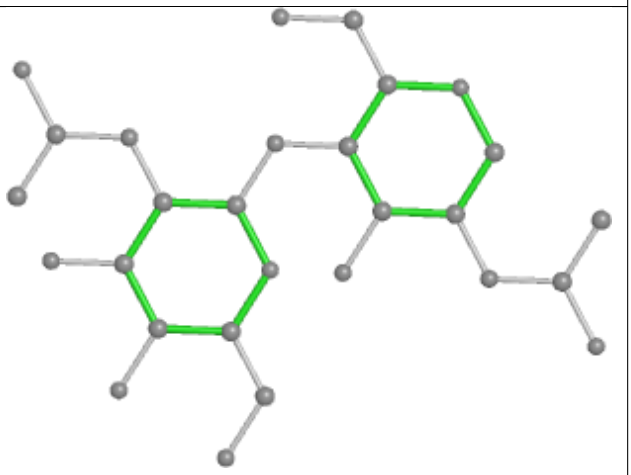
Bond lengths



Bond angles

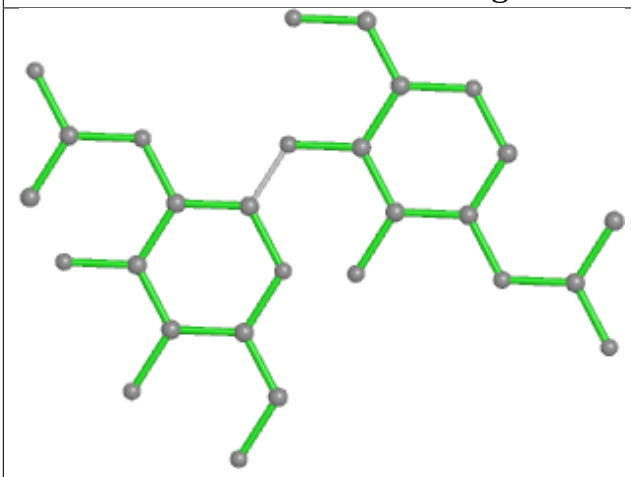


Torsions

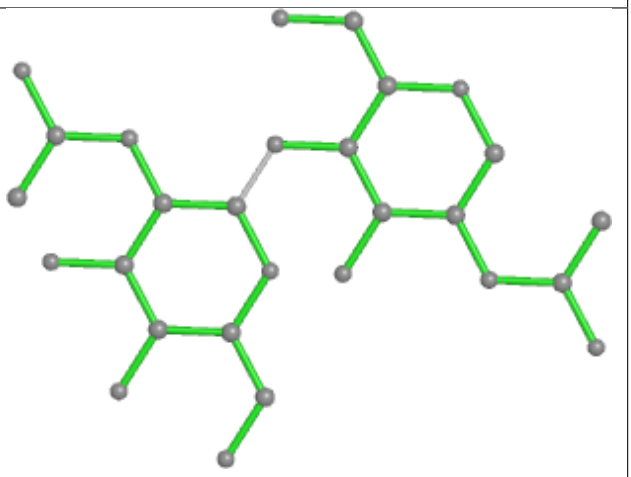


Rings

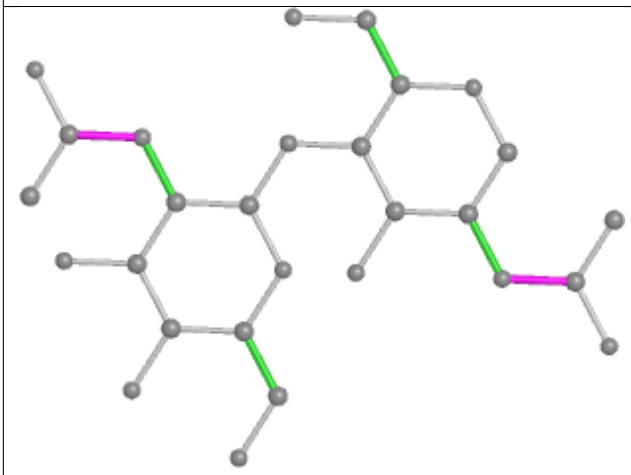
Oligosaccharide Chain M



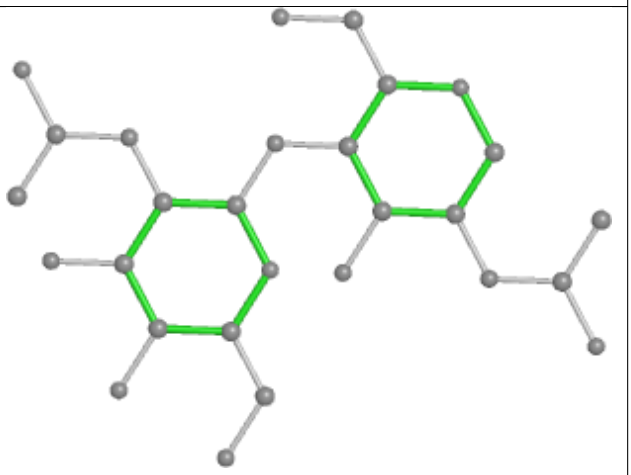
Bond lengths



Bond angles

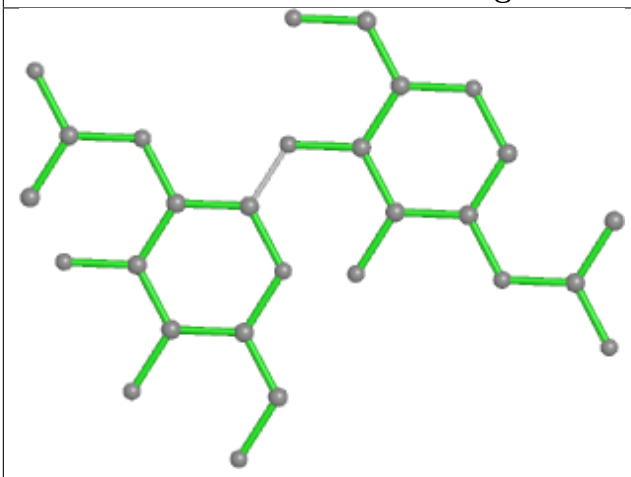


Torsions

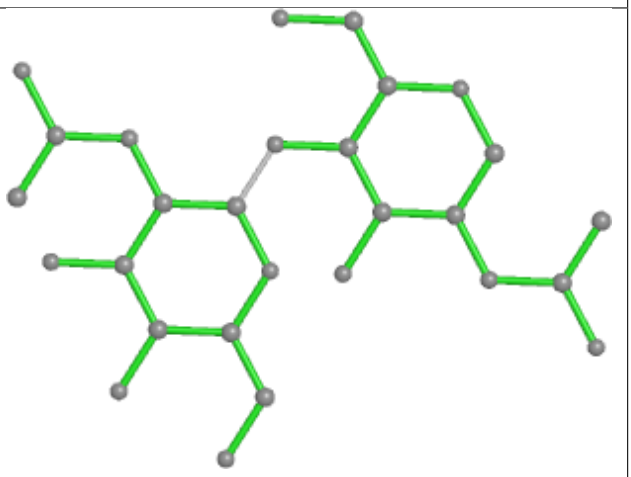


Rings

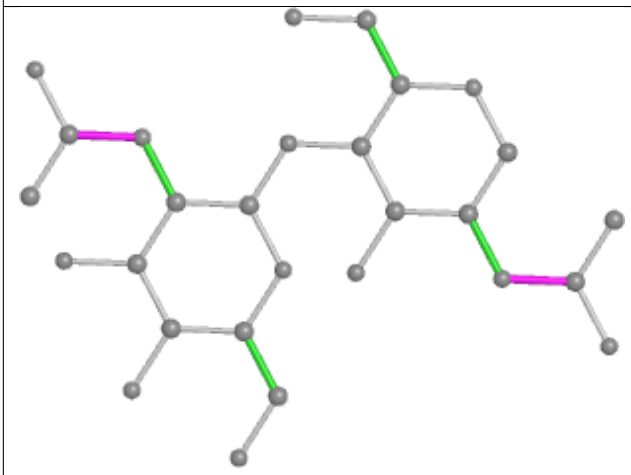
Oligosaccharide Chain N



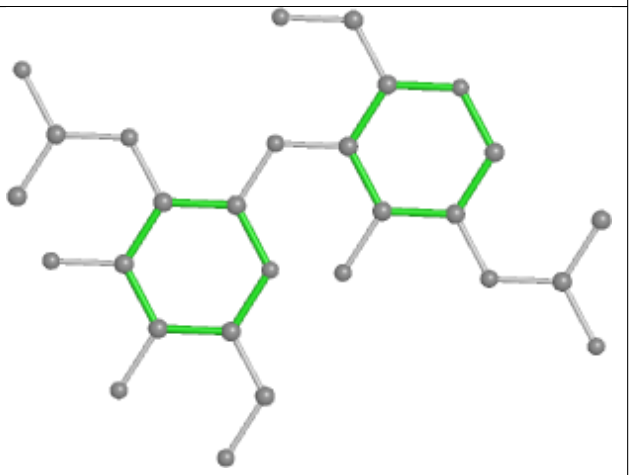
Bond lengths



Bond angles

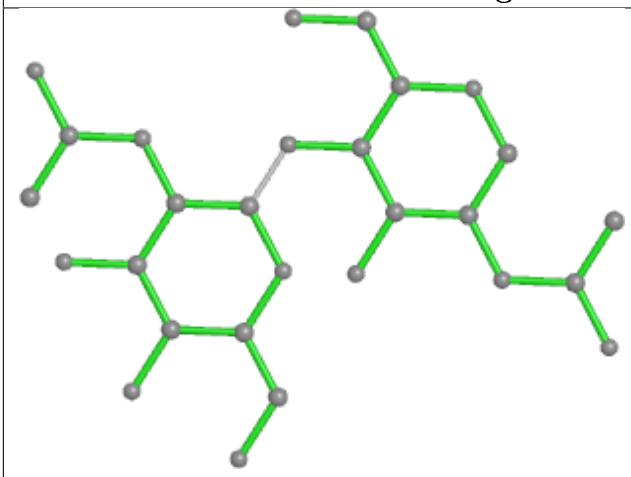


Torsions

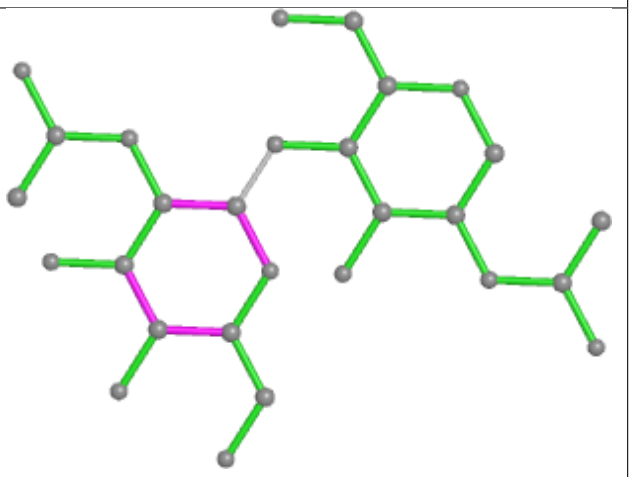


Rings

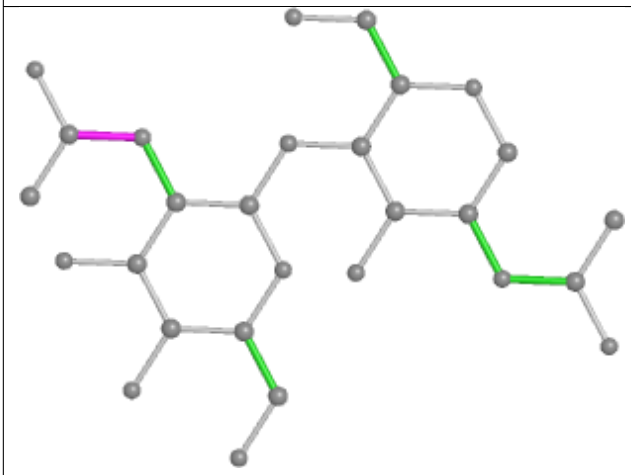
Oligosaccharide Chain P



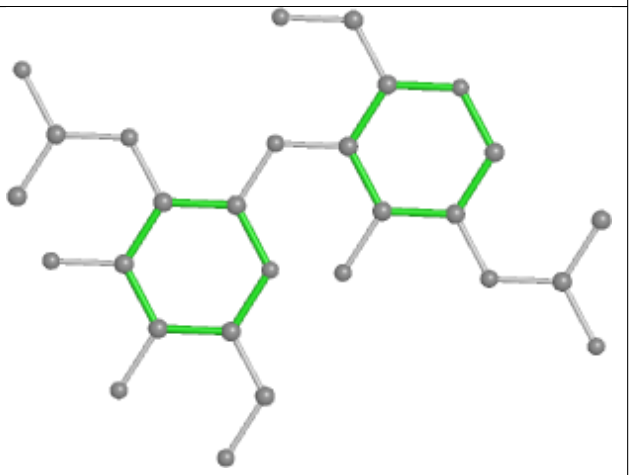
Bond lengths



Bond angles

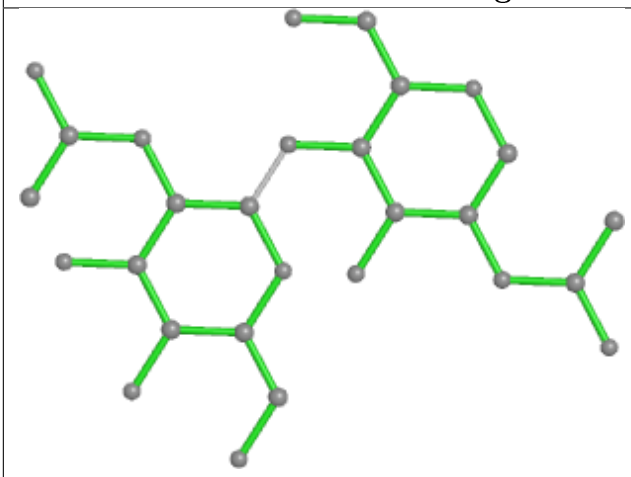


Torsions

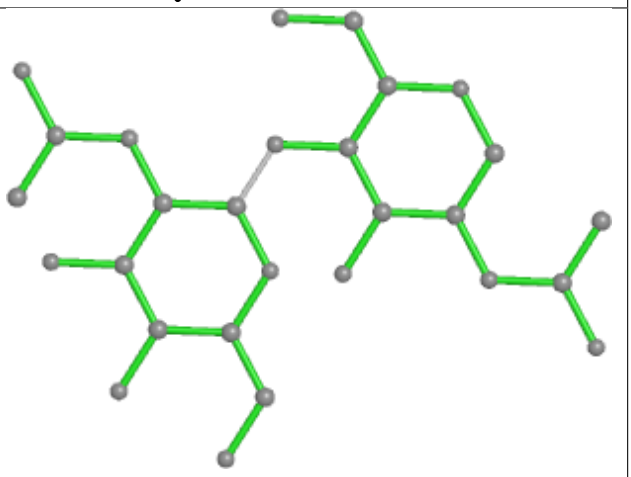


Rings

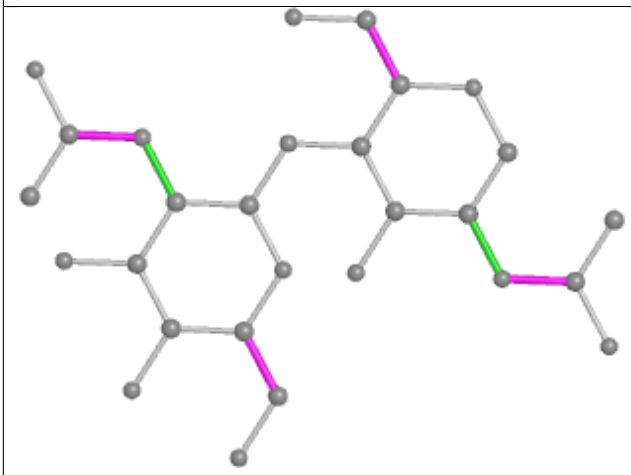
Oligosaccharide Chain Q



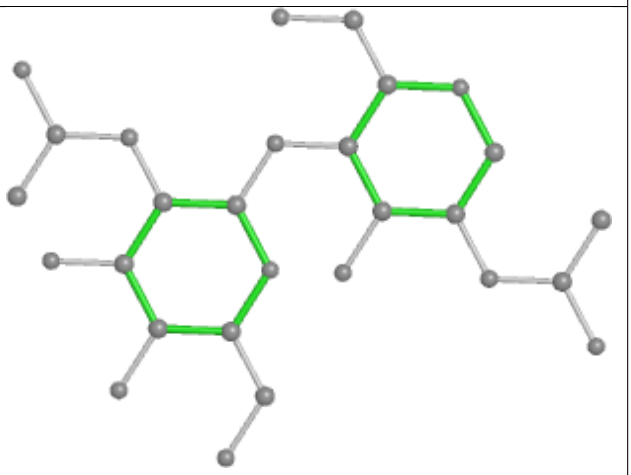
Bond lengths



Bond angles

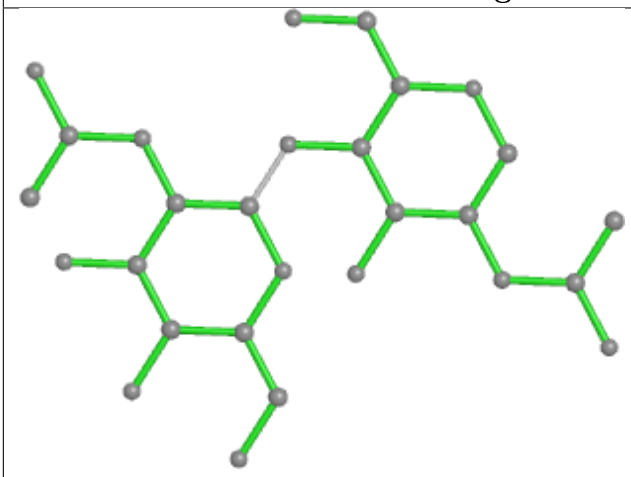


Torsions

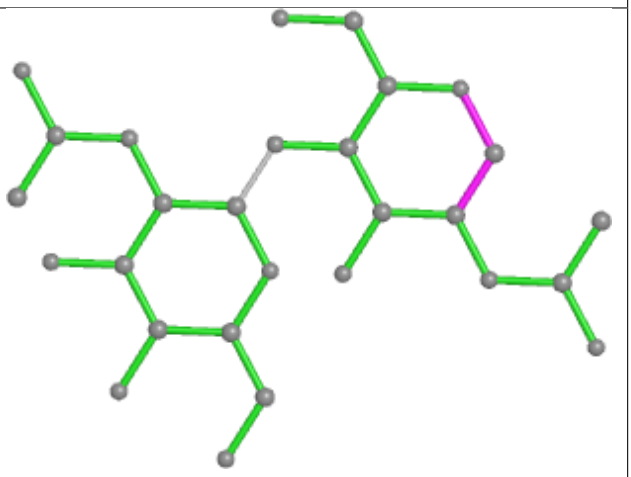


Rings

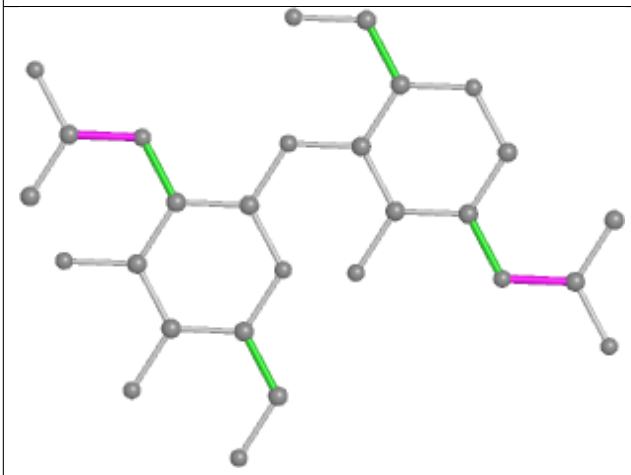
Oligosaccharide Chain V



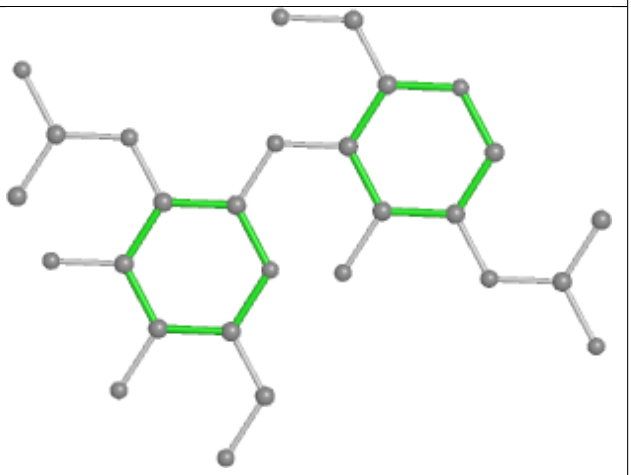
Bond lengths



Bond angles

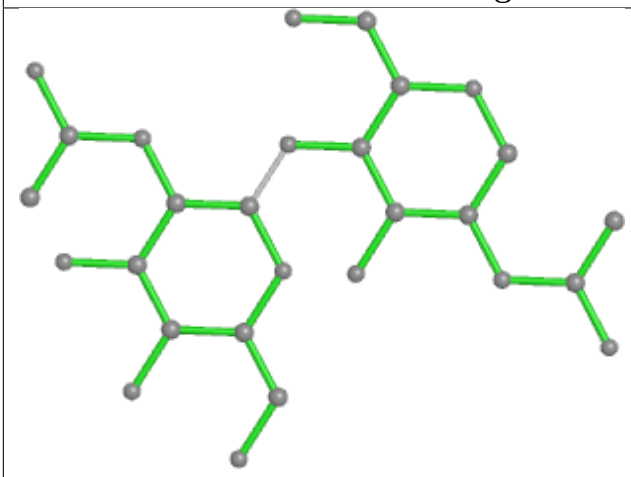


Torsions

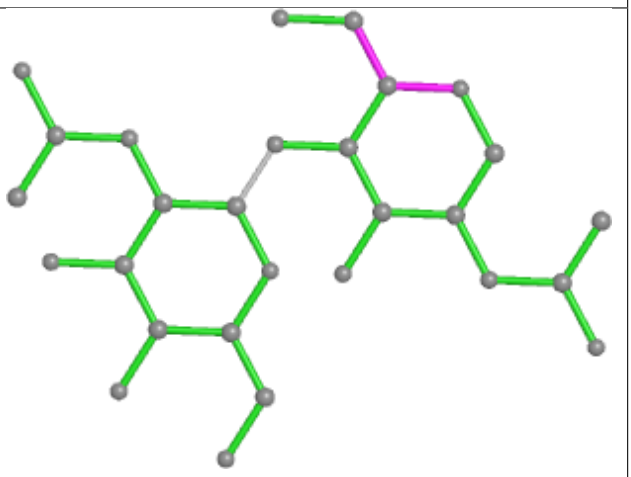


Rings

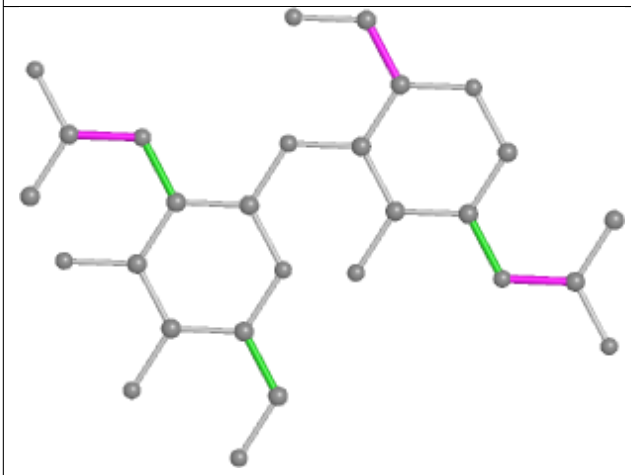
Oligosaccharide Chain X



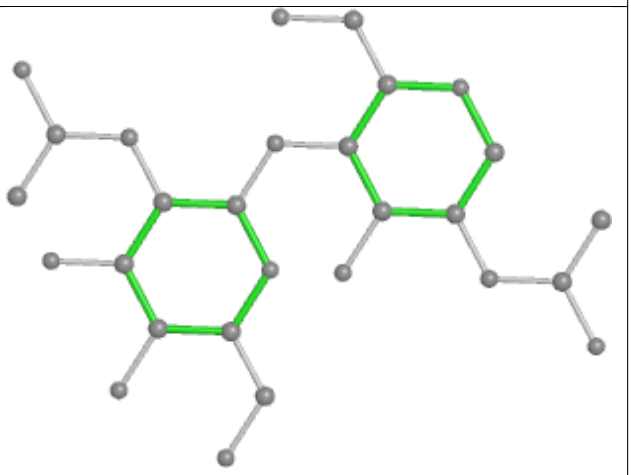
Bond lengths



Bond angles

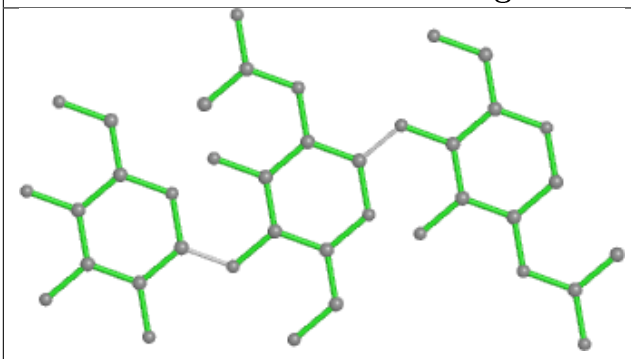


Torsions

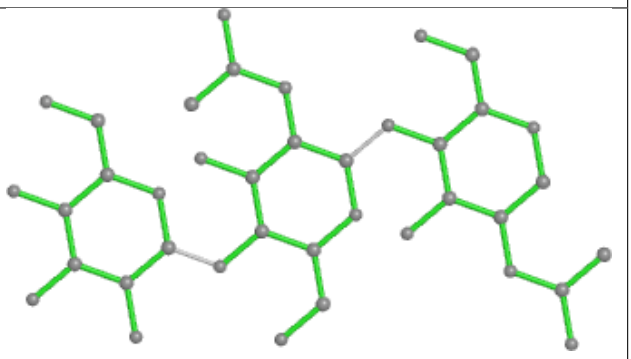


Rings

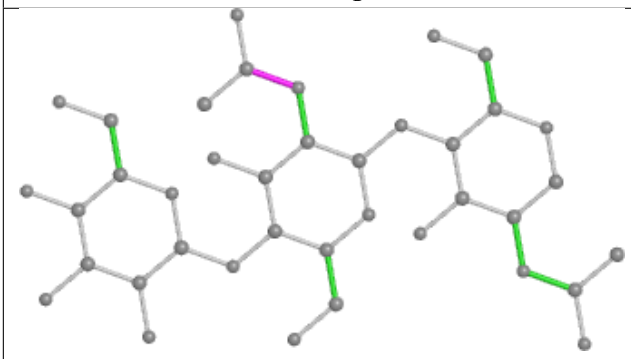
Oligosaccharide Chain H



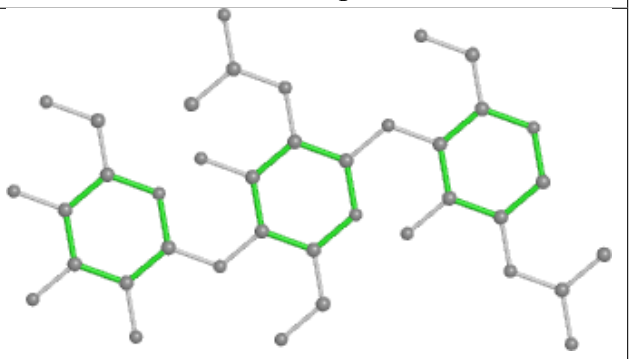
Bond lengths



Bond angles

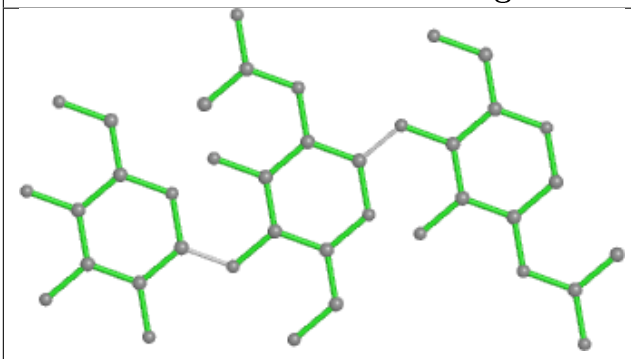


Torsions

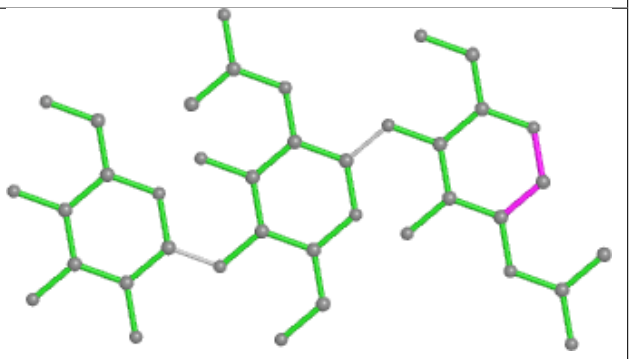


Rings

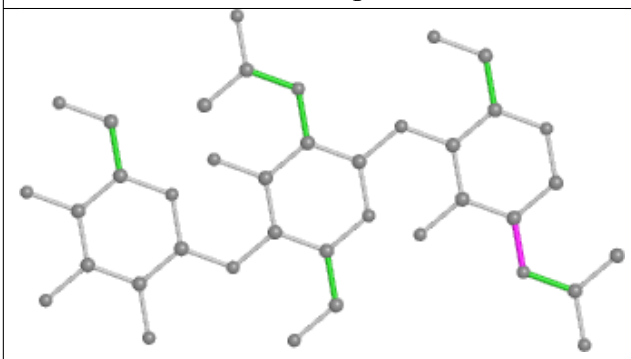
Oligosaccharide Chain O



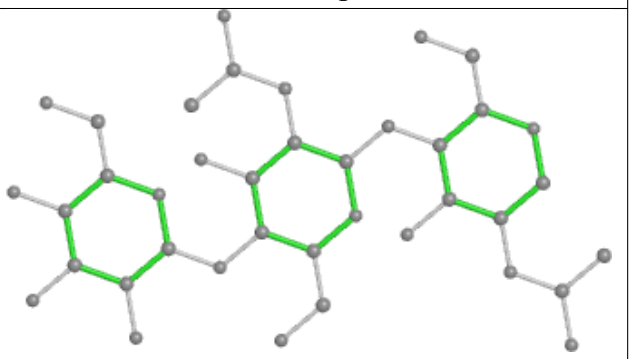
Bond lengths



Bond angles

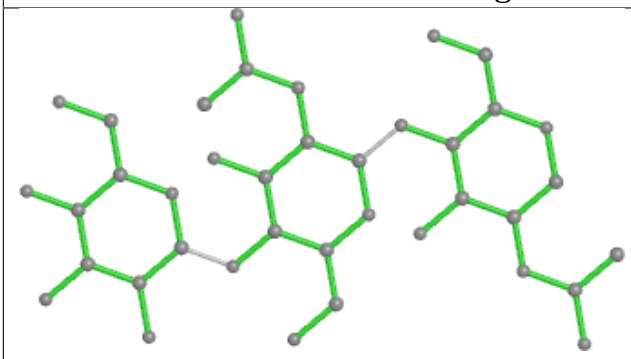


Torsions

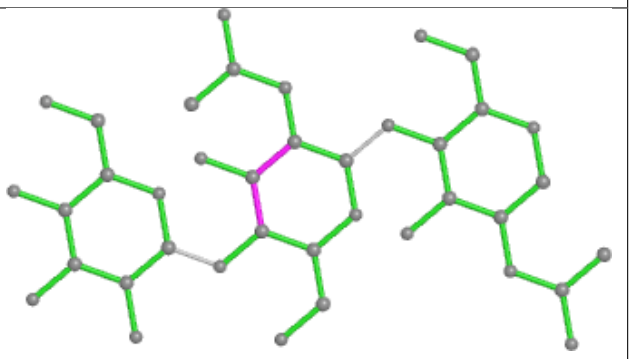


Rings

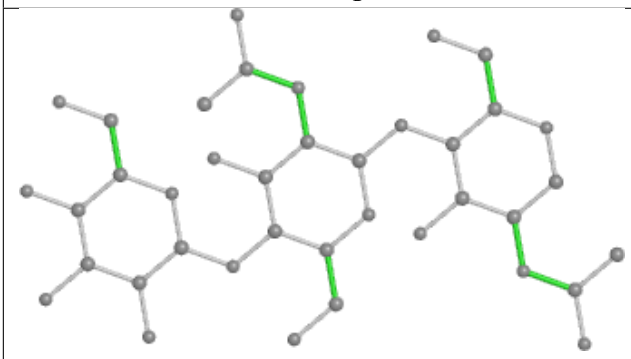
Oligosaccharide Chain U



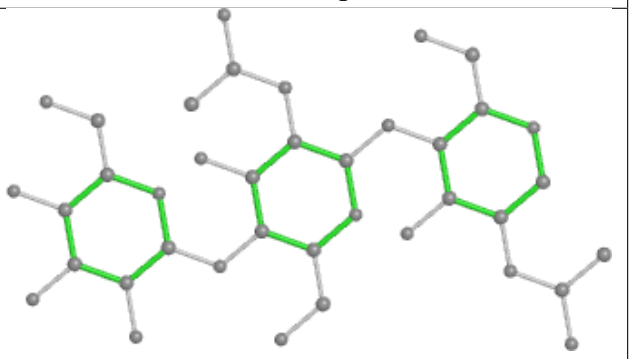
Bond lengths



Bond angles

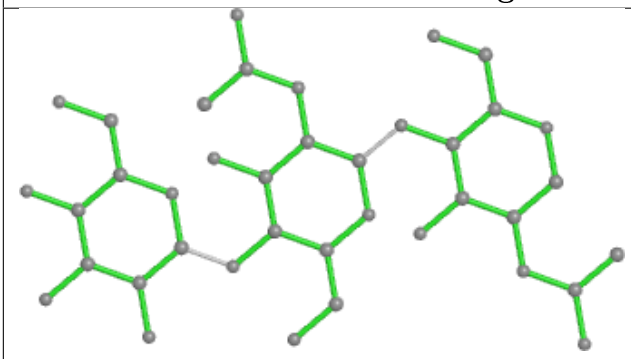


Torsions

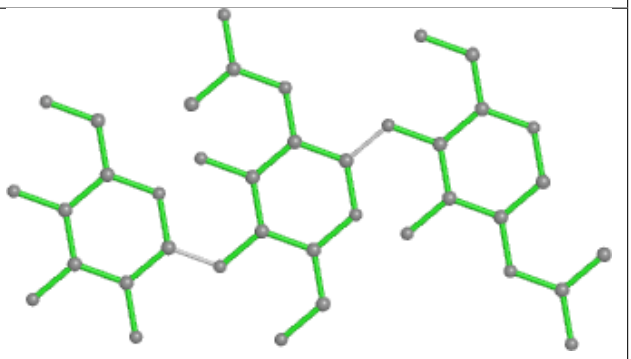


Rings

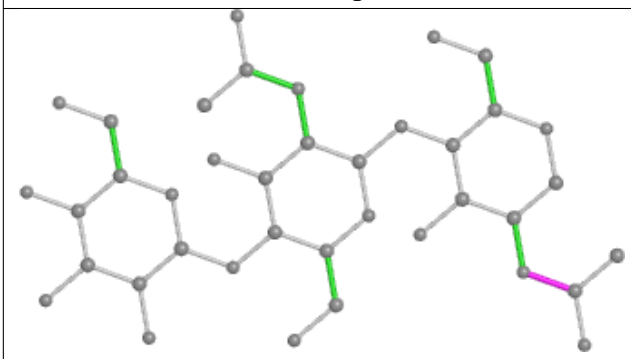
Oligosaccharide Chain Z



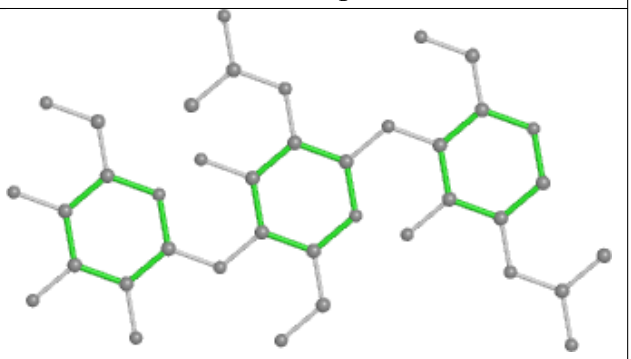
Bond lengths



Bond angles

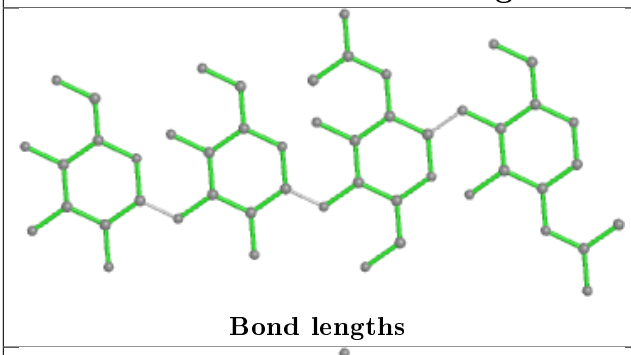


Torsions

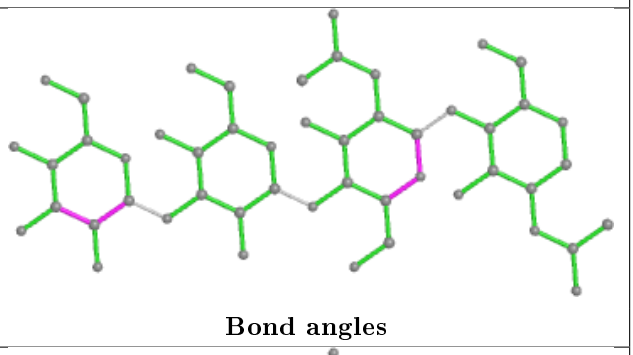


Rings

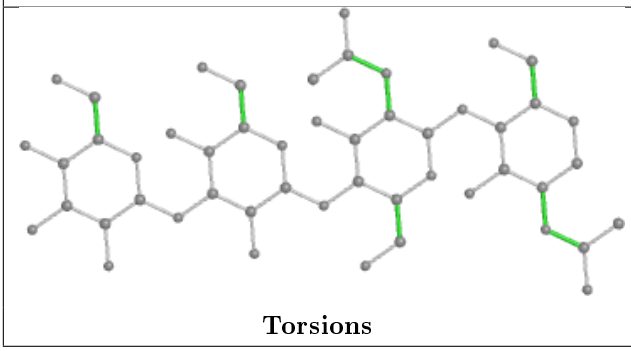
Oligosaccharide Chain T



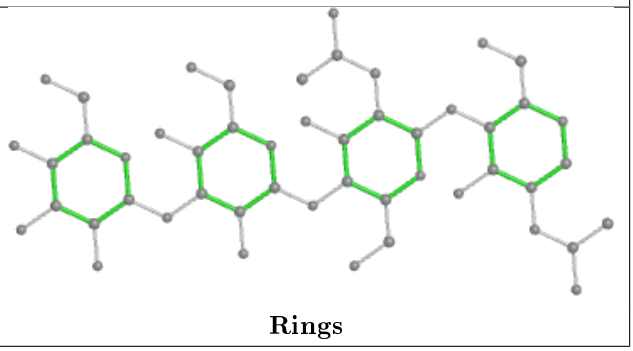
Bond lengths



Bond angles

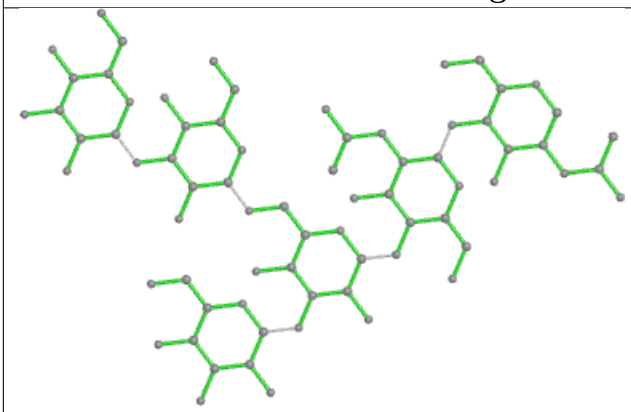


Torsions

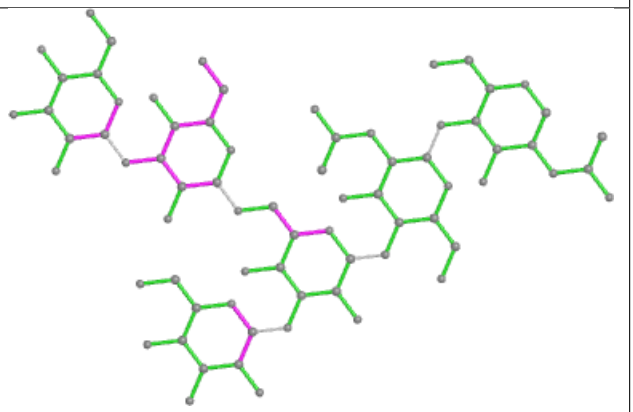


Rings

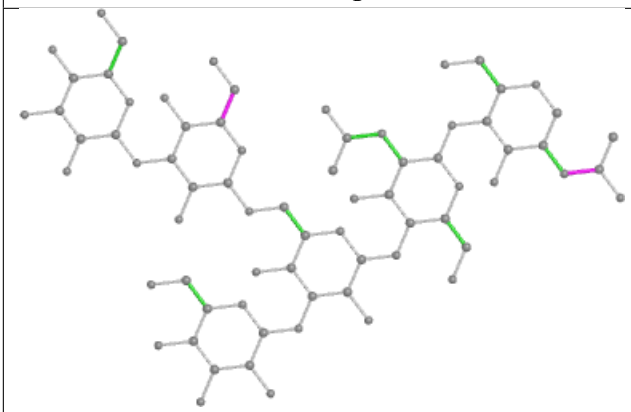
Oligosaccharide Chain W



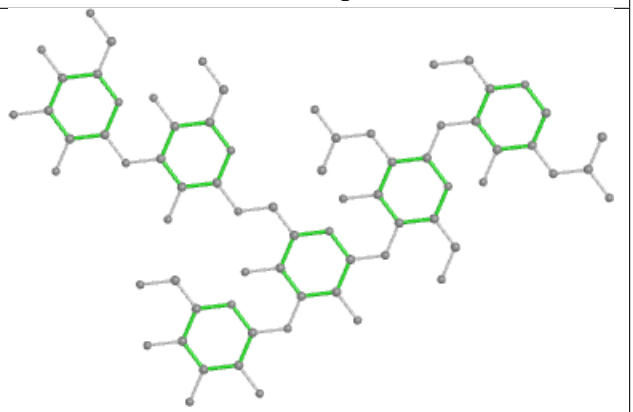
Bond lengths



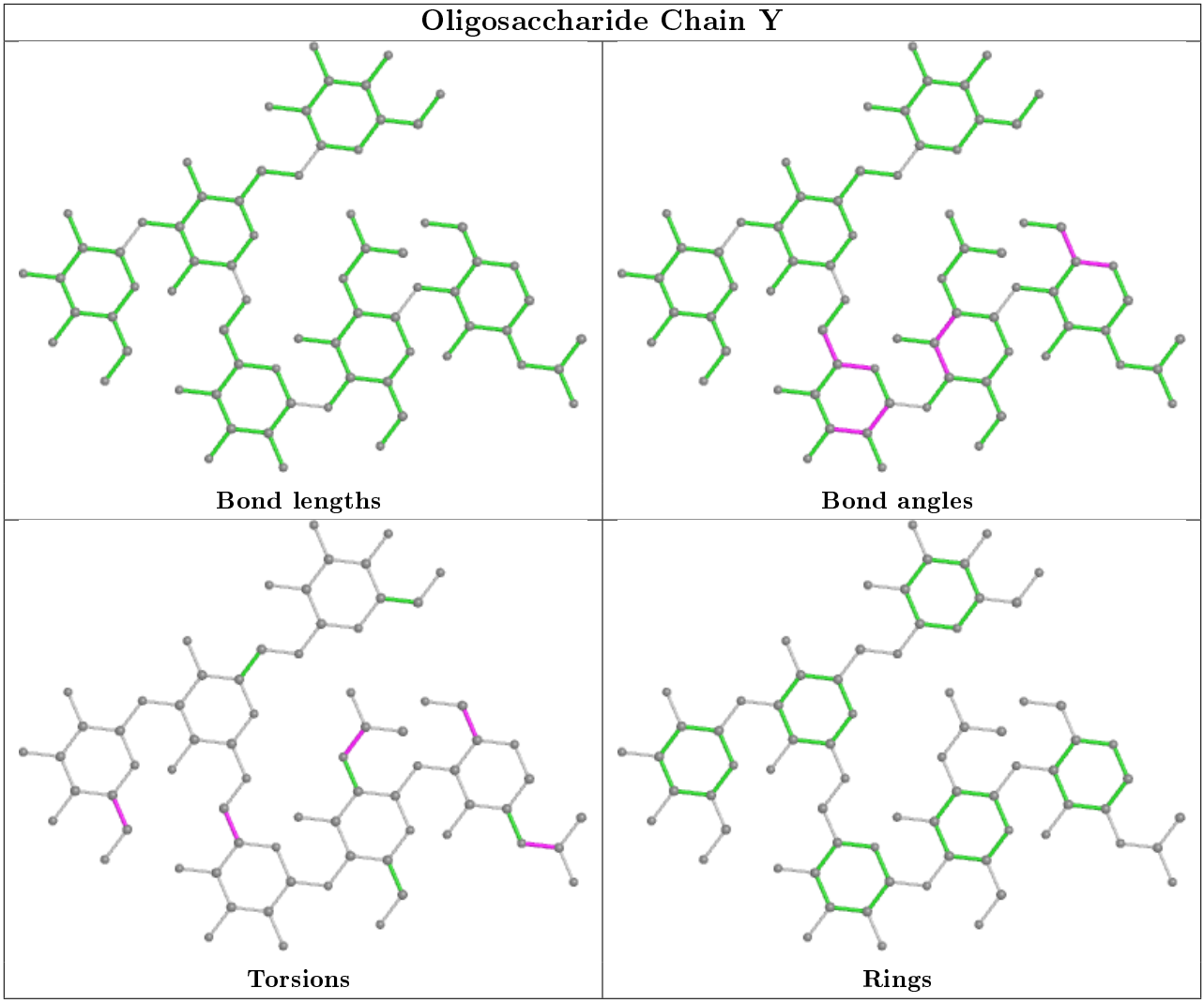
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 4 are monoatomic - leaving 52 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	A	1015	1	14,14,15	0.54	0	17,19,21	0.63	0
9	NAG	D	1025	1	14,14,15	0.54	0	17,19,21	0.66	0
11	EDO	A	1039	-	3,3,3	0.44	0	2,2,2	0.35	0
11	EDO	A	1034	-	3,3,3	0.49	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	EDO	D	1029	-	3,3,3	0.45	0	2,2,2	0.33	0
11	EDO	A	1040	-	3,3,3	0.43	0	2,2,2	0.27	0
11	EDO	A	1026	-	3,3,3	0.46	0	2,2,2	0.34	0
11	EDO	A	1033	-	3,3,3	0.46	0	2,2,2	0.32	0
11	EDO	A	1036	-	3,3,3	0.47	0	2,2,2	0.32	0
11	EDO	A	1038	-	3,3,3	0.46	0	2,2,2	0.33	0
11	EDO	D	1028	-	3,3,3	0.46	0	2,2,2	0.36	0
11	EDO	D	1031	-	3,3,3	0.49	0	2,2,2	0.26	0
11	EDO	A	1024	-	3,3,3	0.47	0	2,2,2	0.31	0
11	EDO	B	1034	-	3,3,3	0.50	0	2,2,2	0.21	0
11	EDO	A	1029	-	3,3,3	0.46	0	2,2,2	0.17	0
11	EDO	D	1030	-	3,3,3	0.48	0	2,2,2	0.22	0
11	EDO	A	1027	-	3,3,3	0.45	0	2,2,2	0.40	0
11	EDO	A	1028	-	3,3,3	0.49	0	2,2,2	0.26	0
11	EDO	C	1140	-	3,3,3	0.51	0	2,2,2	0.20	0
11	EDO	C	1144	-	3,3,3	0.46	0	2,2,2	0.35	0
11	EDO	C	1142	-	3,3,3	0.47	0	2,2,2	0.30	0
11	EDO	C	1143	-	3,3,3	0.47	0	2,2,2	0.32	0
11	EDO	B	1032	-	3,3,3	0.46	0	2,2,2	0.35	0
11	EDO	B	1027	-	3,3,3	0.42	0	2,2,2	0.39	0
9	NAG	D	1016	1	14,14,15	0.48	0	17,19,21	0.78	0
11	EDO	A	1025	-	3,3,3	0.47	0	2,2,2	0.30	0
11	EDO	C	1146	-	3,3,3	0.49	0	2,2,2	0.21	0
11	EDO	B	1030	-	3,3,3	0.49	0	2,2,2	0.27	0
11	EDO	A	1030	-	3,3,3	0.46	0	2,2,2	0.35	0
11	EDO	C	1137	-	3,3,3	0.46	0	2,2,2	0.35	0
9	NAG	B	1021	1	14,14,15	0.56	0	17,19,21	0.91	0
11	EDO	B	1033	-	3,3,3	0.46	0	2,2,2	0.33	0
11	EDO	A	1031	-	3,3,3	0.48	0	2,2,2	0.24	0
11	EDO	C	1138	-	3,3,3	0.46	0	2,2,2	0.35	0
11	EDO	A	1032	-	3,3,3	0.47	0	2,2,2	0.31	0
11	EDO	C	1135	-	3,3,3	0.46	0	2,2,2	0.35	0
11	EDO	A	1037	-	3,3,3	0.45	0	2,2,2	0.36	0
11	EDO	B	1031	-	3,3,3	0.48	0	2,2,2	0.24	0
11	EDO	B	1028	-	3,3,3	0.48	0	2,2,2	0.30	0
9	NAG	A	1022	1	14,14,15	0.48	0	17,19,21	0.76	0
11	EDO	B	1024	-	3,3,3	0.45	0	2,2,2	0.34	0
11	EDO	D	1027	-	3,3,3	0.44	0	2,2,2	0.37	0
9	NAG	C	1117	1	14,14,15	0.53	0	17,19,21	0.74	0
11	EDO	B	1029	-	3,3,3	0.48	0	2,2,2	0.28	0
11	EDO	C	1139	-	3,3,3	0.45	0	2,2,2	0.36	0
11	EDO	B	1025	-	3,3,3	0.42	0	2,2,2	0.48	0
11	EDO	C	1141	-	3,3,3	0.46	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	EDO	A	1035	-	3,3,3	0.46	0	2,2,2	0.39	0
11	EDO	C	1145	-	3,3,3	0.47	0	2,2,2	0.35	0
11	EDO	B	1026	-	3,3,3	0.46	0	2,2,2	0.40	0
11	EDO	C	1136	-	3,3,3	0.45	0	2,2,2	0.35	0
11	EDO	B	1023	-	3,3,3	0.44	0	2,2,2	0.37	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
11	EDO	D	1029	-	-	0/1/1/1	-
9	NAG	D	1025	1	-	2/6/23/26	0/1/1/1
11	EDO	A	1039	-	-	0/1/1/1	-
11	EDO	A	1034	-	-	0/1/1/1	-
9	NAG	A	1015	1	1/1/5/7	3/6/23/26	0/1/1/1
11	EDO	A	1040	-	-	0/1/1/1	-
11	EDO	A	1026	-	-	0/1/1/1	-
11	EDO	A	1033	-	-	0/1/1/1	-
11	EDO	A	1036	-	-	0/1/1/1	-
11	EDO	A	1038	-	-	0/1/1/1	-
11	EDO	D	1028	-	-	0/1/1/1	-
11	EDO	D	1031	-	-	0/1/1/1	-
11	EDO	A	1024	-	-	0/1/1/1	-
11	EDO	B	1034	-	-	1/1/1/1	-
11	EDO	A	1029	-	-	0/1/1/1	-
11	EDO	D	1030	-	-	0/1/1/1	-
11	EDO	A	1027	-	-	1/1/1/1	-
11	EDO	A	1028	-	-	0/1/1/1	-
11	EDO	C	1140	-	-	0/1/1/1	-
11	EDO	C	1144	-	-	0/1/1/1	-
11	EDO	C	1142	-	-	0/1/1/1	-
11	EDO	C	1143	-	-	0/1/1/1	-
11	EDO	B	1032	-	-	0/1/1/1	-
11	EDO	B	1027	-	-	0/1/1/1	-
9	NAG	D	1016	1	-	2/6/23/26	0/1/1/1
11	EDO	A	1025	-	-	0/1/1/1	-
11	EDO	C	1146	-	-	0/1/1/1	-
11	EDO	B	1030	-	-	0/1/1/1	-
11	EDO	A	1030	-	-	0/1/1/1	-
11	EDO	C	1137	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	B	1021	1	-	2/6/23/26	0/1/1/1
11	EDO	B	1033	-	-	0/1/1/1	-
11	EDO	A	1031	-	-	1/1/1/1	-
11	EDO	C	1138	-	-	0/1/1/1	-
11	EDO	A	1032	-	-	0/1/1/1	-
11	EDO	C	1135	-	-	0/1/1/1	-
11	EDO	A	1037	-	-	0/1/1/1	-
11	EDO	B	1031	-	-	0/1/1/1	-
11	EDO	B	1028	-	-	1/1/1/1	-
9	NAG	A	1022	1	-	2/6/23/26	0/1/1/1
11	EDO	B	1024	-	-	0/1/1/1	-
11	EDO	D	1027	-	-	0/1/1/1	-
9	NAG	C	1117	1	1/1/5/7	2/6/23/26	0/1/1/1
11	EDO	B	1029	-	-	0/1/1/1	-
11	EDO	C	1139	-	-	0/1/1/1	-
11	EDO	B	1025	-	-	0/1/1/1	-
11	EDO	C	1141	-	-	0/1/1/1	-
11	EDO	A	1035	-	-	0/1/1/1	-
11	EDO	C	1145	-	-	0/1/1/1	-
11	EDO	B	1026	-	-	0/1/1/1	-
11	EDO	C	1136	-	-	0/1/1/1	-
11	EDO	B	1023	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1015	NAG	C1
9	C	1117	NAG	C1

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1015	NAG	C1-C2-N2-C7
9	A	1015	NAG	C8-C7-N2-C2
9	A	1015	NAG	O7-C7-N2-C2
9	D	1016	NAG	C8-C7-N2-C2
9	D	1016	NAG	O7-C7-N2-C2
9	B	1021	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	1021	NAG	O7-C7-N2-C2
9	A	1022	NAG	C8-C7-N2-C2
9	A	1022	NAG	O7-C7-N2-C2
9	C	1117	NAG	C8-C7-N2-C2
9	C	1117	NAG	O7-C7-N2-C2
9	D	1025	NAG	C8-C7-N2-C2
9	D	1025	NAG	O7-C7-N2-C2
11	B	1034	EDO	O1-C1-C2-O2
11	A	1027	EDO	O1-C1-C2-O2
11	B	1028	EDO	O1-C1-C2-O2
11	A	1031	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1040	EDO	1	0
11	B	1034	EDO	2	0
11	A	1029	EDO	2	0
11	A	1028	EDO	2	0
11	B	1027	EDO	3	0
11	C	1146	EDO	1	0
11	A	1032	EDO	1	0
11	B	1031	EDO	1	0
11	B	1028	EDO	1	0
11	B	1025	EDO	1	0
11	C	1141	EDO	1	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	903/950 (95%)	-0.19	17 (1%)	66	62	31, 55, 87, 120	0
1	B	904/950 (95%)	-0.21	17 (1%)	66	62	31, 51, 83, 124	0
1	C	905/950 (95%)	-0.22	16 (1%)	68	64	34, 53, 85, 126	0
1	D	904/950 (95%)	-0.20	19 (2%)	63	58	33, 55, 85, 123	0
All	All	3616/3800 (95%)	-0.20	69 (1%)	66	62	31, 53, 85, 126	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	895	SER	6.8
1	D	894	GLY	6.8
1	A	63	THR	6.7
1	C	894	GLY	6.7
1	B	64	THR	6.7
1	B	65	LEU	5.3
1	C	202	ASN	5.1
1	A	295	SER	4.9
1	B	295	SER	4.9
1	C	64	THR	4.9
1	C	893	GLY	4.9
1	C	929	GLY	4.8
1	D	64	THR	4.2
1	C	892	GLY	4.0
1	A	64	THR	4.0
1	D	929	GLY	3.7
1	D	895	SER	3.6
1	C	63	THR	3.4
1	B	98	ARG	3.4
1	A	890	ASP	3.4
1	D	223	CYS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	202	ASN	3.2
1	B	892	GLY	3.2
1	C	927	GLU	3.2
1	B	927	GLU	3.1
1	C	98	ARG	2.9
1	A	296	ASN	2.9
1	D	648	ARG	2.9
1	C	65	LEU	2.9
1	D	927	GLU	2.9
1	C	926	GLU	2.8
1	D	122	ILE	2.8
1	A	927	GLU	2.8
1	A	409	LEU	2.8
1	B	202	ASN	2.6
1	D	926	GLU	2.6
1	B	652	ALA	2.5
1	C	923	LYS	2.5
1	A	923	LYS	2.5
1	B	331[A]	HIS	2.5
1	D	259	PRO	2.4
1	A	571	ASP	2.4
1	A	122	ILE	2.4
1	C	617	ASN	2.4
1	A	202	ASN	2.3
1	B	967	LYS	2.3
1	B	893	GLY	2.3
1	A	926	GLU	2.3
1	D	893	GLY	2.3
1	C	97	ASP	2.2
1	D	889	ASN	2.2
1	D	222	PRO	2.2
1	D	262	PRO	2.2
1	A	637	GLU	2.2
1	A	573	ASN	2.1
1	C	223	CYS	2.1
1	A	372	LEU	2.1
1	B	294	ALA	2.1
1	D	738	ASN	2.1
1	C	895	SER	2.1
1	B	571	ASP	2.1
1	D	224	PHE	2.1
1	A	894	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	923	LYS	2.1
1	D	621	LEU	2.0
1	D	413	PHE	2.0
1	A	640	ARG	2.0
1	B	409	LEU	2.0
1	B	935	ARG	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	U	3	11/12	0.39	0.56	123,126,129,132	0
3	BMA	L	4	11/12	0.43	0.47	104,108,110,111	0
5	BMA	H	3	11/12	0.46	0.57	120,127,130,133	0
3	BMA	L	3	11/12	0.49	0.28	94,96,102,106	0
5	BMA	O	3	11/12	0.49	0.46	105,108,114,116	0
4	NAG	f	2	14/15	0.51	0.52	115,120,124,125	0
5	BMA	c	3	11/12	0.54	0.60	138,142,145,148	0
4	NAG	d	2	14/15	0.56	0.79	148,153,158,158	0
3	BMA	F	4	11/12	0.58	0.34	98,100,102,102	0
8	BMA	Y	6	11/12	0.59	0.57	133,143,147,148	0
4	NAG	V	1	14/15	0.60	0.58	149,151,153,156	0
2	BMA	R	3	11/12	0.63	0.60	134,138,146,147	0
4	NAG	V	2	14/15	0.64	0.74	139,156,163,163	0
6	BMA	T	4	11/12	0.65	0.57	127,134,137,138	0
4	NAG	Q	2	14/15	0.65	0.53	118,123,130,132	0
7	BMA	W	4	11/12	0.65	0.67	138,140,141,142	0
2	BMA	K	4	11/12	0.65	0.42	132,138,143,143	0
2	BMA	J	4	11/12	0.65	0.64	120,125,128,129	0
8	BMA	Y	5	11/12	0.66	0.44	138,141,145,145	0
3	BMA	F	5	11/12	0.67	0.47	103,109,113,115	0
5	NAG	c	2	14/15	0.68	0.51	115,122,129,133	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	N	1	14/15	0.69	0.30	92,102,108,113	0
6	BMA	T	3	11/12	0.70	0.38	113,124,129,131	0
7	BMA	W	3	11/12	0.70	0.52	121,129,136,138	0
8	NAG	Y	1	14/15	0.70	0.33	114,122,126,127	0
7	BMA	W	6	11/12	0.70	0.54	122,126,128,129	0
4	NAG	G	2	14/15	0.71	0.51	110,115,121,122	0
2	BMA	E	3	11/12	0.71	0.40	106,108,111,114	0
7	BMA	W	5	11/12	0.71	0.65	131,138,142,143	0
8	BMA	Y	3	11/12	0.71	0.38	138,144,148,148	0
2	NAG	J	1	14/15	0.71	0.25	86,97,102,106	0
8	BMA	Y	4	11/12	0.72	0.25	134,143,145,146	0
4	NAG	g	2	14/15	0.72	0.66	126,131,135,136	0
2	BMA	R	4	11/12	0.72	0.71	146,150,152,153	0
4	NAG	Q	1	14/15	0.72	0.34	100,107,113,116	0
3	BMA	S	5	11/12	0.73	0.43	103,105,114,114	0
4	NAG	d	1	14/15	0.73	0.44	131,138,145,147	0
2	BMA	K	3	11/12	0.74	0.42	129,131,133,137	0
2	NAG	R	2	14/15	0.74	0.58	126,131,133,133	0
5	BMA	Z	3	11/12	0.74	0.69	131,136,139,141	0
4	NAG	g	1	14/15	0.75	0.38	128,131,133,134	0
4	NAG	N	2	14/15	0.75	0.55	108,121,126,126	0
5	BMA	b	3	11/12	0.76	0.43	103,107,110,113	0
2	BMA	E	4	11/12	0.77	0.36	100,107,109,110	0
5	NAG	Z	2	14/15	0.77	0.47	121,128,134,134	0
5	NAG	H	1	14/15	0.78	0.30	76,90,95,99	0
4	NAG	P	2	14/15	0.78	0.34	80,87,99,102	0
7	BMA	a	5	11/12	0.78	0.44	115,117,121,122	0
2	BMA	J	3	11/12	0.78	0.58	126,128,132,134	0
5	NAG	c	1	14/15	0.79	0.29	81,95,105,112	0
5	NAG	O	1	14/15	0.80	0.27	87,89,94,95	0
7	BMA	a	6	11/12	0.80	0.51	107,113,116,117	0
4	NAG	X	2	14/15	0.80	0.47	123,127,133,135	0
7	NAG	W	2	14/15	0.81	0.24	88,94,104,112	0
3	BMA	S	3	11/12	0.81	0.29	85,92,98,99	0
5	NAG	O	2	14/15	0.81	0.48	95,99,103,103	0
5	NAG	U	2	14/15	0.82	0.51	99,109,115,118	0
4	NAG	f	1	14/15	0.82	0.29	103,108,115,117	0
4	NAG	X	1	14/15	0.82	0.25	106,117,122,125	0
2	NAG	J	2	14/15	0.82	0.47	109,114,120,122	0
2	NAG	K	2	14/15	0.82	0.32	99,105,115,124	0
7	BMA	a	3	11/12	0.83	0.30	87,94,100,103	0
5	NAG	U	1	14/15	0.83	0.27	84,96,100,105	0

Continued on next page...

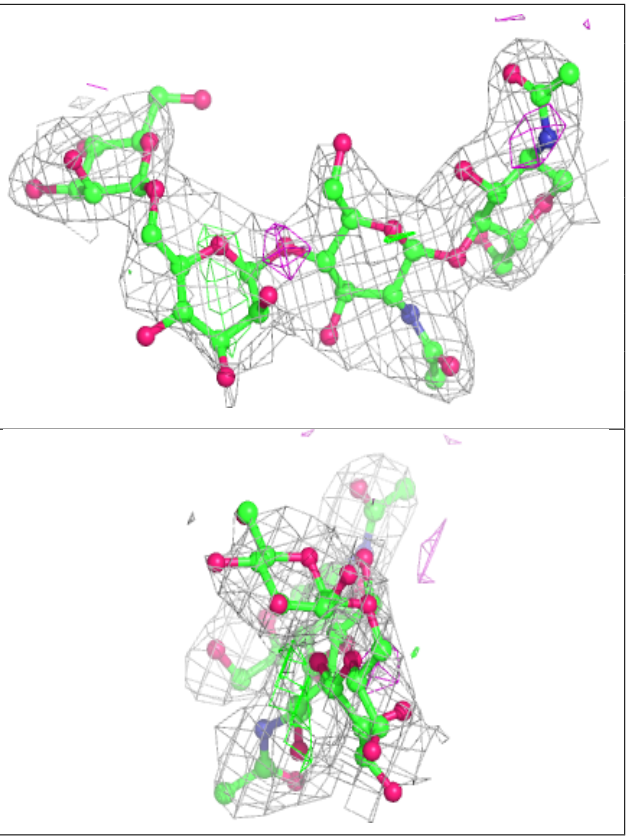
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	H	2	14/15	0.83	0.45	100,105,112,115	0
3	BMA	L	5	11/12	0.83	0.35	99,102,107,108	0
2	NAG	R	1	14/15	0.84	0.29	92,112,119,123	0
4	NAG	I	2	14/15	0.84	0.37	87,94,99,101	0
3	BMA	F	3	11/12	0.85	0.27	85,92,98,102	0
4	NAG	M	2	14/15	0.85	0.45	112,116,121,122	0
8	NAG	Y	2	14/15	0.86	0.50	124,128,135,135	0
4	NAG	e	2	14/15	0.87	0.33	94,97,101,102	0
4	NAG	M	1	14/15	0.87	0.28	81,100,109,109	0
4	NAG	G	1	14/15	0.87	0.27	84,92,98,105	0
3	BMA	S	4	11/12	0.88	0.42	95,103,106,108	0
5	NAG	Z	1	14/15	0.89	0.29	106,114,117,120	0
2	NAG	K	1	14/15	0.90	0.20	80,88,93,98	0
7	BMA	a	4	11/12	0.90	0.32	104,106,109,112	0
3	NAG	L	1	14/15	0.91	0.15	58,59,67,68	0
3	NAG	L	2	14/15	0.91	0.28	67,70,79,85	0
4	NAG	P	1	14/15	0.91	0.19	68,72,79,82	0
2	NAG	E	2	14/15	0.91	0.32	80,88,95,102	0
6	NAG	T	2	14/15	0.91	0.20	86,91,97,104	0
4	NAG	e	1	14/15	0.92	0.20	73,75,79,88	0
3	NAG	S	1	14/15	0.93	0.14	58,61,64,66	0
5	NAG	b	2	14/15	0.93	0.23	90,93,100,100	0
7	NAG	W	1	14/15	0.93	0.17	77,85,87,90	0
3	NAG	F	1	14/15	0.93	0.16	49,55,60,61	0
3	NAG	F	2	14/15	0.94	0.26	63,71,74,80	0
7	NAG	a	2	14/15	0.95	0.28	61,70,74,80	0
7	NAG	a	1	14/15	0.95	0.14	59,63,65,65	0
5	NAG	b	1	14/15	0.95	0.17	67,78,79,85	0
6	NAG	T	1	14/15	0.95	0.16	67,76,81,86	0
3	NAG	S	2	14/15	0.95	0.27	59,64,72,78	0
4	NAG	I	1	14/15	0.96	0.17	67,70,74,81	0
2	NAG	E	1	14/15	0.96	0.19	59,65,69,76	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.

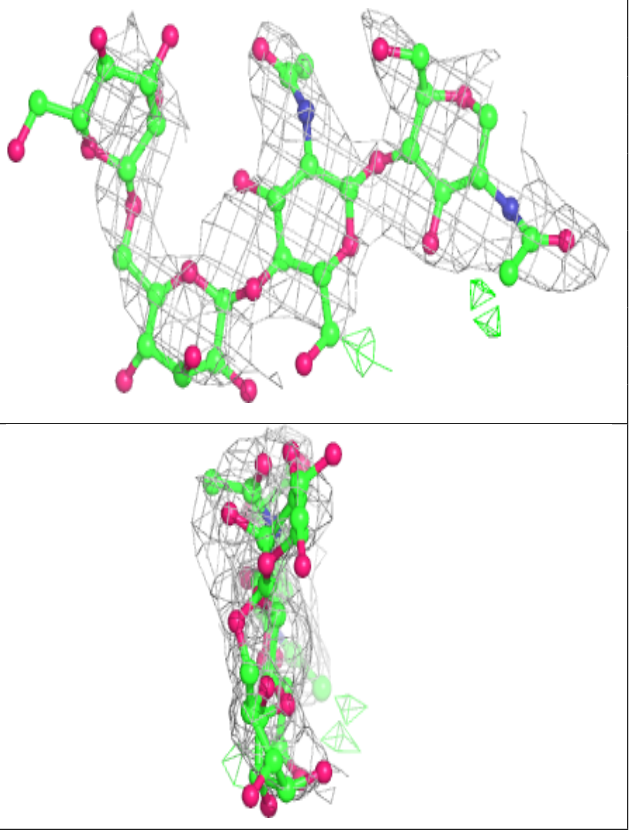
Electron density around Chain E:

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



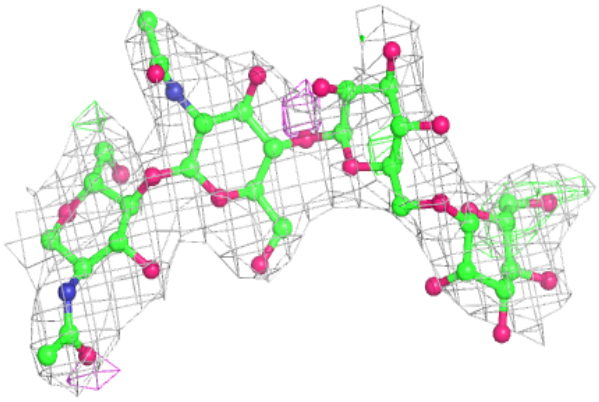
Electron density around Chain J:

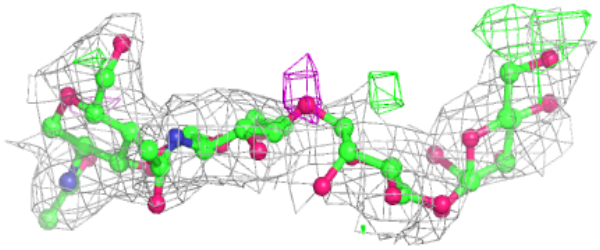
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

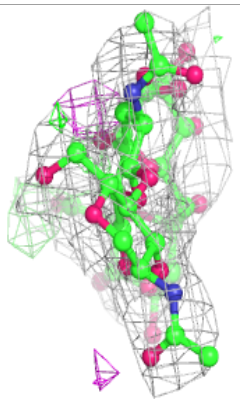


Electron density around Chain K:

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

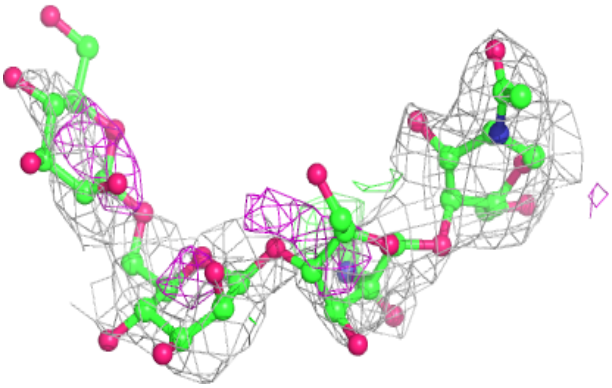


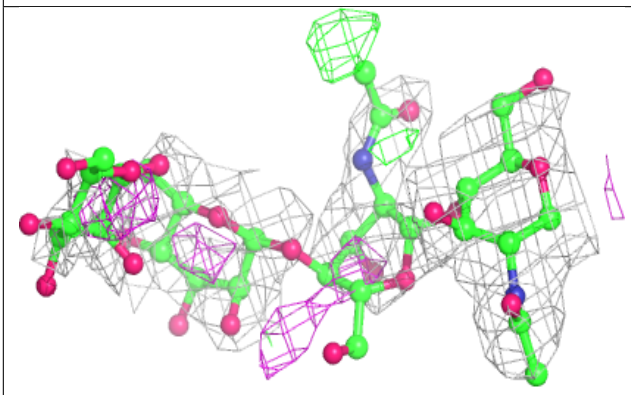


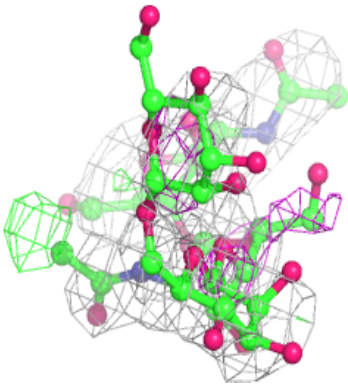


Electron density around Chain R:

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

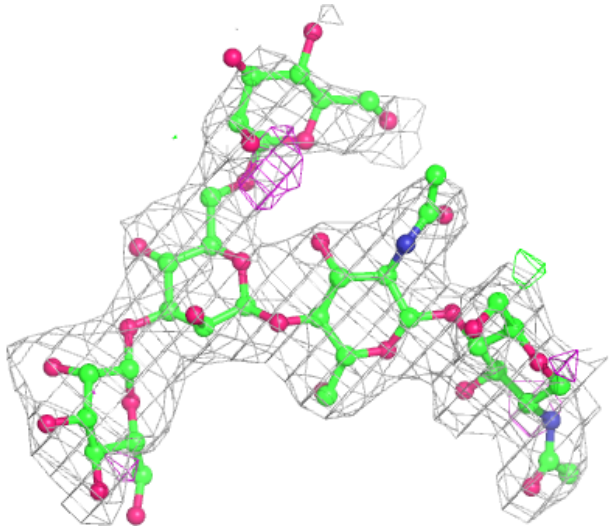


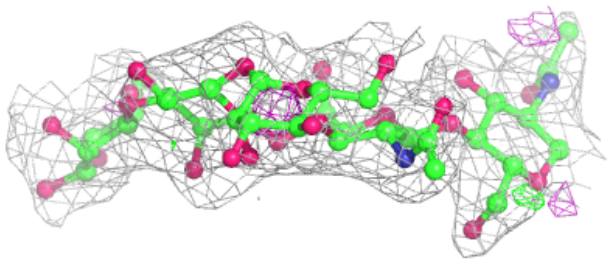


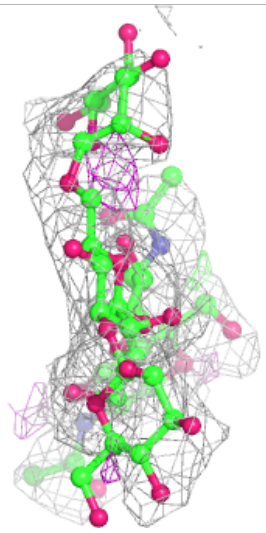


Electron density around Chain F:

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

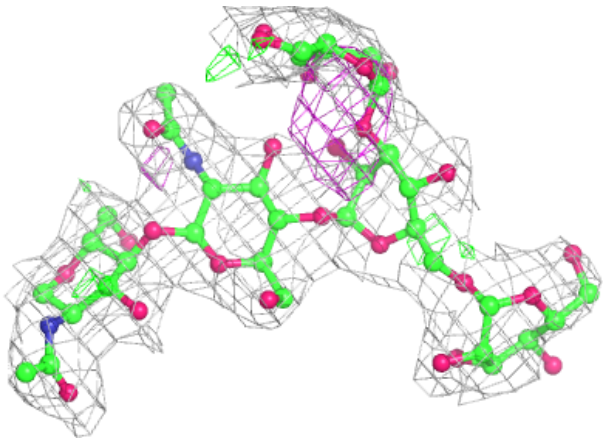


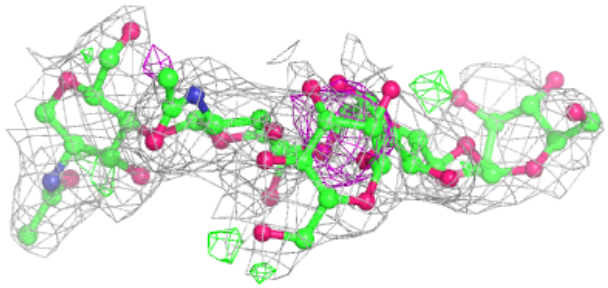


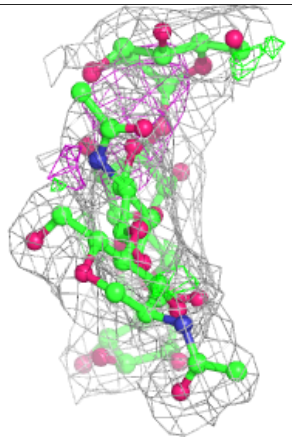


Electron density around Chain L:

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

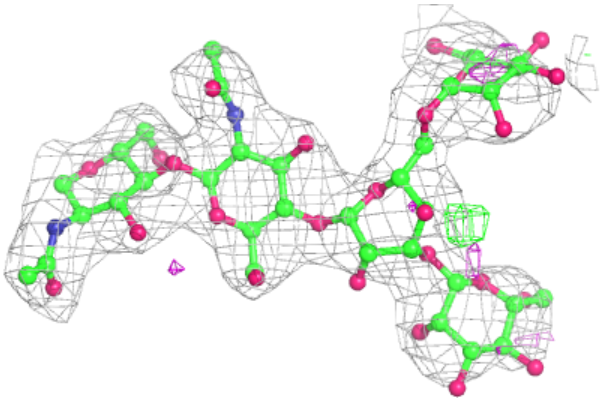


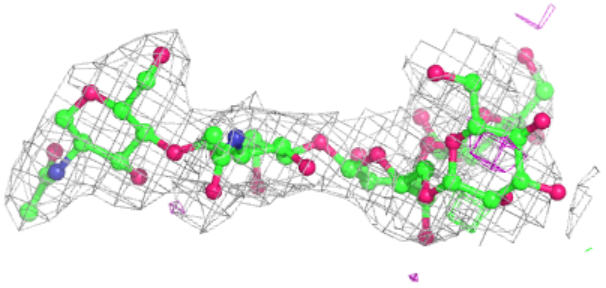


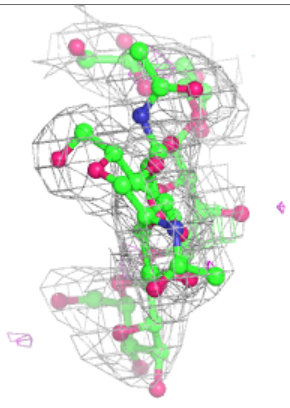


Electron density around Chain S:

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

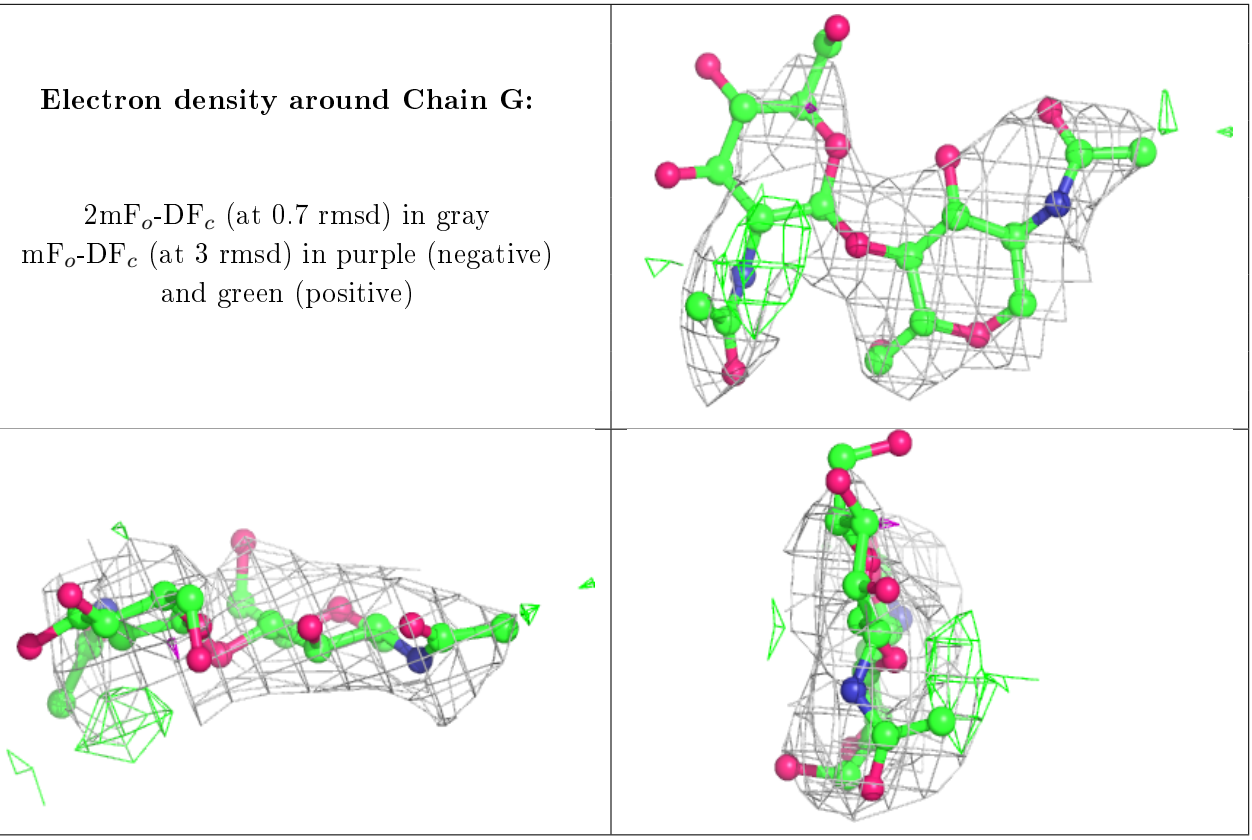






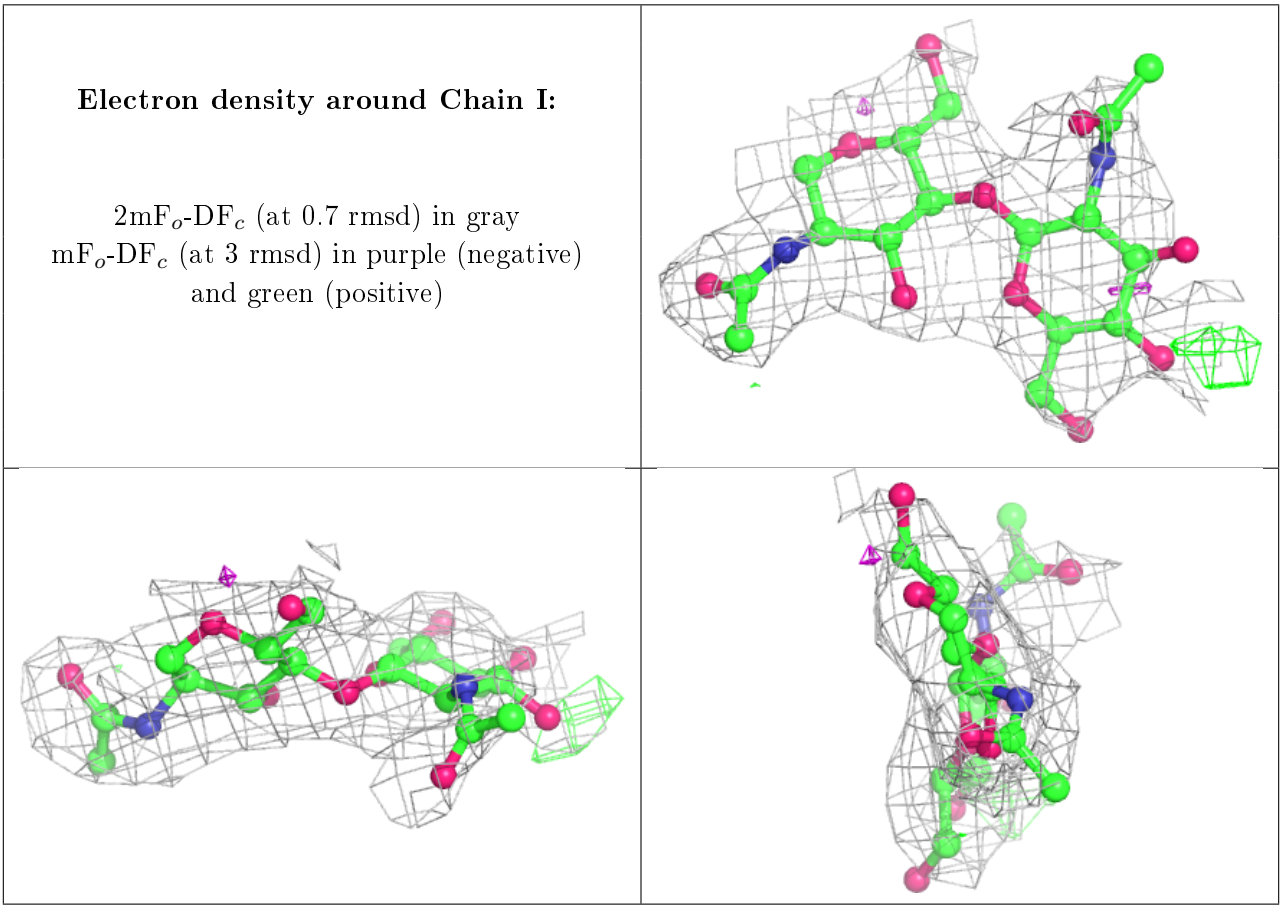
Electron density around Chain G:

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



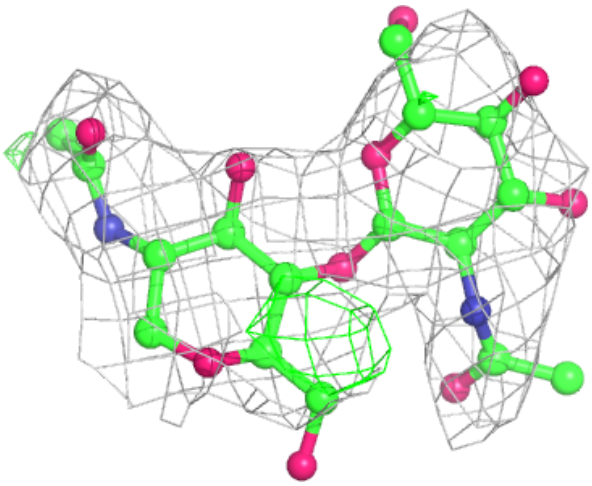
Electron density around Chain I:

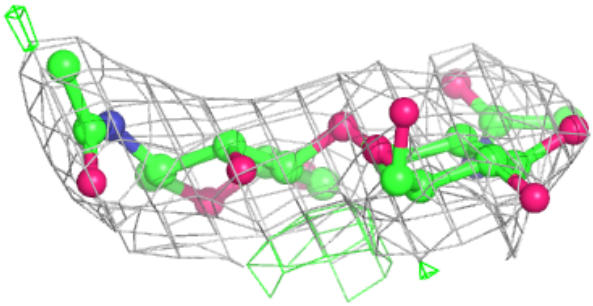
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

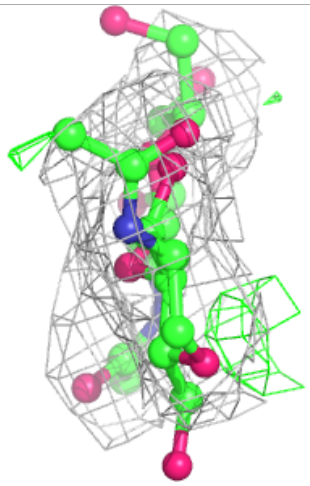


Electron density around Chain M:

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

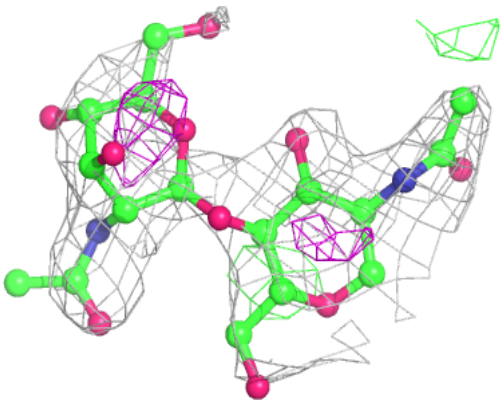


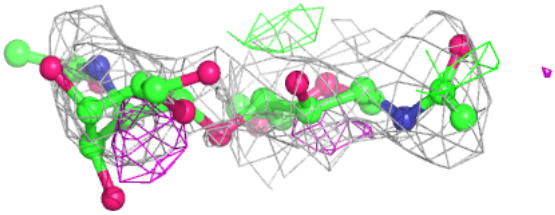


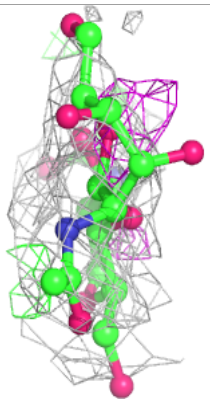


Electron density around Chain N:

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

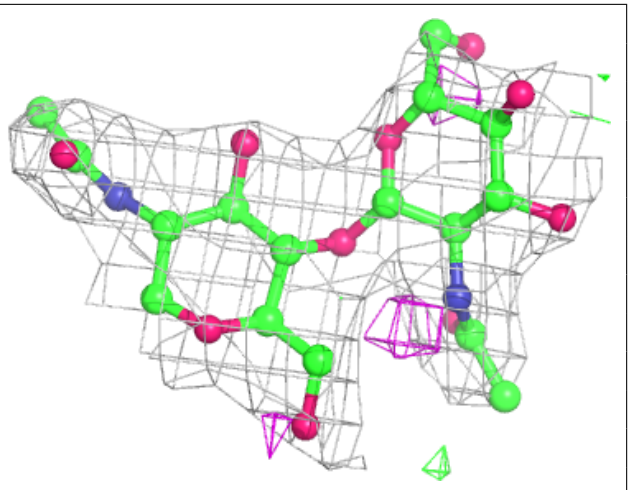


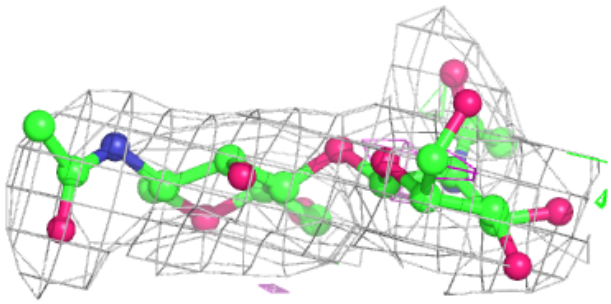


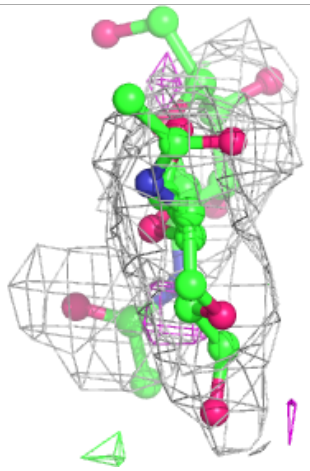


Electron density around Chain P:

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

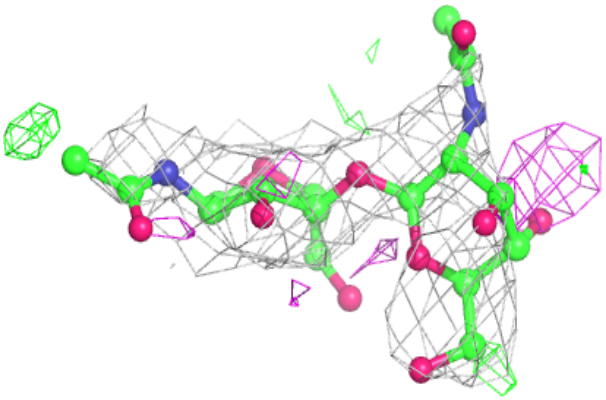


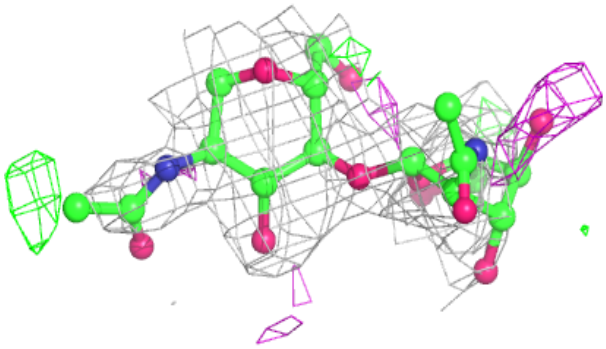


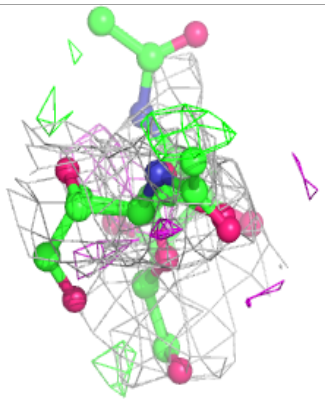


Electron density around Chain Q:

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

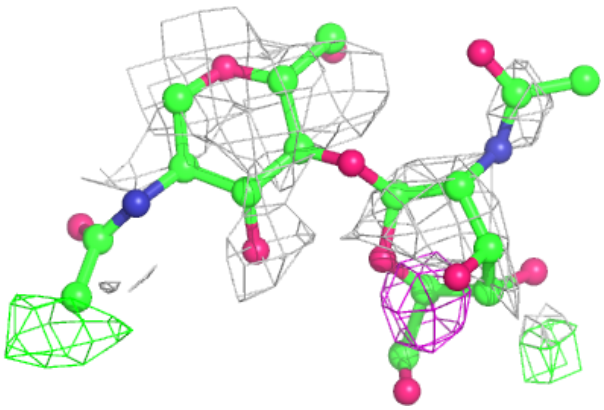


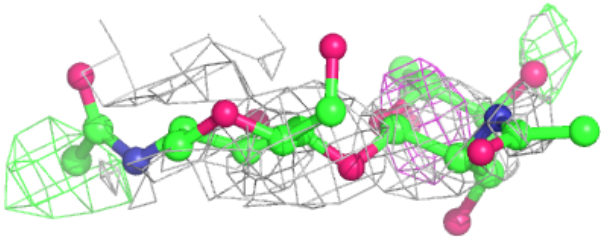


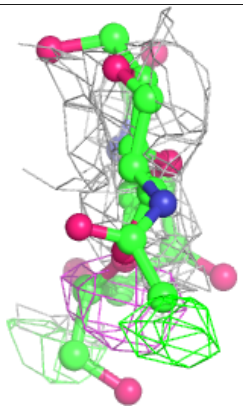


Electron density around Chain V:

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

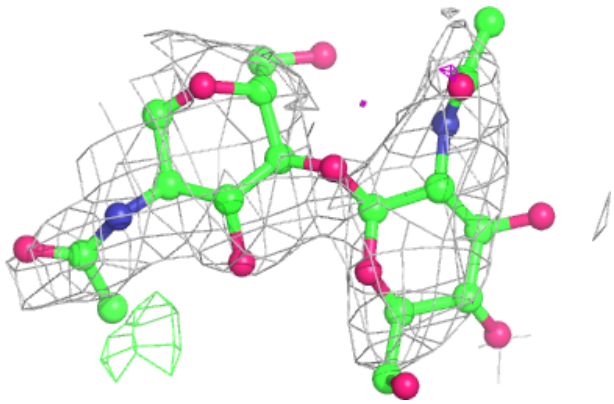


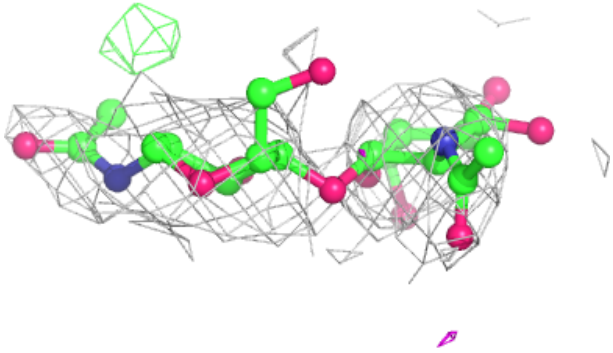


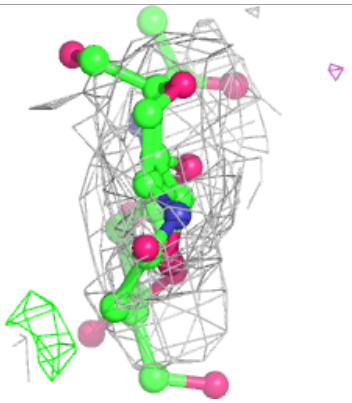


Electron density around Chain X:

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

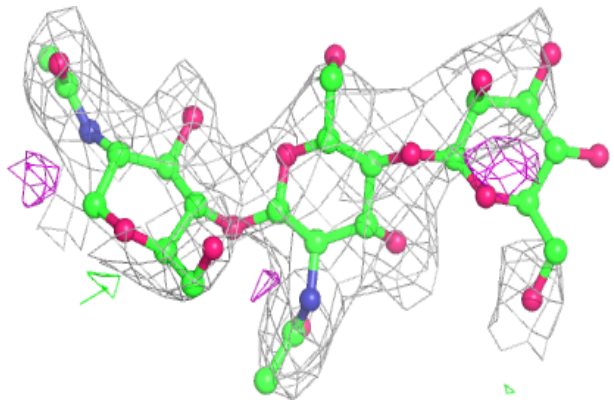


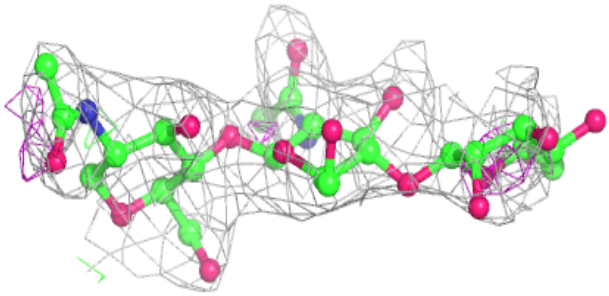


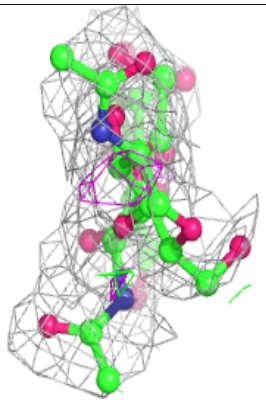


Electron density around Chain H:

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

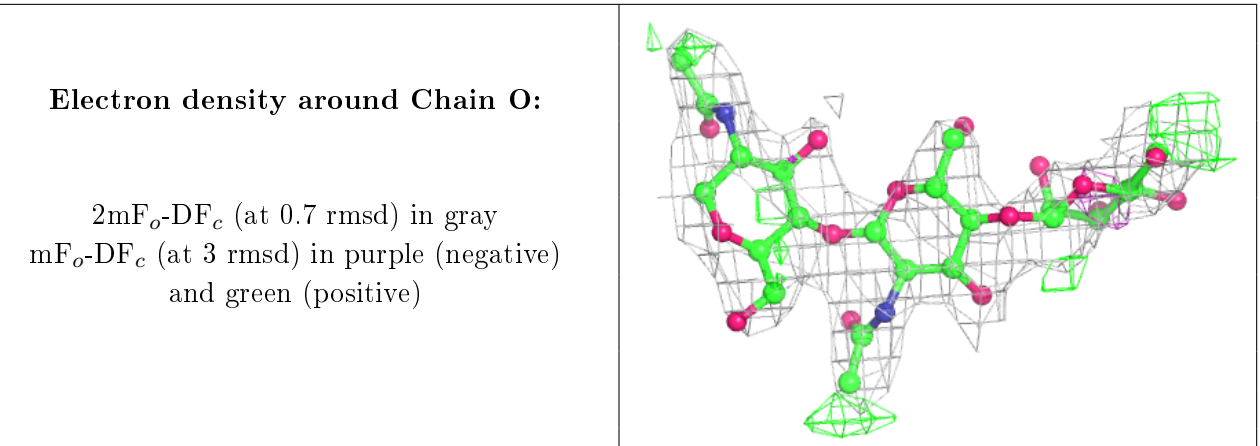






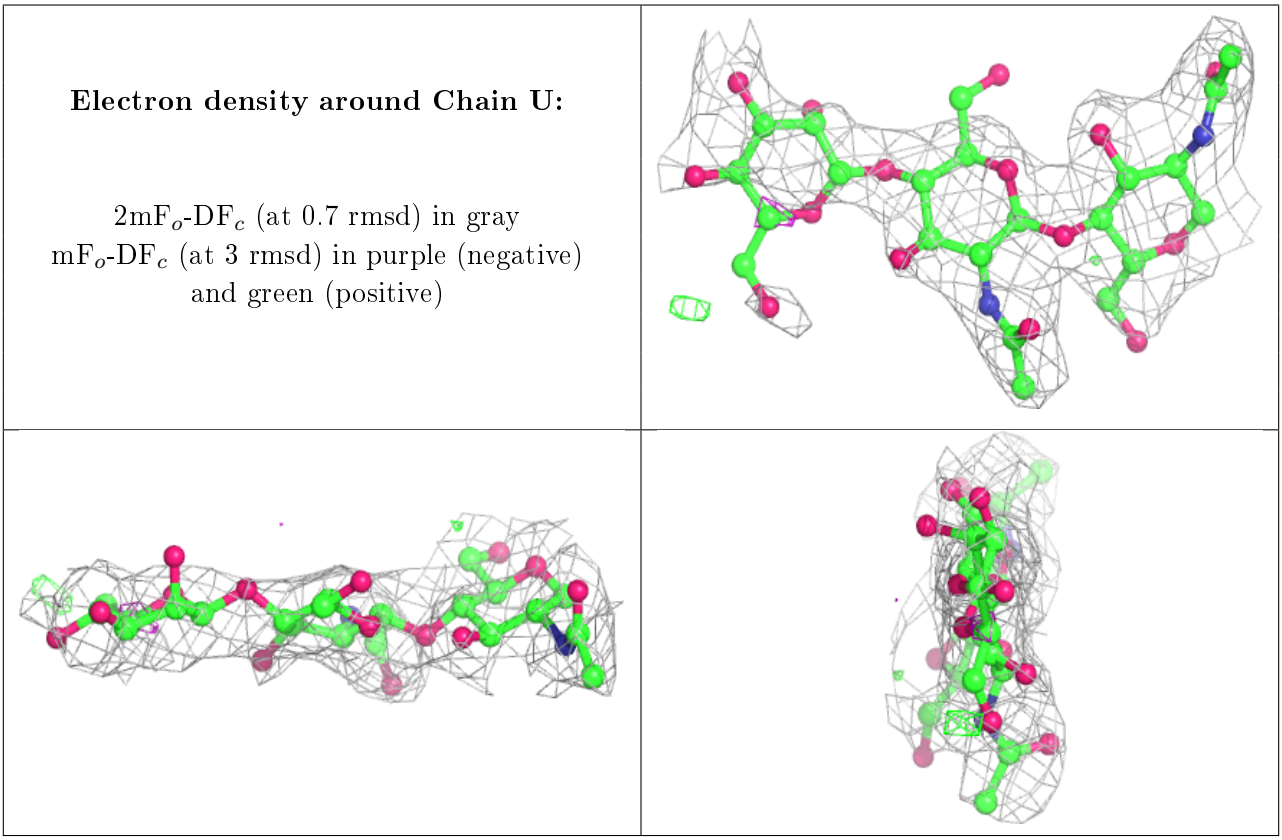
Electron density around Chain O:

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



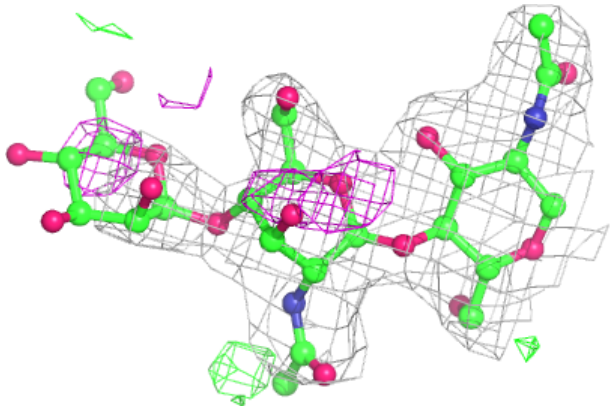
Electron density around Chain U:

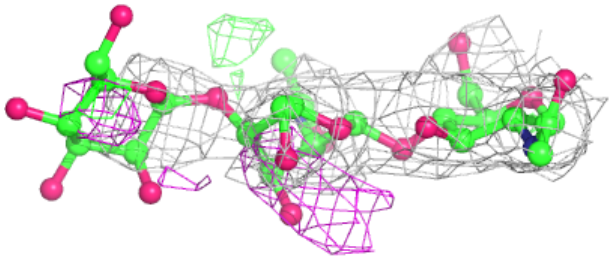
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

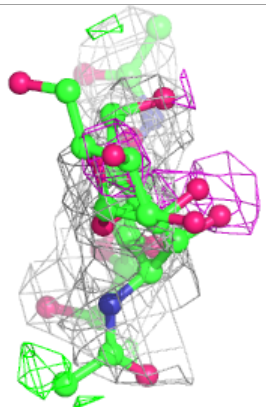


Electron density around Chain Z:

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

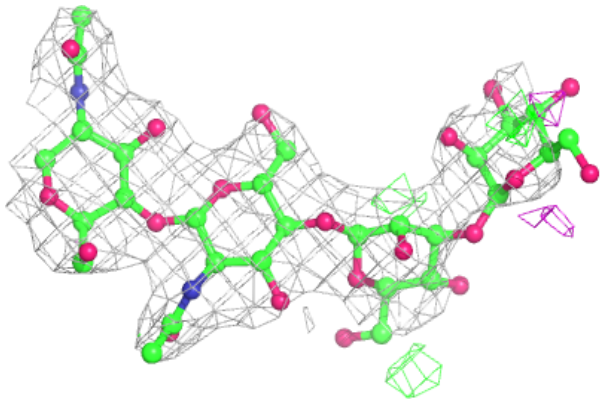


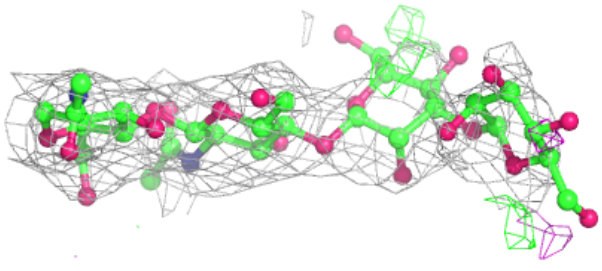




Electron density around Chain T:

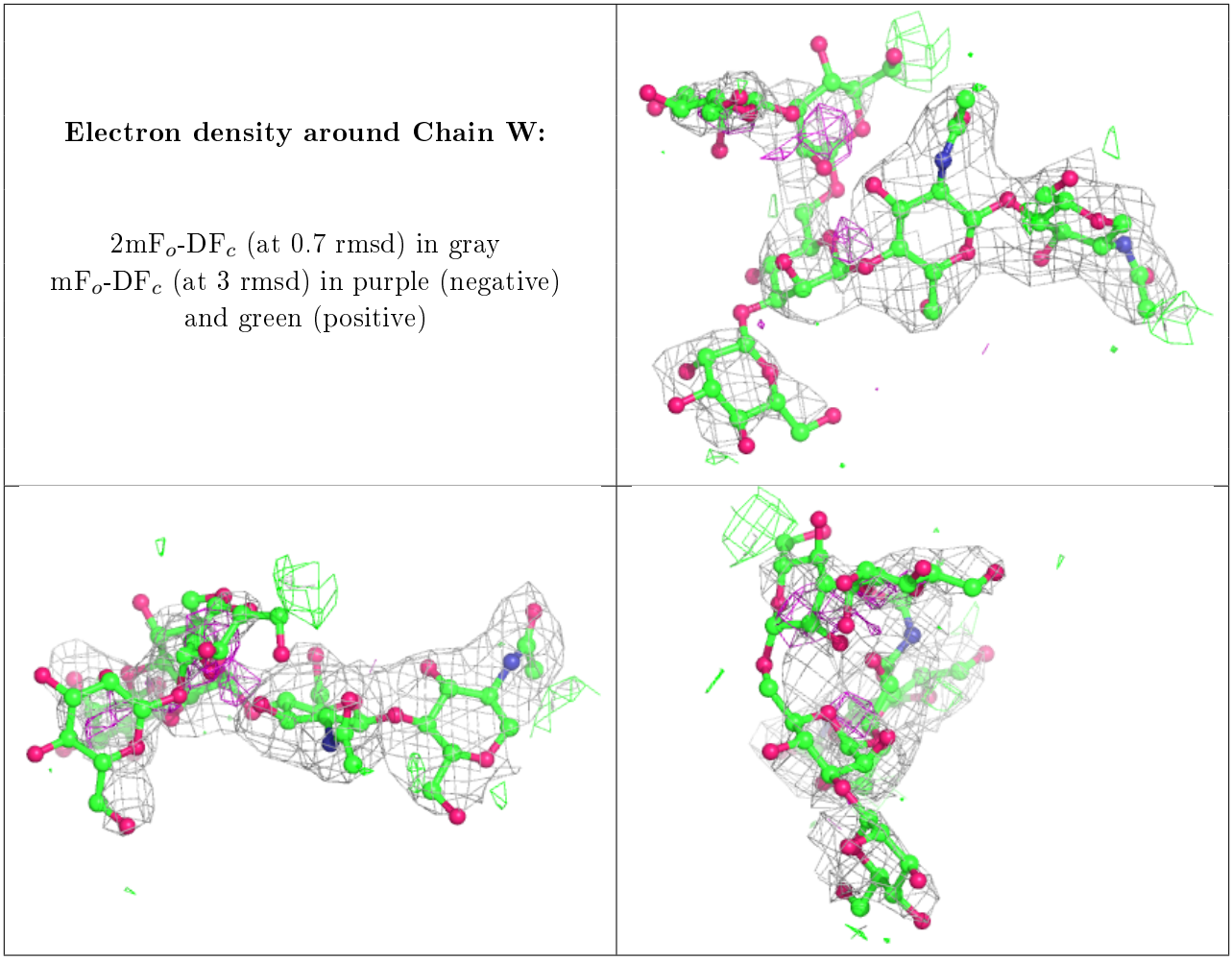
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





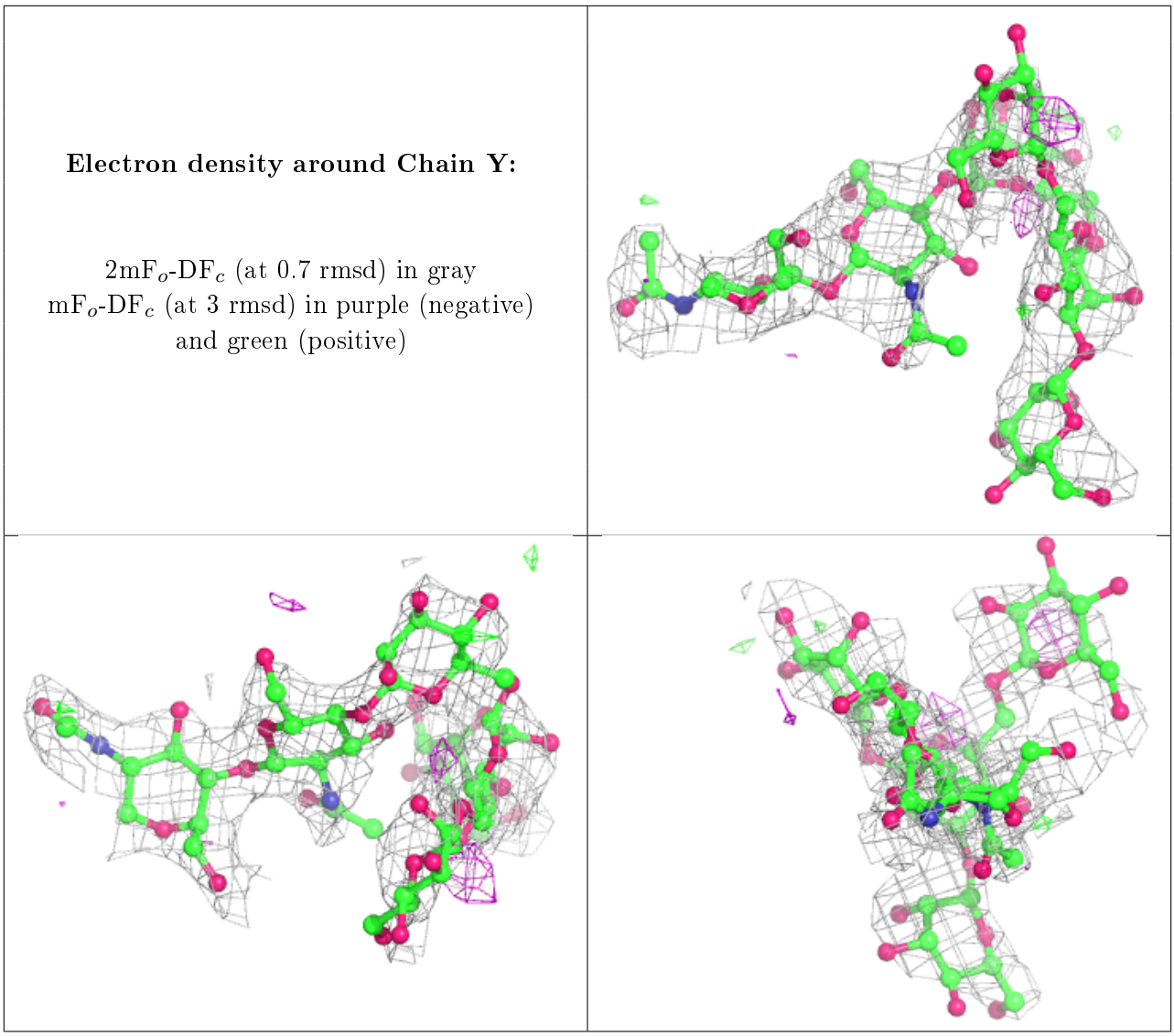
Electron density around Chain W:

$2mF_o$-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)



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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	EDO	B	1030	4/4	0.53	0.41	69,70,71,71	0
9	NAG	A	1022	14/15	0.62	0.61	136,139,145,147	0
9	NAG	D	1025	14/15	0.72	0.49	134,144,148,151	0
11	EDO	C	1141	4/4	0.72	0.29	79,80,82,84	0
11	EDO	A	1035	4/4	0.73	0.33	90,90,91,92	0
9	NAG	D	1016	14/15	0.74	0.38	85,97,99,102	0
11	EDO	B	1034	4/4	0.74	0.47	63,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	EDO	A	1031	4/4	0.75	0.49	57,62,63,67	0
11	EDO	C	1138	4/4	0.75	0.39	77,78,79,79	0
11	EDO	A	1038	4/4	0.76	0.30	72,73,75,77	0
11	EDO	D	1030	4/4	0.76	0.36	65,68,71,72	0
11	EDO	C	1146	4/4	0.77	0.27	72,73,74,74	0
11	EDO	A	1036	4/4	0.77	0.24	73,74,76,77	0
11	EDO	A	1032	4/4	0.79	0.23	61,62,64,64	0
11	EDO	A	1028	4/4	0.79	0.36	63,66,66,69	0
9	NAG	B	1021	14/15	0.80	0.46	129,142,145,148	0
9	NAG	A	1015	14/15	0.80	0.37	97,107,115,116	0
11	EDO	B	1029	4/4	0.80	0.20	68,70,70,71	0
11	EDO	D	1031	4/4	0.80	0.26	64,64,65,66	0
11	EDO	B	1023	4/4	0.81	0.30	65,66,69,70	0
11	EDO	C	1142	4/4	0.82	0.37	73,75,77,77	0
11	EDO	A	1029	4/4	0.83	0.29	59,63,65,68	0
11	EDO	A	1034	4/4	0.83	0.39	65,69,69,70	0
11	EDO	A	1030	4/4	0.83	0.36	73,76,77,78	0
11	EDO	B	1025	4/4	0.84	0.66	79,79,80,81	0
11	EDO	C	1137	4/4	0.86	0.33	75,75,76,76	0
9	NAG	C	1117	14/15	0.86	0.34	94,100,106,107	0
11	EDO	C	1140	4/4	0.86	0.27	68,70,71,71	0
11	EDO	C	1136	4/4	0.87	0.31	67,67,68,71	0
11	EDO	B	1027	4/4	0.87	0.37	57,59,63,66	0
11	EDO	A	1037	4/4	0.88	0.40	77,80,82,84	0
11	EDO	A	1027	4/4	0.89	0.27	73,73,75,75	0
11	EDO	B	1026	4/4	0.89	0.24	67,68,68,68	0
11	EDO	A	1025	4/4	0.89	0.35	63,65,67,68	0
11	EDO	A	1033	4/4	0.90	0.35	71,72,75,76	0
11	EDO	B	1031	4/4	0.90	0.29	58,62,63,63	0
11	EDO	A	1039	4/4	0.91	0.20	81,82,82,83	0
11	EDO	B	1033	4/4	0.91	0.22	69,69,69,70	0
11	EDO	D	1029	4/4	0.91	0.23	58,58,58,58	0
11	EDO	B	1028	4/4	0.91	0.27	54,55,56,57	0
11	EDO	C	1145	4/4	0.92	0.27	58,58,60,62	0
11	EDO	A	1026	4/4	0.92	0.25	81,82,82,83	0
11	EDO	A	1024	4/4	0.92	0.20	71,71,72,73	0
11	EDO	B	1024	4/4	0.93	0.18	60,61,64,67	0
11	EDO	C	1143	4/4	0.93	0.26	65,68,69,71	0
11	EDO	C	1135	4/4	0.93	0.16	67,69,71,71	0
11	EDO	B	1032	4/4	0.94	0.17	81,81,82,82	0
11	EDO	A	1040	4/4	0.94	0.22	54,56,59,61	0
11	EDO	C	1144	4/4	0.94	0.17	62,63,63,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	EDO	D	1028	4/4	0.95	0.15	61,62,64,65	0
11	EDO	C	1139	4/4	0.96	0.19	62,63,64,66	0
11	EDO	D	1027	4/4	0.97	0.19	69,69,70,71	0
10	ZN	D	1026	1/1	0.99	0.10	43,43,43,43	0
10	ZN	B	1022	1/1	0.99	0.09	42,42,42,42	0
10	ZN	A	1023	1/1	0.99	0.09	43,43,43,43	0
10	ZN	C	1134	1/1	1.00	0.09	41,41,41,41	0

6.5 Other polymers

There are no such residues in this entry.