wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 11:04 AM EDT

PDB ID	:	6QXP
Title	:	Protein peptide complex
Authors	:	Moussu, S.; Caroline, C.; Santos-Fernandez, G.; Wehrle, S.; Grossniklaus, U.; Santiago, J.
Deposited on	:	2019-03-07
Resolution	:	3.20 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

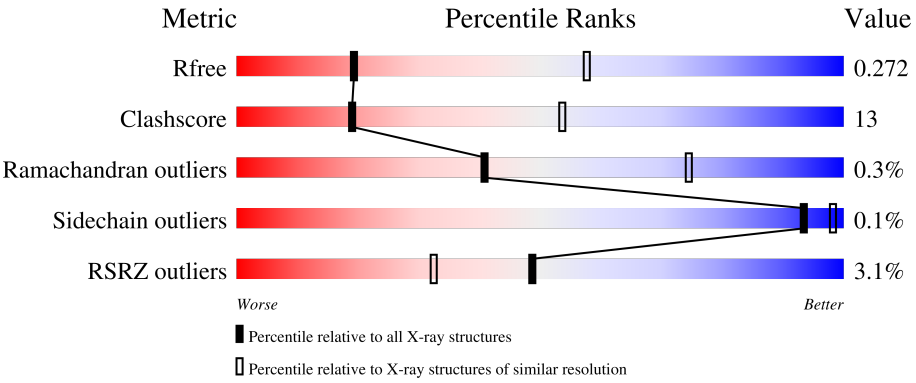
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	361	.% 68% 27% 5%
1	B	361	11% 62% 29% 9%
1	C	361	.% 68% 26% 5%
1	D	361	.% 68% 25% 7%
1	E	361	68% 27% 5%

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Mol	Chain	Length	Quality of chain
1	F	361	2% 71% 22% 7%
1	G	361	68% 26% 5%
1	H	361	9% 60% 29% 10%
2	I	56	61% 23% 16%
2	J	56	7% 64% 18% 18%
2	K	56	61% 20% 20%
2	L	56	70% 14% 16%
2	M	56	2% 61% 23% 16%
2	N	56	70% 12% 18%
2	O	56	61% 23% 16%
2	P	56	5% 71% 9% 20%
3	Q	3	100%
3	R	3	100%
3	T	3	100%
3	V	3	100%
3	X	3	67% 33%
3	a	3	67% 33%
3	f	3	100%
4	S	4	75% 25%
5	U	2	100%
5	W	2	100%
5	Y	2	100%
5	c	2	100%
5	d	2	100%
5	e	2	100%

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Mol	Chain	Length	Quality of chain
6	Z	4	
6	b	4	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 24293 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 Leucine-rich repeat extensin-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2616	1657	441	500	18			
1	B	328	Total	C	N	O	S	0	0	0
			2515	1593	422	482	18			
1	C	343	Total	C	N	O	S	0	0	0
			2636	1671	445	502	18			
1	D	336	Total	C	N	O	S	0	0	0
			2557	1619	429	491	18			
1	E	344	Total	C	N	O	S	0	0	0
			2624	1667	438	501	18			
1	F	336	Total	C	N	O	S	0	0	0
			2573	1633	429	494	17			
1	G	342	Total	C	N	O	S	0	0	0
			2616	1659	441	498	18			
1	H	325	Total	C	N	O	S	0	0	0
			2487	1577	415	479	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	LEU	-	expression tag	UNP O48809
A	387	GLU	-	expression tag	UNP O48809
A	388	ASN	-	expression tag	UNP O48809
A	389	LEU	-	expression tag	UNP O48809
B	386	LEU	-	expression tag	UNP O48809
B	387	GLU	-	expression tag	UNP O48809
B	388	ASN	-	expression tag	UNP O48809
B	389	LEU	-	expression tag	UNP O48809
C	386	LEU	-	expression tag	UNP O48809
C	387	GLU	-	expression tag	UNP O48809
C	388	ASN	-	expression tag	UNP O48809
C	389	LEU	-	expression tag	UNP O48809
D	386	LEU	-	expression tag	UNP O48809

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Chain	Residue	Modelled	Actual	Comment	Reference
D	387	GLU	-	expression tag	UNP O48809
D	388	ASN	-	expression tag	UNP O48809
D	389	LEU	-	expression tag	UNP O48809
E	385	LEU	-	expression tag	UNP O48809
E	386	GLU	-	expression tag	UNP O48809
E	387	ASN	-	expression tag	UNP O48809
E	388	LEU	-	expression tag	UNP O48809
F	386	LEU	-	expression tag	UNP O48809
F	387	GLU	-	expression tag	UNP O48809
F	388	ASN	-	expression tag	UNP O48809
F	389	LEU	-	expression tag	UNP O48809
G	386	LEU	-	expression tag	UNP O48809
G	387	GLU	-	expression tag	UNP O48809
G	388	ASN	-	expression tag	UNP O48809
G	389	LEU	-	expression tag	UNP O48809
H	386	LEU	-	expression tag	UNP O48809
H	387	GLU	-	expression tag	UNP O48809
H	388	ASN	-	expression tag	UNP O48809
H	389	LEU	-	expression tag	UNP O48809

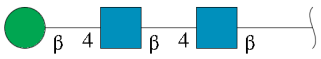
- Molecule 2 is a protein called Protein RALF-like 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	47	Total	C	N	O	S	0	0	0
			370	226	76	64	4			
2	J	46	Total	C	N	O	S	0	0	0
			373	229	77	63	4			
2	K	45	Total	C	N	O	S	0	0	0
			353	217	69	63	4			
2	L	47	Total	C	N	O	S	0	0	0
			364	223	73	64	4			
2	M	47	Total	C	N	O	S	0	0	0
			371	226	76	65	4			
2	N	46	Total	C	N	O	S	0	0	0
			359	220	72	63	4			
2	O	47	Total	C	N	O	S	0	0	0
			364	223	73	64	4			
2	P	45	Total	C	N	O	S	0	0	0
			342	211	65	62	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1052	MET	-	initiating methionine	UNP Q9FZA0
I	1053	GLY	-	expression tag	UNP Q9FZA0
J	1052	MET	-	initiating methionine	UNP Q9FZA0
J	1053	GLY	-	expression tag	UNP Q9FZA0
K	1052	MET	-	initiating methionine	UNP Q9FZA0
K	1053	GLY	-	expression tag	UNP Q9FZA0
L	1052	MET	-	initiating methionine	UNP Q9FZA0
L	1053	GLY	-	expression tag	UNP Q9FZA0
M	1052	MET	-	initiating methionine	UNP Q9FZA0
M	1053	GLY	-	expression tag	UNP Q9FZA0
N	1052	MET	-	initiating methionine	UNP Q9FZA0
N	1053	GLY	-	expression tag	UNP Q9FZA0
O	1052	MET	-	initiating methionine	UNP Q9FZA0
O	1053	GLY	-	expression tag	UNP Q9FZA0
P	1052	MET	-	initiating methionine	UNP Q9FZA0
P	1053	GLY	-	expression tag	UNP Q9FZA0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	R	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	T	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	V	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	a	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	f	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

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

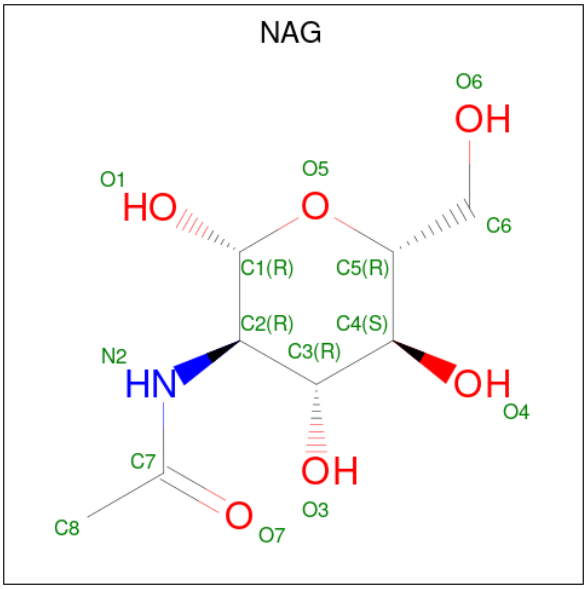
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	U	2	Total C N O 28 16 2 10	0	0	0
5	W	2	Total C N O 28 16 2 10	0	0	0
5	Y	2	Total C N O 28 16 2 10	0	0	0
5	c	2	Total C N O 28 16 2 10	0	0	0
5	d	2	Total C N O 28 16 2 10	0	0	0
5	e	2	Total C N O 28 16 2 10	0	0	0

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

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		

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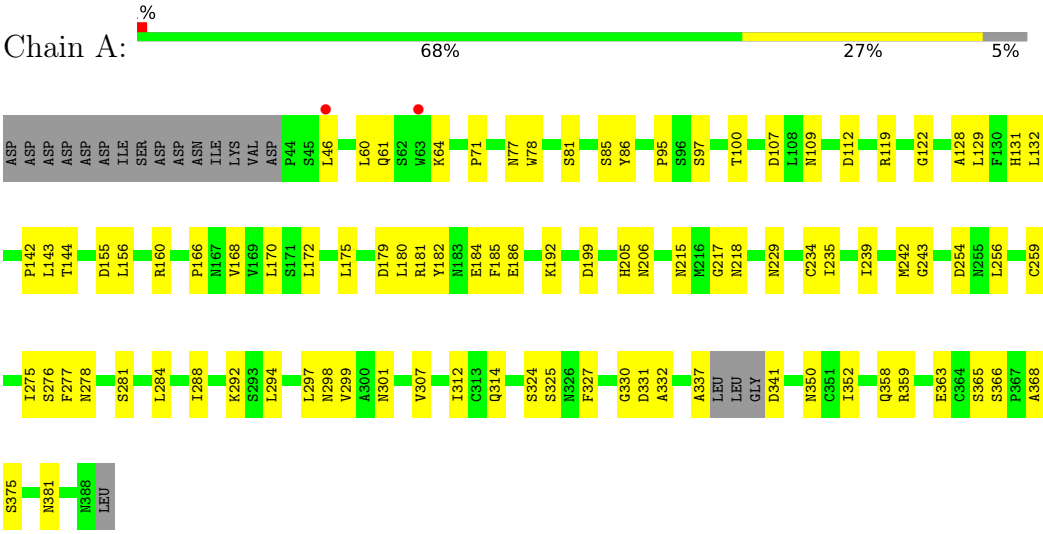
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	H	1	Total	C	N	O	0	0
			14	8	1	5		

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.

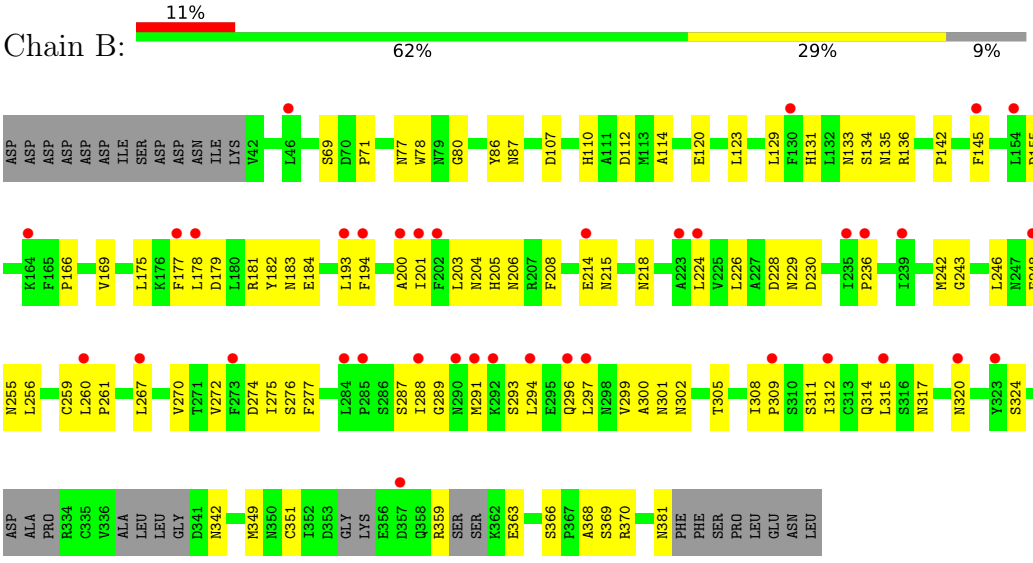
• Molecule 1: Leucine-rich repeat extensin-like protein 2

Chain A:



• Molecule 1: Leucine-rich repeat extensin-like protein 2

Chain B:

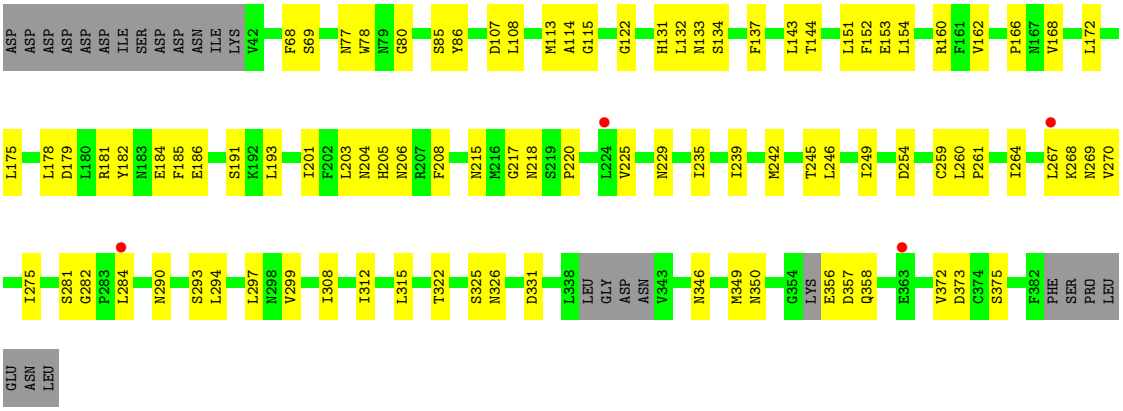


• Molecule 1: Leucine-rich repeat extensin-like protein 2

Chain C:

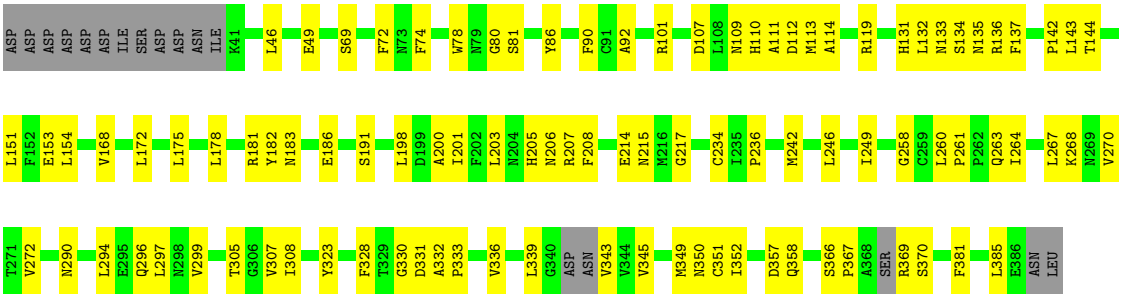
• Molecule 1: Leucine-rich repeat extensin-like protein 2

Chain D:



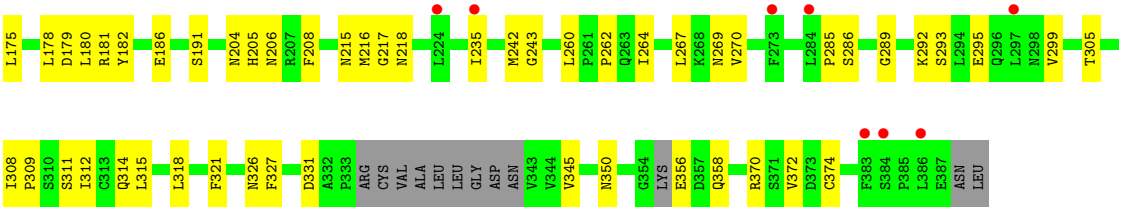
• Molecule 1: Leucine-rich repeat extensin-like protein 2

Chain E:



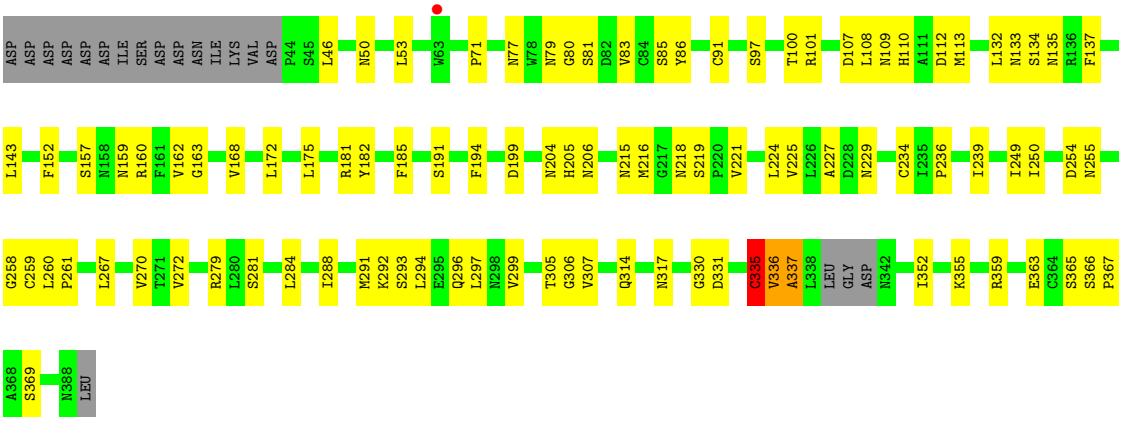
• Molecule 1: Leucine-rich repeat extensin-like protein 2

Chain F:



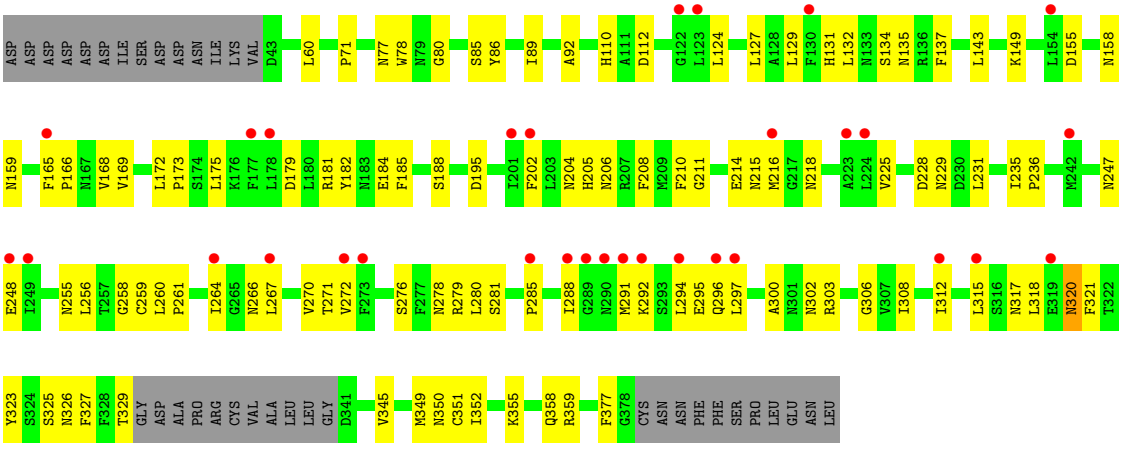
• Molecule 1: Leucine-rich repeat extensin-like protein 2

Chain G:



• Molecule 1: Leucine-rich repeat extensin-like protein 2

Chain H:

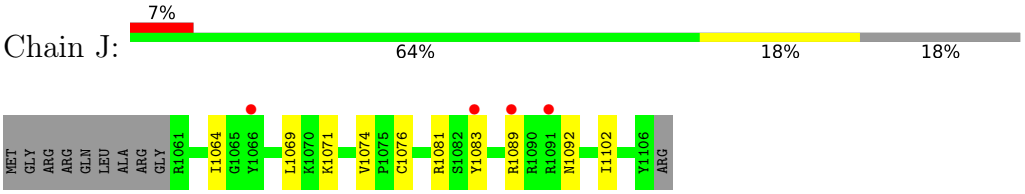


• Molecule 2: Protein RALF-like 4

Chain I:

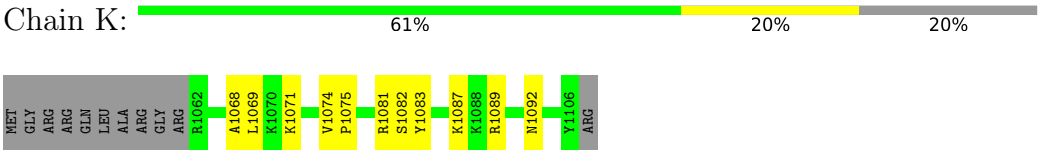
• Molecule 2: Protein RALF-like 4

Chain J:



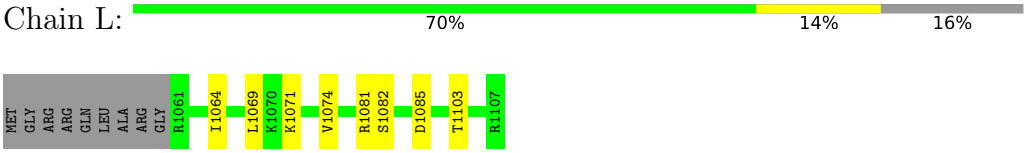
• Molecule 2: Protein RALF-like 4

Chain K:



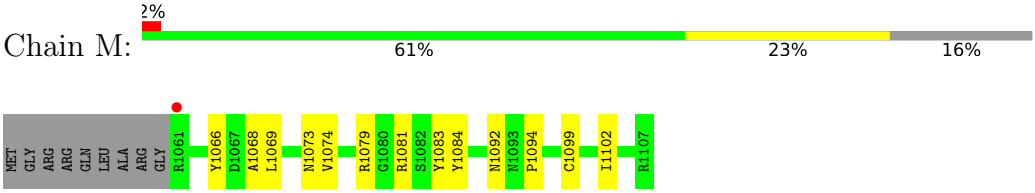
• Molecule 2: Protein RALF-like 4

Chain L:



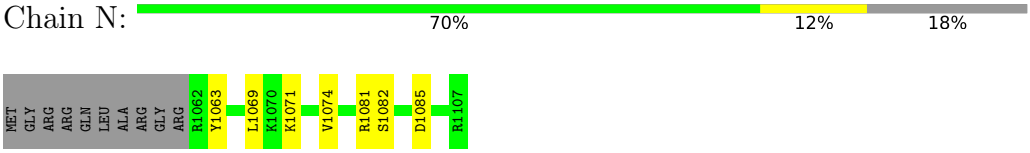
• Molecule 2: Protein RALF-like 4

Chain M:



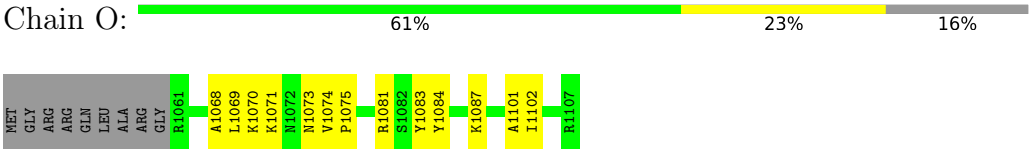
• Molecule 2: Protein RALF-like 4

Chain N:



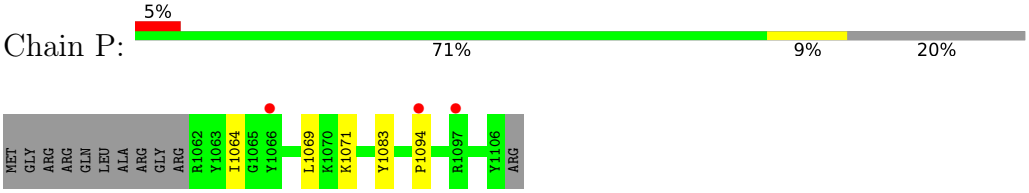
• Molecule 2: Protein RALF-like 4

Chain O:



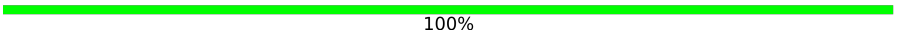
• Molecule 2: Protein RALF-like 4

Chain P:



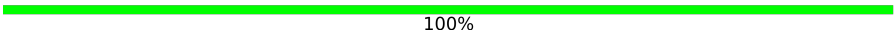
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



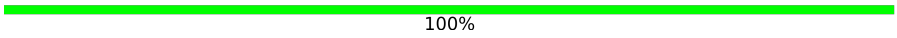
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



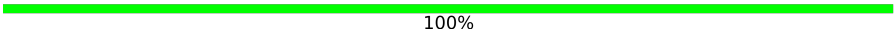
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



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

Chain V:



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

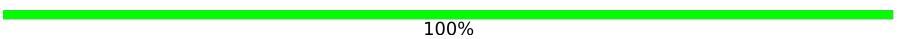
Chain X:

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

Chain a:

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

Chain f:

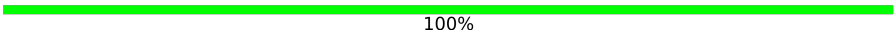


• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

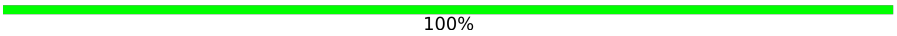
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



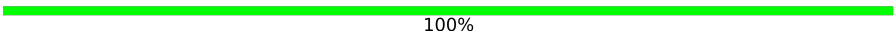
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



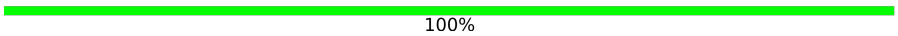
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



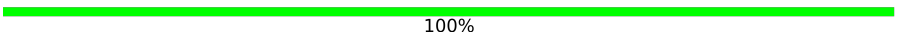
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



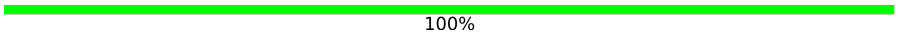
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



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

Chain e:



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

Chain Z:

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

Chain b:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	119.99Å 119.99Å 305.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.99 – 3.20 94.39 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (59.99-3.20) 99.9 (94.39-3.20)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.19Å)	Xtriage
Refinement program	PHENIX v1.14	Depositor
R, R_{free}	0.227 , 0.274 0.223 , 0.272	Depositor DCC
R_{free} test set	3562 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	78.6	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	24293	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/2675	0.50	0/3629
1	B	0.26	0/2567	0.51	0/3480
1	C	0.27	0/2695	0.52	0/3655
1	D	0.26	0/2612	0.49	0/3545
1	E	0.26	0/2683	0.51	1/3642 (0.0%)
1	F	0.27	0/2631	0.50	0/3570
1	G	0.27	0/2675	0.48	0/3629
1	H	0.26	0/2542	0.52	0/3449
2	I	0.27	0/378	0.45	0/509
2	J	0.31	0/381	0.48	0/510
2	K	0.34	0/361	0.50	0/486
2	L	0.25	0/372	0.41	0/502
2	M	0.26	0/379	0.45	0/510
2	N	0.25	0/367	0.42	0/495
2	O	0.26	0/372	0.45	0/502
2	P	0.27	0/350	0.42	0/474
All	All	0.27	0/24040	0.50	1/32587 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	351	CYS	CA-CB-SG	5.43	123.78	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	335	CYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2616	0	2525	80	0
1	B	2515	0	2428	87	1
1	C	2636	0	2560	75	1
1	D	2557	0	2467	69	0
1	E	2624	0	2536	74	0
1	F	2573	0	2483	60	0
1	G	2616	0	2532	69	0
1	H	2487	0	2407	85	0
2	I	370	0	331	17	0
2	J	373	0	353	14	0
2	K	353	0	319	11	0
2	L	364	0	320	8	0
2	M	371	0	334	16	0
2	N	359	0	318	8	0
2	O	364	0	320	12	0
2	P	342	0	294	5	0
3	Q	39	0	34	0	0
3	R	39	0	34	0	0
3	T	39	0	34	0	0
3	V	39	0	34	0	0
3	X	39	0	34	1	0
3	a	39	0	34	0	0
3	f	39	0	34	0	0
4	S	50	0	43	0	0
5	U	28	0	25	0	0
5	W	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	28	0	25	0	0
5	c	28	0	25	0	0
5	d	28	0	25	0	0
5	e	28	0	25	0	0
6	Z	50	0	43	0	0
6	b	50	0	43	0	0
7	A	42	0	39	0	0
7	D	28	0	26	0	0
7	E	42	0	39	0	0
7	F	28	0	26	0	0
7	G	28	0	26	0	0
7	H	14	0	13	0	0
All	All	24293	0	23213	615	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 13.

The worst 5 of 615 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:D:282:GLY:HA2	1:D:372:VAL:HG21	1.41	1.01
1:H:208:PHE:HB2	1:H:229:ASN:HD21	1.24	0.97
1:G:204:ASN:HD21	1:G:225:VAL:HG12	1.31	0.95
1:B:351:CYS:SG	1:B:359:ARG:NH2	2.43	0.92
1:E:111:ALA:O	1:E:135:ASN:ND2	2.09	0.86

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:SER:OG	1:C:342:ASN:OD1[4_654]	1.98	0.22

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	338/361 (94%)	305 (90%)	32 (10%)	1 (0%)	41 74
1	B	318/361 (88%)	289 (91%)	29 (9%)	0	100 100
1	C	339/361 (94%)	297 (88%)	40 (12%)	2 (1%)	25 64
1	D	330/361 (91%)	303 (92%)	27 (8%)	0	100 100
1	E	340/361 (94%)	301 (88%)	38 (11%)	1 (0%)	41 74
1	F	330/361 (91%)	305 (92%)	25 (8%)	0	100 100
1	G	338/361 (94%)	301 (89%)	33 (10%)	4 (1%)	13 49
1	H	321/361 (89%)	293 (91%)	28 (9%)	0	100 100
2	I	45/56 (80%)	42 (93%)	3 (7%)	0	100 100
2	J	44/56 (79%)	40 (91%)	4 (9%)	0	100 100
2	K	43/56 (77%)	38 (88%)	5 (12%)	0	100 100
2	L	45/56 (80%)	44 (98%)	1 (2%)	0	100 100
2	M	45/56 (80%)	41 (91%)	4 (9%)	0	100 100
2	N	44/56 (79%)	43 (98%)	1 (2%)	0	100 100
2	O	45/56 (80%)	42 (93%)	3 (7%)	0	100 100
2	P	43/56 (77%)	42 (98%)	1 (2%)	0	100 100
All	All	3008/3336 (90%)	2726 (91%)	274 (9%)	8 (0%)	41 74

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	344	VAL
1	G	336	VAL
1	A	365	SER
1	E	112	ASP
1	G	335	CYS

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	298/320 (93%)	298 (100%)	0	100	100
1	B	288/320 (90%)	287 (100%)	1 (0%)	92	96
1	C	302/320 (94%)	302 (100%)	0	100	100
1	D	291/320 (91%)	291 (100%)	0	100	100
1	E	298/320 (93%)	298 (100%)	0	100	100
1	F	294/320 (92%)	294 (100%)	0	100	100
1	G	298/320 (93%)	298 (100%)	0	100	100
1	H	284/320 (89%)	283 (100%)	1 (0%)	91	95
2	I	35/48 (73%)	35 (100%)	0	100	100
2	J	37/48 (77%)	37 (100%)	0	100	100
2	K	35/48 (73%)	35 (100%)	0	100	100
2	L	34/48 (71%)	34 (100%)	0	100	100
2	M	36/48 (75%)	36 (100%)	0	100	100
2	N	34/48 (71%)	34 (100%)	0	100	100
2	O	34/48 (71%)	34 (100%)	0	100	100
2	P	32/48 (67%)	32 (100%)	0	100	100
All	All	2630/2944 (89%)	2628 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	342	ASN
1	H	320	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	77	ASN
1	G	204	ASN
1	F	218	ASN
1	F	350	ASN
1	G	317	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

45 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	Q	1	1,3	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	Q	2	3	14,14,15	0.21	0	17,19,21	0.56	0
3	BMA	Q	3	3	11,11,12	0.69	0	15,15,17	0.75	0
3	NAG	R	1	1,3	14,14,15	0.32	0	17,19,21	0.52	0
3	NAG	R	2	3	14,14,15	0.28	0	17,19,21	0.40	0
3	BMA	R	3	3	11,11,12	0.65	0	15,15,17	0.86	0
4	NAG	S	1	4,1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	S	2	4	14,14,15	0.19	0	17,19,21	0.44	0
4	BMA	S	3	4	11,11,12	0.75	0	15,15,17	0.88	0
4	MAN	S	4	4	11,11,12	0.76	0	15,15,17	0.94	1 (6%)
3	NAG	T	1	1,3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	T	2	3	14,14,15	0.29	0	17,19,21	0.53	0
3	BMA	T	3	3	11,11,12	0.72	0	15,15,17	0.72	0
5	NAG	U	1	5,1	14,14,15	0.30	0	17,19,21	0.42	0
5	NAG	U	2	5	14,14,15	0.24	0	17,19,21	0.39	0
3	NAG	V	1	1,3	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	V	2	3	14,14,15	0.23	0	17,19,21	0.38	0
3	BMA	V	3	3	11,11,12	0.59	0	15,15,17	0.85	0
5	NAG	W	1	5,1	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	W	2	5	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	X	1	1,3	14,14,15	0.38	0	17,19,21	0.58	0
3	NAG	X	2	3	14,14,15	0.23	0	17,19,21	0.51	0
3	BMA	X	3	3	11,11,12	0.62	0	15,15,17	0.83	0
5	NAG	Y	1	5,1	14,14,15	0.41	0	17,19,21	0.42	0
5	NAG	Y	2	5	14,14,15	0.17	0	17,19,21	0.46	0
6	NAG	Z	1	1,6	14,14,15	0.20	0	17,19,21	0.47	0
6	NAG	Z	2	6	14,14,15	0.32	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BMA	Z	3	6	11,11,12	0.67	0	15,15,17	0.70	0
6	MAN	Z	4	6	11,11,12	0.65	0	15,15,17	1.07	2 (13%)
3	NAG	a	1	1,3	14,14,15	0.42	0	17,19,21	0.58	0
3	NAG	a	2	3	14,14,15	0.34	0	17,19,21	0.36	0
3	BMA	a	3	3	11,11,12	0.69	0	15,15,17	1.02	1 (6%)
6	NAG	b	1	1,6	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	b	2	6	14,14,15	0.19	0	17,19,21	0.48	0
6	BMA	b	3	6	11,11,12	0.55	0	15,15,17	0.75	0
6	MAN	b	4	6	11,11,12	0.74	1 (9%)	15,15,17	1.09	2 (13%)
5	NAG	c	1	5,1	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	c	2	5	14,14,15	0.30	0	17,19,21	0.46	0
5	NAG	d	1	5,1	14,14,15	0.24	0	17,19,21	0.53	0
5	NAG	d	2	5	14,14,15	0.29	0	17,19,21	0.58	0
5	NAG	e	1	5,1	14,14,15	0.29	0	17,19,21	0.54	0
5	NAG	e	2	5	14,14,15	0.31	0	17,19,21	0.44	0
3	NAG	f	1	1,3	14,14,15	0.22	0	17,19,21	0.38	0
3	NAG	f	2	3	14,14,15	0.22	0	17,19,21	0.49	0
3	BMA	f	3	3	11,11,12	0.63	0	15,15,17	0.73	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
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	4/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	1/6/23/26	0/1/1/1
3	BMA	R	3	3	-	1/2/19/22	0/1/1/1
4	NAG	S	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	BMA	S	3	4	-	2/2/19/22	0/1/1/1
4	MAN	S	4	4	-	2/2/19/22	0/1/1/1
3	NAG	T	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
5	NAG	U	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	b	4	MAN	C1-C2	2.04	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Z	4	MAN	C1-O5-C5	2.75	115.92	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	b	4	MAN	C1-O5-C5	2.60	115.71	112.19
6	Z	4	MAN	O2-C2-C3	-2.19	105.75	110.14
4	S	4	MAN	O2-C2-C3	-2.10	105.92	110.14
6	b	4	MAN	O2-C2-C3	-2.07	105.98	110.14

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	a	1	NAG	O5-C5-C6-O6
4	S	3	BMA	C4-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	f	3	BMA	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6

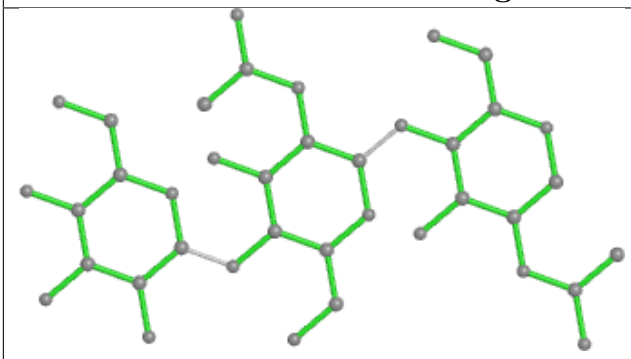
There are no ring outliers.

1 monomer is involved in 1 short contact:

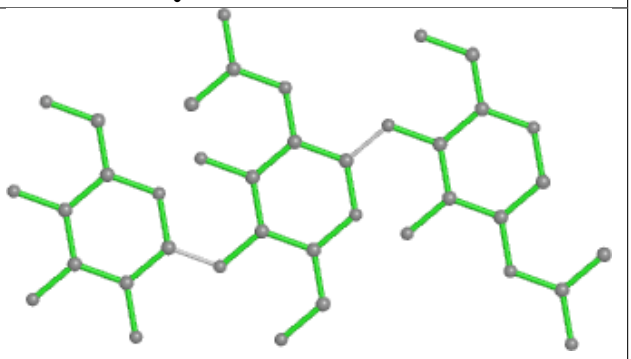
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	2	NAG	1	0

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

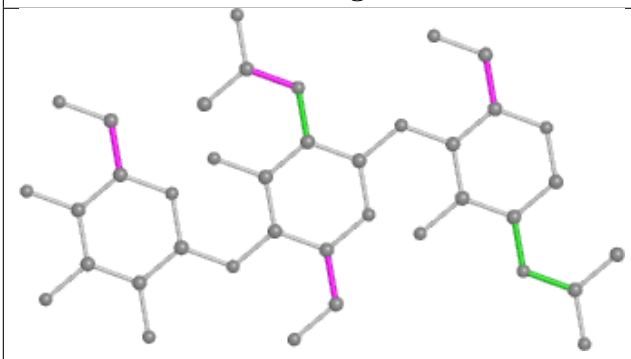
Oligosaccharide Chain Q



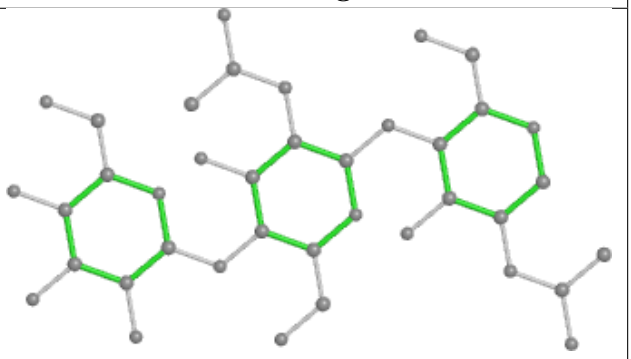
Bond lengths



Bond angles

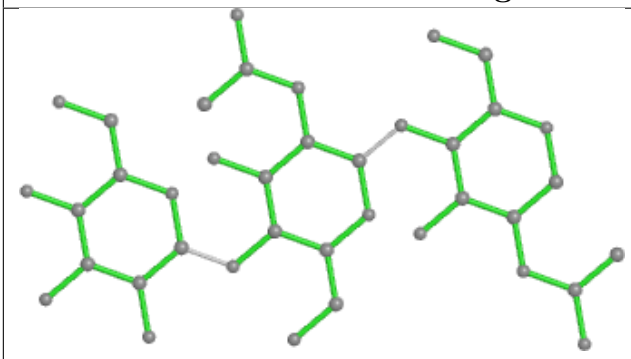


Torsions

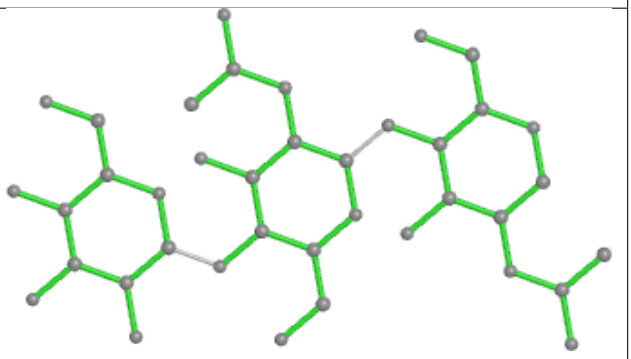


Rings

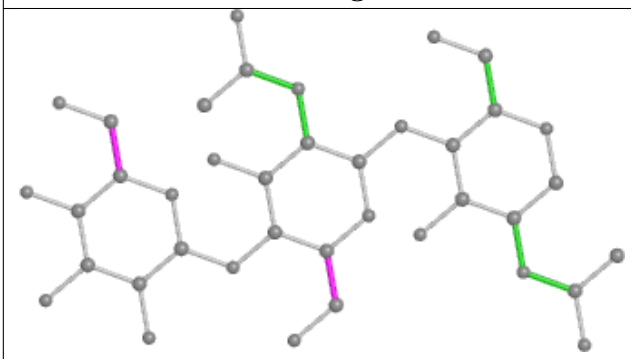
Oligosaccharide Chain R



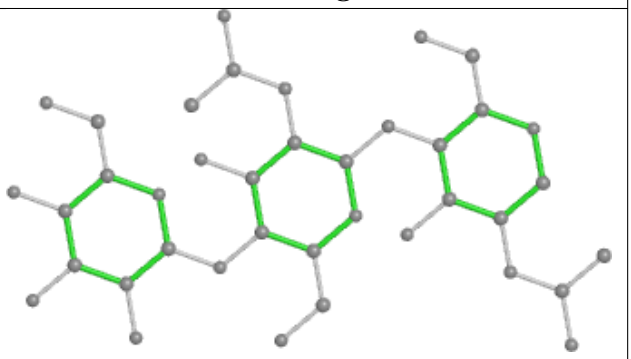
Bond lengths



Bond angles

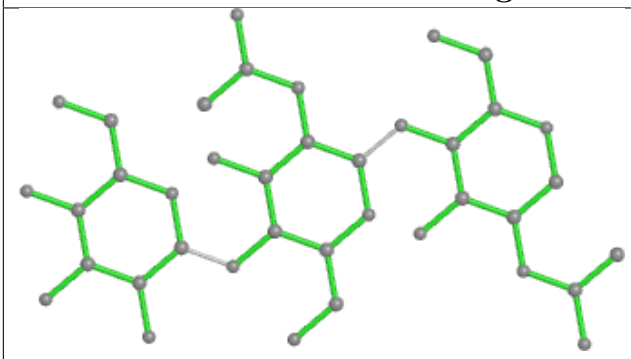


Torsions

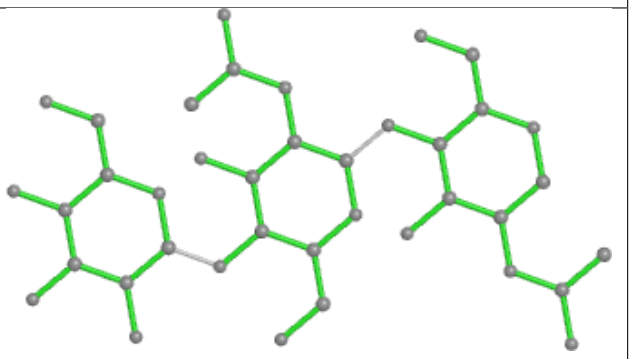


Rings

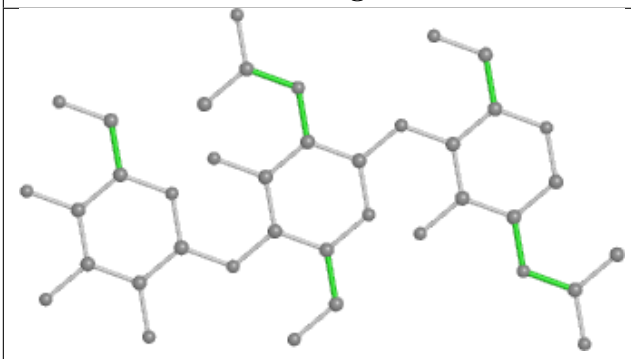
Oligosaccharide Chain T



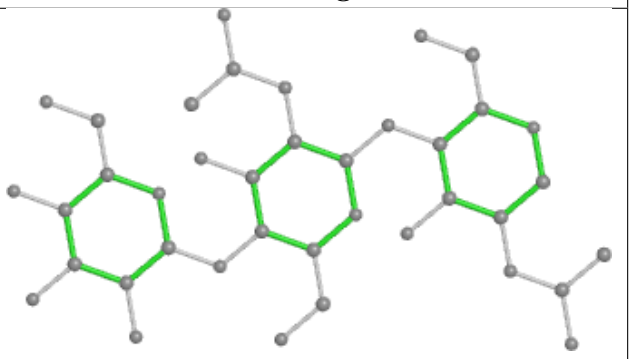
Bond lengths



Bond angles

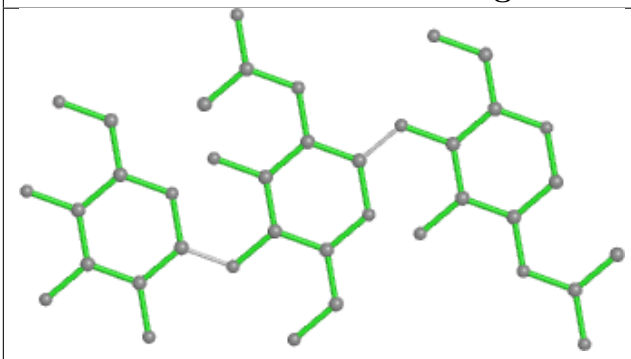


Torsions

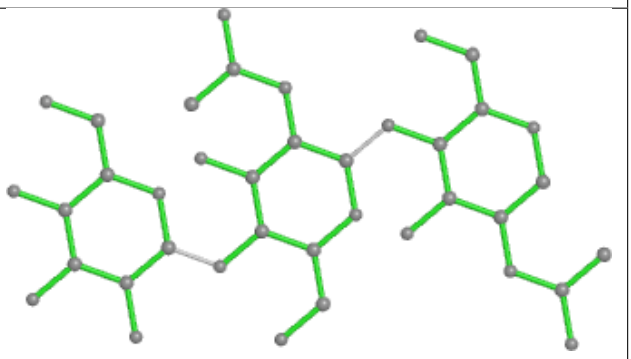


Rings

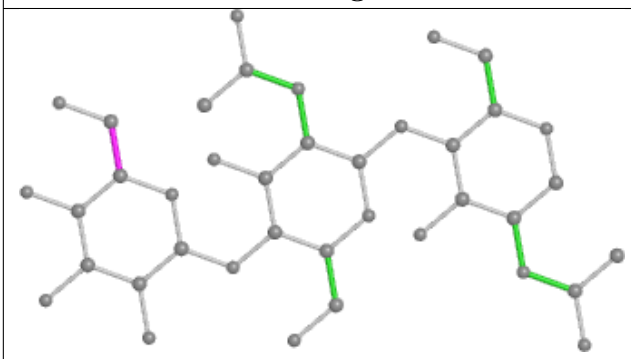
Oligosaccharide Chain V



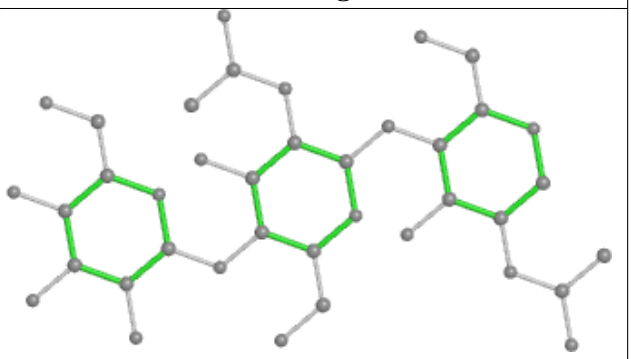
Bond lengths



Bond angles

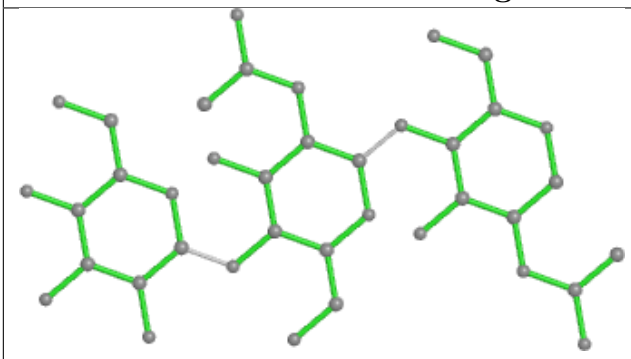


Torsions

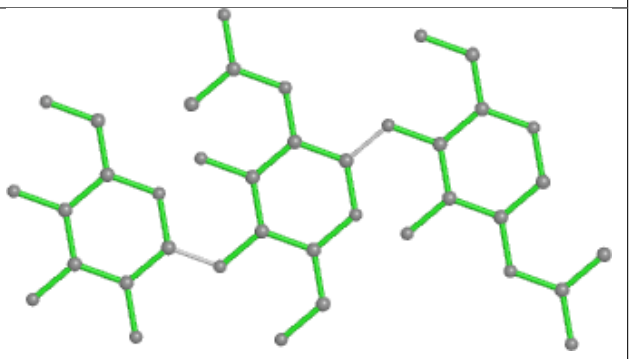


Rings

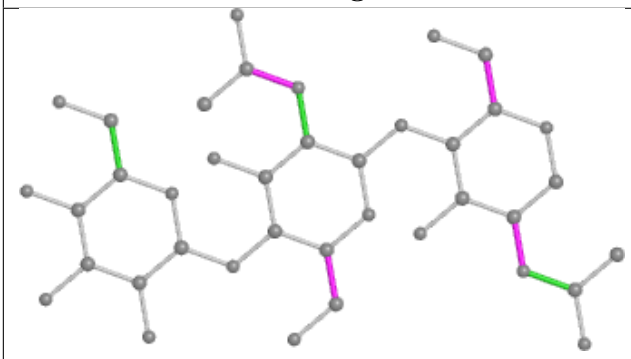
Oligosaccharide Chain X



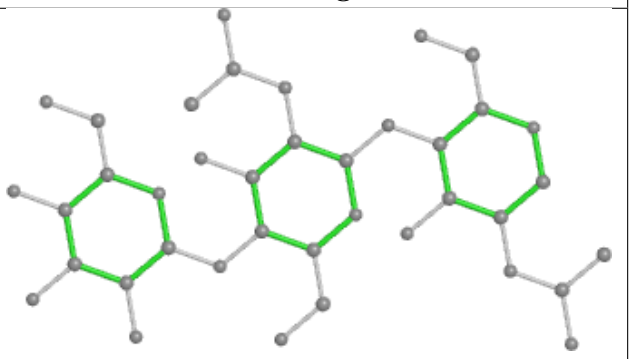
Bond lengths



Bond angles

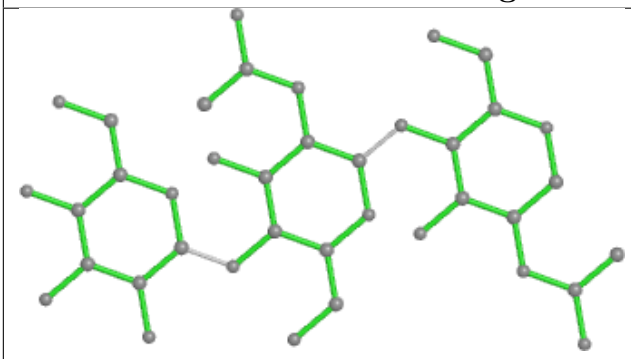


Torsions

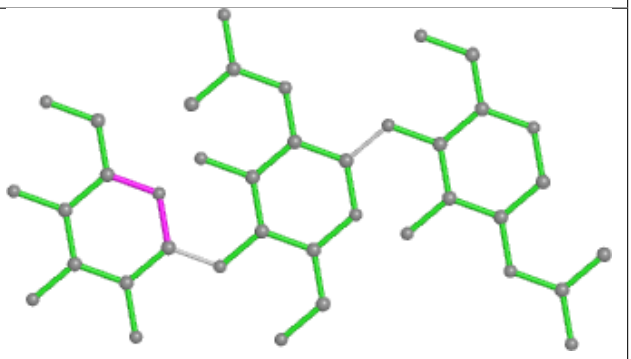


Rings

Oligosaccharide Chain a



Bond lengths



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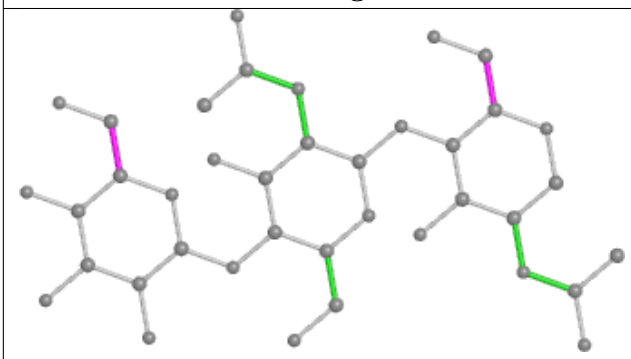

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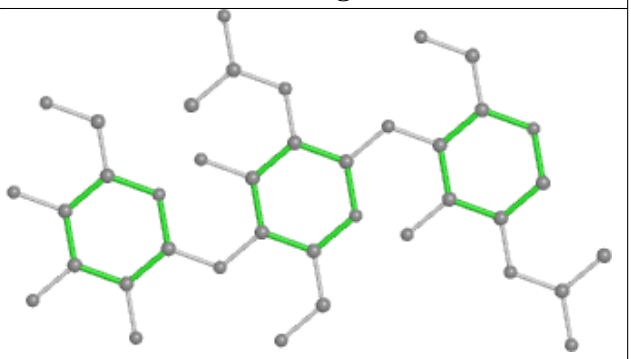
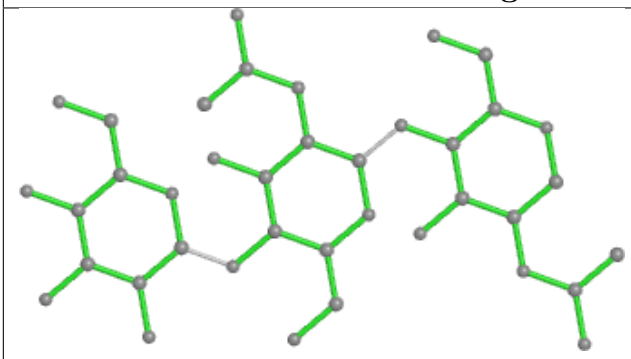
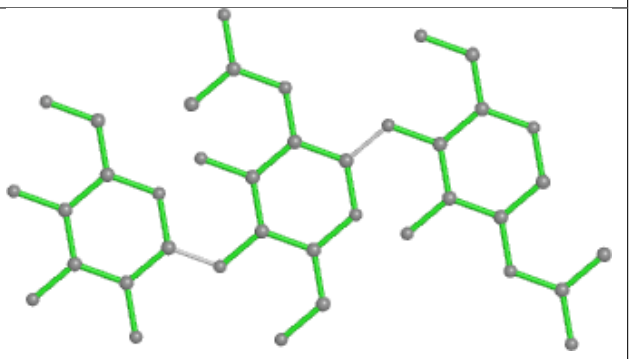


Rings

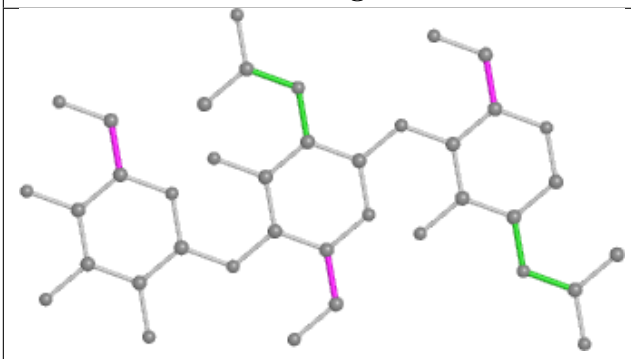
Oligosaccharide Chain f



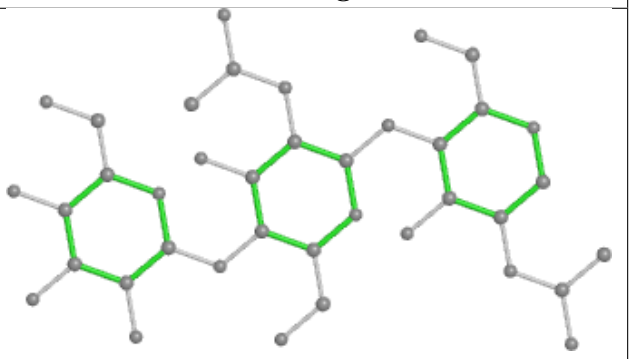
Bond lengths



Bond angles

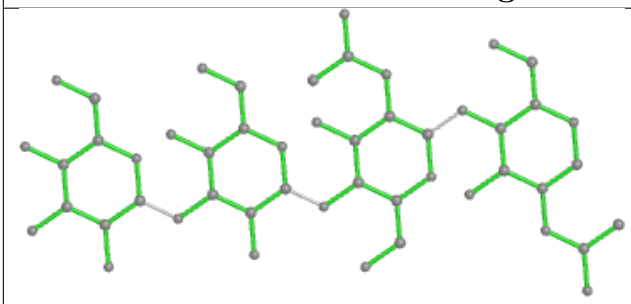


Torsions

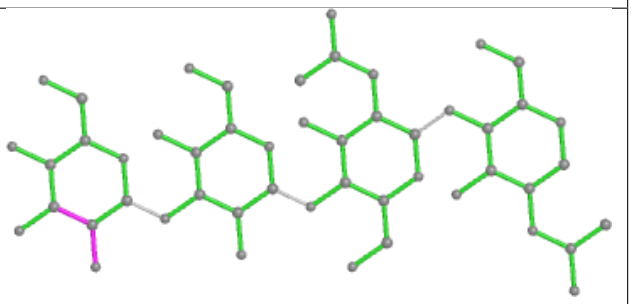


Rings

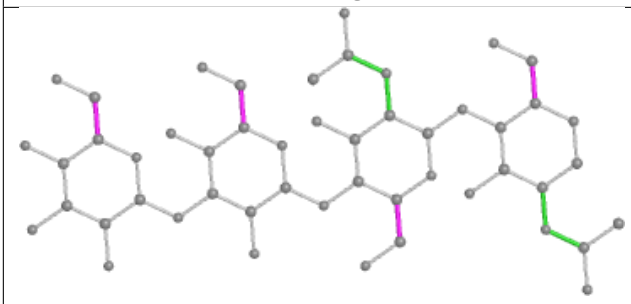
Oligosaccharide Chain S



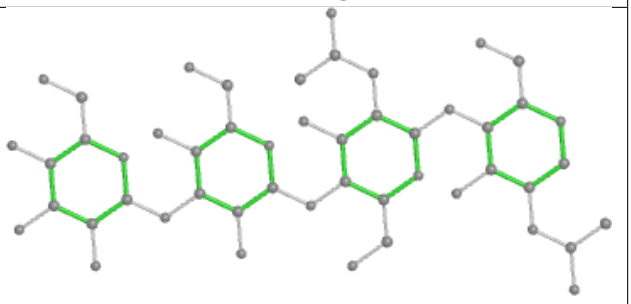
Bond lengths



Bond angles

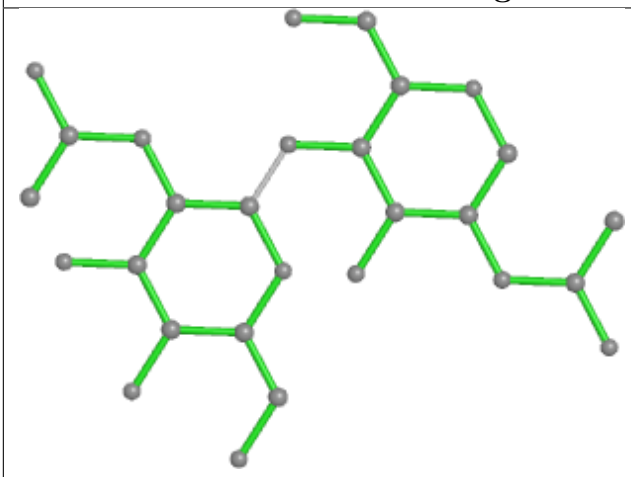


Torsions

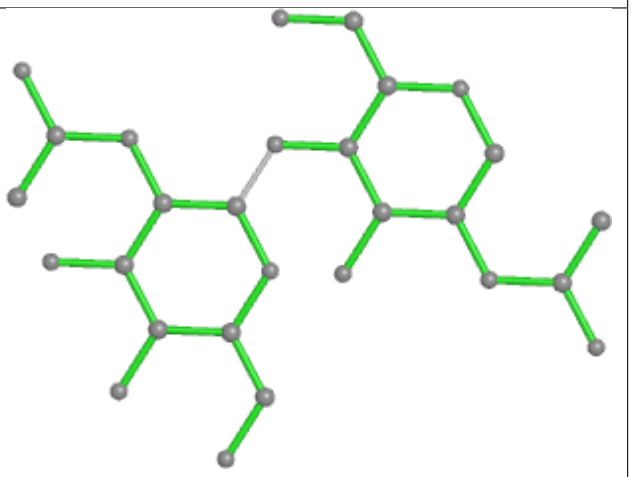


Rings

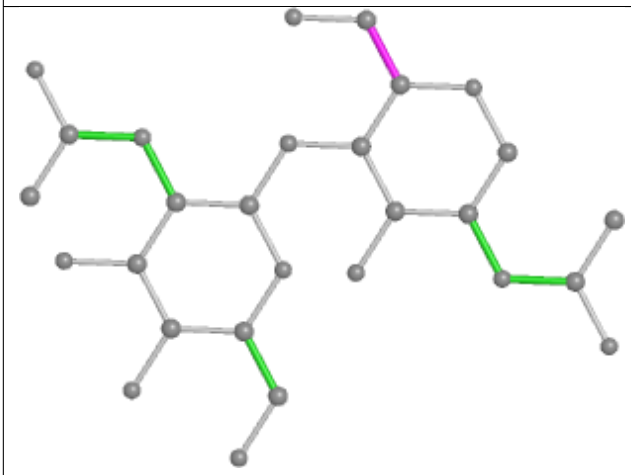
Oligosaccharide Chain U



Bond lengths



Bond angles



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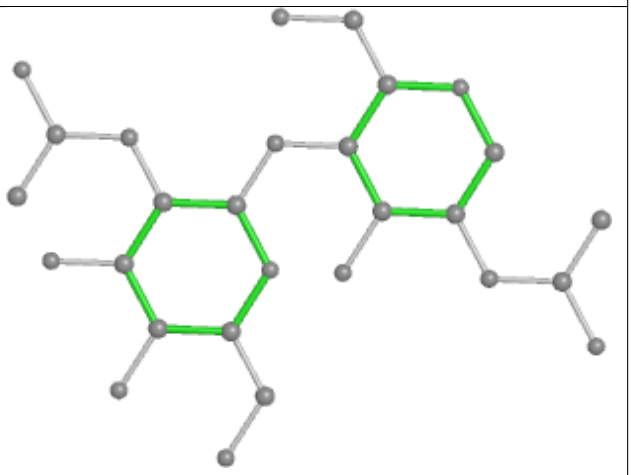
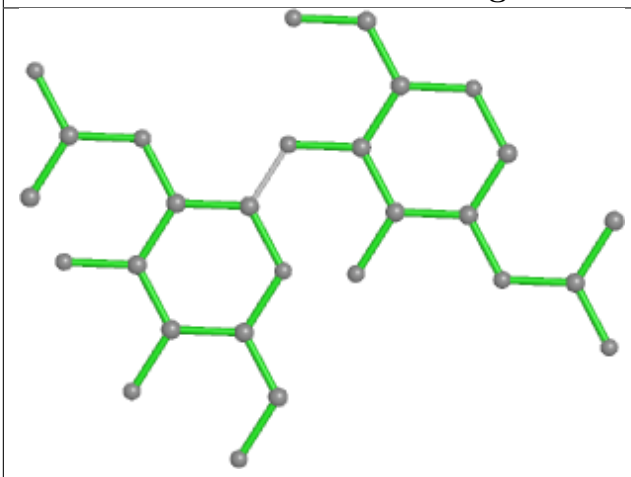
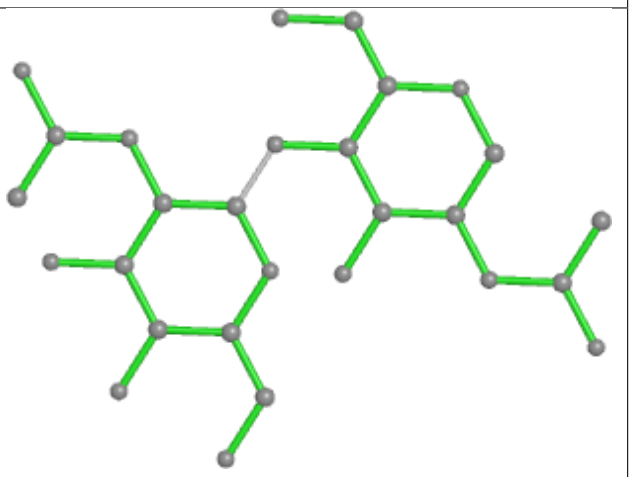


Rings

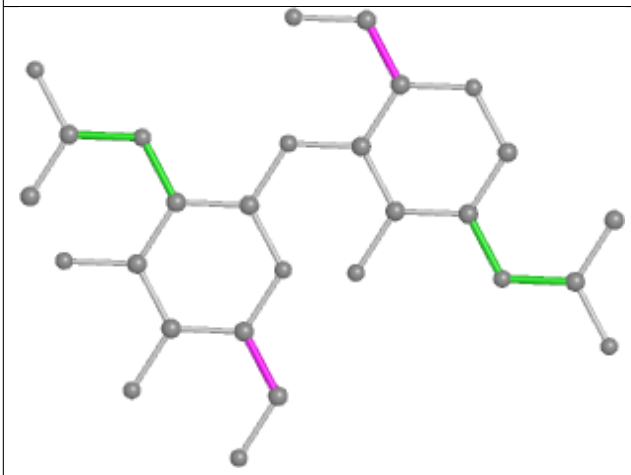
Oligosaccharide Chain W



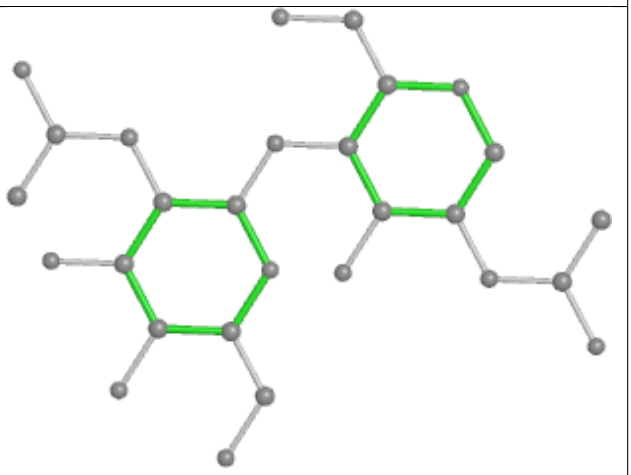
Bond lengths



Bond angles

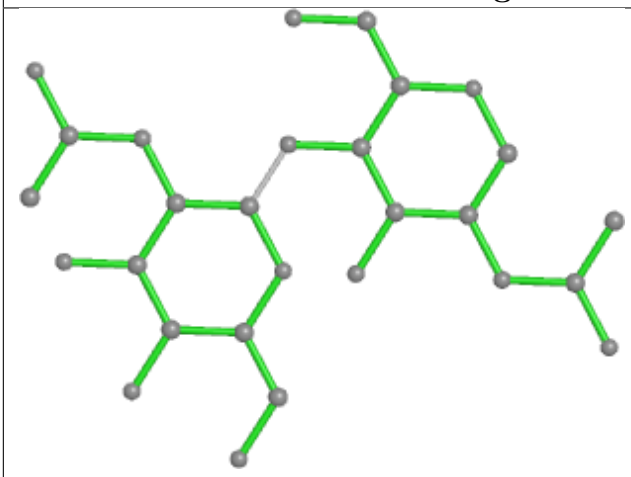


Torsions

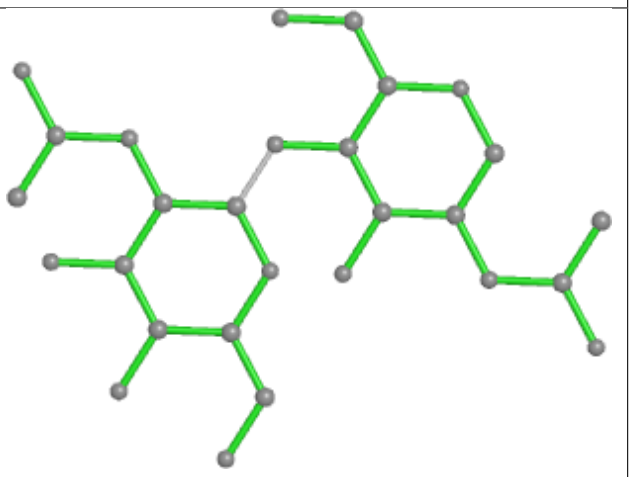


Rings

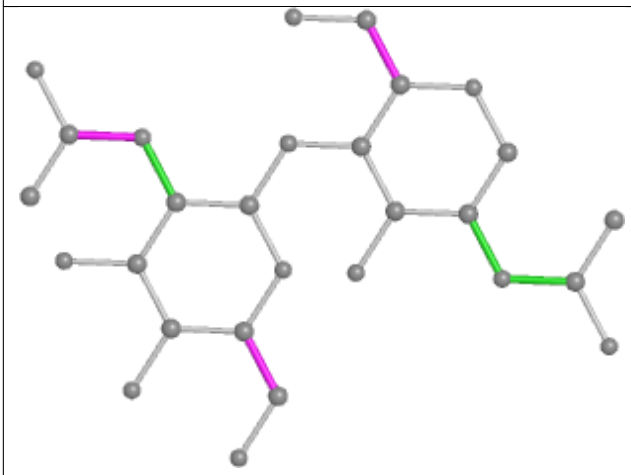
Oligosaccharide Chain Y



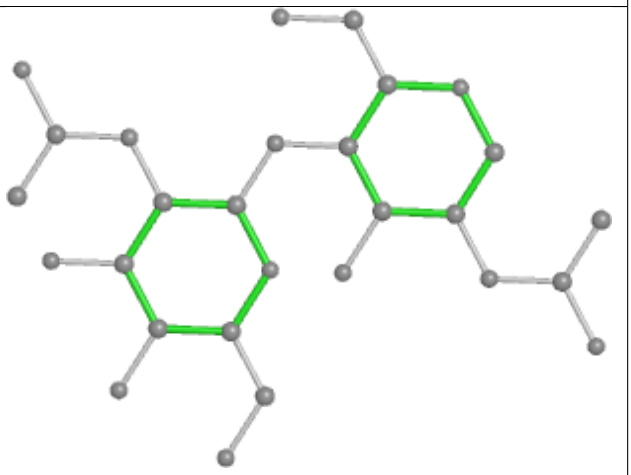
Bond lengths



Bond angles

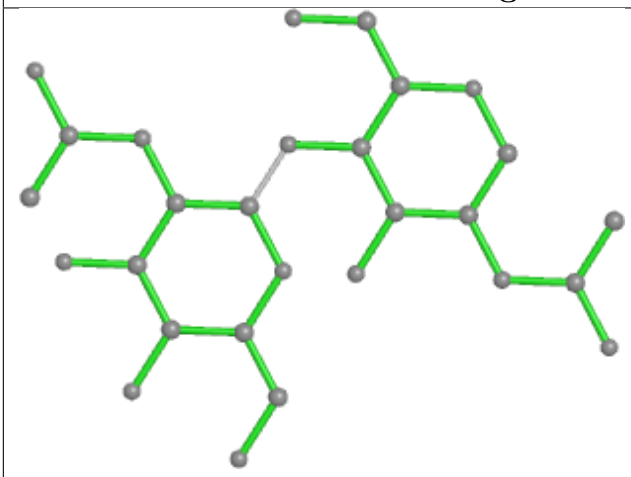


Torsions

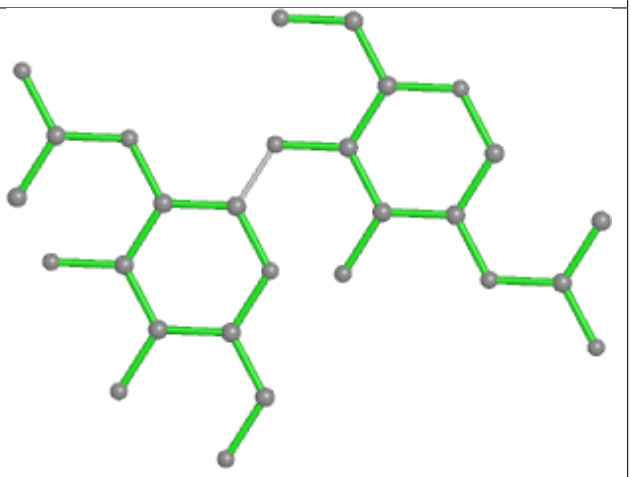


Rings

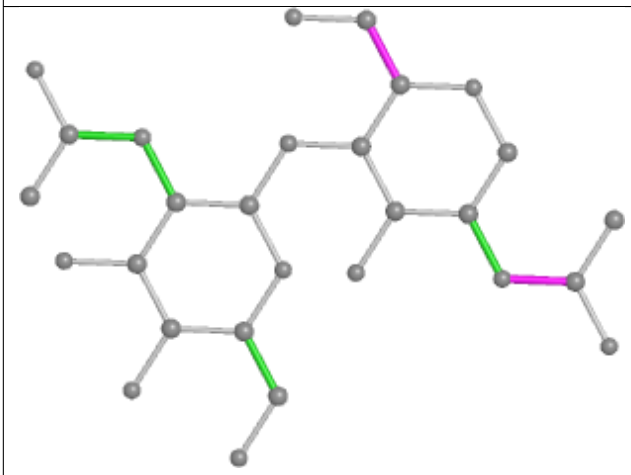
Oligosaccharide Chain c



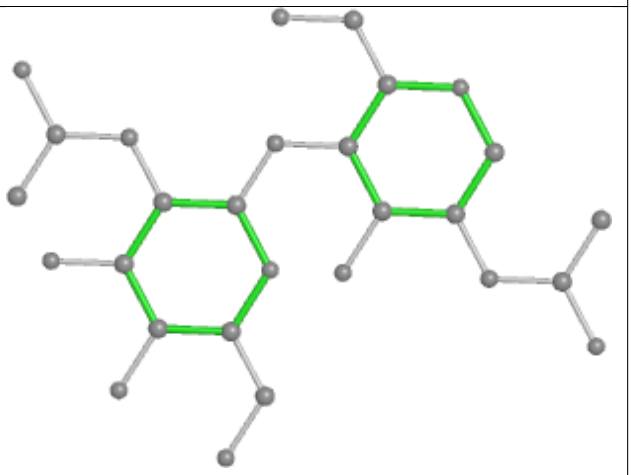
Bond lengths



Bond angles

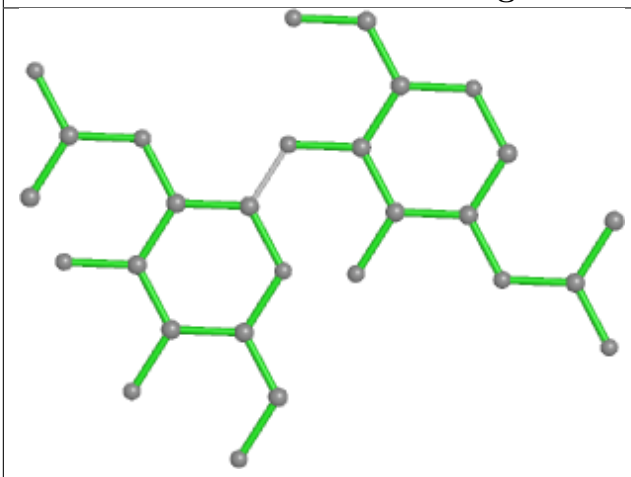


Torsions

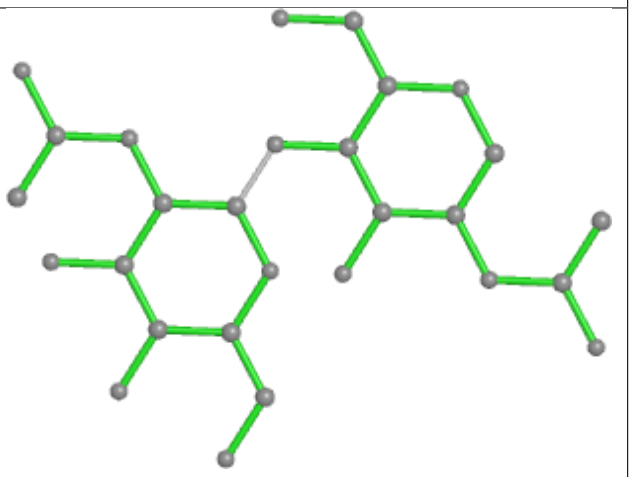


Rings

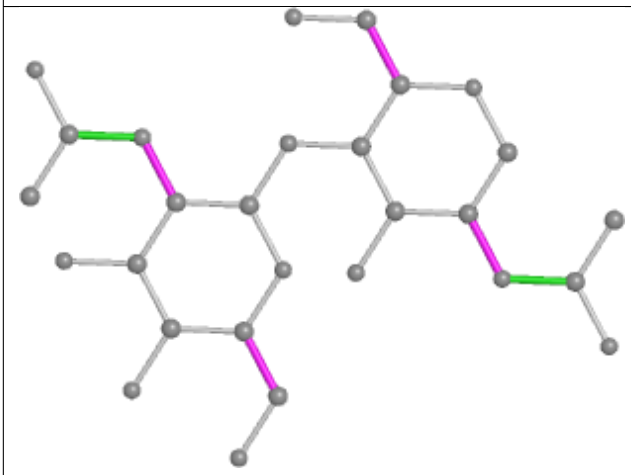
Oligosaccharide Chain d



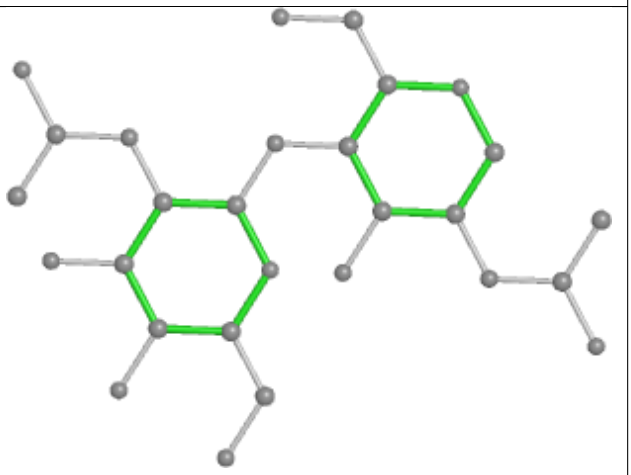
Bond lengths



Bond angles

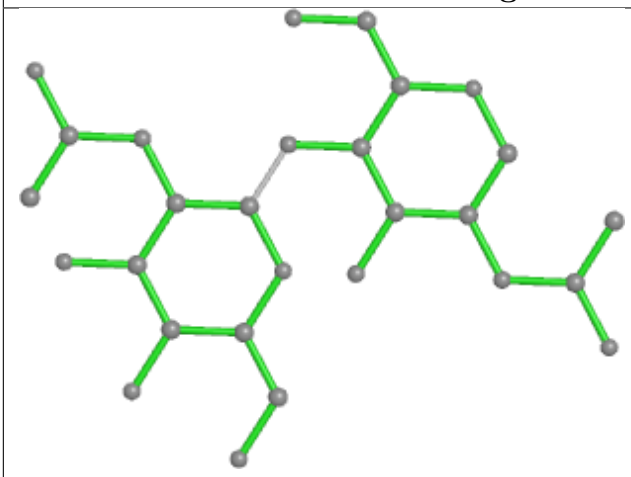


Torsions

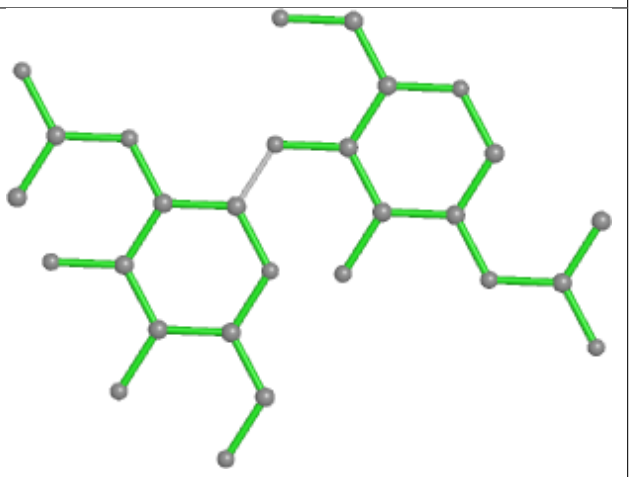


Rings

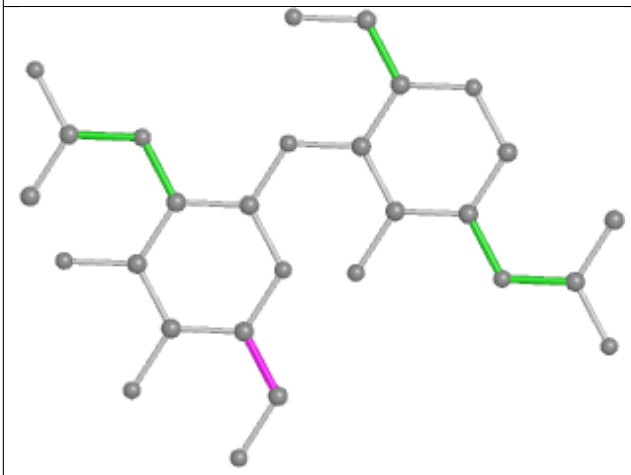
Oligosaccharide Chain e



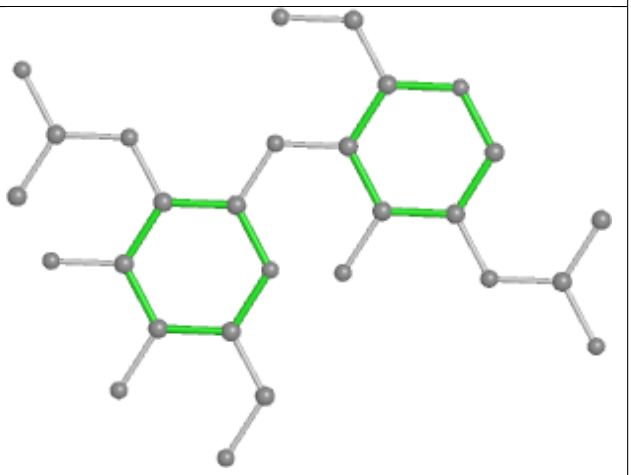
Bond lengths



Bond angles

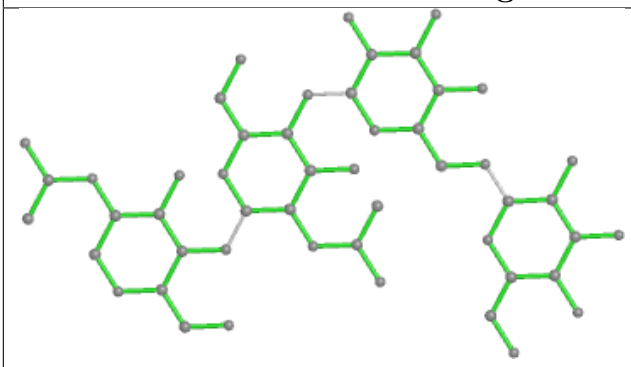


Torsions

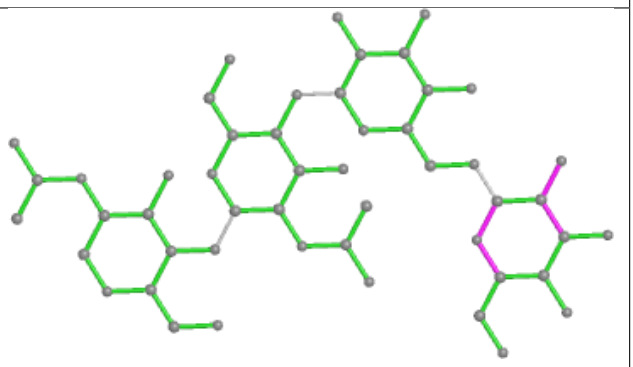


Rings

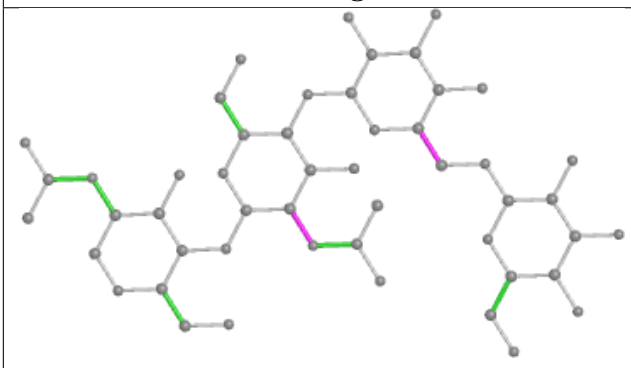
Oligosaccharide Chain Z



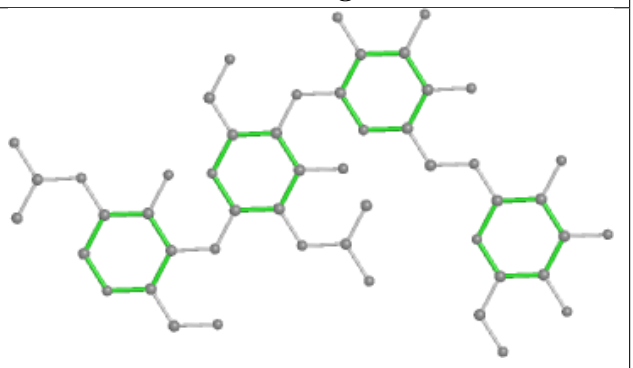
Bond lengths



Bond angles

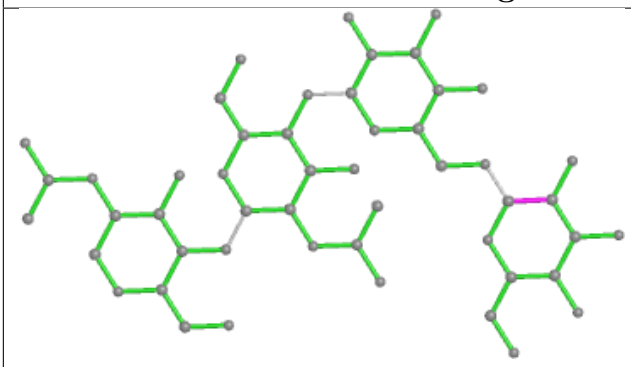


Torsions

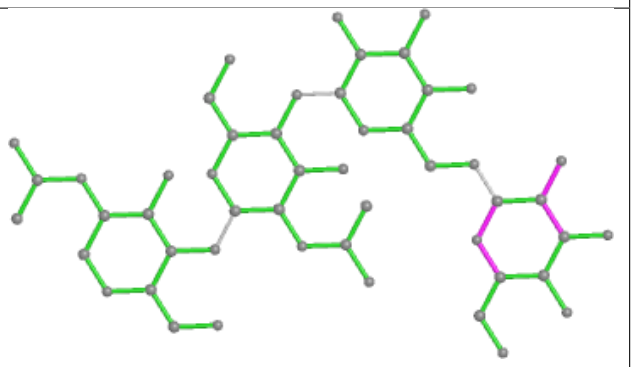


Rings

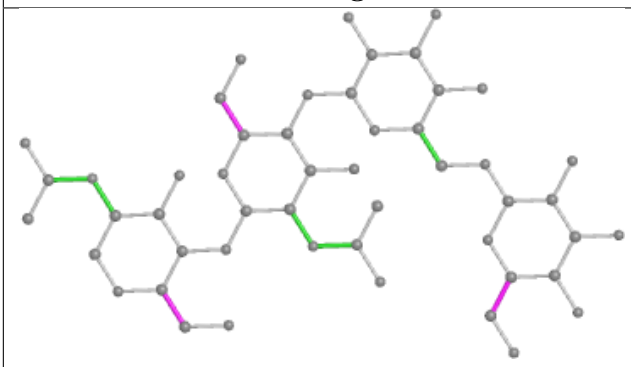
Oligosaccharide Chain b



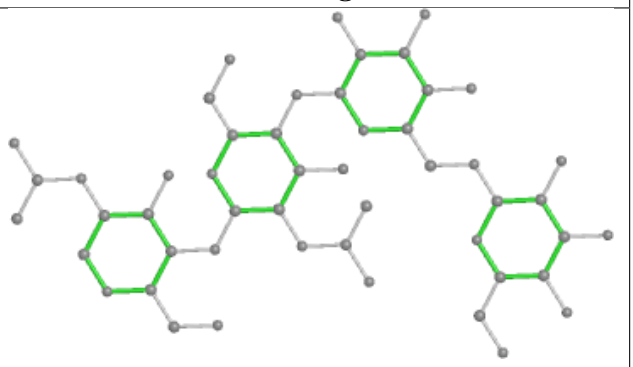
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	H	404	1	14,14,15	0.27	0	17,19,21	0.48	0
7	NAG	G	408	1	14,14,15	0.34	0	17,19,21	0.45	0
7	NAG	D	405	1	14,14,15	0.31	0	17,19,21	0.53	0
7	NAG	A	404	1	14,14,15	0.63	1 (7%)	17,19,21	0.99	1 (5%)
7	NAG	G	405	1	14,14,15	0.35	0	17,19,21	0.61	0
7	NAG	E	410	1	14,14,15	0.28	0	17,19,21	0.48	0
7	NAG	F	405	1	14,14,15	0.30	0	17,19,21	0.44	0
7	NAG	E	406	1	14,14,15	0.26	0	17,19,21	0.41	0
7	NAG	A	405	1	14,14,15	0.37	0	17,19,21	0.60	0
7	NAG	D	404	1	14,14,15	0.27	0	17,19,21	0.39	0
7	NAG	E	405	1	14,14,15	0.35	0	17,19,21	0.52	0
7	NAG	A	409	1	14,14,15	0.37	0	17,19,21	0.48	0
7	NAG	F	406	1	14,14,15	0.40	0	17,19,21	0.47	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
7	NAG	H	404	1	-	0/6/23/26	0/1/1/1
7	NAG	G	408	1	-	1/6/23/26	0/1/1/1
7	NAG	D	405	1	-	1/6/23/26	0/1/1/1
7	NAG	A	404	1	-	2/6/23/26	0/1/1/1
7	NAG	G	405	1	-	3/6/23/26	0/1/1/1
7	NAG	E	410	1	-	1/6/23/26	0/1/1/1
7	NAG	F	405	1	-	3/6/23/26	0/1/1/1
7	NAG	E	406	1	-	0/6/23/26	0/1/1/1
7	NAG	A	405	1	-	3/6/23/26	0/1/1/1
7	NAG	D	404	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	E	405	1	-	2/6/23/26	0/1/1/1
7	NAG	A	409	1	-	1/6/23/26	0/1/1/1
7	NAG	F	406	1	-	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)
7	A	404	NAG	C1-C2	2.07	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	404	NAG	C1-O5-C5	3.54	116.99	112.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	404	NAG	O5-C5-C6-O6
7	A	405	NAG	O5-C5-C6-O6
7	E	405	NAG	O5-C5-C6-O6
7	G	405	NAG	O5-C5-C6-O6
7	F	405	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	342/361 (94%)	0.13	3 (0%) 84 75	39, 71, 118, 197	0
1	B	328/361 (90%)	0.44	38 (11%) 4 3	64, 122, 174, 233	0
1	C	343/361 (95%)	0.08	3 (0%) 84 75	38, 69, 117, 178	0
1	D	336/361 (93%)	0.11	4 (1%) 79 67	32, 82, 160, 196	0
1	E	344/361 (95%)	0.06	0 100 100	34, 67, 113, 175	0
1	F	336/361 (93%)	0.15	8 (2%) 59 44	33, 82, 171, 241	0
1	G	342/361 (94%)	0.10	1 (0%) 94 92	36, 72, 115, 208	0
1	H	325/361 (90%)	0.44	31 (9%) 8 4	69, 123, 188, 257	0
2	I	47/56 (83%)	-0.17	0 100 100	46, 73, 112, 127	0
2	J	46/56 (82%)	0.60	4 (8%) 10 5	93, 134, 172, 265	0
2	K	45/56 (80%)	-0.08	0 100 100	57, 88, 126, 150	0
2	L	47/56 (83%)	0.19	0 100 100	55, 78, 111, 120	0
2	M	47/56 (83%)	-0.04	1 (2%) 63 49	61, 93, 136, 170	0
2	N	46/56 (82%)	-0.06	0 100 100	52, 76, 99, 131	0
2	O	47/56 (83%)	-0.20	0 100 100	50, 74, 117, 139	0
2	P	45/56 (80%)	0.38	3 (6%) 17 10	93, 125, 171, 192	0
All	All	3066/3336 (91%)	0.17	96 (3%) 49 32	32, 85, 162, 265	0

The worst 5 of 96 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	288	ILE	6.3
1	H	291	MET	5.5
1	B	291	MET	5.0
1	H	248	GLU	4.8
1	H	290	ASN	4.8

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
3	BMA	R	3	11/12	0.68	0.25	144,152,167,173	0
6	BMA	Z	3	11/12	0.75	0.16	129,135,151,153	0
5	NAG	W	2	14/15	0.79	0.20	122,150,158,161	0
3	BMA	a	3	11/12	0.79	0.17	110,140,151,152	0
4	BMA	S	3	11/12	0.80	0.14	64,111,130,145	0
3	NAG	V	2	14/15	0.81	0.34	125,148,154,155	0
3	BMA	T	3	11/12	0.83	0.17	69,123,139,139	0
5	NAG	e	2	14/15	0.84	0.23	88,103,110,111	0
3	BMA	V	3	11/12	0.85	0.20	106,142,150,152	0
3	NAG	V	1	14/15	0.85	0.36	131,147,157,157	0
4	MAN	S	4	11/12	0.86	0.18	136,150,155,157	0
3	NAG	R	2	14/15	0.86	0.26	84,110,124,136	0
3	BMA	f	3	11/12	0.86	0.15	41,91,116,121	0
3	BMA	Q	3	11/12	0.86	0.15	118,134,143,149	0
6	BMA	b	3	11/12	0.86	0.18	114,126,139,150	0
5	NAG	c	2	14/15	0.87	0.28	118,138,150,153	0
5	NAG	Y	2	14/15	0.87	0.16	132,148,160,166	0
5	NAG	d	1	14/15	0.88	0.20	117,138,147,152	0
3	NAG	Q	1	14/15	0.88	0.21	97,114,126,134	0
6	NAG	Z	2	14/15	0.88	0.23	129,149,161,163	0
3	NAG	R	1	14/15	0.88	0.33	98,118,129,135	0
5	NAG	W	1	14/15	0.88	0.14	121,135,146,147	0
3	BMA	X	3	11/12	0.89	0.15	94,105,111,117	0
6	MAN	b	4	11/12	0.89	0.20	122,138,145,148	0
3	NAG	a	2	14/15	0.90	0.33	102,129,136,138	0
5	NAG	U	2	14/15	0.90	0.28	122,135,145,146	0
4	NAG	S	2	14/15	0.90	0.14	86,111,129,131	0
3	NAG	f	2	14/15	0.90	0.16	66,108,130,139	0
5	NAG	d	2	14/15	0.91	0.19	132,156,164,165	0
3	NAG	a	1	14/15	0.91	0.32	123,132,139,142	0
3	NAG	Q	2	14/15	0.91	0.33	130,146,155,158	0
3	NAG	T	2	14/15	0.92	0.26	107,135,144,146	0

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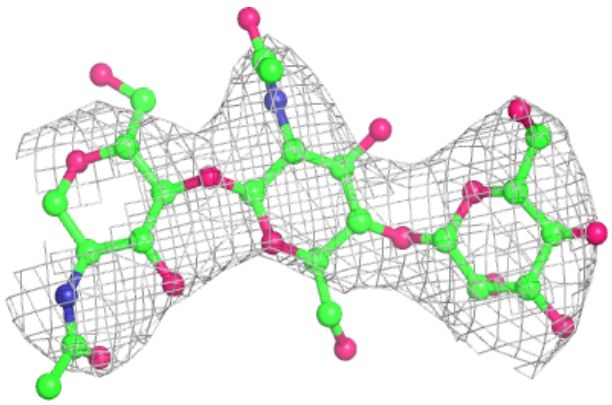
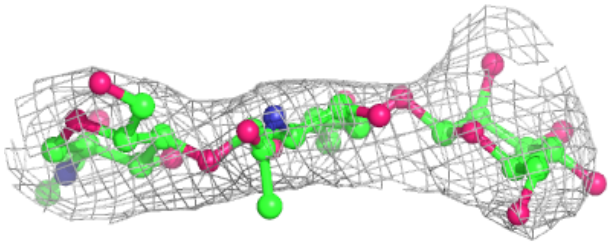
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	X	2	14/15	0.92	0.20	76,92,106,108	0
4	NAG	S	1	14/15	0.92	0.14	69,93,114,114	0
5	NAG	Y	1	14/15	0.93	0.15	127,141,148,155	0
5	NAG	e	1	14/15	0.93	0.25	100,110,118,119	0
6	MAN	Z	4	11/12	0.93	0.13	123,145,152,154	0
5	NAG	c	1	14/15	0.93	0.26	85,105,116,127	0
6	NAG	Z	1	14/15	0.93	0.14	81,99,123,135	0
3	NAG	f	1	14/15	0.94	0.14	68,79,100,113	0
3	NAG	X	1	14/15	0.94	0.17	28,77,104,106	0
3	NAG	T	1	14/15	0.94	0.16	87,106,109,117	0
6	NAG	b	1	14/15	0.95	0.12	19,69,84,92	0
6	NAG	b	2	14/15	0.96	0.17	74,94,113,118	0
5	NAG	U	1	14/15	0.97	0.12	62,74,112,121	0

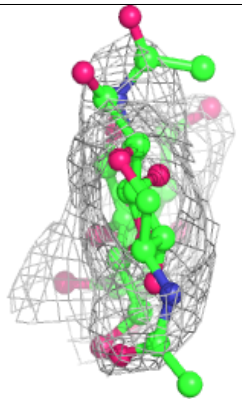
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Q:

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

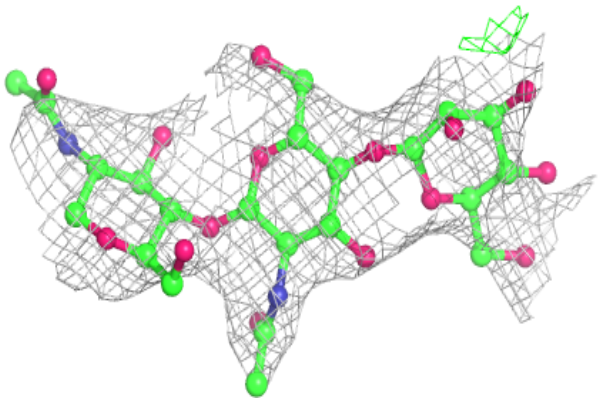


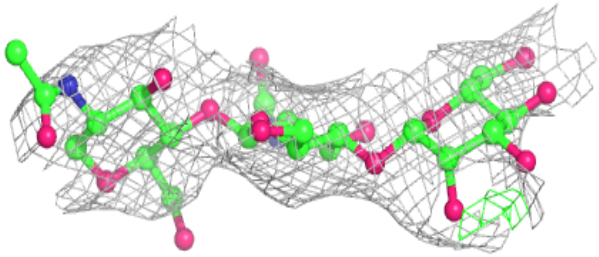


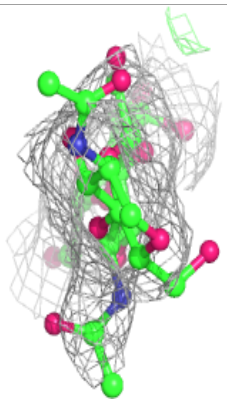


Electron density around Chain R:

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

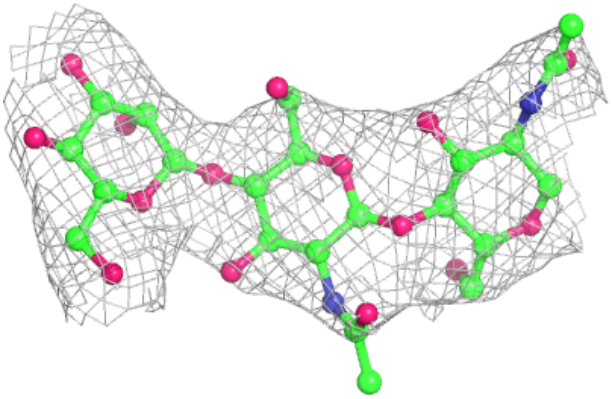


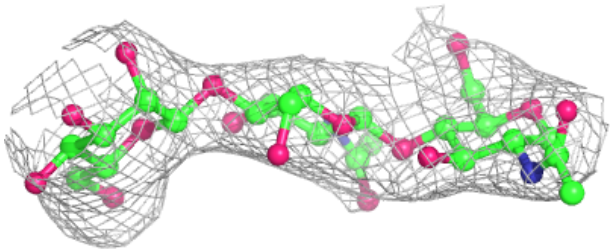


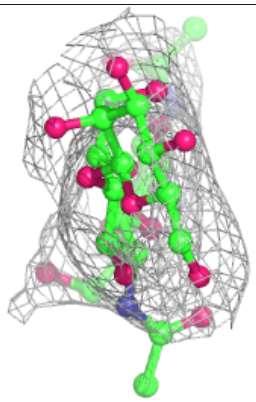


Electron density around Chain T:

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

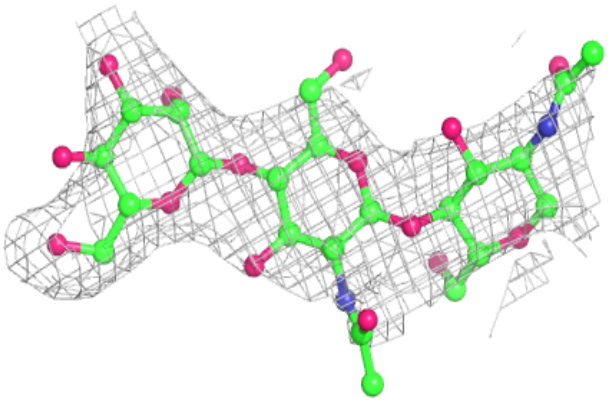


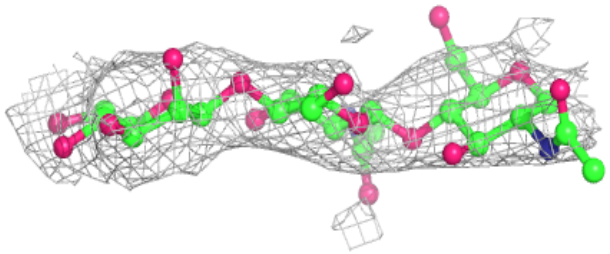


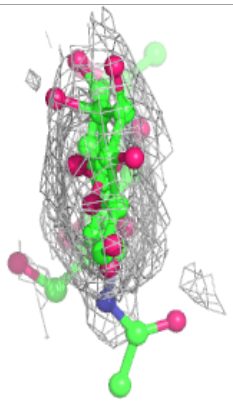


Electron density around Chain V:

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

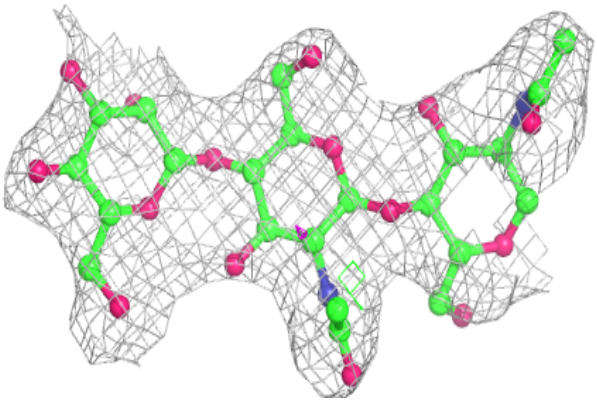


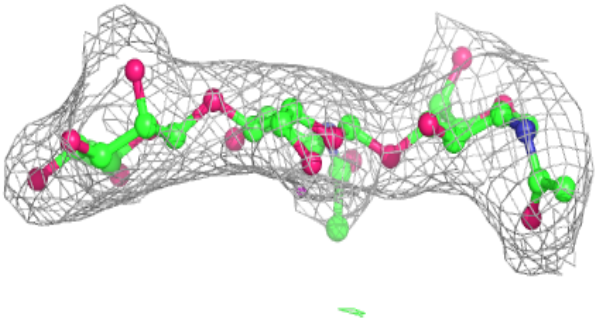


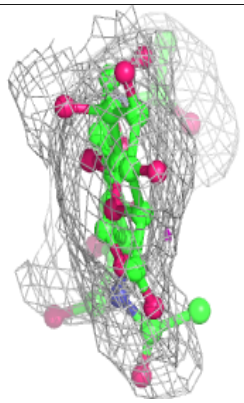


Electron density around Chain X:

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

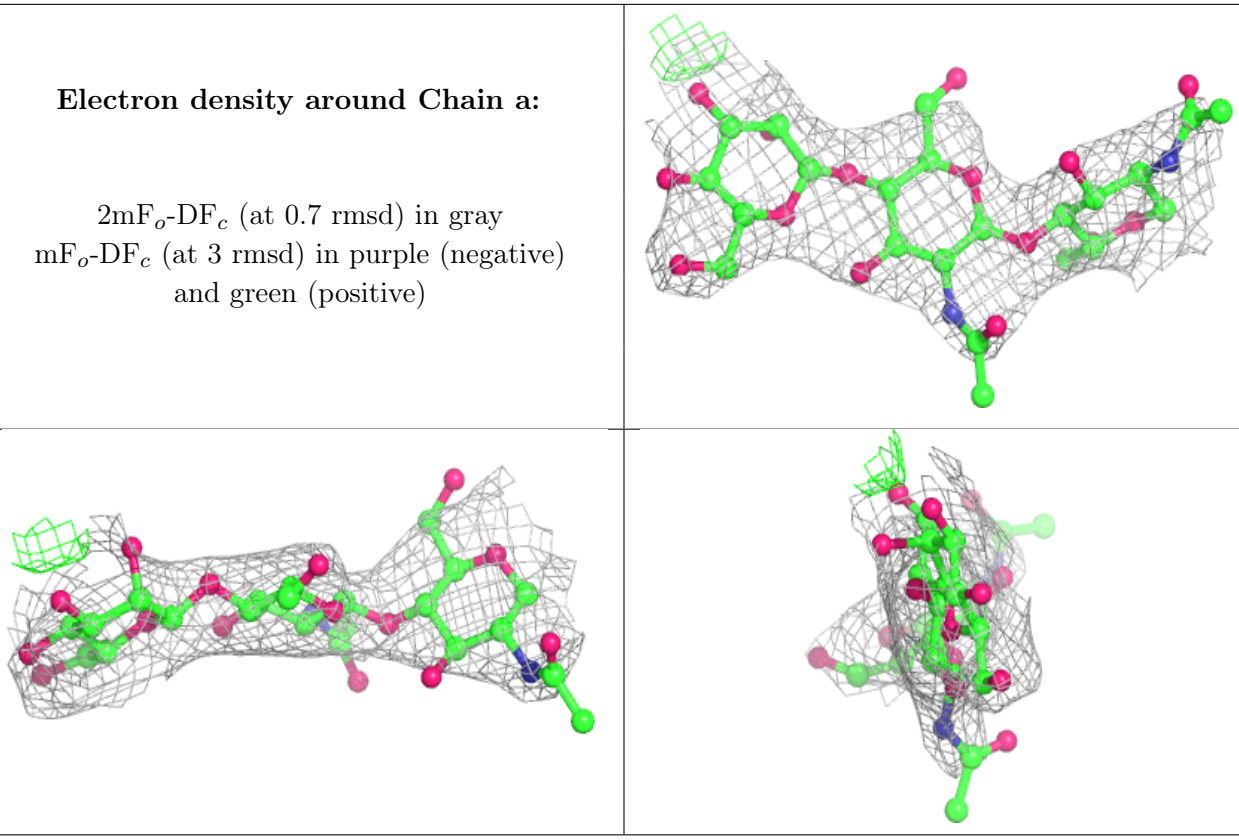






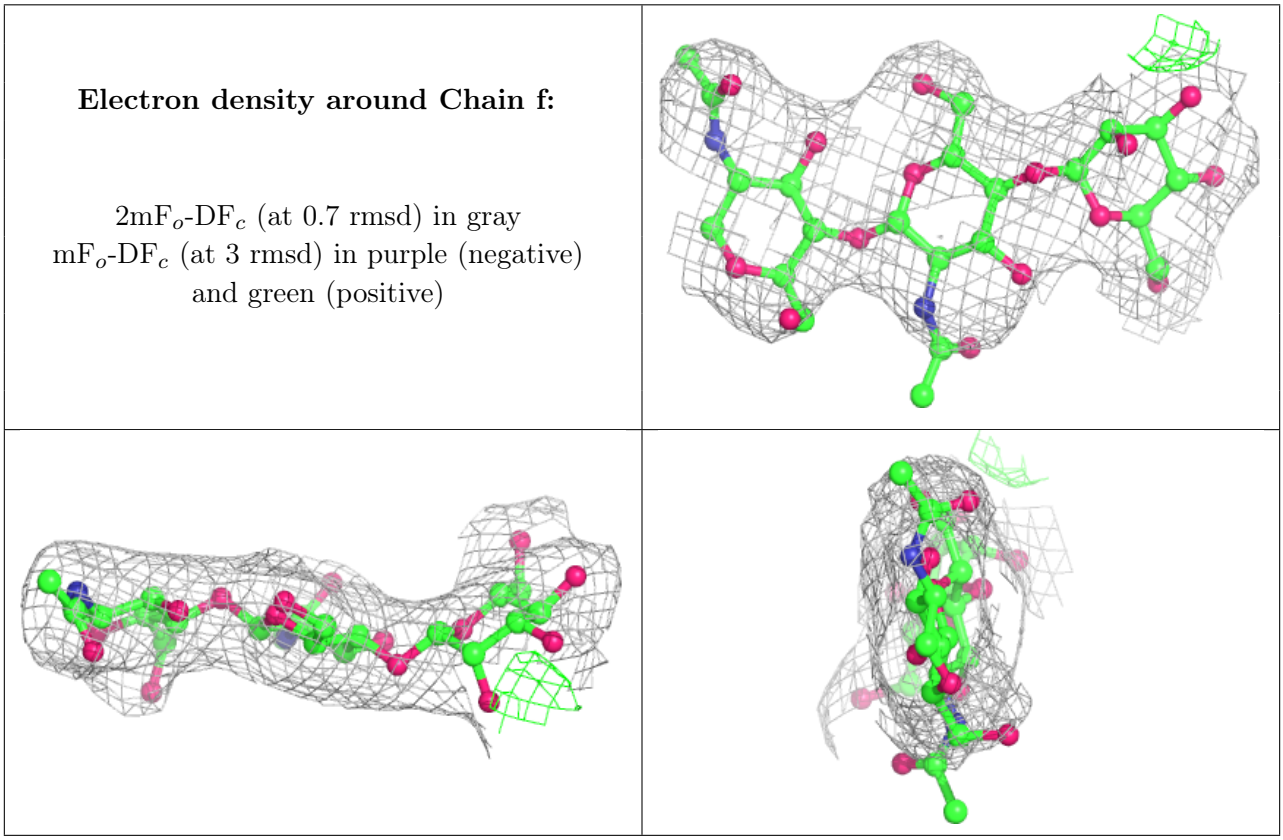
Electron density around Chain a:

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



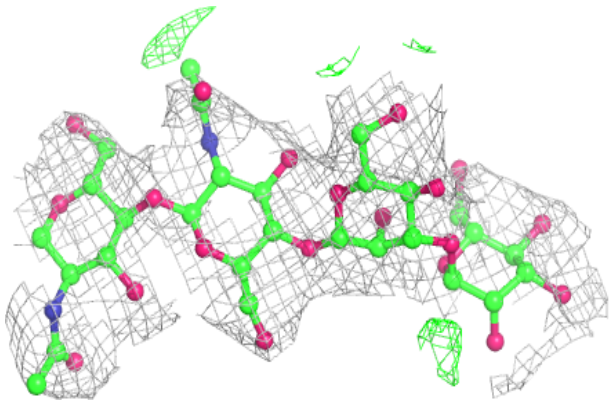
Electron density around Chain f:

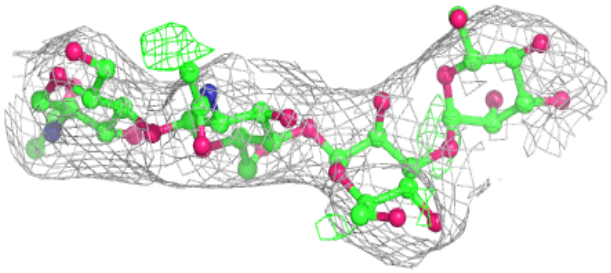
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

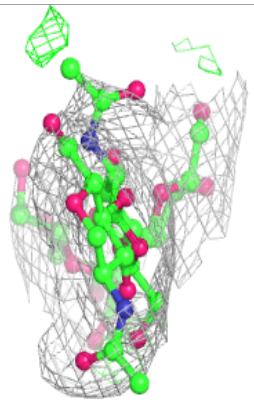


Electron density around Chain S:

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

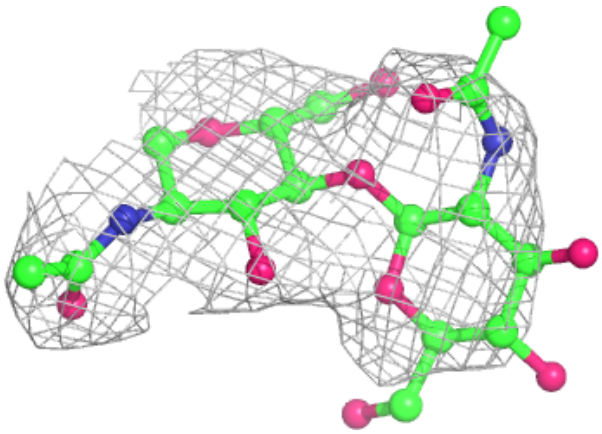


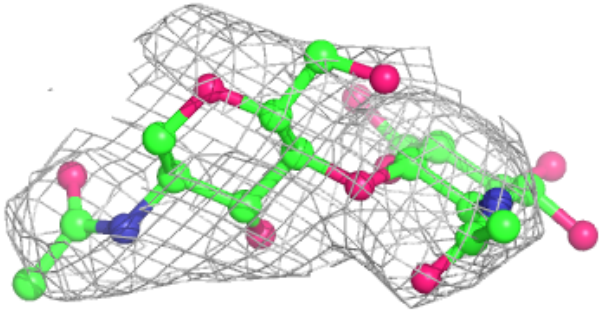


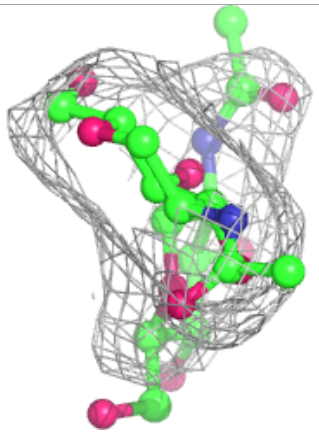


Electron density around Chain U:

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

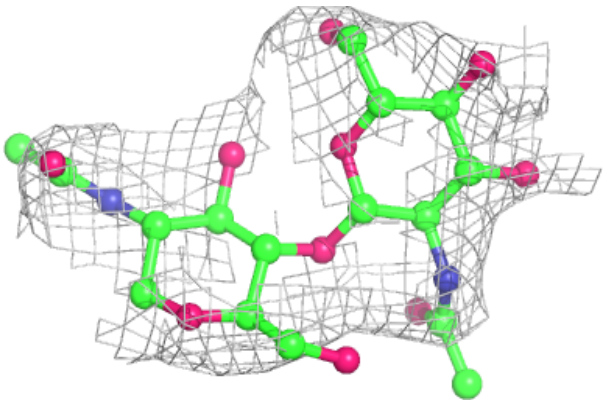


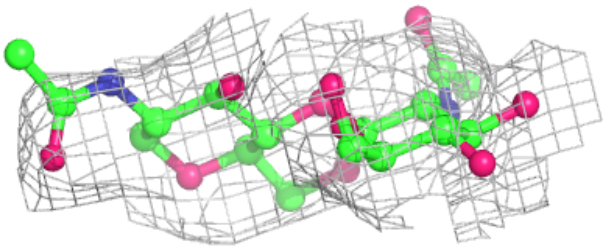


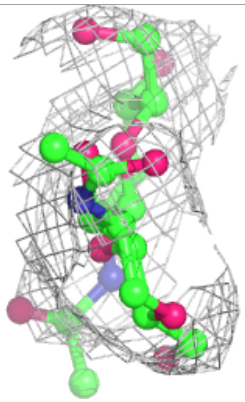


Electron density around Chain W:

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

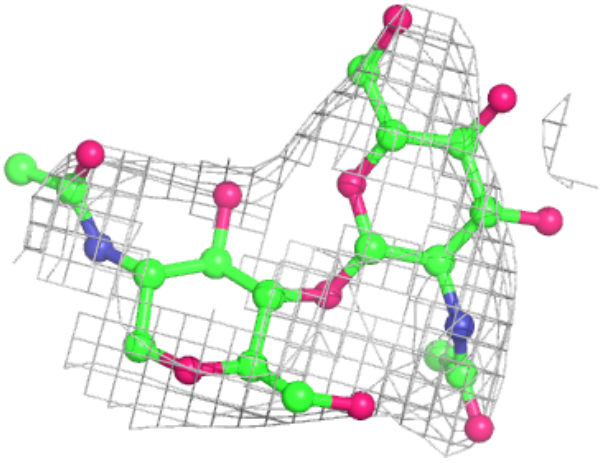


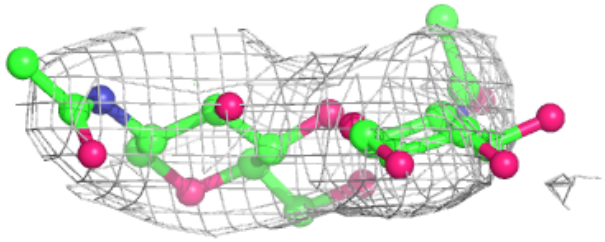


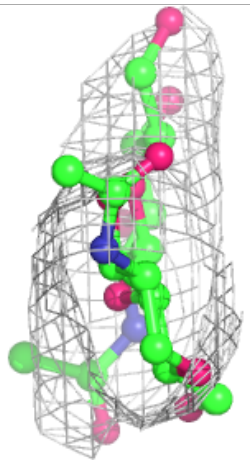


Electron density around Chain Y:

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

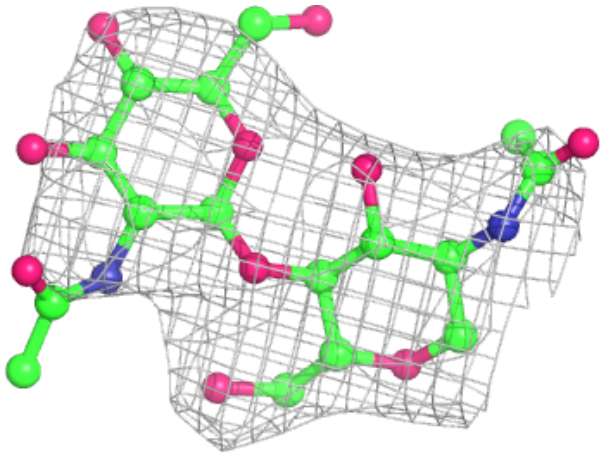


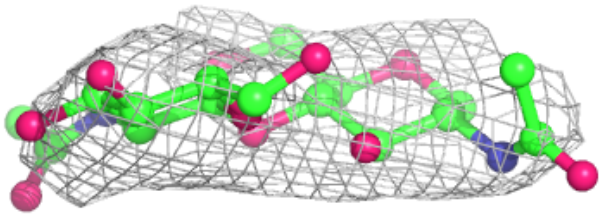


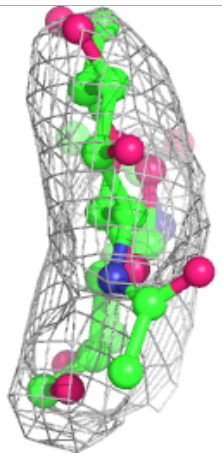


Electron density around Chain c:

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

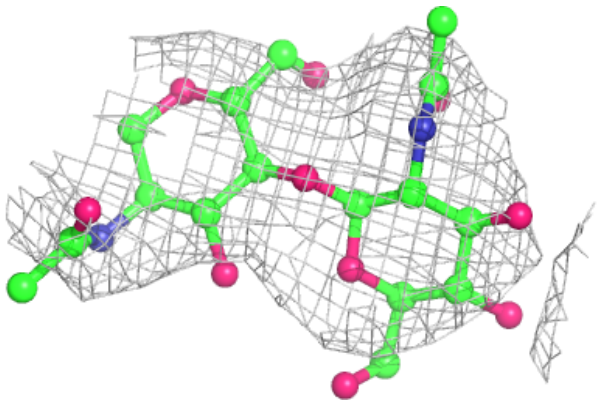


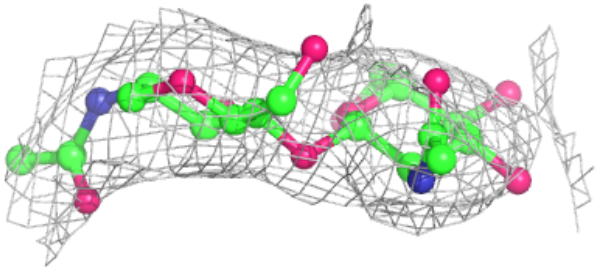


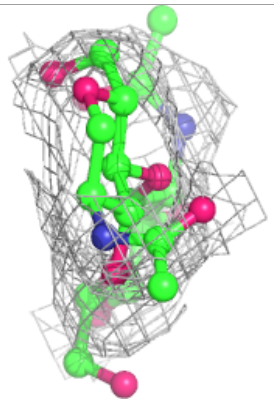


Electron density around Chain d:

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

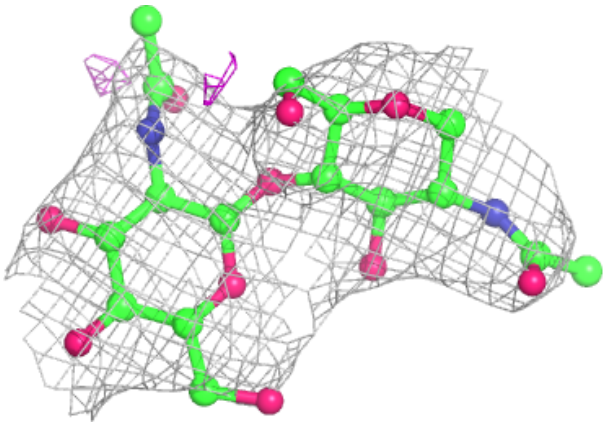


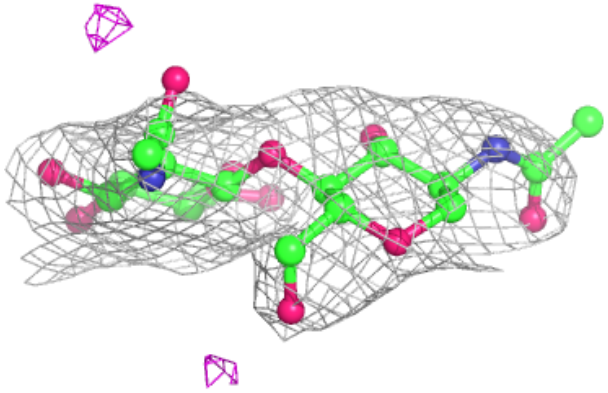


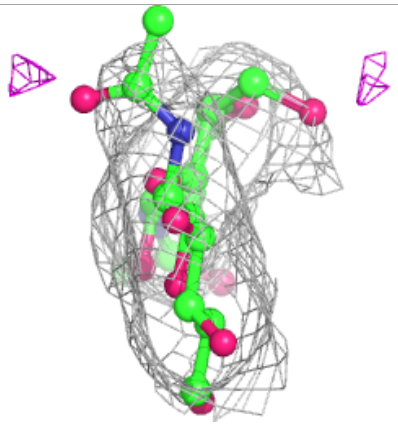


Electron density around Chain e:

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

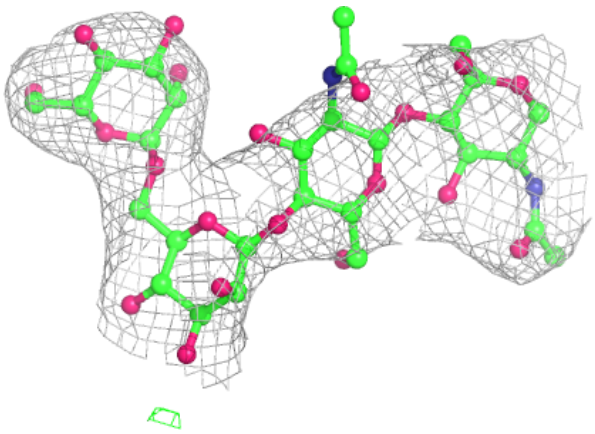


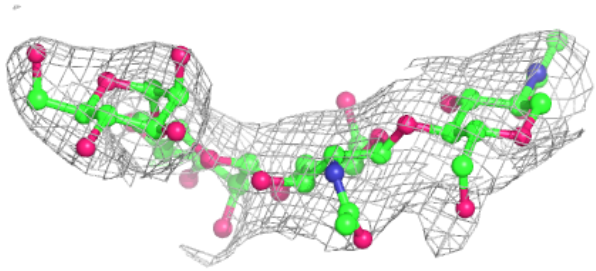


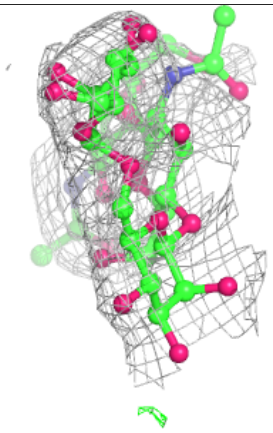


Electron density around Chain Z:

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

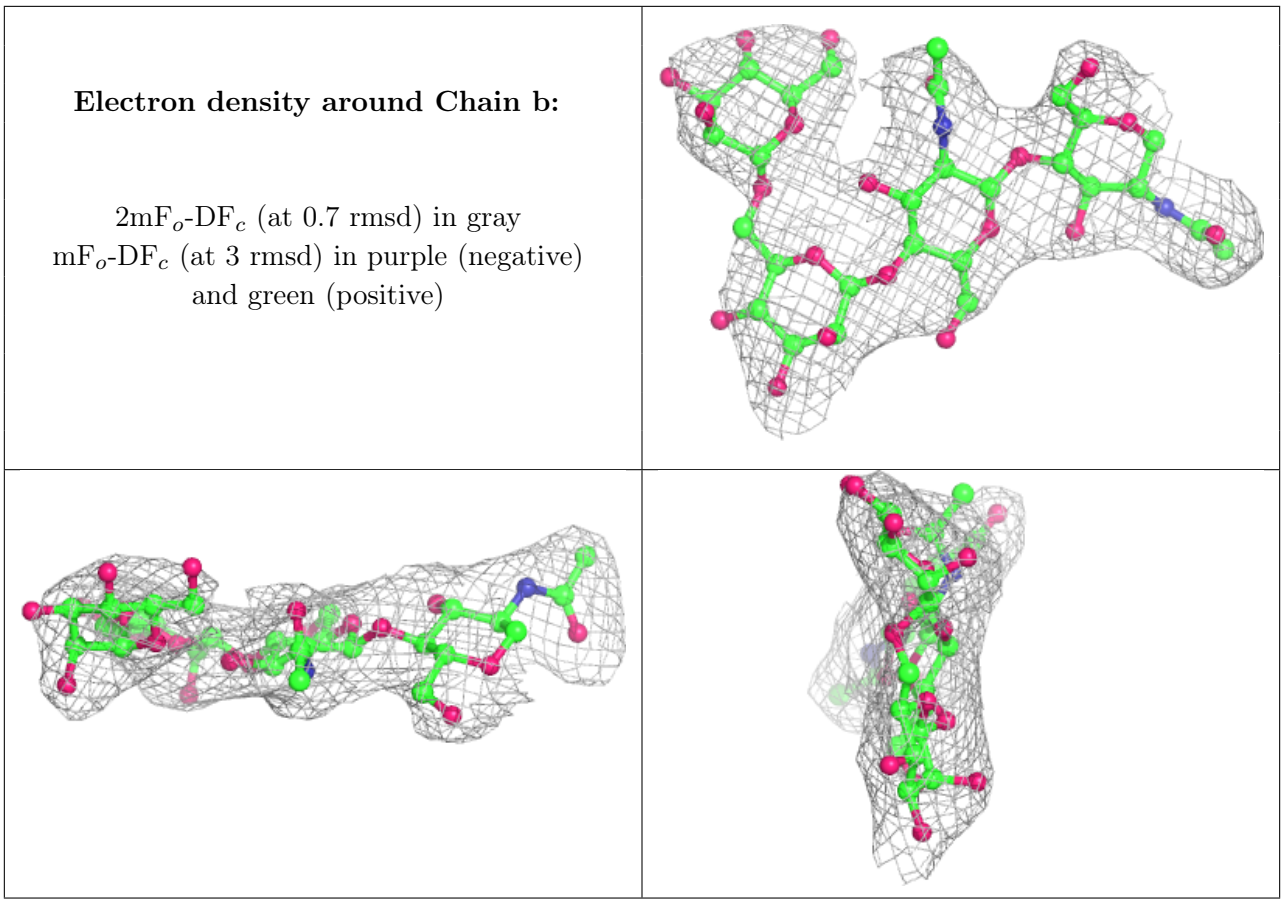






Electron density around Chain b:

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



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
7	NAG	H	404	14/15	0.79	0.24	106,127,133,134	0
7	NAG	F	406	14/15	0.82	0.23	112,130,141,141	0
7	NAG	E	406	14/15	0.82	0.22	88,128,148,153	0
7	NAG	E	410	14/15	0.87	0.16	97,117,128,129	0
7	NAG	F	405	14/15	0.87	0.16	86,108,121,124	0
7	NAG	D	404	14/15	0.87	0.17	111,127,136,136	0
7	NAG	A	409	14/15	0.87	0.18	102,124,135,136	0
7	NAG	D	405	14/15	0.88	0.20	104,127,138,141	0
7	NAG	A	405	14/15	0.88	0.15	86,99,108,112	0
7	NAG	G	405	14/15	0.89	0.19	73,98,118,124	0
7	NAG	G	408	14/15	0.89	0.16	106,126,133,136	0
7	NAG	A	404	14/15	0.89	0.23	100,124,134,145	0
7	NAG	E	405	14/15	0.92	0.15	64,70,75,76	0

6.5 Other polymers (i)

There are no such residues in this entry.