wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2022 – 05:35 pm BST

PDB ID	:	7NUP
Title	:	Endoplasmic reticulum aminopeptidase 2 complexed with a mixed hydroxamic and sulfonyl ligand
Authors	:	Mpakali, A.; Giastas, P.; Stratikos, E.
Deposited on	:	2021-03-12
Resolution	:	3.10 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 following versions of software and data (see references (i)) were used in the production of this report:

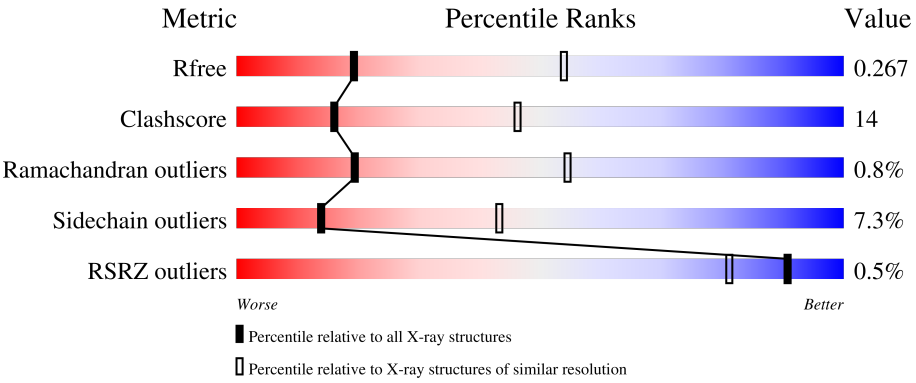
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	966	63% 29% • 5%
1	B	966	% 61% 30% • 6%
1	C	966	56% 33% • 9%
1	D	966	% 55% 34% • 8%
2	E	4	50% 50%

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Mol	Chain	Length	Quality of chain
2	Q	4	25% 75%
3	F	2	50% 50%
3	G	2	50% 50%
3	J	2	100%
3	K	2	50% 50%
3	L	2	50% 50%
3	M	2	50% 50%
3	P	2	50% 50%
3	S	2	100%
4	H	3	33% 33% 33%
4	I	3	100%
4	O	3	67% 33%
4	R	3	33% 67%
5	N	5	20% 80%

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	BR	A	1011	-	-	-	X
11	BR	C	1008	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 29963 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 Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	915	Total	C	N	O	S	0	2	0
			7389	4758	1225	1372	34			
1	B	907	Total	C	N	O	S	0	3	0
			7318	4710	1214	1361	33			
1	C	883	Total	C	N	O	S	0	0	0
			7126	4598	1174	1326	28			
1	D	884	Total	C	N	O	S	0	3	0
			7065	4558	1172	1306	29			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	ASN	LYS	variant	UNP Q6P179
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
A	964	HIS	-	expression tag	UNP Q6P179
A	965	HIS	-	expression tag	UNP Q6P179
A	966	HIS	-	expression tag	UNP Q6P179
B	392	ASN	LYS	variant	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179
B	964	HIS	-	expression tag	UNP Q6P179
B	965	HIS	-	expression tag	UNP Q6P179
B	966	HIS	-	expression tag	UNP Q6P179
C	392	ASN	LYS	variant	UNP Q6P179
C	961	ARG	-	expression tag	UNP Q6P179
C	962	HIS	-	expression tag	UNP Q6P179
C	963	HIS	-	expression tag	UNP Q6P179
C	964	HIS	-	expression tag	UNP Q6P179
C	965	HIS	-	expression tag	UNP Q6P179
C	966	HIS	-	expression tag	UNP Q6P179

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Chain	Residue	Modelled	Actual	Comment	Reference
D	392	ASN	LYS	variant	UNP Q6P179
D	961	ARG	-	expression tag	UNP Q6P179
D	962	HIS	-	expression tag	UNP Q6P179
D	963	HIS	-	expression tag	UNP Q6P179
D	964	HIS	-	expression tag	UNP Q6P179
D	965	HIS	-	expression tag	UNP Q6P179
D	966	HIS	-	expression tag	UNP Q6P179

- Molecule 2 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
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

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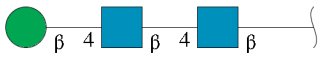
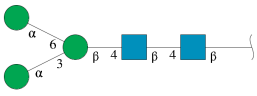
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	P	2	Total C N O 28 16 2 10	0	0	0
3	S	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 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
4	H	3	Total C N O 39 22 2 15	0	0	0
4	I	3	Total C N O 39 22 2 15	0	0	0
4	O	3	Total C N O 39 22 2 15	0	0	0
4	R	3	Total C N O 39 22 2 15	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0
6	B	1	Total Zn 1 1	0	0

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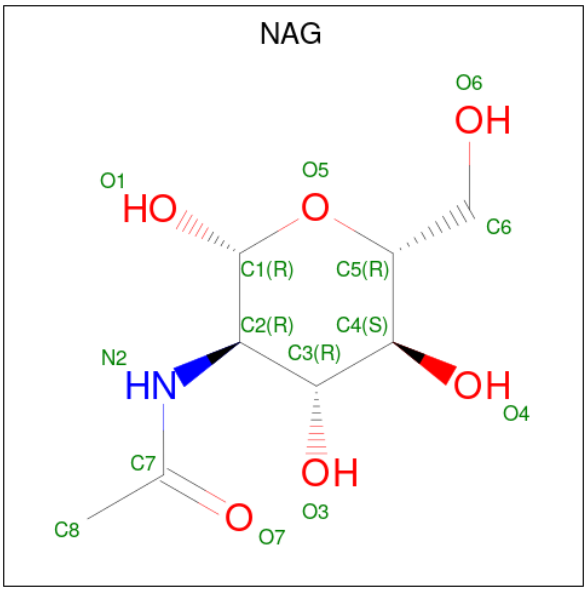
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Zn 1 1	0	0
6	D	1	Total Zn 1 1	0	0

- 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 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0

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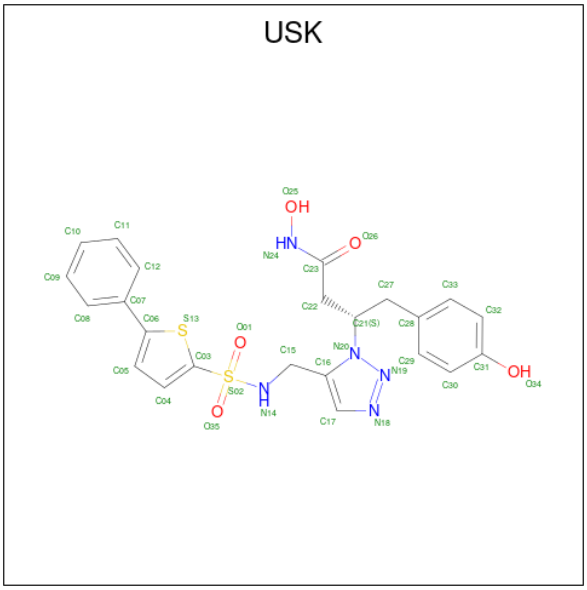
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is (3 {S})-4-(4-hydroxyphenyl)- {N}-oxidanyl-3-[5-[[(5-phenylthiophen-2-yl)sulfonylamino]methyl]-1,2,3-triazol-1-yl]butanamide (three-letter code: USK) (formula: $C_{23}H_{23}N_5O_5S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O S 35 23 5 5 2	0	0
8	B	1	Total C N O S 35 23 5 5 2	0	0

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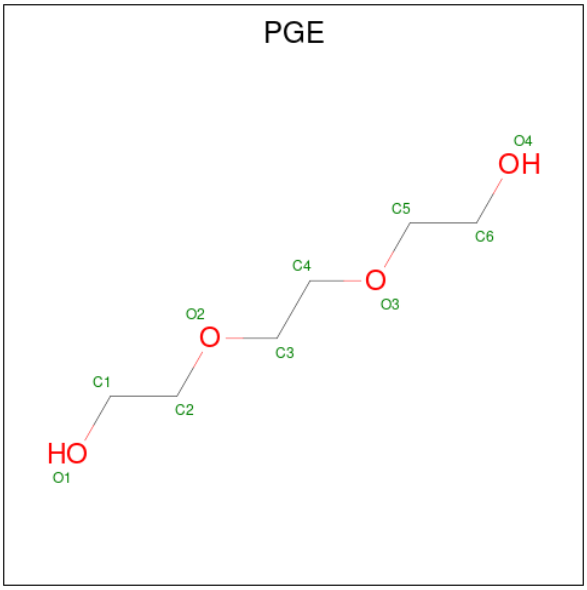
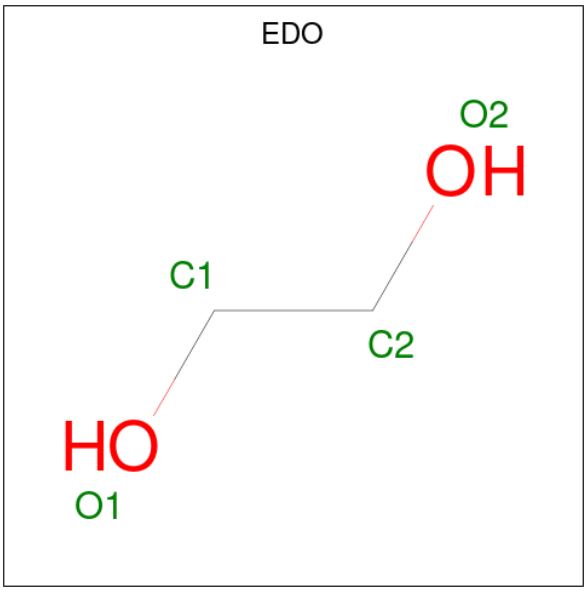
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	S	0	0
			35	23	5	5	2		
8	D	1	Total	C	N	O	S	0	0
			35	23	5	5	2		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	O		0	0
			10	6	4			

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 11 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	8	Total Br 8 8	0	0
11	B	2	Total Br 2 2	0	0
11	C	2	Total Br 2 2	0	0
11	D	1	Total Br 1 1	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	39	Total O 39 39	0	0
12	B	37	Total O 37 37	0	0

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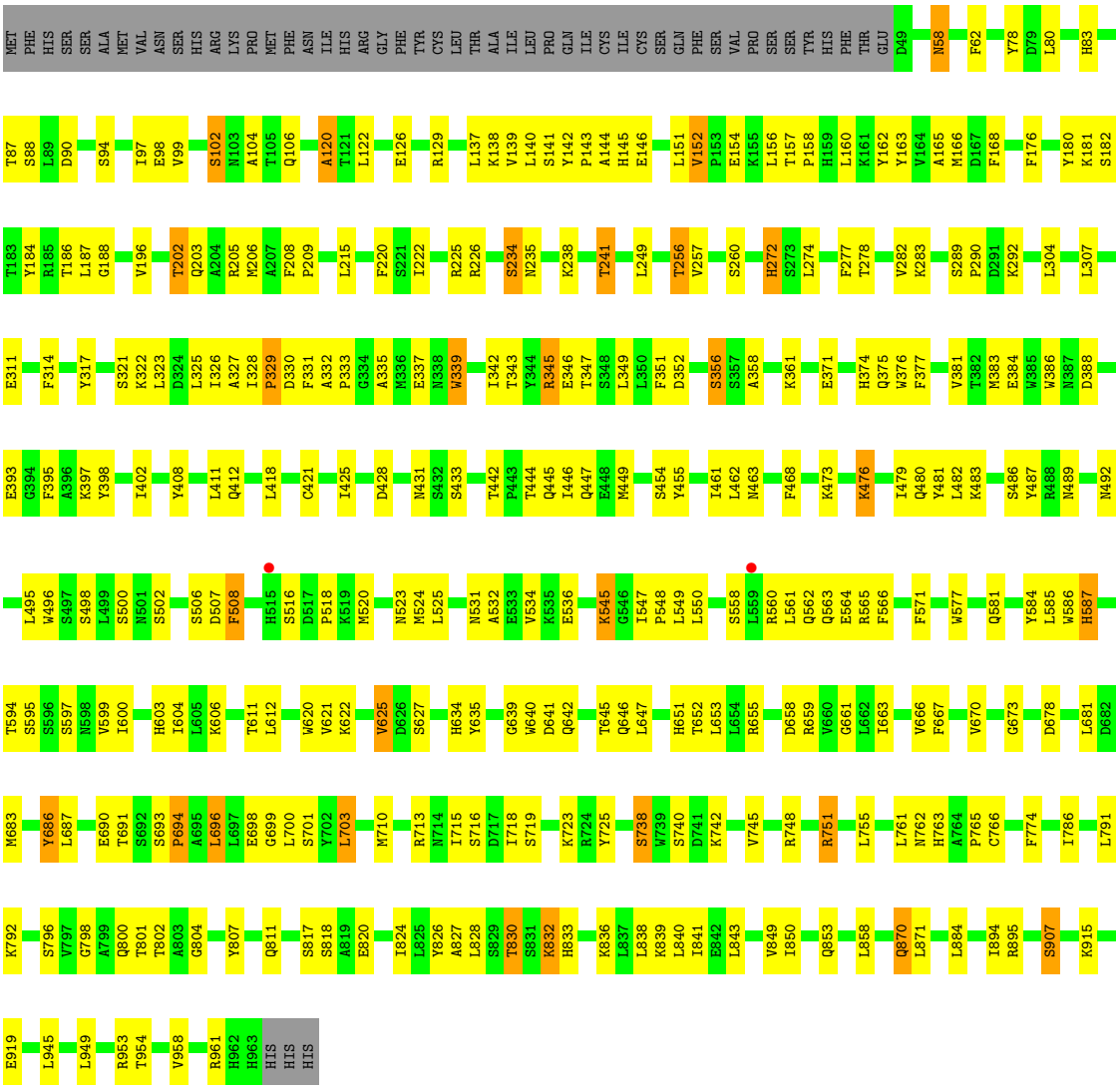
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	21	Total O 21 21	0	0
12	D	10	Total O 10 10	0	0

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.

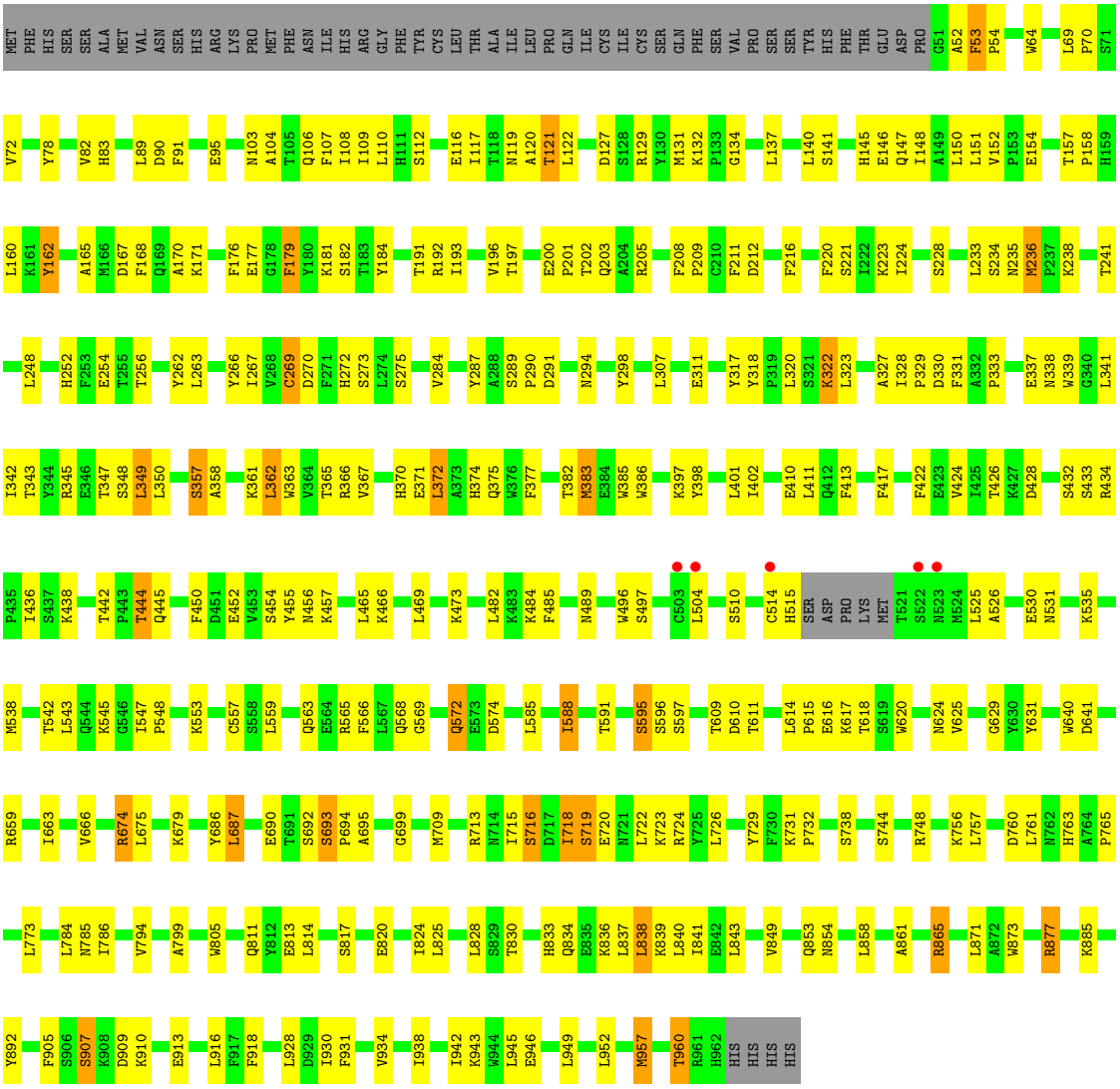
• Molecule 1: Endoplasmic reticulum aminopeptidase 2

Chain A:



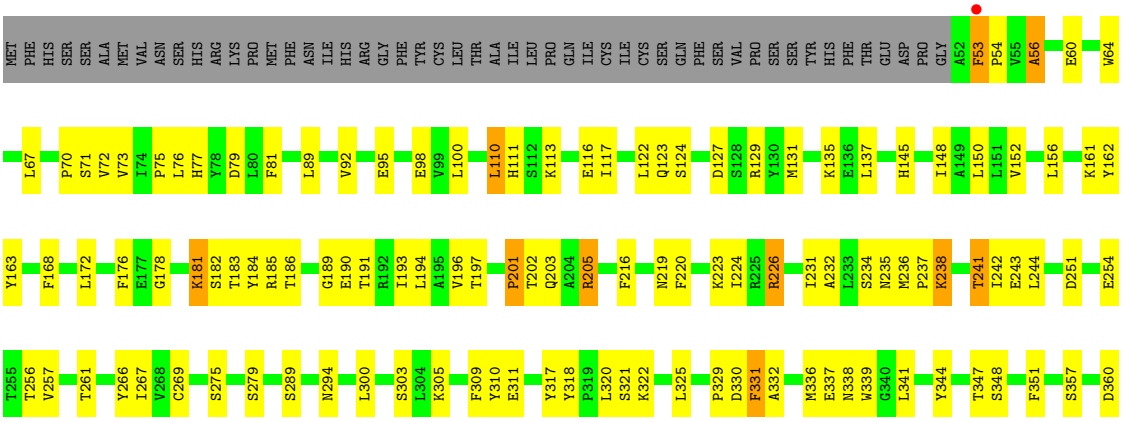
• Molecule 1: Endoplasmic reticulum aminopeptidase 2

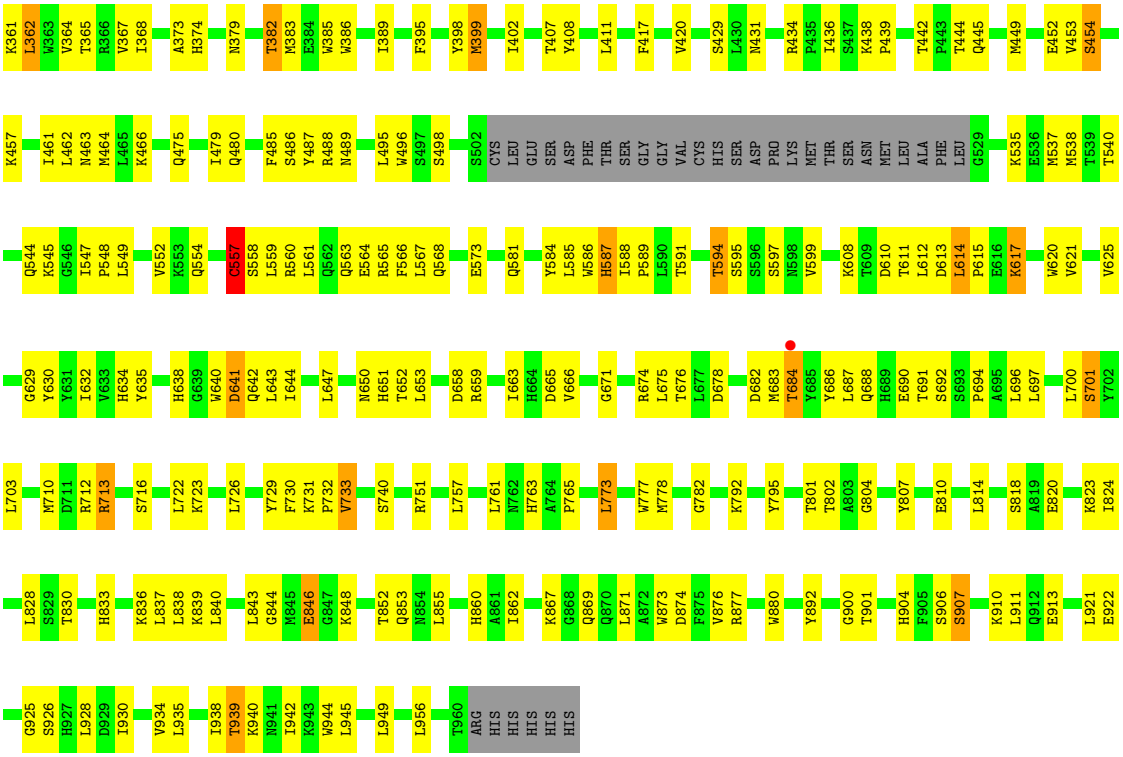
Chain B:



• Molecule 1: Endoplasmic reticulum aminopeptidase 2

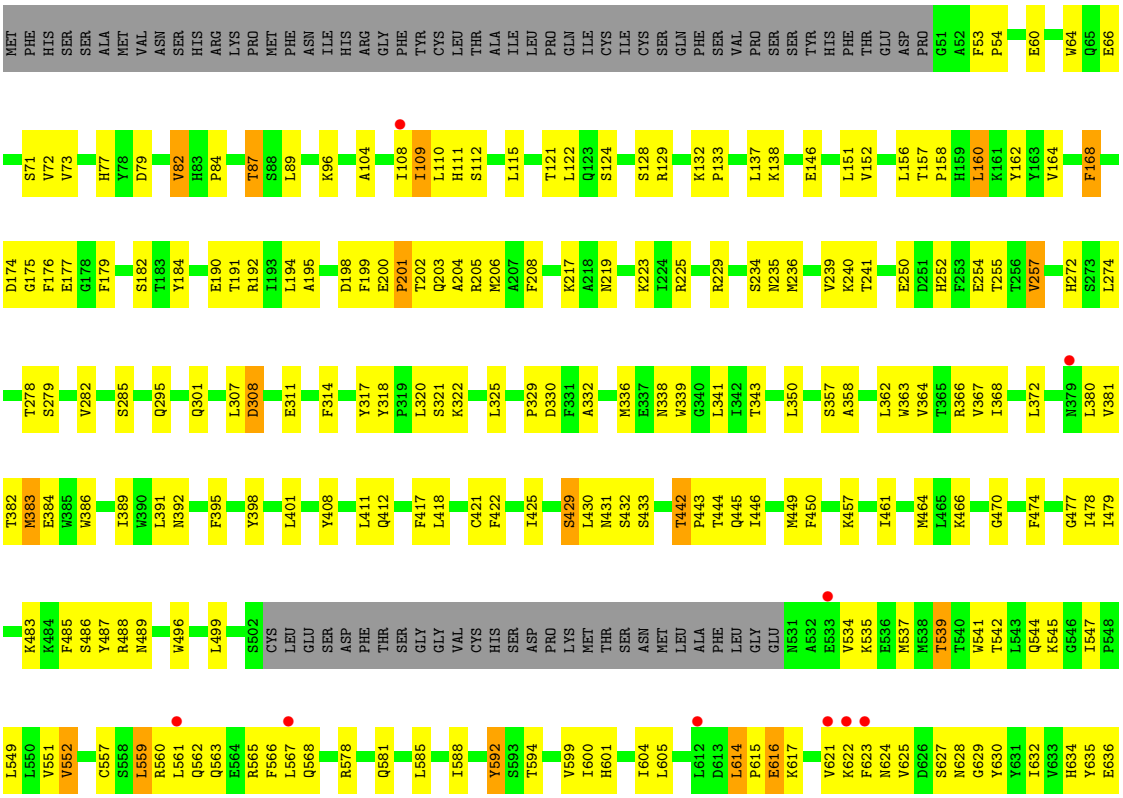
Chain C:

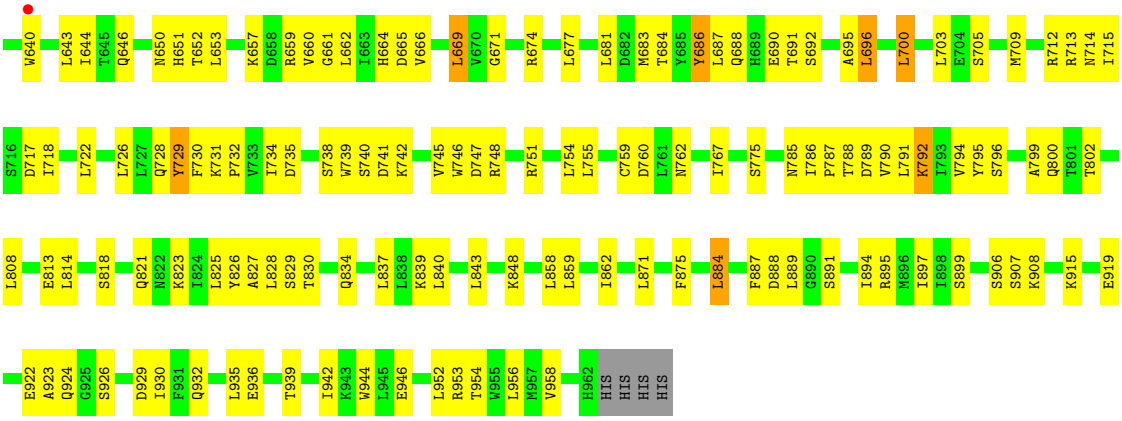




• Molecule 1: Endoplasmic reticulum aminopeptidase 2

Chain D:



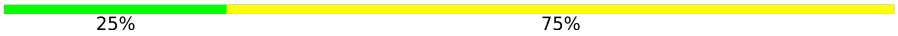


• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain Q:



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

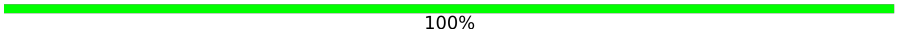
Chain F:

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

Chain G:

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

Chain J:



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

Chain K:

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

Chain L:

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

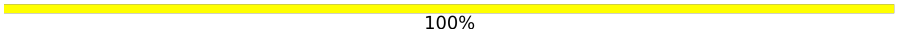
Chain M:

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

Chain P:

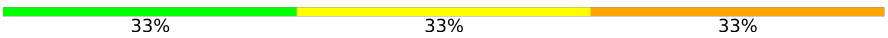
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



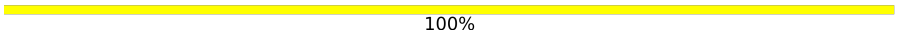
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain I:

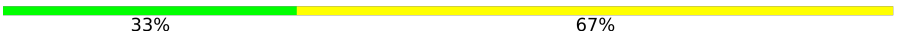


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

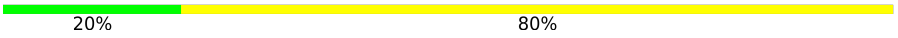
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.27Å 127.19Å 133.41Å 90.92° 90.08° 90.87°	Depositor
Resolution (Å)	48.66 – 3.10 48.66 – 3.10	Depositor EDS
% Data completeness (in resolution range)	83.2 (48.66-3.10) 79.5 (48.66-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.182 , 0.267 0.182 , 0.267	Depositor DCC
R_{free} test set	3482 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,l,-k 0.000 for h,-l,k 0.013 for h,-k,-l 0.001 for -h,k,-l 0.166 for -h,-k,l 0.000 for -h,l,k 0.000 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	29963	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: BR, PGE, NAG, MAN, EDO, ZN, USK, 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	0.52	0/7581	0.67	2/10285 (0.0%)
1	B	0.50	0/7507	0.66	5/10185 (0.0%)
1	C	0.46	0/7305	0.63	0/9916
1	D	0.44	0/7252	0.62	0/9862
All	All	0.48	0/29645	0.64	7/40248 (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	C	0	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	362	LEU	CB-CG-CD2	-6.54	99.88	111.00
1	B	263	LEU	CA-CB-CG	-5.74	102.11	115.30
1	A	274	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	236	MET	CA-CB-CG	-5.41	104.11	113.30
1	A	895	ARG	NE-CZ-NH2	-5.40	117.60	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	557	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	7389	0	7273	204	0
1	B	7318	0	7186	205	0
1	C	7126	0	6990	223	0
1	D	7065	0	6865	226	0
2	E	50	0	43	0	0
2	Q	50	0	43	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	1	0
3	L	28	0	25	1	0
3	M	28	0	25	0	0
3	P	28	0	25	0	0
3	S	28	0	25	0	0
4	H	39	0	34	1	0
4	I	39	0	34	0	0
4	O	39	0	34	0	0
4	R	39	0	34	1	0
5	N	61	0	52	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	84	0	78	1	0
7	B	42	0	39	2	0
7	C	56	0	52	0	0
7	D	56	0	52	2	0
8	A	35	0	0	0	0
8	B	35	0	0	2	0
8	C	35	0	0	2	0
8	D	35	0	0	1	0
9	A	10	0	14	0	0
10	A	4	0	6	0	0
10	B	4	0	6	0	0
10	D	4	0	6	0	0
11	A	8	0	0	3	0
11	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	2	0	0	4	0
11	D	1	0	0	0	0
12	A	39	0	0	2	0
12	B	37	0	0	10	0
12	C	21	0	0	3	0
12	D	10	0	0	2	0
All	All	29963	0	29041	851	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 851 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:220:PHE:H	1:A:256:THR:HG22	1.14	1.06
1:C:659:ARG:HH12	1:C:691:THR:HG22	1.26	0.97
1:C:362:LEU:CD2	11:C:1008:BR:BR	2.68	0.97
1:B:205:ARG:HH21	1:B:212:ASP:HB3	1.31	0.92
1:C:659:ARG:NH1	1:C:690:GLU:OE2	2.03	0.90

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	915/966 (95%)	830 (91%)	77 (8%)	8 (1%)	17	52
1	B	906/966 (94%)	845 (93%)	53 (6%)	8 (1%)	17	52
1	C	879/966 (91%)	821 (93%)	50 (6%)	8 (1%)	17	52
1	D	883/966 (91%)	831 (94%)	49 (6%)	3 (0%)	41	73
All	All	3583/3864 (93%)	3327 (93%)	229 (6%)	27 (1%)	19	54

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	615	PRO
1	B	744	SER
1	D	132	LYS
1	B	216	PHE
1	B	616	GLU

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	812/869 (93%)	763 (94%)	49 (6%)	19 49
1	B	801/869 (92%)	745 (93%)	56 (7%)	15 45
1	C	778/869 (90%)	722 (93%)	56 (7%)	14 44
1	D	758/869 (87%)	689 (91%)	69 (9%)	9 33
All	All	3149/3476 (91%)	2919 (93%)	230 (7%)	14 43

5 of 230 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	241	THR
1	D	775	SER
1	C	658	ASP
1	D	759	CYS
1	D	559	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	563	GLN
1	D	646	GLN
1	B	568	GLN
1	B	563	GLN
1	D	728	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

41 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	2,1	14,14,15	0.59	0	17,19,21	0.73	0
2	NAG	E	2	2	14,14,15	0.52	0	17,19,21	0.52	0
2	BMA	E	3	2	11,11,12	1.96	4 (36%)	15,15,17	0.94	0
2	MAN	E	4	2	11,11,12	1.36	2 (18%)	15,15,17	1.55	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.55	0	17,19,21	0.64	0
3	NAG	F	2	3	14,14,15	0.66	1 (7%)	17,19,21	0.78	0
3	NAG	G	1	1,3	14,14,15	0.93	1 (7%)	17,19,21	0.48	0
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	H	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	0.46	0
4	NAG	H	2	4	14,14,15	0.41	0	17,19,21	0.62	0
4	BMA	H	3	4	11,11,12	1.21	1 (9%)	15,15,17	0.92	1 (6%)
4	NAG	I	1	4,1	14,14,15	0.88	1 (7%)	17,19,21	0.63	0
4	NAG	I	2	4	14,14,15	0.33	0	17,19,21	0.76	1 (5%)
4	BMA	I	3	4	11,11,12	1.06	2 (18%)	15,15,17	0.82	1 (6%)
3	NAG	J	1	1,3	14,14,15	0.54	0	17,19,21	0.65	0
3	NAG	J	2	3	14,14,15	0.49	0	17,19,21	0.53	0
3	NAG	K	1	1,3	14,14,15	0.73	0	17,19,21	1.22	1 (5%)
3	NAG	K	2	3	14,14,15	0.60	0	17,19,21	0.59	0
3	NAG	L	1	1,3	14,14,15	0.24	0	17,19,21	0.63	0
3	NAG	L	2	3	14,14,15	0.72	1 (7%)	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	M	1	1,3	14,14,15	0.79	2 (14%)	17,19,21	1.14	1 (5%)
3	NAG	M	2	3	14,14,15	0.55	0	17,19,21	0.63	0
5	NAG	N	1	1,5	14,14,15	0.37	0	17,19,21	0.55	0
5	NAG	N	2	5	14,14,15	0.85	1 (7%)	17,19,21	0.53	0
5	BMA	N	3	5	11,11,12	1.16	1 (9%)	15,15,17	1.03	1 (6%)
5	MAN	N	4	5	11,11,12	1.04	1 (9%)	15,15,17	1.37	1 (6%)
5	MAN	N	5	5	11,11,12	1.77	5 (45%)	15,15,17	0.89	0
4	NAG	O	1	4,1	14,14,15	0.49	0	17,19,21	0.44	0
4	NAG	O	2	4	14,14,15	0.37	0	17,19,21	0.56	0
4	BMA	O	3	4	11,11,12	2.21	3 (27%)	15,15,17	1.19	1 (6%)
3	NAG	P	1	1,3	14,14,15	0.31	0	17,19,21	0.67	0
3	NAG	P	2	3	14,14,15	0.46	0	17,19,21	1.17	2 (11%)
2	NAG	Q	1	2,1	14,14,15	0.55	0	17,19,21	0.41	0
2	NAG	Q	2	2	14,14,15	0.54	0	17,19,21	0.84	1 (5%)
2	BMA	Q	3	2	11,11,12	1.07	2 (18%)	15,15,17	1.32	2 (13%)
2	MAN	Q	4	2	11,11,12	1.55	2 (18%)	15,15,17	1.17	1 (6%)
4	NAG	R	1	4,1	14,14,15	0.49	0	17,19,21	0.55	0
4	NAG	R	2	4	14,14,15	0.53	0	17,19,21	0.61	0
4	BMA	R	3	4	11,11,12	1.65	3 (27%)	15,15,17	2.15	3 (20%)
3	NAG	S	1	1,3	14,14,15	0.24	0	17,19,21	0.83	1 (5%)
3	NAG	S	2	3	14,14,15	0.92	1 (7%)	17,19,21	0.64	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
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1

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

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	3	BMA	C2-C3	5.11	1.60	1.52
2	Q	4	MAN	C2-C3	3.91	1.58	1.52
2	E	3	BMA	C4-C5	3.53	1.60	1.53
4	R	3	BMA	C1-C2	3.31	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	3	BMA	C4-C5	3.26	1.59	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	3	BMA	C1-O5-C5	6.68	121.25	112.19
2	E	4	MAN	C1-O5-C5	5.07	119.06	112.19
3	M	1	NAG	C1-O5-C5	4.03	117.65	112.19
3	P	2	NAG	C2-N2-C7	3.80	128.31	122.90
5	N	4	MAN	C1-O5-C5	3.47	116.89	112.19

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

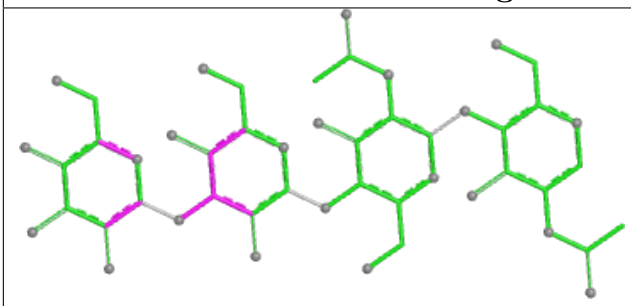
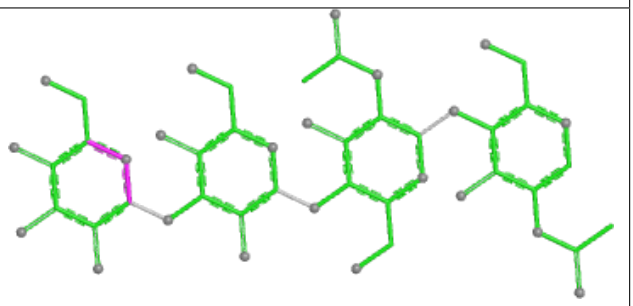
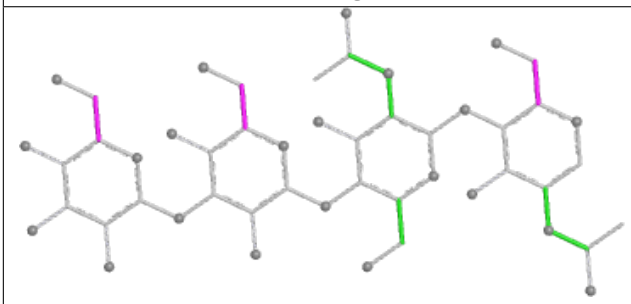
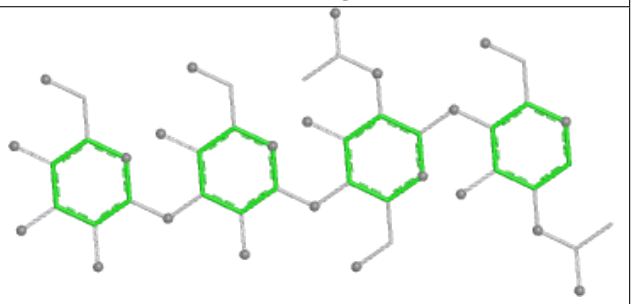
Mol	Chain	Res	Type	Atoms
3	P	2	NAG	C1-C2-N2-C7
3	S	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6

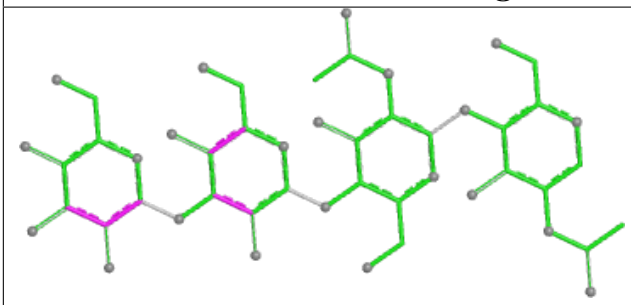
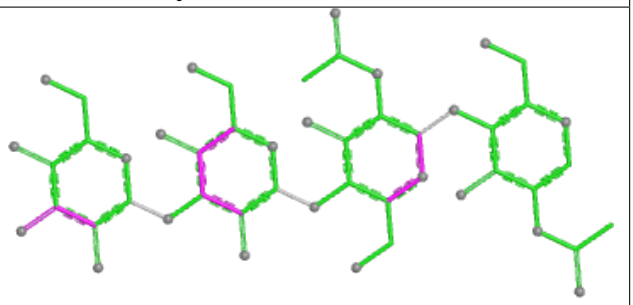
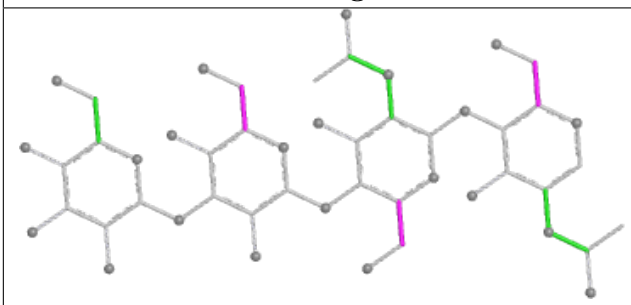
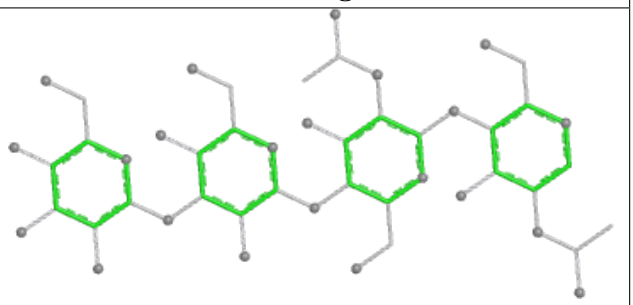
There are no ring outliers.

4 monomers are involved in 4 short contacts:

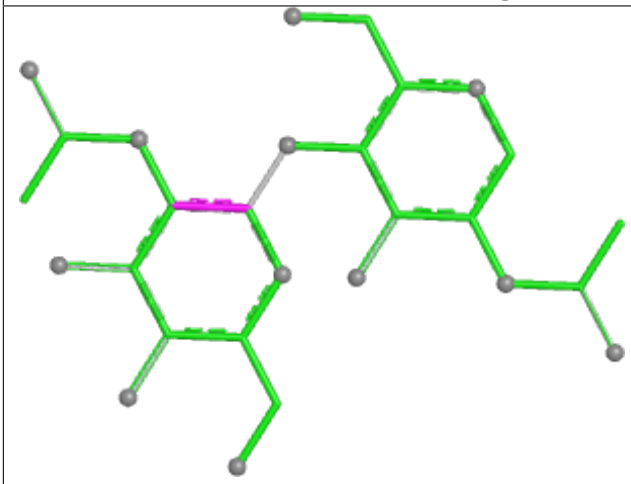
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	1	0
4	R	1	NAG	1	0
3	L	2	NAG	1	0
3	K	1	NAG	1	0

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 Q	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain F



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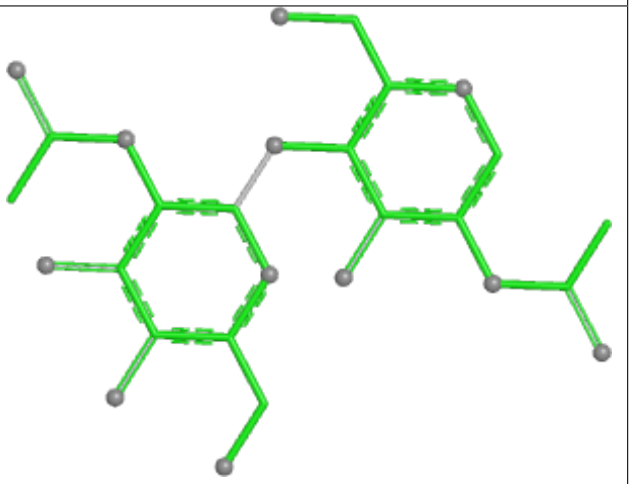

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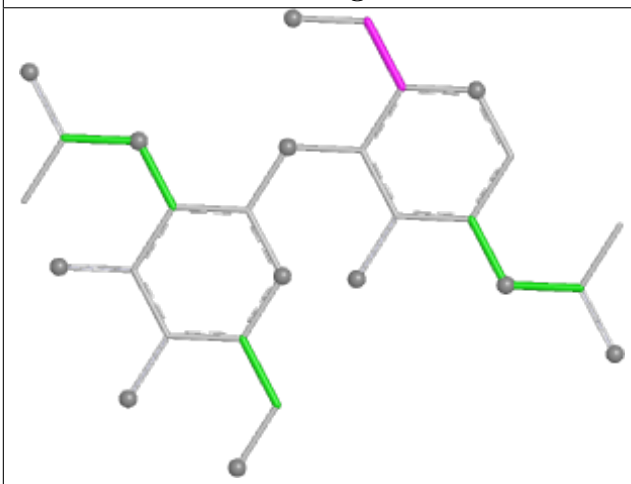
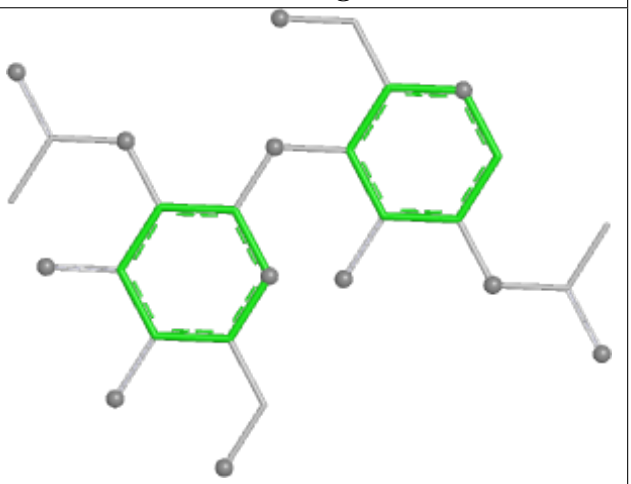
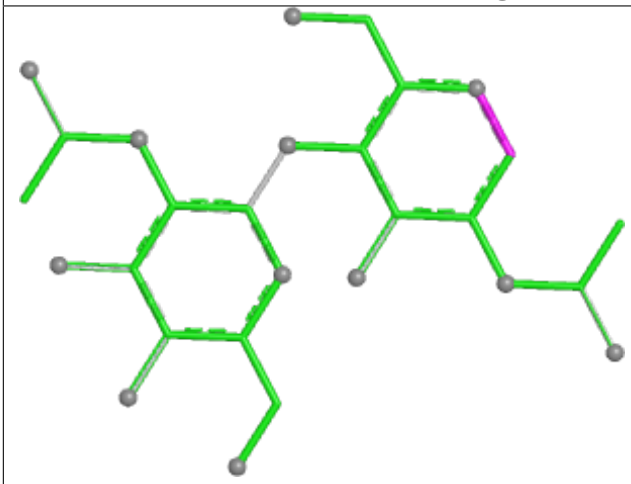


Torsions



Rings

Oligosaccharide Chain G



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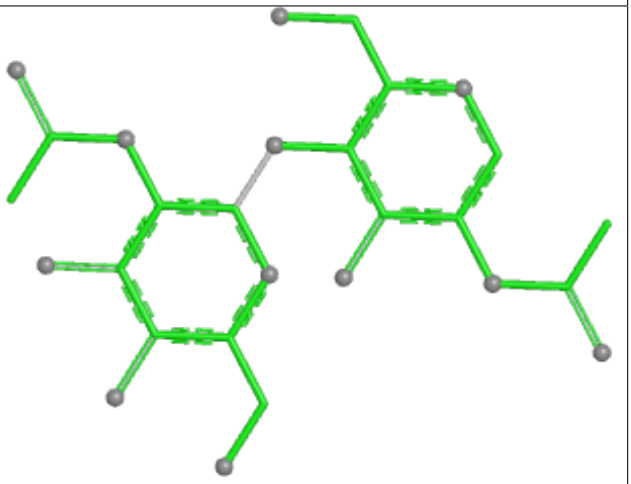
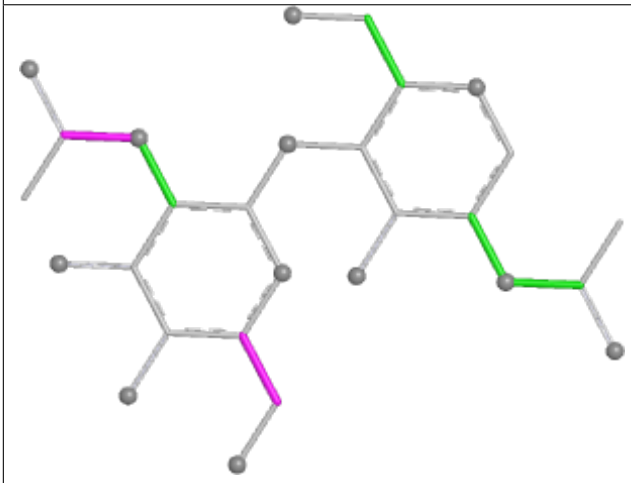
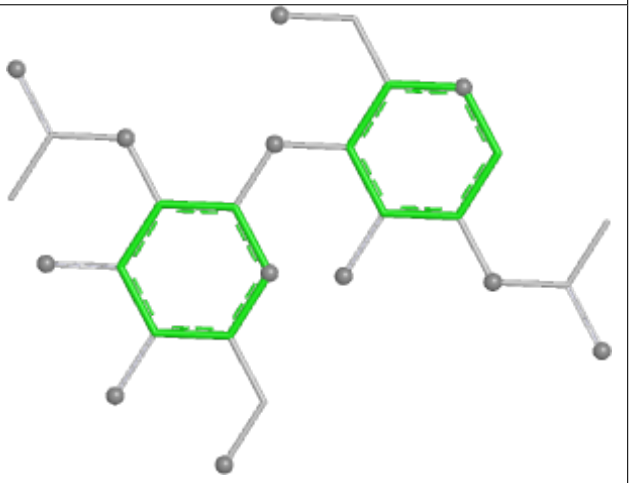


Bond angles

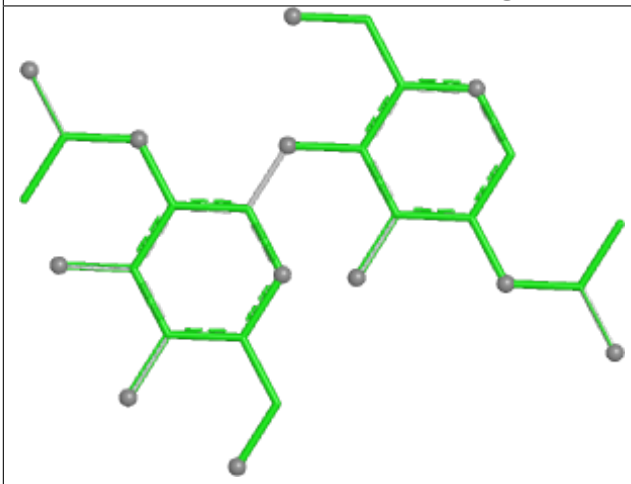


Torsions



Rings

Oligosaccharide Chain J



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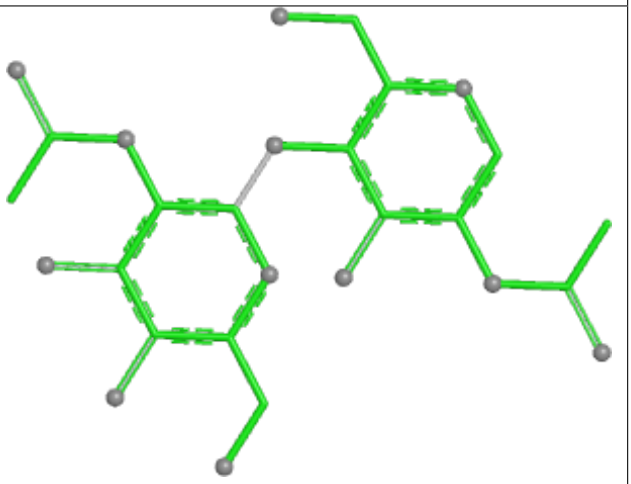
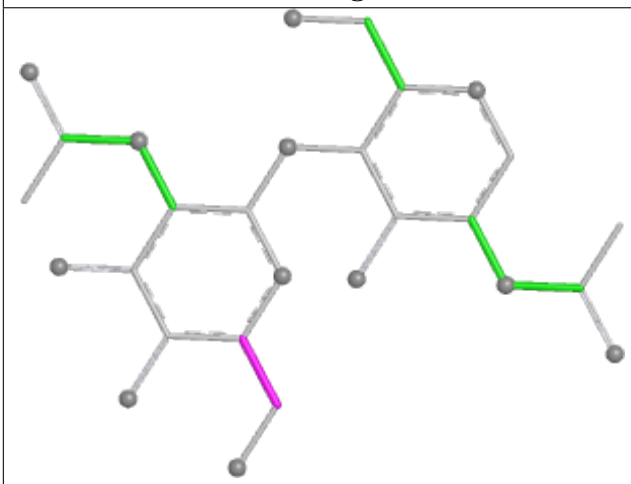
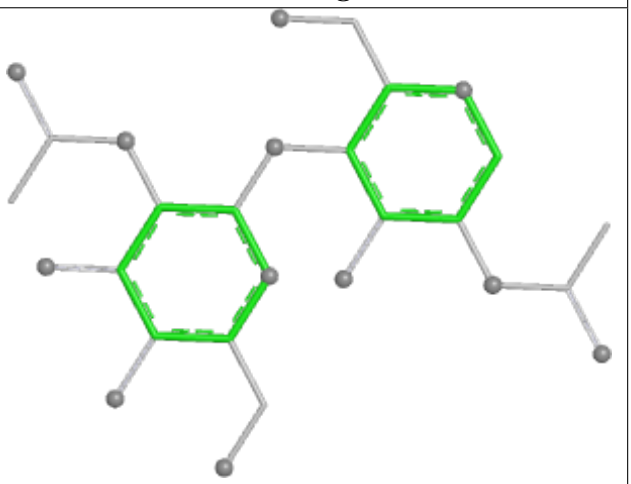


Bond angles

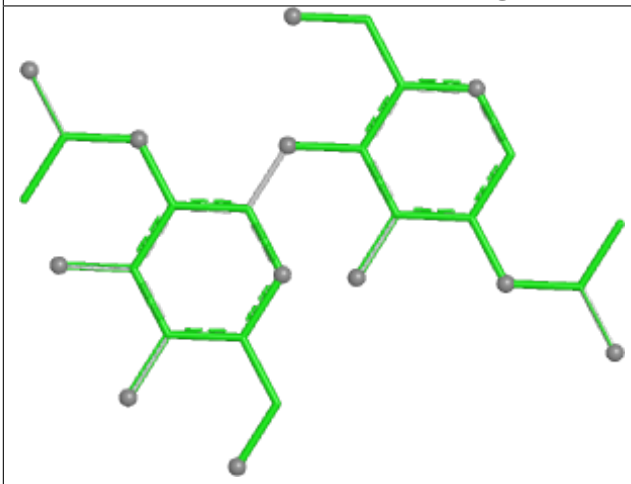


Torsions

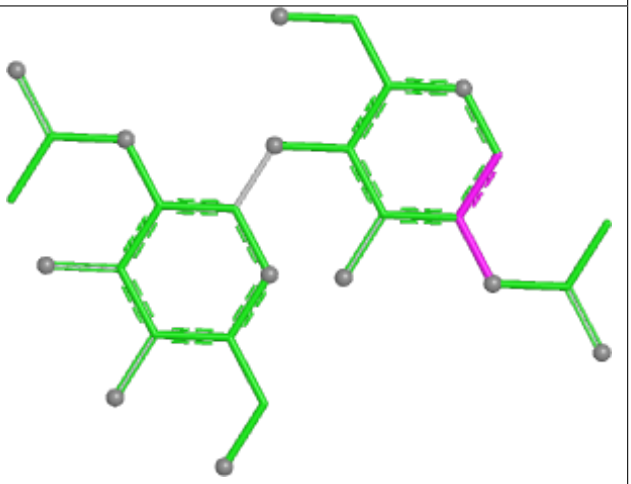


Rings

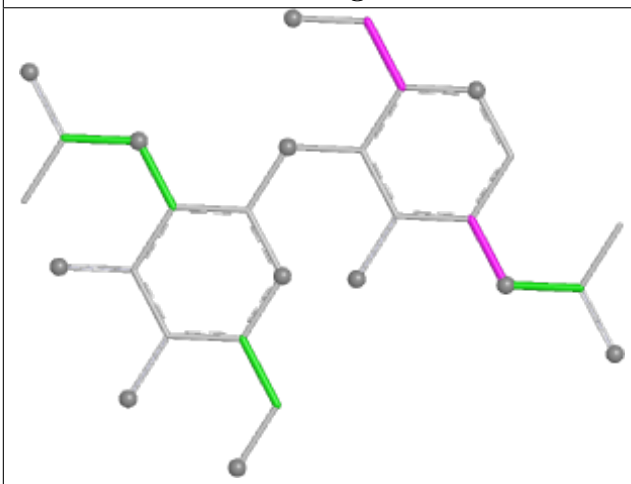
Oligosaccharide Chain K



Bond lengths



Bond angles



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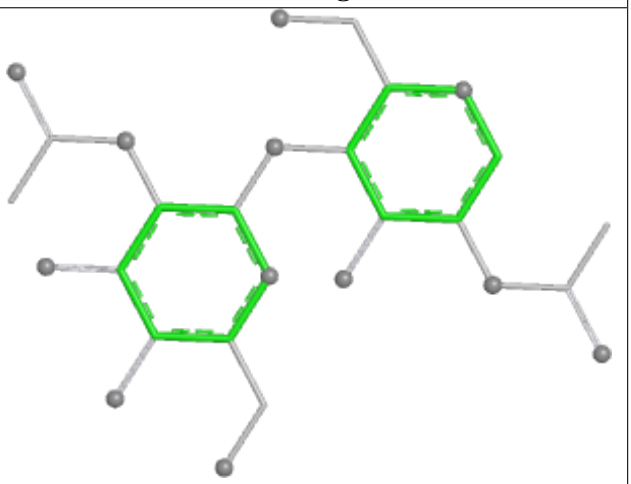
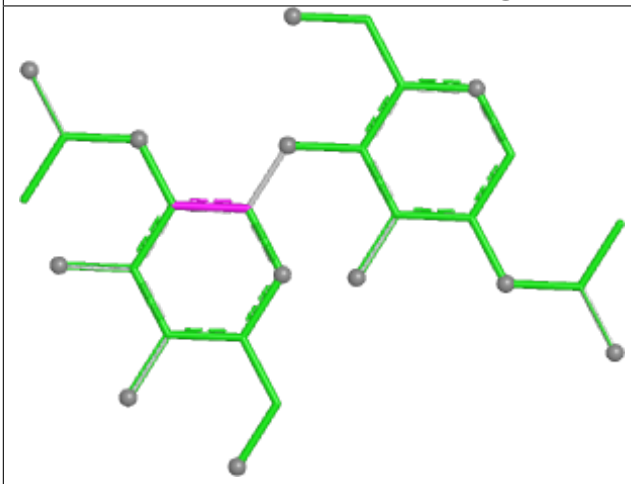
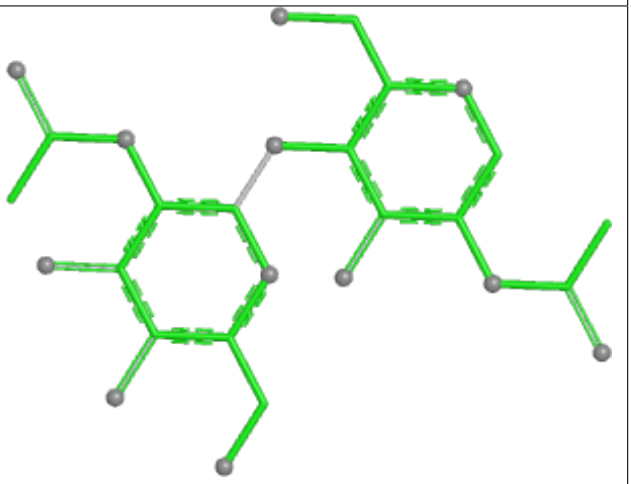


Rings

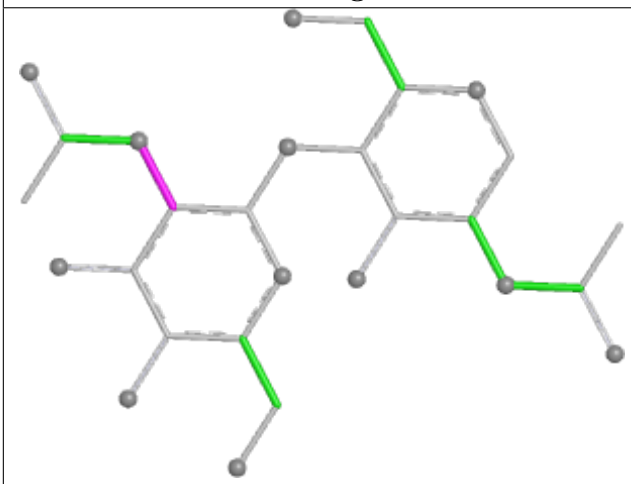
Oligosaccharide Chain L



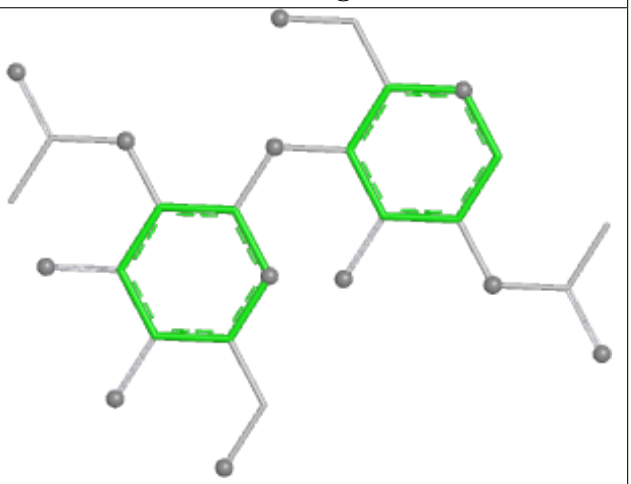
Bond lengths



Bond angles

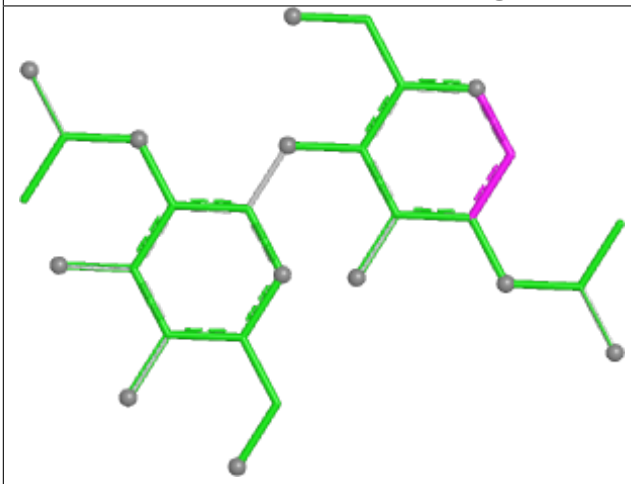


Torsions

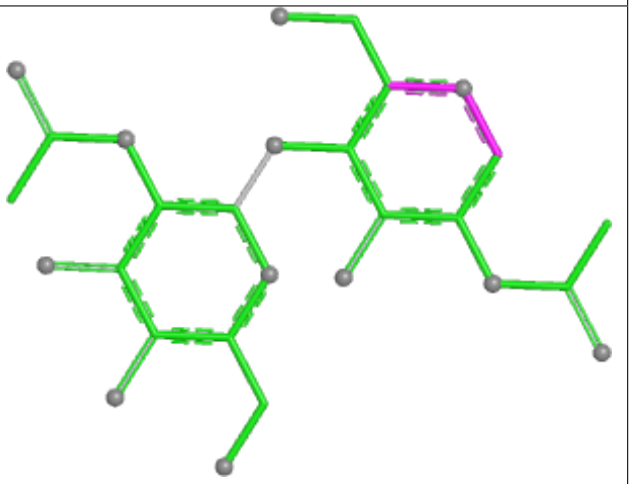


Rings

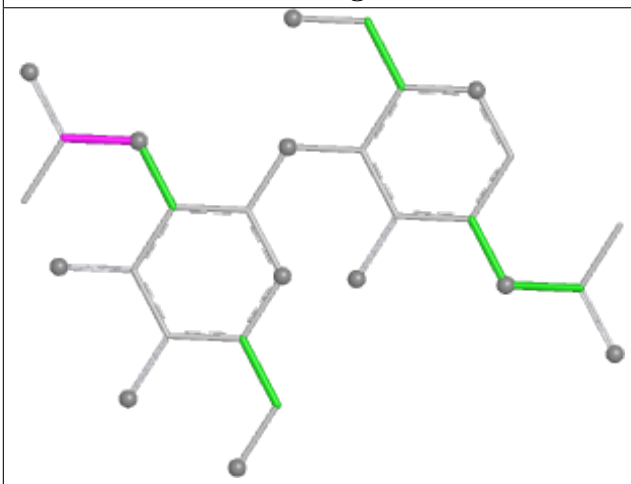
Oligosaccharide Chain M



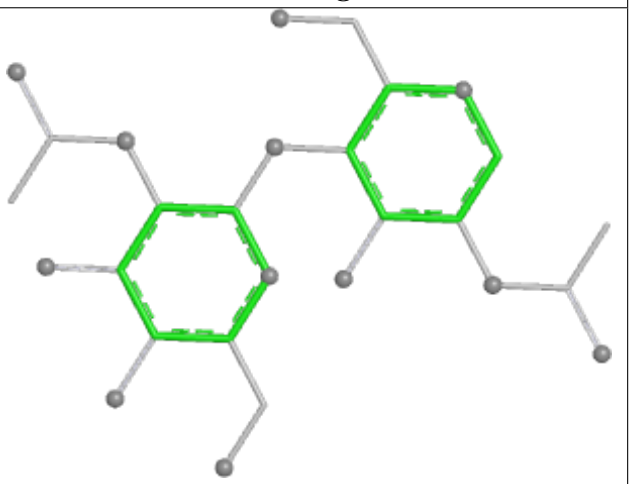
Bond lengths



Bond angles

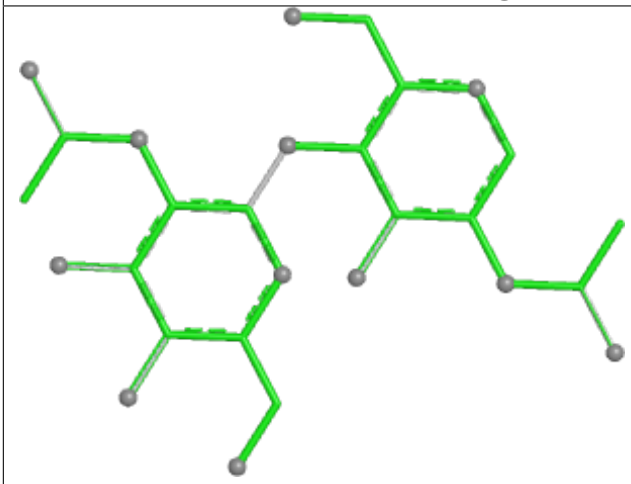


Torsions

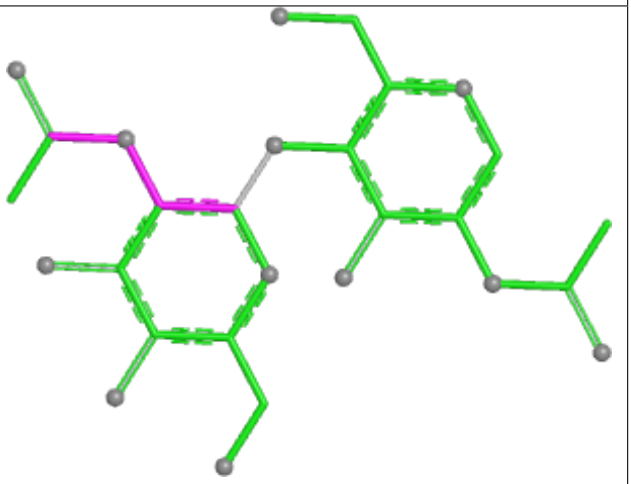


Rings

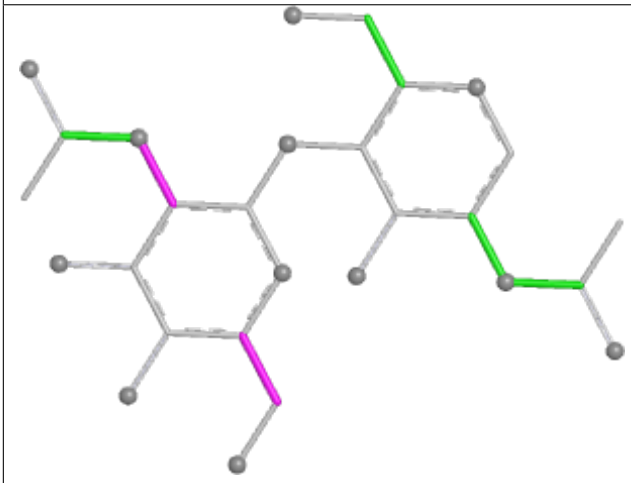
Oligosaccharide Chain P



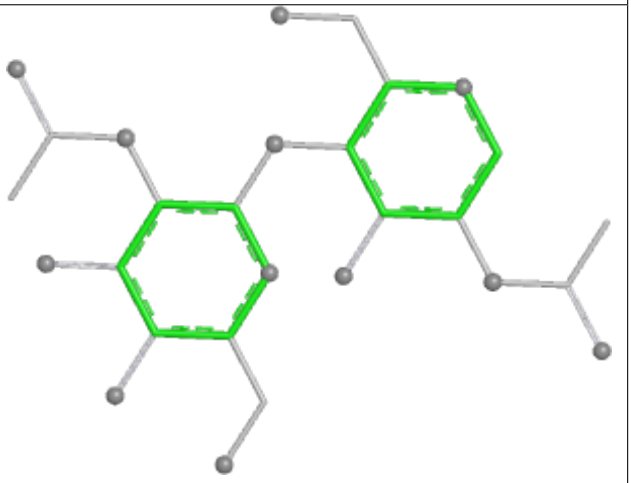
Bond lengths



Bond angles

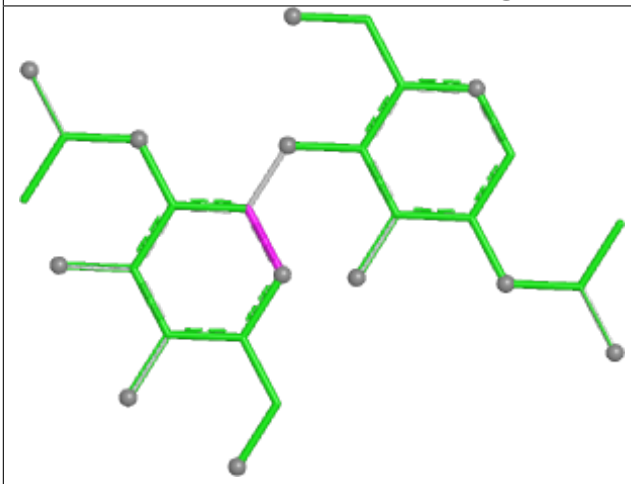


Torsions

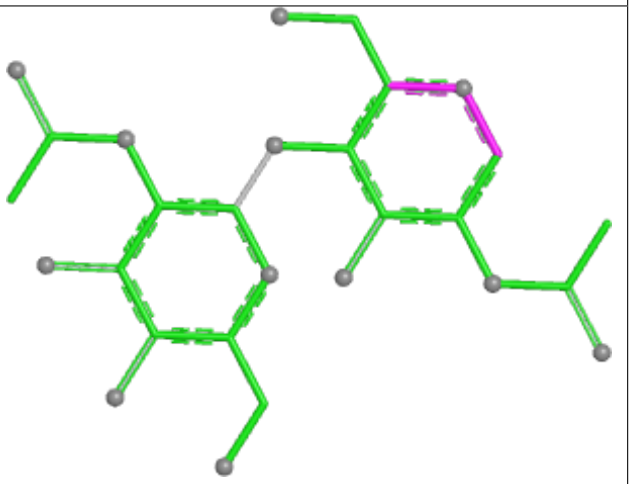


Rings

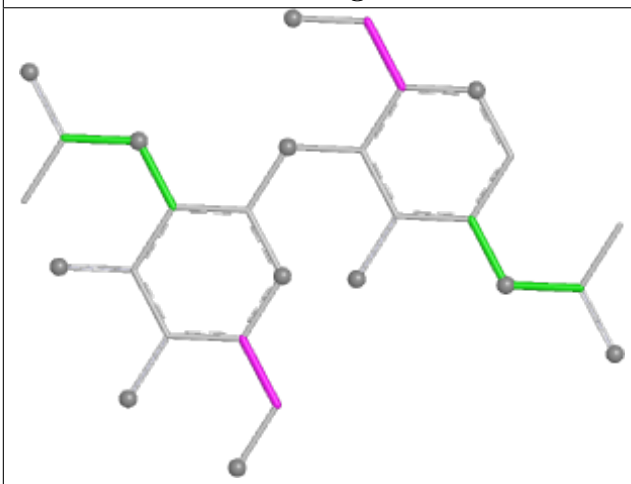
Oligosaccharide Chain S



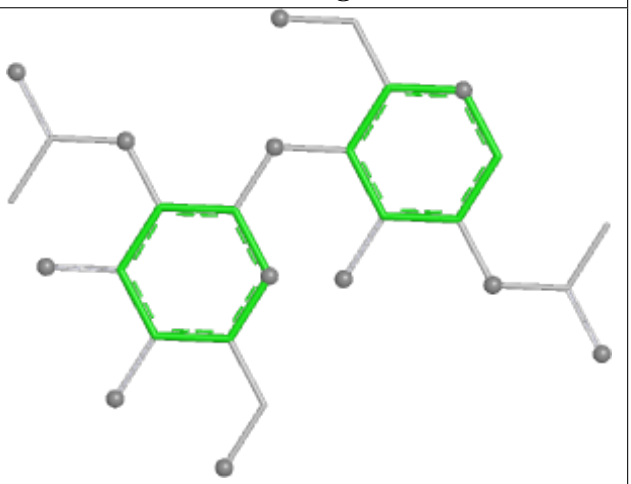
Bond lengths



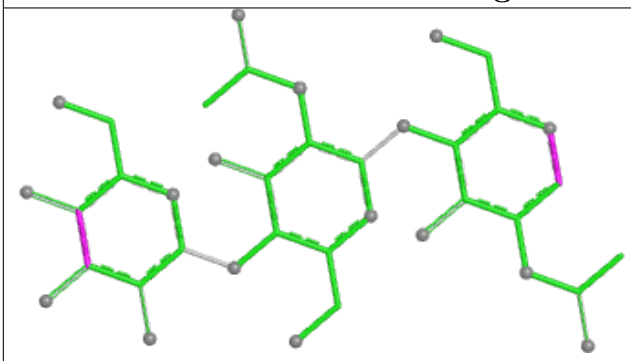
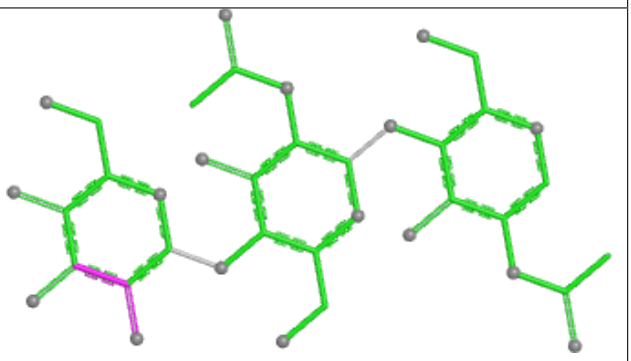
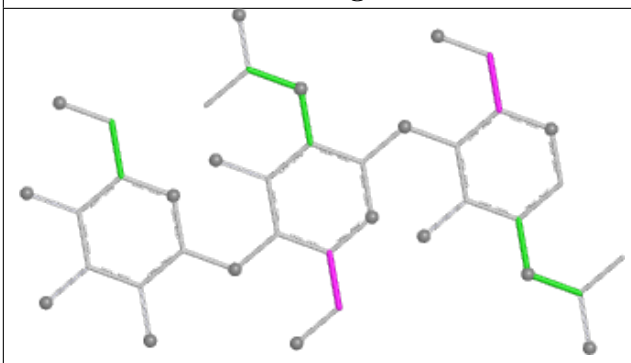
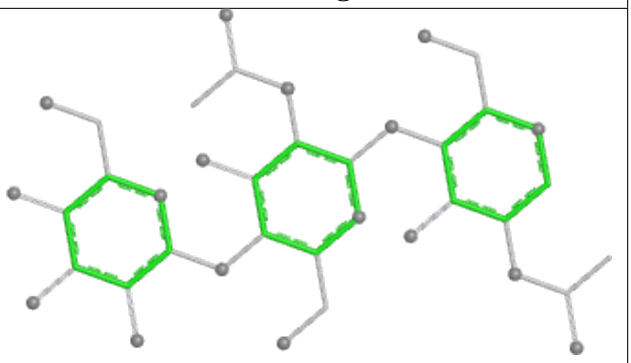
Bond angles

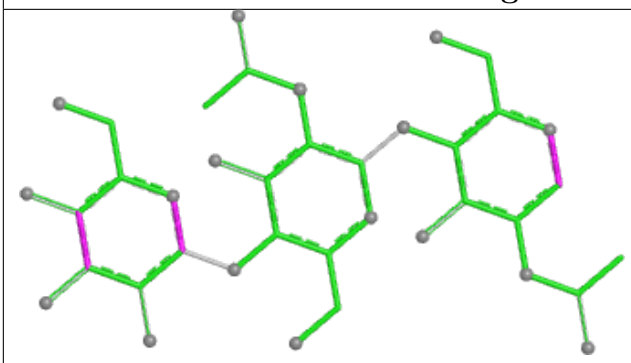
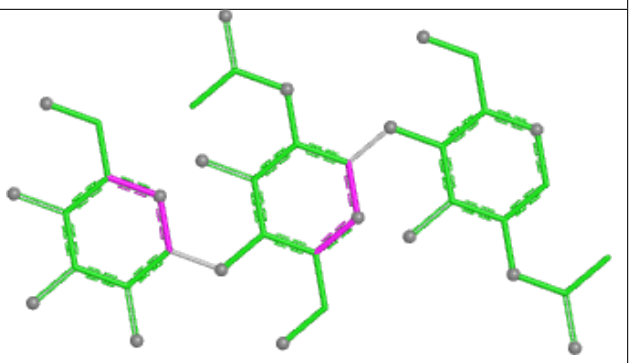
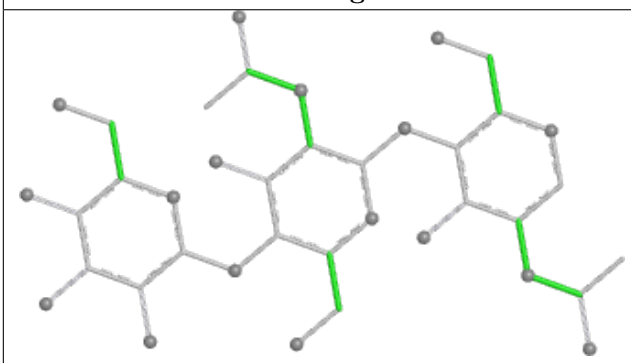
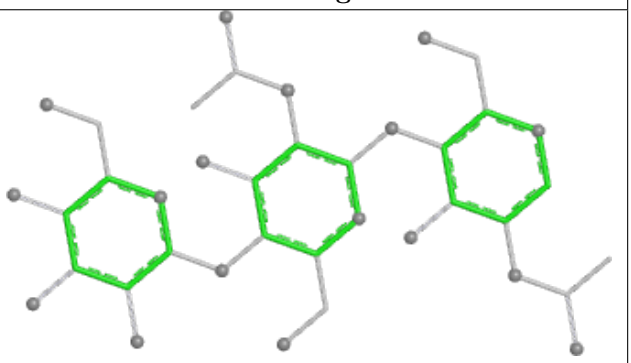


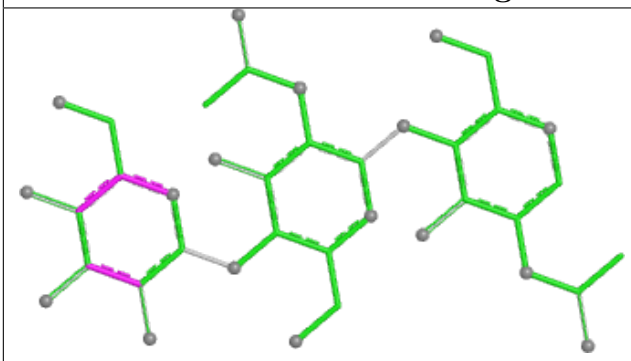
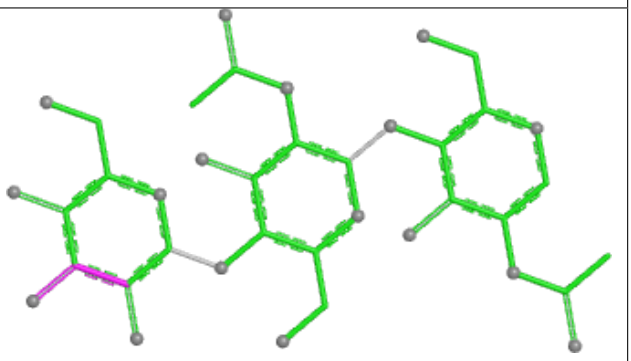
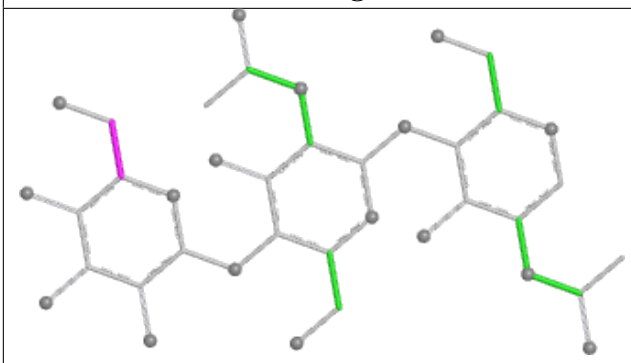
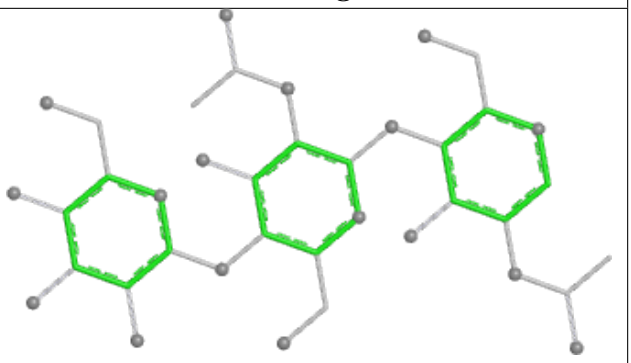
Torsions

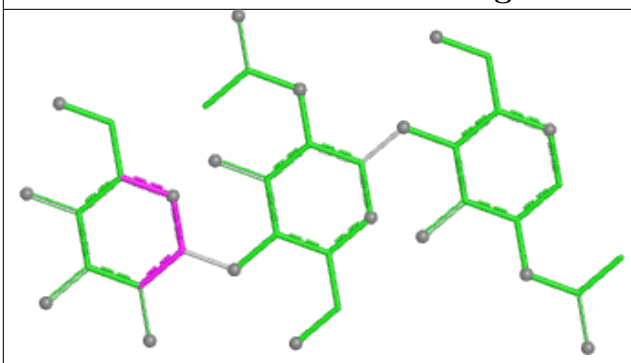
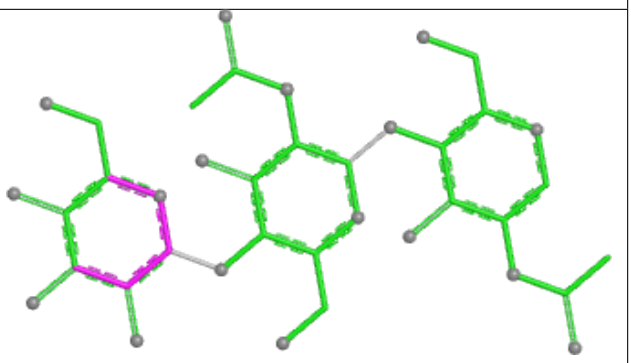
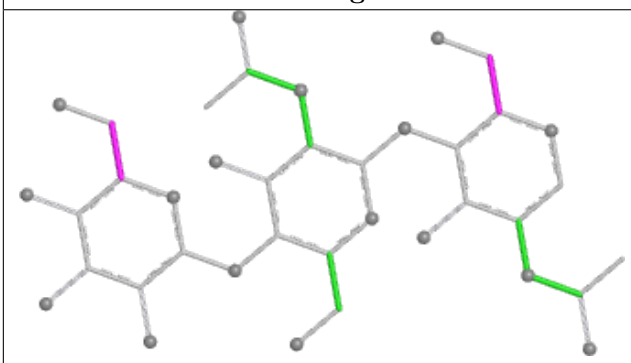
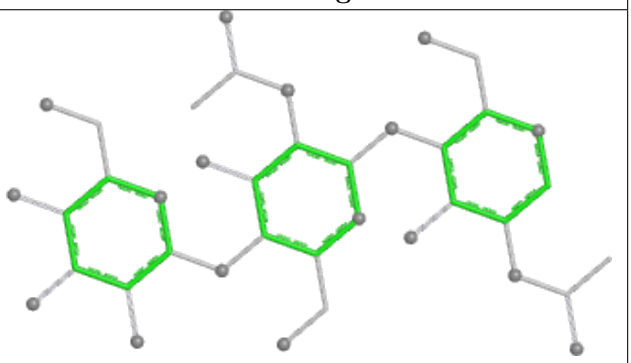


Rings

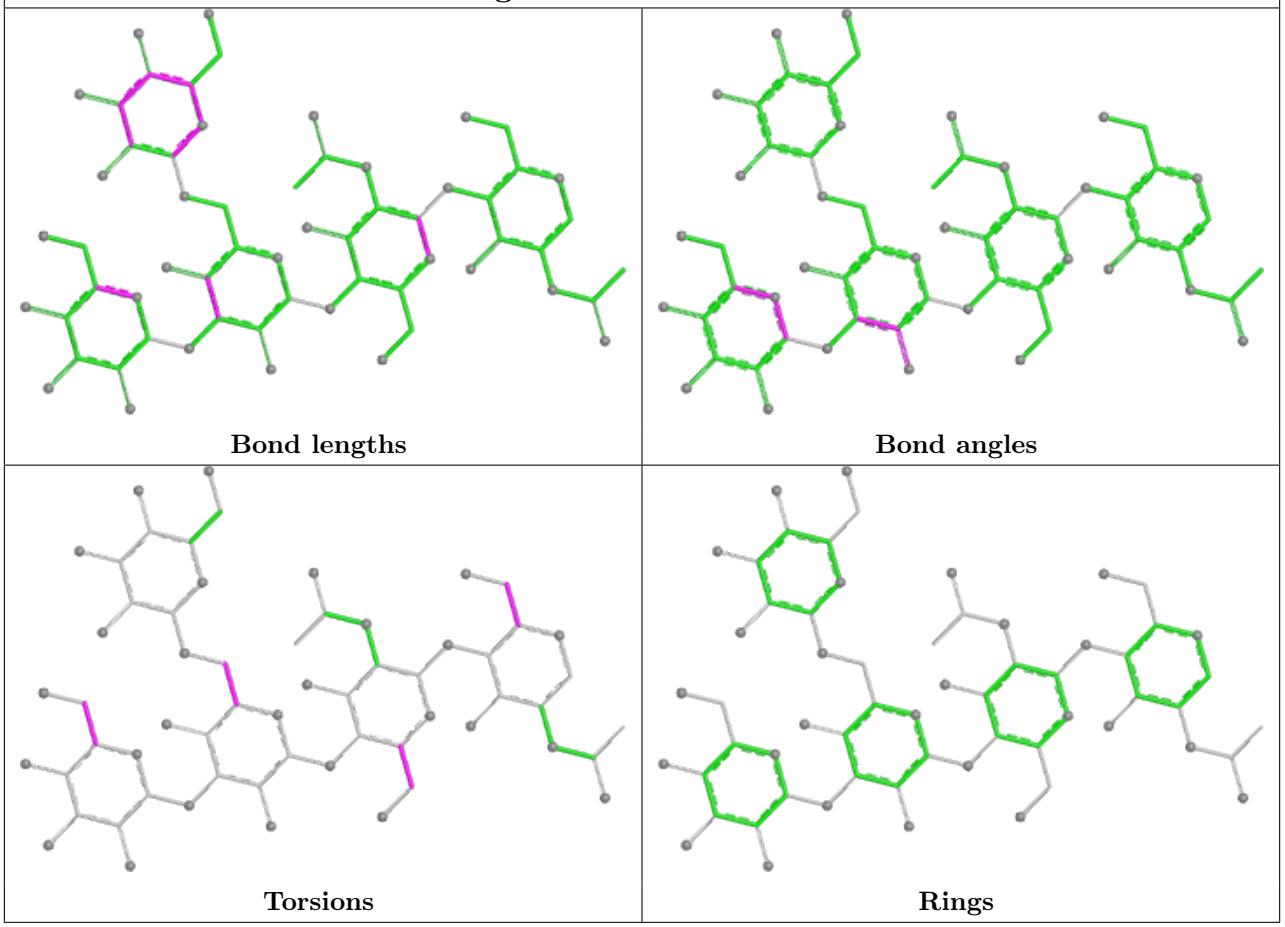
Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain I	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain R	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain N



5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 17 are monoatomic - leaving 25 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	$\#\|Z\| > 2$
7	NAG	C	1003	1	14,14,15	0.73	1 (7%)	17,19,21	0.77	1 (5%)
7	NAG	A	1004	1	14,14,15	0.29	0	17,19,21	0.40	0
7	NAG	B	1003	1	14,14,15	1.33	2 (14%)	17,19,21	1.92	6 (35%)
8	USK	A	1008	6	34,38,38	3.07	14 (41%)	34,53,53	3.36	10 (29%)
8	USK	D	1006	6	34,38,38	2.87	12 (35%)	34,53,53	3.49	12 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	D	1005	1	14,14,15	0.79	1 (7%)	17,19,21	1.35	2 (11%)
7	NAG	D	1004	1	14,14,15	0.97	2 (14%)	17,19,21	0.45	0
10	EDO	B	1006	-	3,3,3	0.58	0	2,2,2	0.03	0
7	NAG	A	1002	1	14,14,15	0.85	1 (7%)	17,19,21	1.40	2 (11%)
7	NAG	C	1004	1	14,14,15	0.66	1 (7%)	17,19,21	0.76	1 (5%)
10	EDO	A	1010	-	3,3,3	0.57	0	2,2,2	0.28	0
7	NAG	B	1002	1	14,14,15	1.09	2 (14%)	17,19,21	0.86	1 (5%)
10	EDO	D	1007	-	3,3,3	0.60	0	2,2,2	0.07	0
7	NAG	A	1003	1	14,14,15	0.85	1 (7%)	17,19,21	1.61	3 (17%)
8	USK	B	1005	6	34,38,38	2.97	12 (35%)	34,53,53	3.57	11 (32%)
7	NAG	A	1007	1	14,14,15	1.04	2 (14%)	17,19,21	0.75	0
7	NAG	B	1004	1	14,14,15	0.43	0	17,19,21	0.47	0
7	NAG	A	1006	1	14,14,15	0.84	1 (7%)	17,19,21	0.57	0
7	NAG	A	1005	1	14,14,15	0.60	0	17,19,21	0.57	0
7	NAG	D	1002	1	14,14,15	0.70	0	17,19,21	1.30	1 (5%)
8	USK	C	1006	6	34,38,38	3.01	15 (44%)	34,53,53	3.59	10 (29%)
7	NAG	C	1005	1	14,14,15	0.41	0	17,19,21	0.91	0
7	NAG	C	1002	1	14,14,15	0.56	0	17,19,21	0.70	0
9	PGE	A	1009	-	9,9,9	0.36	0	8,8,8	0.75	0
7	NAG	D	1003	1	14,14,15	0.97	1 (7%)	17,19,21	0.53	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	C	1003	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1004	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1003	1	-	3/6/23/26	0/1/1/1
8	USK	A	1008	6	-	6/18/30/30	0/4/4/4
8	USK	D	1006	6	-	5/18/30/30	0/4/4/4
7	NAG	D	1005	1	-	5/6/23/26	0/1/1/1
7	NAG	D	1004	1	-	1/6/23/26	0/1/1/1
10	EDO	B	1006	-	-	0/1/1/1	-
7	NAG	A	1002	1	-	4/6/23/26	0/1/1/1
7	NAG	C	1004	1	-	4/6/23/26	0/1/1/1
10	EDO	A	1010	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
10	EDO	D	1007	-	-	1/1/1/1	-
7	NAG	A	1003	1	-	3/6/23/26	0/1/1/1
8	USK	B	1005	6	-	9/18/30/30	0/4/4/4
7	NAG	A	1007	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1004	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
7	NAG	D	1002	1	-	5/6/23/26	0/1/1/1
8	USK	C	1006	6	-	2/18/30/30	0/4/4/4
7	NAG	C	1005	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1002	1	-	0/6/23/26	0/1/1/1
9	PGE	A	1009	-	-	2/7/7/7	-
7	NAG	D	1003	1	-	4/6/23/26	0/1/1/1

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1006	USK	C23-N24	11.60	1.45	1.32
8	B	1005	USK	C23-N24	11.48	1.44	1.32
8	D	1006	USK	C23-N24	11.42	1.44	1.32
8	A	1008	USK	C23-N24	11.38	1.44	1.32
8	C	1006	USK	C03-S13	-6.00	1.61	1.72

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1006	USK	O35-S02-O01	-15.69	100.26	119.55
8	B	1005	USK	O35-S02-O01	-15.57	100.41	119.55
8	D	1006	USK	O35-S02-O01	-15.05	101.05	119.55
8	A	1008	USK	O35-S02-O01	-14.55	101.66	119.55
8	C	1006	USK	C15-C16-C17	-7.16	119.88	129.46

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1003	NAG	C3-C2-N2-C7
7	B	1003	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	A	1008	USK	C05-C06-C07-C08
8	A	1008	USK	C05-C06-C07-C12
8	A	1008	USK	S13-C06-C07-C08

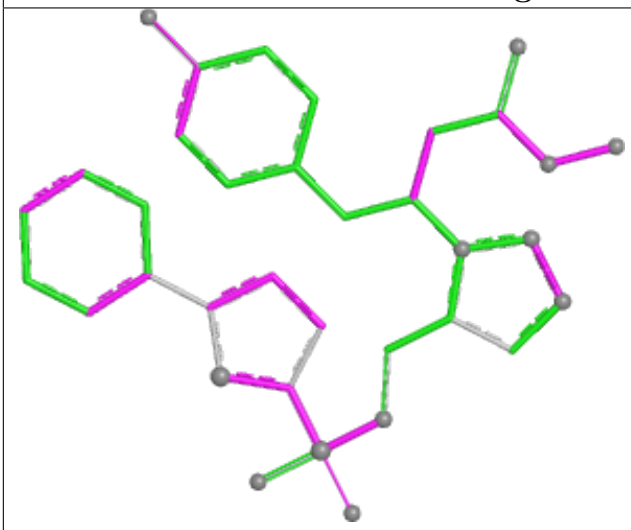
There are no ring outliers.

8 monomers are involved in 10 short contacts:

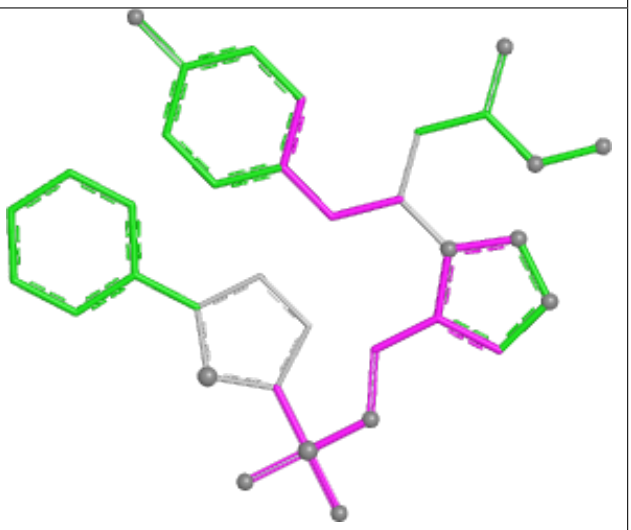
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	1006	USK	1	0
7	D	1005	NAG	1	0
7	A	1002	NAG	1	0
7	B	1002	NAG	1	0
8	B	1005	USK	2	0
7	B	1004	NAG	1	0
7	D	1002	NAG	1	0
8	C	1006	USK	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

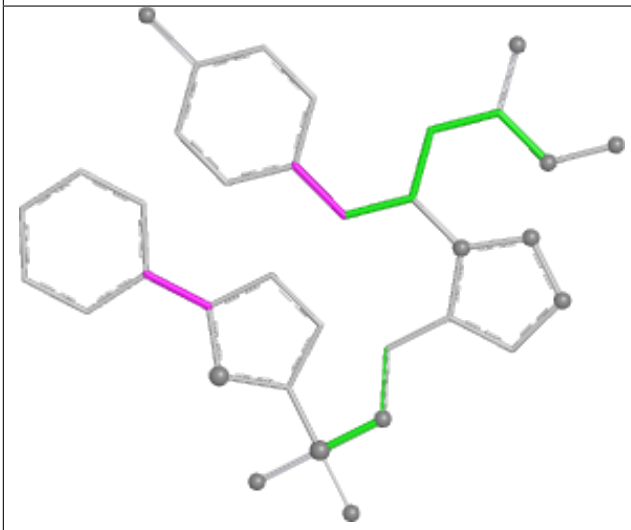
Ligand USK A 1008



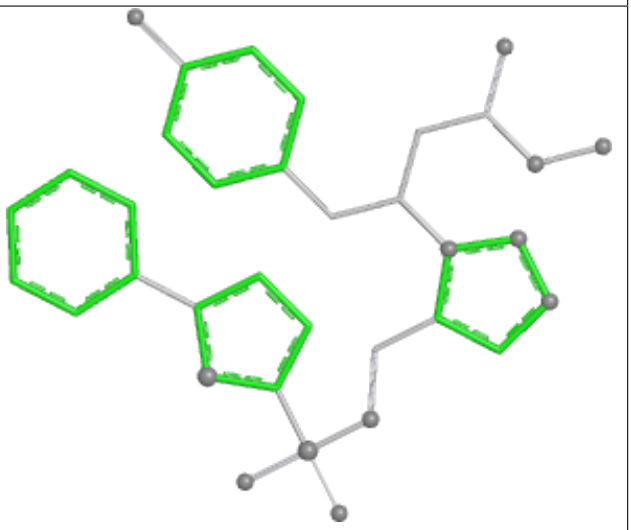
Bond lengths



Bond angles

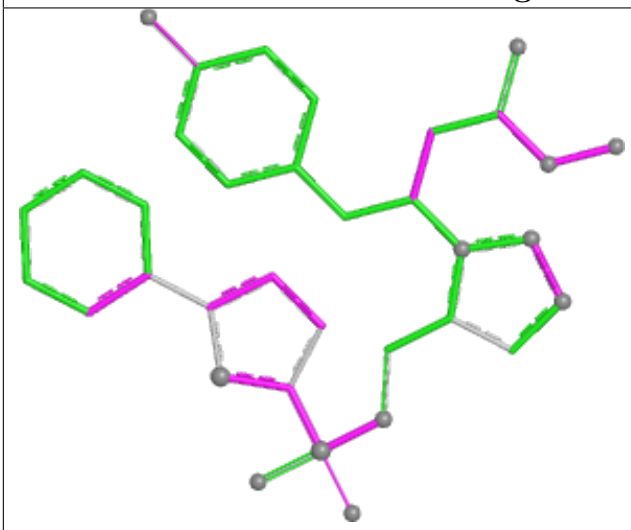


Torsions

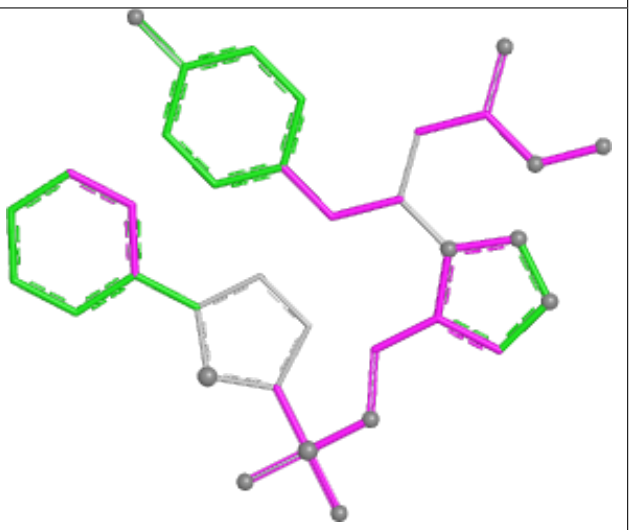


Rings

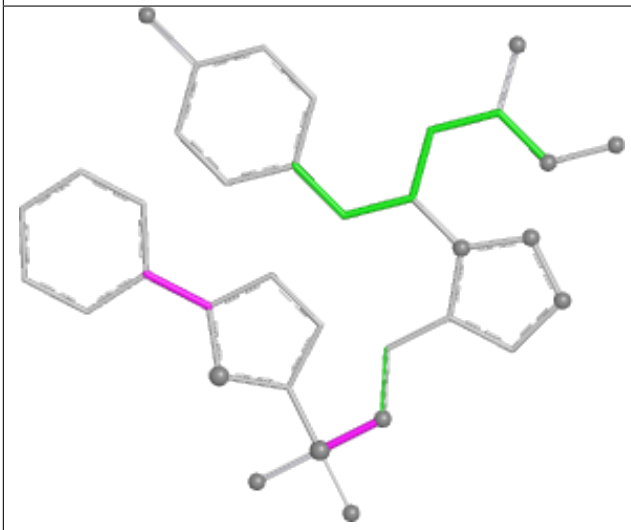
Ligand USK D 1006



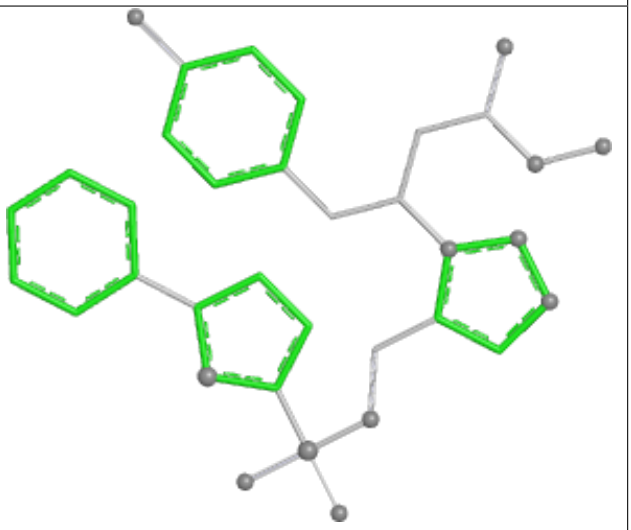
Bond lengths



Bond angles

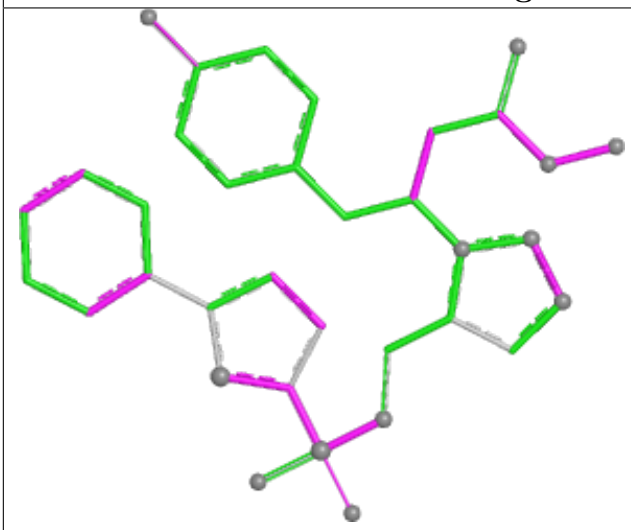


Torsions

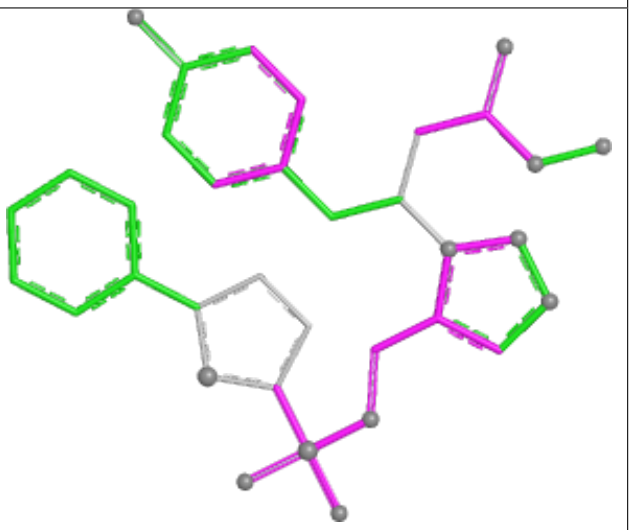


Rings

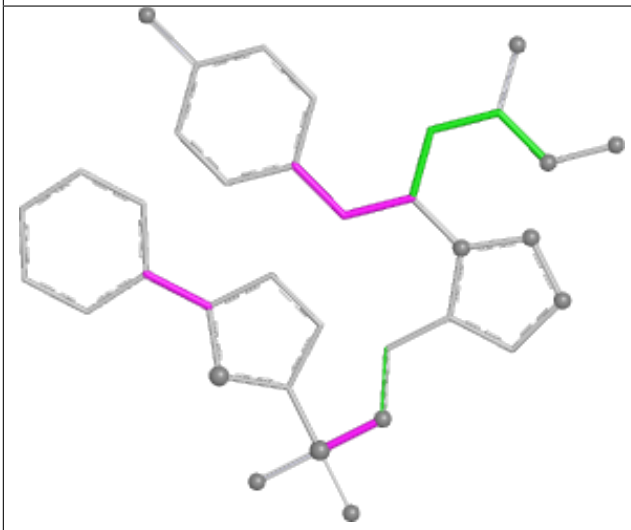
Ligand USK B 1005



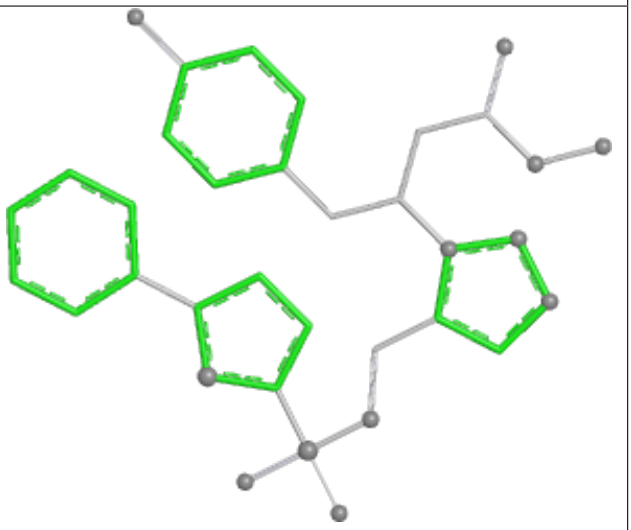
Bond lengths



Bond angles

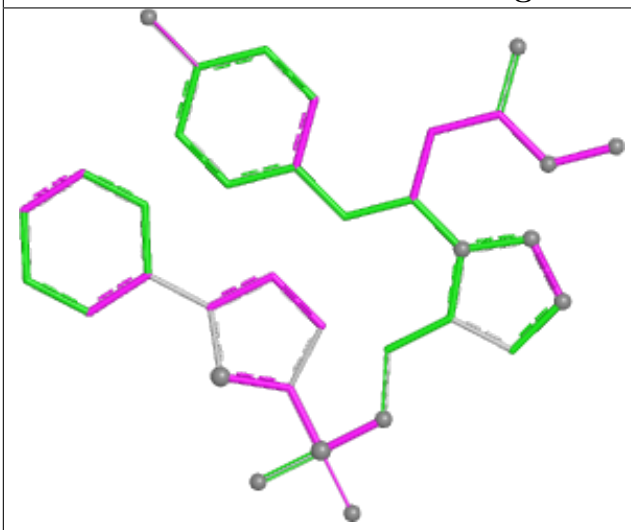


Torsions

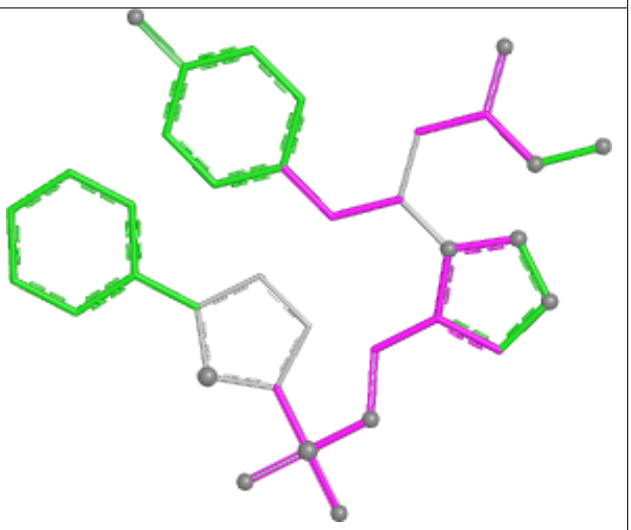


Rings

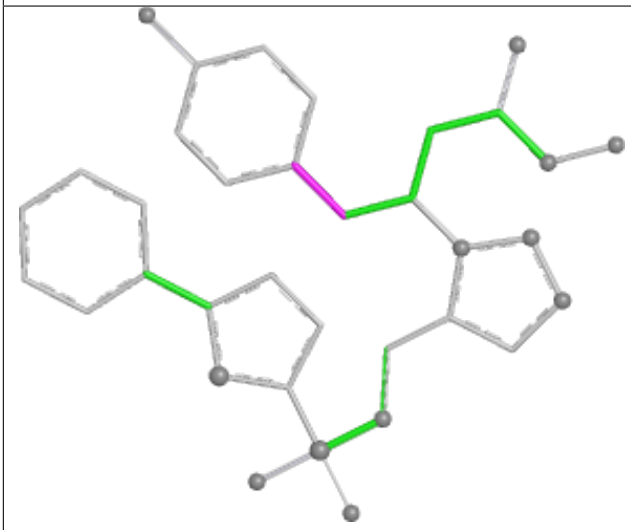
Ligand USK C 1006



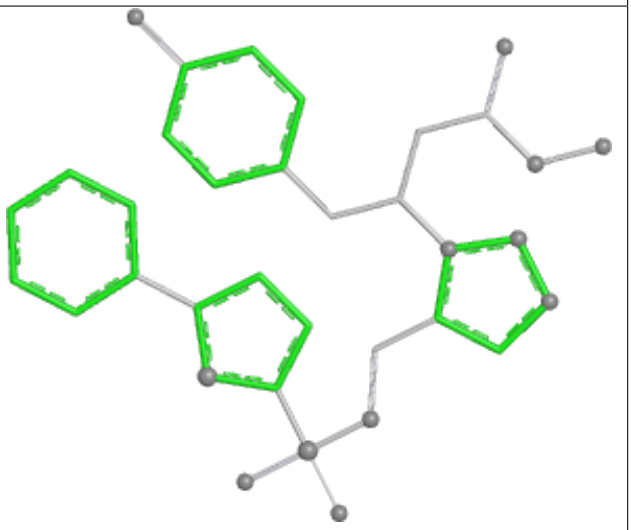
Bond lengths



Bond angles



Torsions



Rings

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	915/966 (94%)	-0.51	2 (0%)	95	90	15, 37, 80, 133	0
1	B	907/966 (93%)	-0.47	5 (0%)	89	78	18, 46, 88, 152	0
1	C	883/966 (91%)	-0.37	2 (0%)	95	90	24, 60, 107, 154	0
1	D	884/966 (91%)	-0.29	10 (1%)	80	64	25, 66, 116, 159	0
All	All	3589/3864 (92%)	-0.41	19 (0%)	91	81	15, 51, 103, 159	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	522	SER	4.2
1	B	503	CYS	3.2
1	D	623	PHE	3.2
1	D	640	TRP	2.8
1	D	621	VAL	2.8

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

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	NAG	M	2	14/15	0.73	0.28	65,117,124,126	0
4	BMA	R	3	11/12	0.78	0.18	89,100,112,118	0

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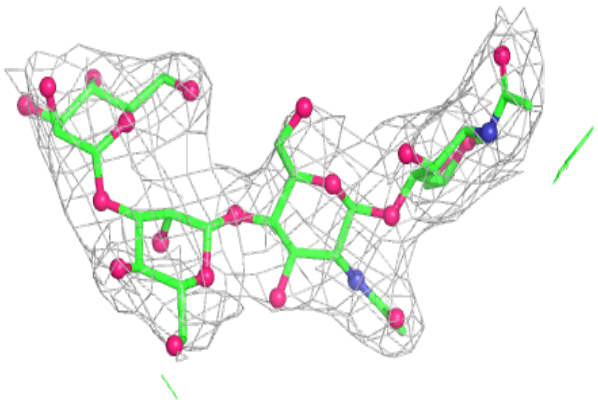
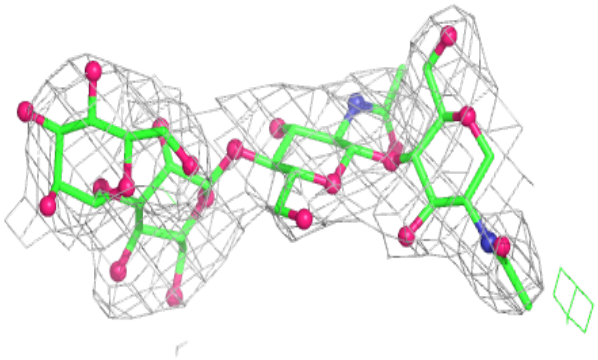
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	S	2	14/15	0.79	0.34	55,102,111,114	0
3	NAG	L	2	14/15	0.79	0.39	87,101,109,111	0
3	NAG	K	2	14/15	0.80	0.35	96,111,115,117	0
3	NAG	M	1	14/15	0.82	0.18	80,101,116,122	0
3	NAG	P	2	14/15	0.82	0.27	89,111,120,122	0
4	BMA	H	3	11/12	0.84	0.18	90,98,103,103	0
4	BMA	O	3	11/12	0.84	0.13	59,75,95,96	0
2	MAN	E	4	11/12	0.84	0.16	77,94,100,113	0
3	NAG	K	1	14/15	0.85	0.15	67,85,109,115	0
4	BMA	I	3	11/12	0.85	0.13	79,95,103,104	0
5	MAN	N	5	11/12	0.85	0.19	67,85,90,92	0
3	NAG	S	1	14/15	0.86	0.24	57,78,107,109	0
2	NAG	Q	2	14/15	0.88	0.17	56,77,81,89	0
4	NAG	R	2	14/15	0.89	0.16	55,86,100,104	0
2	MAN	Q	4	11/12	0.89	0.12	60,72,89,94	0
2	BMA	Q	3	11/12	0.89	0.12	61,78,83,96	0
4	NAG	H	2	14/15	0.90	0.20	73,82,92,100	0
4	NAG	O	1	14/15	0.90	0.18	55,77,93,102	0
3	NAG	J	2	14/15	0.90	0.15	79,93,106,107	0
2	BMA	E	3	11/12	0.92	0.12	75,79,89,89	0
4	NAG	O	2	14/15	0.92	0.14	52,79,100,102	0
3	NAG	G	2	14/15	0.93	0.14	62,81,88,97	0
2	NAG	E	2	14/15	0.93	0.16	44,74,92,93	0
3	NAG	L	1	14/15	0.93	0.19	64,86,91,98	0
4	NAG	H	1	14/15	0.94	0.16	44,53,69,76	0
5	MAN	N	4	11/12	0.94	0.16	38,60,85,97	0
3	NAG	P	1	14/15	0.94	0.21	57,76,104,114	0
4	NAG	R	1	14/15	0.95	0.12	39,62,69,79	0
3	NAG	J	1	14/15	0.95	0.13	48,65,81,101	0
3	NAG	F	2	14/15	0.95	0.15	20,46,67,67	0
5	BMA	N	3	11/12	0.95	0.10	60,72,82,83	0
2	NAG	Q	1	14/15	0.95	0.13	35,52,76,79	0
4	NAG	I	2	14/15	0.95	0.10	26,57,76,84	0
5	NAG	N	2	14/15	0.96	0.12	39,53,76,81	0
3	NAG	F	1	14/15	0.96	0.13	14,36,44,47	0
4	NAG	I	1	14/15	0.97	0.12	23,37,46,51	0
2	NAG	E	1	14/15	0.97	0.14	27,40,59,64	0
3	NAG	G	1	14/15	0.97	0.17	39,55,75,83	0
5	NAG	N	1	14/15	0.97	0.14	30,41,55,68	0

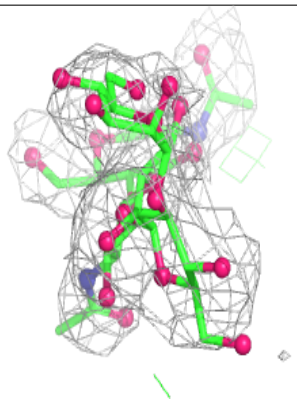
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

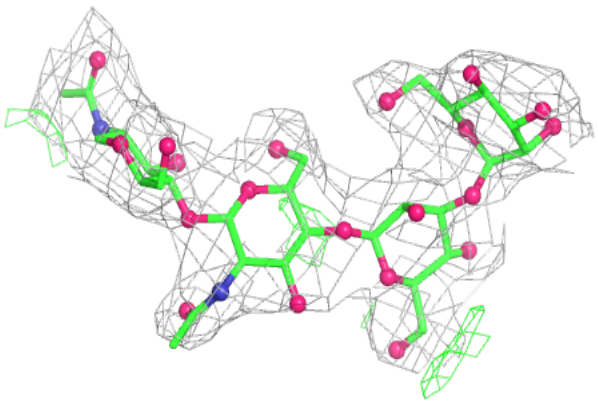


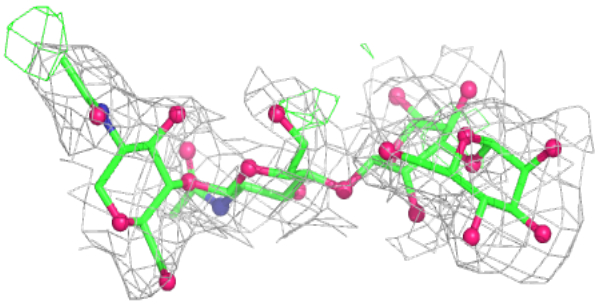


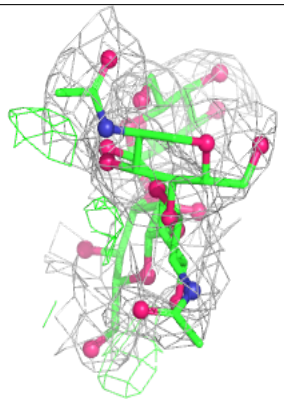


Electron density around Chain Q:

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

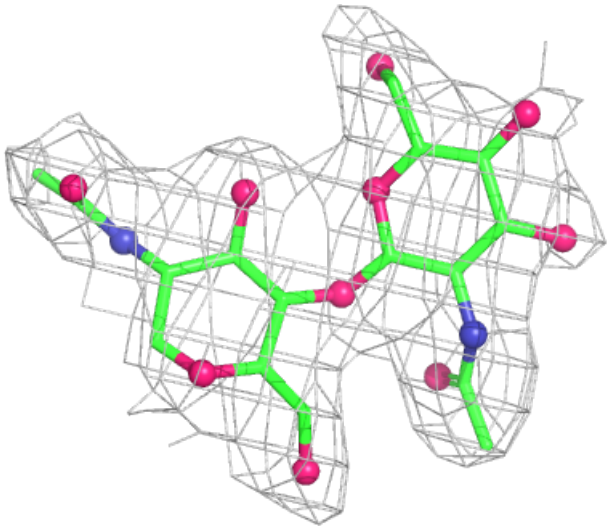


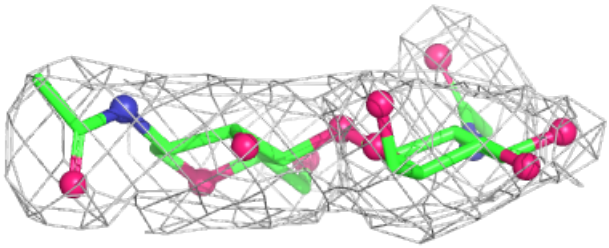


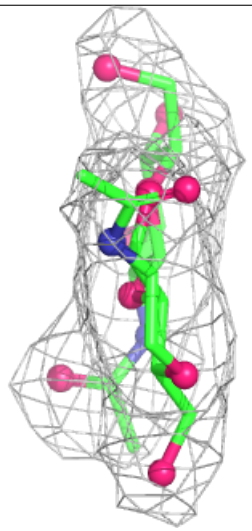


Electron density around Chain F:

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

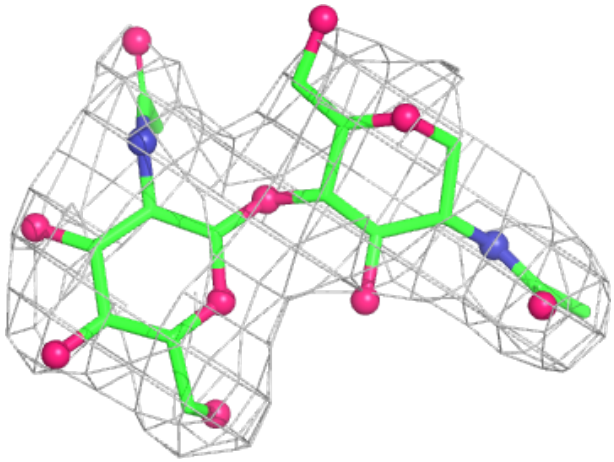


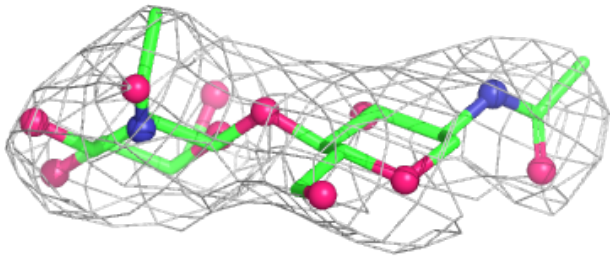


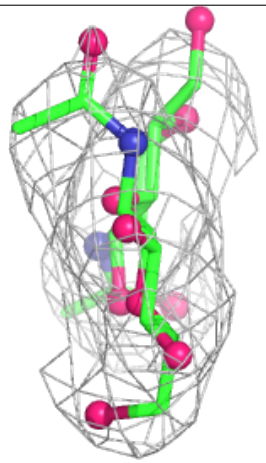


Electron density around Chain G:

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

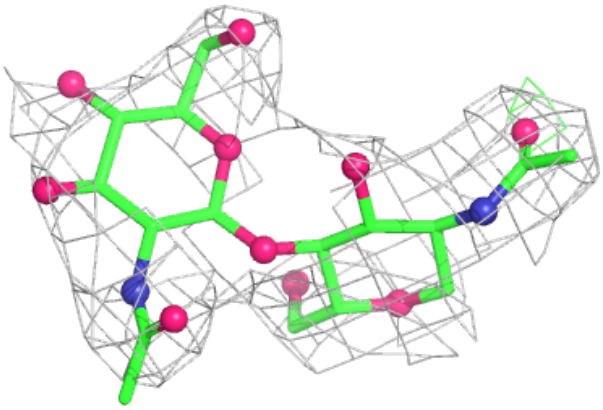


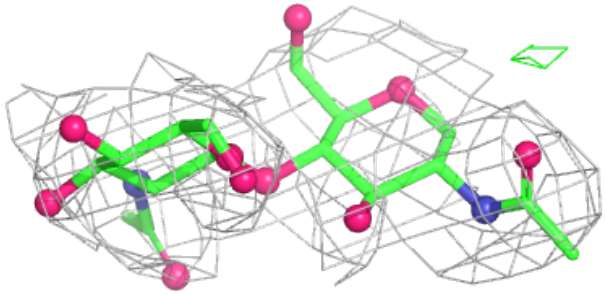


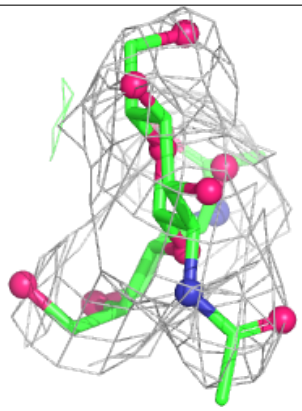


Electron density around Chain J:

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

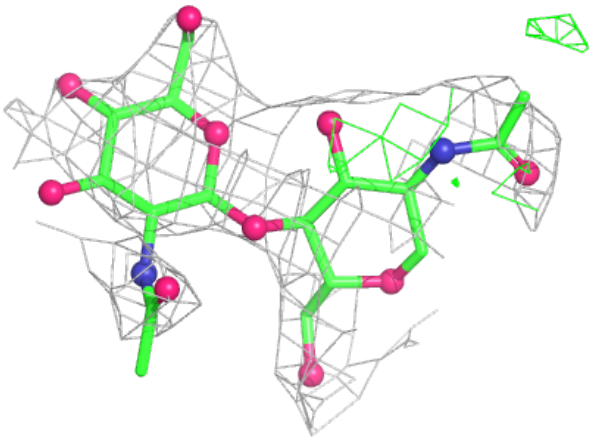


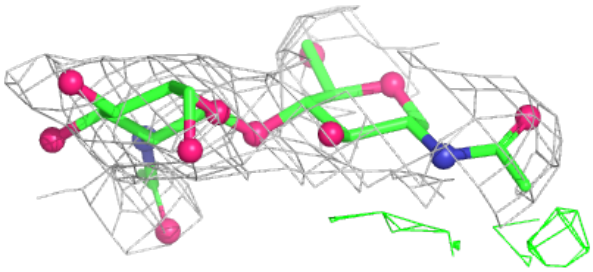


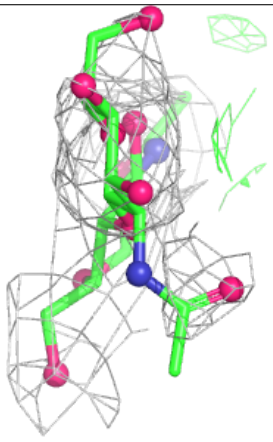


Electron density around Chain K:

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

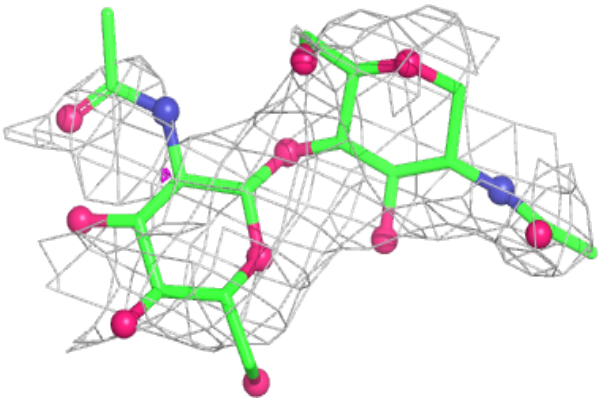


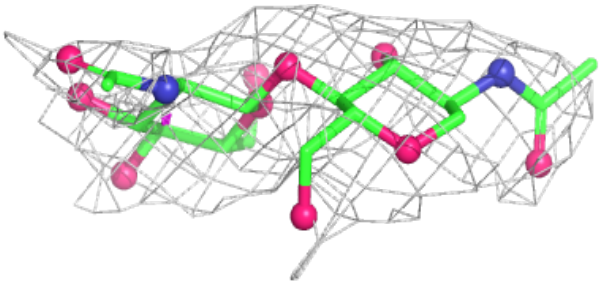


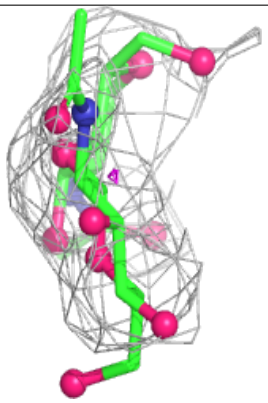


Electron density around Chain L:

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

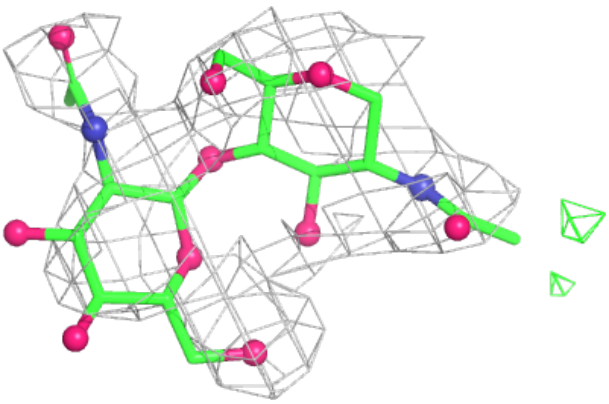


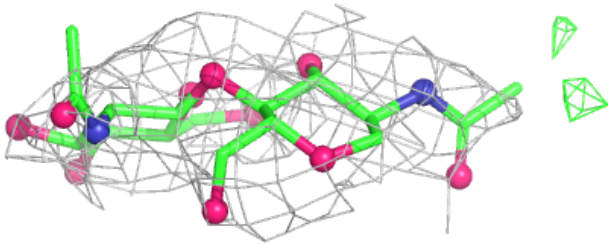


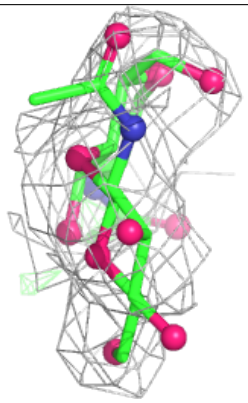


Electron density around Chain M:

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

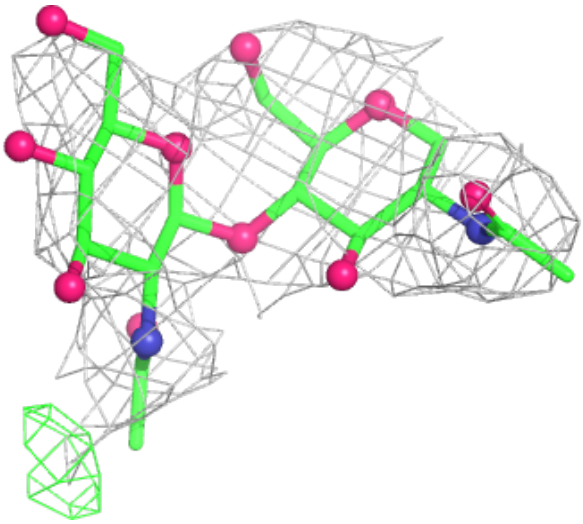


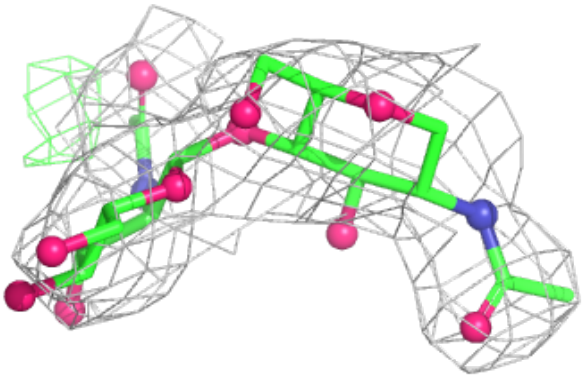


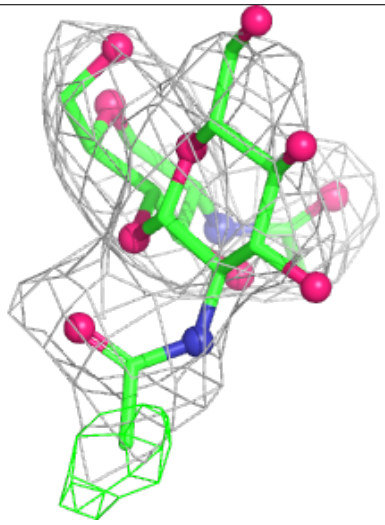


Electron density around Chain P:

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

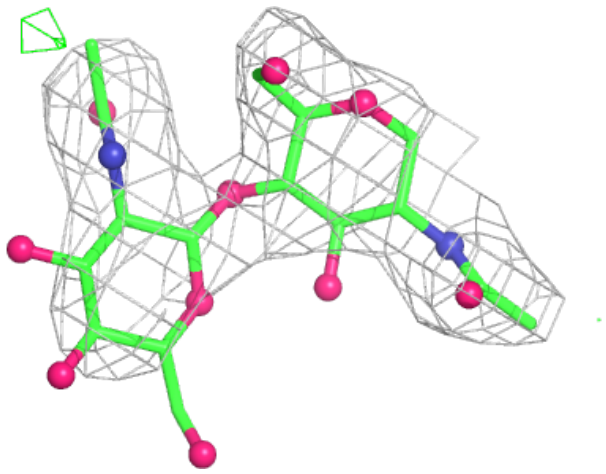


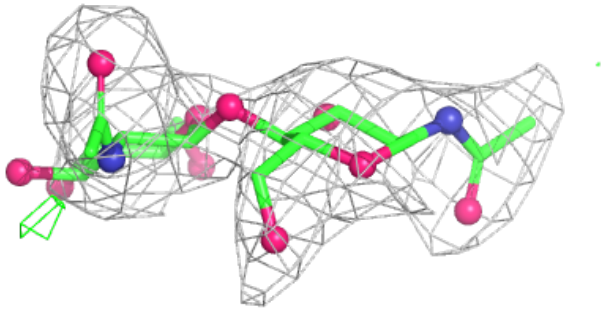


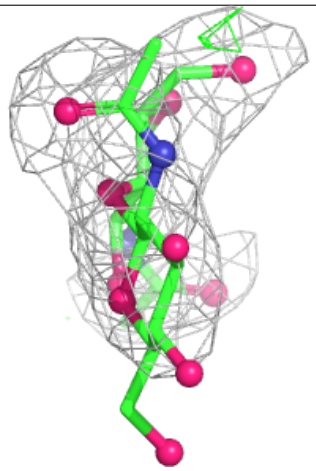


Electron density around Chain S:

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

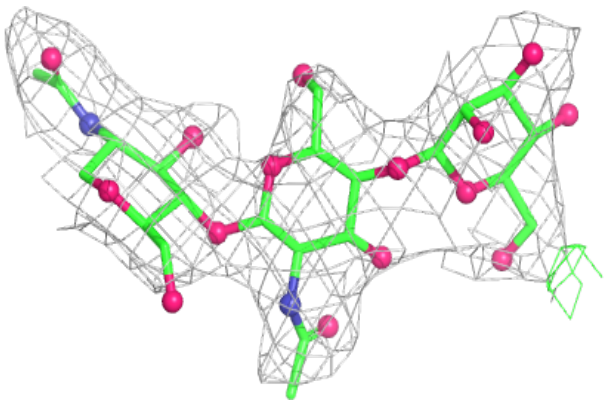


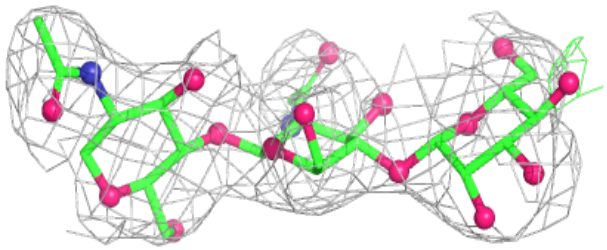


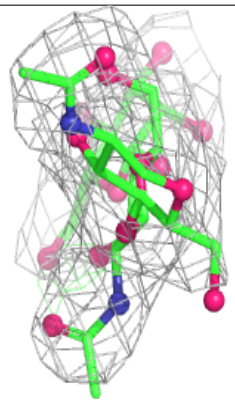


Electron density around Chain H:

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

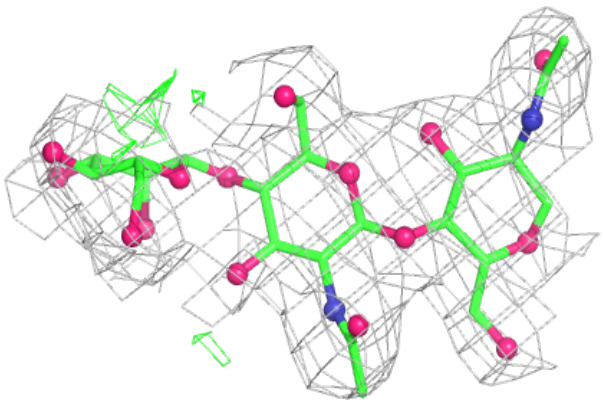


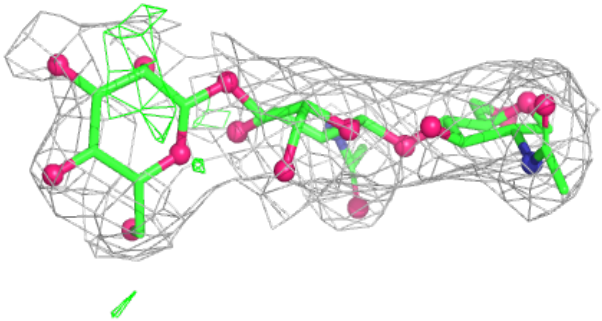


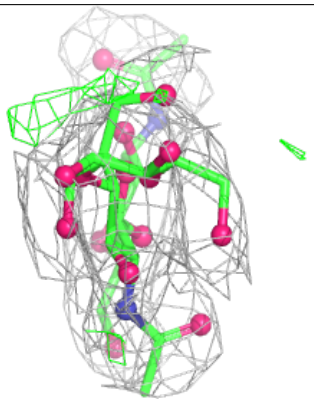


Electron density around Chain I:

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

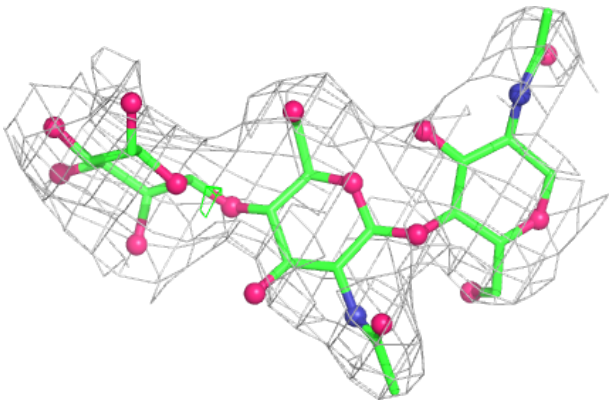


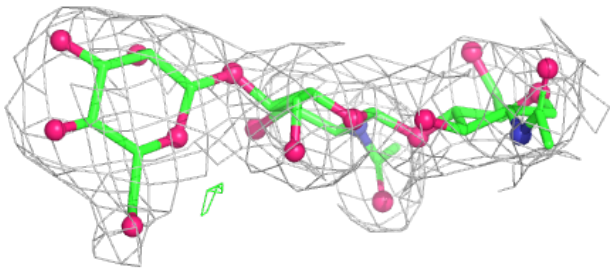


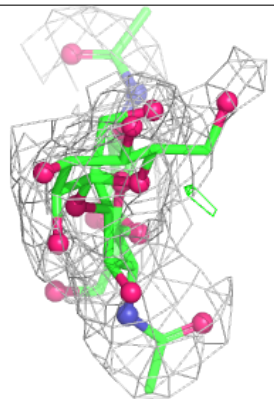


Electron density around Chain O:

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

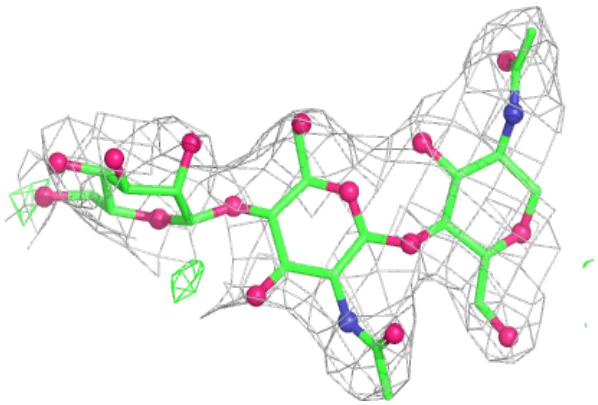


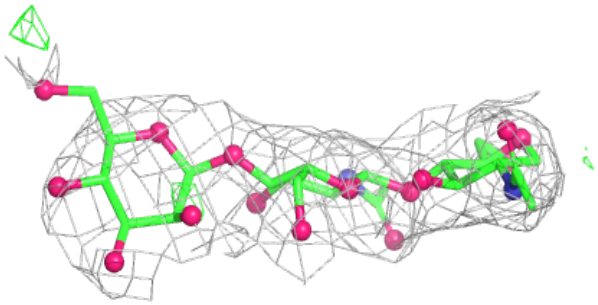


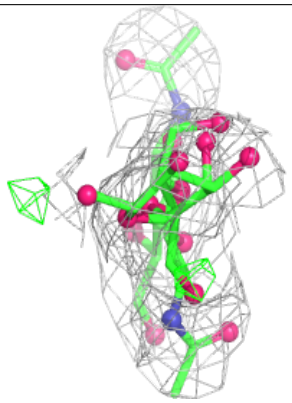


Electron density around Chain R:

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

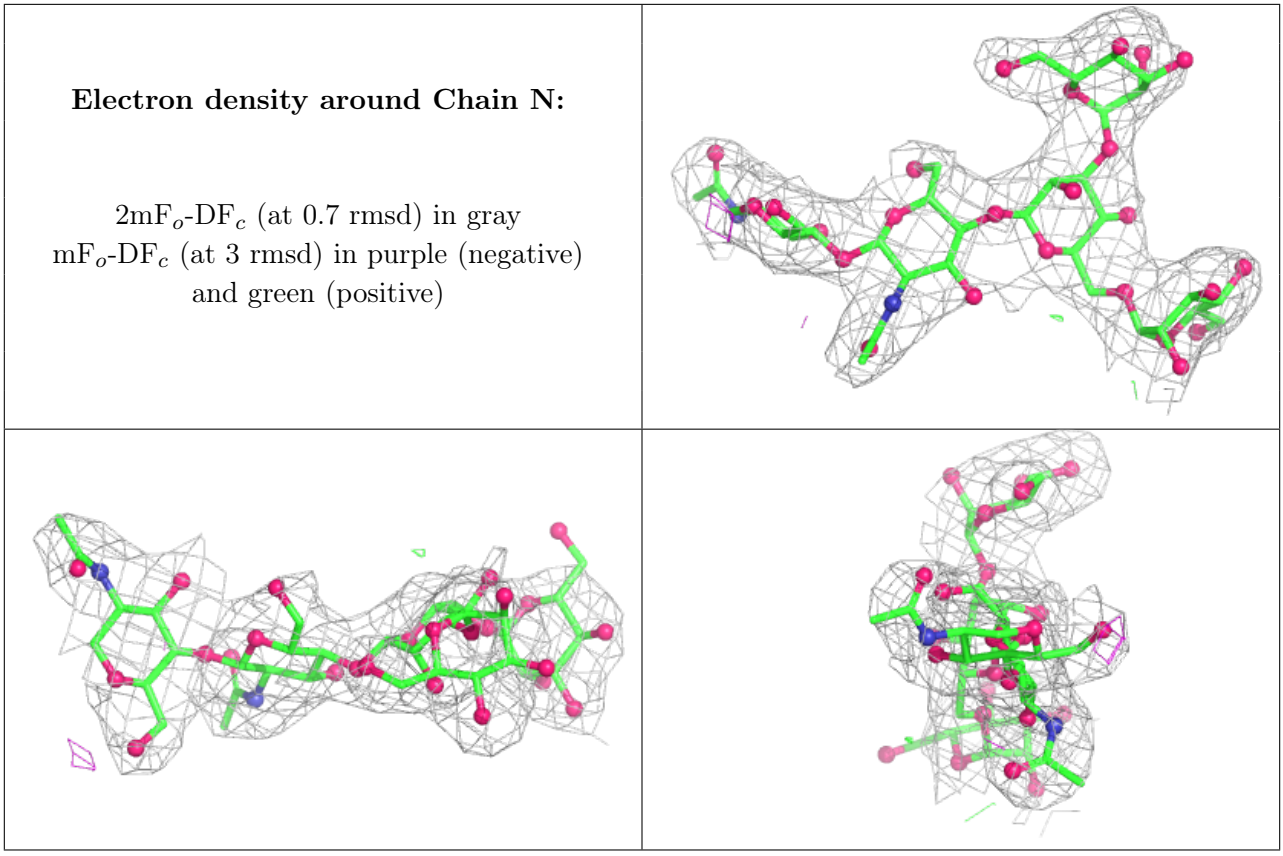






Electron density around Chain N:

$2mF_o$-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	BR	C	1008	1/1	0.28	0.28	240,240,240,240	0
11	BR	A	1013	1/1	0.64	0.36	302,302,302,302	0
11	BR	B	1007	1/1	0.69	0.32	262,262,262,262	0
11	BR	A	1011	1/1	0.70	0.46	299,299,299,299	0
10	EDO	B	1006	4/4	0.75	0.34	70,76,78,79	0
11	BR	A	1017	1/1	0.79	0.33	284,284,284,284	0
7	NAG	A	1003	14/15	0.80	0.16	76,96,106,107	0
7	NAG	A	1002	14/15	0.81	0.17	78,91,97,97	0
7	NAG	C	1002	14/15	0.81	0.20	80,98,101,101	0
11	BR	C	1007	1/1	0.82	0.47	290,290,290,290	0
7	NAG	C	1003	14/15	0.82	0.25	81,93,104,106	0
11	BR	D	1008	1/1	0.82	0.69	354,354,354,354	0
7	NAG	B	1004	14/15	0.83	0.14	76,90,98,98	0
11	BR	A	1015	1/1	0.84	0.36	282,282,282,282	0

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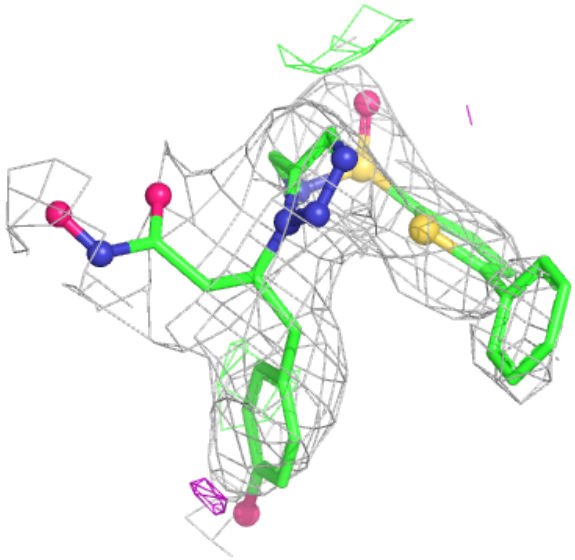
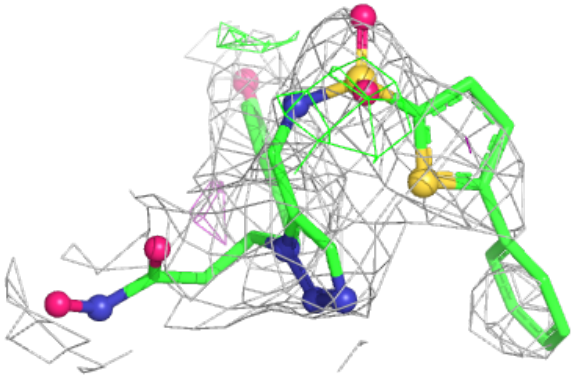
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	A	1006	14/15	0.84	0.21	75,102,118,120	0
11	BR	A	1016	1/1	0.85	0.23	268,268,268,268	0
7	NAG	B	1003	14/15	0.85	0.23	27,27,27,27	0
7	NAG	C	1005	14/15	0.85	0.15	69,88,94,98	0
7	NAG	A	1004	14/15	0.86	0.16	79,95,110,113	0
11	BR	A	1014	1/1	0.87	0.16	170,170,170,170	0
7	NAG	D	1002	14/15	0.87	0.18	70,95,104,106	0
11	BR	B	1008	1/1	0.88	0.45	290,290,290,290	0
7	NAG	B	1002	14/15	0.88	0.13	64,83,93,95	0
7	NAG	A	1005	14/15	0.89	0.14	39,60,86,87	0
7	NAG	D	1004	14/15	0.89	0.12	56,75,89,92	0
10	EDO	D	1007	4/4	0.90	0.31	22,41,42,46	0
7	NAG	C	1004	14/15	0.90	0.15	68,89,96,96	0
7	NAG	D	1003	14/15	0.90	0.12	62,88,94,101	0
7	NAG	D	1005	14/15	0.91	0.25	80,95,101,103	0
8	USK	B	1005	35/35	0.91	0.32	71,94,124,127	0
7	NAG	A	1007	14/15	0.91	0.20	60,83,93,96	0
9	PGE	A	1009	10/10	0.92	0.24	42,55,62,65	0
10	EDO	A	1010	4/4	0.92	0.16	47,62,70,70	0
8	USK	A	1008	35/35	0.92	0.19	36,66,97,106	0
11	BR	A	1018	1/1	0.94	0.20	187,187,187,187	0
8	USK	D	1006	35/35	0.94	0.21	55,92,118,121	0
8	USK	C	1006	35/35	0.95	0.25	39,78,112,118	0
11	BR	A	1012	1/1	0.96	0.33	218,218,218,218	0
6	ZN	D	1001	1/1	0.99	0.17	41,41,41,41	0
6	ZN	B	1001	1/1	0.99	0.18	32,32,32,32	0
6	ZN	C	1001	1/1	0.99	0.18	47,47,47,47	0
6	ZN	A	1001	1/1	1.00	0.21	35,35,35,35	0

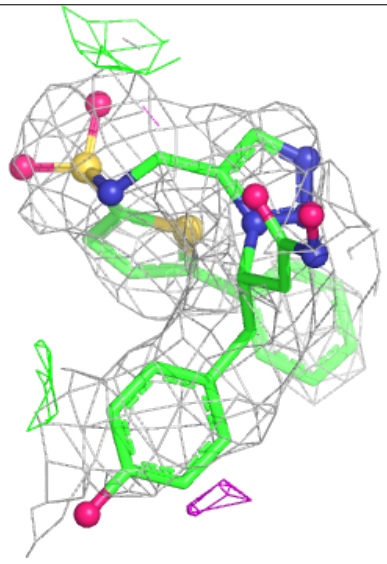
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around USK B 1005:

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

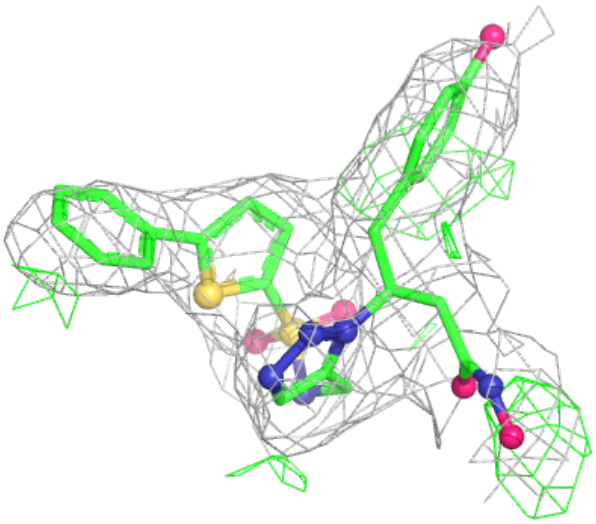


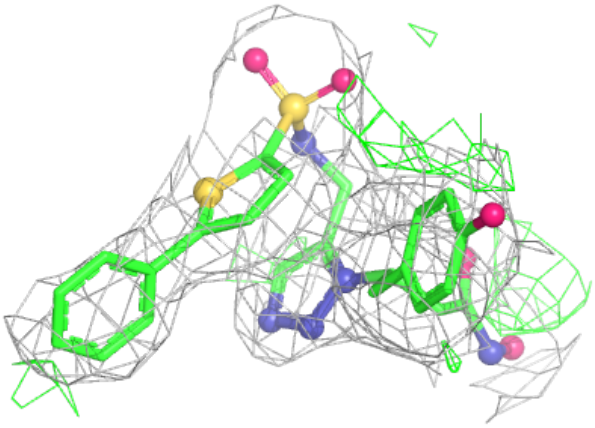


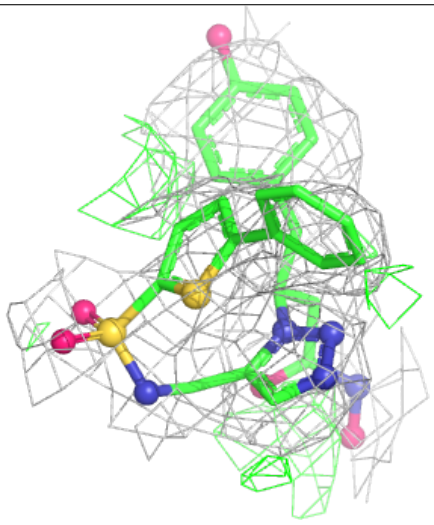


Electron density around USK A 1008:

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

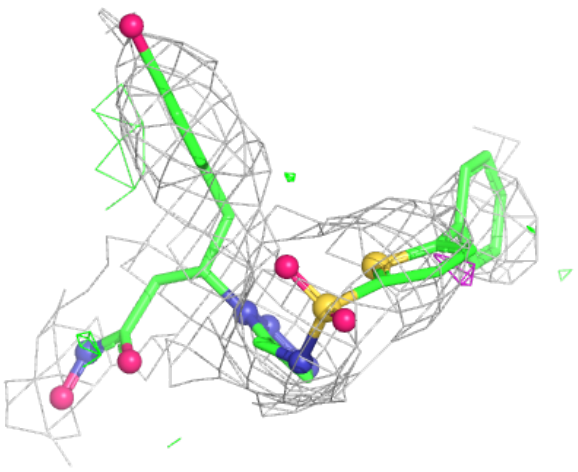


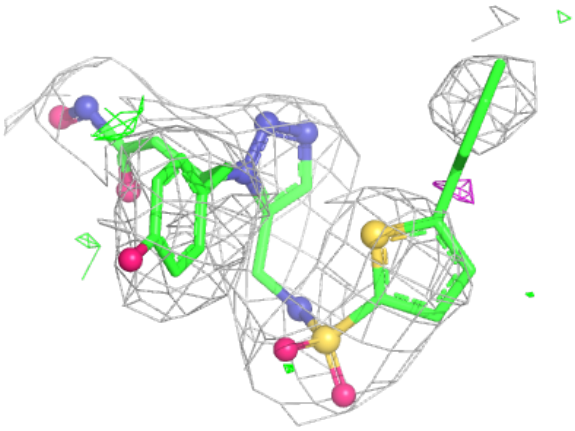


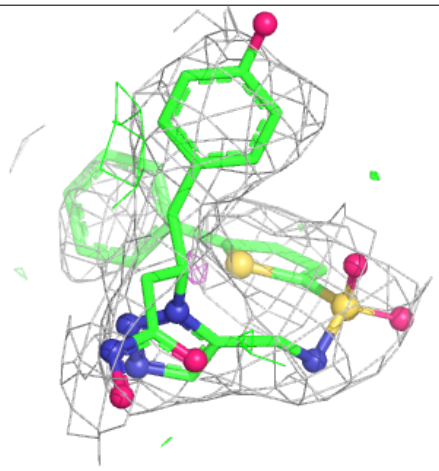


Electron density around USK D 1006:

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

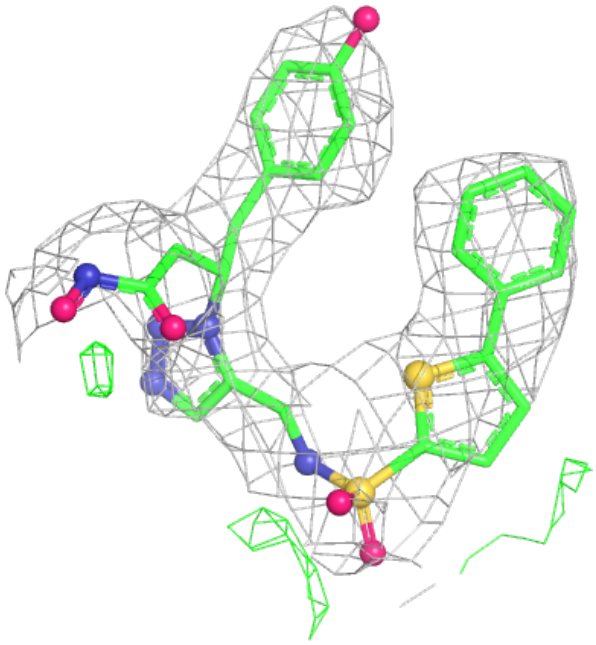


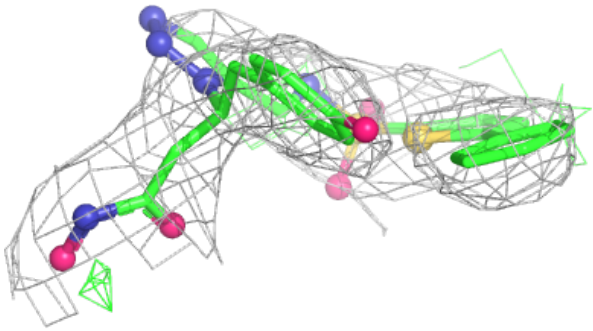


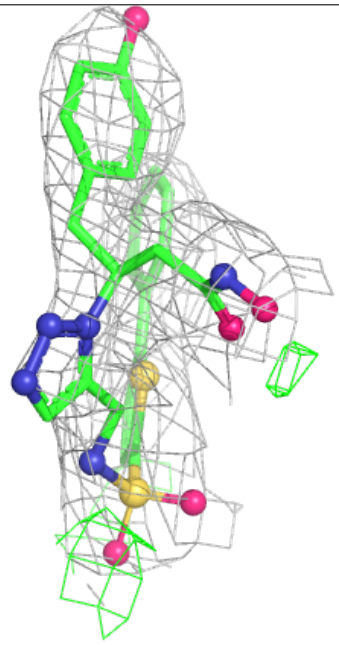


Electron density around USK C 1006:

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







6.5 Other polymers

There are no such residues in this entry.