wwPDB X-ray Structure Validation Summary Report (i)

Jul 14, 2022 – 01:20 pm BST

PDB ID	:	7ZYF
Title	:	Insulin regulated aminopeptidase (IRAP) in complex with a nanomolar alpha hydroxy beta amino acid based inhibitor.
Authors	:	Mpakali, A.; Stratikos, E.; Giastas, P.; Papakyriakou, A.
Deposited on	:	2022-05-24
Resolution	:	2.81 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:

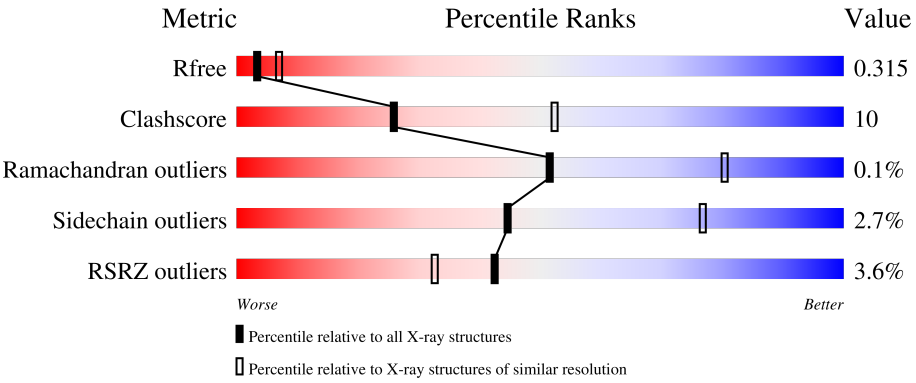
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	871	3% 77% 20%
1	B	871	4% 68% 29%
2	C	4	50% 50%
3	D	2	100%
3	F	2	100%

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Mol	Chain	Length	Quality of chain
3	G	2	100%
3	K	2	50% 50%
4	E	3	33% 67%
4	J	3	100%
5	H	5	100%
5	I	5	40% 60%

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
3	NAG	K	1	-	-	-	X
3	NAG	K	2	-	-	-	X
5	MAN	H	4	-	-	-	X
5	NAG	I	1	-	-	-	X
7	NAG	A	1103	-	-	-	X
7	NAG	B	1803	-	-	-	X
7	NAG	B	1810	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 14588 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.

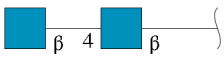
- Molecule 1 is a protein called Leucyl-cystinyl aminopeptidase, pregnancy serum form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	852	Total	C	N	O	S	0	4	0
			6910	4481	1123	1279	27			
1	B	854	Total	C	N	O	S	0	2	0
			6882	4457	1122	1277	26			

- Molecule 2 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
2	C	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	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
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			

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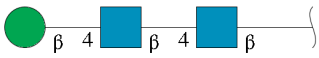
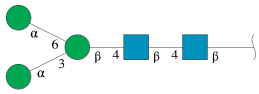
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	K	2	Total C N O 28 16 2 10	0	0	0

- 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	E	3	Total C N O 39 22 2 15	0	0	0
4	J	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.

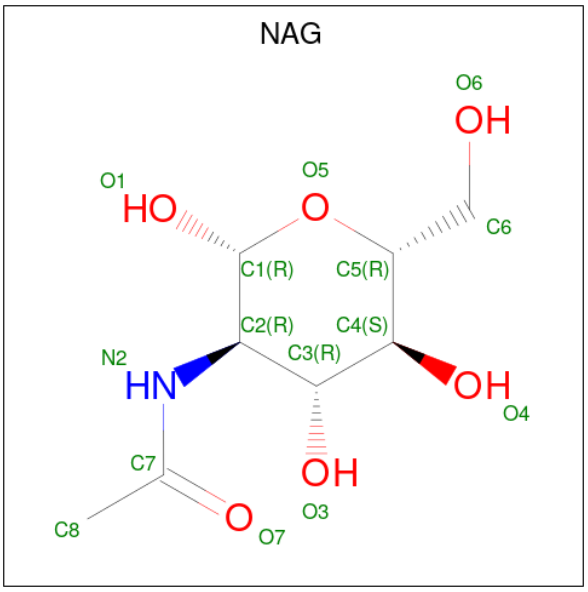


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	H	5	Total C N O 61 34 2 25	0	0	0
5	I	5	Total C N O 61 34 2 25	0	0	0

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

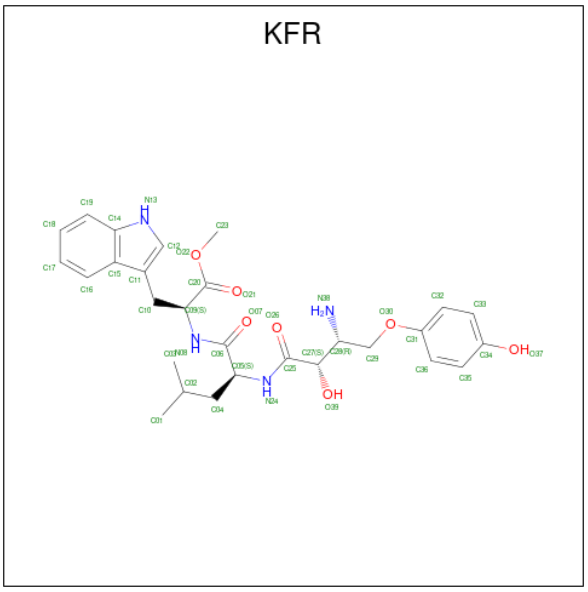
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0
6	B	1	Total Zn 1 1	0	0

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



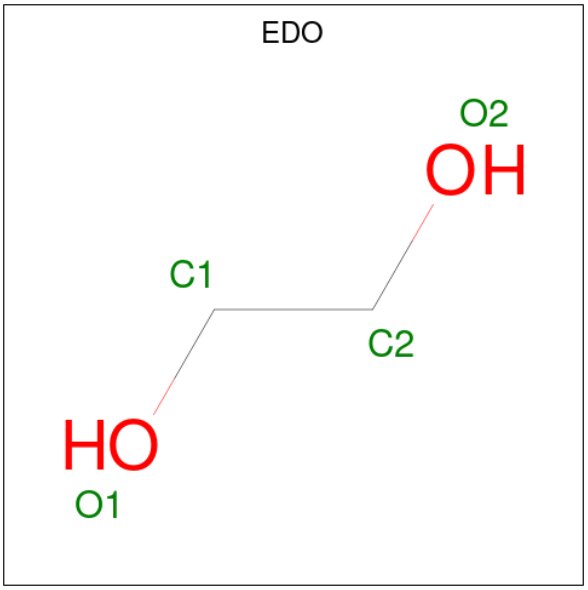
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total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

- Molecule 8 is methyl (2S)-2-[[(2S)-2-[[(2S,3R)-3-azanyl-2-oxidanyl-4-(4-oxidanylphenoxy)butanoyl]amino]-4-methyl-pentanoyl]amino]-3-(1H-indol-3-yl)propanoate (three-letter code: KFR) (formula: $C_{28}H_{36}N_4O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			39	28	4	7		
8	B	1	Total	C	N	O	0	1
			78	56	8	14		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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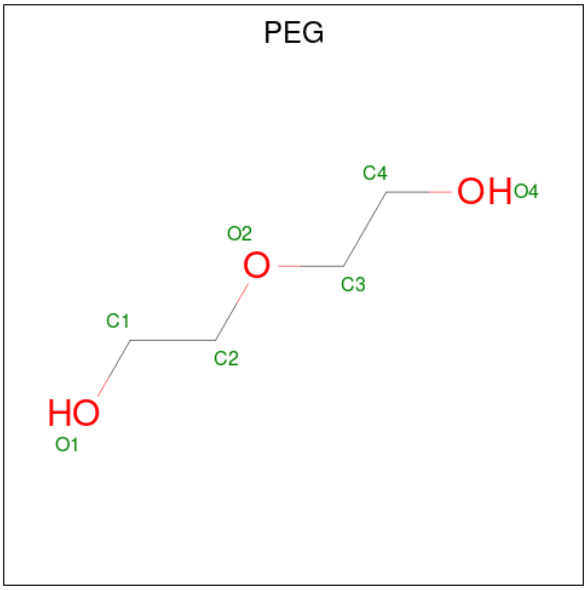
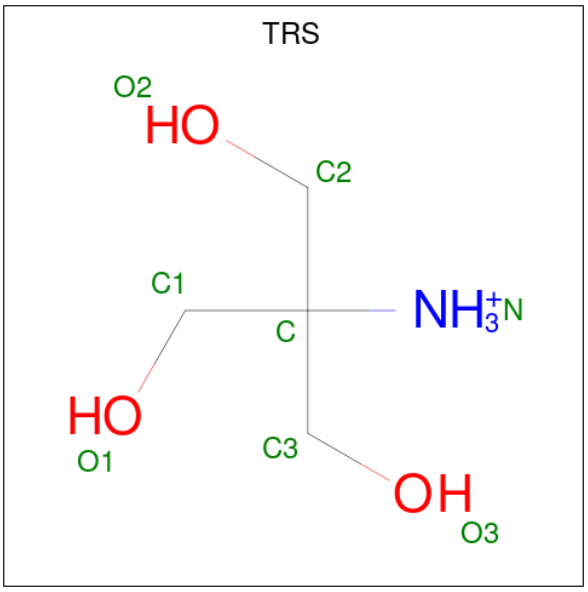
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 7 4 3	0	0
10	A	1	Total C O 7 4 3	0	0
10	B	1	Total C O 7 4 3	0	0

- Molecule 11 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C N O 8 4 1 3	0	0

- Molecule 12 is water.

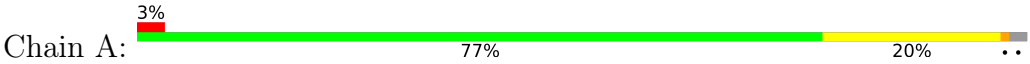
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	51	Total O 51 51	0	0
12	B	53	Total O 53 53	0	0

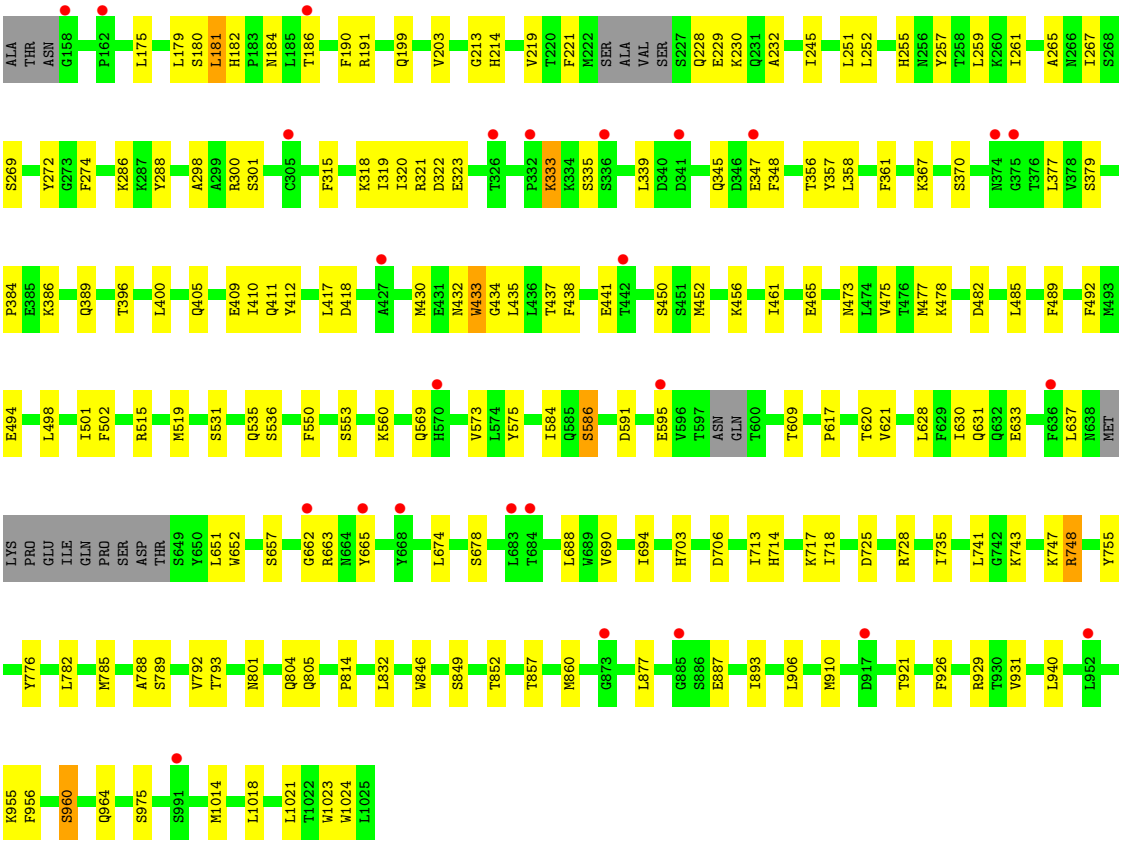
3 Residue-property plots (i)

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: Leucyl-cystinyl aminopeptidase, pregnancy serum form

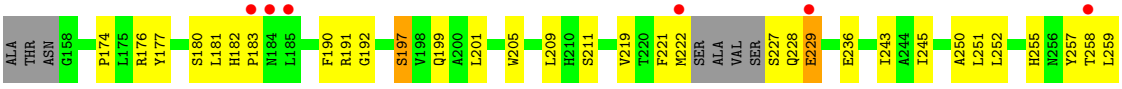
Chain A:

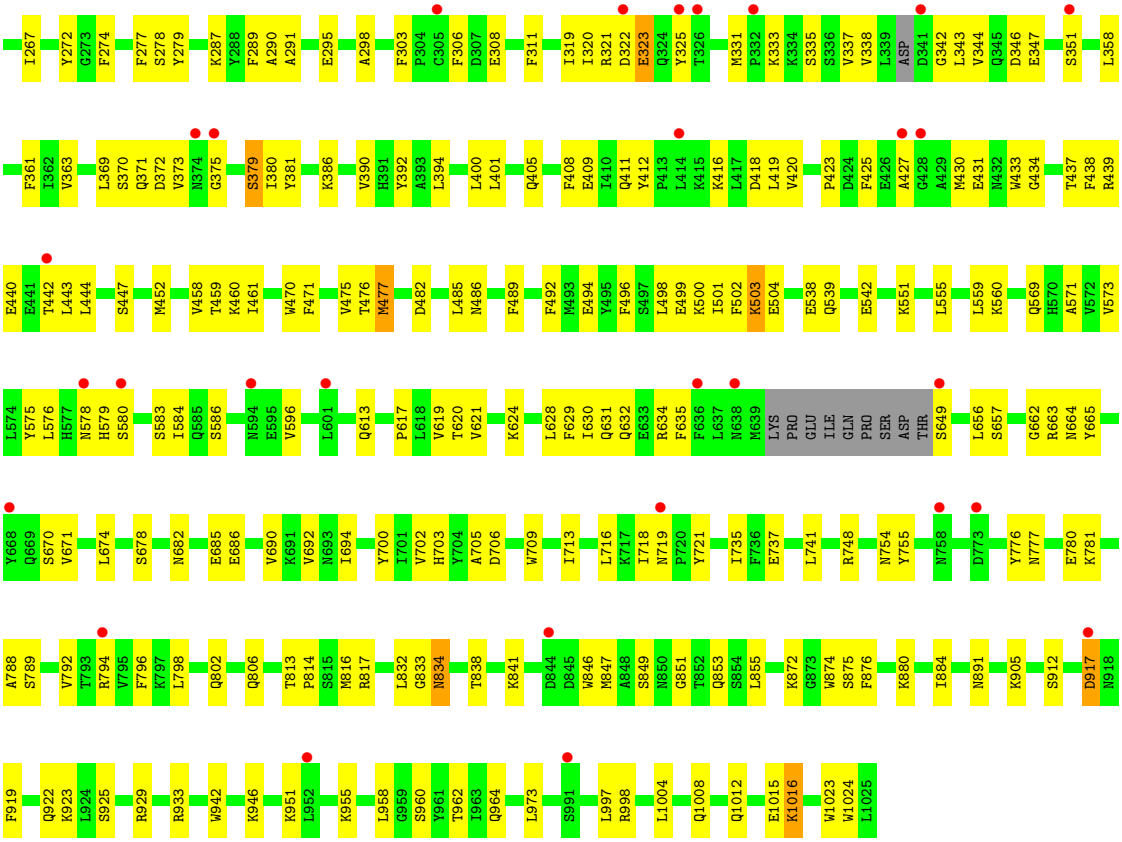




• Molecule 1: Leucyl-cystinyl aminopeptidase, pregnancy serum form

Chain B:



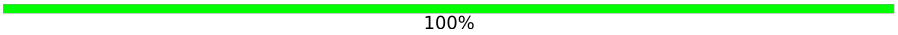


• Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

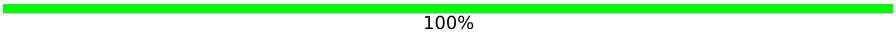
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



• 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

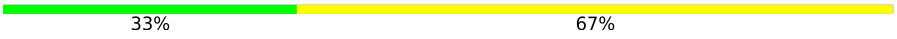
Chain G:

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

Chain K:

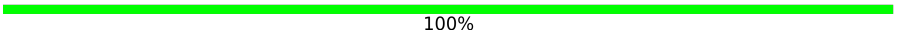
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



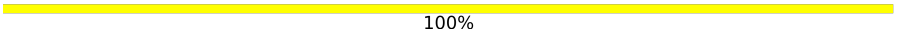
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• 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 H:



• 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 I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.48Å 120.05Å 141.25Å 90.00° 103.28° 90.00°	Depositor
Resolution (Å)	137.47 – 2.81 137.47 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.5 (137.47-2.81) 99.6 (137.47-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.271 , 0.314 0.271 , 0.315	Depositor DCC
R_{free} test set	2883 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	14588	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8538e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.30	0/7091	0.52	0/9615
1	B	0.33	1/7057 (0.0%)	0.55	1/9576 (0.0%)
All	All	0.32	1/14148 (0.0%)	0.53	1/19191 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	236	GLU	CB-CG	-5.95	1.40	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	227	SER	C-N-CA	5.56	135.59	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6910	0	6805	122	0
1	B	6882	0	6717	171	0
2	C	50	0	43	4	0
3	D	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	K	28	0	25	2	0
4	E	39	0	34	0	0
4	J	39	0	34	0	0
5	H	61	0	52	2	0
5	I	61	0	52	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	56	0	52	4	0
7	B	98	0	89	8	0
8	A	39	0	0	0	0
8	B	78	0	0	4	0
9	A	12	0	18	0	0
9	B	16	0	24	0	0
10	A	14	0	20	0	0
10	B	7	0	10	0	0
11	B	8	0	12	0	0
12	A	51	0	0	0	0
12	B	53	0	0	1	0
All	All	14588	0	14062	299	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 10.

The worst 5 of 299 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:441:GLU:HG2	1:A:887:GLU:HB3	1.46	0.97
1:B:735:ILE:HD11	1:B:748:ARG:HG3	1.51	0.92
1:B:833:GLY:HA3	3:K:1:NAG:H82	1.55	0.88
1:A:245:ILE:HD13	1:A:259:LEU:HD21	1.62	0.81
1:B:219:VAL:HG21	1:B:245:ILE:HD12	1.60	0.81

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	848/871 (97%)	821 (97%)	27 (3%)	0	100 100
1	B	848/871 (97%)	812 (96%)	34 (4%)	2 (0%)	47 76
All	All	1696/1742 (97%)	1633 (96%)	61 (4%)	2 (0%)	51 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	229	GLU
1	B	323	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	756/780 (97%)	739 (98%)	17 (2%)	52 81
1	B	745/780 (96%)	720 (97%)	25 (3%)	37 69
All	All	1501/1560 (96%)	1459 (97%)	42 (3%)	44 76

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	477	MET
1	B	737	GLU
1	B	489	PHE
1	B	632	GLN

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Mol	Chain	Res	Type
1	B	794[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	805	GLN
1	B	199	GLN
1	B	486	ASN
1	A	800	GLN
1	A	324	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)

28 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	C	1	2,1	14,14,15	0.59	0	17,19,21	1.44	2 (11%)
2	NAG	C	2	2	14,14,15	1.06	1 (7%)	17,19,21	0.89	1 (5%)
2	BMA	C	3	2	11,11,12	0.83	0	15,15,17	1.95	5 (33%)
2	MAN	C	4	2	11,11,12	0.56	0	15,15,17	0.97	2 (13%)
3	NAG	D	1	3,1	14,14,15	0.48	0	17,19,21	0.52	0
3	NAG	D	2	3	14,14,15	0.32	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	1	4,1	14,14,15	0.46	0	17,19,21	0.75	1 (5%)
4	NAG	E	2	4	14,14,15	0.30	0	17,19,21	0.56	0
4	BMA	E	3	4	11,11,12	1.15	1 (9%)	15,15,17	1.19	2 (13%)
3	NAG	F	1	3,1	14,14,15	0.58	0	17,19,21	0.69	0
3	NAG	F	2	3	14,14,15	0.53	0	17,19,21	0.50	0
3	NAG	G	1	3,1	14,14,15	0.52	0	17,19,21	0.82	0
3	NAG	G	2	3	14,14,15	0.44	0	17,19,21	0.55	0
5	NAG	H	1	5,1	14,14,15	0.30	0	17,19,21	0.79	0
5	NAG	H	2	5	14,14,15	0.20	0	17,19,21	0.50	0
5	BMA	H	3	5	11,11,12	1.50	2 (18%)	15,15,17	1.31	2 (13%)
5	MAN	H	4	5	11,11,12	0.82	1 (9%)	15,15,17	1.54	3 (20%)
5	MAN	H	5	5	11,11,12	0.92	1 (9%)	15,15,17	1.20	2 (13%)
5	NAG	I	1	5,1	14,14,15	0.35	0	17,19,21	0.54	0
5	NAG	I	2	5	14,14,15	0.38	0	17,19,21	0.52	0
5	BMA	I	3	5	11,11,12	0.64	0	15,15,17	0.79	0
5	MAN	I	4	5	11,11,12	0.72	0	15,15,17	1.04	2 (13%)
5	MAN	I	5	5	11,11,12	0.86	0	15,15,17	1.05	2 (13%)
4	NAG	J	1	4,1	14,14,15	0.31	0	17,19,21	0.75	0
4	NAG	J	2	4	14,14,15	0.43	0	17,19,21	0.68	0
4	BMA	J	3	4	11,11,12	0.62	0	15,15,17	0.84	0
3	NAG	K	1	3,1	14,14,15	0.36	0	17,19,21	0.67	0
3	NAG	K	2	3	14,14,15	0.63	0	17,19,21	0.44	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	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	BMA	C2-C3	3.86	1.58	1.52
2	C	2	NAG	O5-C1	-3.70	1.37	1.43
5	H	4	MAN	C1-C2	2.31	1.57	1.52
5	H	3	BMA	O3-C3	2.26	1.48	1.43
5	H	5	MAN	C1-C2	2.14	1.57	1.52

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	O4-C4-C5	-4.25	98.75	109.30
5	H	4	MAN	C1-O5-C5	4.10	117.75	112.19
2	C	3	BMA	C1-O5-C5	3.75	117.27	112.19
5	H	3	BMA	O3-C3-C2	3.72	117.12	109.99
2	C	3	BMA	O5-C1-C2	3.65	116.41	110.77

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

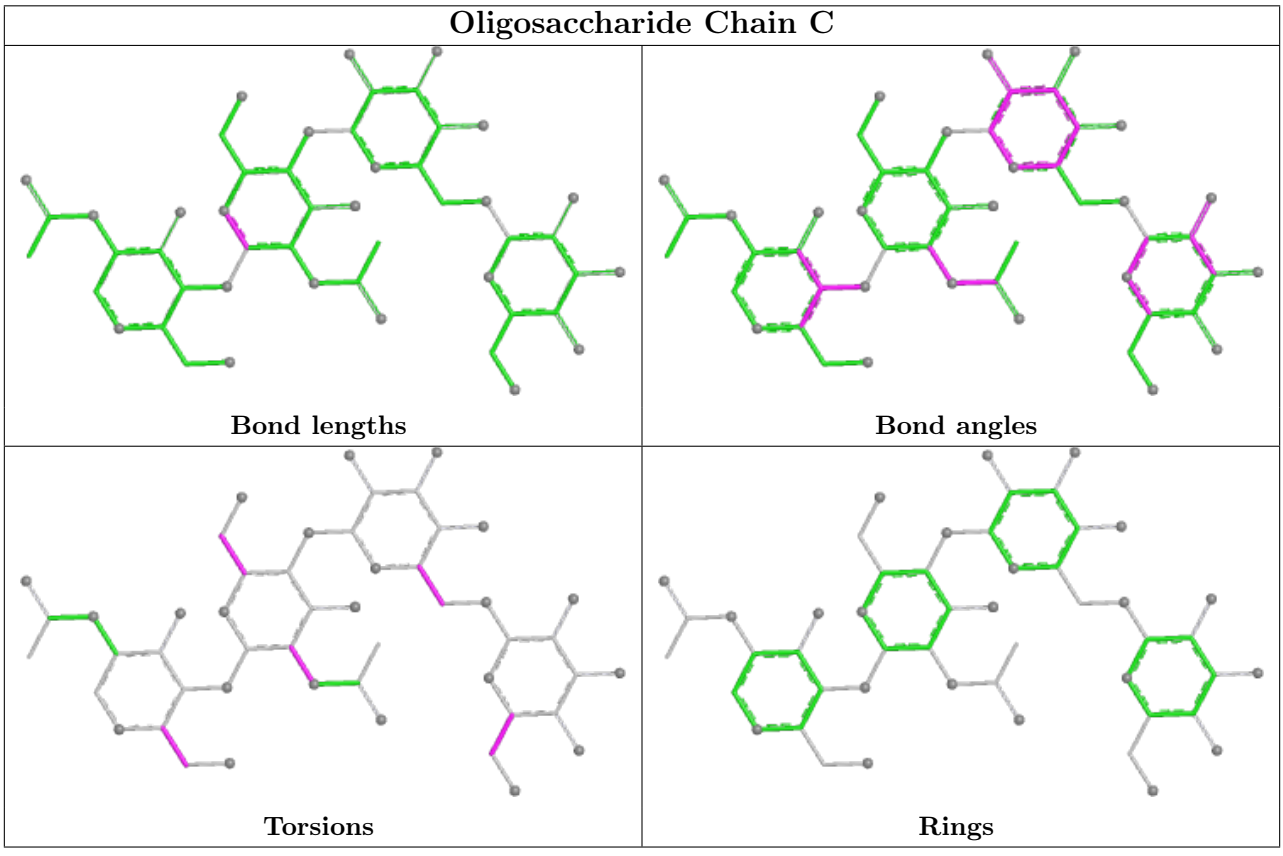
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
5	I	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

There are no ring outliers.

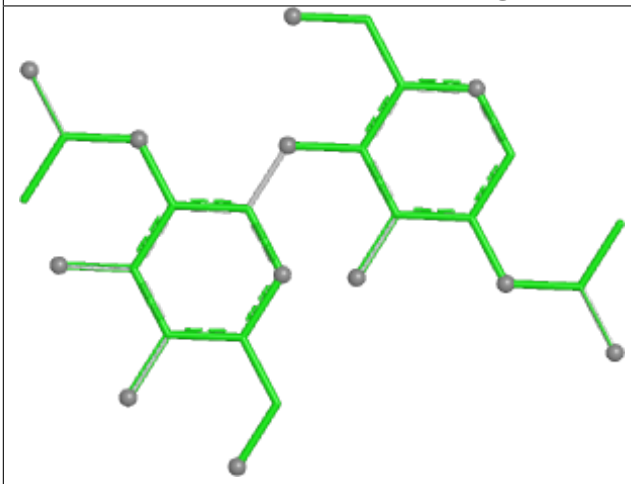
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	NAG	1	0
3	K	1	NAG	2	0
5	I	1	NAG	1	0
2	C	3	BMA	1	0
2	C	2	NAG	4	0
5	H	1	NAG	2	0

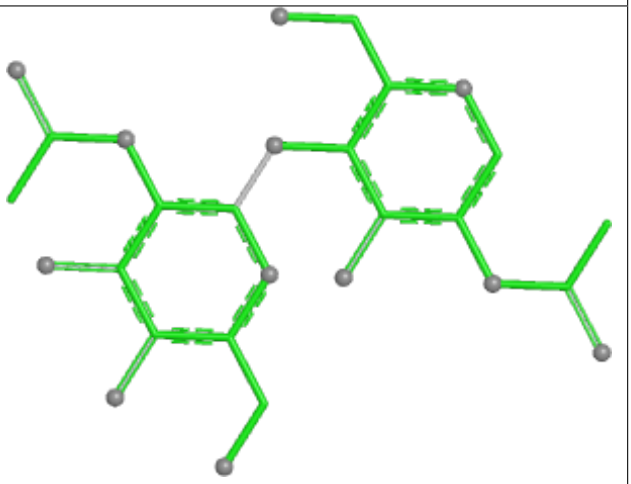
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



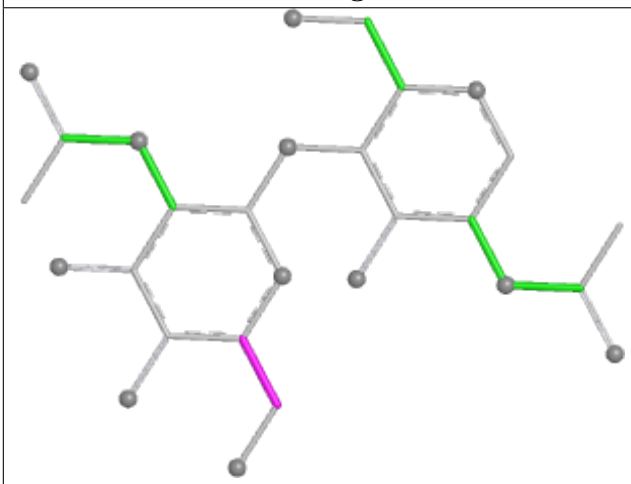
Oligosaccharide Chain D



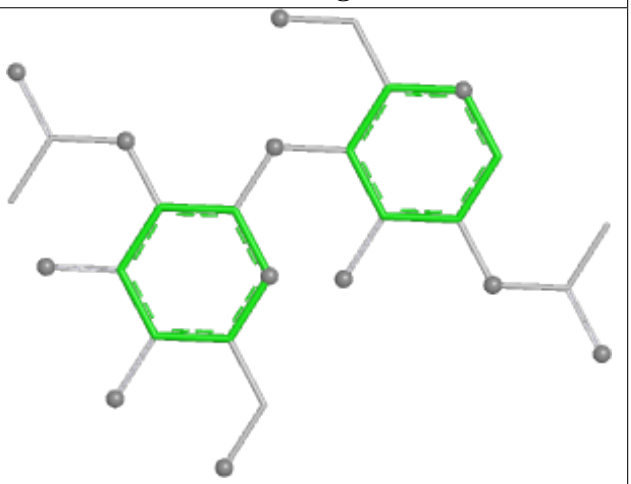
Bond lengths



Bond angles

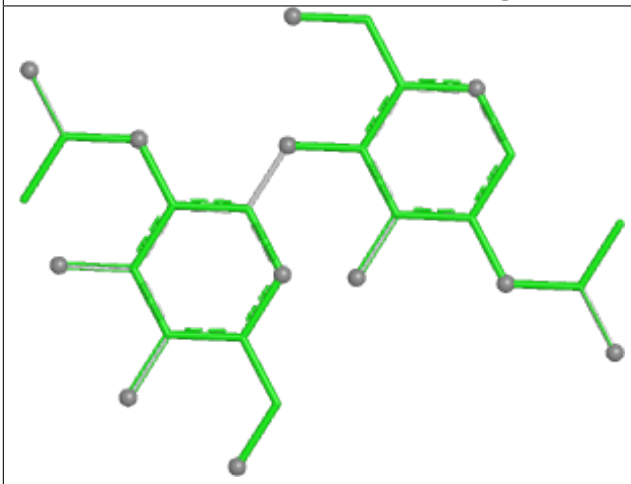


Torsions

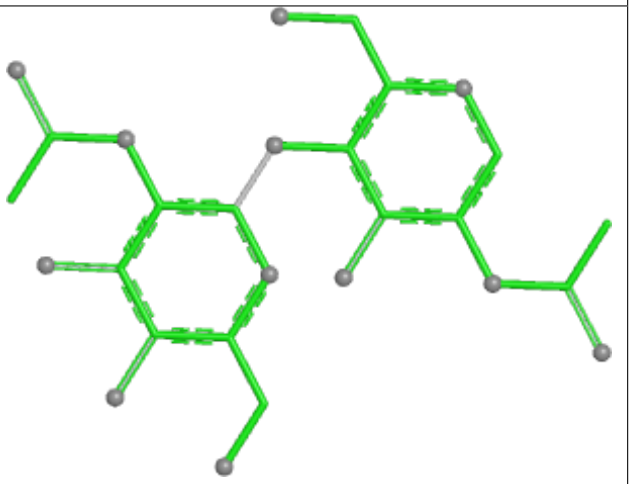


Rings

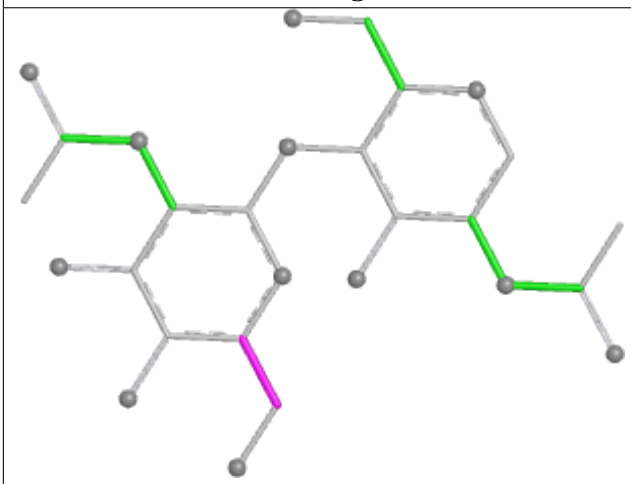
Oligosaccharide Chain F



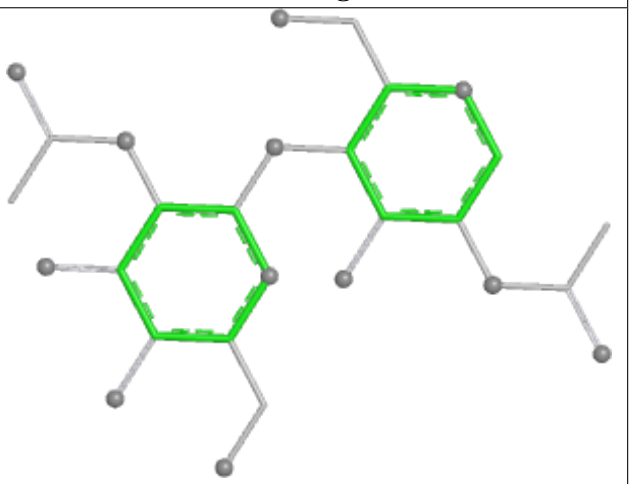
Bond lengths



Bond angles

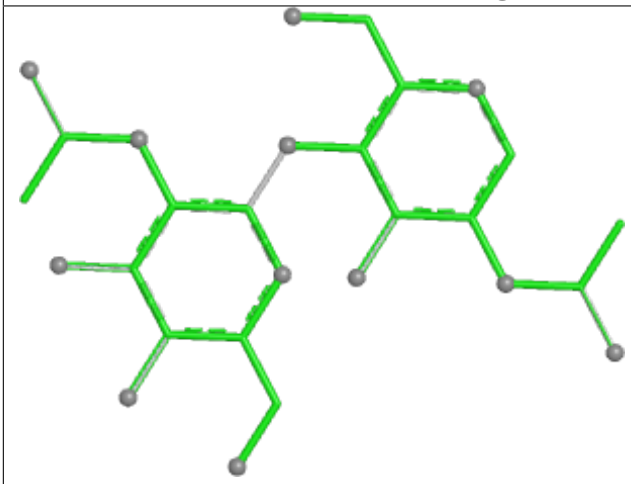


Torsions

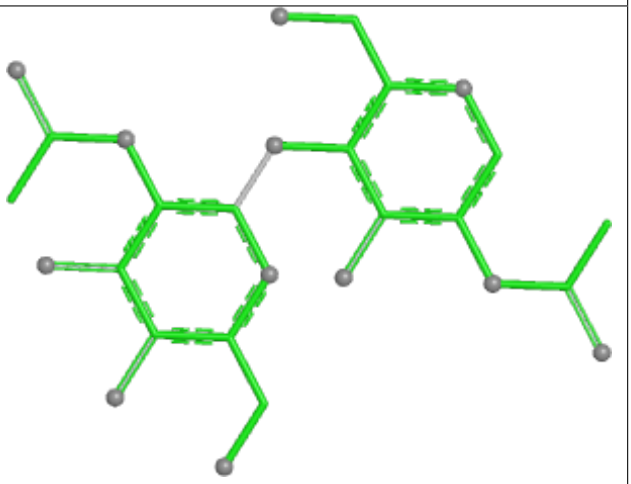


Rings

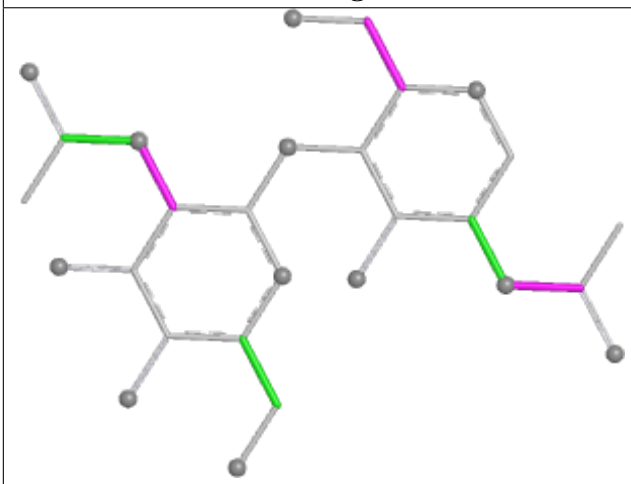
Oligosaccharide Chain G



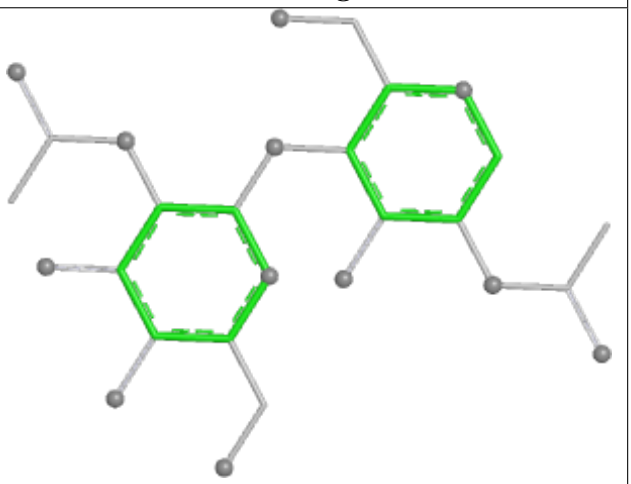
Bond lengths



Bond angles

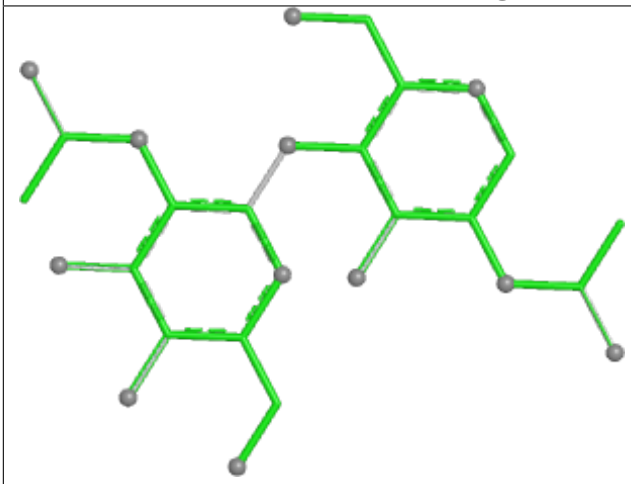


Torsions

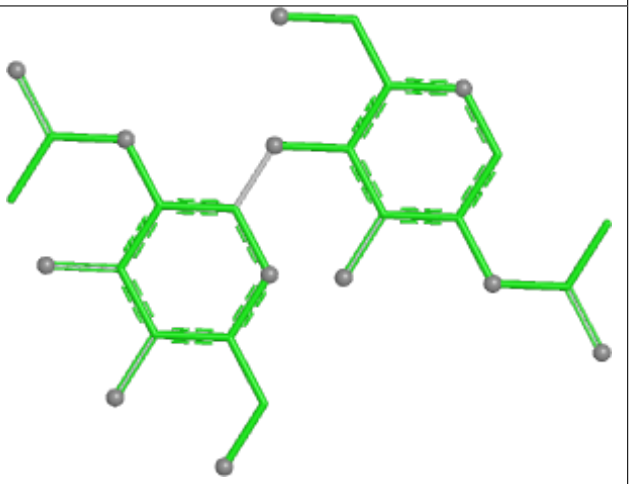


Rings

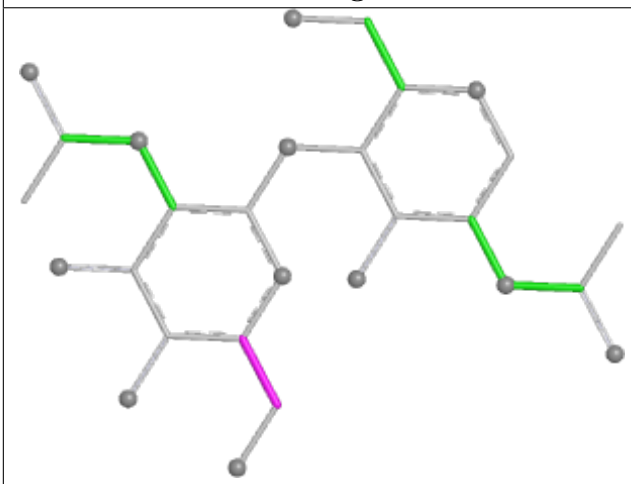
Oligosaccharide Chain K



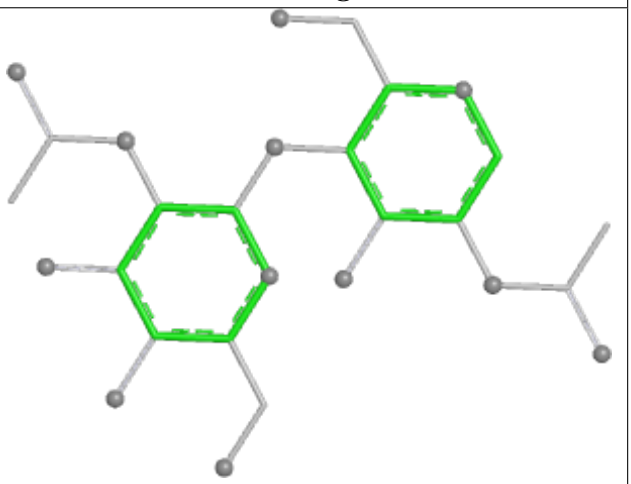
Bond lengths



Bond angles

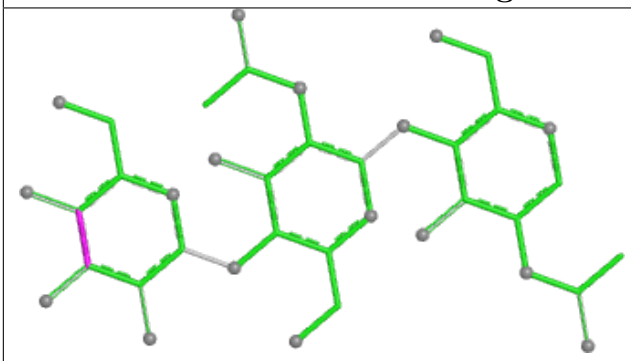


Torsions

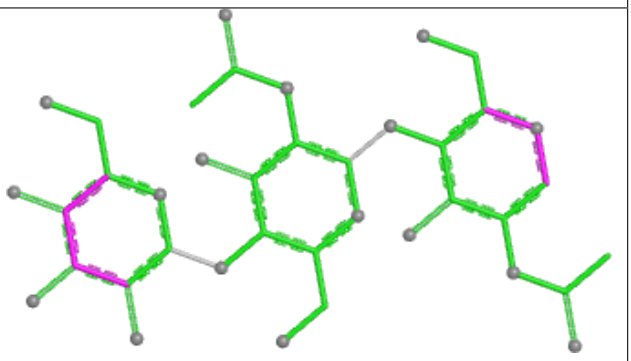


Rings

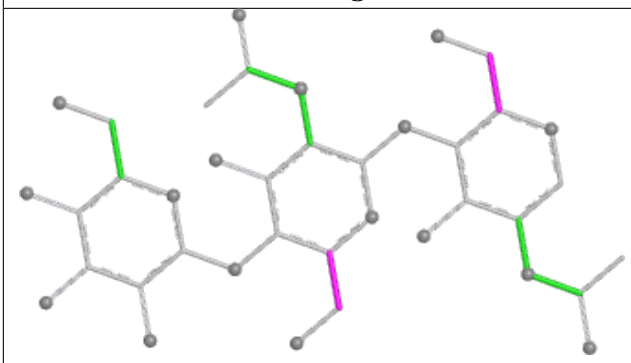
Oligosaccharide Chain E



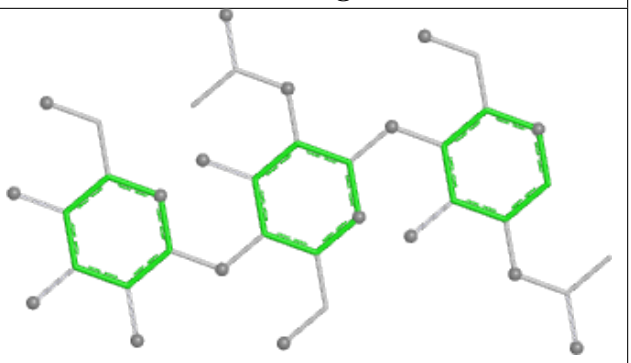
Bond lengths



Bond angles

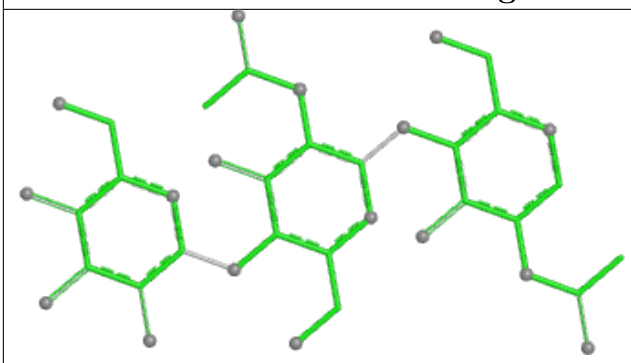


Torsions

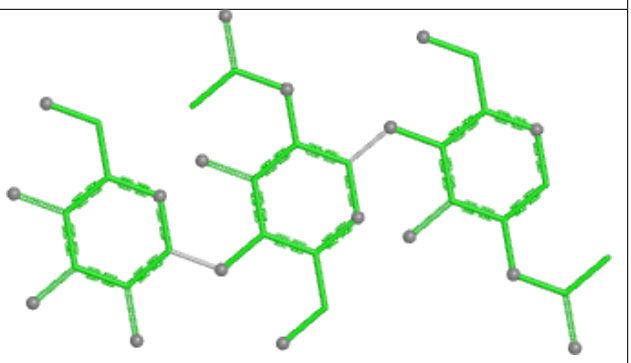


Rings

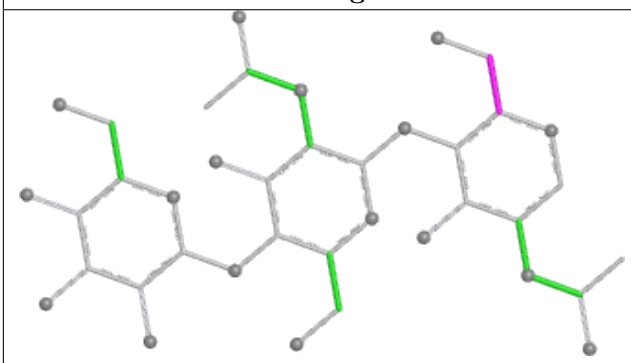
Oligosaccharide Chain J



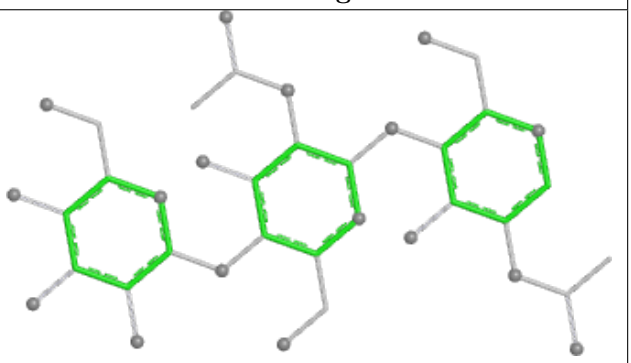
Bond lengths



Bond angles

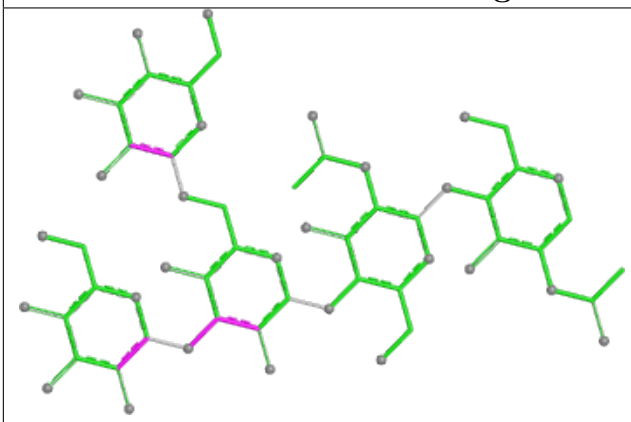


Torsions

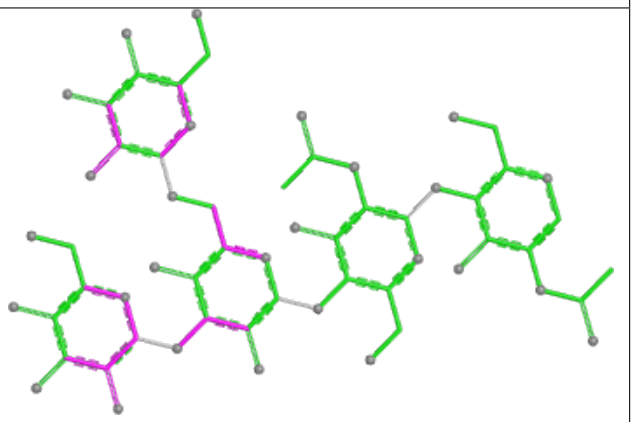


Rings

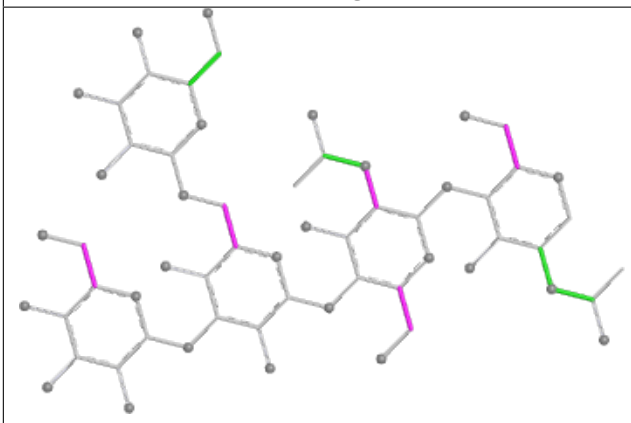
Oligosaccharide Chain H



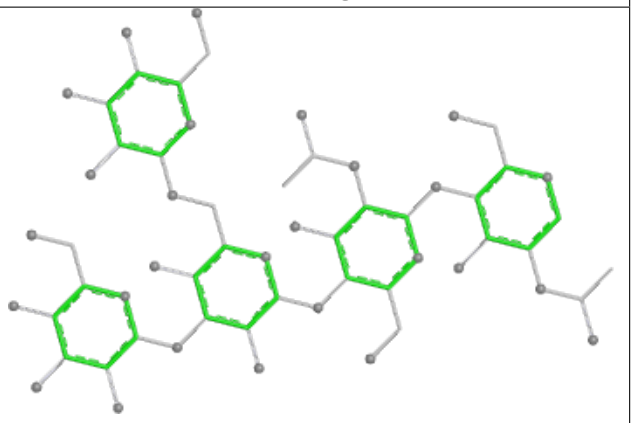
Bond lengths



Bond angles

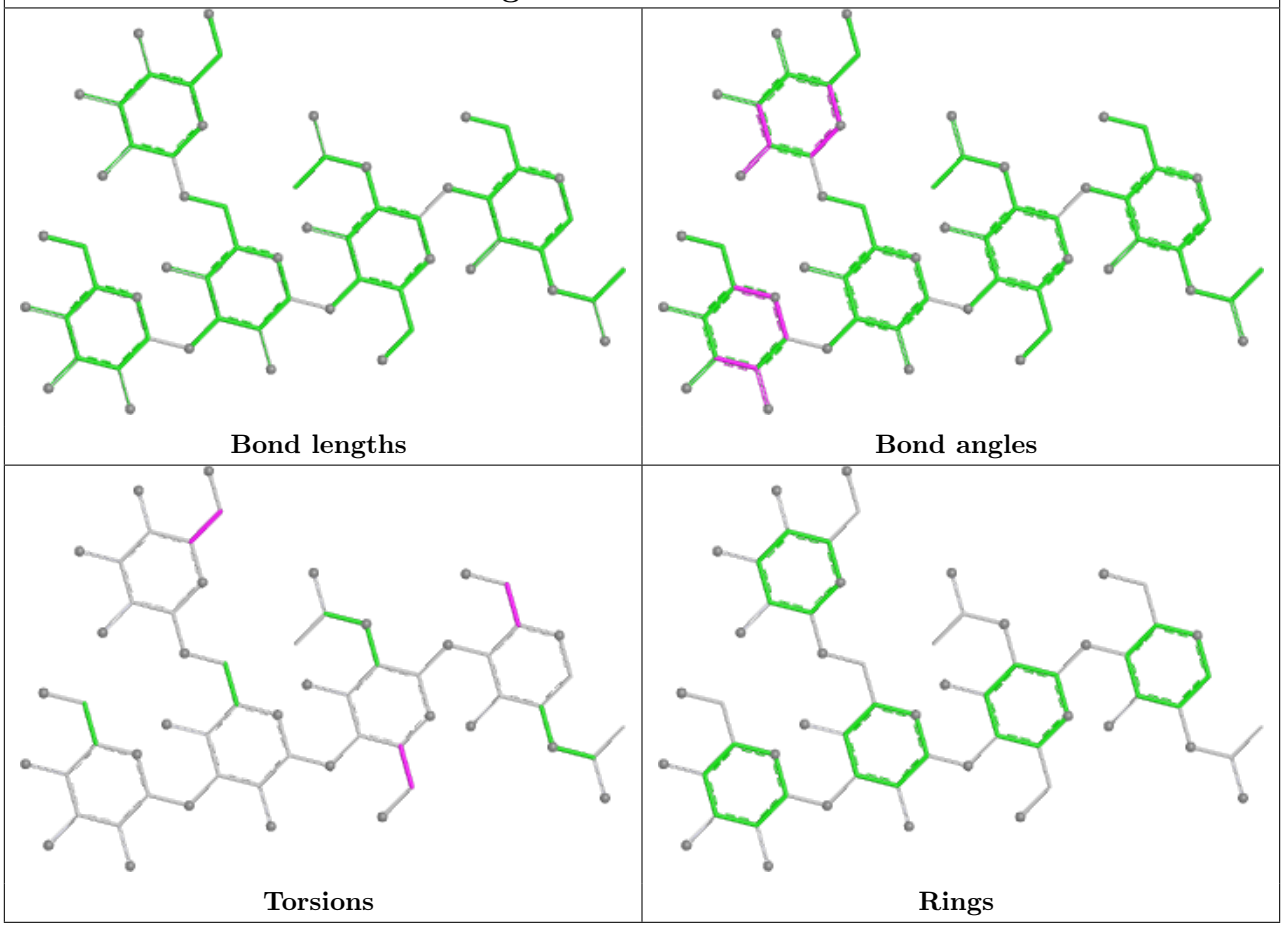


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 2 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	B	1814	1	14,14,15	0.68	0	17,19,21	1.65	1 (5%)
8	KFR	B	1815[A]	6	40,41,41	1.61	7 (17%)	49,56,56	0.94	3 (6%)
9	EDO	A	1108	-	3,3,3	0.45	0	2,2,2	0.35	0
7	NAG	B	1810	7,1	14,14,15	0.79	1 (7%)	17,19,21	1.39	1 (5%)
11	TRS	B	1807	-	7,7,7	0.32	0	9,9,9	0.30	0
7	NAG	B	1802	1	14,14,15	0.95	1 (7%)	17,19,21	0.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	B	1803	1	14,14,15	1.05	2 (14%)	17,19,21	0.82	1 (5%)
9	EDO	B	1804	-	3,3,3	0.47	0	2,2,2	0.37	0
7	NAG	A	1102	1	14,14,15	0.19	0	17,19,21	0.54	0
9	EDO	B	1805	-	3,3,3	0.46	0	2,2,2	0.37	0
10	PEG	A	1110	-	6,6,6	0.49	0	5,5,5	0.30	0
10	PEG	B	1809	-	6,6,6	0.49	0	5,5,5	0.28	0
7	NAG	B	1811	7	14,14,15	0.65	1 (7%)	17,19,21	0.91	0
9	EDO	B	1806	-	3,3,3	0.47	0	2,2,2	0.35	0
8	KFR	A	1106	6	40,41,41	1.59	6 (15%)	49,56,56	0.97	2 (4%)
8	KFR	B	1815[B]	6	40,41,41	1.62	7 (17%)	49,56,56	0.98	3 (6%)
7	NAG	A	1104	1	14,14,15	0.80	1 (7%)	17,19,21	0.86	0
7	NAG	B	1812	7	14,14,15	0.67	1 (7%)	17,19,21	0.67	0
10	PEG	A	1111	-	6,6,6	0.48	0	5,5,5	0.29	0
9	EDO	A	1109	-	3,3,3	0.46	0	2,2,2	0.35	0
9	EDO	B	1808	-	3,3,3	0.45	0	2,2,2	0.38	0
7	NAG	B	1813	7,1	14,14,15	0.45	0	17,19,21	0.82	0
9	EDO	A	1107	-	3,3,3	0.49	0	2,2,2	0.29	0
7	NAG	A	1105	1	14,14,15	0.29	0	17,19,21	0.58	0
7	NAG	A	1103	1	14,14,15	0.34	0	17,19,21	0.45	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	B	1814	1	-	3/6/23/26	0/1/1/1
8	KFR	B	1815[A]	6	-	13/38/48/48	0/3/3/3
9	EDO	A	1108	-	-	0/1/1/1	-
7	NAG	B	1810	7,1	-	4/6/23/26	0/1/1/1
11	TRS	B	1807	-	-	0/9/9/9	-
7	NAG	B	1802	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1803	1	-	2/6/23/26	0/1/1/1
9	EDO	B	1804	-	-	1/1/1/1	-
7	NAG	A	1102	1	-	0/6/23/26	0/1/1/1
9	EDO	B	1805	-	-	0/1/1/1	-
10	PEG	A	1110	-	-	0/4/4/4	-
10	PEG	B	1809	-	-	0/4/4/4	-
7	NAG	B	1811	7	-	1/6/23/26	0/1/1/1
9	EDO	B	1806	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	KFR	A	1106	6	-	15/38/48/48	0/3/3/3
8	KFR	B	1815[B]	6	-	9/38/48/48	0/3/3/3
7	NAG	A	1104	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1812	7	-	1/6/23/26	0/1/1/1
10	PEG	A	1111	-	-	3/4/4/4	-
9	EDO	A	1109	-	-	0/1/1/1	-
9	EDO	B	1808	-	-	0/1/1/1	-
7	NAG	B	1813	7,1	-	1/6/23/26	0/1/1/1
9	EDO	A	1107	-	-	1/1/1/1	-
7	NAG	A	1105	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1103	1	-	2/6/23/26	0/1/1/1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1815[B]	KFR	C06-N08	5.52	1.46	1.34
8	B	1815[A]	KFR	C06-N08	5.45	1.46	1.34
8	B	1815[B]	KFR	C25-N24	5.36	1.45	1.34
8	A	1106	KFR	C06-N08	5.35	1.45	1.34
8	B	1815[A]	KFR	C25-N24	5.25	1.45	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1814	NAG	C2-N2-C7	6.14	131.64	122.90
7	B	1810	NAG	C1-O5-C5	4.51	118.30	112.19
8	B	1815[A]	KFR	O22-C20-C09	3.46	120.36	111.52
8	B	1815[B]	KFR	O22-C20-C09	3.45	120.34	111.52
8	A	1106	KFR	O22-C20-C09	3.27	119.89	111.52

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1814	NAG	C3-C2-N2-C7
8	A	1106	KFR	C25-C27-C28-C29
8	A	1106	KFR	O39-C27-C28-C29
8	A	1106	KFR	C25-C27-C28-N38
8	A	1106	KFR	O39-C27-C28-N38

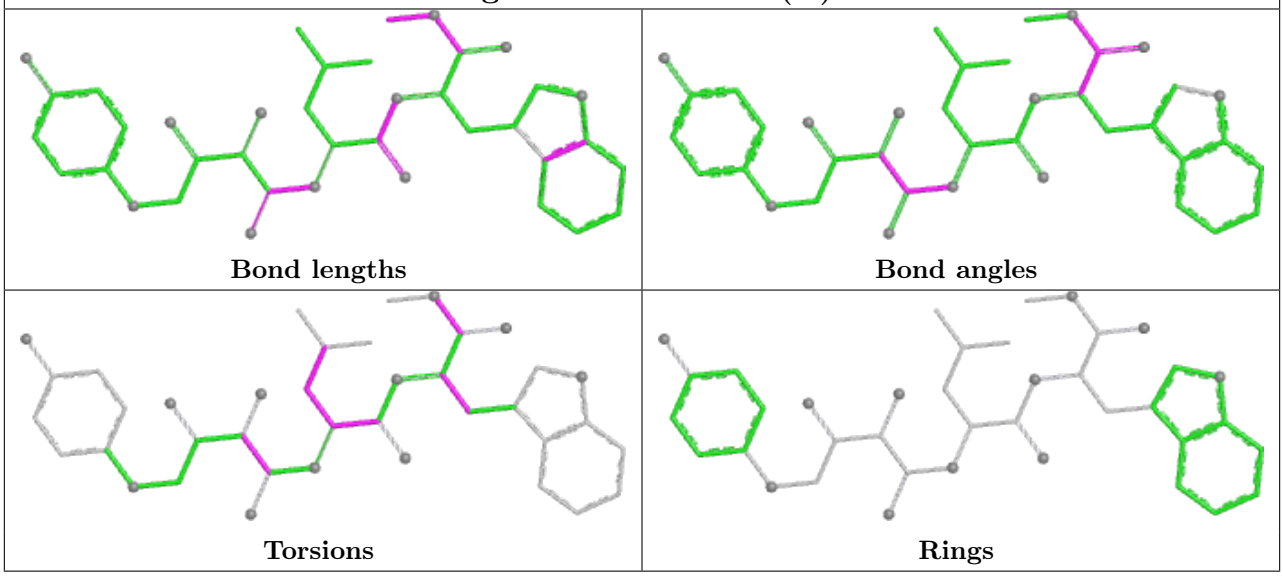
There are no ring outliers.

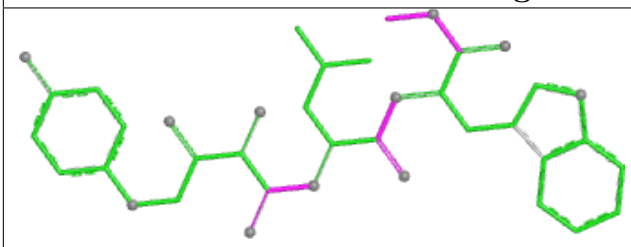
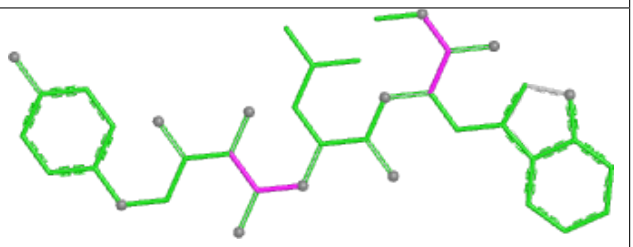
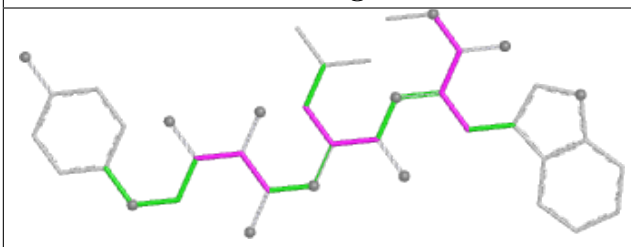
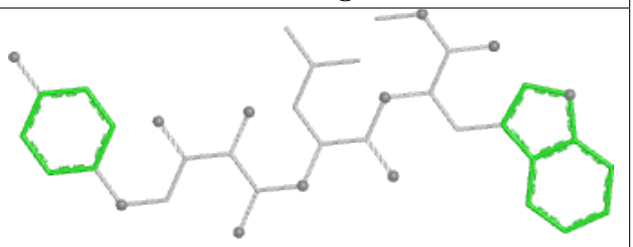
9 monomers are involved in 16 short contacts:

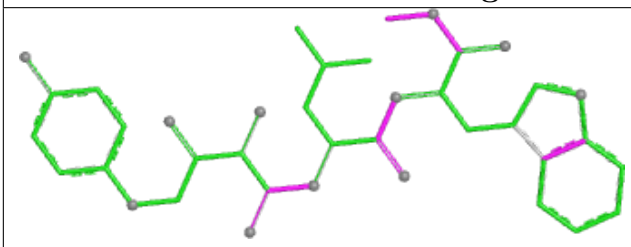
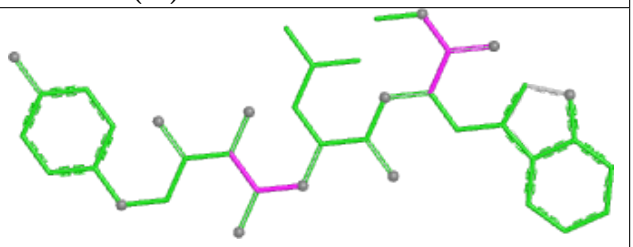
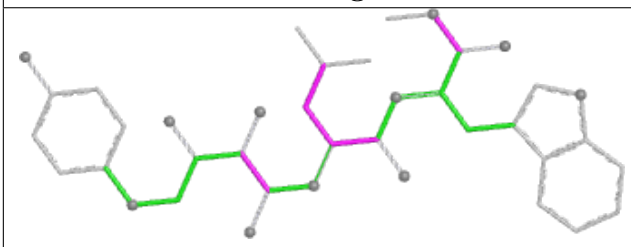
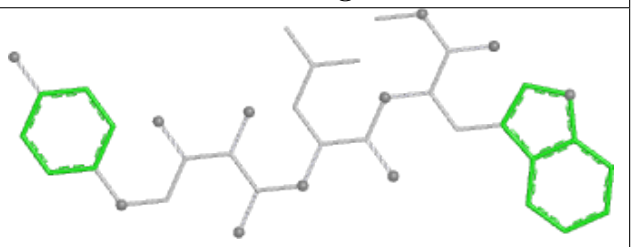
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1814	NAG	3	0
8	B	1815[A]	KFR	2	0
7	B	1810	NAG	2	0
7	B	1802	NAG	1	0
7	A	1102	NAG	1	0
8	B	1815[B]	KFR	2	0
7	A	1104	NAG	2	0
7	B	1813	NAG	2	0
7	A	1103	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 KFR B 1815 (A)



Ligand KFR A 1106	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KFR B 1815 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	852/871 (97%)	0.46	26 (3%)	49	39	8, 33, 62, 96	0
1	B	854/871 (98%)	0.56	35 (4%)	37	27	7, 39, 68, 115	0
All	All	1706/1742 (97%)	0.51	61 (3%)	42	32	7, 36, 66, 115	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	649	SER	5.1
1	A	885	GLY	4.2
1	A	665	TYR	4.0
1	B	375	GLY	3.8
1	B	758	ASN	3.7

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
5	MAN	H	5	11/12	0.36	0.32	83,87,89,89	0
4	BMA	J	3	11/12	0.39	0.36	92,94,97,98	0
3	NAG	G	2	14/15	0.40	0.32	82,87,89,93	0
4	BMA	E	3	11/12	0.41	0.26	73,75,76,77	0
3	NAG	K	1	14/15	0.43	0.51	121,128,131,131	0

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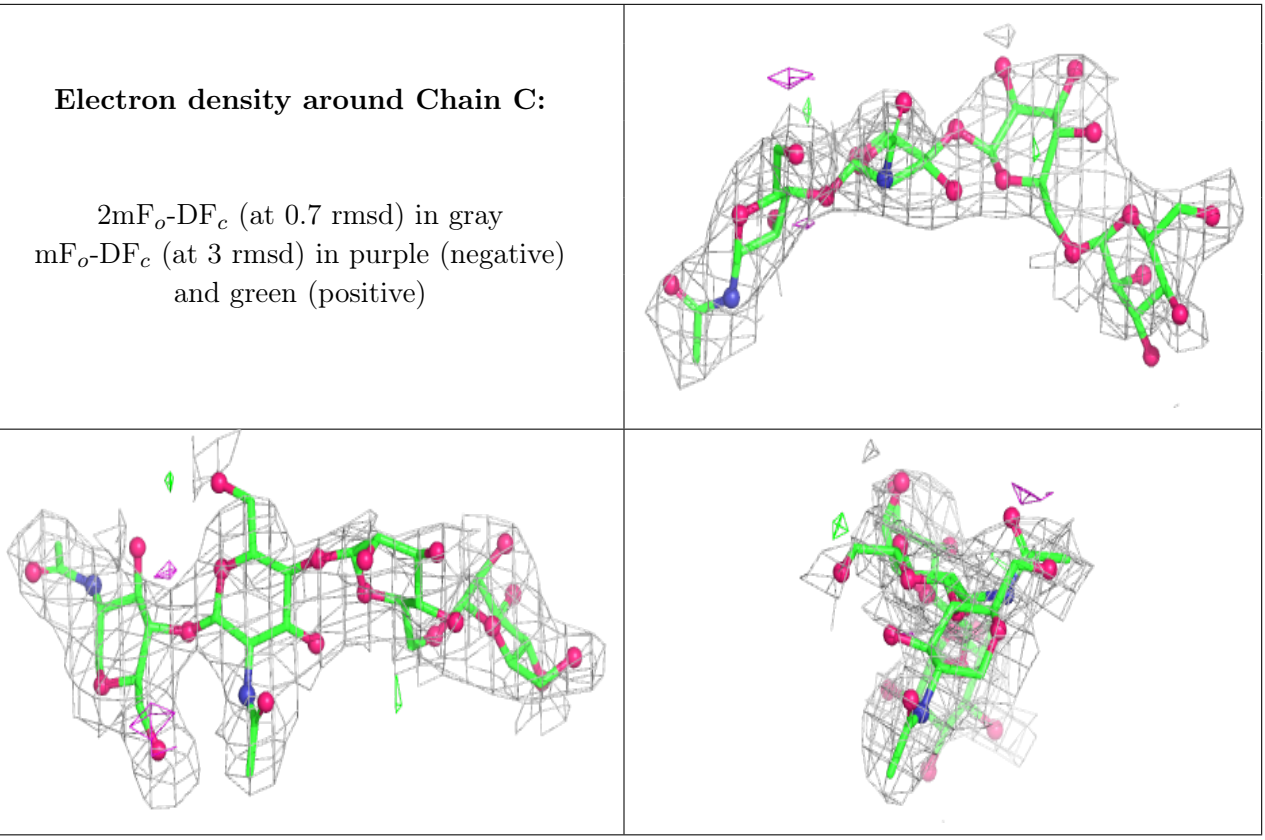
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	H	1	14/15	0.47	0.36	91,103,108,114	0
3	NAG	F	2	14/15	0.53	0.26	60,68,69,72	0
4	NAG	J	2	14/15	0.55	0.34	85,90,91,91	0
5	MAN	H	4	11/12	0.59	0.40	80,82,84,86	0
5	BMA	H	3	11/12	0.59	0.28	90,97,100,100	0
5	MAN	I	5	11/12	0.60	0.34	68,71,73,75	0
5	NAG	H	2	14/15	0.62	0.24	105,113,117,118	0
3	NAG	G	1	14/15	0.63	0.38	104,109,116,117	0
5	NAG	I	1	14/15	0.64	0.47	63,67,75,76	0
5	MAN	I	4	11/12	0.68	0.33	83,86,88,88	0
5	NAG	I	2	14/15	0.68	0.32	47,60,62,65	0
4	NAG	J	1	14/15	0.70	0.23	76,83,89,92	0
2	MAN	C	4	11/12	0.72	0.30	64,68,71,71	0
2	BMA	C	3	11/12	0.73	0.25	76,79,81,82	0
4	NAG	E	2	14/15	0.75	0.23	68,73,76,78	0
3	NAG	F	1	14/15	0.75	0.33	79,87,89,94	0
3	NAG	D	2	14/15	0.77	0.33	59,65,70,71	0
2	NAG	C	2	14/15	0.77	0.28	67,71,74,79	0
3	NAG	K	2	14/15	0.78	0.46	76,89,94,101	0
5	BMA	I	3	11/12	0.79	0.28	68,69,73,78	0
4	NAG	E	1	14/15	0.82	0.25	39,48,52,60	0
3	NAG	D	1	14/15	0.84	0.20	37,43,49,53	0
2	NAG	C	1	14/15	0.85	0.25	42,47,54,61	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.

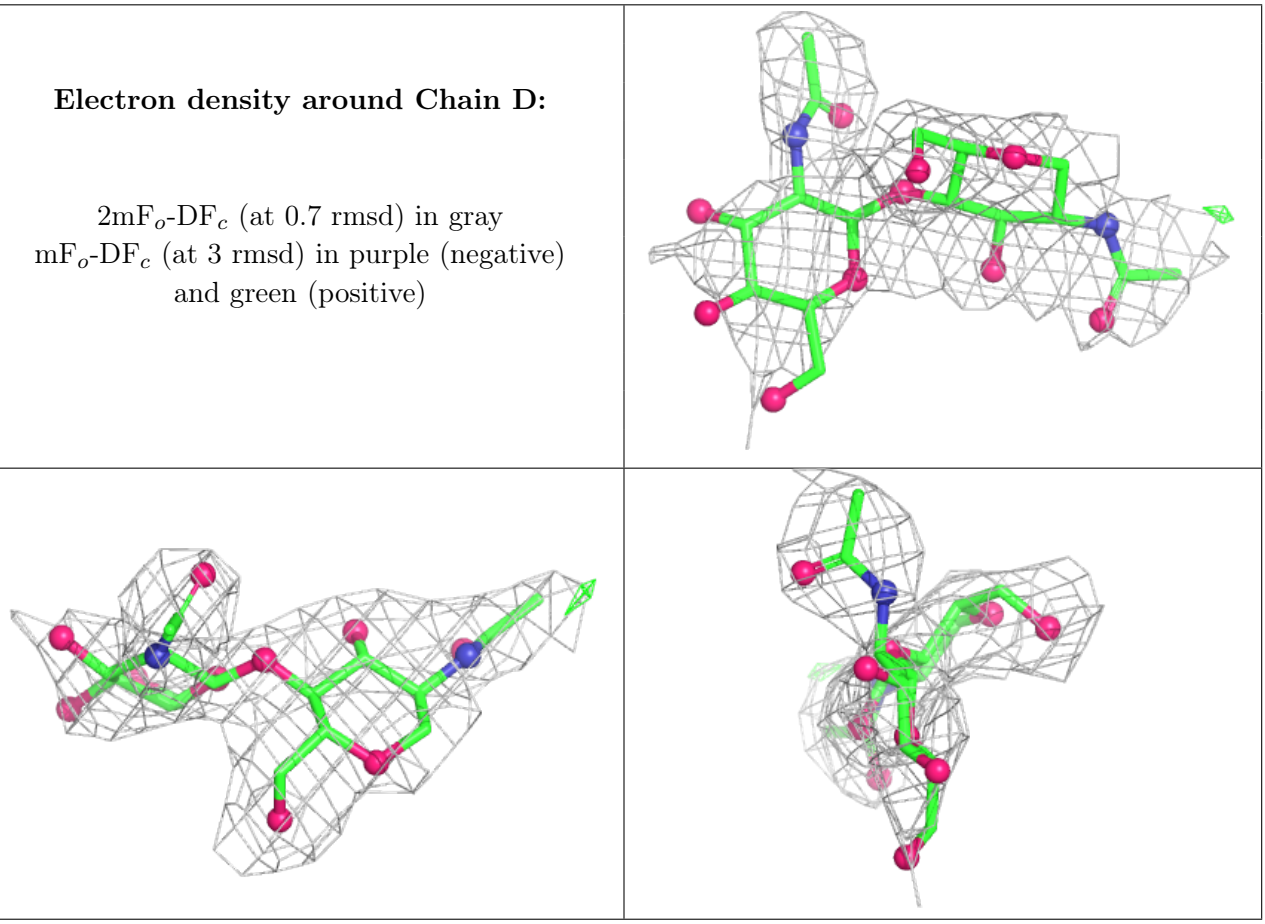
Electron density around Chain C:

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



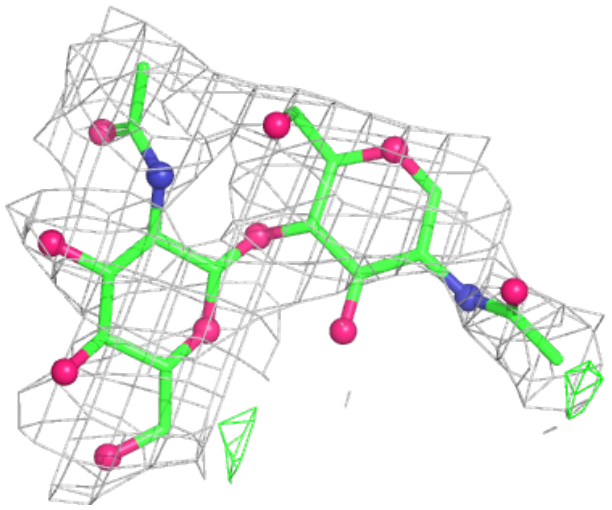
Electron density around Chain D:

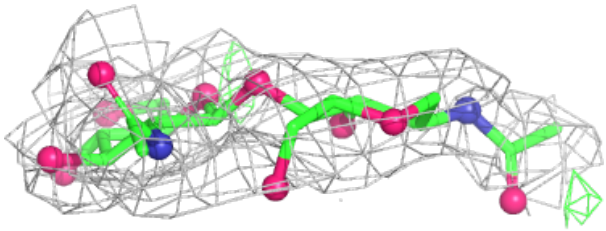
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

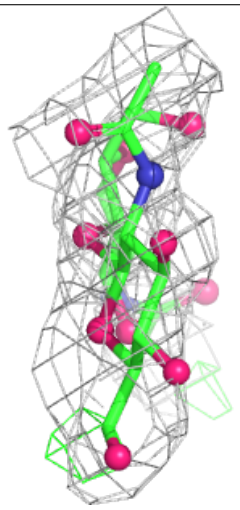


Electron density around Chain F:

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

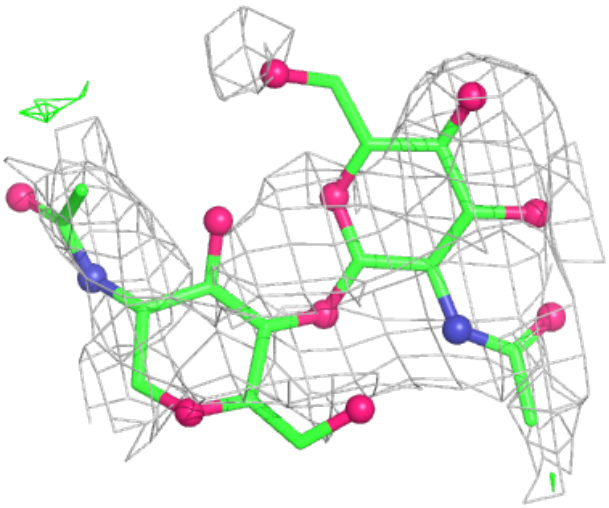


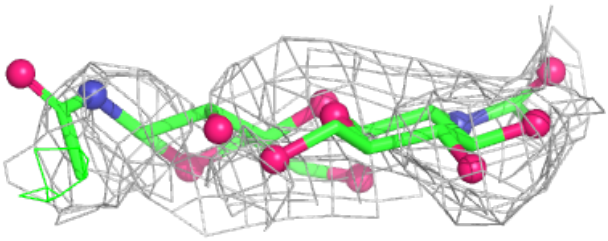


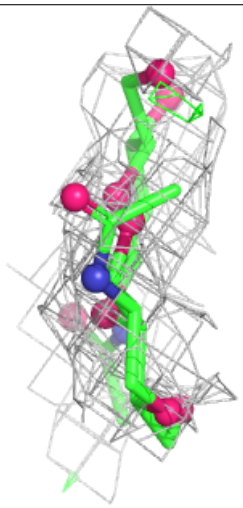


Electron density around Chain G:

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

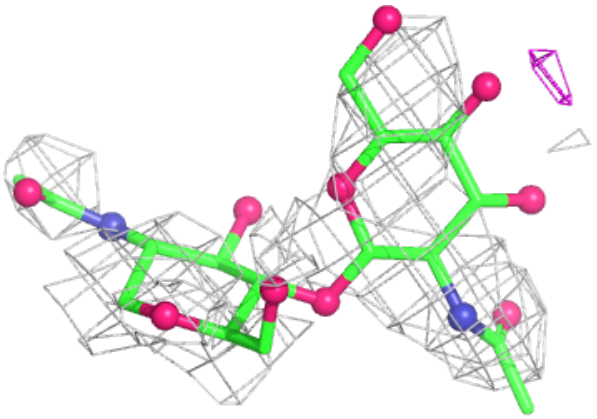


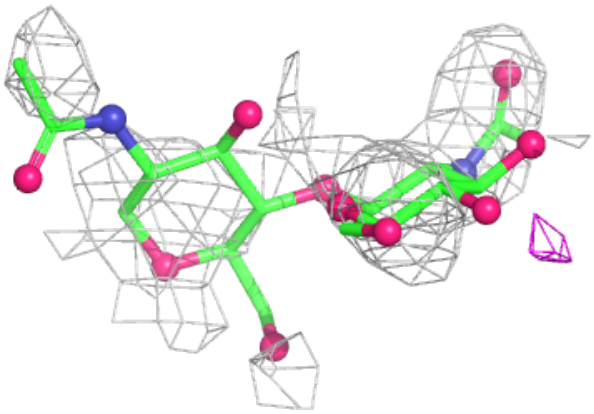


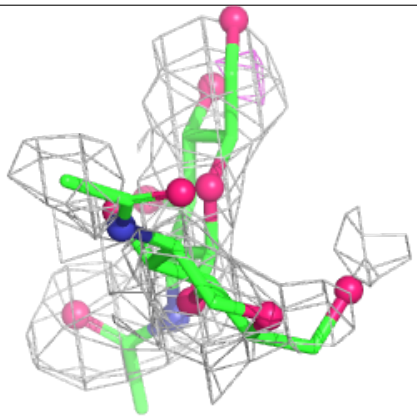


Electron density around Chain K:

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

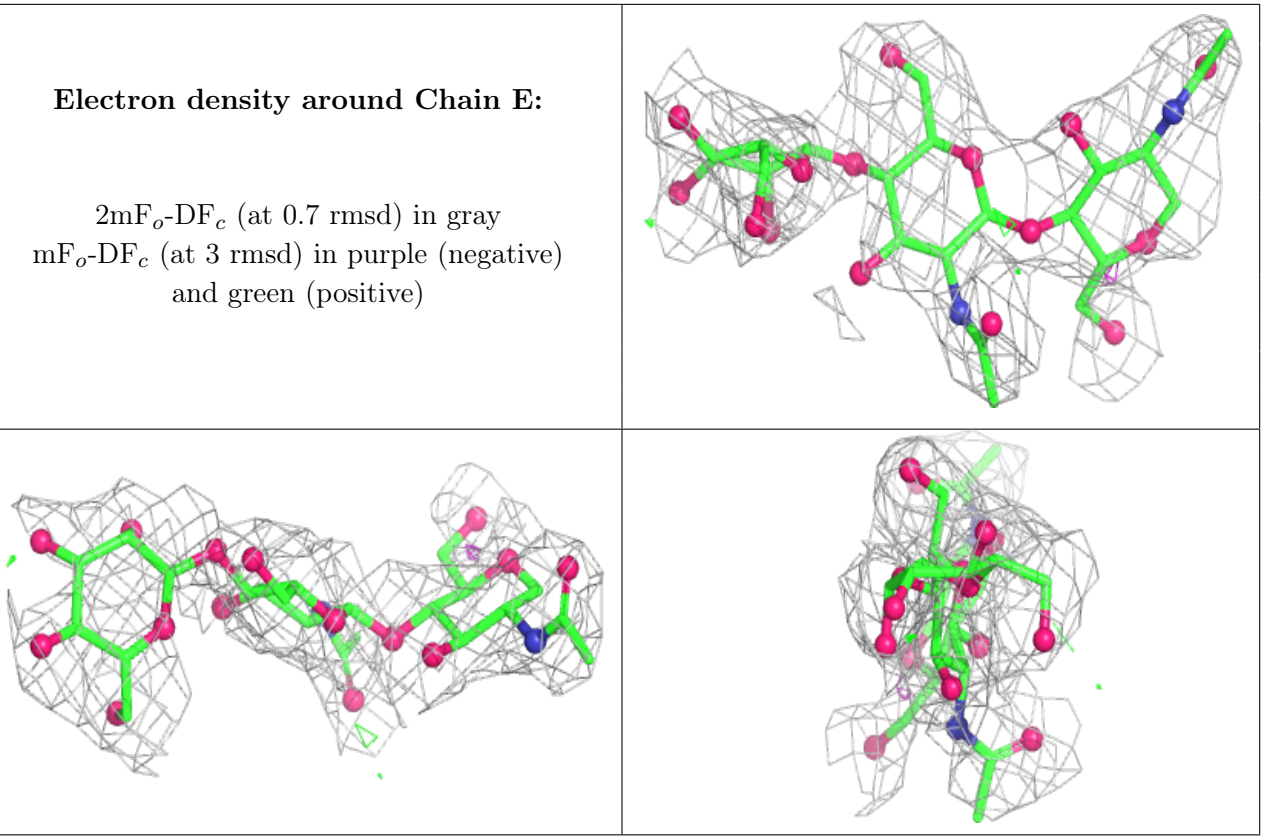






Electron density around Chain E:

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



Electron density around Chain J:

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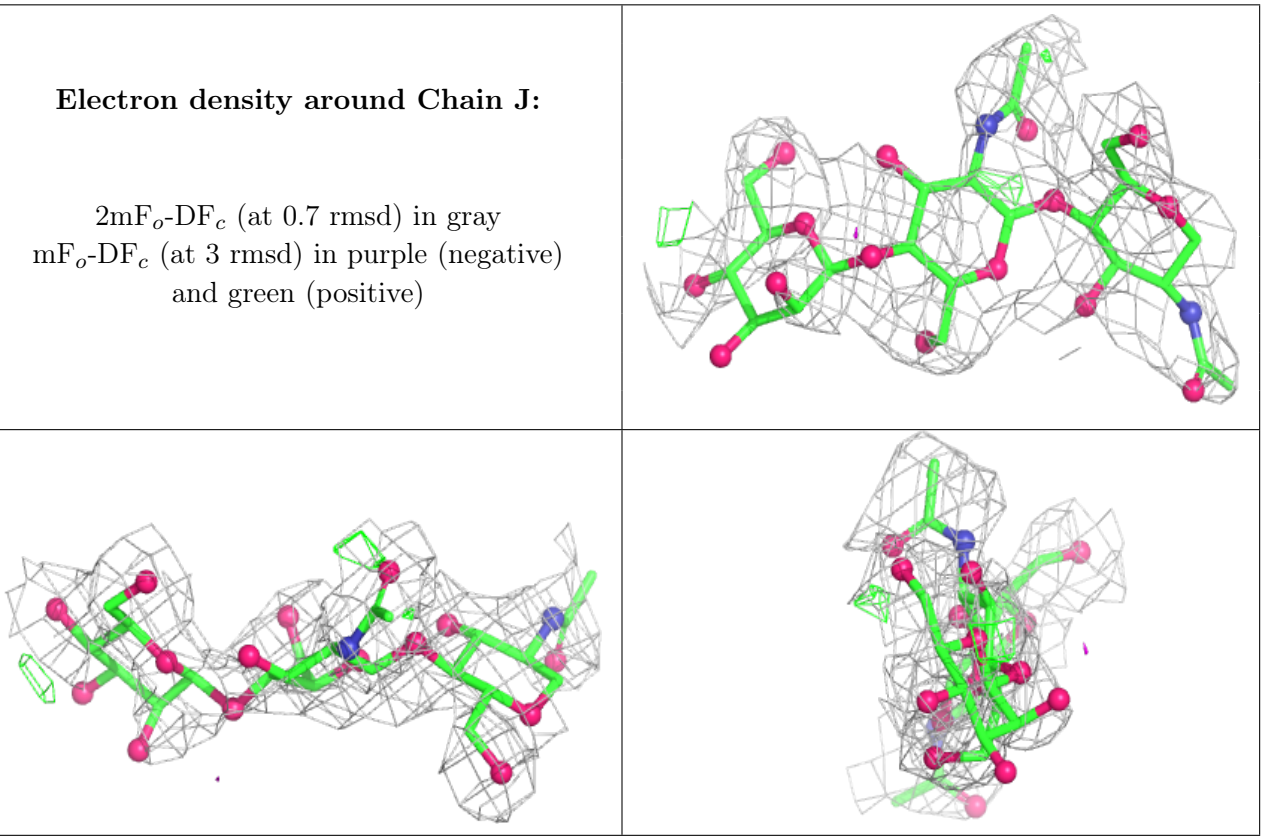
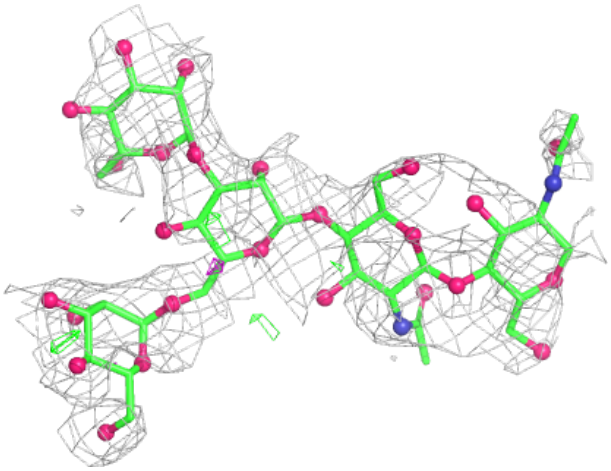
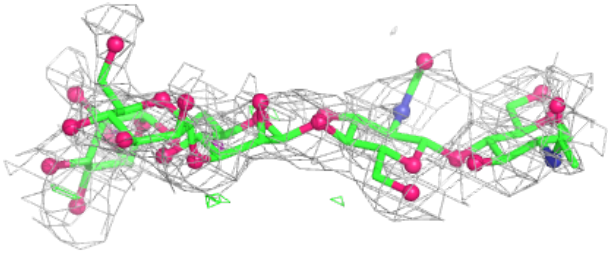
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

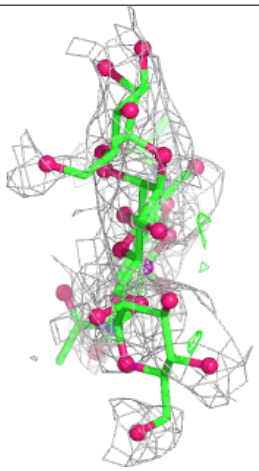


Electron density around Chain H:

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

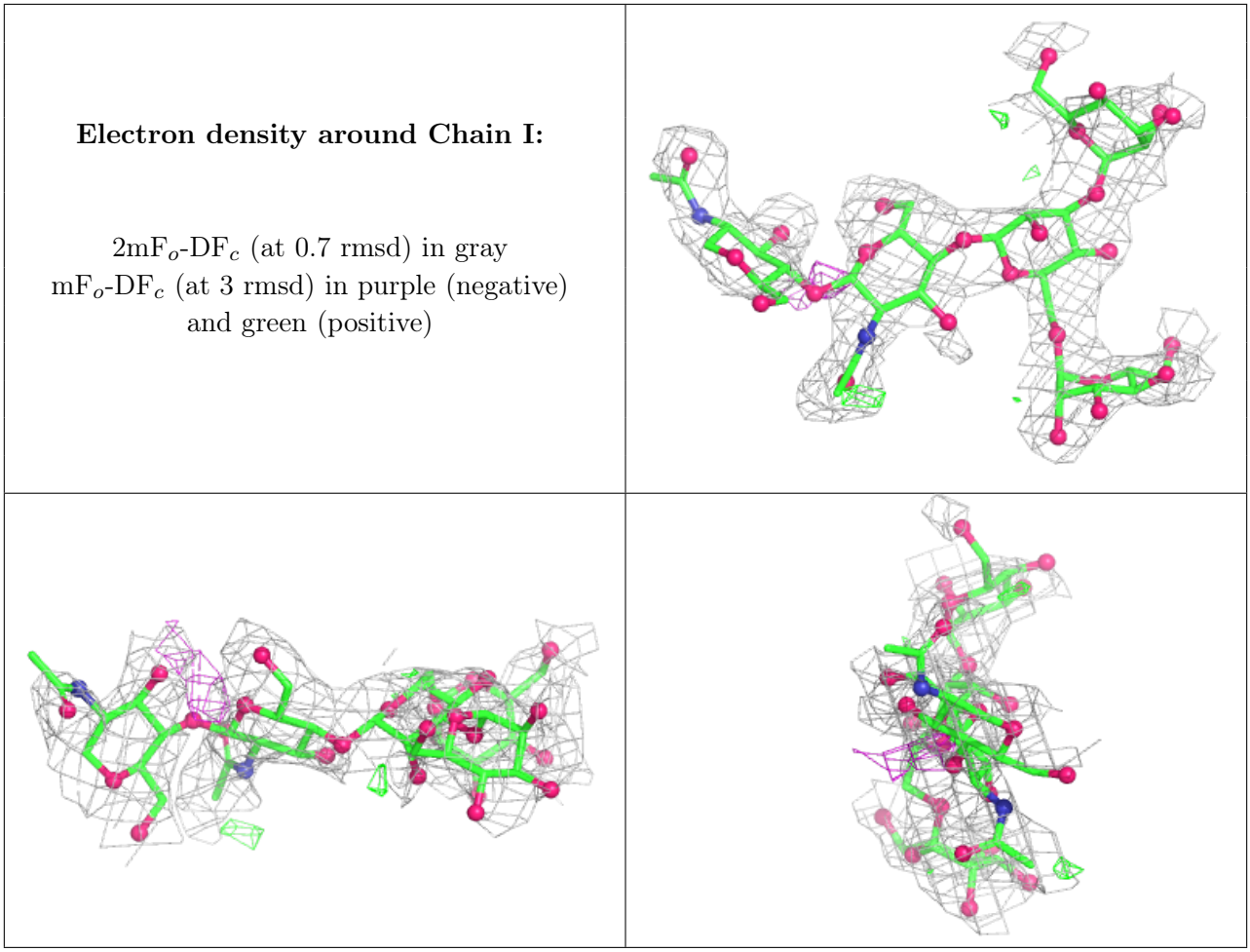






Electron density around Chain I:

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



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	B	1803	14/15	0.55	0.40	70,74,75,76	0
7	NAG	B	1811	14/15	0.57	0.26	62,67,74,77	0
7	NAG	B	1813	14/15	0.57	0.28	63,66,72,78	0
10	PEG	B	1809	7/7	0.59	0.20	55,58,62,63	0
7	NAG	B	1812	14/15	0.64	0.26	82,85,88,88	0
7	NAG	B	1814	14/15	0.65	0.32	74,77,82,89	0
7	NAG	B	1802	14/15	0.65	0.32	78,84,86,86	0
7	NAG	A	1103	14/15	0.66	0.45	64,65,66,68	0
7	NAG	A	1104	14/15	0.70	0.28	65,68,73,73	0
7	NAG	B	1810	14/15	0.71	0.45	77,84,88,88	0
9	EDO	B	1804	4/4	0.72	0.22	31,32,33,33	0

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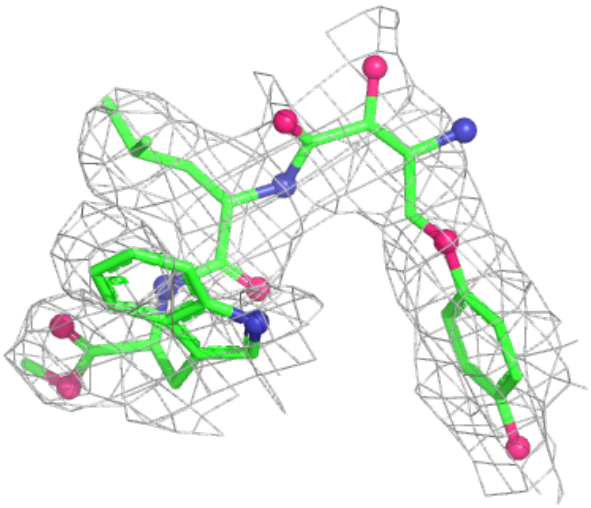
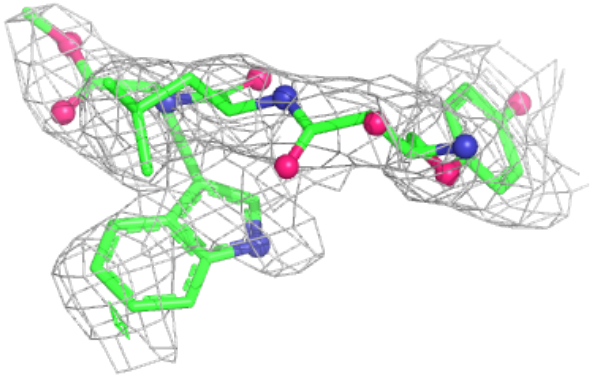
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	TRS	B	1807	8/8	0.75	0.27	34,36,37,37	0
7	NAG	A	1105	14/15	0.78	0.29	78,89,91,91	0
9	EDO	B	1806	4/4	0.81	0.17	42,43,43,43	0
8	KFR	B	1815[A]	39/39	0.83	0.33	36,42,49,52	39
10	PEG	A	1111	7/7	0.83	0.20	50,53,56,58	0
8	KFR	B	1815[B]	39/39	0.83	0.33	37,42,48,50	39
7	NAG	A	1102	14/15	0.83	0.24	68,73,76,76	0
9	EDO	A	1107	4/4	0.84	0.23	44,45,45,45	0
10	PEG	A	1110	7/7	0.87	0.20	34,37,40,41	0
8	KFR	A	1106	39/39	0.87	0.30	34,43,55,58	0
9	EDO	B	1805	4/4	0.88	0.16	36,37,37,38	0
9	EDO	A	1109	4/4	0.91	0.18	31,32,32,33	0
9	EDO	A	1108	4/4	0.93	0.24	40,40,41,41	0
9	EDO	B	1808	4/4	0.93	0.19	40,41,41,41	0
6	ZN	A	1101	1/1	0.99	0.11	25,25,25,25	0
6	ZN	B	1801	1/1	1.00	0.08	29,29,29,29	0

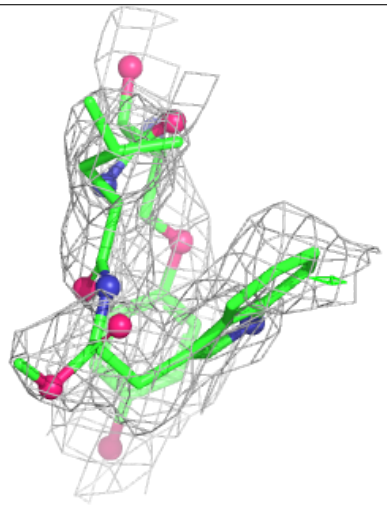
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KFR B 1815 (A):

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

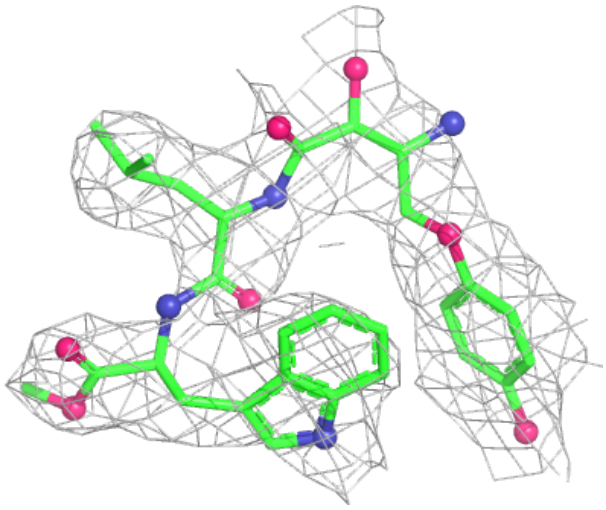


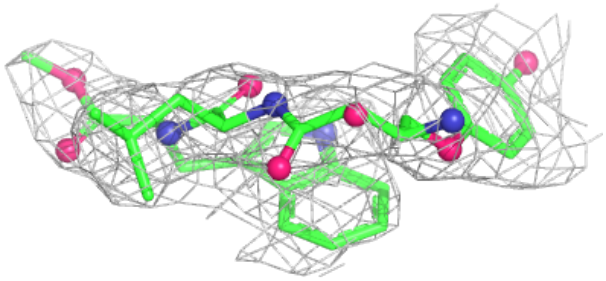


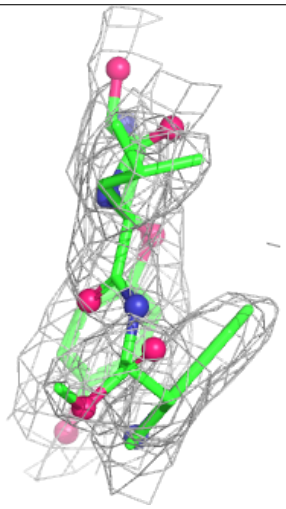


Electron density around KFR B 1815 (B):

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

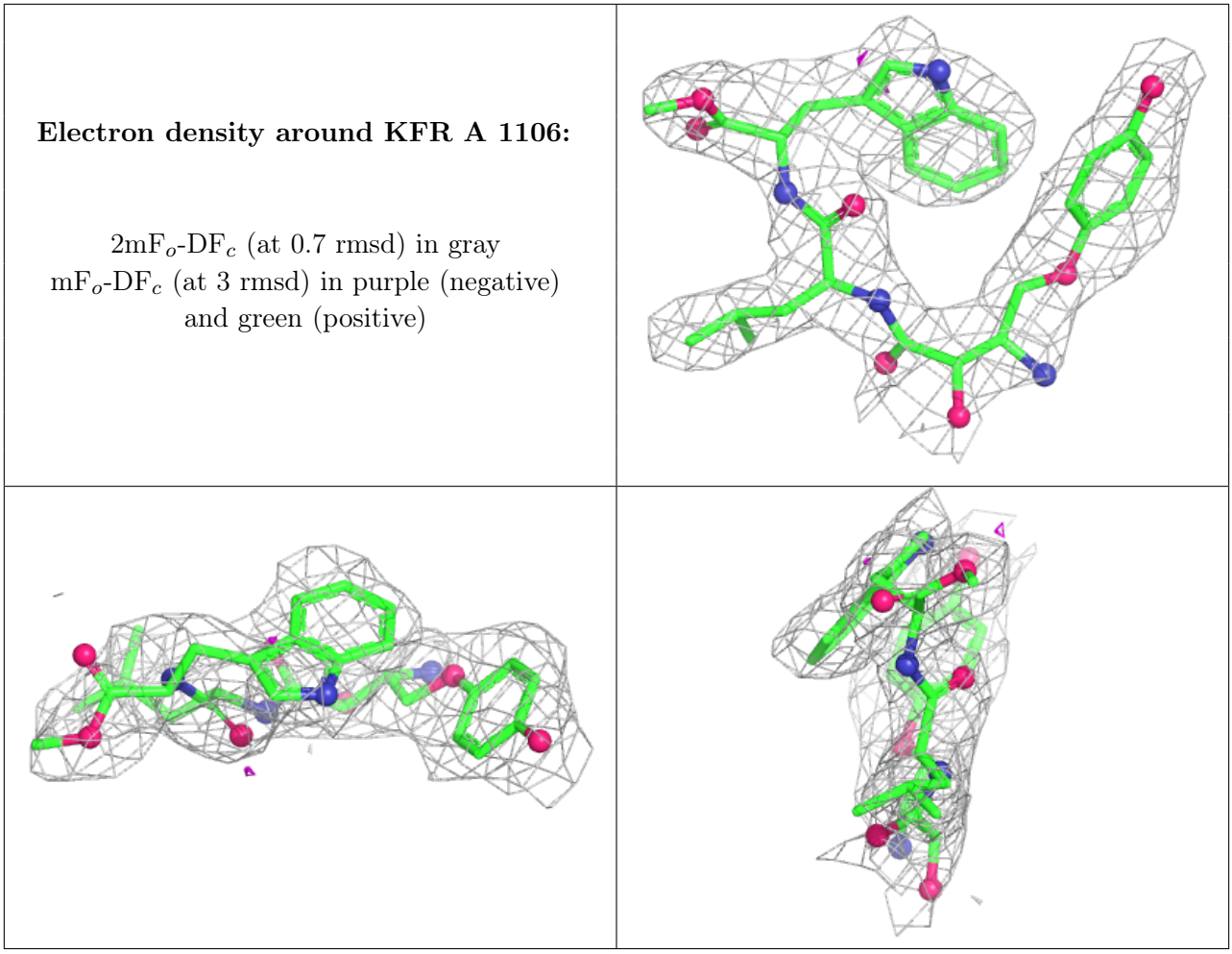






Electron density around KFR A 1106:

$2mF_o$-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 (i)

There are no such residues in this entry.