wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 06:44 pm GMT

PDB ID	:	4A5G
Title	:	Raphanus sativus anionic peroxidase.
Authors	:	Jimenez-Arroyo, N.; Valderrama, B.; Gil-Rodriguez, P.; Rojas-Trejo, S.P.; Rudino-Pinera, E.
Deposited on	:	2011-10-25
Resolution	:	2.05 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:

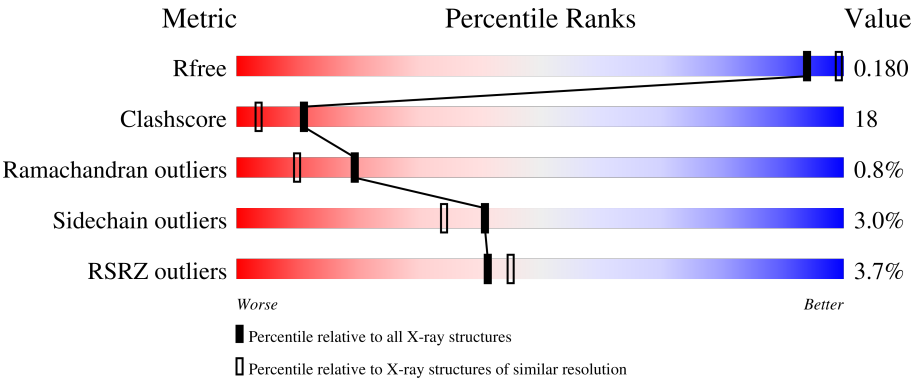
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	308	3% 81% 16% ·
1	B	308	4% 83% 14% ·
2	C	6	67% 33%
2	I	6	67% 33%
3	D	4	100%

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Mol	Chain	Length	Quality of chain
4	E	4	25% 75%
5	F	4	100%
5	L	4	50% 50%
6	G	6	83% 17%
7	H	2	100%
8	J	4	50% 50%
9	K	3	100%

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
12	NAG	B	1326	X	-	-	X
12	NAG	B	1327	-	-	-	X
12	NAG	B	1328	X	-	-	X
13	1PE	B	1330	-	-	X	-
2	NAG	I	2	X	-	-	-
2	BMA	I	3	-	-	-	X
2	MAN	I	5	X	-	-	-
3	BMA	D	3	X	-	-	-
5	NAG	L	1	X	-	-	-
6	NAG	G	1	-	-	-	X
6	NAG	G	2	X	-	-	X
6	BMA	G	3	-	-	-	X
6	BMA	G	5	-	-	-	X
6	FUL	G	6	-	-	-	X
7	NAG	H	2	-	-	-	X
9	FUC	K	2	-	-	-	X
9	NAG	K	3	-	-	-	X

2 Entry composition (i)

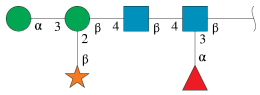
There are 15 unique types of molecules in this entry. The entry contains 5969 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ANIONIC PEROXIDASE.

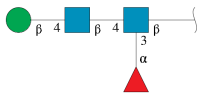
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	7	0
			2277	1395	400	467	15			
1	B	307	Total	C	N	O	S	0	5	0
			2258	1388	395	462	13			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			69	39	2	28			
2	I	6	Total	C	N	O	0	0	0
			69	39	2	28			

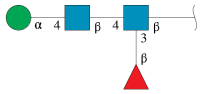
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

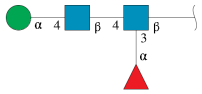
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-

beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



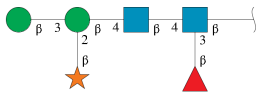
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	4	Total	C	N	O	0	0	0
			49	28	2	19			
5	L	4	Total	C	N	O	0	0	0
			49	28	2	19			

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

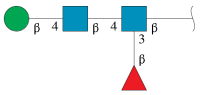


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	6	Total	C	N	O	0	0	0
			69	39	2	28			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

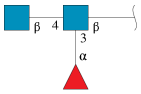
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



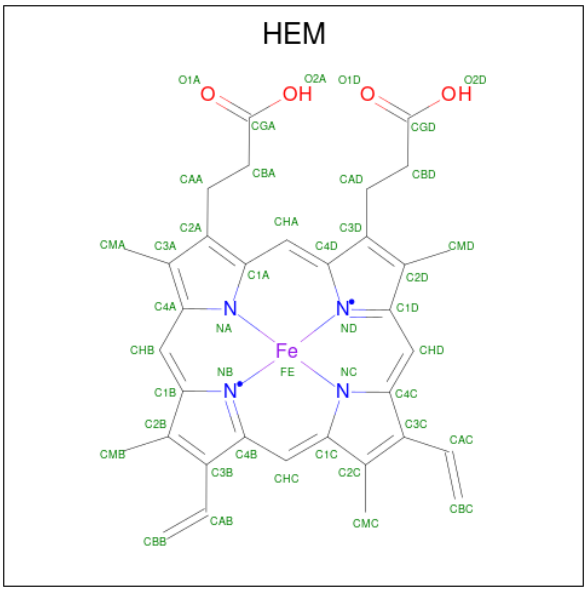
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 9 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

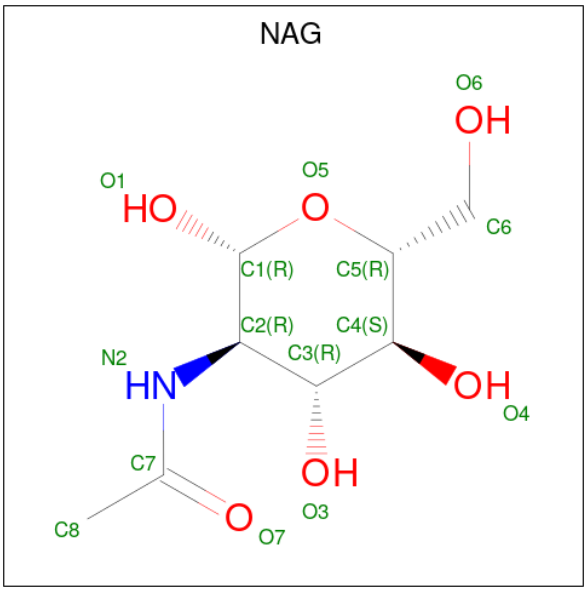


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

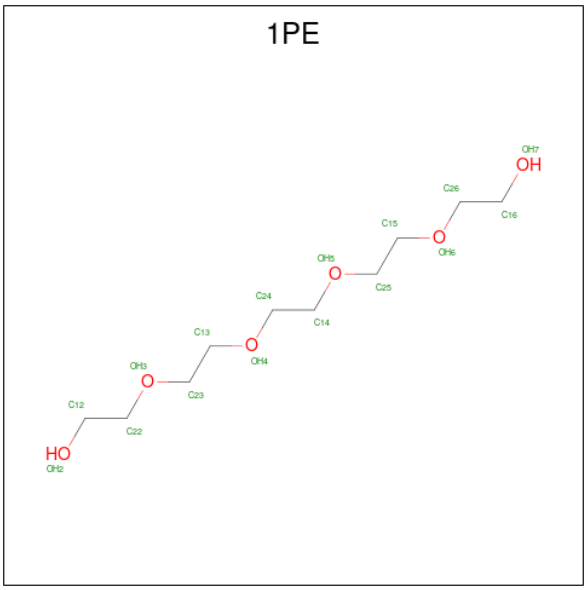
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Ca	0	0
			2	2		
11	B	2	Total	Ca	0	0
			2	2		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



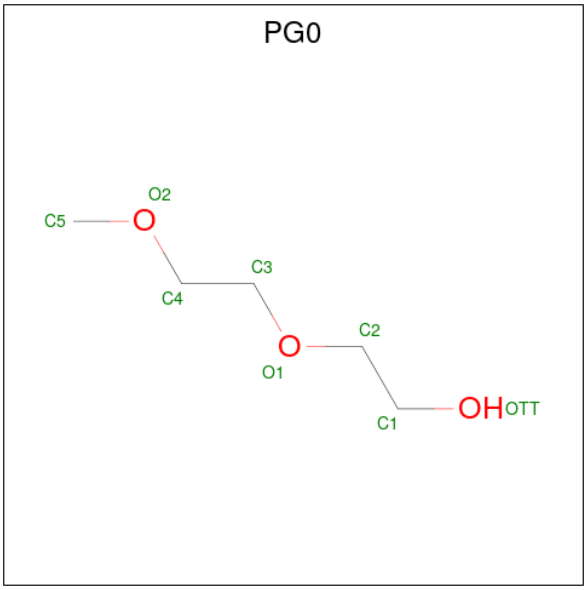
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C N O 14 8 1 5	0	0
12	B	1	Total C N O 14 8 1 5	0	0
12	B	1	Total C N O 14 8 1 5	0	0
12	B	1	Total C N O 14 8 1 5	0	0

- Molecule 13 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 5 3 2	0	0
13	A	1	Total C O 10 6 4	0	0
13	B	1	Total C O 15 10 5	0	0
13	B	1	Total C O 16 10 6	0	0
13	B	1	Total C O 5 3 2	0	0
13	B	1	Total C O 6 4 2	0	0
13	B	1	Total C O 5 3 2	0	0

- Molecule 14 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total C O 8 5 3	0	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	364	Total O 364 364	0	0

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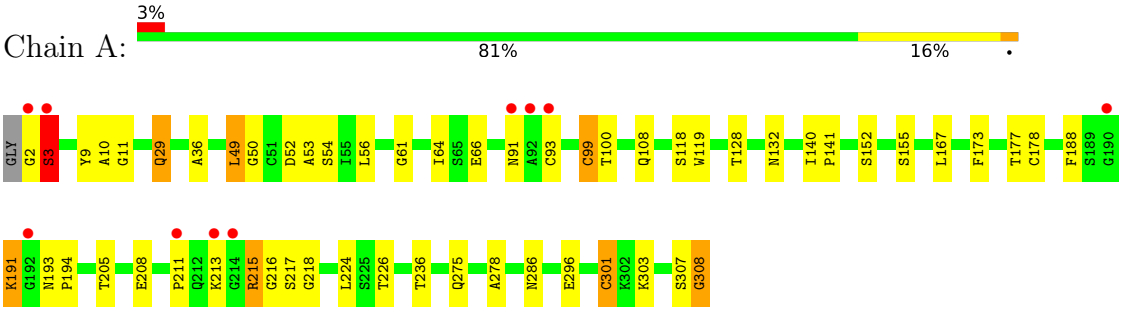
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	336	Total	O	0	0
			336	336		

3 Residue-property plots

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

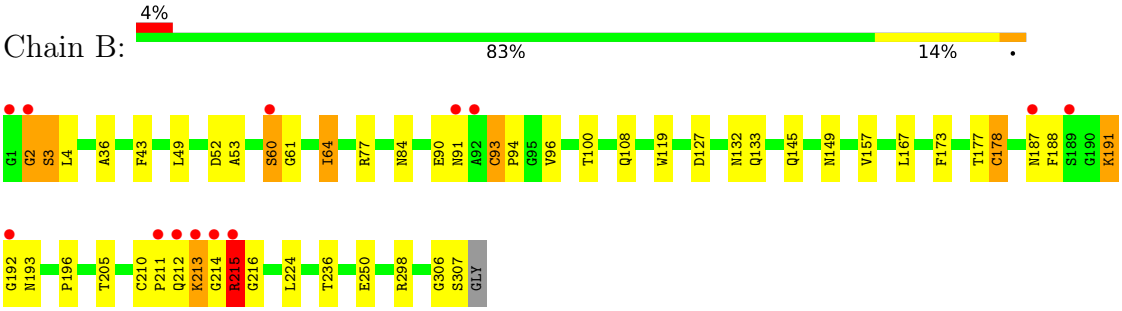
• Molecule 1: ANIONIC PEROXIDASE

Chain A:



• Molecule 1: ANIONIC PEROXIDASE

Chain B:

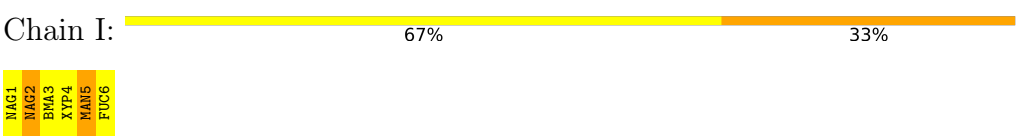


• Molecule 2: beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

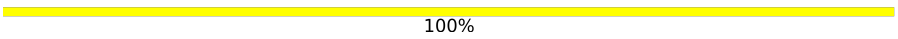
• Molecule 2: beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain D:

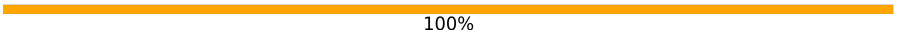


• Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain F:

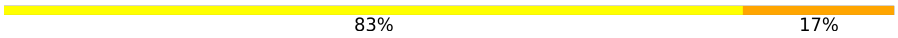


• Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

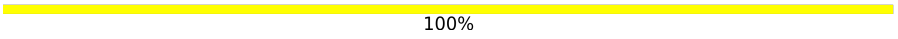
• Molecule 6: beta-D-xylopyranose-(1-2)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

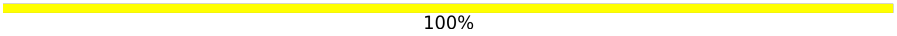


• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 9: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.15Å 41.19Å 137.80Å 90.00° 96.91° 90.00°	Depositor
Resolution (Å)	35.29 – 2.05 35.29 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.29-2.05) 98.6 (35.29-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.163 , 0.185 0.155 , 0.180	Depositor DCC
R_{free} test set	2634 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5969	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.06% 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: FUC, NAG, 1PE, HEM, CA, FUL, MAN, XYP, PG0, 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	1.57	7/2314 (0.3%)	0.79	2/3144 (0.1%)
1	B	1.57	3/2301 (0.1%)	0.83	3/3128 (0.1%)
All	All	1.57	10/4615 (0.2%)	0.81	5/6272 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
All	All	0	7

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	ASN	C-N	-11.08	1.08	1.34
1	B	90	GLU	C-N	-8.77	1.13	1.34
1	A	91	ASN	C-N	-8.60	1.14	1.34
1	B	250	GLU	CD-OE2	-5.56	1.19	1.25
1	A	66	GLU	CD-OE1	-5.41	1.19	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2	GLY	N-CA-C	-6.29	97.39	113.10
1	A	91	ASN	O-C-N	-5.91	113.25	122.70
1	B	157[A]	VAL	CA-C-N	5.27	126.75	116.20
1	B	157[B]	VAL	CA-C-N	5.27	126.75	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	308	GLY	N-CA-C	5.20	126.11	113.10

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3[B]	SER	Mainchain
1	A	301[B]	CYS	Mainchain
1	A	93[B]	CYS	Mainchain
1	A	99[B]	CYS	Mainchain
1	B	212	GLN	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	2277	0	2185	74	0
1	B	2258	0	2177	79	1
2	C	69	0	51	5	0
2	I	69	0	51	5	0
3	D	49	0	43	0	0
4	E	49	0	43	2	0
5	F	49	0	43	2	1
5	L	49	0	43	1	0
6	G	69	0	51	1	0
7	H	28	0	25	0	0
8	J	49	0	43	4	0
9	K	38	0	34	0	0
10	A	43	0	30	2	0
10	B	43	0	30	3	0
11	A	2	0	0	0	0
11	B	2	0	0	0	0
12	A	14	0	13	2	0
12	B	42	0	39	2	0
13	A	15	0	17	5	0
13	B	47	0	55	13	0
14	B	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	364	0	0	32	9
15	B	336	0	0	29	2
All	All	5969	0	4985	182	11

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 18.

The worst 5 of 182 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:177:THR:HG23	15:A:2200:HOH:O	1.22	1.31
1:A:99[B]:CYS:SG	1:A:301[B]:CYS:HB3	1.73	1.27
1:A:56:LEU:CD1	1:A:99[B]:CYS:SG	2.30	1.20
1:B:60:SER:HA	15:B:2089:HOH:O	1.02	1.20
1:A:308:GLY:O	15:A:2328:HOH:O	1.57	1.19

The worst 5 of 11 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:4:FUC:C6	15:B:2137:HOH:O[1_445]	1.72	0.48
15:A:2194:HOH:O	15:A:2212:HOH:O[2_556]	1.95	0.25
1:B:93[B]:CYS:O	15:A:2353:HOH:O[1_665]	2.00	0.20
15:A:2076:HOH:O	15:A:2122:HOH:O[2_556]	2.02	0.18
15:A:2159:HOH:O	15:A:2358:HOH:O[2_656]	2.03	0.17

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	312/308 (101%)	305 (98%)	5 (2%)	2 (1%)	25 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	310/308 (101%)	297 (96%)	7 (2%)	6 (2%)	8 2
All	All	622/616 (101%)	602 (97%)	12 (2%)	8 (1%)	19 4

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	215	ARG
1	A	3[A]	SER
1	A	3[B]	SER
1	B	94	PRO
1	B	178[A]	CYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	257/250 (103%)	251 (98%)	6 (2%)	50 44
1	B	255/250 (102%)	246 (96%)	9 (4%)	36 29
All	All	512/500 (102%)	497 (97%)	15 (3%)	41 35

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43	PHE
1	B	215	ARG
1	B	60	SER
1	B	224	LEU
1	B	191	LYS

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

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)

43 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	1,2	14,14,15	1.92	4 (28%)	17,19,21	1.15	2 (11%)
2	NAG	C	2	2	14,14,15	1.96	6 (42%)	17,19,21	1.30	2 (11%)
2	BMA	C	3	2	11,11,12	2.01	2 (18%)	15,15,17	0.91	0
2	XYP	C	4	2	9,9,10	2.25	3 (33%)	10,12,14	1.16	1 (10%)
2	MAN	C	5	2	11,11,12	1.90	2 (18%)	15,15,17	0.91	1 (6%)
2	FUC	C	6	2	10,10,11	1.98	2 (20%)	14,14,16	0.92	0
3	NAG	D	1	1,3	14,14,15	1.86	4 (28%)	17,19,21	1.14	0
3	NAG	D	2	3	14,14,15	1.92	5 (35%)	17,19,21	1.14	0
3	BMA	D	3	3	11,11,12	1.85	2 (18%)	15,15,17	1.13	0
3	FUC	D	4	3	10,10,11	1.92	2 (20%)	14,14,16	0.77	0
4	NAG	E	1	1,4	14,14,15	1.97	4 (28%)	17,19,21	1.76	3 (17%)
4	NAG	E	2	4	14,14,15	2.03	4 (28%)	17,19,21	1.10	1 (5%)
4	MAN	E	3	4	11,11,12	2.09	2 (18%)	15,15,17	1.18	1 (6%)
4	FUL	E	4	4	10,10,11	2.07	2 (20%)	14,14,16	1.00	1 (7%)
5	NAG	F	1	1,5	14,14,15	1.85	4 (28%)	17,19,21	0.94	1 (5%)
5	NAG	F	2	5	14,14,15	1.91	5 (35%)	17,19,21	1.46	3 (17%)
5	MAN	F	3	5	11,11,12	1.86	2 (18%)	15,15,17	1.19	2 (13%)
5	FUC	F	4	5	10,10,11	1.98	2 (20%)	14,14,16	1.23	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	G	1	1,6	14,14,15	1.94	4 (28%)	17,19,21	1.47	5 (29%)
6	NAG	G	2	6	14,14,15	1.96	5 (35%)	17,19,21	1.18	2 (11%)
6	BMA	G	3	6	11,11,12	1.87	2 (18%)	15,15,17	0.86	0
6	XYP	G	4	6	9,9,10	2.24	3 (33%)	10,12,14	1.04	1 (10%)
6	BMA	G	5	6	11,11,12	1.78	2 (18%)	15,15,17	1.06	1 (6%)
6	FUL	G	6	6	10,10,11	1.99	2 (20%)	14,14,16	1.12	0
7	NAG	H	1	1,7	14,14,15	1.98	5 (35%)	17,19,21	1.07	1 (5%)
7	NAG	H	2	7	14,14,15	1.92	5 (35%)	17,19,21	1.22	3 (17%)
2	NAG	I	1	1,2	14,14,15	1.93	4 (28%)	17,19,21	1.27	2 (11%)
2	NAG	I	2	2	14,14,15	1.90	5 (35%)	17,19,21	1.65	5 (29%)
2	BMA	I	3	2	11,11,12	1.92	2 (18%)	15,15,17	0.80	0
2	XYP	I	4	2	9,9,10	2.31	3 (33%)	10,12,14	1.33	2 (20%)
2	MAN	I	5	2	11,11,12	1.83	2 (18%)	15,15,17	0.95	0
2	FUC	I	6	2	10,10,11	1.94	2 (20%)	14,14,16	1.14	1 (7%)
8	NAG	J	1	1,8	14,14,15	1.94	4 (28%)	17,19,21	1.21	2 (11%)
8	NAG	J	2	8	14,14,15	1.95	4 (28%)	17,19,21	1.38	2 (11%)
8	BMA	J	3	8	11,11,12	1.84	2 (18%)	15,15,17	1.06	1 (6%)
8	FUL	J	4	8	10,10,11	2.07	2 (20%)	14,14,16	0.88	1 (7%)
9	NAG	K	1	1,9	14,14,15	1.93	4 (28%)	17,19,21	1.37	2 (11%)
9	FUC	K	2	9	10,10,11	2.02	2 (20%)	14,14,16	0.75	0
9	NAG	K	3	9	14,14,15	1.95	5 (35%)	17,19,21	1.22	2 (11%)
5	NAG	L	1	1,5	14,14,15	1.91	5 (35%)	17,19,21	1.69	5 (29%)
5	NAG	L	2	5	14,14,15	1.93	5 (35%)	17,19,21	1.26	2 (11%)
5	MAN	L	3	5	11,11,12	1.85	2 (18%)	15,15,17	1.37	2 (13%)
5	FUC	L	4	5	10,10,11	1.92	2 (20%)	14,14,16	0.97	1 (7%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	XYP	C	4	2	-	-	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	C	6	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	1/1/4/5	2/2/19/22	0/1/1/1
3	FUC	D	4	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	MAN	E	3	4	-	2/2/19/22	0/1/1/1
4	FUL	E	4	4	-	-	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	MAN	F	3	5	-	0/2/19/22	0/1/1/1
5	FUC	F	4	5	-	-	0/1/1/1
6	NAG	G	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	1/1/5/7	2/6/23/26	0/1/1/1
6	BMA	G	3	6	-	2/2/19/22	0/1/1/1
6	XYP	G	4	6	-	-	0/1/1/1
6	BMA	G	5	6	-	0/2/19/22	1/1/1/1
6	FUL	G	6	6	-	-	0/1/1/1
7	NAG	H	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	H	2	7	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	1/1/5/7	0/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	XYP	I	4	2	-	-	0/1/1/1
2	MAN	I	5	2	1/1/4/5	2/2/19/22	1/1/1/1
2	FUC	I	6	2	-	-	0/1/1/1
8	NAG	J	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	1/6/23/26	0/1/1/1
8	BMA	J	3	8	-	2/2/19/22	0/1/1/1
8	FUL	J	4	8	-	-	0/1/1/1
9	NAG	K	1	1,9	-	0/6/23/26	0/1/1/1
9	FUC	K	2	9	-	-	0/1/1/1
9	NAG	K	3	9	-	0/6/23/26	0/1/1/1
5	NAG	L	1	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	MAN	L	3	5	-	2/2/19/22	0/1/1/1
5	FUC	L	4	5	-	-	0/1/1/1

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	MAN	C2-C3	-5.71	1.44	1.52
2	C	3	BMA	C2-C3	-5.60	1.44	1.52
4	E	4	FUL	C2-C3	-5.49	1.44	1.52
8	J	4	FUL	C2-C3	-5.44	1.44	1.52
6	G	6	FUL	C2-C3	-5.31	1.44	1.52

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1	NAG	C2-N2-C7	-3.82	117.46	122.90
4	E	1	NAG	C1-O5-C5	-3.77	107.09	112.19
2	C	2	NAG	C2-N2-C7	-3.56	117.83	122.90
8	J	2	NAG	C2-N2-C7	-3.43	118.02	122.90
5	F	2	NAG	C2-N2-C7	-3.41	118.05	122.90

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	2	NAG	C1
2	I	5	MAN	C1
3	D	3	BMA	C1
5	L	1	NAG	C1
6	G	2	NAG	C1

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	3	MAN	C4-C5-C6-O6
5	L	3	MAN	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
6	G	2	NAG	C4-C5-C6-O6
4	E	3	MAN	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	5	BMA	C1-C2-C3-C4-C5-O5
2	I	5	MAN	C1-C2-C3-C4-C5-O5

16 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	5	BMA	1	0

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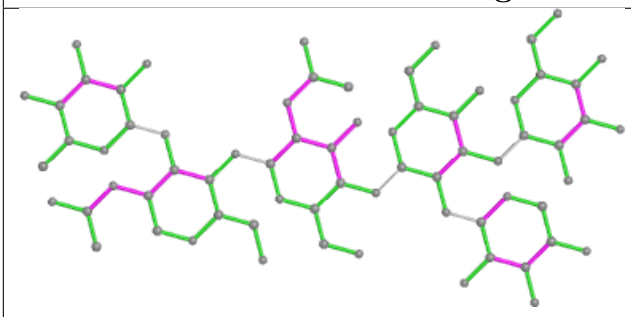
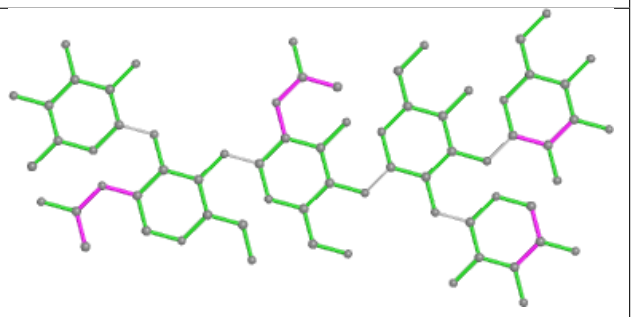
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	XYP	5	0
8	J	3	BMA	2	0
5	F	2	NAG	1	0
5	L	2	NAG	1	0
4	E	1	NAG	1	0
2	I	5	MAN	4	0
8	J	2	NAG	2	0
5	L	4	FUC	1	0
5	F	4	FUC	0	1
2	C	5	MAN	1	0
2	I	2	NAG	1	0
5	F	1	NAG	1	0
4	E	4	FUL	1	0
4	E	3	MAN	1	0
5	F	3	MAN	1	0

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

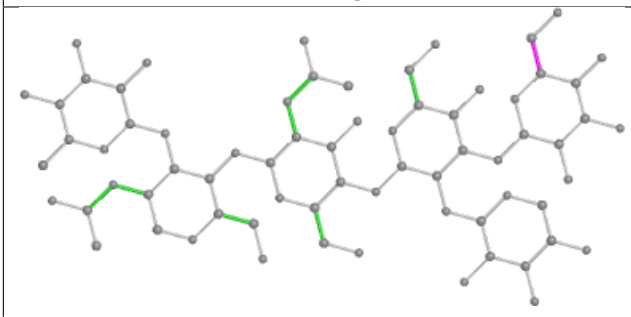
Oligosaccharide Chain C



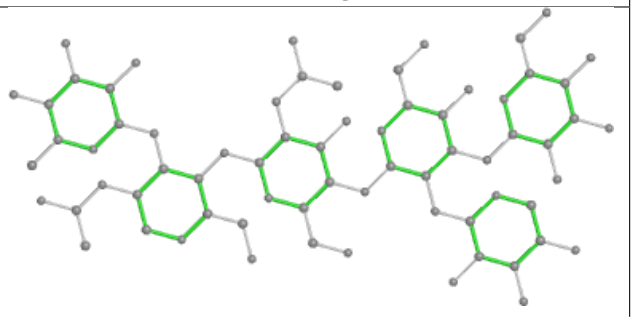
Bond lengths



Bond angles

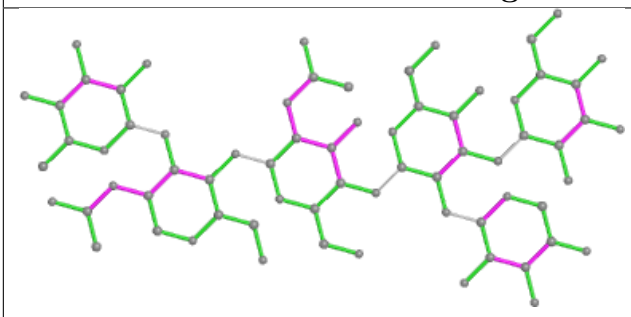


Torsions

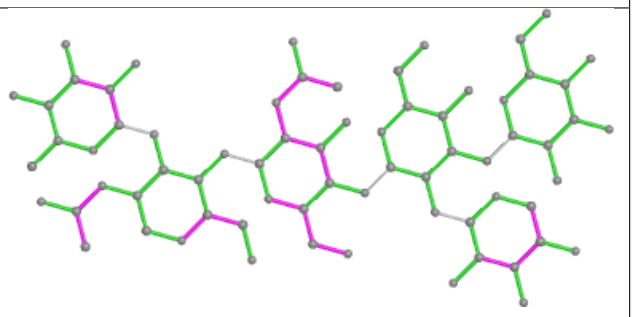


Rings

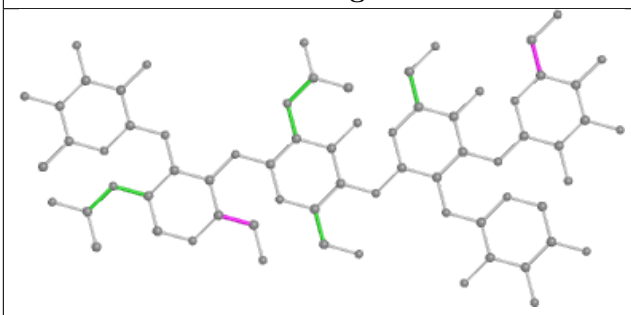
Oligosaccharide Chain I



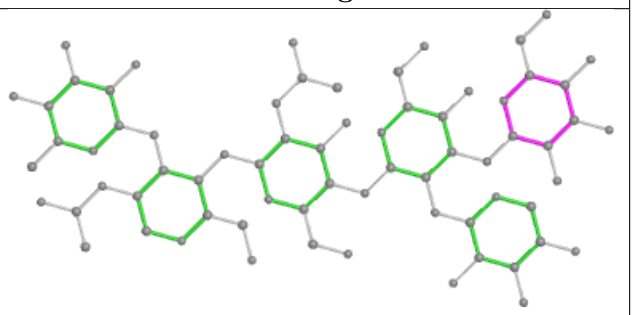
Bond lengths



Bond angles

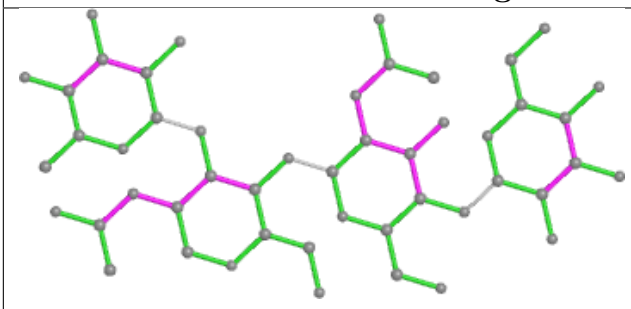


Torsions

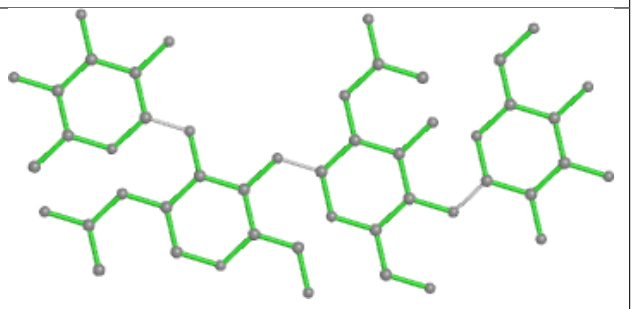


Rings

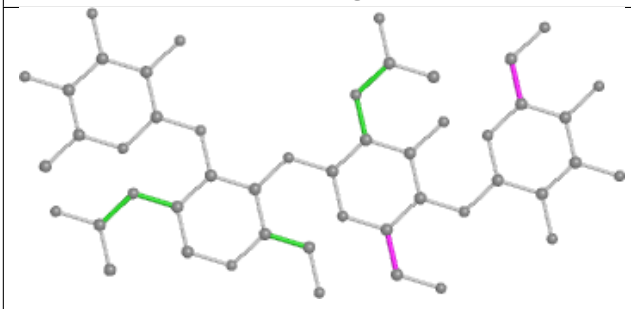
Oligosaccharide Chain D



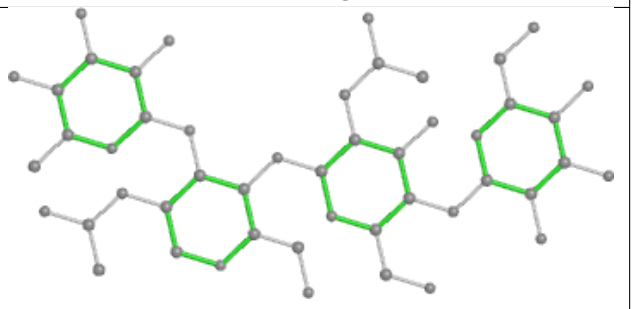
Bond lengths



Bond angles

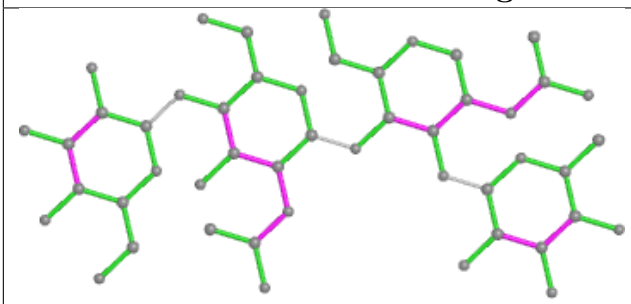


Torsions

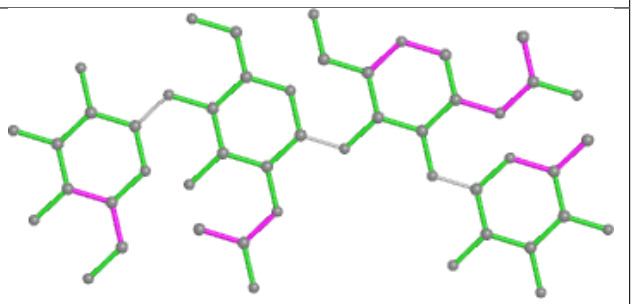


Rings

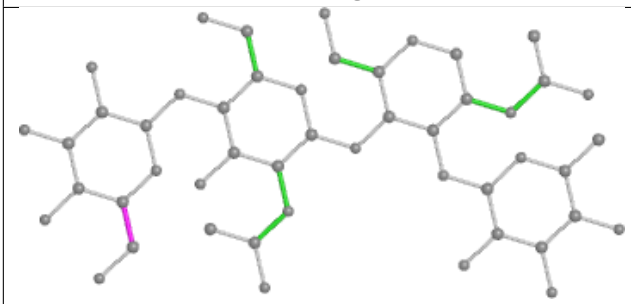
Oligosaccharide Chain E



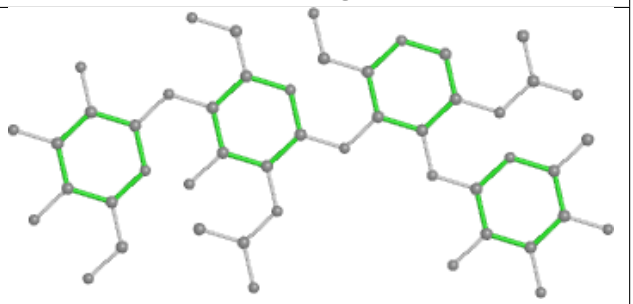
Bond lengths



Bond angles

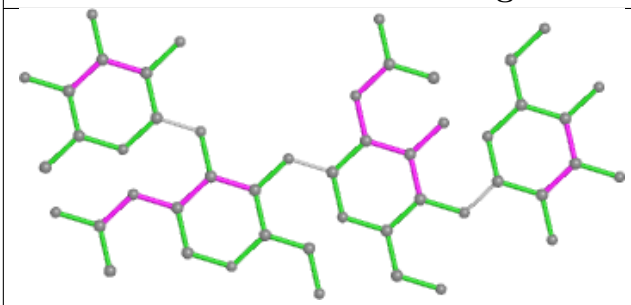


Torsions

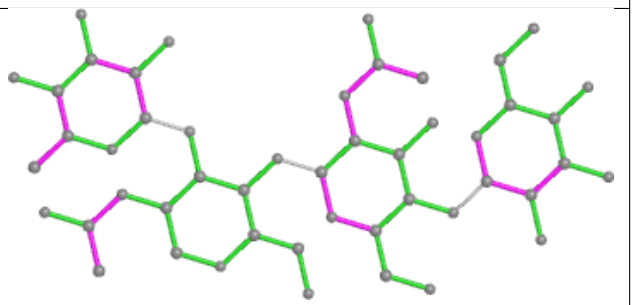


Rings

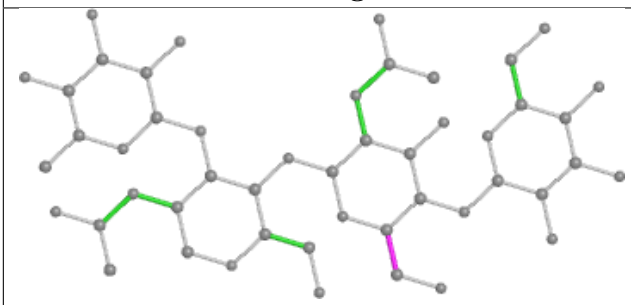
Oligosaccharide Chain F



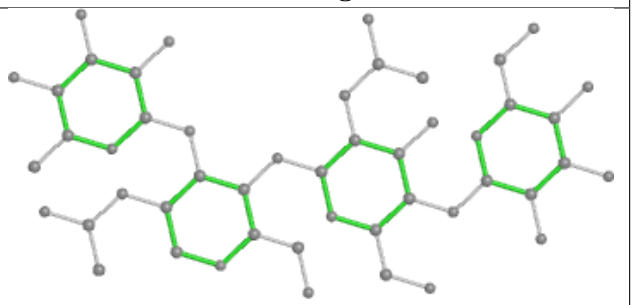
Bond lengths



Bond angles

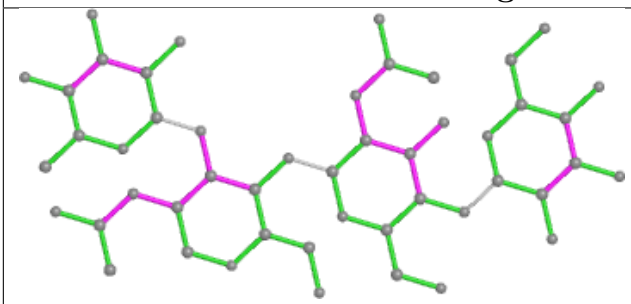


Torsions

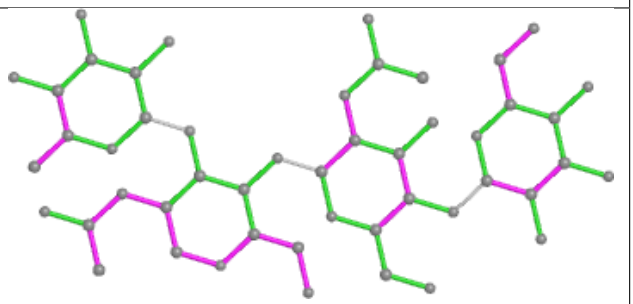


Rings

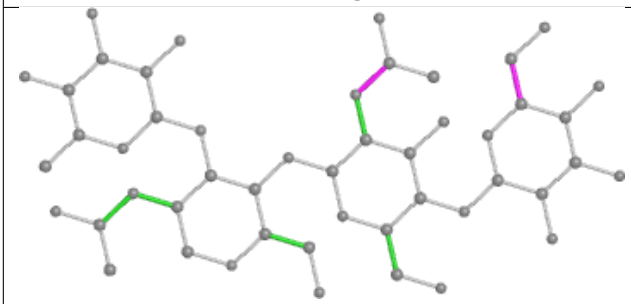
Oligosaccharide Chain L



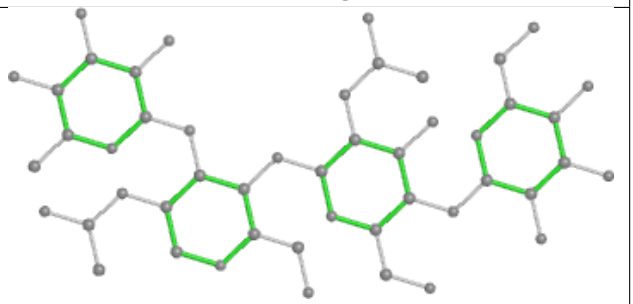
Bond lengths



Bond angles

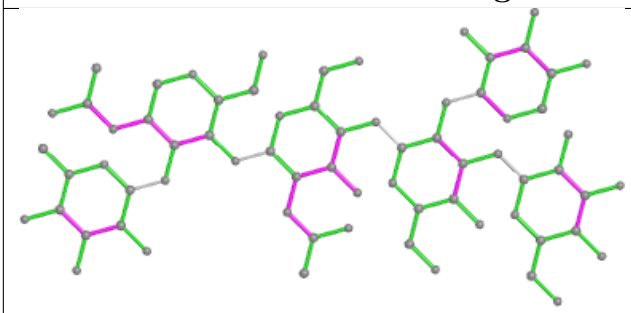


Torsions

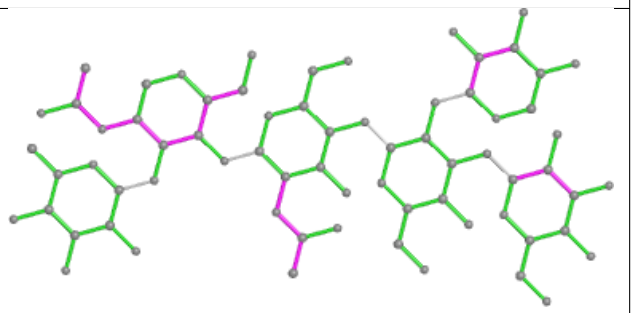


Rings

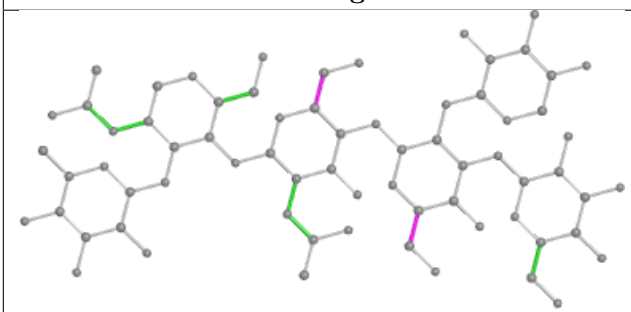
Oligosaccharide Chain G



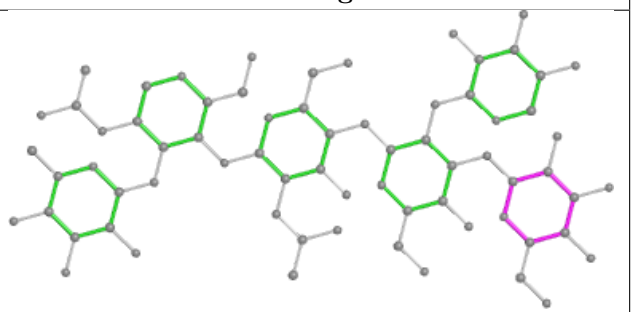
Bond lengths



Bond angles

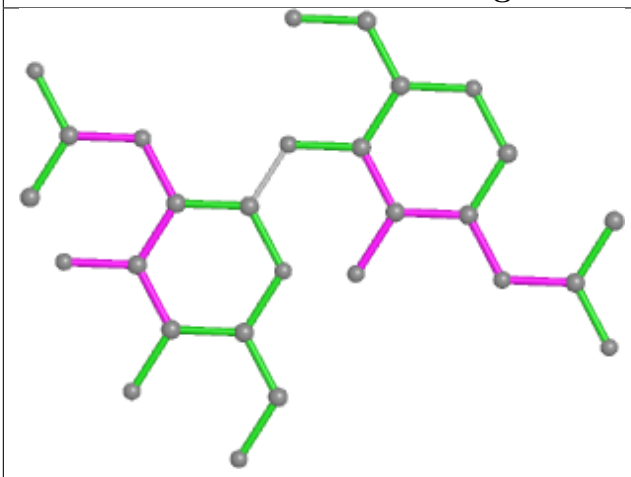


Torsions

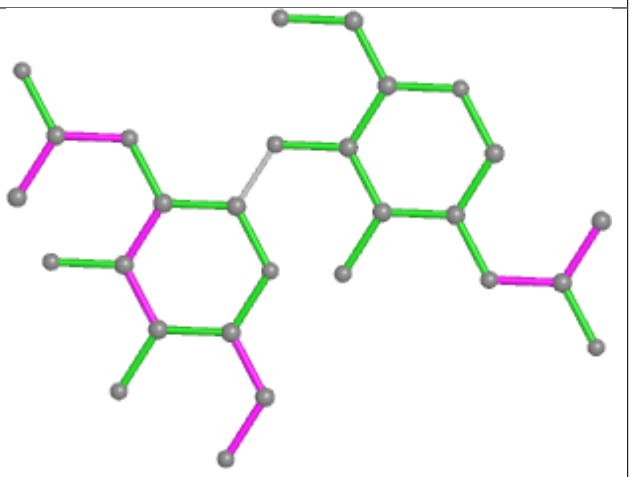


Rings

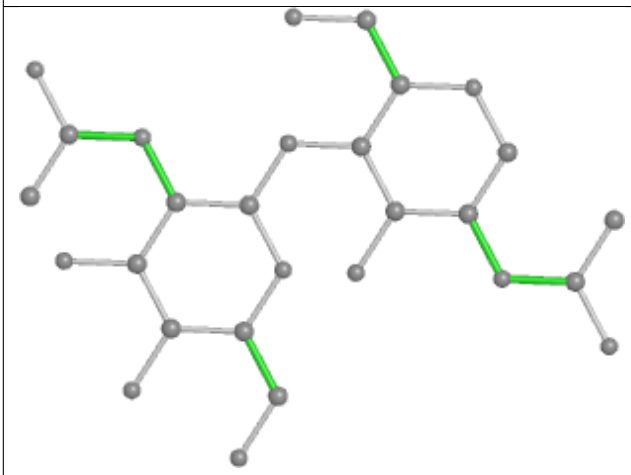
Oligosaccharide Chain H



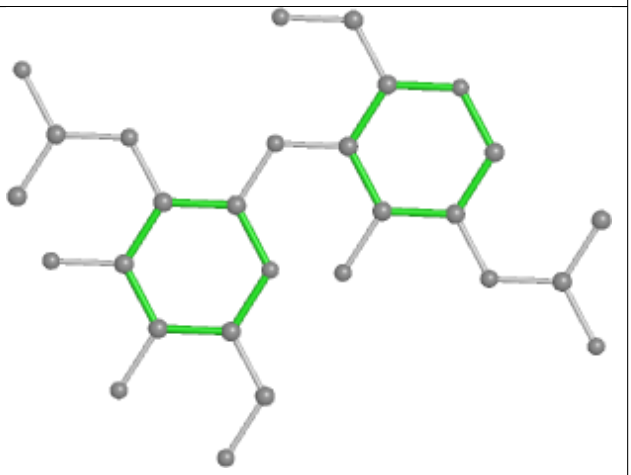
Bond lengths



Bond angles

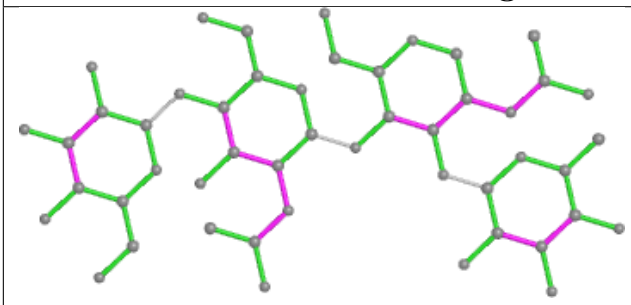


Torsions

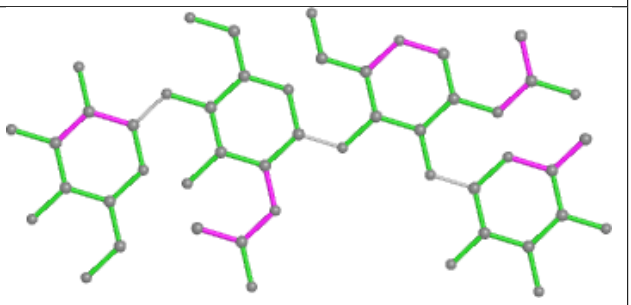


Rings

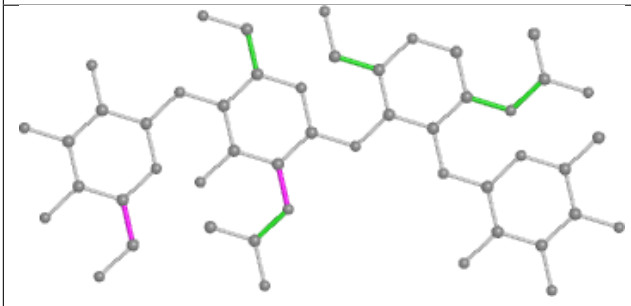
Oligosaccharide Chain J



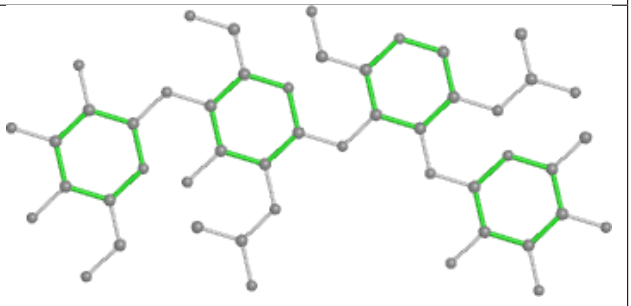
Bond lengths



Bond angles

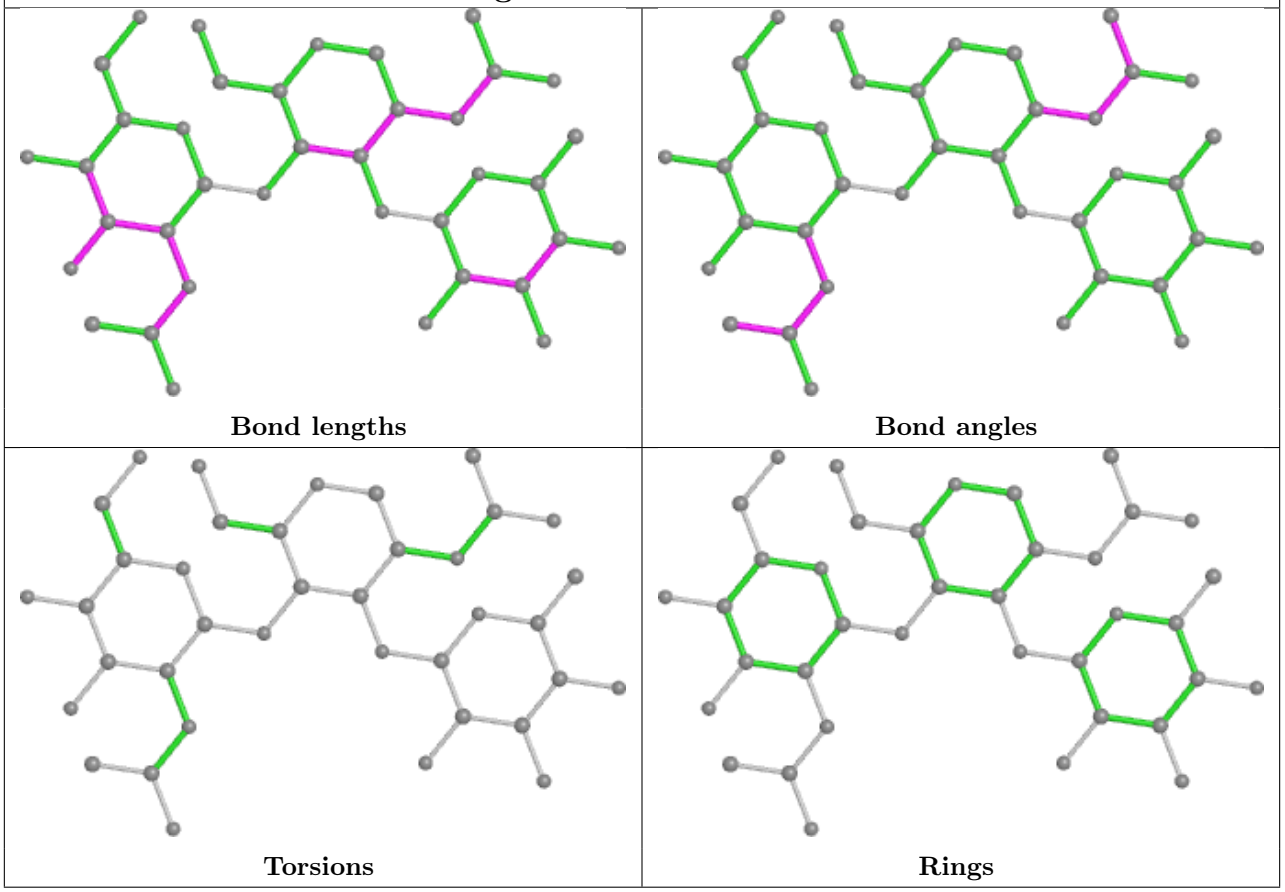


Torsions



Rings

Oligosaccharide Chain K



5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
13	1PE	A	1338	-	9,9,15	0.64	0	8,8,14	1.48	0
13	1PE	B	1333	-	5,5,15	0.56	0	4,4,14	1.23	0
13	1PE	B	1334	-	4,4,15	0.56	0	3,3,14	0.71	0
12	NAG	B	1326	1	14,14,15	1.92	5 (35%)	17,19,21	1.28	3 (17%)
10	HEM	A	1307	1	41,50,50	1.94	7 (17%)	45,82,82	1.86	7 (15%)
12	NAG	A	1336	-	14,14,15	2.09	5 (35%)	17,19,21	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	NAG	B	1327	1	14,14,15	1.94	5 (35%)	17,19,21	1.36	2 (11%)
13	1PE	B	1329	-	14,14,15	0.63	0	13,13,14	1.61	1 (7%)
13	1PE	B	1332	-	4,4,15	0.51	0	3,3,14	0.86	0
12	NAG	B	1328	1	14,14,15	1.93	5 (35%)	17,19,21	1.35	2 (11%)
10	HEM	B	1306	1	41,50,50	1.94	6 (14%)	45,82,82	1.87	9 (20%)
14	PG0	B	1331	-	7,7,7	0.34	0	6,6,6	0.61	0
13	1PE	A	1337	-	4,4,15	0.53	0	3,3,14	0.77	0
13	1PE	B	1330	-	15,15,15	0.66	0	14,14,14	1.61	1 (7%)

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
13	1PE	A	1338	-	-	1/7/7/13	-
13	1PE	B	1333	-	-	2/3/3/13	-
13	1PE	B	1334	-	-	1/2/2/13	-
12	NAG	B	1326	1	1/1/5/7	1/6/23/26	0/1/1/1
10	HEM	A	1307	1	-	3/12/54/54	-
12	NAG	A	1336	-	-	2/6/23/26	0/1/1/1
12	NAG	B	1327	1	-	3/6/23/26	0/1/1/1
13	1PE	B	1329	-	-	7/12/12/13	-
13	1PE	B	1332	-	-	1/2/2/13	-
12	NAG	B	1328	1	1/1/5/7	2/6/23/26	0/1/1/1
10	HEM	B	1306	1	-	2/12/54/54	-
14	PG0	B	1331	-	-	4/5/5/5	-
13	1PE	A	1337	-	-	2/2/2/13	-
13	1PE	B	1330	-	-	6/13/13/13	-

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1307	HEM	C3D-C2D	7.93	1.53	1.36
10	B	1306	HEM	C3D-C2D	7.80	1.53	1.36
12	B	1327	NAG	C7-N2	4.17	1.48	1.34
12	A	1336	NAG	C7-N2	4.16	1.48	1.34
12	B	1326	NAG	C7-N2	4.03	1.48	1.34

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1307	HEM	C4D-ND-C1D	6.42	111.70	105.07
10	B	1306	HEM	C4D-ND-C1D	6.17	111.44	105.07
10	B	1306	HEM	C4C-CHD-C1D	4.19	128.09	122.56
10	A	1307	HEM	CBD-CAD-C3D	-4.14	101.11	112.63
10	B	1306	HEM	CBD-CAD-C3D	-4.07	101.32	112.63

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	B	1326	NAG	C1
12	B	1328	NAG	C1

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	1327	NAG	O5-C5-C6-O6
12	B	1327	NAG	C4-C5-C6-O6
13	B	1334	1PE	OH4-C13-C23-OH3
12	B	1328	NAG	O5-C5-C6-O6
13	B	1329	1PE	OH5-C14-C24-OH4

There are no ring outliers.

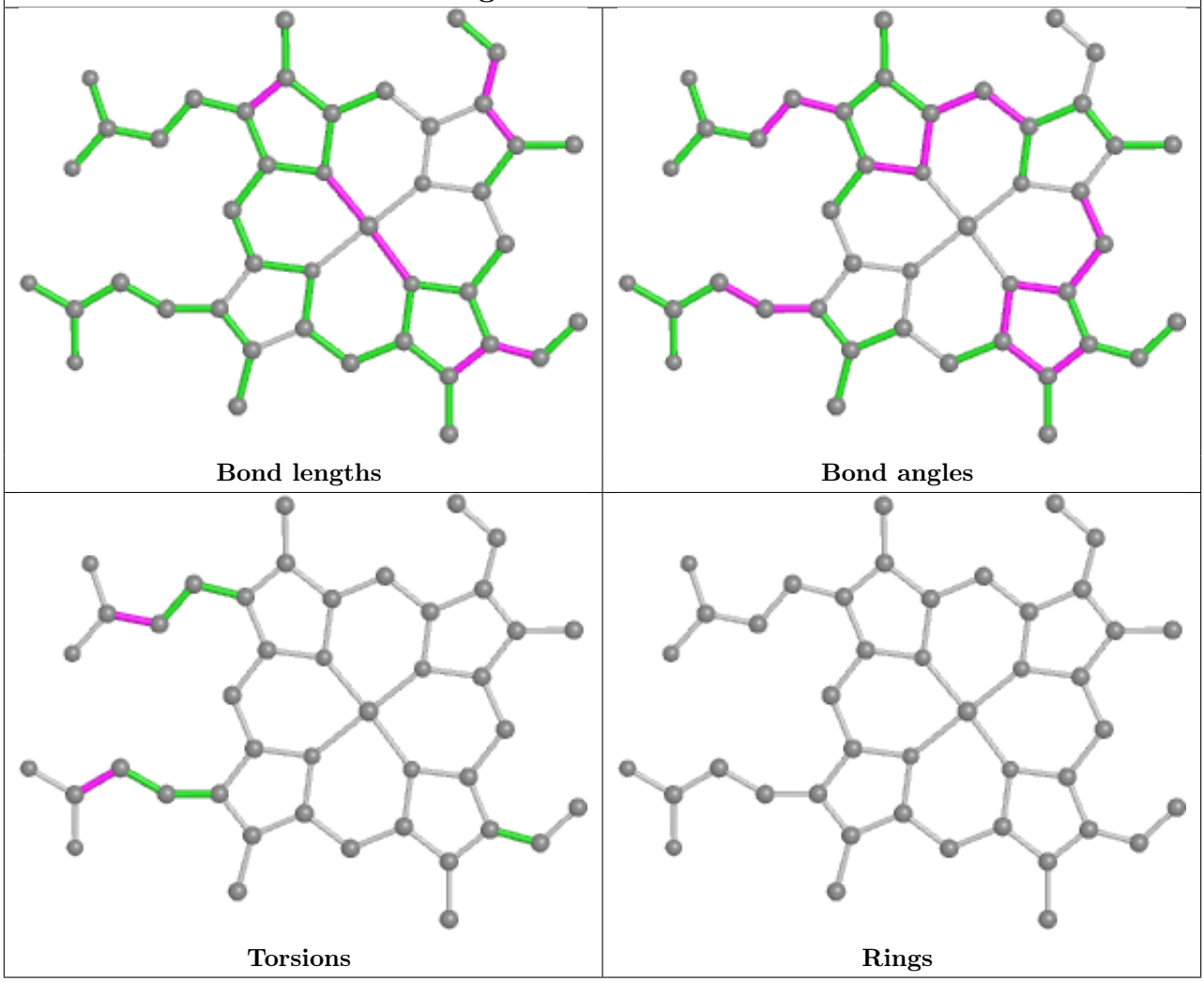
10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1333	1PE	3	0
13	B	1334	1PE	3	0
12	B	1326	NAG	1	0
10	A	1307	HEM	2	0
12	A	1336	NAG	2	0
12	B	1327	NAG	1	0
10	B	1306	HEM	3	0
14	B	1331	PG0	1	0
13	A	1337	1PE	5	0
13	B	1330	1PE	8	0

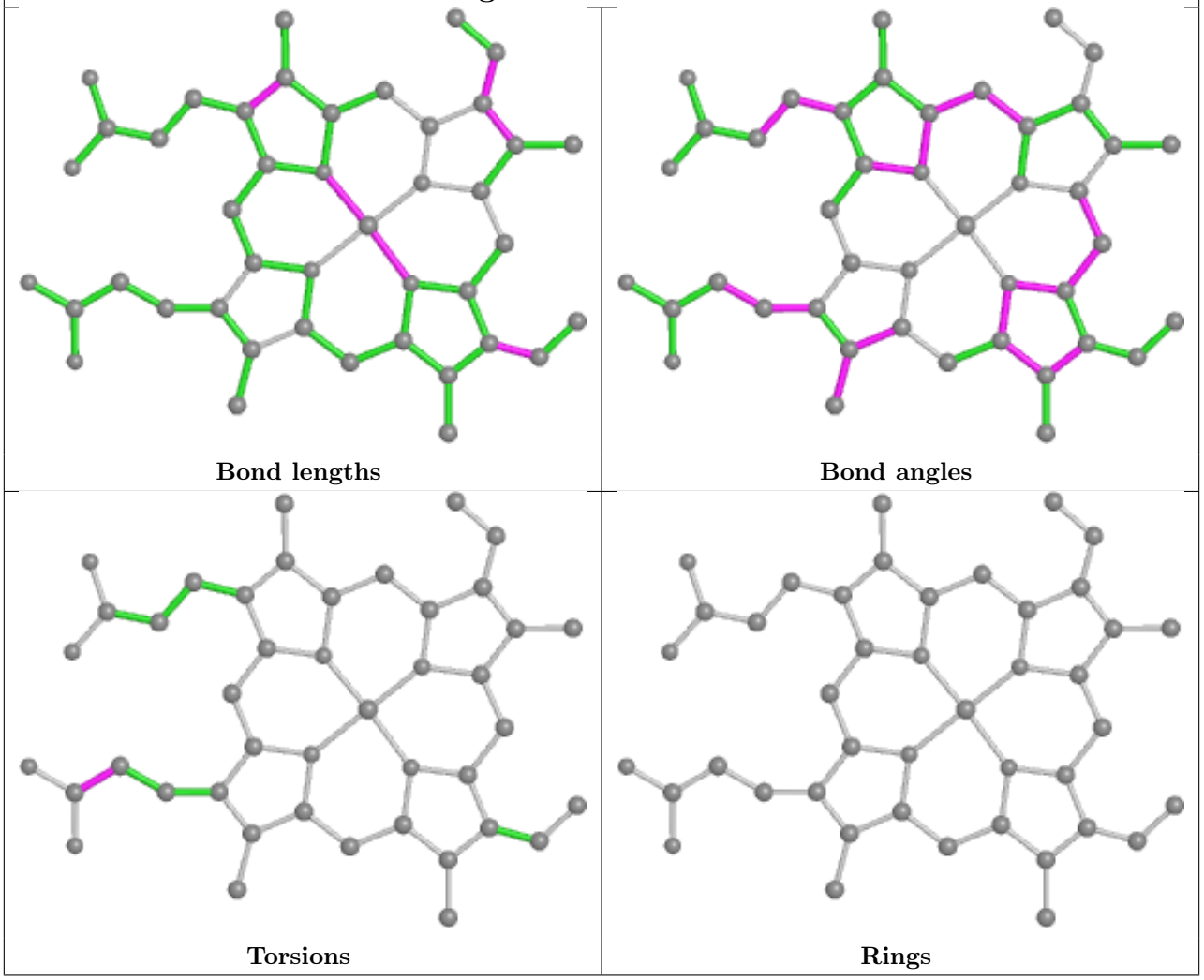
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 HEM A 1307



Ligand HEM B 1306



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	91:ASN	C	92:ALA	N	1.14
1	B	90:GLU	C	91:ASN	N	1.13
1	B	91:ASN	C	92:ALA	N	1.08

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	307/308 (99%)	-0.14	10 (3%)	46	50	18, 23, 35, 50	0
1	B	307/308 (99%)	-0.12	13 (4%)	36	39	17, 25, 41, 67	0
All	All	614/616 (99%)	-0.13	23 (3%)	41	45	17, 24, 39, 67	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	GLY	5.8
1	B	215	ARG	5.6
1	B	212	GLN	4.5
1	B	189	SER	4.0
1	B	91	ASN	3.9

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

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	H	1	14/15	0.42	0.36	52,61,67,72	0
2	BMA	I	3	11/12	0.52	0.56	52,60,67,70	0
2	NAG	I	2	14/15	0.53	0.29	29,52,59,61	0
8	BMA	J	3	11/12	0.56	0.27	52,63,67,68	0
5	MAN	L	3	11/12	0.58	0.38	73,77,80,86	0

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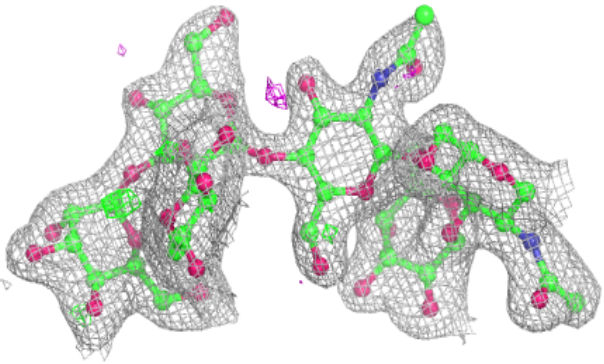
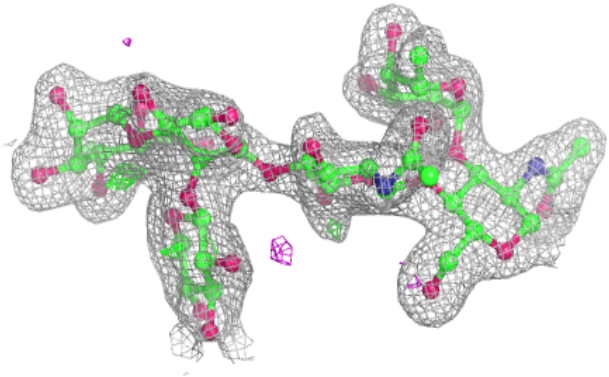
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	FUC	K	2	10/11	0.63	0.47	66,71,77,82	0
6	NAG	G	1	14/15	0.65	0.41	47,53,60,62	0
6	XYP	G	4	9/10	0.67	0.34	56,64,70,70	0
3	BMA	D	3	11/12	0.68	0.28	61,70,75,78	0
7	NAG	H	2	14/15	0.69	0.40	57,72,88,88	0
5	MAN	F	3	11/12	0.71	0.29	47,56,60,61	0
5	NAG	L	2	14/15	0.72	0.17	36,50,60,63	0
3	NAG	D	2	14/15	0.73	0.33	36,51,63,75	0
5	FUC	L	4	10/11	0.74	0.35	56,64,71,77	0
9	NAG	K	3	14/15	0.74	0.49	60,71,82,86	0
6	BMA	G	5	11/12	0.77	0.46	55,60,65,70	0
2	MAN	I	5	11/12	0.78	0.24	43,50,61,63	0
5	NAG	L	1	14/15	0.78	0.26	37,50,58,60	0
6	FUL	G	6	10/11	0.78	0.63	59,63,68,69	0
6	NAG	G	2	14/15	0.78	0.41	52,60,66,68	0
6	BMA	G	3	11/12	0.79	0.47	58,61,64,64	0
8	FUL	J	4	10/11	0.80	0.16	30,41,53,55	0
4	MAN	E	3	11/12	0.81	0.27	55,63,71,72	0
2	NAG	I	1	14/15	0.81	0.16	23,32,49,51	0
5	NAG	F	2	14/15	0.84	0.21	31,37,46,49	0
4	FUL	E	4	10/11	0.84	0.15	30,43,51,57	0
9	NAG	K	1	14/15	0.86	0.42	46,56,64,66	0
8	NAG	J	2	14/15	0.87	0.17	32,48,53,60	0
2	XYP	C	4	9/10	0.87	0.13	35,44,49,49	0
2	MAN	C	5	11/12	0.87	0.09	32,36,39,44	0
2	XYP	I	4	9/10	0.88	0.17	41,47,52,56	0
2	NAG	C	2	14/15	0.89	0.14	31,38,41,44	0
4	NAG	E	2	14/15	0.89	0.17	32,42,49,53	0
5	FUC	F	4	10/11	0.89	0.31	28,37,41,49	0
5	NAG	F	1	14/15	0.90	0.19	25,30,35,40	0
3	FUC	D	4	10/11	0.90	0.24	39,48,50,52	0
2	NAG	C	1	14/15	0.91	0.10	25,27,32,37	0
2	FUC	I	6	10/11	0.91	0.11	30,37,42,43	0
2	FUC	C	6	10/11	0.92	0.09	26,31,33,35	0
3	NAG	D	1	14/15	0.92	0.22	29,36,40,48	0
2	BMA	C	3	11/12	0.93	0.18	42,44,49,56	0
8	NAG	J	1	14/15	0.94	0.09	23,30,35,37	0
4	NAG	E	1	14/15	0.95	0.09	21,28,33,38	0

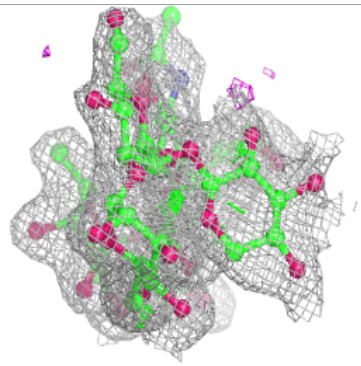
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

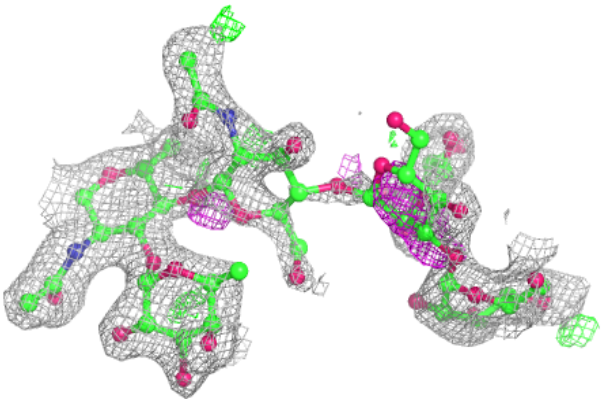


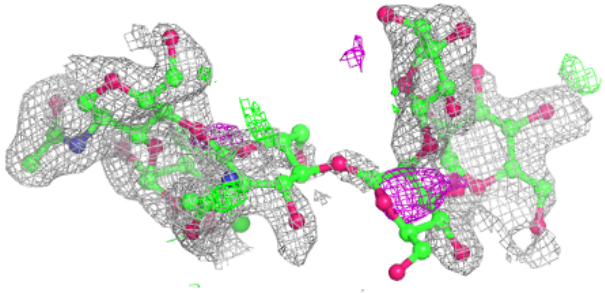


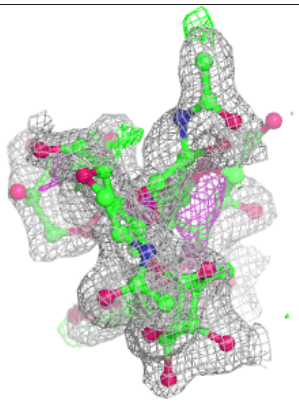


Electron density around Chain I:

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

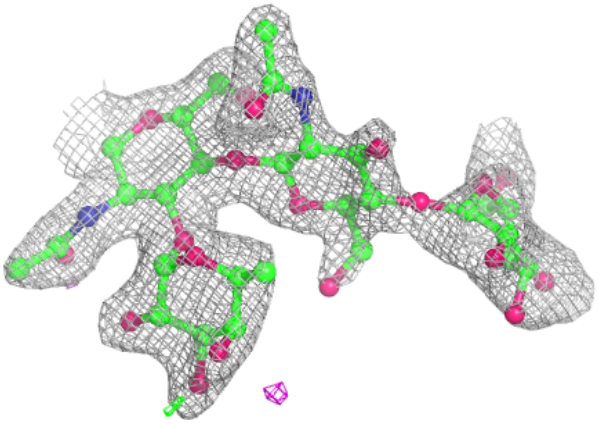


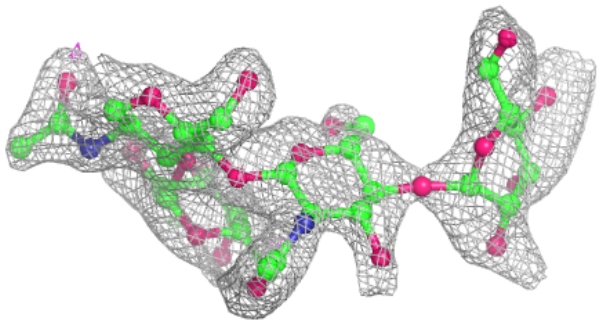


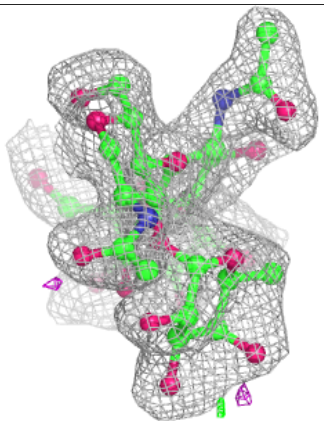


Electron density around Chain D:

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

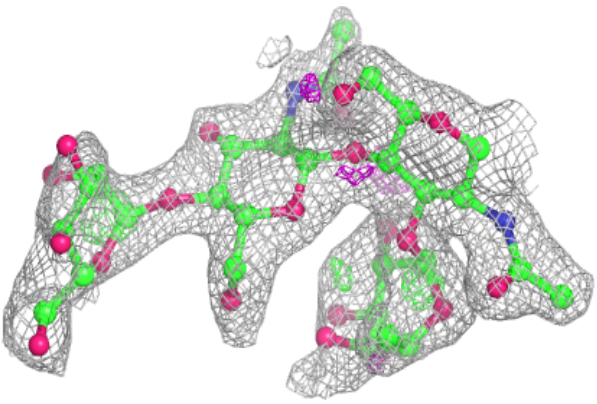


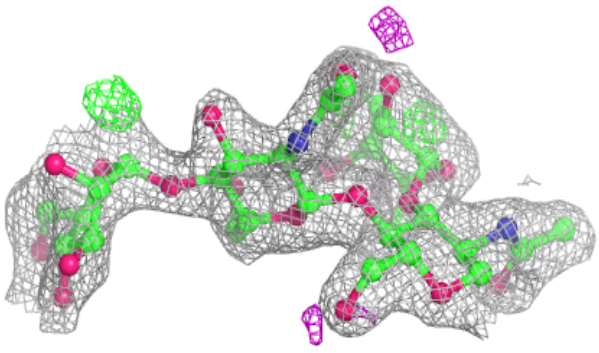


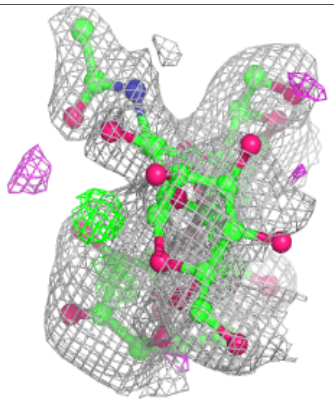


Electron density around Chain E:

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

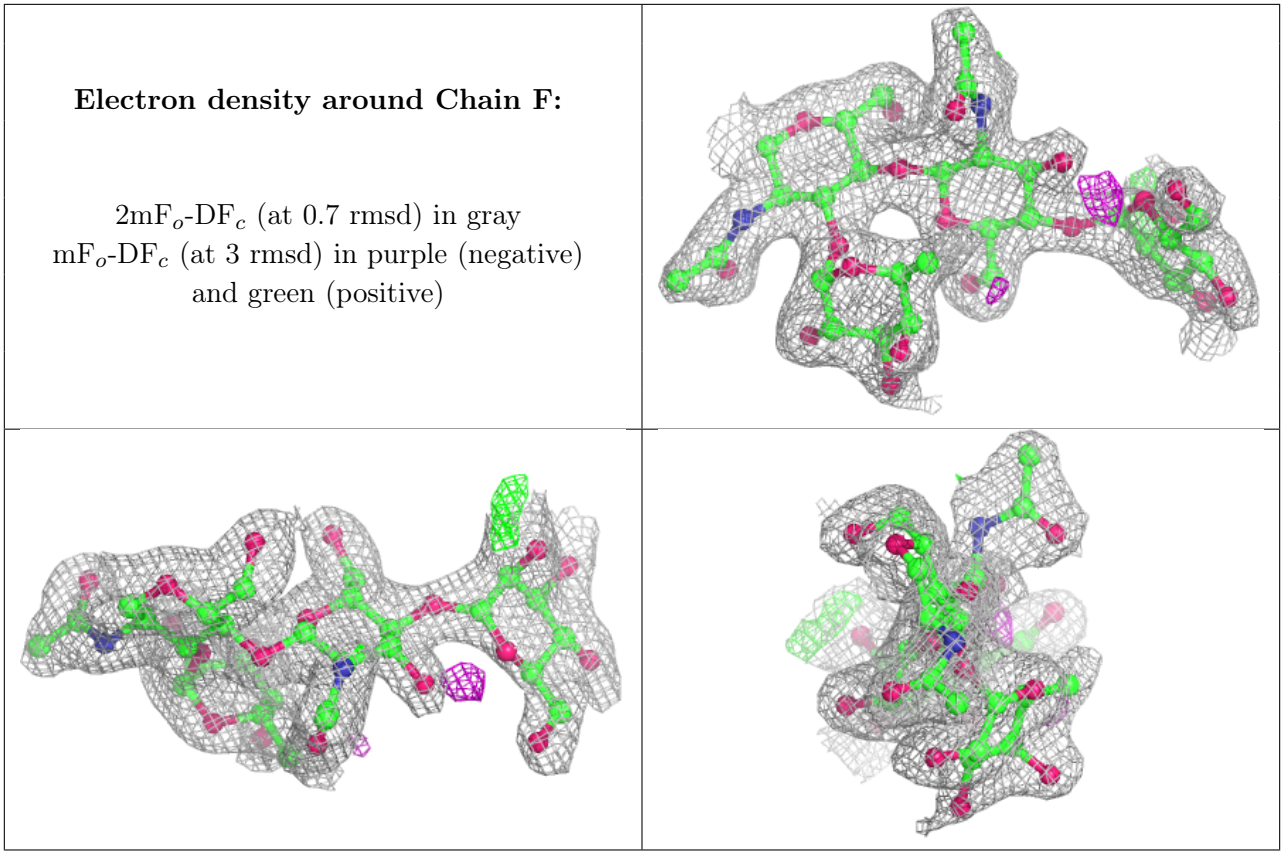






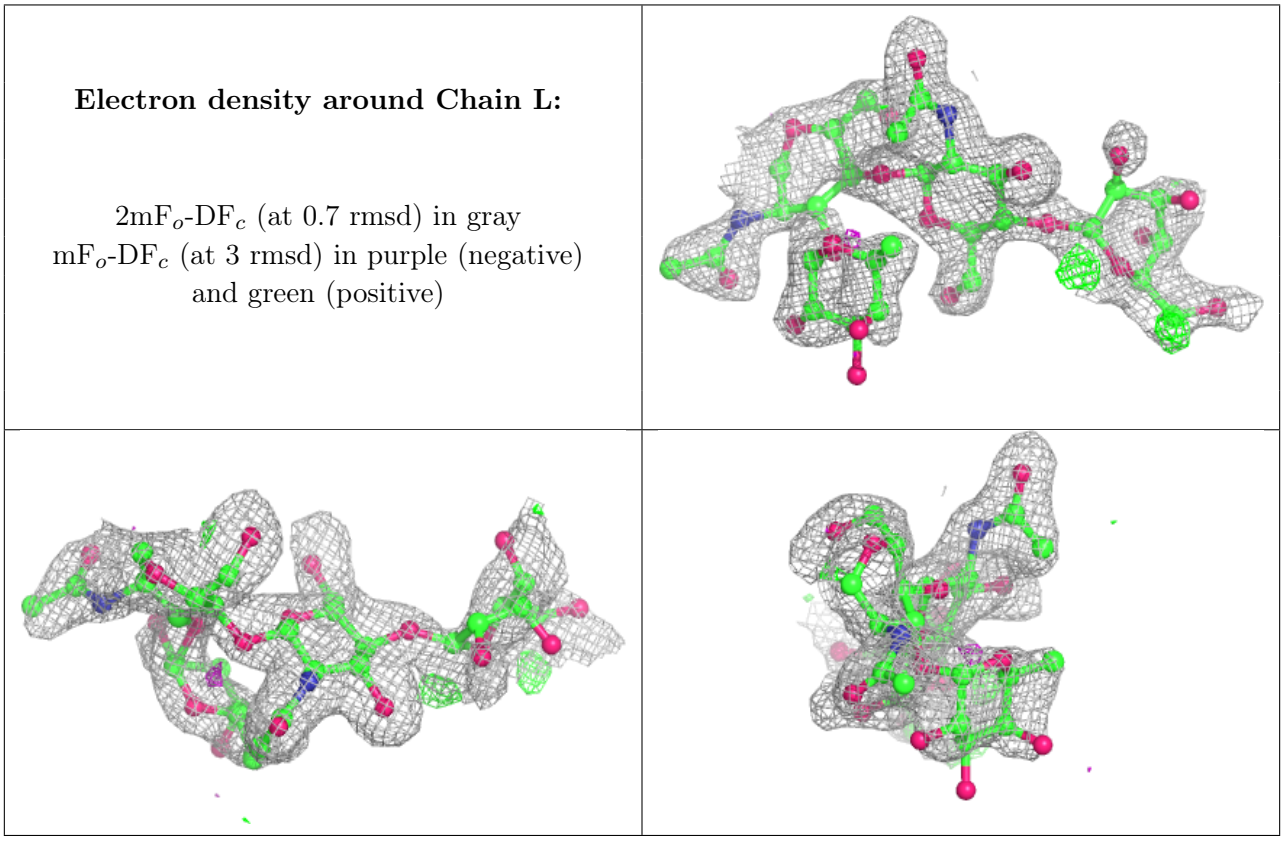
Electron density around Chain F:

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



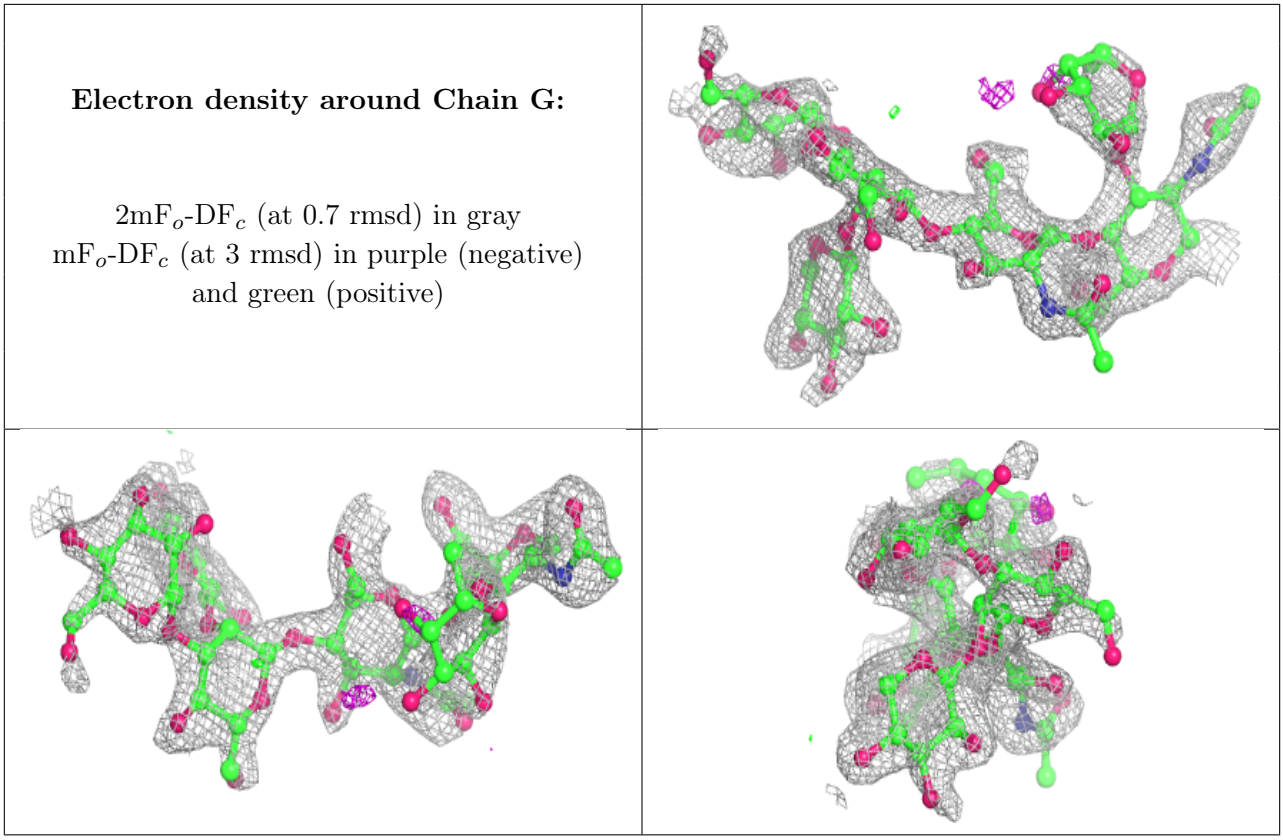
Electron density around Chain L:

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



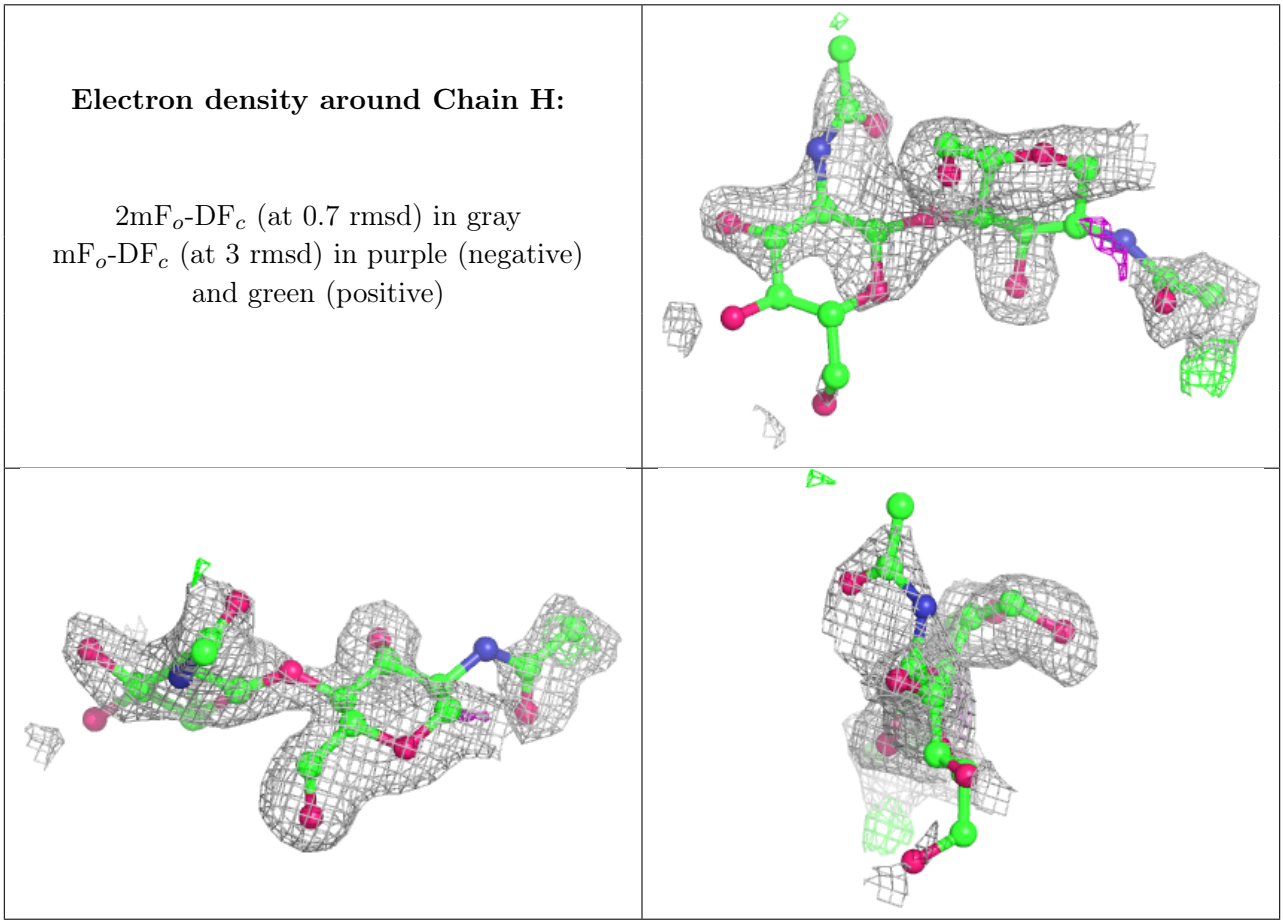
Electron density around Chain G:

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



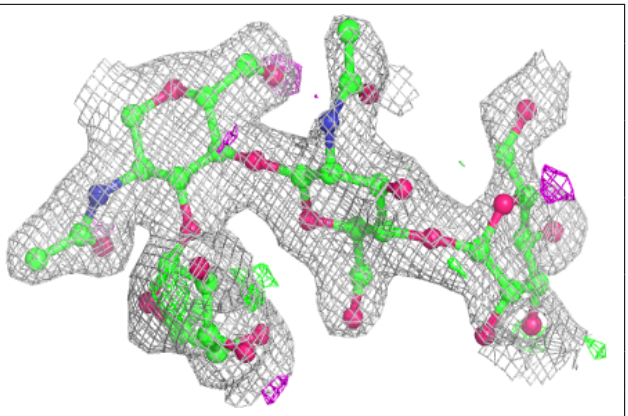
Electron density around Chain H:

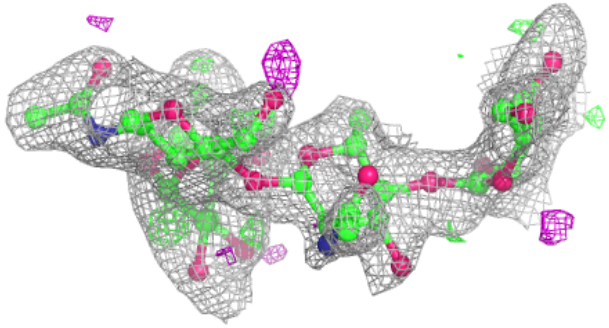
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

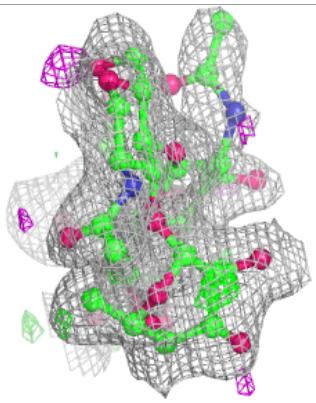


Electron density around Chain J:

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

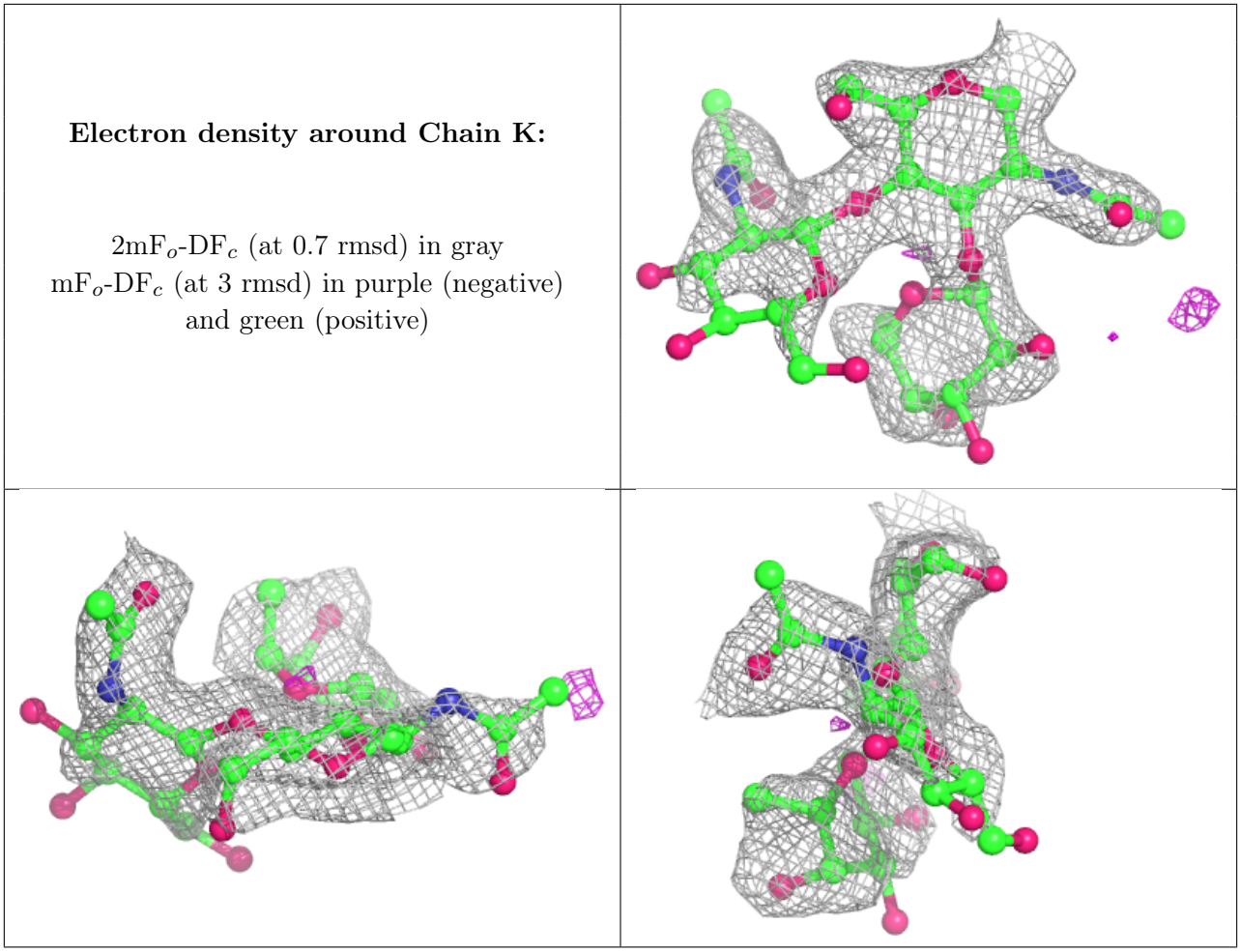






Electron density around Chain K:

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



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
12	NAG	B	1326	14/15	0.55	0.52	57,65,72,75	0
12	NAG	B	1327	14/15	0.61	0.42	49,66,75,78	0
12	NAG	B	1328	14/15	0.74	0.47	59,74,80,85	0
13	1PE	B	1334	5/16	0.75	0.23	49,50,57,60	0
12	NAG	A	1336	14/15	0.78	0.35	48,61,67,86	0
13	1PE	B	1329	15/16	0.81	0.17	32,42,54,61	0
13	1PE	A	1338	10/16	0.81	0.15	32,37,46,47	0
13	1PE	B	1330	16/16	0.83	0.16	41,49,57,57	0
14	PG0	B	1331	8/8	0.86	0.15	41,52,54,55	0
13	1PE	B	1332	5/16	0.91	0.28	40,48,50,59	0

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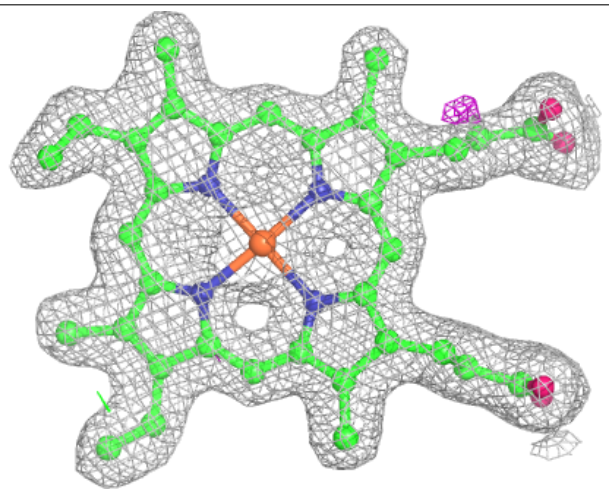
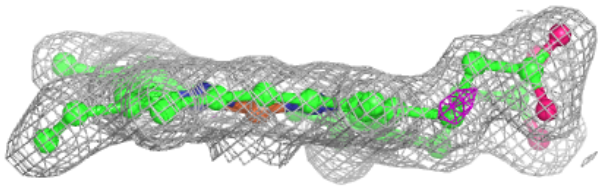
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	1PE	B	1333	6/16	0.92	0.14	30,43,51,55	0
13	1PE	A	1337	5/16	0.93	0.14	31,31,42,48	0
10	HEM	A	1307	43/43	0.94	0.12	14,18,24,29	0
10	HEM	B	1306	43/43	0.95	0.11	15,21,26,35	0
11	CA	B	1307	1/1	0.98	0.10	25,25,25,25	0
11	CA	A	1309	1/1	0.99	0.11	20,20,20,20	0
11	CA	A	1308	1/1	0.99	0.10	22,22,22,22	0
11	CA	B	1308	1/1	0.99	0.09	22,22,22,22	0

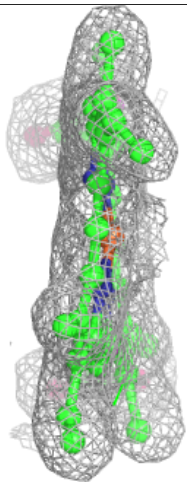
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM A 1307:

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

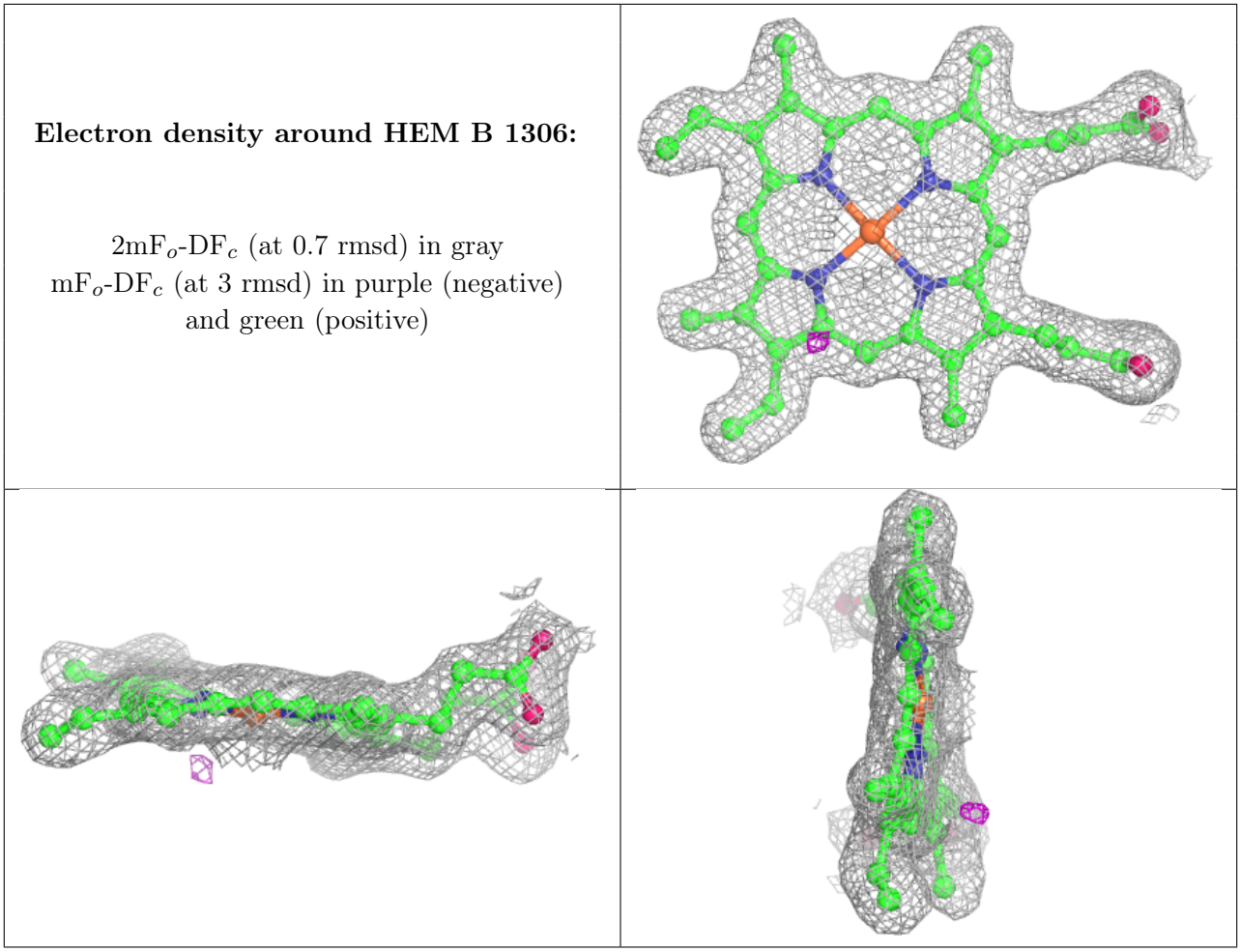






Electron density around HEM B 1306:

$2mF_o$-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.