Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 10:01 PM JST

PDB ID	:	7X36
Title	:	Crystal Structure of hetero-Diels-Alderase EupfF
Authors	:	Zhou, J.; Lu, J.
Deposited on	:	2022-02-28
Resolution	:	1.92 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

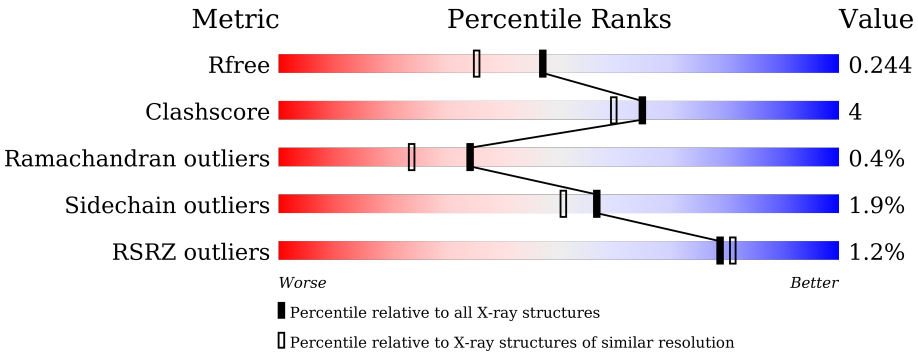
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	373	82% 9% 9%
1	B	373	82% 9% 9%
1	C	373	78% 12% 9%
1	D	373	80% 10% 9%
2	E	2	50% 50%
2	F	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	H	2	100%
2	I	2	50% 50%
2	J	2	100%
2	K	2	100%
2	N	2	100%
2	O	2	50% 50%
2	P	2	100%
2	Q	2	100%
3	G	3	33% 67%
3	M	3	33% 67%
4	L	4	50% 50%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 12420 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 EupfF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2676	1712	449	508	7			
1	B	338	Total	C	N	O	S	0	1	0
			2665	1705	446	507	7			
1	C	339	Total	C	N	O	S	0	0	0
			2672	1709	449	507	7			
1	D	339	Total	C	N	O	S	0	1	0
			2675	1711	449	508	7			

- Molecule 2 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
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

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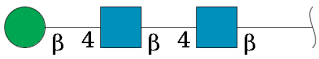
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	P	2	Total C N O 28 16 2 10	0	0	0
2	Q	2	Total C N O 28 16 2 10	0	0	0

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

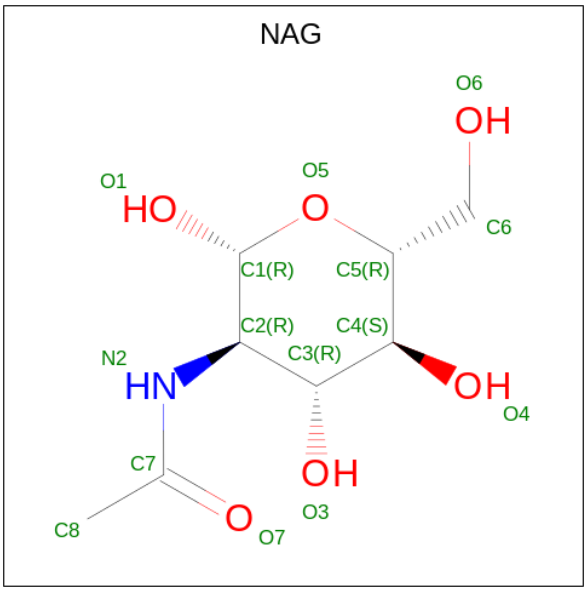


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	G	3	Total C N O 39 22 2 15	0	0	0
3	M	3	Total C N O 39 22 2 15	0	0	0

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

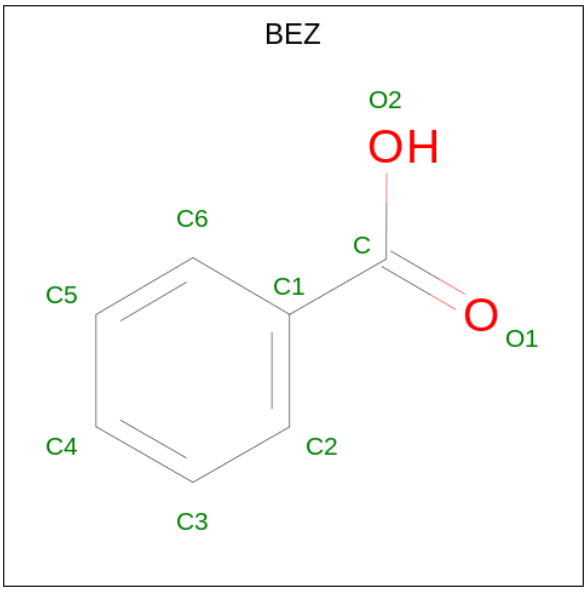


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

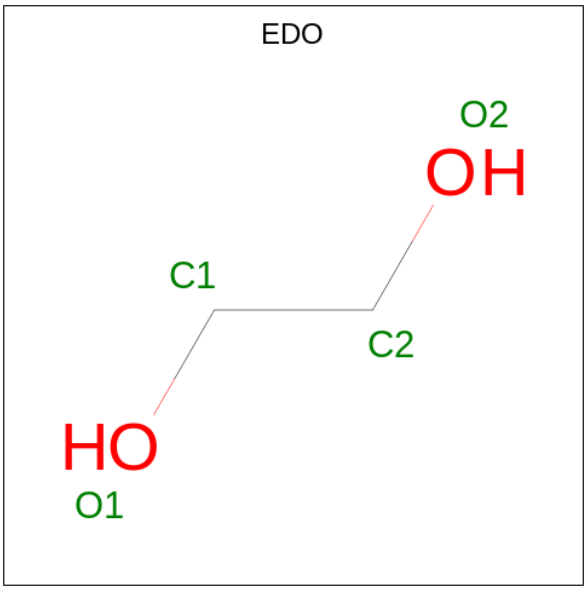
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0

- Molecule 7 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 9 7 2	0	0
7	B	1	Total C O 9 7 2	0	0
7	C	1	Total C O 9 7 2	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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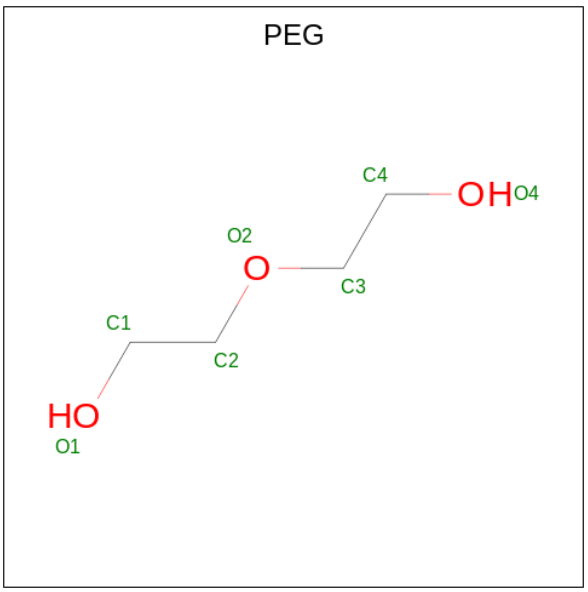
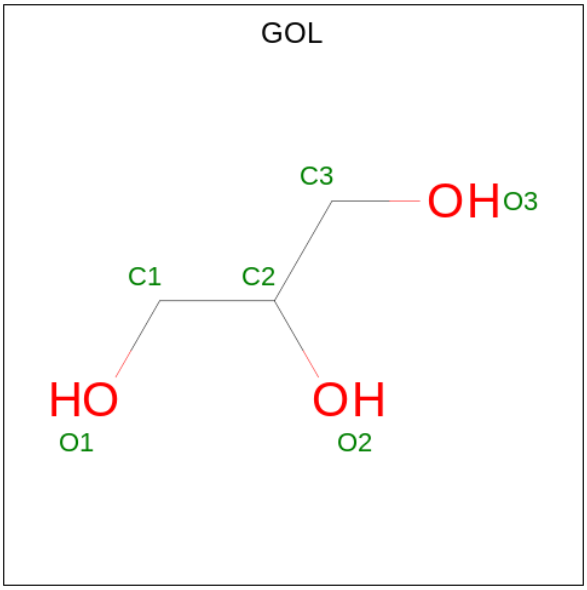
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



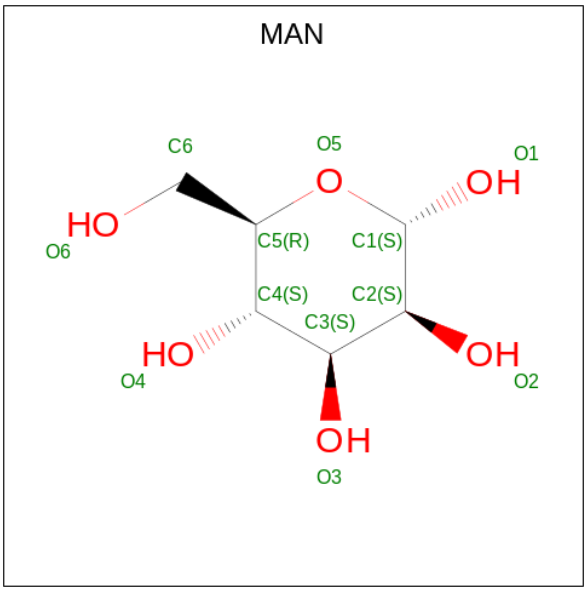
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total C O 6 3 3	0	0

- Molecule 11 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total C O 12 6 6	0	0

- Molecule 12 is water.

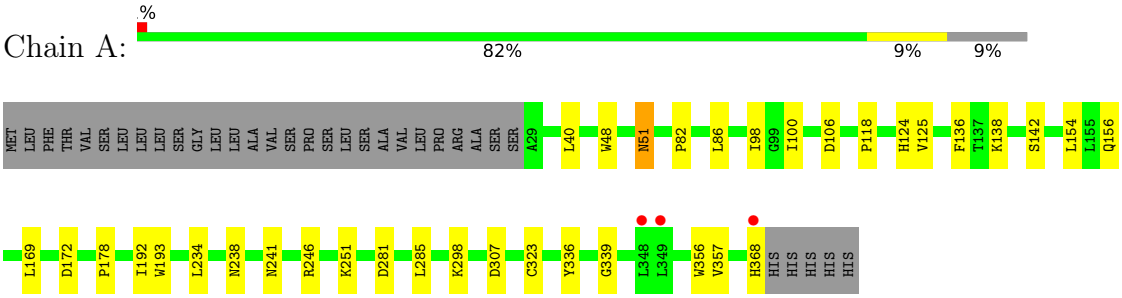
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	326	Total O 326 326	0	0
12	B	304	Total O 304 304	0	0
12	C	267	Total O 267 267	0	0
12	D	249	Total O 249 249	0	0

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.

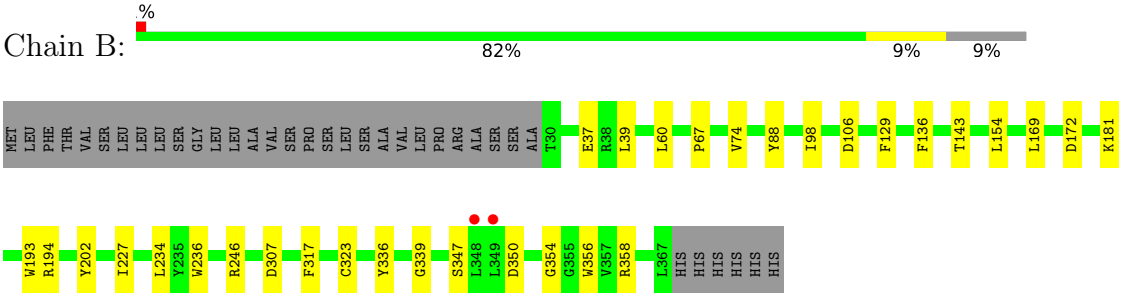
• Molecule 1: EupfF

Chain A:



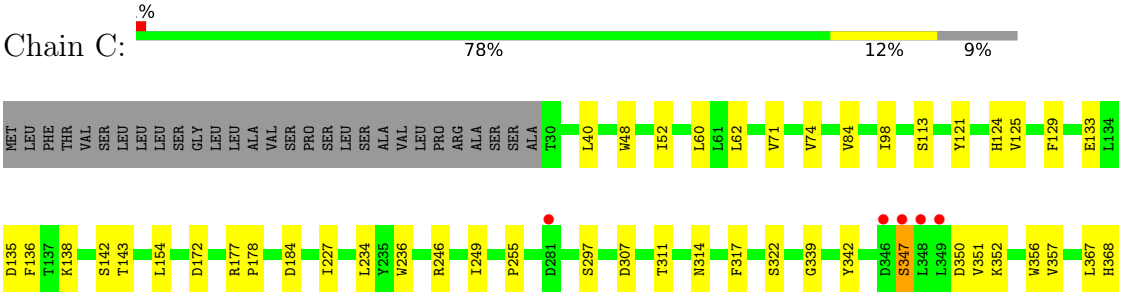
• Molecule 1: EupfF

Chain B:



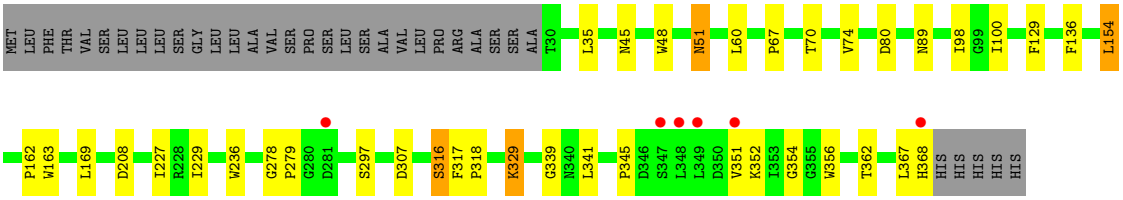
• Molecule 1: EupfF

Chain C:



• Molecule 1: EupfF

Chain D:



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

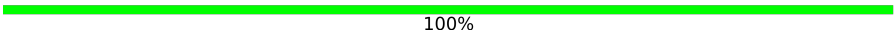
Chain E:

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

Chain F:

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

Chain H:

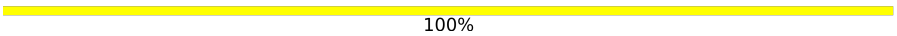


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

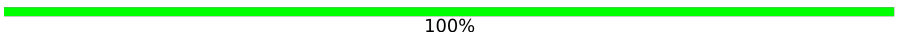
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



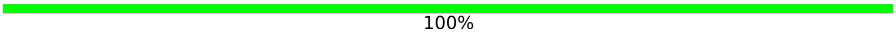
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain N:

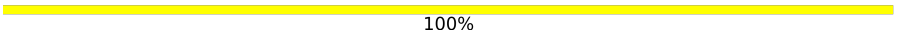


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

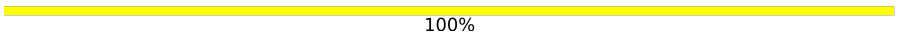
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



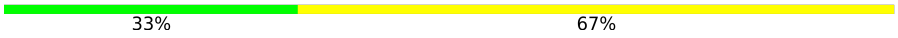
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



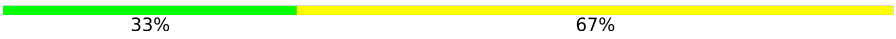
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain M:



• Molecule 4: 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 L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.94Å 76.53Å 147.78Å 90.00° 104.03° 90.00°	Depositor
Resolution (Å)	46.90 – 1.92 46.90 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.90-1.92) 98.8 (46.90-1.92)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.47 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.204 , 0.245 0.203 , 0.244	Depositor DCC
R_{free} test set	7190 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.905	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12420	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: PEG, CA, BEZ, GOL, MAN, NAG, BMA, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/2758	0.64	0/3785
1	B	0.42	0/2749	0.59	0/3774
1	C	0.42	0/2754	0.60	0/3780
1	D	0.41	0/2760	0.57	0/3789
All	All	0.44	0/11021	0.60	0/15128

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2676	0	2563	24	0
1	B	2665	0	2560	16	0
1	C	2672	0	2561	25	0
1	D	2675	0	2567	22	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	1	0
2	P	28	0	25	0	0
2	Q	28	0	25	1	0
3	G	39	0	34	0	0
3	M	39	0	34	2	0
4	L	50	0	43	0	0
5	A	14	0	13	2	0
5	C	42	0	39	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	9	0	5	1	0
7	B	9	0	5	0	0
7	C	9	0	5	0	0
8	A	32	0	48	6	0
8	B	8	0	12	0	0
8	C	8	0	12	0	0
8	D	4	0	6	1	0
9	B	7	0	10	0	0
9	D	14	0	20	1	0
10	D	6	0	8	0	0
11	D	12	0	12	0	0
12	A	326	0	0	2	0
12	B	304	0	0	0	0
12	C	267	0	0	0	0
12	D	249	0	0	0	0
All	All	12420	0	10807	91	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 4.

All (91) 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:285:LEU:HD13	1:A:298:LYS:HG3	1.76	0.68
1:C:121:TYR:OH	1:C:351:VAL:HG21	1.97	0.64
1:D:345:PRO:HA	9:D:405:PEG:H31	1.79	0.64
1:C:135:ASP:OD2	1:C:138:LYS:NZ	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:SER:HB3	1:B:350:ASP:OD2	2.02	0.60
1:A:285:LEU:CD1	1:A:298:LYS:CG	2.82	0.57
1:A:339:GLY:HA3	1:A:356:TRP:CZ2	2.39	0.57
1:A:285:LEU:HD13	1:A:298:LYS:CG	2.34	0.57
1:A:138:LYS:HE3	8:A:408:EDO:H12	1.88	0.55
1:D:329:LYS:H	1:D:329:LYS:CE	2.22	0.53
1:D:60:LEU:HB2	1:D:74:VAL:HB	1.90	0.53
1:D:329:LYS:H	1:D:329:LYS:HE2	1.72	0.53
1:A:154:LEU:O	1:A:172:ASP:HA	2.09	0.52
1:B:37:GLU:HG3	1:B:317:PHE:CZ	2.45	0.52
1:D:208:ASP:O	8:D:403:EDO:O1	2.26	0.52
1:A:118:PRO:O	8:A:407:EDO:H12	2.10	0.52
1:C:40:LEU:HB2	1:C:357:VAL:HG13	1.92	0.52
1:D:67:PRO:HB2	2:O:1:NAG:H82	1.92	0.52
5:A:401:NAG:H83	5:A:401:NAG:H3	1.92	0.51
1:C:249:ILE:HA	1:C:255:PRO:HA	1.92	0.51
8:A:406:EDO:H12	8:A:411:EDO:O1	2.09	0.51
1:A:192:ILE:HD13	1:A:234:LEU:HD21	1.94	0.50
1:D:169:LEU:HD12	1:D:229:ILE:HD11	1.93	0.50
1:C:307:ASP:HB3	1:C:317:PHE:CE2	2.47	0.50
1:B:154:LEU:O	1:B:172:ASP:HA	2.12	0.49
1:C:347:SER:O	1:C:350:ASP:HB2	2.12	0.49
1:D:341:LEU:HD22	1:D:351:VAL:CG1	2.43	0.48
1:D:227:ILE:HG22	1:D:236:TRP:HB3	1.96	0.48
1:A:86:LEU:CD2	8:A:410:EDO:H22	2.44	0.47
1:A:285:LEU:CD1	1:A:298:LYS:HG2	2.43	0.47
1:A:339:GLY:HA3	1:A:356:TRP:CE2	2.50	0.47
5:A:401:NAG:H62	12:A:741:HOH:O	2.14	0.47
1:C:177:ARG:NH1	1:C:184:ASP:OD2	2.48	0.47
1:B:339:GLY:HA3	1:B:356:TRP:CZ2	2.49	0.47
1:D:339:GLY:HA3	1:D:356:TRP:CZ2	2.50	0.46
1:C:339:GLY:HA3	1:C:356:TRP:CZ2	2.51	0.46
1:D:35:LEU:HD13	1:D:362:THR:HA	1.96	0.46
1:C:367:LEU:HD12	3:M:1:NAG:H5	1.98	0.46
1:B:60:LEU:HB2	1:B:74:VAL:HB	1.98	0.45
1:C:367:LEU:O	1:C:368:HIS:HB2	2.17	0.45
1:A:285:LEU:HD11	1:A:298:LYS:HG2	1.98	0.45
1:B:234:LEU:O	1:B:246:ARG:HA	2.16	0.45
1:C:133:GLU:O	1:C:143:THR:HA	2.16	0.45
1:D:162:PRO:HD2	1:D:163:TRP:CZ3	2.52	0.45
1:B:323:CYS:HA	1:B:336:TYR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LEU:HB2	1:C:74:VAL:HB	1.99	0.45
1:C:342:TYR:CE2	5:C:401:NAG:H5	2.52	0.45
8:A:409:EDO:O1	5:C:402:NAG:O4	2.26	0.45
1:C:74:VAL:HG13	1:C:84:VAL:HG12	2.00	0.44
1:A:82:PRO:O	12:A:501:HOH:O	2.21	0.44
1:A:169:LEU:HA	1:A:193:TRP:O	2.17	0.44
1:D:351:VAL:HG12	1:D:352:LYS:N	2.32	0.44
1:D:45:ASN:HB3	1:D:352:LYS:HE3	2.00	0.44
1:A:234:LEU:O	1:A:246:ARG:HA	2.18	0.43
1:A:238:ASN:HB3	1:A:241:ASN:OD1	2.17	0.43
1:C:227:ILE:HG22	1:C:236:TRP:HB3	2.00	0.43
1:D:129:PHE:CE2	1:D:154:LEU:HA	2.53	0.43
1:A:156:GLN:HE22	7:A:403:BEZ:H5	1.83	0.43
1:C:62:LEU:O	1:C:71:VAL:HA	2.19	0.43
1:D:368:HIS:NE2	2:Q:1:NAG:H3	2.33	0.43
1:C:154:LEU:O	1:C:172:ASP:HA	2.18	0.43
1:D:70:THR:HG22	1:D:89:ASN:HA	1.99	0.43
1:D:278:GLY:HA3	1:D:279:PRO:HA	1.93	0.42
1:C:297:SER:HB2	1:C:367:LEU:HD11	2.00	0.42
1:B:181:LYS:HD3	1:B:181:LYS:HA	1.74	0.42
1:C:113:SER:HB3	1:C:129:PHE:CG	2.55	0.42
1:B:227:ILE:HG22	1:B:236:TRP:HB3	2.01	0.42
1:C:311:THR:O	1:C:314:ASN:HB3	2.20	0.41
1:A:86:LEU:HD21	8:A:410:EDO:H22	2.02	0.41
3:M:1:NAG:O7	3:M:1:NAG:H3	2.19	0.41
1:A:51:ASN:HB3	1:A:100:ILE:HG22	2.01	0.41
1:A:124:HIS:NE2	1:A:178:PRO:HG3	2.36	0.41
1:B:169:LEU:HA	1:B:193:TRP:O	2.20	0.41
1:D:316:SER:C	1:D:318:PRO:HD3	2.41	0.41
1:B:37:GLU:HG3	1:B:317:PHE:CE2	2.56	0.41
1:B:88:TYR:CD2	1:B:143:THR:HG21	2.56	0.41
1:B:129:PHE:CE2	1:B:154:LEU:HA	2.56	0.40
1:B:194:ARG:O	1:B:202:TYR:HA	2.21	0.40
1:C:352:LYS:HG2	5:C:401:NAG:H62	2.03	0.40
1:D:297:SER:HB2	1:D:367:LEU:HD11	2.02	0.40
1:A:40:LEU:HB2	1:A:357:VAL:HG13	2.03	0.40
1:A:125:VAL:HG11	1:C:125:VAL:HG11	2.04	0.40
1:C:124:HIS:O	1:C:178:PRO:HB2	2.20	0.40
1:B:39:LEU:HA	1:B:358:ARG:HG2	2.04	0.40
1:B:67:PRO:HG3	2:I:1:NAG:H82	2.03	0.40
1:C:234:LEU:O	1:C:246:ARG:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ASN:HB3	1:D:100:ILE:HG22	2.04	0.40
1:A:251:LYS:HA	1:A:251:LYS:HD3	1.88	0.40
1:A:323:CYS:HA	1:A:336:TYR:O	2.22	0.40
1:C:52:ILE:HG22	1:C:322:SER:HB3	2.03	0.40
1:D:307:ASP:HB3	1:D:317:PHE:CE1	2.57	0.40

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	338/373 (91%)	315 (93%)	22 (6%)	1 (0%)	41	31
1	B	337/373 (90%)	314 (93%)	21 (6%)	2 (1%)	25	14
1	C	337/373 (90%)	319 (95%)	17 (5%)	1 (0%)	41	31
1	D	338/373 (91%)	318 (94%)	18 (5%)	2 (1%)	25	14
All	All	1350/1492 (90%)	1266 (94%)	78 (6%)	6 (0%)	34	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	ILE
1	A	98	ILE
1	B	354	GLY
1	C	98	ILE
1	D	98	ILE
1	D	354	GLY

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	293/322 (91%)	285 (97%)	8 (3%)	44	36
1	B	293/322 (91%)	290 (99%)	3 (1%)	76	75
1	C	293/322 (91%)	289 (99%)	4 (1%)	67	63
1	D	294/322 (91%)	287 (98%)	7 (2%)	49	41
All	All	1173/1288 (91%)	1151 (98%)	22 (2%)	57	51

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	TRP
1	A	51	ASN
1	A	106	ASP
1	A	136	PHE
1	A	142	SER
1	A	281	ASP
1	A	307	ASP
1	A	368	HIS
1	B	106	ASP
1	B	136	PHE
1	B	307	ASP
1	C	48	TRP
1	C	136	PHE
1	C	142	SER
1	C	347	SER
1	D	48	TRP
1	D	51	ASN
1	D	80	ASP
1	D	136	PHE
1	D	154	LEU
1	D	316	SER
1	D	329	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)

30 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	2,1	14,14,15	0.63	1 (7%)	17,19,21	0.48	0
2	NAG	E	2	2	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	F	1	2,1	14,14,15	0.55	0	17,19,21	0.93	1 (5%)
2	NAG	F	2	2	14,14,15	0.46	0	17,19,21	0.58	0
3	NAG	G	1	3,1	14,14,15	0.83	1 (7%)	17,19,21	0.61	0
3	NAG	G	2	3	14,14,15	0.89	1 (7%)	17,19,21	0.49	0
3	BMA	G	3	3	11,11,12	0.63	0	15,15,17	0.79	0
2	NAG	H	1	2,1	14,14,15	0.27	0	17,19,21	0.44	0
2	NAG	H	2	2	14,14,15	0.24	0	17,19,21	0.55	0
2	NAG	I	1	2,1	14,14,15	0.25	0	17,19,21	0.67	1 (5%)
2	NAG	I	2	2	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	J	1	2,1	14,14,15	0.45	0	17,19,21	0.85	1 (5%)
2	NAG	J	2	2	14,14,15	0.41	0	17,19,21	0.59	1 (5%)
2	NAG	K	1	2,1	14,14,15	0.58	0	17,19,21	0.58	0
2	NAG	K	2	2	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	L	1	1,4	14,14,15	0.55	0	17,19,21	0.66	0
4	NAG	L	2	4	14,14,15	0.45	0	17,19,21	0.51	0
4	BMA	L	3	4	11,11,12	0.49	0	15,15,17	0.91	1 (6%)
4	MAN	L	4	4	11,11,12	0.97	0	15,15,17	0.92	1 (6%)
3	NAG	M	1	3,1	14,14,15	0.73	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	M	2	3	14,14,15	0.50	0	17,19,21	0.47	0
3	BMA	M	3	3	11,11,12	1.29	2 (18%)	15,15,17	1.65	2 (13%)
2	NAG	N	1	2,1	14,14,15	0.41	0	17,19,21	0.44	0
2	NAG	N	2	2	14,14,15	0.31	0	17,19,21	0.47	0
2	NAG	O	1	2,1	14,14,15	0.22	0	17,19,21	0.75	1 (5%)
2	NAG	O	2	2	14,14,15	0.38	0	17,19,21	0.62	0
2	NAG	P	1	2,1	14,14,15	0.54	0	17,19,21	0.76	1 (5%)
2	NAG	P	2	2	14,14,15	0.81	1 (7%)	17,19,21	0.59	0
2	NAG	Q	1	2,1	14,14,15	0.51	0	17,19,21	0.67	0
2	NAG	Q	2	2	14,14,15	0.75	1 (7%)	17,19,21	0.40	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	4/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	NAG	O5-C1	-2.94	1.39	1.43
2	P	2	NAG	O5-C1	-2.92	1.39	1.43
3	M	3	BMA	C4-C5	2.80	1.58	1.53
3	G	1	NAG	C1-C2	2.38	1.55	1.52
2	Q	2	NAG	O5-C1	2.36	1.47	1.43
3	M	3	BMA	C1-C2	2.28	1.57	1.52
2	E	1	NAG	C1-C2	2.24	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	3	BMA	C1-O5-C5	4.54	118.35	112.19
2	F	1	NAG	C1-O5-C5	3.04	116.31	112.19
2	J	1	NAG	C1-O5-C5	2.52	115.60	112.19
3	M	3	BMA	O5-C1-C2	2.49	114.61	110.77
2	P	1	NAG	C1-O5-C5	2.43	115.49	112.19
4	L	3	BMA	C1-O5-C5	2.31	115.32	112.19
2	I	1	NAG	C1-O5-C5	2.12	115.06	112.19
4	L	4	MAN	C1-O5-C5	2.10	115.04	112.19
2	O	1	NAG	C1-O5-C5	2.10	115.03	112.19
2	J	2	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	M	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	M	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	O	2	NAG	C8-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2
2	P	1	NAG	C8-C7-N2-C2
2	P	1	NAG	O7-C7-N2-C2
2	P	2	NAG	C8-C7-N2-C2
2	P	2	NAG	O7-C7-N2-C2
2	K	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	M	3	BMA	C4-C5-C6-O6
3	M	1	NAG	C3-C2-N2-C7
3	G	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	K	1	NAG	C3-C2-N2-C7

All (1) ring outliers are listed below:

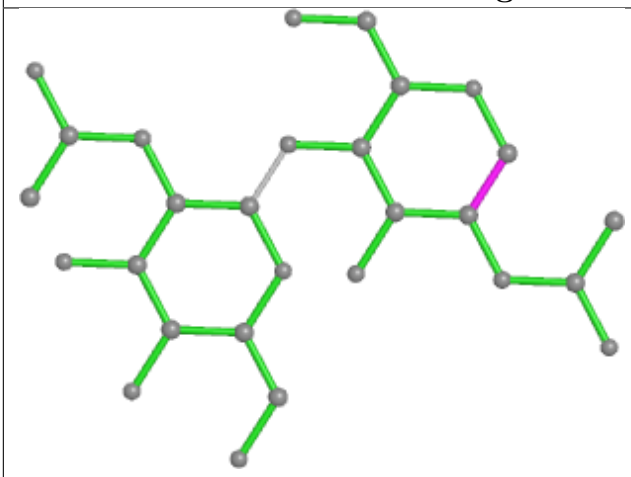
Mol	Chain	Res	Type	Atoms
3	M	3	BMA	C1-C2-C3-C4-C5-O5

4 monomers are involved in 5 short contacts:

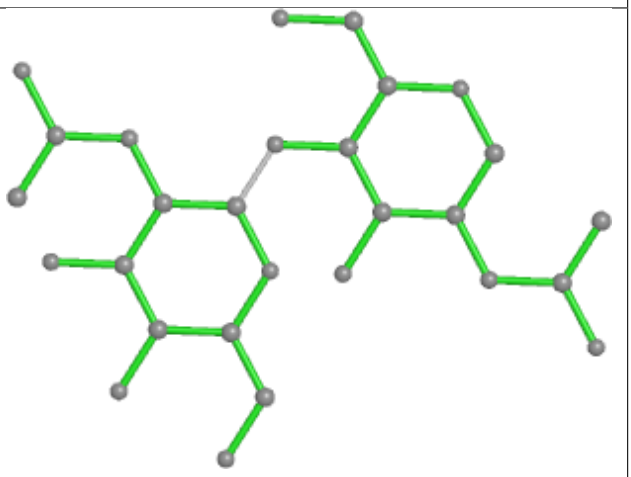
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	NAG	1	0
2	Q	1	NAG	1	0
2	O	1	NAG	1	0
3	M	1	NAG	2	0

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

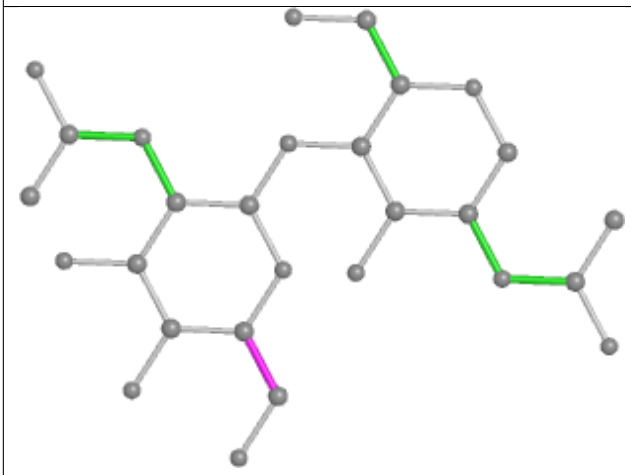
Oligosaccharide Chain E



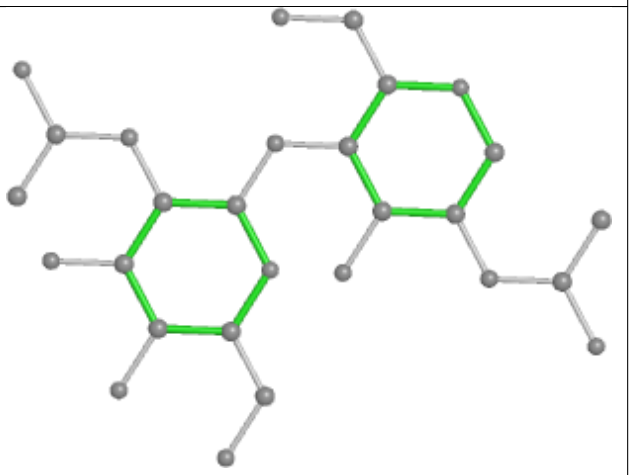
Bond lengths



Bond angles

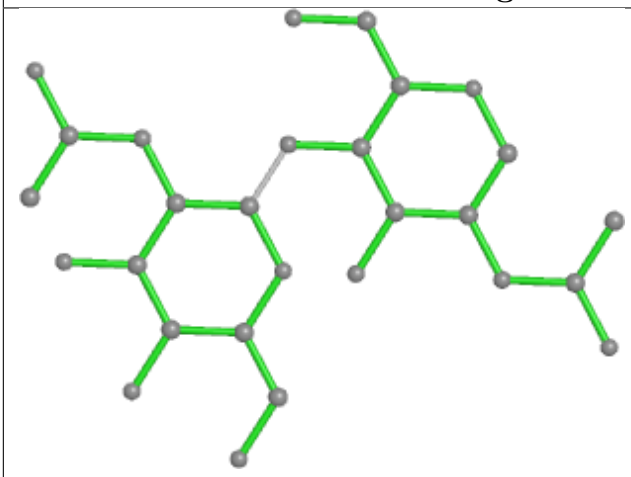


Torsions

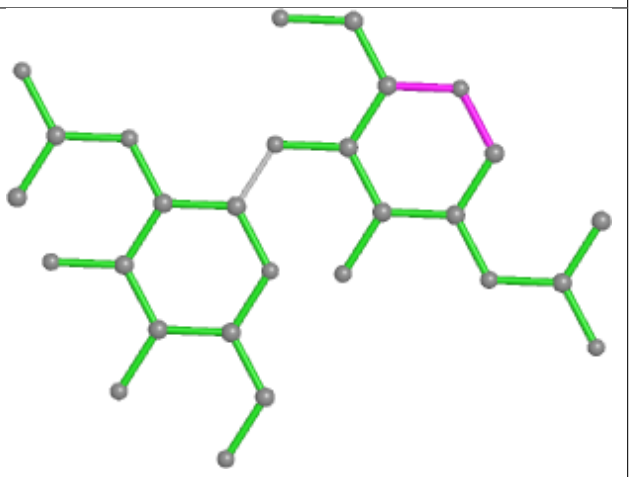


Rings

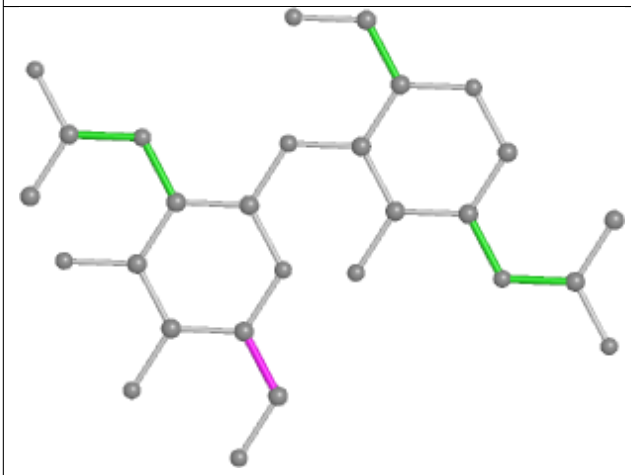
Oligosaccharide Chain F



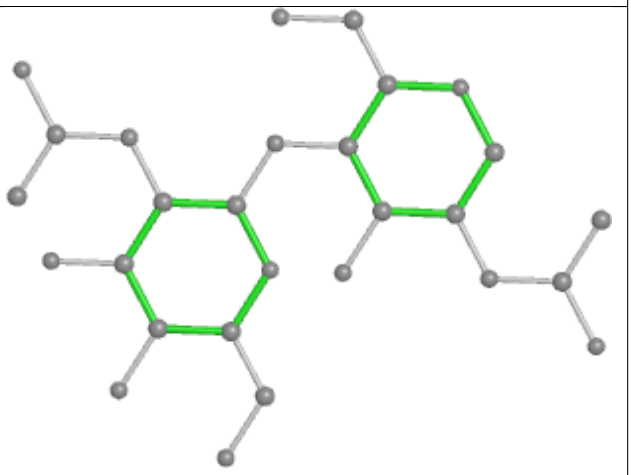
Bond lengths



Bond angles

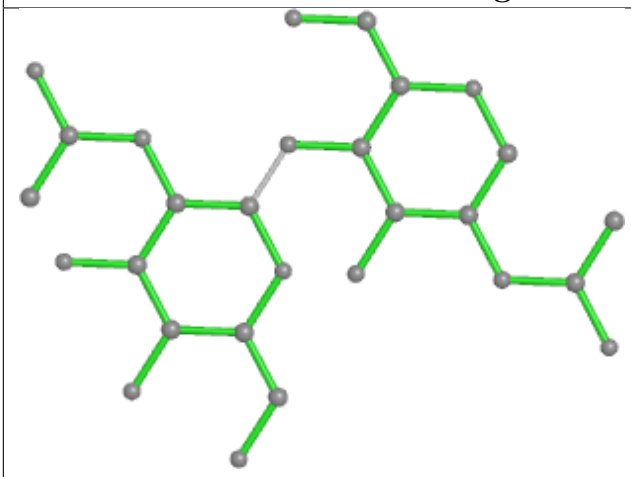


Torsions

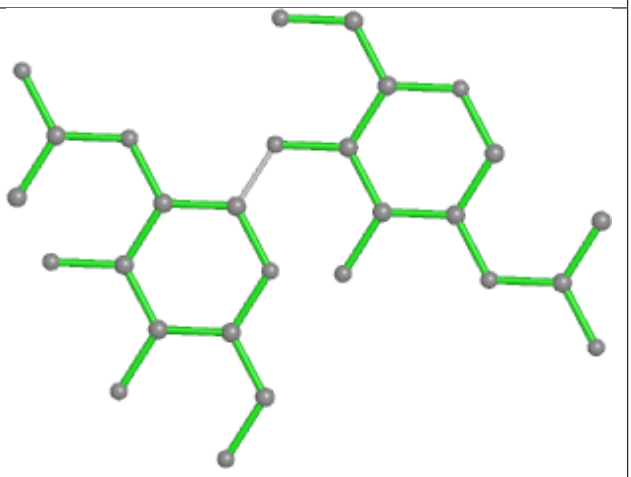


Rings

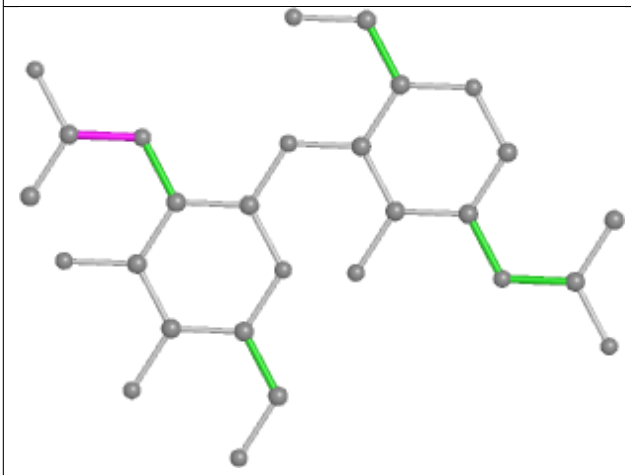
Oligosaccharide Chain H



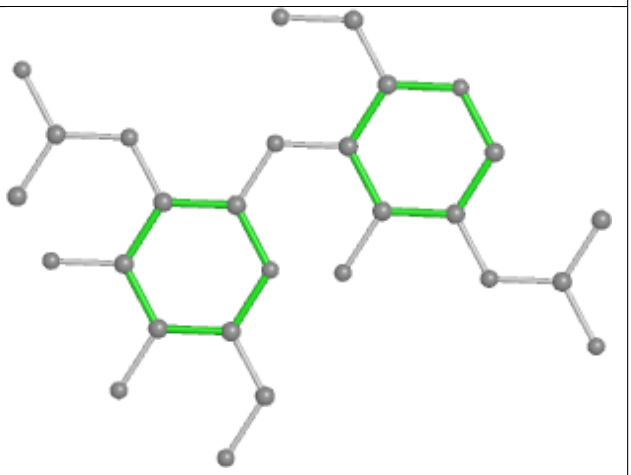
Bond lengths



Bond angles

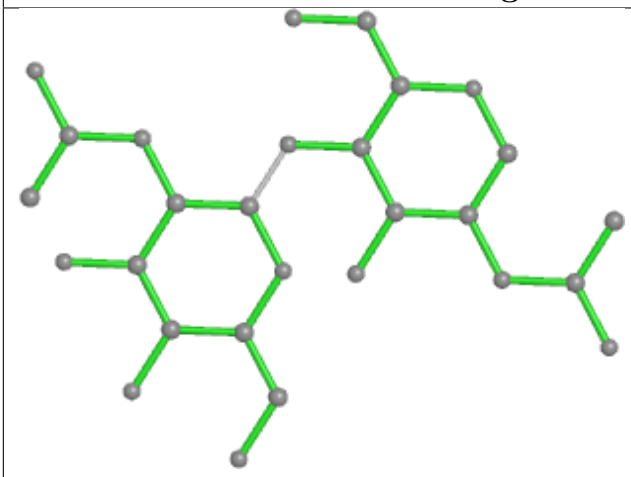


Torsions

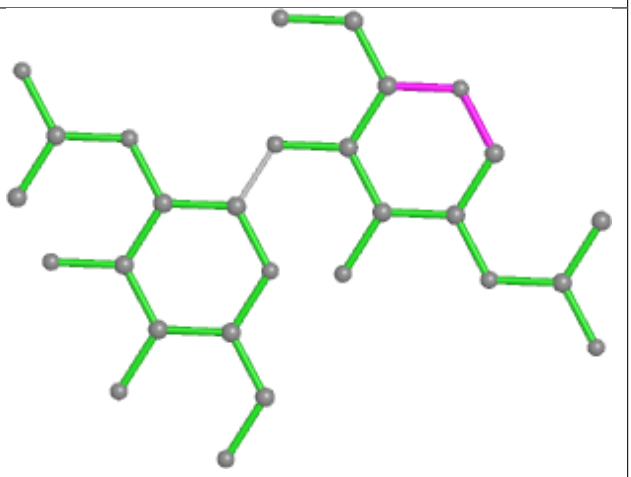


Rings

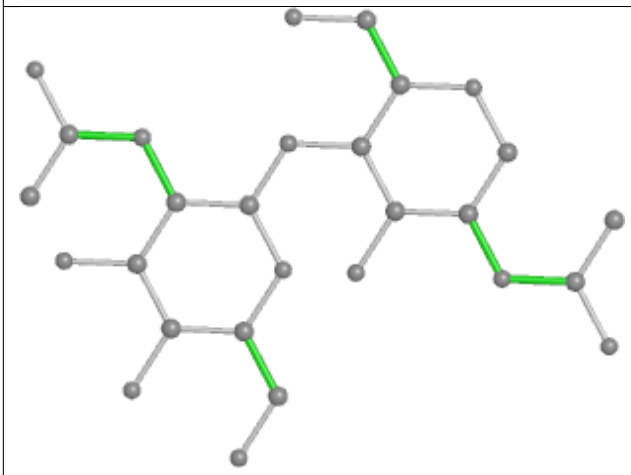
Oligosaccharide Chain I



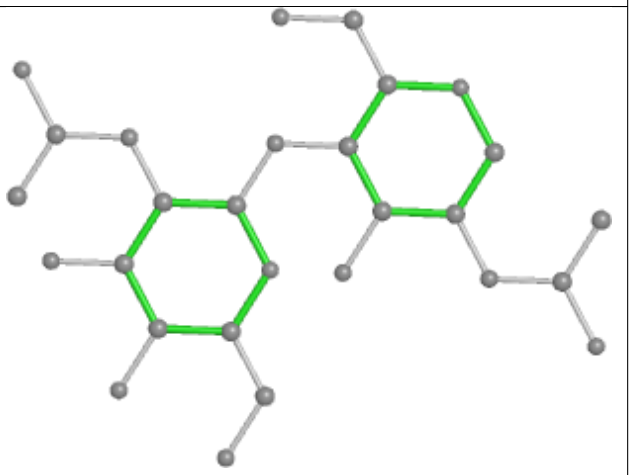
Bond lengths



Bond angles

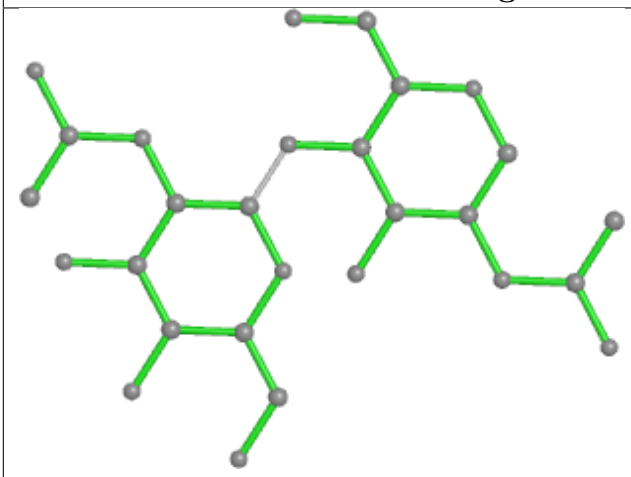


Torsions

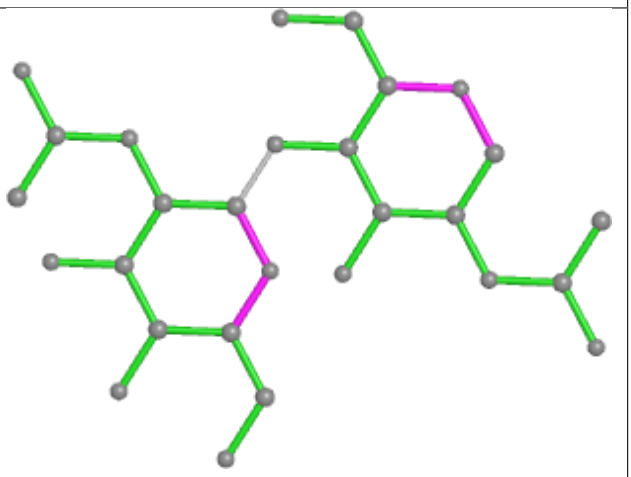


Rings

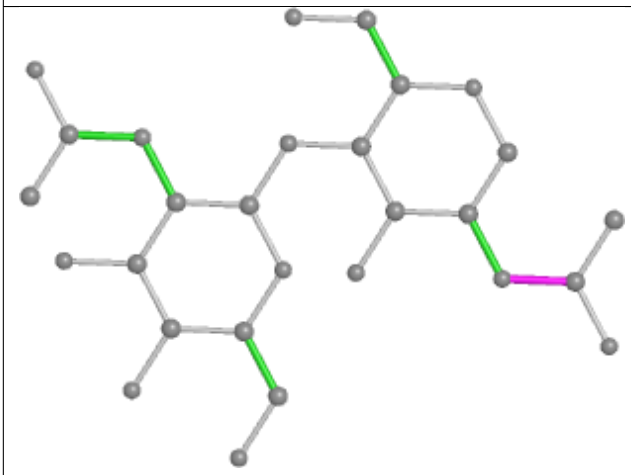
Oligosaccharide Chain J



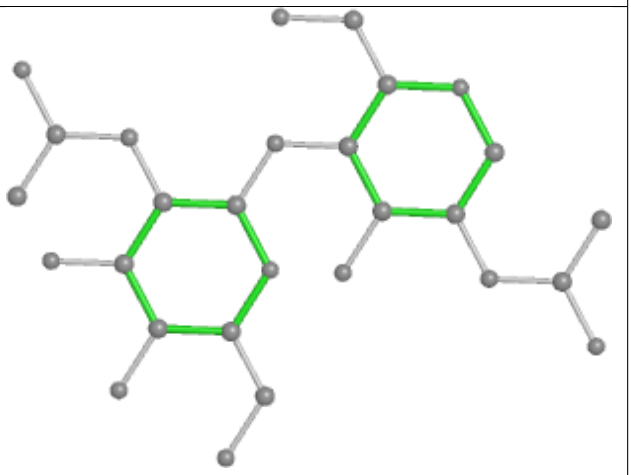
Bond lengths



Bond angles

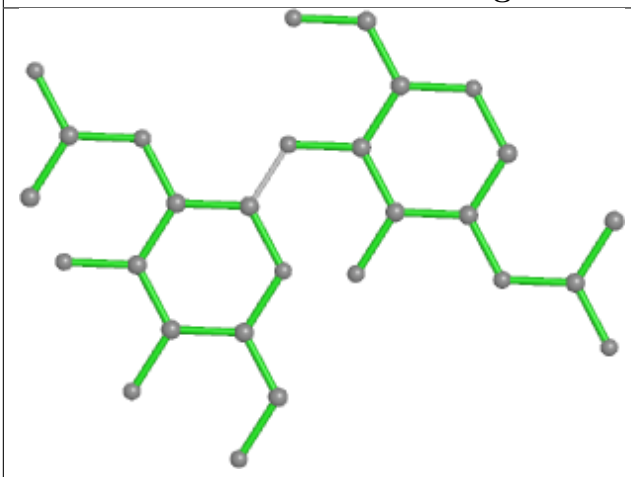


Torsions

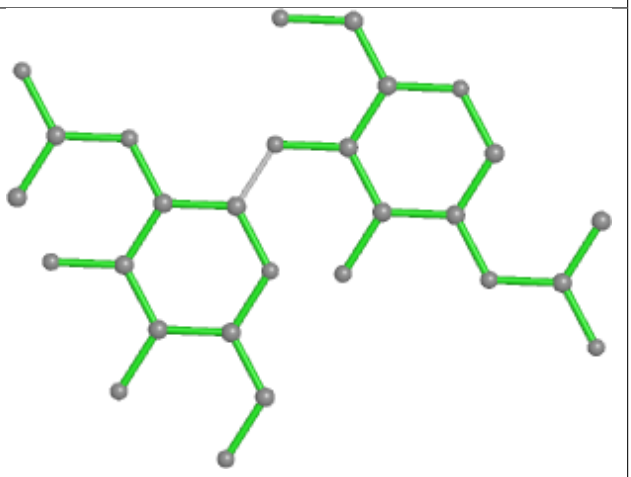


Rings

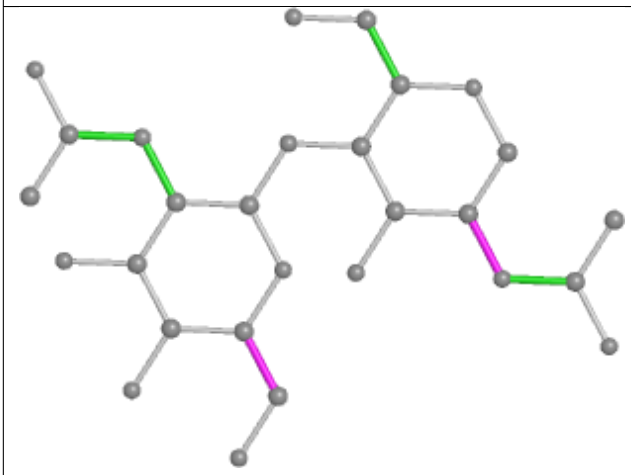
Oligosaccharide Chain K



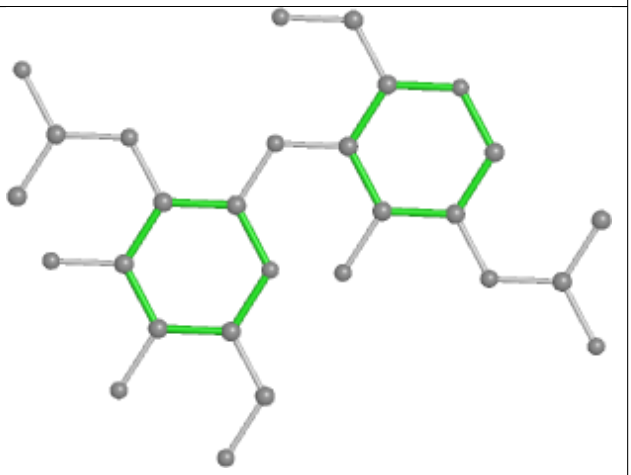
Bond lengths



Bond angles

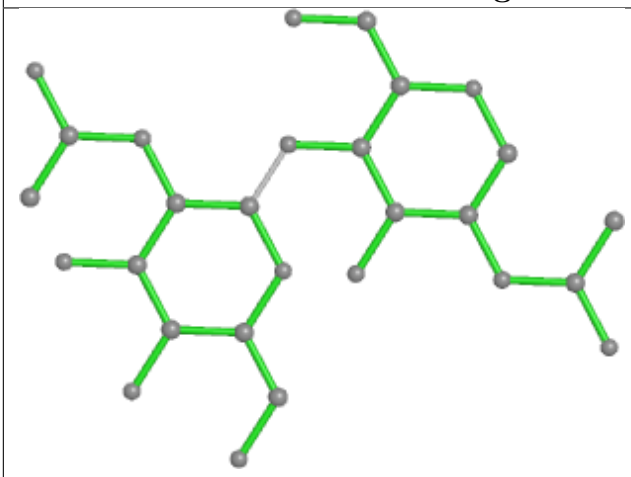


Torsions

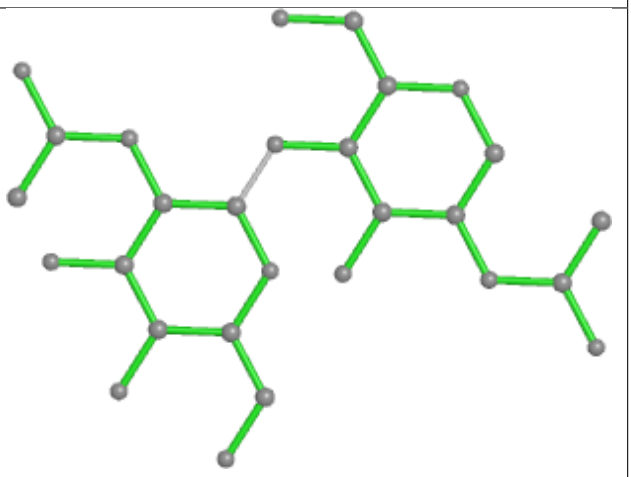


Rings

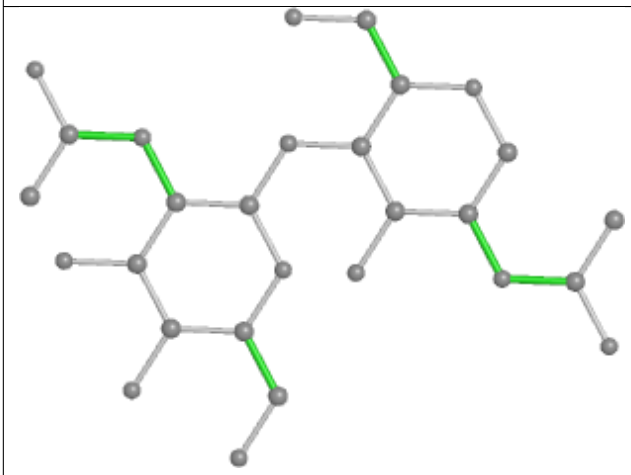
Oligosaccharide Chain N



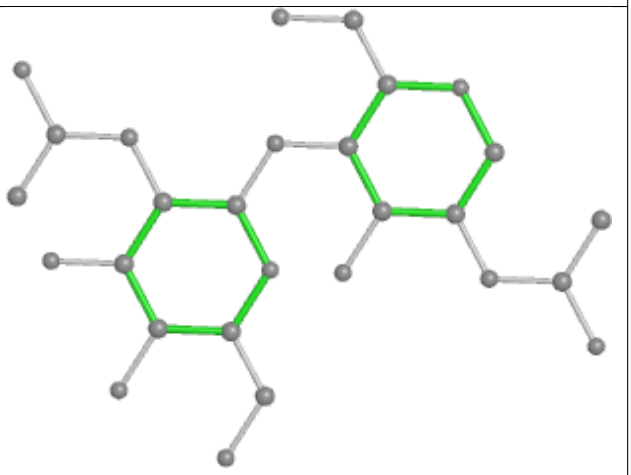
Bond lengths



Bond angles

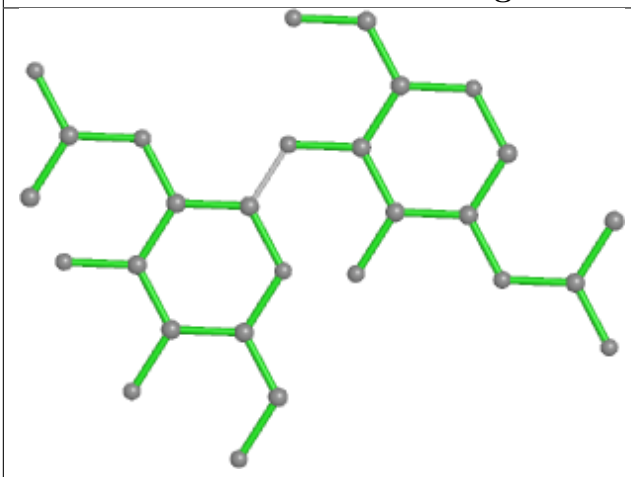


Torsions

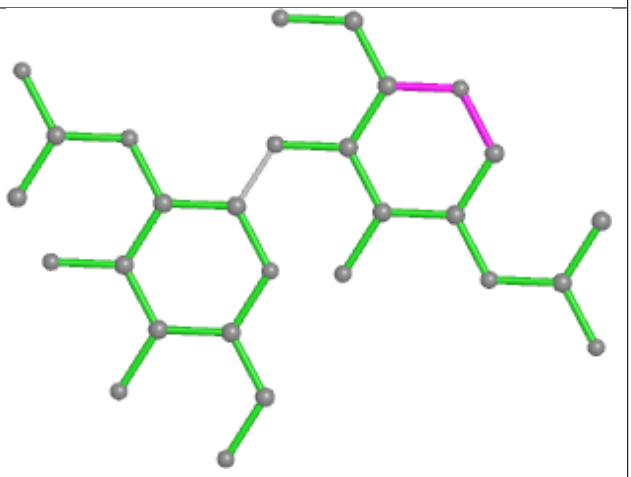


Rings

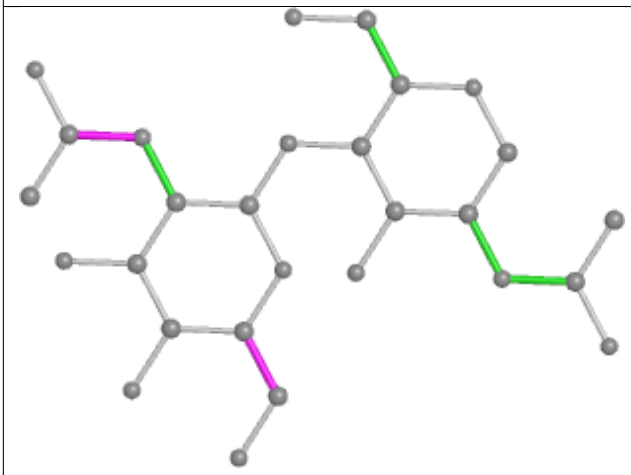
Oligosaccharide Chain O



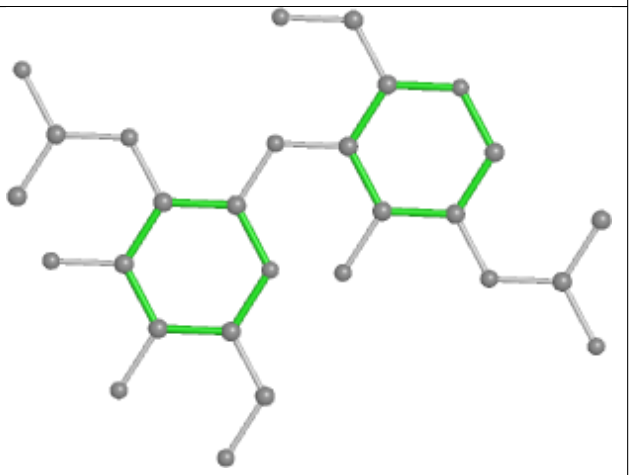
Bond lengths



Bond angles

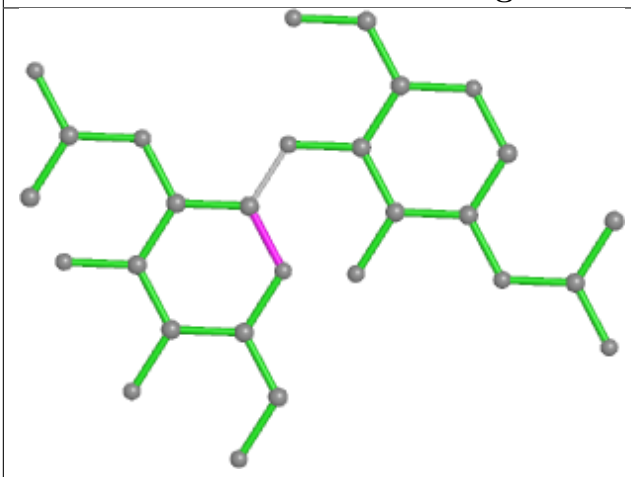


Torsions

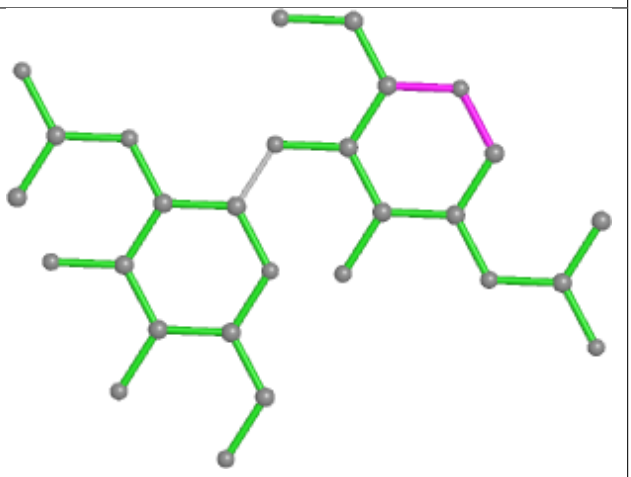


Rings

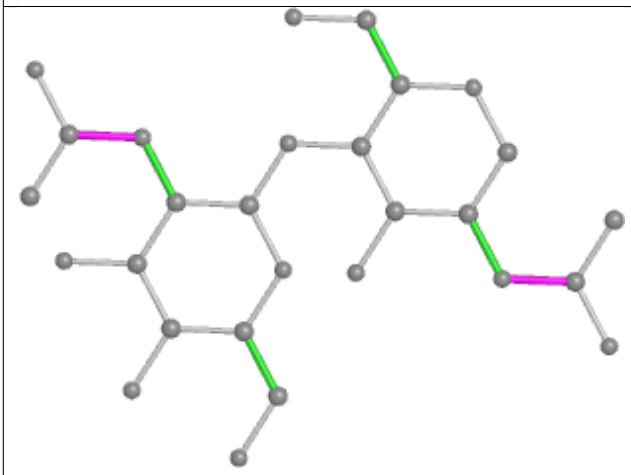
Oligosaccharide Chain P



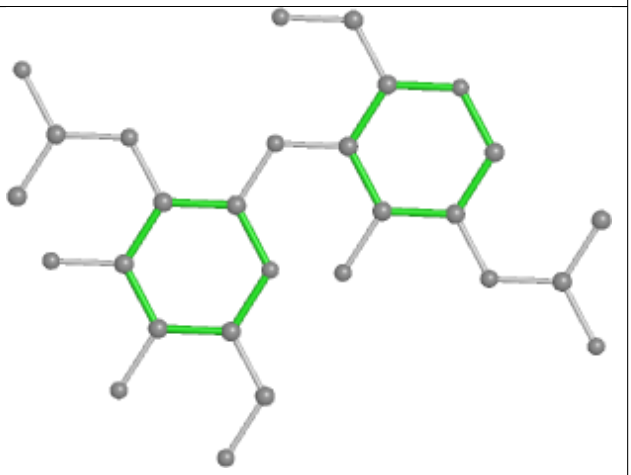
Bond lengths



Bond angles

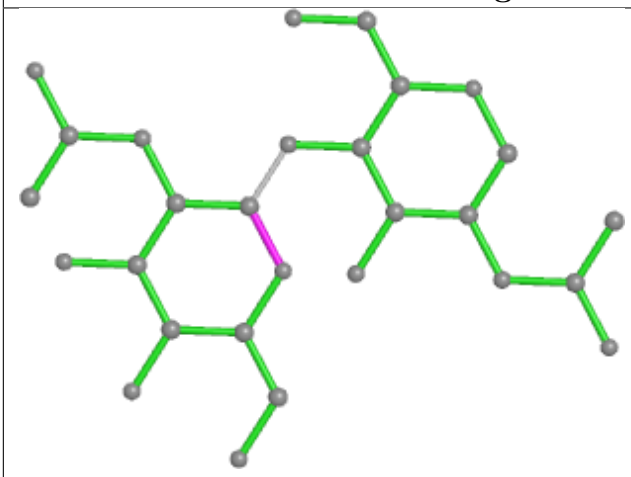


Torsions

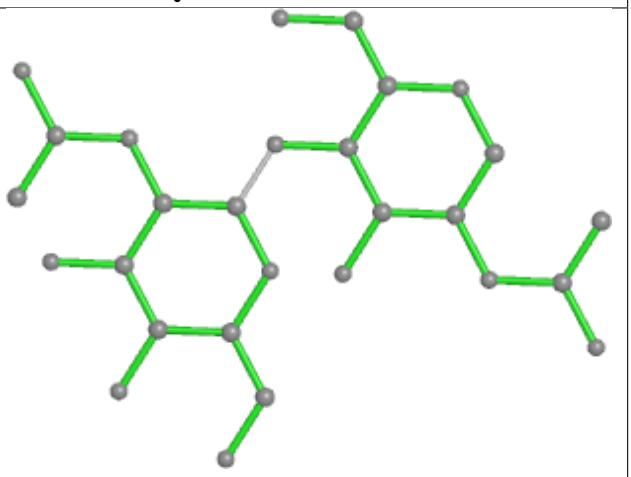


Rings

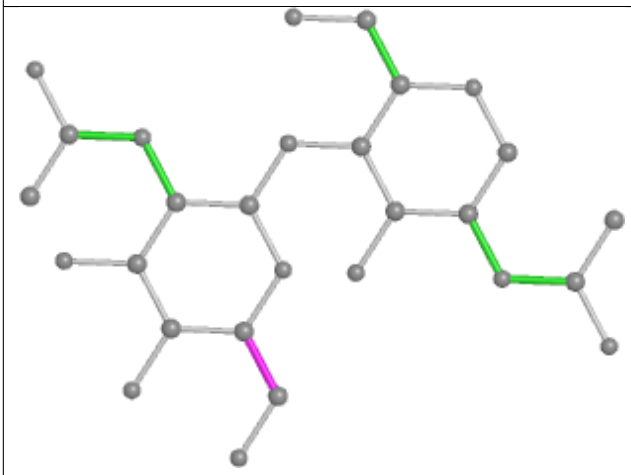
Oligosaccharide Chain Q



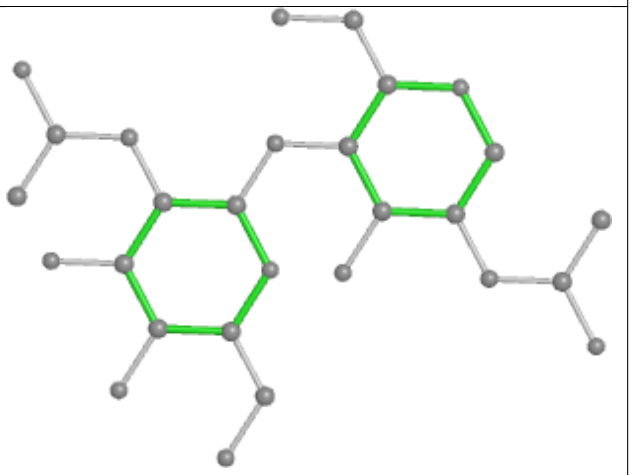
Bond lengths



Bond angles

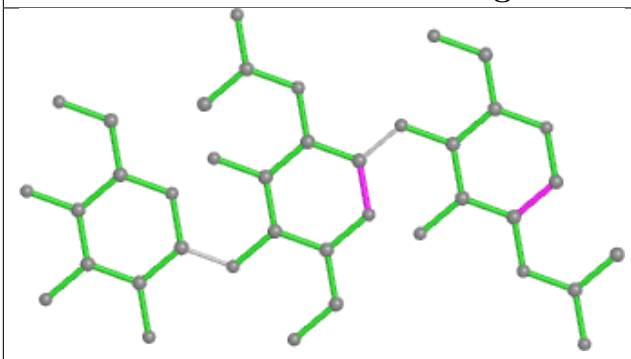


Torsions

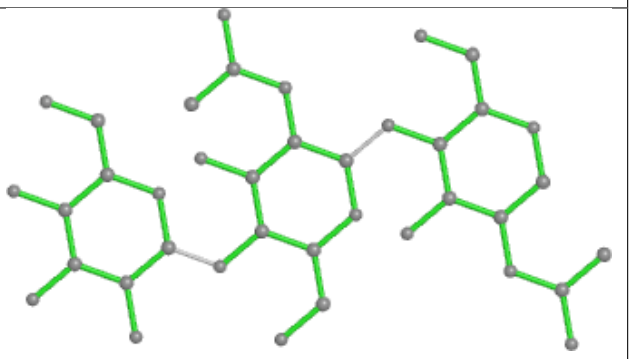


Rings

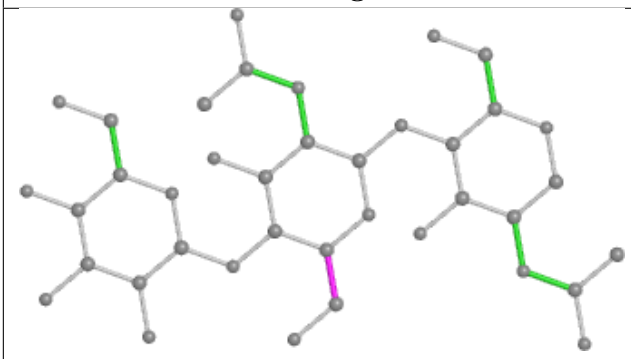
Oligosaccharide Chain G



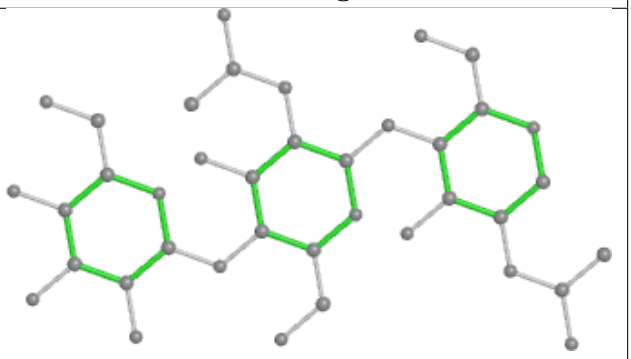
Bond lengths



Bond angles

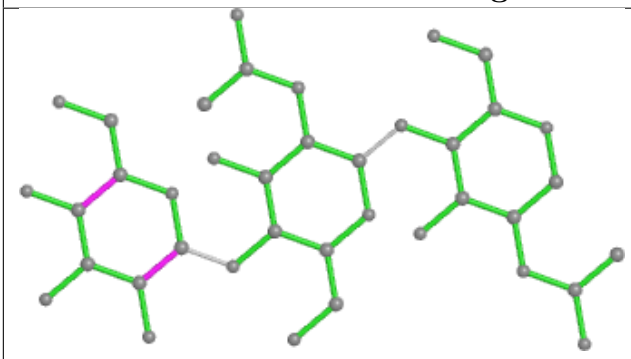


Torsions

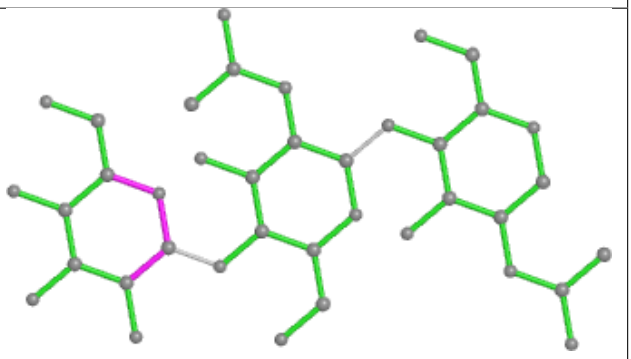


Rings

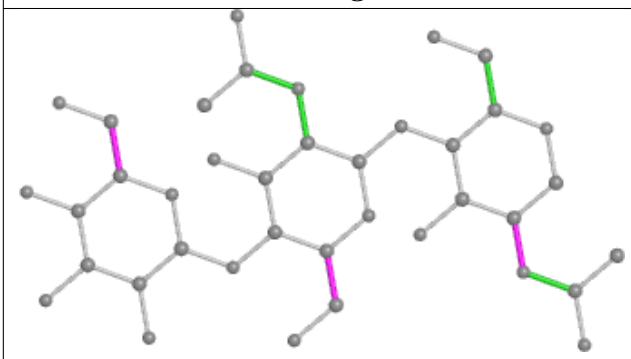
Oligosaccharide Chain M



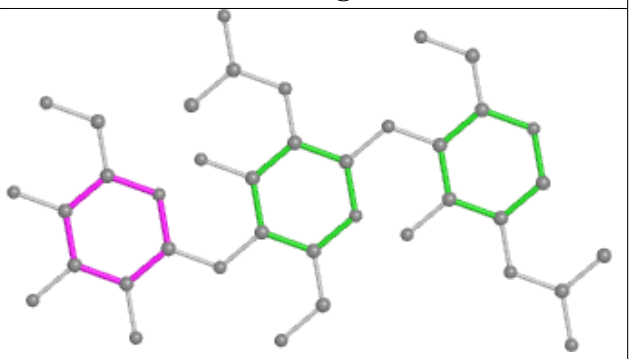
Bond lengths



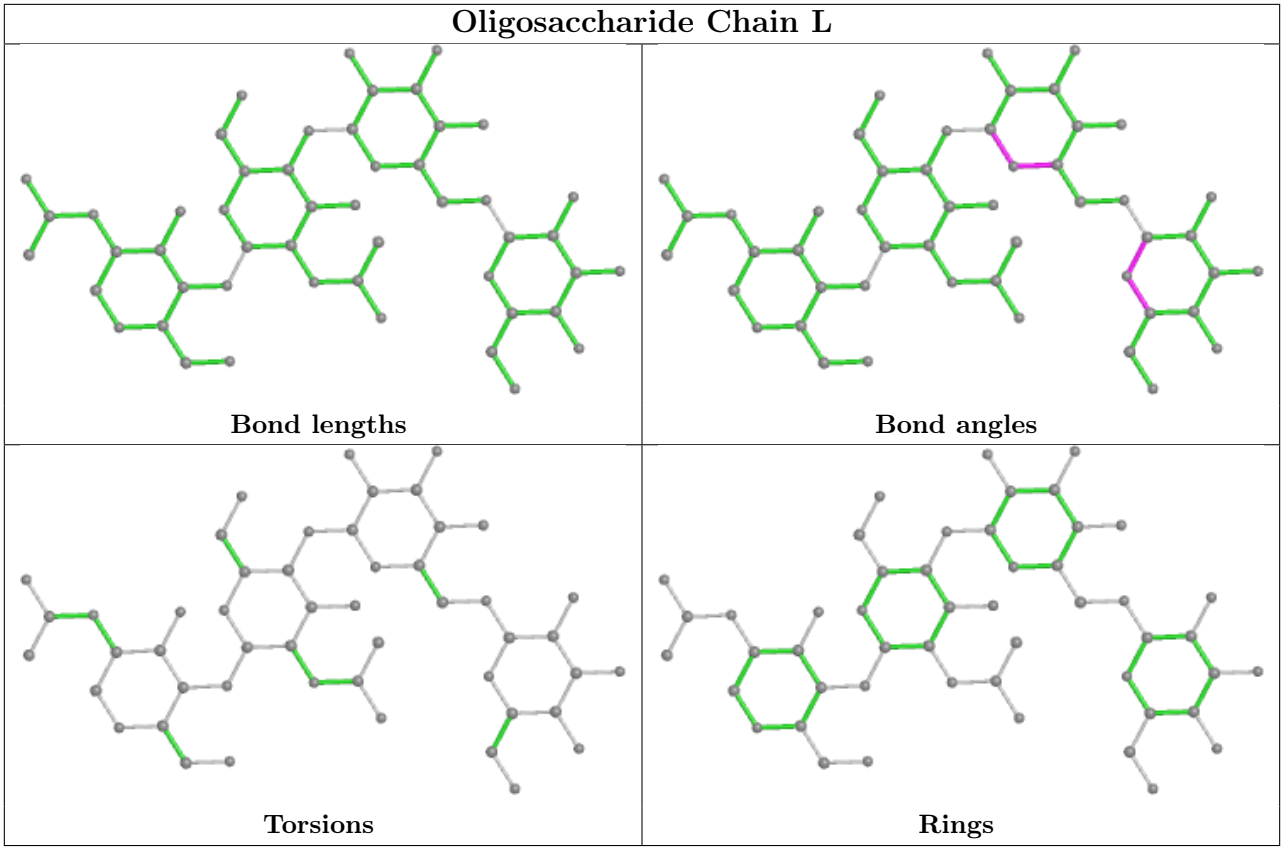
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
8	EDO	A	406	-	3,3,3	0.50	0	2,2,2	0.42	0
8	EDO	D	403	-	3,3,3	0.46	0	2,2,2	0.45	0
7	BEZ	A	403	-	9,9,9	1.04	0	11,11,11	1.22	2 (18%)
7	BEZ	C	405	-	9,9,9	0.81	0	11,11,11	1.11	1 (9%)
8	EDO	A	408	-	3,3,3	0.54	0	2,2,2	0.33	0
5	NAG	A	401	1	14,14,15	0.49	0	17,19,21	1.38	2 (11%)
8	EDO	A	409	-	3,3,3	0.51	0	2,2,2	0.35	0
5	NAG	C	403	1	14,14,15	0.23	0	17,19,21	0.43	0
7	BEZ	B	402	-	9,9,9	0.66	0	11,11,11	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	EDO	A	405	-	3,3,3	0.75	0	2,2,2	0.32	0
5	NAG	C	401	1	14,14,15	0.38	0	17,19,21	0.62	1 (5%)
8	EDO	A	404	-	3,3,3	0.48	0	2,2,2	0.30	0
11	MAN	D	404	-	12,12,12	0.92	0	17,17,17	1.04	1 (5%)
8	EDO	A	407	-	3,3,3	0.50	0	2,2,2	0.25	0
8	EDO	B	403	-	3,3,3	0.48	0	2,2,2	0.49	0
10	GOL	D	402	-	5,5,5	0.87	0	5,5,5	0.93	0
8	EDO	C	406	-	3,3,3	0.52	0	2,2,2	0.23	0
8	EDO	A	410	-	3,3,3	0.43	0	2,2,2	0.35	0
5	NAG	C	402	1	14,14,15	0.22	0	17,19,21	0.68	1 (5%)
8	EDO	A	411	-	3,3,3	0.44	0	2,2,2	0.58	0
9	PEG	D	405	-	6,6,6	0.45	0	5,5,5	0.39	0
9	PEG	D	406	-	6,6,6	0.51	0	5,5,5	0.25	0
9	PEG	B	405	-	6,6,6	0.47	0	5,5,5	0.25	0
8	EDO	C	407	-	3,3,3	0.47	0	2,2,2	0.38	0
8	EDO	B	404	-	3,3,3	0.51	0	2,2,2	0.20	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
8	EDO	A	406	-	-	0/1/1/1	-
8	EDO	D	403	-	-	1/1/1/1	-
7	BEZ	A	403	-	-	0/4/4/4	0/1/1/1
7	BEZ	C	405	-	-	0/4/4/4	0/1/1/1
8	EDO	A	408	-	-	0/1/1/1	-
5	NAG	A	401	1	-	5/6/23/26	0/1/1/1
8	EDO	A	409	-	-	0/1/1/1	-
5	NAG	C	403	1	-	0/6/23/26	0/1/1/1
7	BEZ	B	402	-	-	0/4/4/4	0/1/1/1
8	EDO	A	405	-	-	0/1/1/1	-
5	NAG	C	401	1	-	2/6/23/26	0/1/1/1
8	EDO	A	404	-	-	0/1/1/1	-
11	MAN	D	404	-	-	0/2/22/22	0/1/1/1
8	EDO	A	407	-	-	0/1/1/1	-
8	EDO	B	403	-	-	0/1/1/1	-
10	GOL	D	402	-	-	2/4/4/4	-
8	EDO	C	406	-	-	0/1/1/1	-
8	EDO	A	410	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	402	1	-	0/6/23/26	0/1/1/1
8	EDO	A	411	-	-	1/1/1/1	-
9	PEG	D	405	-	-	0/4/4/4	-
9	PEG	D	406	-	-	2/4/4/4	-
9	PEG	B	405	-	-	1/4/4/4	-
8	EDO	C	407	-	-	1/1/1/1	-
8	EDO	B	404	-	-	0/1/1/1	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	401	NAG	C2-N2-C7	4.39	129.16	122.90
7	A	403	BEZ	O2-C-O1	-2.78	117.17	123.35
7	A	403	BEZ	O2-C-C1	2.74	121.95	114.85
11	D	404	MAN	C4-C3-C2	2.53	115.23	110.82
5	C	402	NAG	C1-O5-C5	2.35	115.37	112.19
7	C	405	BEZ	O2-C-C1	2.20	120.55	114.85
5	C	401	NAG	C1-O5-C5	2.05	114.97	112.19
5	A	401	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	NAG	C8-C7-N2-C2
5	A	401	NAG	O7-C7-N2-C2
5	C	401	NAG	C8-C7-N2-C2
5	C	401	NAG	O7-C7-N2-C2
9	B	405	PEG	O1-C1-C2-O2
5	A	401	NAG	C4-C5-C6-O6
8	A	411	EDO	O1-C1-C2-O2
8	C	407	EDO	O1-C1-C2-O2
8	D	403	EDO	O1-C1-C2-O2
9	D	406	PEG	O2-C3-C4-O4
5	A	401	NAG	O5-C5-C6-O6
9	D	406	PEG	C4-C3-O2-C2
10	D	402	GOL	O1-C1-C2-O2
8	A	410	EDO	O1-C1-C2-O2
10	D	402	GOL	O1-C1-C2-C3
5	A	401	NAG	C3-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	406	EDO	1	0
8	D	403	EDO	1	0
7	A	403	BEZ	1	0
8	A	408	EDO	1	0
5	A	401	NAG	2	0
8	A	409	EDO	1	0
5	C	401	NAG	2	0
8	A	407	EDO	1	0
8	A	410	EDO	2	0
5	C	402	NAG	1	0
8	A	411	EDO	1	0
9	D	405	PEG	1	0

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	340/373 (91%)	-0.48	3 (0%)	84	85	18, 25, 40, 66	0
1	B	338/373 (90%)	-0.47	2 (0%)	89	90	20, 28, 41, 70	0
1	C	339/373 (90%)	-0.40	5 (1%)	73	76	19, 29, 45, 83	0
1	D	339/373 (90%)	-0.42	6 (1%)	68	71	20, 31, 46, 69	0
All	All	1356/1492 (90%)	-0.44	16 (1%)	79	81	18, 28, 44, 83	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	LEU	6.9
1	D	349	LEU	6.5
1	B	349	LEU	5.7
1	D	348	LEU	4.7
1	C	348	LEU	4.6
1	A	349	LEU	4.6
1	D	281	ASP	3.0
1	A	368	HIS	2.9
1	C	346	ASP	2.7
1	B	348	LEU	2.6
1	A	348	LEU	2.6
1	C	281	ASP	2.5
1	D	347	SER	2.5
1	D	368	HIS	2.4
1	D	351	VAL	2.4
1	C	347	SER	2.2

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 (i)

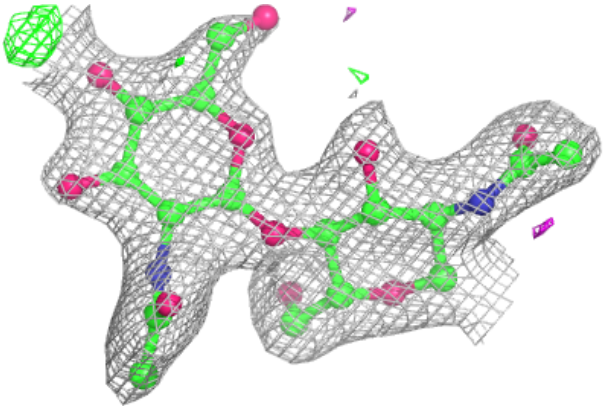
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

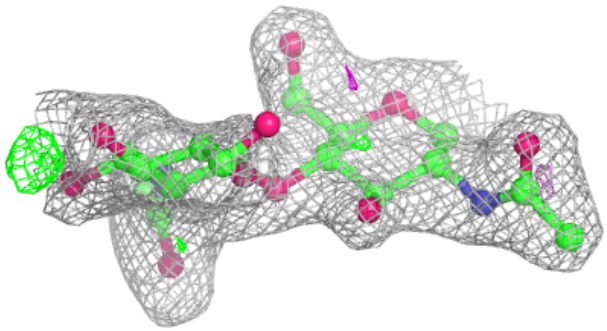
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	L	4	11/12	0.72	0.23	59,62,70,71	0
4	BMA	L	3	11/12	0.74	0.27	56,64,70,71	0
2	NAG	H	2	14/15	0.75	0.21	48,61,71,72	0
2	NAG	P	2	14/15	0.77	0.15	46,52,56,56	0
2	NAG	N	2	14/15	0.78	0.16	57,64,74,74	0
3	BMA	M	3	11/12	0.78	0.15	61,65,71,73	0
2	NAG	O	2	14/15	0.81	0.15	40,55,61,63	0
2	NAG	E	2	14/15	0.82	0.17	49,58,65,70	0
2	NAG	Q	2	14/15	0.83	0.17	37,44,50,54	0
2	NAG	F	2	14/15	0.83	0.19	44,50,59,60	0
3	BMA	G	3	11/12	0.84	0.20	55,62,73,73	0
2	NAG	J	2	14/15	0.85	0.18	41,48,53,61	0
2	NAG	I	2	14/15	0.87	0.18	47,65,72,76	0
2	NAG	N	1	14/15	0.88	0.11	40,48,54,54	0
2	NAG	O	1	14/15	0.88	0.12	38,45,51,54	0
3	NAG	M	2	14/15	0.88	0.14	33,45,62,63	0
4	NAG	L	2	14/15	0.91	0.12	35,43,47,57	0
2	NAG	K	2	14/15	0.91	0.14	36,50,57,60	0
2	NAG	J	1	14/15	0.91	0.09	24,32,40,41	0
2	NAG	K	1	14/15	0.92	0.08	33,38,45,46	0
2	NAG	I	1	14/15	0.92	0.09	38,48,56,56	0
3	NAG	G	2	14/15	0.92	0.10	30,35,50,53	0
2	NAG	P	1	14/15	0.93	0.08	26,33,38,46	0
2	NAG	E	1	14/15	0.93	0.10	34,43,53,55	0
4	NAG	L	1	14/15	0.94	0.08	24,28,34,34	0
3	NAG	M	1	14/15	0.94	0.10	24,30,37,37	0
2	NAG	Q	1	14/15	0.94	0.08	27,33,41,42	0
2	NAG	H	1	14/15	0.94	0.10	39,48,54,58	0
2	NAG	F	1	14/15	0.95	0.09	24,30,37,43	0
3	NAG	G	1	14/15	0.97	0.07	22,25,27,27	0

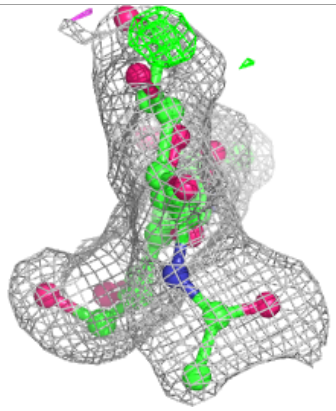
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

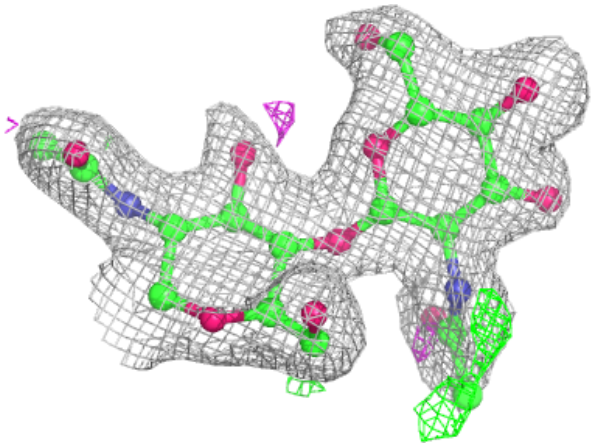


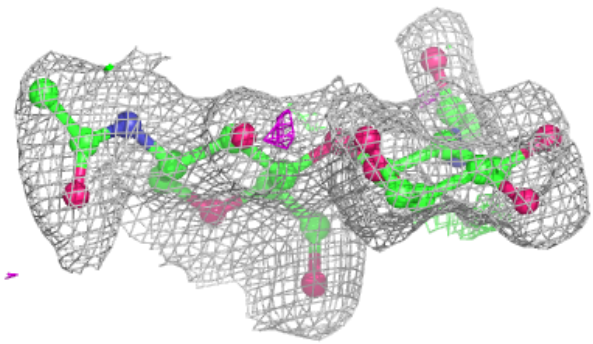


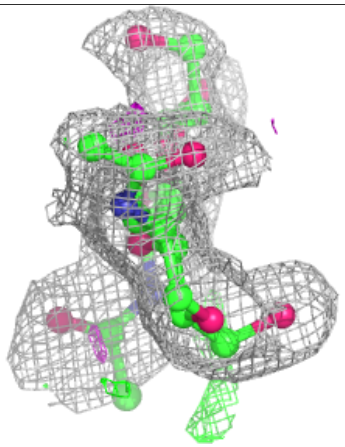


Electron density around Chain F:

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

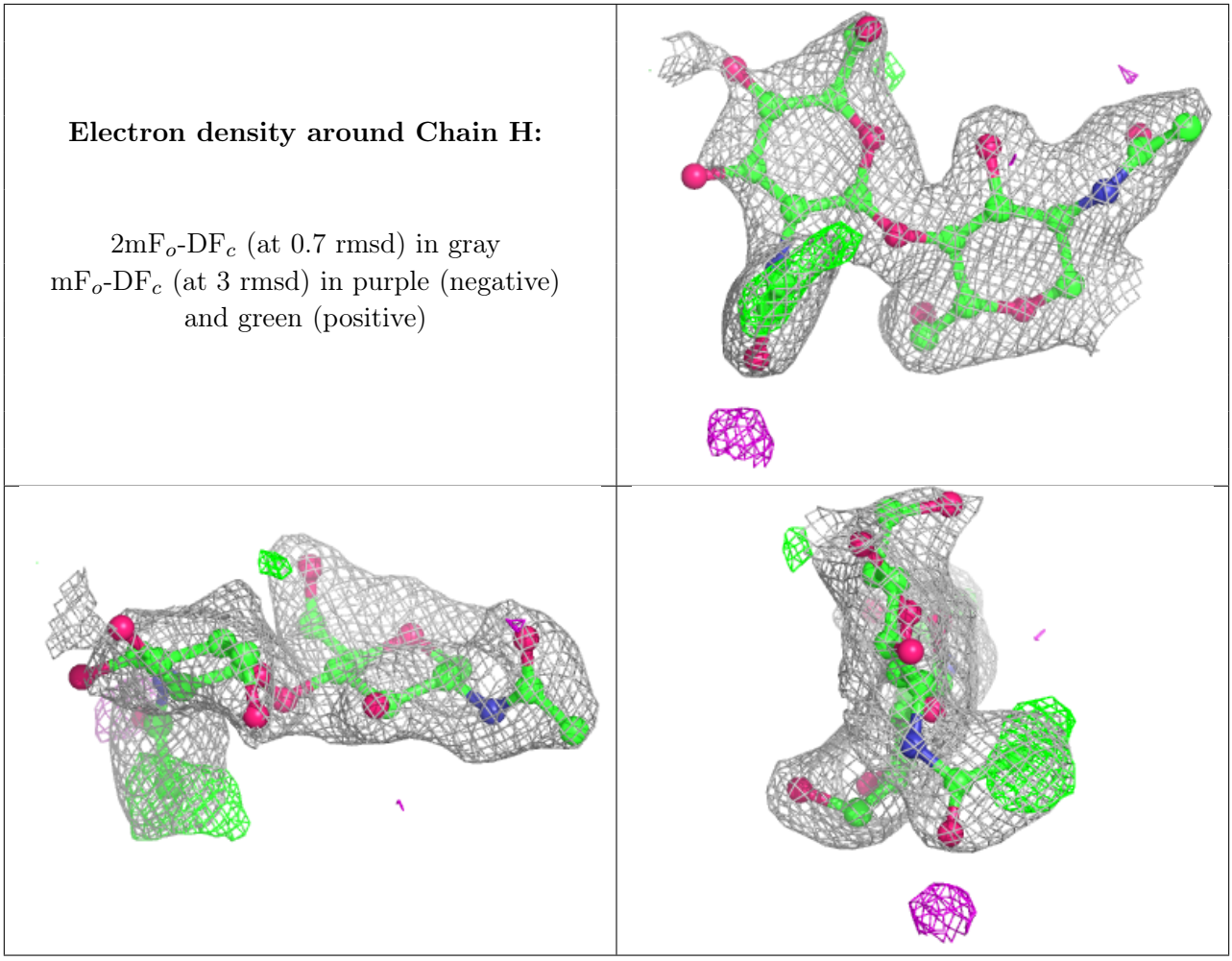






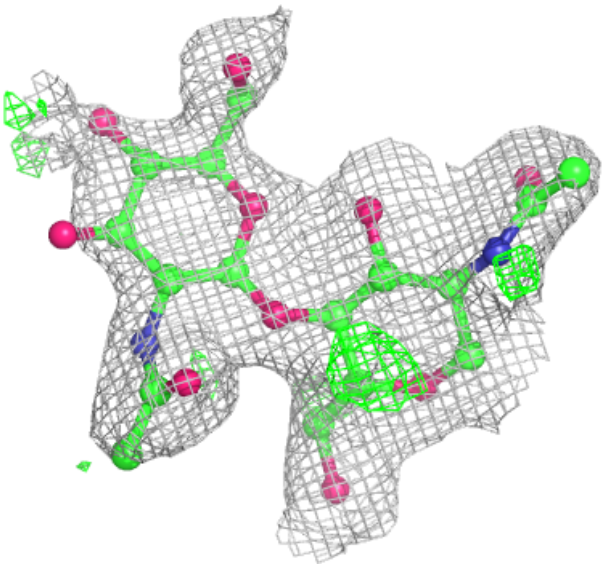
Electron density around Chain H:

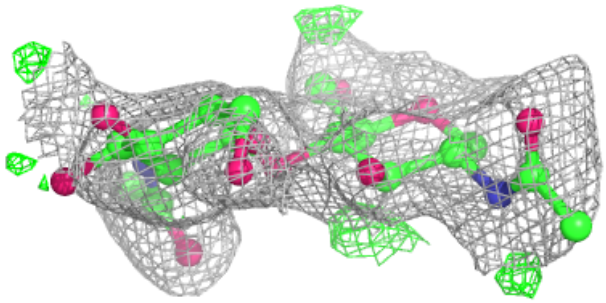
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

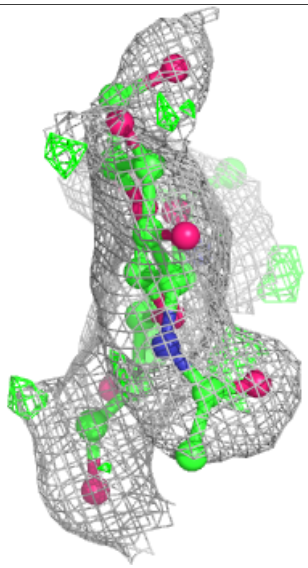


Electron density around Chain I:

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

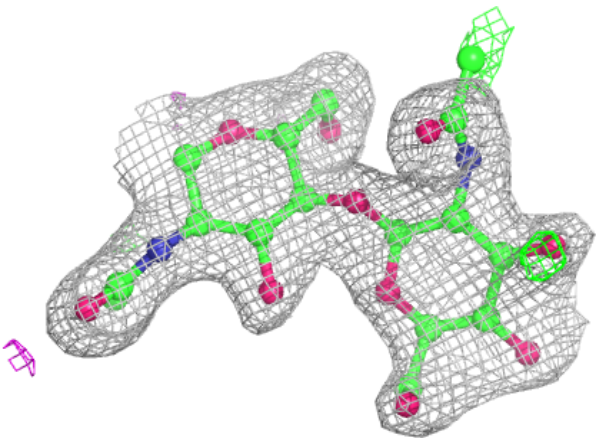


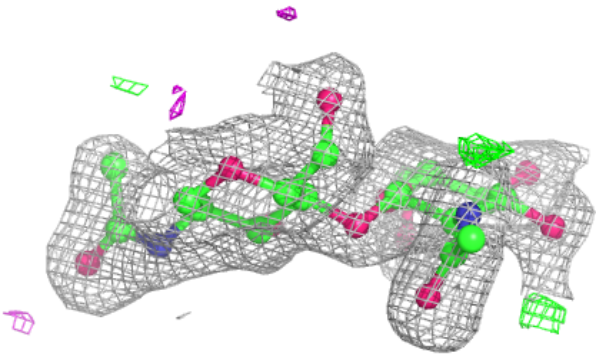


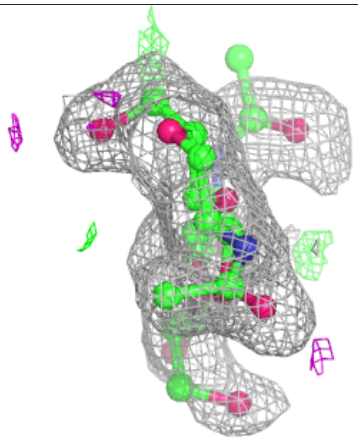


Electron density around Chain J:

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

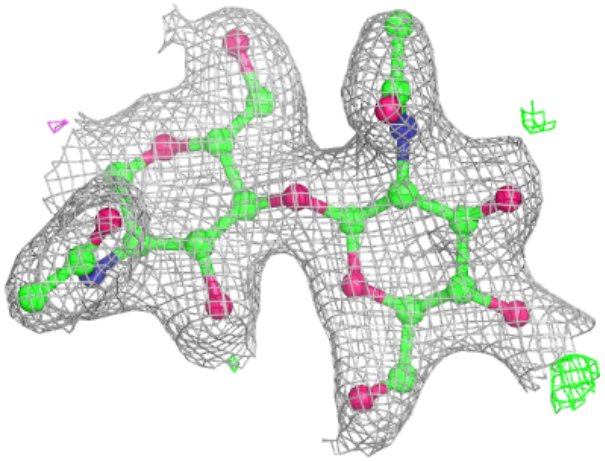


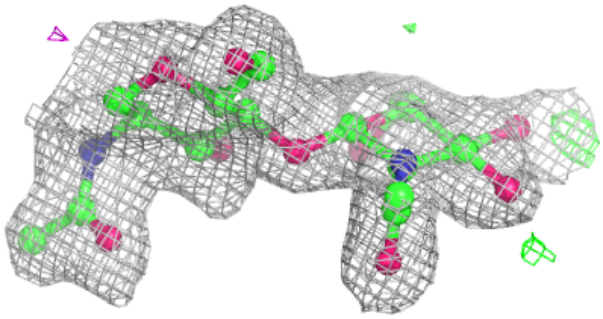


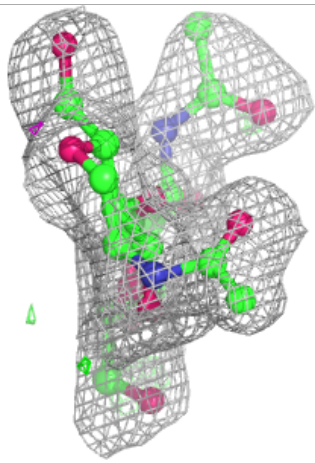


Electron density around Chain K:

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

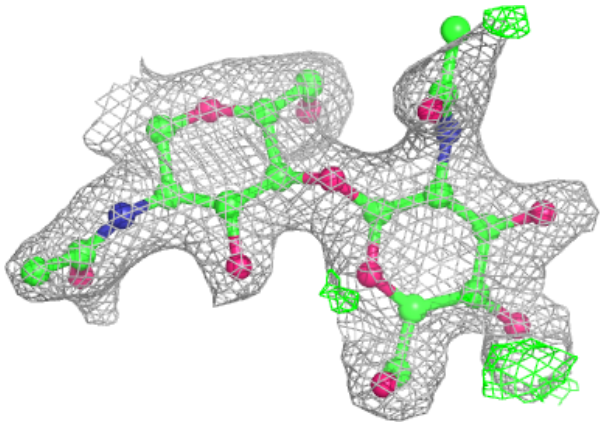


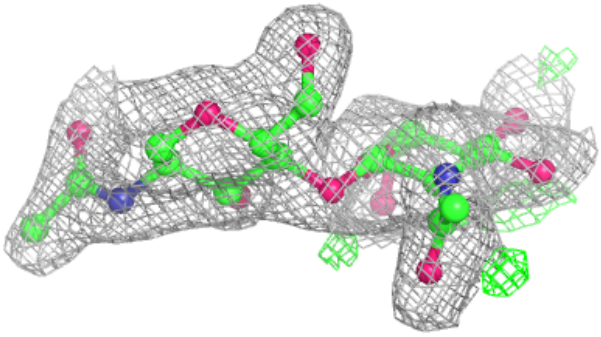


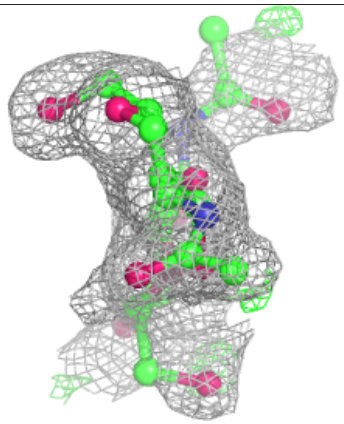


Electron density around Chain N:

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

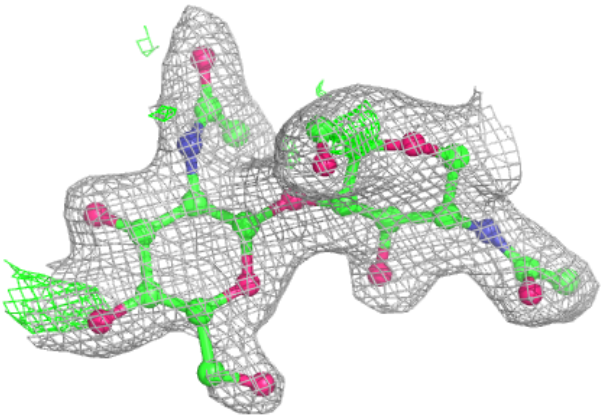


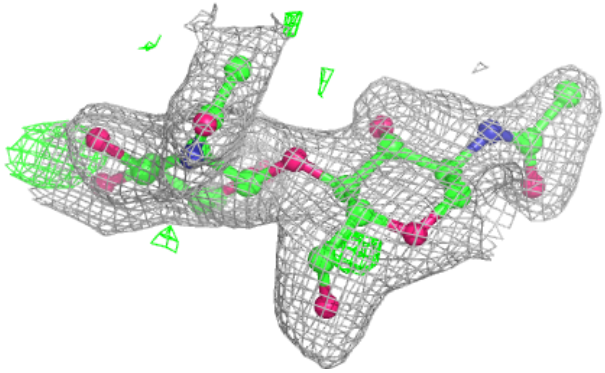


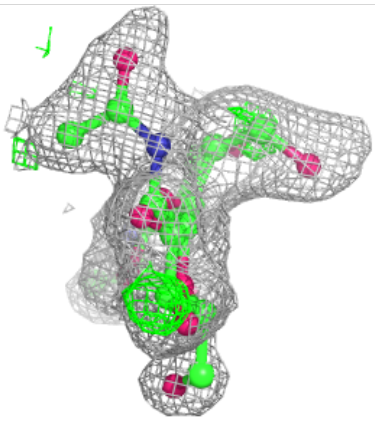


Electron density around Chain O:

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

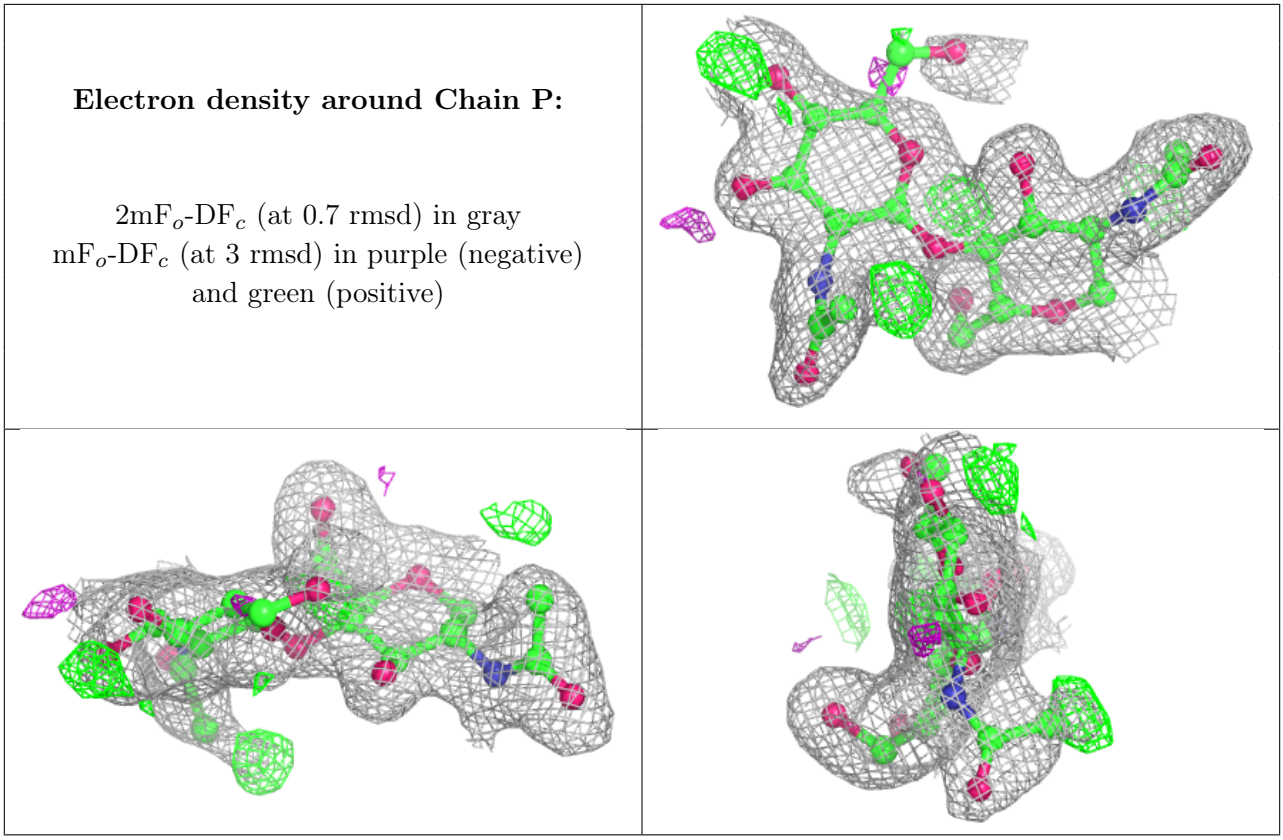






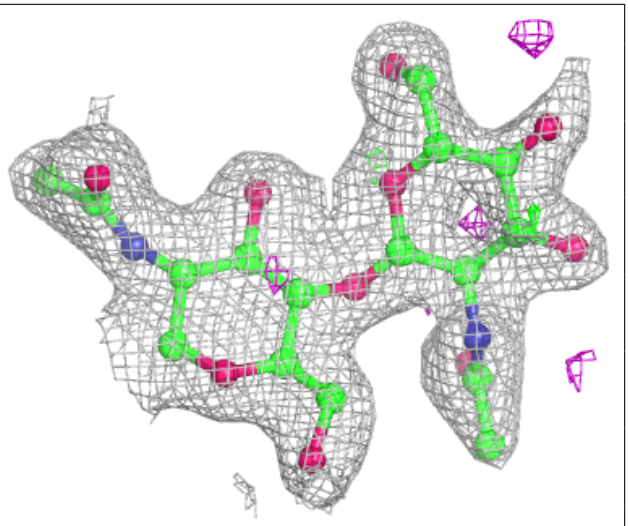
Electron density around Chain P:

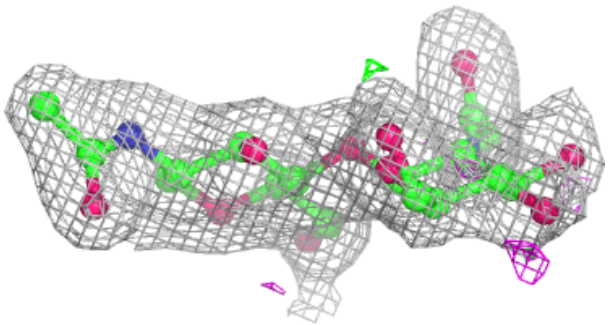
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

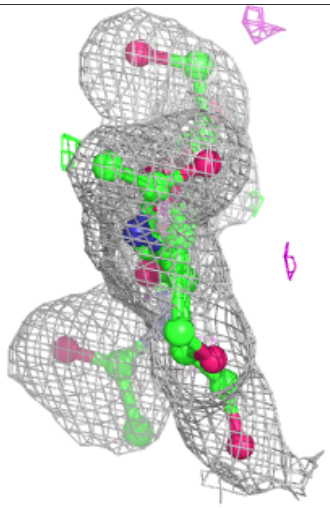


Electron density around Chain Q:

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

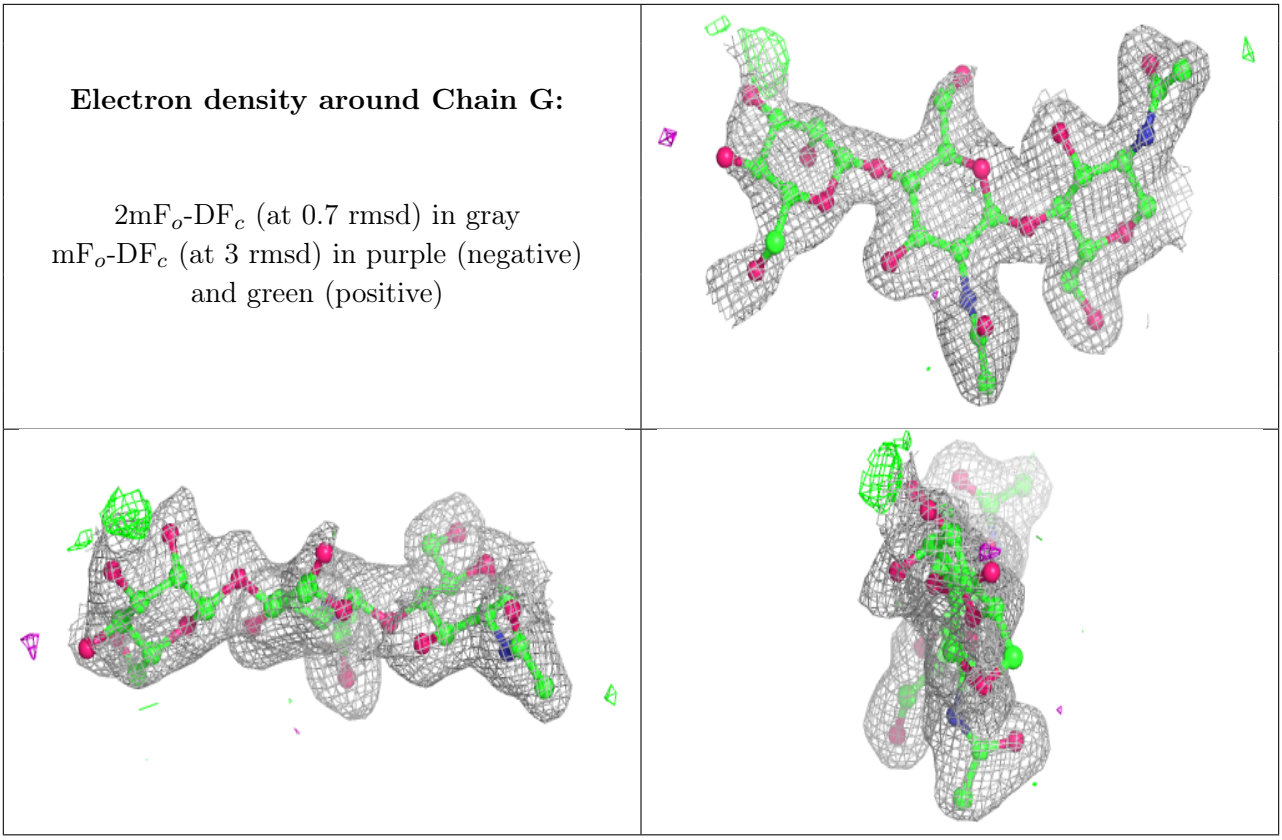






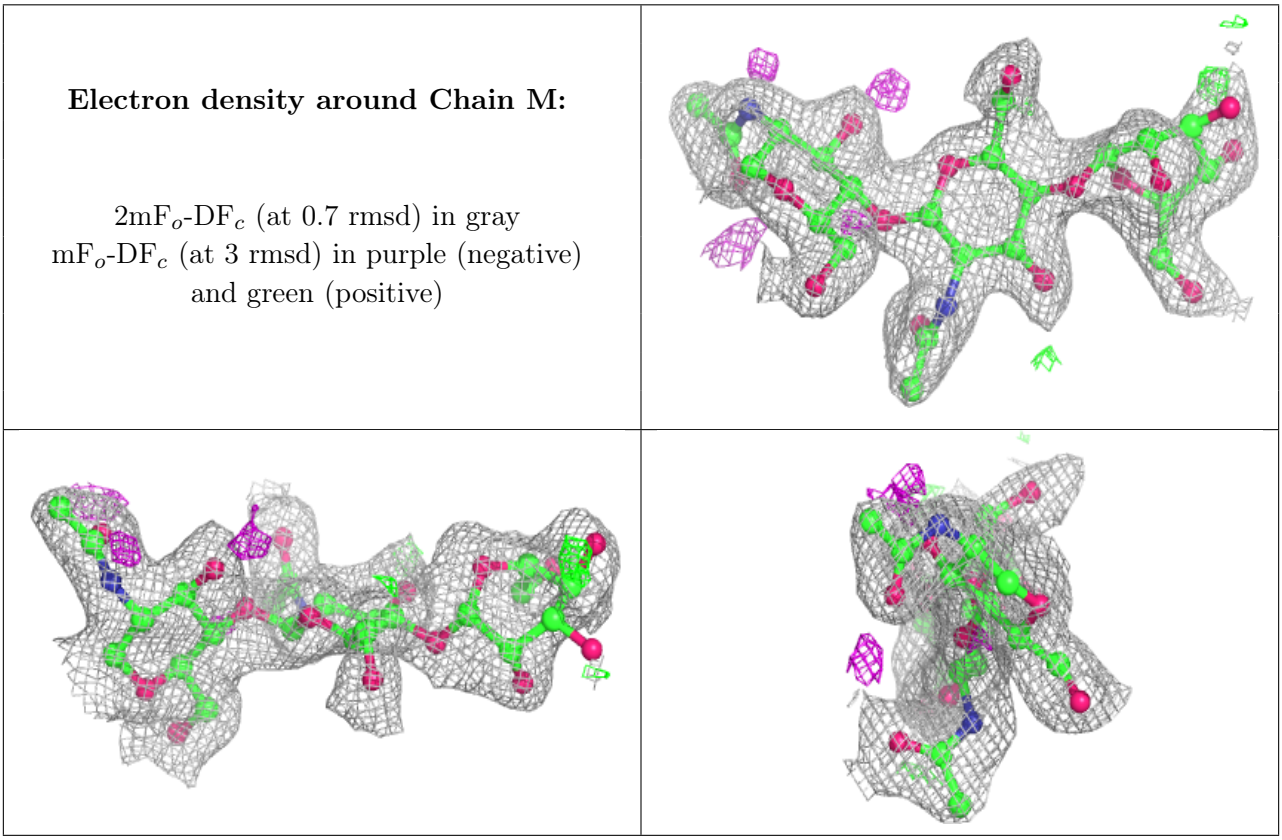
Electron density around Chain G:

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



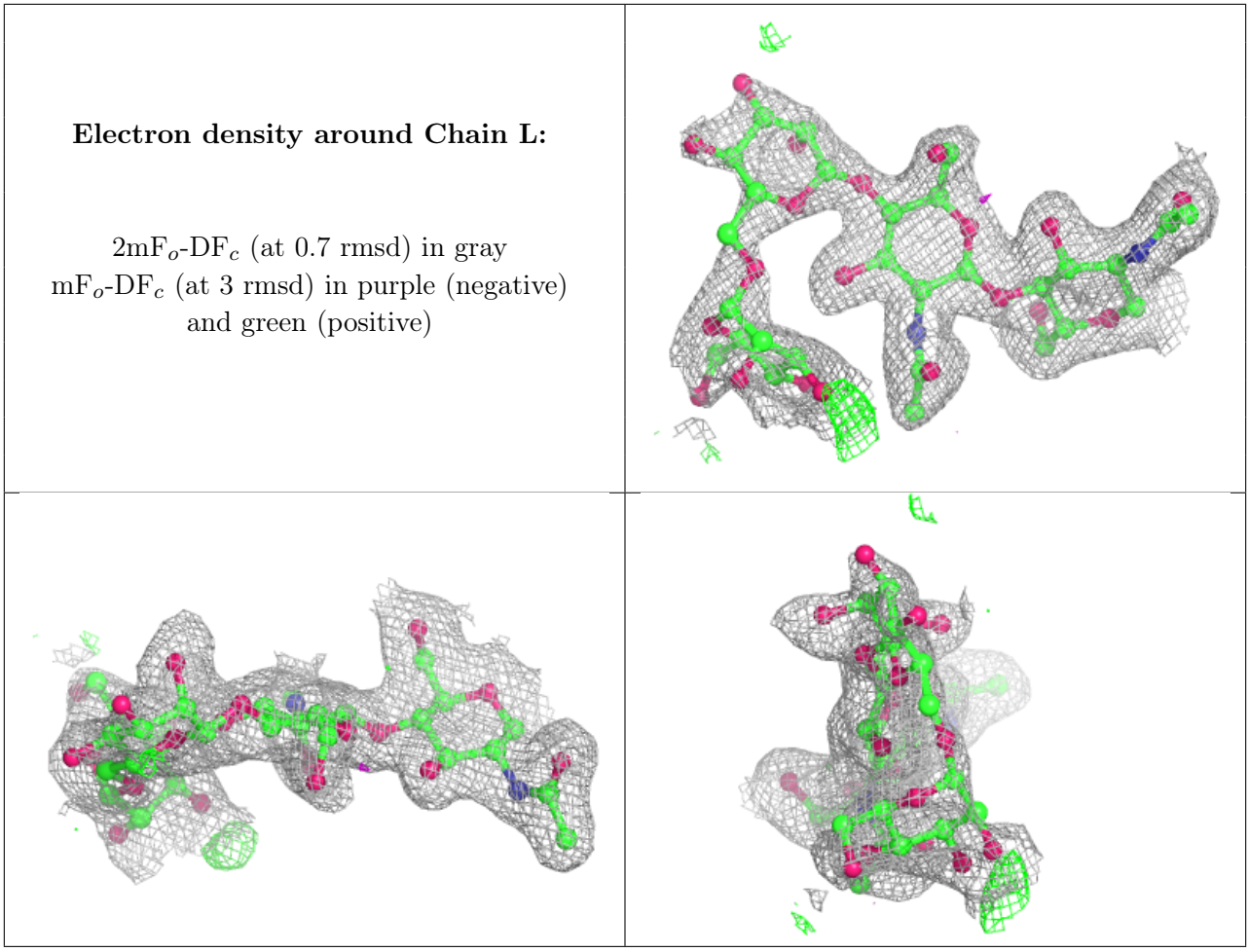
Electron density around Chain M:

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



Electron density around Chain L:

$2mF_o$-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
8	EDO	A	409	4/4	0.65	0.19	47,51,54,61	0
8	EDO	C	406	4/4	0.70	0.36	36,42,46,48	0
8	EDO	B	404	4/4	0.79	0.32	46,46,46,50	0
8	EDO	A	406	4/4	0.79	0.20	38,42,52,52	0
9	PEG	B	405	7/7	0.79	0.15	31,36,44,46	7
5	NAG	C	403	14/15	0.81	0.25	56,66,74,76	0
11	MAN	D	404	12/12	0.82	0.23	68,76,80,80	0
9	PEG	D	406	7/7	0.84	0.16	45,47,52,53	0
9	PEG	D	405	7/7	0.84	0.14	51,55,57,64	0
5	NAG	C	401	14/15	0.85	0.16	42,52,58,62	0
8	EDO	C	407	4/4	0.85	0.21	41,48,48,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	C	402	14/15	0.86	0.14	39,53,60,64	0
8	EDO	A	410	4/4	0.88	0.22	36,38,42,48	0
7	BEZ	B	402	9/9	0.88	0.14	31,37,39,40	0
8	EDO	A	407	4/4	0.89	0.17	32,37,41,47	0
5	NAG	A	401	14/15	0.89	0.13	36,44,62,63	0
7	BEZ	C	405	9/9	0.90	0.14	29,34,42,44	0
8	EDO	A	404	4/4	0.91	0.19	36,42,44,50	0
8	EDO	A	411	4/4	0.92	0.14	27,30,35,47	0
8	EDO	A	405	4/4	0.92	0.10	20,27,29,44	0
10	GOL	D	402	6/6	0.93	0.14	39,40,41,43	0
7	BEZ	A	403	9/9	0.93	0.16	24,35,38,39	0
8	EDO	D	403	4/4	0.94	0.09	40,42,44,52	0
8	EDO	A	408	4/4	0.94	0.18	34,35,39,44	0
8	EDO	B	403	4/4	0.95	0.09	30,31,33,50	0
6	CA	B	401	1/1	0.98	0.03	26,26,26,26	0
6	CA	A	402	1/1	0.99	0.03	24,24,24,24	0
6	CA	C	404	1/1	0.99	0.07	26,26,26,26	0
6	CA	D	401	1/1	0.99	0.04	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.