Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 07:18 PM JST

PDB ID	:	7VPP
Title	:	Structures of a deltacoronavirus spike protein bound to porcine and human receptors indicate the risk of virus adaptation to humans
Authors	:	Ji, W.; Xu, Y.; Zhang, S.
Deposited on	:	2021-10-17
Resolution	:	2.69 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 ⓘ 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 ⓘ) were used in the production of this report:

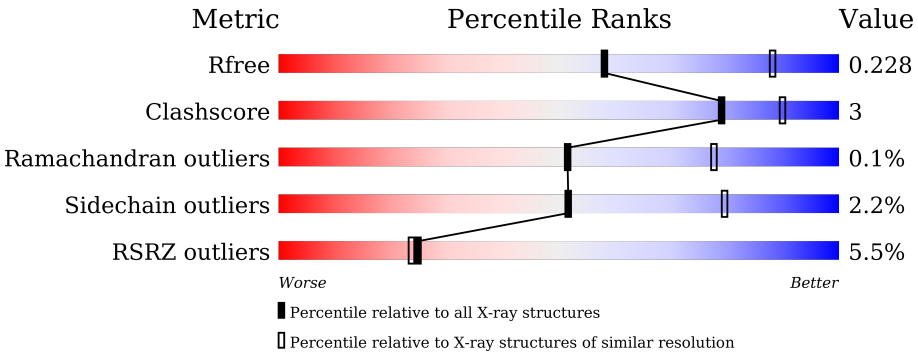
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	911	4% 90% 9%
1	C	911	4% 91% 8%
2	B	127	28% 51% 19% 29%
3	D	2	50% 50%
3	E	2	100%
3	F	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	G	2	100%
3	H	2	50% 50%
3	I	2	100%
3	J	2	100%
3	K	2	50% 50%
3	M	2	50% 50%
4	L	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	G	2	-	-	-	X
3	NAG	M	2	-	-	-	X
7	NAG	B	501	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15615 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 Aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	904	Total	C	N	O	S	0	0	0
			7266	4640	1216	1380	30			
1	C	898	Total	C	N	O	S	0	0	0
			7222	4613	1206	1373	30			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	962	GLY	-	expression tag	UNP K7GMF9
A	963	HIS	-	expression tag	UNP K7GMF9
A	964	HIS	-	expression tag	UNP K7GMF9
A	965	HIS	-	expression tag	UNP K7GMF9
A	966	HIS	-	expression tag	UNP K7GMF9
A	967	HIS	-	expression tag	UNP K7GMF9
A	968	HIS	-	expression tag	UNP K7GMF9
C	962	GLY	-	expression tag	UNP K7GMF9
C	963	HIS	-	expression tag	UNP K7GMF9
C	964	HIS	-	expression tag	UNP K7GMF9
C	965	HIS	-	expression tag	UNP K7GMF9
C	966	HIS	-	expression tag	UNP K7GMF9
C	967	HIS	-	expression tag	UNP K7GMF9
C	968	HIS	-	expression tag	UNP K7GMF9

- Molecule 2 is a protein called Spike protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	90	Total	C	N	O	S	0	0	0
			710	444	119	139	8			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	420	GLY	-	expression tag	UNP A0A4P8D758
B	421	HIS	-	expression tag	UNP A0A4P8D758
B	422	HIS	-	expression tag	UNP A0A4P8D758
B	423	HIS	-	expression tag	UNP A0A4P8D758
B	424	HIS	-	expression tag	UNP A0A4P8D758
B	425	HIS	-	expression tag	UNP A0A4P8D758
B	426	HIS	-	expression tag	UNP A0A4P8D758

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	2	Total C N O 28 16 2 10	0	0	0
3	E	2	Total C N O 28 16 2 10	0	0	0
3	F	2	Total C N O 28 16 2 10	0	0	0
3	G	2	Total C N O 28 16 2 10	0	0	0
3	H	2	Total C N O 28 16 2 10	0	0	0
3	I	2	Total C N O 28 16 2 10	0	0	0
3	J	2	Total C N O 28 16 2 10	0	0	0
3	K	2	Total C N O 28 16 2 10	0	0	0
3	M	2	Total C N O 28 16 2 10	0	0	0

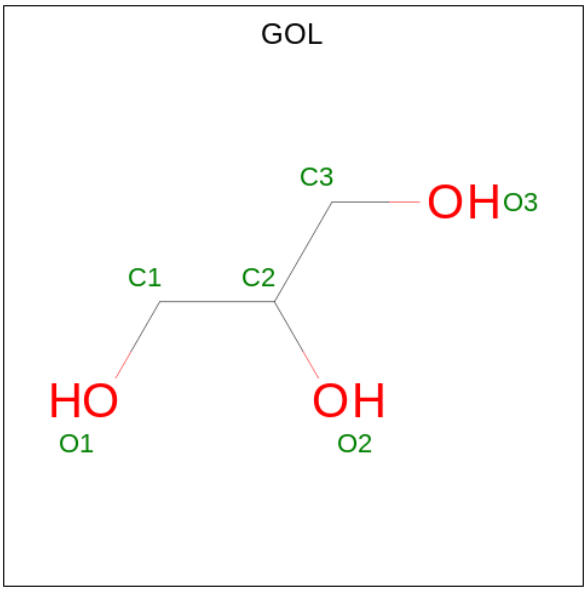
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

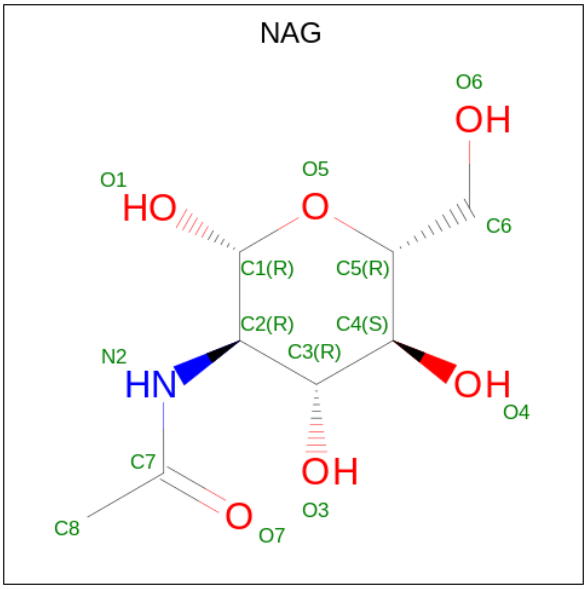
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	C	1	Total Zn 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is water.

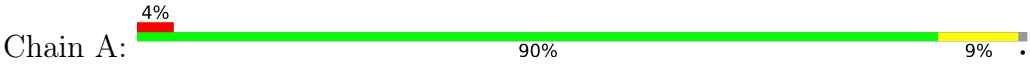
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	18	Total O 18 18	0	0
8	C	17	Total O 17 17	0	0

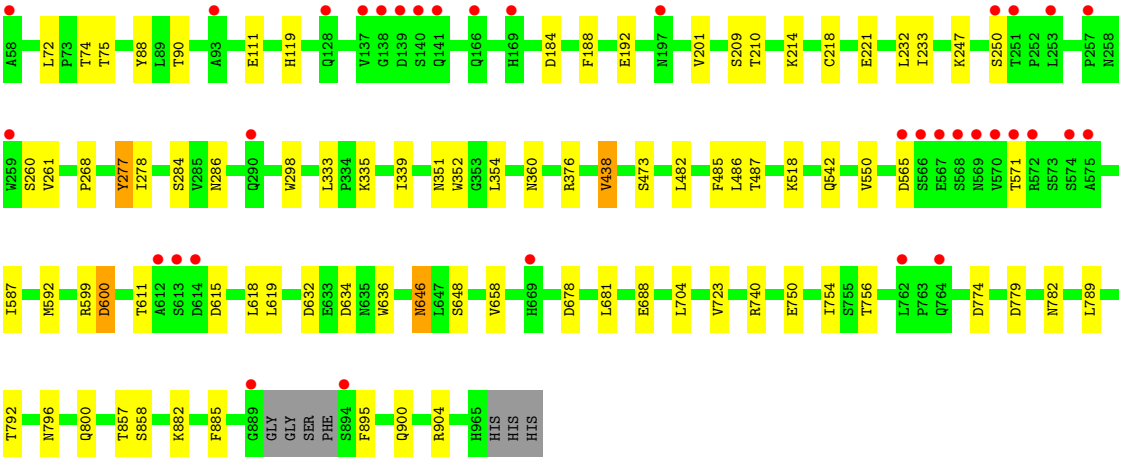
3 Residue-property plots (i)

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: Aminopeptidase

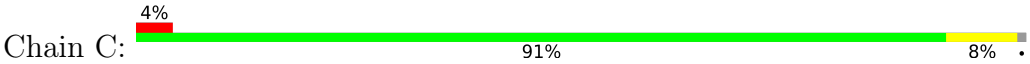
Chain A:

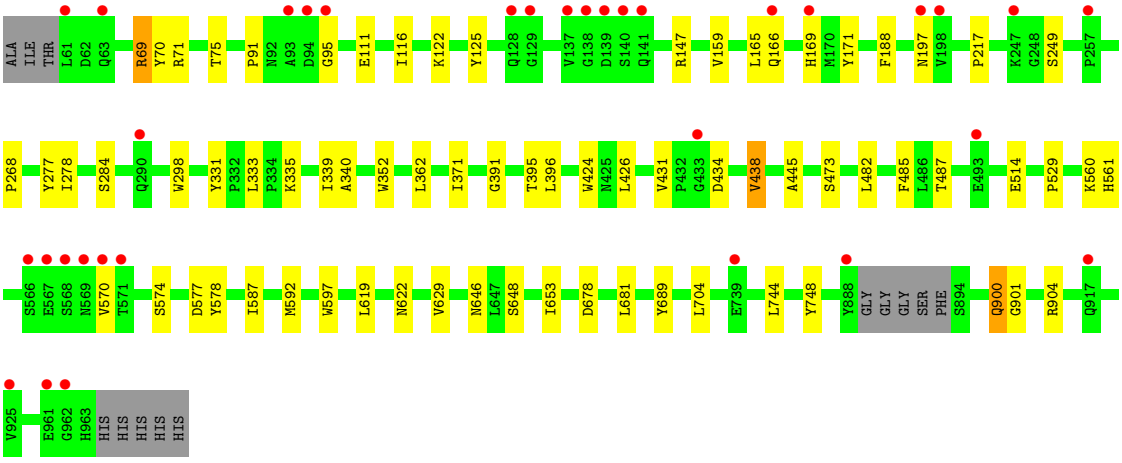




• Molecule 1: Aminopeptidase

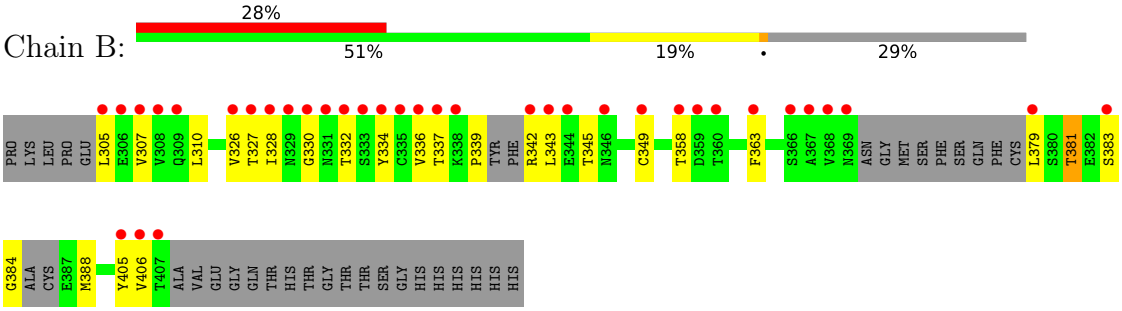
Chain C:





• Molecule 2: Spike protein

Chain B:

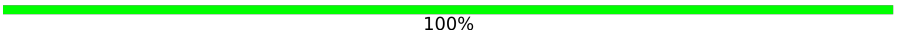


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

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

Chain E:

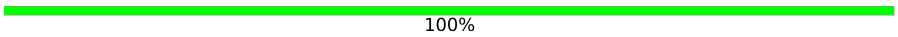


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

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

Chain G:



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

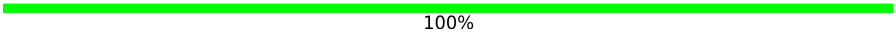
Chain H:

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

Chain I:

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

Chain J:



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

Chain K:

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

Chain M:

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

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	186.64Å 186.64Å 173.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.65 – 2.69 42.65 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.65-2.69) 99.1 (42.65-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.198 , 0.230 0.195 , 0.228	Depositor DCC
R_{free} test set	4278 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	70.5	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15615	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: ZN, GOL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.24	0/7455	0.45	0/10161
1	C	0.24	0/7409	0.45	0/10098
2	B	0.25	0/717	0.53	0/968
All	All	0.24	0/15581	0.46	0/21227

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	7266	0	7026	38	0
1	C	7222	0	6985	35	0
2	B	710	0	695	12	0
3	D	28	0	25	1	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	28	0	25	0	0
3	M	28	0	25	0	0
4	L	28	0	25	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	18	0	24	0	0
6	C	12	0	16	0	0
7	A	28	0	26	0	0
7	B	14	0	13	0	0
7	C	28	0	26	0	0
8	A	18	0	0	0	0
8	C	17	0	0	0	0
All	All	15615	0	15061	85	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 3.

All (85) 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:599:ARG:HG2	1:A:600:ASP:H	1.59	0.67
2:B:328:ILE:HD13	2:B:379:LEU:HB3	1.74	0.67
2:B:307:VAL:HG22	2:B:342:ARG:HD2	1.78	0.65
2:B:305:LEU:N	2:B:334:TYR:HH	1.96	0.63
1:A:611:THR:HB	1:A:615:ASP:HB2	1.83	0.61
2:B:310:LEU:HD23	2:B:345:THR:HG22	1.83	0.60
1:A:268:PRO:HG3	1:A:333:LEU:HD21	1.84	0.59
1:C:901:GLY:HA2	1:C:904:ARG:HD2	1.85	0.58
1:A:885:PHE:HA	1:A:895:PHE:CZ	2.39	0.58
1:C:704:LEU:HD13	1:C:904:ARG:HB3	1.87	0.57
1:A:882:LYS:HD2	1:A:882:LYS:H	1.70	0.57
1:A:796:ASN:OD1	1:A:800:GLN:NE2	2.34	0.56
1:A:636:TRP:HZ3	1:A:658:VAL:HG13	1.71	0.56
1:C:438:VAL:HG13	1:C:473:SER:HB2	1.86	0.56
1:A:740:ARG:NH1	1:A:750:GLU:OE2	2.38	0.56
1:A:779:ASP:OD2	1:A:782:ASN:HB2	2.06	0.56
1:C:278:ILE:HD13	1:C:339:ILE:HD13	1.89	0.55
1:C:166:GLN:HB2	1:C:169:HIS:ND1	2.20	0.55
2:B:327:THR:HB	2:B:330:GLY:HA2	1.89	0.55
1:A:247:LYS:NZ	3:D:1:NAG:O6	2.41	0.53
1:C:900:GLN:O	1:C:904:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:VAL:HG13	1:A:473:SER:HB2	1.90	0.53
1:A:209:SER:OG	1:A:210:THR:N	2.41	0.52
1:C:622:ASN:OD1	1:C:653:ILE:HB	2.09	0.52
1:C:116:ILE:HB	1:C:159:VAL:HB	1.92	0.52
1:C:69:ARG:HD3	1:C:71:ARG:H	1.75	0.52
1:A:646:ASN:O	1:A:648:SER:N	2.42	0.52
1:A:704:LEU:HD13	1:A:904:ARG:HB3	1.93	0.51
1:C:284:SER:HB3	1:C:298:TRP:CD2	2.46	0.51
1:C:529:PRO:HG3	1:C:597:TRP:CD2	2.45	0.51
1:A:360:ASN:OD1	1:A:376:ARG:NH1	2.42	0.51
1:C:587:ILE:HG22	1:C:592:MET:HA	1.93	0.50
1:A:250:SER:HB3	1:A:260:SER:OG	2.11	0.49
1:C:69:ARG:HD3	1:C:70:TYR:N	2.27	0.49
1:A:351:ASN:HB2	1:A:354:LEU:O	2.13	0.49
1:C:445:ALA:HB1	1:C:570:VAL:HA	1.95	0.48
1:A:885:PHE:HA	1:A:895:PHE:HZ	1.78	0.48
1:A:754:ILE:HD12	1:A:789:LEU:HD22	1.97	0.47
1:A:900:GLN:O	1:A:904:ARG:HG3	2.15	0.47
1:C:268:PRO:HG3	1:C:333:LEU:HD21	1.96	0.47
1:A:75:THR:HG22	1:A:111:GLU:HB2	1.98	0.46
1:A:284:SER:HB3	1:A:298:TRP:CD2	2.51	0.46
1:C:622:ASN:ND2	4:L:1:NAG:O7	2.49	0.46
1:A:232:LEU:HD11	1:A:277:TYR:HB2	1.98	0.45
1:A:754:ILE:HG22	1:A:792:THR:HG21	1.98	0.45
1:C:561:HIS:HB2	1:C:578:TYR:HB3	1.98	0.45
2:B:337:THR:O	2:B:339:PRO:HD3	2.17	0.45
1:A:550:VAL:HG21	1:A:619:LEU:HD11	1.98	0.45
1:A:72:LEU:HD12	1:A:221:GLU:HG3	1.98	0.44
1:C:482:LEU:HA	1:C:485:PHE:CE2	2.53	0.44
1:C:434:ASP:O	1:C:438:VAL:HG22	2.17	0.44
1:C:340:ALA:HB2	1:C:362:LEU:HD23	1.99	0.44
1:A:119:HIS:HB2	1:A:218:CYS:O	2.18	0.43
1:A:192:GLU:HG2	1:A:201:VAL:HG22	2.00	0.43
1:C:75:THR:HG22	1:C:111:GLU:HB2	2.00	0.43
1:A:678:ASP:HA	1:A:681:LEU:HG	2.00	0.43
1:A:88:TYR:O	1:A:90:THR:N	2.52	0.43
1:A:184:ASP:OD2	1:A:214:LYS:NZ	2.51	0.43
1:C:125:TYR:OH	1:C:217:PRO:HG3	2.18	0.43
2:B:383:SER:OG	2:B:384:GLY:N	2.49	0.43
1:C:391:GLY:O	1:C:395:THR:HG22	2.19	0.43
1:C:424:TRP:CD2	1:C:744:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ILE:HD13	1:A:339:ILE:HD13	2.00	0.43
1:C:165:LEU:HD22	1:C:171:TYR:CZ	2.54	0.42
1:A:587:ILE:HG22	1:A:592:MET:HA	2.00	0.42
1:C:619:LEU:HB2	1:C:629:VAL:HG11	2.01	0.42
1:C:678:ASP:HA	1:C:681:LEU:HG	2.01	0.42
1:A:233:ILE:HG12	1:A:261:VAL:HG22	2.01	0.42
2:B:358:THR:HG22	2:B:388:MET:HG2	2.01	0.42
2:B:383:SER:HB3	2:B:405:TYR:HB2	2.00	0.42
1:C:560:LYS:HD3	1:C:561:HIS:N	2.35	0.42
2:B:336:VAL:O	2:B:337:THR:OG1	2.29	0.42
1:C:574:SER:HB2	1:C:578:TYR:CZ	2.55	0.41
1:C:91:PRO:HB2	1:C:95:GLY:HA2	2.01	0.41
1:C:331:TYR:CE2	1:C:333:LEU:HB2	2.55	0.41
1:A:518:LYS:HA	1:A:518:LYS:HD2	1.81	0.41
1:C:689:TYR:CD1	1:C:748:TYR:HB3	2.56	0.41
1:C:371:ILE:HD11	1:C:744:LEU:HD12	2.02	0.41
1:A:482:LEU:HA	1:A:485:PHE:CE2	2.56	0.41
1:A:723:VAL:HG21	1:A:756:THR:HB	2.03	0.41
2:B:332:THR:HG23	2:B:381:THR:HG23	2.03	0.41
1:C:646:ASN:OD1	1:C:648:SER:OG	2.35	0.41
1:C:122:LYS:HE2	1:C:122:LYS:HB3	1.87	0.40
1:A:632:ASP:OD2	1:A:634:ASP:HB2	2.21	0.40
2:B:363:PHE:CE2	2:B:406:VAL:HG11	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	900/911 (99%)	867 (96%)	32 (4%)	1 (0%)	51 78
1	C	894/911 (98%)	854 (96%)	39 (4%)	1 (0%)	51 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	82/127 (65%)	70 (85%)	12 (15%)	0	100 100
All	All	1876/1949 (96%)	1791 (96%)	83 (4%)	2 (0%)	51 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	LEU
1	C	487	THR

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	799/804 (99%)	781 (98%)	18 (2%)	50 78
1	C	795/804 (99%)	780 (98%)	15 (2%)	57 82
2	B	83/114 (73%)	79 (95%)	4 (5%)	25 53
All	All	1677/1722 (97%)	1640 (98%)	37 (2%)	52 79

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	THR
1	A	188	PHE
1	A	277	TYR
1	A	286	ASN
1	A	335	LYS
1	A	352	TRP
1	A	438	VAL
1	A	487	THR
1	A	542	GLN
1	A	565	ASP
1	A	571	THR
1	A	600	ASP
1	A	618	LEU

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Mol	Chain	Res	Type
1	A	646	ASN
1	A	688	GLU
1	A	774	ASP
1	A	857	THR
1	A	858	SER
2	B	326	VAL
2	B	343	LEU
2	B	349	CYS
2	B	381	THR
1	C	69	ARG
1	C	147	ARG
1	C	188	PHE
1	C	197	ASN
1	C	249	SER
1	C	277	TYR
1	C	335	LYS
1	C	352	TRP
1	C	396	LEU
1	C	426	LEU
1	C	431	VAL
1	C	438	VAL
1	C	514	GLU
1	C	577	ASP
1	C	900	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	814	GLN
1	A	921	ASN
1	C	206	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

20 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	D	1	1,3	14,14,15	0.29	0	17,19,21	0.40	0
3	NAG	D	2	3	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	E	1	1,3	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	E	2	3	14,14,15	0.33	0	17,19,21	0.54	0
3	NAG	F	1	1,3	14,14,15	0.42	0	17,19,21	0.75	1 (5%)
3	NAG	F	2	3	14,14,15	0.27	0	17,19,21	0.41	0
3	NAG	G	1	1,3	14,14,15	0.21	0	17,19,21	0.39	0
3	NAG	G	2	3	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	H	1	1,3	14,14,15	1.40	1 (7%)	17,19,21	1.26	2 (11%)
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	0.39	0
3	NAG	I	1	1,3	14,14,15	0.26	0	17,19,21	0.43	0
3	NAG	I	2	3	14,14,15	0.34	0	17,19,21	0.44	0
3	NAG	J	1	1,3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	J	2	3	14,14,15	0.35	0	17,19,21	0.49	0
3	NAG	K	1	1,3	14,14,15	0.40	0	17,19,21	0.72	1 (5%)
3	NAG	K	2	3	14,14,15	0.31	0	17,19,21	0.41	0
4	NAG	L	1	1,4	14,14,15	1.07	2 (14%)	17,19,21	0.89	0
4	NAG	L	2	4	14,14,15	0.62	0	17,19,21	0.35	0
3	NAG	M	1	1,3	14,14,15	0.61	1 (7%)	17,19,21	0.66	0
3	NAG	M	2	3	14,14,15	0.51	0	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
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	-5.07	1.35	1.43
4	L	1	NAG	C1-C2	2.72	1.56	1.52
4	L	1	NAG	O5-C1	-2.61	1.39	1.43
3	M	1	NAG	O5-C1	-2.16	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	NAG	C3-C4-C5	3.53	116.54	110.24
3	F	1	NAG	C1-O5-C5	2.56	115.67	112.19
3	K	1	NAG	C1-O5-C5	2.48	115.55	112.19
3	H	1	NAG	C4-C3-C2	2.35	114.46	111.02

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	2	NAG	C1-C2-N2-C7
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6

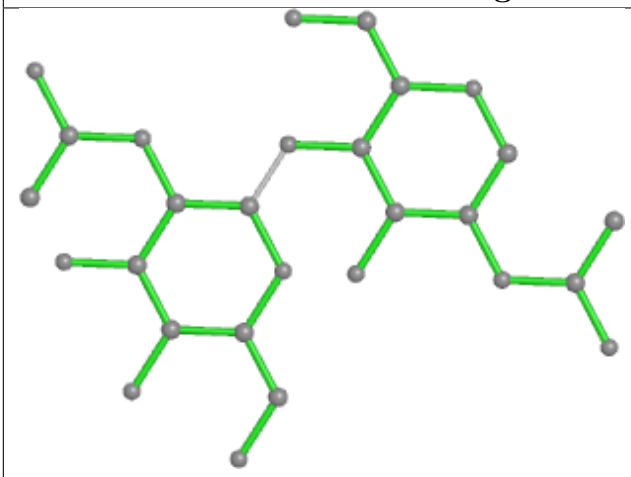
There are no ring outliers.

2 monomers are involved in 2 short contacts:

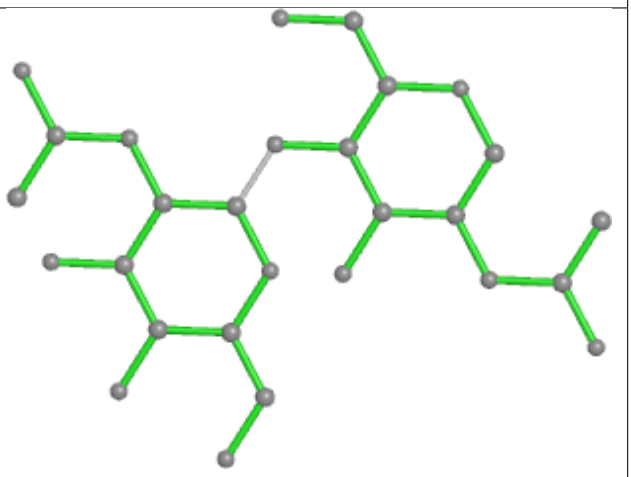
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1	NAG	1	0
3	D	1	NAG	1	0

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

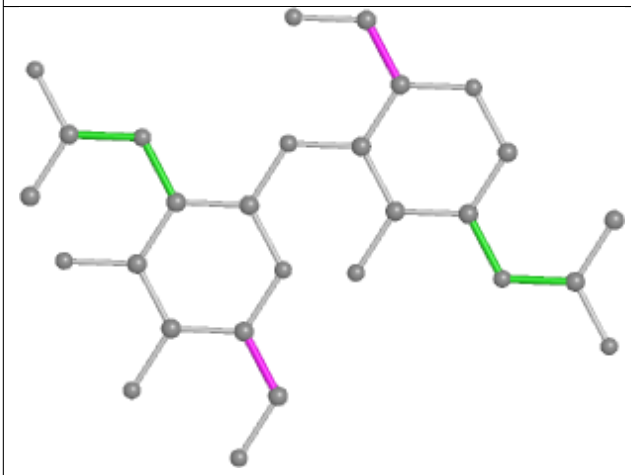
Oligosaccharide Chain D



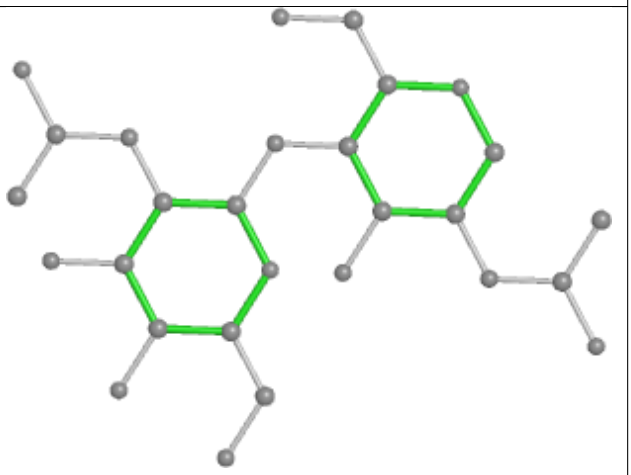
Bond lengths



Bond angles

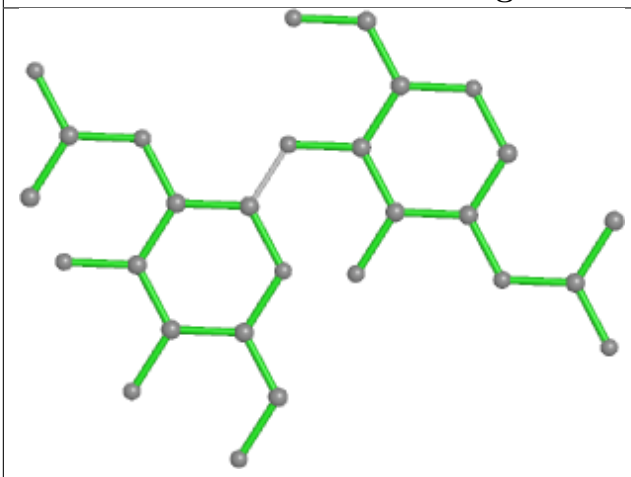


Torsions

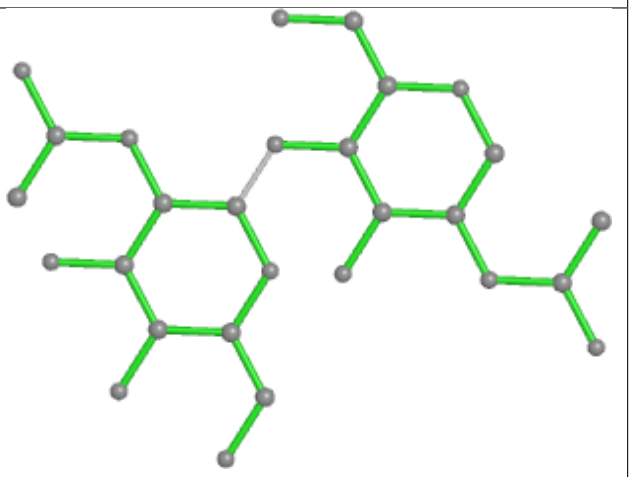


Rings

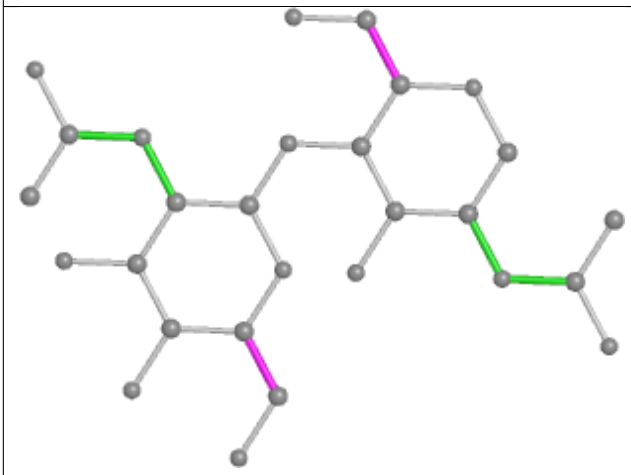
Oligosaccharide Chain E



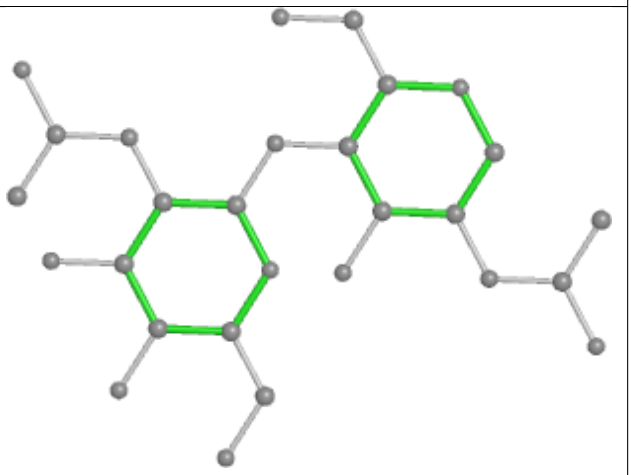
Bond lengths



Bond angles

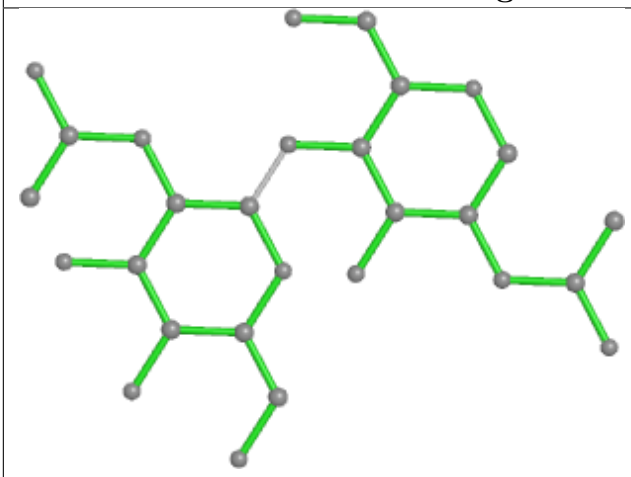


Torsions

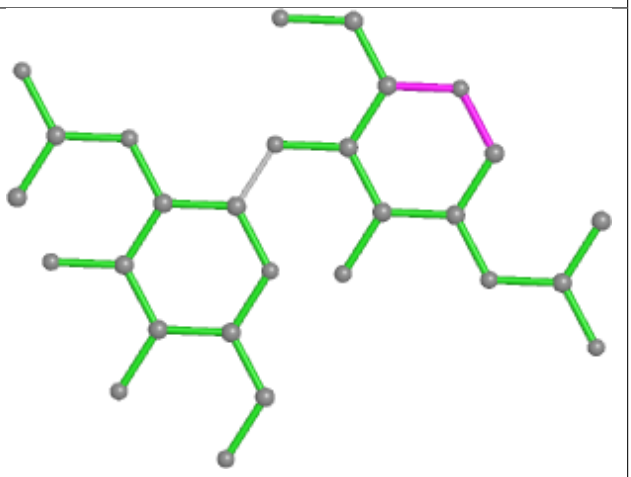


Rings

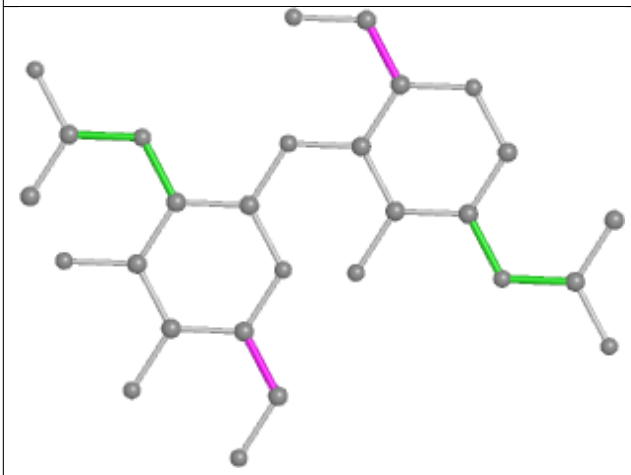
Oligosaccharide Chain F



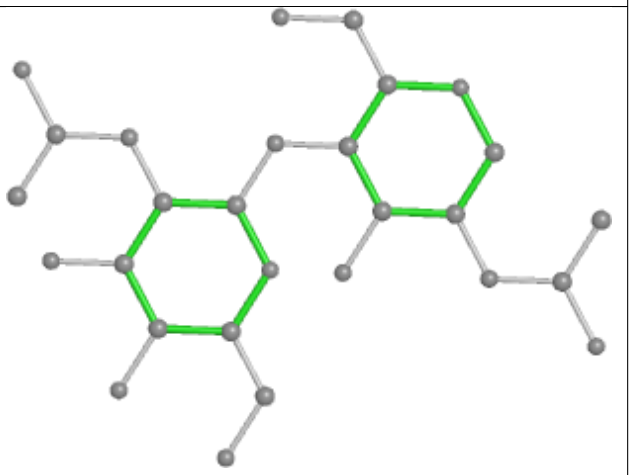
Bond lengths



Bond angles

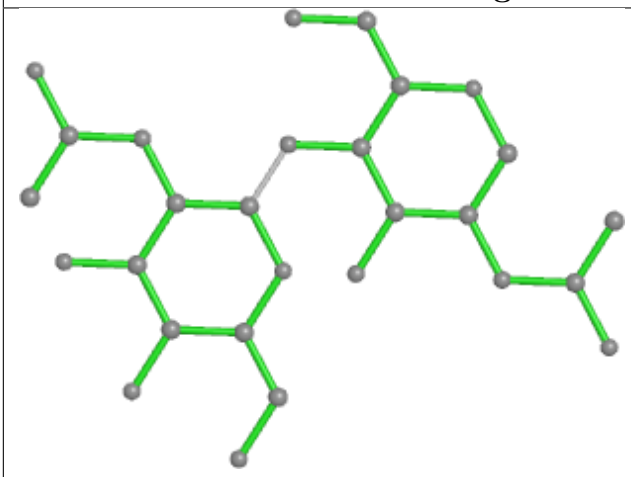


Torsions

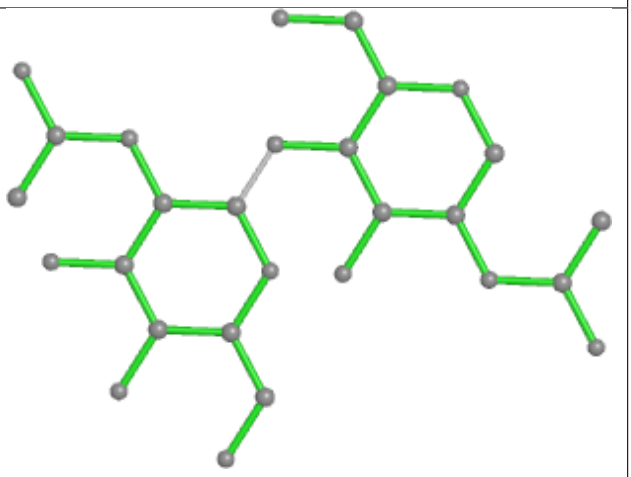


Rings

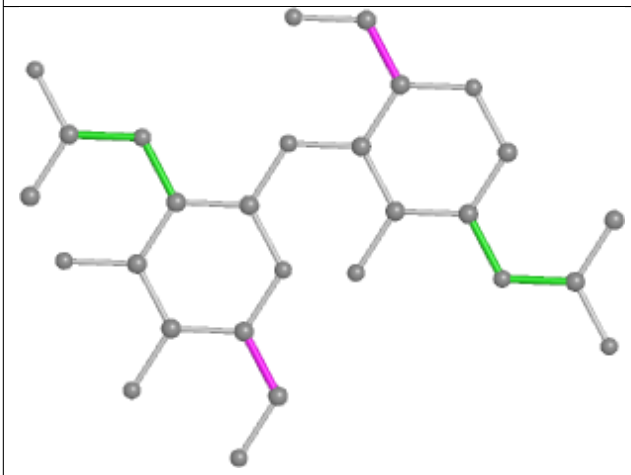
Oligosaccharide Chain G



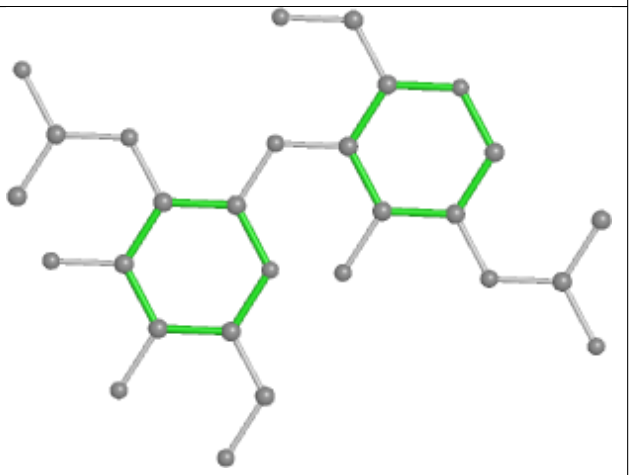
Bond lengths



Bond angles

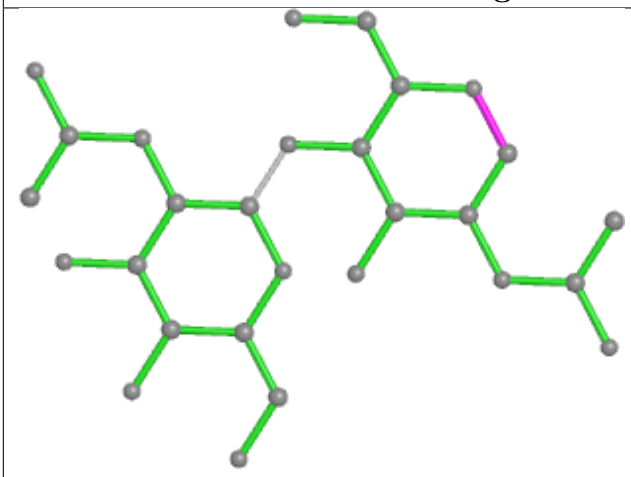


Torsions

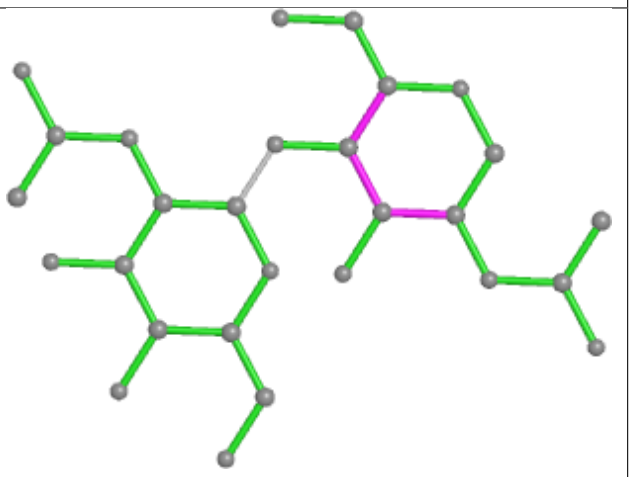


Rings

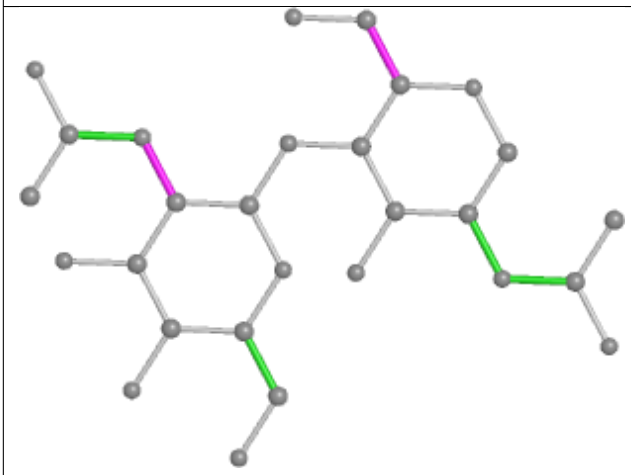
Oligosaccharide Chain H



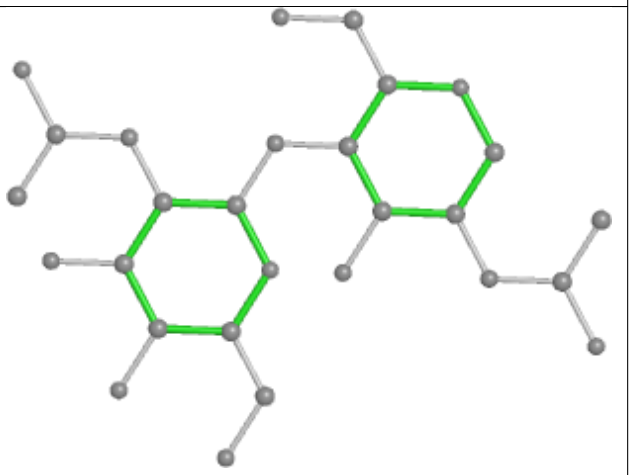
Bond lengths



Bond angles

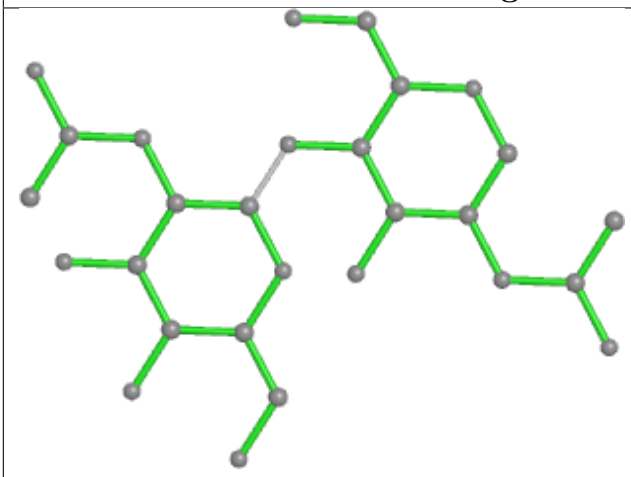


Torsions

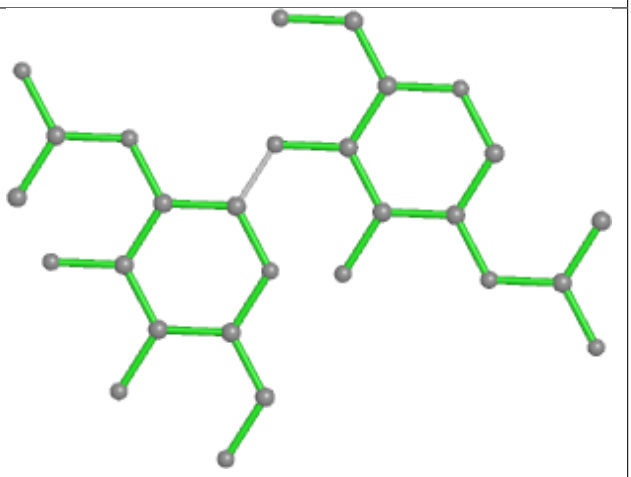


Rings

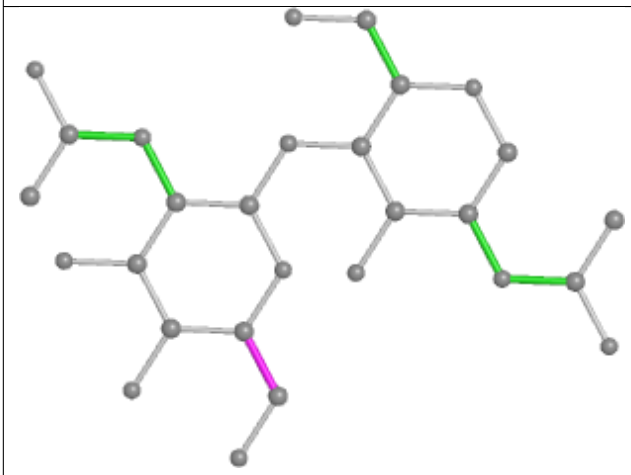
Oligosaccharide Chain I



Bond lengths



Bond angles



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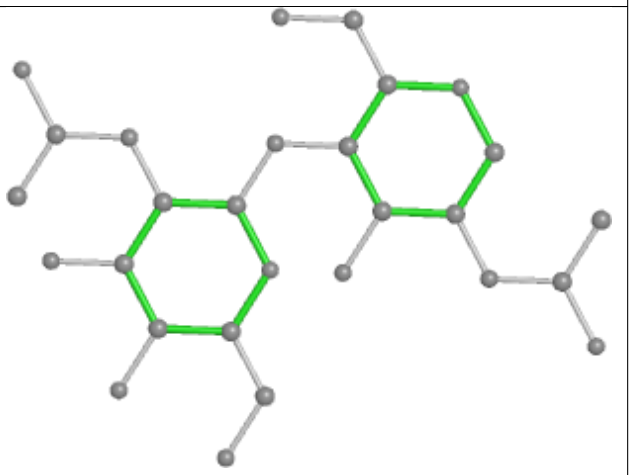
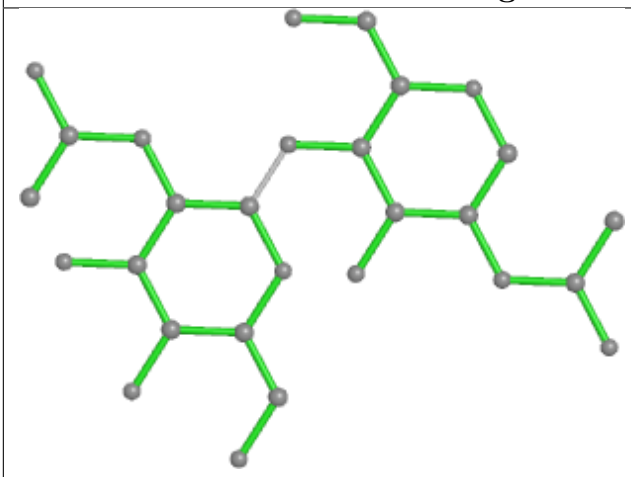
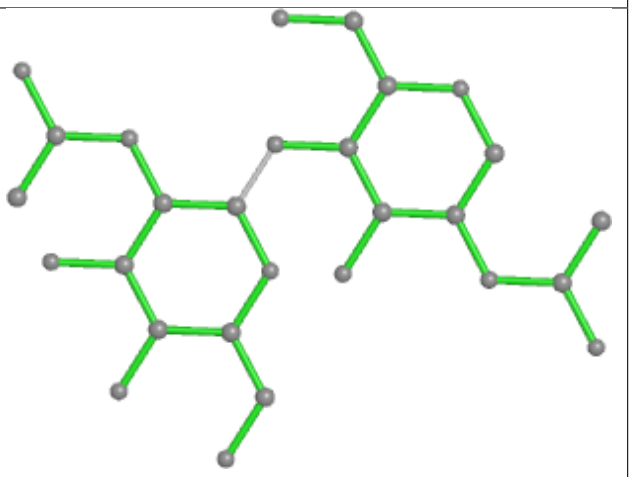


Rings

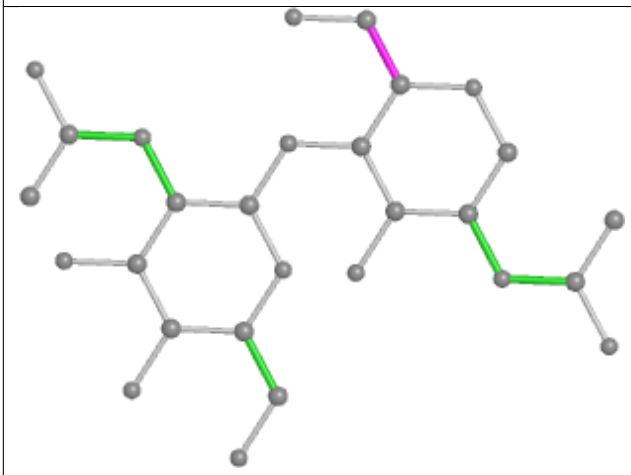
Oligosaccharide Chain J



Bond lengths



Bond angles



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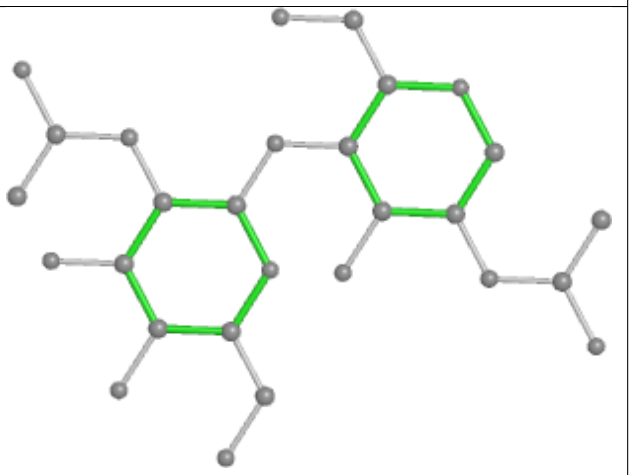
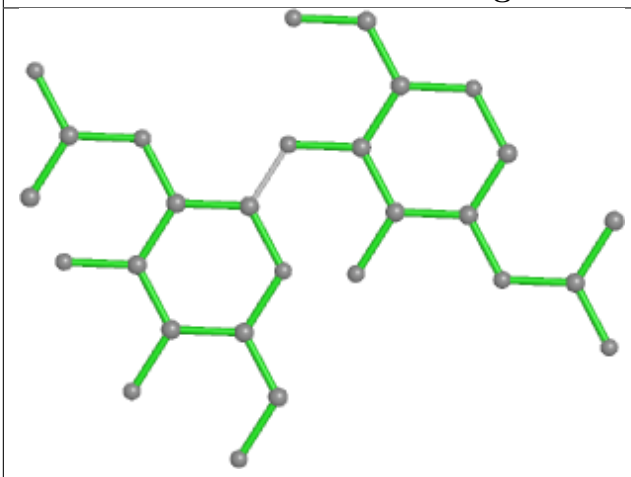


Rings

Oligosaccharide Chain K



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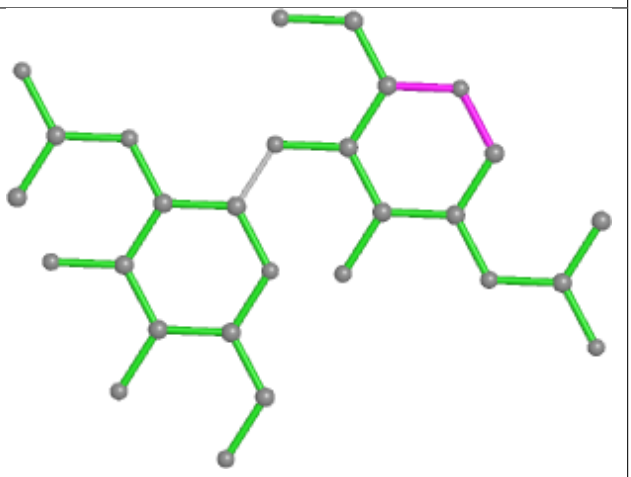
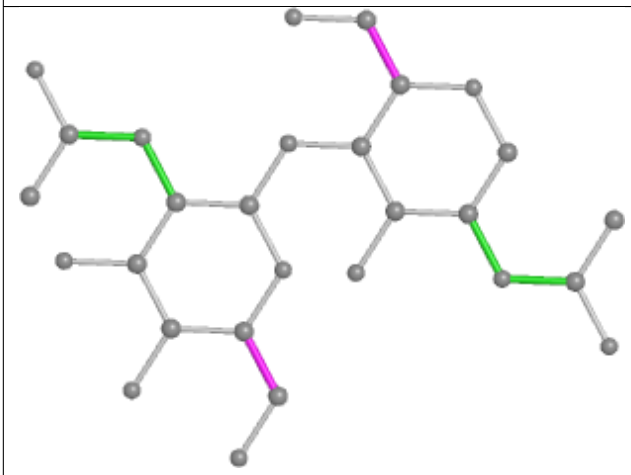


Bond angles



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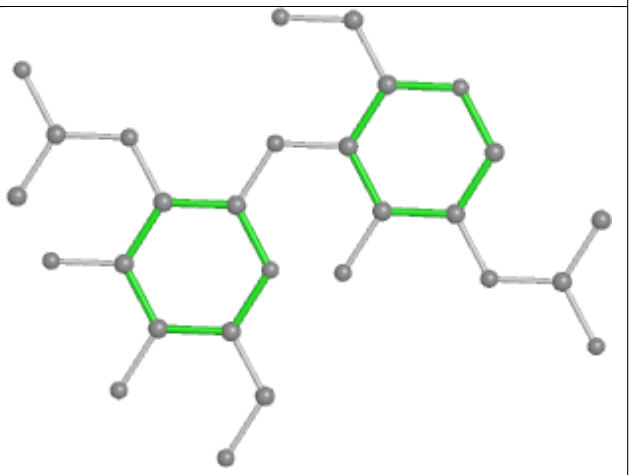
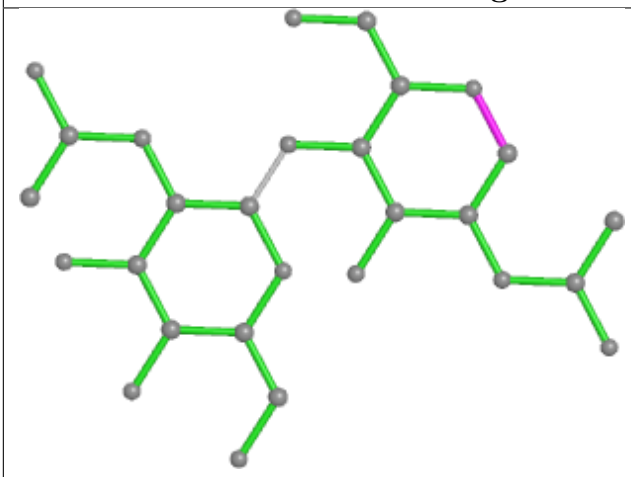
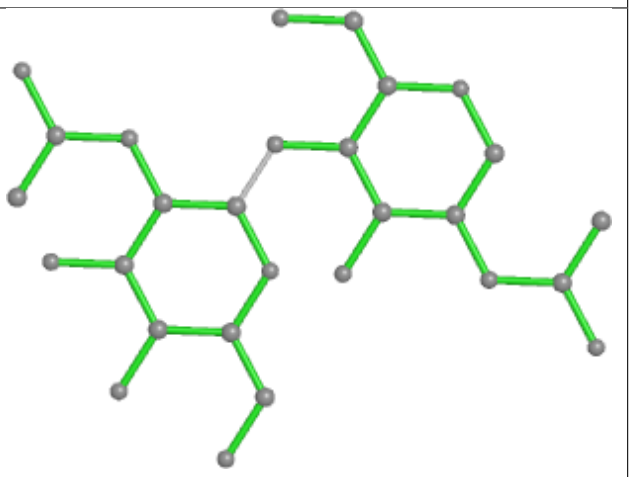


Rings

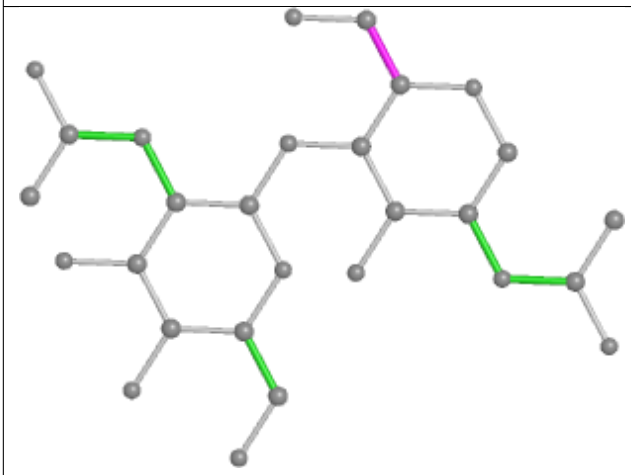
Oligosaccharide Chain M



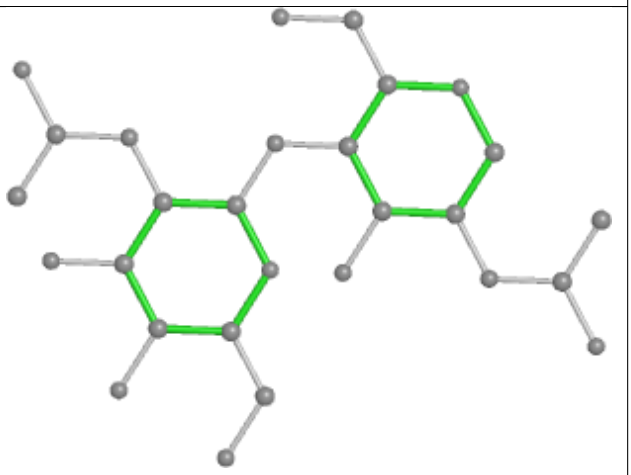
Bond lengths



Bond angles

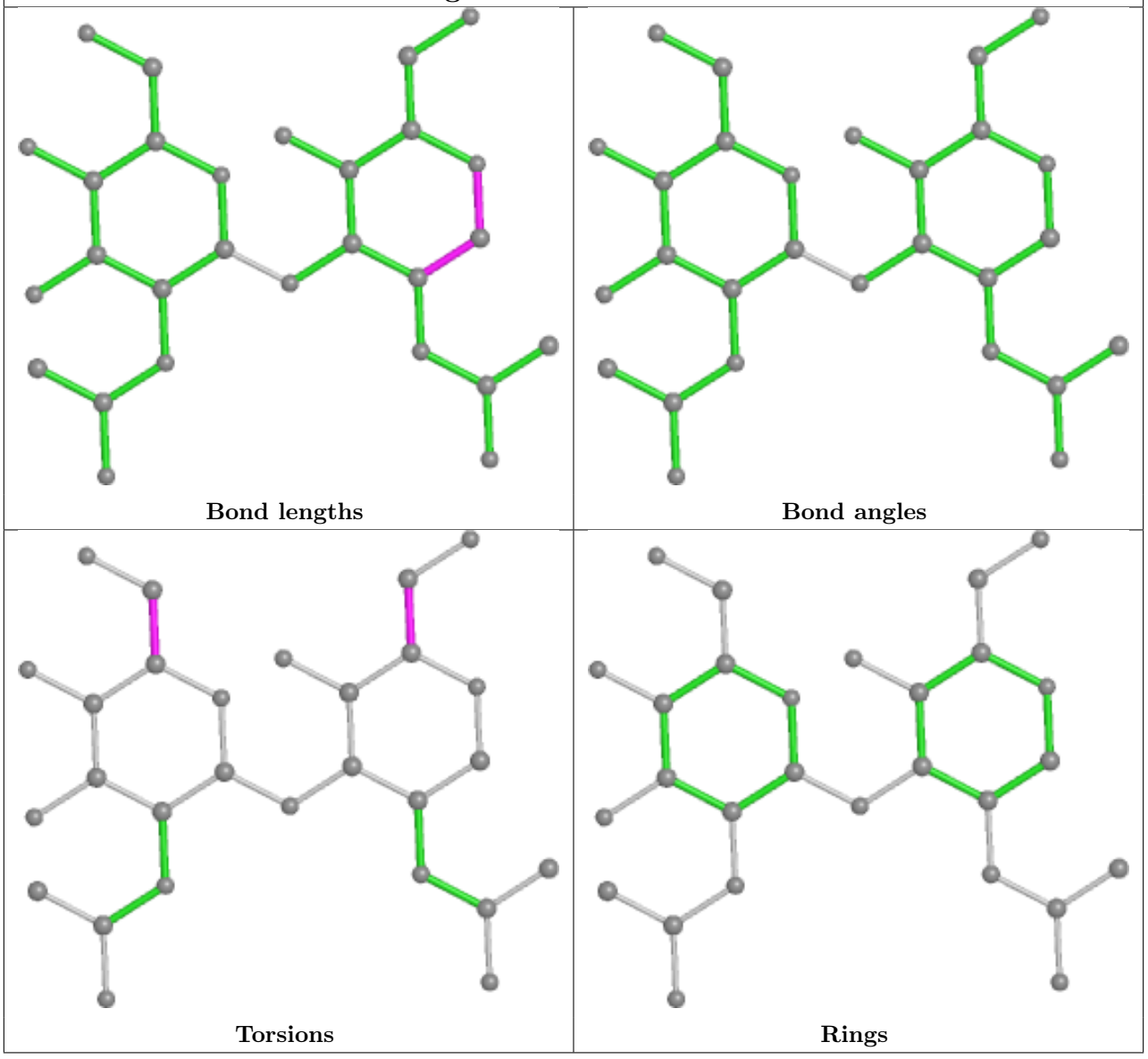


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\#\|Z\|>2$
6	GOL	A	1004	-	5,5,5	0.95	0	5,5,5	0.98	0
7	NAG	C	1005	1	14,14,15	0.37	0	17,19,21	0.60	1 (5%)
6	GOL	C	1003	-	5,5,5	0.91	0	5,5,5	1.01	0
7	NAG	A	1005	1	14,14,15	0.37	0	17,19,21	0.50	0
7	NAG	B	501	2	14,14,15	0.49	0	17,19,21	0.59	0
7	NAG	A	1006	1	14,14,15	0.28	0	17,19,21	0.54	0
6	GOL	A	1003	-	5,5,5	0.91	0	5,5,5	1.00	0
7	NAG	C	1004	1	14,14,15	0.27	0	17,19,21	0.51	0
6	GOL	A	1002	-	5,5,5	1.01	0	5,5,5	0.97	0
6	GOL	C	1002	-	5,5,5	0.91	0	5,5,5	0.95	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
6	GOL	A	1004	-	-	2/4/4/4	-
7	NAG	C	1005	1	-	0/6/23/26	0/1/1/1
6	GOL	C	1003	-	-	2/4/4/4	-
7	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
7	NAG	B	501	2	-	4/6/23/26	0/1/1/1
7	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
6	GOL	A	1003	-	-	0/4/4/4	-
7	NAG	C	1004	1	-	0/6/23/26	0/1/1/1
6	GOL	A	1002	-	-	0/4/4/4	-
6	GOL	C	1002	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1005	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1003	GOL	O1-C1-C2-C3
7	B	501	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

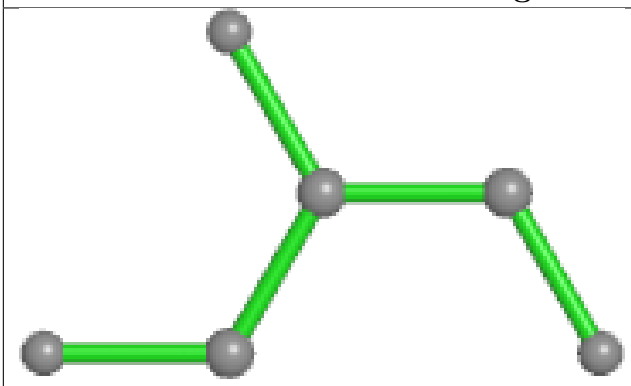
Mol	Chain	Res	Type	Atoms
7	B	501	NAG	O7-C7-N2-C2
7	B	501	NAG	C4-C5-C6-O6
6	A	1004	GOL	O1-C1-C2-C3
7	B	501	NAG	O5-C5-C6-O6
6	C	1002	GOL	O2-C2-C3-O3
6	A	1004	GOL	O1-C1-C2-O2
6	C	1002	GOL	C1-C2-C3-O3
6	C	1003	GOL	O1-C1-C2-O2

There are no ring outliers.

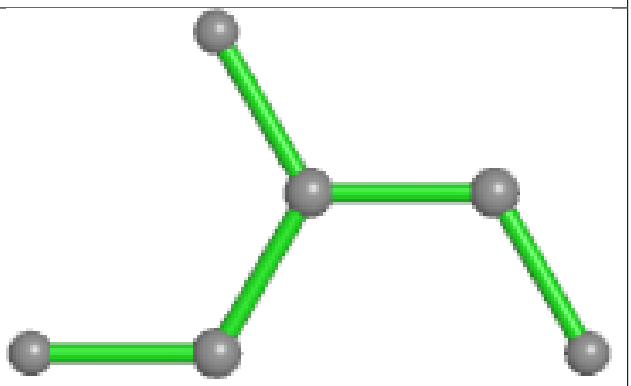
No monomer is involved in short contacts.

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.

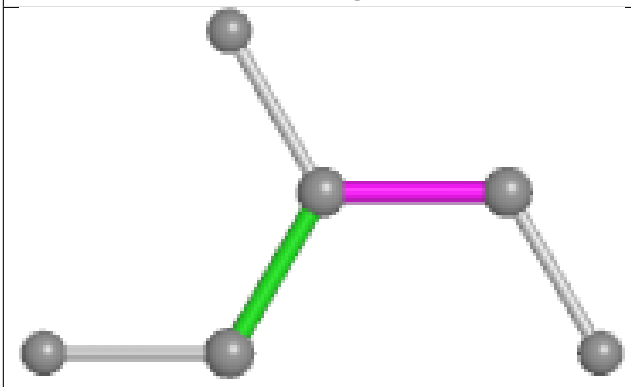
Ligand GOL A 1004



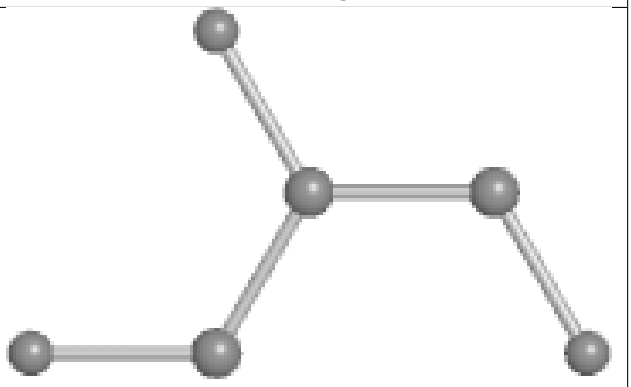
Bond lengths



Bond angles

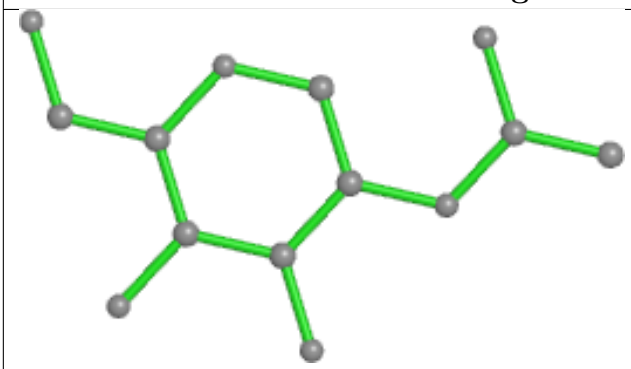


Torsions

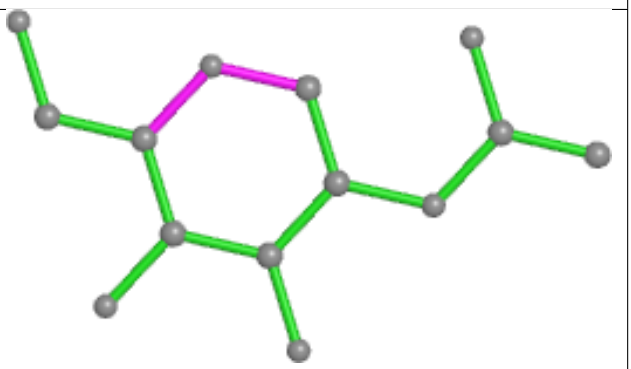


Rings

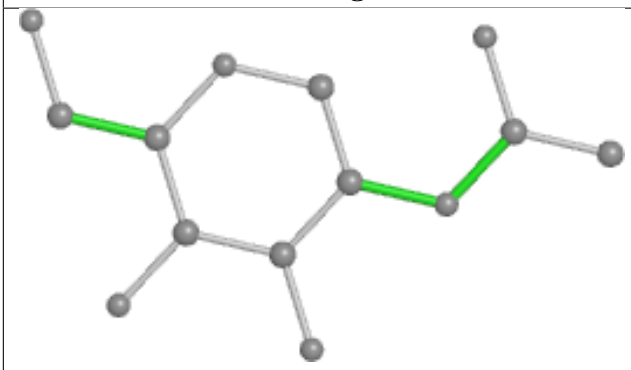
Ligand NAG C 1005



Bond lengths



Bond angles



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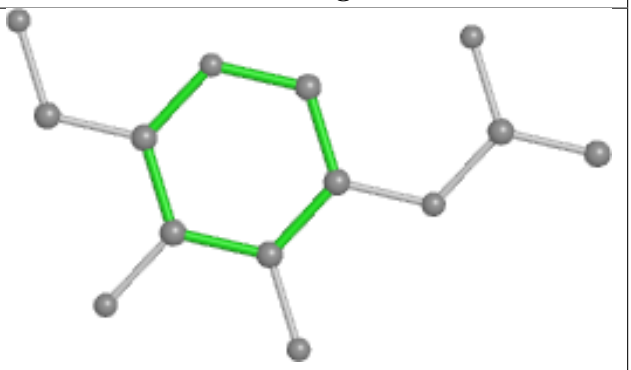
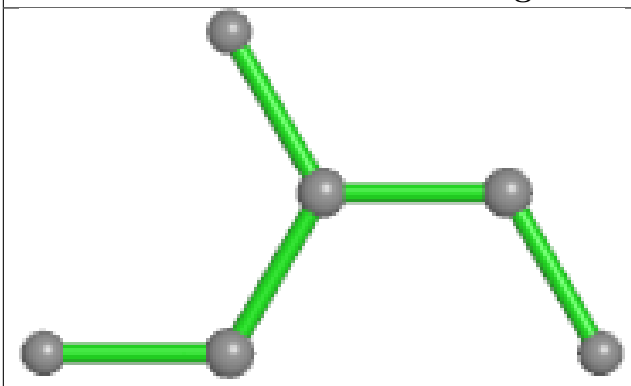
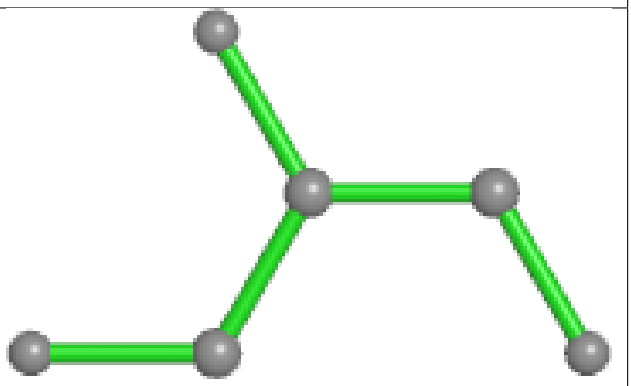


Rings

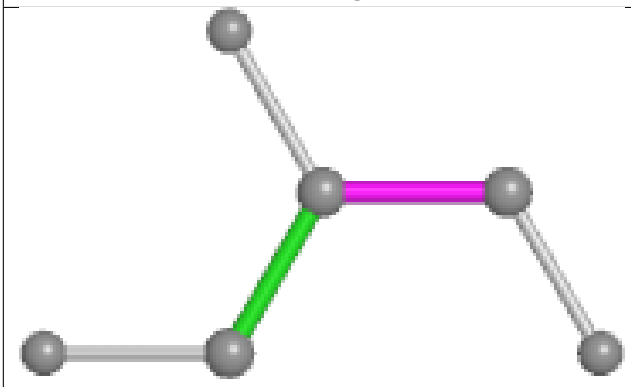
Ligand GOL C 1003



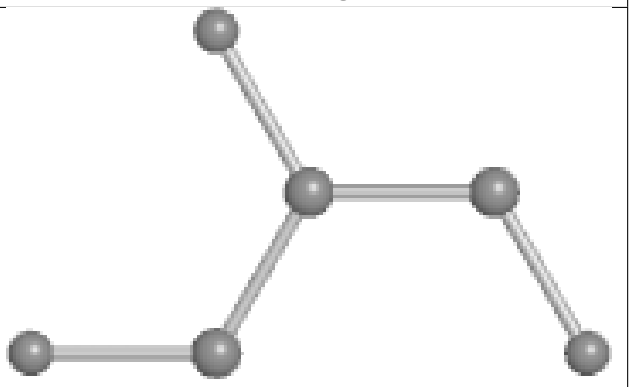
Bond lengths



Bond angles

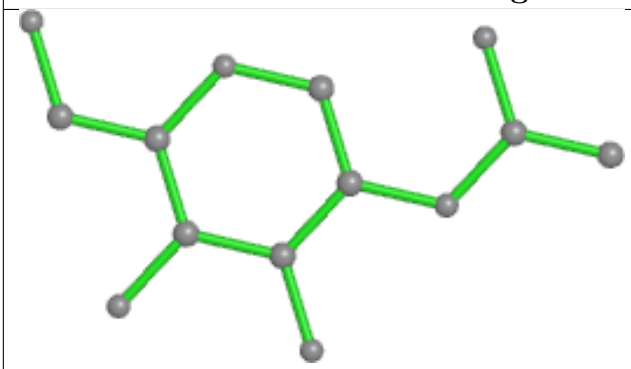


Torsions

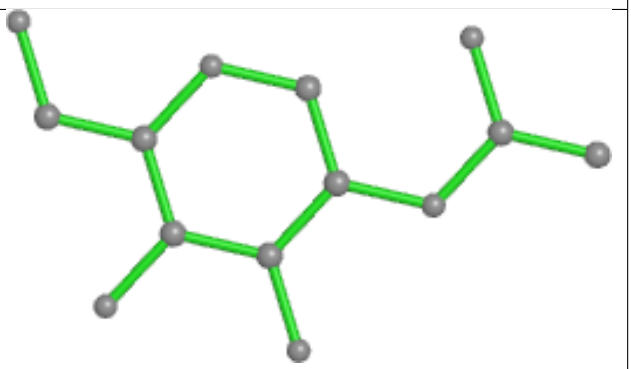


Rings

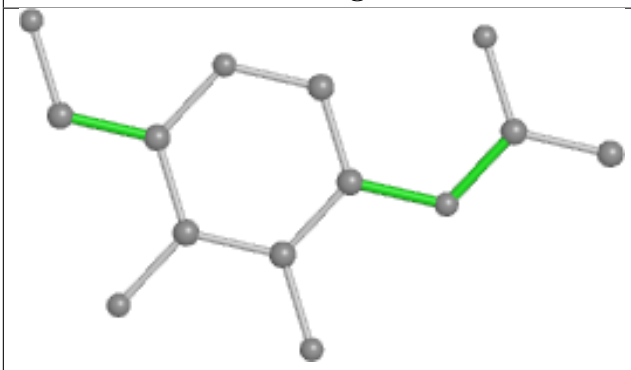
Ligand NAG A 1005



Bond lengths



Bond angles



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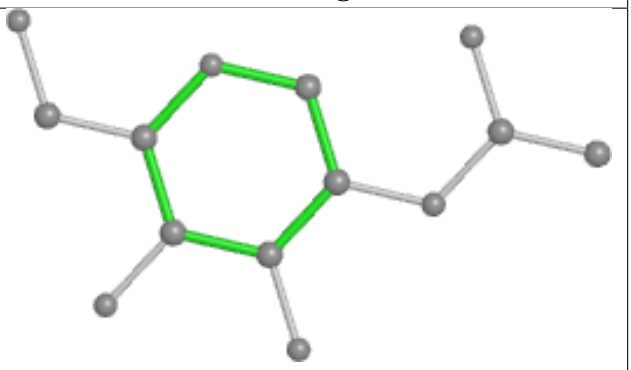
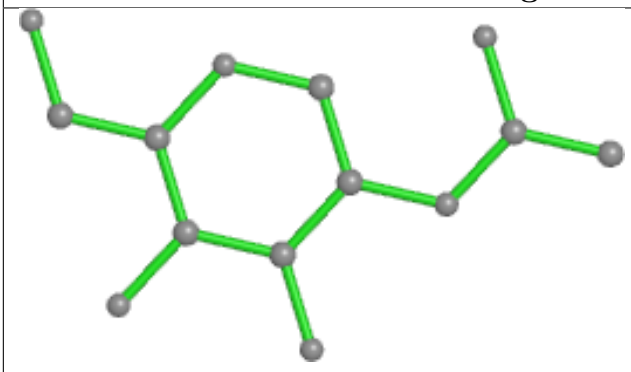
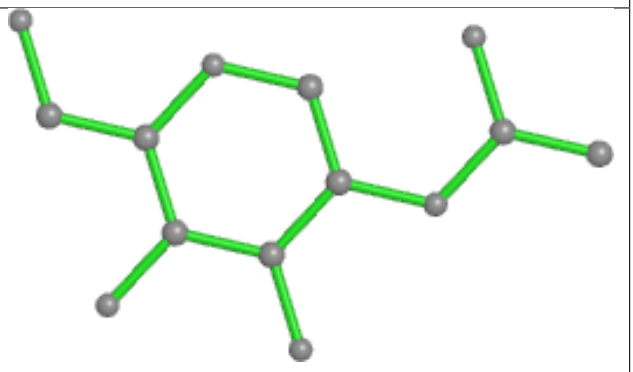


Rings

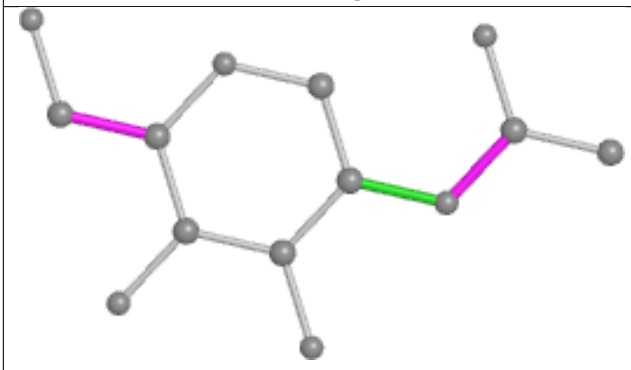
Ligand NAG B 501



Bond lengths



Bond angles



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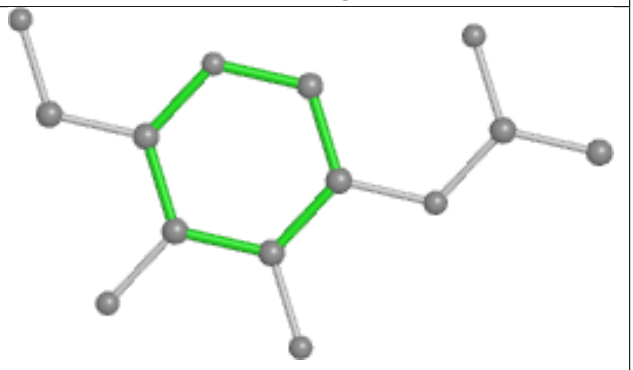
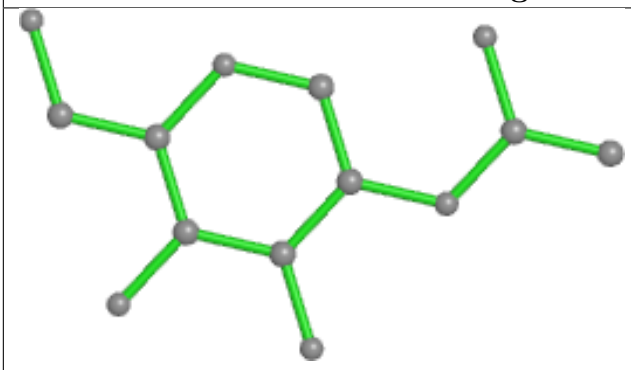
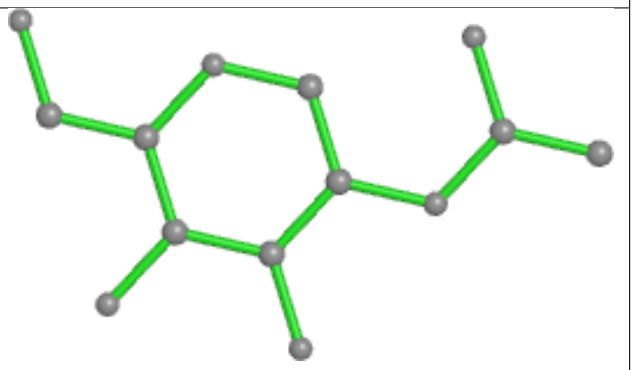


Rings

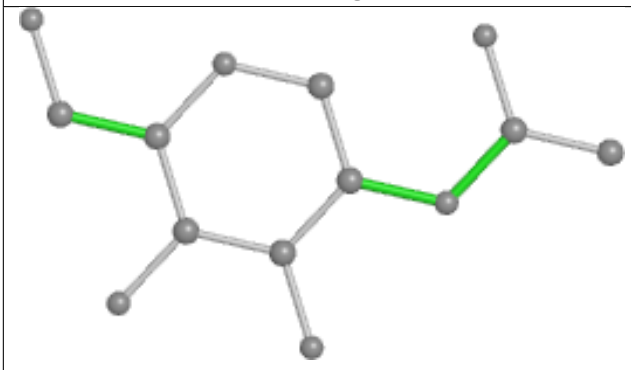
Ligand NAG A 1006



Bond lengths



Bond angles



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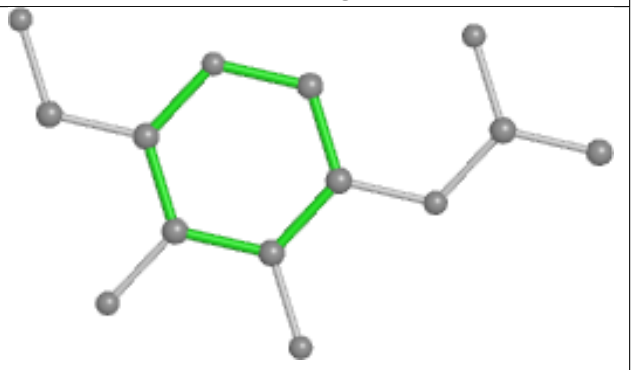
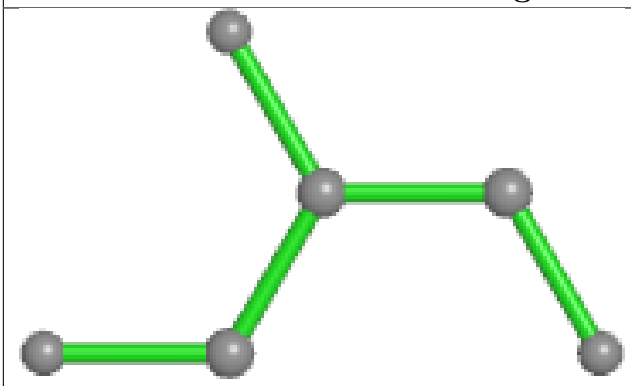
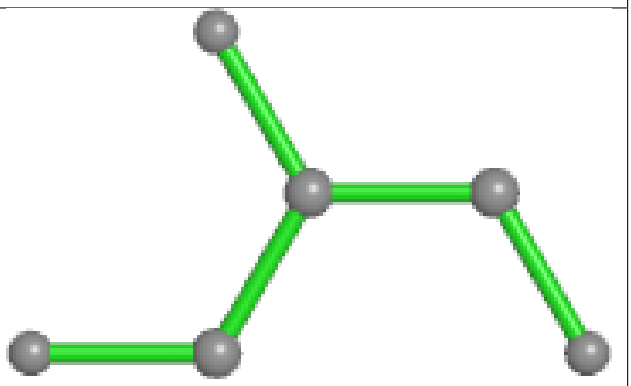


Rings

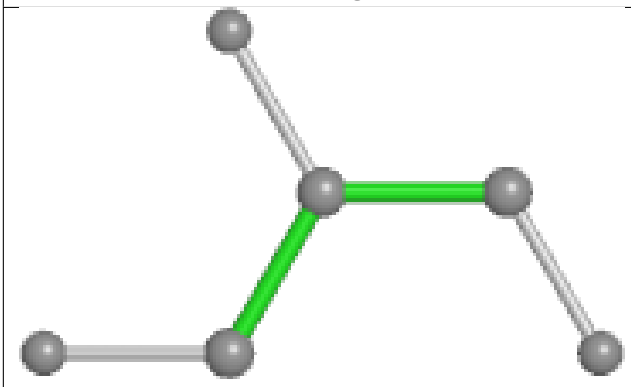
Ligand GOL A 1003



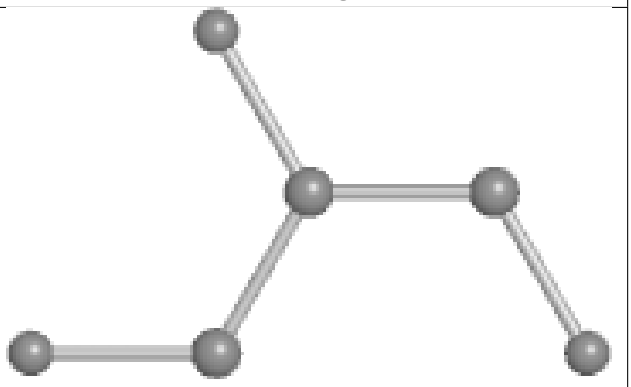
Bond lengths



Bond angles

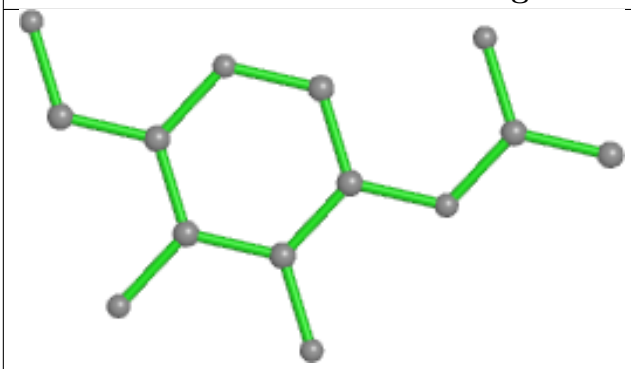


Torsions

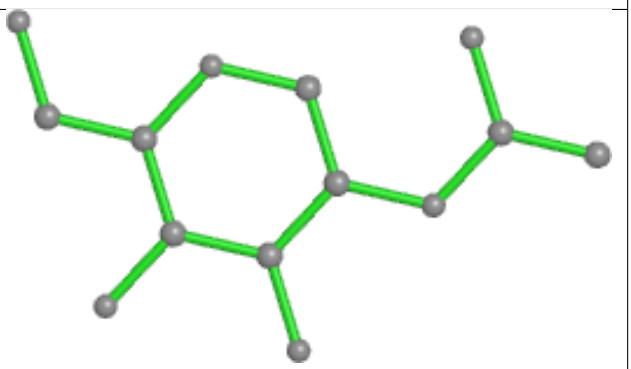


Rings

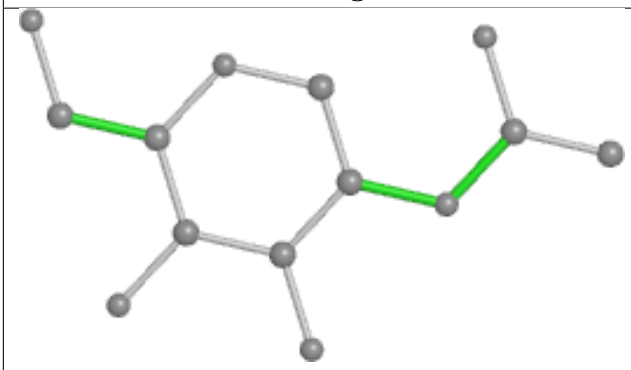
Ligand NAG C 1004



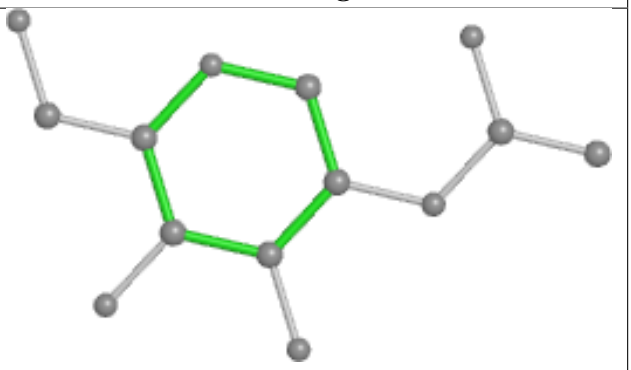
Bond lengths



Bond angles

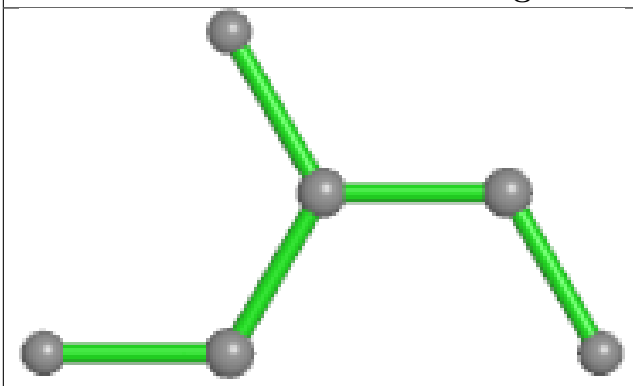


Torsions

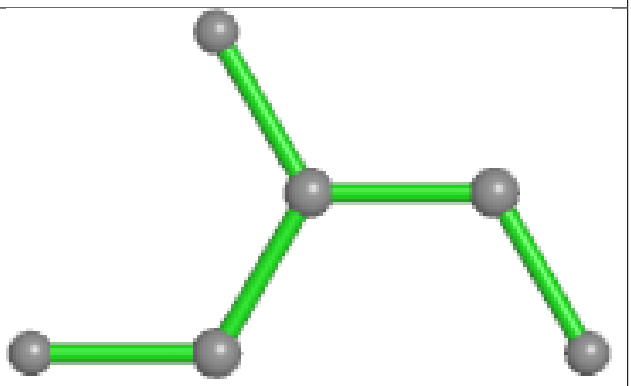


Rings

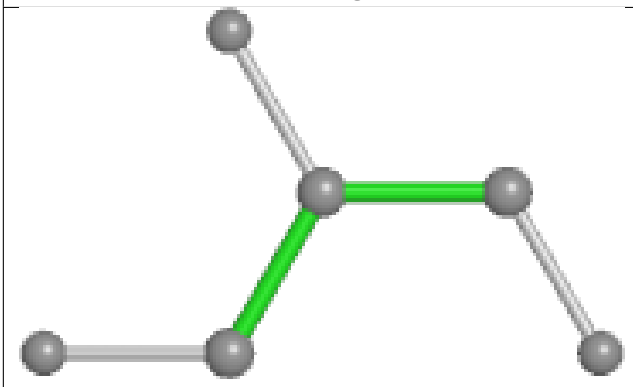
Ligand GOL A 1002



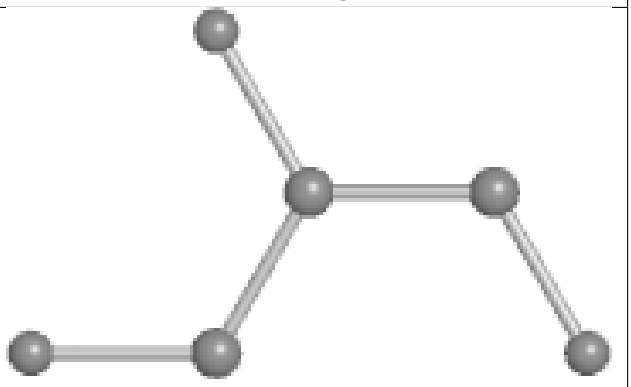
Bond lengths



Bond angles

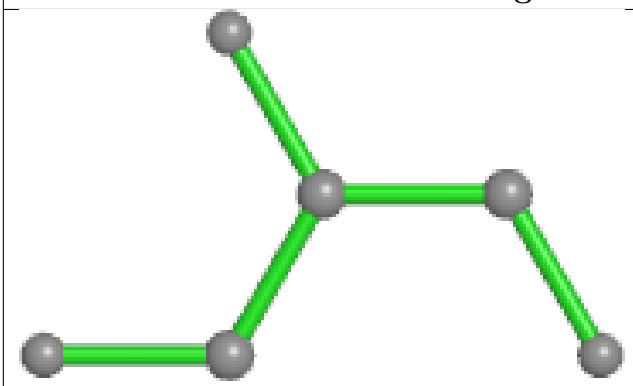


Torsions

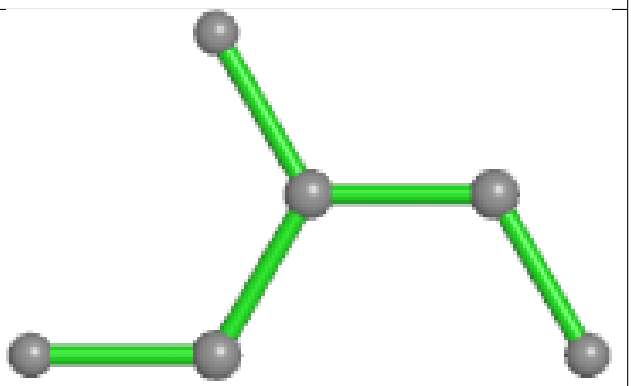


Rings

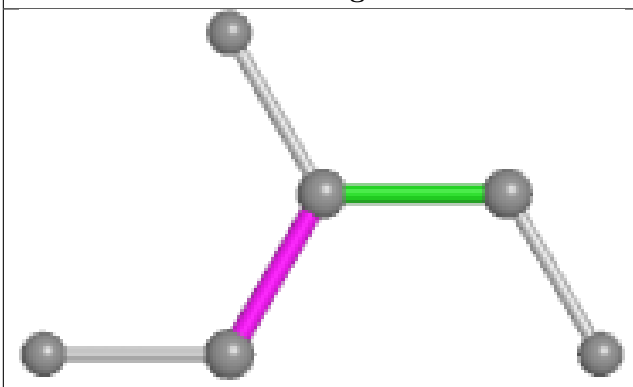
Ligand GOL C 1002



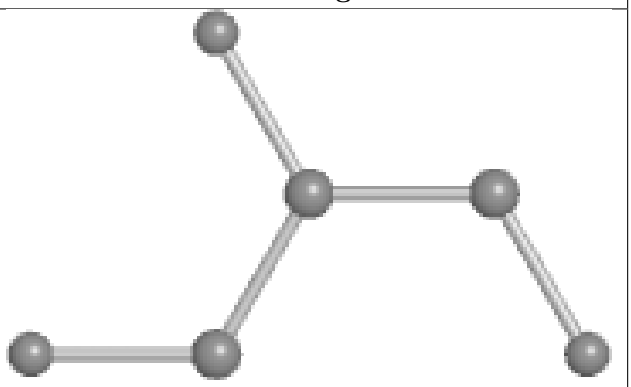
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	904/911 (99%)	0.08	35 (3%)	39	38	43, 59, 88, 148	0
1	C	898/911 (98%)	0.17	33 (3%)	41	41	43, 61, 91, 147	0
2	B	90/127 (70%)	1.90	36 (40%)	0	0	63, 107, 135, 141	0
All	All	1892/1949 (97%)	0.21	104 (5%)	25	24	43, 60, 100, 148	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	334	TYR	8.7
1	C	567	GLU	8.3
1	C	566	SER	8.0
2	B	307	VAL	7.6
1	A	567	GLU	7.5
2	B	368	VAL	6.8
1	A	568	SER	6.7
2	B	305	LEU	6.6
1	A	570	VAL	6.5
2	B	343	LEU	6.4
1	A	569	ASN	6.0
2	B	328	ILE	5.9
1	C	568	SER	5.9
1	A	140	SER	5.8
1	A	139	ASP	5.8
1	C	139	ASP	5.7
2	B	363	PHE	5.6
2	B	335	CYS	5.4
2	B	367	ALA	5.3
1	A	141	GLN	5.3
1	C	141	GLN	5.2
2	B	369	ASN	5.1
1	A	138	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	571	THR	5.0
1	A	566	SER	4.9
2	B	308	VAL	4.7
2	B	327	THR	4.5
2	B	332	THR	4.5
1	C	569	ASN	4.2
2	B	306	GLU	4.2
2	B	337	THR	4.0
1	A	571	THR	3.9
2	B	359	ASP	3.9
2	B	383	SER	3.8
2	B	309	GLN	3.8
2	B	336	VAL	3.8
1	C	140	SER	3.8
2	B	331	ASN	3.7
1	C	129	GLY	3.7
1	C	94	ASP	3.7
1	A	166	GLN	3.7
1	A	889	GLY	3.6
1	C	93	ALA	3.6
2	B	360	THR	3.6
1	A	574	SER	3.5
2	B	338	LYS	3.5
2	B	342	ARG	3.5
1	A	565	ASP	3.5
1	C	197	ASN	3.5
2	B	358	THR	3.3
1	C	95	GLY	3.3
2	B	346	ASN	3.3
1	C	888	TYR	3.2
2	B	407	THR	3.1
1	A	169	HIS	3.1
1	C	166	GLN	3.1
1	A	614	ASP	3.1
1	C	925	VAL	3.0
1	A	257	PRO	3.0
2	B	330	GLY	2.9
2	B	329	ASN	2.9
1	A	764	GLN	2.8
2	B	344	GLU	2.8
1	A	572	ARG	2.8
1	C	570	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	612	ALA	2.8
1	A	137	VAL	2.8
1	C	198	VAL	2.8
1	C	290	GLN	2.8
1	A	290	GLN	2.7
2	B	379	LEU	2.7
1	C	137	VAL	2.7
1	C	61	LEU	2.7
2	B	333	SER	2.7
2	B	406	VAL	2.7
1	C	739	GLU	2.6
1	A	669	HIS	2.6
1	C	961	GLU	2.6
2	B	366	SER	2.6
1	A	613	SER	2.5
2	B	405	TYR	2.5
1	A	250	SER	2.4
1	C	433	GLY	2.4
1	A	762	LEU	2.3
1	C	138	GLY	2.3
1	A	251	THR	2.3
1	C	247	LYS	2.3
1	C	493	GLU	2.2
1	A	894	SER	2.2
1	A	128	GLN	2.2
1	C	63	GLN	2.2
1	A	259	TRP	2.2
1	A	575	ALA	2.2
2	B	349	CYS	2.1
1	C	128	GLN	2.1
1	C	169	HIS	2.1
2	B	326	VAL	2.1
1	C	257	PRO	2.1
1	C	962	GLY	2.1
1	A	93	ALA	2.0
1	C	917	GLN	2.0
1	A	58	ALA	2.0
1	A	253	LEU	2.0
1	A	197	ASN	2.0

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

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

6.3 Carbohydrates (i)

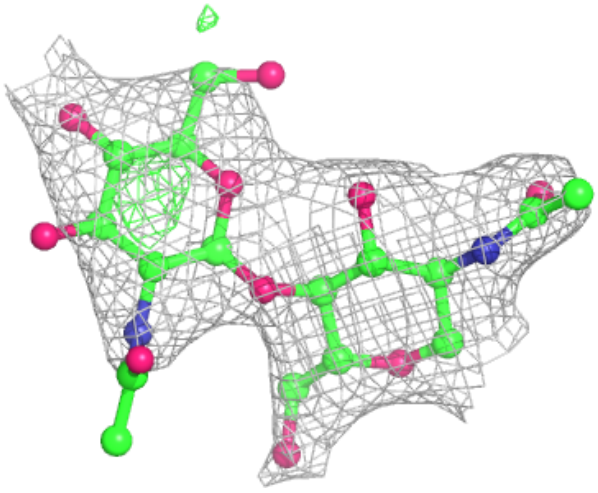
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

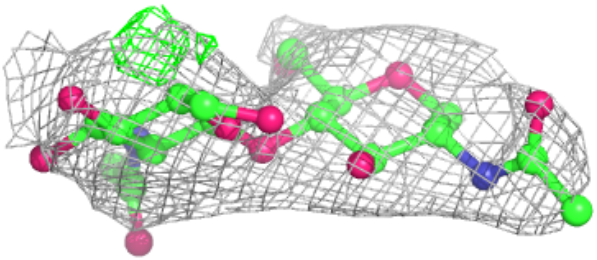
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	L	2	14/15	0.55	0.35	87,104,114,118	0
3	NAG	M	2	14/15	0.77	0.40	93,116,125,126	0
3	NAG	G	2	14/15	0.79	0.49	92,106,112,117	0
3	NAG	M	1	14/15	0.80	0.25	80,99,118,121	0
3	NAG	I	2	14/15	0.81	0.44	90,104,114,123	0
3	NAG	F	2	14/15	0.83	0.27	72,92,110,111	0
3	NAG	H	2	14/15	0.83	0.22	93,107,111,117	0
3	NAG	D	2	14/15	0.85	0.34	98,109,113,116	0
3	NAG	I	1	14/15	0.86	0.28	66,88,90,92	0
3	NAG	G	1	14/15	0.87	0.45	68,98,112,119	0
4	NAG	L	1	14/15	0.89	0.26	57,83,108,109	0
3	NAG	E	2	14/15	0.89	0.31	76,88,99,99	0
3	NAG	F	1	14/15	0.90	0.19	46,72,89,89	0
3	NAG	K	2	14/15	0.90	0.22	82,104,114,116	0
3	NAG	H	1	14/15	0.90	0.25	54,88,109,110	0
3	NAG	J	2	14/15	0.93	0.24	70,93,100,106	0
3	NAG	D	1	14/15	0.93	0.21	68,84,95,109	0
3	NAG	K	1	14/15	0.96	0.12	47,70,87,97	0
3	NAG	J	1	14/15	0.97	0.17	50,62,75,90	0
3	NAG	E	1	14/15	0.97	0.16	56,66,75,90	0

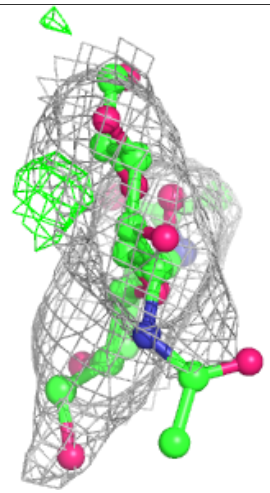
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

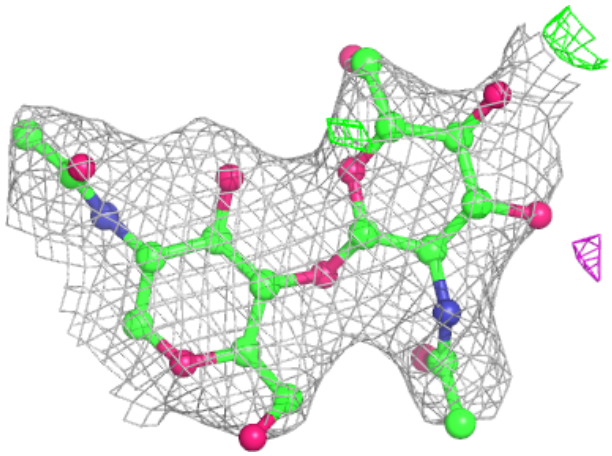


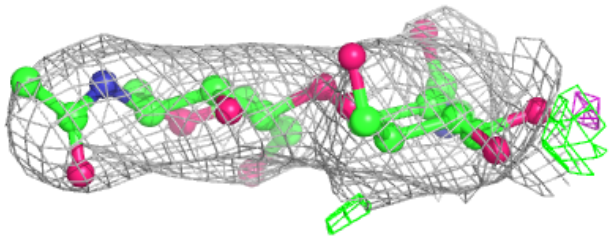


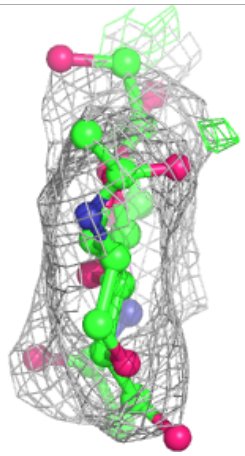


Electron density around Chain E:

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

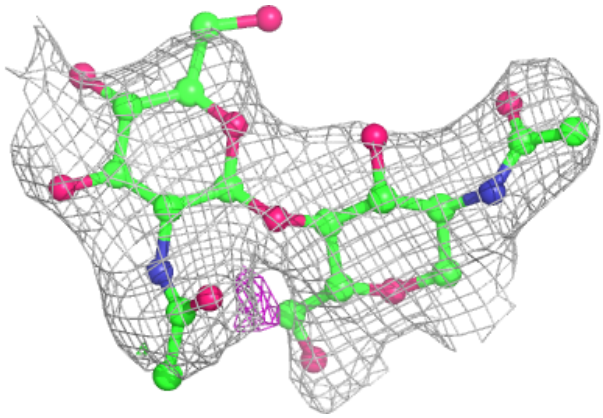


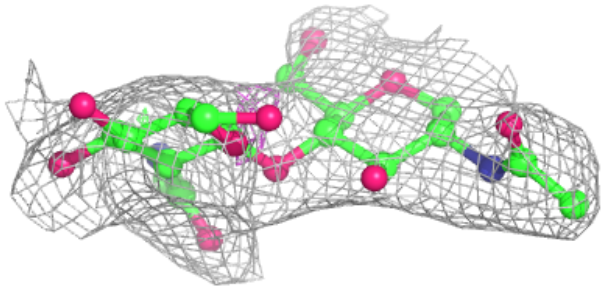


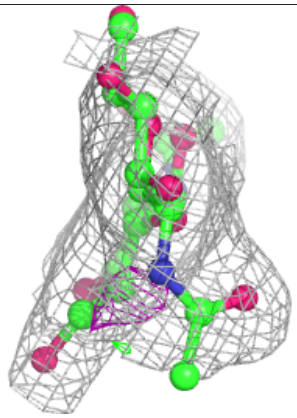


Electron density around Chain F:

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

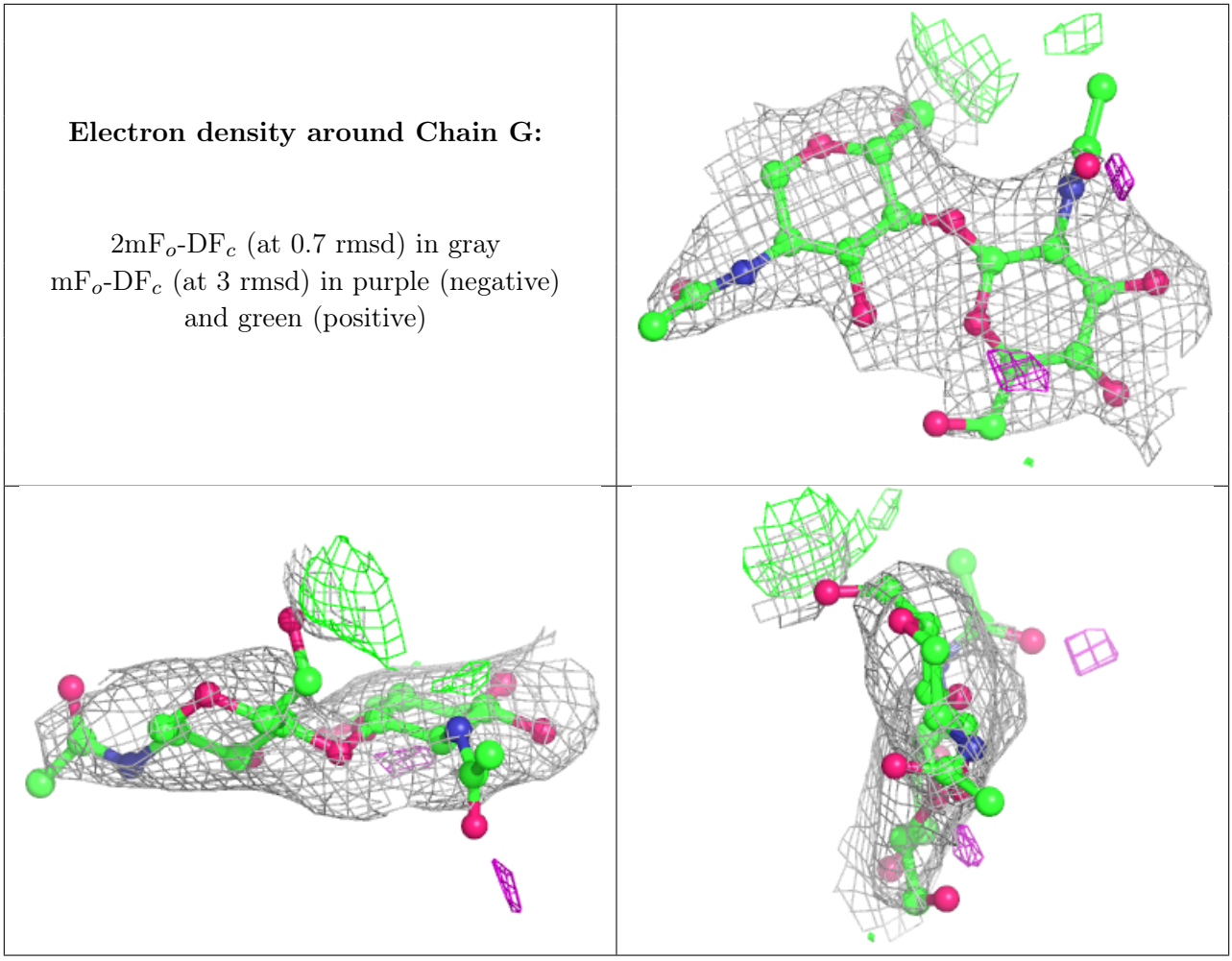






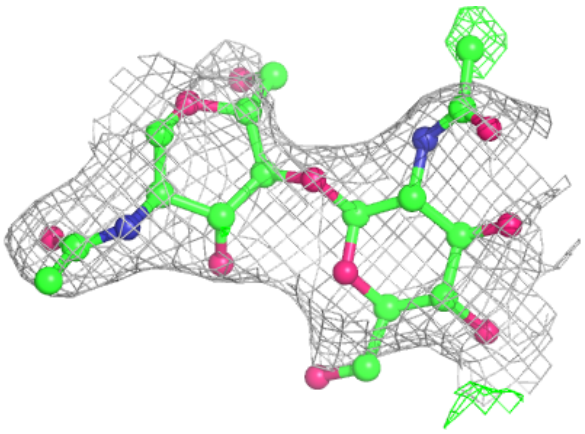
Electron density around Chain G:

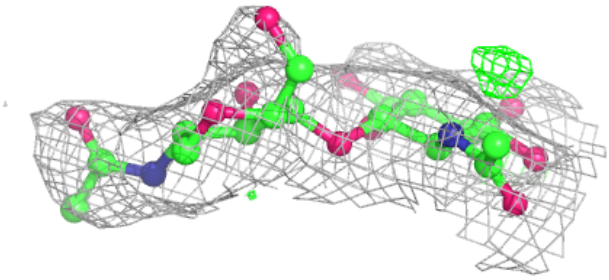
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

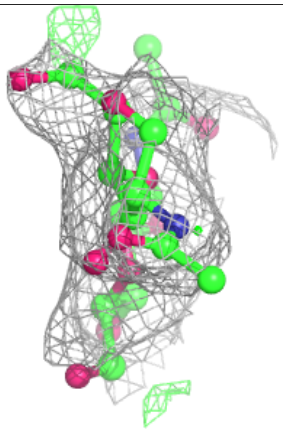


Electron density around Chain H:

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

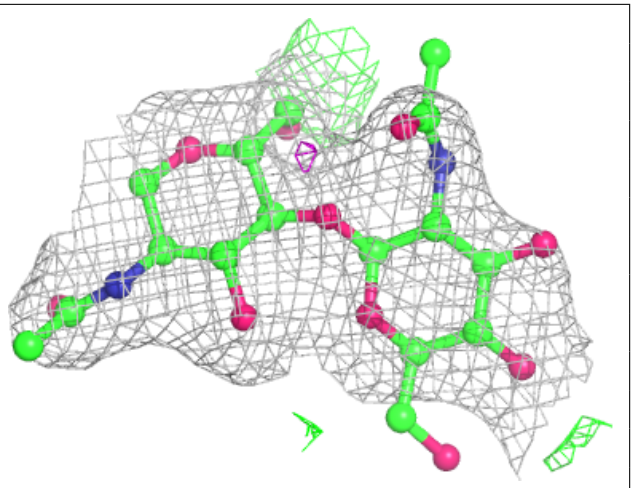


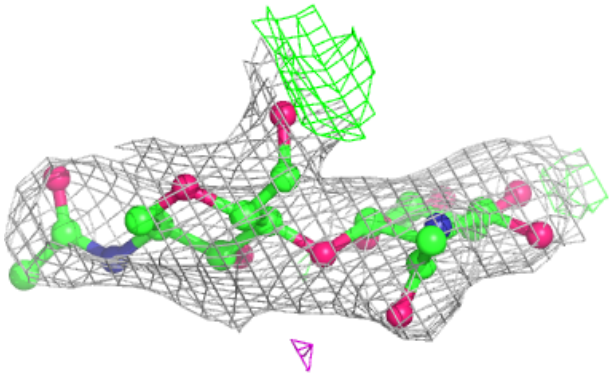


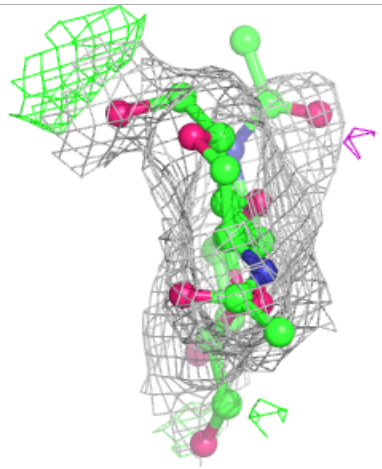


Electron density around Chain I:

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

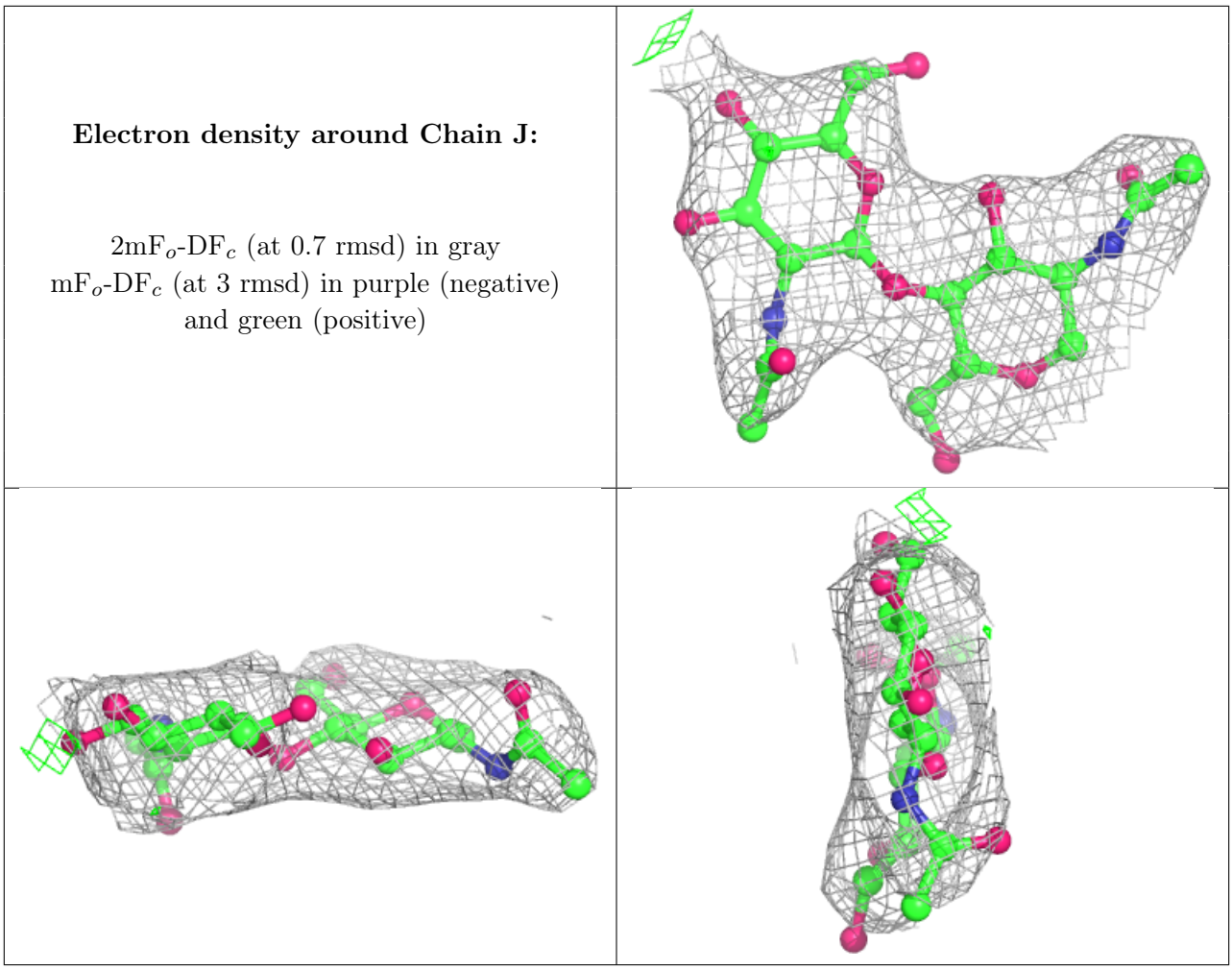






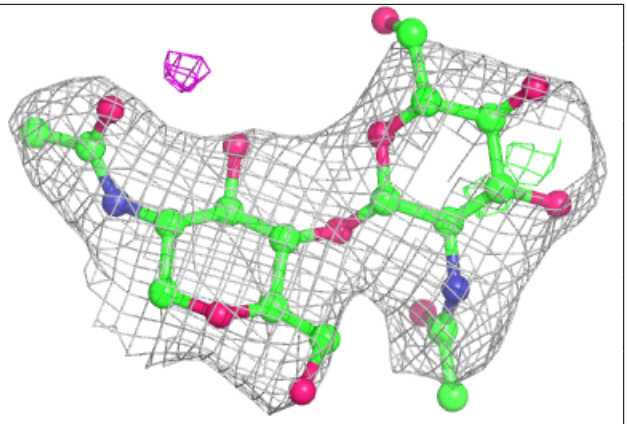
Electron density around Chain J:

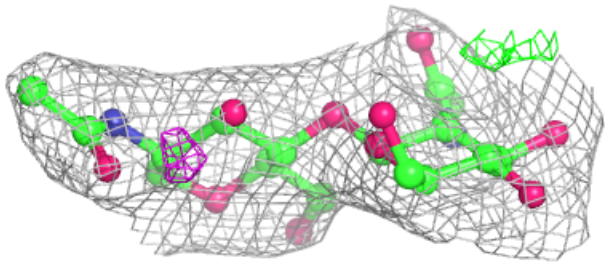
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

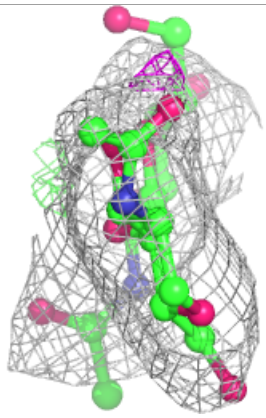


Electron density around Chain K:

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

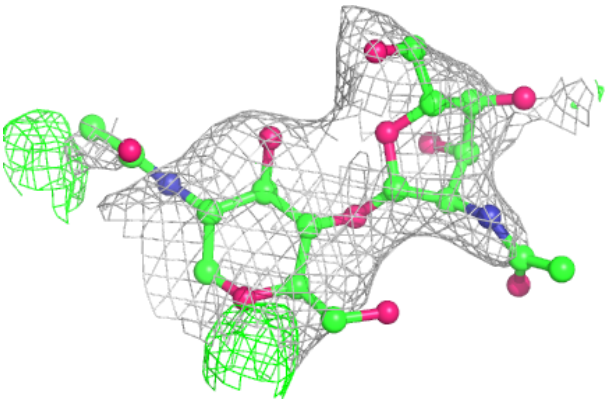


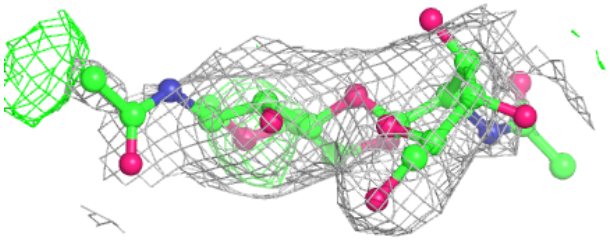


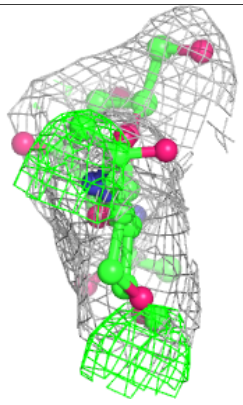


Electron density around Chain M:

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

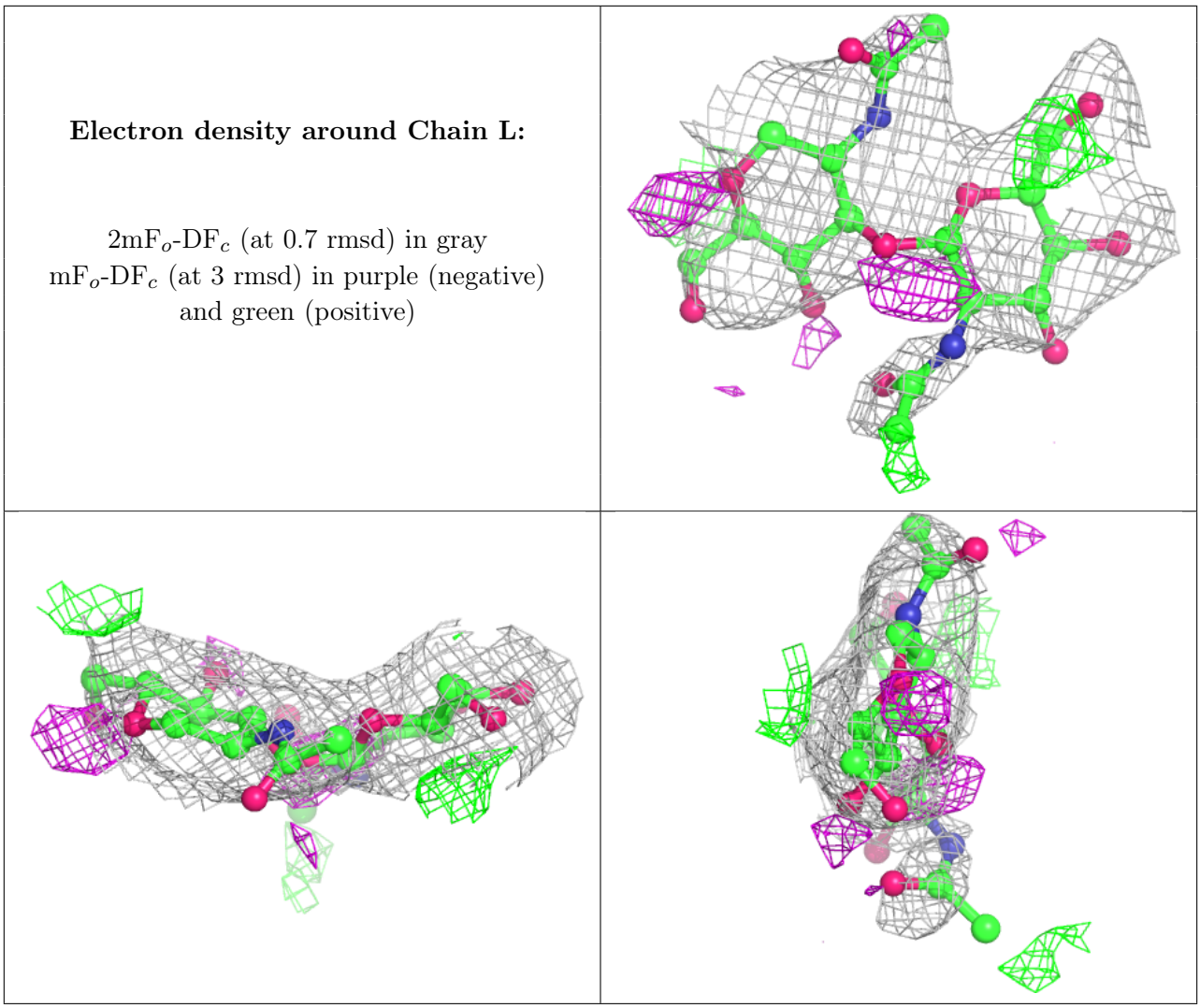






Electron density around Chain L:

$2mF_o$-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
7	NAG	B	501	14/15	0.74	0.60	103,115,131,138	0
6	GOL	A	1003	6/6	0.81	0.30	53,69,93,94	0
6	GOL	C	1003	6/6	0.86	0.70	62,73,89,93	0
6	GOL	A	1004	6/6	0.86	0.18	66,74,77,86	0
7	NAG	C	1005	14/15	0.86	0.23	59,93,100,102	0
6	GOL	C	1002	6/6	0.87	0.46	49,58,67,84	0
6	GOL	A	1002	6/6	0.87	0.33	46,57,60,74	0
7	NAG	A	1005	14/15	0.90	0.15	52,66,83,85	0

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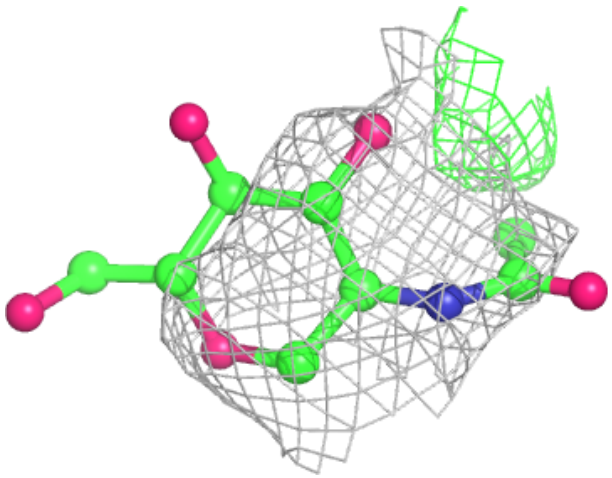
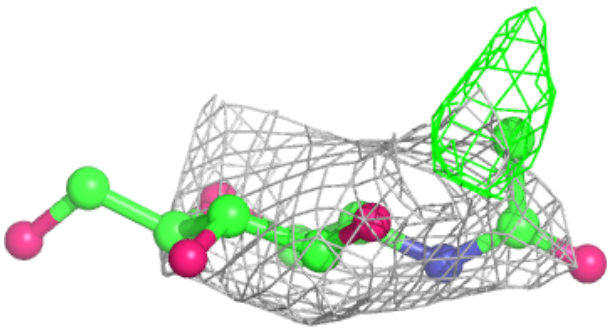
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	A	1006	14/15	0.90	0.19	75,94,100,101	0
7	NAG	C	1004	14/15	0.92	0.22	68,82,88,98	0
5	ZN	A	1001	1/1	0.98	0.20	49,49,49,49	0
5	ZN	C	1001	1/1	0.99	0.23	54,54,54,54	0

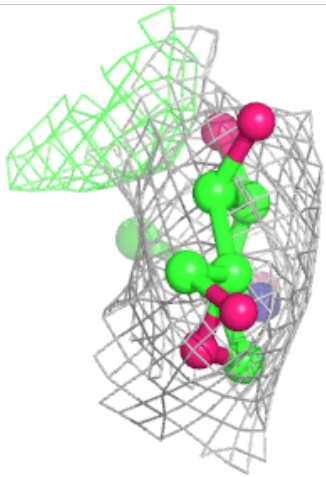
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG B 501:

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

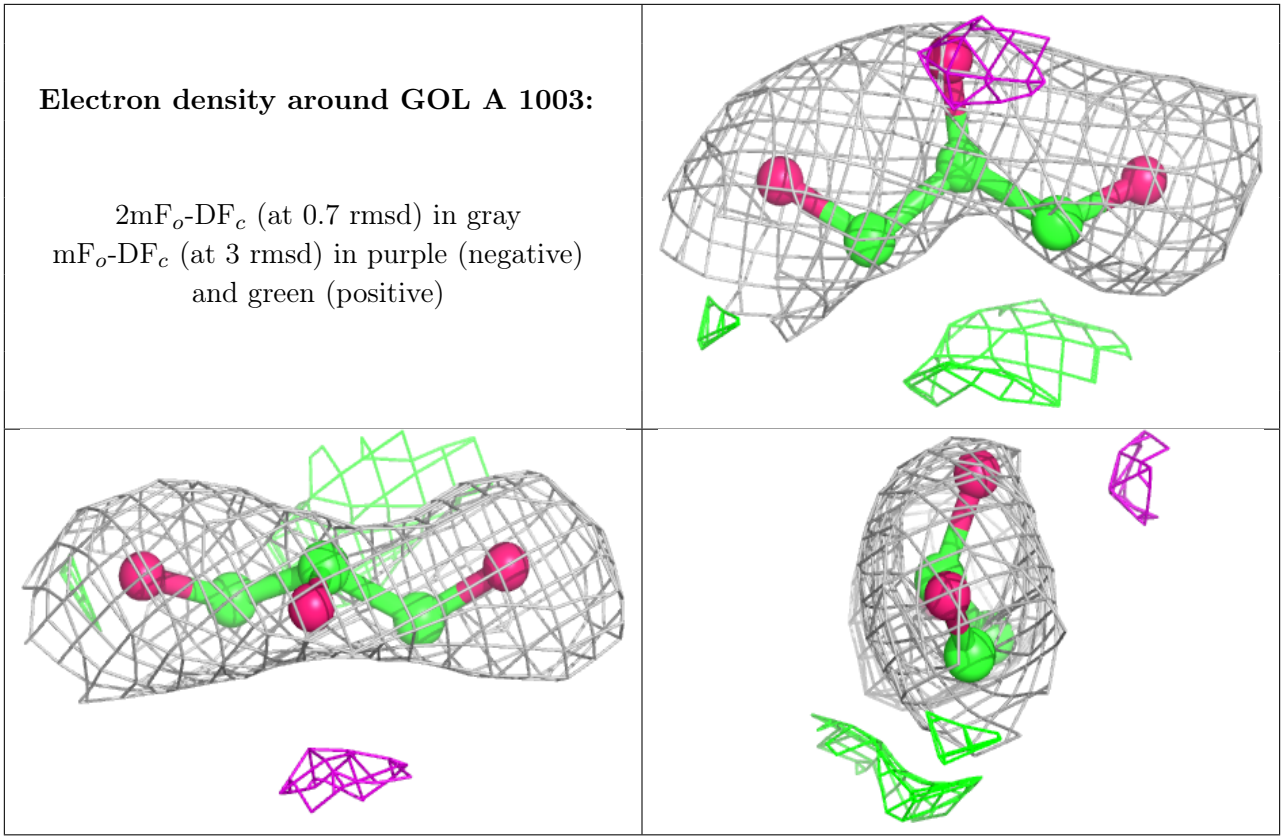






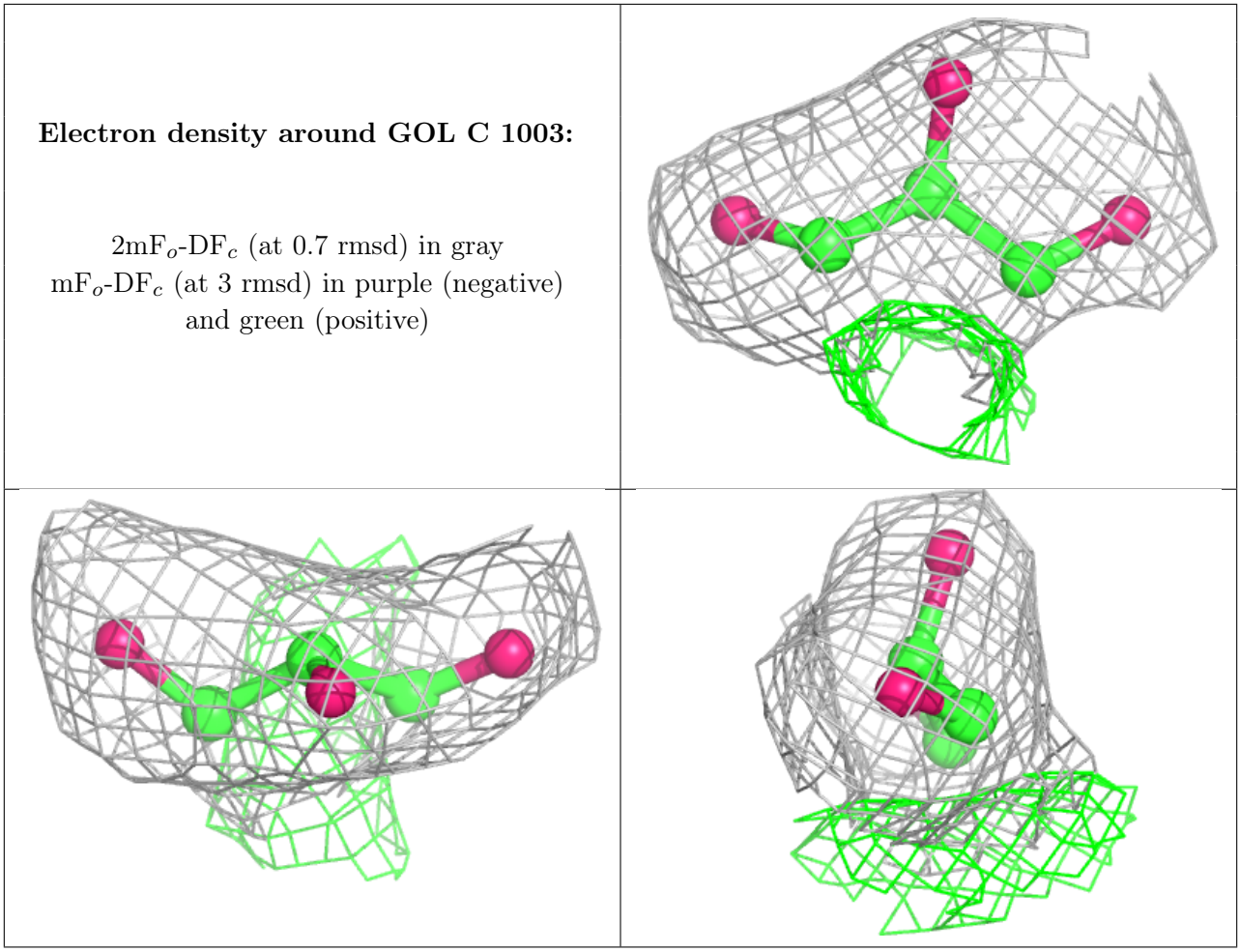
Electron density around GOL A 1003:

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



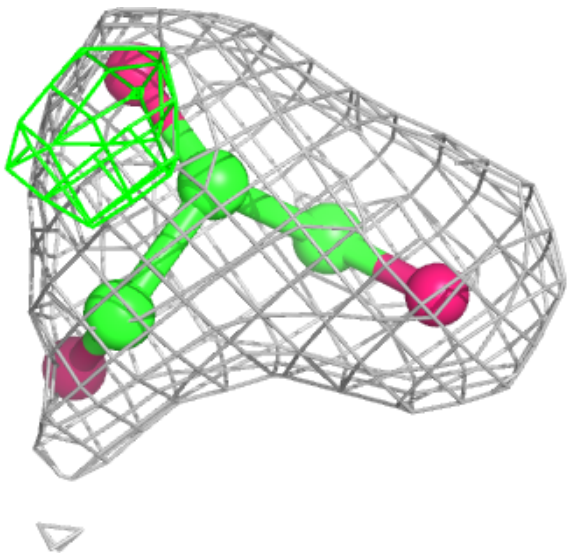
Electron density around GOL C 1003:

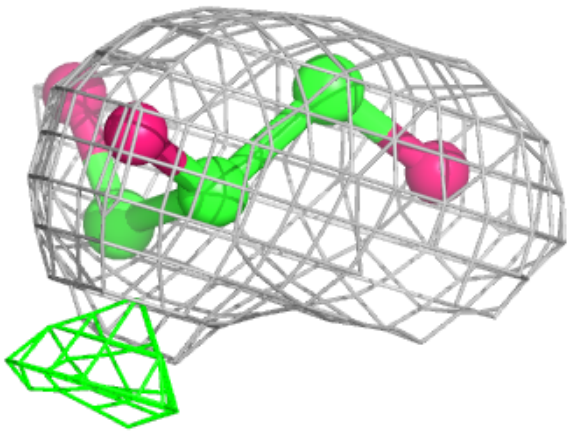
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

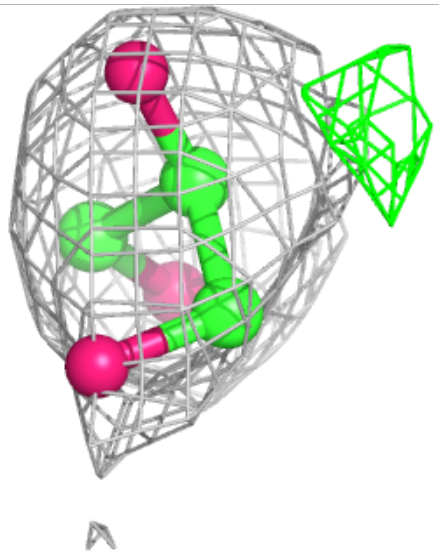


Electron density around GOL A 1004:

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

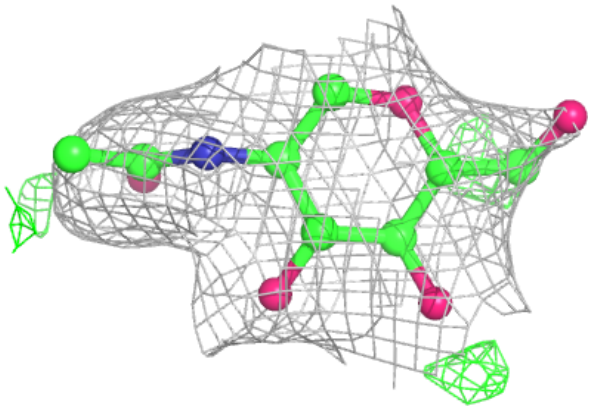


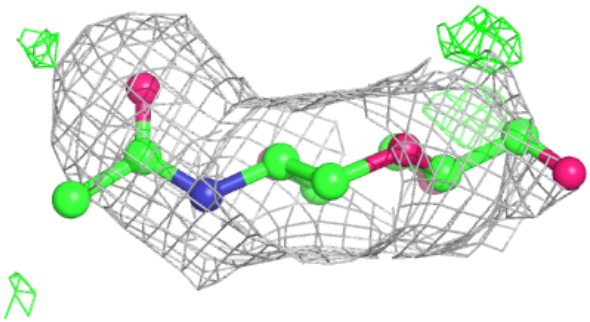


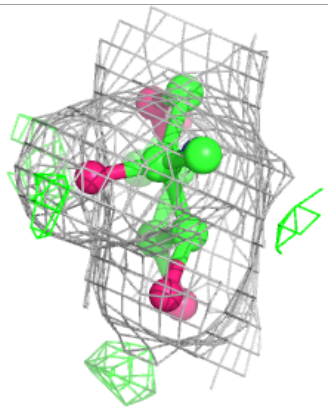


Electron density around NAG C 1005:

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

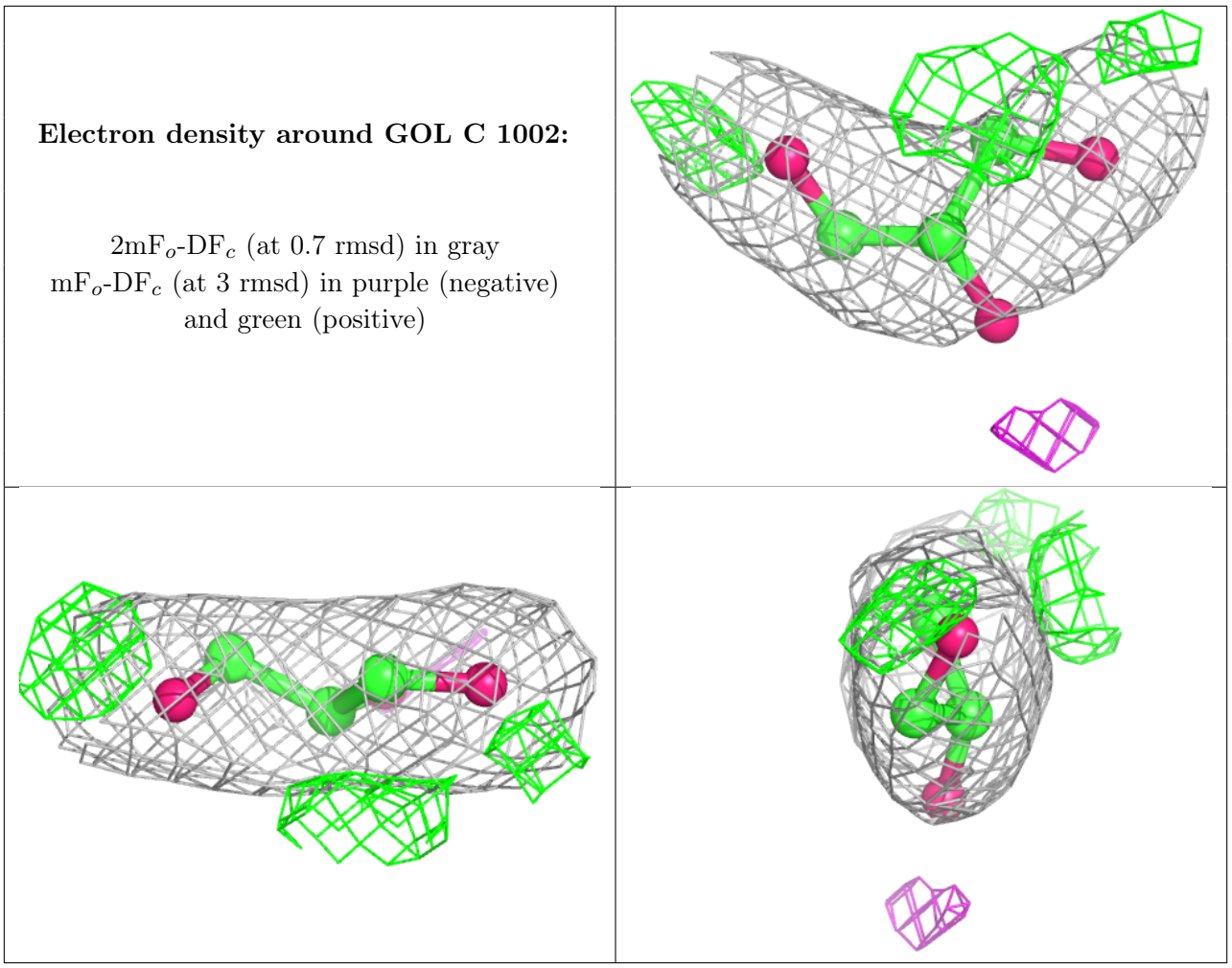






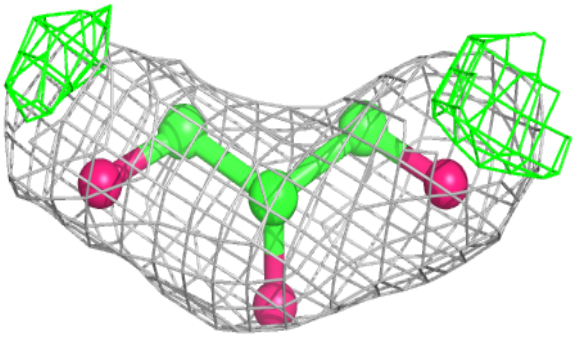
Electron density around GOL C 1002:

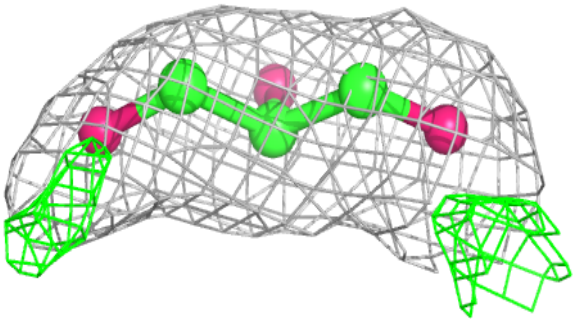
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

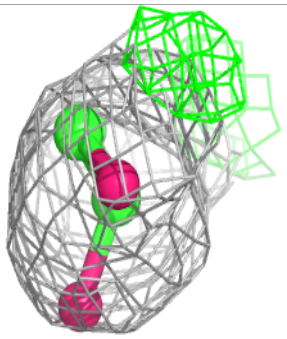


Electron density around GOL A 1002:

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

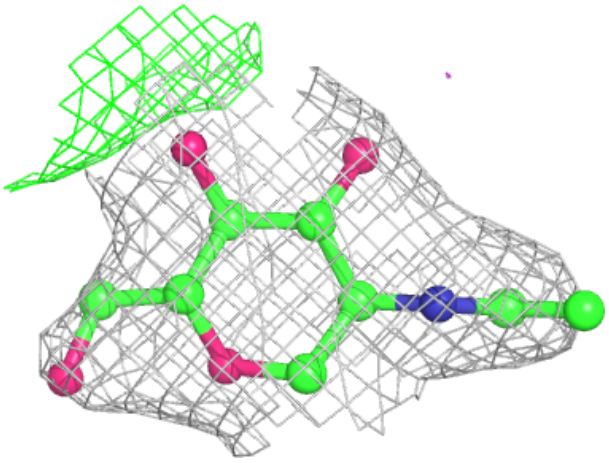


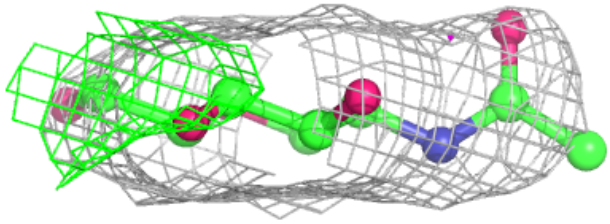


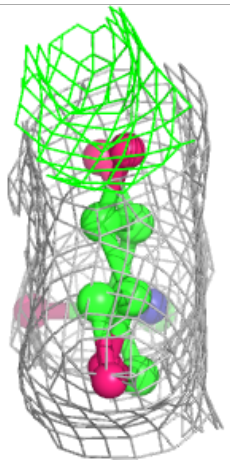


Electron density around NAG A 1005:

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

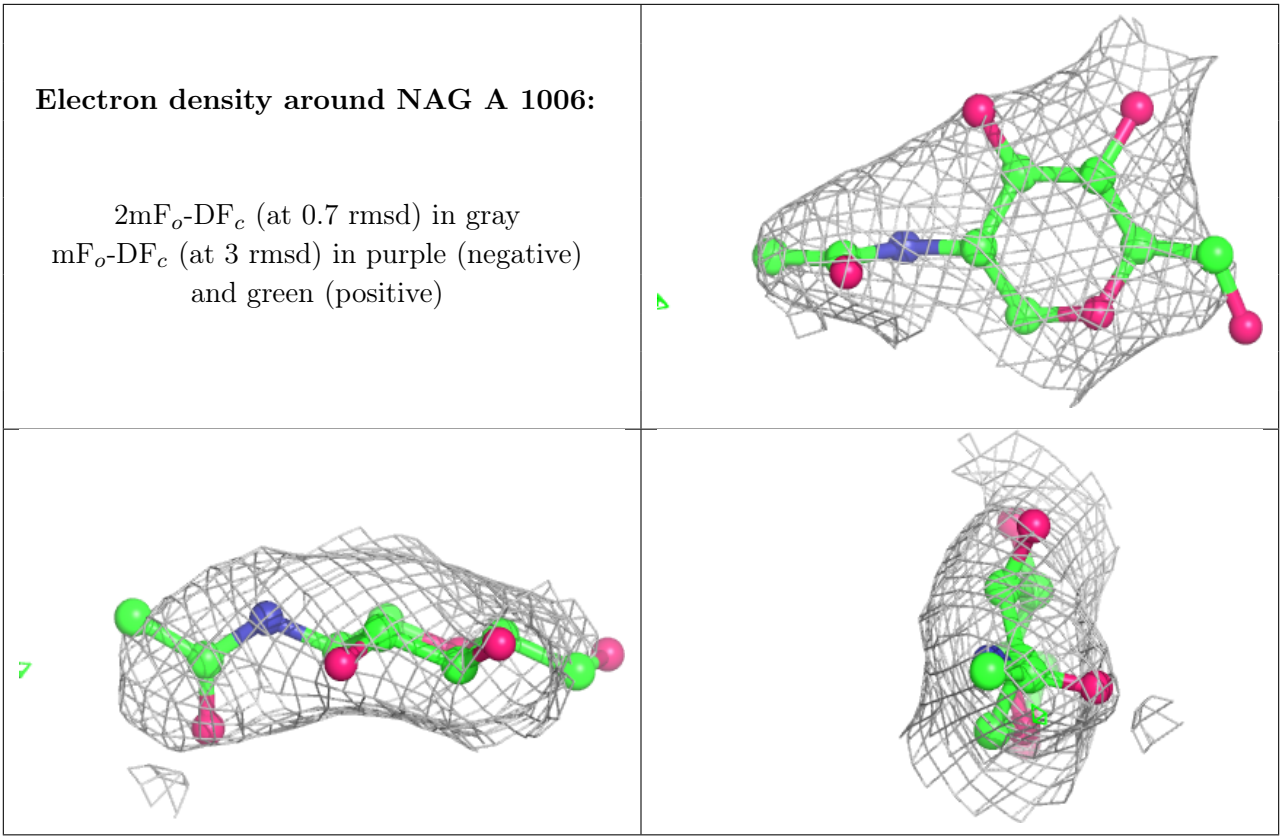






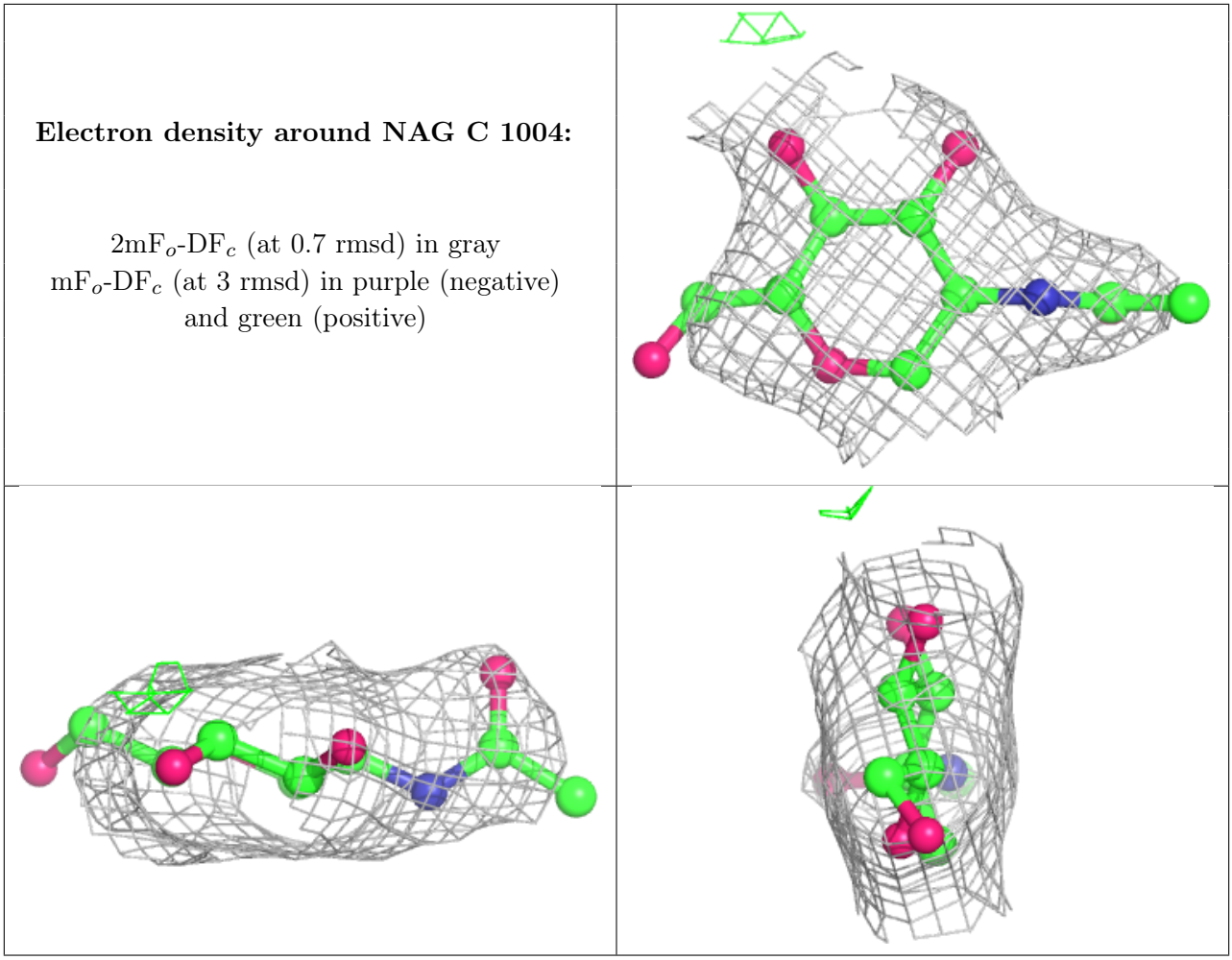
Electron density around NAG A 1006:

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



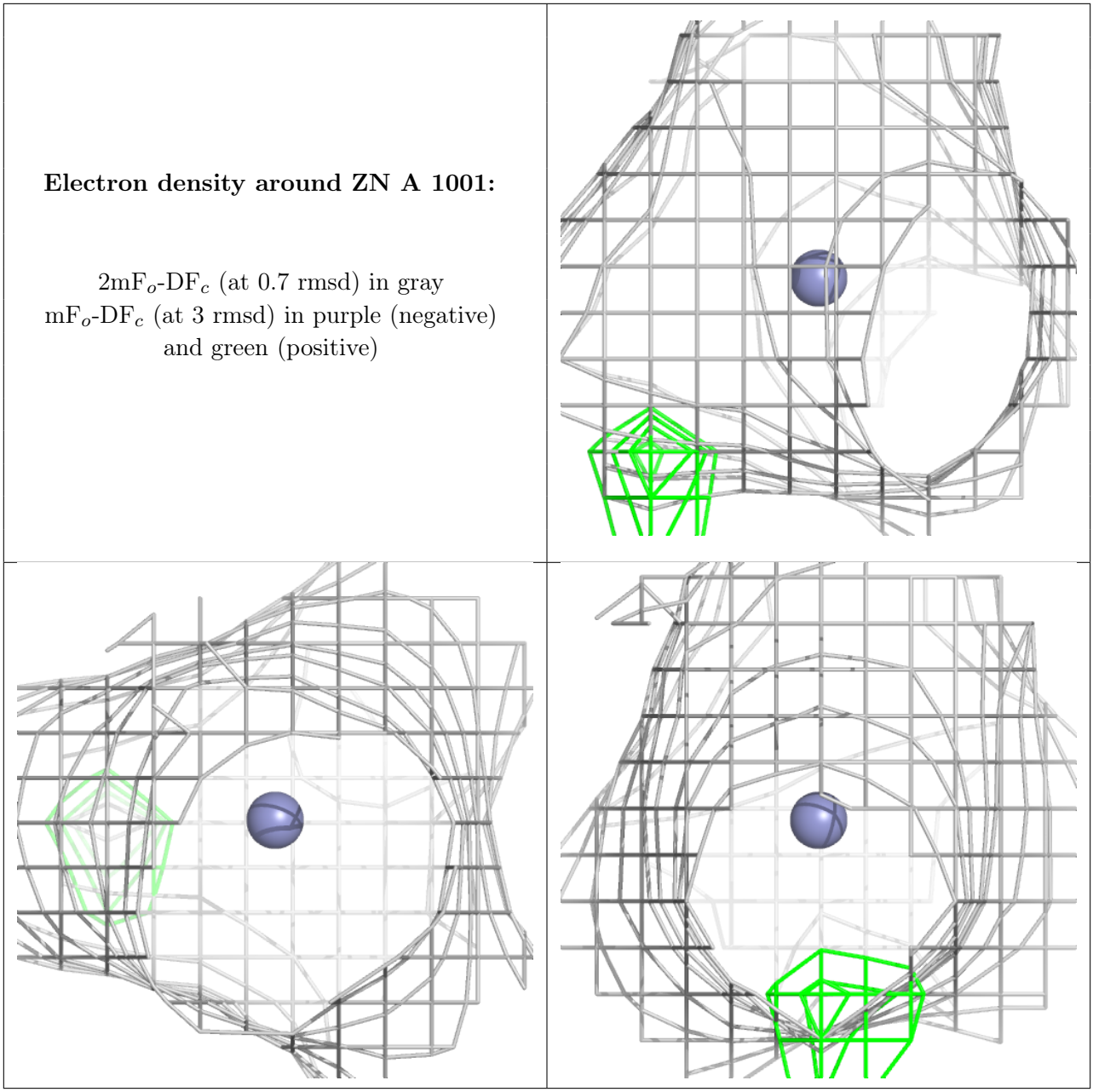
Electron density around NAG C 1004:

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



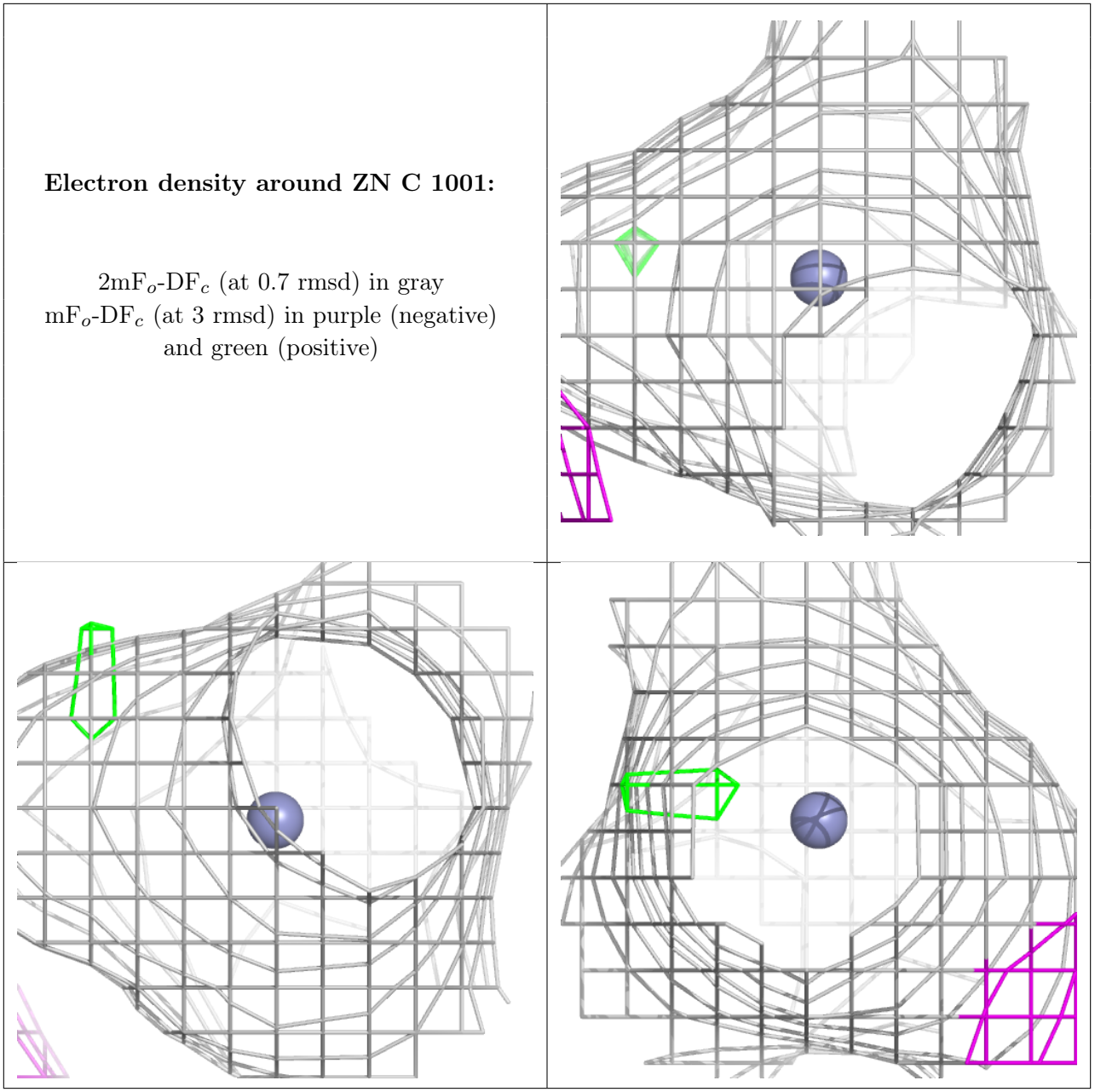
Electron density around ZN A 1001:

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



Electron density around ZN C 1001:

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



6.5 Other polymers

There are no such residues in this entry.