Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2026 – 12:19 AM UTC

PDB ID	:	8WDR / pdb_00008wdr
Title	:	Crystal structure of BQ.1.1 RBD complexed with human ACE2
Authors	:	Li, W.; Xie, Y.
Deposited on	:	2023-09-16
Resolution	:	3.47 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 (i)) were used in the production of this report:

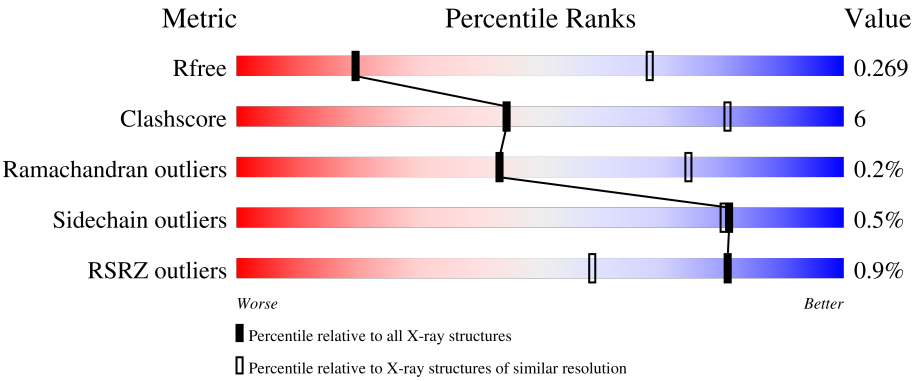
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.47 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}	180053	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	805	64% 10% 26%
1	C	805	62% 12% 26%
2	B	247	2% 64% 15% 21%
2	D	247	2% 69% 10% 21%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	G	2	100%
3	H	2	50% 50%
4	F	3	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13055 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			
1	C	596	Total	C	N	O	S	0	1	0
			4857	3110	801	917	29			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	1	0
			1558	1004	261	285	8			
2	D	195	Total	C	N	O	S	0	1	0
			1555	1003	260	284	8			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	301	MET	-	initiating methionine	UNP P0DTC2
B	302	HIS	-	expression tag	UNP P0DTC2
B	303	SER	-	expression tag	UNP P0DTC2
B	304	SER	-	expression tag	UNP P0DTC2
B	305	ALA	-	expression tag	UNP P0DTC2
B	306	LEU	-	expression tag	UNP P0DTC2
B	307	LEU	-	expression tag	UNP P0DTC2
B	308	CYS	-	expression tag	UNP P0DTC2
B	309	CYS	-	expression tag	UNP P0DTC2
B	310	LEU	-	expression tag	UNP P0DTC2
B	311	VAL	-	expression tag	UNP P0DTC2
B	312	LEU	-	expression tag	UNP P0DTC2
B	313	LEU	-	expression tag	UNP P0DTC2
B	314	THR	-	expression tag	UNP P0DTC2
B	315	GLY	-	expression tag	UNP P0DTC2
B	316	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	317	ARG	-	expression tag	UNP P0DTC2
B	318	ALA	-	expression tag	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	444	THR	LYS	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
D	301	MET	-	initiating methionine	UNP P0DTC2
D	302	HIS	-	expression tag	UNP P0DTC2
D	303	SER	-	expression tag	UNP P0DTC2
D	304	SER	-	expression tag	UNP P0DTC2
D	305	ALA	-	expression tag	UNP P0DTC2
D	306	LEU	-	expression tag	UNP P0DTC2
D	307	LEU	-	expression tag	UNP P0DTC2
D	308	CYS	-	expression tag	UNP P0DTC2
D	309	CYS	-	expression tag	UNP P0DTC2
D	310	LEU	-	expression tag	UNP P0DTC2
D	311	VAL	-	expression tag	UNP P0DTC2
D	312	LEU	-	expression tag	UNP P0DTC2
D	313	LEU	-	expression tag	UNP P0DTC2
D	314	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	315	GLY	-	expression tag	UNP P0DTC2
D	316	VAL	-	expression tag	UNP P0DTC2
D	317	ARG	-	expression tag	UNP P0DTC2
D	318	ALA	-	expression tag	UNP P0DTC2
D	339	ASP	GLY	variant	UNP P0DTC2
D	346	THR	ARG	variant	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	376	ALA	THR	variant	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	444	THR	LYS	variant	UNP P0DTC2
D	452	ARG	LEU	variant	UNP P0DTC2
D	460	LYS	ASN	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	486	VAL	PHE	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2
D	542	HIS	-	expression tag	UNP P0DTC2
D	543	HIS	-	expression tag	UNP P0DTC2
D	544	HIS	-	expression tag	UNP P0DTC2
D	545	HIS	-	expression tag	UNP P0DTC2
D	546	HIS	-	expression tag	UNP P0DTC2
D	547	HIS	-	expression tag	UNP P0DTC2

- 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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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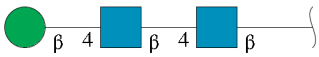
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	G	2	Total C N O 28 16 2 10	0	0	0
3	H	2	Total C N O 28 16 2 10	0	0	0

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

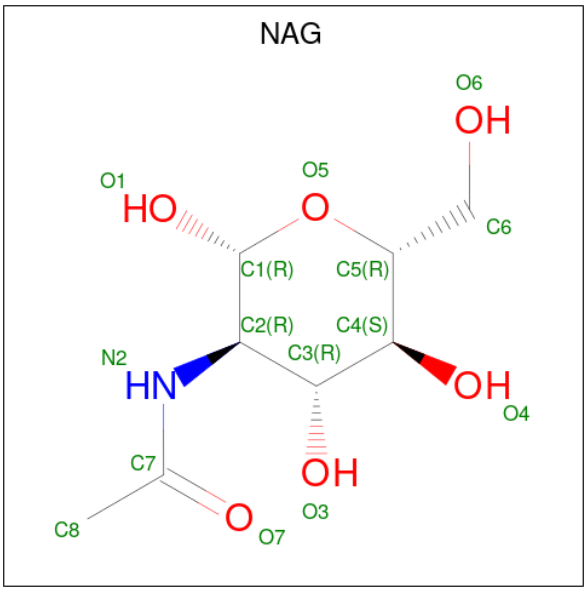


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	3	Total C N O 39 22 2 15	0	0	0

- Molecule 5 is ZINC ION (CCD ID: 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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



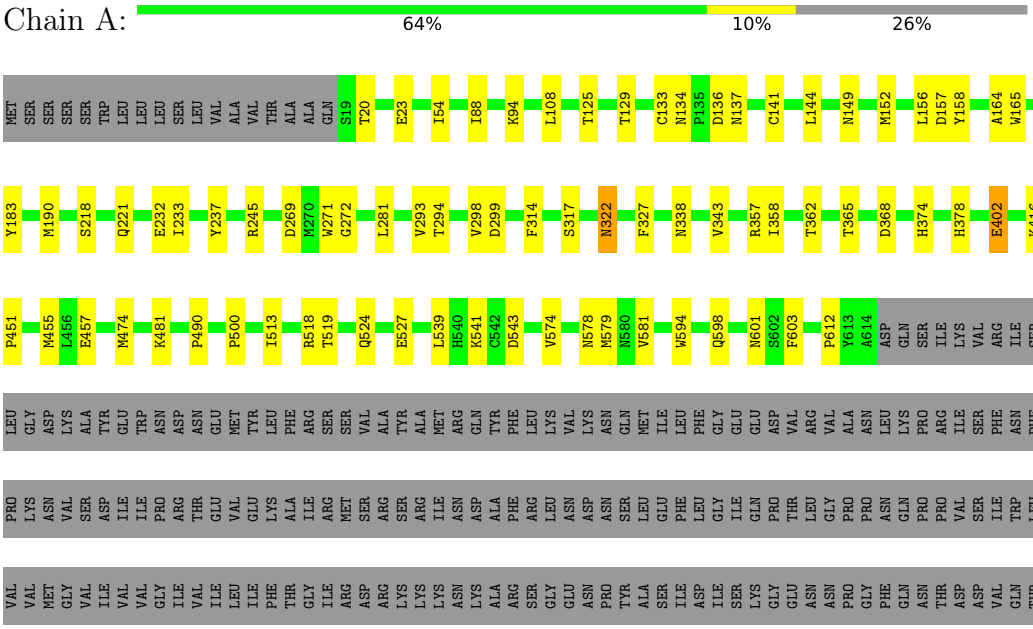
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0

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.

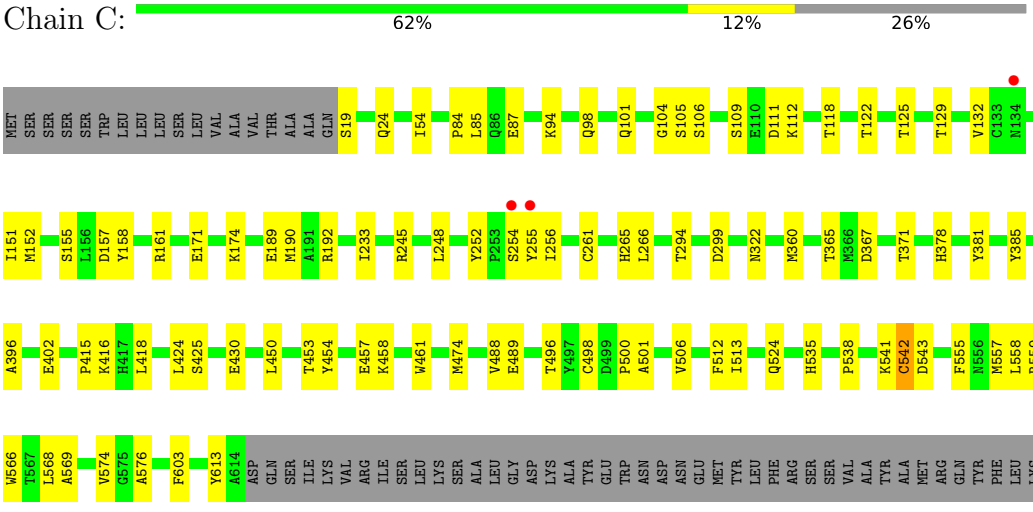
• Molecule 1: Angiotensin-converting enzyme 2

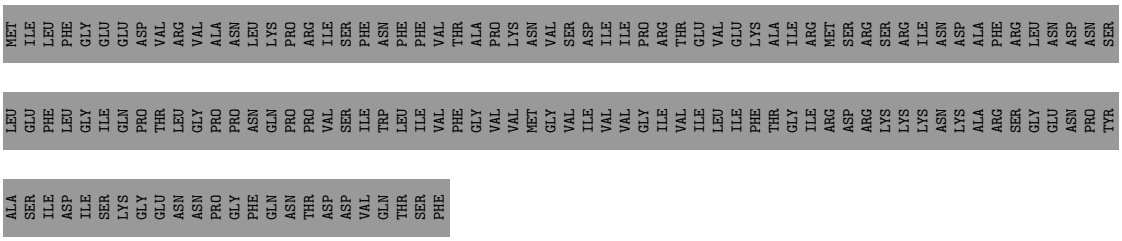
Chain A:



• Molecule 1: Angiotensin-converting enzyme 2

Chain C:

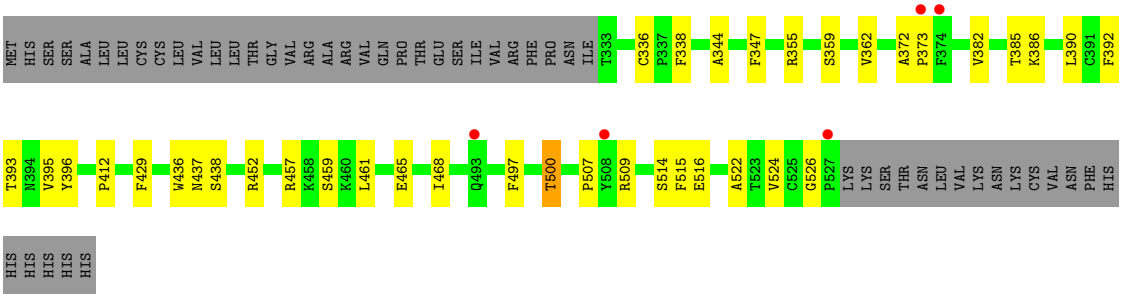




• Molecule 2: Spike protein S1

Chain B:

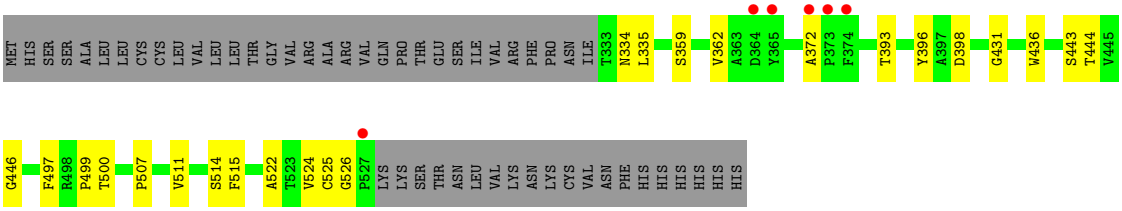




• Molecule 2: Spike protein S1

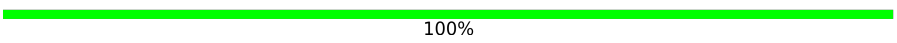
Chain D:





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

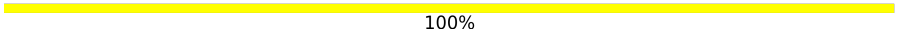
Chain E:





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

Chain G:





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

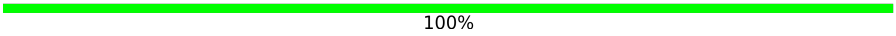
Chain H:





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

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.58Å 135.41Å 154.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.47 29.75 – 3.47	Depositor EDS
% Data completeness (in resolution range)	95.7 (29.75-3.47) 95.6 (29.75-3.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.211 , 0.269 0.211 , 0.269	Depositor DCC
R_{free} test set	1646 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	82.3	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13055	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, BMA, 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	0.10	0/4999	0.29	0/6792
1	C	0.16	0/4998	0.33	0/6793
2	B	0.14	0/1605	0.38	0/2187
2	D	0.12	0/1605	0.34	0/2187
All	All	0.13	0/13207	0.32	0/17959

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	4862	0	4635	45	1
1	C	4857	0	4618	69	1
2	B	1558	0	1478	26	0
2	D	1555	0	1480	13	0
3	E	28	0	25	0	0
3	G	28	0	25	1	0
3	H	28	0	25	1	0
4	F	39	0	34	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
6	A	42	0	39	0	0
6	B	14	0	13	0	0
6	C	42	0	39	2	0
All	All	13055	0	12411	153	1

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 6.

All (153) 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:C:252:TYR:HD1	1:C:255:TYR:HH	1.00	0.97
1:C:252:TYR:HB3	1:C:255:TYR:CE1	2.11	0.86
1:A:455:MET:HE2	1:A:481:LYS:HG2	1.65	0.79
1:C:252:TYR:HD1	1:C:255:TYR:OH	1.69	0.75
1:C:157:ASP:OD1	1:C:158:TYR:N	2.22	0.72
2:B:359:SER:HA	2:B:524:VAL:HG22	1.73	0.69
2:D:362:VAL:HG23	2:D:526:GLY:HA3	1.75	0.67
2:D:359:SER:HA	2:D:524:VAL:HG22	1.78	0.66
1:A:245:ARG:NH2	1:A:603:PHE:O	2.30	0.64
1:C:252:TYR:HB3	1:C:255:TYR:CZ	2.33	0.64
1:A:294:THR:HG23	1:A:365:THR:HA	1.80	0.63
1:C:85:LEU:O	1:C:94:LYS:NZ	2.30	0.63
1:A:134:ASN:OD1	1:A:136:ASP:N	2.32	0.62
2:D:393:THR:HA	2:D:522:ALA:HA	1.81	0.61
1:C:261:CYS:HB2	1:C:488:VAL:HB	1.83	0.60
1:C:457:GLU:HG2	1:C:513:ILE:HB	1.84	0.60
2:B:362:VAL:HG23	2:B:526:GLY:HA3	1.84	0.59
1:C:132:VAL:HG22	1:C:148:LEU:HD11	1.84	0.59
2:B:393:THR:HA	2:B:522:ALA:HA	1.85	0.59
2:B:347:PHE:CE1	2:B:509:ARG:HD3	2.39	0.58
1:C:104:GLY:O	1:C:106:SER:N	2.37	0.58
1:C:416:LYS:HD2	1:C:543:ASP:HB3	1.84	0.58
1:A:157:ASP:OD1	1:A:158:TYR:N	2.37	0.58
1:A:416:LYS:HD2	1:A:543:ASP:HB3	1.85	0.58
1:A:474:MET:HE1	1:A:500:PRO:HD2	1.84	0.58
1:C:85:LEU:HD21	1:C:98:GLN:HB2	1.86	0.58
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.85	0.58
1:C:245:ARG:NH2	1:C:603:PHE:O	2.37	0.57
1:C:118:THR:O	1:C:122:THR:OG1	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ILE:HD13	1:C:450:LEU:HD13	1.86	0.56
2:B:468:ILE:HG13	1:C:425:SER:HB3	1.88	0.56
1:C:294:THR:HG23	1:C:365:THR:HA	1.88	0.56
1:C:255:TYR:CD1	1:C:256:ILE:HG13	2.41	0.55
1:C:535:HIS:CD2	1:C:542:CYS:HB2	2.42	0.55
2:B:452:ARG:HD2	1:C:299:ASP:OD2	2.06	0.55
1:A:108:LEU:HD11	1:A:190:MET:HB2	1.87	0.55
1:C:498:CYS:O	1:C:501:ALA:N	2.40	0.55
2:B:373:PRO:HG2	2:B:437:ASN:HB3	1.89	0.54
1:C:524:GLN:HB3	1:C:574:VAL:HG11	1.91	0.53
1:C:125:THR:O	1:C:129:THR:OG1	2.22	0.53
1:A:20:THR:HG23	1:A:23:GLU:H	1.74	0.53
1:A:54:ILE:HD11	1:A:343:VAL:HG23	1.91	0.53
1:A:152:MET:HE3	1:A:164:ALA:HB3	1.90	0.52
1:C:255:TYR:CE1	1:C:256:ILE:HG13	2.44	0.52
1:C:367:ASP:O	1:C:371:THR:OG1	2.22	0.52
6:C:904:NAG:H83	6:C:904:NAG:H3	1.91	0.52
1:C:255:TYR:CD1	1:C:256:ILE:N	2.77	0.52
1:A:88:ILE:HG22	1:A:94:LYS:HG3	1.90	0.51
1:A:322:ASN:N	1:A:322:ASN:OD1	2.41	0.51
2:D:444:THR:HG22	2:D:446:GLY:H	1.76	0.51
2:B:385:THR:O	2:B:386:LYS:HG2	2.10	0.51
2:B:395:VAL:HG22	2:B:515:PHE:CD1	2.46	0.51
2:B:395:VAL:HG22	2:B:515:PHE:HD1	1.76	0.51
1:C:489:GLU:HG3	1:C:613:TYR:HE2	1.76	0.51
1:C:252:TYR:HB3	1:C:255:TYR:HE1	1.68	0.50
2:B:396:TYR:HB2	2:B:514:SER:HB3	1.93	0.50
1:A:402:GLU:HA	1:A:402:GLU:OE1	2.11	0.50
3:G:1:NAG:H61	3:G:2:NAG:C7	2.42	0.50
1:A:133:CYS:HA	1:A:141:CYS:HA	1.94	0.50
1:C:418:LEU:HB3	1:C:424:LEU:HD13	1.92	0.50
1:C:500:PRO:HB2	1:C:506:VAL:HG11	1.94	0.49
2:B:457:ARG:HG2	2:B:459:SER:O	2.12	0.49
1:C:396:ALA:HB1	1:C:566:TRP:HA	1.94	0.49
1:C:415:PRO:HG2	1:C:430:GLU:HG2	1.95	0.49
1:C:104:GLY:C	1:C:106:SER:H	2.20	0.49
2:B:336:CYS:O	2:B:338:PHE:N	2.42	0.49
2:B:461:LEU:HG	2:B:465:GLU:HB3	1.94	0.49
1:A:180:TYR:HA	1:A:183:TYR:HB3	1.95	0.48
1:C:489:GLU:HG3	1:C:613:TYR:CE2	2.48	0.48
2:D:362:VAL:HA	2:D:525:CYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:372:ALA:CB	2:D:436:TRP:HB2	2.43	0.48
1:C:378:HIS:HE1	1:C:402:GLU:HA	1.78	0.48
1:C:161:ARG:HE	1:C:266:LEU:HA	1.79	0.48
1:C:555:PHE:O	1:C:559:ARG:HG2	2.14	0.48
2:B:372:ALA:CB	2:B:436:TRP:HB2	2.43	0.47
1:A:269:ASP:OD1	1:A:272:GLY:N	2.31	0.47
1:C:158:TYR:CD2	1:C:255:TYR:CZ	3.01	0.47
1:C:151:ILE:O	1:C:155:SER:HB3	2.14	0.47
2:D:497:PHE:CD2	2:D:507:PRO:HB3	2.50	0.47
1:A:218:SER:OG	1:A:221:GLN:HG3	2.15	0.47
2:D:396:TYR:HB2	2:D:514:SER:HB2	1.97	0.46
1:A:125:THR:O	1:A:129:THR:OG1	2.31	0.46
6:C:902:NAG:O7	6:C:902:NAG:O3	2.31	0.46
1:C:557:MET:HG2	1:C:569:ALA:HB1	1.96	0.46
2:B:372:ALA:HB3	2:B:436:TRP:HB2	1.96	0.46
1:C:109:SER:O	1:C:111:ASP:N	2.48	0.46
1:A:362:THR:HG23	1:A:368:ASP:HB3	1.97	0.46
1:A:524:GLN:HB3	1:A:574:VAL:HG11	1.98	0.46
2:D:431:GLY:HA2	2:D:515:PHE:CD2	2.51	0.46
2:B:359:SER:HA	2:B:524:VAL:CG2	2.42	0.46
1:C:105:SER:H	1:C:190:MET:CG	2.28	0.46
2:B:392:PHE:HB3	2:B:516:GLU:O	2.16	0.45
1:C:101:GLN:O	3:H:1:NAG:H82	2.17	0.45
1:A:294:THR:O	1:A:298:VAL:HG23	2.16	0.45
1:A:293:VAL:HG11	1:A:418:LEU:HD22	1.99	0.45
1:C:161:ARG:HD3	1:C:266:LEU:HD23	1.98	0.45
2:B:392:PHE:CD1	2:B:515:PHE:HB3	2.50	0.45
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.99	0.44
1:A:594:TRP:CZ2	1:A:598:GLN:HG3	2.52	0.44
1:A:402:GLU:HB3	1:A:518:ARG:HG3	1.98	0.44
1:A:232:GLU:HB2	1:A:581:VAL:HG11	2.00	0.44
1:C:360:MET:HE1	1:C:371:THR:HB	2.00	0.44
1:C:564:GLU:HB3	1:C:568:LEU:HD23	1.99	0.44
1:C:152:MET:HE1	1:C:161:ARG:HA	2.00	0.44
1:A:374:HIS:CE1	1:A:402:GLU:OE1	2.70	0.44
1:A:578:ASN:OD1	1:A:579:MET:N	2.49	0.44
2:D:335:LEU:HD23	2:D:362:VAL:HG13	1.98	0.44
1:C:574:VAL:HG23	1:C:576:ALA:H	1.82	0.44
1:A:541:LYS:HE2	1:A:541:LYS:HB3	1.75	0.43
1:C:19:SER:O	1:C:24:GLN:NE2	2.49	0.43
1:C:109:SER:O	1:C:112:LYS:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ARG:NE	1:C:265:HIS:O	2.52	0.43
1:A:314:PHE:O	1:A:317:SER:OG	2.32	0.42
1:A:134:ASN:OD1	1:A:137:ASN:N	2.52	0.42
1:A:327:PHE:HE2	1:A:358:ILE:HG13	1.85	0.42
1:C:132:VAL:HG12	1:C:171:GLU:OE1	2.19	0.42
1:C:418:LEU:CB	1:C:424:LEU:HD13	2.49	0.42
1:C:538:PRO:HD2	1:C:541:LYS:HD3	2.01	0.42
1:A:144:LEU:O	1:A:149:ASN:HB2	2.19	0.42
1:C:457:GLU:HG3	1:C:461:TRP:CE2	2.54	0.42
1:A:455:MET:C	1:A:455:MET:SD	3.02	0.42
1:C:474:MET:HE1	1:C:500:PRO:HD2	2.01	0.42
1:C:174:LYS:HA	1:C:496:THR:O	2.19	0.42
1:A:527:GLU:HG3	1:A:539:LEU:HD22	2.02	0.42
1:A:169:ARG:HH22	1:A:271:TRP:HA	1.85	0.42
1:C:385:TYR:CE1	1:C:393:ARG:HB3	2.55	0.41
1:A:165:TRP:CH2	1:A:490:PRO:HD2	2.55	0.41
1:A:378:HIS:HE1	1:A:402:GLU:HA	1.85	0.41
2:D:334:ASN:O	2:D:362:VAL:HG12	2.21	0.41
2:B:382:VAL:HG23	2:B:390:LEU:HD12	2.02	0.41
2:D:398:ASP:O	2:D:511:VAL:HA	2.20	0.41
1:C:84:PRO:HB2	1:C:87:GLU:HG3	2.03	0.41
1:C:454:TYR:O	1:C:458:LYS:HB2	2.20	0.41
2:B:355:ARG:HE	2:B:396:TYR:HB3	1.86	0.41
2:B:395:VAL:CG2	2:B:524:VAL:HG11	2.51	0.41
2:B:497:PHE:CE2	2:B:507:PRO:HB3	2.56	0.41
1:C:255:TYR:HD1	1:C:256:ILE:N	2.17	0.41
1:A:156:LEU:HD22	1:A:281:LEU:HD11	2.02	0.41
1:C:392:LEU:HD13	1:C:563:SER:HA	2.03	0.41
1:A:237:TYR:CZ	1:A:451:PRO:HG2	2.56	0.40
1:C:381:TYR:CE1	1:C:558:LEU:HA	2.56	0.40
1:C:453:THR:HG23	1:C:512:PHE:CD2	2.56	0.40
1:C:535:HIS:CG	1:C:542:CYS:HB2	2.57	0.40
1:A:357:ARG:NH2	2:B:500:THR:OG1	2.54	0.40
1:A:450:LEU:HD21	1:A:519:THR:HG21	2.04	0.40
2:B:412:PRO:HG3	2:B:429:PHE:HB3	2.02	0.40
1:C:394:ASN:OD1	1:C:395:GLY:N	2.53	0.40
1:A:233:ILE:HG13	1:A:581:VAL:HG21	2.03	0.40
2:D:443:SER:HB3	2:D:499:PRO:N	2.35	0.40
2:B:438:SER:OG	2:B:509:ARG:HG3	2.21	0.40
1:C:189:GLU:HG2	1:C:192:ARG:HH12	1.85	0.40
1:C:248:LEU:HB3	1:C:256:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:TYR:C	1:C:385:TYR:CD1	3.00	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ASN:ND2	1:C:254:SER:O[4_444]	2.15	0.05

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	594/805 (74%)	577 (97%)	16 (3%)	1 (0%)	43	74
1	C	595/805 (74%)	563 (95%)	31 (5%)	1 (0%)	43	74
2	B	194/247 (78%)	176 (91%)	17 (9%)	1 (0%)	24	58
2	D	194/247 (78%)	178 (92%)	16 (8%)	0	100	100
All	All	1577/2104 (75%)	1494 (95%)	80 (5%)	3 (0%)	43	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
2	B	344	ALA
1	C	54	ILE

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	526/711 (74%)	523 (99%)	3 (1%)	78	79
1	C	525/711 (74%)	523 (100%)	2 (0%)	84	81
2	B	168/216 (78%)	167 (99%)	1 (1%)	78	79
2	D	168/216 (78%)	167 (99%)	1 (1%)	78	79
All	All	1387/1854 (75%)	1380 (100%)	7 (0%)	81	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	ASP
1	A	322	ASN
1	A	402	GLU
2	B	500	THR
1	C	322	ASN
1	C	542	CYS
2	D	500	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	33	ASN
1	A	42	GLN
1	A	76	GLN
1	A	96	GLN
1	A	210	ASN
1	A	472	GLN
1	A	535	HIS
1	A	552	GLN
2	B	505	HIS
1	C	154	ASN
1	C	194	ASN
1	C	522	GLN
1	C	552	GLN
2	D	394	ASN

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)

9 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	E	1	1,3	14,14,15	0.27	0	17,19,21	0.46	0
3	NAG	E	2	3	14,14,15	0.31	0	17,19,21	0.63	0
4	NAG	F	1	1,4	14,14,15	0.18	0	17,19,21	0.50	0
4	NAG	F	2	4	14,14,15	0.28	0	17,19,21	0.53	0
4	BMA	F	3	4	11,11,12	0.64	0	15,15,17	0.72	0
3	NAG	G	1	1,3	14,14,15	0.22	0	17,19,21	0.73	0
3	NAG	G	2	3	14,14,15	0.31	0	17,19,21	0.47	0
3	NAG	H	1	1,3	14,14,15	0.15	0	17,19,21	0.53	0
3	NAG	H	2	3	14,14,15	0.25	0	17,19,21	0.47	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	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	3	BMA	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C1-C2-N2-C7
3	G	1	NAG	C1-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7
3	G	1	NAG	C3-C2-N2-C7

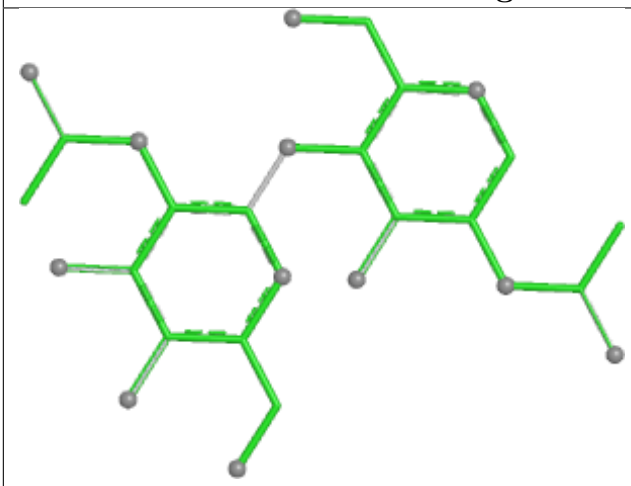
There are no ring outliers.

3 monomers are involved in 2 short contacts:

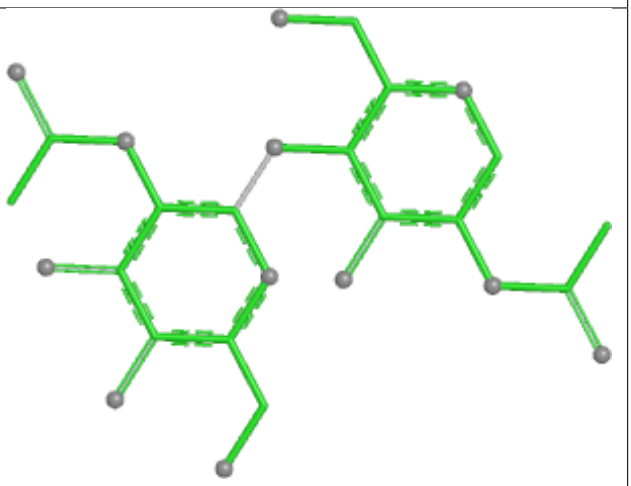
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
3	G	2	NAG	1	0
3	G	1	NAG	1	0

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

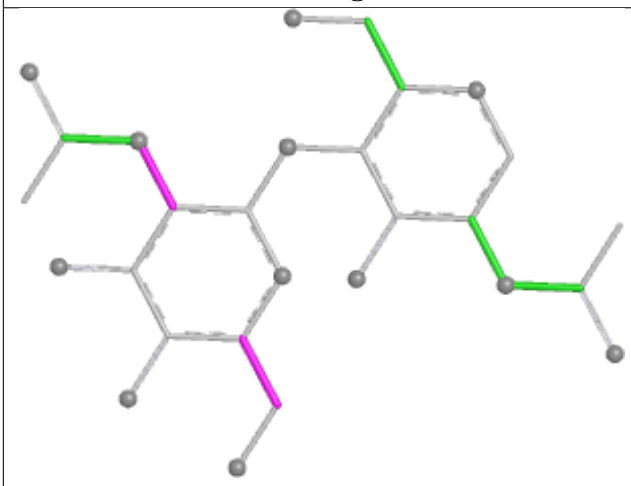
Oligosaccharide Chain E



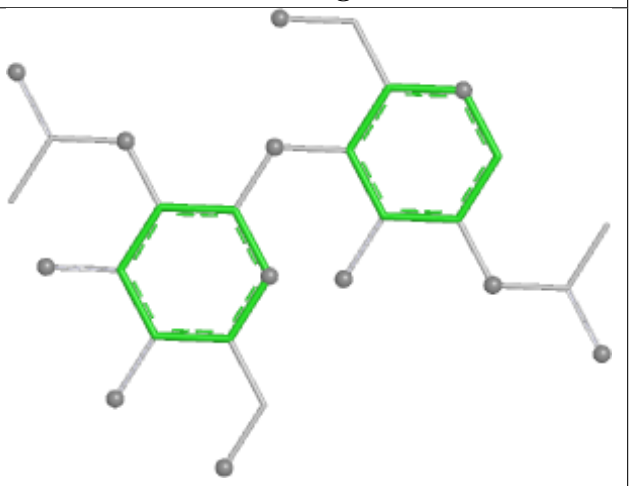
Bond lengths



Bond angles

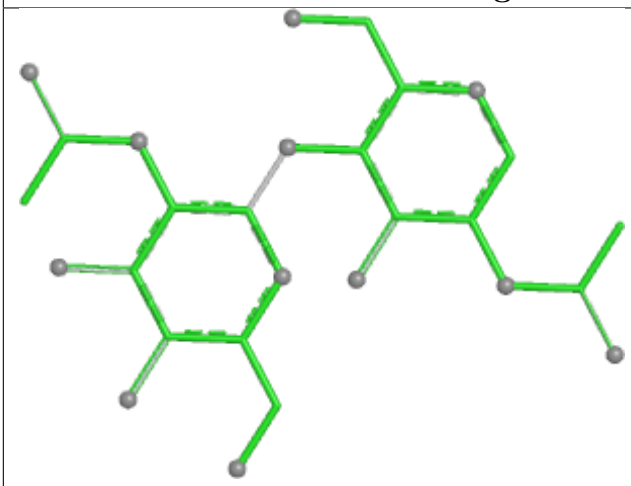


Torsions

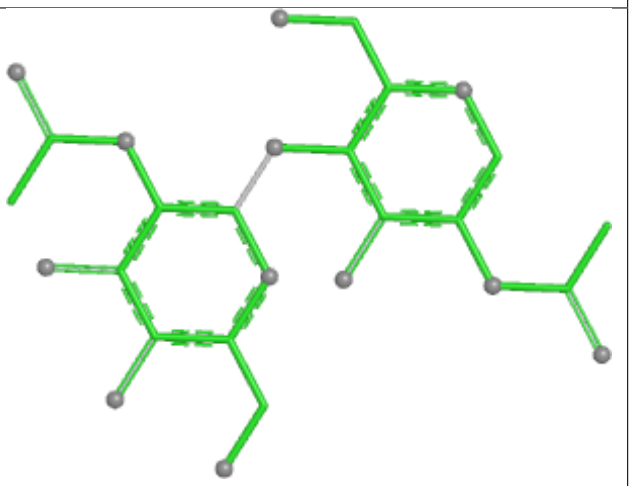


Rings

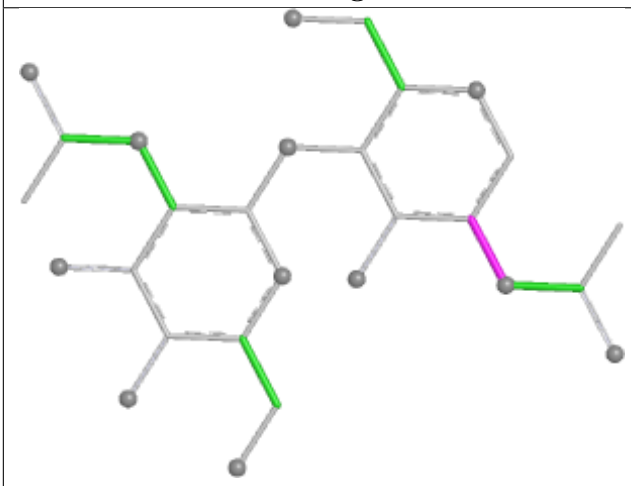
Oligosaccharide Chain G



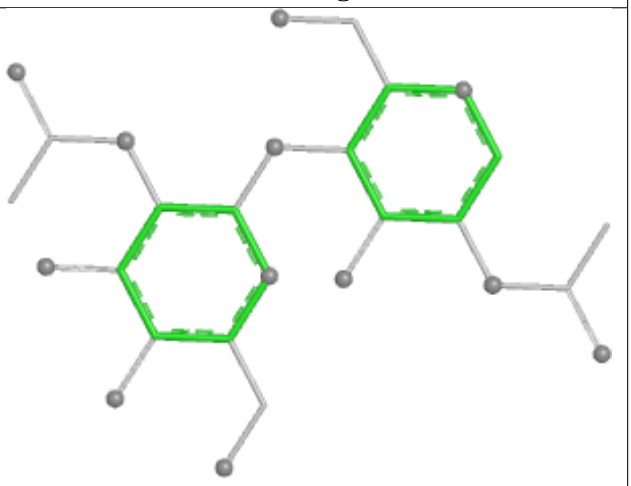
Bond lengths



Bond angles

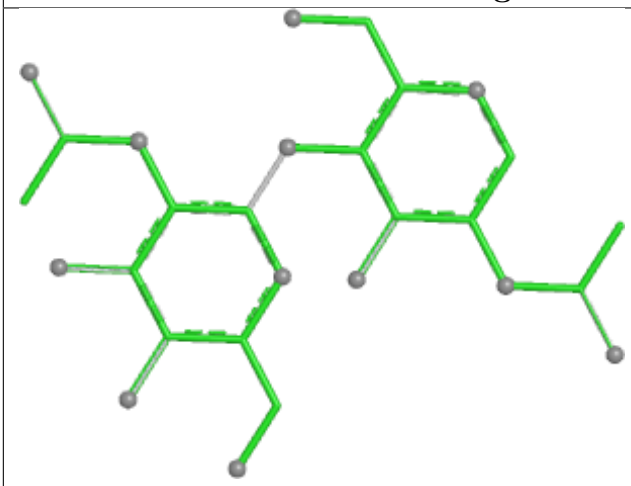


Torsions

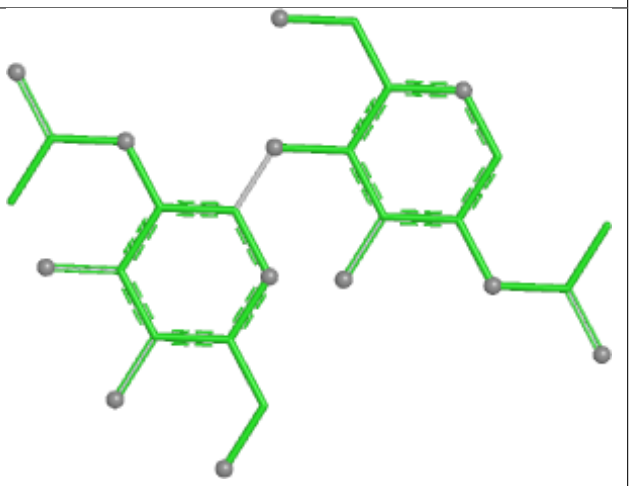


Rings

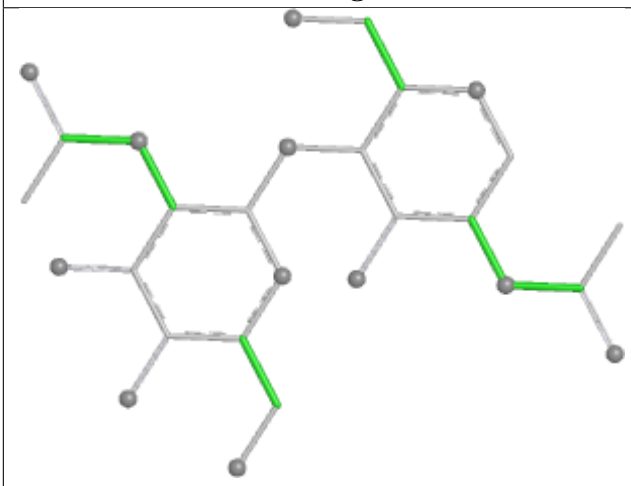
Oligosaccharide Chain H



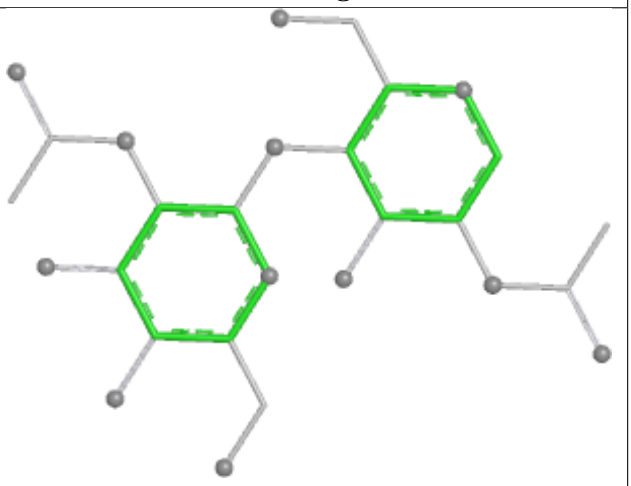
Bond lengths



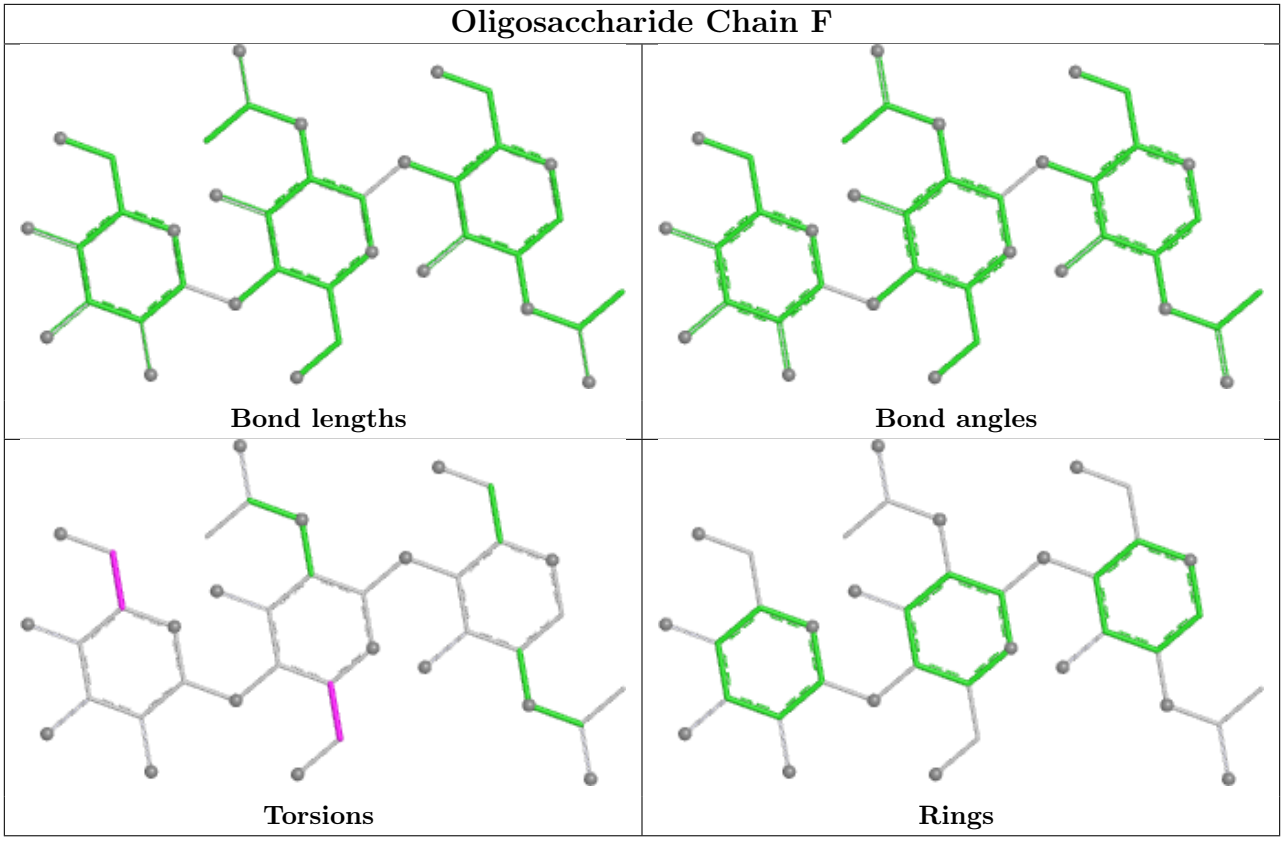
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	NAG	A	903	1	14,14,15	0.20	0	17,19,21	0.47	0
6	NAG	B	601	2	14,14,15	0.15	0	17,19,21	0.36	0
6	NAG	C	904	1	14,14,15	0.30	0	17,19,21	1.36	2 (11%)
6	NAG	C	902	1	14,14,15	0.62	1 (7%)	17,19,21	0.55	0
6	NAG	C	903	1	14,14,15	0.76	1 (7%)	17,19,21	0.58	0
6	NAG	A	904	1	14,14,15	0.35	0	17,19,21	0.46	0
6	NAG	A	902	1	14,14,15	0.35	0	17,19,21	0.46	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	NAG	A	903	1	-	2/6/23/26	0/1/1/1
6	NAG	B	601	2	-	2/6/23/26	0/1/1/1
6	NAG	C	904	1	-	6/6/23/26	0/1/1/1
6	NAG	C	902	1	-	1/6/23/26	0/1/1/1
6	NAG	C	903	1	-	2/6/23/26	0/1/1/1
6	NAG	A	904	1	-	0/6/23/26	0/1/1/1
6	NAG	A	902	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	903	NAG	C1-C2	2.62	1.55	1.52
6	C	902	NAG	C1-C2	2.13	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	904	NAG	C2-N2-C7	4.67	129.16	122.90
6	C	904	NAG	C1-C2-N2	2.17	113.86	110.43

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	902	NAG	O5-C5-C6-O6
6	A	902	NAG	C4-C5-C6-O6
6	A	903	NAG	C4-C5-C6-O6
6	B	601	NAG	C8-C7-N2-C2
6	B	601	NAG	O7-C7-N2-C2
6	C	904	NAG	C8-C7-N2-C2
6	C	904	NAG	O7-C7-N2-C2
6	A	903	NAG	O5-C5-C6-O6
6	C	903	NAG	O5-C5-C6-O6
6	C	904	NAG	C4-C5-C6-O6
6	C	903	NAG	C4-C5-C6-O6
6	C	904	NAG	O5-C5-C6-O6
6	C	902	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	C	904	NAG	C1-C2-N2-C7
6	C	904	NAG	C3-C2-N2-C7

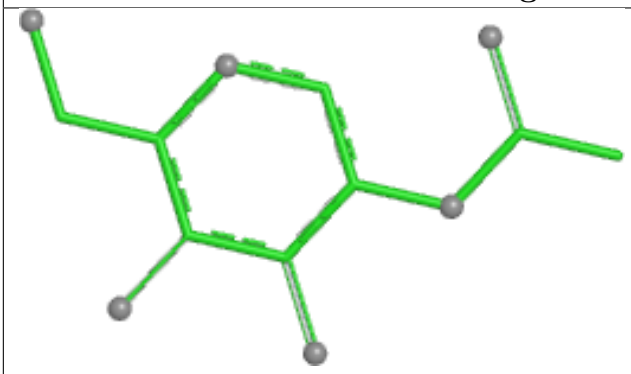
There are no ring outliers.

2 monomers are involved in 2 short contacts:

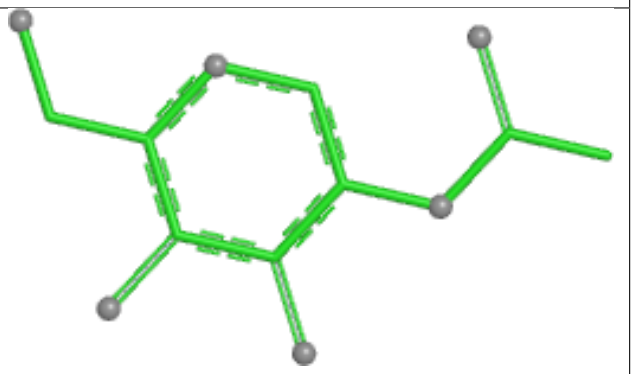
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	904	NAG	1	0
6	C	902	NAG	1	0

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

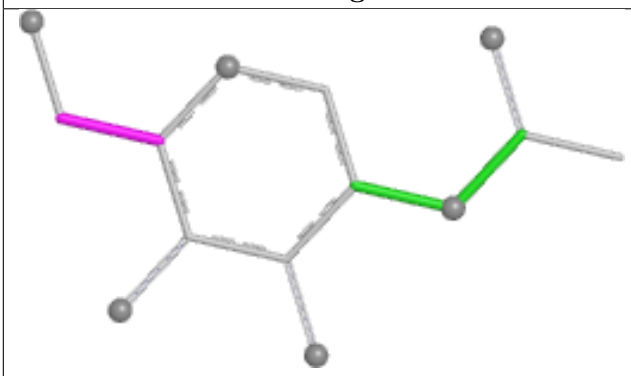
Ligand NAG A 903



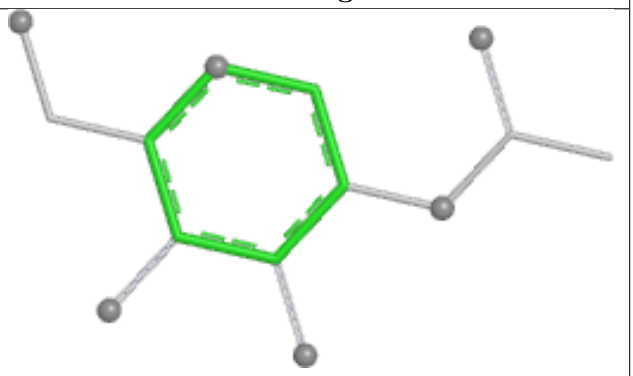
Bond lengths



Bond angles

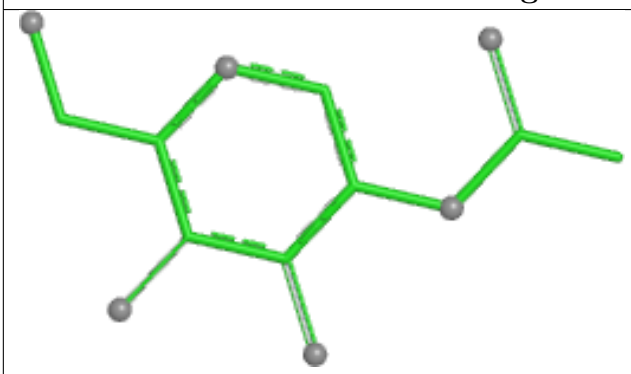


Torsions

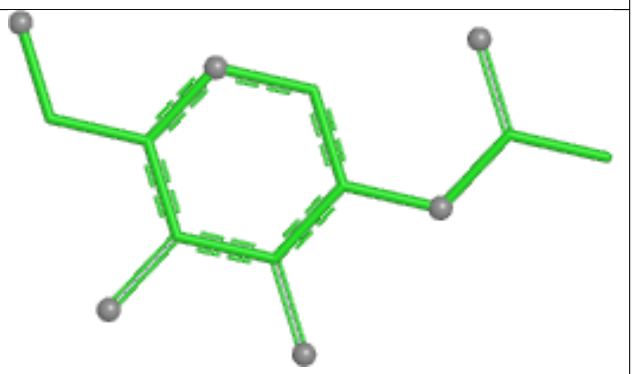


Rings

Ligand NAG B 601



Bond lengths



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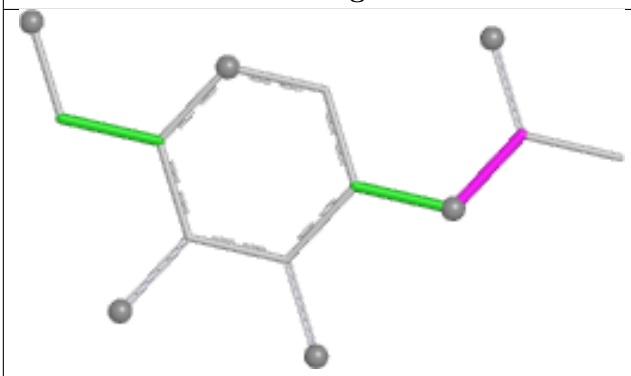

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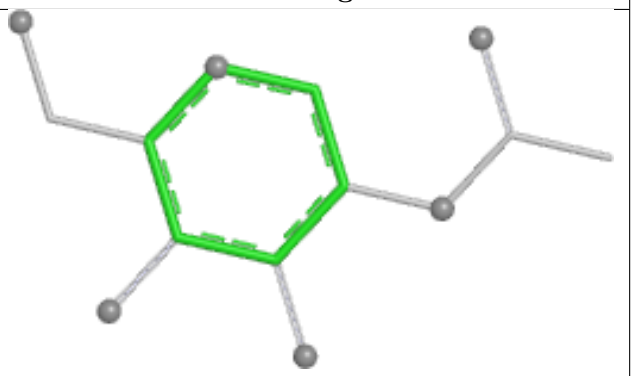
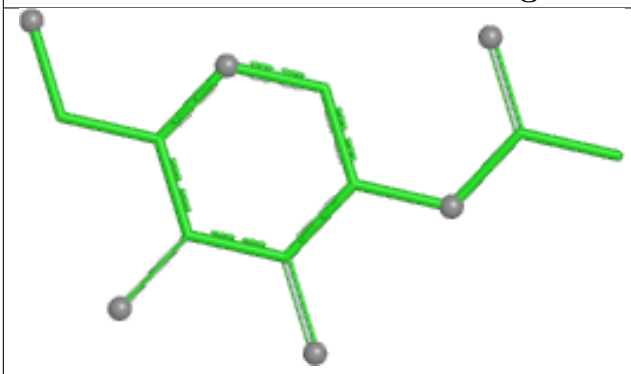
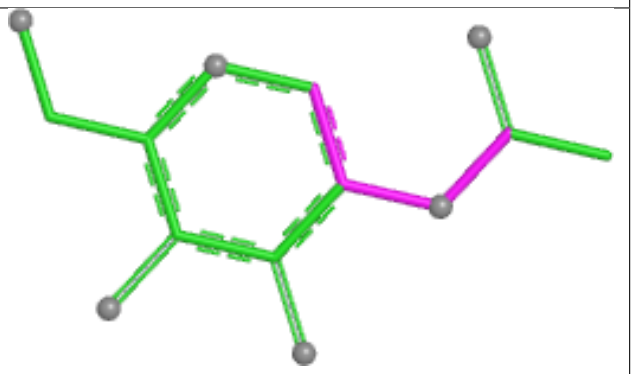


Rings

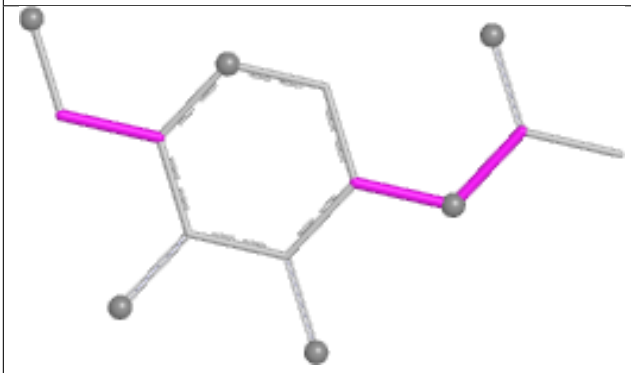
Ligand NAG C 904



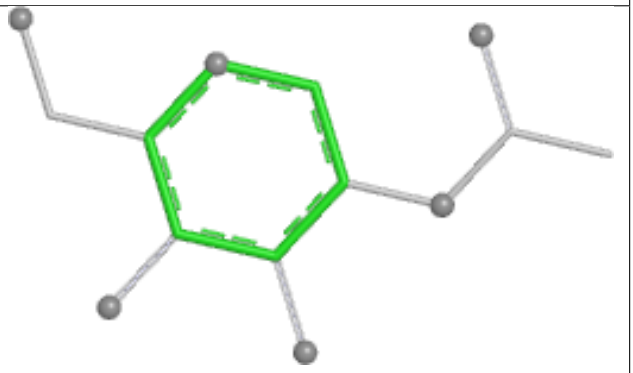
Bond lengths



Bond angles

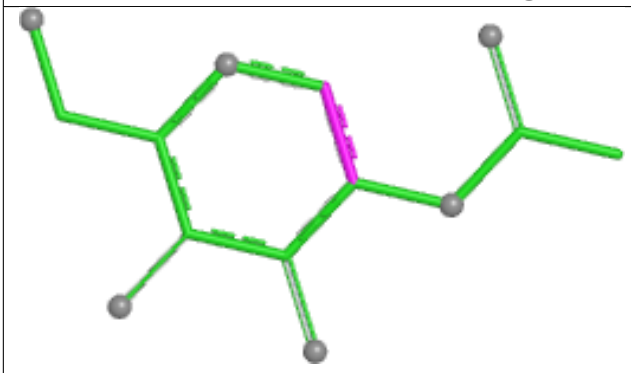


Torsions

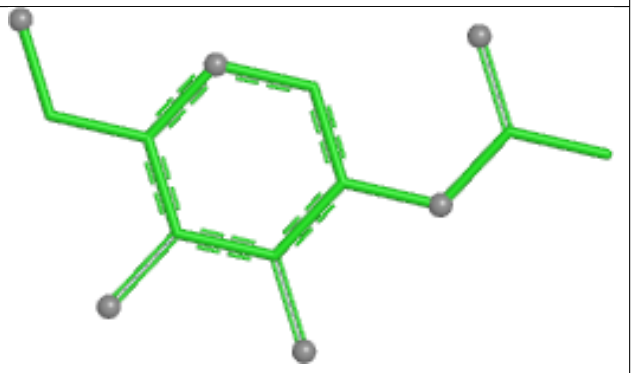


Rings

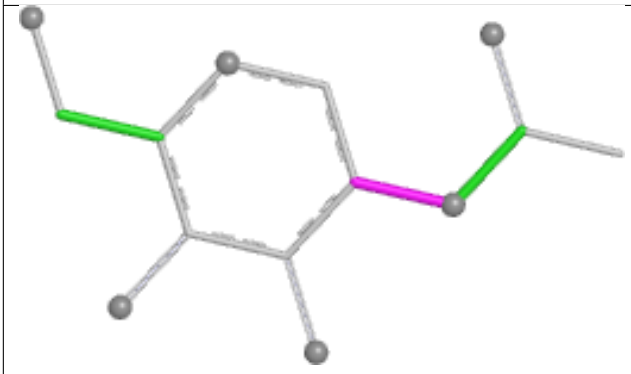
Ligand NAG C 902



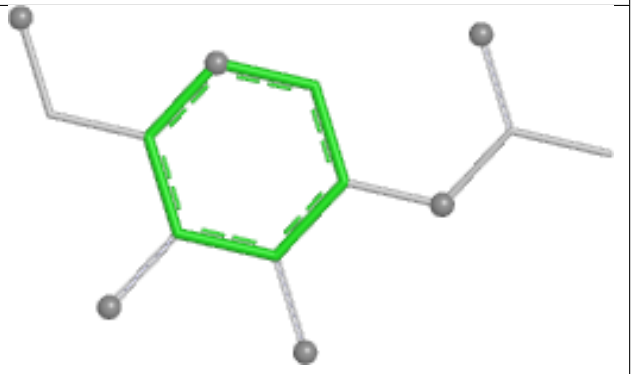
Bond lengths



Bond angles

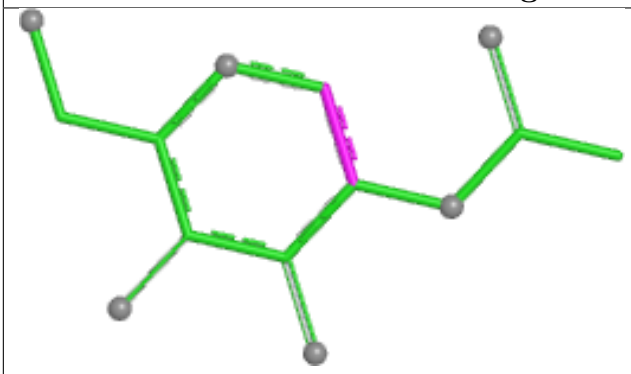


Torsions



Rings

Ligand NAG C 903



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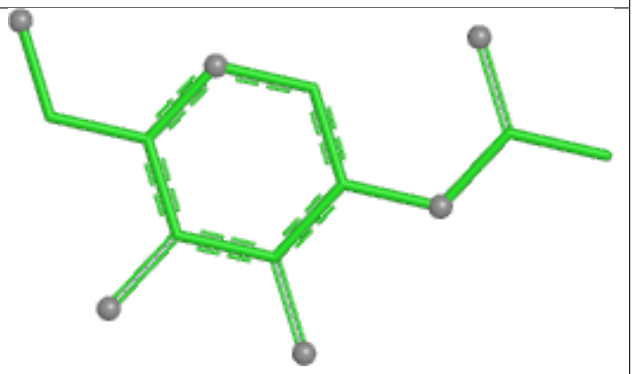

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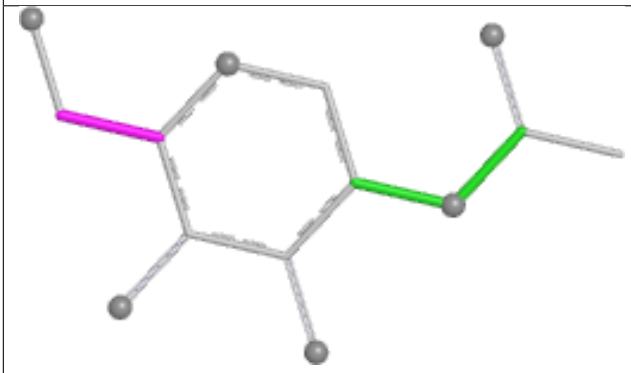

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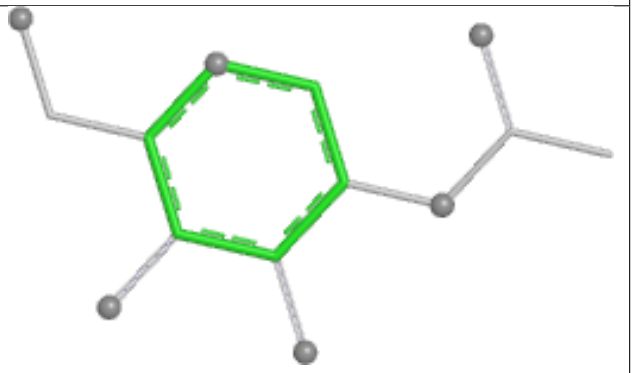
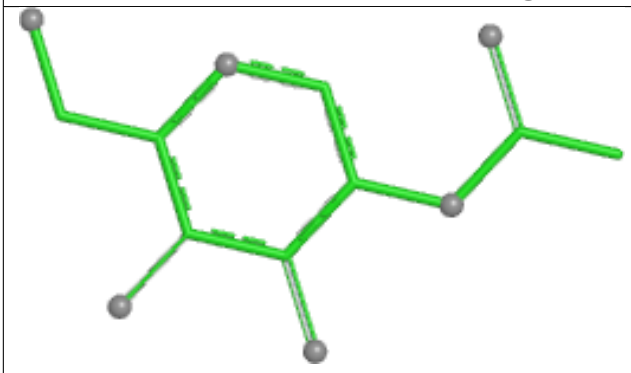


Rings

Ligand NAG A 904



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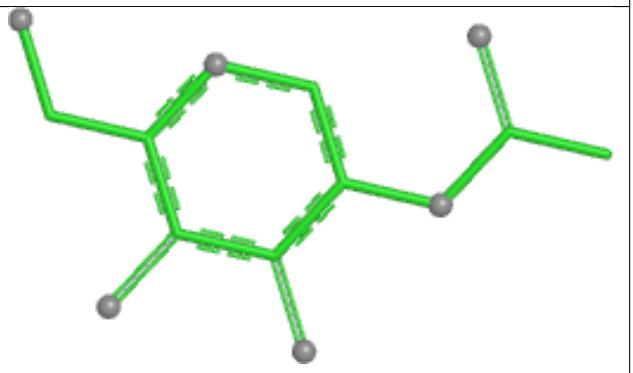
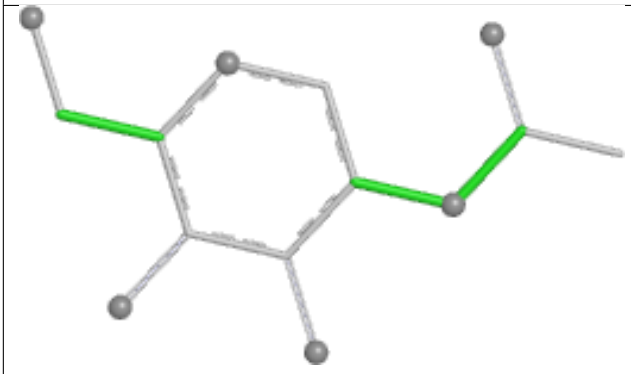
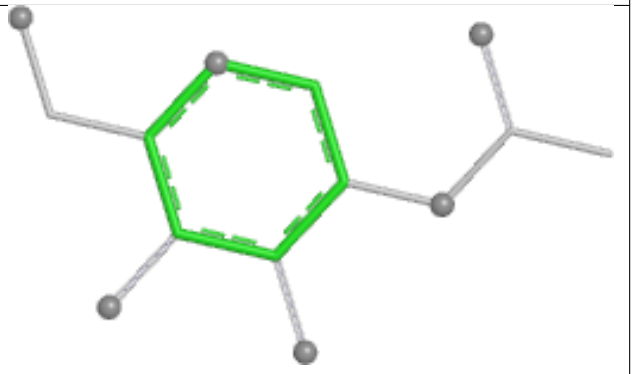


Bond angles

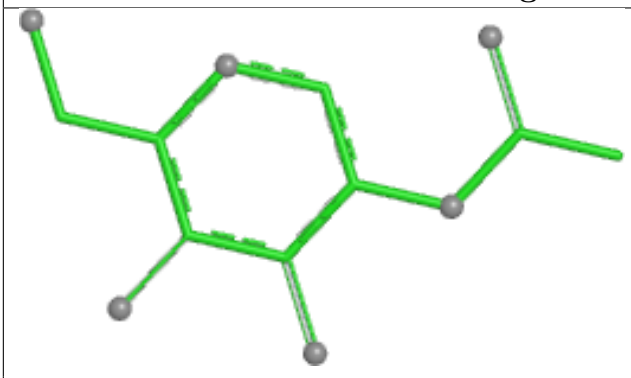


Torsions

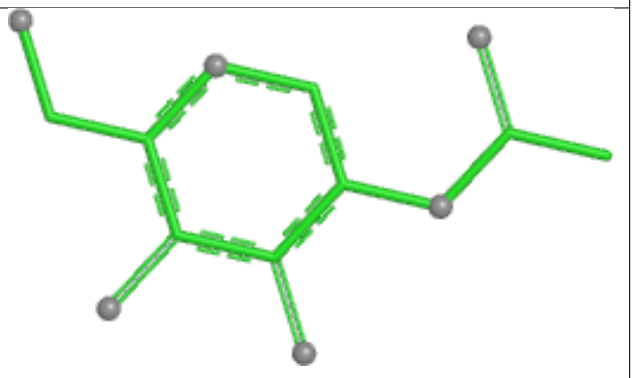


Rings

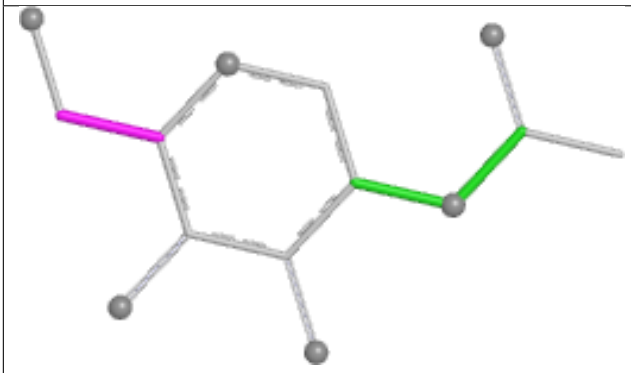
Ligand NAG A 902



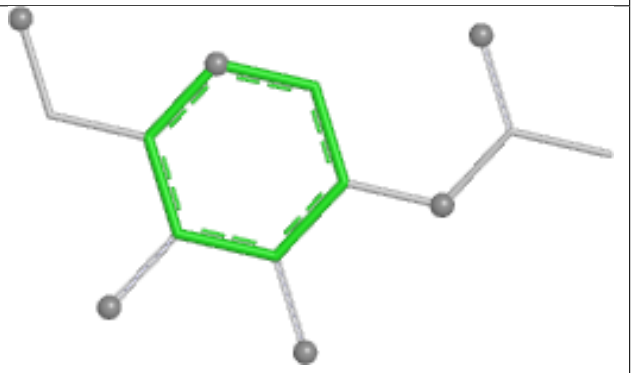
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	596/805 (74%)	-0.42	0 100 100	46, 78, 133, 196	0
1	C	596/805 (74%)	-0.29	4 (0%) 84 63	42, 82, 143, 270	1 (0%)
2	B	195/247 (78%)	0.02	5 (2%) 57 34	38, 99, 212, 280	1 (0%)
2	D	195/247 (78%)	0.08	6 (3%) 51 30	57, 96, 212, 267	1 (0%)
All	All	1582/2104 (75%)	-0.25	15 (0%) 81 58	38, 83, 175, 280	3 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	493[A]	GLN	4.3
2	B	527	PRO	4.3
1	C	255	TYR	4.3
2	D	365	TYR	3.4
2	D	364	ASP	2.9
2	D	372	ALA	2.8
2	B	374	PHE	2.8
2	D	527	PRO	2.6
2	D	373	PRO	2.4
1	C	134	ASN	2.3
1	C	254	SER	2.2
2	B	508	TYR	2.1
2	D	374	PHE	2.1
2	B	373	PRO	2.1
1	C	144	LEU	2.0

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)

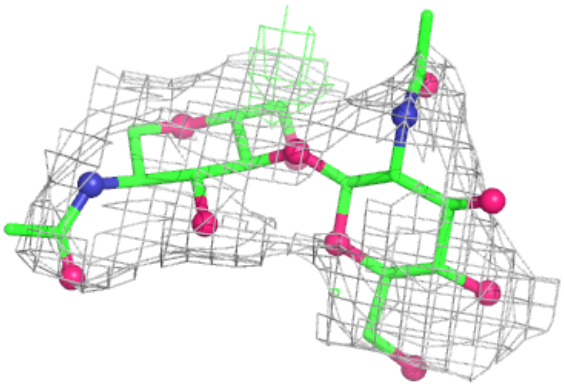
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

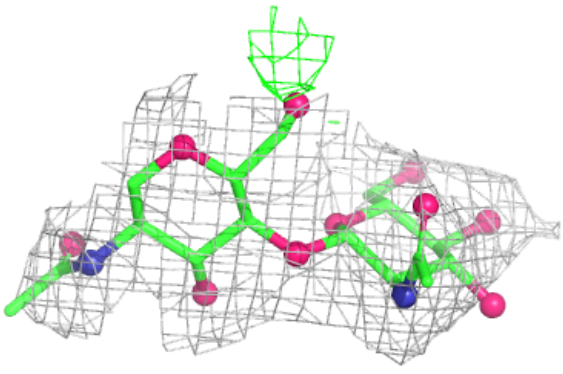
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	H	2	14/15	0.42	0.12	131,157,165,165	0
4	BMA	F	3	11/12	0.50	0.09	133,159,169,170	0
3	NAG	E	2	14/15	0.71	0.10	104,118,131,131	0
3	NAG	G	2	14/15	0.75	0.09	100,118,128,128	0
3	NAG	H	1	14/15	0.79	0.10	117,128,142,146	0
4	NAG	F	2	14/15	0.83	0.07	137,146,159,163	0
3	NAG	G	1	14/15	0.84	0.10	77,94,102,105	0
4	NAG	F	1	14/15	0.85	0.09	83,104,121,124	0
3	NAG	E	1	14/15	0.90	0.08	74,80,87,93	0

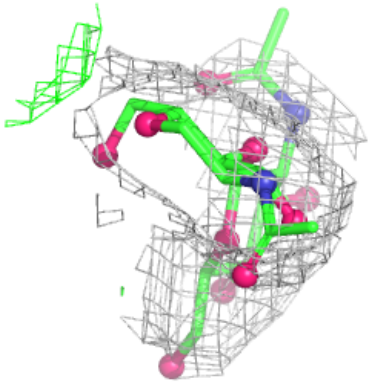
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

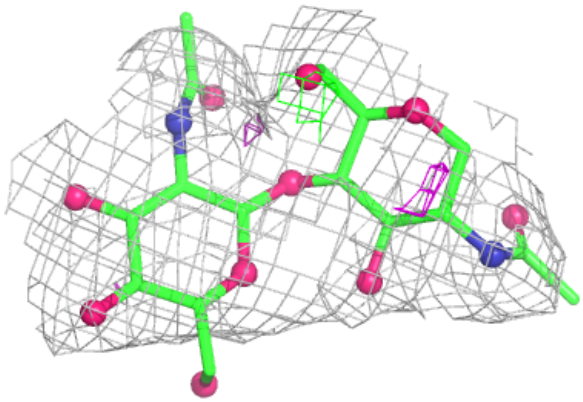


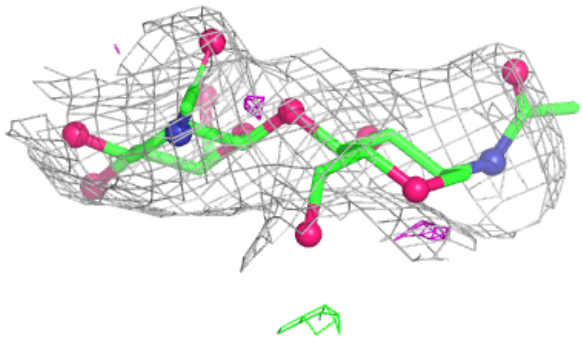


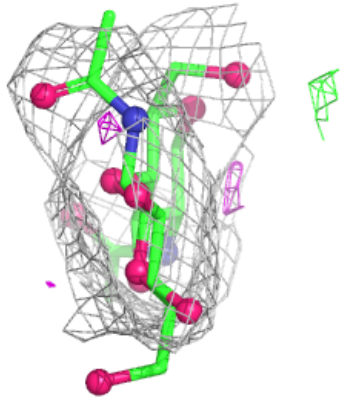


Electron density around Chain G:

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

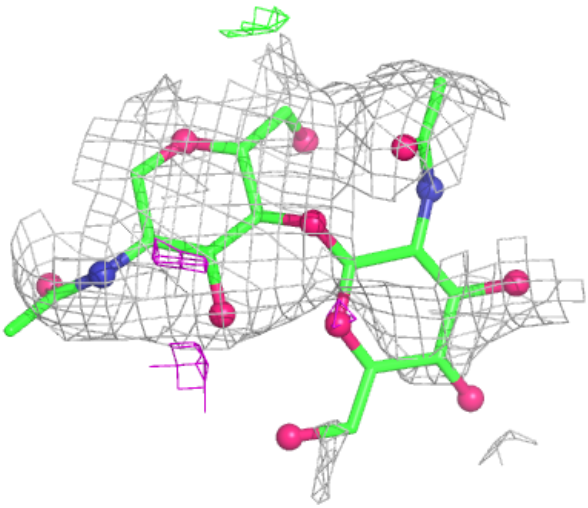


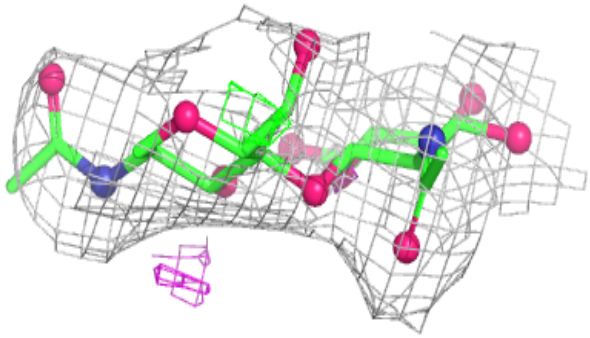


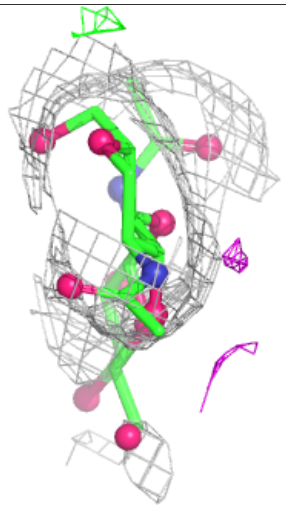


Electron density around Chain H:

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

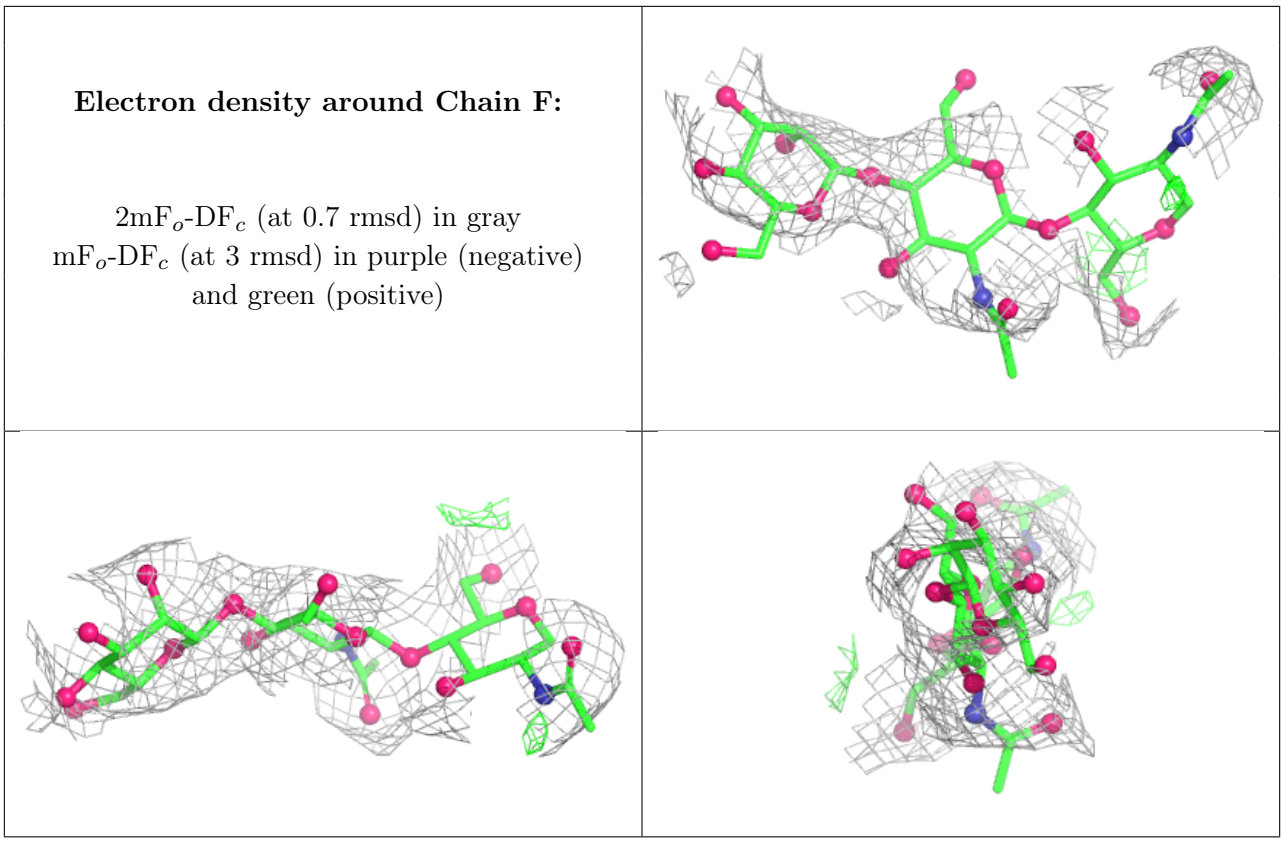






Electron density around Chain F:

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



6.4 Ligands

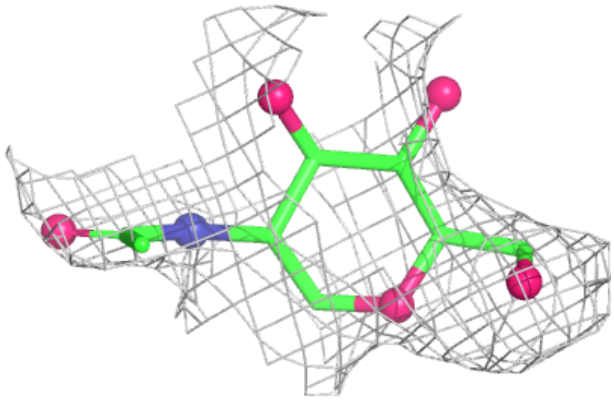
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

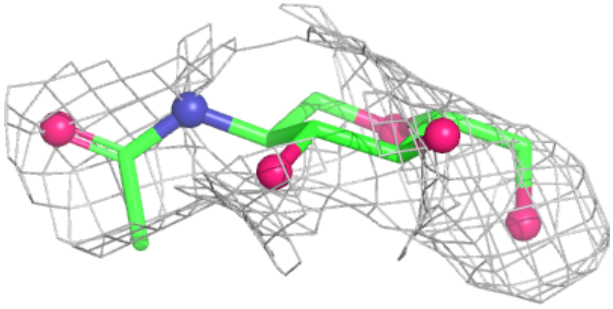
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	B	601	14/15	0.46	0.11	139,159,166,167	0
6	NAG	C	904	14/15	0.56	0.12	117,132,141,150	0
6	NAG	C	902	14/15	0.59	0.14	153,177,186,189	0
6	NAG	A	903	14/15	0.61	0.14	166,184,193,205	0
6	NAG	A	902	14/15	0.63	0.12	113,123,131,144	0
6	NAG	C	903	14/15	0.65	0.14	102,123,134,139	0
6	NAG	A	904	14/15	0.78	0.10	135,158,174,178	0
5	ZN	A	901	1/1	0.98	0.03	74,74,74,74	0
5	ZN	C	901	1/1	0.99	0.03	58,58,58,58	0

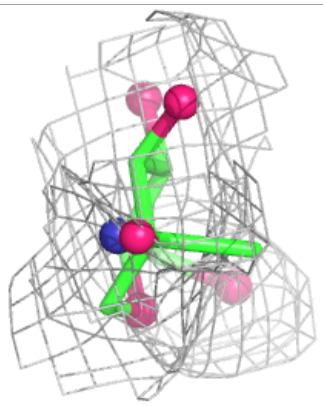
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG B 601:

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

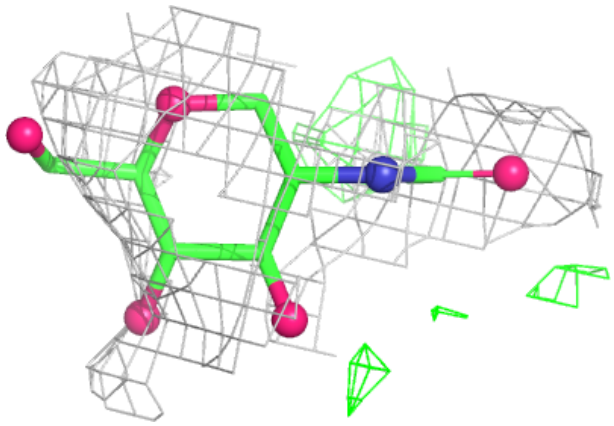


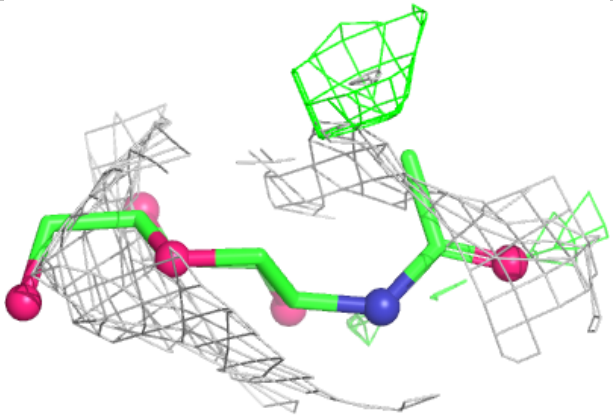


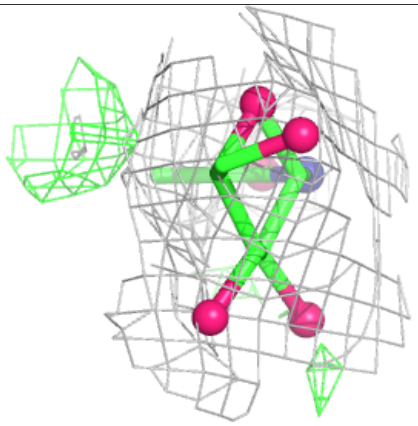


Electron density around NAG C 904:

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

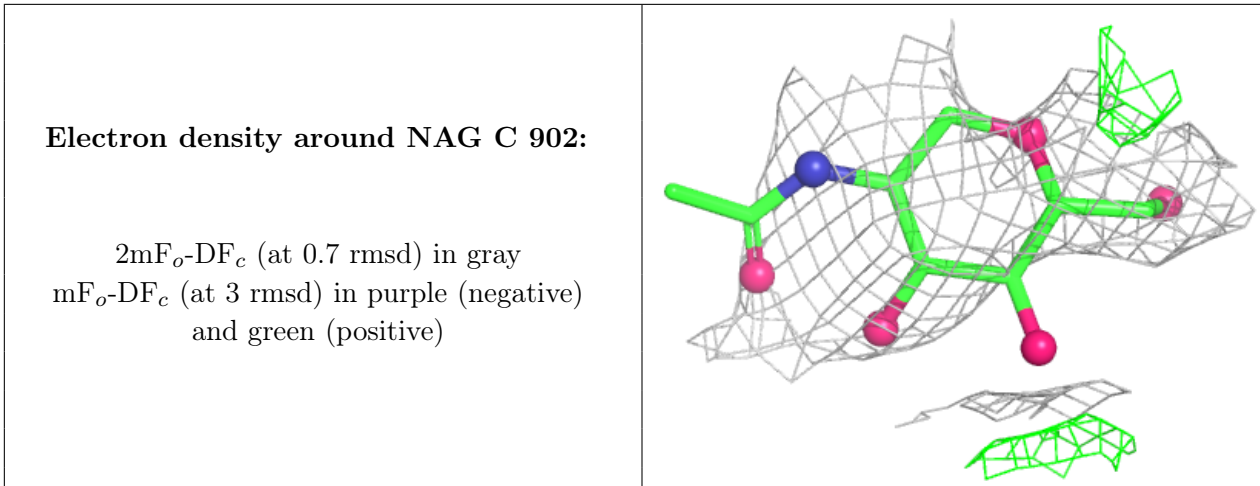


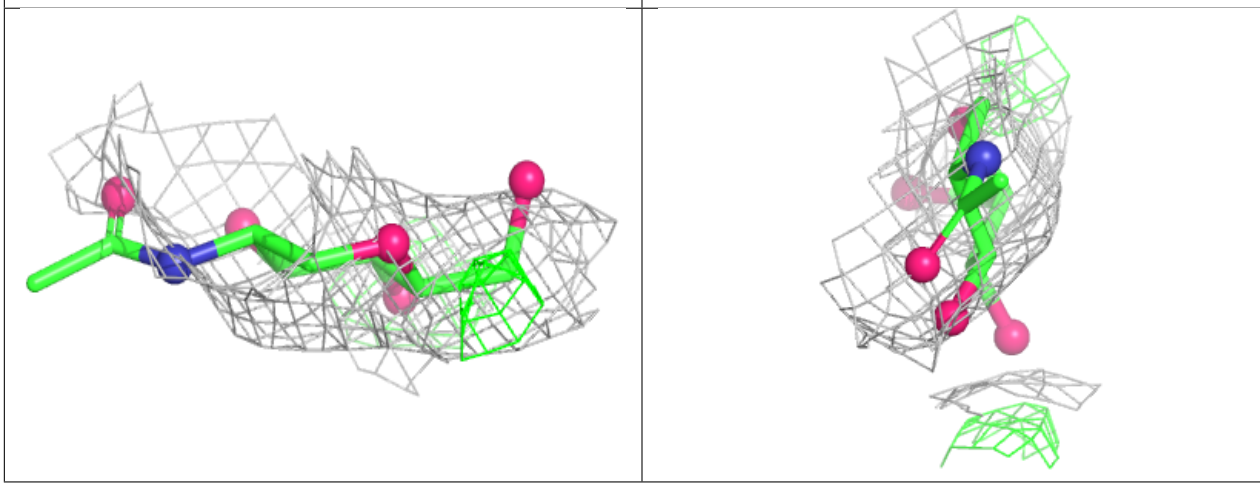




Electron density around NAG C 902:

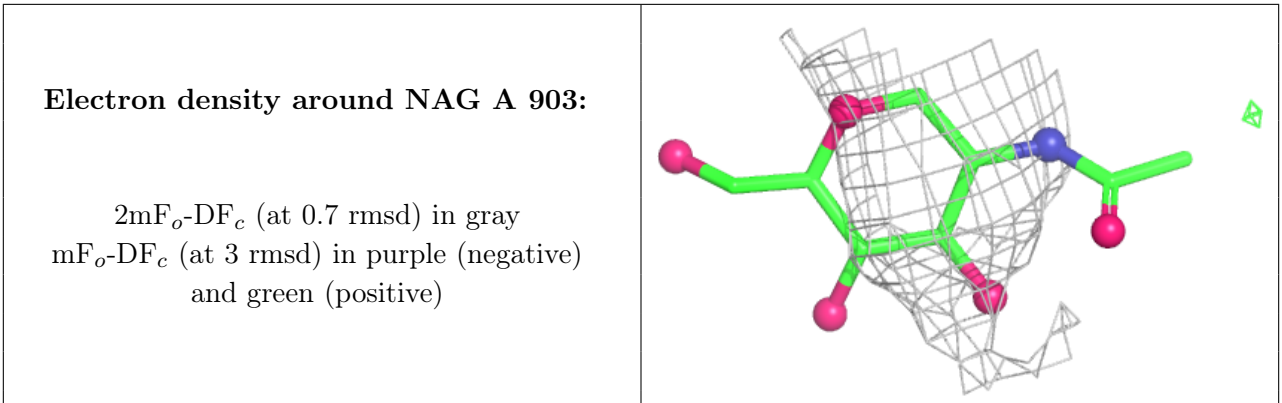
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

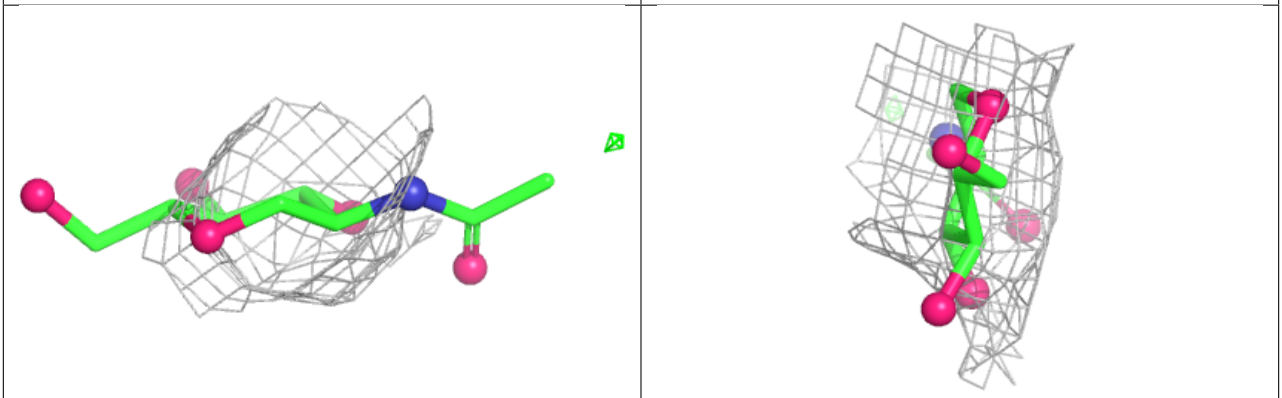




Electron density around NAG A 903:

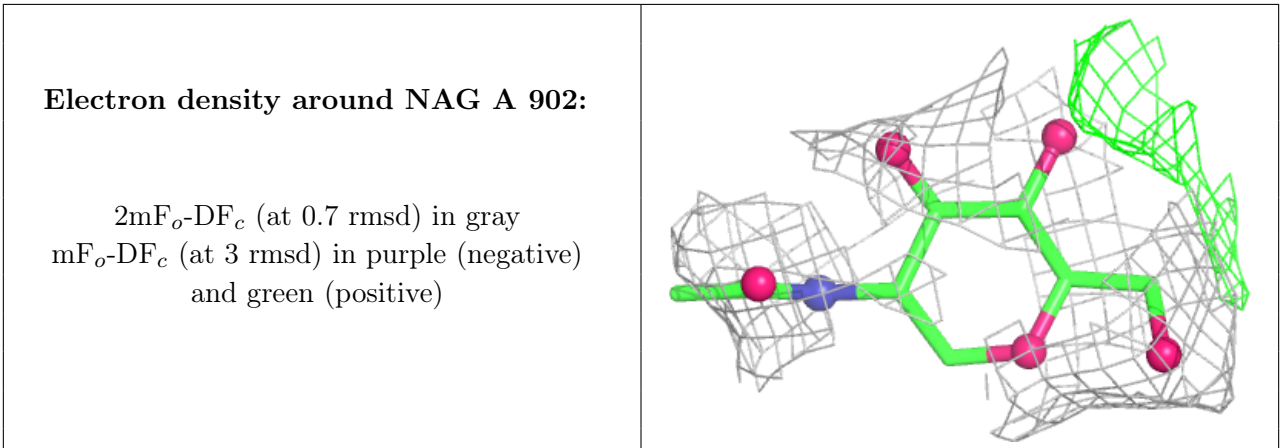
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

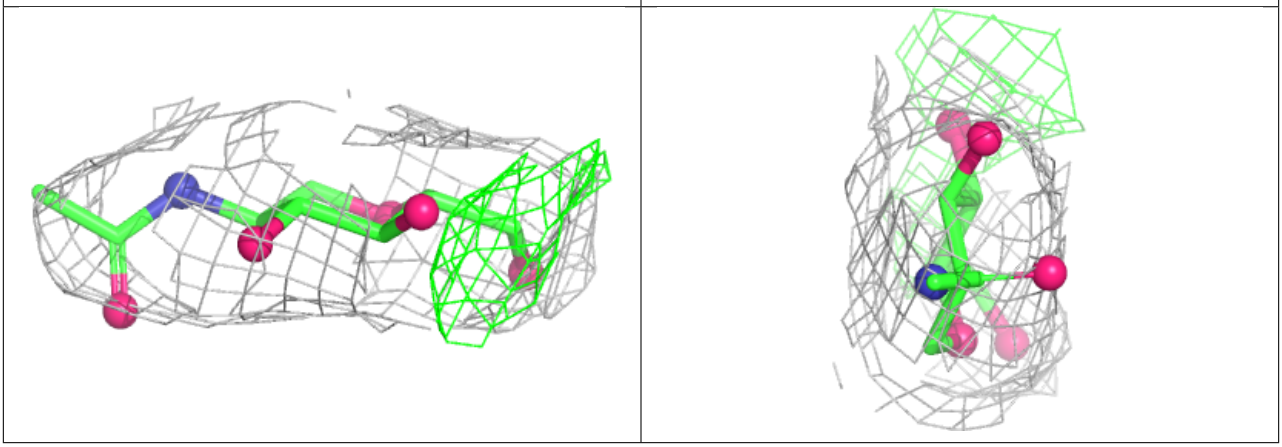




Electron density around NAG A 902:

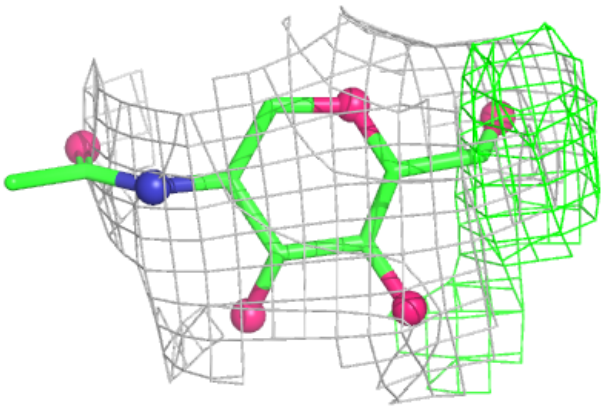
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

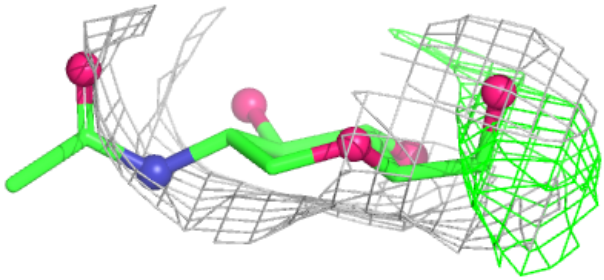


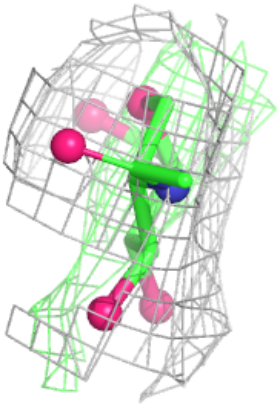


Electron density around NAG C 903:

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

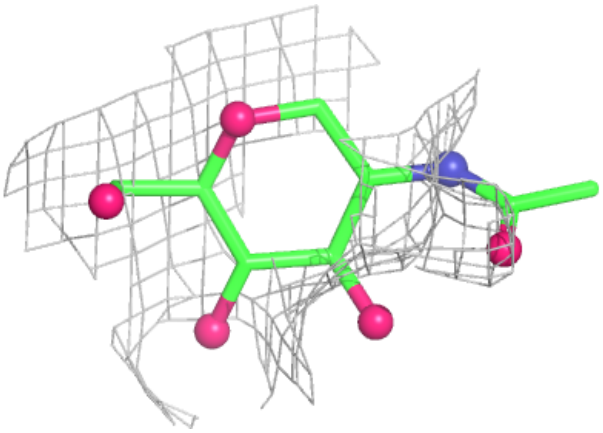


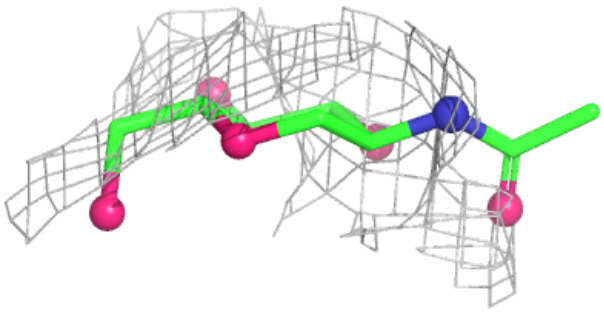


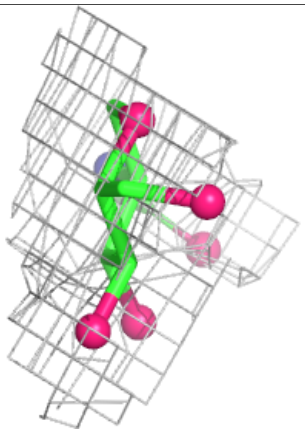


Electron density around NAG A 904:

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

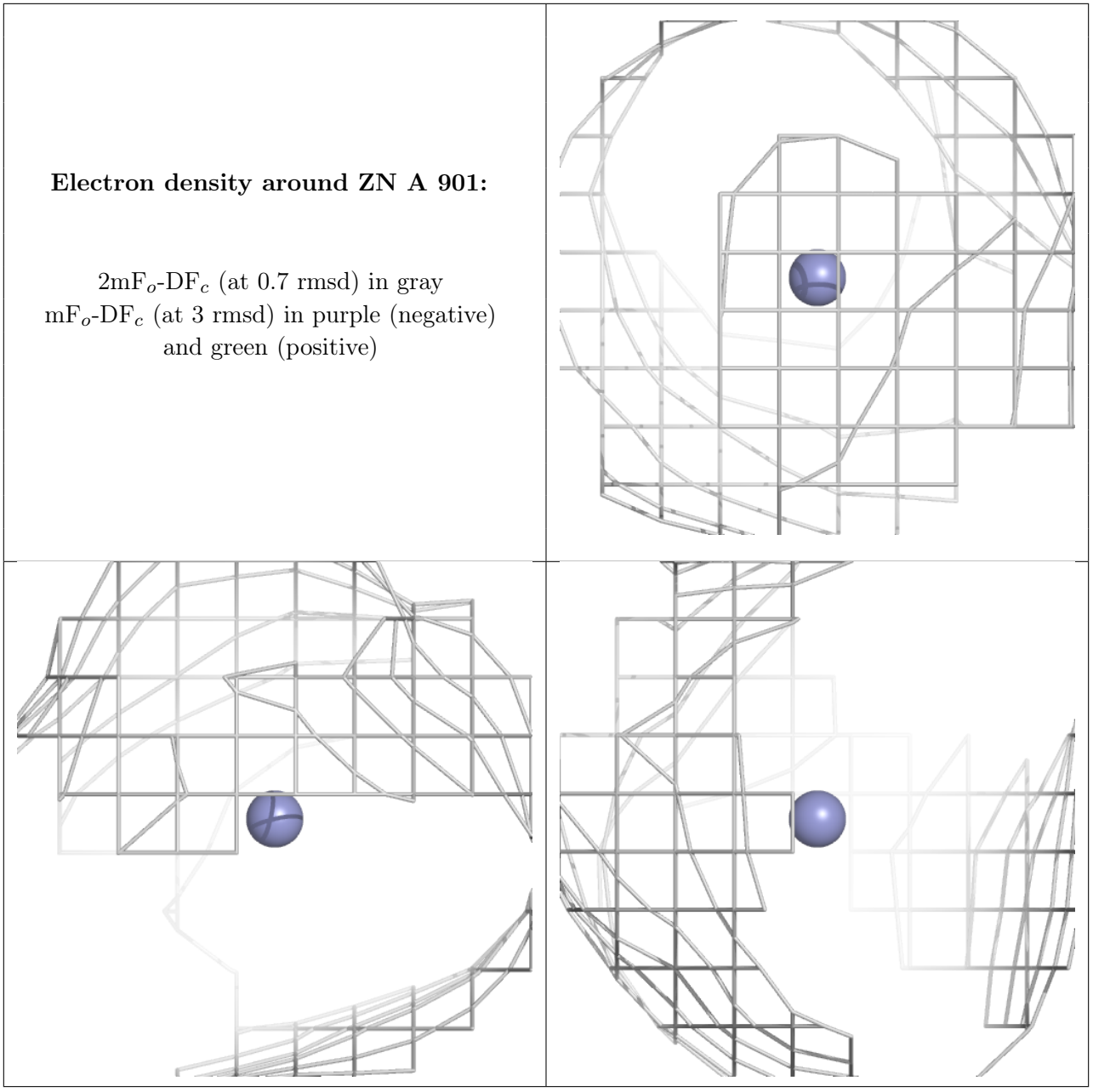






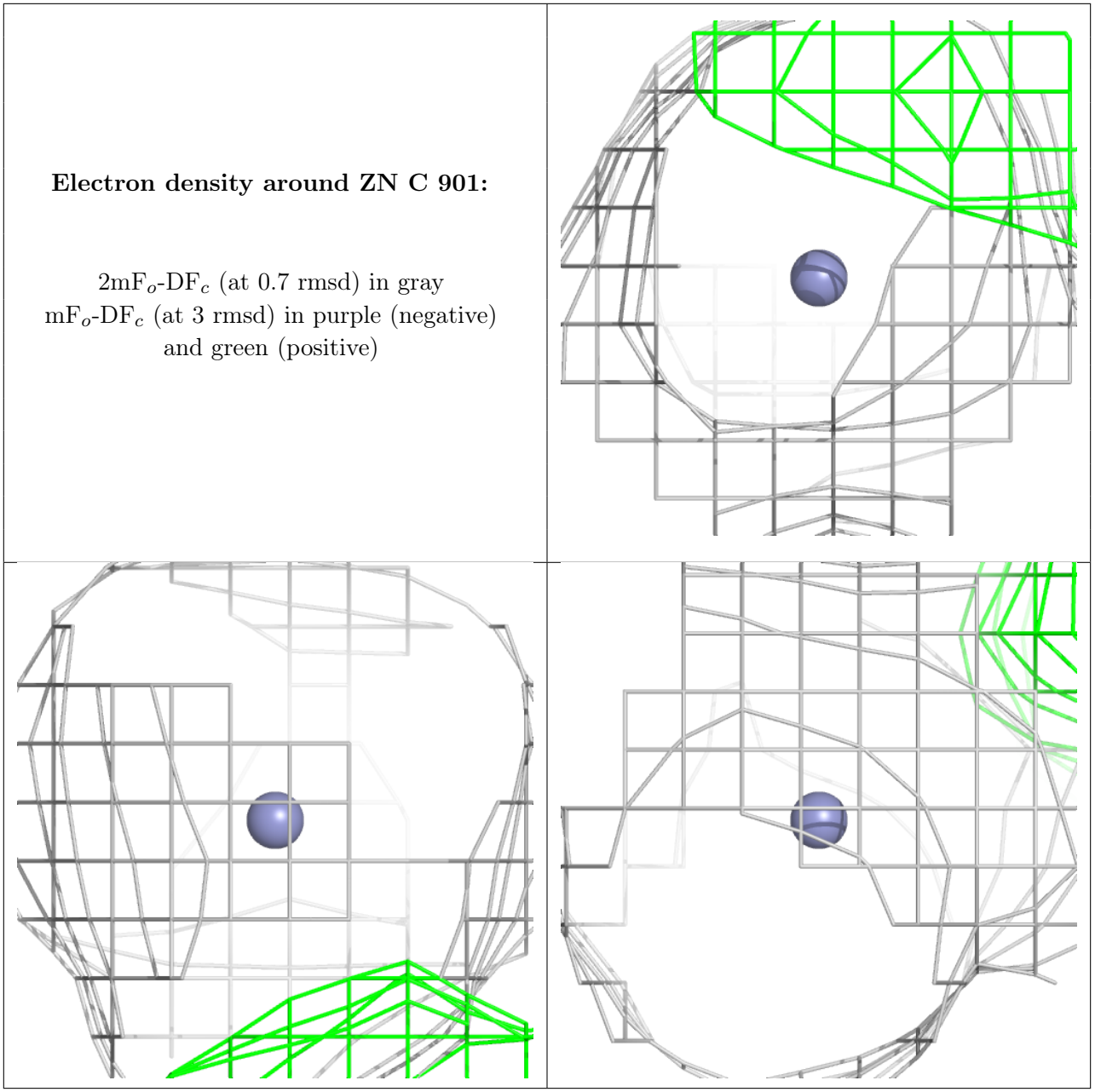
Electron density around ZN A 901:

$2mF_o$-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 901:

$2mF_o$-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.