



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2025 – 10:12 AM EDT

PDB ID : 9NR5 / pdb_00009nr5
Title : Crystal structure of H5 hemagglutinin Q226L mutant from the influenza virus A/black swan/Akita/1/2016 with LSTc
Authors : Lin, T.H.; Zhu, Y.; Wilson, I.A.
Deposited on : 2025-03-14
Resolution : 2.52 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

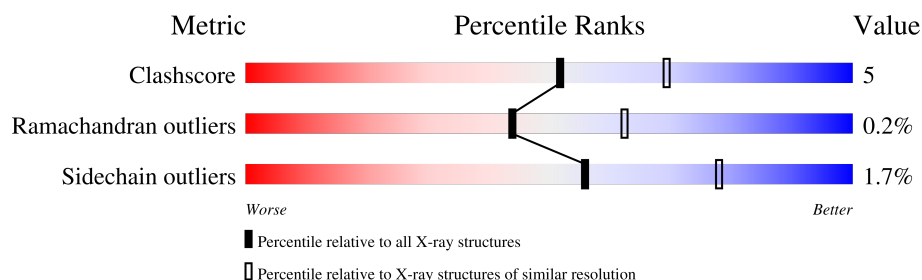
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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))
Clashscore	180529	7778 (2.54-2.50)
Ramachandran outliers	177936	7674 (2.54-2.50)
Sidechain outliers	177891	7676 (2.54-2.50)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	324	86% 11% ..
1	C	324	85% 14%
1	E	324	84% 15% .
2	B	177	84% 15% .
2	D	177	90% 8% .
2	F	177	86% 14%
3	G	2	100%
3	H	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	J	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>
4	I	3	<div><div></div><div>100%</div><div></div></div>
5	K	3	<div><div></div><div>33%</div><div></div><div>67%</div></div>
5	L	3	<div><div></div><div>33%</div><div></div><div>33%</div><div></div><div>33%</div></div>
5	M	3	<div><div></div><div>33%</div><div></div><div>67%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12294 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2537	1605	439	477	16			
1	C	323	Total	C	N	O	S	0	0	0
			2556	1617	444	479	16			
1	E	321	Total	C	N	O	S	0	0	0
			2537	1605	439	477	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP A0A1L7N0F8
A	10	GLY	-	expression tag	UNP A0A1L7N0F8
A	226	LEU	GLN	engineered mutation	UNP A0A1L7N0F8
C	9	PRO	-	expression tag	UNP A0A1L7N0F8
C	10	GLY	-	expression tag	UNP A0A1L7N0F8
C	226	LEU	GLN	engineered mutation	UNP A0A1L7N0F8
E	9	PRO	-	expression tag	UNP A0A1L7N0F8
E	10	GLY	-	expression tag	UNP A0A1L7N0F8
E	226	LEU	GLN	engineered mutation	UNP A0A1L7N0F8

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1414	878	247	281	8			
2	D	174	Total	C	N	O	S	0	0	0
			1414	878	247	281	8			
2	F	177	Total	C	N	O	S	0	0	0
			1435	889	253	285	8			

There are 9 discrepancies between the modelled and reference sequences:

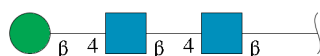
Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A1L7N0F8
B	176	GLY	-	expression tag	UNP A0A1L7N0F8
B	177	ARG	-	expression tag	UNP A0A1L7N0F8
D	175	SER	-	expression tag	UNP A0A1L7N0F8
D	176	GLY	-	expression tag	UNP A0A1L7N0F8
D	177	ARG	-	expression tag	UNP A0A1L7N0F8
F	175	SER	-	expression tag	UNP A0A1L7N0F8
F	176	GLY	-	expression tag	UNP A0A1L7N0F8
F	177	ARG	-	expression tag	UNP A0A1L7N0F8

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



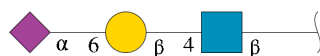
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



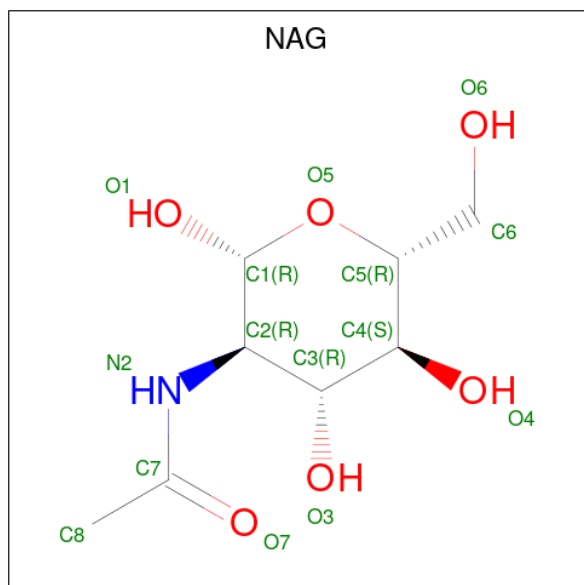
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	3	Total	C	N	O	0	0	0
			46	25	2	19			
5	L	3	Total	C	N	O	0	0	0
			46	25	2	19			
5	M	3	Total	C	N	O	0	0	0
			46	25	2	19			

- 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	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

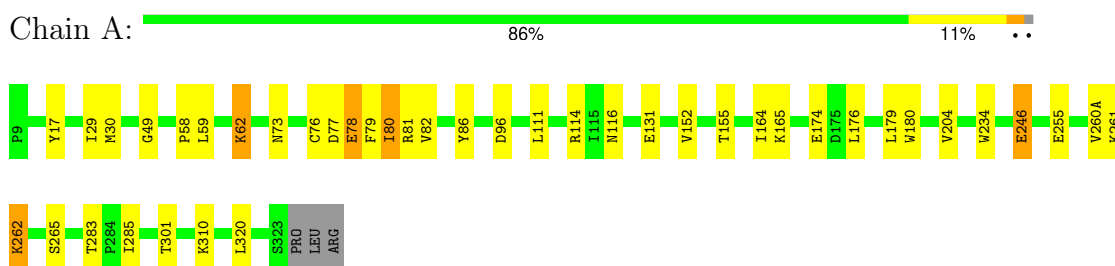
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	18	Total 18	O 18	0	0
7	B	7	Total 7	O 7	0	0
7	C	6	Total 6	O 6	0	0
7	D	5	Total 5	O 5	0	0
7	E	14	Total 14	O 14	0	0
7	F	6	Total 6	O 6	0	0

3 Residue-property plots [i](#)

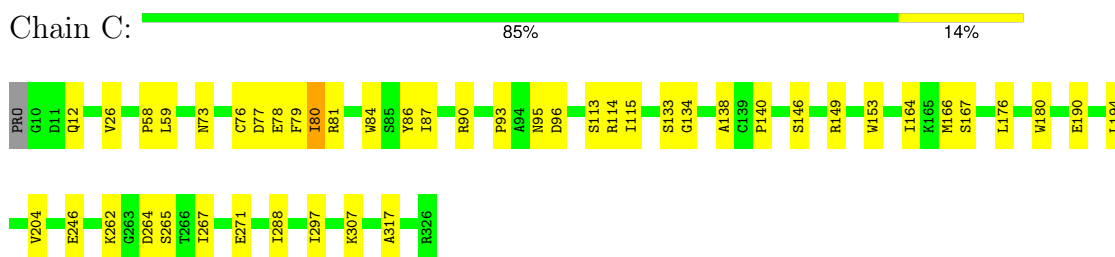
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

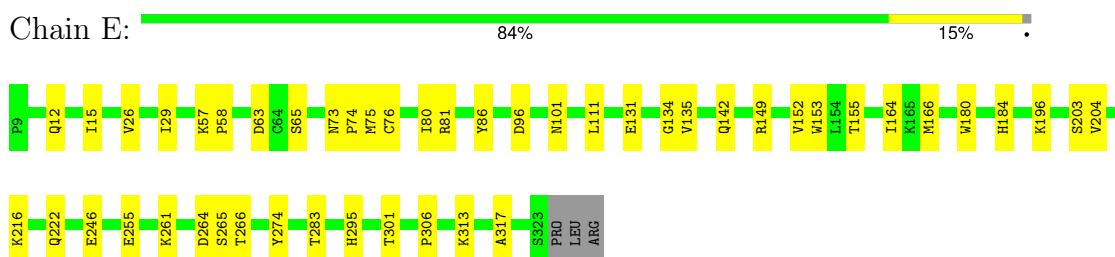
• Molecule 1: Hemagglutinin HA1



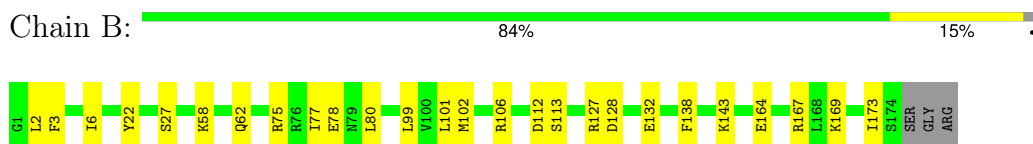
• Molecule 1: Hemagglutinin HA1




• Molecule 1: Hemagglutinin HA1




• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2

Chain D:  90% 8%

• Molecule 2: Hemagglutinin HA2

Chain F:  86% 14%

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

Chain G:  100%

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

Chain H:  50% 50%

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

Chain J:  50% 50%

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

Chain I:  100%

• Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  33% 67%



- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.08Å 99.83Å 132.06Å 90.00° 126.19° 90.00°	Depositor
Resolution (Å)	39.68 – 2.52	Depositor
% Data completeness (in resolution range)	97.5 (39.68-2.52)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.200 , 0.257	Depositor
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.397	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12294	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, NAG, SIA, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.26	0/2601	0.49	0/3538
1	C	0.26	0/2620	0.50	0/3564
1	E	0.27	0/2601	0.50	0/3538
2	B	0.31	0/1441	0.50	0/1937
2	D	0.28	0/1441	0.48	0/1937
2	F	0.27	0/1462	0.49	0/1964
All	All	0.27	0/12166	0.50	0/16478

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2537	0	2479	28	0
1	C	2556	0	2504	26	0
1	E	2537	0	2480	26	0
2	B	1414	0	1319	17	0
2	D	1414	0	1318	14	0
2	F	1435	0	1339	22	0
3	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	28	0	25	1	0
3	J	28	0	25	0	0
4	I	39	0	34	0	0
5	K	46	0	40	0	0
5	L	46	0	40	3	0
5	M	46	0	40	0	0
6	A	42	0	39	0	0
6	C	28	0	26	0	0
6	E	14	0	13	0	0
7	A	18	0	0	0	0
7	B	7	0	0	0	0
7	C	6	0	0	0	0
7	D	5	0	0	0	0
7	E	14	0	0	0	0
7	F	6	0	0	0	0
All	All	12294	0	11746	119	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 5.

All (119) 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:E:184:HIS:HD2	1:E:216:LYS:H	1.19	0.89
1:A:131:GLU:HB3	1:A:155:THR:HG23	1.69	0.75
1:E:73:ASN:HB3	1:E:76:CYS:HB2	1.73	0.70
2:D:30:GLN:HE21	2:D:145:ASP:HB2	1.58	0.68
1:A:29:ILE:HG23	1:A:30:MET:HG3	1.79	0.64
2:B:75:ARG:NH1	2:B:78:GLU:OE2	2.31	0.64
1:E:80:ILE:HG22	1:E:81:ARG:H	1.63	0.64
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.79	0.62
1:A:165:LYS:HG2	1:A:246:GLU:HG2	1.82	0.60
2:D:133:LEU:HD21	2:D:139:GLU:HB2	1.84	0.60
1:A:80:ILE:HG13	1:A:81:ARG:H	1.66	0.60
1:E:75:MET:HE1	1:E:142:GLN:H	1.65	0.60
1:E:283:THR:HG22	1:E:301:THR:HG22	1.84	0.59
2:D:30:GLN:NE2	2:D:145:ASP:HB2	2.17	0.58
1:C:166:MET:SD	1:C:167:SER:N	2.77	0.58
2:B:58:LYS:HD2	2:D:97:GLU:HB3	1.86	0.57
2:D:19:ASP:OD2	2:D:19:ASP:N	2.37	0.57
2:B:77:ILE:HD13	2:D:77:ILE:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:GLU:HG2	1:C:194:LEU:HD13	1.88	0.55
1:A:29:ILE:HG21	2:F:106:ARG:NH2	2.21	0.55
2:B:6:ILE:HG13	2:B:112:ASP:HA	1.88	0.55
2:B:75:ARG:HH11	2:B:78:GLU:CD	2.10	0.55
2:F:128:ASP:OD1	2:F:159:TYR:OH	2.17	0.54
1:E:26:VAL:HG21	1:E:317:ALA:HB2	1.88	0.54
1:A:73:ASN:ND2	1:A:96:ASP:O	2.41	0.53
1:C:26:VAL:HG21	1:C:317:ALA:HB2	1.90	0.53
5:L:3:SIA:O6	5:L:3:SIA:O8	2.25	0.53
1:C:288:ILE:HG21	1:C:297:ILE:HG13	1.90	0.53
1:A:111:LEU:HD12	1:A:261:LYS:HD2	1.92	0.52
1:A:283:THR:HG22	1:A:301:THR:HG22	1.92	0.52
1:E:164:ILE:O	1:E:246:GLU:HA	2.10	0.52
2:F:133:LEU:HD21	2:F:139:GLU:HB2	1.92	0.52
2:F:55:ILE:HD11	2:F:103:GLU:HG3	1.91	0.51
1:E:184:HIS:CD2	1:E:216:LYS:H	2.11	0.50
2:B:2:LEU:O	2:F:113:SER:OG	2.26	0.50
2:B:101:LEU:HD11	2:F:58:LYS:HE3	1.92	0.50
1:E:131:GLU:HB3	1:E:155:THR:HB	1.93	0.50
1:C:133:SER:OG	1:C:133:SER:O	2.27	0.50
2:B:173:ILE:H	2:B:173:ILE:HD12	1.77	0.49
2:B:102:MET:O	2:B:106:ARG:HG2	2.13	0.49
1:C:59:LEU:HD12	1:C:84:TRP:CE2	2.48	0.49
1:C:77:ASP:N	1:C:77:ASP:OD1	2.45	0.48
1:C:180:TRP:NE1	1:C:204:VAL:HG21	2.28	0.48
1:E:153:TRP:HH2	5:L:3:SIA:H91	1.78	0.48
1:A:62:LYS:HB2	1:A:79:PHE:HE1	1.77	0.48
1:A:179:LEU:CD2	1:A:234:TRP:HB3	2.44	0.48
2:F:171:GLU:OE2	2:F:177:ARG:NH2	2.47	0.48
1:E:265:SER:OG	1:E:266:THR:N	2.46	0.48
1:A:59:LEU:HD13	1:A:82:VAL:HG11	1.95	0.47
2:F:167:ARG:HG2	2:F:167:ARG:HH11	1.79	0.47
1:E:74:PRO:O	1:E:149:ARG:NH2	2.47	0.47
1:A:310:LYS:HD3	2:F:60:ASN:HD21	1.78	0.47
1:E:57:LYS:HD2	1:E:274:TYR:CZ	2.49	0.47
1:E:203:SER:OG	1:E:246:GLU:HB3	2.15	0.47
1:C:79:PHE:O	1:C:80:ILE:HD12	2.15	0.47
1:C:149:ARG:HG3	1:C:149:ARG:NH1	2.30	0.47
1:A:17:TYR:HB2	1:A:320:LEU:HD22	1.97	0.47
1:A:114:ARG:HB2	1:A:265:SER:HB2	1.96	0.47
1:A:310:LYS:HD3	2:F:60:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:ILE:HG22	1:E:81:ARG:N	2.29	0.46
1:A:58:PRO:HB3	1:A:86:TYR:CE1	2.50	0.46
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.96	0.46
2:F:19:ASP:OD1	2:F:19:ASP:N	2.42	0.46
1:E:180:TRP:NE1	1:E:204:VAL:HG21	2.31	0.46
1:C:114:ARG:HB2	1:C:265:SER:HB2	1.97	0.46
1:C:73:ASN:HB3	1:C:76:CYS:SG	2.56	0.46
1:E:58:PRO:HB3	1:E:86:TYR:CE1	2.51	0.45
1:C:78:GLU:OE2	1:C:81:ARG:NH2	2.45	0.45
1:C:113:SER:HB2	1:C:265:SER:HB3	1.98	0.45
2:B:106:ARG:CZ	2:F:106:ARG:HD3	2.46	0.45
2:F:164:GLU:OE2	2:F:167:ARG:NH2	2.50	0.45
2:B:132:GLU:HG2	2:B:138:PHE:CE2	2.52	0.45
1:E:295:HIS:CD2	1:E:306:PRO:HG2	2.52	0.45
1:C:58:PRO:HB3	1:C:86:TYR:CE1	2.53	0.44
2:D:40:SER:HA	2:D:43:LYS:HE2	1.99	0.44
2:B:62:GLN:OE1	2:D:86:ASP:HB3	2.18	0.44
1:E:15:ILE:HD11	2:F:122:VAL:HG21	2.00	0.44
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.99	0.44
2:B:77:ILE:O	2:B:80:LEU:HB3	2.18	0.44
2:F:3:PHE:O	2:F:116:LYS:HD2	2.19	0.43
1:A:174:GLU:HG2	1:A:260(A):VAL:HG22	1.99	0.43
1:A:152:VAL:HG23	1:A:255:GLU:HB2	2.00	0.43
1:C:164:ILE:O	1:C:246:GLU:HA	2.18	0.43
1:C:90:ARG:HG2	1:C:271:GLU:HG3	2.01	0.43
1:A:164:ILE:O	1:A:246:GLU:HA	2.19	0.42
2:B:3:PHE:CE1	2:B:113:SER:HB2	2.54	0.42
2:D:127:ARG:HH21	2:F:132:GLU:HB2	1.83	0.42
1:C:262:LYS:HD2	1:C:262:LYS:HA	1.92	0.42
1:E:111:LEU:HD12	1:E:261:LYS:HD2	2.01	0.42
1:A:73:ASN:HB3	1:A:76:CYS:SG	2.59	0.42
1:A:79:PHE:O	1:A:80:ILE:HG22	2.20	0.42
1:C:87:ILE:HB	1:C:267:ILE:HD13	2.01	0.42
2:F:167:ARG:HG2	2:F:167:ARG:NH1	2.34	0.42
2:B:169:LYS:O	2:B:173:ILE:HD12	2.20	0.42
1:A:180:TRP:NE1	1:A:204:VAL:HG21	2.35	0.42
2:F:143:LYS:HA	2:F:143:LYS:HD3	1.64	0.42
1:E:152:VAL:HG23	1:E:255:GLU:HB2	2.02	0.42
1:E:65:SER:OG	1:E:96:ASP:OD1	2.32	0.41
1:C:115:ILE:HD13	1:C:115:ILE:HA	1.83	0.41
1:C:307:LYS:HA	1:C:307:LYS:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:ARG:NH2	2:F:132:GLU:H	2.18	0.41
1:E:29:ILE:HG12	2:F:101:LEU:HB3	2.03	0.41
2:D:151:SER:HB3	3:H:1:NAG:H62	2.03	0.41
2:D:170:ARG:O	2:D:173:ILE:HG22	2.21	0.41
1:A:80:ILE:HG13	1:A:81:ARG:N	2.33	0.41
1:E:135:VAL:H	5:L:3:SIA:H113	1.84	0.41
1:A:116:ASN:ND2	1:A:262:LYS:HD3	2.36	0.41
2:B:164:GLU:OE2	2:B:167:ARG:NH2	2.46	0.41
1:C:12:GLN:HG2	2:D:139:GLU:HA	2.03	0.41
2:D:43:LYS:HE2	2:D:43:LYS:HB2	1.64	0.41
1:E:12:GLN:HA	2:F:138:PHE:O	2.21	0.41
2:F:103:GLU:OE1	2:F:106:ARG:NH2	2.55	0.40
1:A:77:ASP:O	1:A:78:GLU:HB2	2.21	0.40
1:A:176:LEU:HD12	1:A:176:LEU:HA	1.94	0.40
1:C:176:LEU:HD12	1:C:176:LEU:HA	1.92	0.40
2:B:127:ARG:HB3	2:B:128:ASP:H	1.70	0.40
1:A:49:GLY:HA2	1:A:285:ILE:O	2.22	0.40
1:C:138:ALA:C	1:C:140:PRO:HD3	2.42	0.40
1:C:149:ARG:HG3	1:C:149:ARG:HH11	1.85	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	319/324 (98%)	307 (96%)	10 (3%)	2 (1%)	22	37
1	C	321/324 (99%)	313 (98%)	7 (2%)	1 (0%)	37	54
1	E	319/324 (98%)	309 (97%)	10 (3%)	0	100	100
2	B	172/177 (97%)	168 (98%)	4 (2%)	0	100	100
2	D	172/177 (97%)	169 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
All	All	1478/1503 (98%)	1438 (97%)	37 (2%)	3 (0%)	44	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	80	ILE
1	C	80	ILE

5.3.2 Protein sidechains ⓘ

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	286/289 (99%)	283 (99%)	3 (1%)	73	87
1	C	288/289 (100%)	283 (98%)	5 (2%)	56	78
1	E	286/289 (99%)	279 (98%)	7 (2%)	44	68
2	B	149/151 (99%)	145 (97%)	4 (3%)	40	65
2	D	149/151 (99%)	149 (100%)	0	100	100
2	F	151/151 (100%)	148 (98%)	3 (2%)	50	74
All	All	1309/1320 (99%)	1287 (98%)	22 (2%)	56	78

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

Mol	Chain	Res	Type
1	A	62	LYS
1	A	246	GLU
1	A	262	LYS
2	B	22	TYR
2	B	27	SER
2	B	99	LEU
2	B	143	LYS
1	C	93	PRO

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Mol	Chain	Res	Type
1	C	95	ASN
1	C	96	ASP
1	C	146	SER
1	C	264	ASP
1	E	63	ASP
1	E	101	ASN
1	E	166	MET
1	E	196	LYS
1	E	222	GLN
1	E	264	ASP
1	E	313	LYS
2	F	22	TYR
2	F	75	ARG
2	F	89	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	ASN
1	C	222	GLN
2	D	30	GLN
1	E	101	ASN
1	E	184	HIS
2	F	60	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](#)

18 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	G	1	3,1	14,14,15	0.76	0	17,19,21	1.19	2 (11%)
3	NAG	G	2	3	14,14,15	0.72	0	17,19,21	1.10	1 (5%)
3	NAG	H	1	2,3	14,14,15	0.69	0	17,19,21	1.00	2 (11%)
3	NAG	H	2	3	14,14,15	0.71	0	17,19,21	0.92	0
4	NAG	I	1	4,1	14,14,15	0.77	0	17,19,21	1.31	2 (11%)
4	NAG	I	2	4	14,14,15	0.68	0	17,19,21	1.26	2 (11%)
4	BMA	I	3	4	11,11,12	0.85	0	15,15,17	2.24	2 (13%)
3	NAG	J	1	2,3	14,14,15	0.69	0	17,19,21	0.90	1 (5%)
3	NAG	J	2	3	14,14,15	0.71	0	17,19,21	0.96	0
5	NAG	K	1	5	15,15,15	0.57	0	21,21,21	0.65	0
5	GAL	K	2	5	11,11,12	0.80	0	15,15,17	1.23	1 (6%)
5	SIA	K	3	5	20,20,21	1.54	2 (10%)	21,28,31	1.55	3 (14%)
5	NAG	L	1	5	15,15,15	0.55	0	21,21,21	0.68	0
5	GAL	L	2	5	11,11,12	0.76	0	15,15,17	1.07	1 (6%)
5	SIA	L	3	5	20,20,21	1.65	2 (10%)	21,28,31	1.57	3 (14%)
5	NAG	M	1	5	15,15,15	0.54	0	21,21,21	0.75	0
5	GAL	M	2	5	11,11,12	0.78	0	15,15,17	1.18	1 (6%)
5	SIA	M	3	5	20,20,21	1.66	2 (10%)	21,28,31	1.53	3 (14%)

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	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	1/2/19/22	0/1/1/1
3	NAG	J	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	K	1	5	-	2/6/26/26	0/1/1/1
5	GAL	K	2	5	-	2/2/19/22	0/1/1/1
5	SIA	K	3	5	-	4/18/34/38	0/1/1/1
5	NAG	L	1	5	-	0/6/26/26	0/1/1/1
5	GAL	L	2	5	-	0/2/19/22	0/1/1/1
5	SIA	L	3	5	-	4/18/34/38	0/1/1/1
5	NAG	M	1	5	-	0/6/26/26	0/1/1/1
5	GAL	M	2	5	-	0/2/19/22	0/1/1/1
5	SIA	M	3	5	-	1/18/34/38	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	3	SIA	C2-C1	5.82	1.59	1.52
5	L	3	SIA	C2-C1	5.73	1.59	1.52
5	K	3	SIA	C2-C1	5.42	1.58	1.52
5	L	3	SIA	O6-C2	2.19	1.47	1.43
5	M	3	SIA	O6-C2	2.19	1.47	1.43
5	K	3	SIA	O6-C2	2.08	1.47	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	3	BMA	C1-O5-C5	7.32	121.99	112.19
5	K	3	SIA	O1A-C1-C2	-4.67	112.76	122.85
5	L	3	SIA	O1A-C1-C2	-4.66	112.77	122.85
5	M	3	SIA	O1A-C1-C2	-4.36	113.43	122.85
4	I	2	NAG	C2-N2-C7	3.27	127.28	122.90
3	G	2	NAG	C2-N2-C7	3.11	127.06	122.90
5	M	2	GAL	C1-O5-C5	3.03	116.25	112.19
4	I	1	NAG	C1-O5-C5	2.90	116.08	112.19
5	K	2	GAL	C1-O5-C5	2.74	115.86	112.19
5	K	3	SIA	O1B-C1-O1A	2.61	130.01	124.08
3	H	1	NAG	O5-C1-C2	-2.60	107.27	111.29
4	I	2	NAG	O5-C1-C2	-2.52	107.39	111.29
5	L	2	GAL	C1-O5-C5	2.46	115.48	112.19
5	L	3	SIA	O1B-C1-O1A	2.40	129.53	124.08
3	G	1	NAG	C2-N2-C7	2.37	126.08	122.90
5	M	3	SIA	O1B-C1-O1A	2.37	129.46	124.08
5	K	3	SIA	O6-C2-C1	2.36	112.17	107.72
3	J	1	NAG	O5-C1-C2	-2.17	107.94	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C1-O5-C5	2.04	114.92	112.19
4	I	3	BMA	O4-C4-C3	-2.04	105.58	110.38
5	L	3	SIA	O6-C2-C1	2.03	111.55	107.72
5	M	3	SIA	O6-C2-C3	-2.02	107.83	110.56
4	I	1	NAG	O4-C4-C3	-2.02	105.62	110.38
3	H	1	NAG	O4-C4-C3	-2.01	105.65	110.38

There are no chirality outliers.

All (26) torsion outliers are listed below:

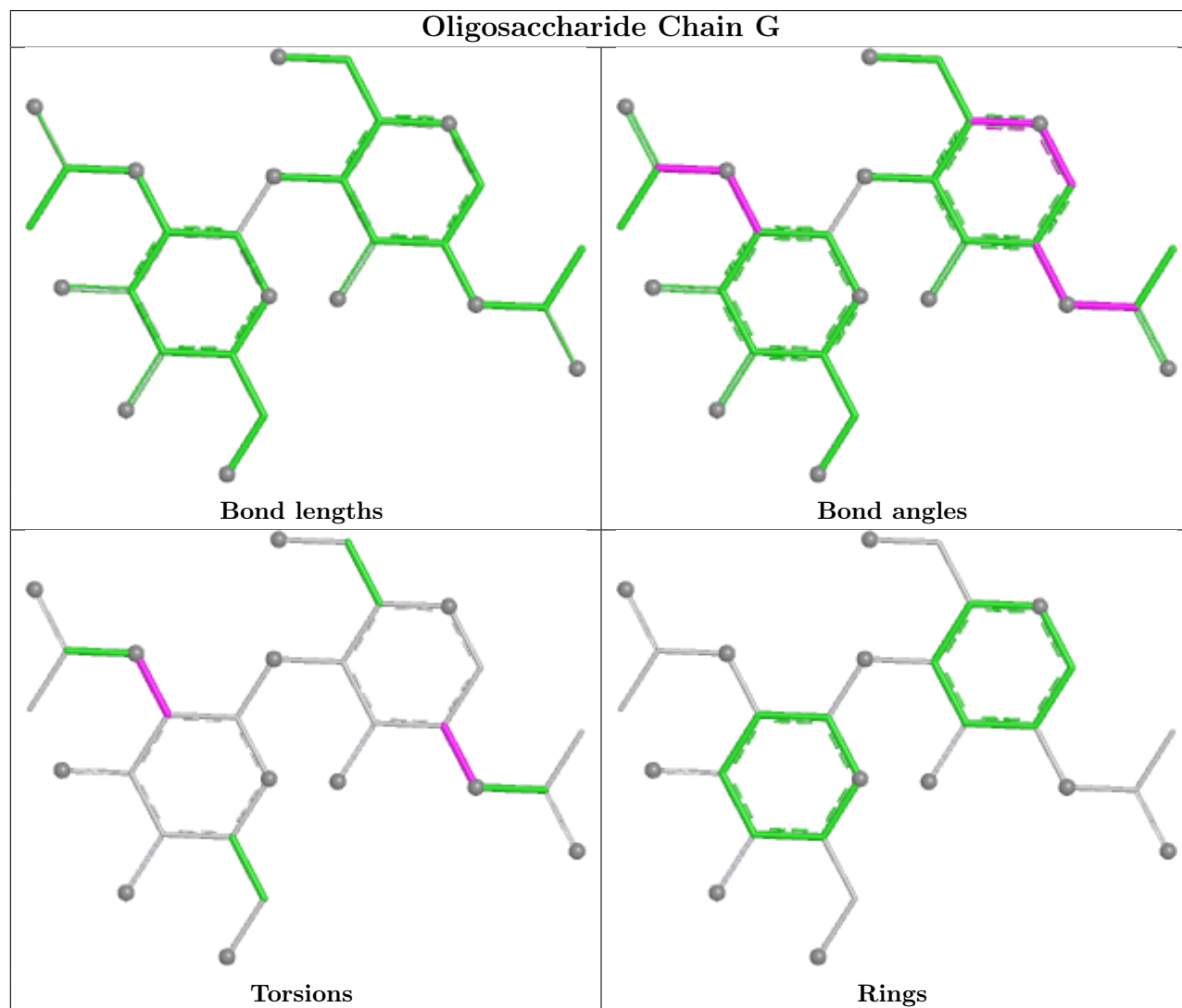
Mol	Chain	Res	Type	Atoms
5	K	3	SIA	C6-C7-C8-C9
5	K	3	SIA	C6-C7-C8-O8
5	K	3	SIA	O7-C7-C8-C9
5	K	3	SIA	O7-C7-C8-O8
5	L	3	SIA	C6-C7-C8-C9
5	L	3	SIA	C6-C7-C8-O8
5	L	3	SIA	O7-C7-C8-C9
5	L	3	SIA	O7-C7-C8-O8
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
5	K	2	GAL	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7
4	I	2	NAG	C1-C2-N2-C7
5	M	3	SIA	C6-C7-C8-O8
3	H	1	NAG	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C3-C2-N2-C7
3	G	2	NAG	C3-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7
5	K	2	GAL	C4-C5-C6-O6
4	I	3	BMA	C4-C5-C6-O6

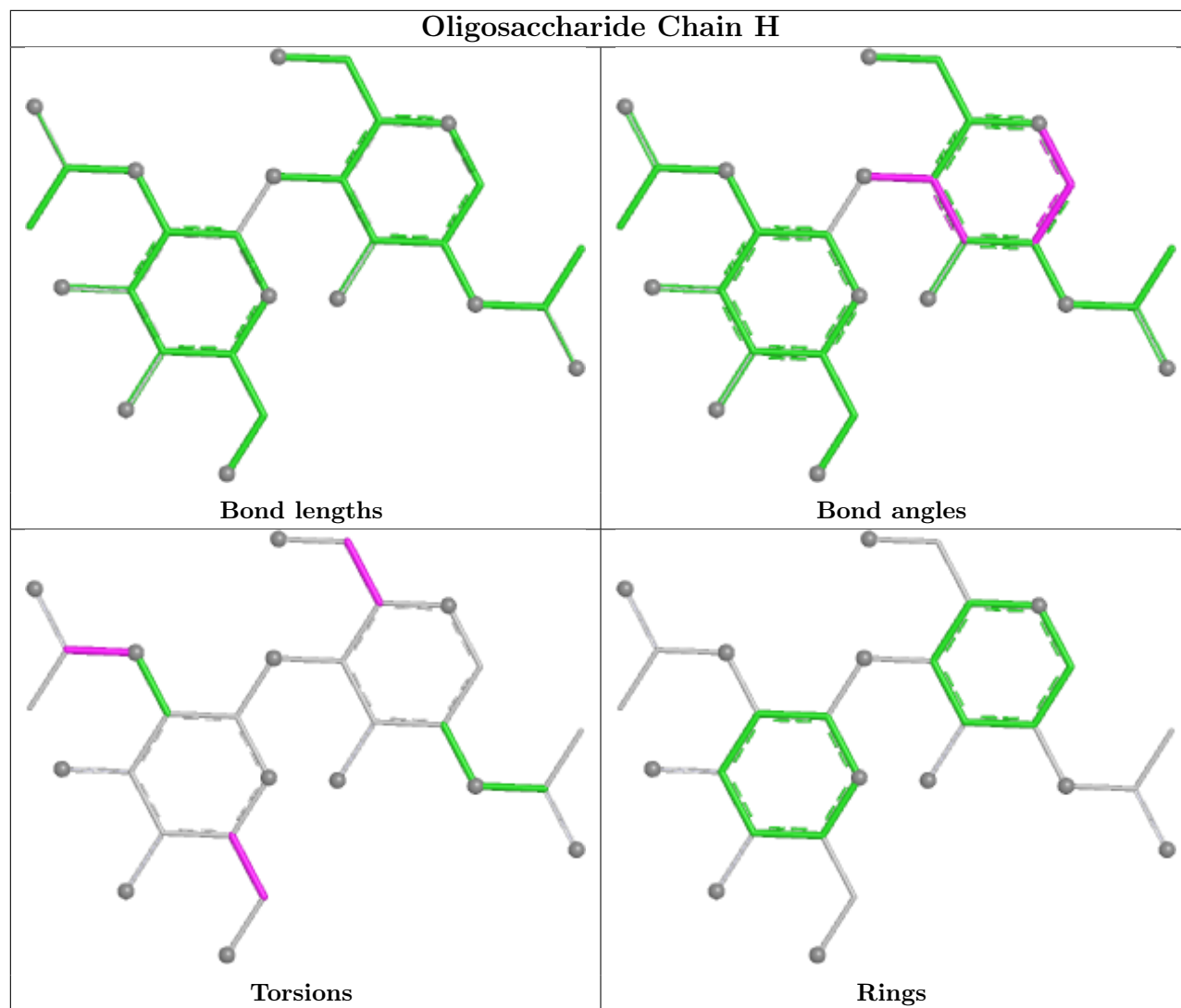
There are no ring outliers.

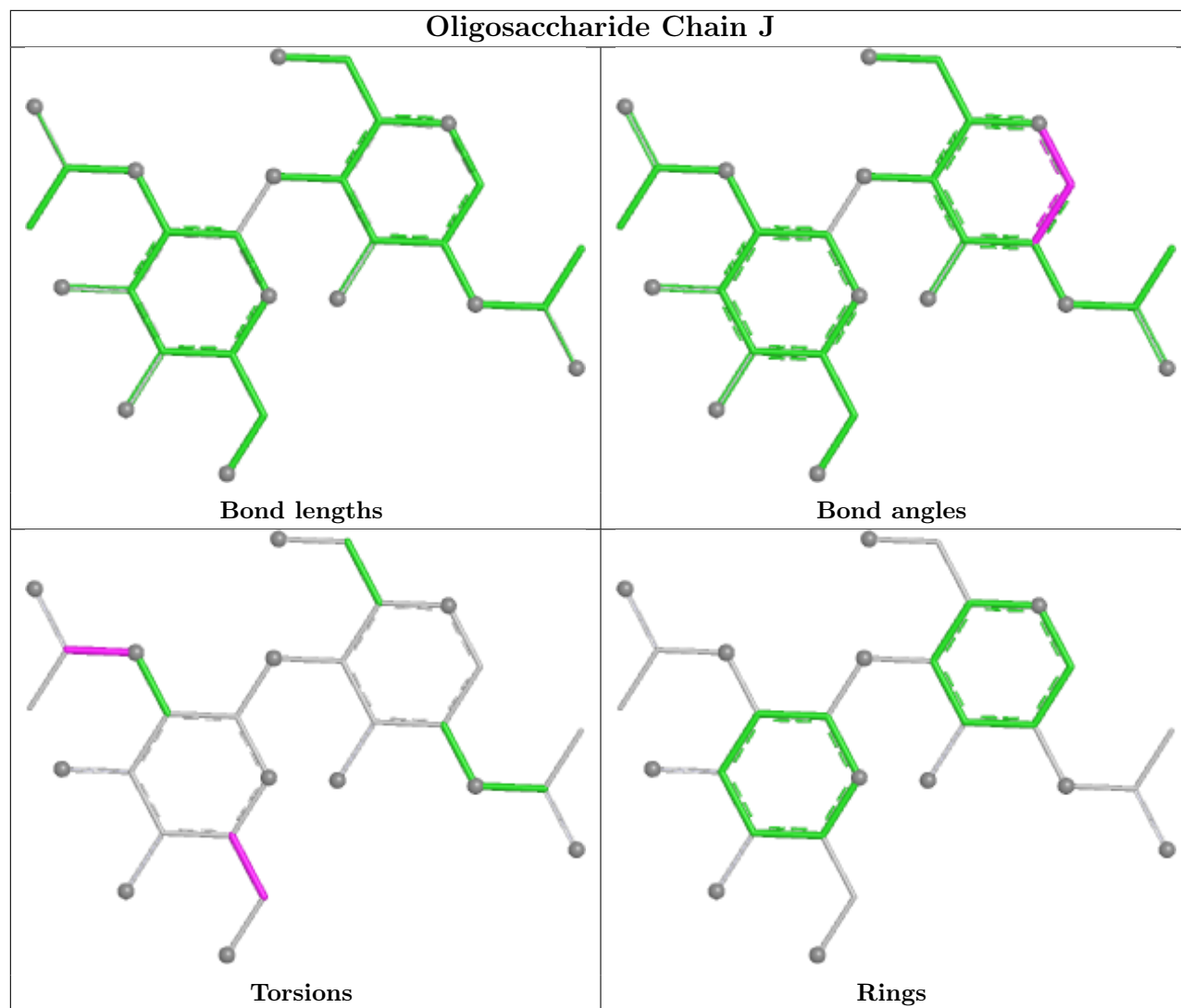
2 monomers are involved in 4 short contacts:

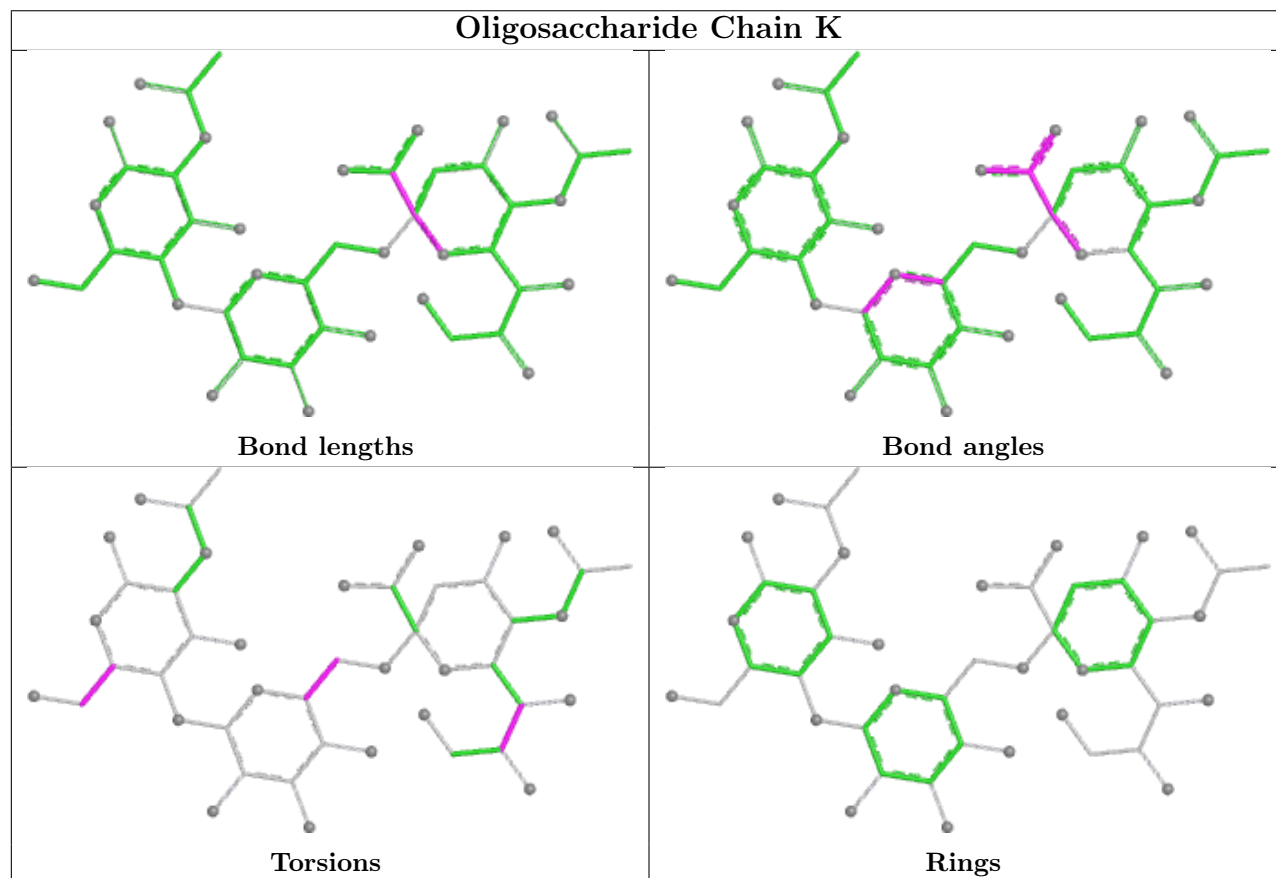
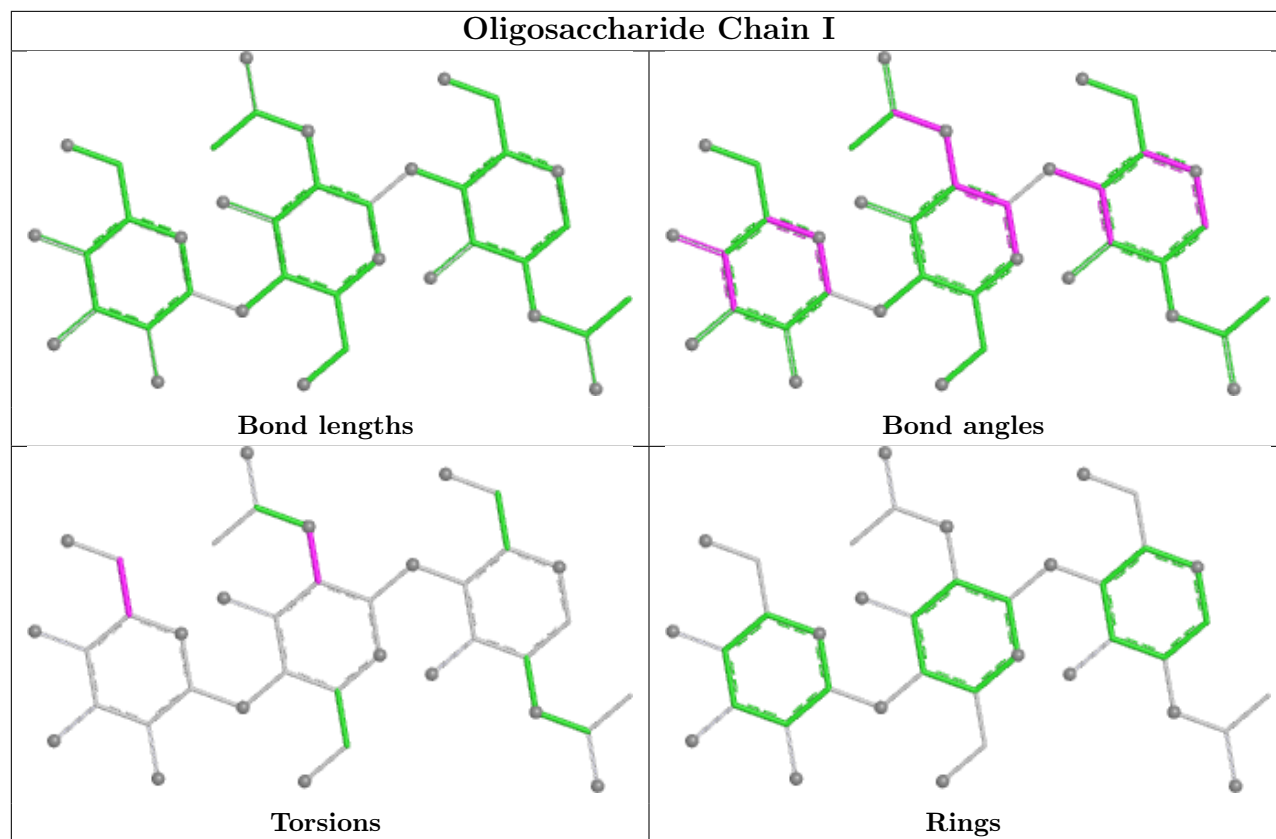
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
5	L	3	SIA	3	0

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

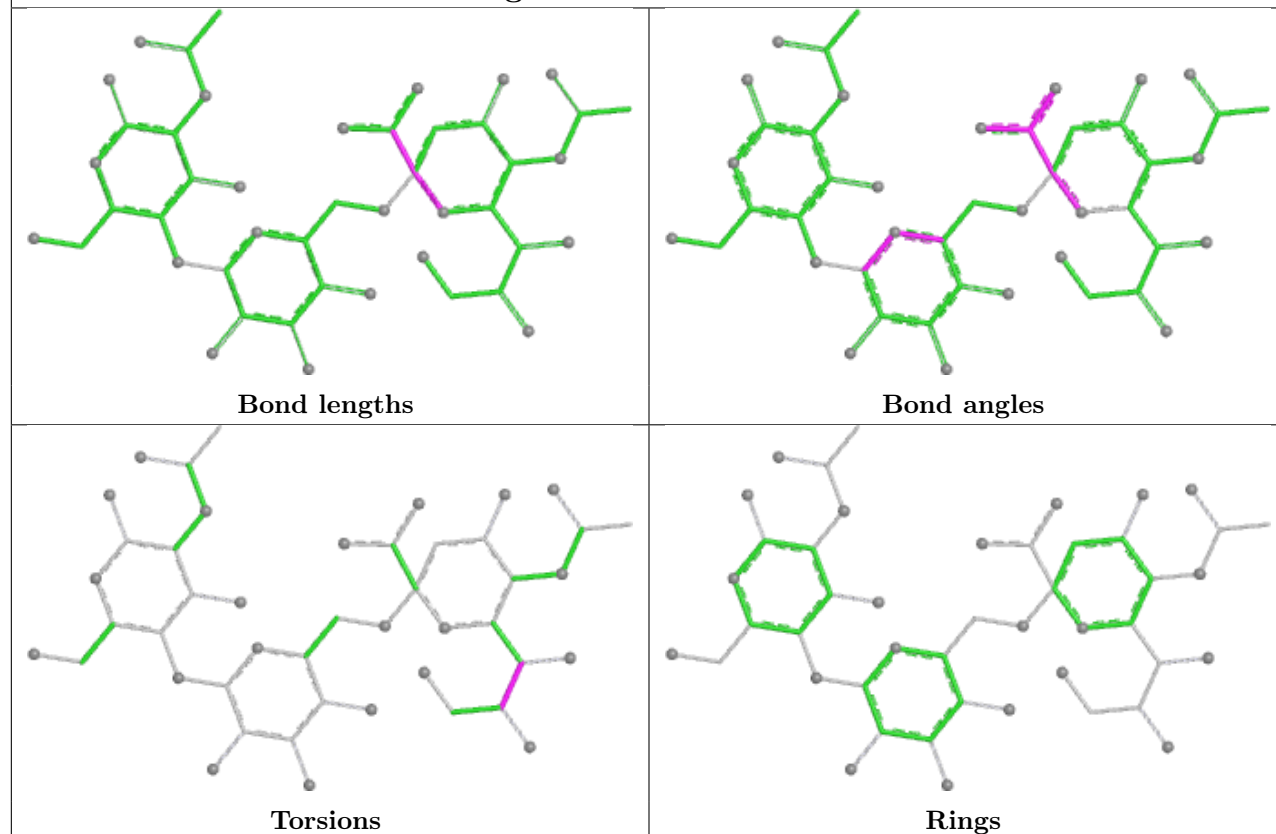




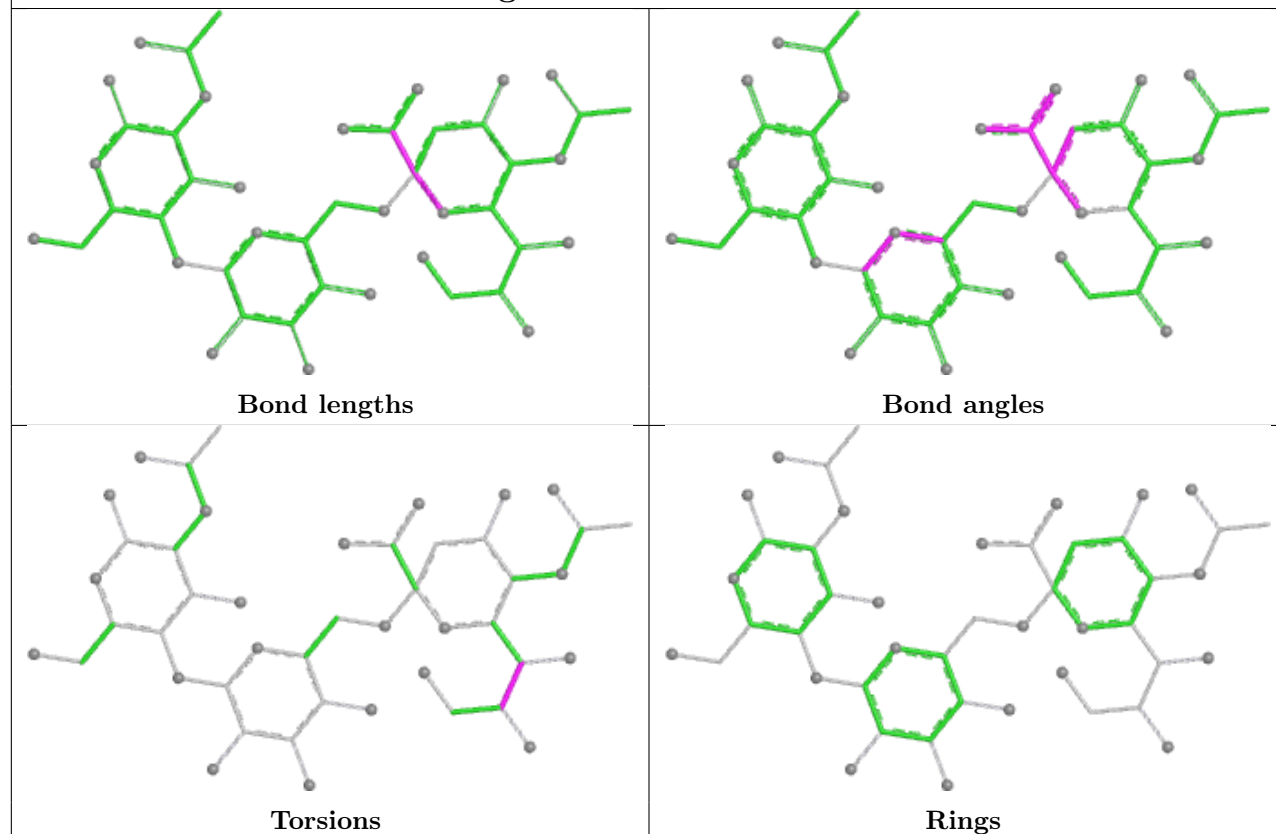




Oligosaccharide Chain L



Oligosaccharide Chain M



5.6 Ligand geometry

6 ligands 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	$\# Z > 2$
6	NAG	E	401	1	14,14,15	0.68	0	17,19,21	0.83	0
6	NAG	C	402	1	14,14,15	0.71	0	17,19,21	0.92	0
6	NAG	A	403	1	14,14,15	0.72	0	17,19,21	0.90	0
6	NAG	C	401	1	14,14,15	0.67	0	17,19,21	0.91	0
6	NAG	A	402	1	14,14,15	0.70	0	17,19,21	0.91	1 (5%)
6	NAG	A	401	1	14,14,15	0.72	0	17,19,21	0.98	1 (5%)

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	E	401	1	-	1/6/23/26	0/1/1/1
6	NAG	C	402	1	-	2/6/23/26	0/1/1/1
6	NAG	A	403	1	-	4/6/23/26	0/1/1/1
6	NAG	C	401	1	-	2/6/23/26	0/1/1/1
6	NAG	A	402	1	-	0/6/23/26	0/1/1/1
6	NAG	A	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	401	NAG	C1-O5-C5	2.72	115.83	112.19
6	A	402	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

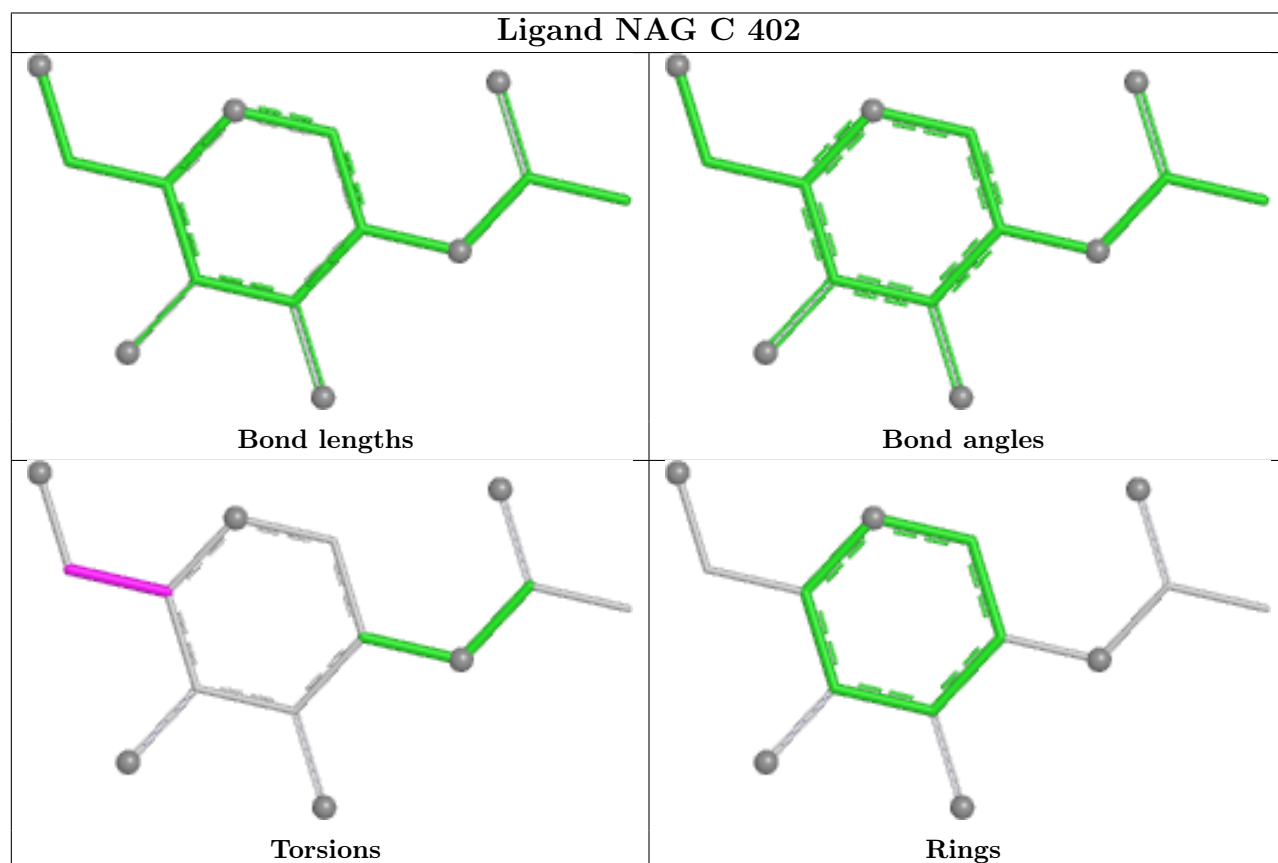
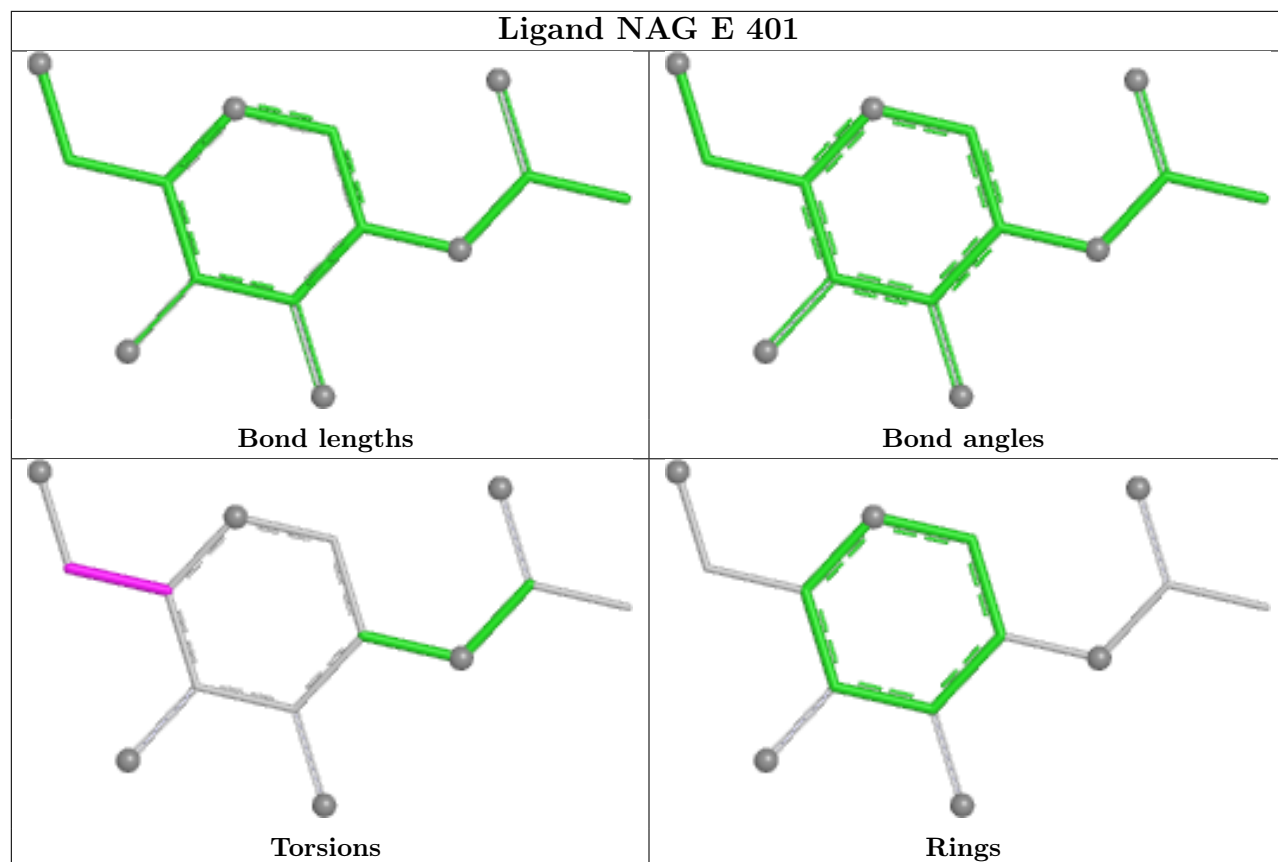
All (11) torsion outliers are listed below:

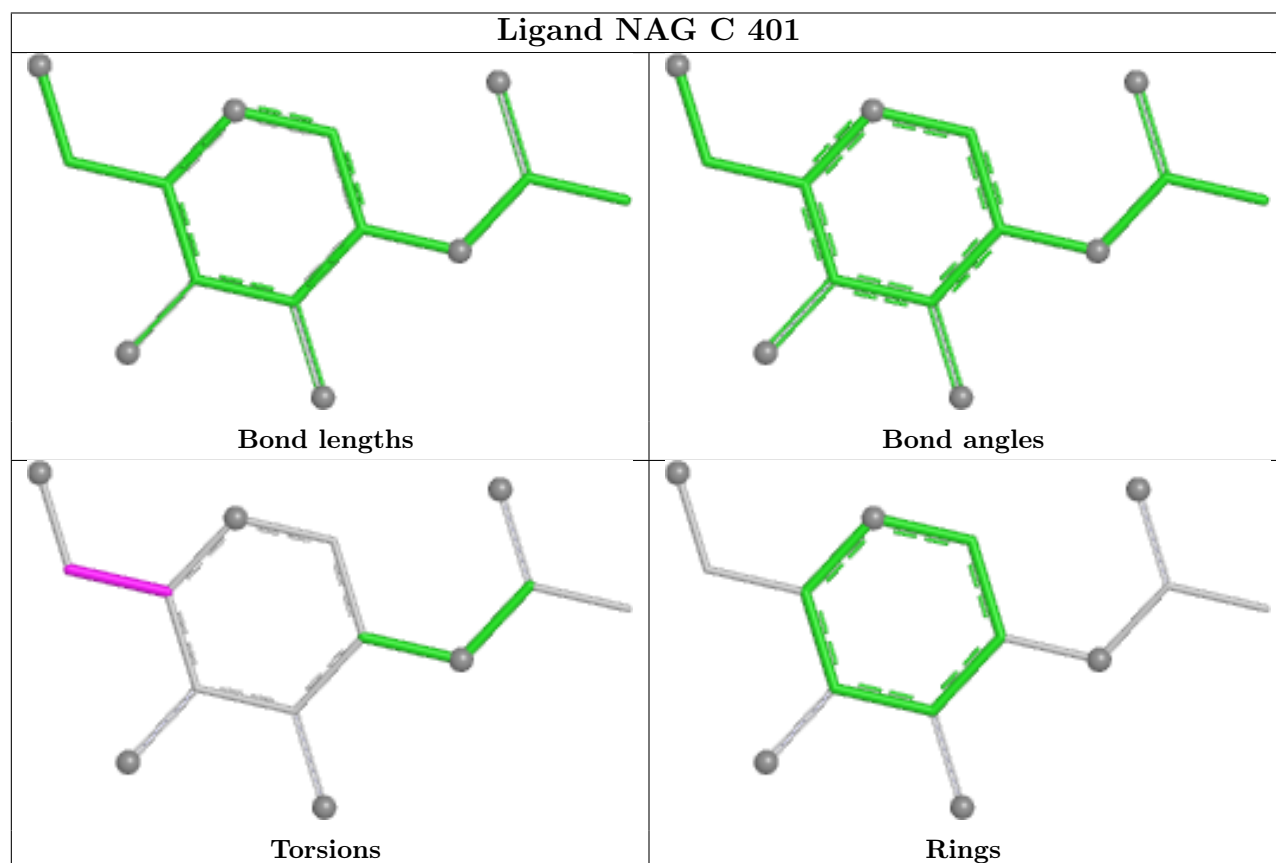
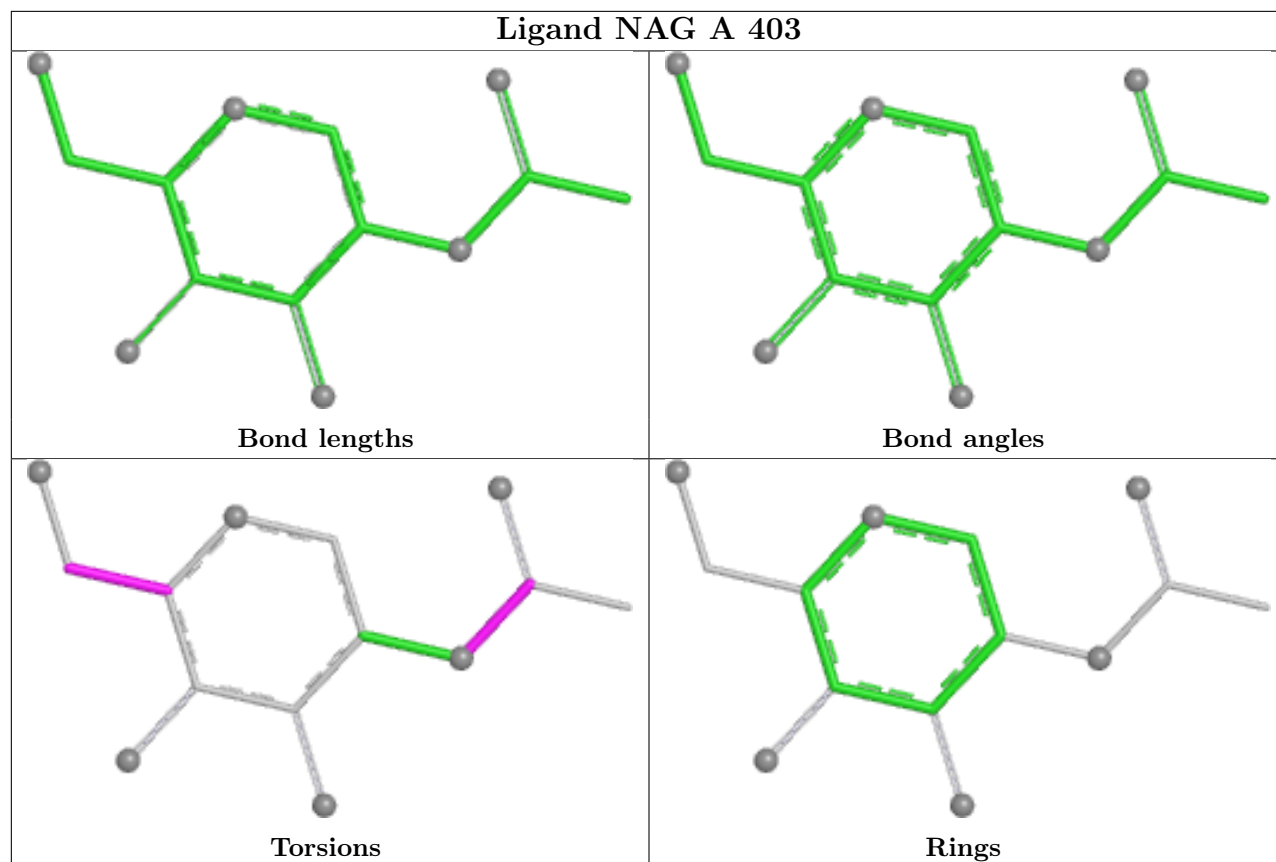
Mol	Chain	Res	Type	Atoms
6	C	402	NAG	O5-C5-C6-O6
6	A	403	NAG	O5-C5-C6-O6
6	A	403	NAG	C4-C5-C6-O6
6	A	403	NAG	C8-C7-N2-C2
6	A	403	NAG	O7-C7-N2-C2
6	C	402	NAG	C4-C5-C6-O6
6	C	401	NAG	O5-C5-C6-O6
6	A	401	NAG	C4-C5-C6-O6
6	A	401	NAG	O5-C5-C6-O6
6	C	401	NAG	C4-C5-C6-O6
6	E	401	NAG	C4-C5-C6-O6

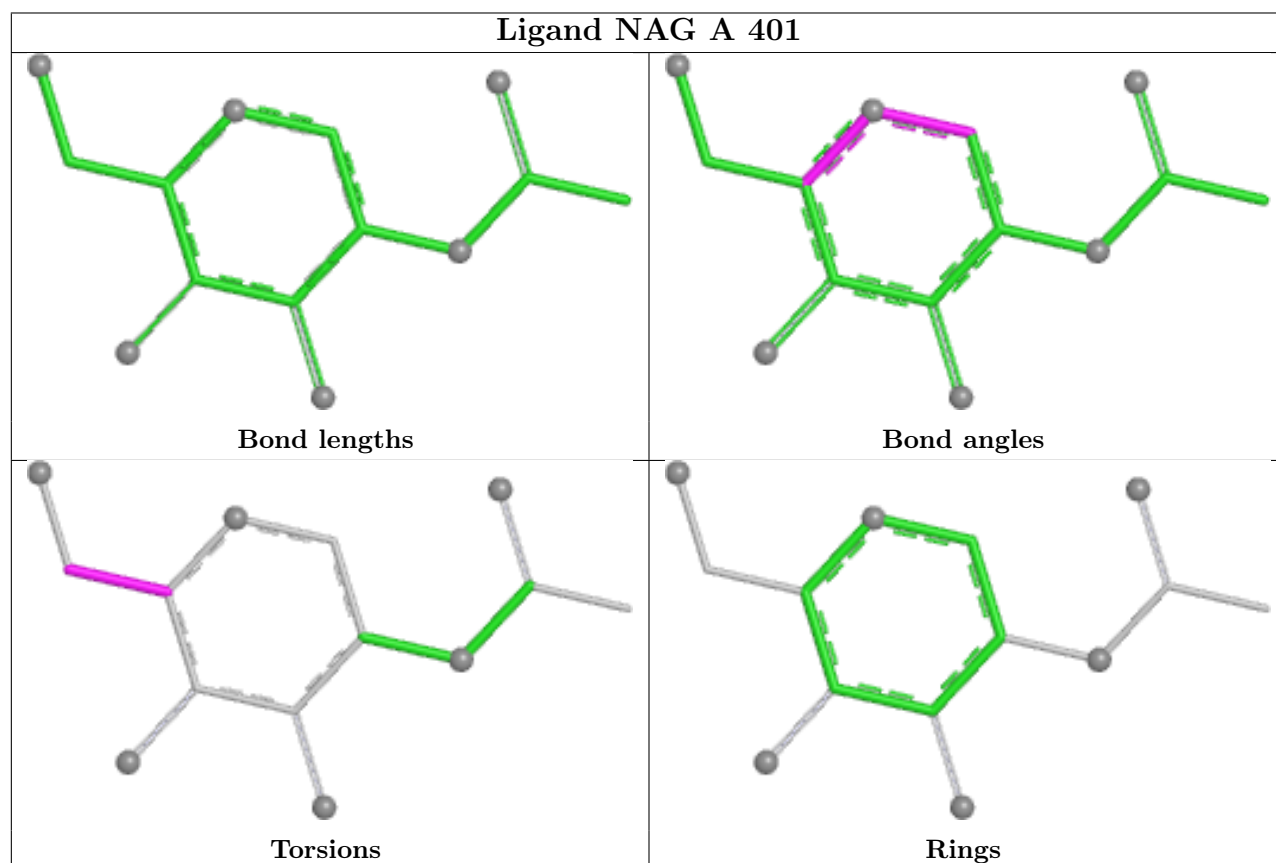
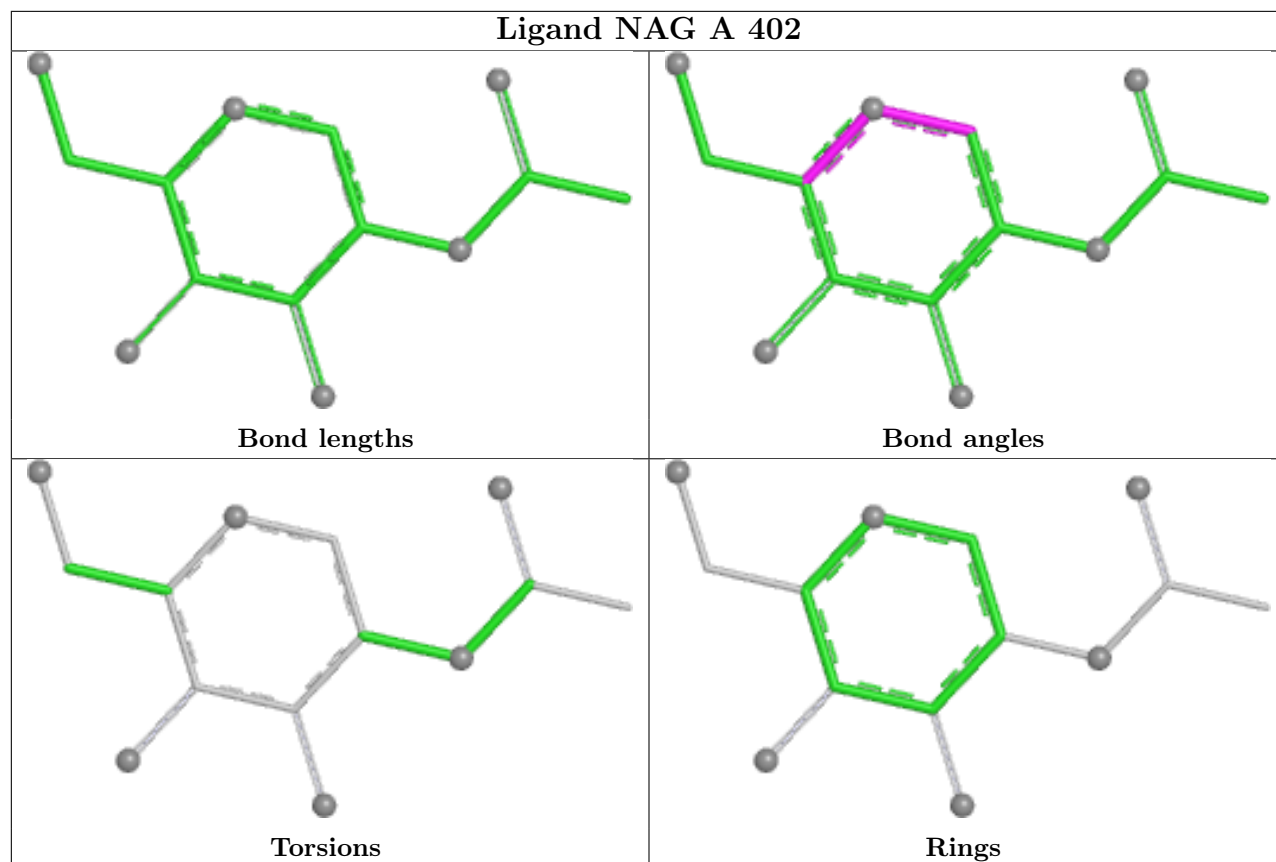
There are no ring outliers.

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 than 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.







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

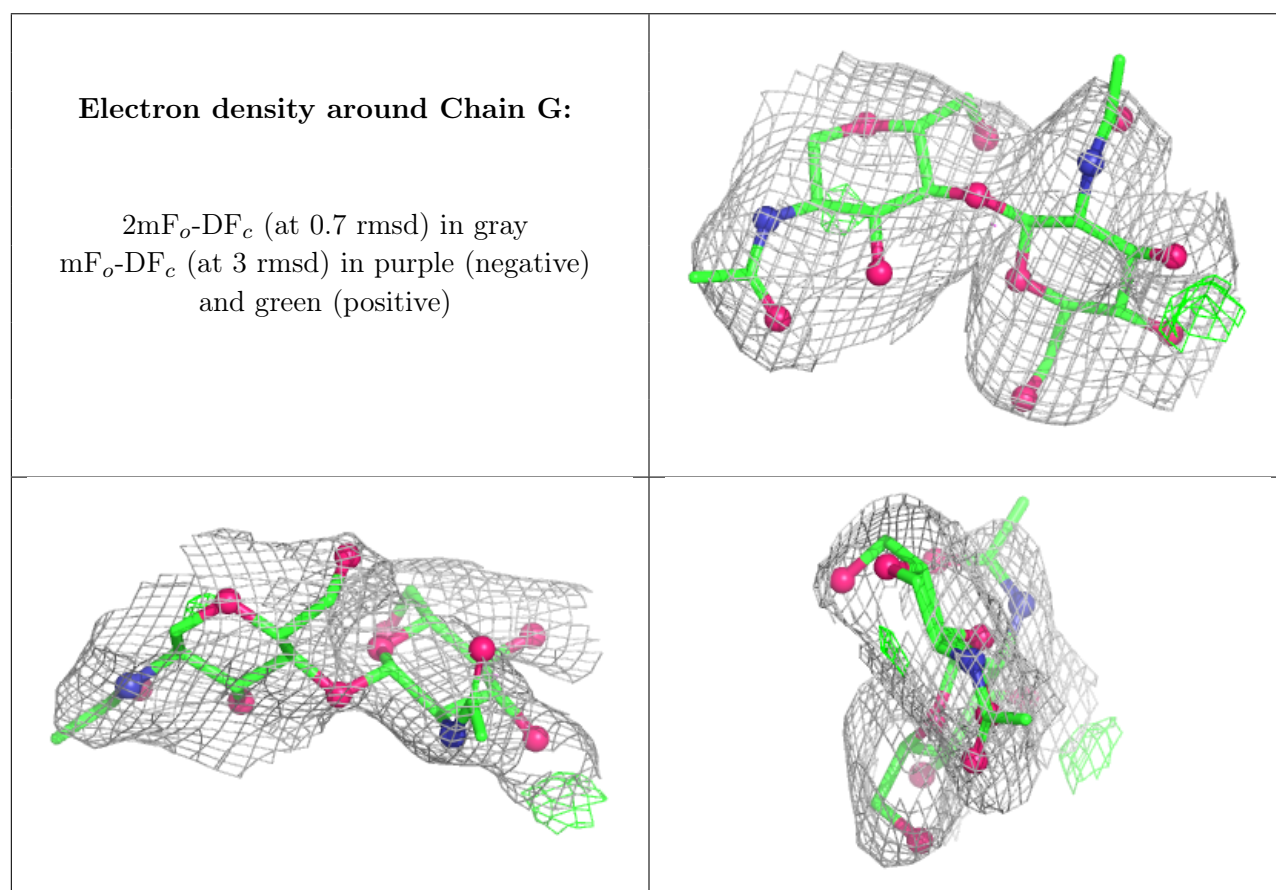
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

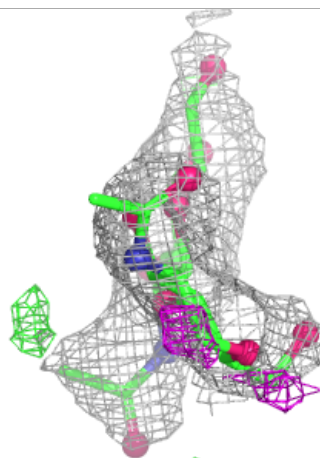
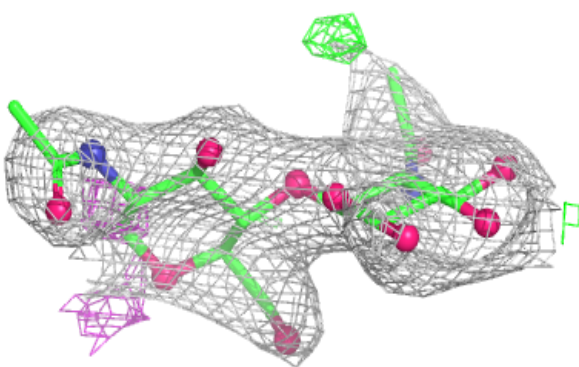
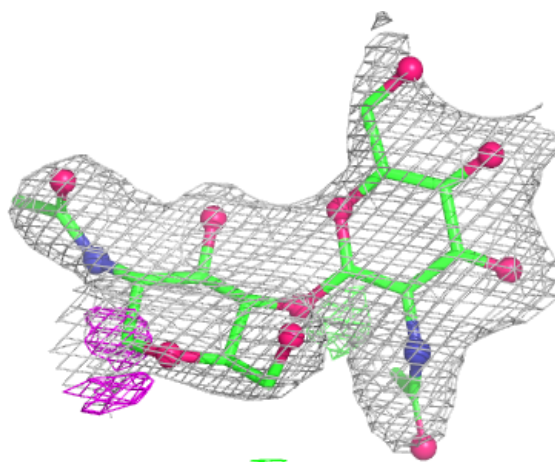
EDS failed to run properly - this section is therefore empty.

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.



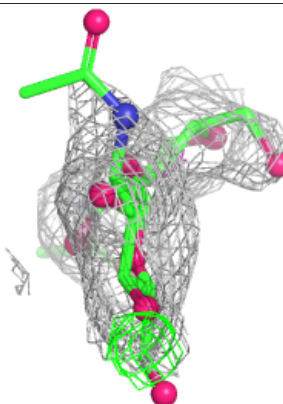
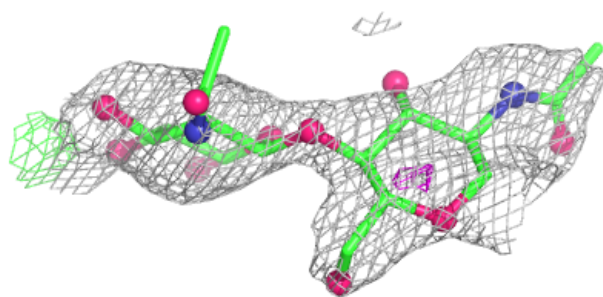
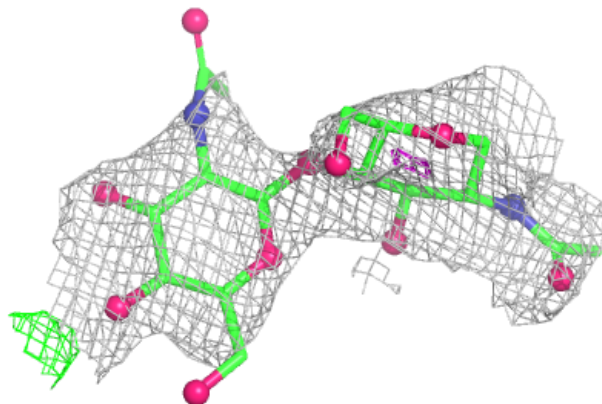
Electron density around Chain H:

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

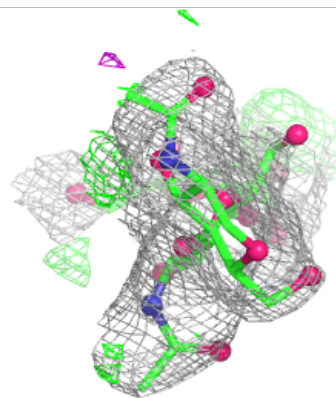
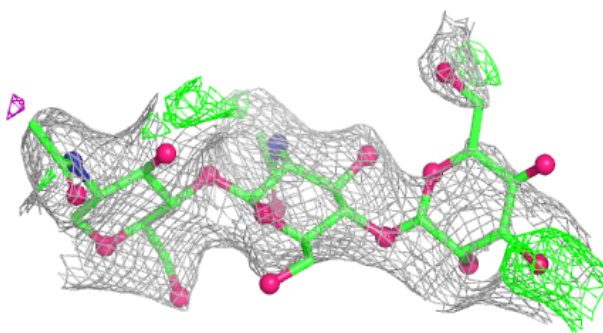
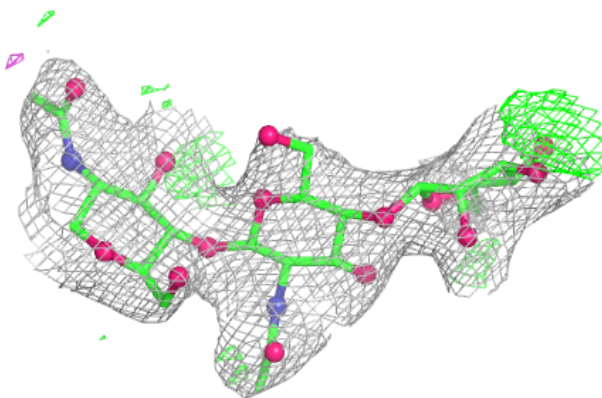


Electron density around Chain J:

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

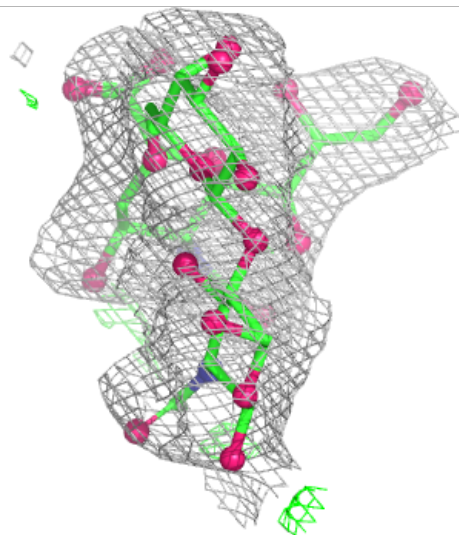
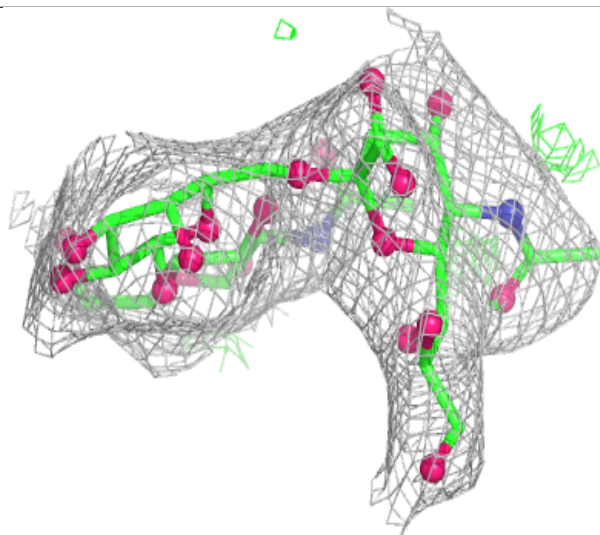
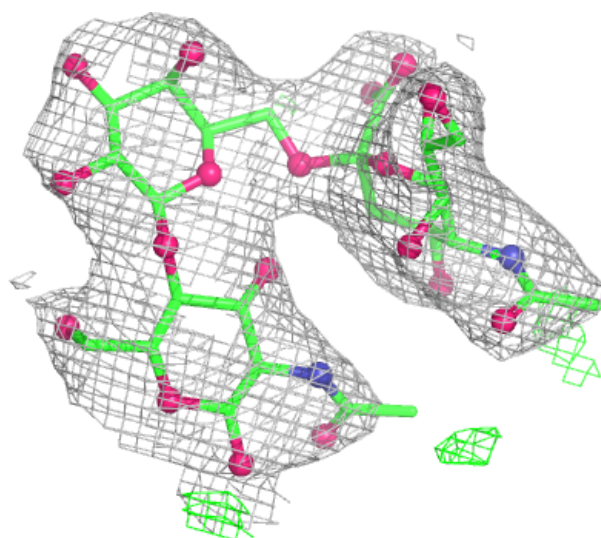
**Electron density around Chain I:**

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



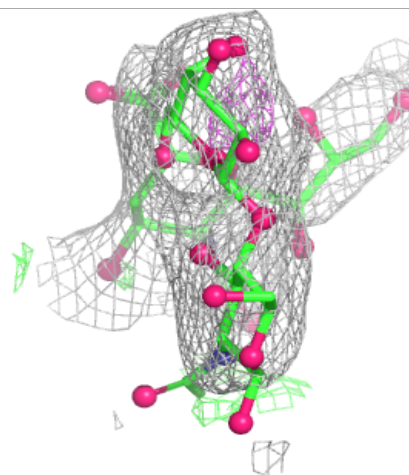
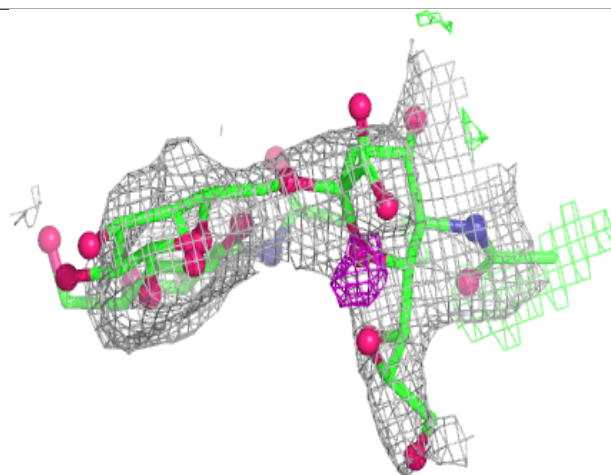
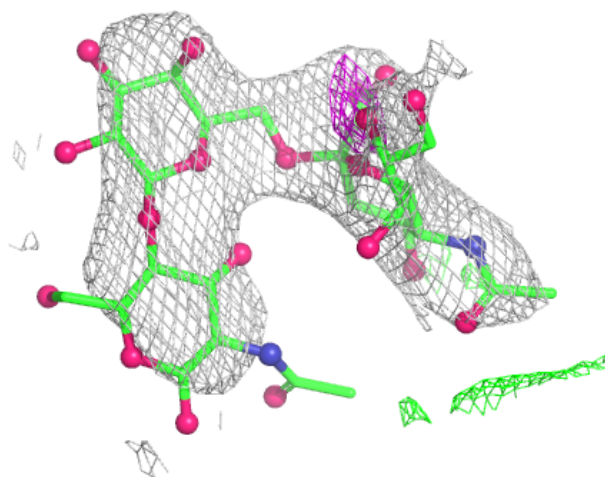
Electron density around Chain K:

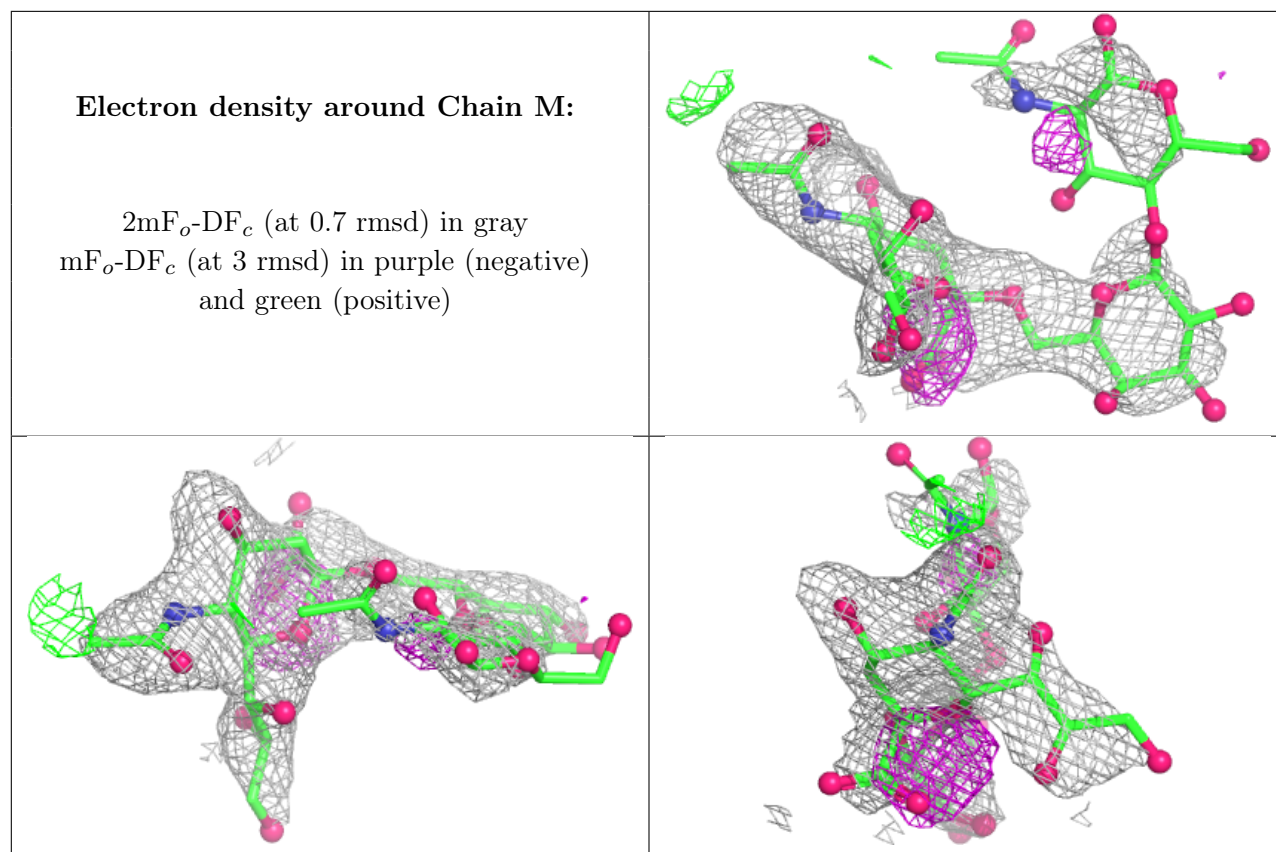
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

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





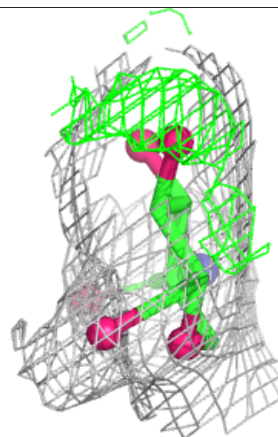
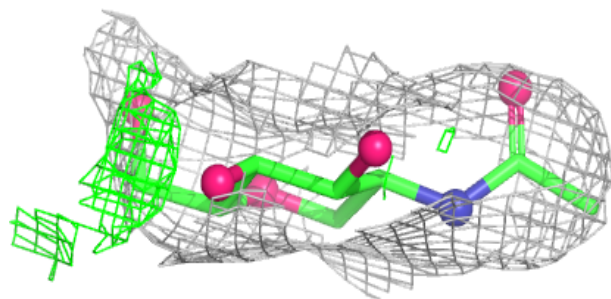
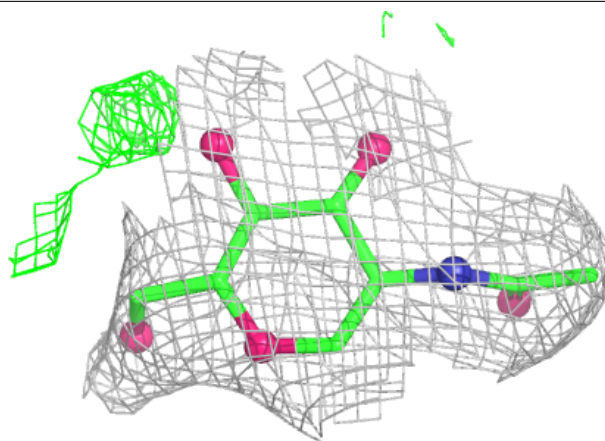
6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

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.

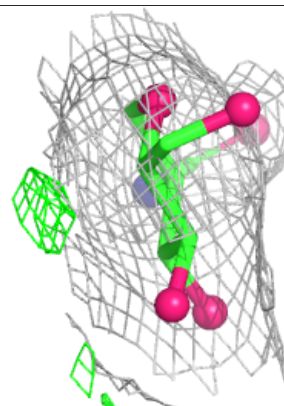
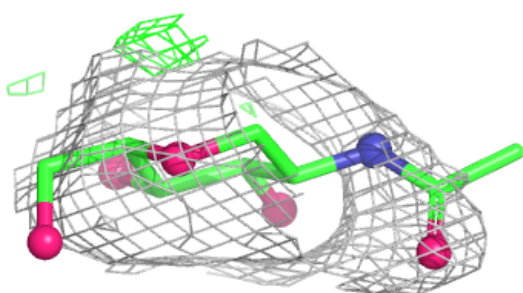
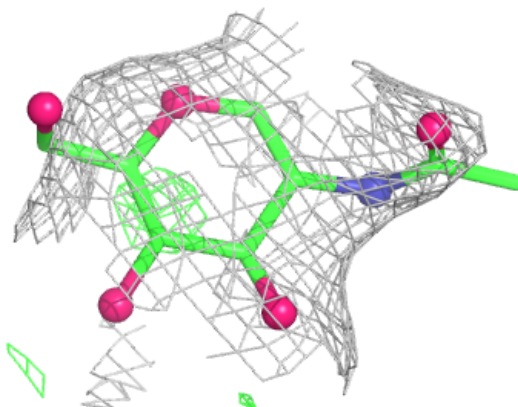
Electron density around NAG A 401:

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

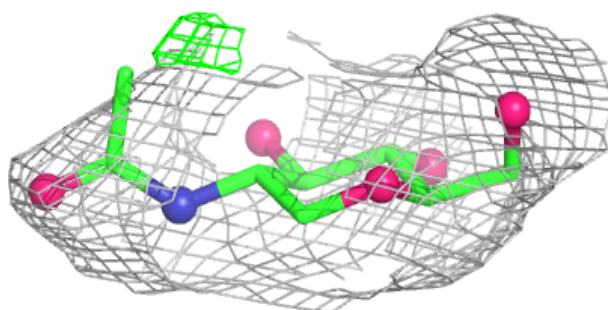
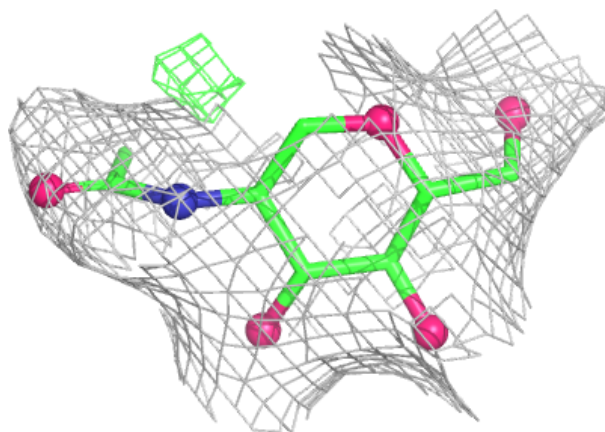


Electron density around NAG A 402:

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

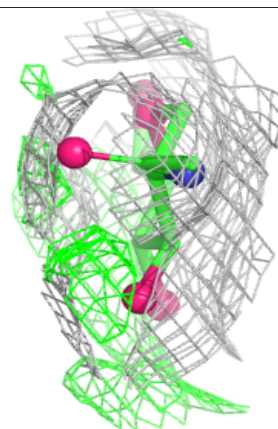
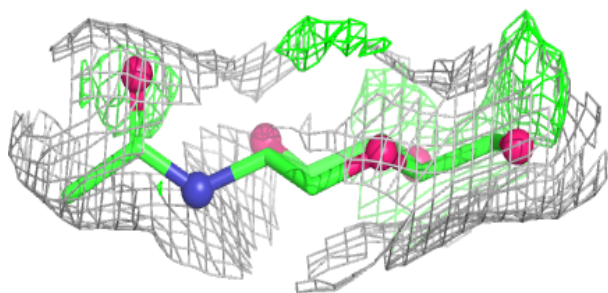
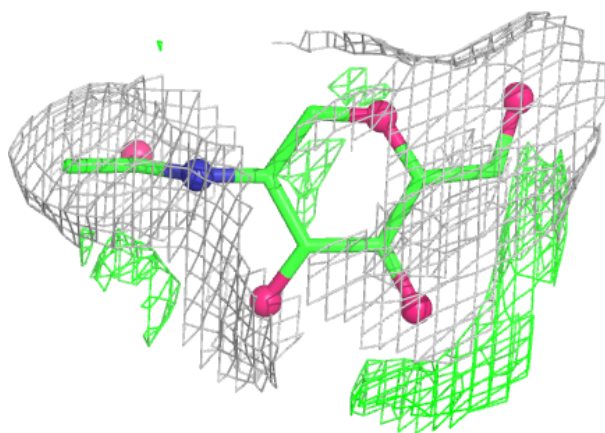
**Electron density around NAG A 403:**

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

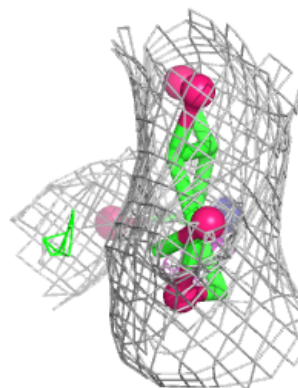
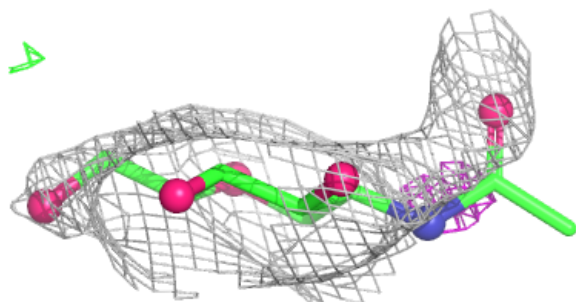
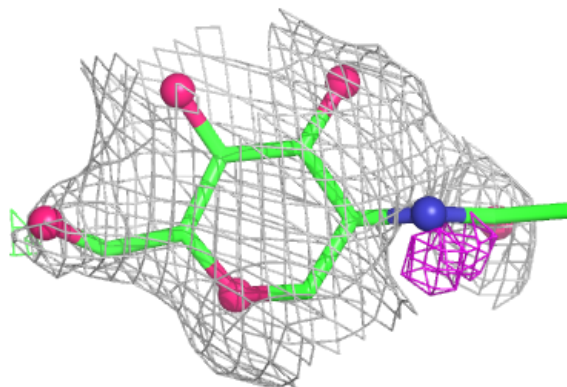


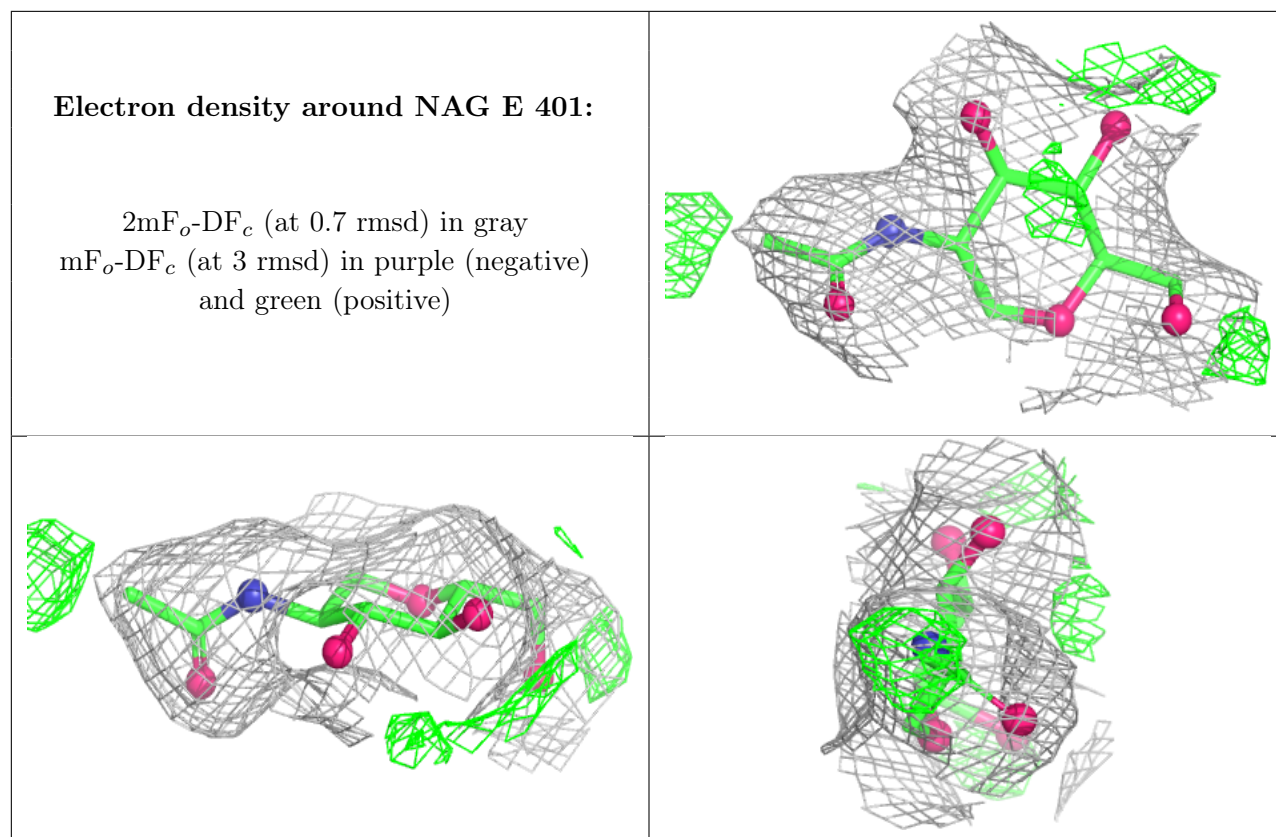
Electron density around NAG C 401:

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

**Electron density around NAG C 402:**

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





6.5 Other polymers [i](#)

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