



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2022 – 12:12 AM EST

PDB ID : 7TPS
Title : Crystal structure of ALPN-202 (engineered CD80 vIgD) in complex with PD-L1
Authors : Demonte, D.W.; Maurer, M.F.; Akutsu, M.; Kimbung, Y.R.; Logan, D.T.; Walse, B.
Deposited on : 2022-01-26
Resolution : 3.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

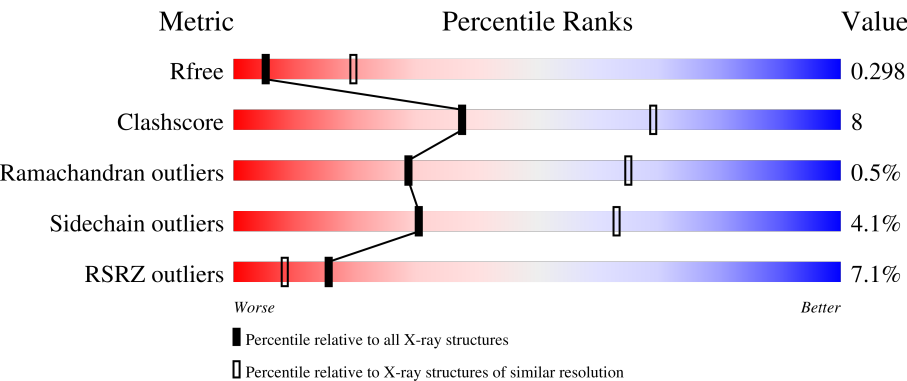
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




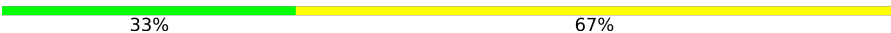
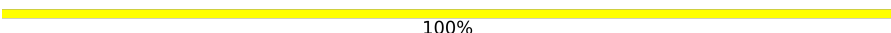
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 $\leq 5\%$. 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	106	<div><div></div><div>76%24%</div></div>
1	C	106	<div><div>23%</div><div>75%15%8%</div></div>
2	B	209	<div><div>6%</div><div>73%25%</div></div>
3	D	209	<div><div>3%</div><div>81%18%</div></div>
4	E	3	<div><div></div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
4	G	3	 33% 67%
4	H	3	 33% 67%
5	F	3	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	F	2	-	-	-	X
5	FUC	F	3	-	-	-	X
6	NAG	C	201	-	-	-	X
7	GOL	D	303	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5316 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 T-lymphocyte activation antigen CD80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			856	547	141	162	6			
1	C	97	Total	C	N	O	S	0	0	0
			795	510	131	148	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	TYR	HIS	engineered mutation	UNP P33681
A	60	GLU	ALA	engineered mutation	UNP P33681
A	69	ASP	GLU	engineered mutation	UNP P33681
A	81	LEU	MET	engineered mutation	UNP P33681
A	102	MET	VAL	engineered mutation	UNP P33681
A	105	GLY	ALA	engineered mutation	UNP P33681
A	124	GLY	ASP	engineered mutation	UNP P33681
C	52	TYR	HIS	engineered mutation	UNP P33681
C	60	GLU	ALA	engineered mutation	UNP P33681
C	69	ASP	GLU	engineered mutation	UNP P33681
C	81	LEU	MET	engineered mutation	UNP P33681
C	102	MET	VAL	engineered mutation	UNP P33681
C	105	GLY	ALA	engineered mutation	UNP P33681
C	124	GLY	ASP	engineered mutation	UNP P33681

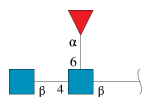
- Molecule 2 is a protein called Programmed cell death 1 ligand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	P S	0	0	0
			1687	1064	286	329	1 7			

- Molecule 3 is a protein called Programmed cell death 1 ligand 1.

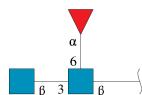
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	209	Total	C	N	O	S	0	0	0
			1683	1064	286	326	7			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



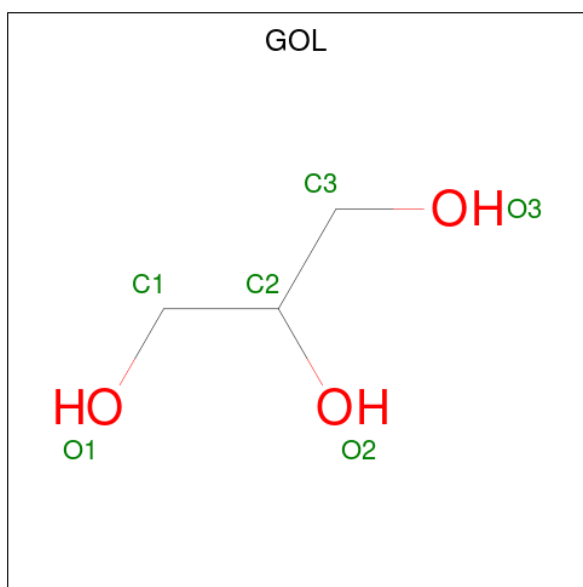
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (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	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	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	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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


- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	10	Total	O	0	0
			10	10		
8	B	30	Total	O	0	0
			30	30		
8	C	2	Total	O	0	0
			2	2		
8	D	11	Total	O	0	0
			11	11		

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.

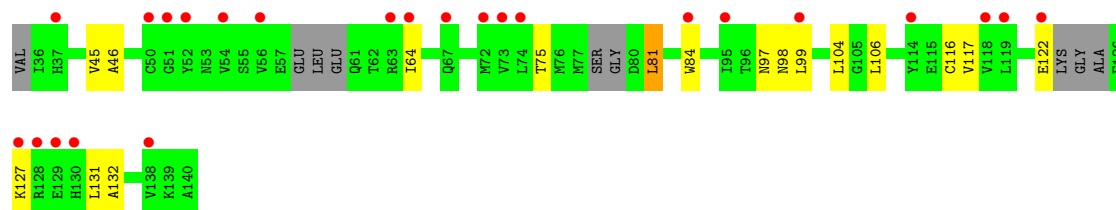
- Molecule 1: T-lymphocyte activation antigen CD80

Chain A: 



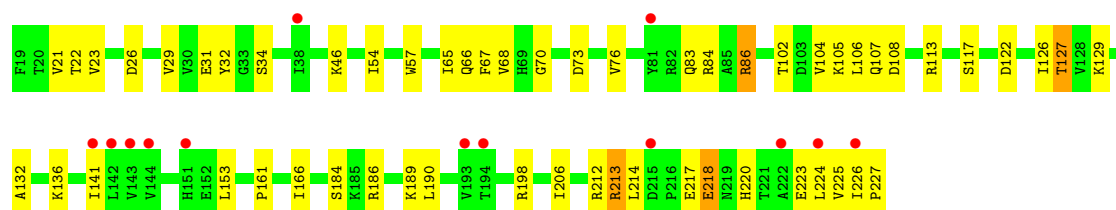
- Molecule 1: T-lymphocyte activation antigen CD80

Chain C: 




- Molecule 2: Programmed cell death 1 ligand 1

Chain B: 



- Molecule 3: Programmed cell death 1 ligand 1

Chain D: 





- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 67%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 67%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.93Å 122.15Å 152.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.34 – 3.15 76.34 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (76.34-3.15) 99.0 (76.34-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.11.8 (11-DEC-2020)	Depositor
R, R_{free}	0.247 , 0.291 0.245 , 0.298	Depositor DCC
R_{free} test set	991 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	89.5	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5316	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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: GOL, NAG, TPO, FUC

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	0.47	0/870	0.64	0/1174
1	C	0.41	0/806	0.64	0/1084
2	B	0.43	0/1706	0.61	0/2313
3	D	0.39	0/1714	0.60	0/2326
All	All	0.42	0/5096	0.62	0/6897

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	856	0	869	11	0
1	C	795	0	805	9	0
2	B	1687	0	1668	35	0
3	D	1683	0	1670	30	0
4	E	38	0	34	0	0
4	G	38	0	34	0	0
4	H	38	0	34	0	0
5	F	38	0	34	1	0
6	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	28	0	26	0	0
6	C	14	0	13	1	0
6	D	28	0	26	0	0
7	D	6	0	8	7	0
8	A	10	0	0	0	0
8	B	30	0	0	0	0
8	C	2	0	0	0	0
8	D	11	0	0	0	0
All	All	5316	0	5234	81	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 8.

All (81) 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)
3:D:24:PRO:HG3	3:D:41:LYS:HZ2	1.29	0.94
3:D:24:PRO:HG3	3:D:41:LYS:NZ	1.86	0.90
2:B:86:ARG:HE	7:D:303:GOL:H2	1.40	0.87
3:D:89:LYS:NZ	7:D:303:GOL:H12	1.98	0.79
3:D:106:LEU:HD22	3:D:189:LYS:HD3	1.71	0.71
3:D:86:ARG:HE	7:D:303:GOL:H11	1.56	0.71
2:B:23:VAL:HG11	2:B:126:ILE:HD11	1.73	0.70
2:B:31:GLU:O	2:B:34:SER:HB3	1.92	0.69
1:C:104:LEU:HD12	3:D:117:SER:HB2	1.76	0.67
3:D:31:GLU:O	3:D:34:SER:HB3	1.94	0.67
3:D:23:VAL:HG11	3:D:126:ILE:HD11	1.77	0.65
1:A:64:ILE:HB	1:A:76:MET:HB3	1.78	0.64
1:A:46:ALA:HB2	1:A:106:LEU:HD11	1.81	0.61
2:B:86:ARG:NE	7:D:303:GOL:H2	2.11	0.61
2:B:84:ARG:NH2	2:B:108:ASP:OD2	2.26	0.61
2:B:206:ILE:HD11	2:B:223:GLU:HB2	1.83	0.60
3:D:89:LYS:HZ2	7:D:303:GOL:H12	1.65	0.60
2:B:29:VAL:HG22	2:B:129:LYS:HB2	1.84	0.59
3:D:89:LYS:HZ3	7:D:303:GOL:H12	1.66	0.59
3:D:29:VAL:HG22	3:D:129:LYS:HB2	1.85	0.59
3:D:135:ASN:HD22	3:D:220:HIS:CE1	2.20	0.58
3:D:106:LEU:HD11	3:D:160:TYR:CB	2.34	0.57
1:C:75:THR:HG23	1:C:84:TRP:HE1	1.68	0.57
1:A:35:VAL:HB	1:A:133:GLU:HB3	1.86	0.56
3:D:161:PRO:HD2	3:D:213:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:HD12	2:B:117:SER:HB2	1.88	0.55
2:B:57:TRP:HB2	2:B:65:ILE:HB	1.89	0.55
3:D:57:TRP:HB2	3:D:65:ILE:HB	1.89	0.55
3:D:66:GLN:HB3	3:D:76:VAL:HG11	1.89	0.55
1:C:81:LEU:O	1:C:81:LEU:HG	2.08	0.53
2:B:66:GLN:HB3	2:B:76:VAL:HG11	1.90	0.53
1:A:116:CYS:HB3	1:A:132:ALA:HB3	1.91	0.52
2:B:26:ASP:O	2:B:127:TPO:O1P	2.28	0.52
1:C:64:ILE:HG12	1:C:99:LEU:HD13	1.91	0.51
2:B:107:GLN:NE2	2:B:108:ASP:OD1	2.44	0.51
2:B:102:THR:HG21	5:F:3:FUC:H5	1.93	0.51
2:B:105:LYS:HB2	2:B:107:GLN:HG3	1.93	0.51
1:C:116:CYS:HB3	1:C:132:ALA:HB3	1.92	0.51
3:D:54:ILE:HB	3:D:117:SER:HB3	1.92	0.50
3:D:213:ARG:NH2	3:D:216:PRO:HD2	2.27	0.50
3:D:218:GLU:OE1	3:D:220:HIS:NE2	2.43	0.50
2:B:54:ILE:HB	2:B:117:SER:HB3	1.93	0.49
3:D:86:ARG:HE	7:D:303:GOL:C1	2.25	0.49
2:B:34:SER:O	2:B:104:VAL:HG13	2.12	0.49
2:B:213:ARG:NH2	2:B:214:LEU:O	2.46	0.49
3:D:106:LEU:HD11	3:D:160:TYR:HB2	1.96	0.47
1:A:113:THR:HG23	1:A:135:THR:HG22	1.97	0.47
2:B:161:PRO:HD2	2:B:213:ARG:HG3	1.97	0.47
3:D:67:PHE:CZ	3:D:70:GLY:HA2	2.50	0.47
3:D:213:ARG:HB3	3:D:218:GLU:HG3	1.96	0.47
3:D:54:ILE:HG23	3:D:68:VAL:HG12	1.97	0.46
1:C:122:GLU:HB2	1:C:127:LYS:HD2	1.97	0.46
3:D:213:ARG:HH22	3:D:216:PRO:HD2	1.81	0.46
2:B:67:PHE:CZ	2:B:70:GLY:HA2	2.51	0.45
1:A:52:TYR:HE2	1:A:120:LYS:NZ	2.15	0.45
1:A:56:VAL:HA	1:A:59:LEU:HD12	1.99	0.45
1:A:35:VAL:CG2	1:A:37:HIS:CE1	2.99	0.45
1:C:46:ALA:HB2	1:C:106:LEU:HD11	1.99	0.45
2:B:106:LEU:HD12	2:B:189:LYS:HB3	1.99	0.45
2:B:54:ILE:HG23	2:B:68:VAL:HG12	1.99	0.44
2:B:106:LEU:HD21	2:B:132:ALA:HB2	2.01	0.43
2:B:153:LEU:HD23	2:B:224:LEU:HD22	1.99	0.43
2:B:166:ILE:HD11	2:B:212:ARG:HE	1.84	0.43
2:B:73:ASP:O	2:B:76:VAL:HG12	2.18	0.43
2:B:218:GLU:OE2	2:B:220:HIS:NE2	2.46	0.42
2:B:23:VAL:CG1	2:B:126:ILE:HD11	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ARG:NH1	2:B:217:GLU:OE2	2.52	0.42
2:B:83:GLN:HE21	3:D:90:ASP:HA	1.83	0.42
2:B:32:TYR:OH	2:B:186:ARG:HD2	2.20	0.41
3:D:73:ASP:O	3:D:76:VAL:HG12	2.20	0.41
2:B:184:SER:HB3	2:B:190:LEU:HB3	2.01	0.41
1:A:111:GLU:HG3	1:A:136:LEU:O	2.21	0.41
1:A:121:TYR:HB2	1:A:126:PHE:CE2	2.55	0.41
1:C:45:VAL:HG22	3:D:56:TYR:CE2	2.55	0.41
3:D:158:GLU:HA	3:D:191:PHE:O	2.20	0.41
2:B:206:ILE:HD13	2:B:225:VAL:HG22	2.03	0.41
2:B:21:VAL:HG23	2:B:122:ASP:HB3	2.02	0.40
2:B:141:ILE:HD11	2:B:224:LEU:HB3	2.04	0.40
2:B:226:ILE:HA	2:B:227:PRO:HD3	1.96	0.40
1:C:97:ASN:HA	6:C:201:NAG:H61	2.03	0.40
3:D:153:LEU:N	3:D:153:LEU:HD12	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	104/106 (98%)	99 (95%)	4 (4%)	1 (1%)	15	51
1	C	89/106 (84%)	84 (94%)	5 (6%)	0	100	100
2	B	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29	65
3	D	207/209 (99%)	196 (95%)	10 (5%)	1 (0%)	29	65
All	All	606/630 (96%)	577 (95%)	26 (4%)	3 (0%)	29	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	LYS
2	B	46	LYS
3	D	46	LYS

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	97/97 (100%)	93 (96%)	4 (4%)	30	63
1	C	91/97 (94%)	87 (96%)	4 (4%)	28	61
2	B	189/189 (100%)	182 (96%)	7 (4%)	34	66
3	D	190/190 (100%)	182 (96%)	8 (4%)	30	62
All	All	567/573 (99%)	544 (96%)	23 (4%)	30	63

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	95	ILE
1	A	117	VAL
1	A	131	LEU
2	B	22	THR
2	B	86	ARG
2	B	113	ARG
2	B	136	LYS
2	B	198	ARG
2	B	213	ARG
2	B	218	GLU
1	C	81	LEU
1	C	98	ASN
1	C	117	VAL
1	C	131	LEU
3	D	19	PHE
3	D	60	GLU
3	D	86	ARG
3	D	135	ASN

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Mol	Chain	Res	Type
3	D	171	ASP
3	D	184	SER
3	D	198	ARG
3	D	218	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	83	GLN
1	C	98	ASN
3	D	83	GLN
3	D	135	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TPO	B	127	2	8,10,11	2.54	1 (12%)	10,14,16	2.53	4 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	B	127	2	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	127	TPO	P-OG1	6.63	1.71	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	127	TPO	O2P-P-O1P	-5.28	90.01	110.68
2	B	127	TPO	CG2-CB-CA	-3.23	106.79	113.16
2	B	127	TPO	O3P-P-O2P	2.74	118.11	107.64
2	B	127	TPO	OG1-P-O1P	2.21	117.90	109.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	127	TPO	CB-OG1-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	127	TPO	1	0

5.5 Carbohydrates ⓘ

12 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	$\# Z > 2$
4	NAG	E	1	4,1	14,14,15	0.34	0	17,19,21	1.05	2 (11%)
4	NAG	E	2	4	14,14,15	0.28	0	17,19,21	0.90	1 (5%)
4	FUC	E	3	4	10,10,11	0.63	0	14,14,16	1.28	3 (21%)
5	NAG	F	1	2,5	14,14,15	0.40	0	17,19,21	0.99	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	F	2	5	14,14,15	0.48	0	17,19,21	1.41	3 (17%)
5	FUC	F	3	5	10,10,11	0.35	0	14,14,16	0.67	0
4	NAG	G	1	4,1	14,14,15	0.35	0	17,19,21	0.85	1 (5%)
4	NAG	G	2	4	14,14,15	0.27	0	17,19,21	0.92	1 (5%)
4	FUC	G	3	4	10,10,11	0.33	0	14,14,16	1.01	0
4	NAG	H	1	4,3	14,14,15	0.29	0	17,19,21	0.87	1 (5%)
4	NAG	H	2	4	14,14,15	0.28	0	17,19,21	0.71	0
4	FUC	H	3	4	10,10,11	0.72	0	14,14,16	1.38	3 (21%)

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
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	FUC	E	3	4	-	-	0/1/1/1
5	NAG	F	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	FUC	F	3	5	-	-	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	FUC	G	3	4	-	-	0/1/1/1
4	NAG	H	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	FUC	H	3	4	-	-	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	2	NAG	C1-O5-C5	3.88	117.45	112.19
4	H	3	FUC	C1-O5-C5	3.43	120.55	112.78
4	E	2	NAG	C1-C2-N2	2.82	115.31	110.49
4	H	1	NAG	O5-C1-C2	-2.79	106.88	111.29
5	F	2	NAG	O5-C1-C2	2.78	115.68	111.29
4	G	2	NAG	C1-C2-N2	2.75	115.18	110.49
5	F	1	NAG	C1-C2-N2	-2.73	105.83	110.49
5	F	1	NAG	O3-C3-C2	2.46	114.56	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	O5-C1-C2	-2.46	107.40	111.29
4	H	3	FUC	C1-C2-C3	2.36	112.56	109.67
4	H	3	FUC	C2-C3-C4	2.34	114.94	110.89
4	E	1	NAG	C1-C2-N2	-2.32	106.52	110.49
4	E	3	FUC	O2-C2-C1	2.30	113.86	109.15
4	E	3	FUC	C6-C5-C4	2.12	116.99	113.07
4	E	3	FUC	C1-C2-C3	2.08	112.22	109.67
4	E	1	NAG	O5-C1-C2	-2.06	108.03	111.29
5	F	2	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

All (9) torsion outliers are listed below:

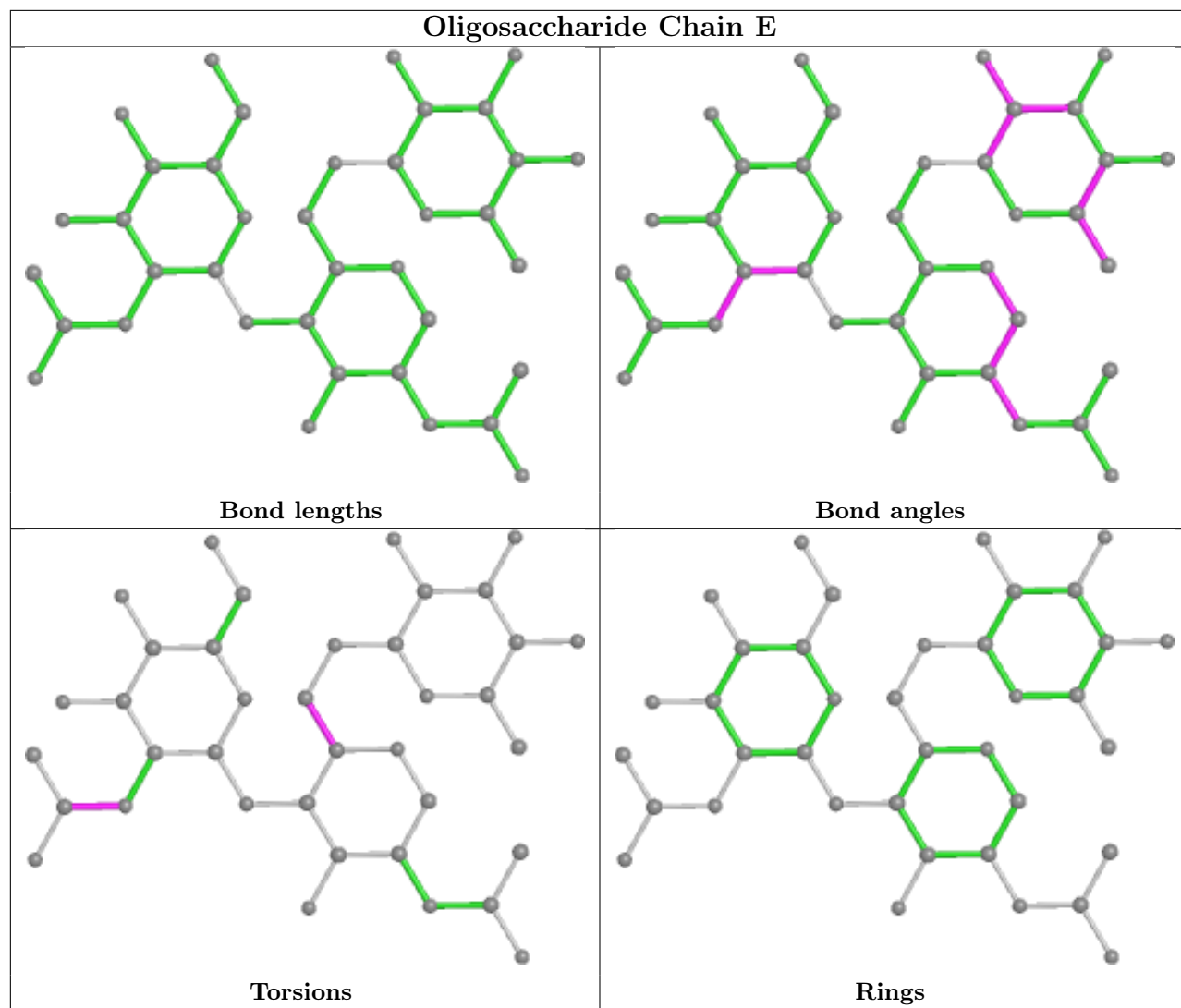
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C8-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	H	2	NAG	O5-C5-C6-O6

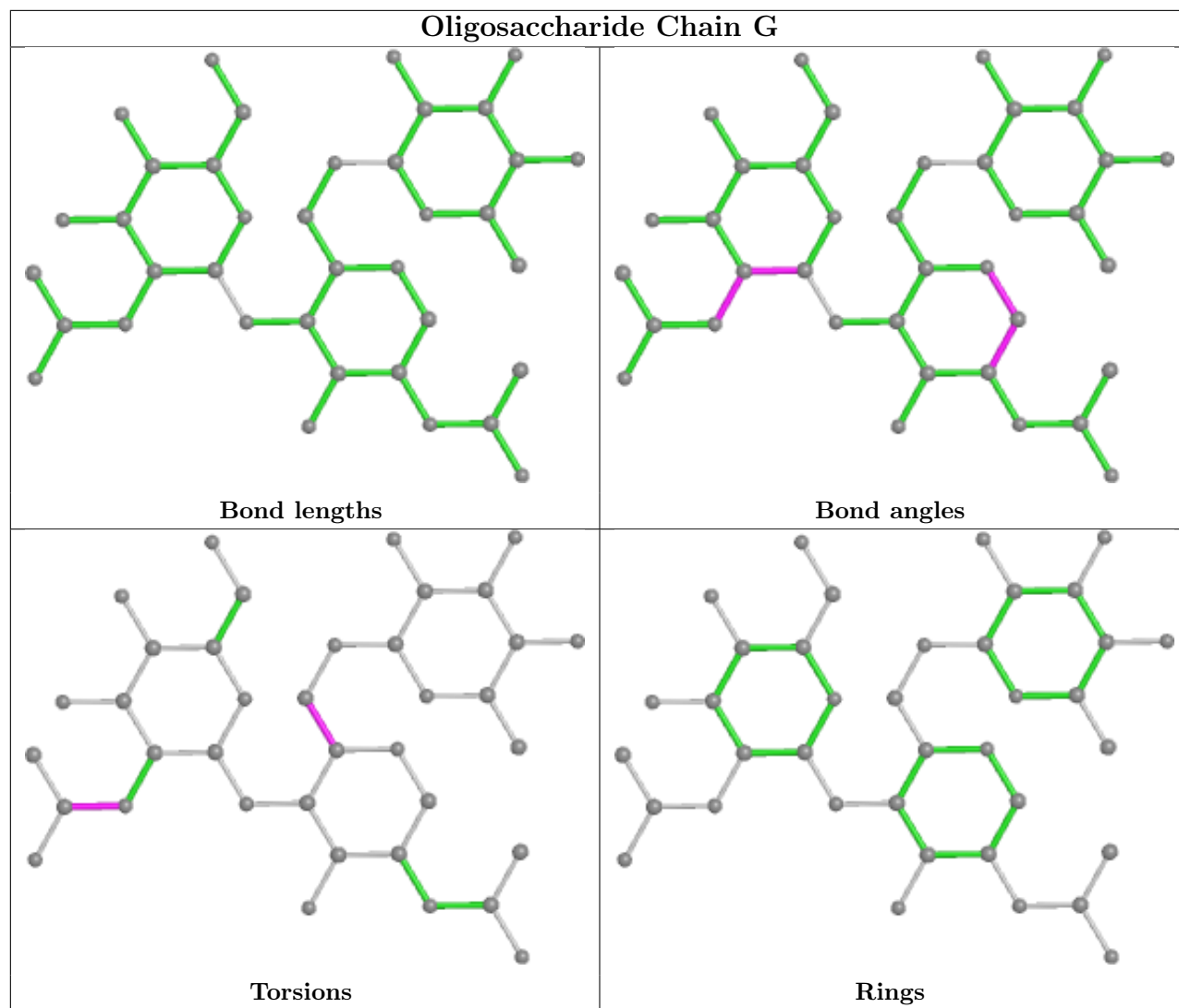
There are no ring outliers.

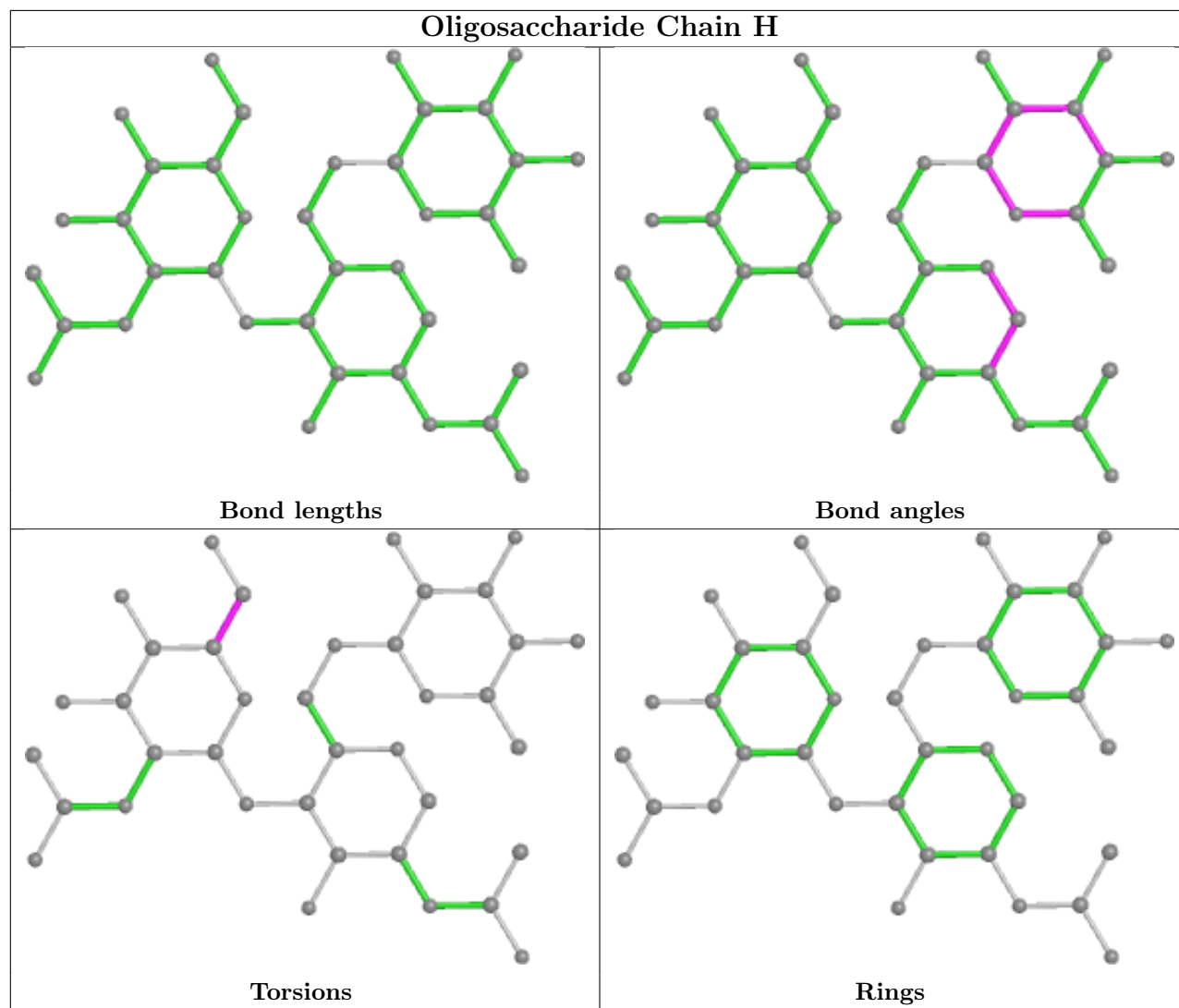
1 monomer is involved in 1 short contact:

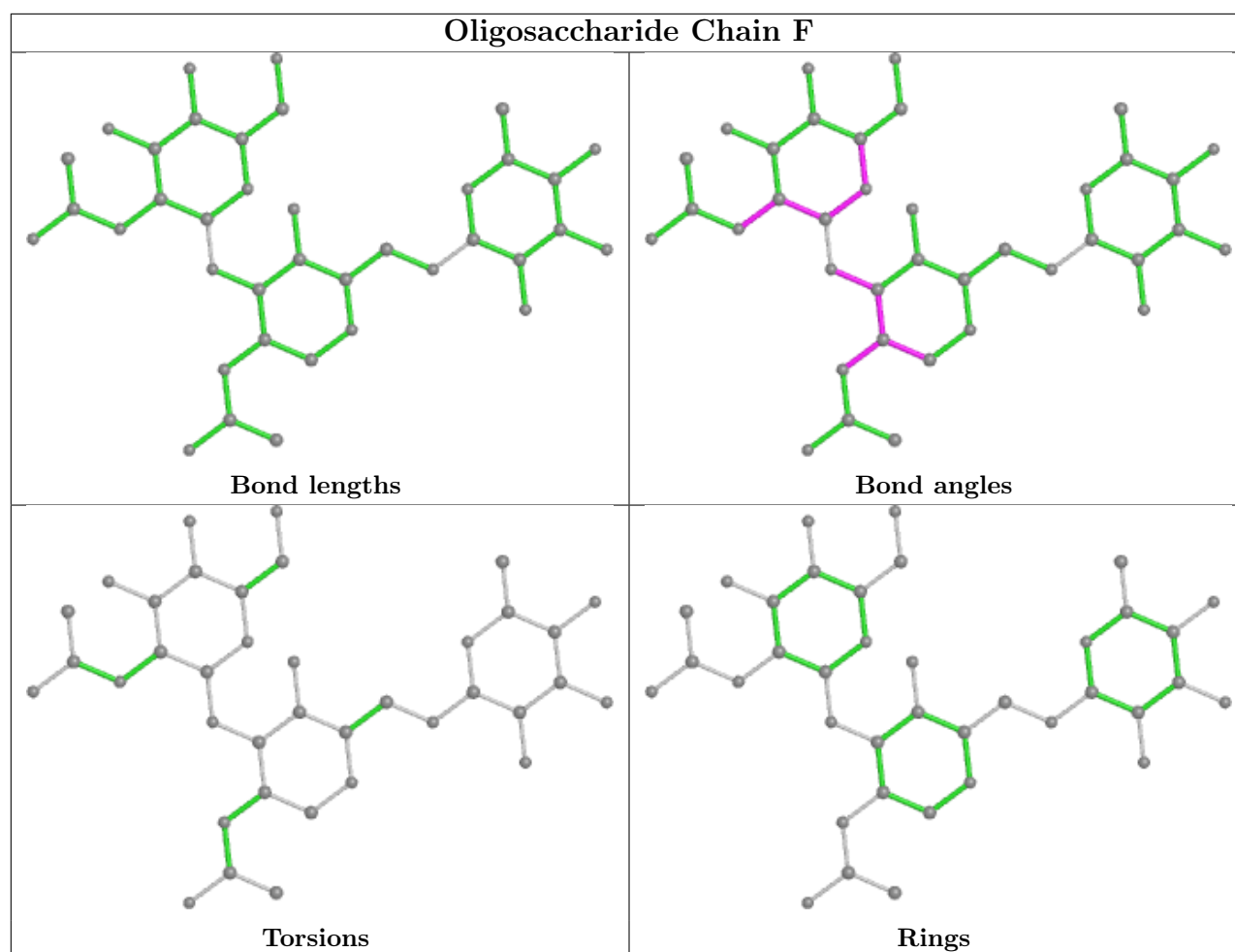
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	3	FUC	1	0

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









5.6 Ligand geometry [i](#)

7 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	B	301	2	14,14,15	0.27	0	17,19,21	0.84	1 (5%)
6	NAG	A	201	1	14,14,15	0.57	0	17,19,21	1.32	2 (11%)
6	NAG	D	302	3	14,14,15	0.35	0	17,19,21	0.93	2 (11%)
7	GOL	D	303	-	5,5,5	0.17	0	5,5,5	0.38	0
6	NAG	B	302	2	14,14,15	0.47	0	17,19,21	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	201	1	14,14,15	0.34	0	17,19,21	0.61	0
6	NAG	D	301	3	14,14,15	0.28	0	17,19,21	0.80	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	B	301	2	-	0/6/23/26	0/1/1/1
6	NAG	A	201	1	-	2/6/23/26	0/1/1/1
6	NAG	D	302	3	-	1/6/23/26	0/1/1/1
7	GOL	D	303	-	-	0/4/4/4	-
6	NAG	B	302	2	-	0/6/23/26	0/1/1/1
6	NAG	C	201	1	-	0/6/23/26	0/1/1/1
6	NAG	D	301	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	201	NAG	C1-O5-C5	3.46	116.88	112.19
6	D	302	NAG	C1-C2-N2	2.65	115.01	110.49
6	B	302	NAG	O5-C1-C2	2.62	115.43	111.29
6	B	302	NAG	C3-C4-C5	2.61	114.90	110.24
6	A	201	NAG	O5-C1-C2	2.57	115.35	111.29
6	B	301	NAG	C1-O5-C5	2.49	115.56	112.19
6	D	301	NAG	C1-O5-C5	2.42	115.47	112.19
6	D	302	NAG	C2-N2-C7	2.12	125.93	122.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

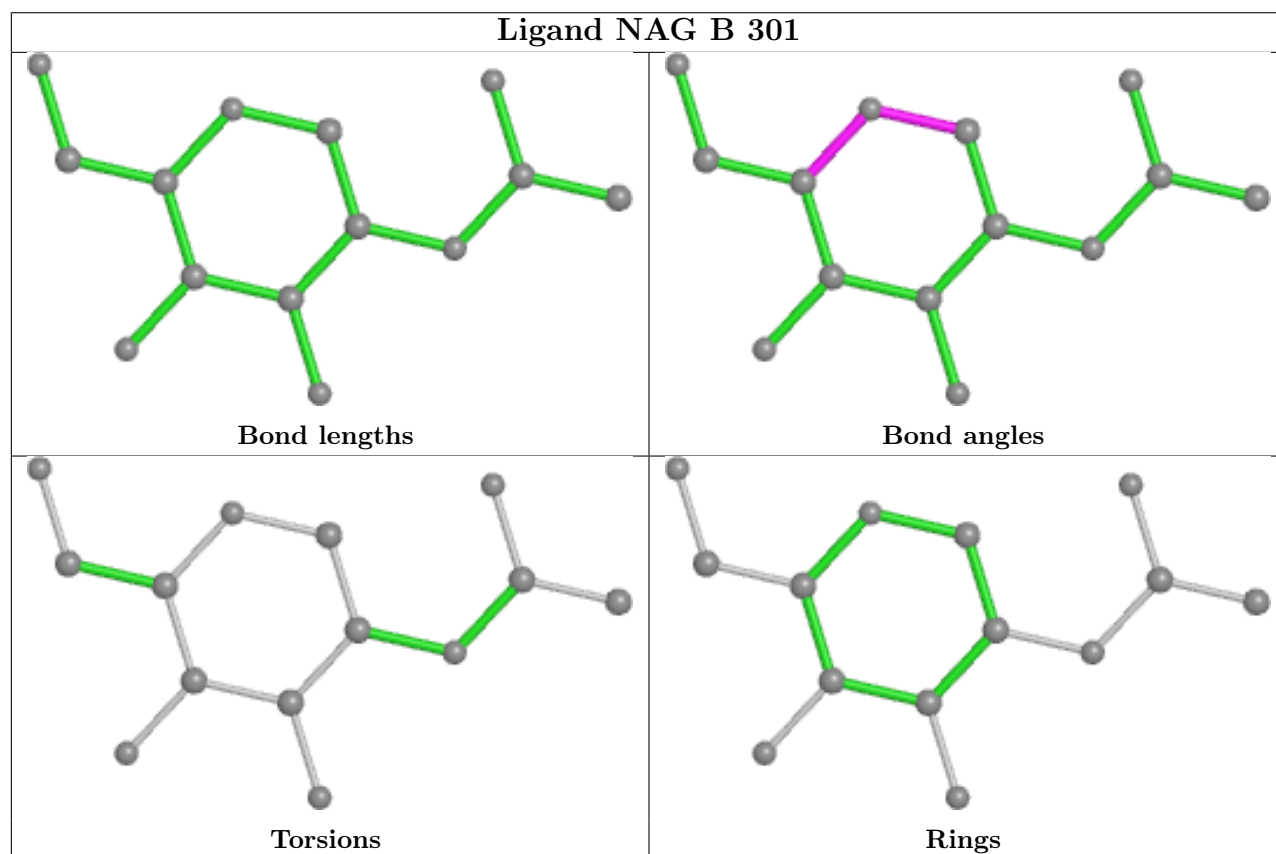
Mol	Chain	Res	Type	Atoms
6	A	201	NAG	O5-C5-C6-O6
6	A	201	NAG	C4-C5-C6-O6
6	D	302	NAG	C1-C2-N2-C7

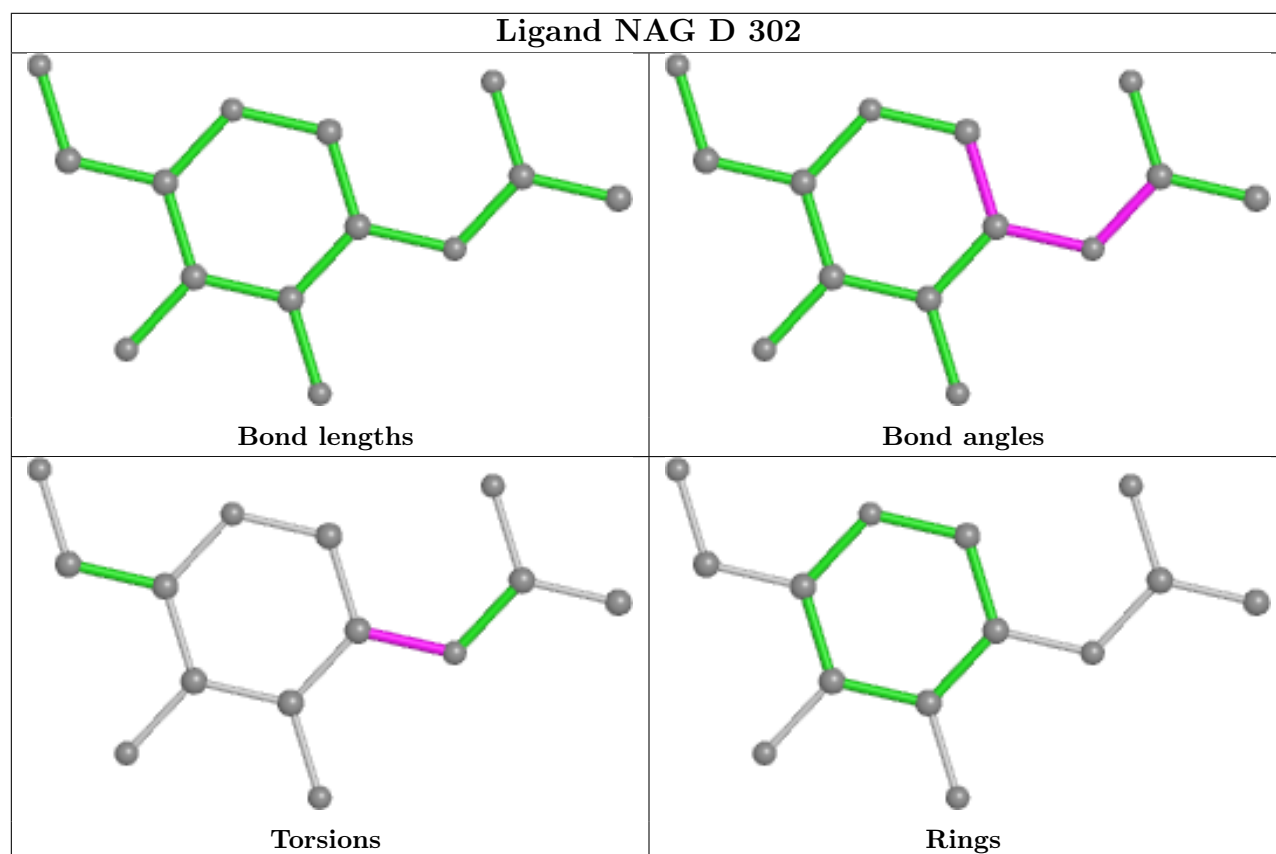
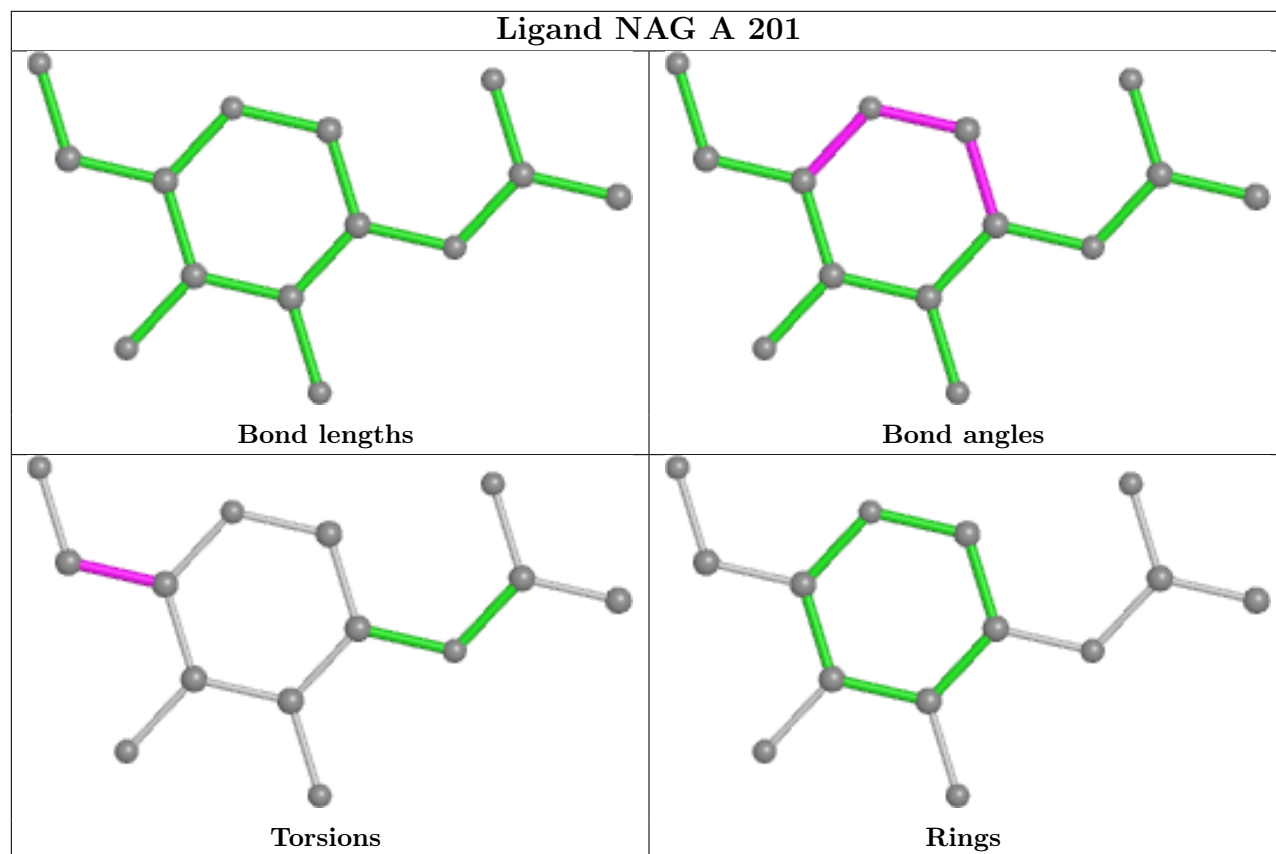
There are no ring outliers.

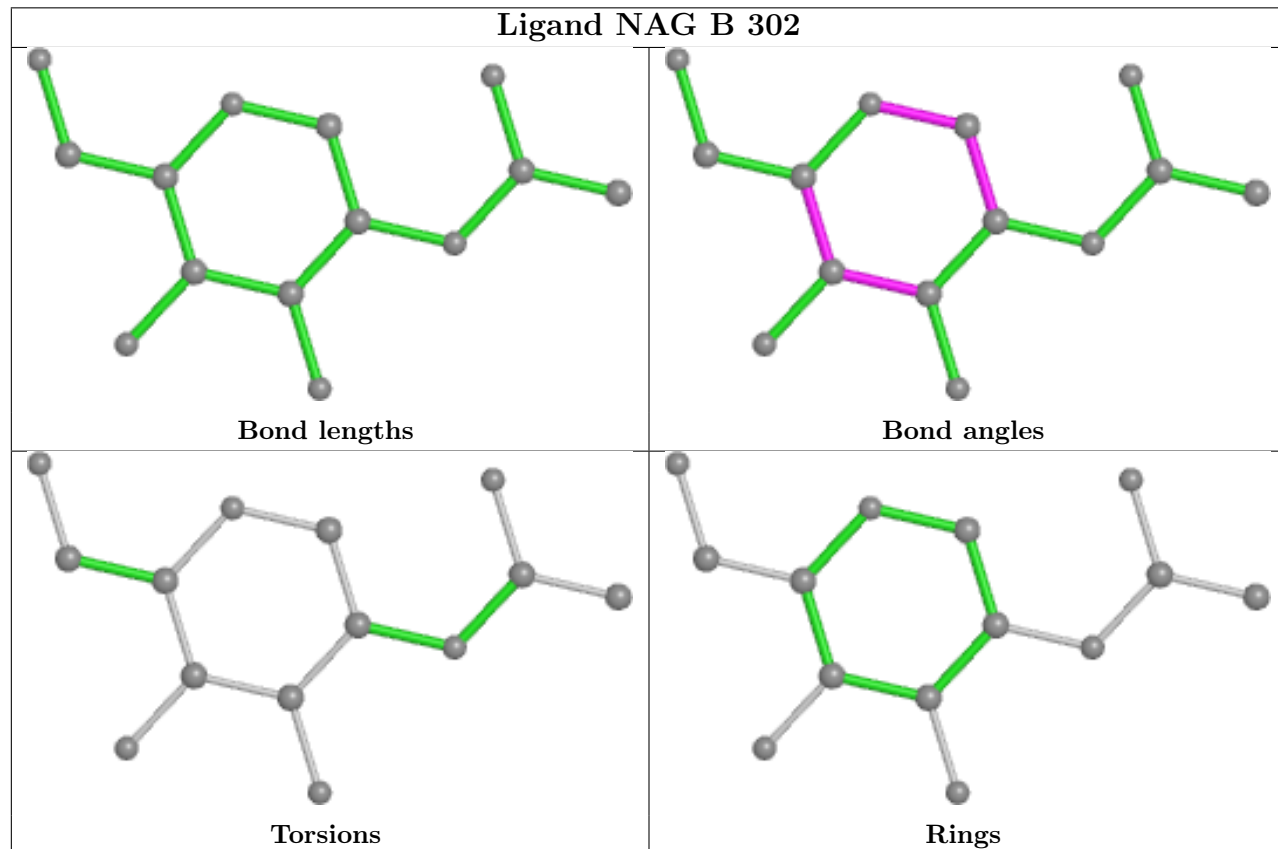
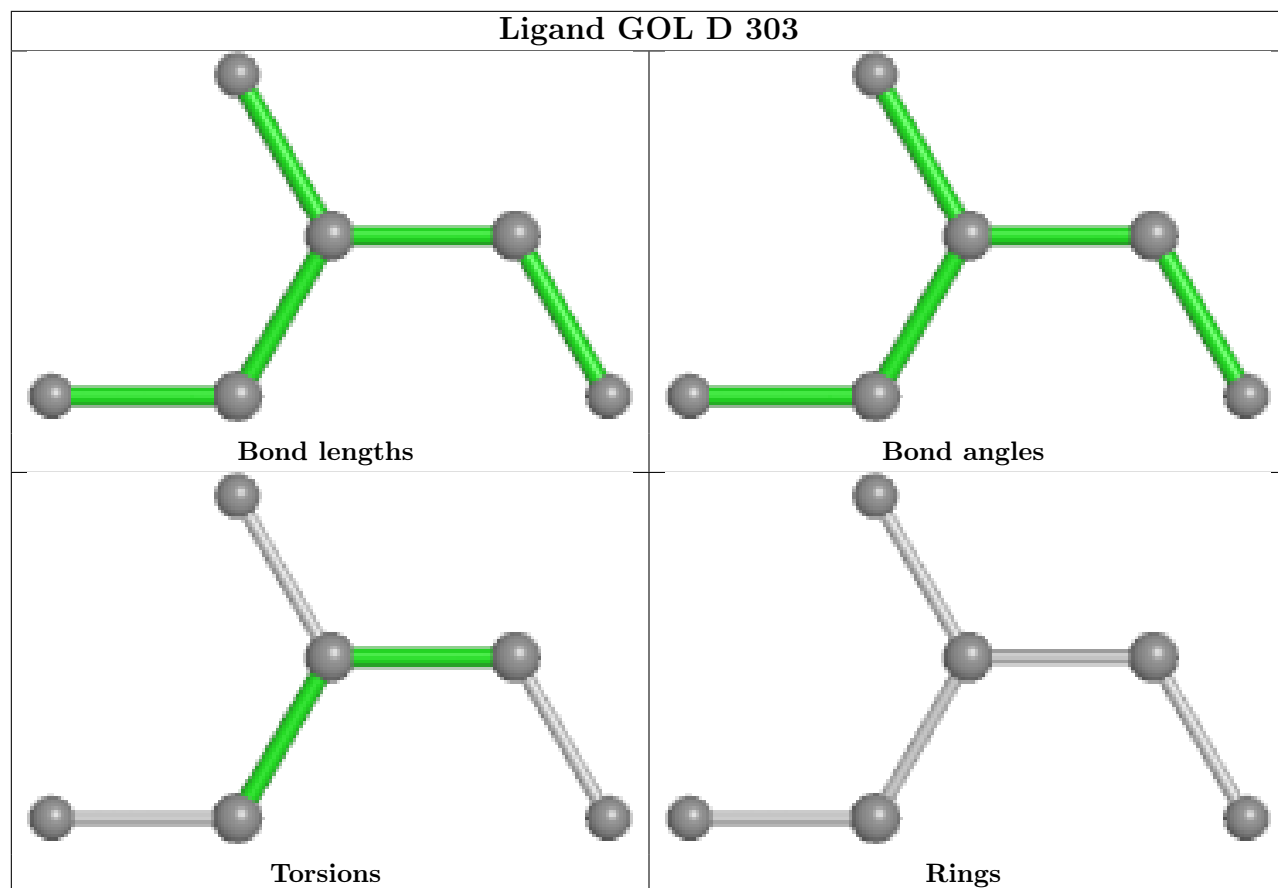
2 monomers are involved in 8 short contacts:

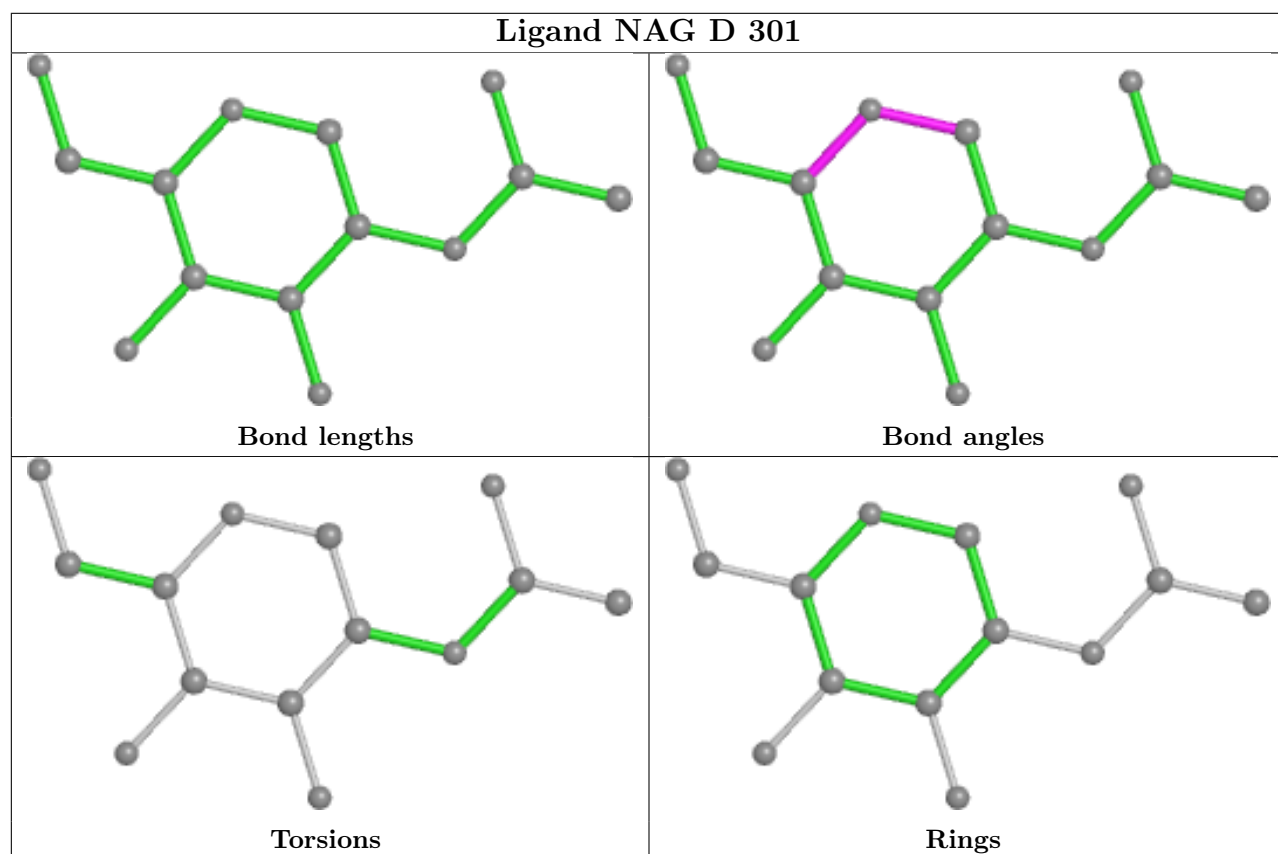
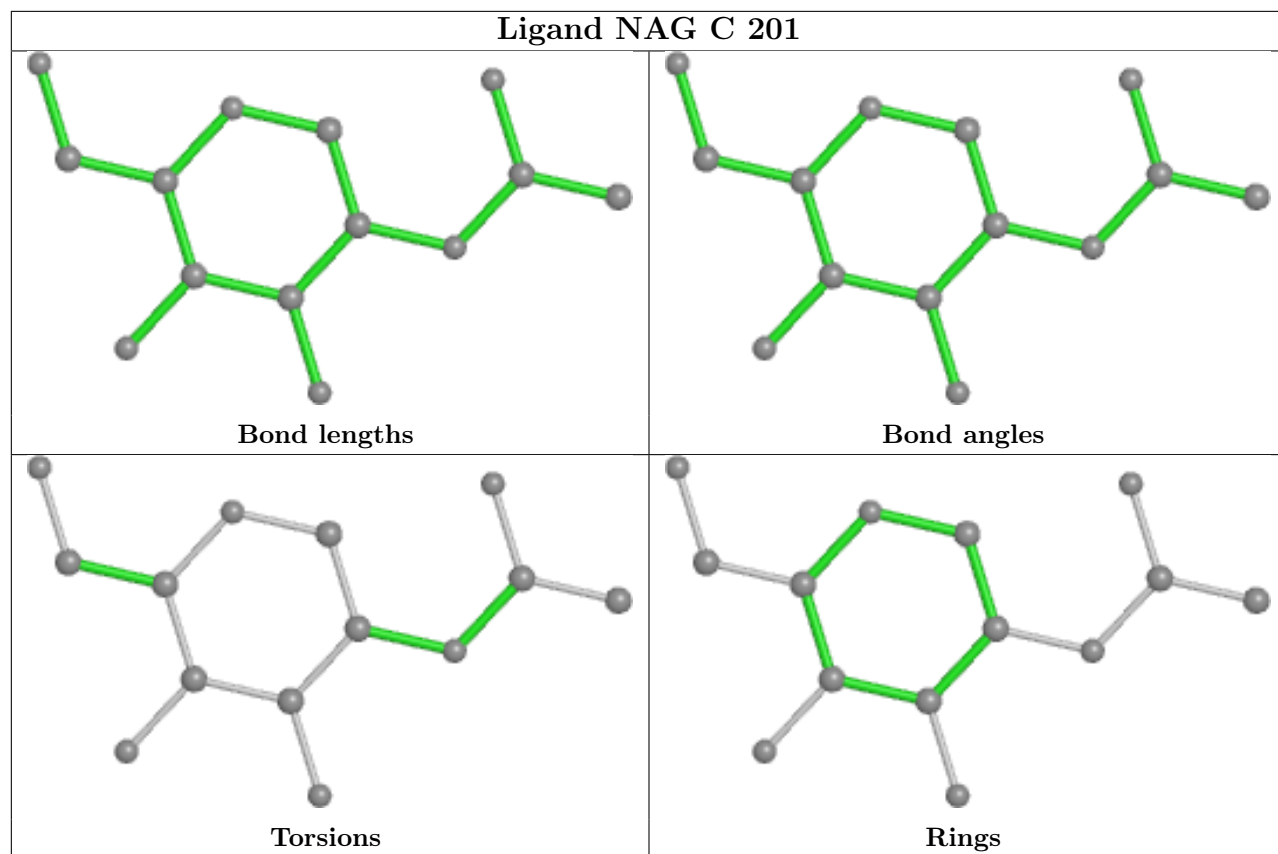
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	303	GOL	7	0
6	C	201	NAG	1	0

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 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

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	106/106 (100%)	0.54	0 100 100	73, 89, 109, 122	0
1	C	97/106 (91%)	1.23	24 (24%) 0 0	125, 157, 181, 189	0
2	B	208/209 (99%)	0.63	13 (6%) 20 10	70, 89, 134, 151	0
3	D	209/209 (100%)	0.48	7 (3%) 46 29	95, 113, 133, 142	0
All	All	620/630 (98%)	0.66	44 (7%) 16 8	70, 105, 165, 189	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	50	CYS	5.0
2	B	151	HIS	5.0
1	C	73	VAL	4.9
1	C	118	VAL	4.9
1	C	64	ILE	4.1
1	C	52	TYR	4.0
1	C	72	MET	3.8
1	C	129	GLU	3.5
1	C	130	HIS	3.5
1	C	99	LEU	3.4
1	C	37	HIS	3.4
3	D	223	GLU	3.3
1	C	56	VAL	3.1
1	C	138	VAL	3.1
2	B	222	ALA	3.0
1	C	119	LEU	3.0
3	D	42	PHE	3.0
1	C	51	GLY	3.0
2	B	226	ILE	2.9
2	B	143	VAL	2.9
1	C	54	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	74	LEU	2.7
2	B	142	LEU	2.6
1	C	122	GLU	2.6
2	B	224	LEU	2.5
1	C	84	TRP	2.5
3	D	207	PHE	2.4
3	D	190	LEU	2.3
2	B	38	ILE	2.3
2	B	194	THR	2.3
2	B	81	TYR	2.3
1	C	63	ARG	2.3
3	D	43	PRO	2.3
1	C	127	LYS	2.3
2	B	193	VAL	2.3
2	B	144	VAL	2.2
1	C	114	TYR	2.2
3	D	72	GLU	2.1
2	B	215	ASP	2.1
1	C	67	GLN	2.1
3	D	38	ILE	2.1
2	B	141	ILE	2.0
1	C	95	ILE	2.0
1	C	128	ARG	2.0

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

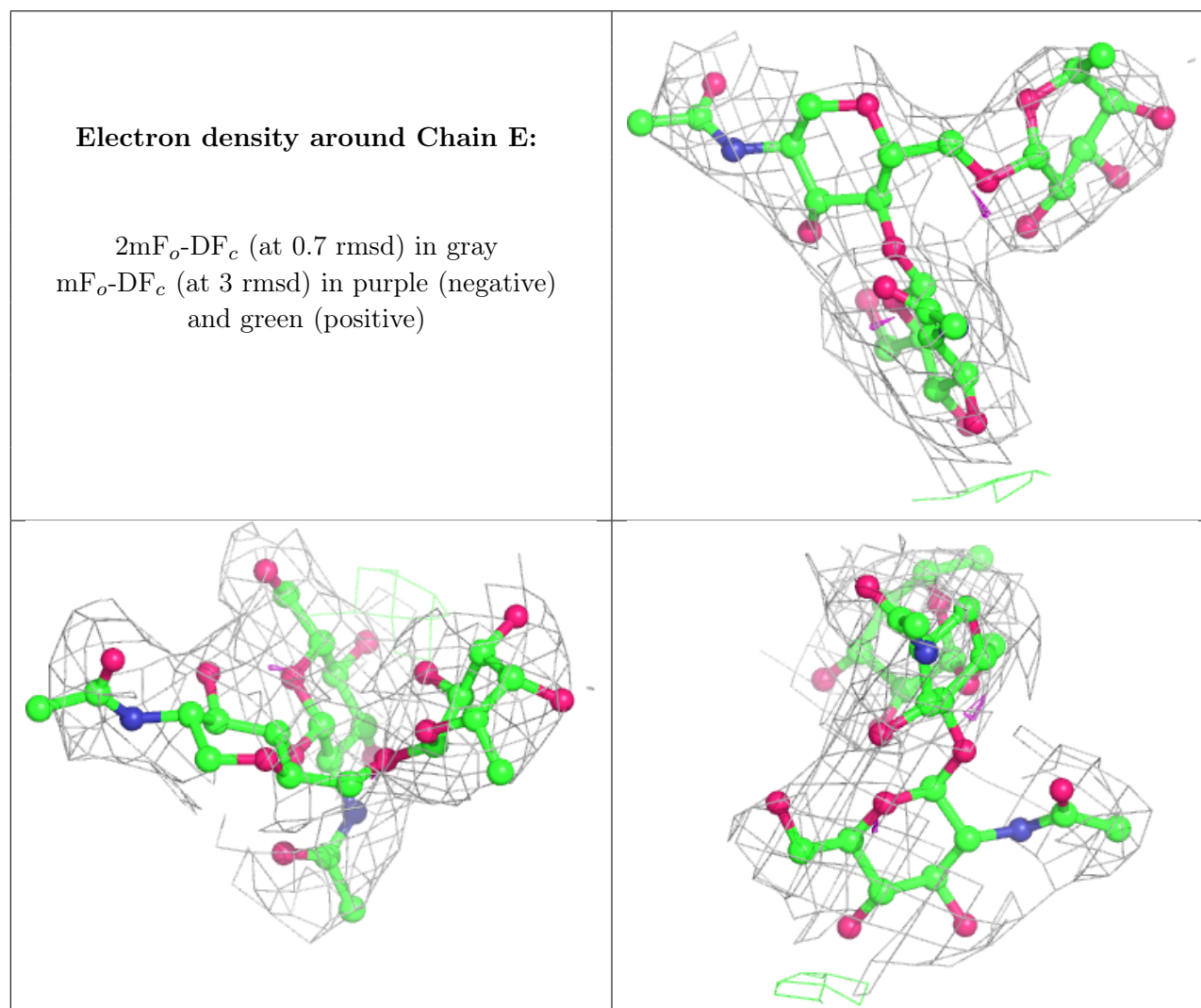
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TPO	B	127	11/12	0.81	0.28	82,87,127,138	0

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.

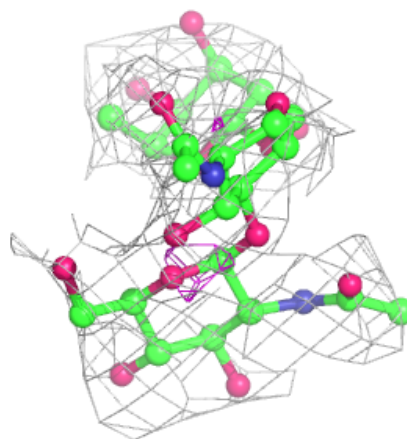
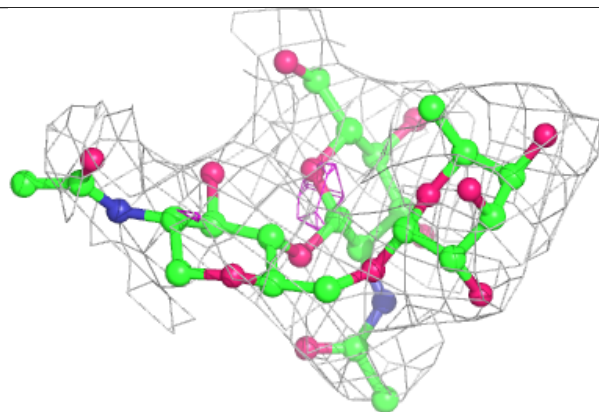
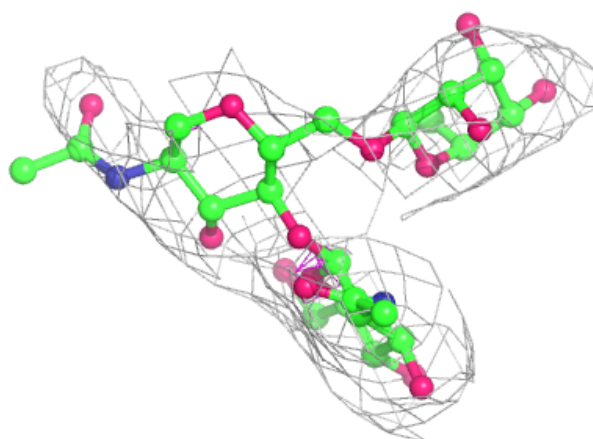
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	F	2	14/15	0.62	0.48	132,133,134,134	0
5	NAG	F	1	14/15	0.72	0.32	123,126,130,131	0
5	FUC	F	3	10/11	0.73	0.75	133,134,135,136	0
4	NAG	H	2	14/15	0.78	0.19	141,141,143,143	0
4	NAG	G	2	14/15	0.79	0.20	156,157,157,157	0
4	NAG	G	1	14/15	0.81	0.23	154,155,156,156	0
4	FUC	G	3	10/11	0.82	0.31	155,156,156,156	0
4	FUC	H	3	10/11	0.83	0.56	142,142,143,143	0
4	NAG	E	2	14/15	0.83	0.17	110,111,112,113	0
4	NAG	H	1	14/15	0.84	0.16	136,137,140,141	0
4	FUC	E	3	10/11	0.94	0.26	105,105,106,106	0
4	NAG	E	1	14/15	0.94	0.18	104,106,107,108	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.



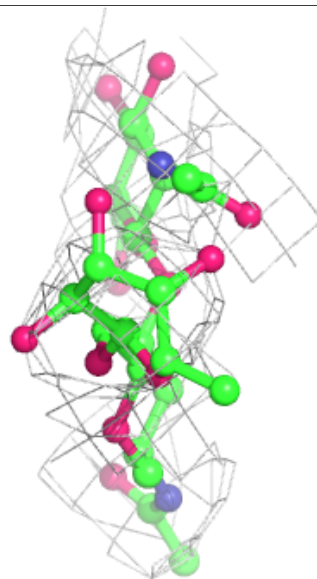
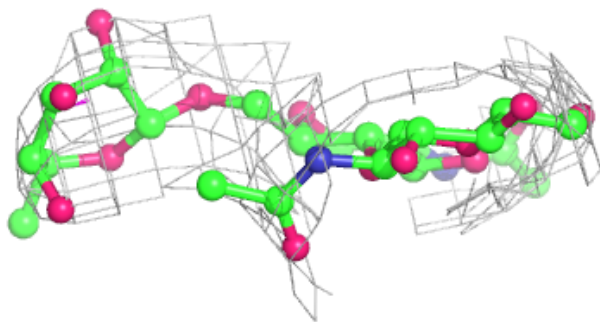
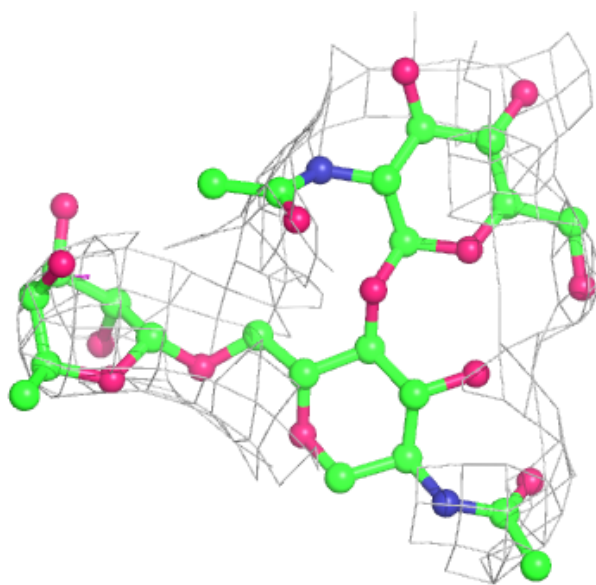
Electron density around Chain G:

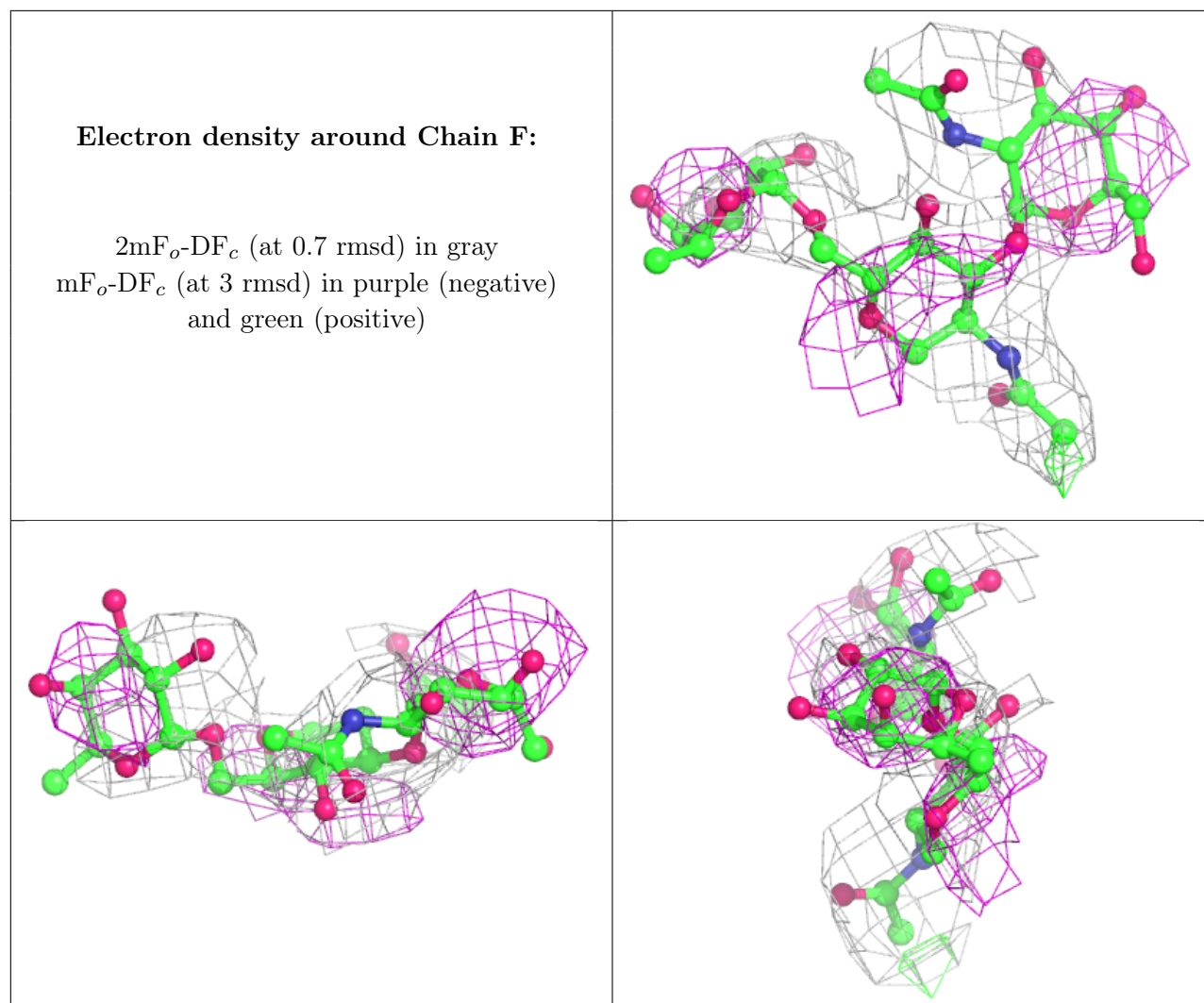
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





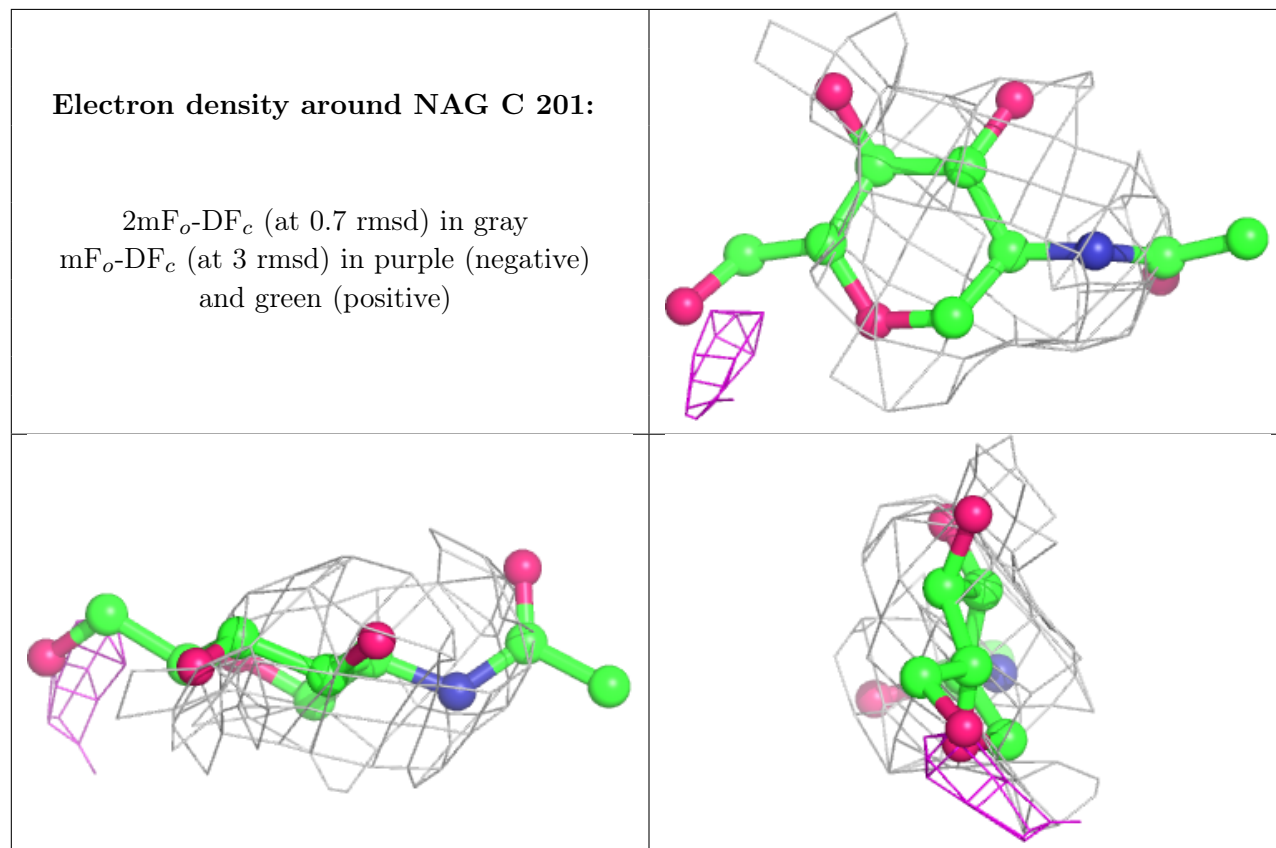
6.4 Ligands ⓘ

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	C	201	14/15	0.33	0.56	183,183,184,184	0
6	NAG	A	201	14/15	0.48	0.34	124,125,126,126	0
6	NAG	B	302	14/15	0.63	0.26	148,149,151,151	0
6	NAG	D	301	14/15	0.74	0.26	121,122,123,123	0
6	NAG	D	302	14/15	0.74	0.24	131,131,132,132	0
6	NAG	B	301	14/15	0.81	0.35	102,102,104,104	0
7	GOL	D	303	6/6	0.92	0.29	77,77,78,79	0

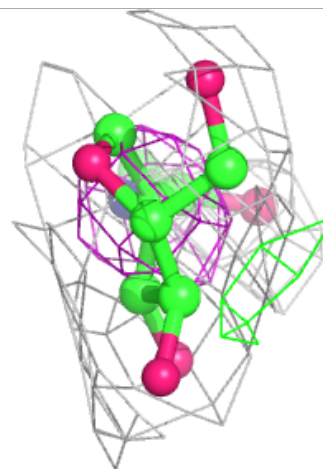
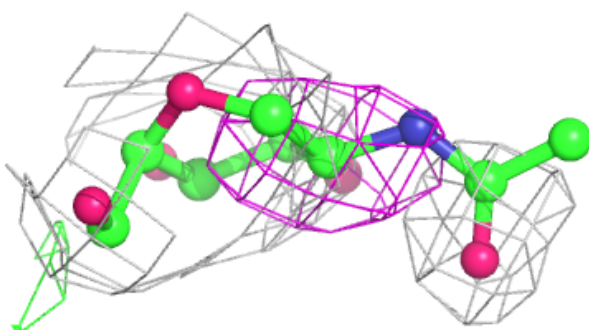
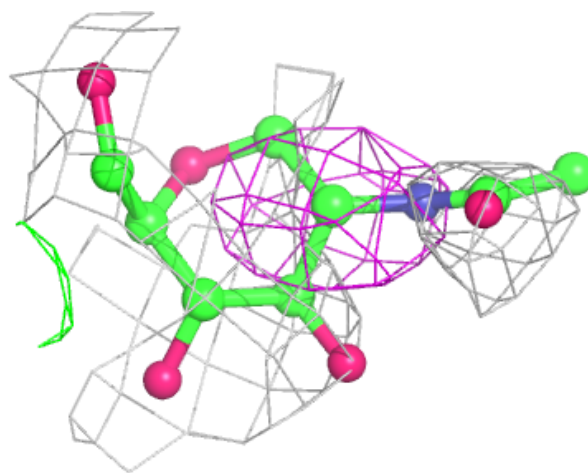
The following is a graphical depiction of the model fit to experimental electron density of all

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.



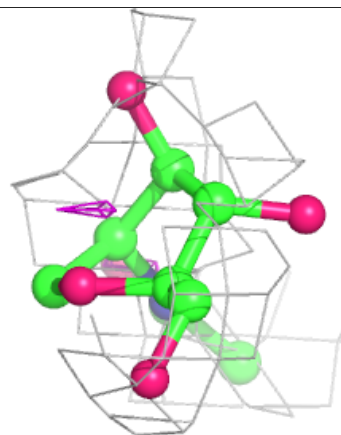
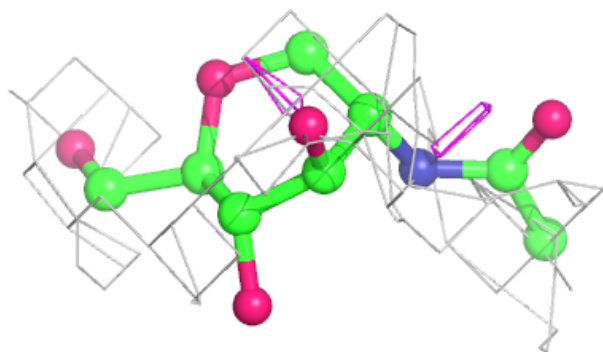
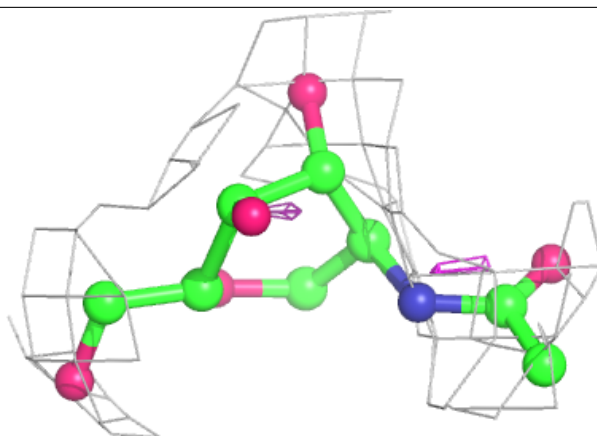
Electron density around NAG A 201:

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

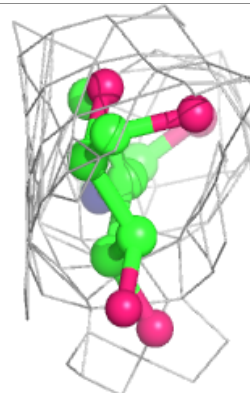
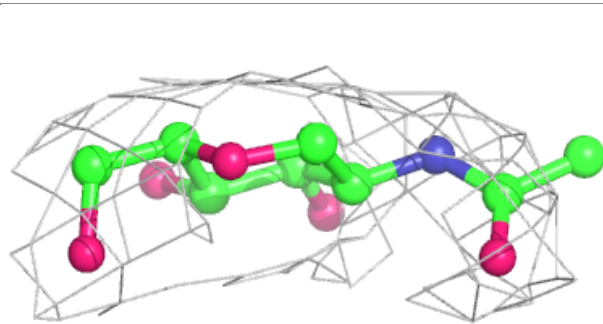
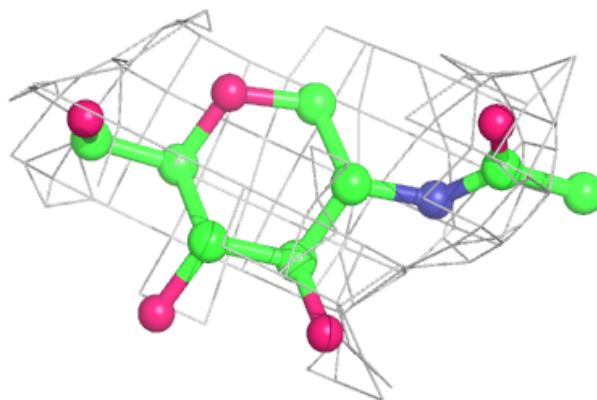


Electron density around NAG B 302:

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

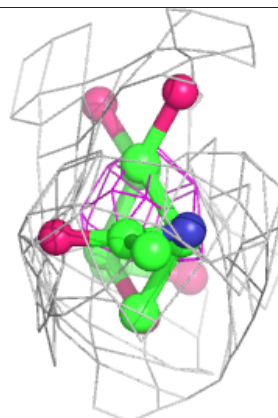
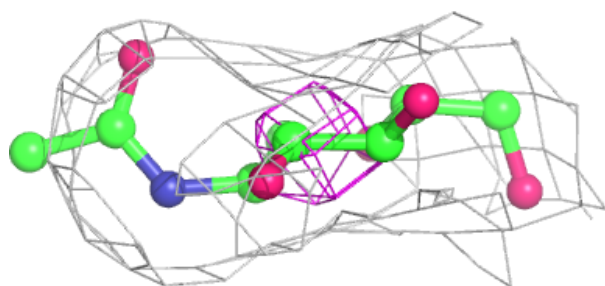
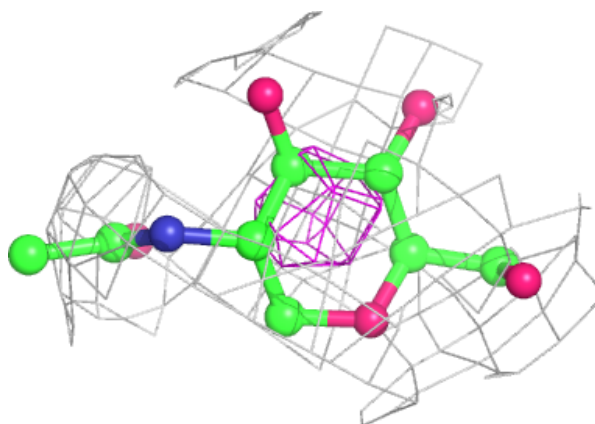
**Electron density around NAG D 301:**

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



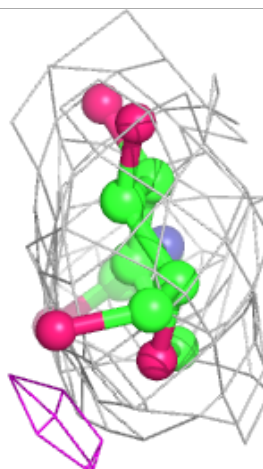
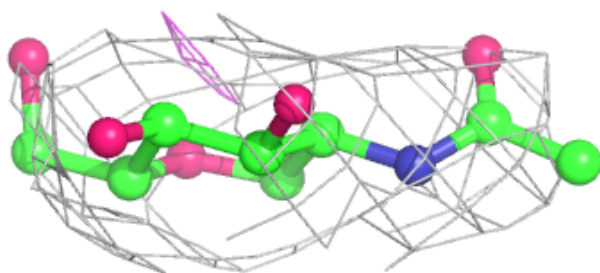
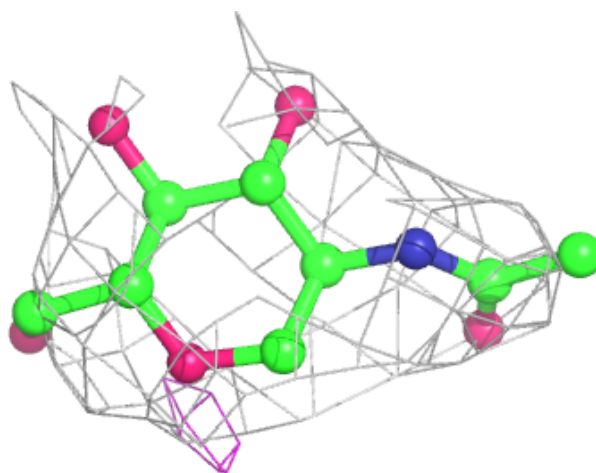
Electron density around NAG D 302:

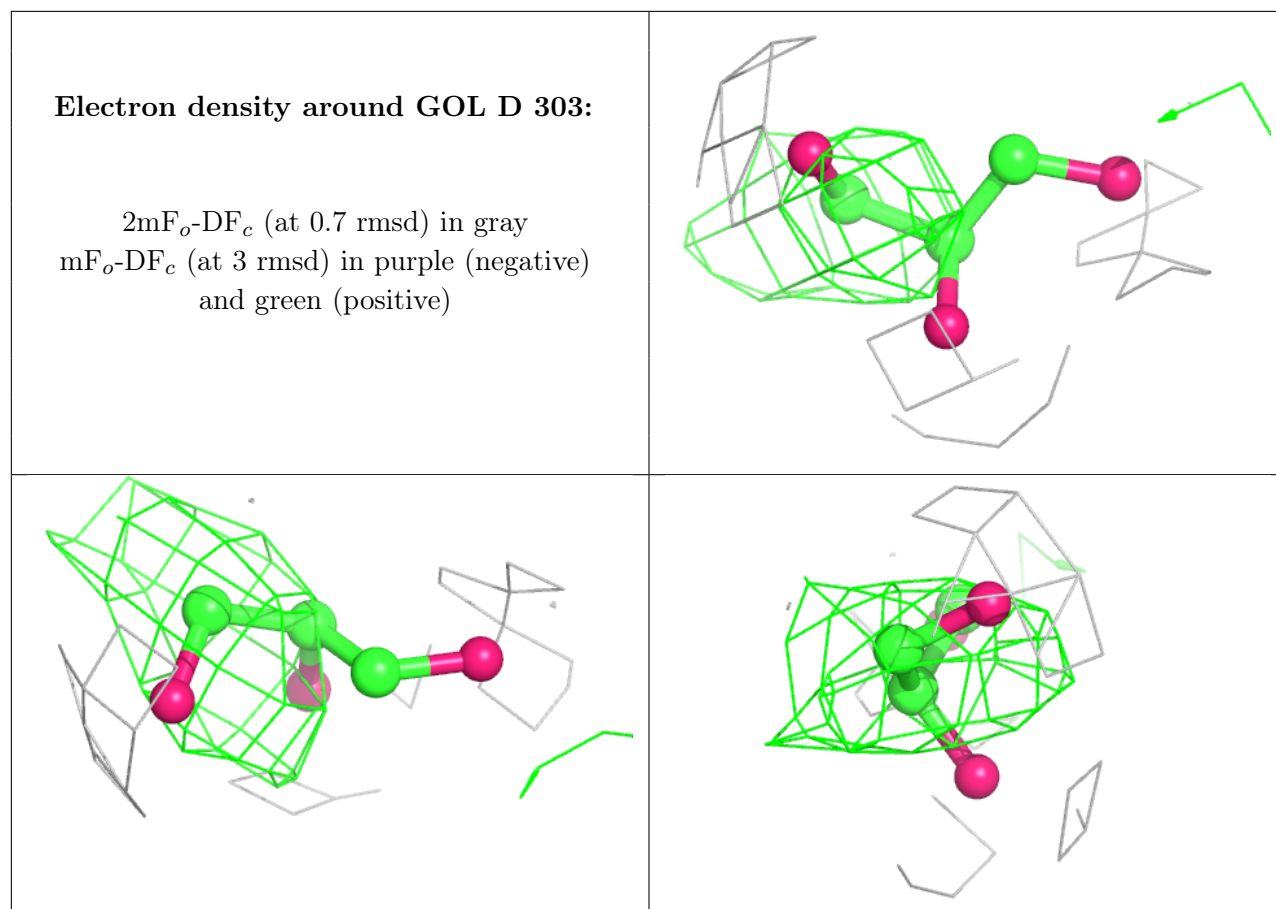
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAG B 301:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.