



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:46 AM UTC

PDB ID : 8ZWY / pdb_00008zwy
Title : Structure-Based Mechanism and Specificity of Human Galactosyltransferase B3GalT5
Authors : Lo, J.M.; Ma, C.
Deposited on : 2024-06-13
Resolution : 1.95 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 : 4-5-2 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

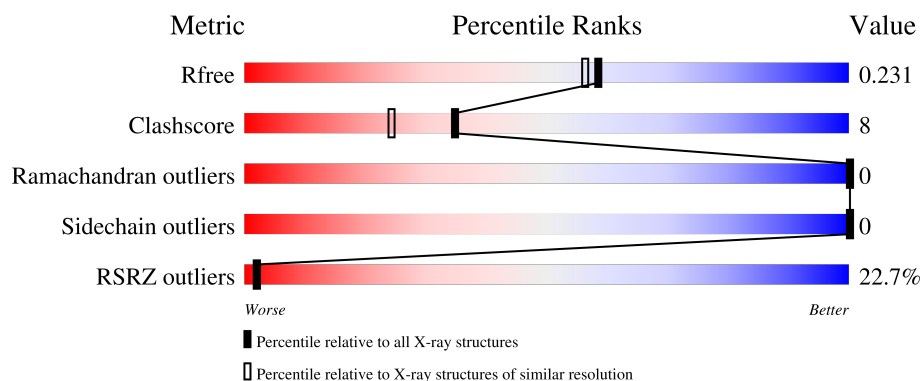
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	278	8% 82% 13% ••
1	B	278	36% 74% 21% •
2	E	2	100%
2	G	2	100%
3	F	2	100%

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Mol	Chain	Length	Quality of chain
4	H	6	 67% 33%
5	I	2	 50% 50%
5	J	2	 50% 50%

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 5179 atoms, of which 261 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 Beta-1,3-galactosyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	3	0
			2206	1432	371	390	13			
1	B	266	Total	C	N	O	S	0	0	0
			2189	1418	370	388	13			

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



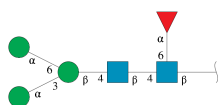
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	G	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	2	Total	C	H	N	O	0	0	0
			36	14	12	1	9			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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	H	6	Total	C	H	N	O	0	0	0
			138	40	67	2	29			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-methyl beta-D-galactopyranoside.

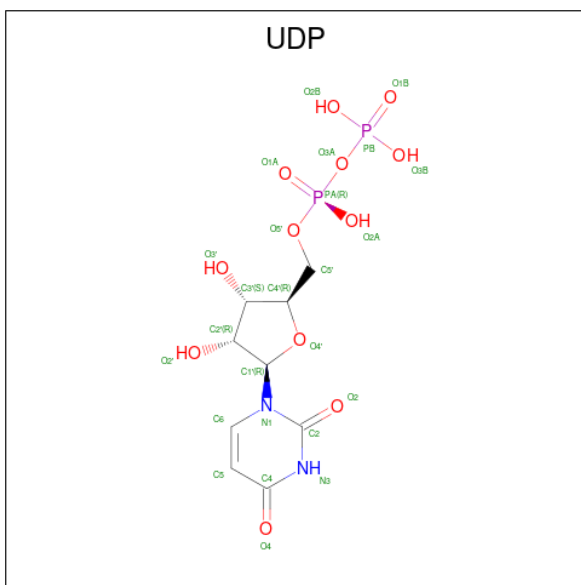


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	2	Total	C	H	N	O	0	0	0
			54	15	27	1	11			
5	J	2	Total	C	H	N	O	0	0	0
			54	15	27	1	11			

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

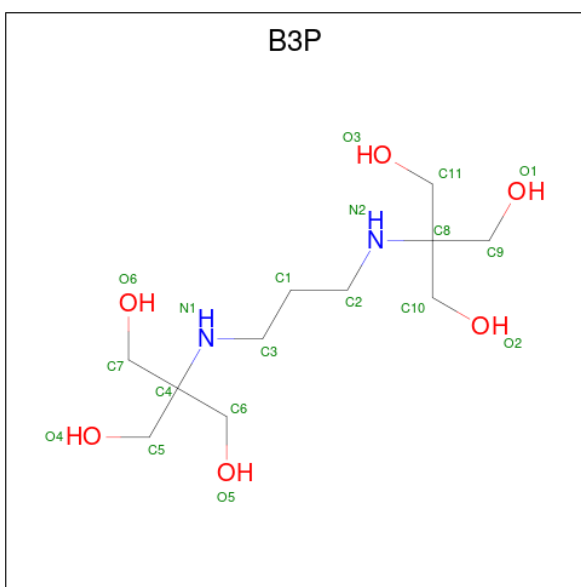
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mn	0	0
			1	1		
6	B	1	Total	Mn	0	0
			1	1		

- Molecule 7 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: C₉H₁₄N₂O₁₂P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0
7	B	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0

- Molecule 8 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	0	0
			45	11	26	2	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	0	0
			45	11	26	2	6		

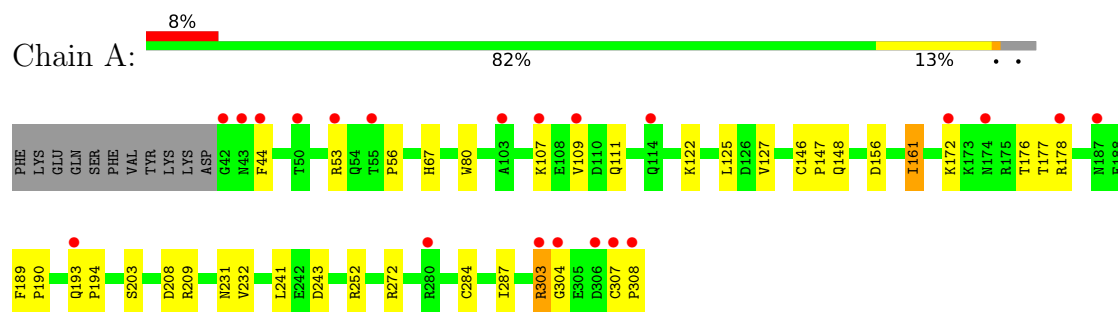
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	171	Total	O	0	0
			171	171		
9	B	57	Total	O	0	0
			57	57		

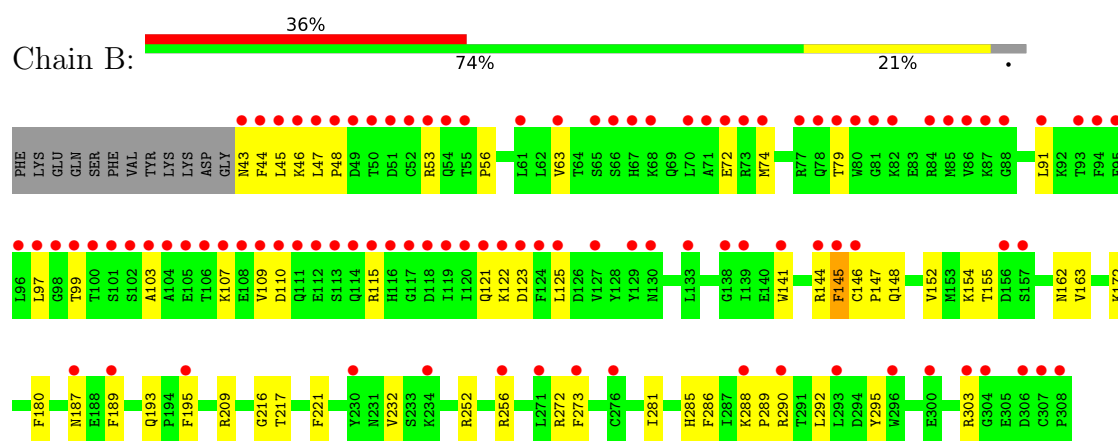
3 Residue-property plots [i](#)

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.

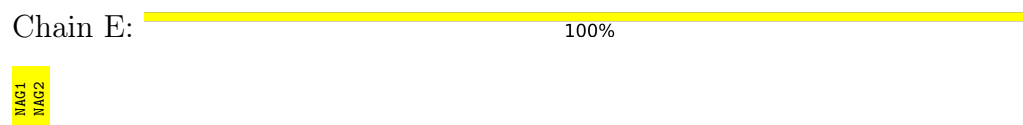
- Molecule 1: Beta-1,3-galactosyltransferase 5



- Molecule 1: Beta-1,3-galactosyltransferase 5



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



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





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

Chain F:  100%



- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  67% 33%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-methyl beta-D-galactopyranoside

Chain I:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-methyl beta-D-galactopyranoside

Chain J:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.65Å 86.70Å 87.00Å 90.00° 95.25° 90.00°	Depositor
Resolution (Å)	47.44 – 1.95 47.44 – 1.95	Depositor EDS
% Data completeness (in resolution range)	92.8 (47.44-1.95) 92.9 (47.44-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.48 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.208 , 0.227 (Not available) , 0.231	Depositor DCC
R_{free} test set	2274 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5179	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MBG, BMA, FUC, MN, UDP, MAN, B3P, 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	0.94	4/2274 (0.2%)	1.18	8/3075 (0.3%)
1	B	0.61	0/2248	0.87	1/3040 (0.0%)
All	All	0.79	4/4522 (0.1%)	1.04	9/6115 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	6
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161[A]	ILE	C-O	5.65	1.30	1.24
1	A	161[B]	ILE	C-O	5.65	1.30	1.24
1	A	203[A]	SER	C-O	5.38	1.30	1.24
1	A	203[B]	SER	C-O	5.38	1.30	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	PRO	N-CA-C	6.88	122.79	113.84
1	A	156	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	303	ARG	CA-C-N	-6.10	114.85	123.08
1	A	303	ARG	C-N-CA	-6.10	114.85	123.08
1	B	145	PHE	N-CA-CB	-5.58	102.19	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203[A]	SER	CA-C-O	5.49	126.23	120.42
1	A	203[B]	SER	CA-C-O	5.49	126.23	120.42
1	A	243	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	193	GLN	CB-CA-C	5.22	118.25	109.85

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	ARG	Sidechain
1	A	272	ARG	Sidechain
1	A	53	ARG	Sidechain
1	B	115	ARG	Sidechain
1	B	144	ARG	Sidechain
1	B	256	ARG	Sidechain
1	B	272	ARG	Sidechain
1	B	303	ARG	Sidechain
1	B	53	ARG	Sidechain

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	2206	0	2205	23	0
1	B	2189	0	2175	44	0
2	E	28	27	25	0	0
2	G	28	27	25	4	0
3	F	24	12	22	0	0
4	H	71	67	61	0	0
5	I	27	27	26	2	0
5	J	27	27	26	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	25	11	11	0	0
7	B	25	11	11	0	0
8	A	19	26	26	0	0
8	B	19	26	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	171	0	0	3	0
9	B	57	0	0	0	0
All	All	4918	261	4639	70	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 (70) 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:B:288:LYS:HE3	1:B:290:ARG:HB3	1.57	0.85
1:B:46:LYS:NZ	1:B:110:ASP:HA	1.93	0.83
1:A:107:LYS:HA	1:A:107:LYS:HE2	1.70	0.74
1:B:47:LEU:HD12	1:B:48:PRO:HD2	1.69	0.73
1:B:193:GLN:HE21	1:B:195:PHE:HZ	1.37	0.72
1:B:46:LYS:HZ3	1:B:110:ASP:HA	1.58	0.68
1:B:56:PRO:HB3	1:B:148:GLN:HB3	1.74	0.68
1:A:232:VAL:HG21	1:A:252:ARG:HG2	1.75	0.66
1:B:46:LYS:HZ1	1:B:110:ASP:HA	1.63	0.63
1:A:232:VAL:CG2	1:A:252:ARG:HG2	2.29	0.62
1:B:79:THR:HG21	1:B:292:LEU:HG	1.82	0.62
1:B:193:GLN:NE2	1:B:195:PHE:CZ	2.63	0.60
1:A:189:PHE:CE1	1:A:209:ARG:HG2	2.36	0.60
1:B:46:LYS:HZ2	1:B:109:VAL:HG12	1.69	0.58
1:B:154:LYS:NZ	1:B:216:GLY:O	2.35	0.58
1:B:288:LYS:CE	1:B:290:ARG:HB3	2.33	0.56
2:G:1:NAG:H4	2:G:2:NAG:H83	1.87	0.56
1:B:187:ASN:OD1	1:B:209:ARG:NH2	2.37	0.56
1:A:107:LYS:O	1:A:111:GLN:HG3	2.05	0.56
1:B:193:GLN:NE2	1:B:195:PHE:HZ	2.03	0.56
1:A:307:CYS:O	1:A:308:PRO:C	2.49	0.54
1:A:56:PRO:HB3	1:A:148:GLN:HB3	1.89	0.54
1:B:232:VAL:HG21	1:B:252:ARG:HG2	1.89	0.54
1:A:303:ARG:HD3	1:A:304:GLY:N	2.23	0.53
1:B:189:PHE:CE1	1:B:209:ARG:HG2	2.44	0.52
1:A:231:ASN:HB2	9:A:620:HOH:O	2.10	0.51
1:B:152:VAL:HB	1:B:221:PHE:CE1	2.45	0.51
1:B:180:PHE:CD2	1:B:221:PHE:HB3	2.46	0.50
1:A:80:TRP:CZ3	1:A:161[B]:ILE:HD12	2.47	0.50
1:A:67:HIS:CD2	1:A:109:VAL:HG21	2.47	0.50
1:A:232:VAL:HG21	1:A:252:ARG:CG	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLU:HA	1:B:289:PRO:HG3	1.94	0.49
1:B:217:THR:HG23	5:J:2:NAG:H81	1.94	0.49
1:B:232:VAL:CG2	1:B:252:ARG:HG2	2.43	0.48
1:A:172:LYS:HG3	9:A:534:HOH:O	2.13	0.48
1:B:99:THR:HG21	1:B:123:ASP:HA	1.95	0.48
1:B:99:THR:CG2	1:B:123:ASP:HA	2.43	0.48
1:B:141:TRP:CD1	1:B:145:PHE:HD2	2.32	0.47
1:A:107:LYS:O	1:A:107:LYS:HD3	2.14	0.47
1:B:45:LEU:HB2	1:B:121:GLN:HG2	1.97	0.47
1:B:125:LEU:HD22	2:G:2:NAG:H81	1.97	0.46
1:B:97:LEU:O	1:B:121:GLN:HA	2.15	0.46
1:B:46:LYS:HB2	1:B:121:GLN:HB3	1.98	0.46
1:A:80:TRP:CH2	1:A:161[B]:ILE:HD12	2.50	0.46
1:A:189:PHE:CD1	1:A:209:ARG:HG2	2.51	0.45
1:B:63:VAL:HG22	1:B:155:THR:CG2	2.46	0.45
1:B:74:MET:HE3	1:B:74:MET:HA	1.98	0.45
1:B:56:PRO:HB3	1:B:148:GLN:CB	2.46	0.44
1:B:44:PHE:HB3	1:B:47:LEU:HD13	1.99	0.44
1:B:189:PHE:HE1	1:B:209:ARG:HG2	1.81	0.44
1:A:146:CYS:N	1:A:147:PRO:CD	2.81	0.44
1:A:190:PRO:HD2	1:A:208:ASP:O	2.17	0.44
2:G:1:NAG:H61	2:G:2:NAG:H4	2.00	0.44
1:A:284:CYS:O	1:A:287[B]:ILE:HD12	2.18	0.43
1:B:99:THR:HG21	1:B:123:ASP:OD1	2.17	0.43
1:B:46:LYS:HZ1	1:B:110:ASP:CA	2.28	0.43
1:A:241:LEU:HD13	5:I:2:NAG:H62	2.00	0.43
1:A:125:LEU:HG	1:A:127:VAL:HG13	1.99	0.43
1:B:43:ASN:O	1:B:122:LYS:HG2	2.18	0.43
1:B:172:LYS:HE3	1:B:172:LYS:HB2	1.73	0.42
1:B:273:PHE:HB2	1:B:295:TYR:CZ	2.55	0.42
1:B:103:ALA:O	1:B:107:LYS:HG3	2.19	0.42
9:A:615:HOH:O	5:I:2:NAG:H83	2.19	0.42
1:A:44:PHE:HA	1:A:122:LYS:HG2	2.02	0.42
1:A:176:THR:HG23	1:A:177:THR:HG23	2.02	0.42
1:B:146:CYS:N	1:B:147:PRO:CD	2.83	0.42
1:B:285:HIS:CD2	1:B:286:PHE:H	2.37	0.42
1:B:91:LEU:HD13	1:B:163:VAL:HG11	2.01	0.41
1:B:125:LEU:HB3	2:G:1:NAG:H2	2.03	0.41
1:B:162:ASN:HB3	1:B:281:ILE:O	2.21	0.41

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	268/278 (96%)	262 (98%)	6 (2%)	0	100	100
1	B	264/278 (95%)	254 (96%)	10 (4%)	0	100	100
All	All	532/556 (96%)	516 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	150/255 (59%)	150 (100%)	0	100	100
1	B	244/255 (96%)	244 (100%)	0	100	100
All	All	394/510 (77%)	394 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	B	228	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

16 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	0.44	0	17,19,21	0.95	1 (5%)
2	NAG	E	2	2	14,14,15	0.73	1 (7%)	17,19,21	0.55	0
3	NAG	F	1	1,3	14,14,15	0.45	0	17,19,21	0.49	0
3	FUC	F	2	3	10,10,11	0.86	0	14,14,16	0.89	0
2	NAG	G	1	1,2	14,14,15	0.42	0	17,19,21	1.48	1 (5%)
2	NAG	G	2	2	14,14,15	0.40	0	17,19,21	0.73	1 (5%)
4	NAG	H	1	1,4	14,14,15	0.43	0	17,19,21	1.05	1 (5%)
4	NAG	H	2	4	14,14,15	0.44	0	17,19,21	0.91	1 (5%)
4	BMA	H	3	4	11,11,12	0.57	0	15,15,17	0.51	0
4	MAN	H	4	4	11,11,12	0.32	0	15,15,17	0.56	0
4	MAN	H	5	4	11,11,12	0.33	0	15,15,17	0.72	0
4	FUC	H	6	4	10,10,11	0.30	0	14,14,16	0.43	0
5	MBG	I	1	5	13,13,13	0.25	0	18,18,18	0.39	0
5	NAG	I	2	5	14,14,15	0.41	0	17,19,21	0.68	0
5	MBG	J	1	5	13,13,13	0.44	0	18,18,18	0.96	1 (5%)
5	NAG	J	2	5	14,14,15	0.45	0	17,19,21	1.79	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	5/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	MAN	H	5	4	-	2/2/19/22	0/1/1/1
4	FUC	H	6	4	-	-	0/1/1/1
5	MBG	I	1	5	-	0/4/24/24	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	MBG	J	1	5	-	4/4/24/24	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C1-C2	2.02	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	2	NAG	O5-C1-C2	-6.03	101.96	111.29
2	G	1	NAG	O5-C1-C2	-5.40	102.93	111.29
4	H	1	NAG	C2-N2-C7	3.02	126.95	122.90
2	G	2	NAG	C1-O5-C5	2.68	115.78	112.19
2	E	1	NAG	C2-N2-C7	2.27	125.94	122.90
4	H	2	NAG	C2-N2-C7	2.12	125.74	122.90
5	J	2	NAG	C1-C2-N2	2.11	113.75	110.43
5	J	1	MBG	C1-O5-C5	-2.10	109.62	113.72

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C8-C7-N2-C2

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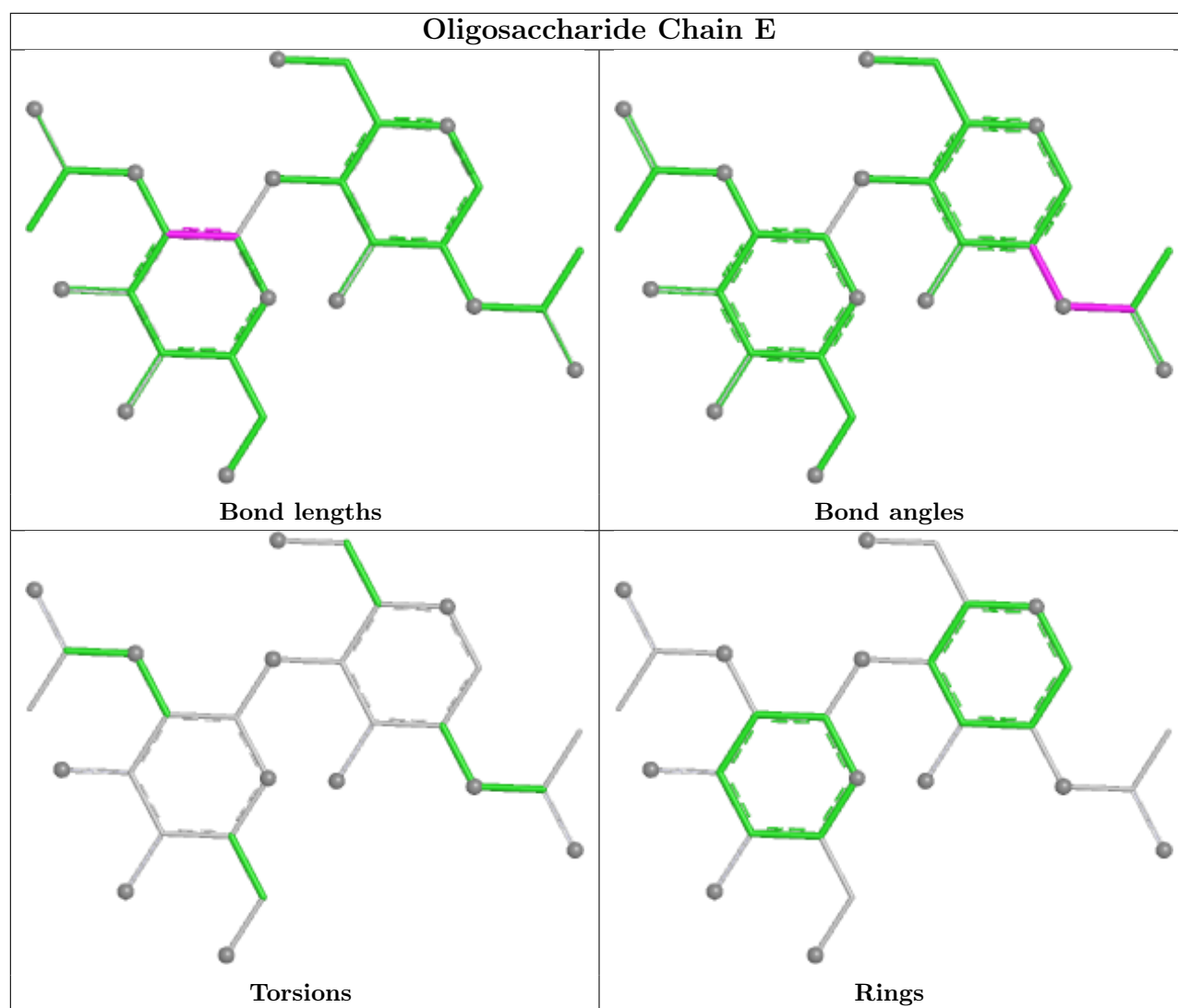
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	1	MBG	O5-C1-O1-C7
5	J	1	MBG	C2-C1-O1-C7
2	G	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
5	J	1	MBG	C4-C5-C6-O6
4	H	5	MAN	C4-C5-C6-O6
4	H	5	MAN	O5-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
5	J	1	MBG	O5-C5-C6-O6
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C1-C2-N2-C7

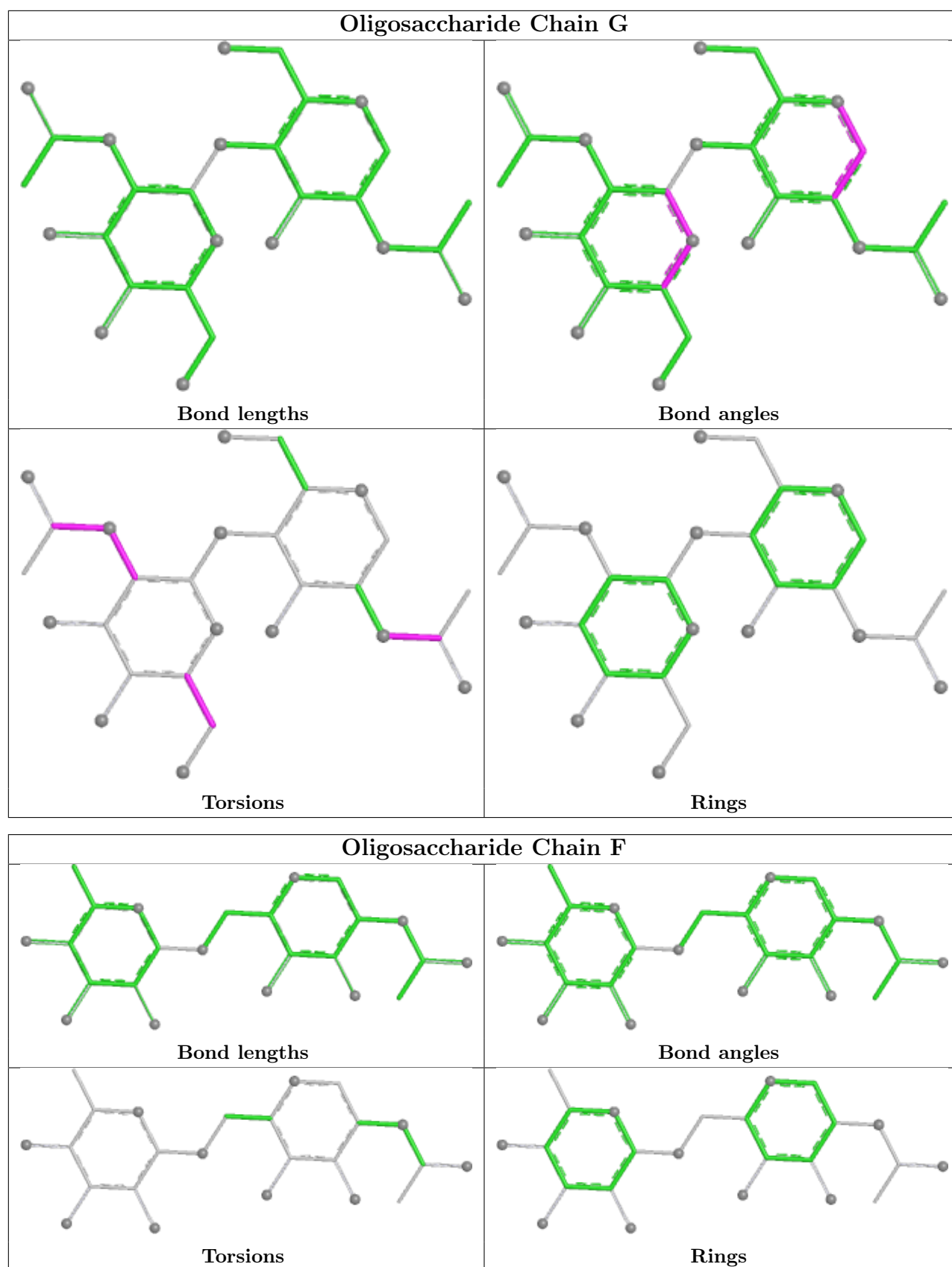
There are no ring outliers.

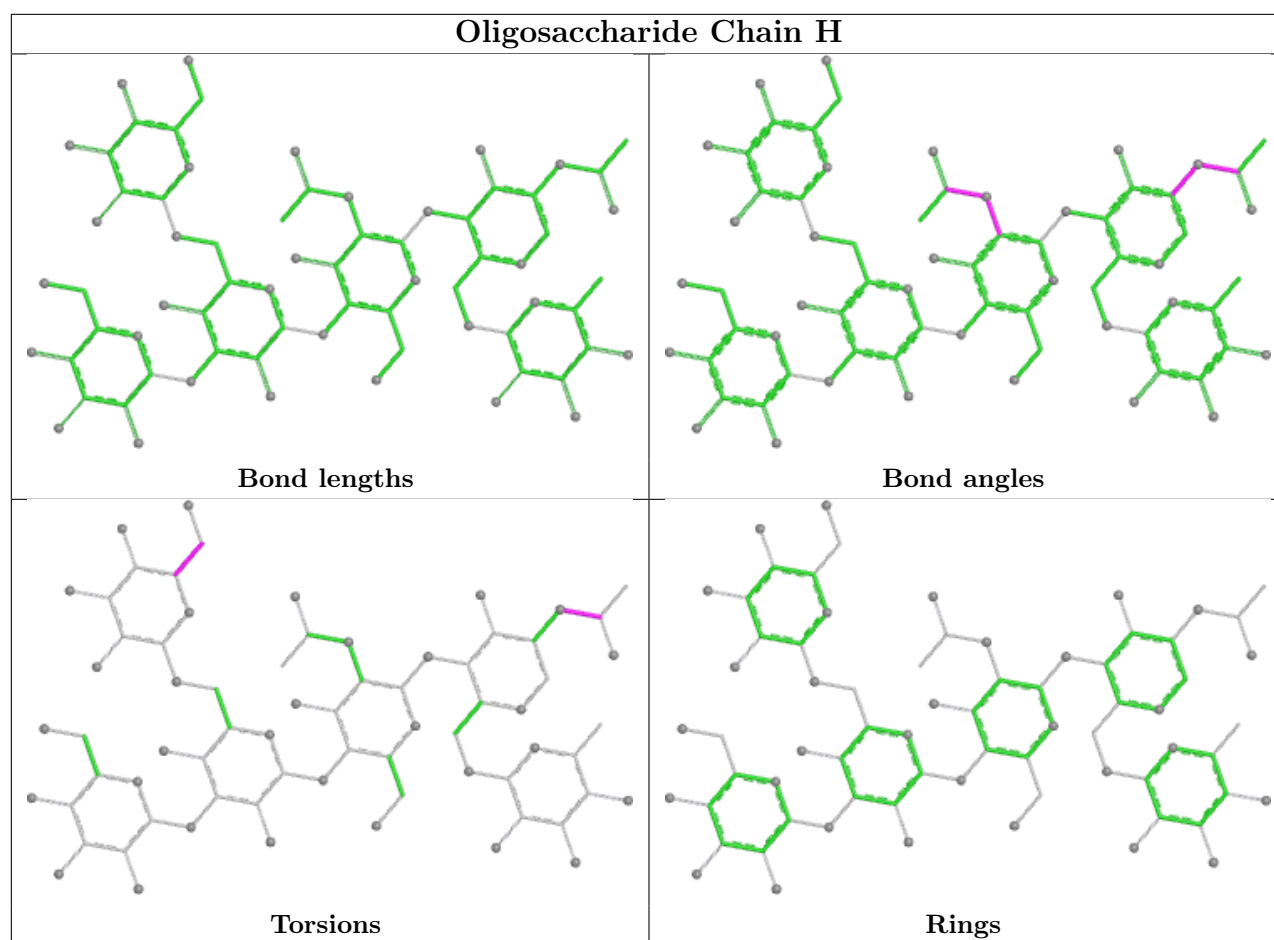
4 monomers are involved in 7 short contacts:

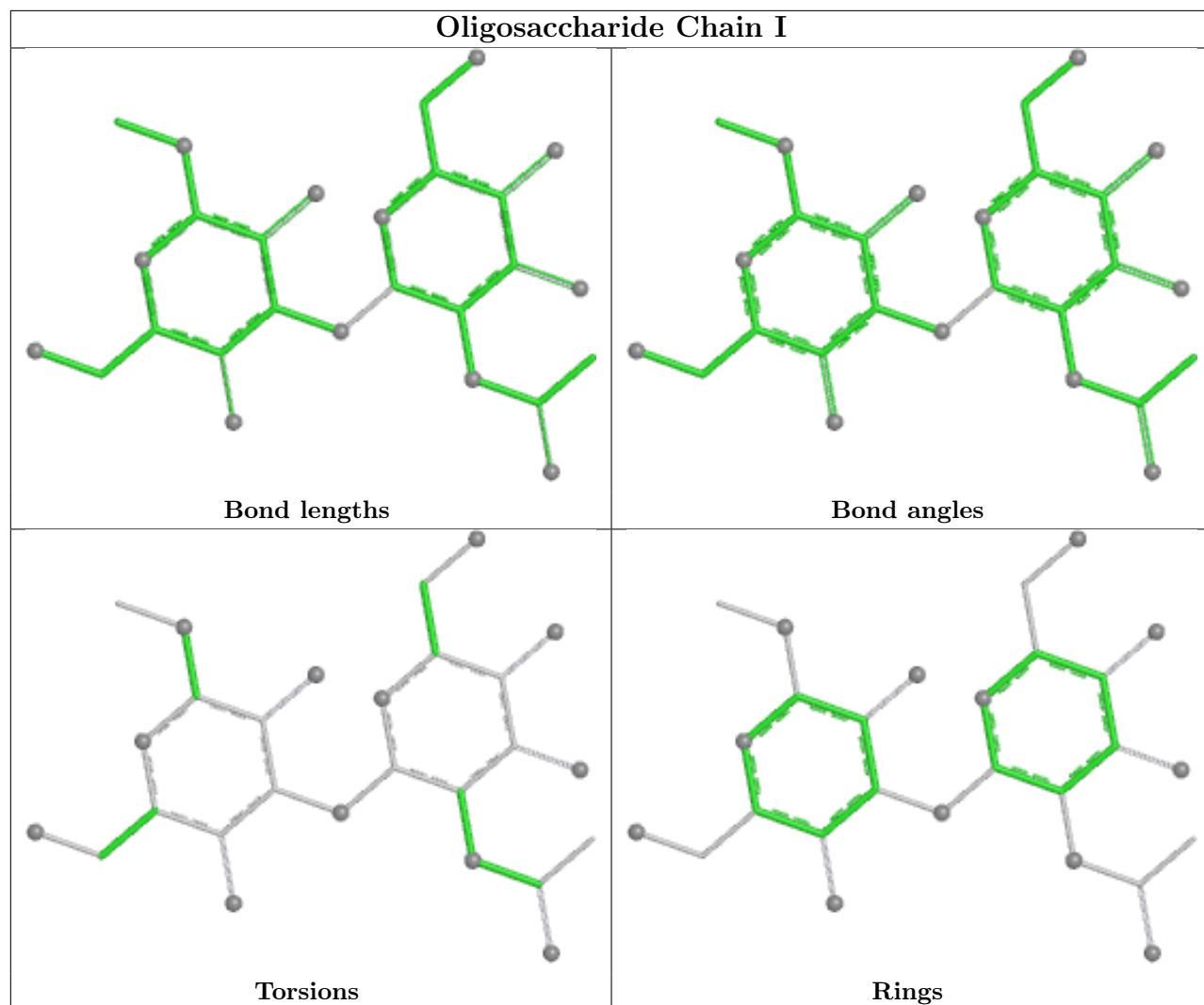
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	3	0
5	I	2	NAG	2	0
5	J	2	NAG	1	0
2	G	1	NAG	3	0

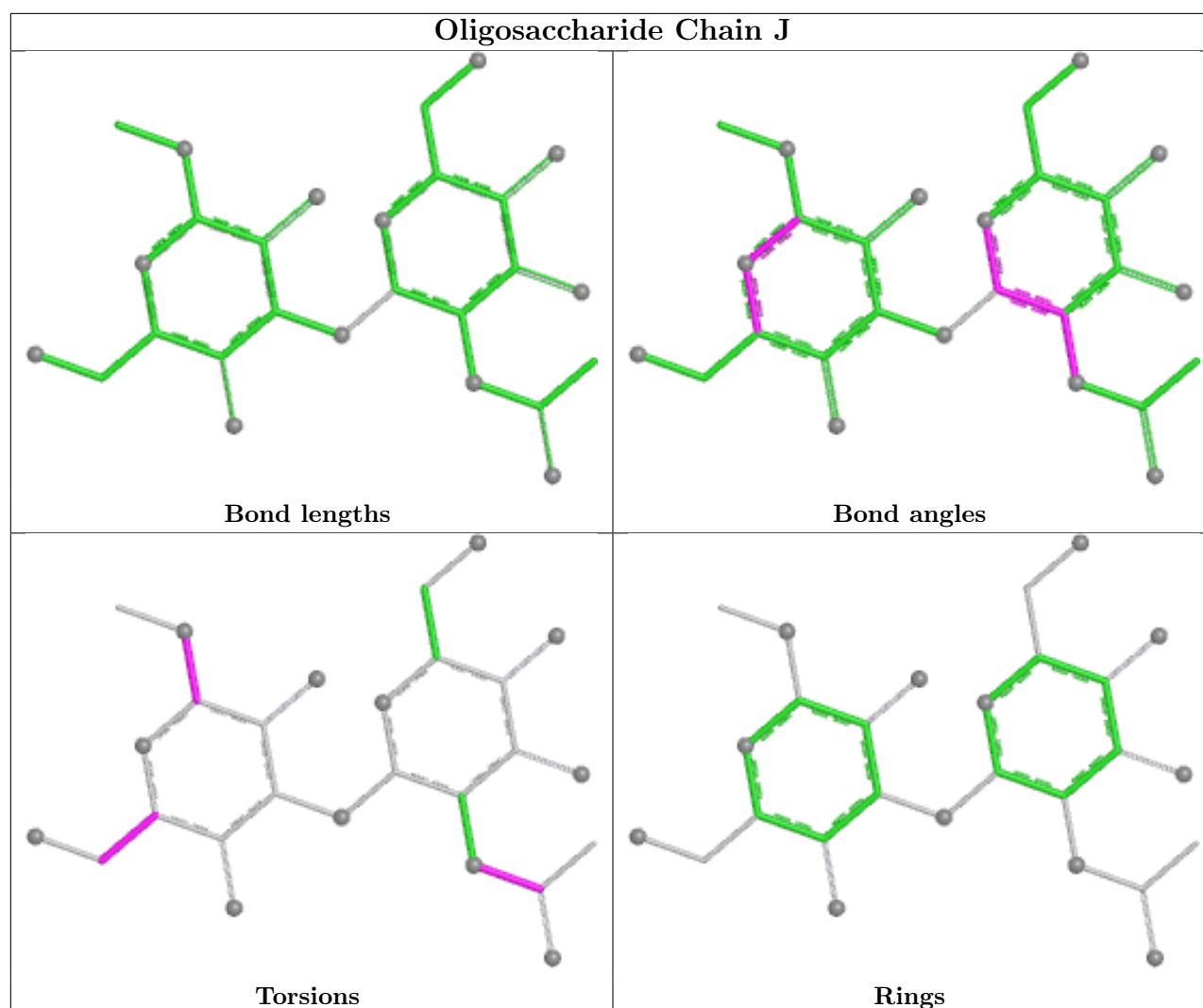
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	B3P	B	403	-	18,18,18	0.76	0	23,23,23	1.49	4 (17%)
7	UDP	B	402	6	25,26,26	0.58	0	38,40,40	0.52	0
8	B3P	A	403	-	18,18,18	1.00	0	23,23,23	1.42	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	UDP	A	402	6	25,26,26	1.66	2 (8%)	38,40,40	0.61	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	B3P	B	403	-	-	3/28/28/28	-
7	UDP	B	402	6	-	8/16/32/32	0/2/2/2
8	B3P	A	403	-	-	0/28/28/28	-
7	UDP	A	402	6	-	2/16/32/32	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	402	UDP	PB-O1B	7.42	1.73	1.50
7	A	402	UDP	PA-O3A	-2.70	1.56	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	403	B3P	C2-N2-C8	-3.96	110.37	116.17
8	A	403	B3P	C7-C4-C5	-3.33	102.72	110.02
8	B	403	B3P	O1-C9-C8	-2.81	105.96	111.68
8	A	403	B3P	O1-C9-C8	-2.36	106.89	111.68
8	A	403	B3P	C3-N1-C4	-2.21	112.94	116.17
8	B	403	B3P	O2-C10-C8	-2.21	107.19	111.68
7	A	402	UDP	O2B-PB-O1B	2.19	119.39	110.83
8	B	403	B3P	C3-N1-C4	-2.04	113.18	116.17

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	402	UDP	C5'-O5'-PA-O1A
7	B	402	UDP	C5'-O5'-PA-O3A
7	B	402	UDP	PB-O3A-PA-O5'
8	B	403	B3P	N1-C4-C6-O5
8	B	403	B3P	C5-C4-C6-O5

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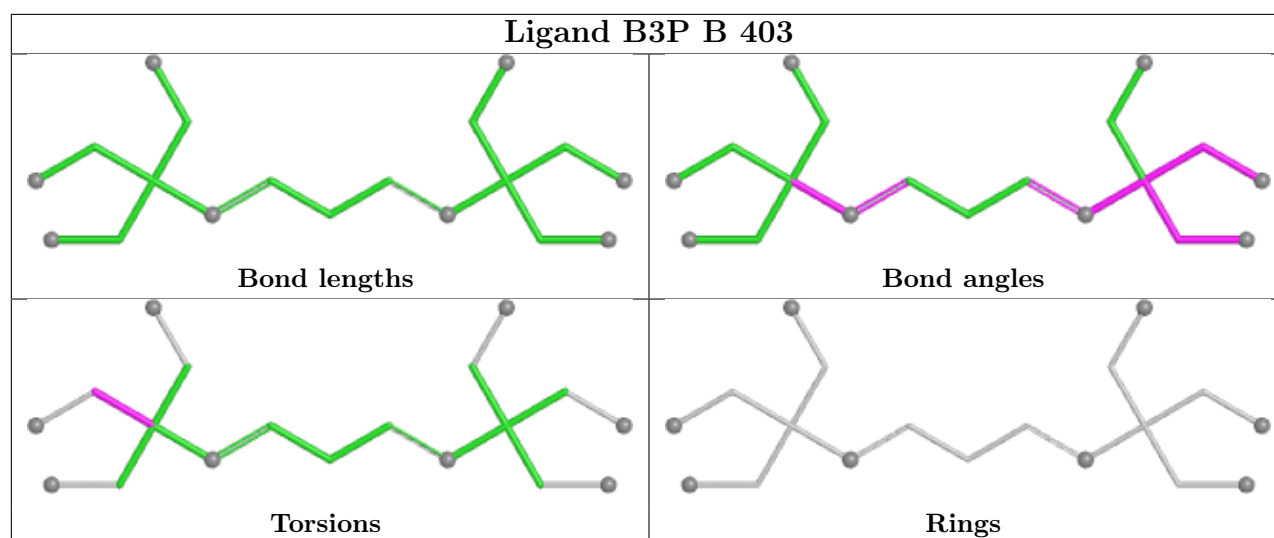
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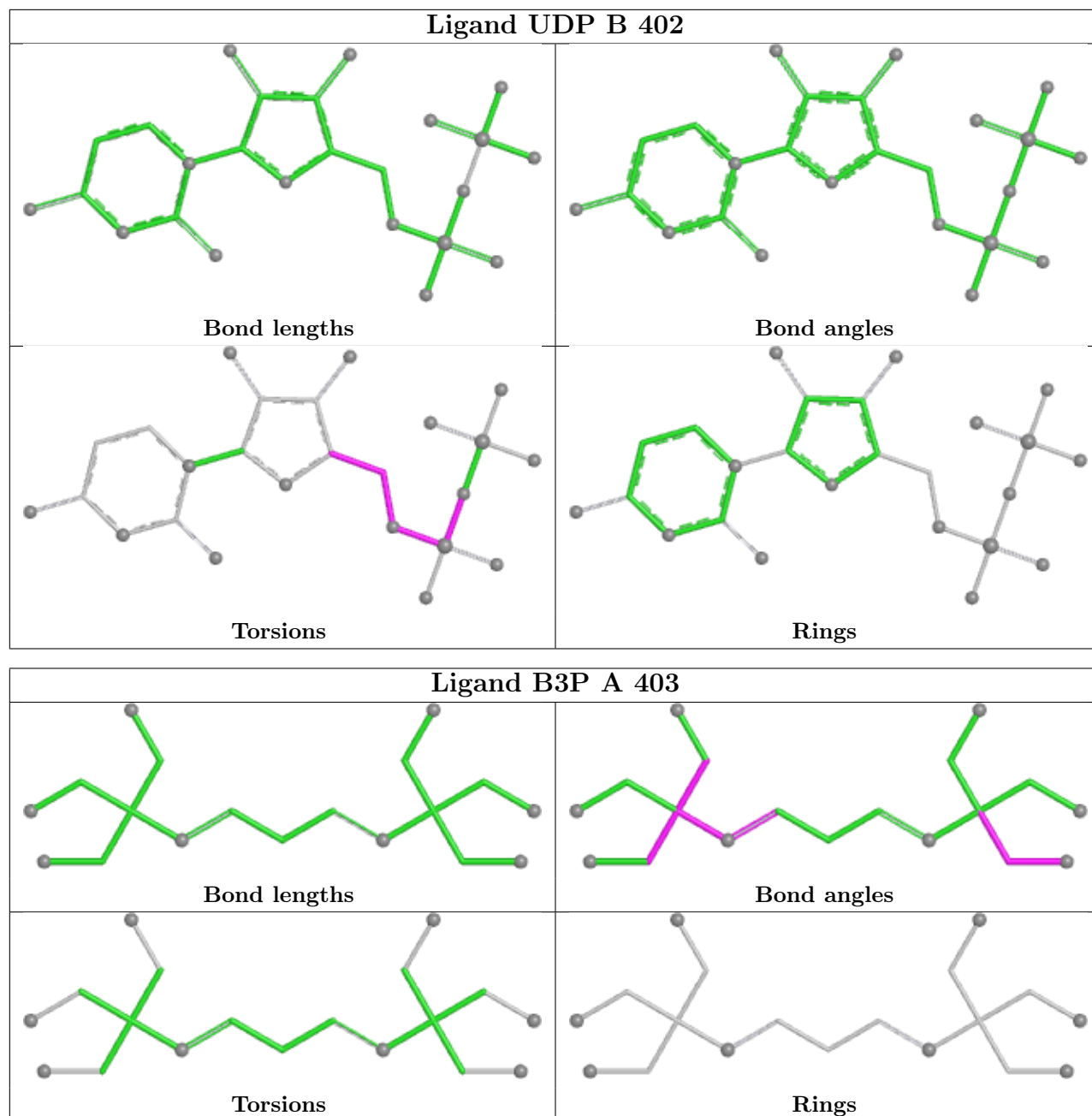
Mol	Chain	Res	Type	Atoms
8	B	403	B3P	C7-C4-C6-O5
7	B	402	UDP	O4'-C4'-C5'-O5'
7	B	402	UDP	C5'-O5'-PA-O2A
7	A	402	UDP	PB-O3A-PA-O1A
7	B	402	UDP	C4'-C5'-O5'-PA
7	A	402	UDP	PB-O3A-PA-O2A
7	B	402	UDP	PB-O3A-PA-O1A
7	B	402	UDP	PB-O3A-PA-O2A

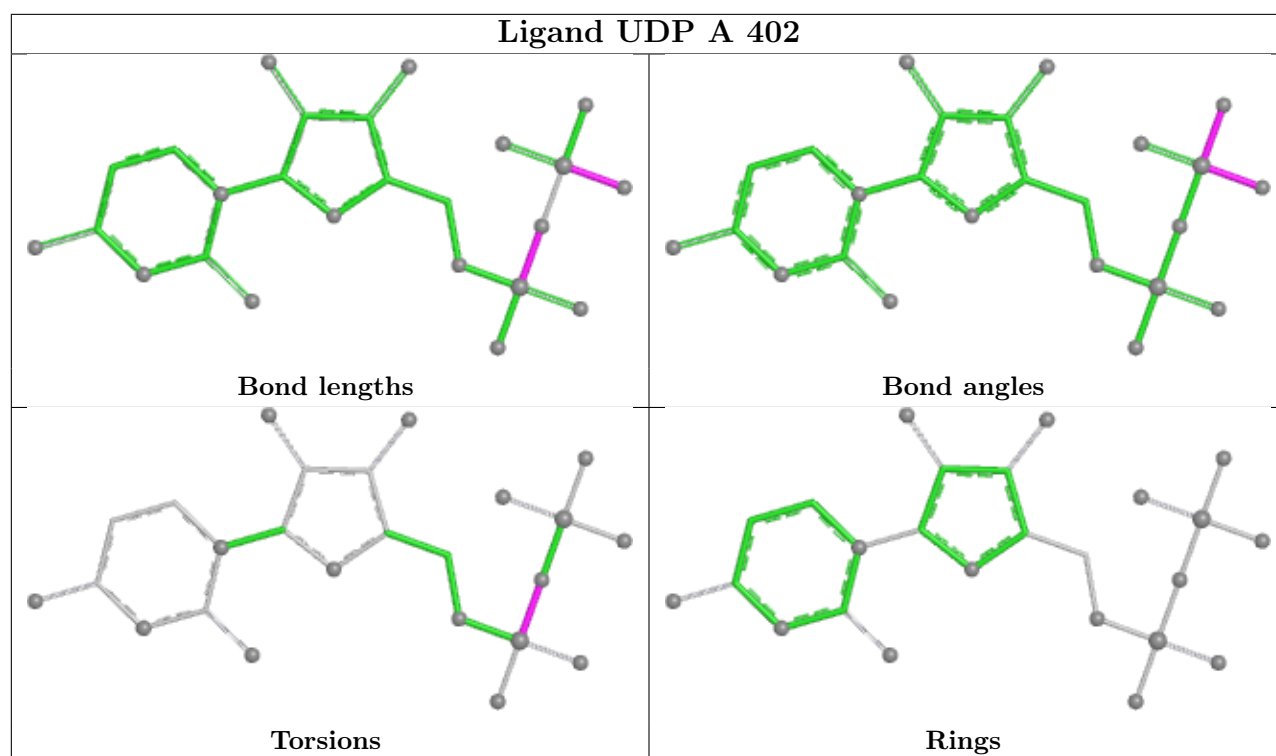
There are no ring outliers.

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

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	267/278 (96%)	0.50	21 (7%) 18 21	7, 18, 49, 66	3 (1%)
1	B	266/278 (95%)	1.85	100 (37%) 1 0	26, 41, 75, 92	0
All	All	533/556 (95%)	1.17	121 (22%) 2 2	7, 32, 70, 92	3 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	VAL	7.5
1	B	103	ALA	6.6
1	B	45	LEU	6.3
1	B	124	PHE	6.1
1	B	107	LYS	6.1
1	B	119	ILE	5.7
1	B	70	LEU	5.5
1	B	97	LEU	5.3
1	A	308	PRO	5.3
1	B	106	THR	5.2
1	B	47	LEU	5.0
1	B	187	ASN	4.9
1	B	145	PHE	4.7
1	B	104	ALA	4.7
1	B	54	GLN	4.7
1	B	111	GLN	4.7
1	B	256	ARG	4.5
1	A	44	PHE	4.4
1	B	308	PRO	4.3
1	B	141	TRP	4.1
1	B	49	ASP	4.0
1	B	114	GLN	4.0
1	B	48	PRO	4.0
1	B	121	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	110	ASP	4.0
1	B	120	ILE	4.0
1	B	139	ILE	4.0
1	B	98	GLY	3.9
1	B	118	ASP	3.9
1	B	94	PHE	3.8
1	B	125	LEU	3.8
1	B	53	ARG	3.7
1	B	67	HIS	3.7
1	B	123	ASP	3.7
1	A	187	ASN	3.7
1	B	99	THR	3.7
1	B	117	GLY	3.6
1	A	307	CYS	3.6
1	B	307	CYS	3.5
1	B	79	THR	3.5
1	B	55	THR	3.4
1	B	44	PHE	3.4
1	B	273	PHE	3.4
1	B	133	LEU	3.4
1	A	55	THR	3.4
1	A	42	GLY	3.4
1	B	71	ALA	3.4
1	B	80	TRP	3.4
1	B	101	SER	3.4
1	A	303	ARG	3.4
1	B	51	ASP	3.3
1	A	304	GLY	3.3
1	B	116	HIS	3.3
1	B	129	TYR	3.2
1	A	174	ASN	3.2
1	B	115	ARG	3.2
1	B	105	GLU	3.2
1	B	84	ARG	3.2
1	B	43	ASN	3.1
1	A	172	LYS	3.1
1	B	52	CYS	3.1
1	B	91	LEU	3.1
1	B	96	LEU	3.1
1	B	74	MET	3.1
1	B	66	SER	3.1
1	B	72	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	293	LEU	3.0
1	B	127	VAL	2.9
1	B	234	LYS	2.9
1	B	81	GLY	2.9
1	B	304	GLY	2.9
1	B	78	GLN	2.9
1	B	68	LYS	2.8
1	B	108	GLU	2.8
1	B	306	ASP	2.8
1	B	46	LYS	2.8
1	B	50	THR	2.7
1	A	109	VAL	2.7
1	A	306	ASP	2.7
1	B	122	LYS	2.7
1	B	100	THR	2.6
1	A	178	ARG	2.6
1	B	288	LYS	2.6
1	B	130	ASN	2.6
1	B	195	PHE	2.6
1	A	43	ASN	2.6
1	B	85	MET	2.5
1	B	95	PHE	2.5
1	B	230	TYR	2.5
1	B	102	SER	2.5
1	A	107	LYS	2.5
1	B	87	LYS	2.5
1	B	290	ARG	2.4
1	B	271	LEU	2.4
1	A	114	GLN	2.4
1	A	50	THR	2.4
1	B	86	VAL	2.4
1	B	63	VAL	2.4
1	B	146	CYS	2.4
1	B	61	LEU	2.3
1	A	193	GLN	2.3
1	A	280	ARG	2.2
1	B	113	SER	2.2
1	B	303	ARG	2.2
1	B	156	ASP	2.2
1	B	93	THR	2.2
1	B	276	CYS	2.2
1	B	82	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	296	TRP	2.2
1	B	112	GLU	2.2
1	A	53	ARG	2.2
1	B	189	PHE	2.1
1	B	88	GLY	2.1
1	B	138	GLY	2.1
1	A	103	ALA	2.1
1	B	300	GLU	2.1
1	B	77	ARG	2.1
1	B	65	SER	2.0
1	B	144	ARG	2.0
1	B	157	SER	2.0
1	B	73	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

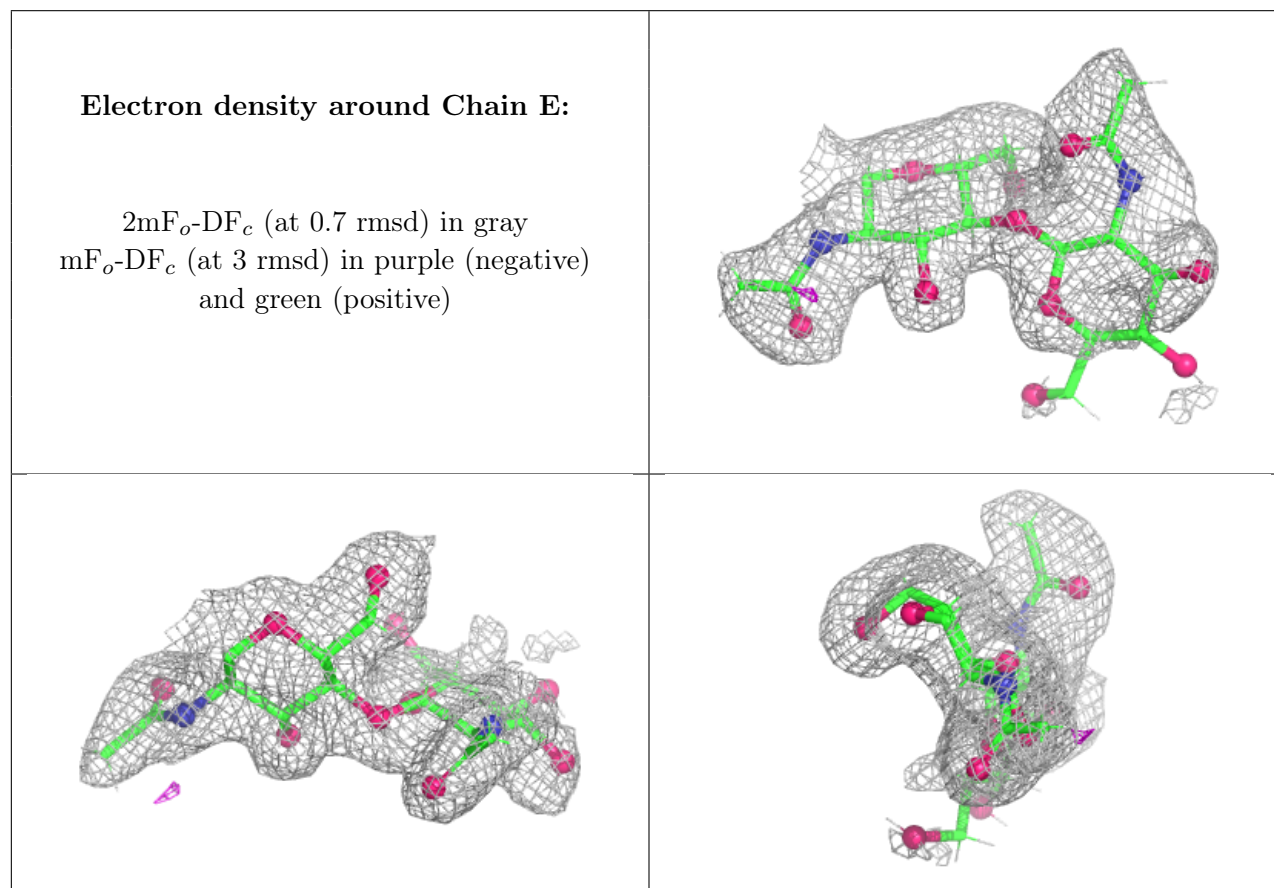
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.49	0.19	38,67,93,97	0
2	NAG	E	1	14/15	0.69	0.19	22,28,34,40	0
2	NAG	G	1	14/15	-	-	66,82,101,111	0
3	NAG	F	1	14/15	0.88	0.13	44,64,76,80	0
4	NAG	H	2	14/15	0.89	0.11	39,42,50,50	0
3	FUC	F	2	10/11	-	-	55,76,85,102	0
4	NAG	H	1	14/15	-	-	37,41,47,49	0
2	NAG	G	2	14/15	0.97	0.05	85,109,131,133	0
4	BMA	H	3	11/12	-	-	40,44,51,55	0
4	MAN	H	4	11/12	-	-	39,55,66,69	0
4	MAN	H	5	11/12	-	-	43,51,55,62	0
4	FUC	H	6	10/11	-	-	54,78,93,102	0
5	MBG	I	1	13/13	-	-	10,20,33,33	0
5	NAG	I	2	14/15	-	-	9,14,19,19	0
5	MBG	J	1	13/13	-	-	30,41,49,54	0

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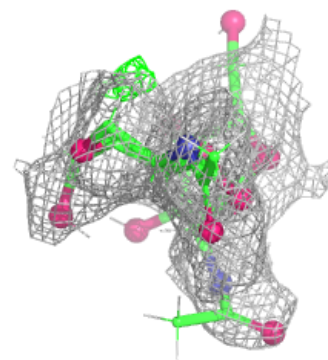
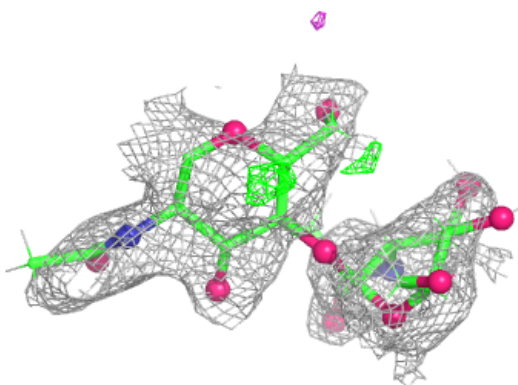
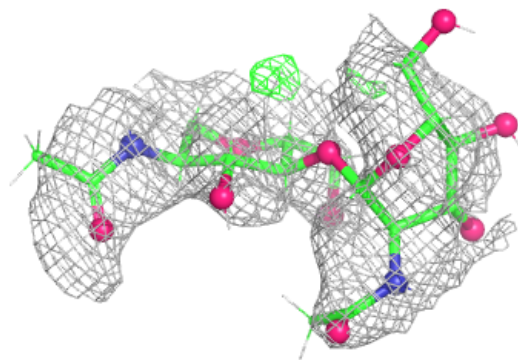
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	J	2	14/15	-	-	23,35,57,57	0

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.

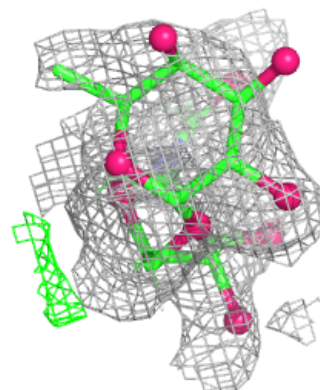
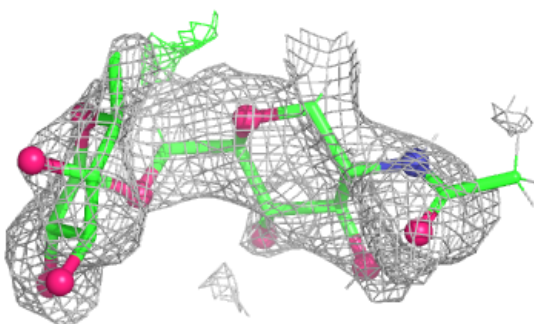
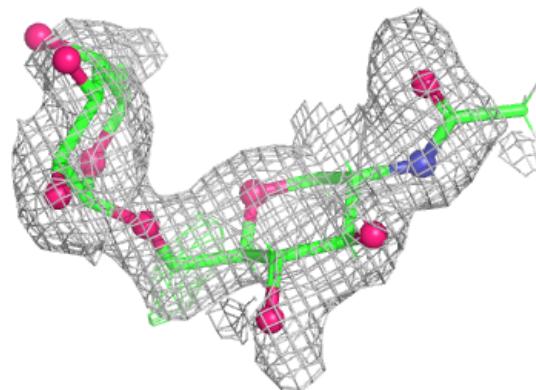


Electron density around Chain G:

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

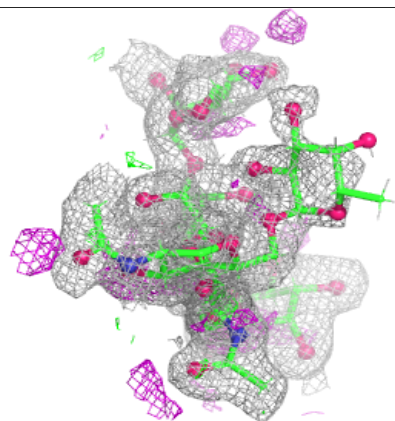
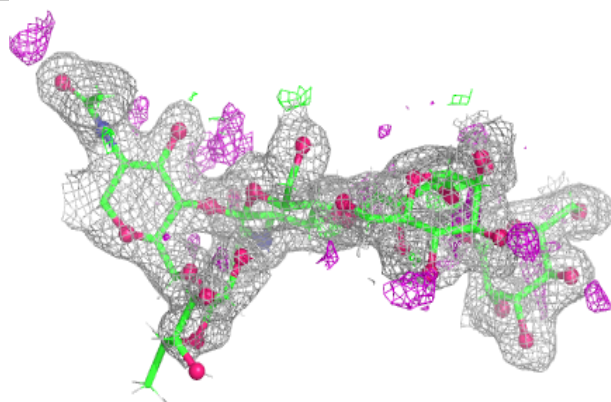
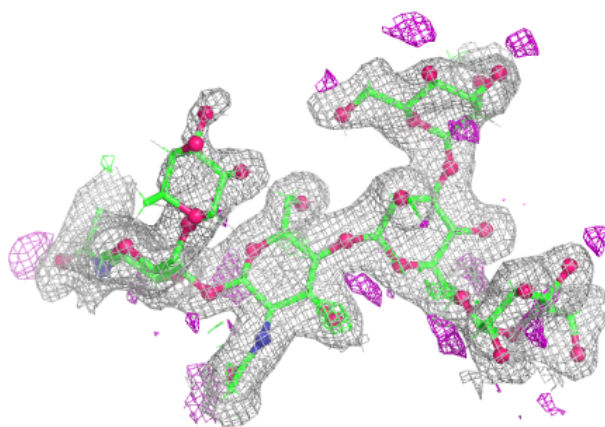
**Electron density around Chain F:**

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



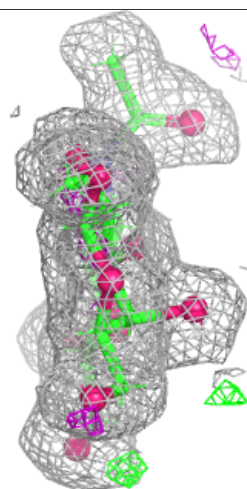
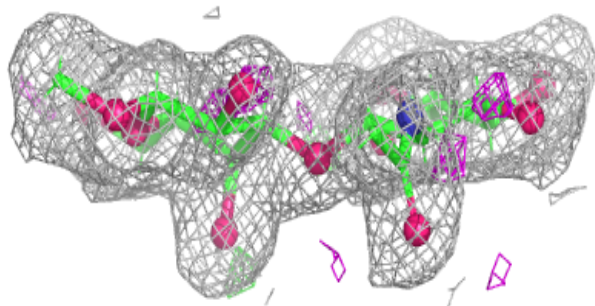
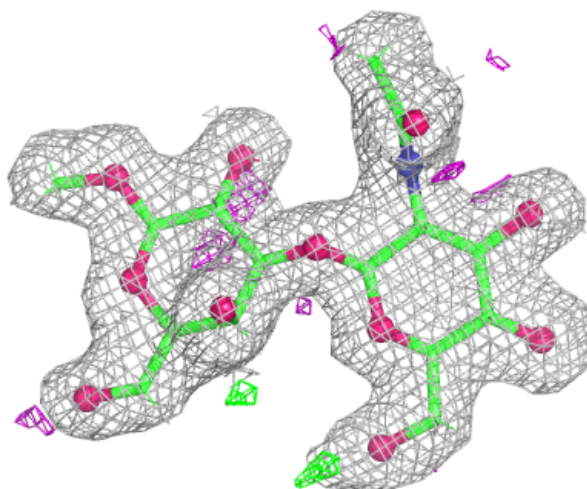
Electron density around Chain H:

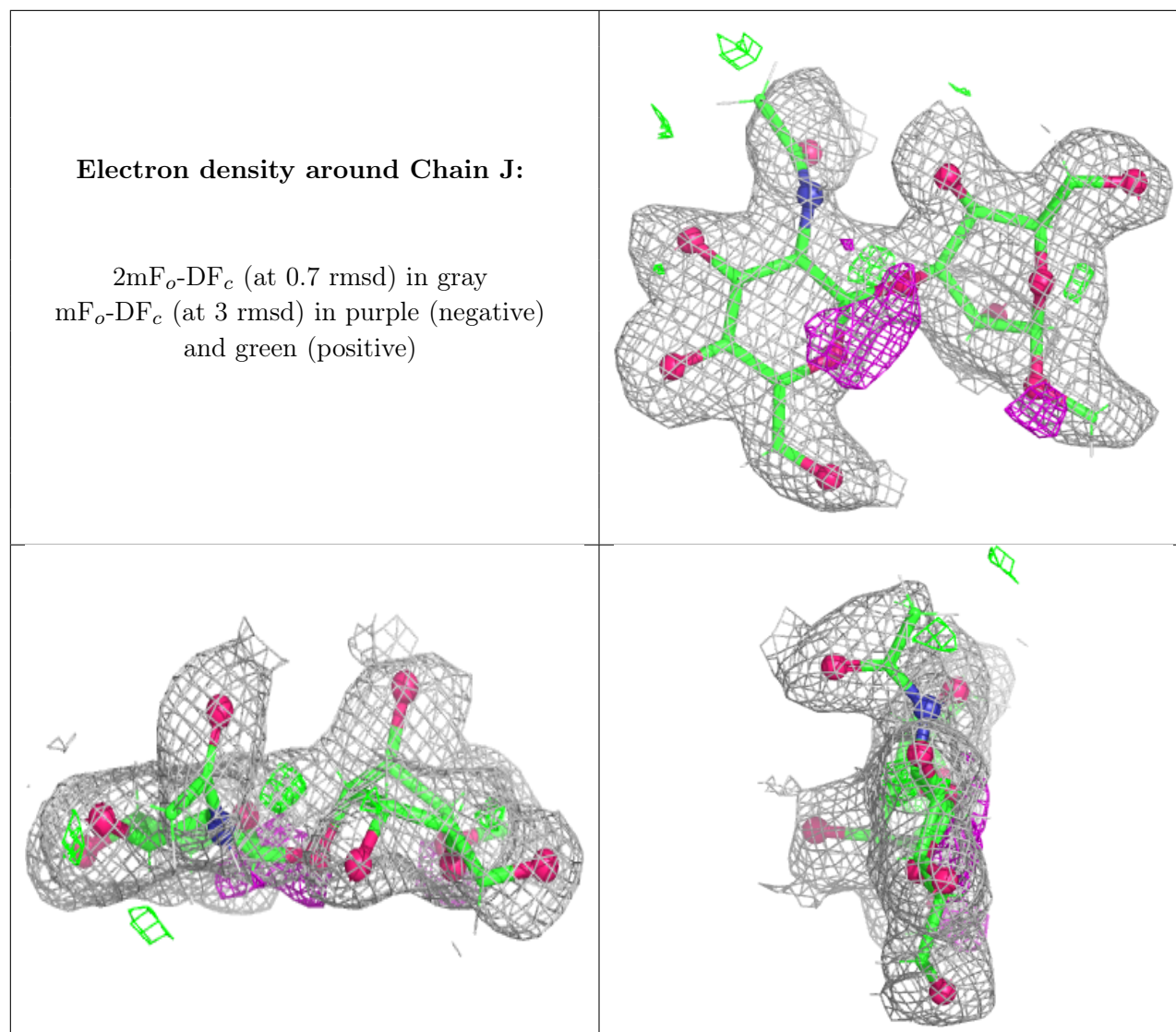
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

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



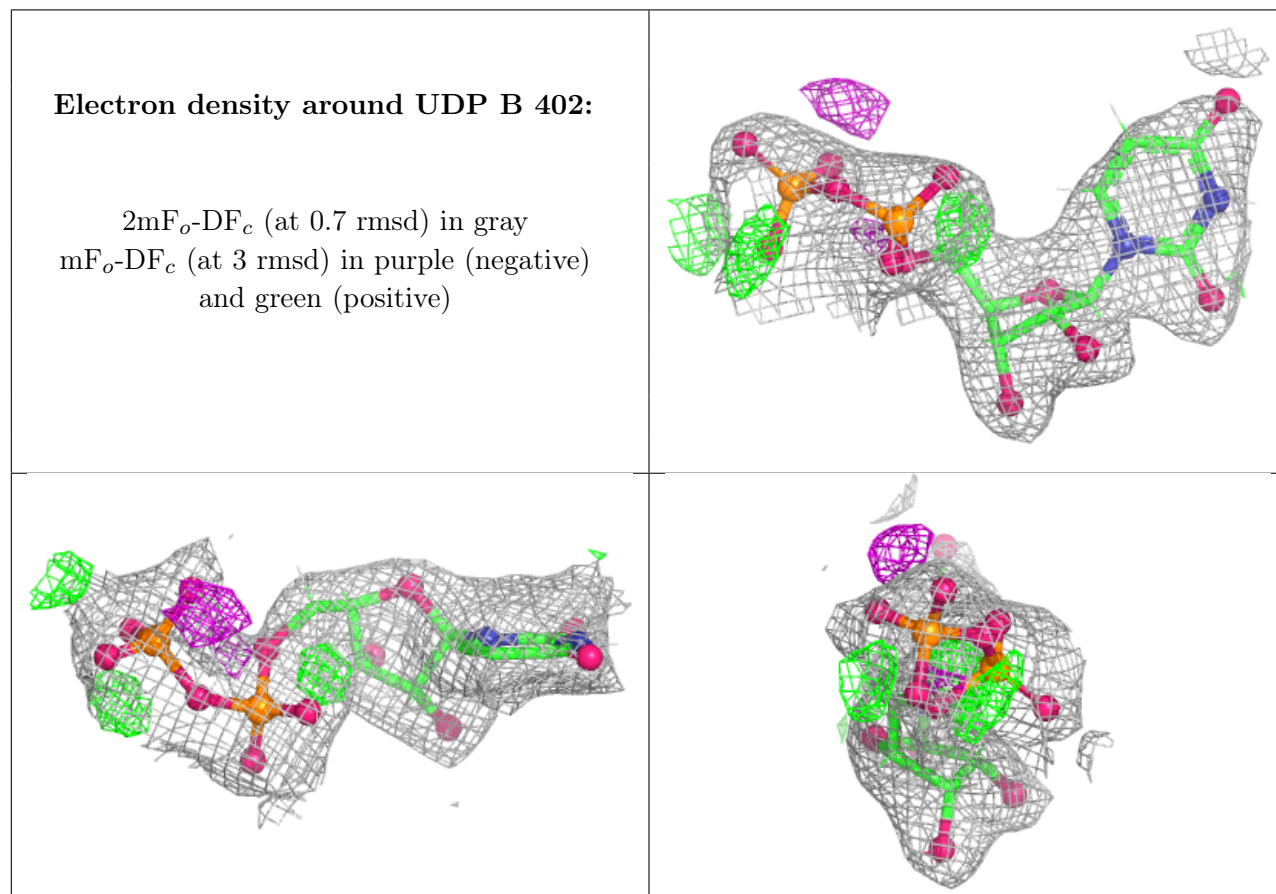


6.4 Ligands [i](#)

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.

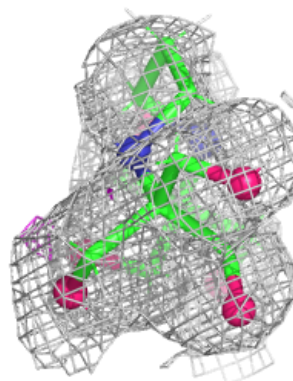
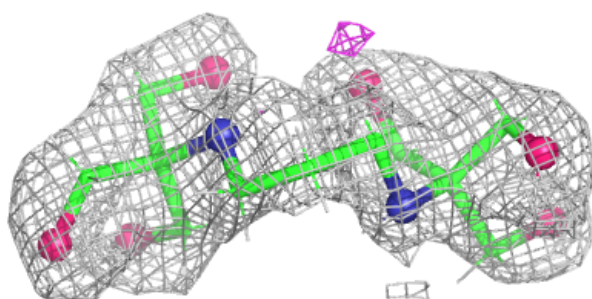
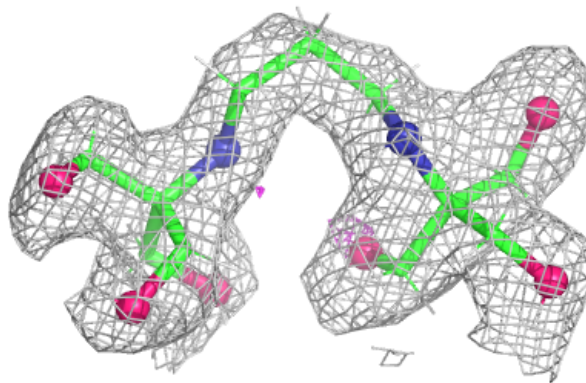
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	UDP	B	402	25/25	0.86	0.13	41,53,63,66	0
8	B3P	B	403	19/19	0.87	0.12	34,52,65,66	0
8	B3P	A	403	19/19	0.97	0.05	9,15,23,25	0
7	UDP	A	402	25/25	0.97	0.06	11,18,25,37	0
6	MN	A	401	1/1	0.99	0.03	20,20,20,20	0
6	MN	B	401	1/1	0.99	0.03	43,43,43,43	0

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.

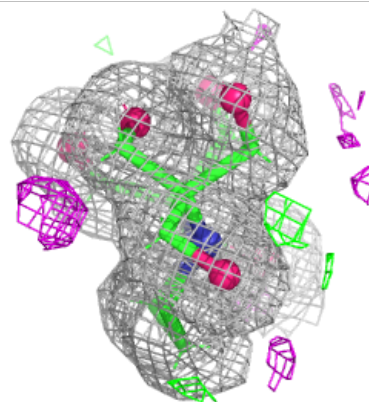
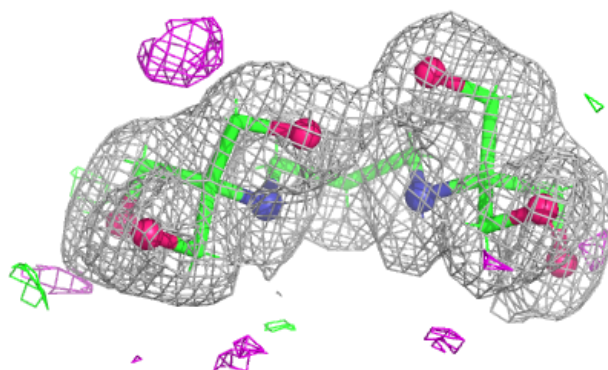
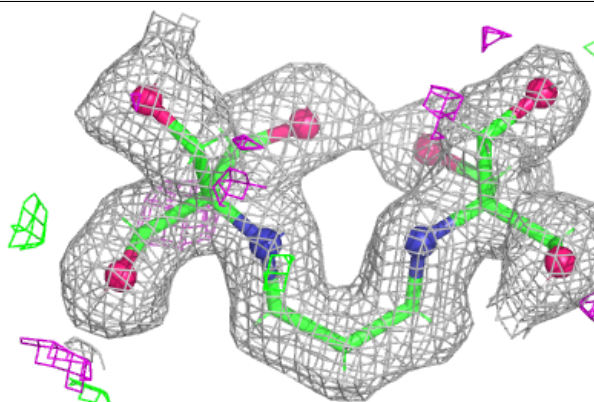


Electron density around B3P B 403:

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

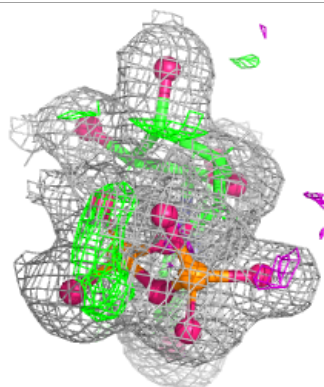
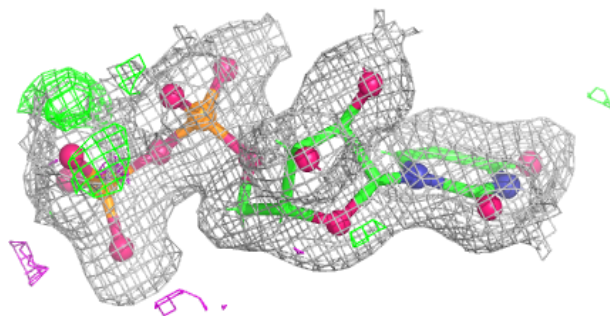
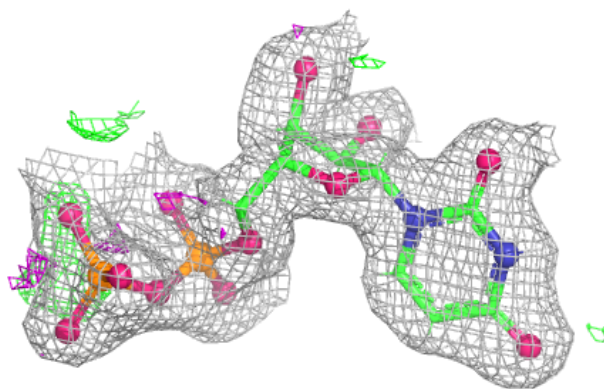
**Electron density around B3P A 403:**

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



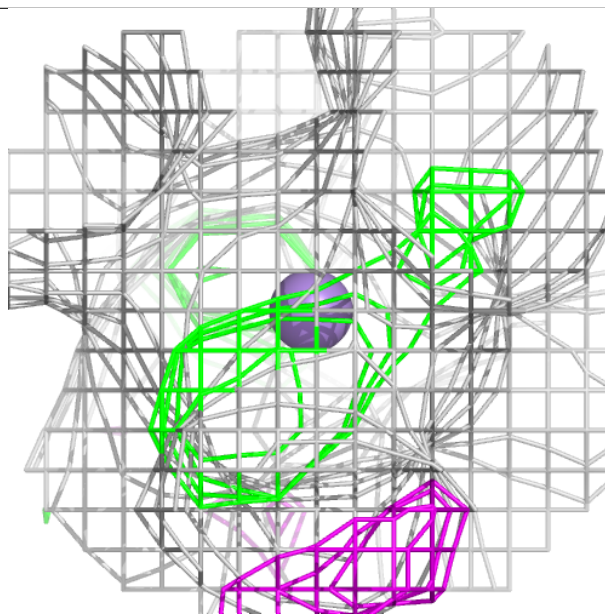
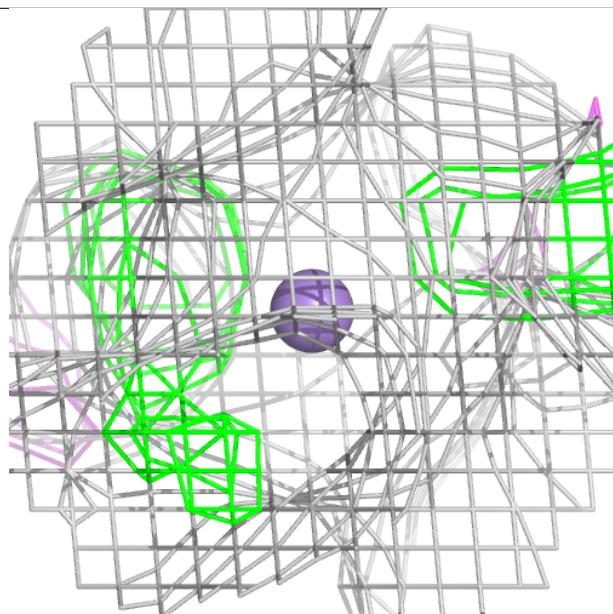
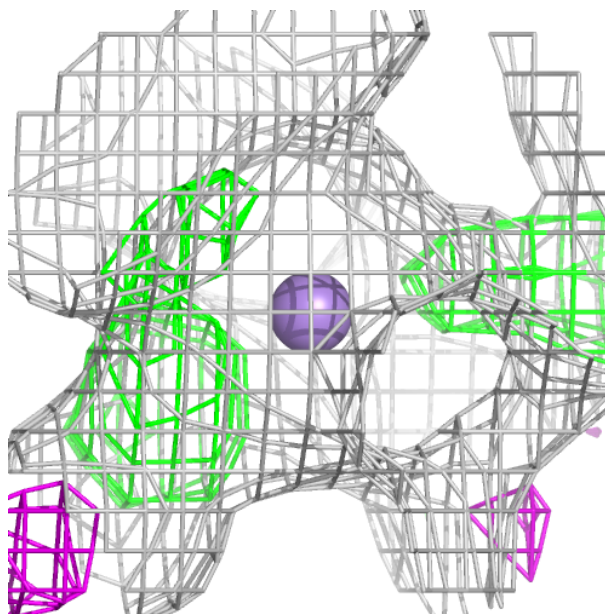
Electron density around UDP A 402:

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



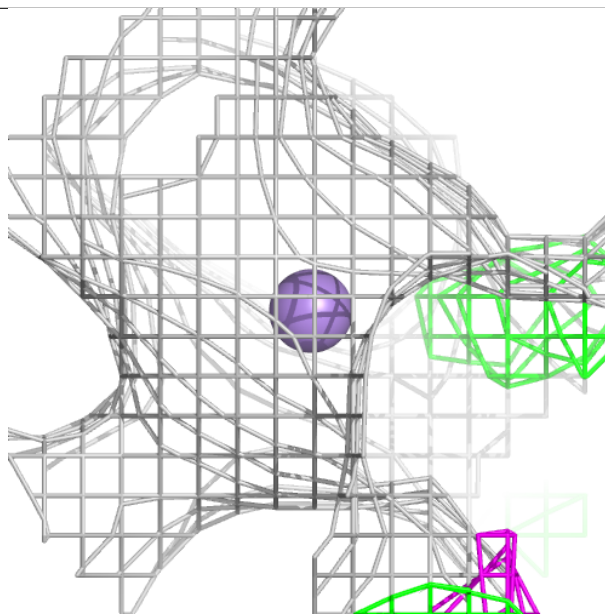
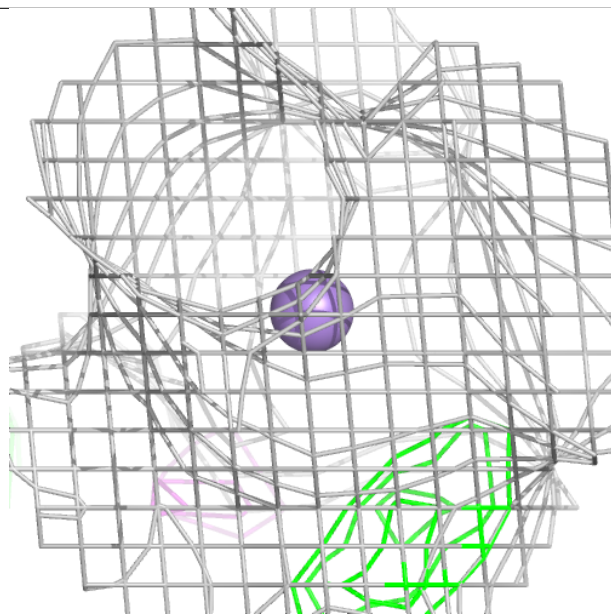
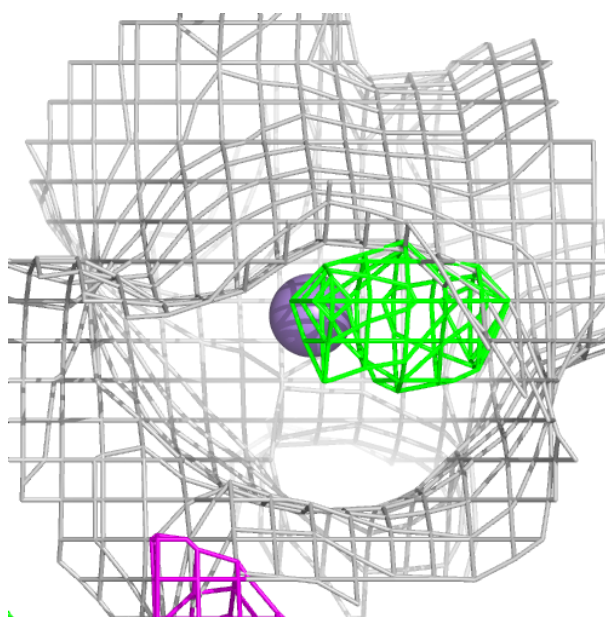
Electron density around MN A 401:

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



Electron density around MN B 401:

$2mF_o-DF_c$ (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.