



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 07:23 PM UTC

PDB ID : 8P0I / pdb_00008p0i
Title : Crystal structure of the open conformation of insulin-regulated aminopeptidase
in complex with a small-MW inhibitor
Authors : Mpakali, A.; Giastas, P.; Stratikos, E.
Deposited on : 2023-05-10
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

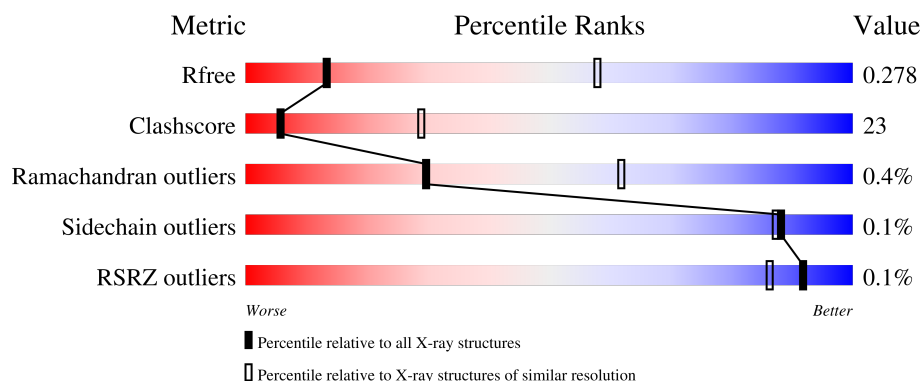
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

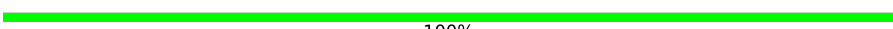
The reported resolution of this entry is 3.50 Å.

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.



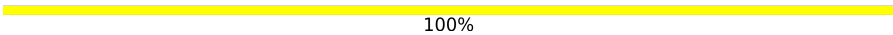
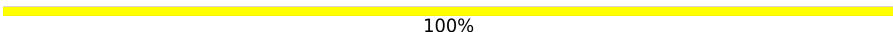
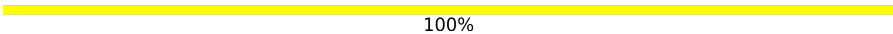
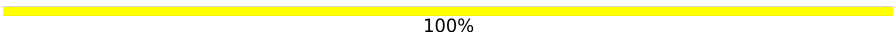
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	871	
1	B	871	
2	C	3	
2	E	3	
2	G	3	

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Mol	Chain	Length	Quality of chain
2	I	3	 67% 33%
3	D	4	 50% 50%
3	F	4	 75% 25%
4	H	2	 100%
4	J	2	 100%
4	K	2	 100%
4	L	2	 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
6	WC3	B	1107	-	X	-	-

2 Entry composition [i](#)

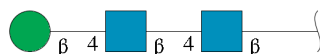
There are 7 unique types of molecules in this entry. The entry contains 13992 atoms, of which 56 are hydrogens and 0 are deuteriums.

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 Leucyl-cystinyl aminopeptidase, pregnancy serum form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	857	Total	C	N	O	S	0	0	0
			6700	4328	1091	1255	26			
1	B	851	Total	C	N	O	S	0	0	0
			6614	4290	1061	1239	24			

- Molecule 2 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
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



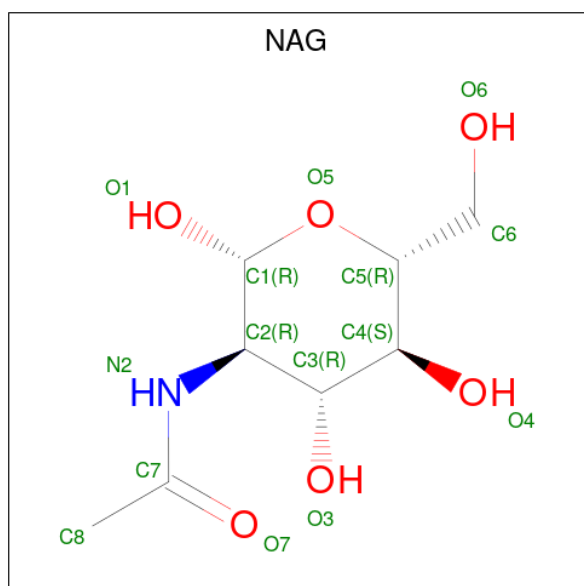
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



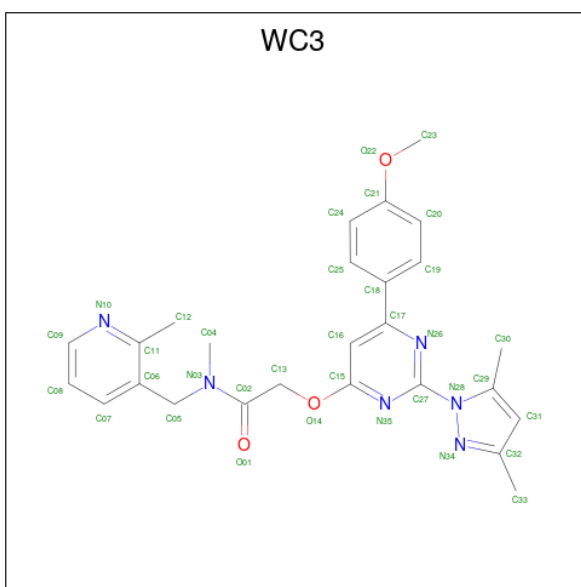
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is 2-[2-(3,5-dimethylpyrazol-1-yl)-6-(4-methoxyphenyl)pyrimidin-4-yl]oxy-N-methyl-N-[(2-methylpyridin-3-yl)methyl]ethanamide (CCD ID: WC3) (formula: C₂₆H₂₈N₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 63	C 26	H 28	N 6	O 3	0	0
6	B	1	Total 63	C 26	H 28	N 6	O 3	0	0

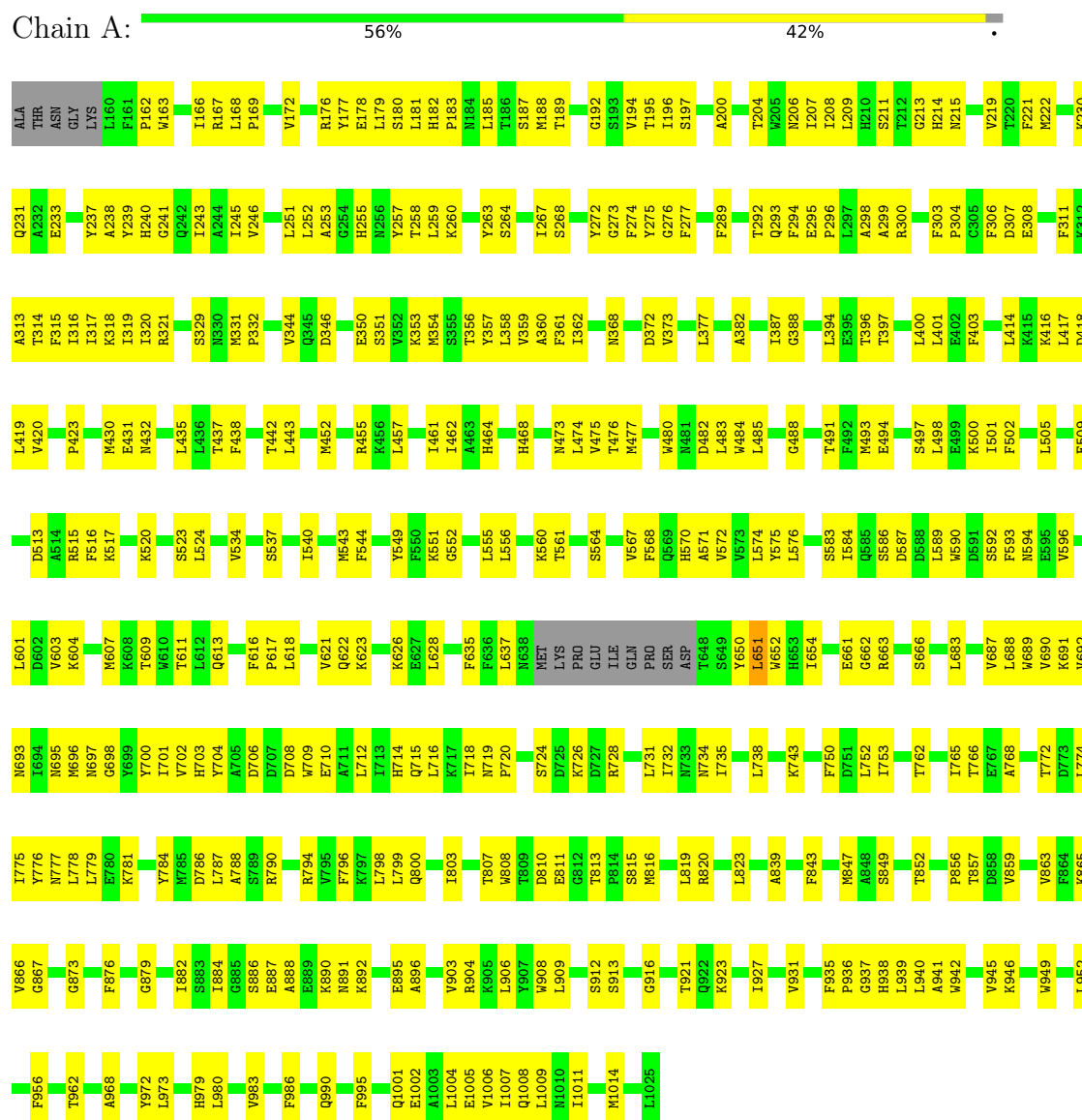
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Zn 1 1	0	0
7	B	1	Total Zn 1 1	0	0

3 Residue-property plots

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: Leucyl-cystinyl aminopeptidase, pregnancy serum form



- Molecule 1: Leucyl-cystinyl aminopeptidase, pregnancy serum form



Chain G:  100%



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

Chain I:  67% 33%



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

Chain D:  50% 50%

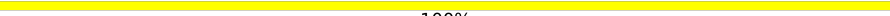


- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  75% 25%

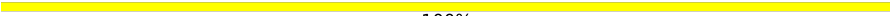


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

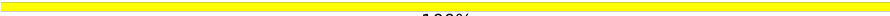


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



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

Chain K:  100%



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

Chain L:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.23Å 255.12Å 73.27Å 90.00° 110.00° 90.00°	Depositor
Resolution (Å)	64.11 – 3.50 64.11 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (64.11-3.50) 99.7 (64.11-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.240 , 0.277 0.242 , 0.278	Depositor DCC
R_{free} test set	1695 reflections (5.73%)	wwPDB-VP
Wilson B-factor (Å ²)	117.4	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 86.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13992	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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: BMA, WC3, NAG, MAN, ZN

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	0.32	0/6867	0.65	1/9360 (0.0%)
1	B	0.29	0/6778	0.65	2/9245 (0.0%)
All	All	0.30	0/13645	0.65	3/18605 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	651	LEU	CD1-CG-CD2	-10.82	87.00	110.80
1	B	169	PRO	CA-C-N	5.41	131.88	121.54
1	B	169	PRO	C-N-CA	5.41	131.88	121.54

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	6700	0	6340	311	0
1	B	6614	0	6240	312	0
2	C	39	0	34	0	0
2	E	39	0	34	1	0
2	G	39	0	34	0	0
2	I	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	50	0	43	3	0
3	F	50	0	43	1	0
4	H	28	0	25	0	0
4	J	28	0	25	1	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
5	A	98	0	91	1	0
5	B	84	0	78	3	0
6	A	35	28	0	0	0
6	B	35	28	0	3	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
All	All	13936	56	13071	627	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 23.

The worst 5 of 627 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:THR:HG21	1:A:652:TRP:HA	1.41	1.00
1:A:571:ALA:HA	1:A:596:VAL:HG21	1.44	0.97
1:B:661:GLU:HA	1:B:666:SER:HB3	1.49	0.93
1:B:910:MET:HE3	1:B:928:ILE:HG12	1.48	0.93
1:B:762:THR:HG22	1:B:819:LEU:HB2	1.53	0.90

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	853/871 (98%)	784 (92%)	64 (8%)	5 (1%)	21	54
1	B	844/871 (97%)	775 (92%)	67 (8%)	2 (0%)	43	74
All	All	1697/1742 (97%)	1559 (92%)	131 (8%)	7 (0%)	30	62

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	601	LEU
1	A	388	GLY
1	B	183	PRO
1	A	183	PRO
1	A	213	GLY

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	701/780 (90%)	701 (100%)	0	100	100
1	B	688/780 (88%)	687 (100%)	1 (0%)	88	87
All	All	1389/1560 (89%)	1388 (100%)	1 (0%)	88	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	673	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	734	ASN
1	B	830	HIS
1	B	1017	ASN
1	B	631	GLN
1	B	632	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 ⓘ

28 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	C	1	1,2	14,14,15	0.64	1 (7%)	17,19,21	0.69	0
2	NAG	C	2	2	14,14,15	0.45	0	17,19,21	0.52	0
2	BMA	C	3	2	11,11,12	0.72	0	15,15,17	0.75	0
3	NAG	D	1	1,3	14,14,15	0.40	0	17,19,21	0.48	0
3	NAG	D	2	3	14,14,15	0.74	1 (7%)	17,19,21	0.82	0
3	BMA	D	3	3	11,11,12	1.27	0	15,15,17	1.07	1 (6%)
3	MAN	D	4	3	11,11,12	0.80	0	15,15,17	1.29	2 (13%)
2	NAG	E	1	1,2	14,14,15	0.25	0	17,19,21	0.80	0
2	NAG	E	2	2	14,14,15	0.41	0	17,19,21	1.53	3 (17%)
2	BMA	E	3	2	11,11,12	0.41	0	15,15,17	0.99	1 (6%)
3	NAG	F	1	1,3	14,14,15	1.34	1 (7%)	17,19,21	2.04	5 (29%)
3	NAG	F	2	3	14,14,15	0.79	1 (7%)	17,19,21	1.09	2 (11%)
3	BMA	F	3	3	11,11,12	1.13	0	15,15,17	0.92	0
3	MAN	F	4	3	11,11,12	1.83	3 (27%)	15,15,17	1.40	2 (13%)
2	NAG	G	1	1,2	14,14,15	0.51	0	17,19,21	0.54	0
2	NAG	G	2	2	14,14,15	0.54	0	17,19,21	0.47	0
2	BMA	G	3	2	11,11,12	0.68	0	15,15,17	0.73	0
4	NAG	H	1	1,4	14,14,15	0.62	1 (7%)	17,19,21	0.99	2 (11%)
4	NAG	H	2	4	14,14,15	1.11	1 (7%)	17,19,21	2.09	3 (17%)
2	NAG	I	1	1,2	14,14,15	1.02	1 (7%)	17,19,21	1.18	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	I	2	2	14,14,15	0.38	0	17,19,21	0.56	0
2	BMA	I	3	2	11,11,12	0.56	0	15,15,17	0.90	1 (6%)
4	NAG	J	1	1,4	14,14,15	0.37	0	17,19,21	0.58	0
4	NAG	J	2	4	14,14,15	1.31	1 (7%)	17,19,21	0.68	0
4	NAG	K	1	1,4	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
4	NAG	K	2	4	14,14,15	0.39	0	17,19,21	0.98	1 (5%)
4	NAG	L	1	1,4	14,14,15	0.83	0	17,19,21	1.94	2 (11%)
4	NAG	L	2	4	14,14,15	0.90	1 (7%)	17,19,21	1.47	3 (17%)

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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	1/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	1/1/1/1
2	NAG	G	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	-4.84	1.35	1.43
3	F	4	MAN	O5-C5	4.68	1.52	1.43
4	J	2	NAG	C1-C2	4.43	1.58	1.52
4	H	2	NAG	C1-C2	3.72	1.57	1.52
2	I	1	NAG	C1-C2	3.64	1.57	1.52

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1	NAG	C2-N2-C7	6.70	131.88	122.90
4	H	2	NAG	C2-N2-C7	6.59	131.73	122.90
3	F	1	NAG	C1-O5-C5	-4.44	106.24	112.19
2	E	2	NAG	C1-O5-C5	4.03	117.59	112.19
4	H	2	NAG	C1-C2-N2	3.86	116.51	110.43

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C1-C2-N2-C7
2	I	1	NAG	C1-C2-N2-C7
4	H	2	NAG	C1-C2-N2-C7
4	L	1	NAG	C3-C2-N2-C7
4	H	1	NAG	C4-C5-C6-O6

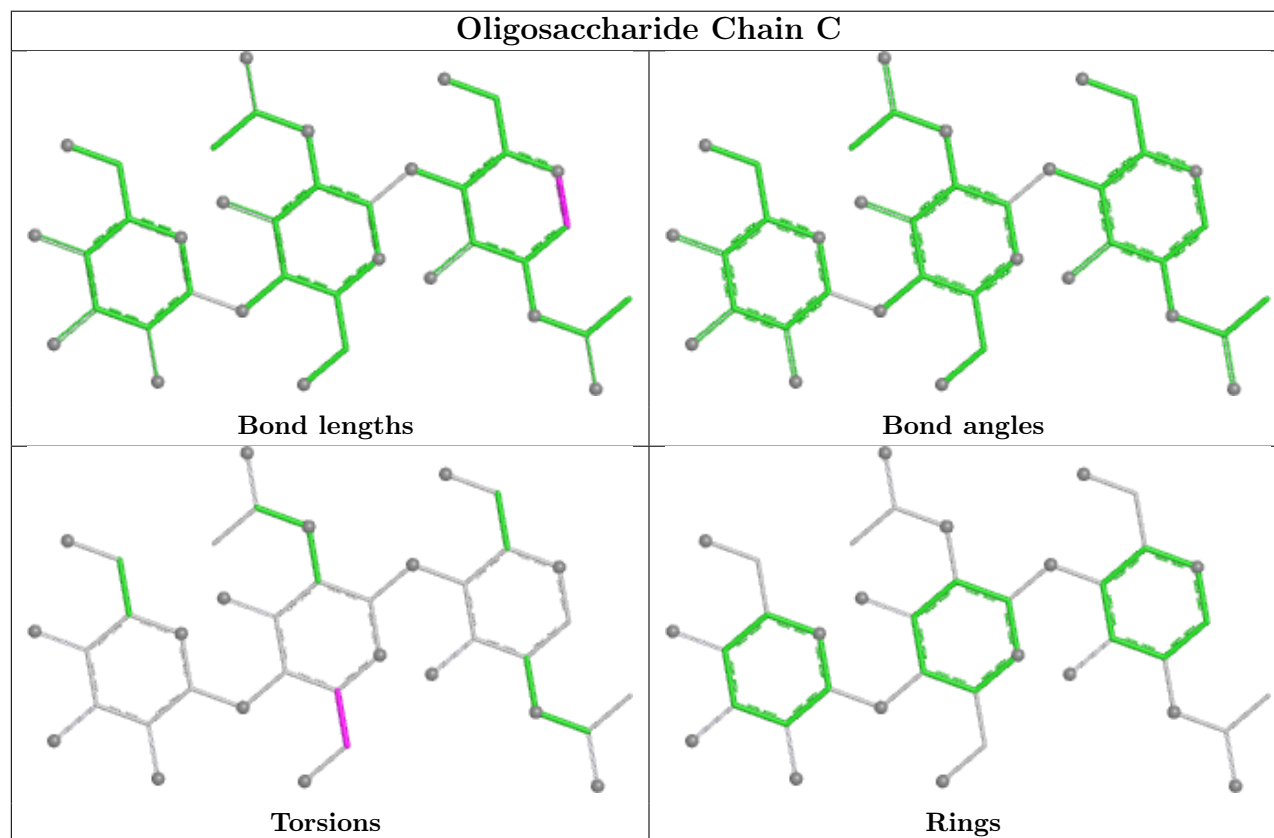
All (1) ring outliers are listed below:

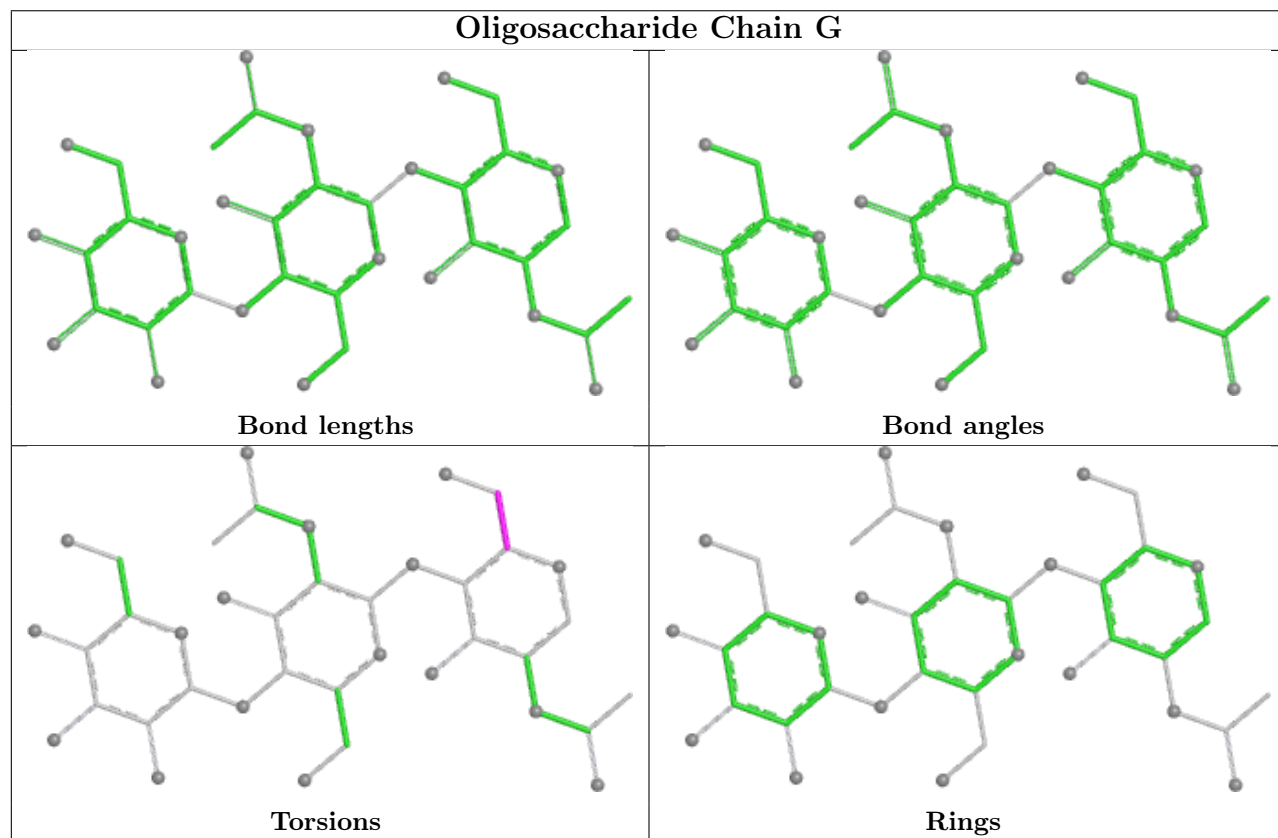
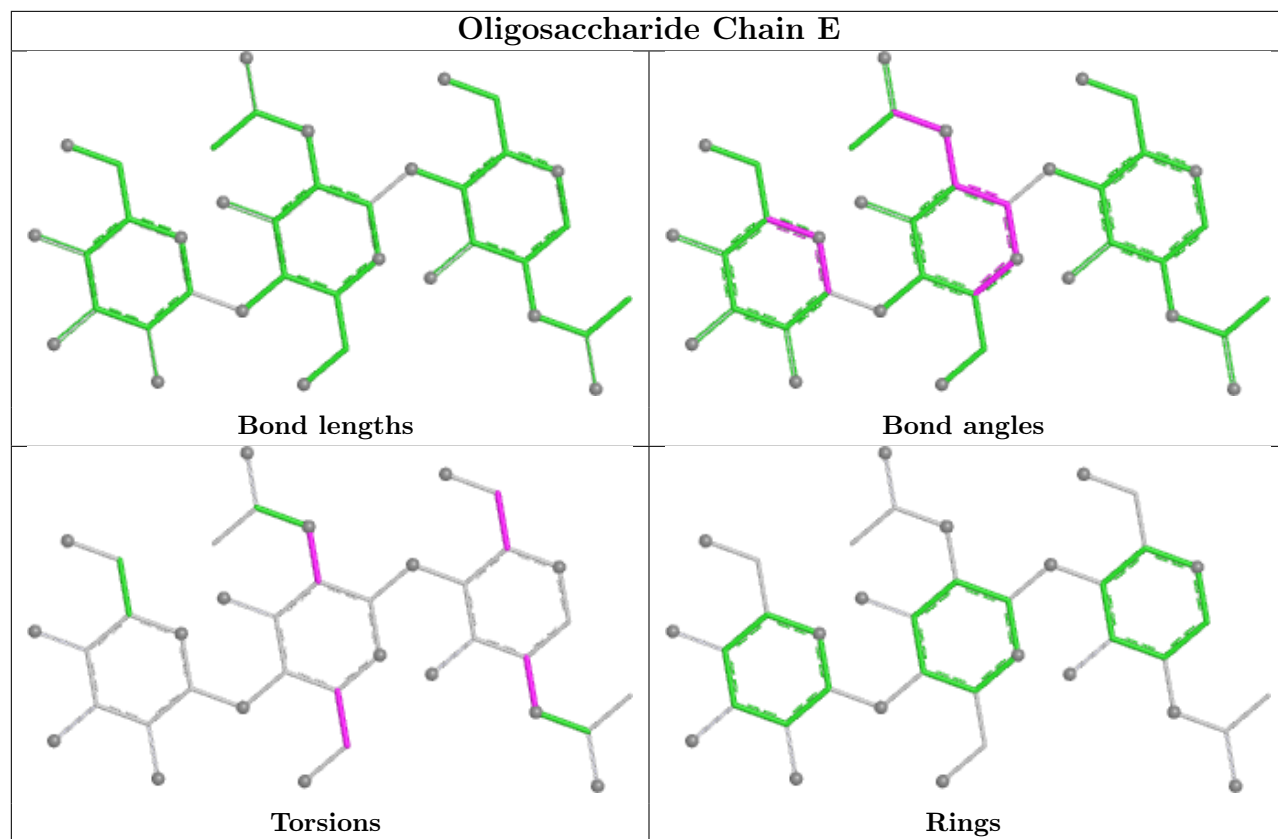
Mol	Chain	Res	Type	Atoms
3	F	4	MAN	C1-C2-C3-C4-C5-O5

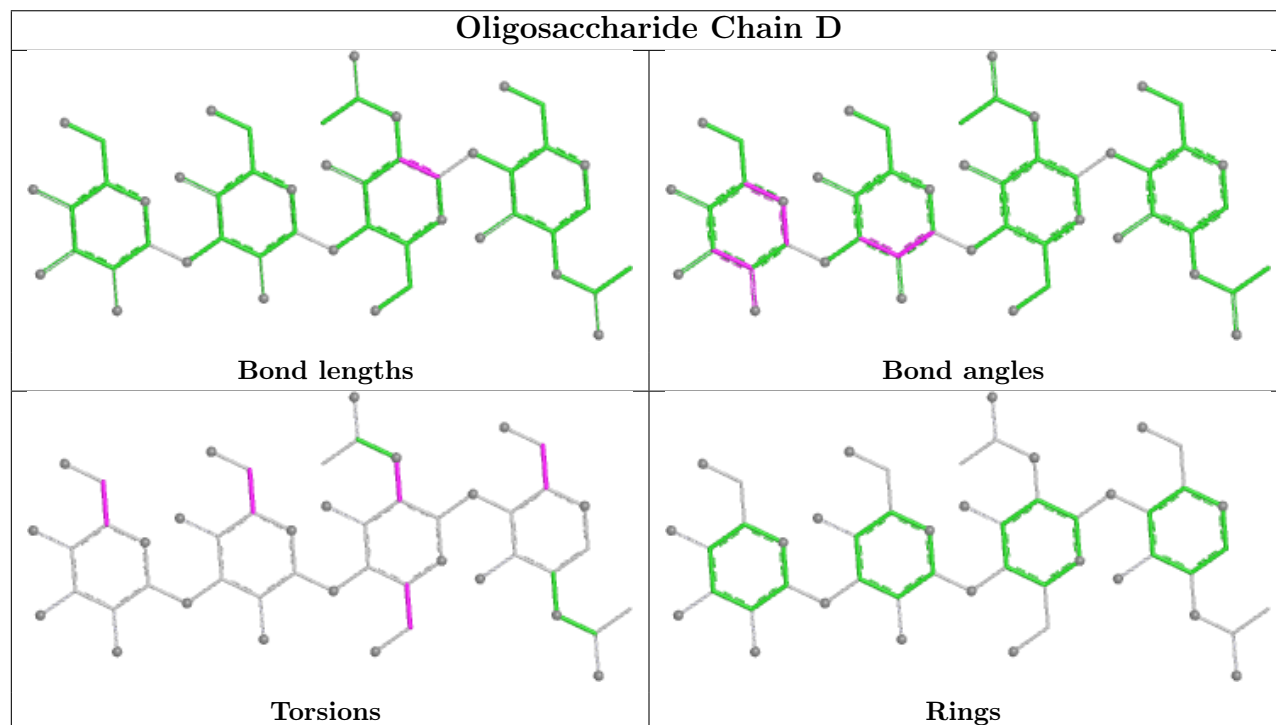
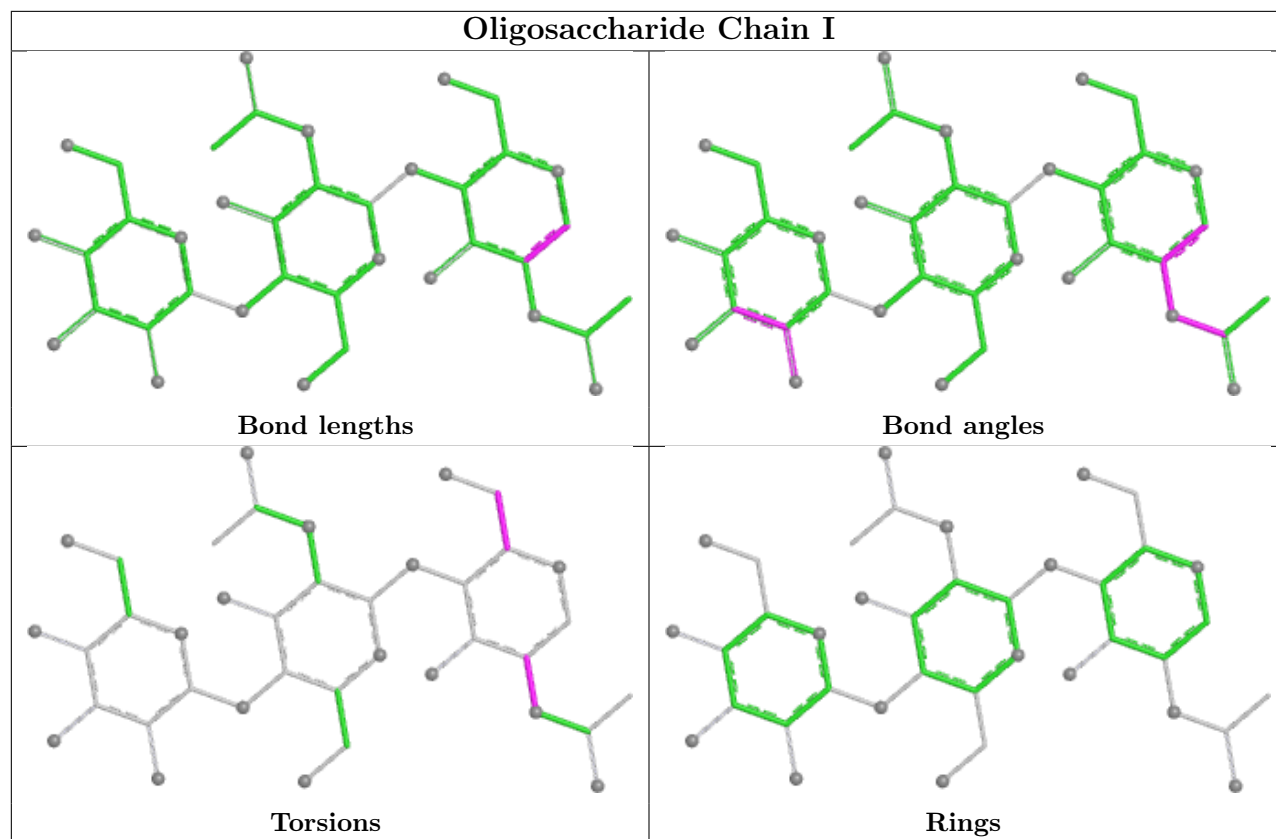
10 monomers are involved in 7 short contacts:

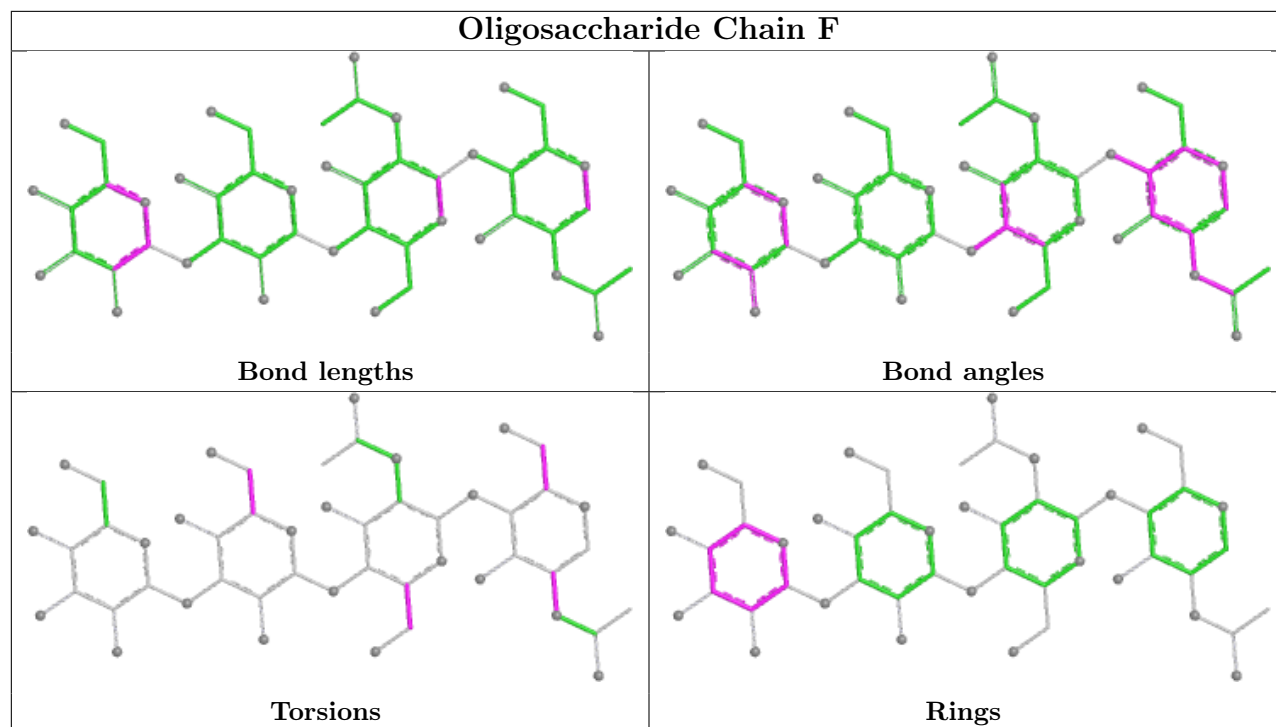
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	BMA	1	0
3	D	2	NAG	2	0
2	I	3	BMA	1	0
3	F	3	BMA	1	0
4	J	1	NAG	1	0
2	I	2	NAG	1	0
3	D	1	NAG	2	0
3	D	3	BMA	1	0
3	F	4	MAN	1	0
2	E	2	NAG	1	0

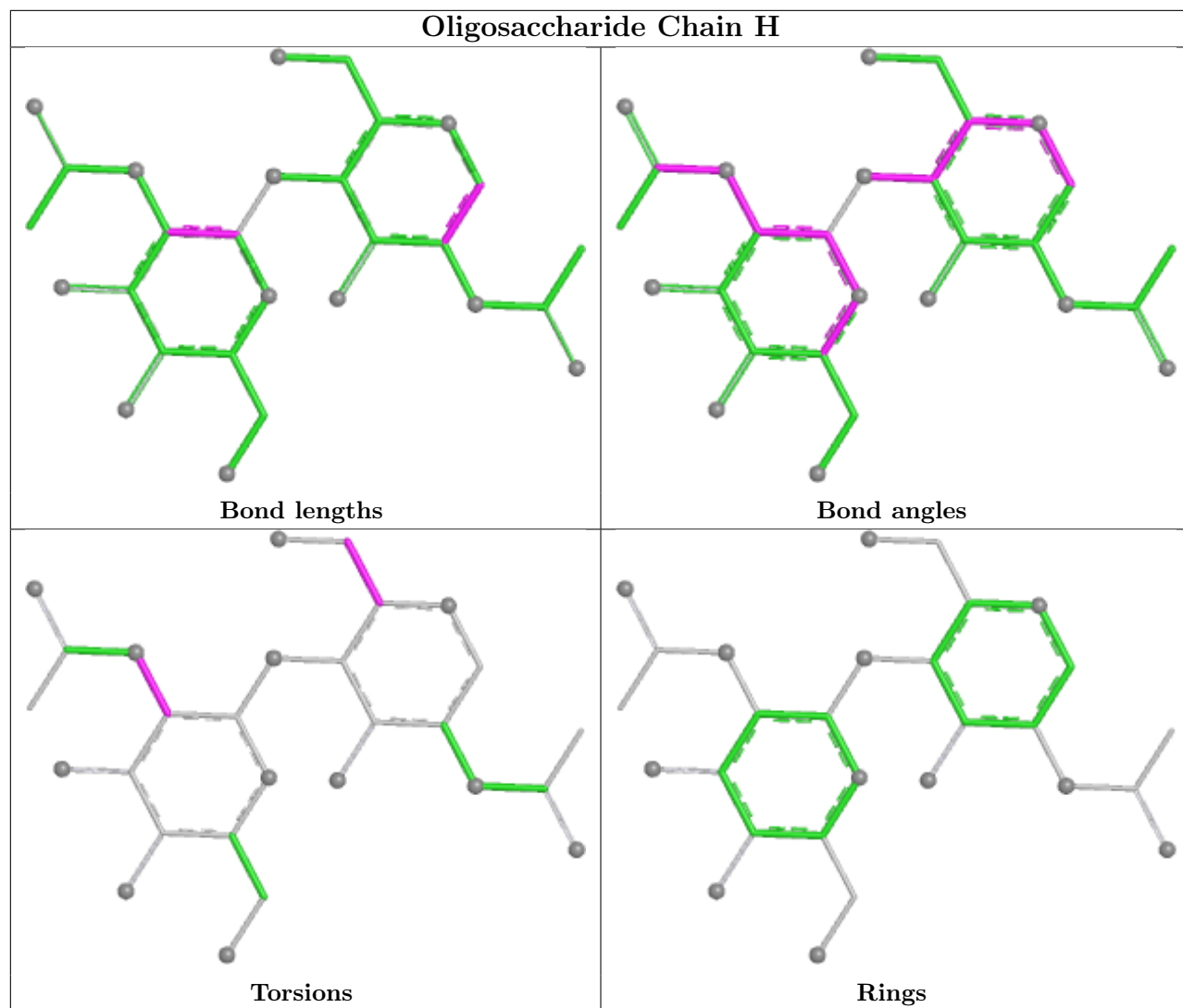
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

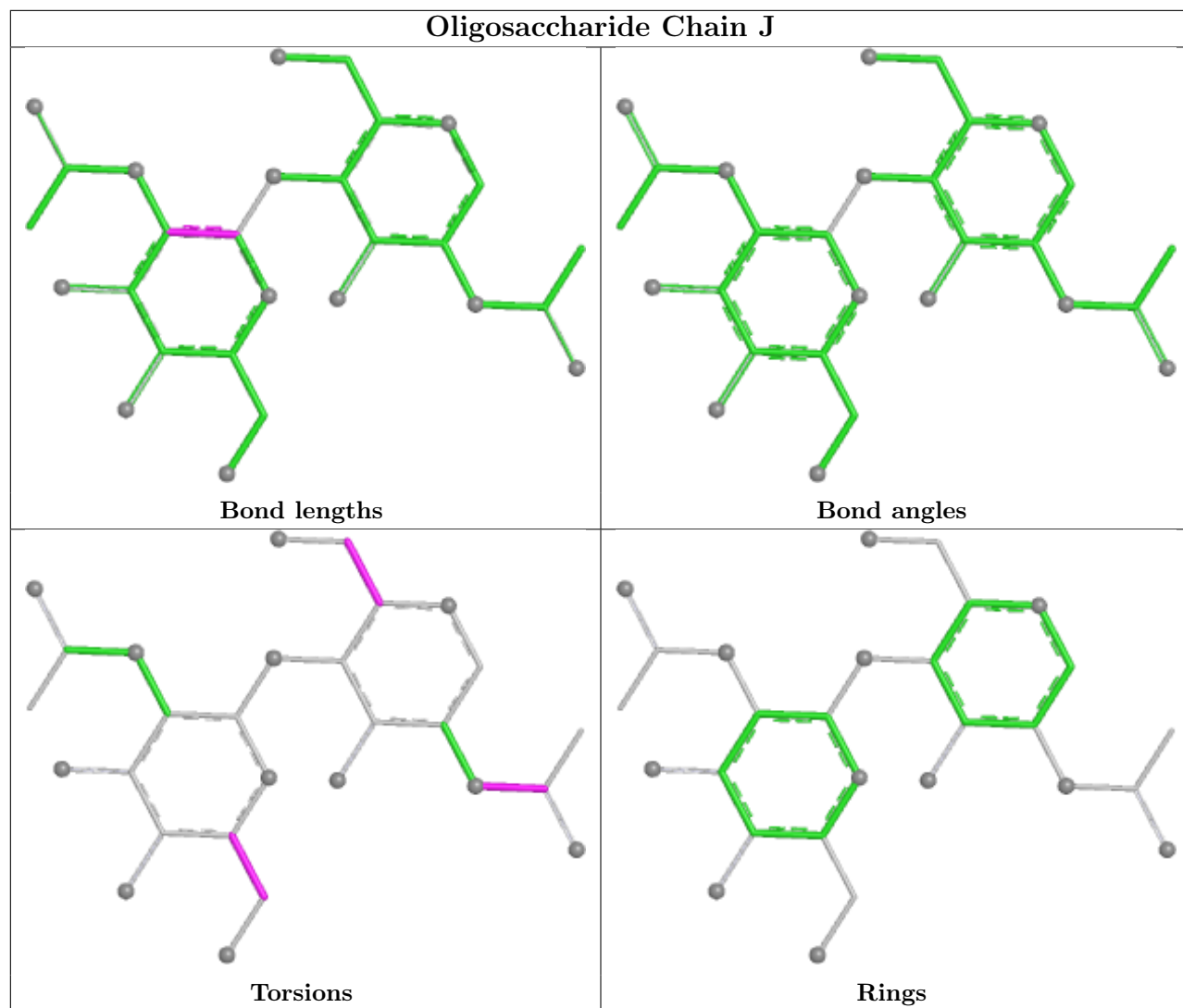


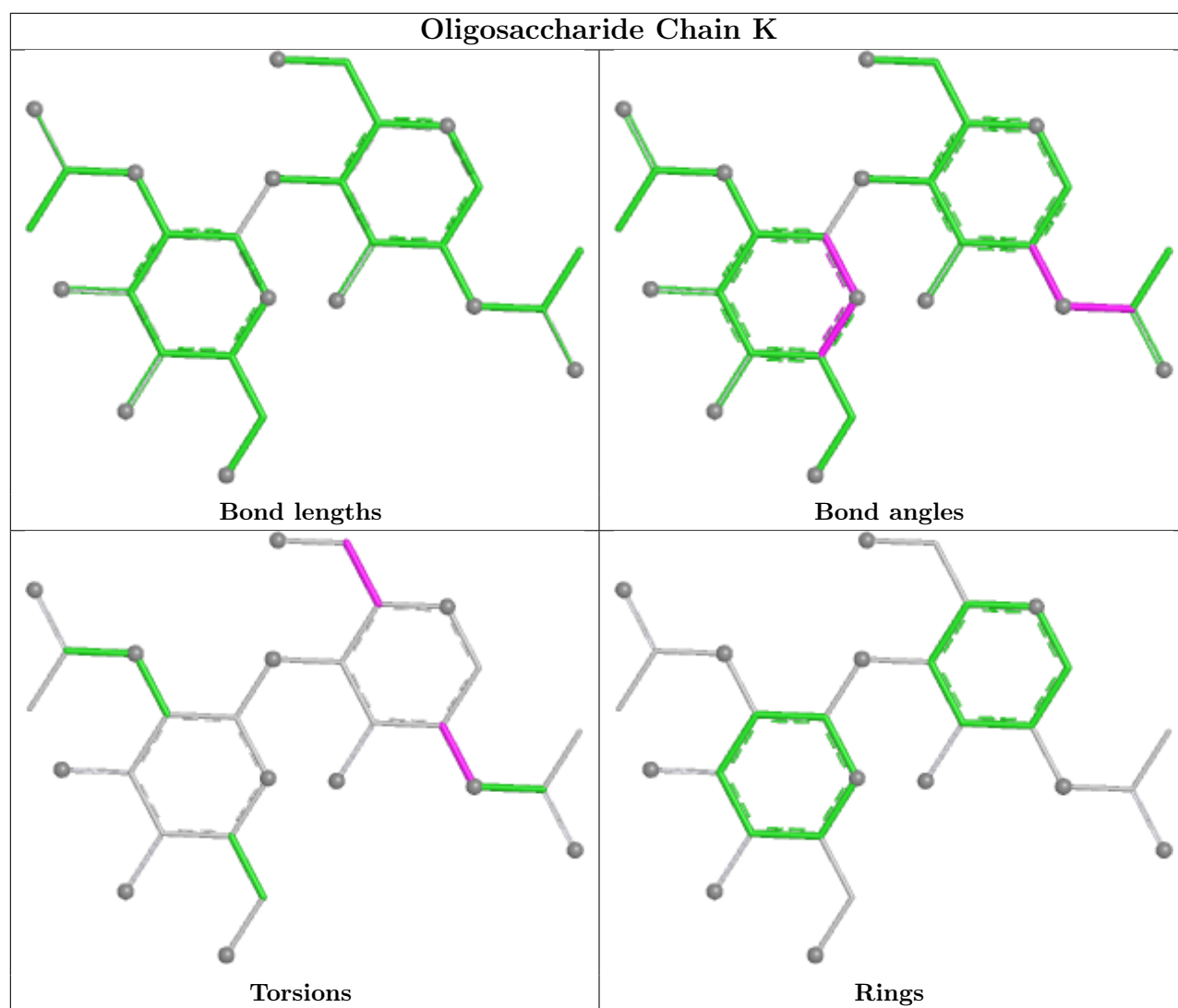


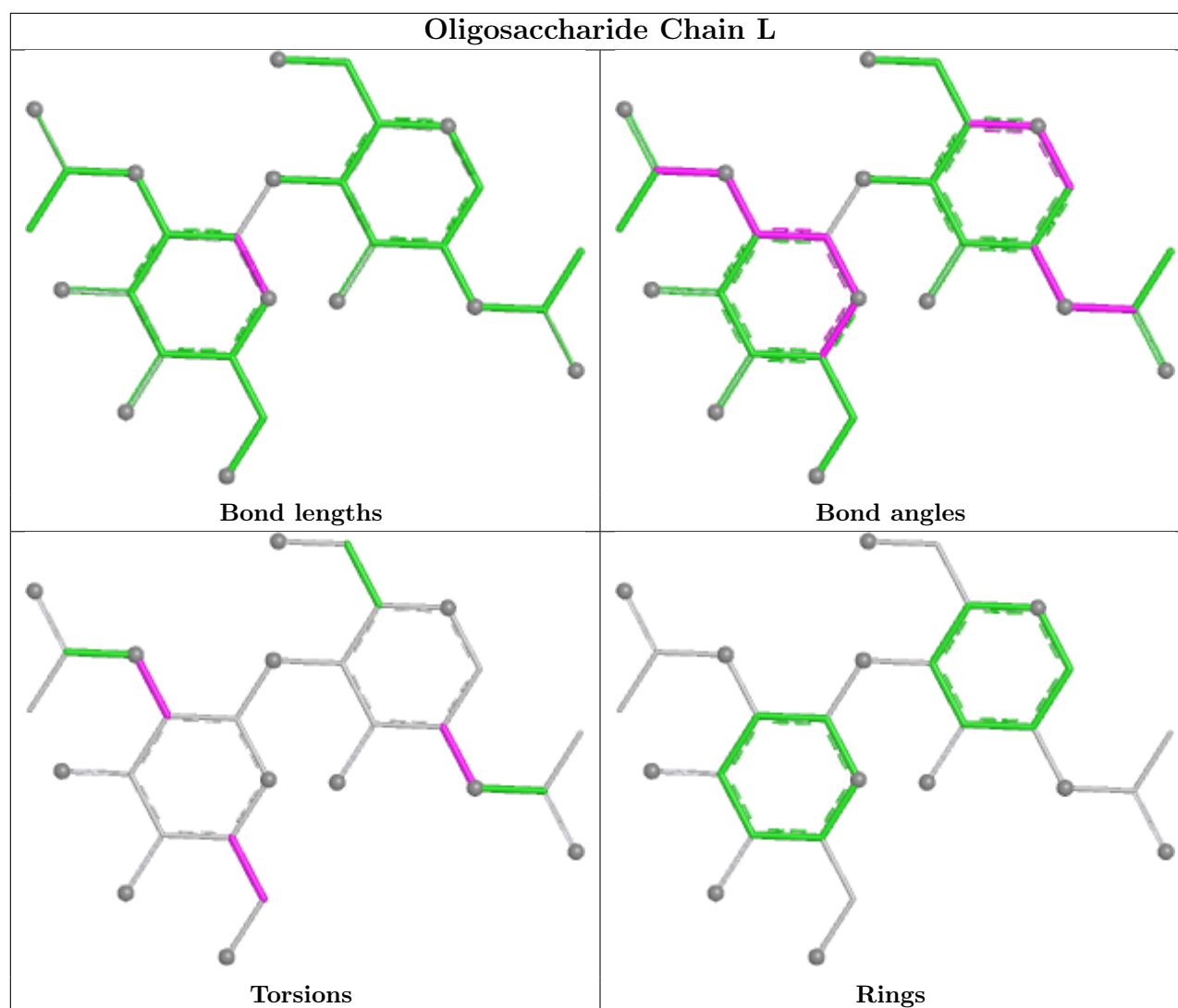












5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\# Z > 2$
5	NAG	A	1105	1	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	A	1109	1	14,14,15	1.12	1 (7%)	17,19,21	1.77	2 (11%)
5	NAG	B	1104	1	14,14,15	0.45	0	17,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1101	1	14,14,15	1.88	2 (14%)	17,19,21	2.14	3 (17%)
5	NAG	A	1103	1	14,14,15	0.36	0	17,19,21	0.57	0
5	NAG	B	1103	1	14,14,15	0.30	0	17,19,21	0.47	0
5	NAG	A	1106	1	14,14,15	0.62	1 (7%)	17,19,21	0.56	0
5	NAG	B	1106	1	14,14,15	0.33	0	17,19,21	1.54	2 (11%)
5	NAG	A	1102	1	14,14,15	0.47	0	17,19,21	1.70	1 (5%)
5	NAG	A	1104	1	14,14,15	0.19	0	17,19,21	0.96	1 (5%)
5	NAG	B	1102	1	14,14,15	0.42	0	17,19,21	0.45	0
6	WC3	A	1107	7	38,38,38	3.14	5 (13%)	51,53,53	4.18	24 (47%)
5	NAG	A	1101	1	14,14,15	1.02	1 (7%)	17,19,21	1.38	2 (11%)
6	WC3	B	1107	7	38,38,38	3.04	9 (23%)	51,53,53	4.41	26 (50%)
5	NAG	B	1105	1	14,14,15	0.56	0	17,19,21	0.71	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
5	NAG	A	1105	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1109	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1104	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1101	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1103	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1103	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1106	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1106	1	-	6/6/23/26	0/1/1/1
5	NAG	A	1102	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1104	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1102	1	-	1/6/23/26	0/1/1/1
6	WC3	A	1107	7	-	12/23/23/23	0/4/4/4
5	NAG	A	1101	1	-	2/6/23/26	0/1/1/1
6	WC3	B	1107	7	-	14/23/23/23	0/4/4/4
5	NAG	B	1105	1	-	0/6/23/26	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1107	WC3	C02-N03	16.43	1.54	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1107	WC3	C02-N03	15.12	1.52	1.34
6	A	1107	WC3	C27-N28	6.26	1.49	1.40
5	B	1101	NAG	O5-C1	6.09	1.53	1.43
6	B	1107	WC3	C27-N28	5.99	1.49	1.40

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1107	WC3	C12-C11-C06	12.82	132.06	121.80
6	A	1107	WC3	O01-C02-N03	12.54	140.37	122.19
6	B	1107	WC3	C27-N28-N34	9.69	130.07	118.49
6	A	1107	WC3	C29-N28-N34	-9.49	105.82	111.97
6	A	1107	WC3	C32-N34-N28	8.94	110.39	104.57

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1101	NAG	C1-C2-N2-C7
5	A	1102	NAG	C3-C2-N2-C7
5	A	1109	NAG	C1-C2-N2-C7
5	B	1101	NAG	C8-C7-N2-C2
5	B	1104	NAG	C1-C2-N2-C7

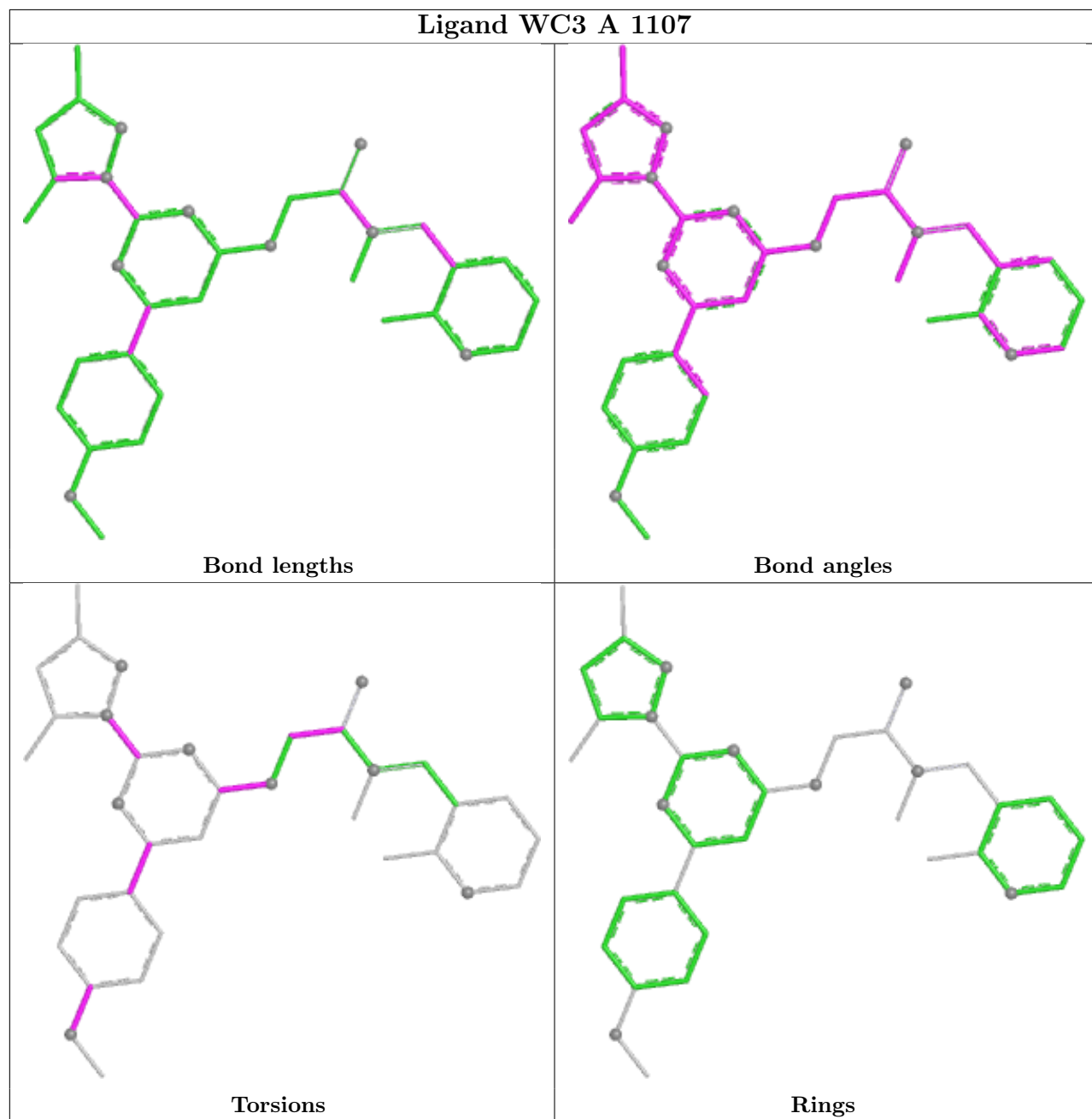
There are no ring outliers.

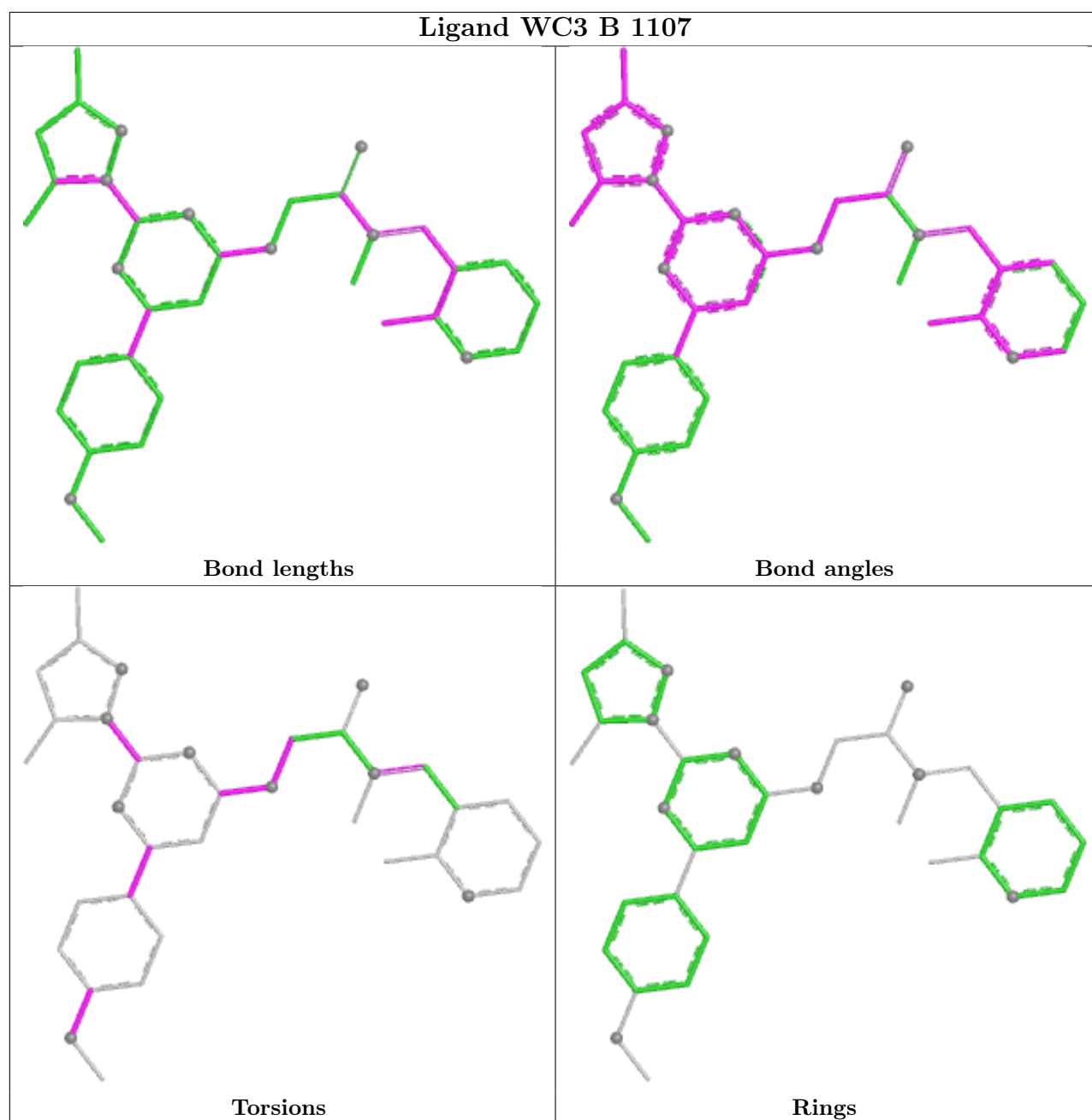
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1101	NAG	2	0
5	B	1106	NAG	1	0
5	A	1104	NAG	1	0
6	B	1107	WC3	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 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](#)

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	857/871 (98%)	-0.41	0 100 100	83, 112, 140, 156	1 (0%)
1	B	851/871 (97%)	-0.40	2 (0%) 91 82	92, 118, 144, 165	0
All	All	1708/1742 (98%)	-0.40	2 (0%) 92 86	83, 115, 142, 165	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	ALA	3.0
1	B	327	ALA	2.7

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
4	NAG	H	2	14/15	0.33	0.08	159,168,174,174	0
3	NAG	F	1	14/15	0.35	0.11	155,168,178,180	0
2	BMA	G	3	11/12	0.35	0.10	141,160,167,170	0
3	BMA	D	3	11/12	0.38	0.08	165,177,181,183	0
3	MAN	D	4	11/12	0.38	0.08	154,178,181,184	0
2	NAG	G	2	14/15	0.47	0.08	143,157,160,162	0
3	BMA	F	3	11/12	0.49	0.13	129,149,156,158	0

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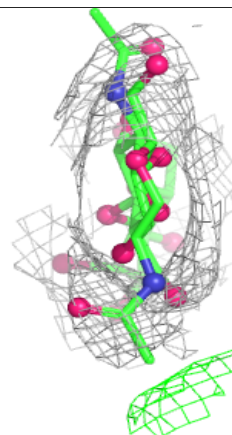
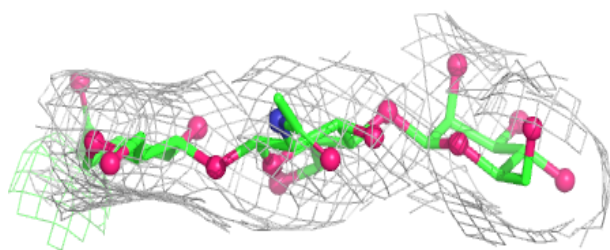
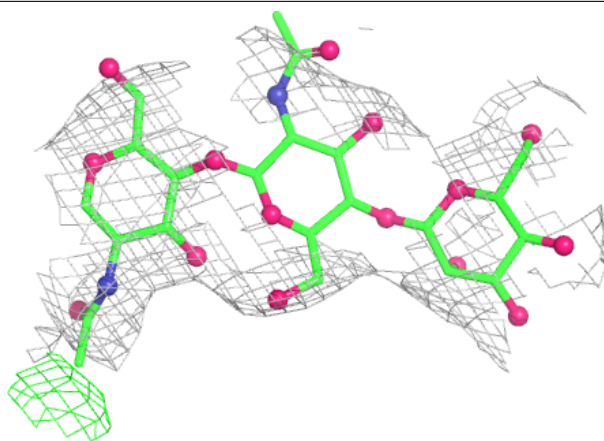
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	1	14/15	0.49	0.11	127,139,148,150	0
2	BMA	E	3	11/12	0.50	0.07	134,136,139,144	0
4	NAG	K	1	14/15	0.54	0.09	142,156,162,172	0
2	BMA	C	3	11/12	0.57	0.07	138,146,151,152	0
4	NAG	J	1	14/15	0.59	0.10	125,138,143,144	0
4	NAG	H	1	14/15	0.60	0.08	134,160,170,174	0
3	NAG	D	1	14/15	0.61	0.07	115,143,159,164	0
3	NAG	F	2	14/15	0.64	0.08	145,157,163,166	0
3	MAN	F	4	11/12	0.66	0.11	126,139,145,148	0
4	NAG	K	2	14/15	0.66	0.07	132,155,164,167	0
2	NAG	G	1	14/15	0.67	0.09	135,149,156,156	0
4	NAG	J	2	14/15	0.70	0.07	147,157,164,165	0
2	BMA	I	3	11/12	0.71	0.05	139,142,144,144	0
2	NAG	C	2	14/15	0.73	0.06	132,156,168,191	0
3	NAG	D	2	14/15	0.76	0.07	146,166,175,177	0
4	NAG	L	2	14/15	0.77	0.07	135,146,150,151	0
2	NAG	E	1	14/15	0.78	0.08	124,127,131,134	0
2	NAG	E	2	14/15	0.81	0.07	131,136,143,144	0
2	NAG	I	1	14/15	0.82	0.09	138,145,152,153	0
2	NAG	I	2	14/15	0.87	0.06	120,143,148,153	0
4	NAG	L	1	14/15	0.90	0.08	147,152,157,160	0

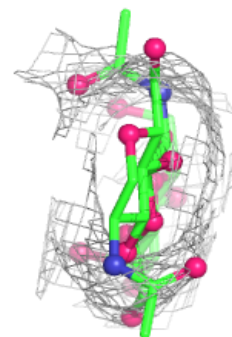
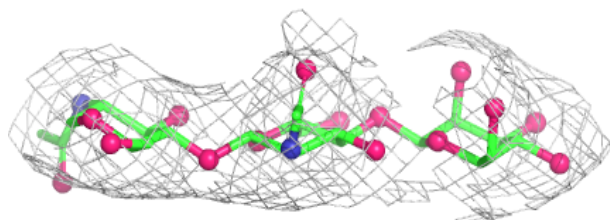
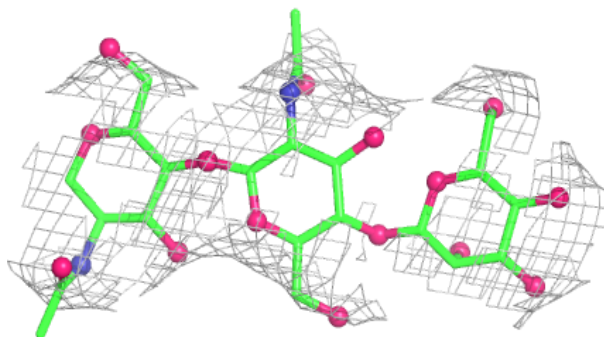
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

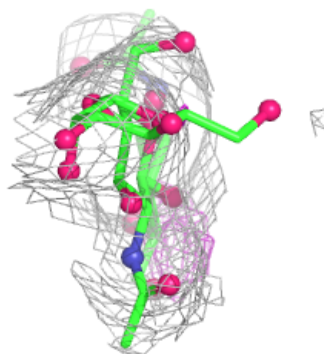
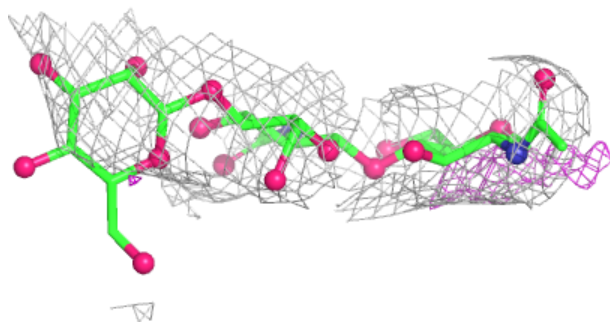
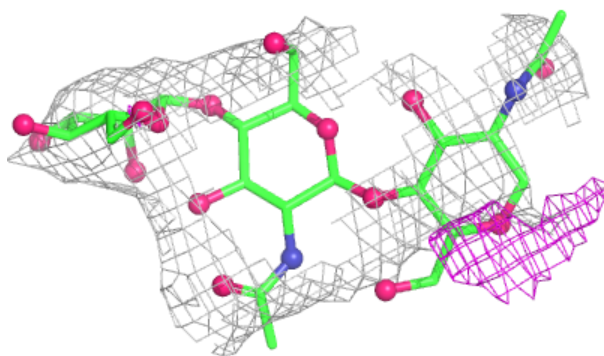
**Electron density around Chain E:**

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

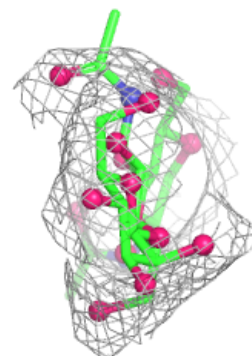
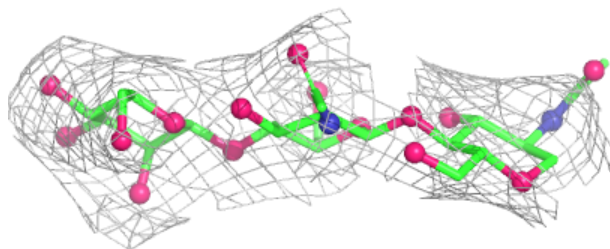
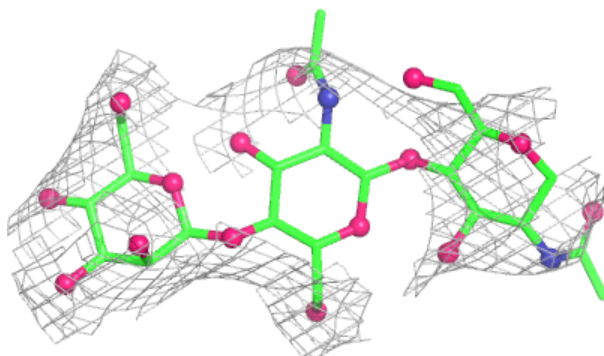


Electron density around Chain G:

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

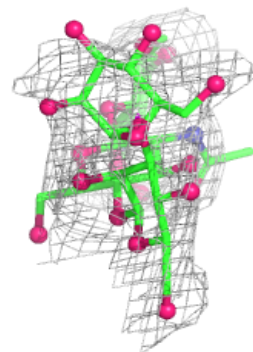
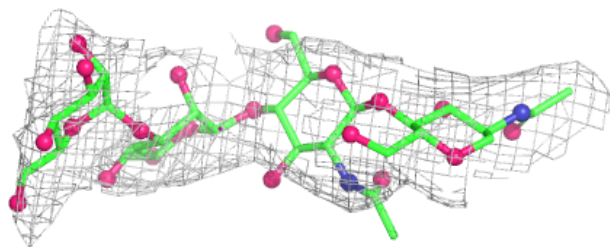
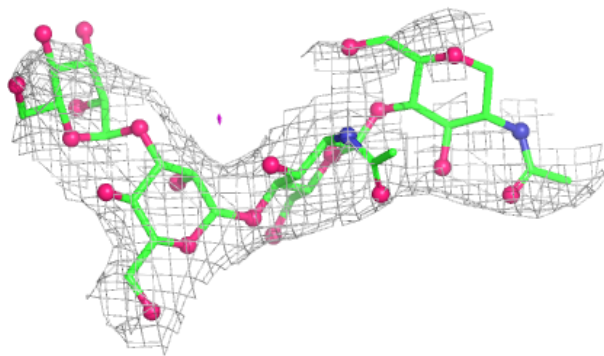
**Electron density around Chain I:**

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



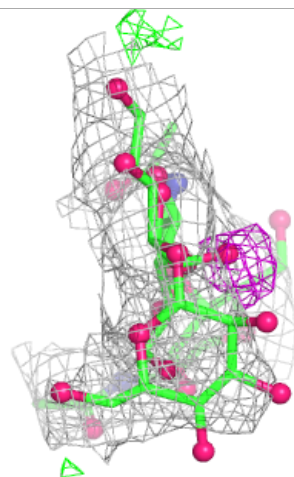
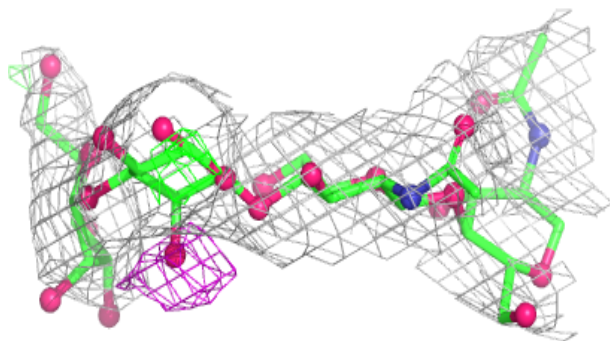
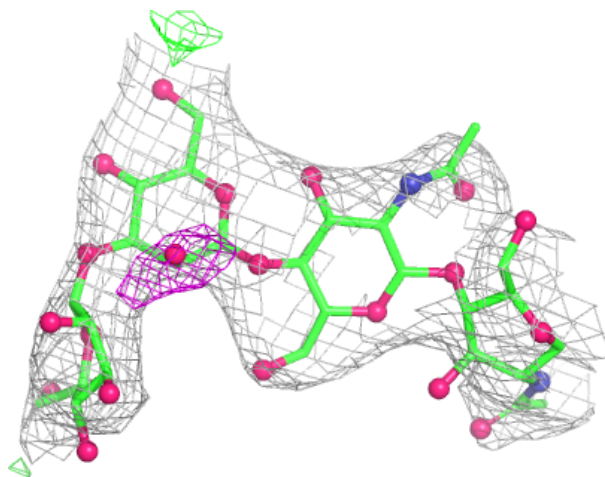
Electron density around Chain D:

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



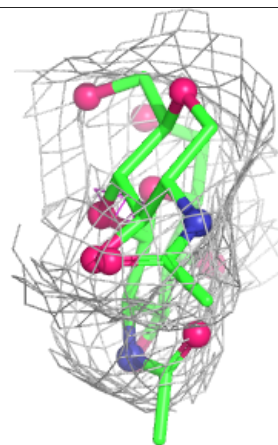
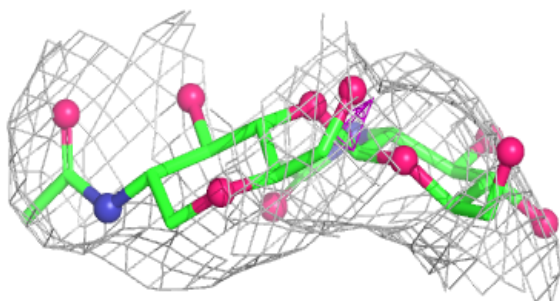
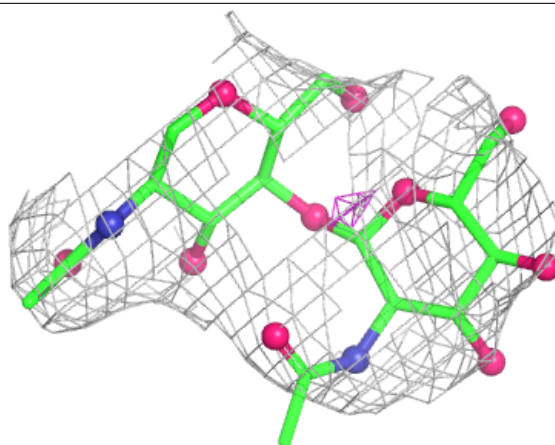
Electron density around Chain F:

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



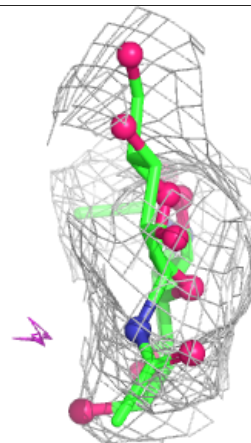
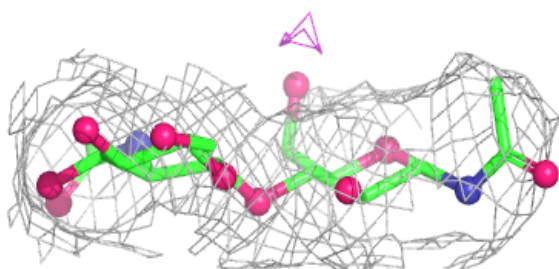
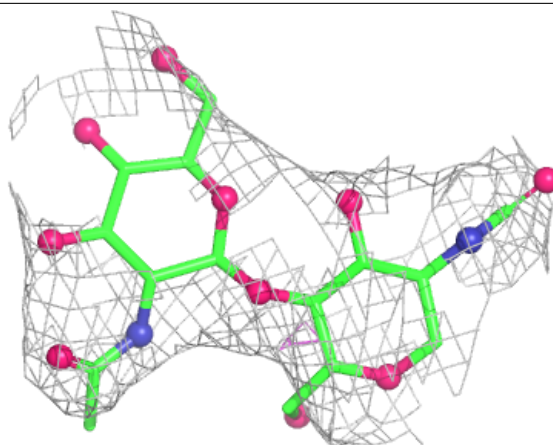
Electron density around Chain H:

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



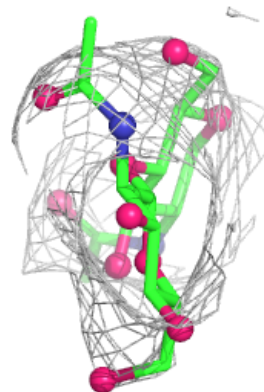
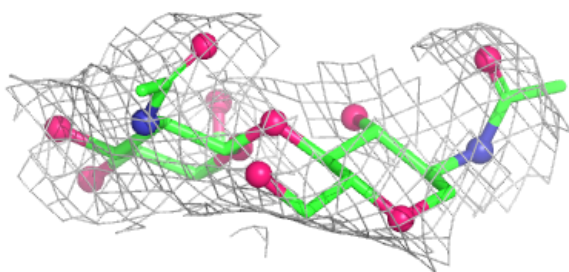
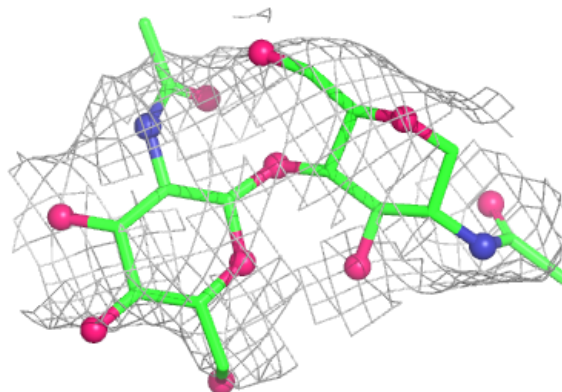
Electron density around Chain J:

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

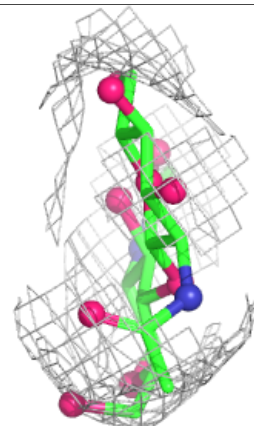
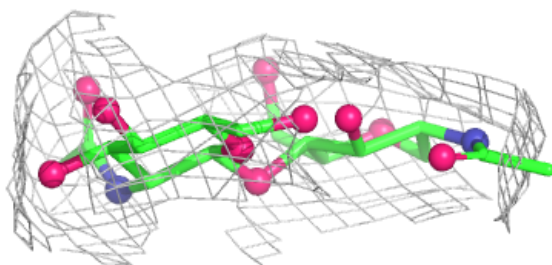
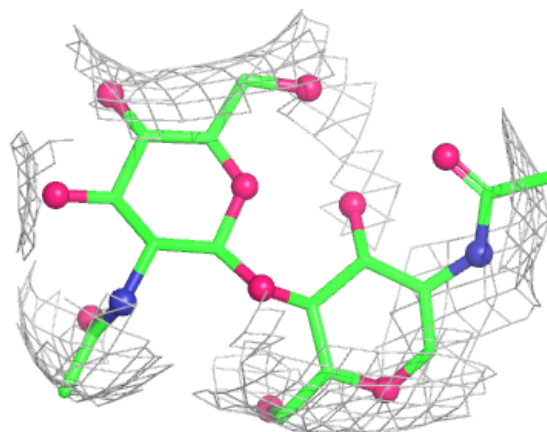


Electron density around Chain K:

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

**Electron density around Chain L:**

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



6.4 Ligands

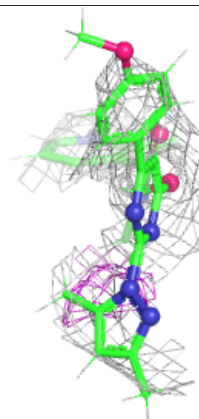
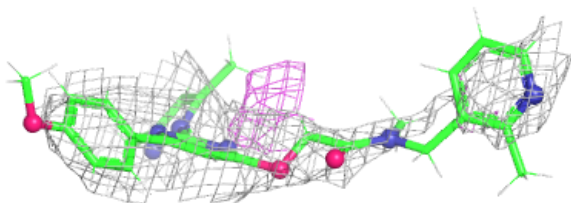
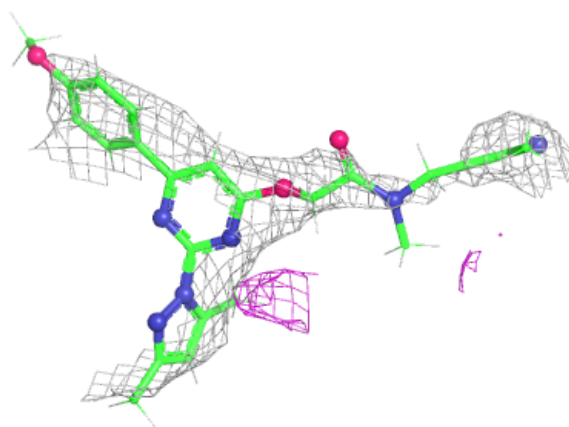
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	1106	14/15	0.43	0.08	153,162,168,172	0
5	NAG	B	1105	14/15	0.51	0.08	146,166,170,171	0
5	NAG	A	1105	14/15	0.51	0.10	137,154,169,179	0
5	NAG	A	1104	14/15	0.62	0.07	135,154,158,159	0
5	NAG	B	1101	14/15	0.63	0.08	141,159,163,167	0
5	NAG	A	1102	14/15	0.64	0.08	141,158,169,172	0
5	NAG	B	1104	14/15	0.64	0.07	147,162,167,168	0
5	NAG	A	1109	14/15	0.65	0.08	130,139,149,150	0
5	NAG	A	1106	14/15	0.70	0.07	142,150,158,160	0
5	NAG	B	1102	14/15	0.79	0.07	109,134,142,144	0
5	NAG	A	1101	14/15	0.81	0.06	139,146,149,150	0
5	NAG	B	1103	14/15	0.85	0.06	123,132,141,147	0
6	WC3	A	1107	35/35	0.85	0.10	120,144,172,175	0
6	WC3	B	1107	35/35	0.85	0.11	126,158,194,209	0
5	NAG	A	1103	14/15	0.91	0.07	107,115,124,127	0
7	ZN	B	1108	1/1	0.98	0.03	105,105,105,105	0
7	ZN	A	1108	1/1	0.99	0.03	114,114,114,114	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.

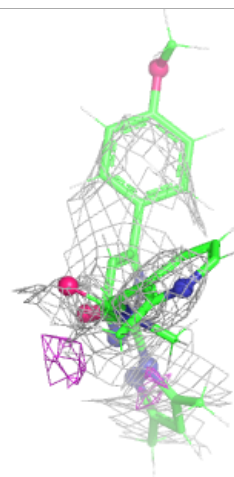
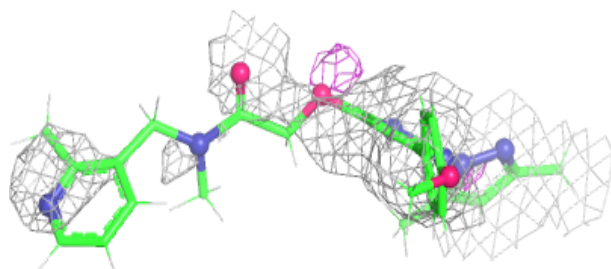
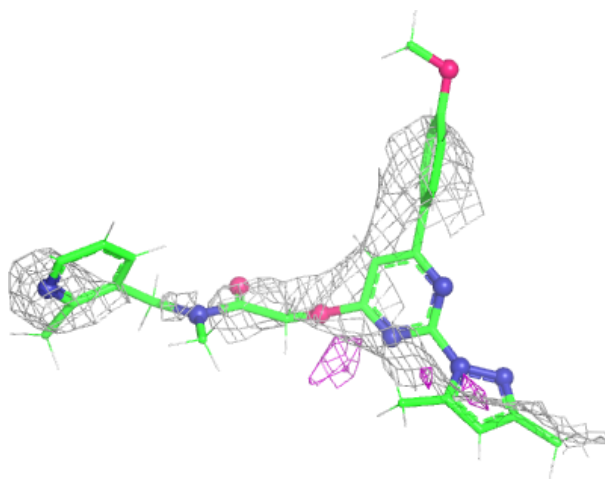
Electron density around WC3 A 1107:

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



Electron density around WC3 B 1107:

$2mF_o-DF_c$ (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.