



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 09:30 AM BST

PDB ID : 5T6N
Title : Crystal structure of the A/Hong Kong/1/1968 (H3N2) influenza virus hemagglutinin in complex with the antiviral drug arbidol
Authors : Kadam, R.U.; Wilson, I.A.
Deposited on : 2016-09-01
Resolution : 2.54 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 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	:	2.13.1
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)	:	2.13.1

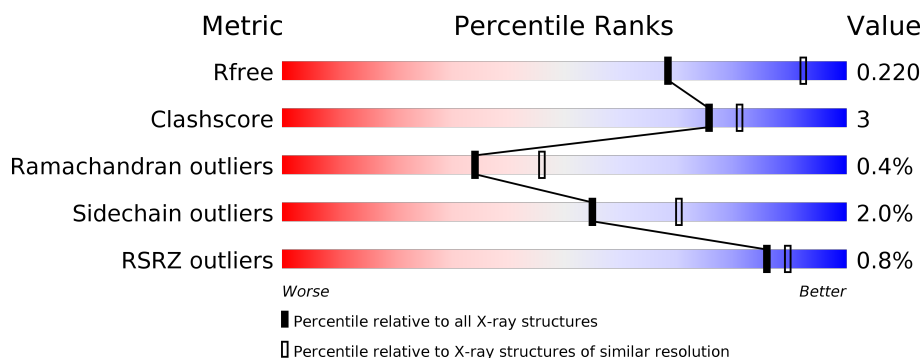
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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.






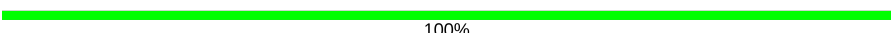

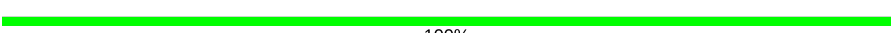



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 on 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	323	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>..</div> </div> </div>
1	C	323	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>5%</div> <div>..</div> </div> </div>
1	E	323	<div> <div></div> <div> <div></div> <div>90%</div> <div>7%</div> <div>..</div> </div> </div>
2	B	174	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
2	D	174	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
2	F	174	<div> <div></div> <div> <div></div> <div>89%</div> <div>7%</div> <div>...</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	4	 50%50%
4	H	2	 50%50%
4	I	2	 100%
4	J	2	 100%
4	L	2	 100%
4	M	2	 100%
4	O	2	 100%
5	K	3	 67%33%
6	N	5	 60%40%

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
3	MAN	G	4	-	-	-	X
6	MAN	N	5	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 12992 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	8	0
			2519	1578	443	484	14			
1	C	317	Total	C	N	O	S	0	8	0
			2506	1567	443	482	14			
1	E	318	Total	C	N	O	S	0	9	0
			2533	1587	447	485	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q91MA7
A	8	ASP	-	expression tag	UNP Q91MA7
A	9	PRO	-	expression tag	UNP Q91MA7
A	10	GLY	-	expression tag	UNP Q91MA7
C	7	ALA	-	expression tag	UNP Q91MA7
C	8	ASP	-	expression tag	UNP Q91MA7
C	9	PRO	-	expression tag	UNP Q91MA7
C	10	GLY	-	expression tag	UNP Q91MA7
E	7	ALA	-	expression tag	UNP Q91MA7
E	8	ASP	-	expression tag	UNP Q91MA7
E	9	PRO	-	expression tag	UNP Q91MA7
E	10	GLY	-	expression tag	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	5	0
			1429	889	248	285	7			
2	D	171	Total	C	N	O	S	0	5	0
			1419	883	246	283	7			
2	F	171	Total	C	N	O	S	0	7	0
			1435	893	248	287	7			

There are 3 discrepancies between the modelled and reference sequences:

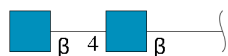
Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	conflict	UNP P03436
D	123	GLY	ARG	conflict	UNP P03436
F	123	GLY	ARG	conflict	UNP P03436

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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	G	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.



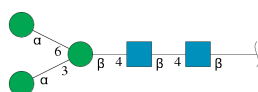
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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.



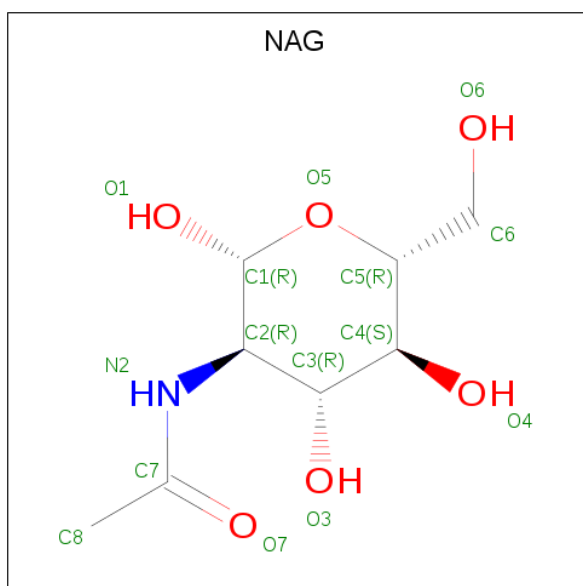
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	N	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



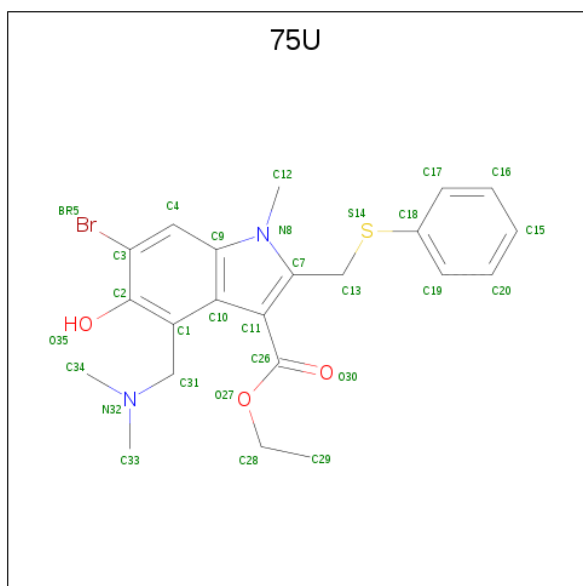
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 8 is ethyl 6-bromo-4-[(dimethylamino)methyl]-5-hydroxy-1-methyl-2-[(phenylsulfonyl)methyl]-1H-indole-3-carboxylate (three-letter code: 75U) (formula: C₂₂H₂₅BrN₂O₃S).



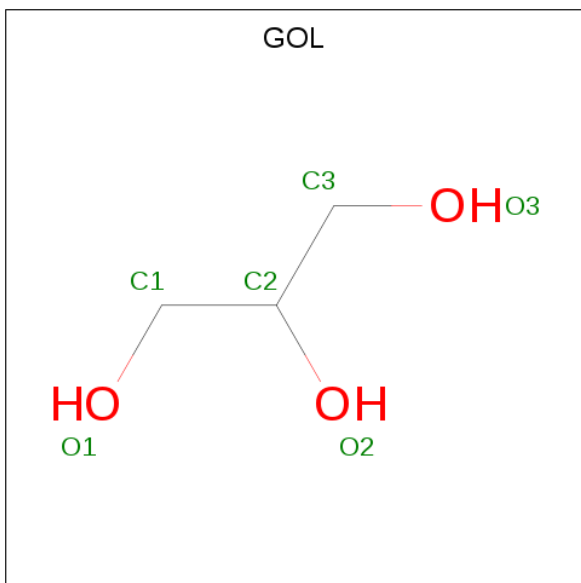
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	Br	C	N	O	S	0	0
			29	1	22	2	3	1		
8	D	1	Total	Br	C	N	O	S	0	0
			29	1	22	2	3	1		
8	D	1	Total	Br	C	N	O	S	0	0
			29	1	22	2	3	1		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			6	3	3		
10	E	1	Total	C	O	0	0
			6	3	3		

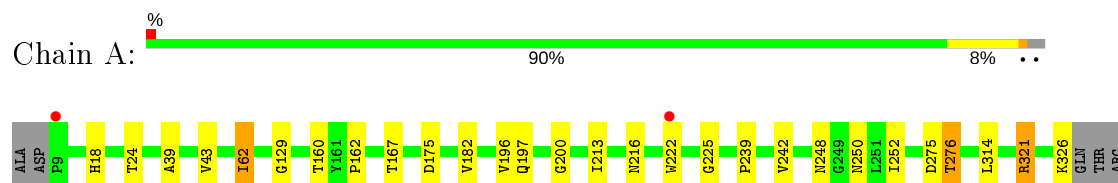
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	107	Total	O	0	0
			107	107		
11	B	99	Total	O	0	0
			99	99		
11	C	122	Total	O	0	0
			122	122		
11	D	103	Total	O	0	0
			103	103		
11	E	112	Total	O	0	0
			112	112		
11	F	74	Total	O	0	0
			74	74		

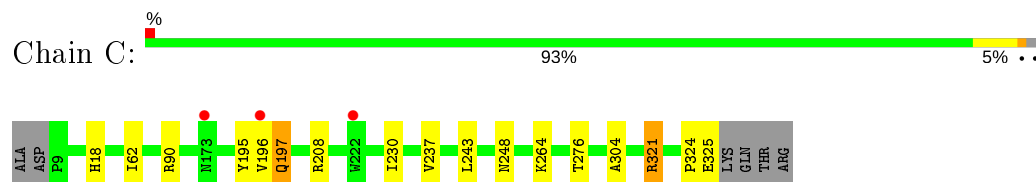
3 Residue-property plots

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.

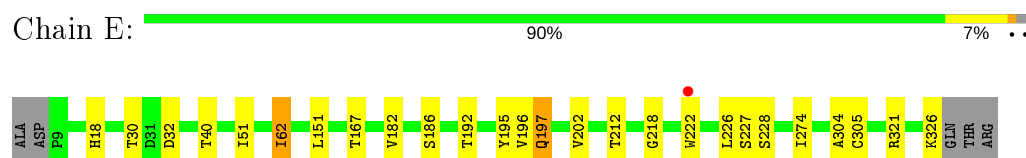
- Molecule 1: Hemagglutinin HA1



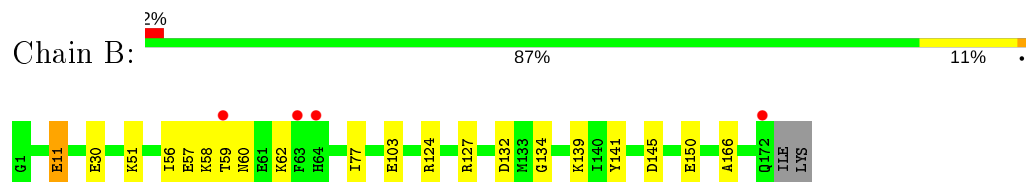
- Molecule 1: Hemagglutinin HA1



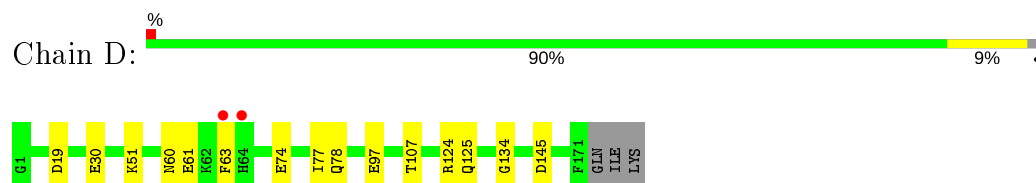
- Molecule 1: Hemagglutinin HA1




- Molecule 2: Hemagglutinin HA2



- Molecule 2: Hemagglutinin HA2




- Molecule 2: Hemagglutinin HA2

Chain F:  89% 7% ...



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

Chain G:  50% 50%



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

Chain H:  50% 50%



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

Chain I:  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 L:  100%



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

Chain M:  100%



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

Chain O:  100%




- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67% 33%



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

Chain N:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	105.94Å 151.81Å 349.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 2.54 48.22 – 2.54	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.22-2.54) 98.3 (48.22-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.180 , 0.220 0.180 , 0.220	Depositor DCC
R_{free} test set	4464 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12992	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: GOL, BMA, NAG, 75U, SO4, MAN

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	0.63	1/2578 (0.0%)	0.68	0/3512
1	C	0.62	0/2563	0.68	0/3491
1	E	0.63	0/2592	0.68	0/3530
2	B	0.65	0/1453	0.75	1/1953 (0.1%)
2	D	0.68	0/1443	0.72	0/1940
2	F	0.71	1/1459 (0.1%)	0.77	1/1962 (0.1%)
All	All	0.65	2/12088 (0.0%)	0.70	2/16388 (0.0%)

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
2	D	0	1
2	F	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	103	GLU	CG-CD	-5.16	1.44	1.51
1	A	252	ILE	C-N	-5.14	1.22	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	90	ASP	CB-CG-OD1	5.75	123.48	118.30
2	B	132	ASP	CB-CG-OD1	5.52	123.27	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	60	ASN	Peptide
2	F	60	ASN	Peptide
2	F	62	LYS	Peptide

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	2519	0	2457	18	0
1	C	2506	0	2451	10	0
1	E	2533	0	2475	18	0
2	B	1429	0	1348	13	0
2	D	1419	0	1338	14	0
2	F	1435	0	1351	13	0
3	G	50	0	43	4	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	O	28	0	25	0	0
5	K	39	0	34	0	0
6	N	60	0	49	6	0
7	A	42	0	39	0	0
7	B	14	0	13	0	0
7	E	28	0	26	0	0
7	F	14	0	13	0	0
8	B	29	0	0	0	0
8	D	58	0	0	1	0
9	B	10	0	0	2	0
9	C	5	0	0	0	0
9	D	5	0	0	0	0
10	C	6	0	8	1	0
10	E	6	0	8	0	0
11	A	107	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	99	0	0	0	0
11	C	122	0	0	1	0
11	D	103	0	0	1	0
11	E	112	0	0	1	0
11	F	74	0	0	2	0
All	All	12992	0	11803	74	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 3.

The worst 5 of 74 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:326:LYS:HD2	2:B:11:GLU:HG2	1.65	0.77
2:B:77:ILE:HD12	2:D:77[A]:ILE:HD11	1.69	0.74
2:D:51:LYS:HG3	1:E:30[A]:THR:HG22	1.73	0.69
6:N:3:BMA:H2	6:N:4:MAN:H5	1.77	0.66
1:E:196:VAL:HG22	1:E:197:GLN:OE1	1.99	0.63

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	324/323 (100%)	313 (97%)	10 (3%)	1 (0%)	41	51
1	C	323/323 (100%)	311 (96%)	10 (3%)	2 (1%)	25	34
1	E	325/323 (101%)	314 (97%)	10 (3%)	1 (0%)	41	51
2	B	175/174 (101%)	166 (95%)	9 (5%)	0	100	100
2	D	174/174 (100%)	164 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	176/174 (101%)	164 (93%)	10 (6%)	2 (1%)	14	19
All	All	1497/1491 (100%)	1432 (96%)	59 (4%)	6 (0%)	34	46

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	62	ILE
2	F	57	GLU
2	F	60	ASN
1	A	62	ILE
1	C	62	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/283 (101%)	281 (98%)	6 (2%)	53	68
1	C	286/283 (101%)	280 (98%)	6 (2%)	53	68
1	E	288/283 (102%)	281 (98%)	7 (2%)	49	64
2	B	151/148 (102%)	146 (97%)	5 (3%)	38	51
2	D	150/148 (101%)	149 (99%)	1 (1%)	84	90
2	F	152/148 (103%)	149 (98%)	3 (2%)	55	70
All	All	1314/1293 (102%)	1286 (98%)	28 (2%)	55	68

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	197	GLN
1	C	321[A]	ARG
2	F	51	LYS
1	C	208	ARG
1	C	276	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	G	1	1,3	14,14,15	0.51	0	17,19,21	0.62	0
3	NAG	G	2	3	14,14,15	1.17	1 (7%)	17,19,21	1.56	2 (11%)
3	BMA	G	3	3	11,11,12	0.43	0	15,15,17	2.30	6 (40%)
3	MAN	G	4	3	11,11,12	0.80	0	15,15,17	1.06	2 (13%)
4	NAG	H	1	1,4	14,14,15	0.38	0	17,19,21	0.49	0
4	NAG	H	2	4	14,14,15	0.18	0	17,19,21	0.62	1 (5%)
4	NAG	I	1	1,4	14,14,15	0.43	0	17,19,21	0.54	0
4	NAG	I	2	4	14,14,15	0.23	0	17,19,21	0.47	0
4	NAG	J	1	1,4	14,14,15	0.28	0	17,19,21	0.70	0
4	NAG	J	2	4	14,14,15	0.31	0	17,19,21	0.41	0
5	NAG	K	1	1,5	14,14,15	0.54	0	17,19,21	0.46	0
5	NAG	K	2	5	14,14,15	0.42	0	17,19,21	0.39	0
5	BMA	K	3	5	11,11,12	0.92	1 (9%)	15,15,17	1.31	3 (20%)
4	NAG	L	1	1,4	14,14,15	0.43	0	17,19,21	0.48	0
4	NAG	L	2	4	14,14,15	0.34	0	17,19,21	0.41	0
4	NAG	M	1	2,4	14,14,15	0.43	0	17,19,21	0.50	0
4	NAG	M	2	4	14,14,15	0.23	0	17,19,21	0.33	0
6	NAG	N	1	1,6	14,14,15	0.26	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	N	2	6	14,14,15	0.31	0	17,19,21	0.51	0
6	BMA	N	3	6	11,11,12	0.90	0	15,15,17	1.58	2 (13%)
6	MAN	N	4	6	10,10,12	0.66	0	14,14,17	1.11	2 (14%)
6	MAN	N	5	6	11,11,12	0.76	0	15,15,17	0.95	1 (6%)
4	NAG	O	1	1,4	14,14,15	0.56	0	17,19,21	0.46	0
4	NAG	O	2	4	14,14,15	0.27	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	NAG	M	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
6	NAG	N	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	-	0/1/1/1
6	MAN	N	5	6	-	2/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	NAG	O5-C1	4.17	1.50	1.43
5	K	3	BMA	C1-C2	2.64	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C1-O5-C5	5.37	119.47	112.19
3	G	3	BMA	C1-O5-C5	4.87	118.79	112.19
6	N	3	BMA	O3-C3-C2	4.27	118.16	109.99
3	G	3	BMA	C1-C2-C3	3.67	114.18	109.67
3	G	3	BMA	C3-C4-C5	-3.39	104.20	110.24

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

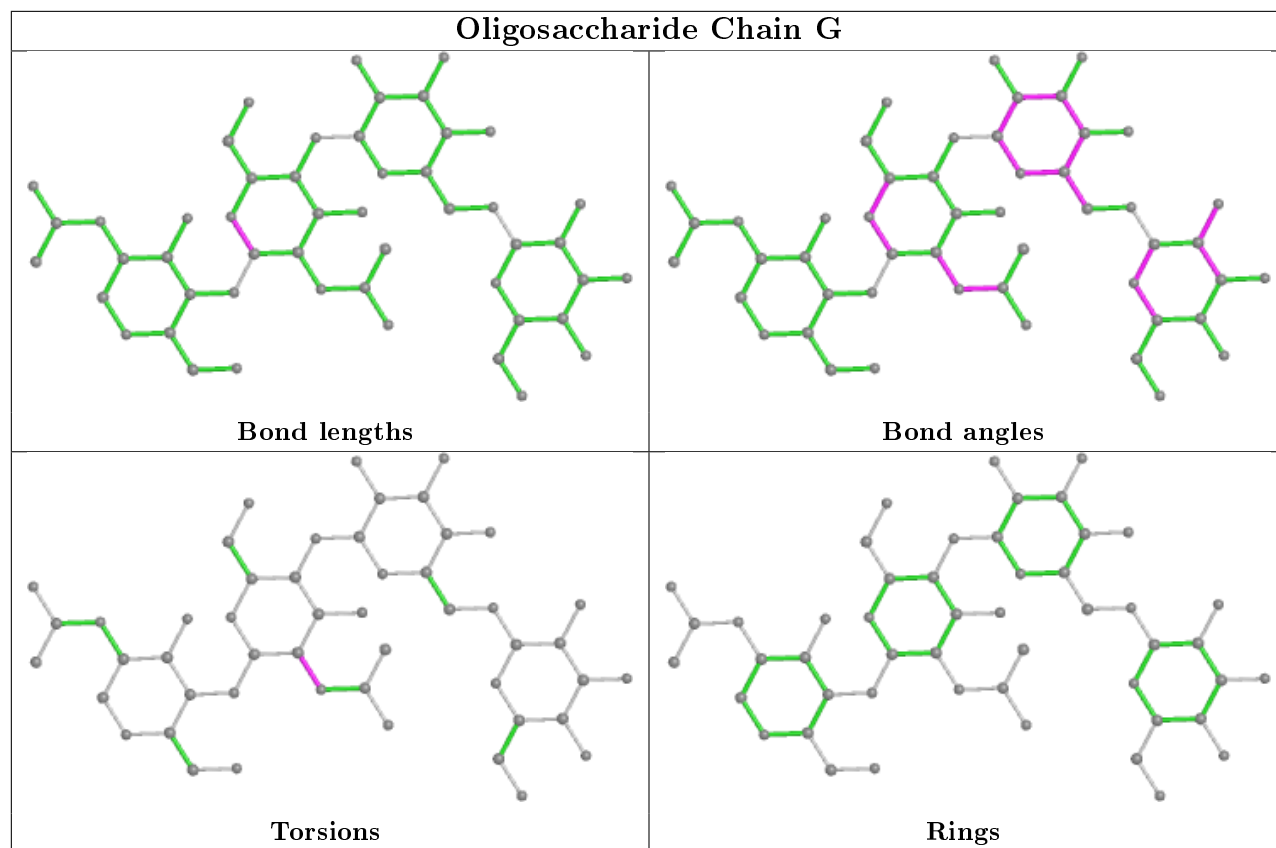
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C3-C2-N2-C7
4	I	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6

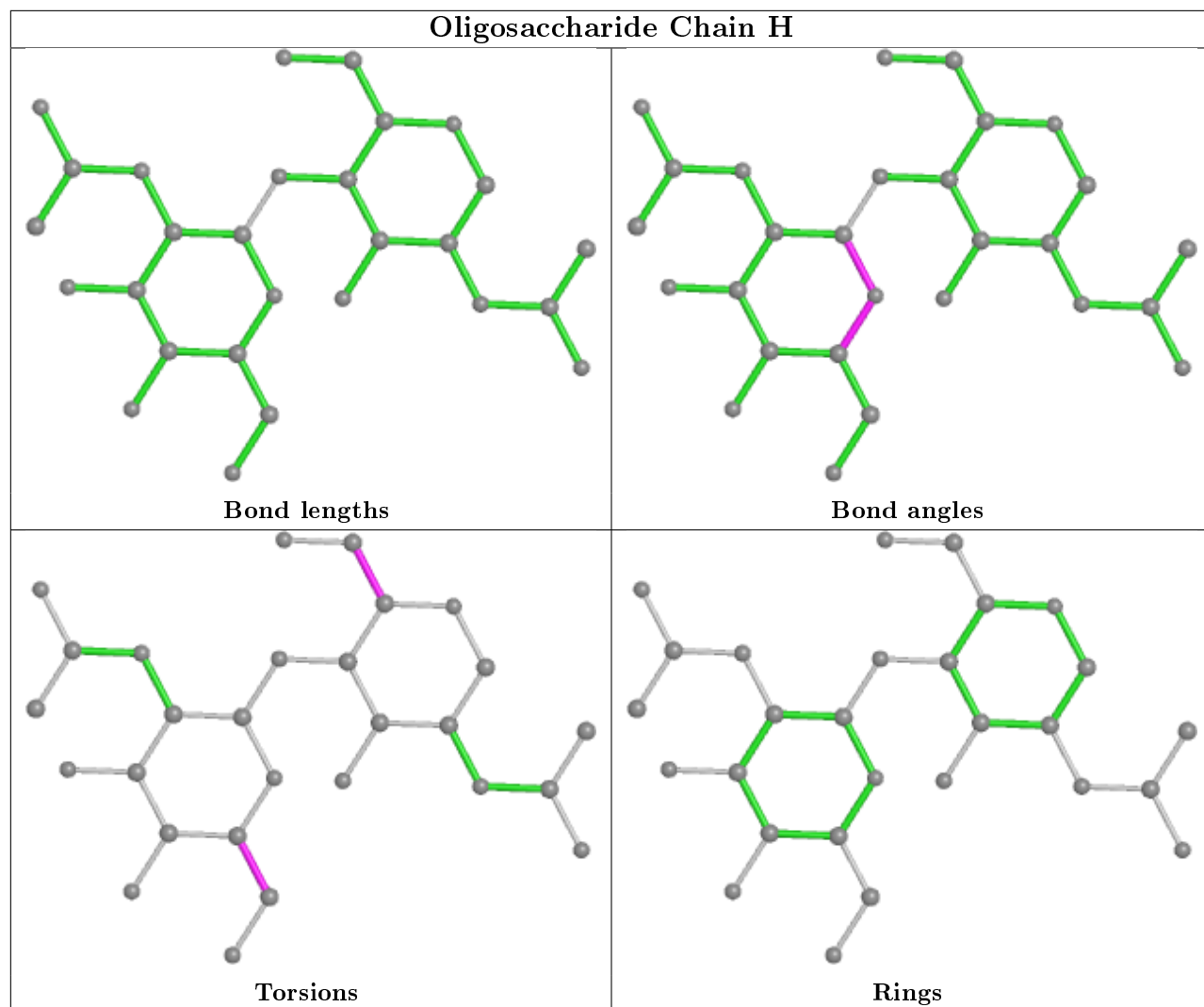
There are no ring outliers.

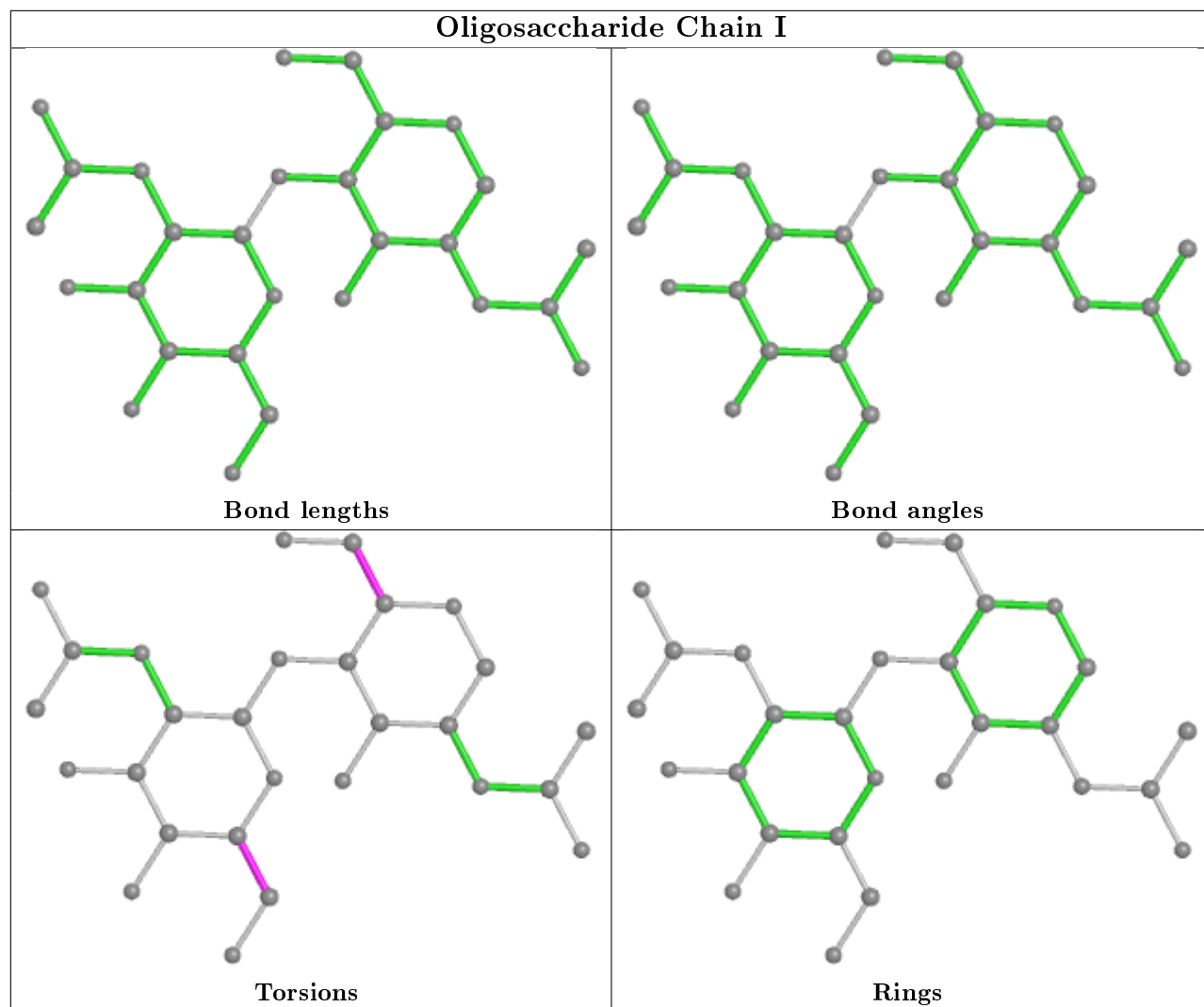
7 monomers are involved in 10 short contacts:

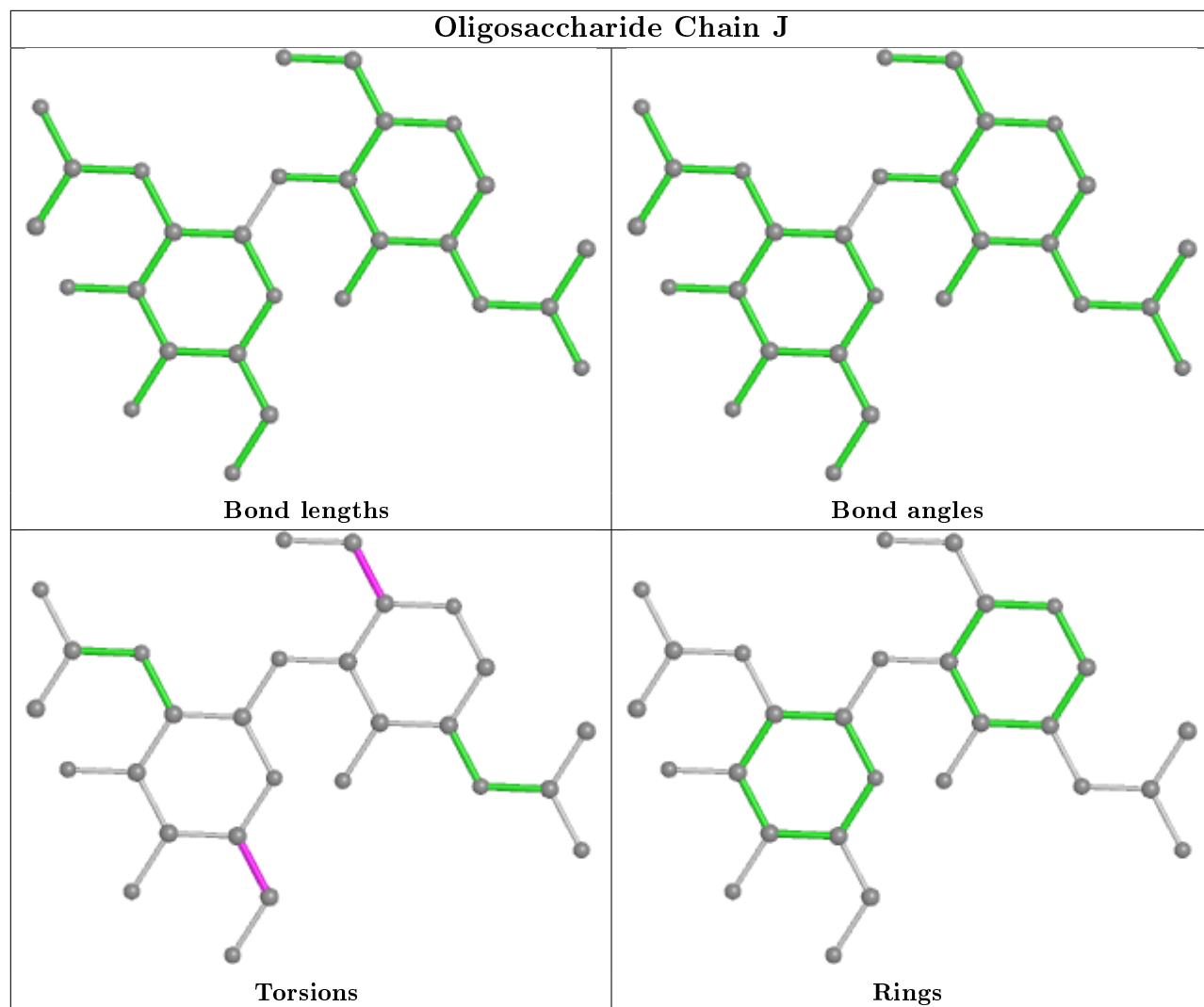
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	2	0
3	G	2	NAG	3	0
6	N	1	NAG	1	0
6	N	4	MAN	2	0
6	N	2	NAG	1	0
6	N	3	BMA	4	0
3	G	3	BMA	2	0

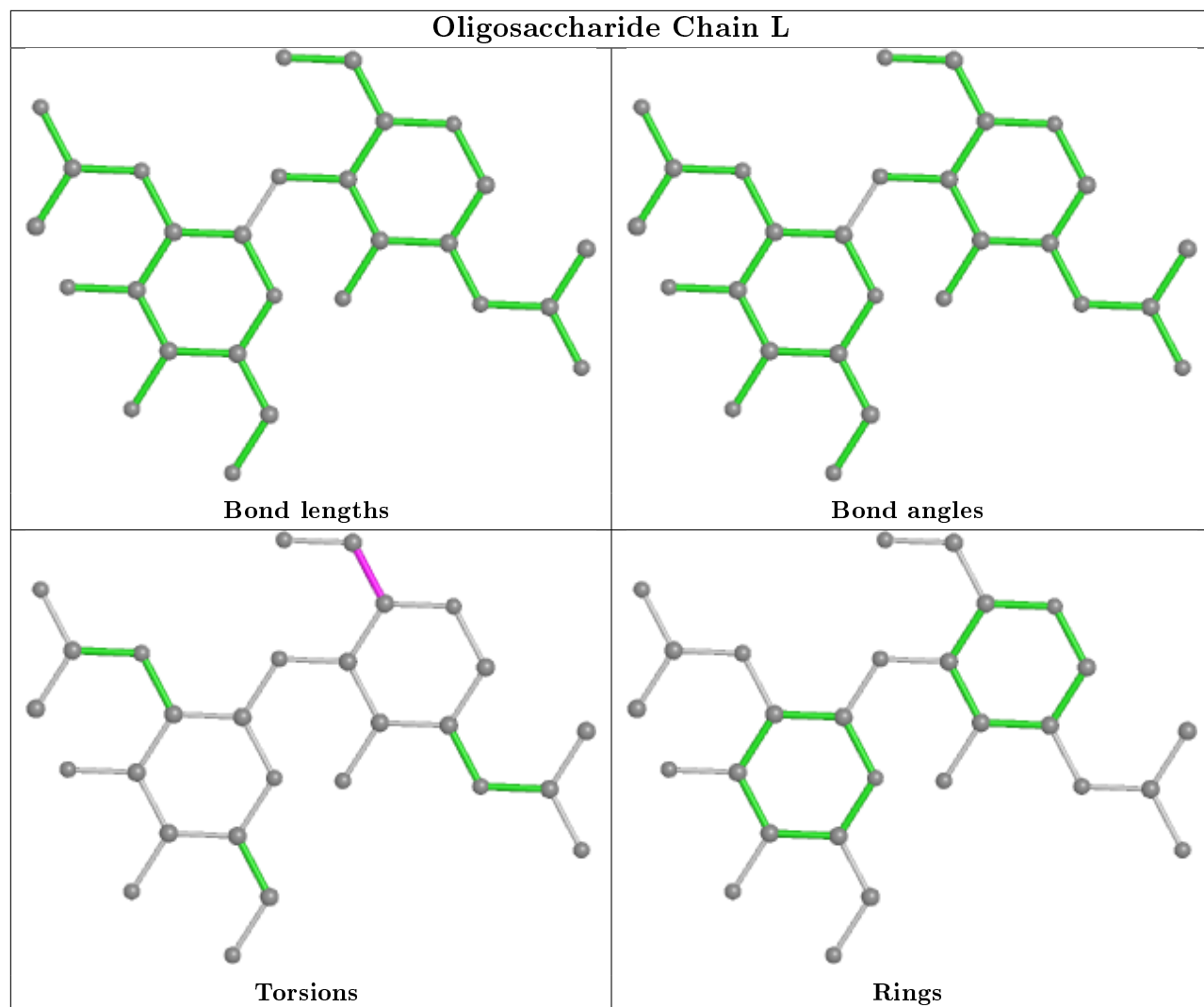
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

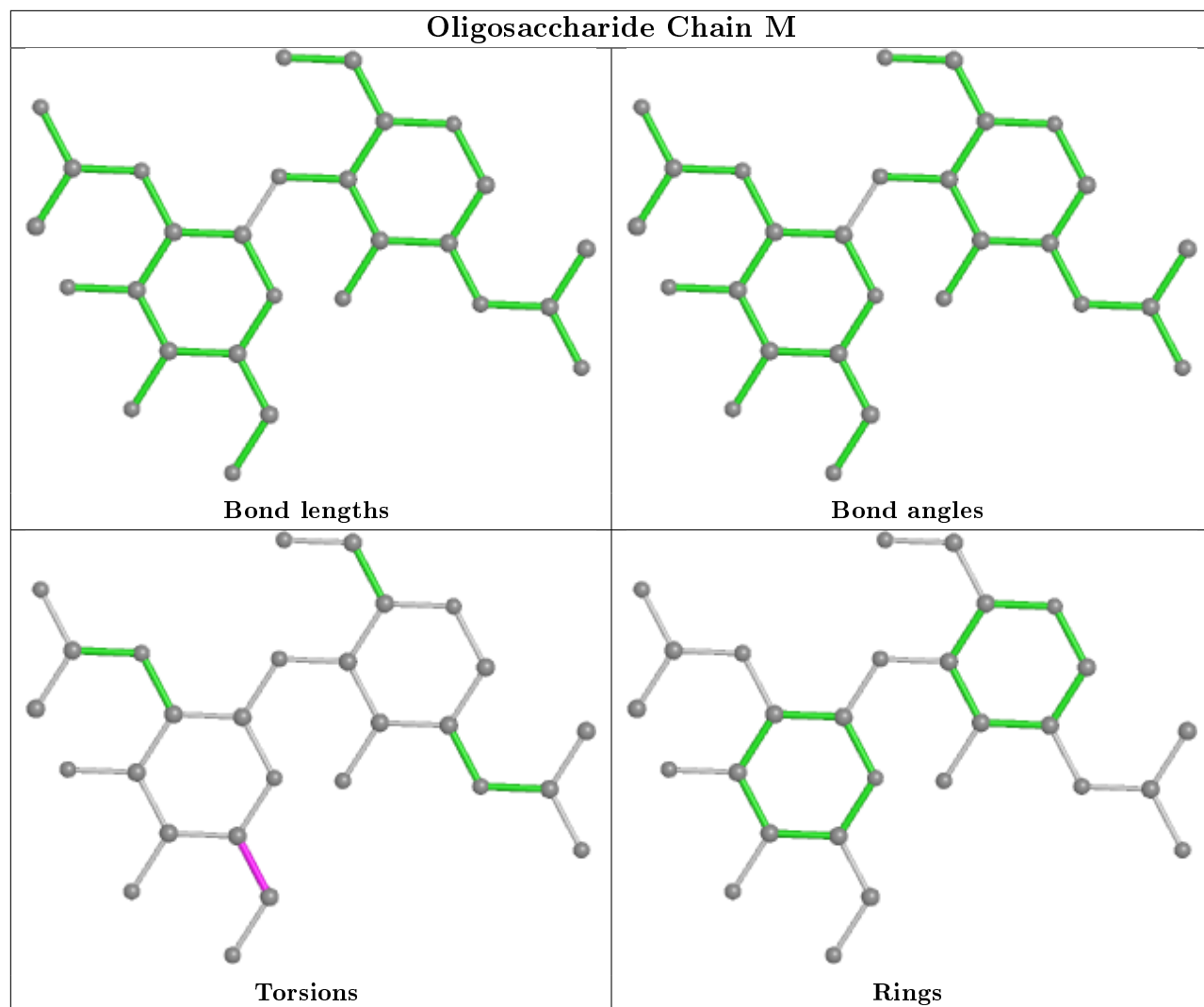


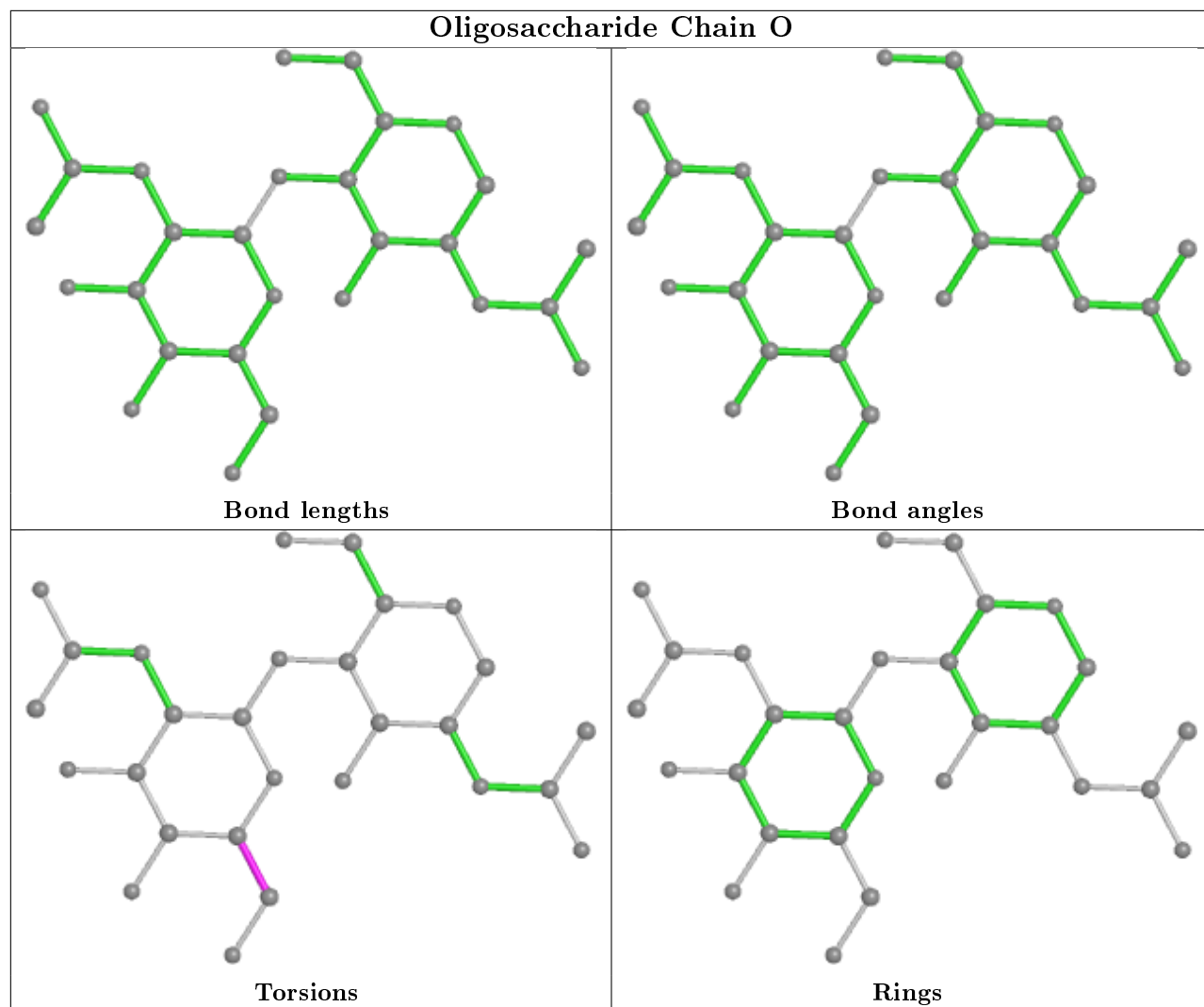


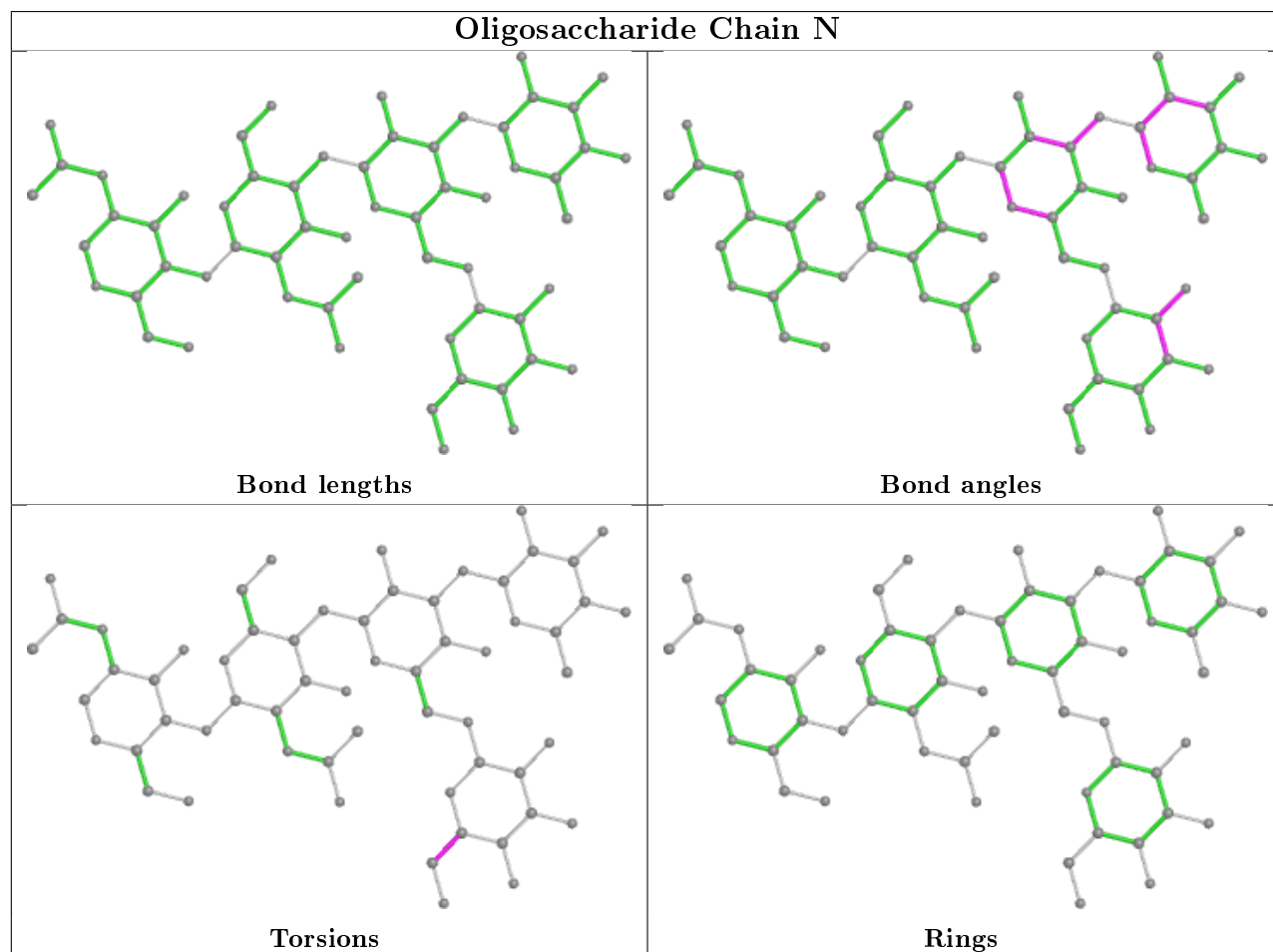
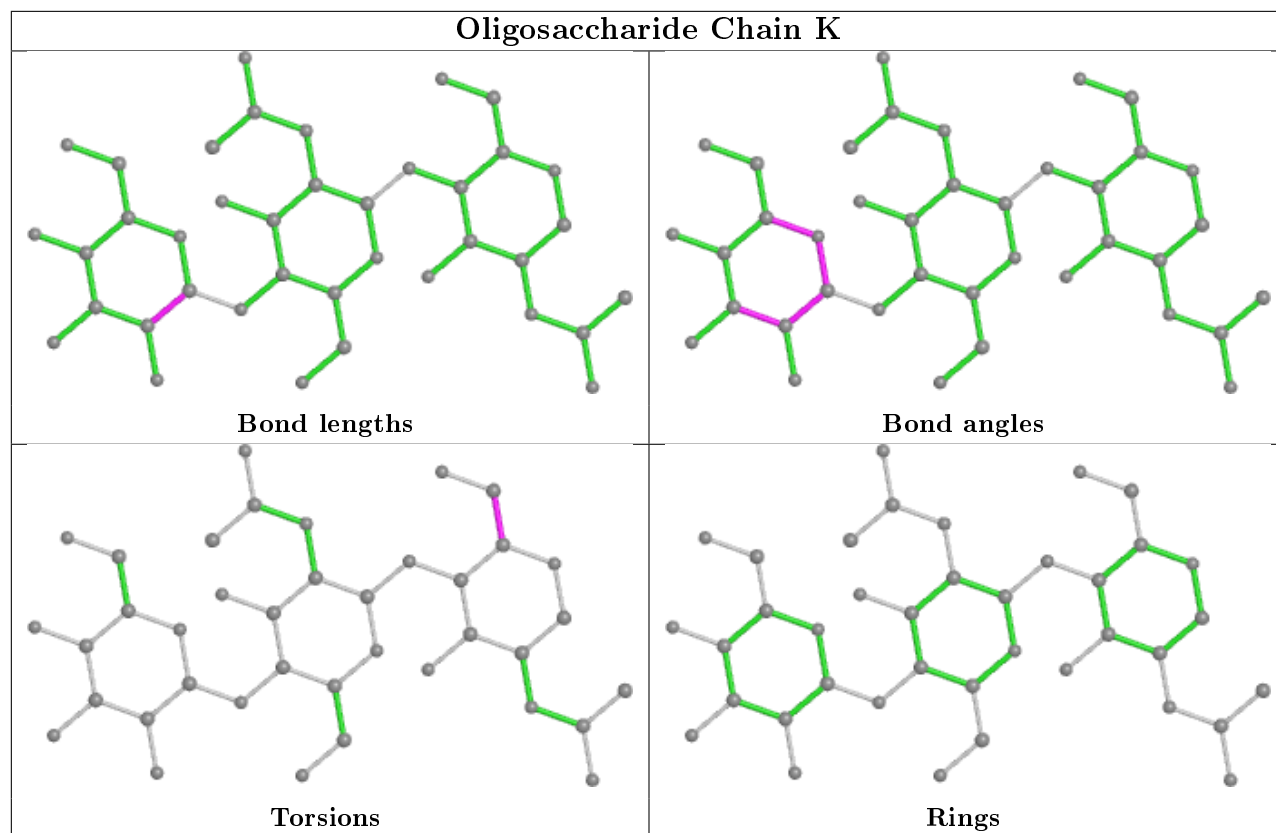












5.6 Ligand geometry

16 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
10	GOL	C	411	-	5,5,5	0.35	0	5,5,5	0.35	0
7	NAG	A	401	1	14,14,15	0.32	0	17,19,21	0.50	0
9	SO4	B	203	-	4,4,4	0.21	0	6,6,6	0.14	0
8	75U	D	202	-	28,31,31	3.54	7 (25%)	35,44,44	2.27	10 (28%)
7	NAG	E	401	1	14,14,15	0.30	0	17,19,21	0.76	1 (5%)
7	NAG	A	402	1	14,14,15	0.15	0	17,19,21	0.64	1 (5%)
9	SO4	C	410	-	4,4,4	0.10	0	6,6,6	0.27	0
9	SO4	B	204	-	4,4,4	0.18	0	6,6,6	0.21	0
9	SO4	D	205	-	4,4,4	0.20	0	6,6,6	0.07	0
8	75U	B	201	-	28,31,31	3.08	6 (21%)	35,44,44	2.48	12 (34%)
7	NAG	B	202	2	14,14,15	0.33	0	17,19,21	0.44	0
10	GOL	E	410	-	5,5,5	0.38	0	5,5,5	0.26	0
7	NAG	F	201	2	14,14,15	0.42	0	17,19,21	0.64	1 (5%)
7	NAG	A	403	1	14,14,15	0.46	0	17,19,21	0.79	1 (5%)
8	75U	D	201	-	28,31,31	3.54	7 (25%)	35,44,44	2.24	10 (28%)
7	NAG	E	402	1	14,14,15	0.62	1 (7%)	17,19,21	0.73	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
10	GOL	C	411	-	-	2/4/4/4	-
7	NAG	A	401	1	-	2/6/23/26	0/1/1/1
7	NAG	F	201	2	-	1/6/23/26	0/1/1/1
7	NAG	E	401	1	-	0/6/23/26	0/1/1/1
7	NAG	A	402	1	-	0/6/23/26	0/1/1/1
10	GOL	E	410	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	75U	B	201	-	-	5/16/16/16	0/3/3/3
7	NAG	B	202	2	-	0/6/23/26	0/1/1/1
8	75U	D	202	-	-	4/16/16/16	0/3/3/3
7	NAG	A	403	1	-	2/6/23/26	0/1/1/1
8	75U	D	201	-	-	4/16/16/16	0/3/3/3
7	NAG	E	402	1	-	2/6/23/26	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	202	75U	C31-C1	-15.57	1.41	1.51
8	D	201	75U	C31-C1	-15.49	1.41	1.51
8	B	201	75U	C31-C1	-13.00	1.42	1.51
8	D	201	75U	C11-C26	-5.55	1.35	1.50
8	D	202	75U	C10-C9	-5.33	1.36	1.42

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	202	75U	C4-C3-C2	-7.42	115.30	121.58
8	D	201	75U	C4-C3-C2	-6.71	115.90	121.58
8	B	201	75U	C4-C3-C2	-6.25	116.28	121.58
8	B	201	75U	C31-C1-C10	5.72	127.86	120.96
8	B	201	75U	BR5-C3-C2	5.39	124.84	118.80

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	411	GOL	O1-C1-C2-C3
10	E	410	GOL	O1-C1-C2-C3
8	D	201	75U	C11-C26-O27-C28
7	A	403	NAG	O5-C5-C6-O6
7	E	402	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

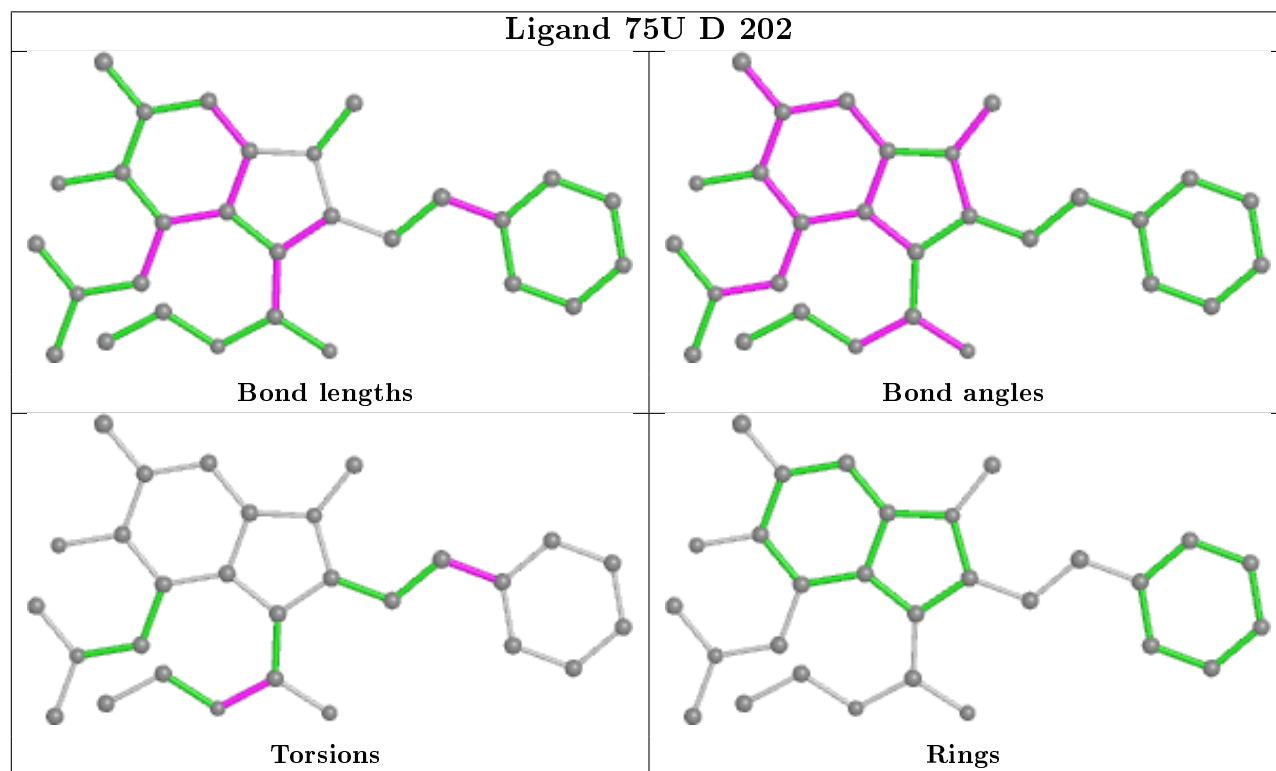
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	411	GOL	1	0

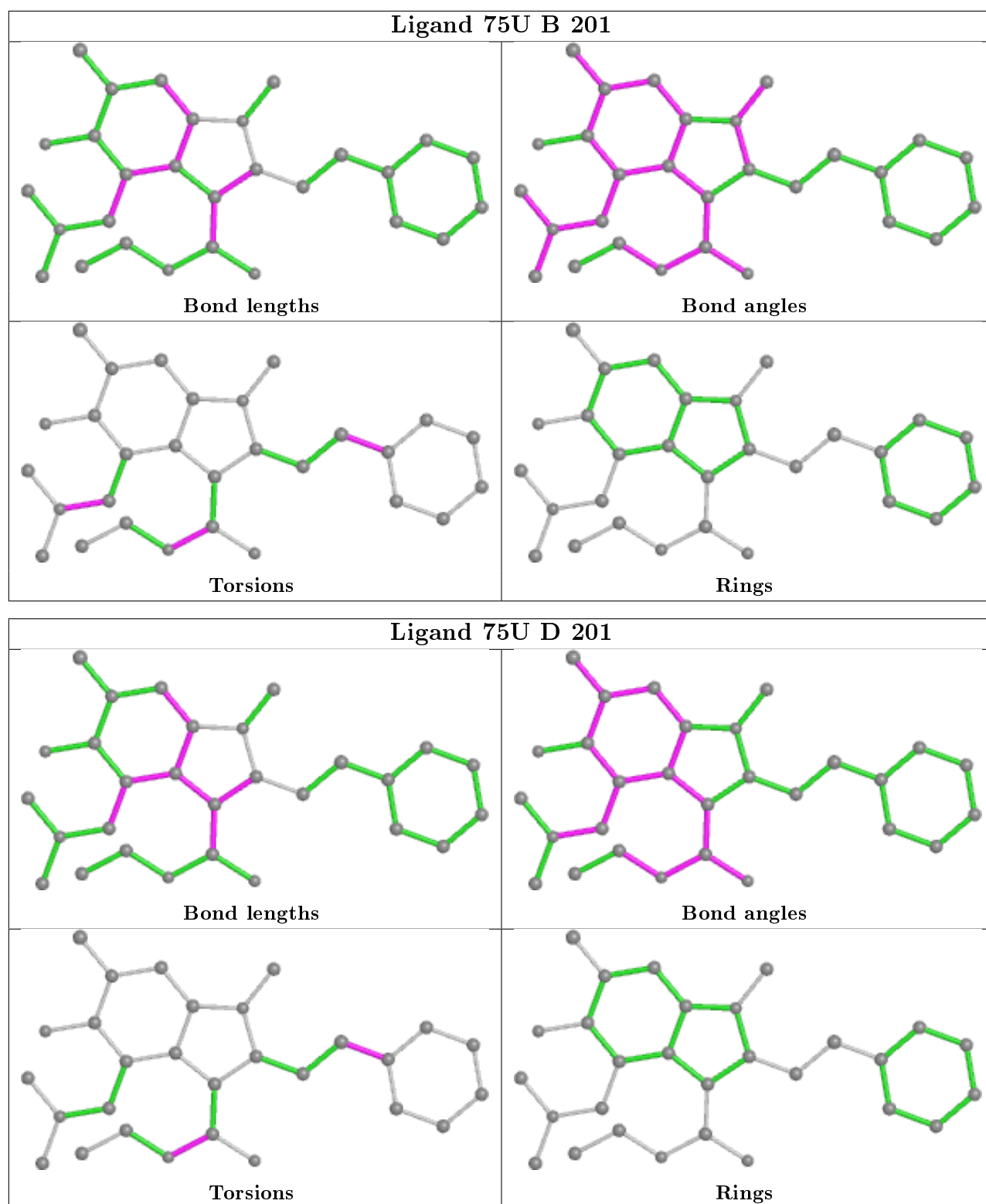
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	203	SO4	1	0
9	B	204	SO4	1	0
8	D	201	75U	1	0

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 ⓘ

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	318/323 (98%)	-0.42	2 (0%) 89 92	15, 31, 55, 82	0
1	C	317/323 (98%)	-0.41	3 (0%) 84 88	15, 32, 57, 81	0
1	E	318/323 (98%)	-0.50	1 (0%) 94 96	14, 30, 52, 79	0
2	B	172/174 (98%)	-0.31	4 (2%) 60 67	15, 27, 63, 99	0
2	D	171/174 (98%)	-0.38	2 (1%) 79 84	13, 27, 54, 81	0
2	F	171/174 (98%)	-0.33	0 100 100	12, 27, 55, 87	0
All	All	1467/1491 (98%)	-0.41	12 (0%) 86 89	12, 30, 55, 99	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	222	TRP	3.6
2	D	64	HIS	3.1
1	C	173	ASN	2.7
2	B	63	PHE	2.7
1	C	196	VAL	2.5

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](#)

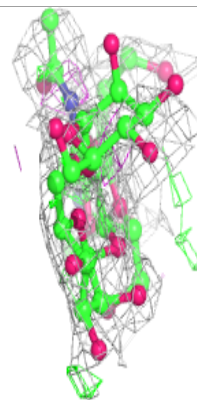
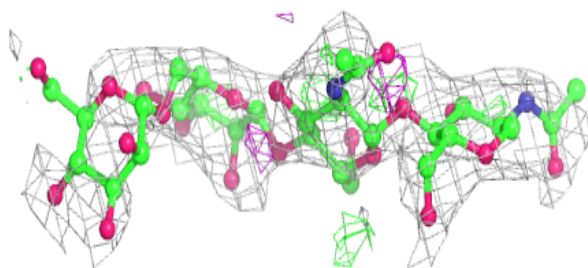
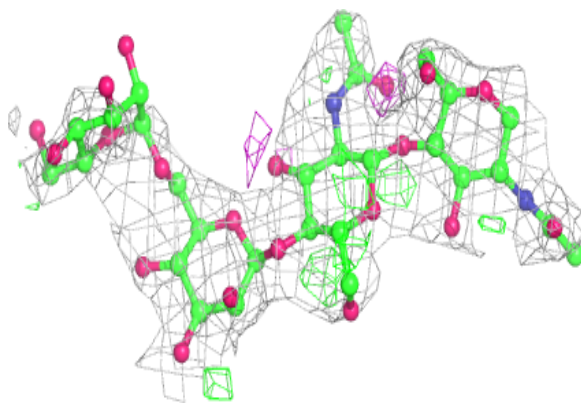
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	G	4	11/12	0.46	0.44	145,158,164,170	0
6	MAN	N	5	11/12	0.51	0.56	146,153,158,159	0
6	MAN	N	4	10/12	0.64	0.33	112,130,139,143	0
3	NAG	G	2	14/15	0.74	0.32	58,97,112,115	0
4	NAG	I	2	14/15	0.74	0.31	52,103,126,132	0
4	NAG	J	2	14/15	0.76	0.35	74,99,116,116	0
5	BMA	K	3	11/12	0.79	0.21	70,83,86,86	0
4	NAG	O	2	14/15	0.81	0.25	60,80,90,92	0
3	BMA	G	3	11/12	0.82	0.32	110,119,128,141	0
4	NAG	H	2	14/15	0.83	0.29	66,87,103,105	0
4	NAG	I	1	14/15	0.84	0.19	61,71,98,102	0
4	NAG	J	1	14/15	0.88	0.21	33,64,76,93	0
6	BMA	N	3	11/12	0.88	0.34	96,109,125,139	0
4	NAG	M	2	14/15	0.88	0.44	99,118,136,147	0
4	NAG	M	1	14/15	0.88	0.32	50,66,91,108	0
4	NAG	L	2	14/15	0.89	0.29	62,80,89,95	0
3	NAG	G	1	14/15	0.90	0.24	61,72,76,80	0
4	NAG	L	1	14/15	0.93	0.19	36,47,59,61	0
4	NAG	H	1	14/15	0.94	0.14	36,47,56,71	0
6	NAG	N	2	14/15	0.94	0.22	41,68,79,88	0
5	NAG	K	2	14/15	0.94	0.17	37,59,80,80	0
4	NAG	O	1	14/15	0.95	0.15	36,48,61,68	0
5	NAG	K	1	14/15	0.95	0.14	45,54,64,64	0
6	NAG	N	1	14/15	0.95	0.19	43,56,67,69	0

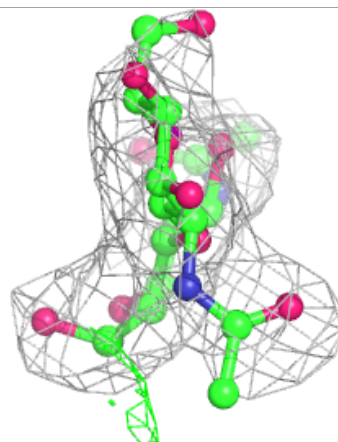
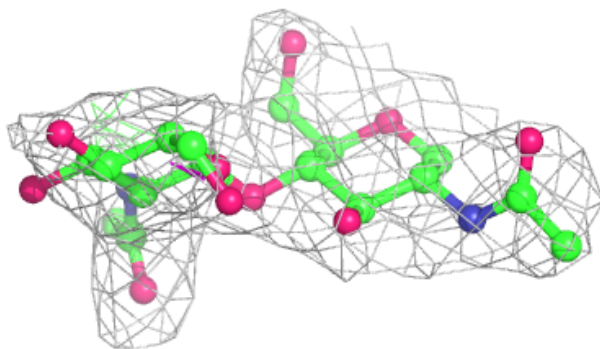
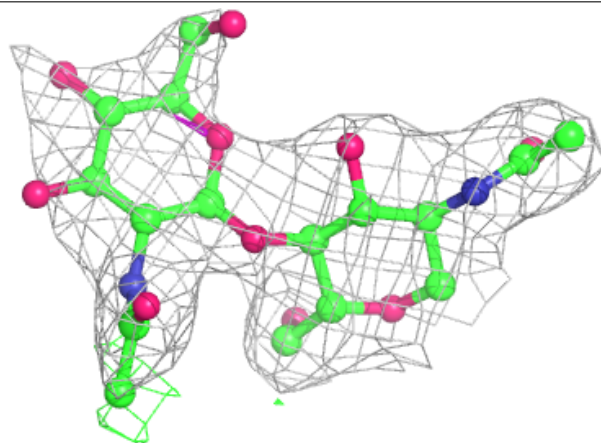
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

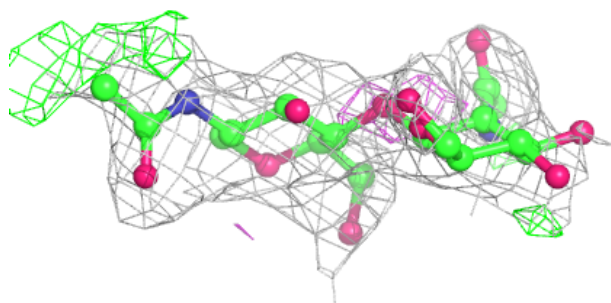
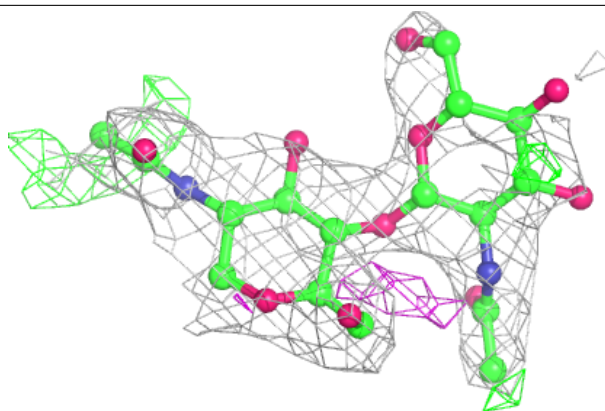
**Electron density around Chain H:**

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

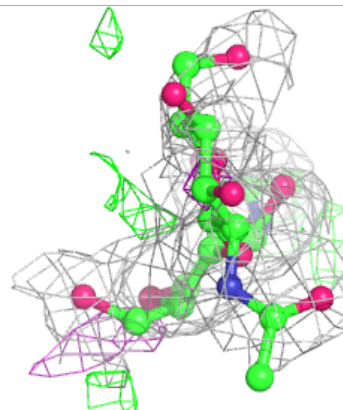
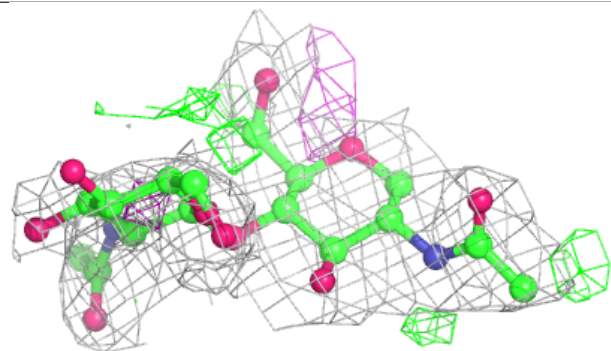
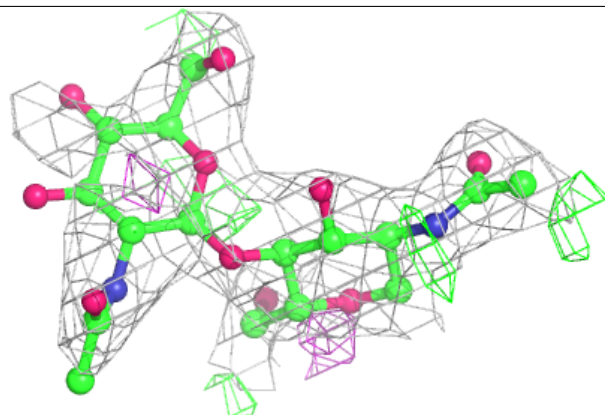


Electron density around Chain I:

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

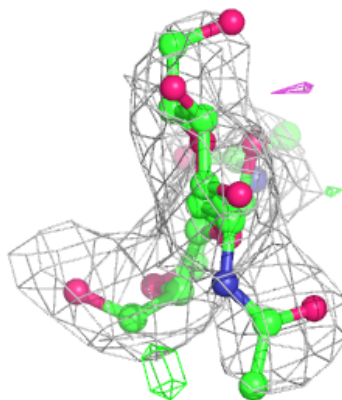
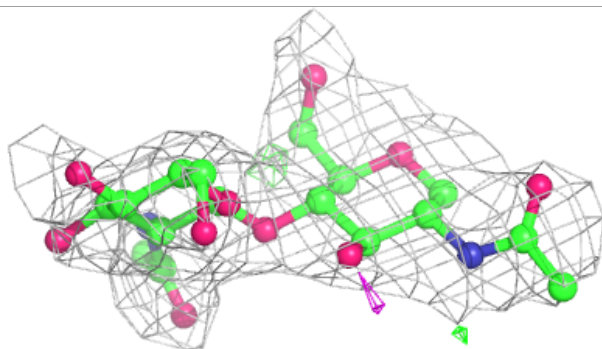
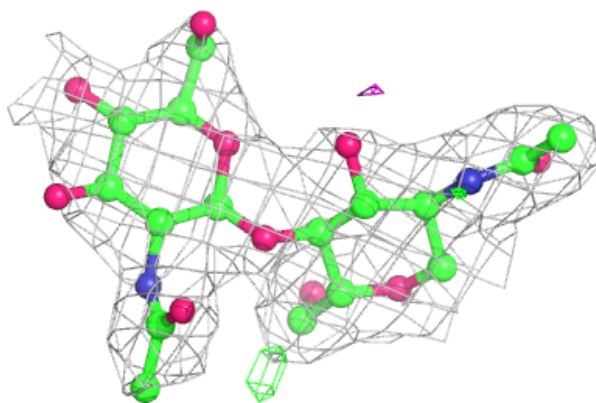
**Electron density around Chain J:**

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



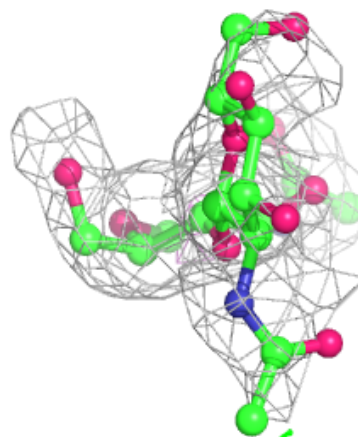
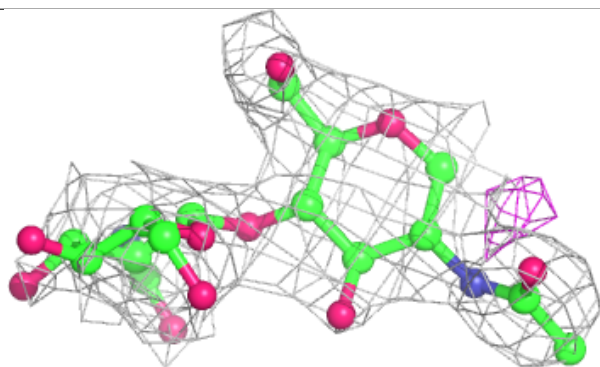
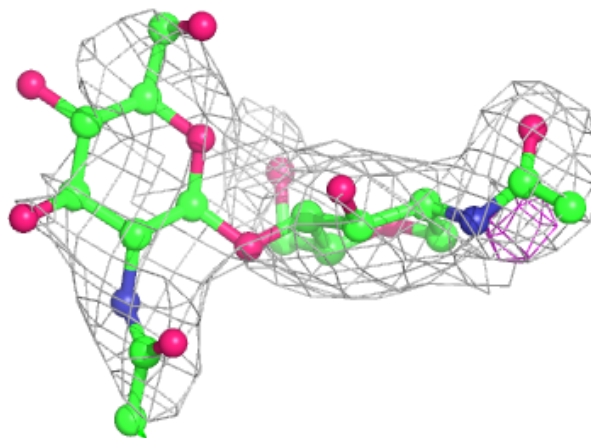
Electron density around Chain L:

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



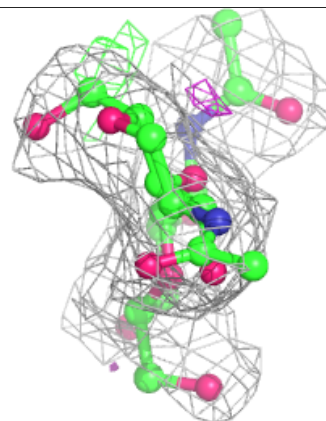
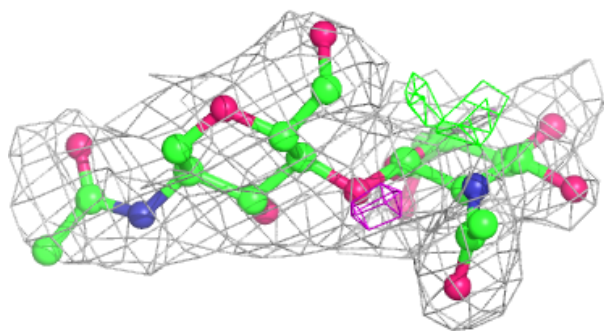
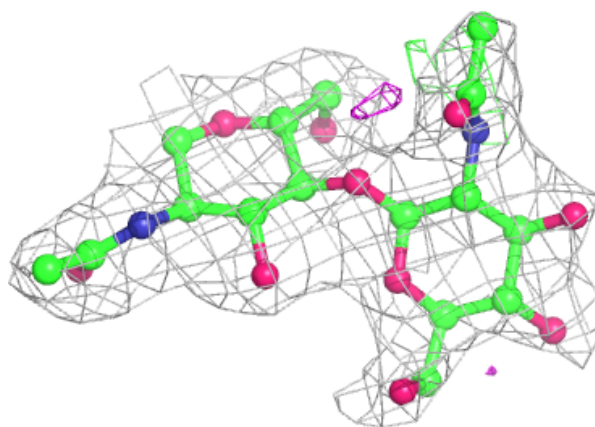
Electron density around Chain M:

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

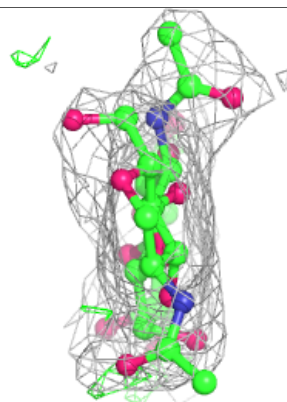
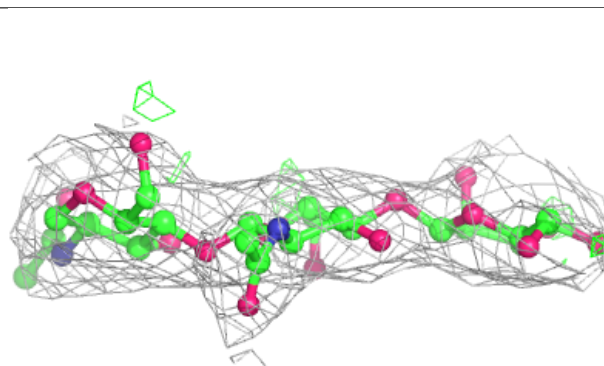
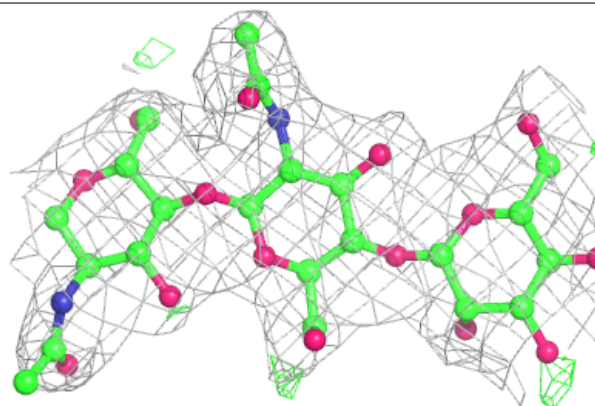


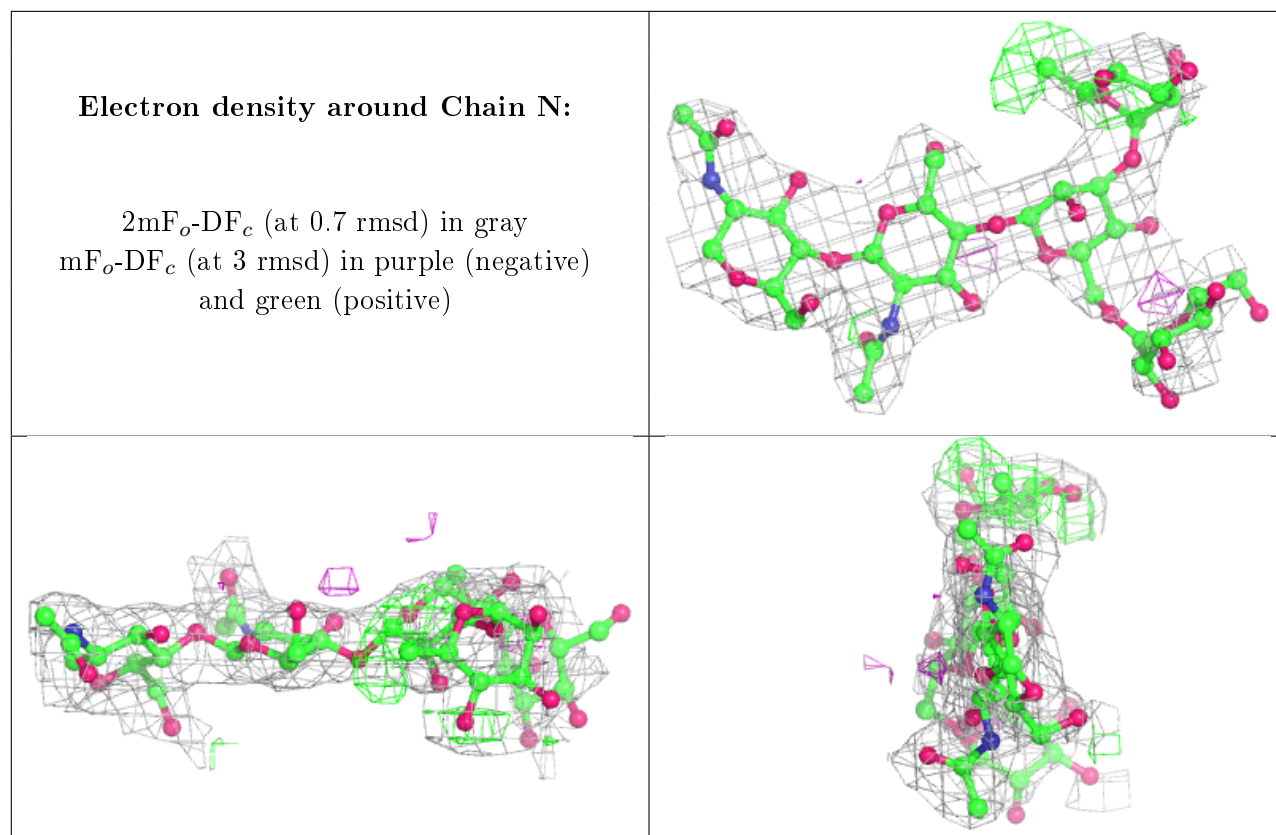
Electron density around Chain O:

$2mF_o-DF_c$ (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)





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
7	NAG	A	401	14/15	0.73	0.28	59,82,87,88	0
7	NAG	A	402	14/15	0.86	0.17	42,59,70,70	0
10	GOL	E	410	6/6	0.87	0.56	52,54,59,69	0
7	NAG	F	201	14/15	0.88	0.31	47,62,71,72	0
8	75U	B	201	29/29	0.89	0.20	30,53,70,152	0
9	SO4	C	410	5/5	0.89	0.29	72,79,100,117	0
7	NAG	E	401	14/15	0.90	0.16	43,52,63,64	0
7	NAG	B	202	14/15	0.91	0.25	48,56,61,70	0
7	NAG	A	403	14/15	0.91	0.16	41,56,63,65	0
8	75U	D	202	29/29	0.92	0.19	27,47,65,157	0
10	GOL	C	411	6/6	0.92	0.44	44,50,67,84	0
8	75U	D	201	29/29	0.92	0.20	31,41,59,166	0
7	NAG	E	402	14/15	0.93	0.19	43,54,60,61	0
9	SO4	D	205	5/5	0.97	0.12	56,56,61,62	0

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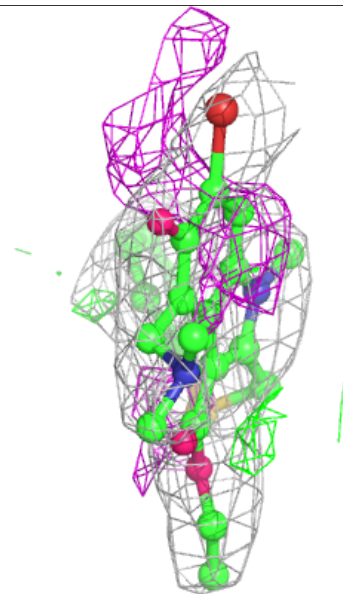
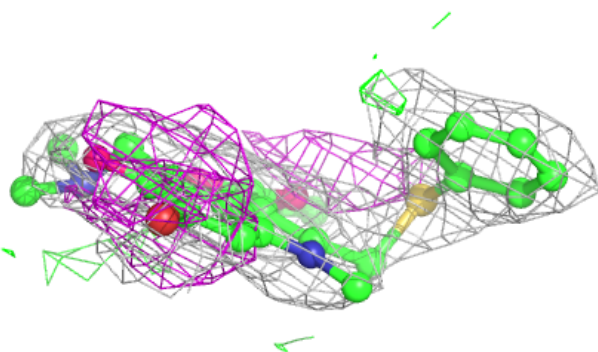
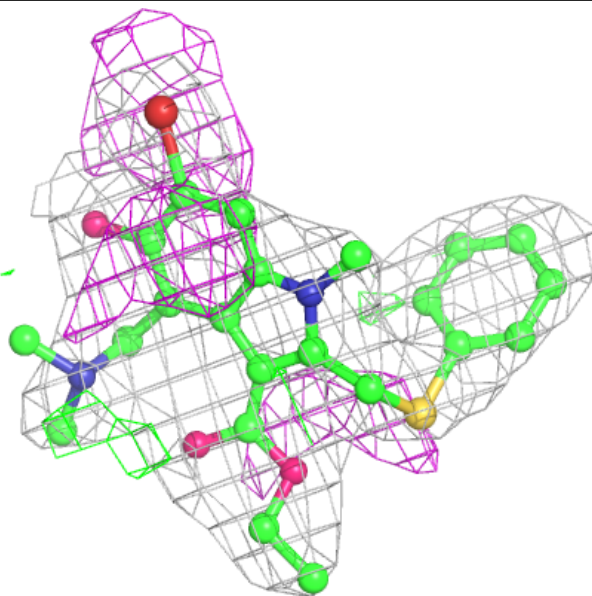
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	SO4	B	203	5/5	0.97	0.10	51,56,68,86	0
9	SO4	B	204	5/5	0.99	0.10	47,53,62,62	0

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.

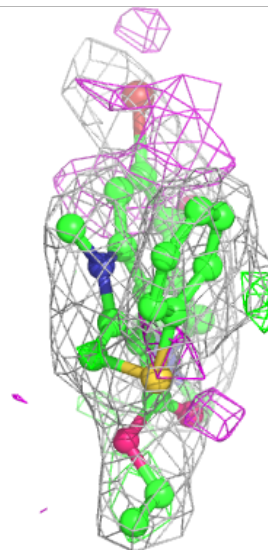
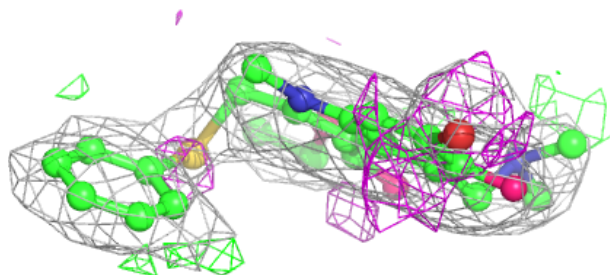
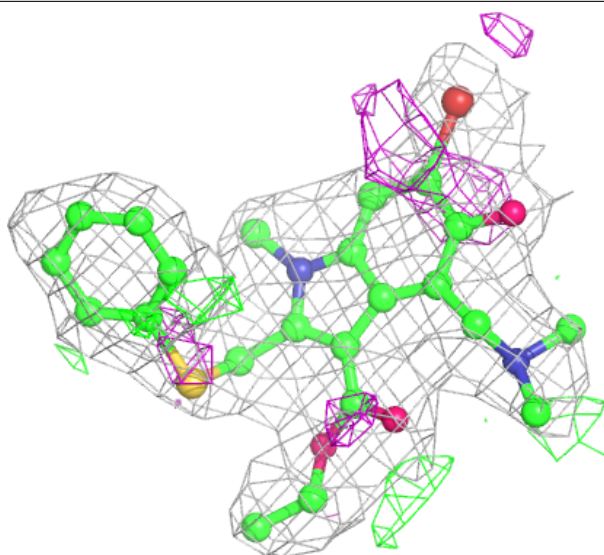
Electron density around 75U B 201:

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



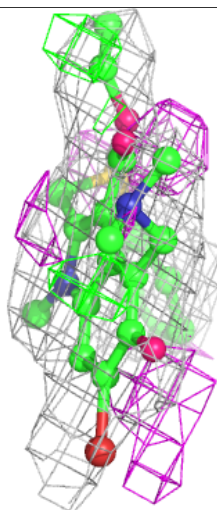
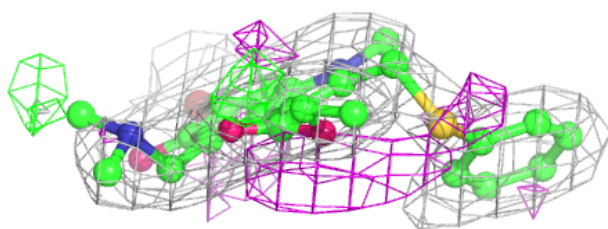
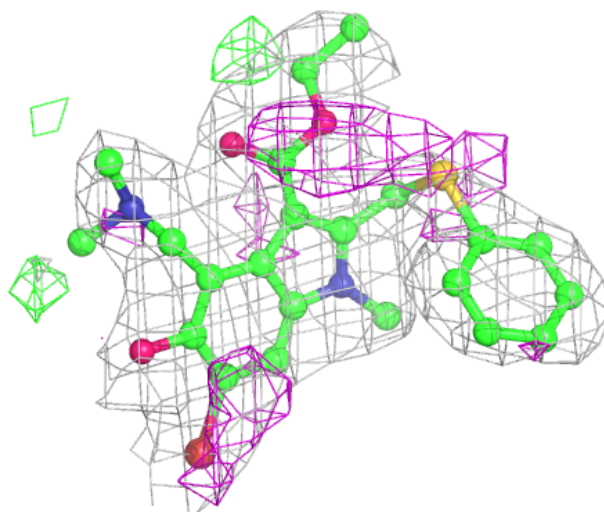
Electron density around 75U D 202:

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



Electron density around 75U D 201:

$2mF_o-DF_c$ (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.