



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 07:04 PM BST

PDB ID : 1XMN
Title : Crystal structure of thrombin bound to heparin
Authors : Carter, W.J.; Cama, E.; Huntington, J.A.
Deposited on : 2004-10-04
Resolution : 1.85 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

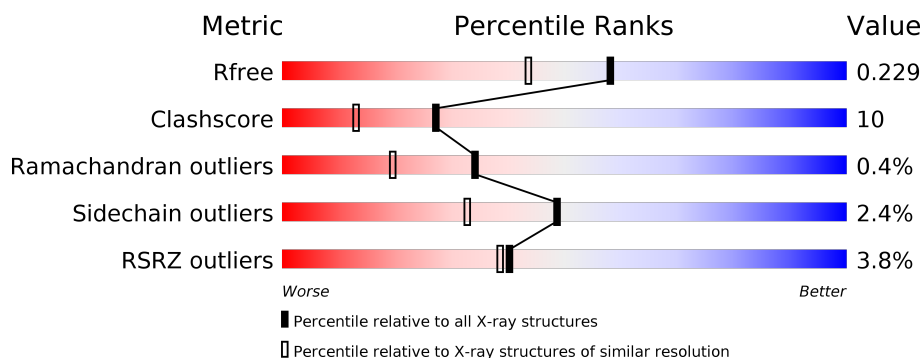
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	36	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>14%</div> </div> </div>
1	C	36	<div> <div>17%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>11%</div> </div> </div>
1	E	36	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>6%</div> <div>19%</div> </div> </div>
1	G	36	<div> <div>11%</div> <div> <div></div> <div>83%</div> <div>•</div> <div>14%</div> </div> </div>
2	B	259	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>••</div> </div> </div>
2	D	259	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	259	
2	H	259	
3	I	6	
4	J	2	
5	K	5	
6	L	2	
6	M	2	
7	N	5	

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
4	NAG	J	1	X	-	-	-
4	NAG	J	2	-	-	-	X
6	NAG	L	1	X	-	-	-
6	NDG	L	2	-	-	-	X
6	NAG	M	1	X	-	-	-
6	NDG	M	2	-	-	-	X
7	NAG	N	1	X	-	-	-
7	NAG	N	2	-	-	-	X
7	BMA	N	3	-	-	-	X
7	MAN	N	4	-	-	-	X
7	MAN	N	5	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 10416 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.

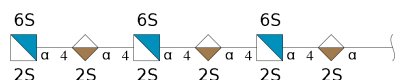
- Molecule 1 is a protein called Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	31	Total	C	N	O	S	0	0	0
			249	154	40	54	1			
1	C	32	Total	C	N	O	S	0	0	0
			248	154	41	52	1			
1	E	29	Total	C	N	O	S	0	0	0
			236	148	38	49	1			
1	G	31	Total	C	N	O	S	0	0	0
			247	153	40	53	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			2053	1310	360	369	14			
2	D	254	Total	C	N	O	S	0	0	0
			2048	1307	360	367	14			
2	F	254	Total	C	N	O	S	0	0	0
			2039	1302	354	369	14			
2	H	253	Total	C	N	O	S	0	0	0
			2035	1300	356	365	14			

- Molecule 3 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid.



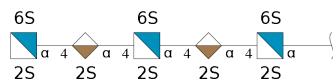
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	6	Total	C	N	O	S	0	0	0
			105	36	3	57	9			

- 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	J	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 5 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	5	Total	C	N	O	S	0	0	0
			89	30	3	48	8			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	2	Total	C	N	O		0	0	0
			28	16	2	10				
6	M	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 7 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-a

- Molecule 8 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (three-letter code: 0G6) (formula: $\text{C}_{21}\text{H}_{34}\text{ClN}_6\text{O}_3$).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Na	0	0
			1	1		
9	D	1	Total	Na	0	0
			1	1		
9	F	1	Total	Na	0	0
			1	1		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	F	1	Total	C	O	0	0
			6	3	3		
10	F	1	Total	C	O	0	0
			6	3	3		
10	F	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	18	Total 18	O 18	0	0
11	B	188	Total 188	O 188	0	0
11	C	20	Total 20	O 20	0	0
11	D	199	Total 199	O 199	0	0
11	E	20	Total 20	O 20	0	0
11	F	133	Total 133	O 133	0	0
11	G	18	Total 18	O 18	0	0
11	H	154	Total 154	O 154	0	0

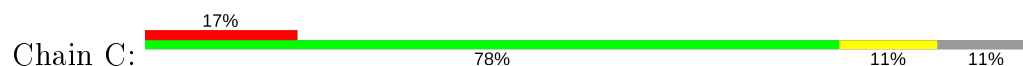
3 Residue-property plots [i](#)

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

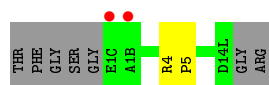
- Molecule 1: Thrombin light chain



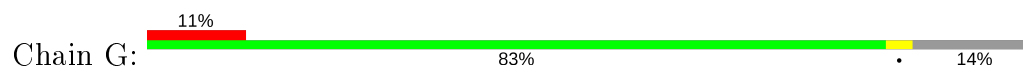
- Molecule 1: Thrombin light chain



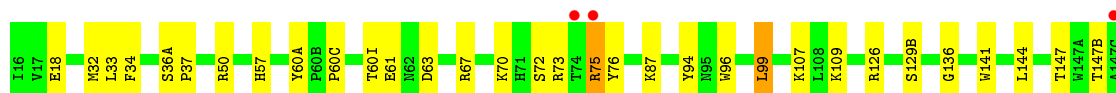
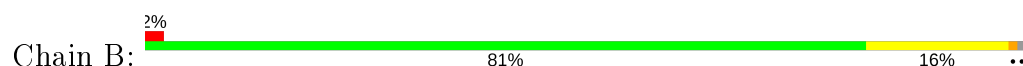
- Molecule 1: Thrombin light chain



- Molecule 1: Thrombin light chain

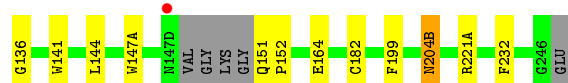
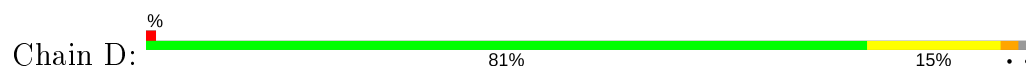


- Molecule 2: Thrombin heavy chain

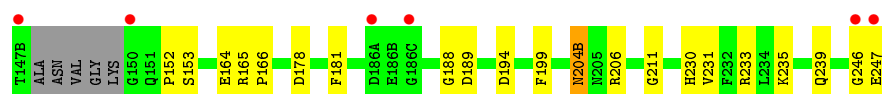
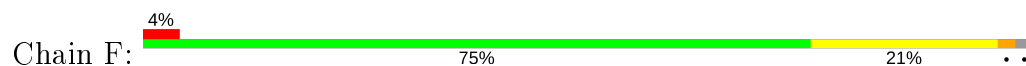




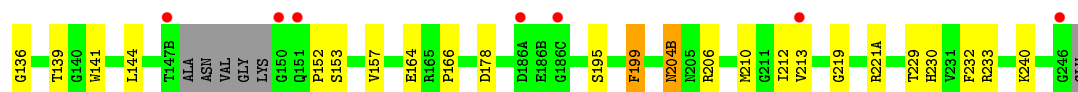
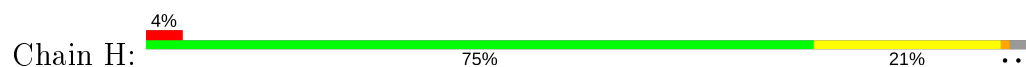
- Molecule 2: Thrombin heavy chain



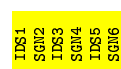
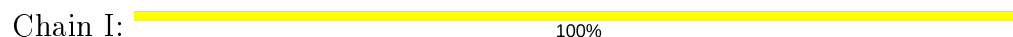
- Molecule 2: Thrombin heavy chain



- Molecule 2: Thrombin heavy chain



- Molecule 3: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid



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

Chain J:  100%

MAG1
MAG2

- Molecule 5: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain K:  100%

SGN1
IDS2
SGN3
IDS4
SGN5

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

Chain L:  50% 50%


MAG1
MAG2

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

Chain M:  100%

MAG1
MAG2

- Molecule 7: 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:  20% 40% 40%

MAG1
MAG2
BMA3
MAIM4
MAIM5

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.91Å 80.84Å 114.14Å 90.00° 101.05° 90.00°	Depositor
Resolution (Å)	36.60 – 1.85 36.60 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.1 (36.60-1.85) 96.1 (36.60-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.85Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.234 0.203 , 0.229	Depositor DCC
R_{free} test set	2411 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.2	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	0.95	EDS
Total number of atoms	10416	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, NA, IDS, NDG, 0G6, SGN, 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	0.32	0/251	0.60	0/334
1	C	0.34	0/250	0.61	0/333
1	E	0.32	0/238	0.62	0/317
1	G	0.35	0/249	0.60	0/331
2	B	0.35	0/2107	0.66	2/2853 (0.1%)
2	D	0.36	0/2102	0.65	0/2846
2	F	0.33	0/2093	0.63	0/2833
2	H	0.35	0/2089	0.67	2/2828 (0.1%)
All	All	0.35	0/9379	0.65	4/12675 (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	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	195	SER	O-C-N	5.48	132.51	123.20
2	B	195	SER	CA-C-N	-5.22	105.76	116.20
2	H	199	PHE	N-CA-C	-5.22	96.90	111.00
2	H	73	ARG	NE-CZ-NH1	-5.05	117.77	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	57	HIS	Mainchain
2	D	57	HIS	Mainchain
2	F	57	HIS	Mainchain
2	H	57	HIS	Mainchain

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	249	0	243	3	0
1	C	248	0	239	2	0
1	E	236	0	233	1	0
1	G	247	0	241	1	0
2	B	2053	0	1994	40	0
2	D	2048	0	1993	37	0
2	F	2039	0	1975	52	0
2	H	2035	0	1981	56	0
3	I	105	0	33	0	0
4	J	28	0	25	0	0
5	K	89	0	29	0	0
6	L	28	0	24	0	0
6	M	28	0	24	0	0
7	N	61	0	52	5	0
8	B	30	0	31	1	0
8	D	30	0	31	1	0
8	F	30	0	31	2	0
8	H	30	0	31	1	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
9	F	1	0	0	0	0
9	H	1	0	0	0	0
10	B	12	0	16	1	0
10	D	12	0	16	1	0
10	F	18	0	24	1	0
10	H	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	18	0	0	0	0
11	B	188	0	0	1	0
11	C	20	0	0	0	0
11	D	199	0	0	3	0
11	E	20	0	0	0	0
11	F	133	0	0	3	0
11	G	18	0	0	0	0
11	H	154	0	0	6	0
All	All	10416	0	9274	192	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 10.

The worst 5 of 192 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)
2:F:40:LEU:HB2	2:F:73:ARG:HH21	1.19	1.05
7:N:3:BMA:H2	7:N:4:MAN:H2	1.40	1.03
2:H:73:ARG:HB2	2:H:141:TRP:CD1	2.08	0.89
2:H:73:ARG:HG3	11:H:3115:HOH:O	1.78	0.82
2:H:139:THR:HG22	2:H:157:VAL:HG22	1.60	0.81

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	29/36 (81%)	26 (90%)	3 (10%)	0	100	100
1	C	30/36 (83%)	27 (90%)	3 (10%)	0	100	100
1	E	27/36 (75%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	29/36 (81%)	27 (93%)	2 (7%)	0	100	100
2	B	252/259 (97%)	245 (97%)	7 (3%)	0	100	100
2	D	250/259 (96%)	246 (98%)	4 (2%)	0	100	100
2	F	250/259 (96%)	234 (94%)	13 (5%)	3 (1%)	13	3
2	H	249/259 (96%)	241 (97%)	6 (2%)	2 (1%)	19	7
All	All	1116/1180 (95%)	1072 (96%)	39 (4%)	5 (0%)	34	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	76	TYR
2	F	77(A)	ARG
2	H	73	ARG
2	H	76	TYR
2	F	73	ARG

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	28/31 (90%)	28 (100%)	0	100	100
1	C	26/31 (84%)	26 (100%)	0	100	100
1	E	26/31 (84%)	26 (100%)	0	100	100
1	G	27/31 (87%)	27 (100%)	0	100	100
2	B	218/225 (97%)	211 (97%)	7 (3%)	39	22
2	D	218/225 (97%)	212 (97%)	6 (3%)	43	27
2	F	217/225 (96%)	213 (98%)	4 (2%)	59	45
2	H	217/225 (96%)	211 (97%)	6 (3%)	43	27
All	All	977/1024 (95%)	954 (98%)	23 (2%)	49	33

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	99	LEU
2	D	204(B)	ASN
2	H	153	SER
2	D	182	CYS
2	F	33	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	143	ASN
2	F	151	GLN
2	H	71	HIS
2	F	38	GLN
2	F	71	HIS

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 ⓘ

22 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	IDS	I	1	3	14,17,17	1.22	1 (7%)	17,26,26	4.24	4 (23%)
3	SGN	I	2	3	18,19,20	1.47	2 (11%)	22,29,31	2.15	5 (22%)
3	IDS	I	3	3	13,16,17	1.36	2 (15%)	15,24,26	2.57	3 (20%)
3	SGN	I	4	3	18,19,20	1.54	2 (11%)	22,29,31	2.04	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IDS	I	5	3	13,16,17	1.42	2 (15%)	15,24,26	2.81	4 (26%)
3	SGN	I	6	3	17,18,20	1.55	3 (17%)	18,27,31	1.25	1 (5%)
4	NAG	J	1	2,4	14,14,15	0.67	0	17,19,21	0.77	1 (5%)
4	NAG	J	2	4	14,14,15	0.65	0	17,19,21	0.91	2 (11%)
5	SGN	K	1	5	19,20,20	1.37	3 (15%)	24,31,31	1.81	2 (8%)
5	IDS	K	2	5	13,16,17	1.37	2 (15%)	15,24,26	2.62	3 (20%)
5	SGN	K	3	5	18,19,20	1.44	2 (11%)	22,29,31	1.89	5 (22%)
5	IDS	K	4	5	13,16,17	1.26	2 (15%)	15,24,26	2.47	3 (20%)
5	SGN	K	5	5	17,18,20	1.57	3 (17%)	18,27,31	1.25	1 (5%)
6	NAG	L	1	2,6	14,14,15	0.58	0	17,19,21	0.75	1 (5%)
6	NDG	L	2	6	14,14,15	0.60	0	17,19,21	0.67	0
6	NAG	M	1	2,6	14,14,15	0.69	0	17,19,21	0.71	1 (5%)
6	NDG	M	2	6	14,14,15	0.65	0	17,19,21	0.70	1 (5%)
7	NAG	N	1	2,7	14,14,15	0.55	0	17,19,21	0.87	0
7	NAG	N	2	7	14,14,15	0.53	0	17,19,21	0.75	1 (5%)
7	BMA	N	3	7	11,11,12	0.56	0	15,15,17	0.36	0
7	MAN	N	4	7	11,11,12	0.60	0	15,15,17	0.61	0
7	MAN	N	5	7	11,11,12	0.56	0	15,15,17	0.78	1 (6%)

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	IDS	I	1	3	-	1/5/29/29	0/1/1/1
3	SGN	I	2	3	-	9/11/28/31	0/1/1/1
3	IDS	I	3	3	-	1/5/26/29	0/1/1/1
3	SGN	I	4	3	-	5/11/28/31	0/1/1/1
3	IDS	I	5	3	-	0/5/26/29	0/1/1/1
3	SGN	I	6	3	-	6/11/24/31	0/1/1/1
4	NAG	J	1	2,4	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
5	SGN	K	1	5	-	2/11/31/31	0/1/1/1
5	IDS	K	2	5	-	3/5/26/29	0/1/1/1
5	SGN	K	3	5	-	2/11/28/31	0/1/1/1
5	IDS	K	4	5	-	0/5/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SGN	K	5	5	-	3/11/24/31	0/1/1/1
6	NAG	L	1	2,6	1/1/5/7	4/6/23/26	0/1/1/1
6	NDG	L	2	6	-	4/6/23/26	0/1/1/1
6	NAG	M	1	2,6	1/1/5/7	4/6/23/26	0/1/1/1
6	NDG	M	2	6	-	4/6/23/26	0/1/1/1
7	NAG	N	1	2,7	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	N	2	7	-	4/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
7	MAN	N	4	7	-	2/2/19/22	1/1/1/1
7	MAN	N	5	7	-	2/2/19/22	1/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	4	SGN	S1-N2	4.51	1.65	1.59
5	K	5	SGN	S1-N2	4.21	1.65	1.59
3	I	6	SGN	S1-N2	4.12	1.65	1.59
5	K	3	SGN	S1-N2	4.08	1.65	1.59
5	K	1	SGN	S1-N2	3.85	1.64	1.59

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	IDS	O4-C4-C5	12.88	134.65	110.05
3	I	1	IDS	O4-C4-C3	-8.79	90.02	110.35
5	K	2	IDS	C2-O2-S	8.42	128.90	117.91
5	K	4	IDS	C2-O2-S	8.21	128.62	117.91
3	I	3	IDS	C2-O2-S	8.20	128.60	117.91

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	J	1	NAG	C1
7	N	1	NAG	C1
6	L	1	NAG	C1
6	M	1	NAG	C1

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	6	SGN	C2-N2-S1-O2S
3	I	6	SGN	C2-N2-S1-O3S
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
5	K	2	IDS	C2-O2-S-O1S

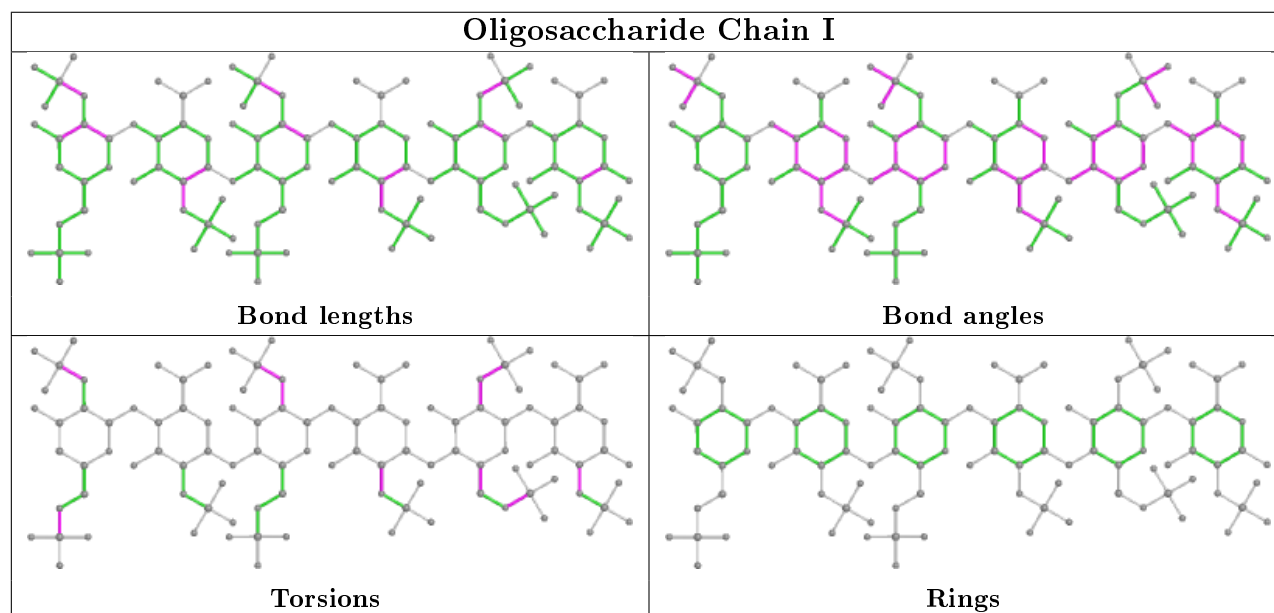
All (2) ring outliers are listed below:

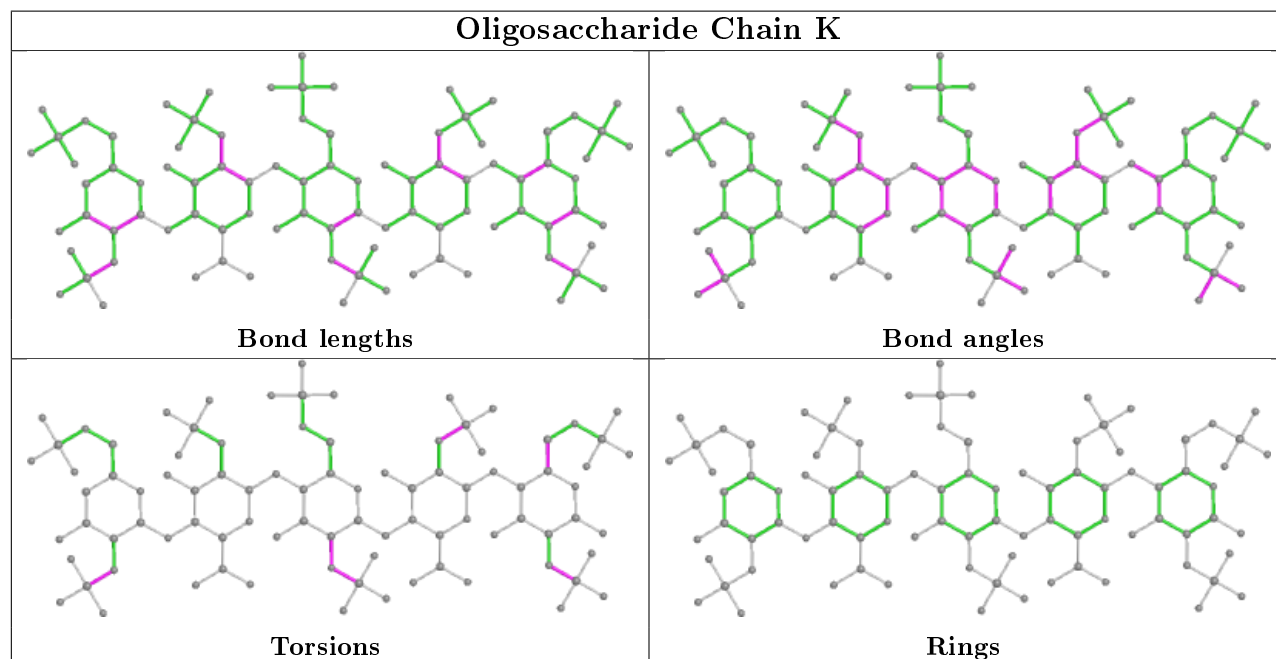
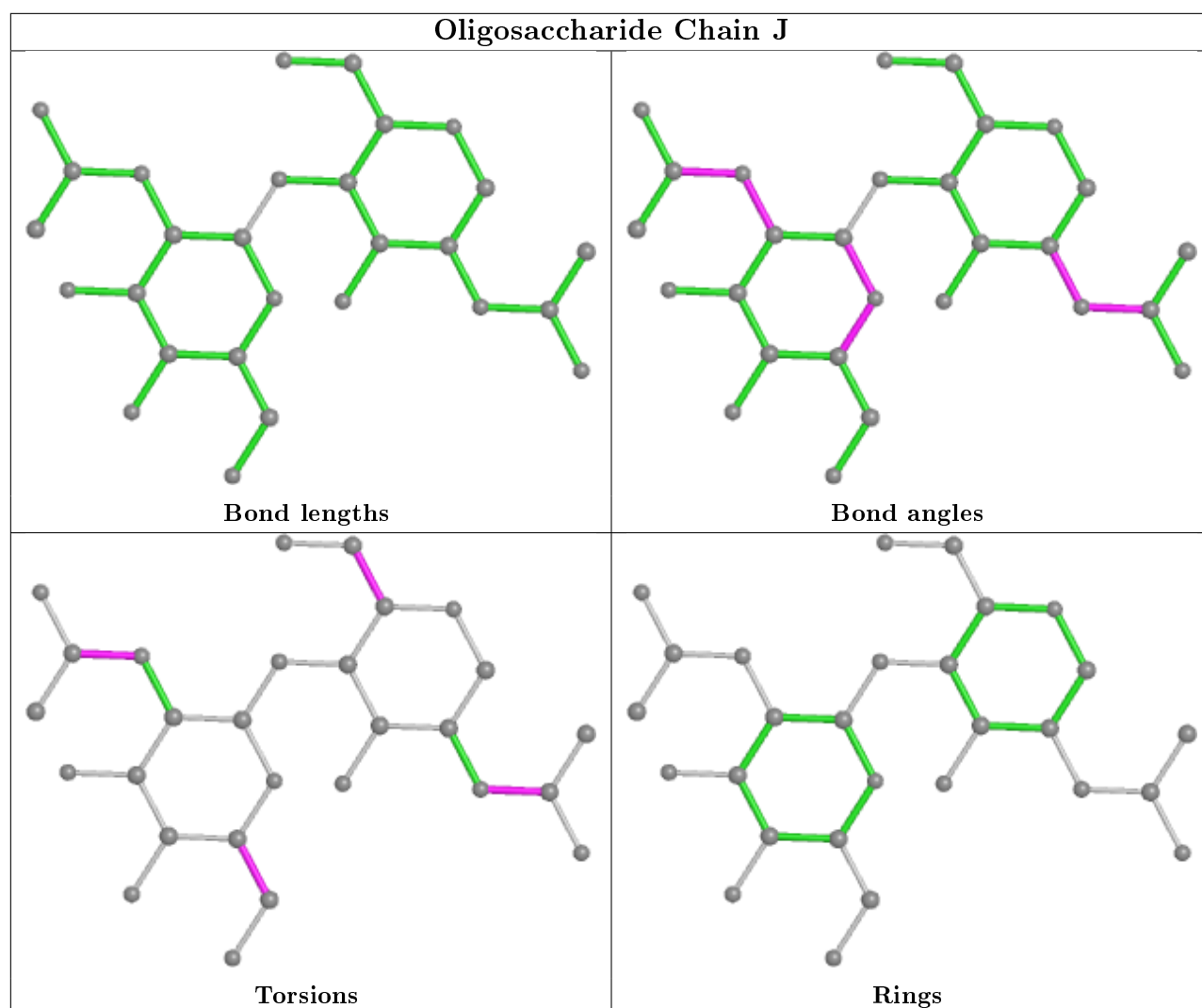
Mol	Chain	Res	Type	Atoms
7	N	4	MAN	C1-C2-C3-C4-C5-O5
7	N	5	MAN	C1-C2-C3-C4-C5-O5

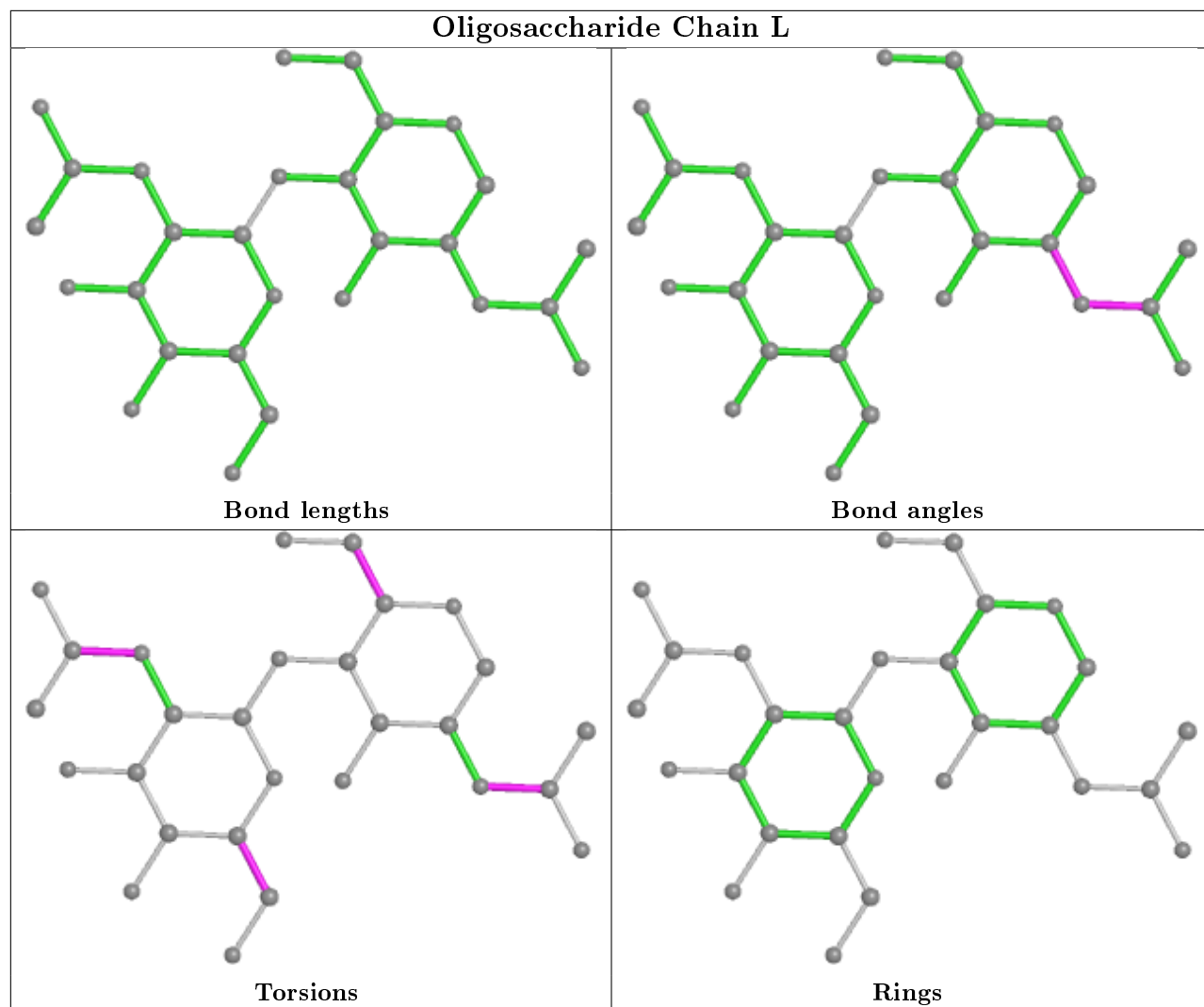
4 monomers are involved in 5 short contacts:

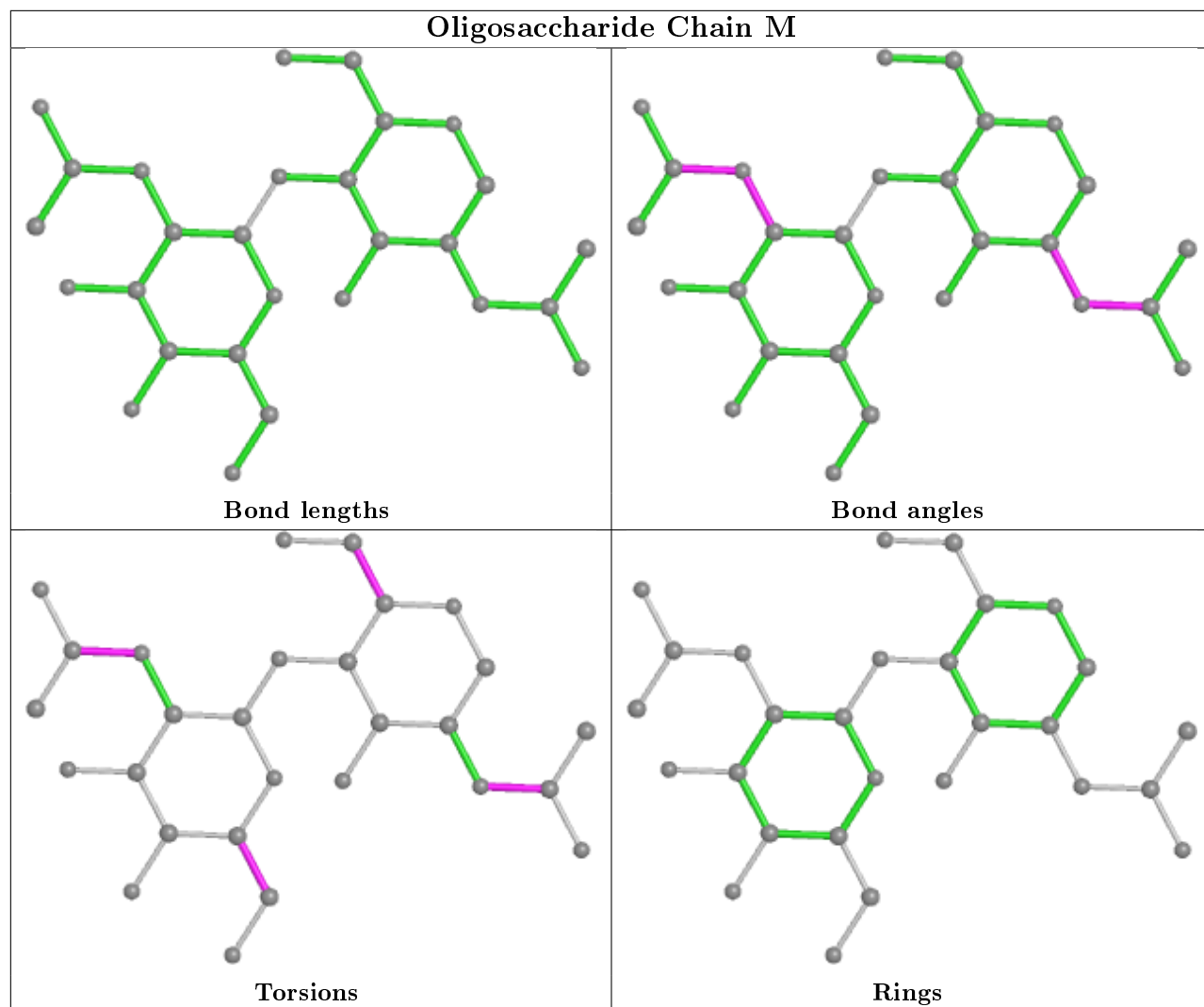
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	N	2	NAG	1	0
7	N	3	BMA	4	0
7	N	4	MAN	4	0
7	N	5	MAN	1	0

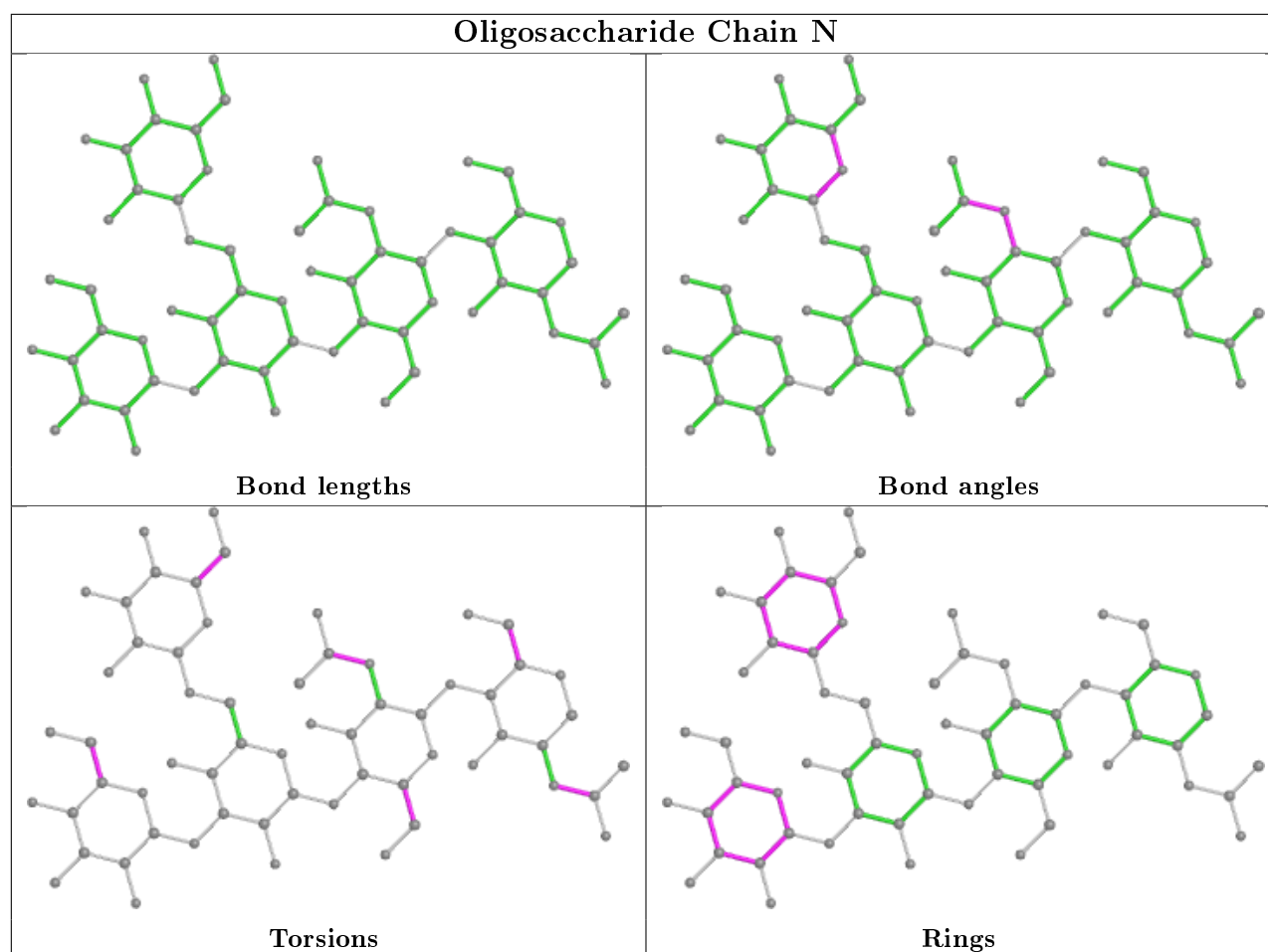
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
10	GOL	D	1004	-	5,5,5	0.72	0	5,5,5	0.42	0
10	GOL	H	1005	-	5,5,5	0.71	0	5,5,5	0.47	0
10	GOL	B	1008	-	5,5,5	0.70	0	5,5,5	0.46	0
10	GOL	F	1007	-	5,5,5	0.67	0	5,5,5	0.40	0
10	GOL	F	1003	-	5,5,5	0.72	0	5,5,5	0.43	0
10	GOL	D	1002	-	5,5,5	0.68	0	5,5,5	0.47	0
10	GOL	F	1006	-	5,5,5	0.75	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	0G6	H	1	2	30,31,32	0.98	0	37,41,42	1.04	2 (5%)
8	0G6	F	1	2	30,31,32	0.99	0	37,41,42	1.07	3 (8%)
10	GOL	B	1001	-	5,5,5	0.69	0	5,5,5	0.43	0
8	0G6	D	1	2	30,31,32	0.97	0	37,41,42	1.04	2 (5%)
8	0G6	B	1	2	30,31,32	0.98	1 (3%)	37,41,42	1.01	2 (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	D	1004	-	-	2/4/4/4	-
10	GOL	H	1005	-	-	3/4/4/4	-
10	GOL	B	1008	-	-	1/4/4/4	-
10	GOL	F	1007	-	-	2/4/4/4	-
10	GOL	F	1003	-	-	0/4/4/4	-
10	GOL	D	1002	-	-	4/4/4/4	-
10	GOL	F	1006	-	-	1/4/4/4	-
8	0G6	H	1	2	-	1/31/41/43	0/2/2/2
8	0G6	F	1	2	-	1/31/41/43	0/2/2/2
10	GOL	B	1001	-	-	0/4/4/4	-
8	0G6	D	1	2	-	1/31/41/43	0/2/2/2
8	0G6	B	1	2	-	1/31/41/43	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1	0G6	O-C	2.14	1.26	1.22

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	1	0G6	O-C-CA	-2.58	114.97	119.66
8	F	1	0G6	O-C-CA	-2.48	115.15	119.66
8	F	1	0G6	CA-C-N1	2.47	123.26	118.65
8	D	1	0G6	CA-C-N1	2.45	123.22	118.65
8	H	1	0G6	O-C-CA	-2.41	115.28	119.66

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	1002	GOL	O1-C1-C2-C3
10	F	1007	GOL	O1-C1-C2-C3
8	F	1	0G6	O2-C2-CA2-CB2
8	D	1	0G6	O2-C2-CA2-CB2
8	B	1	0G6	O2-C2-CA2-CB2

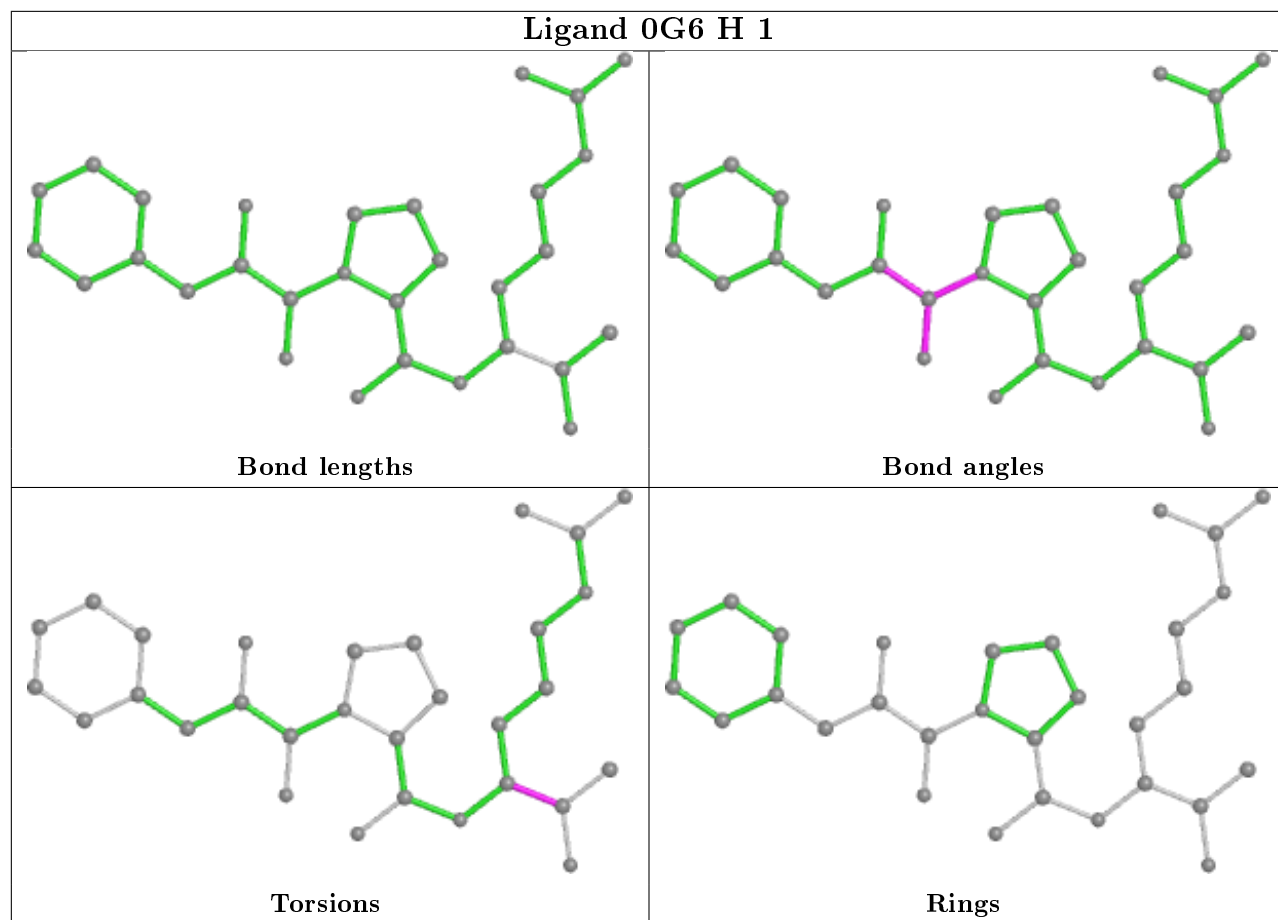
There are no ring outliers.

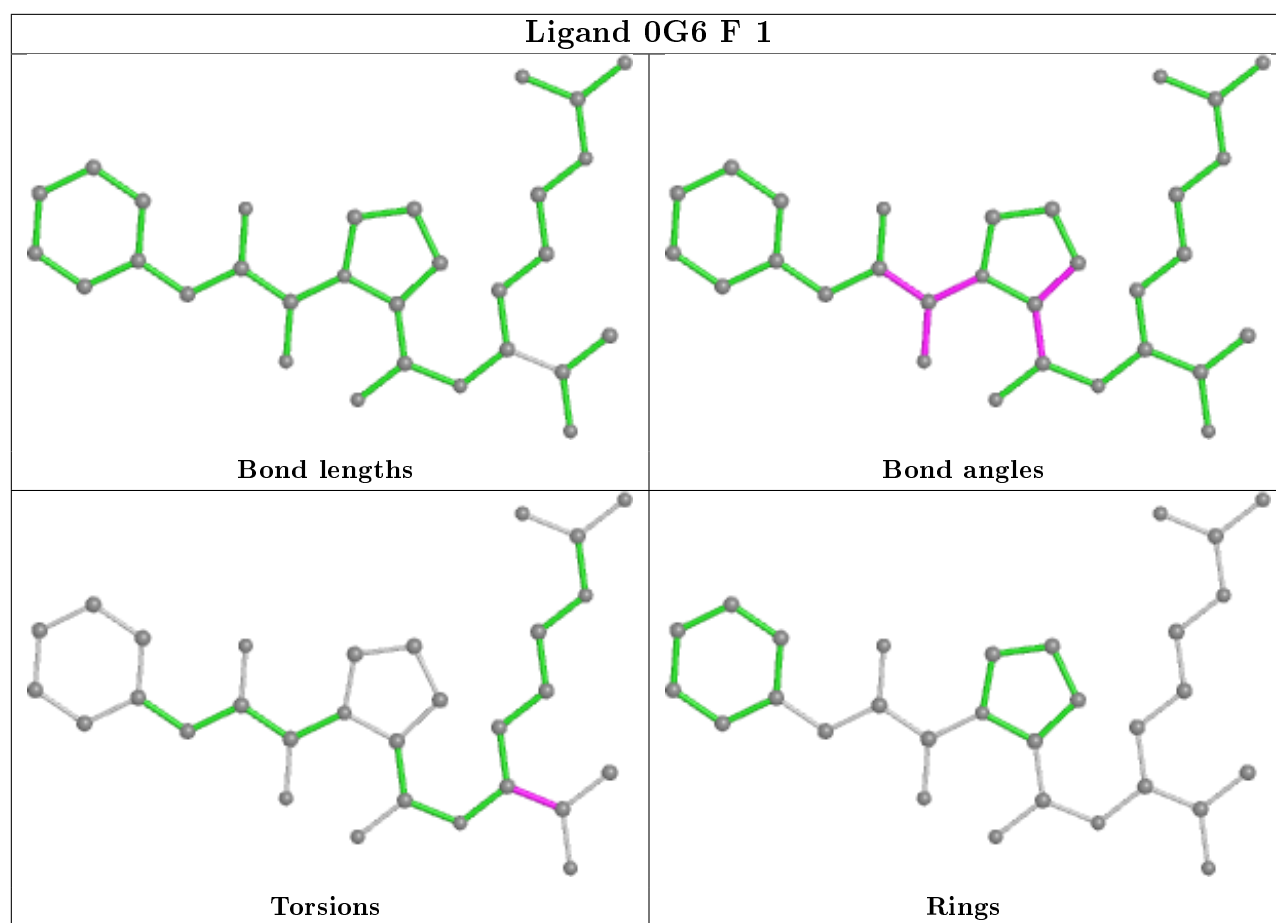
7 monomers are involved in 8 short contacts:

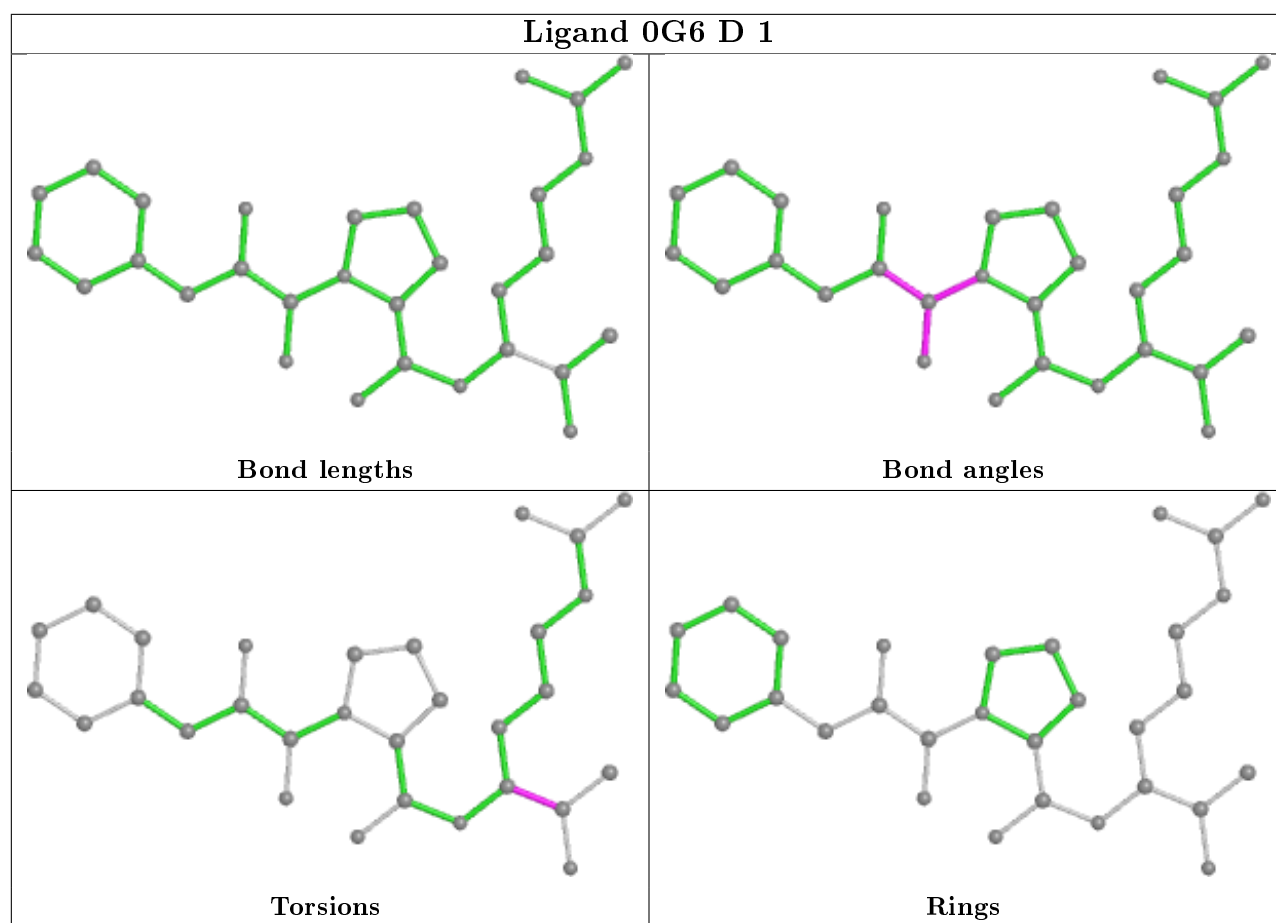
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1004	GOL	1	0
10	B	1008	GOL	1	0
10	F	1007	GOL	1	0
8	H	1	0G6	1	0
8	F	1	0G6	2	0
8	D	1	0G6	1	0
8	B	1	0G6	1	0

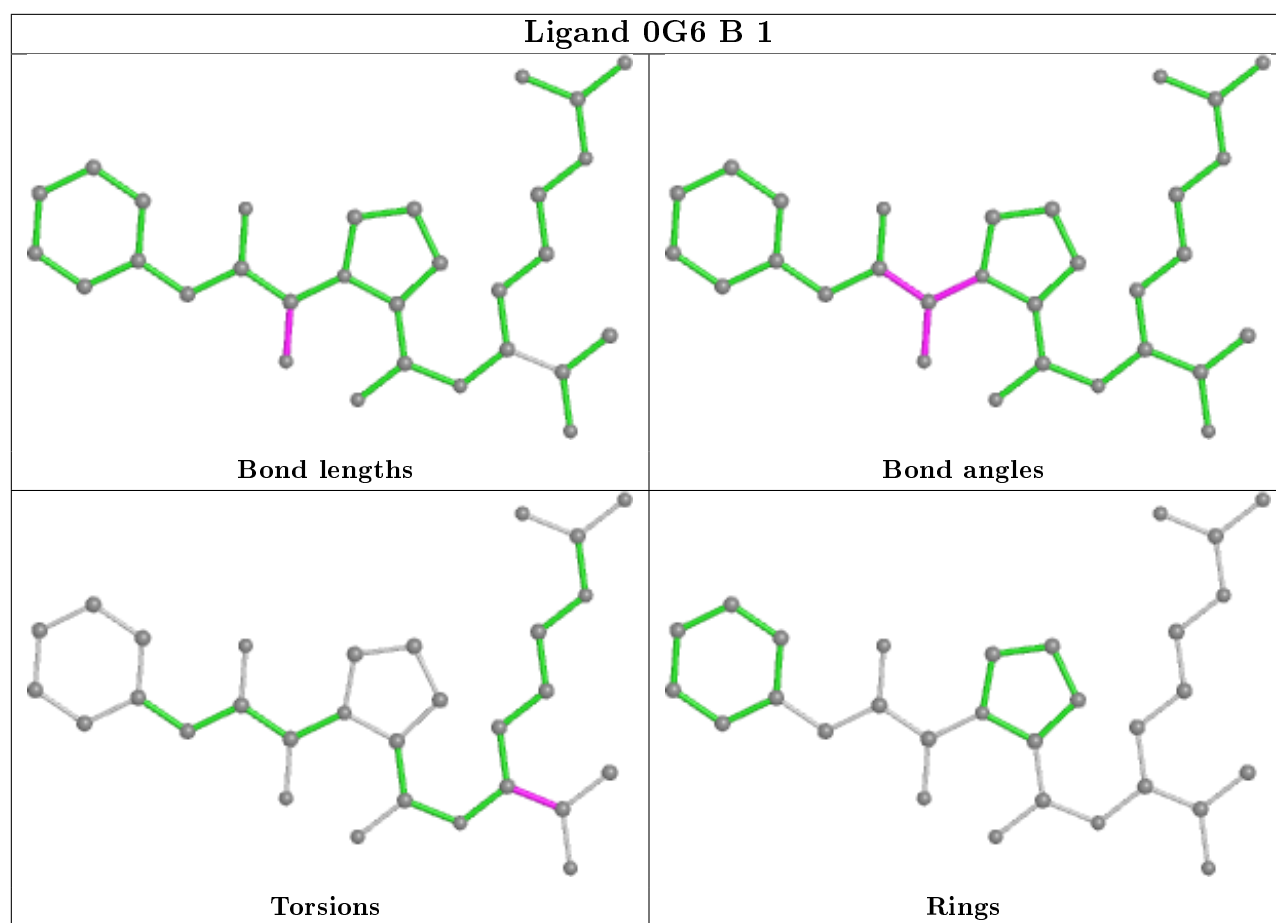
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 0G6 H 1









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	31/36 (86%)	0.18	3 (9%) 7 7	21, 28, 60, 64	0
1	C	32/36 (88%)	0.37	6 (18%) 1 1	20, 30, 53, 56	0
1	E	29/36 (80%)	0.05	2 (6%) 16 16	24, 32, 44, 55	0
1	G	31/36 (86%)	0.31	4 (12%) 3 3	20, 28, 51, 57	0
2	B	256/259 (98%)	-0.13	5 (1%) 65 64	14, 24, 41, 65	0
2	D	254/259 (98%)	-0.13	2 (0%) 86 86	14, 24, 41, 60	0
2	F	254/259 (98%)	0.03	10 (3%) 39 38	16, 30, 49, 65	0
2	H	253/259 (97%)	0.12	11 (4%) 35 33	14, 28, 47, 62	0
All	All	1140/1180 (96%)	0.00	43 (3%) 40 38	14, 27, 47, 65	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	74	THR	5.3
2	H	150	GLY	4.7
1	A	1(D)	GLY	4.3
2	F	150	GLY	4.2
1	C	1(D)	GLY	4.2

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

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

6.3 Carbohydrates ⓘ

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,

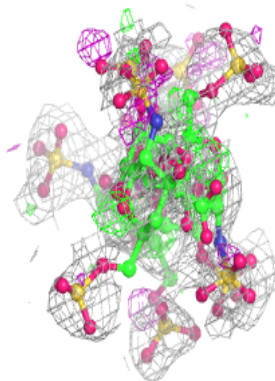
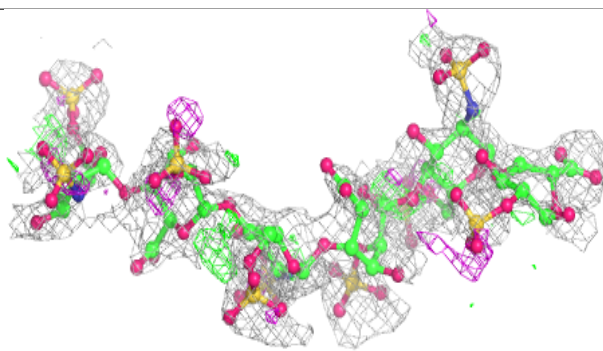
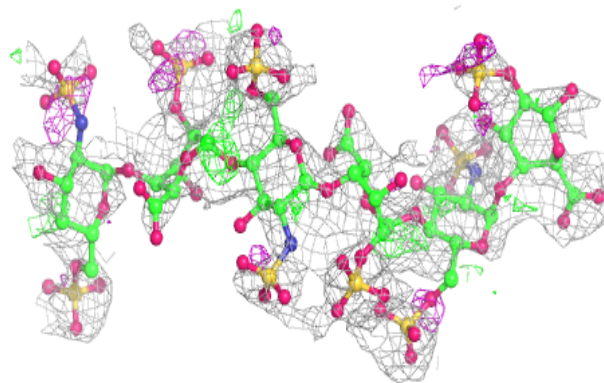
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SGN	K	3	19/20	0.37	0.35	98,100,102,103	0
7	MAN	N	4	11/12	0.45	0.53	106,107,108,108	0
5	SGN	K	1	20/20	0.48	0.32	105,110,116,116	0
3	SGN	I	6	18/20	0.50	0.34	102,104,105,105	0
7	MAN	N	5	11/12	0.54	0.68	110,112,112,112	0
3	SGN	I	2	19/20	0.55	0.24	94,97,101,101	0
3	IDS	I	3	16/17	0.56	0.27	97,98,101,101	0
5	IDS	K	2	16/17	0.58	0.33	100,103,105,105	0
3	SGN	I	4	19/20	0.58	0.30	96,98,101,101	0
3	IDS	I	5	16/17	0.61	0.32	99,100,102,102	0
6	NDG	L	2	14/15	0.62	0.44	65,68,69,69	0
5	SGN	K	5	18/20	0.66	0.40	100,102,103,104	0
5	IDS	K	4	16/17	0.69	0.25	97,98,98,100	0
7	BMA	N	3	11/12	0.70	0.53	100,103,106,108	0
3	IDS	I	1	17/17	0.71	0.33	98,100,103,104	0
4	NAG	J	2	14/15	0.72	0.44	69,72,75,75	0
6	NDG	M	2	14/15	0.72	0.42	68,70,70,72	0
4	NAG	J	1	14/15	0.77	0.23	51,54,58,64	0
7	NAG	N	2	14/15	0.77	0.48	83,87,90,94	0
7	NAG	N	1	14/15	0.78	0.36	63,68,71,77	0
6	NAG	M	1	14/15	0.79	0.33	54,58,64,65	0
6	NAG	L	1	14/15	0.82	0.22	49,53,59,61	0

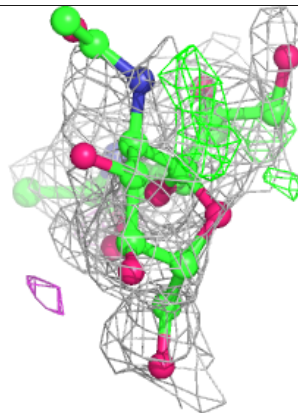
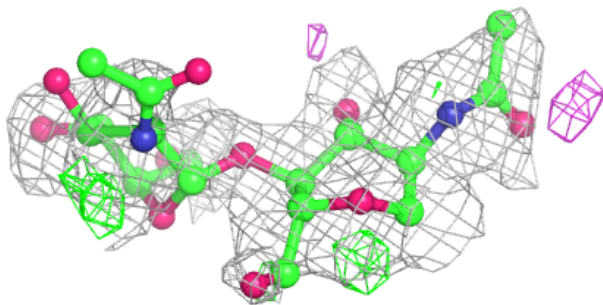
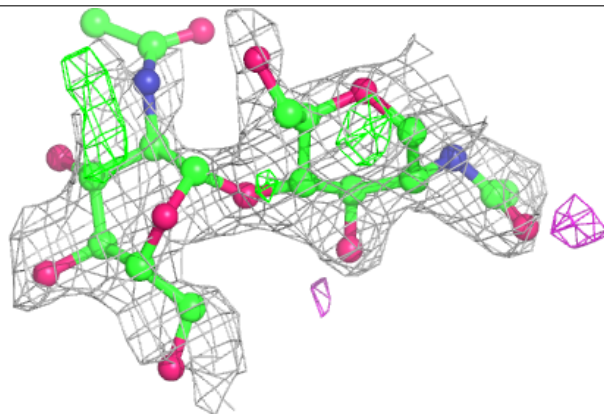
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

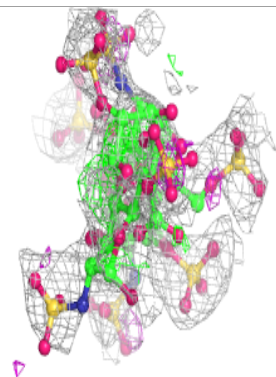
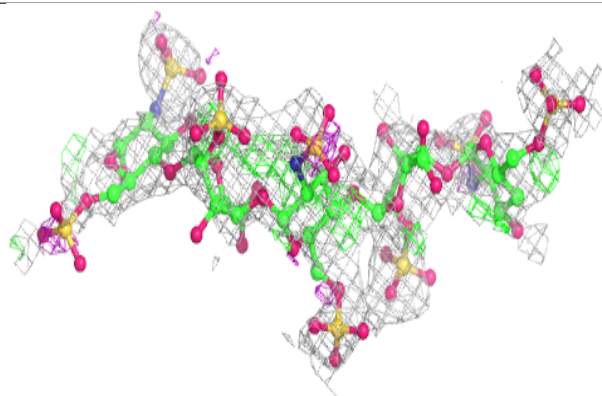
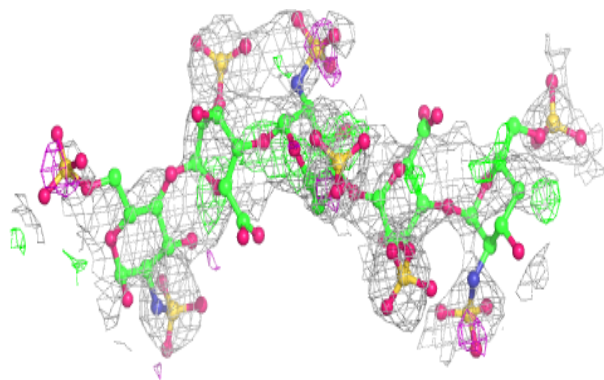
**Electron density around Chain J:**

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

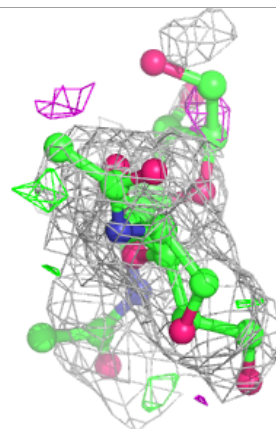
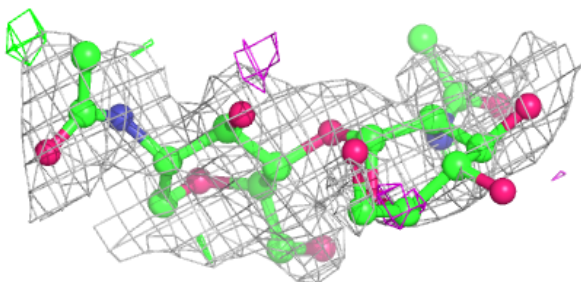
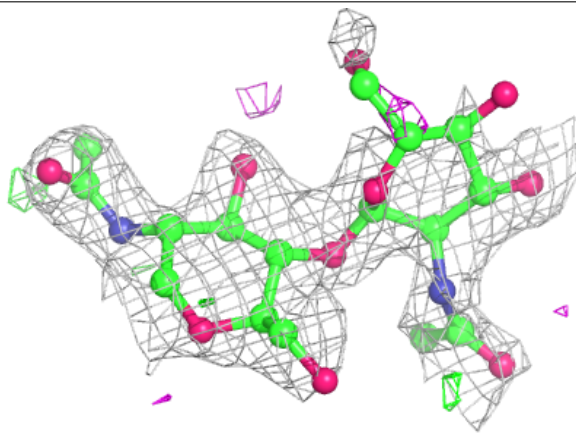


Electron density around Chain K:

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

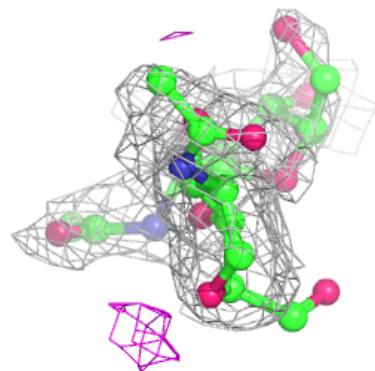
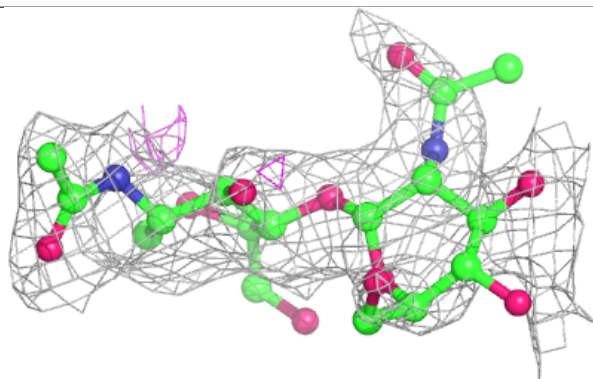
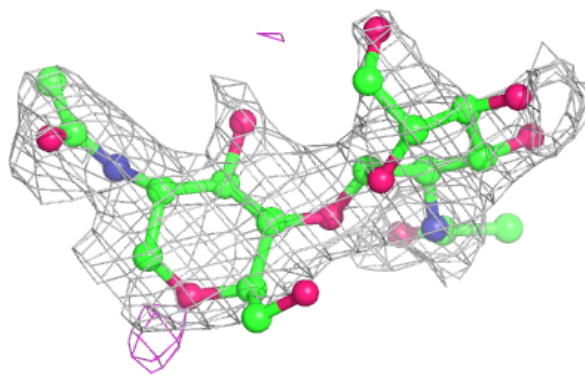
**Electron density around Chain L:**

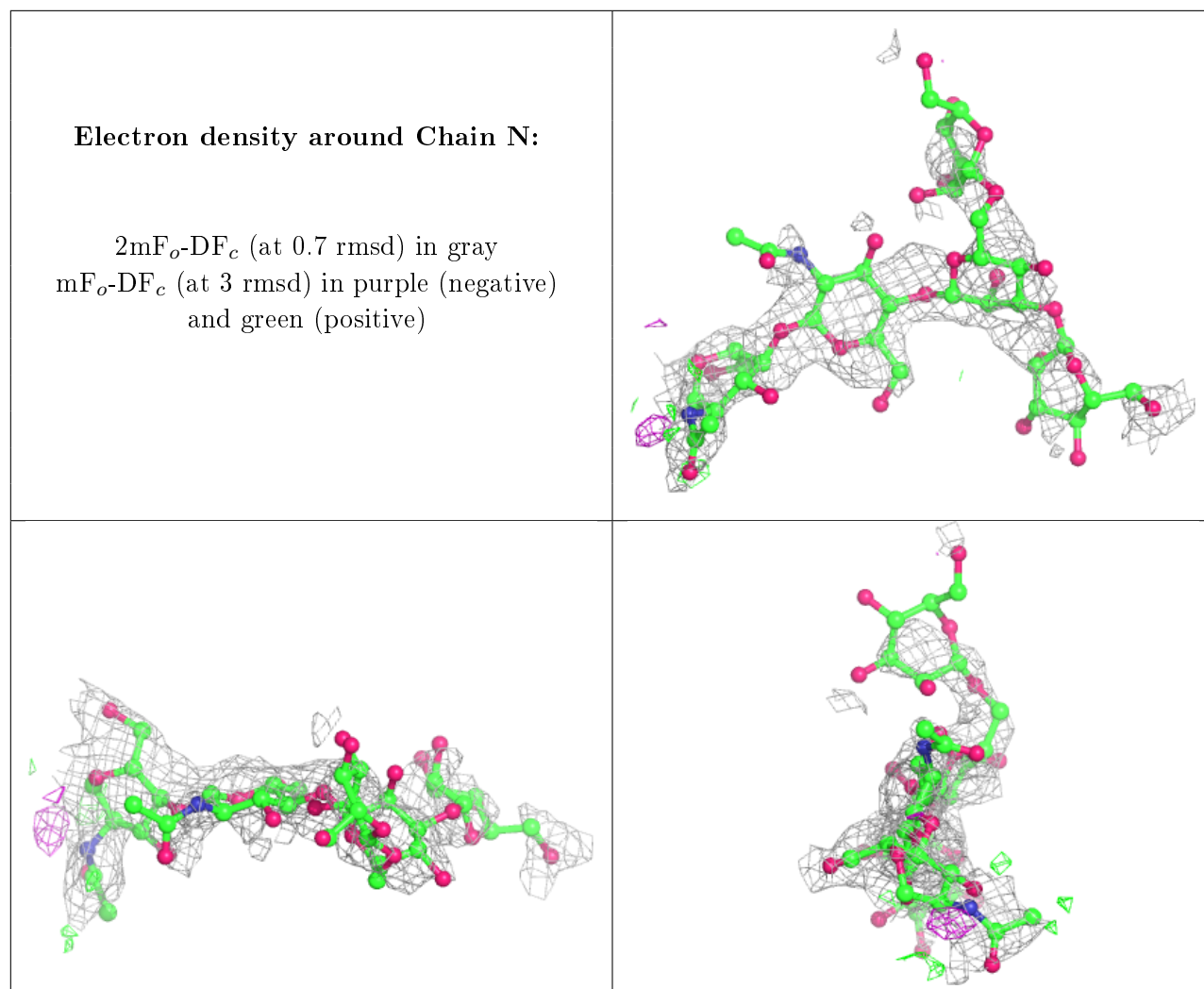
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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(\AA^2)	Q<0.9
10	GOL	D	1004	6/6	0.34	0.34	66,67,68,68	0
10	GOL	F	1006	6/6	0.59	0.23	55,57,58,59	0
10	GOL	F	1007	6/6	0.77	0.16	50,53,54,55	0
10	GOL	F	1003	6/6	0.82	0.17	38,40,42,43	0
10	GOL	B	1008	6/6	0.84	0.15	58,58,59,59	0
10	GOL	B	1001	6/6	0.87	0.14	29,32,34,35	0
10	GOL	H	1005	6/6	0.89	0.16	37,41,41,44	0
10	GOL	D	1002	6/6	0.92	0.14	27,32,33,34	0
8	OG6	F	1	30/31	0.92	0.12	25,28,30,31	0

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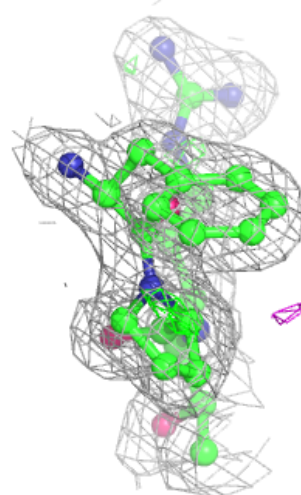
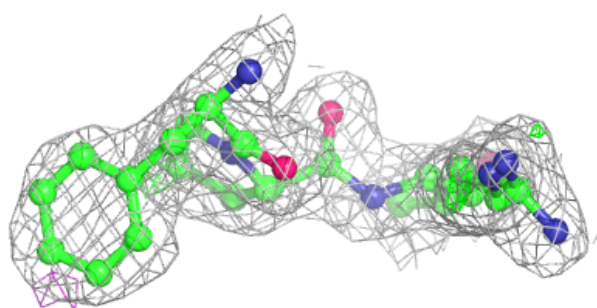
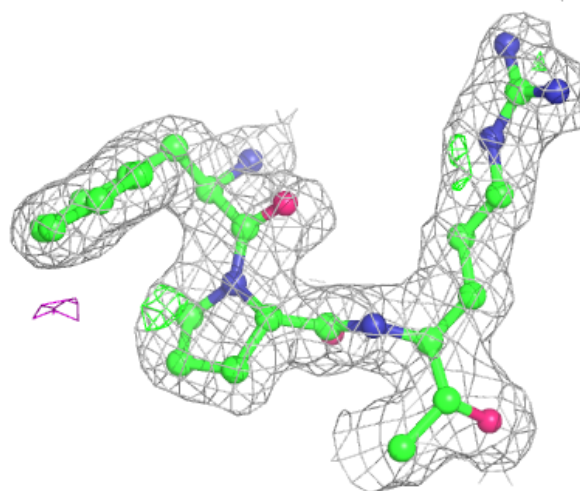
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	NA	F	3002	1/1	0.92	0.11	37,37,37,37	0
8	0G6	H	1	30/31	0.94	0.12	20,22,26,26	0
9	NA	B	3004	1/1	0.95	0.10	28,28,28,28	0
8	0G6	B	1	30/31	0.96	0.10	17,19,24,24	0
9	NA	H	3003	1/1	0.96	0.09	30,30,30,30	0
8	0G6	D	1	30/31	0.96	0.11	14,19,21,22	0
9	NA	D	3001	1/1	0.98	0.09	26,26,26,26	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.

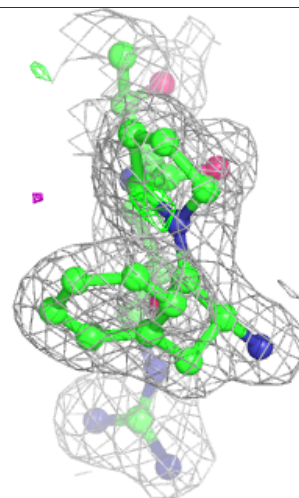
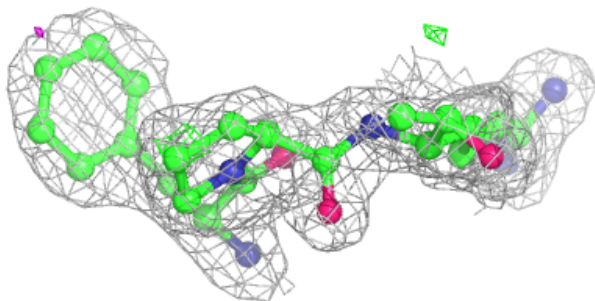
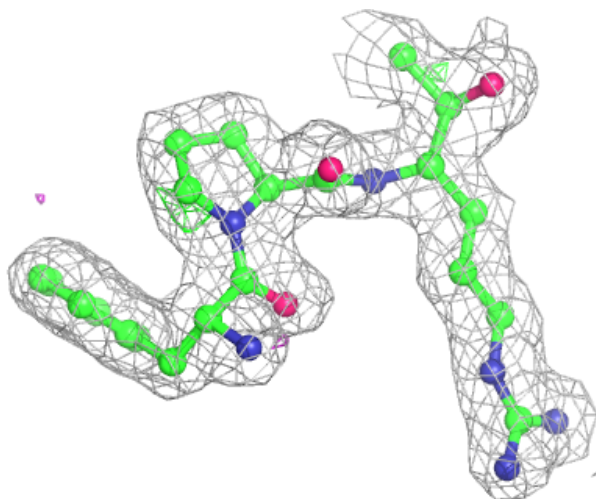
Electron density around 0G6 F 1:

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



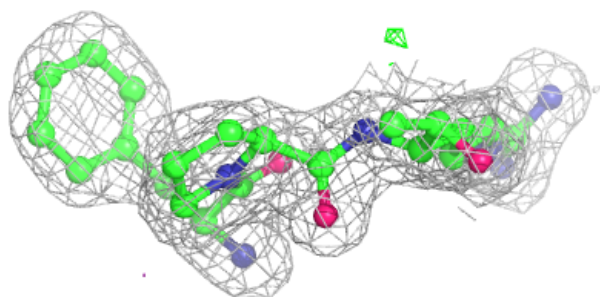
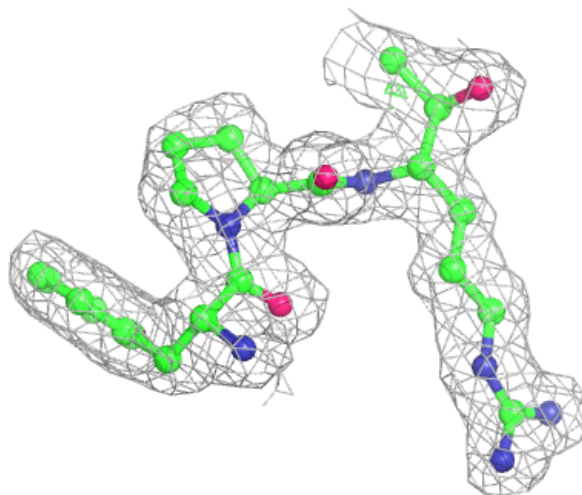
Electron density around 0G6 H 1:

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



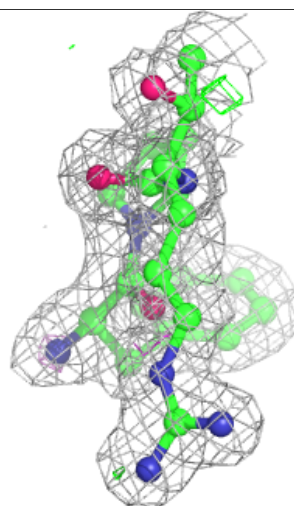
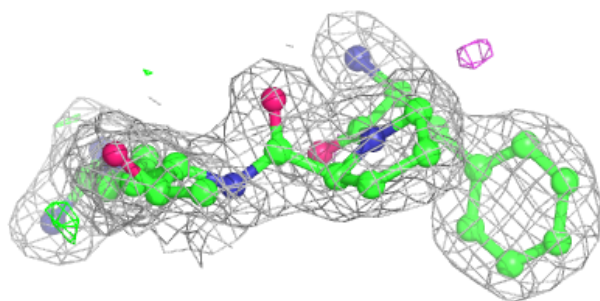
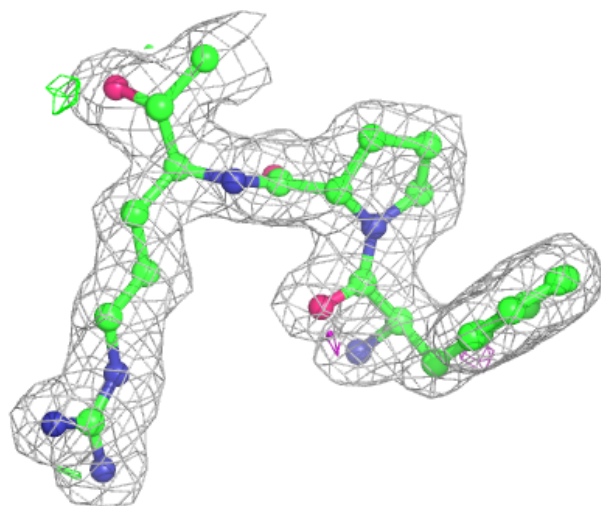
Electron density around 0G6 B 1:

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



Electron density around 0G6 D 1:

$2mF_o-DF_c$ (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.