



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 04:20 PM BST

PDB ID : 5MJ6
Title : Ligand-induced conformational change of Insulin-regulated aminopeptidase:
insights on catalytic mechanism and active site plasticity.
Authors : Mpakali, A.; Stratikos, E.; Saridakis, E.; Giastas, P.
Deposited on : 2016-11-30
Resolution : 2.53 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

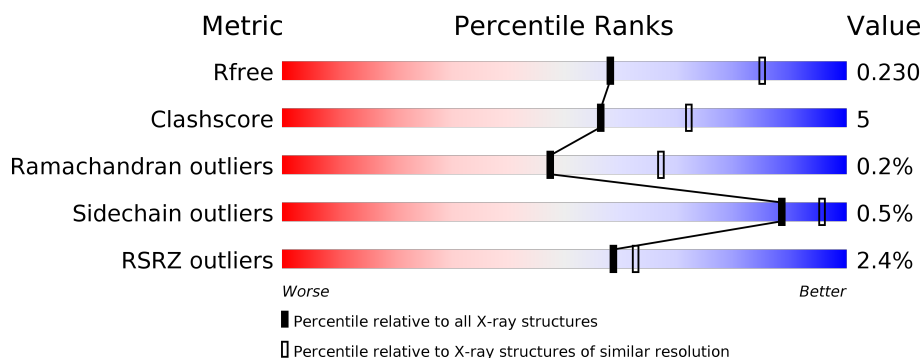
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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.




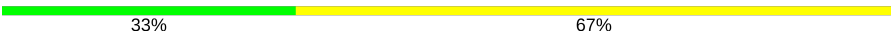

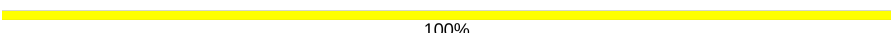

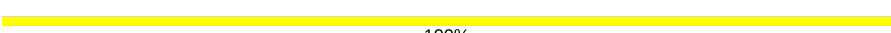






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	881	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div></div> </div> </div>
1	B	881	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div></div> </div> </div>
2	C	4	<div> <div></div> <div> <div>75%</div> <div>25%</div> </div> </div>
2	R	4	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
3	D	3	<div> <div></div> <div>100%</div> </div>
3	F	3	<div> <div></div> <div>100%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	K	3	
3	N	3	
3	P	3	
4	E	2	
4	H	2	
4	J	2	
4	L	2	
4	M	2	
4	O	2	
4	Q	2	
5	G	5	
5	I	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
3	BMA	D	3	-	-	-	X
4	NAG	J	2	-	-	-	X
4	NAG	L	2	-	-	-	X
4	NAG	M	2	-	-	-	X
4	NAG	Q	2	-	-	-	X
5	MAN	I	4	-	-	-	X
5	MAN	I	5	-	-	-	X
6	NAG	A	1132	-	-	-	X
6	NAG	B	1122	-	-	-	X
6	NAG	B	1123	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15376 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.

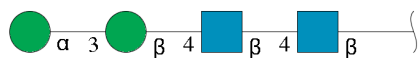
- Molecule 1 is a protein called Leucyl-cystinyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	870	Total	C	N	O	S	0	12	0
			7131	4607	1165	1331	28			
1	B	866	Total	C	N	O	S	0	13	0
			7115	4603	1161	1324	27			

There are 20 discrepancies between the modelled and reference sequences:

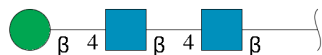
Chain	Residue	Modelled	Actual	Comment	Reference
A	1026	ARG	-	expression tag	UNP Q9UIQ6
A	1027	THR	-	expression tag	UNP Q9UIQ6
A	1028	GLU	-	expression tag	UNP Q9UIQ6
A	1029	THR	-	expression tag	UNP Q9UIQ6
A	1030	SER	-	expression tag	UNP Q9UIQ6
A	1031	GLN	-	expression tag	UNP Q9UIQ6
A	1032	VAL	-	expression tag	UNP Q9UIQ6
A	1033	ALA	-	expression tag	UNP Q9UIQ6
A	1034	PRO	-	expression tag	UNP Q9UIQ6
A	1035	ALA	-	expression tag	UNP Q9UIQ6
B	1026	ARG	-	expression tag	UNP Q9UIQ6
B	1027	THR	-	expression tag	UNP Q9UIQ6
B	1028	GLU	-	expression tag	UNP Q9UIQ6
B	1029	THR	-	expression tag	UNP Q9UIQ6
B	1030	SER	-	expression tag	UNP Q9UIQ6
B	1031	GLN	-	expression tag	UNP Q9UIQ6
B	1032	VAL	-	expression tag	UNP Q9UIQ6
B	1033	ALA	-	expression tag	UNP Q9UIQ6
B	1034	PRO	-	expression tag	UNP Q9UIQ6
B	1035	ALA	-	expression tag	UNP Q9UIQ6

- Molecule 2 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.



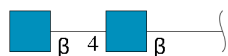
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	P	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



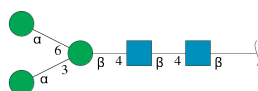
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

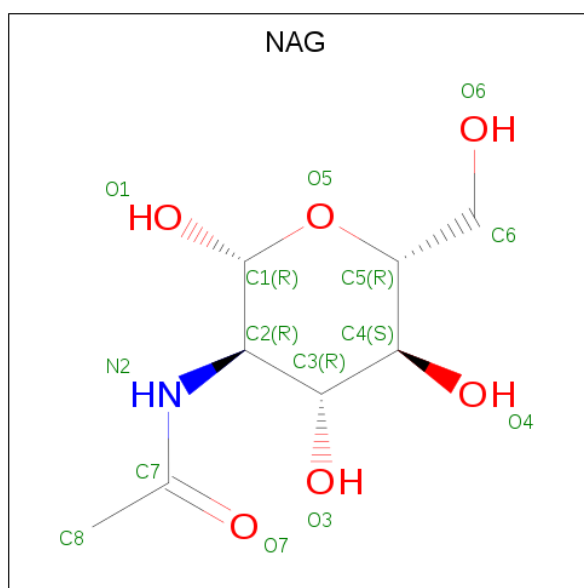
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

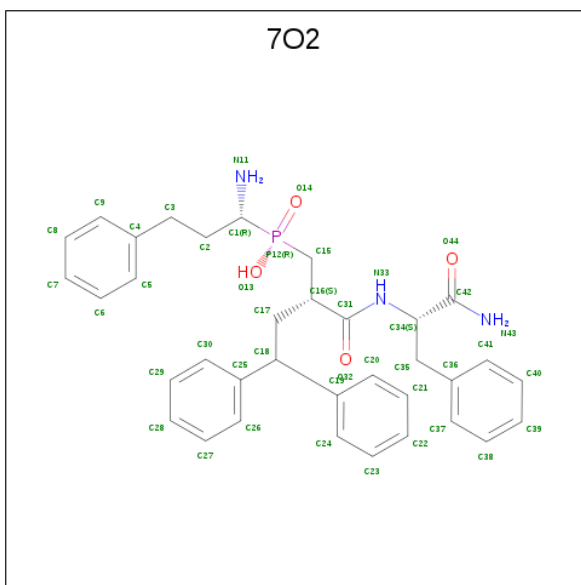


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is [(2 {S})-2-[(2 {S})-1-azanyl-1-oxidanylidene-3-phenyl-propan-2-yl]carbamoyl]-4,4-diphenyl-butyl)-[(1 {R})-1-azanyl-3-phenyl-propyl]phosphinic acid (three-letter code: 7O2) (formula: C₃₅H₄₀N₃O₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			43	35	3	4	1		
8	B	1	Total	C	N	O	P	0	0
			43	35	3	4	1		

- Molecule 9 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	6	Total	Br	0	0
			6	6		
9	A	15	Total	Br	0	0
			15	15		

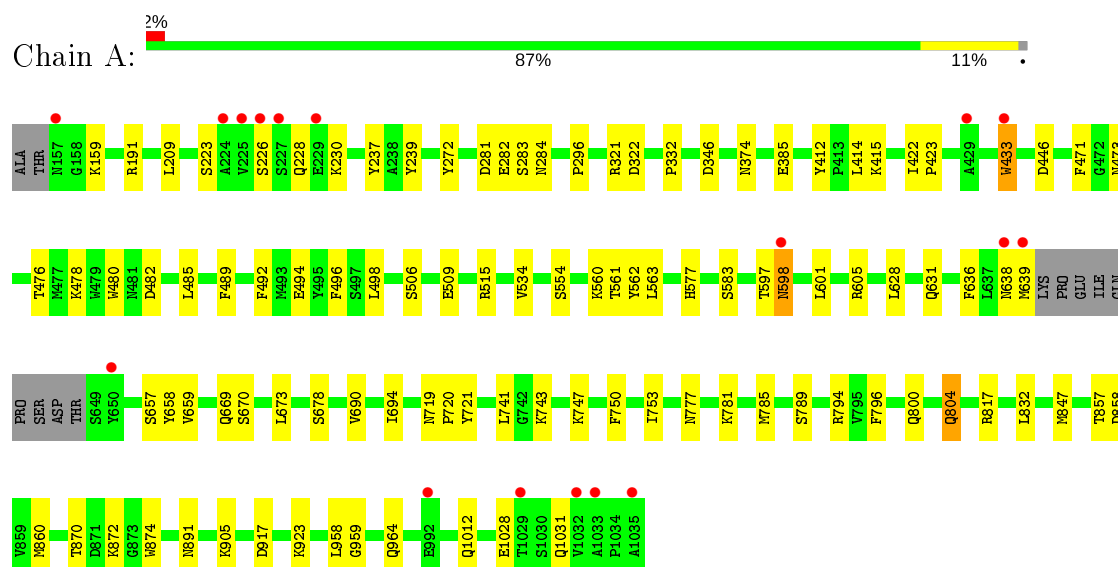
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	152	Total	O	0	0
			152	152		
10	B	88	Total	O	0	0
			88	88		

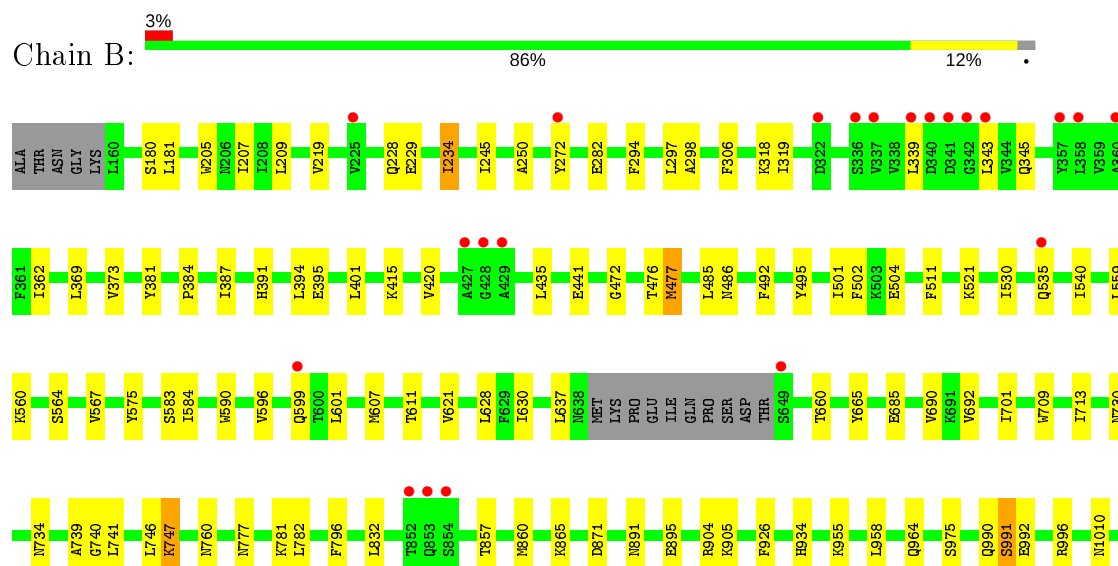
3 Residue-property plots [i](#)

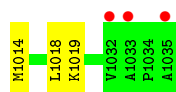
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Leucyl-cystinyl aminopeptidase





- Molecule 2: 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 C: 75% 25%



- Molecule 2: 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 R: 50% 50%



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

Chain D: 100%



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

Chain F: 100%



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

Chain K: 33% 67%



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

Chain N: 33% 67%



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

Chain P:  67% 33%

 NAG1
NAG2
BNA3

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

Chain E:  100%

 NAG1
NAG2

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

Chain H:  100%

 NAG1
NAG2

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

Chain J:  100%

 NAG1
NAG2

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

Chain L:  50% 50%

 NAG1
NAG2

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

Chain M:  50% 50%

 NAG1
NAG2

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

Chain O:  50% 50%



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

Chain Q:  100%



- Molecule 5: 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 G:  20% 80%



- Molecule 5: 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 I:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.24Å 143.17Å 148.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.80 – 2.53 40.80 – 2.53	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.80-2.53) 100.0 (40.80-2.53)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.174 , 0.229 0.176 , 0.230	Depositor DCC
R_{free} test set	3983 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15376	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: ZN, BMA, NAG, 7O2, BR, 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	0.50	0/7339	0.62	3/9945 (0.0%)
1	B	0.47	2/7328 (0.0%)	0.60	2/9934 (0.0%)
All	All	0.49	2/14667 (0.0%)	0.61	5/19879 (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
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	GLU	CD-OE1	5.61	1.31	1.25
1	B	282	GLU	CD-OE2	5.05	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	TRP	CA-CB-CG	7.80	128.53	113.70
1	B	477	MET	CA-CB-CG	-5.43	104.08	113.30
1	B	958	LEU	CA-CB-CG	5.38	127.69	115.30
1	A	209	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	A	804	GLN	N-CA-C	5.15	124.90	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	598	ASN	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7131	0	7052	72	0
1	B	7115	0	7039	74	0
2	C	50	0	43	1	0
2	R	50	0	43	0	0
3	D	39	0	34	0	0
3	F	39	0	34	1	0
3	K	39	0	34	0	0
3	N	39	0	34	0	0
3	P	39	0	34	0	0
4	E	28	0	25	0	0
4	H	28	0	25	0	0
4	J	28	0	25	0	0
4	L	28	0	25	3	0
4	M	28	0	25	1	0
4	O	28	0	25	0	0
4	Q	28	0	25	0	0
5	G	61	0	52	0	0
5	I	61	0	52	2	0
6	A	56	0	52	1	0
6	B	112	0	104	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	43	0	0	1	0
8	B	43	0	0	0	0
9	A	15	0	0	2	0
9	B	6	0	0	0	0
10	A	152	0	0	4	0
10	B	88	0	0	3	0
All	All	15376	0	14782	149	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 5.

The worst 5 of 149 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:GLY:HA2	1:B:486:ASN:HD22	1.29	0.98
1:B:219:VAL:HG21	1:B:234:ILE:HG13	1.63	0.80
1:A:230:LYS:HD3	1:A:230:LYS:N	1.99	0.77
1:B:701:ILE:HG23	1:B:734:ASN:HD22	1.51	0.75
1:B:234:ILE:HD11	1:B:245:ILE:HD13	1.69	0.75

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	878/881 (100%)	839 (96%)	37 (4%)	2 (0%)	47	67
1	B	875/881 (99%)	849 (97%)	24 (3%)	2 (0%)	47	67
All	All	1753/1762 (100%)	1688 (96%)	61 (4%)	4 (0%)	47	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	991	SER
1	A	917	ASP
1	B	747	LYS
1	A	563	LEU

5.3.2 Protein sidechains [i](#)

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	790/788 (100%)	787 (100%)	3 (0%)	91	97
1	B	788/788 (100%)	782 (99%)	6 (1%)	81	92
All	All	1578/1576 (100%)	1569 (99%)	9 (1%)	88	94

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	272[A]	TYR
1	B	782	LEU
1	B	535[A]	GLN
1	A	964	GLN
1	B	272[B]	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	A	486	ASN
1	A	1012	GLN
1	B	730	ASN
1	B	734	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

47 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	0.71	1 (7%)	17,19,21	0.83	1 (5%)
2	NAG	C	2	2	14,14,15	1.17	1 (7%)	17,19,21	1.28	2 (11%)
2	BMA	C	3	2	11,11,12	0.79	0	15,15,17	1.99	4 (26%)
2	MAN	C	4	2	11,11,12	1.58	4 (36%)	15,15,17	1.25	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.81	1 (7%)	17,19,21	0.59	0
3	NAG	D	2	3	14,14,15	0.62	0	17,19,21	1.02	1 (5%)
3	BMA	D	3	3	11,11,12	2.58	3 (27%)	15,15,17	2.79	6 (40%)
4	NAG	E	1	1,4	14,14,15	0.38	0	17,19,21	1.59	3 (17%)
4	NAG	E	2	4	14,14,15	1.05	1 (7%)	17,19,21	0.85	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.24	0	17,19,21	0.76	1 (5%)
3	NAG	F	2	3	14,14,15	0.51	0	17,19,21	0.55	0
3	BMA	F	3	3	11,11,12	1.17	1 (9%)	15,15,17	0.91	0
5	NAG	G	1	1,5	14,14,15	0.52	0	17,19,21	0.57	0
5	NAG	G	2	5	14,14,15	0.80	1 (7%)	17,19,21	0.45	0
5	BMA	G	3	5	11,11,12	0.79	0	15,15,17	1.28	2 (13%)
5	MAN	G	4	5	11,11,12	1.24	2 (18%)	15,15,17	1.38	3 (20%)
5	MAN	G	5	5	11,11,12	1.52	4 (36%)	15,15,17	1.46	3 (20%)
4	NAG	H	1	1,4	14,14,15	0.42	0	17,19,21	0.51	0
4	NAG	H	2	4	14,14,15	0.40	0	17,19,21	0.39	0
5	NAG	I	1	1,5	14,14,15	0.34	0	17,19,21	1.36	2 (11%)
5	NAG	I	2	5	14,14,15	0.71	1 (7%)	17,19,21	0.68	0
5	BMA	I	3	5	11,11,12	1.68	4 (36%)	15,15,17	2.82	4 (26%)
5	MAN	I	4	5	11,11,12	2.26	4 (36%)	15,15,17	2.13	3 (20%)
5	MAN	I	5	5	11,11,12	2.88	6 (54%)	15,15,17	2.20	6 (40%)
4	NAG	J	1	1,4	14,14,15	0.82	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	J	2	4	14,14,15	0.98	1 (7%)	17,19,21	1.14	2 (11%)
3	NAG	K	1	1,3	14,14,15	0.95	1 (7%)	17,19,21	1.00	1 (5%)
3	NAG	K	2	3	14,14,15	0.56	0	17,19,21	0.53	0
3	BMA	K	3	3	11,11,12	1.20	1 (9%)	15,15,17	1.18	1 (6%)
4	NAG	L	1	1,4	14,14,15	0.48	0	17,19,21	0.78	1 (5%)
4	NAG	L	2	4	14,14,15	1.09	1 (7%)	17,19,21	2.12	4 (23%)
4	NAG	M	1	1,4	14,14,15	0.27	0	17,19,21	0.66	0
4	NAG	M	2	4	14,14,15	0.40	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	N	1	1,3	14,14,15	0.26	0	17,19,21	0.77	1 (5%)
3	NAG	N	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	BMA	N	3	3	11,11,12	1.33	1 (9%)	15,15,17	1.00	0
4	NAG	O	1	1,4	14,14,15	0.64	1 (7%)	17,19,21	0.58	0
4	NAG	O	2	4	14,14,15	0.45	0	17,19,21	0.58	0
3	NAG	P	1	1,3	14,14,15	0.51	0	17,19,21	0.59	0
3	NAG	P	2	3	14,14,15	0.79	0	17,19,21	0.88	0
3	BMA	P	3	3	11,11,12	2.03	5 (45%)	15,15,17	2.10	3 (20%)
4	NAG	Q	1	1,4	14,14,15	0.24	0	17,19,21	0.62	0
4	NAG	Q	2	4	14,14,15	0.34	0	17,19,21	0.43	0
2	NAG	R	1	1,2	14,14,15	0.60	0	17,19,21	0.60	0
2	NAG	R	2	2	14,14,15	0.50	0	17,19,21	0.72	0
2	BMA	R	3	2	11,11,12	1.01	1 (9%)	15,15,17	2.74	6 (40%)
2	MAN	R	4	2	11,11,12	2.27	3 (27%)	15,15,17	2.32	8 (53%)

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
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	1/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	5	MAN	C1-C2	5.85	1.65	1.52
2	R	4	MAN	C4-C3	5.39	1.66	1.52
5	I	4	MAN	C4-C3	5.35	1.65	1.52
3	D	3	BMA	O5-C1	-5.05	1.35	1.43
3	D	3	BMA	C4-C5	4.93	1.63	1.53

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	3	BMA	C1-C2-C3	-8.49	99.24	109.67
3	D	3	BMA	C1-C2-C3	-8.04	99.78	109.67
4	L	2	NAG	C2-N2-C7	7.24	133.22	122.90
2	R	3	BMA	O3-C3-C2	-6.31	97.92	109.99
3	P	3	BMA	C1-O5-C5	-5.15	105.22	112.19

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	2	NAG	C3-C2-N2-C7
3	P	2	NAG	O5-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6

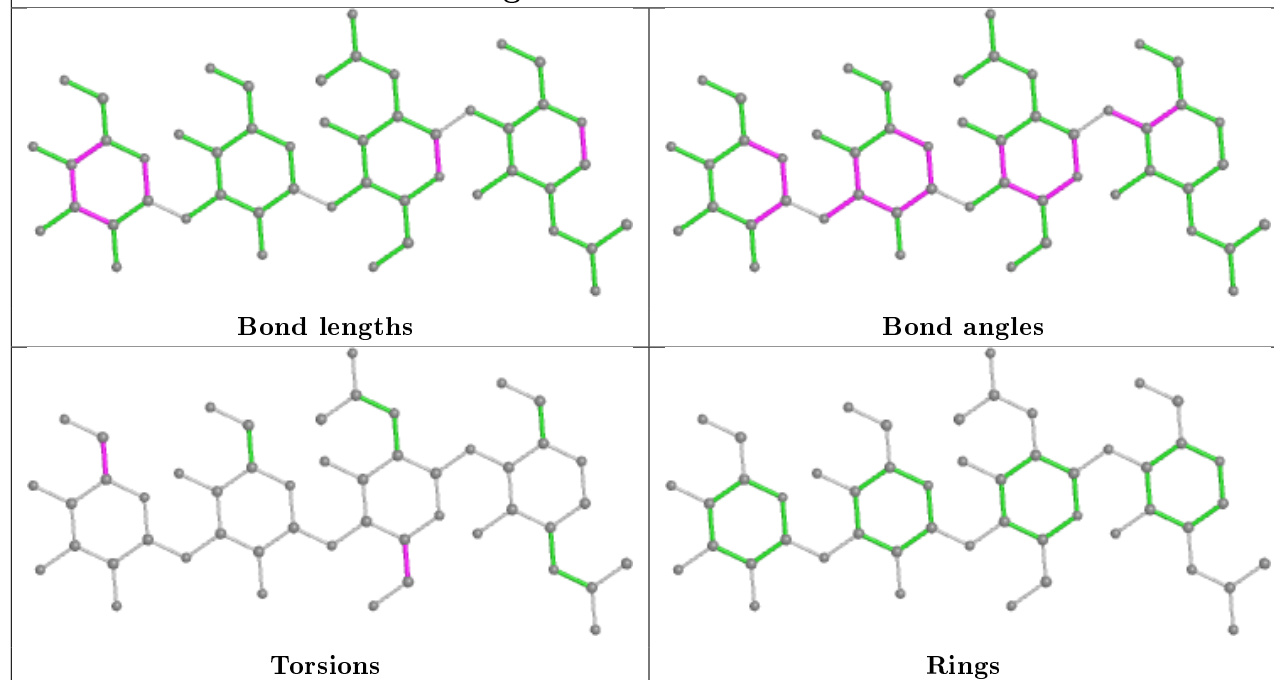
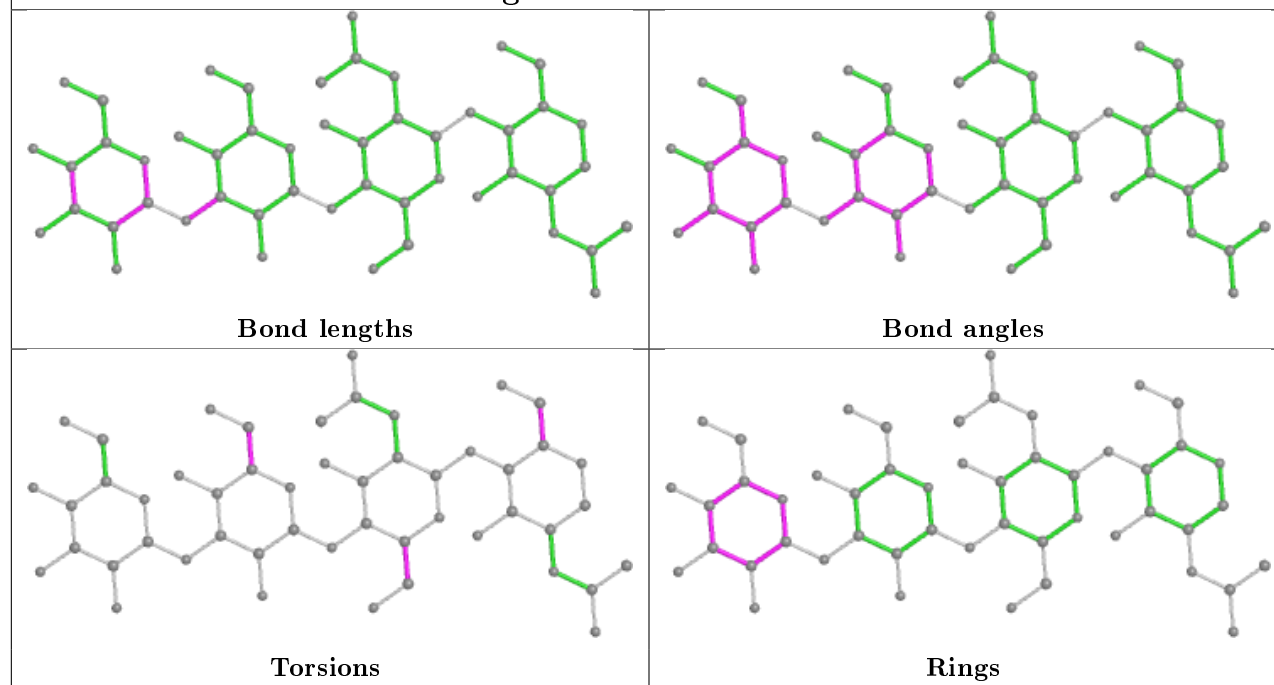
All (1) ring outliers are listed below:

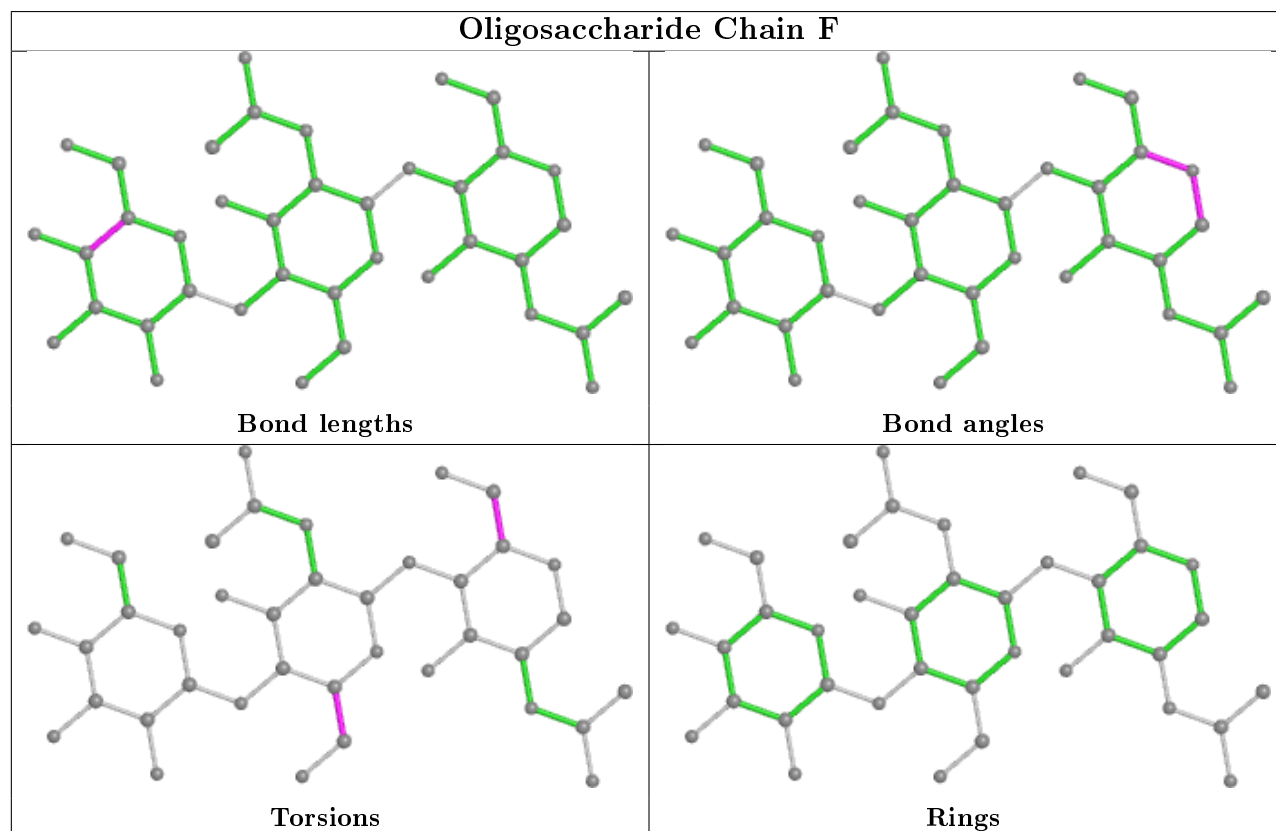
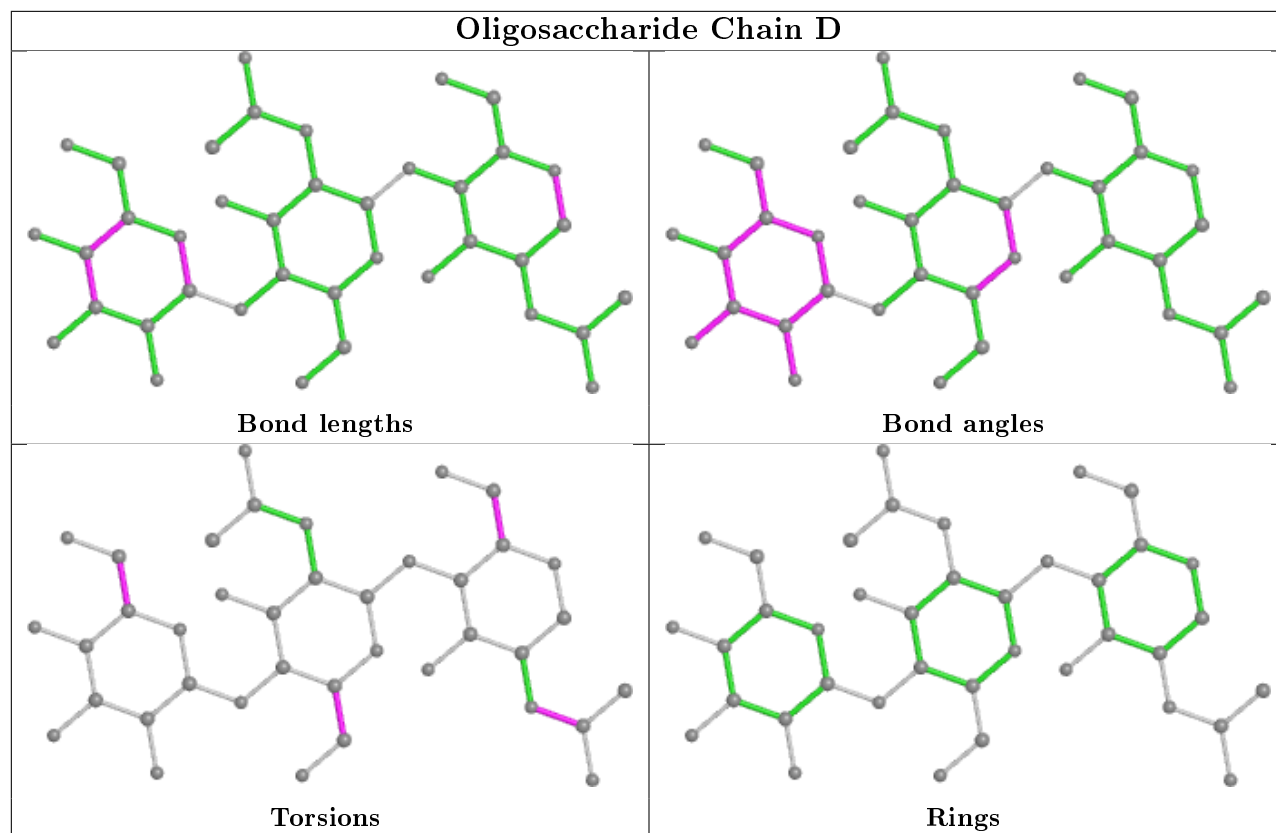
Mol	Chain	Res	Type	Atoms
2	R	4	MAN	C1-C2-C3-C4-C5-O5

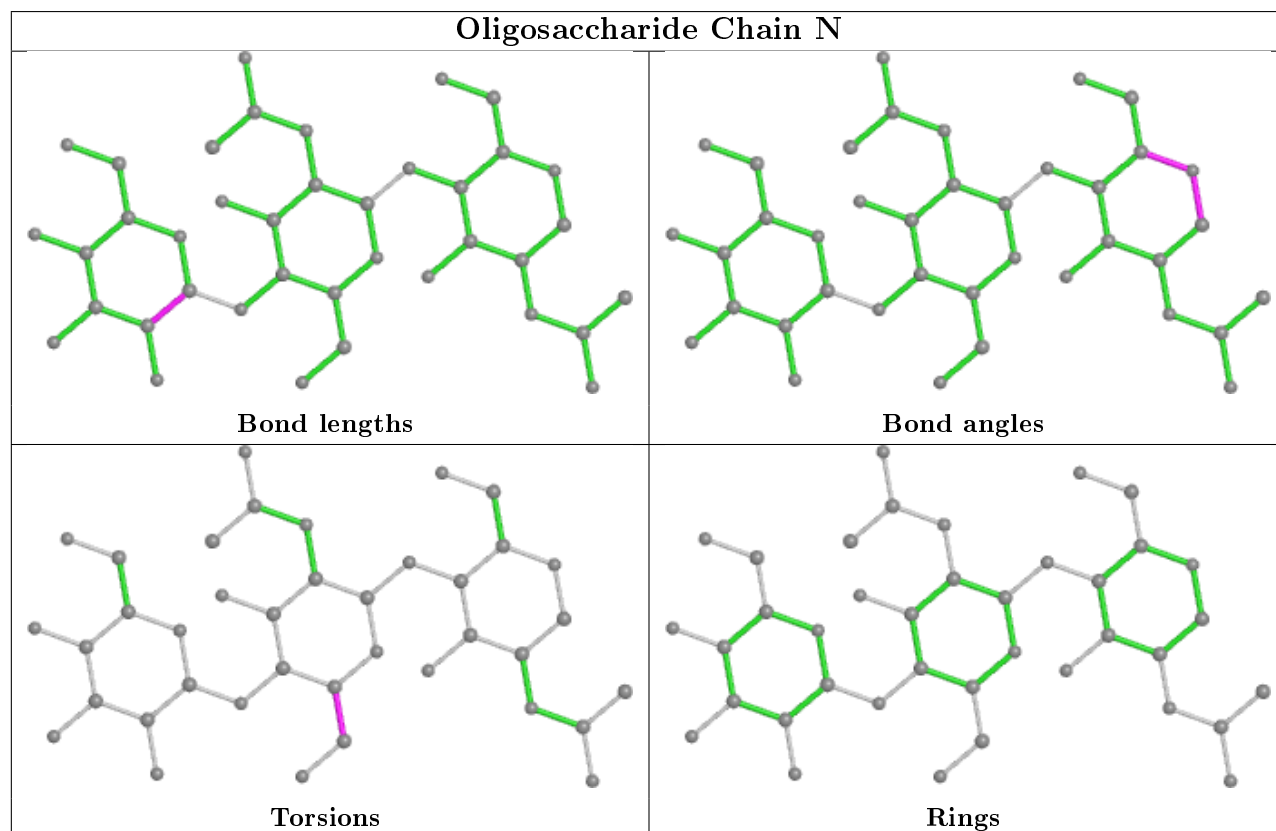
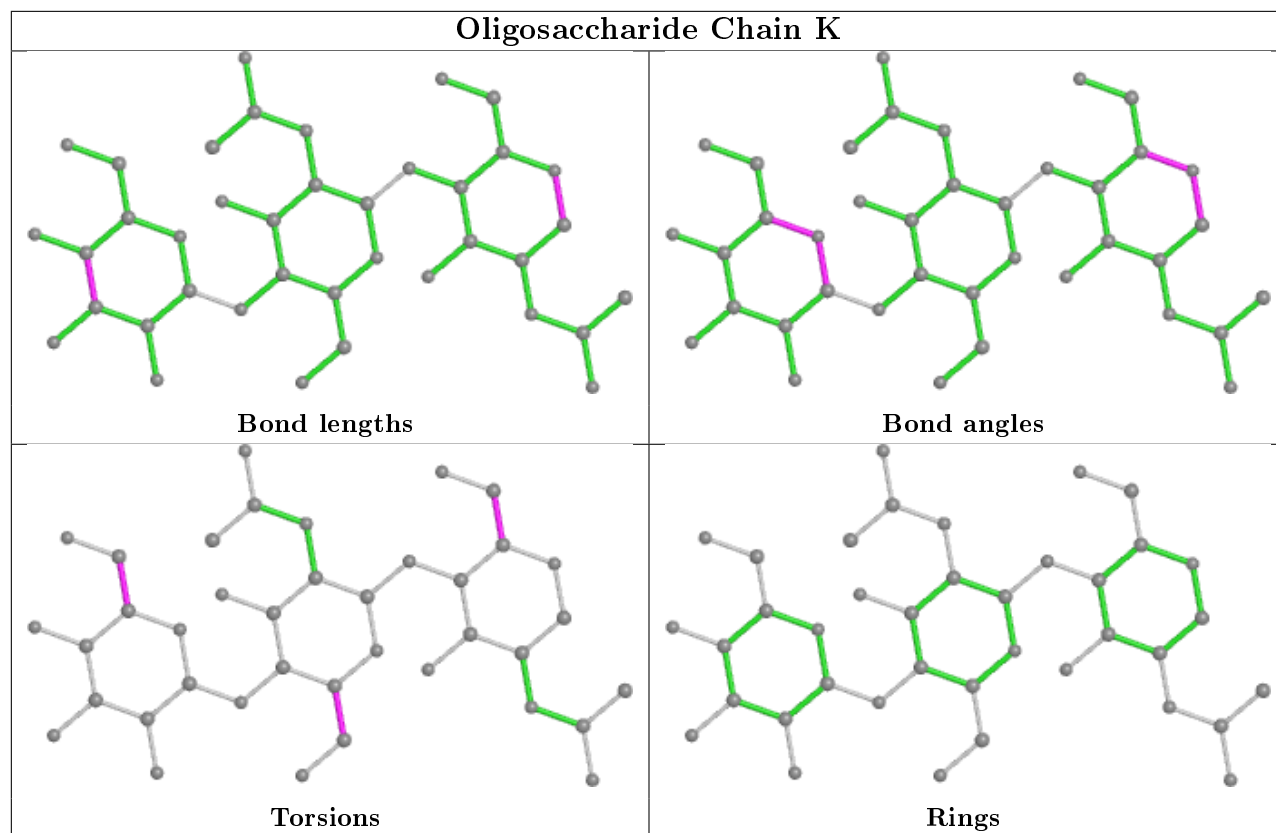
6 monomers are involved in 8 short contacts:

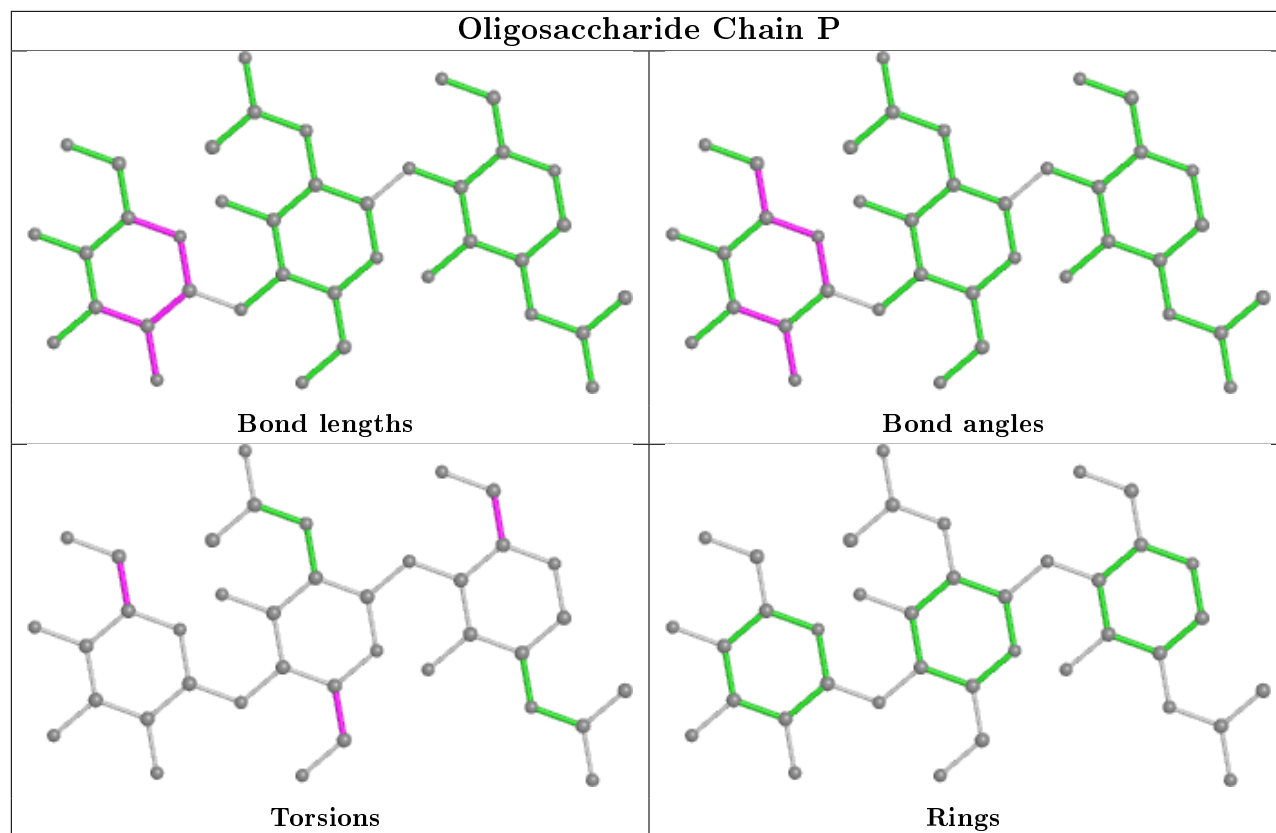
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	2	NAG	3	0
2	C	2	NAG	1	0
3	F	2	NAG	1	0
5	I	1	NAG	1	0
4	M	1	NAG	1	0
5	I	4	MAN	1	0

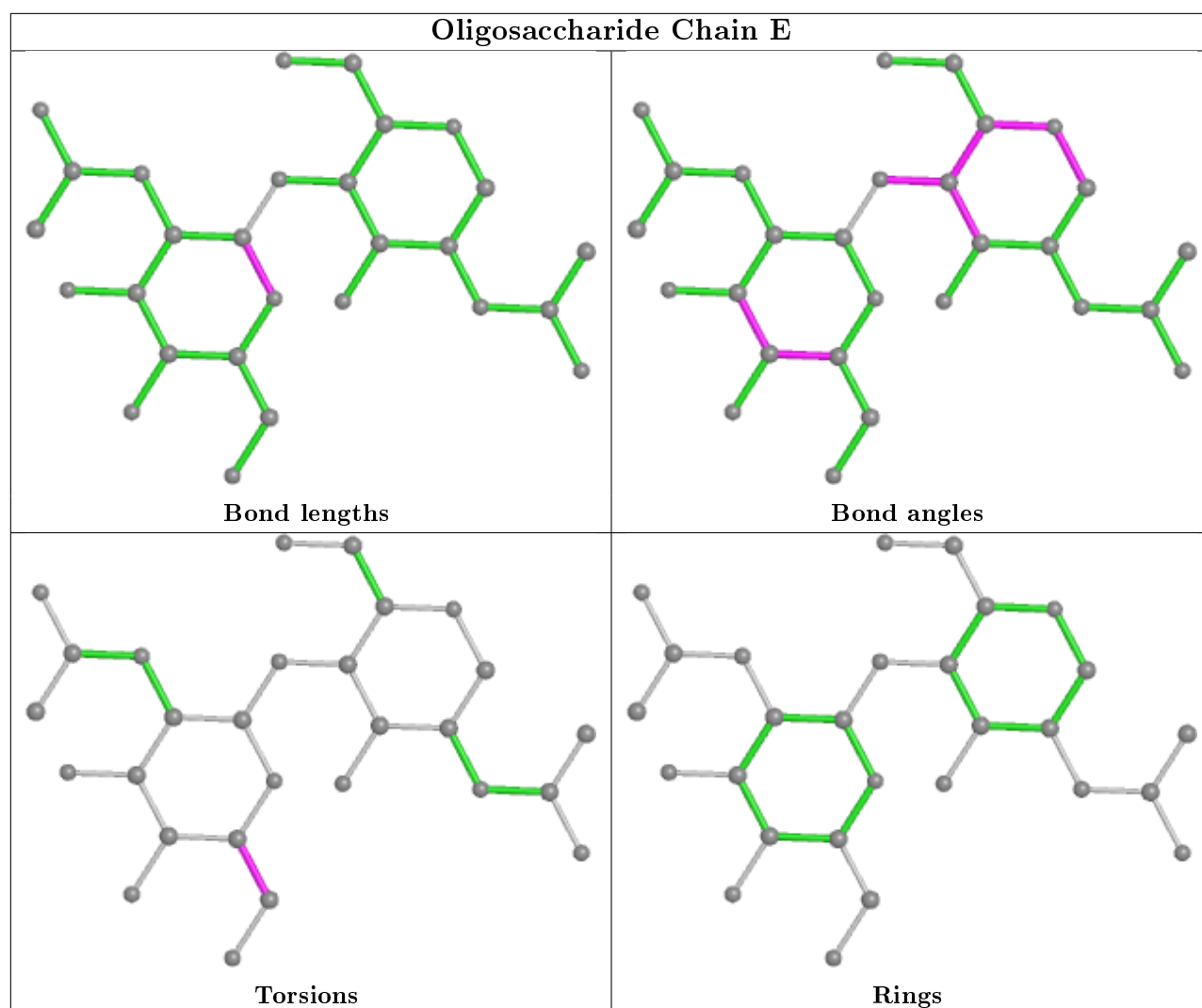
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

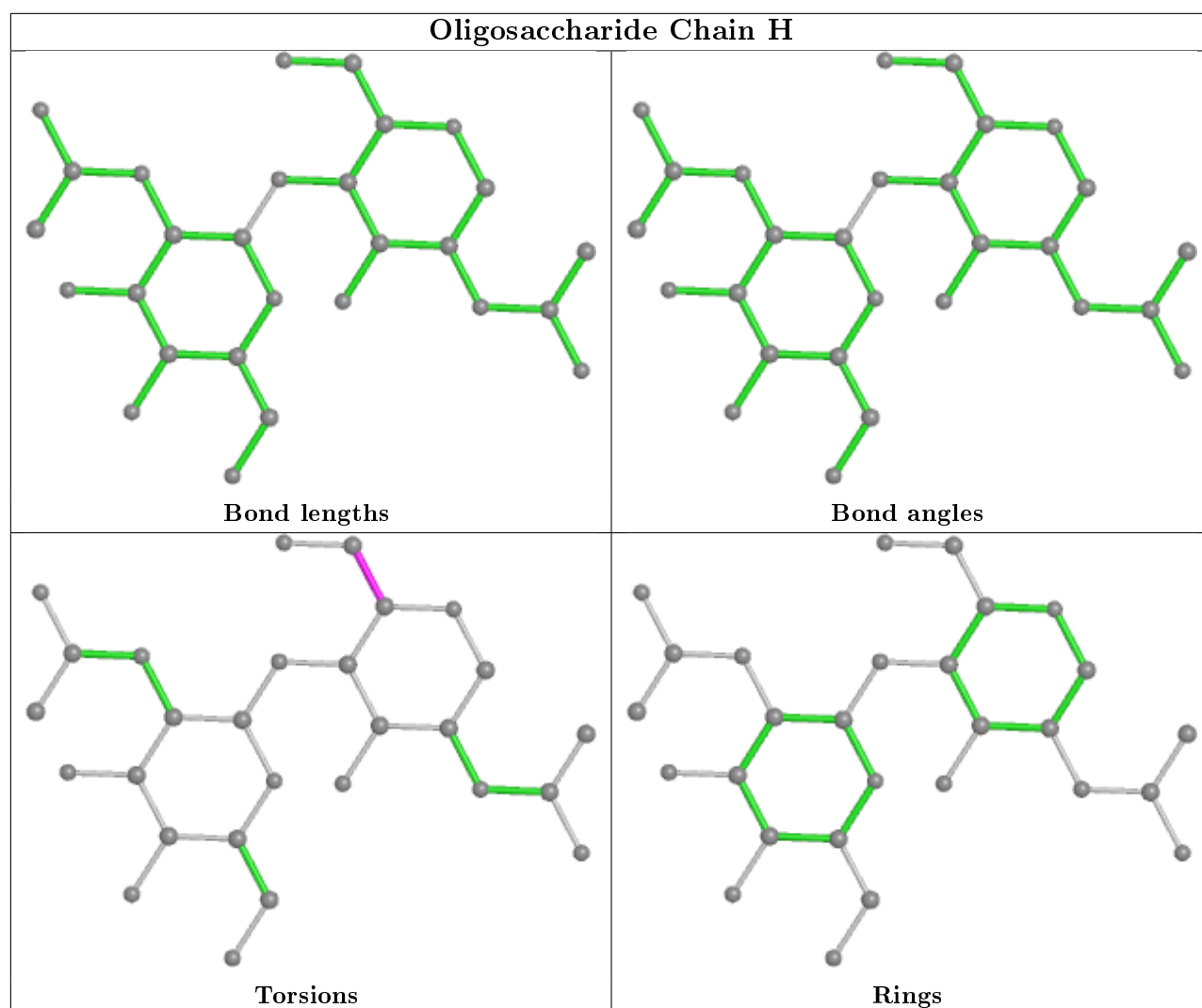
Oligosaccharide Chain C**Oligosaccharide Chain R**

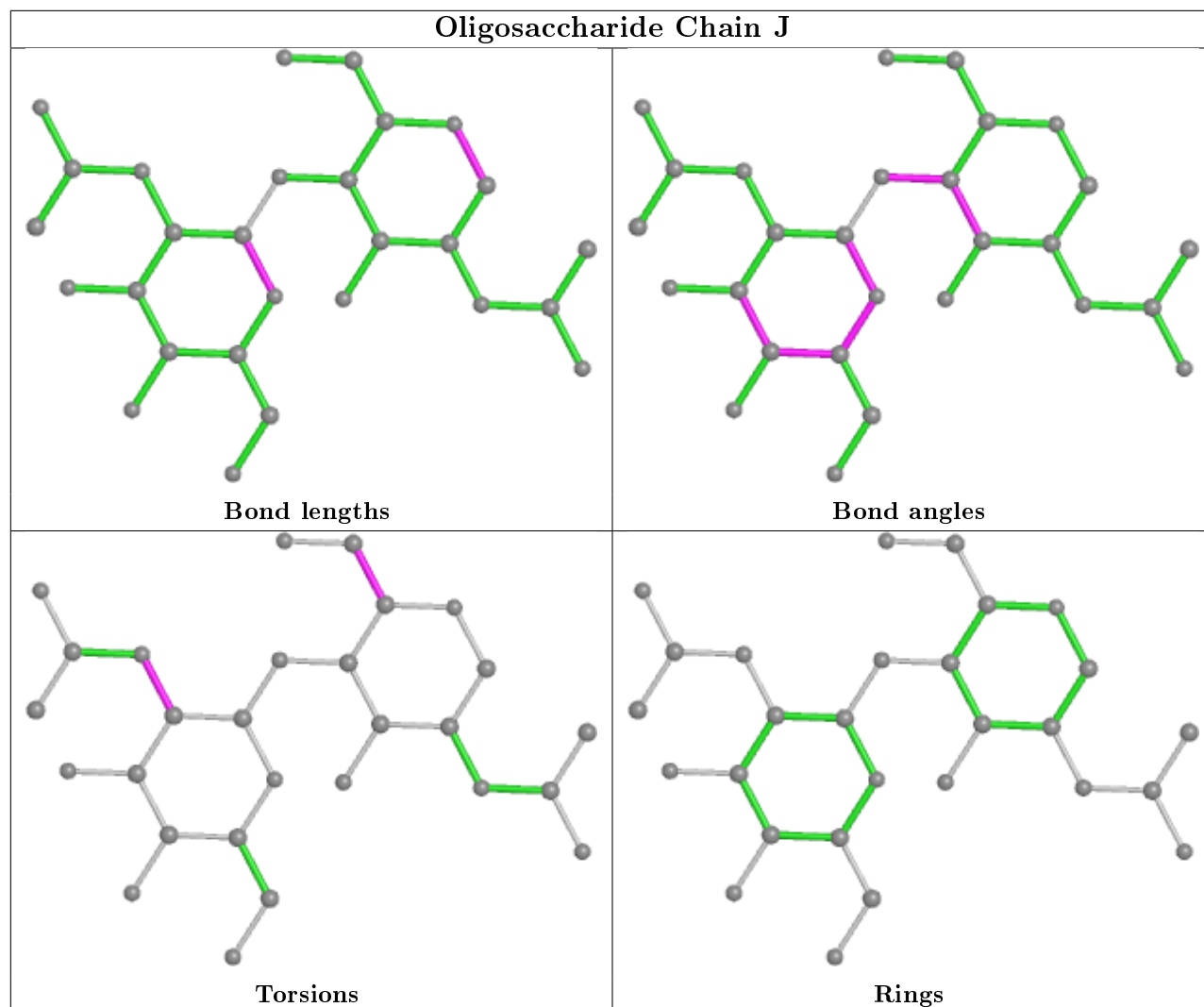


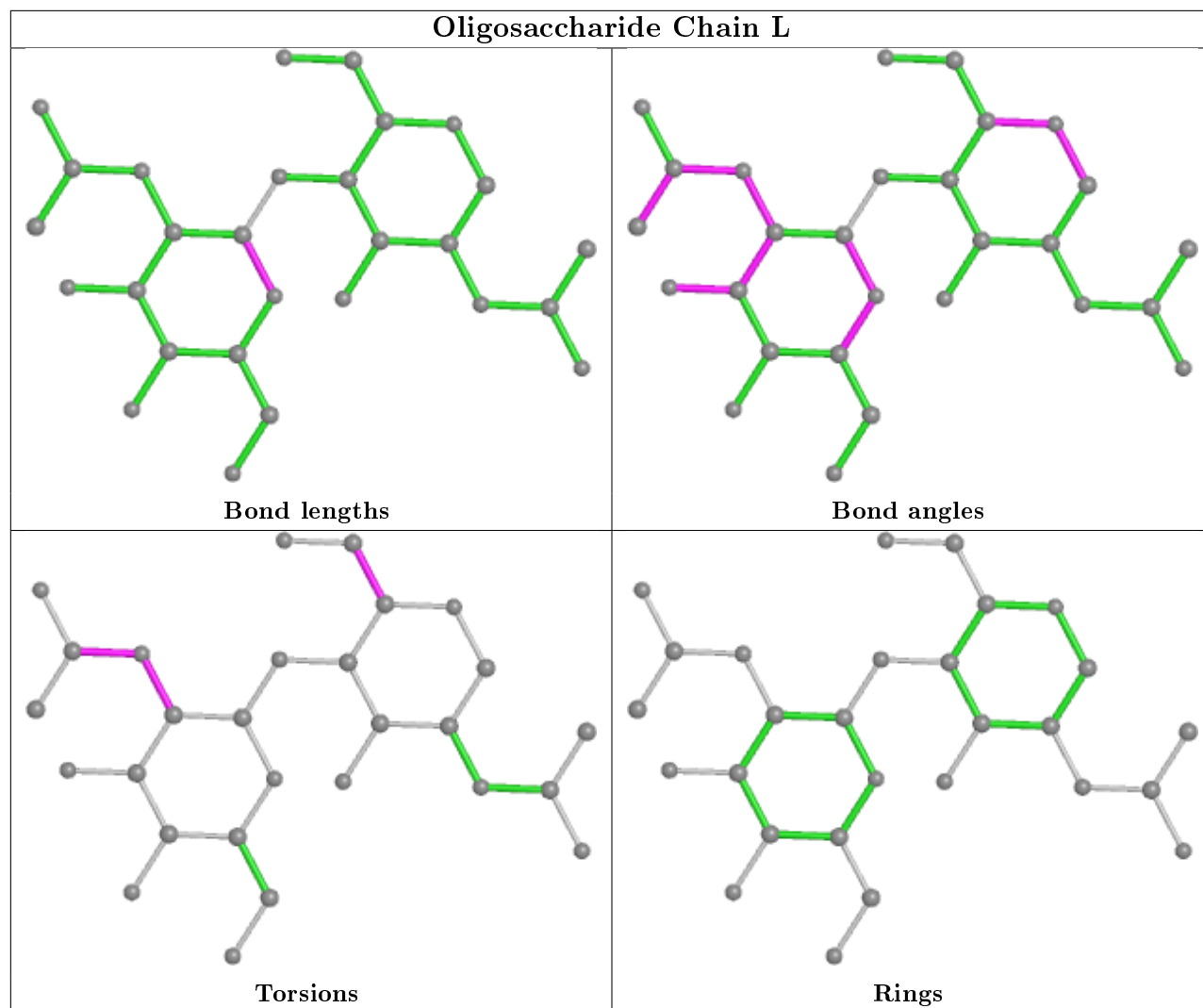


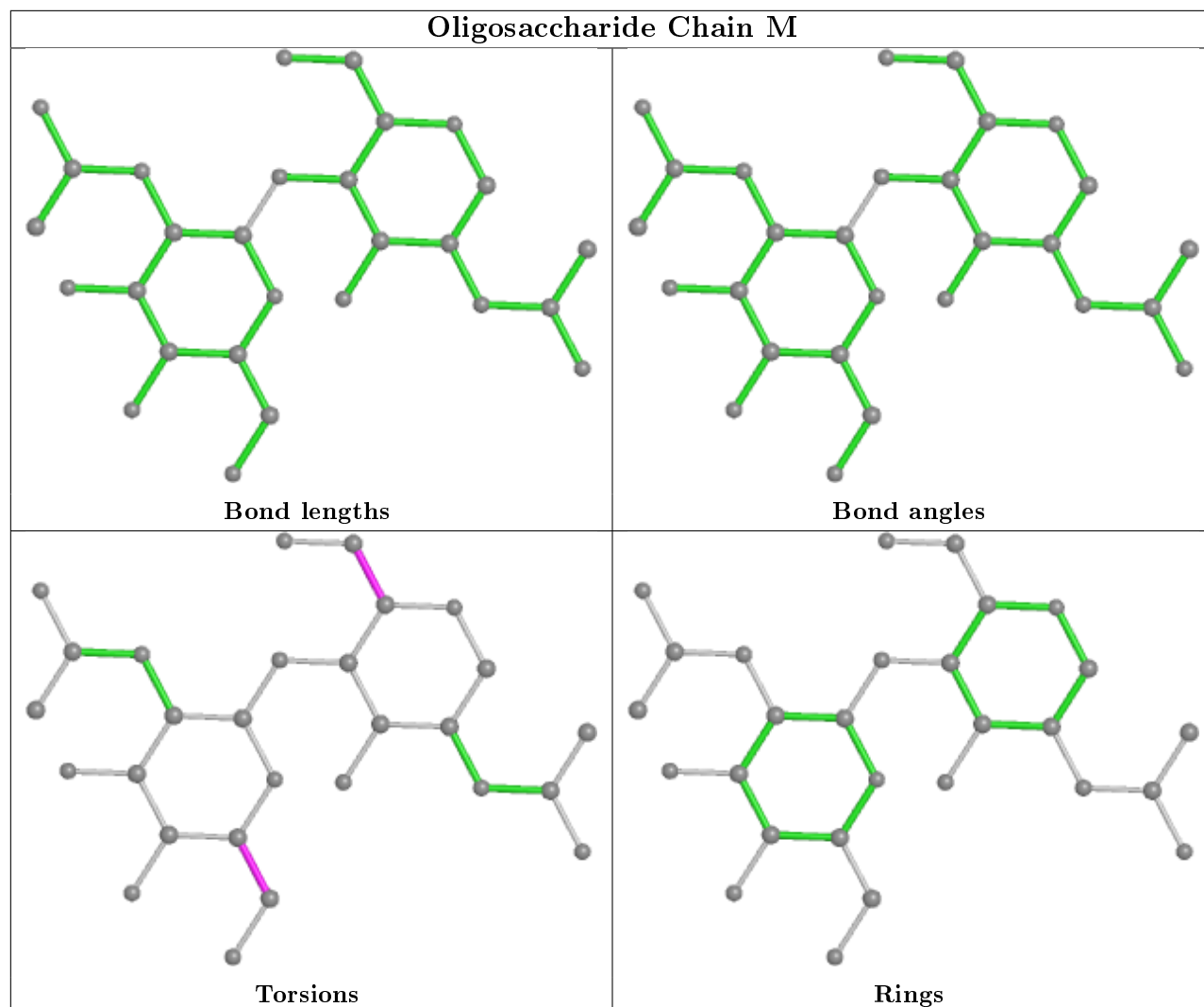


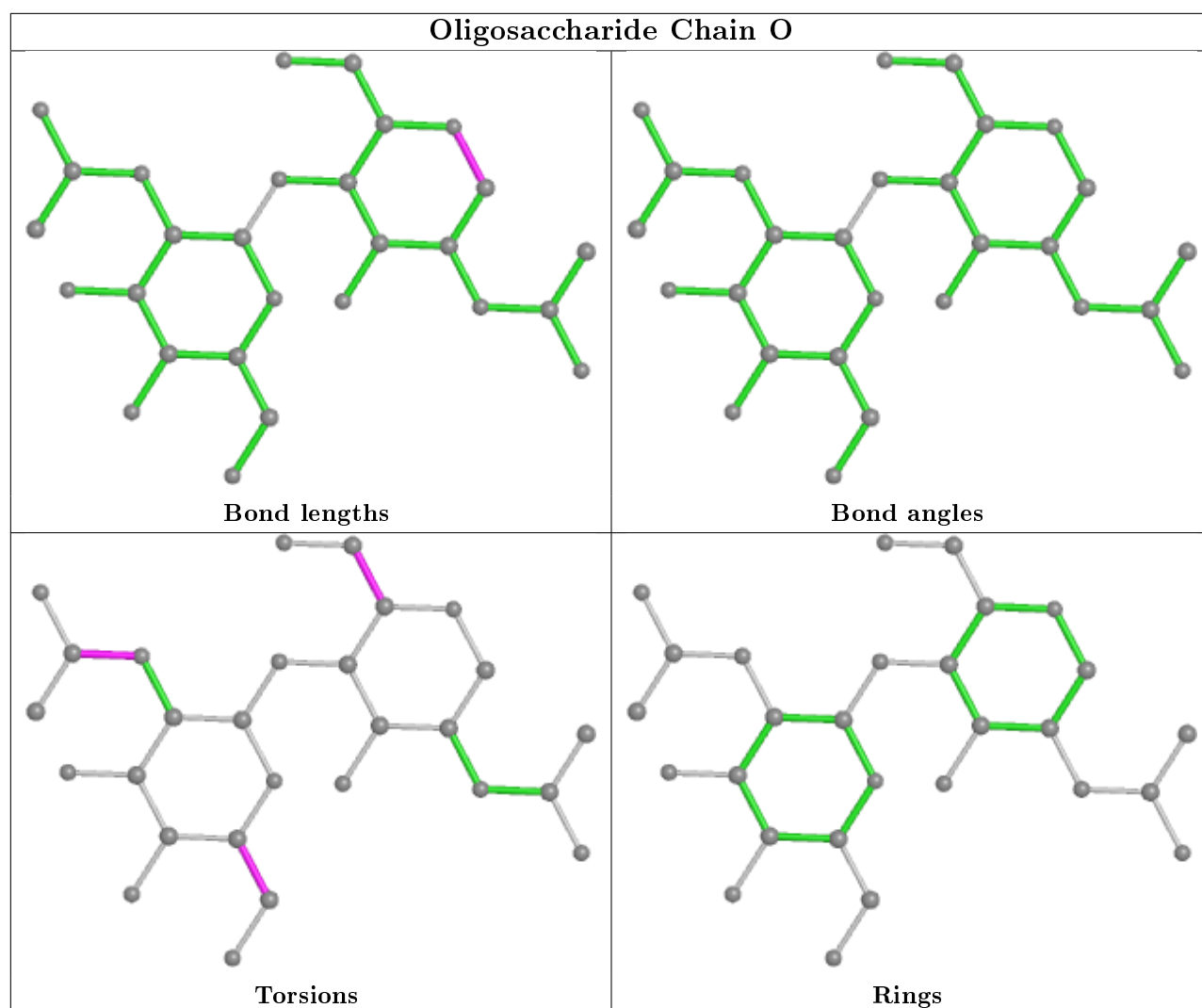


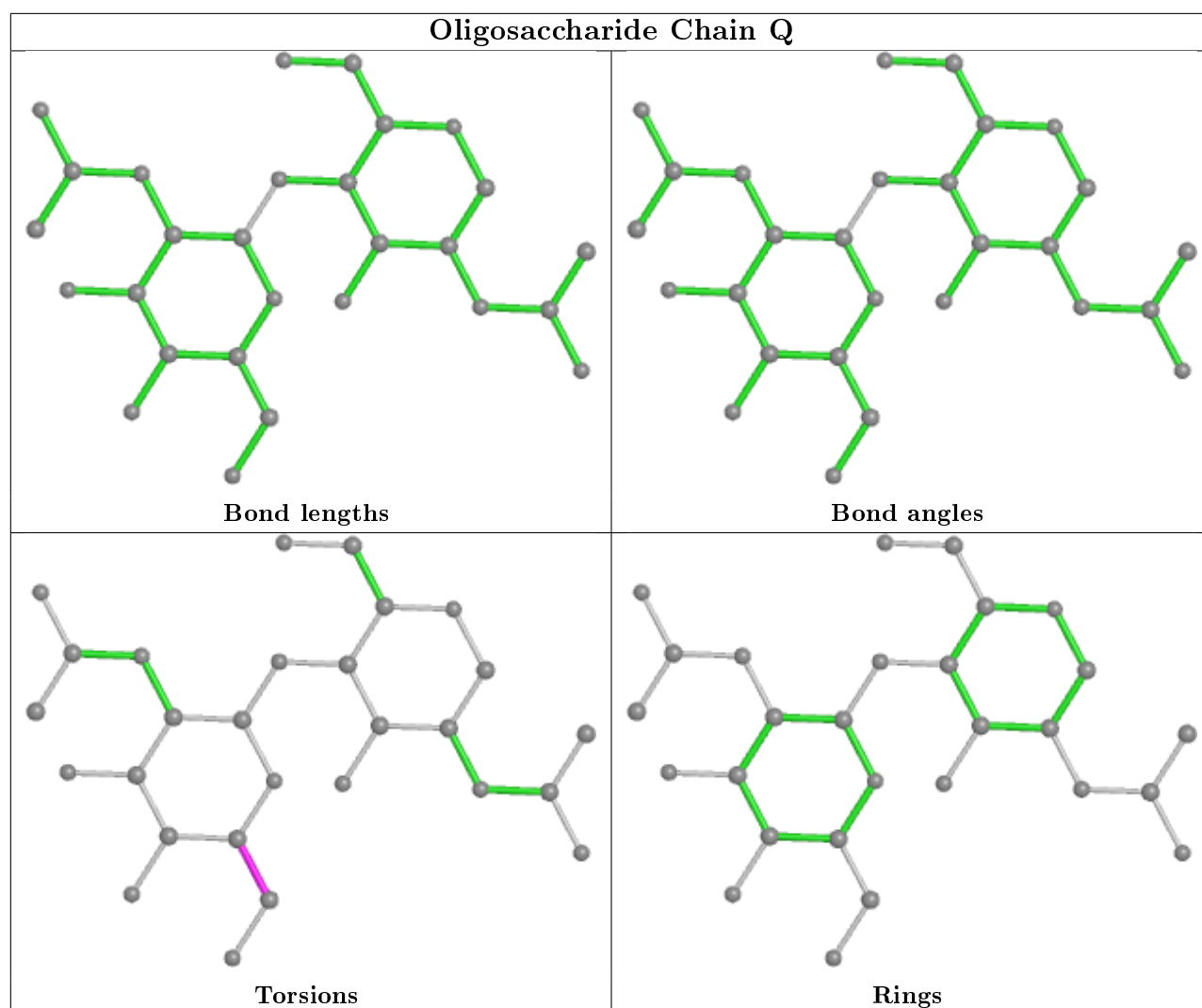


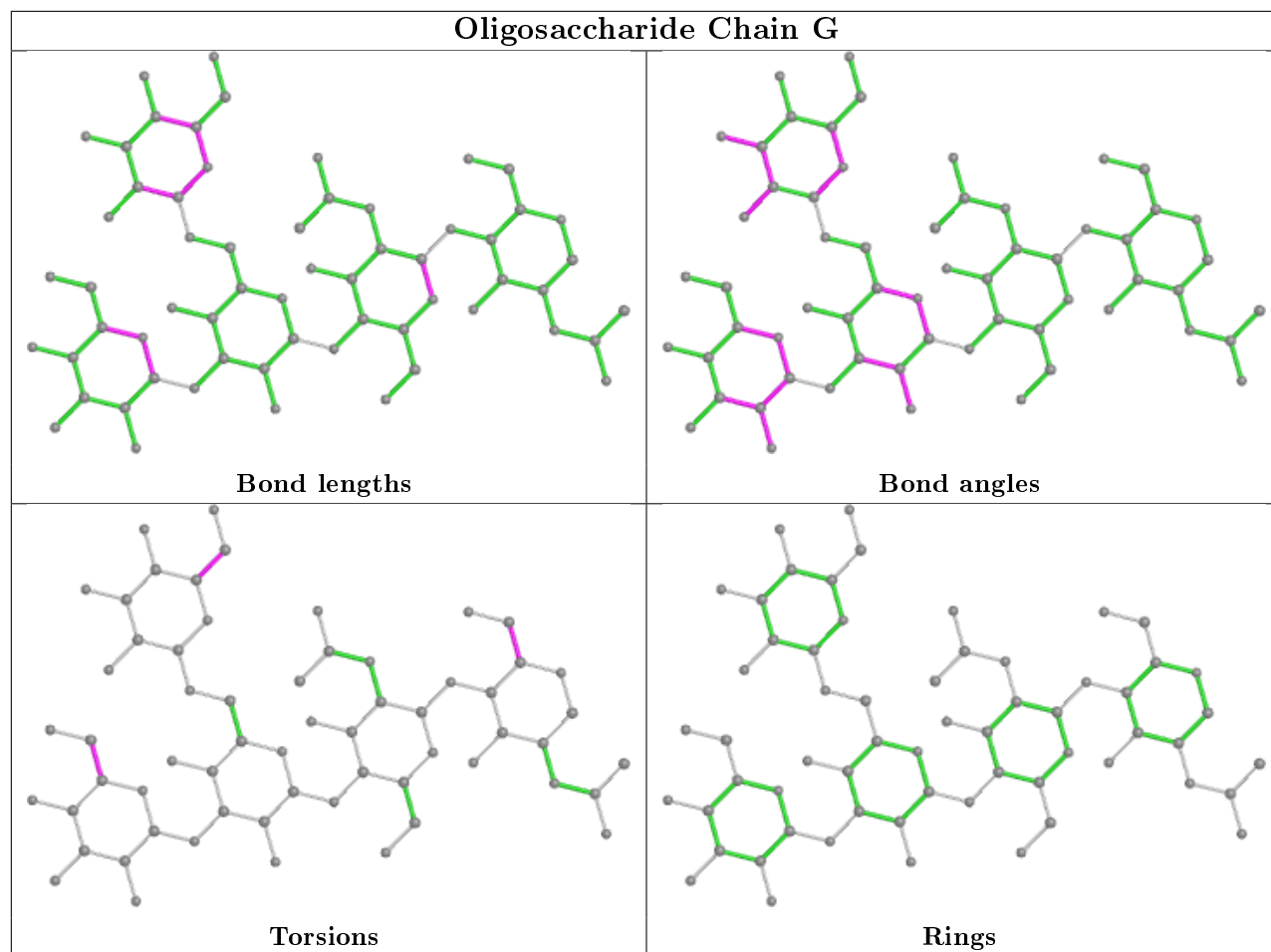


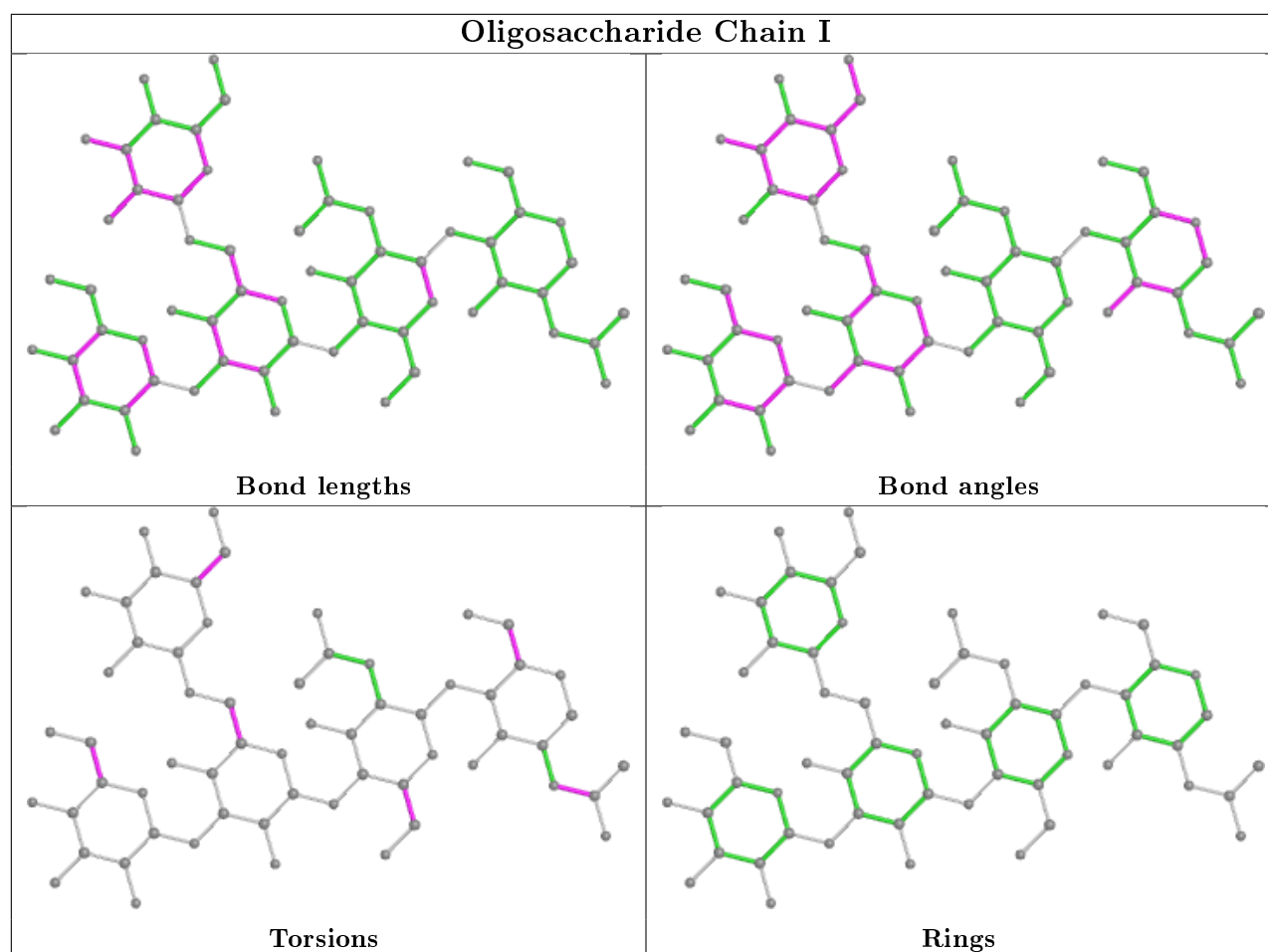












5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 23 are monoatomic - leaving 14 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	$\# Z > 2$
6	NAG	B	1122	1	14,14,15	0.67	0	17,19,21	0.81	1 (5%)
8	7O2	B	1127	7	42,46,46	0.89	1 (2%)	48,62,62	0.65	0
6	NAG	A	1134	1	14,14,15	0.48	0	17,19,21	0.82	1 (5%)
8	7O2	A	1137	7	42,46,46	0.89	1 (2%)	48,62,62	0.99	2 (4%)
6	NAG	B	1102	1	14,14,15	0.45	0	17,19,21	0.40	0
6	NAG	A	1133	1	14,14,15	0.22	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	1124	1	14,14,15	0.18	0	17,19,21	0.41	0
6	NAG	B	1123	1	14,14,15	1.35	1 (7%)	17,19,21	0.71	0
6	NAG	B	1108	1	14,14,15	0.35	0	17,19,21	0.46	0
6	NAG	A	1135	1	14,14,15	0.68	0	17,19,21	0.55	0
6	NAG	B	1109	1	14,14,15	0.17	0	17,19,21	0.69	1 (5%)
6	NAG	A	1132	1	14,14,15	0.60	0	17,19,21	0.66	1 (5%)
6	NAG	B	1117	1	14,14,15	0.63	0	17,19,21	0.61	0
6	NAG	B	1125	1	14,14,15	1.25	1 (7%)	17,19,21	1.67	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1122	1	-	0/6/23/26	0/1/1/1
8	7O2	B	1127	7	-	7/38/44/44	0/4/4/4
6	NAG	A	1134	1	-	4/6/23/26	0/1/1/1
8	7O2	A	1137	7	-	6/38/44/44	0/4/4/4
6	NAG	B	1102	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1133	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1124	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1123	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1108	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1135	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1109	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1132	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1117	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1125	1	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1125	NAG	C1-C2	4.54	1.59	1.52
6	B	1123	NAG	O5-C1	-4.50	1.36	1.43
8	A	1137	7O2	C42-N43	3.74	1.42	1.32
8	B	1127	7O2	C42-N43	3.46	1.41	1.32

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1125	NAG	C1-O5-C5	4.57	118.38	112.19
6	B	1125	NAG	C4-C3-C2	-3.76	105.51	111.02
8	A	1137	7O2	C25-C18-C19	-3.13	102.24	111.84
6	A	1134	NAG	C1-O5-C5	2.61	115.72	112.19
6	B	1109	NAG	C1-O5-C5	2.36	115.39	112.19

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

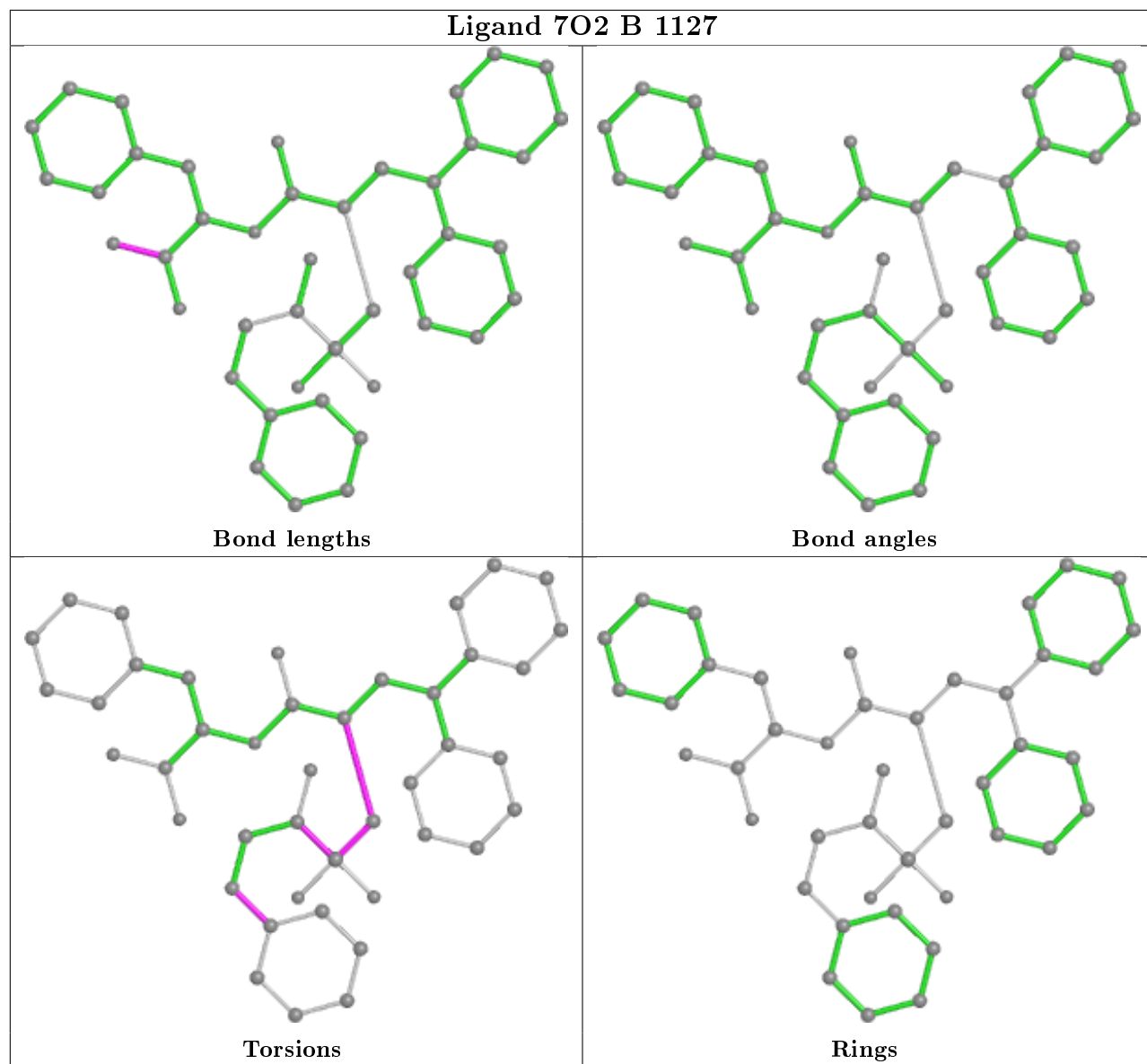
Mol	Chain	Res	Type	Atoms
8	A	1137	7O2	C16-C15-P12-O13
8	A	1137	7O2	C16-C15-P12-O14
8	B	1127	7O2	C2-C1-P12-O14
8	B	1127	7O2	P12-C15-C16-C31
8	B	1127	7O2	C16-C15-P12-O13

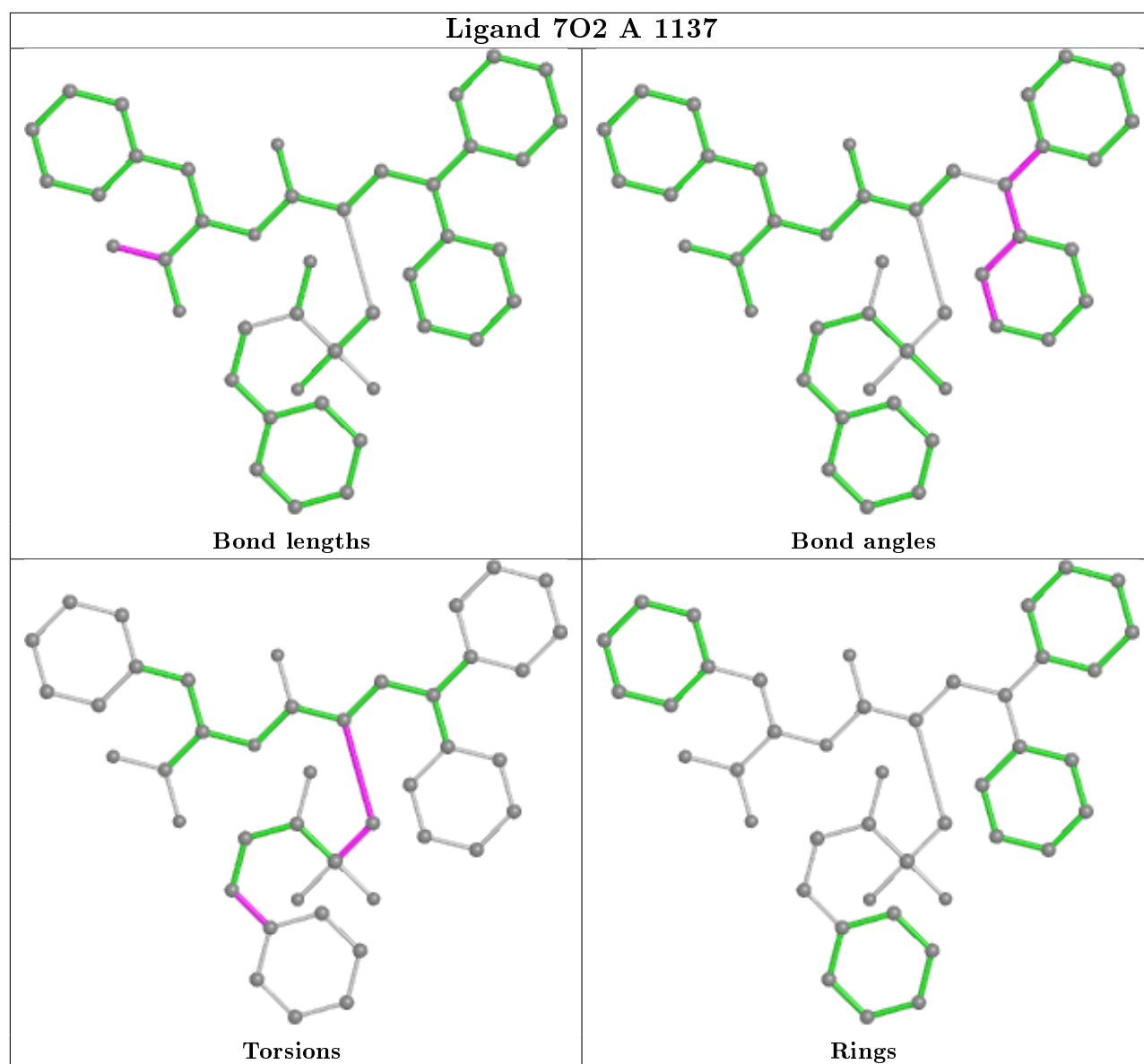
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1137	7O2	1	0
6	A	1132	NAG	1	0
6	B	1117	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	870/881 (98%)	-0.18	17 (1%) 65 68	30, 45, 71, 115	0
1	B	866/881 (98%)	-0.01	25 (2%) 51 55	32, 52, 77, 109	0
All	All	1736/1762 (98%)	-0.10	42 (2%) 59 62	30, 48, 75, 115	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1035	ALA	6.7
1	B	340	ASP	5.3
1	B	649	SER	5.1
1	A	1033	ALA	4.8
1	A	224	ALA	4.4

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

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

6.3 Carbohydrates [i](#)

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

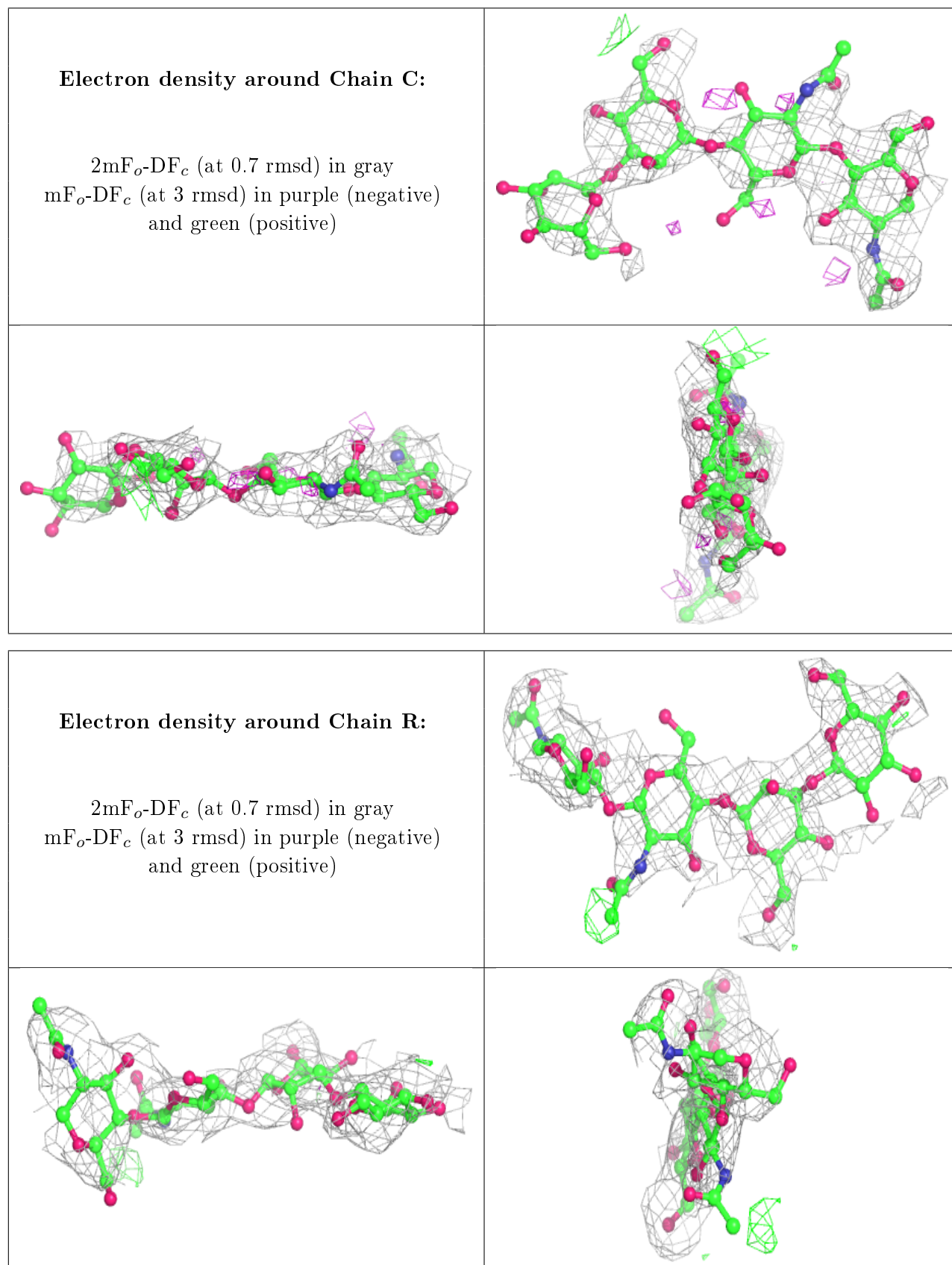
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	R	3	11/12	0.45	0.31	91,124,128,130	0
3	BMA	D	3	11/12	0.58	0.47	122,134,141,145	0
4	NAG	M	2	14/15	0.64	0.45	97,116,120,123	0
3	BMA	K	3	11/12	0.67	0.38	96,104,113,114	0
2	MAN	R	4	11/12	0.67	0.34	102,112,122,125	0

Continued on next page...

Continued from previous page...

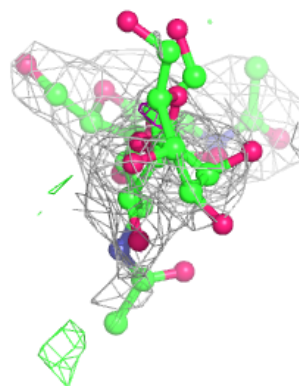
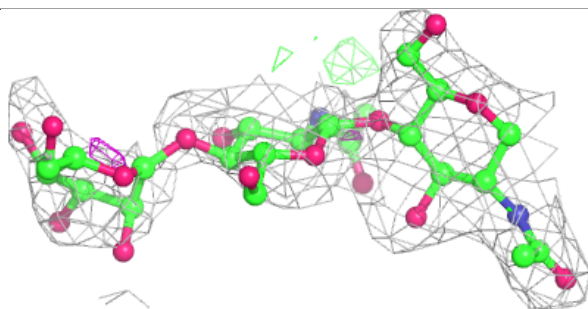
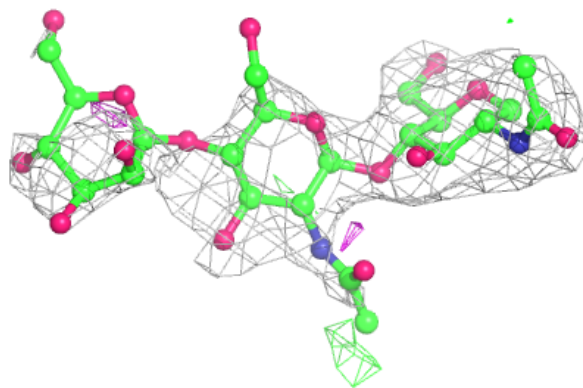
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	I	4	11/12	0.70	0.44	84,97,112,120	0
3	NAG	D	2	14/15	0.70	0.36	93,113,125,133	0
5	MAN	I	5	11/12	0.71	0.44	98,108,118,122	0
2	BMA	C	3	11/12	0.73	0.24	96,105,112,115	0
4	NAG	L	2	14/15	0.74	0.60	84,106,109,109	0
4	NAG	E	2	14/15	0.75	0.31	65,92,99,101	0
4	NAG	Q	2	14/15	0.75	0.43	90,103,114,115	0
2	MAN	C	4	11/12	0.75	0.40	100,109,119,123	0
4	NAG	L	1	14/15	0.76	0.40	88,104,110,111	0
5	BMA	I	3	11/12	0.78	0.39	99,107,118,121	0
4	NAG	O	2	14/15	0.78	0.40	103,115,124,128	0
4	NAG	H	2	14/15	0.78	0.36	92,111,116,120	0
4	NAG	J	2	14/15	0.78	0.52	108,120,131,138	0
5	NAG	I	2	14/15	0.80	0.36	94,103,110,114	0
2	NAG	R	2	14/15	0.80	0.38	111,121,127,128	0
3	BMA	P	3	11/12	0.81	0.24	103,112,120,124	0
3	NAG	F	2	14/15	0.82	0.25	68,93,100,103	0
5	MAN	G	5	11/12	0.83	0.16	75,81,86,90	0
3	BMA	N	3	11/12	0.83	0.27	79,95,103,105	0
2	NAG	R	1	14/15	0.85	0.24	82,99,114,123	0
4	NAG	O	1	14/15	0.85	0.20	66,79,96,111	0
3	BMA	F	3	11/12	0.85	0.16	79,91,103,104	0
2	NAG	C	2	14/15	0.86	0.43	80,95,107,108	0
4	NAG	J	1	14/15	0.87	0.21	84,91,105,114	0
3	NAG	K	1	14/15	0.88	0.28	62,79,87,92	0
4	NAG	H	1	14/15	0.90	0.29	91,99,104,105	0
3	NAG	D	1	14/15	0.92	0.15	58,75,91,103	0
5	NAG	I	1	14/15	0.92	0.22	80,84,94,94	0
3	NAG	K	2	14/15	0.92	0.42	77,88,97,99	0
3	NAG	P	2	14/15	0.92	0.20	64,84,93,105	0
5	BMA	G	3	11/12	0.92	0.14	61,71,79,80	0
4	NAG	E	1	14/15	0.93	0.14	48,58,68,68	0
3	NAG	N	1	14/15	0.93	0.17	60,79,85,86	0
4	NAG	M	1	14/15	0.93	0.26	68,84,97,106	0
3	NAG	F	1	14/15	0.93	0.26	58,72,82,84	0
4	NAG	Q	1	14/15	0.93	0.25	81,86,91,101	0
2	NAG	C	1	14/15	0.94	0.15	44,56,67,68	0
5	MAN	G	4	11/12	0.94	0.09	57,64,72,80	0
3	NAG	N	2	14/15	0.94	0.16	70,79,87,95	0
3	NAG	P	1	14/15	0.95	0.15	57,72,82,86	0
5	NAG	G	1	14/15	0.96	0.11	41,53,57,67	0
5	NAG	G	2	14/15	0.97	0.12	52,57,69,70	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.

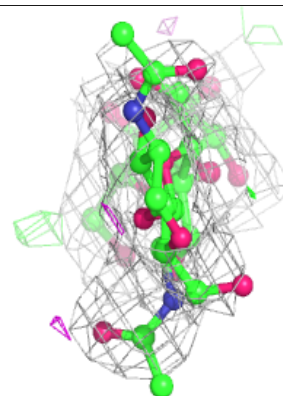
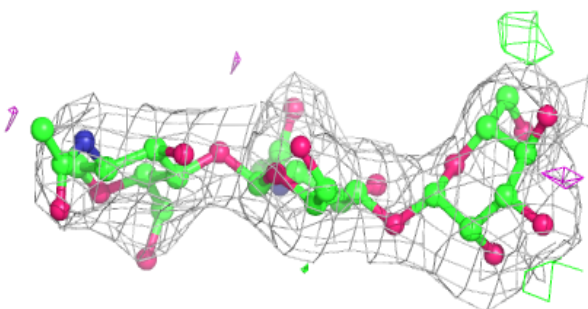
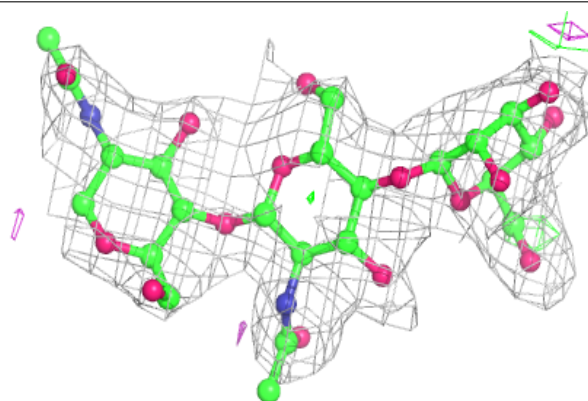


Electron density around Chain D:

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

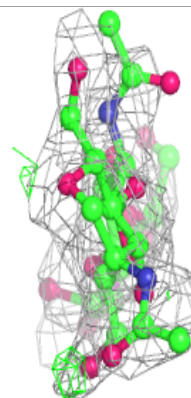
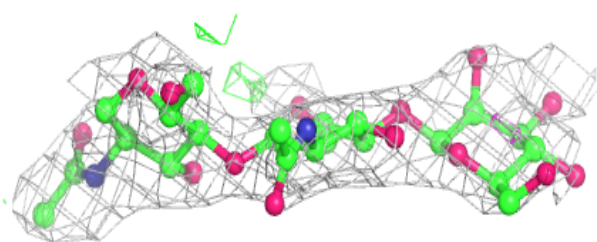
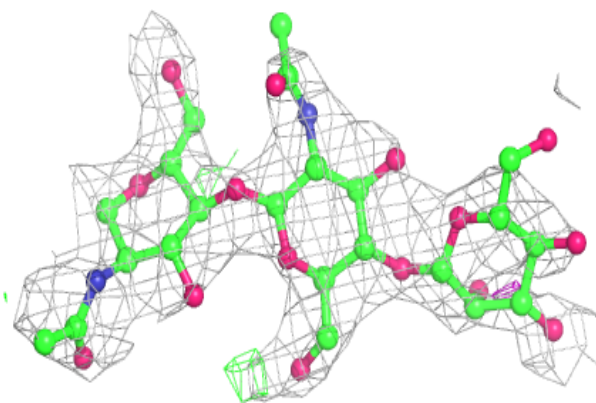
**Electron density around Chain F:**

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

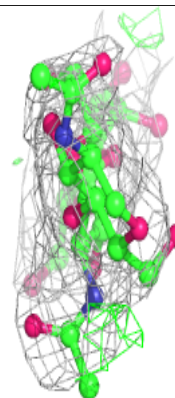
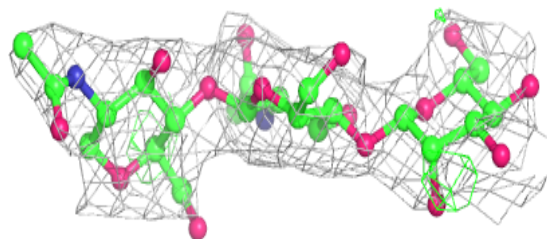
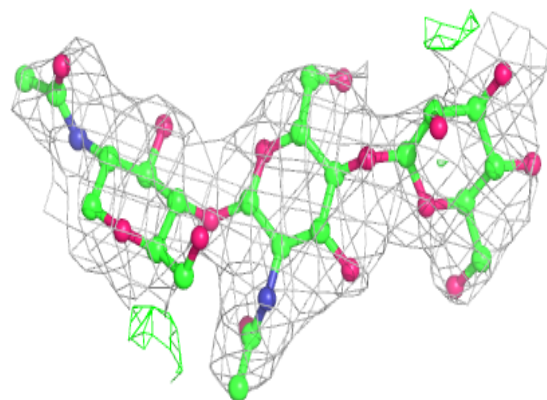


Electron density around Chain K:

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

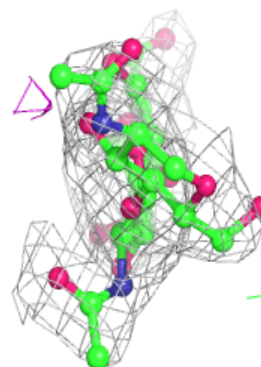
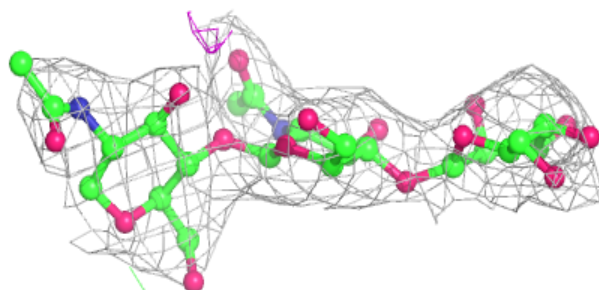
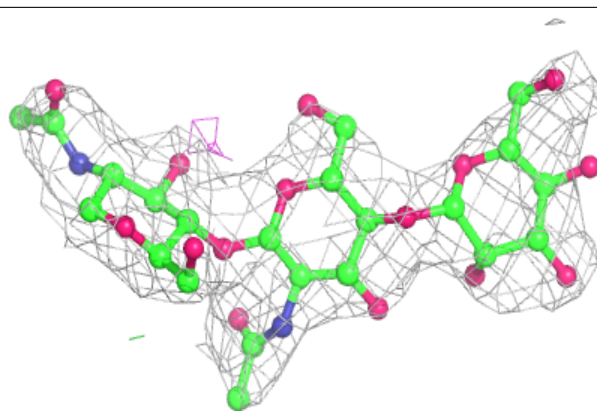
**Electron density around Chain N:**

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

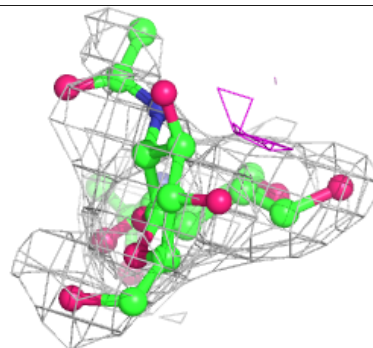
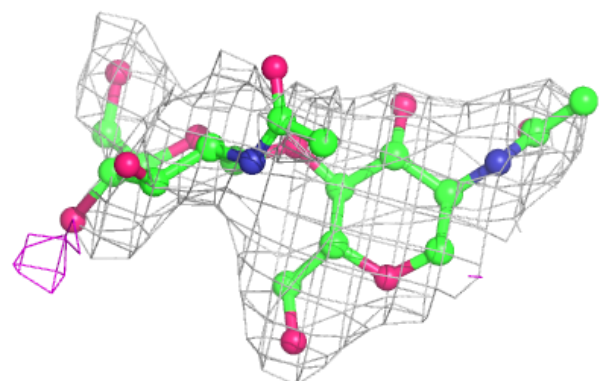
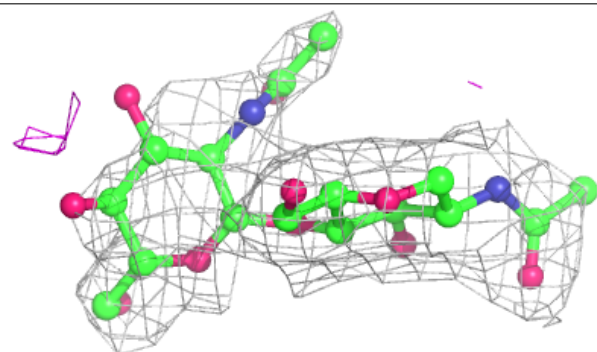


Electron density around Chain P:

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

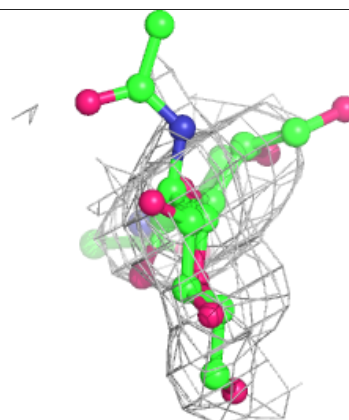
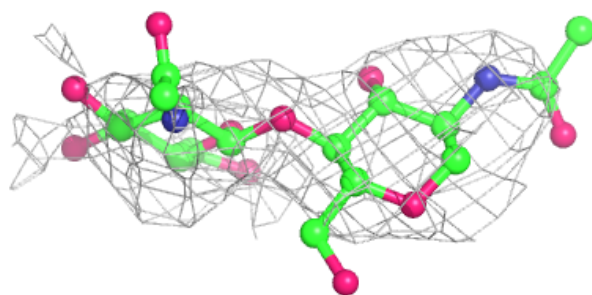
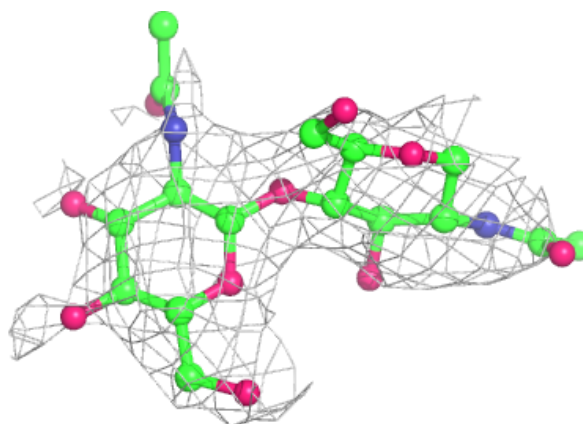
**Electron density around Chain E:**

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



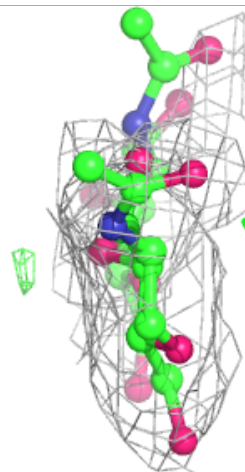
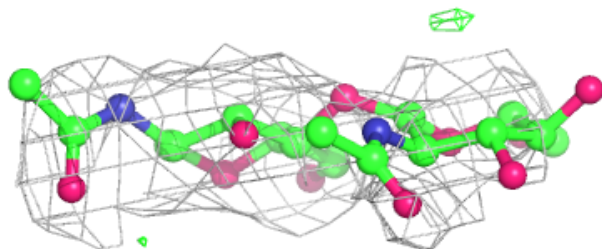
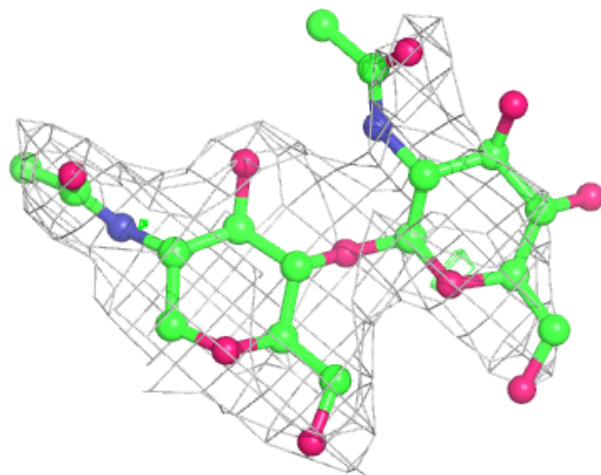
Electron density around Chain H:

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



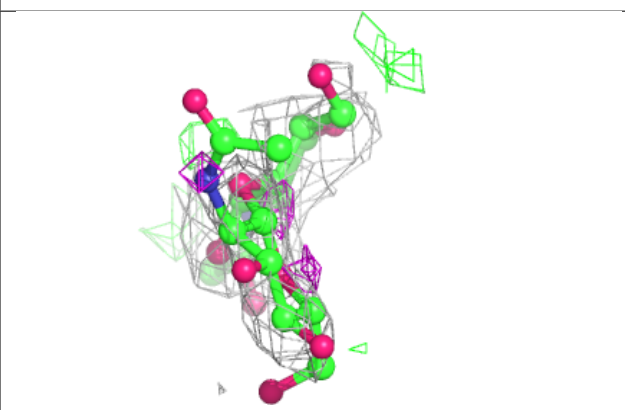
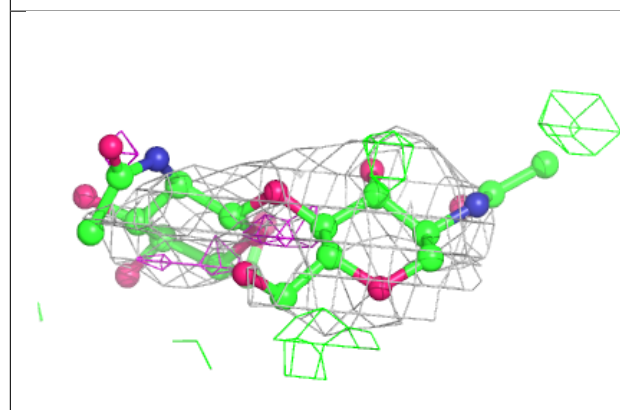
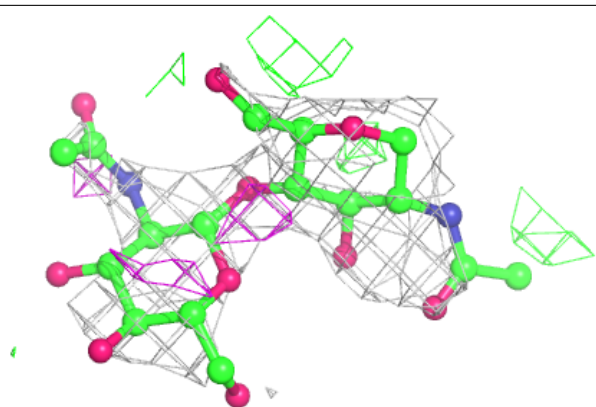
Electron density around Chain J:

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



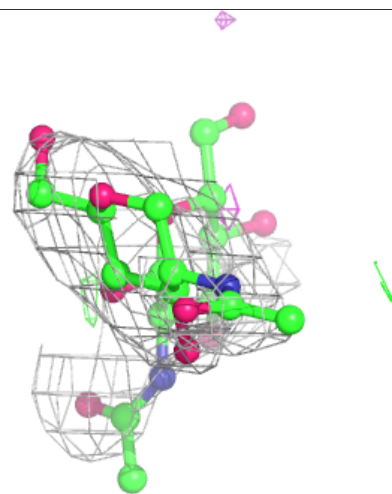
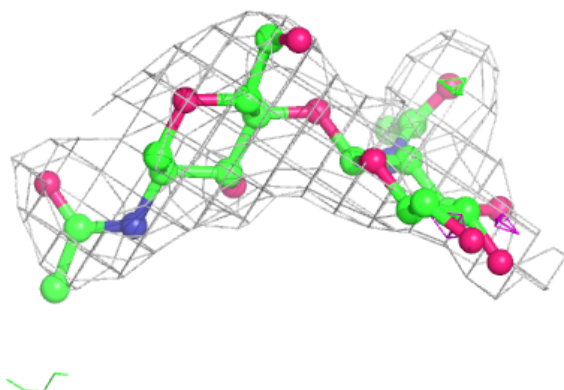
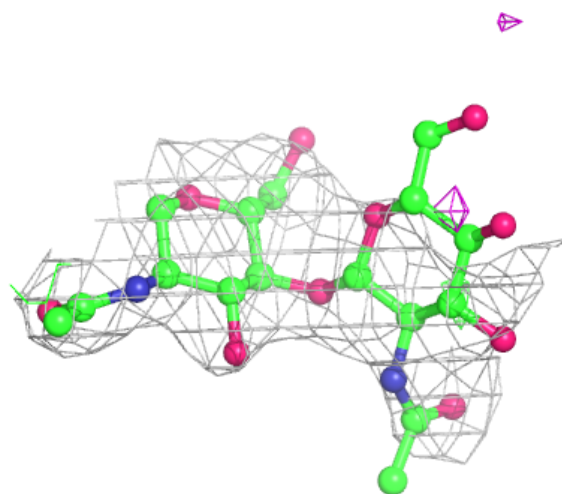
Electron density around Chain L:

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



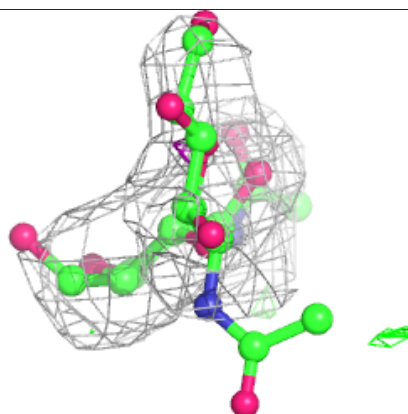
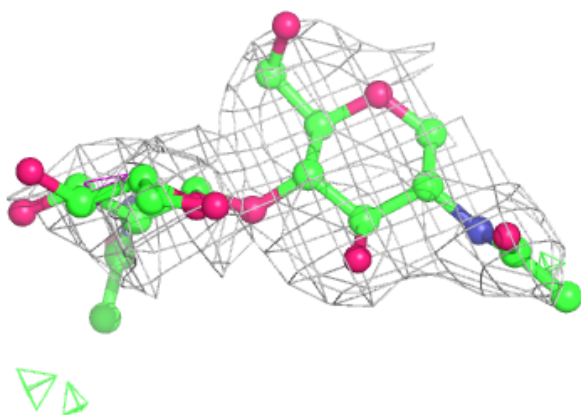
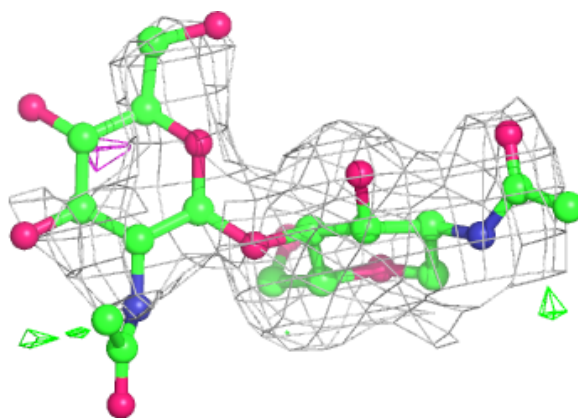
Electron density around Chain M:

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



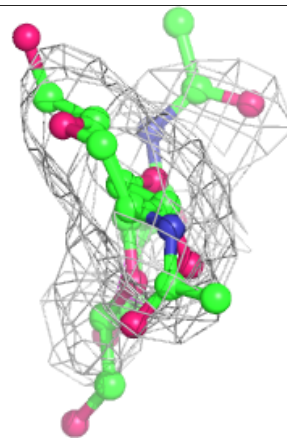
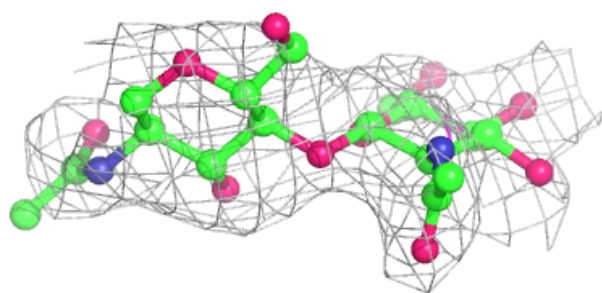
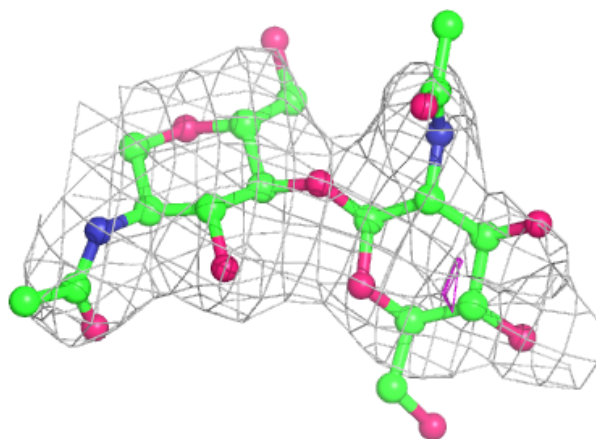
Electron density around Chain O:

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



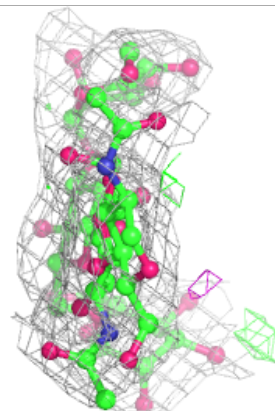
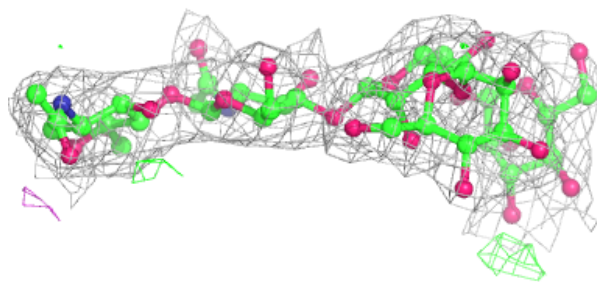
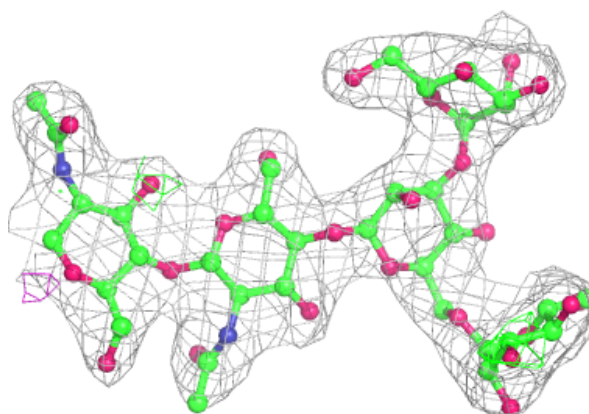
Electron density around Chain Q:

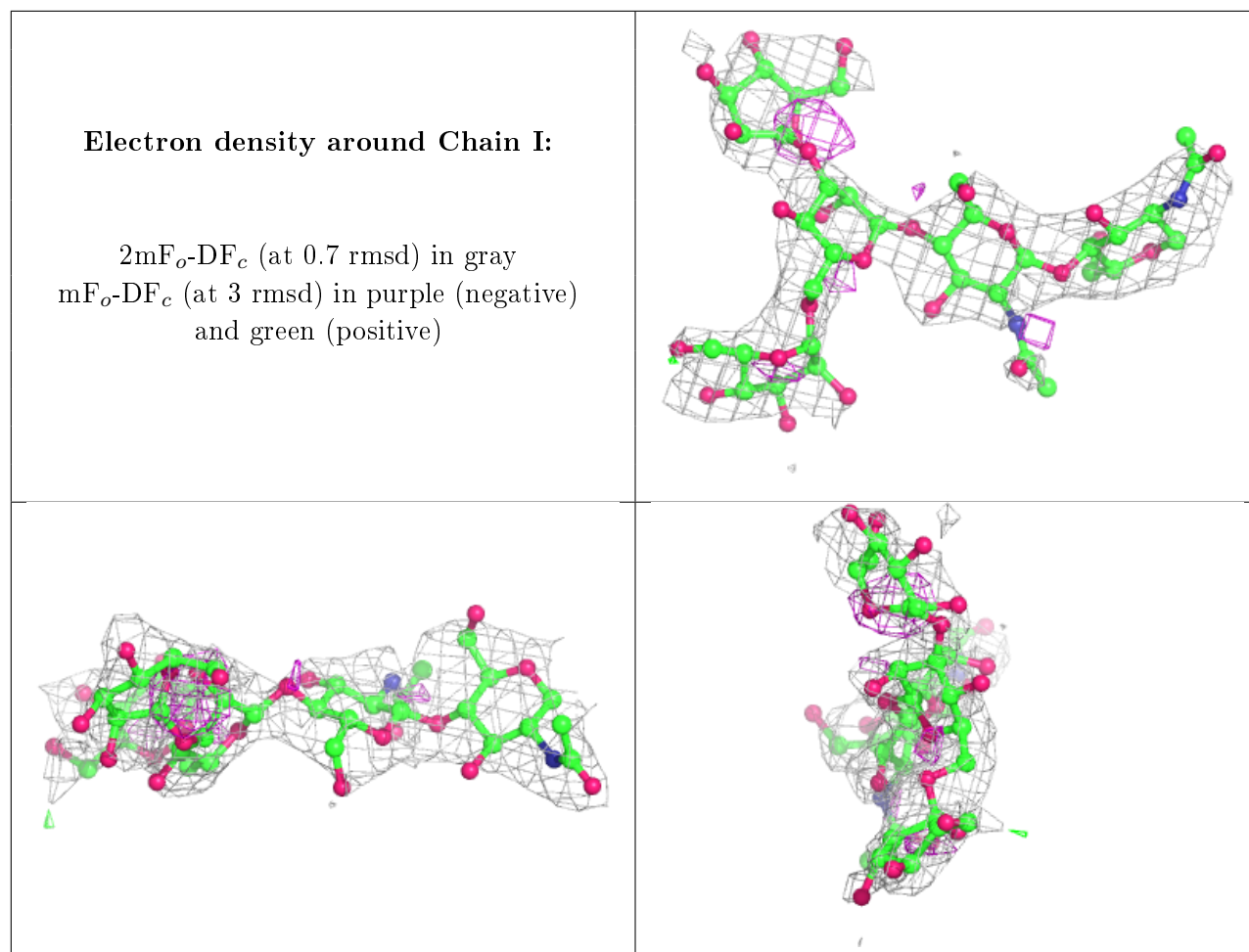
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
9	BR	B	1132	1/1	0.10	0.26	151,151,151,151	0
9	BR	B	1131	1/1	0.60	0.17	149,149,149,149	0
6	NAG	B	1125	14/15	0.61	0.27	91,102,108,122	0
6	NAG	B	1123	14/15	0.66	0.52	94,111,121,122	0
9	BR	A	1150	1/1	0.68	0.26	158,158,158,158	0
6	NAG	B	1122	14/15	0.69	0.41	110,114,120,122	0
6	NAG	A	1132	14/15	0.74	0.42	93,106,113,115	0
6	NAG	A	1134	14/15	0.76	0.39	61,89,103,105	0
9	BR	A	1144	1/1	0.76	0.12	126,126,126,126	0
6	NAG	B	1117	14/15	0.76	0.33	97,108,114,114	0
6	NAG	A	1135	14/15	0.78	0.32	84,99,106,106	0

Continued on next page...

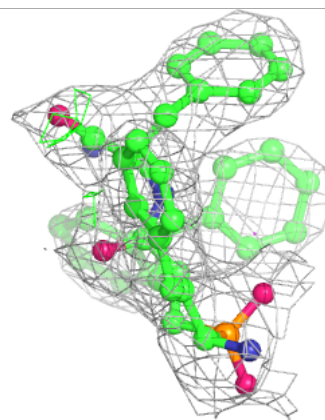
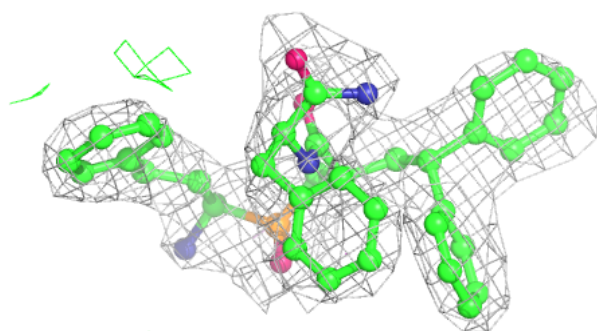
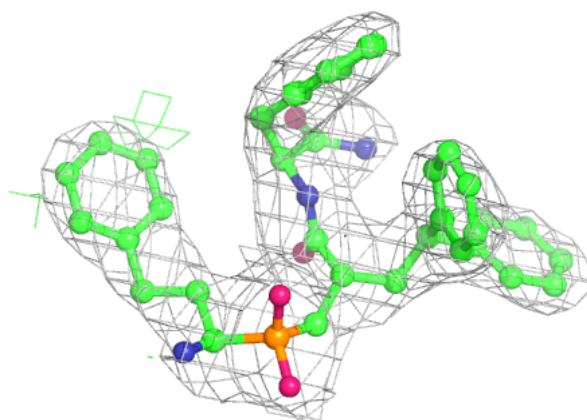
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	BR	A	1143	1/1	0.79	0.17	109,109,109,109	0
6	NAG	B	1102	14/15	0.81	0.39	100,117,122,123	0
9	BR	A	1149	1/1	0.82	0.25	143,143,143,143	0
6	NAG	B	1124	14/15	0.83	0.55	113,127,133,134	0
6	NAG	A	1133	14/15	0.86	0.21	70,89,96,103	0
6	NAG	B	1109	14/15	0.87	0.21	62,83,91,99	0
9	BR	A	1151	1/1	0.90	0.14	140,140,140,140	0
9	BR	B	1130	1/1	0.90	0.12	119,119,119,119	0
6	NAG	B	1108	14/15	0.90	0.34	91,100,104,109	0
9	BR	B	1101	1/1	0.91	0.13	106,106,106,106	0
9	BR	A	1146	1/1	0.93	0.26	151,151,151,151	0
9	BR	B	1129	1/1	0.93	0.10	99,99,99,99	0
9	BR	A	1152	1/1	0.95	0.14	106,106,106,106	0
8	7O2	B	1127	43/43	0.96	0.23	37,46,54,63	0
9	BR	A	1141	1/1	0.96	0.12	105,105,105,105	0
9	BR	B	1128	1/1	0.96	0.05	94,94,94,94	0
9	BR	A	1139	1/1	0.96	0.06	94,94,94,94	0
9	BR	A	1142	1/1	0.97	0.04	74,74,74,74	0
8	7O2	A	1137	43/43	0.97	0.20	31,39,48,53	0
9	BR	A	1147	1/1	0.97	0.06	66,66,66,66	0
9	BR	A	1145	1/1	0.97	0.06	83,83,83,83	0
9	BR	A	1138	1/1	0.98	0.06	71,71,71,71	0
9	BR	A	1140	1/1	0.98	0.08	107,107,107,107	0
9	BR	A	1148	1/1	0.98	0.10	76,76,76,76	0
7	ZN	B	1126	1/1	0.99	0.17	36,36,36,36	0
7	ZN	A	1136	1/1	1.00	0.16	31,31,31,31	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.

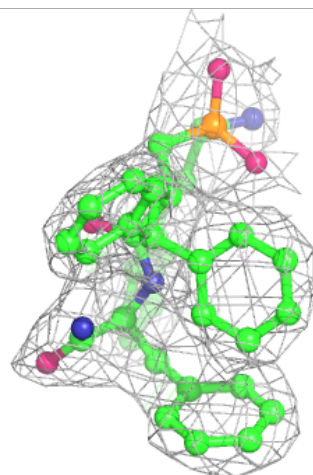
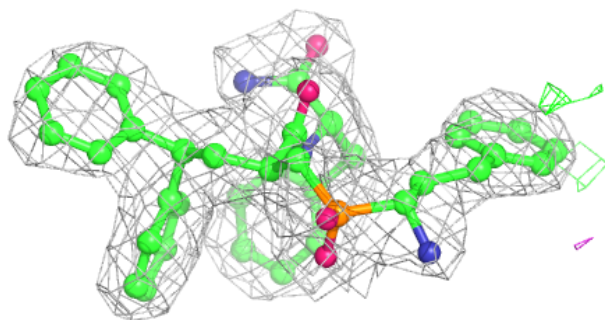
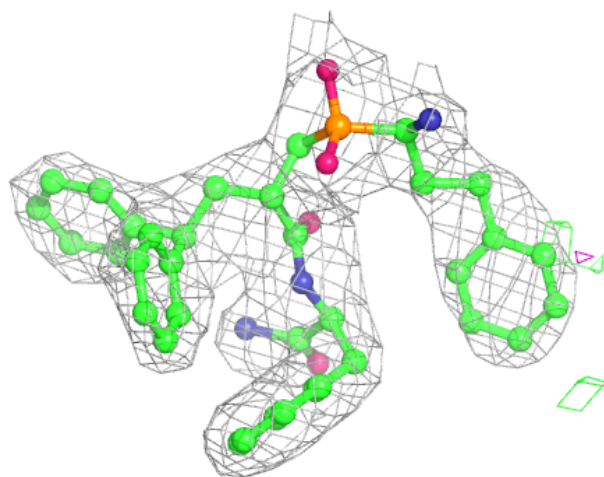
Electron density around 7O2 B 1127:

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



Electron density around 7O2 A 1137:

$2mF_o-DF_c$ (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.