



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 15, 2025 – 02:42 PM JST

PDB ID : 9W2C / pdb_00009w2c
Title : Crystal structure of Aedes aegypti Dopachrome Conversion Enzyme with L-Dopamine.
Authors : Guo, Y.; Zhang, L.; Guo, D.; Li, J.; Deng, J.; Han, Q.
Deposited on : 2025-07-27
Resolution : 3.39 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

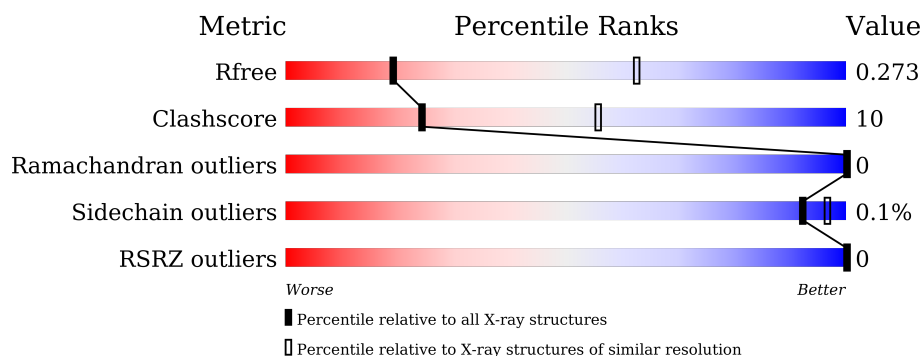
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	463	<div> <div>69%</div> <div>17%</div> <div>15%</div> </div>
1	B	463	<div> <div>69%</div> <div>17%</div> <div>14%</div> </div>
1	C	463	<div> <div>69%</div> <div>16%</div> <div>15%</div> </div>
1	D	463	<div> <div>71%</div> <div>14%</div> <div>14%</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> </div>
3	F	3	<div> <div>33%</div> <div>67%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	3	 67%33%
5	H	6	 50%50%
6	I	4	 75%25%
7	J	2	 50%50%
8	K	2	 100%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 13263 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 Dopachrome conversion enzyme.

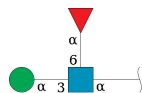
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3213	2068	539	595	11			
1	B	398	Total	C	N	O	S	0	0	0
			3243	2085	548	599	11			
1	C	395	Total	C	N	O	S	0	0	0
			3213	2068	539	595	11			
1	D	396	Total	C	N	O	S	0	0	0
			3223	2074	542	596	11			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			24	14	1	9			

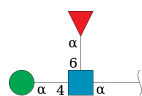
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			35	20	1	14			

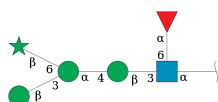
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-[alpha-L-fucopyranose

-(1-6)]2-acetamido-2-deoxy-alpha-D-glucopyranose.



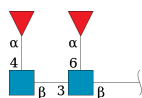
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			35	20	1	14			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-L-arabinopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-alpha-D-glucopyranose.



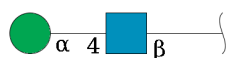
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	6	Total	C	N	O	0	0	0
			66	37	1	28			

- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	4	Total	C	N	O	0	0	0
			48	28	2	18			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose.

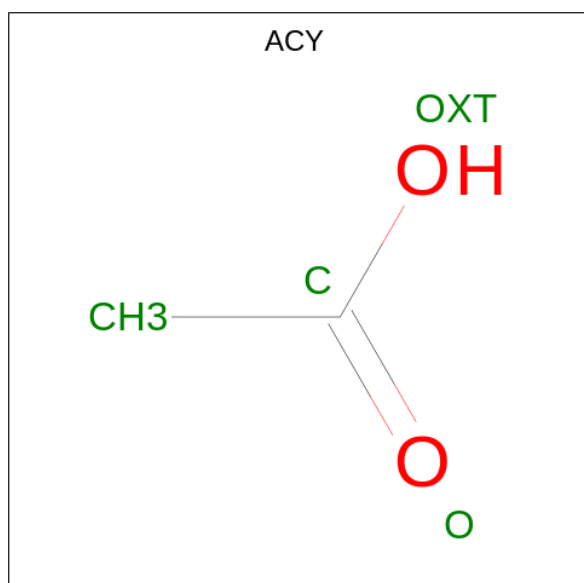


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	K	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

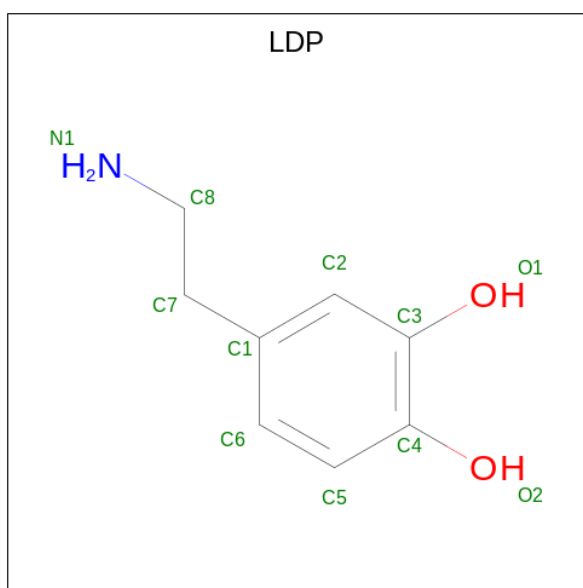
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	Ca	0	0
			2	2		
9	B	2	Total	Ca	0	0
			2	2		
9	C	2	Total	Ca	0	0
			2	2		
9	D	1	Total	Ca	0	0
			1	1		

- Molecule 10 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



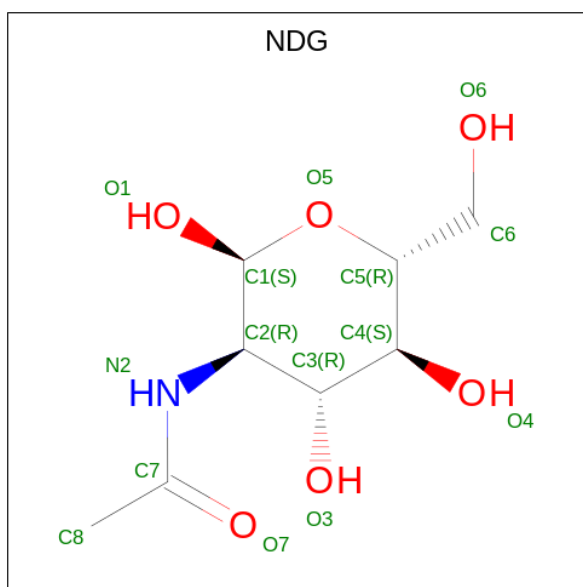
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	B	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0

- Molecule 11 is L-DOPAMINE (CCD ID: LDP) (formula: $C_8H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C N O 11 8 1 2	0	0
11	B	1	Total C N O 11 8 1 2	0	0
11	C	1	Total C N O 11 8 1 2	0	0
11	D	1	Total C N O 11 8 1 2	0	0

- Molecule 12 is 2-acetamido-2-deoxy- α -D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



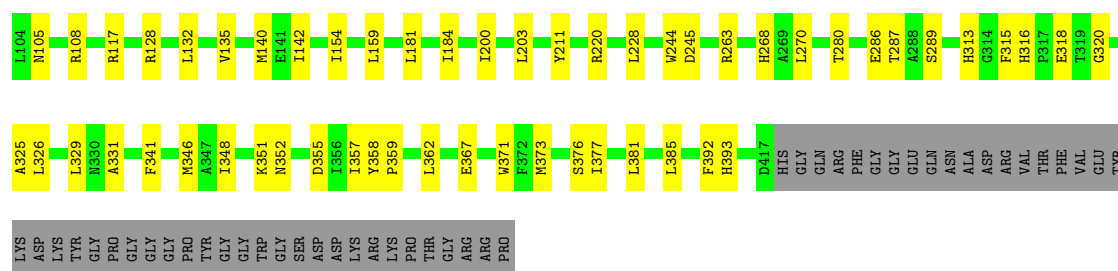
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	9	Total	O	0	0
			9	9		
13	B	4	Total	O	0	0
			4	4		
13	C	8	Total	O	0	0
			8	8		
13	D	7	Total	O	0	0
			7	7		

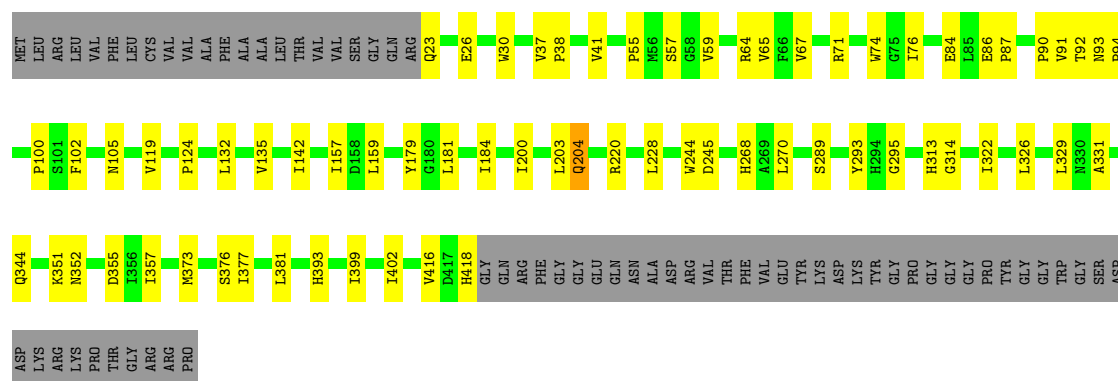
- Molecule 1: Dopachrome conversion enzyme





- Molecule 1: Dopachrome conversion enzyme

Chain D: 71% 14% 14%



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

Chain E: 50% 50%



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

Chain F: 33% 67%



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

Chain G: 67% 33%



- Molecule 5: beta-D-mannopyranose-(1-3)-[beta-L-arabinopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain H:  50% 50%



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

Chain I:  75% 25%



- Molecule 7: α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%



- Molecule 8: α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain K:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.31Å 103.87Å 99.03Å 90.00° 110.35° 90.00°	Depositor
Resolution (Å)	29.66 – 3.39 29.66 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.66-3.39) 99.2 (29.66-3.39)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 3.39Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.194 , 0.274 0.195 , 0.273	Depositor DCC
R_{free} test set	1196 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13263	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: NDG, ARB, MAN, CA, FUC, NAG, LDP, ACY, BMA

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	0.51	0/3308	0.81	2/4517 (0.0%)
1	B	0.51	0/3339	0.81	0/4558
1	C	0.49	0/3308	0.80	0/4517
1	D	0.51	0/3319	0.82	1/4532 (0.0%)
All	All	0.50	0/13274	0.81	3/18124 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	92	THR	CA-CB-OG1	-6.31	100.14	109.60
1	A	89	TYR	CB-CA-C	5.45	117.28	109.11
1	A	114	ASP	CA-CB-CG	5.43	118.03	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	72	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3213	0	3113	64	0
1	B	3243	0	3141	69	0
1	C	3213	0	3113	69	0
1	D	3223	0	3120	50	0
2	E	24	0	22	0	0
3	F	35	0	30	2	0
4	G	35	0	30	0	0
5	H	66	0	55	0	0
6	I	48	0	43	3	0
7	J	25	0	22	0	0
8	K	25	0	21	1	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
9	C	2	0	0	0	0
9	D	1	0	0	0	0
10	A	8	0	6	0	0
10	B	4	0	3	0	0
10	D	8	0	6	0	0
11	A	11	0	11	1	0
11	B	11	0	11	1	0
11	C	11	0	11	1	0
11	D	11	0	11	2	0
12	D	14	0	12	0	0
13	A	9	0	0	2	0
13	B	4	0	0	0	0
13	C	8	0	0	2	0
13	D	7	0	0	1	0
All	All	13263	0	12781	254	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 254 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:C:357:ILE:HD12	1:C:358:TYR:N	1.68	1.07
1:A:268:HIS:NE2	1:A:313:HIS:HD2	1.68	0.91
1:B:154:ILE:HD11	1:B:170:ILE:HD11	1.56	0.88
1:B:51:ILE:HD13	1:B:387:LEU:HD11	1.55	0.87
1:A:268:HIS:NE2	1:A:313:HIS:CD2	2.46	0.83

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	393/463 (85%)	373 (95%)	20 (5%)	0	100	100
1	B	396/463 (86%)	376 (95%)	20 (5%)	0	100	100
1	C	393/463 (85%)	376 (96%)	17 (4%)	0	100	100
1	D	394/463 (85%)	373 (95%)	21 (5%)	0	100	100
All	All	1576/1852 (85%)	1498 (95%)	78 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	361/413 (87%)	360 (100%)	1 (0%)	91	95
1	B	364/413 (88%)	364 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	361/413 (87%)	361 (100%)	0	100	100
1	D	362/413 (88%)	361 (100%)	1 (0%)	91	95
All	All	1448/1652 (88%)	1446 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ARG
1	D	204	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	268	HIS
1	C	294	HIS
1	D	344	GLN
1	D	150	GLN
1	D	216	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues 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	FUC	F	3	3	10,10,11	0.46	0	14,14,16	0.48	0
5	FUC	H	6	5	10,10,11	0.30	0	14,14,16	0.63	0
6	NAG	I	1	6,1	14,14,15	0.50	0	17,19,21	1.76	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUC	G	3	4	10,10,11	0.24	0	14,14,16	0.48	0
6	FUC	I	3	6	10,10,11	0.33	0	14,14,16	0.56	0
6	NAG	I	2	6	14,14,15	0.40	0	17,19,21	0.62	0
2	NAG	E	1	1,2	14,14,15	0.31	0	17,19,21	0.99	1 (5%)
7	NAG	J	1	1,7	14,14,15	0.31	0	17,19,21	0.72	0
6	FUC	I	4	6	10,10,11	0.25	0	14,14,16	1.16	2 (14%)

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	FUC	F	3	3	-	-	0/1/1/1
5	FUC	H	6	5	-	-	0/1/1/1
6	NAG	I	1	6,1	-	4/6/23/26	0/1/1/1
4	FUC	G	3	4	-	-	0/1/1/1
6	FUC	I	3	6	-	-	0/1/1/1
6	NAG	I	2	6	-	1/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
7	NAG	J	1	1,7	-	3/6/23/26	0/1/1/1
6	FUC	I	4	6	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	1	NAG	O5-C1-C2	-4.90	103.55	111.29
2	E	1	NAG	C1-O5-C5	3.32	116.70	112.19
6	I	1	NAG	C3-C4-C5	3.28	116.08	110.24
6	I	4	FUC	C1-C2-C3	3.25	113.66	109.67
6	I	1	NAG	C4-C3-C2	3.13	115.61	111.02

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6
7	J	1	NAG	C8-C7-N2-C2
7	J	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	3	FUC	1	0
6	I	2	NAG	1	0
6	I	4	FUC	2	0

5.5 Carbohydrates [i](#)

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	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	0.31	0	17,19,21	0.99	1 (5%)
2	FUC	E	2	2	10,10,11	0.49	0	14,14,16	0.59	0
3	NDG	F	1	3	14,14,15	0.74	0	17,19,21	1.07	1 (5%)
3	MAN	F	2	3	11,11,12	1.30	1 (9%)	15,15,17	1.73	2 (13%)
3	FUC	F	3	3	10,10,11	0.46	0	14,14,16	0.48	0
4	NDG	G	1	4	14,14,15	0.41	0	17,19,21	0.68	0
4	MAN	G	2	4	11,11,12	0.20	0	15,15,17	0.70	1 (6%)
4	FUC	G	3	4	10,10,11	0.24	0	14,14,16	0.48	0
5	NDG	H	1	5	14,14,15	0.44	0	17,19,21	0.78	0
5	BMA	H	2	5	11,11,12	0.66	0	15,15,17	1.82	2 (13%)
5	MAN	H	3	5	11,11,12	0.50	0	15,15,17	1.31	1 (6%)
5	BMA	H	4	5	11,11,12	0.62	0	15,15,17	1.29	1 (6%)
5	ARB	H	5	5	9,9,10	0.18	0	10,12,14	0.60	0
5	FUC	H	6	5	10,10,11	0.30	0	14,14,16	0.63	0
6	NAG	I	1	6,1	14,14,15	0.50	0	17,19,21	1.76	3 (17%)
6	NAG	I	2	6	14,14,15	0.40	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FUC	I	3	6	10,10,11	0.33	0	14,14,16	0.56	0
6	FUC	I	4	6	10,10,11	0.25	0	14,14,16	1.16	2 (14%)
7	NAG	J	1	1,7	14,14,15	0.31	0	17,19,21	0.72	0
7	MAN	J	2	7	11,11,12	1.16	2 (18%)	15,15,17	1.36	2 (13%)
8	NDG	K	1	8	14,14,15	0.74	0	17,19,21	0.86	0
8	MAN	K	2	8	11,11,12	1.00	1 (9%)	15,15,17	1.03	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
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1
3	NDG	F	1	3	-	3/6/23/26	0/1/1/1
3	MAN	F	2	3	-	0/2/19/22	0/1/1/1
3	FUC	F	3	3	-	-	0/1/1/1
4	NDG	G	1	4	-	2/6/23/26	0/1/1/1
4	MAN	G	2	4	-	0/2/19/22	0/1/1/1
4	FUC	G	3	4	-	-	0/1/1/1
5	NDG	H	1	5	-	6/6/23/26	0/1/1/1
5	BMA	H	2	5	-	1/2/19/22	0/1/1/1
5	MAN	H	3	5	-	0/2/19/22	0/1/1/1
5	BMA	H	4	5	-	0/2/19/22	1/1/1/1
5	ARB	H	5	5	-	-	0/1/1/1
5	FUC	H	6	5	-	-	0/1/1/1
6	NAG	I	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	I	2	6	-	1/6/23/26	0/1/1/1
6	FUC	I	3	6	-	-	0/1/1/1
6	FUC	I	4	6	-	-	0/1/1/1
7	NAG	J	1	1,7	-	3/6/23/26	0/1/1/1
7	MAN	J	2	7	-	2/2/19/22	0/1/1/1
8	NDG	K	1	8	-	4/6/23/26	0/1/1/1
8	MAN	K	2	8	-	0/2/19/22	1/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	MAN	C1-C2	3.91	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	2	MAN	O5-C5	2.58	1.48	1.43
7	J	2	MAN	C4-C5	2.40	1.58	1.53
7	J	2	MAN	O5-C5	2.07	1.47	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2	BMA	C1-C2-C3	5.31	116.19	109.67
6	I	1	NAG	O5-C1-C2	-4.90	103.55	111.29
3	F	2	MAN	O5-C1-C2	4.79	118.17	110.77
5	H	4	BMA	C1-O5-C5	4.39	118.14	112.19
7	J	2	MAN	C1-C2-C3	-4.15	104.57	109.67

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	1	NDG	C3-C2-N2-C7
8	K	1	NDG	C8-C7-N2-C2
8	K	1	NDG	O7-C7-N2-C2
2	E	1	NAG	C4-C5-C6-O6
7	J	1	NAG	C8-C7-N2-C2

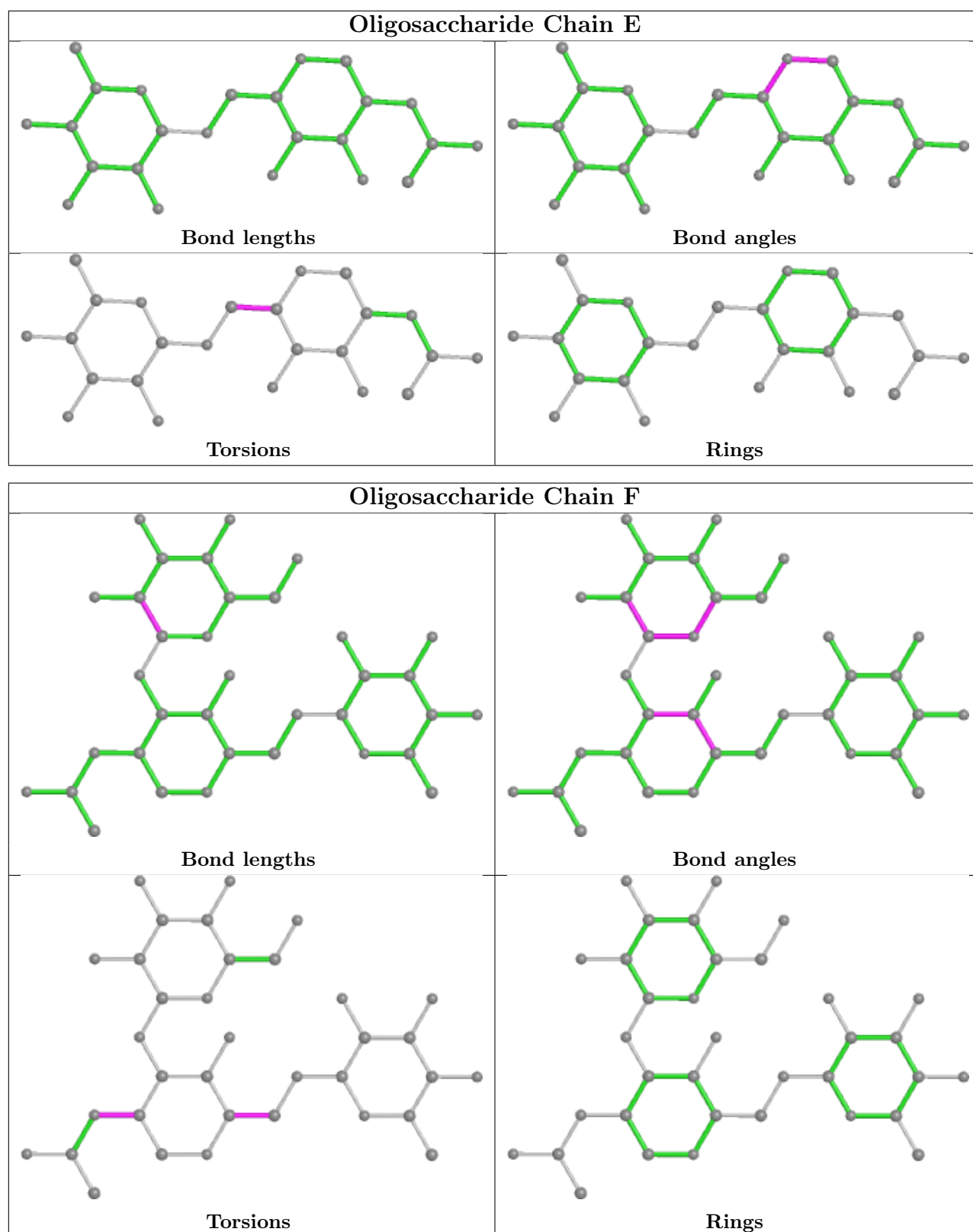
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	4	BMA	C1-C2-C3-C4-C5-O5
8	K	2	MAN	C1-C2-C3-C4-C5-O5

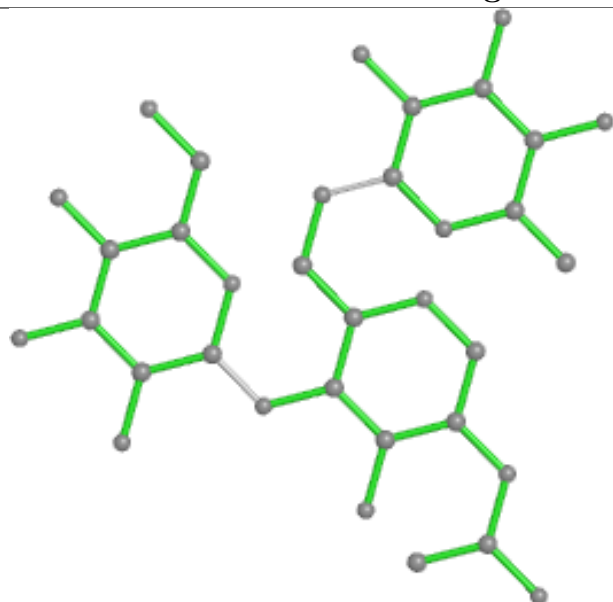
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NDG	2	0
6	I	2	NAG	1	0
6	I	4	FUC	2	0
6	I	3	FUC	1	0
8	K	1	NDG	1	0
3	F	2	MAN	2	0

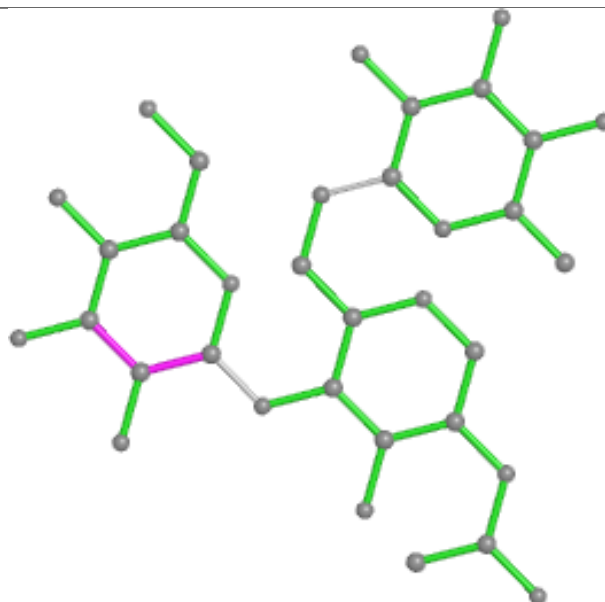
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



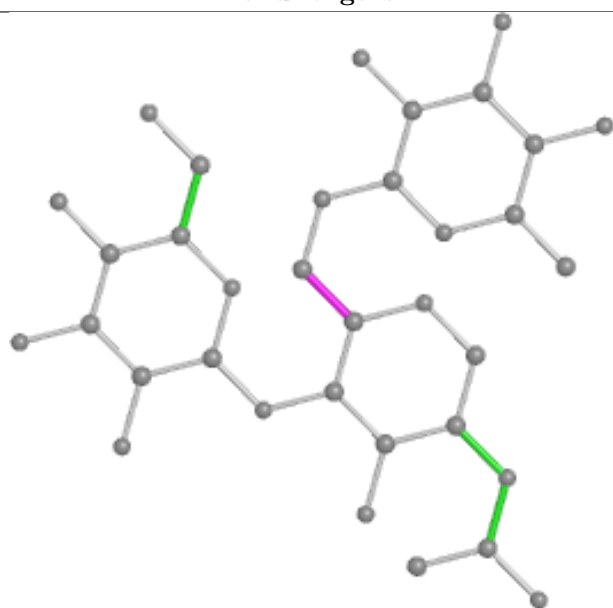
Oligosaccharide Chain G



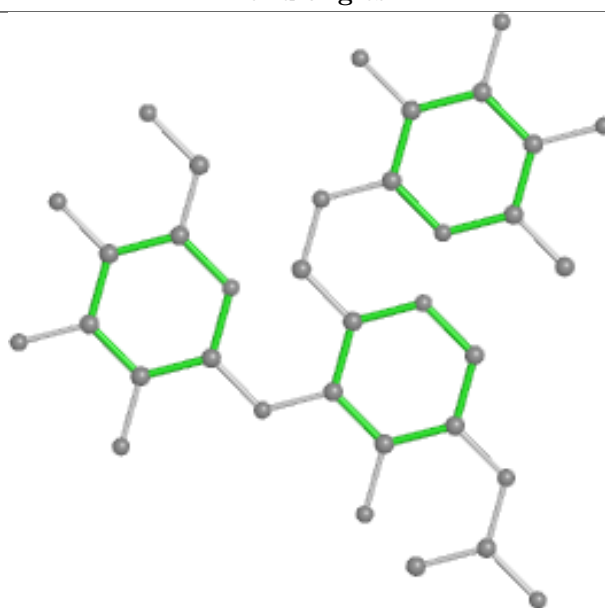
Bond lengths



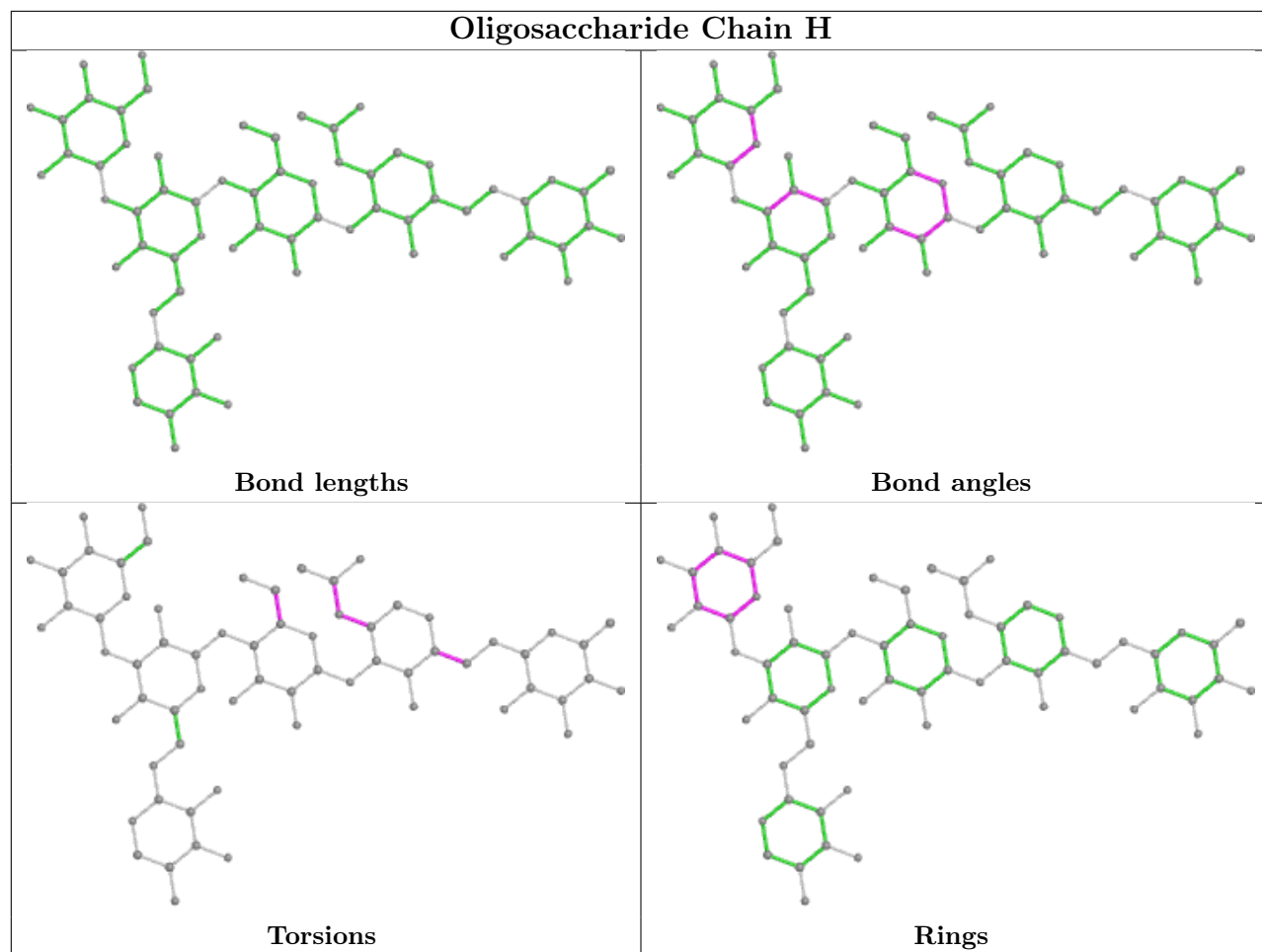
Bond angles

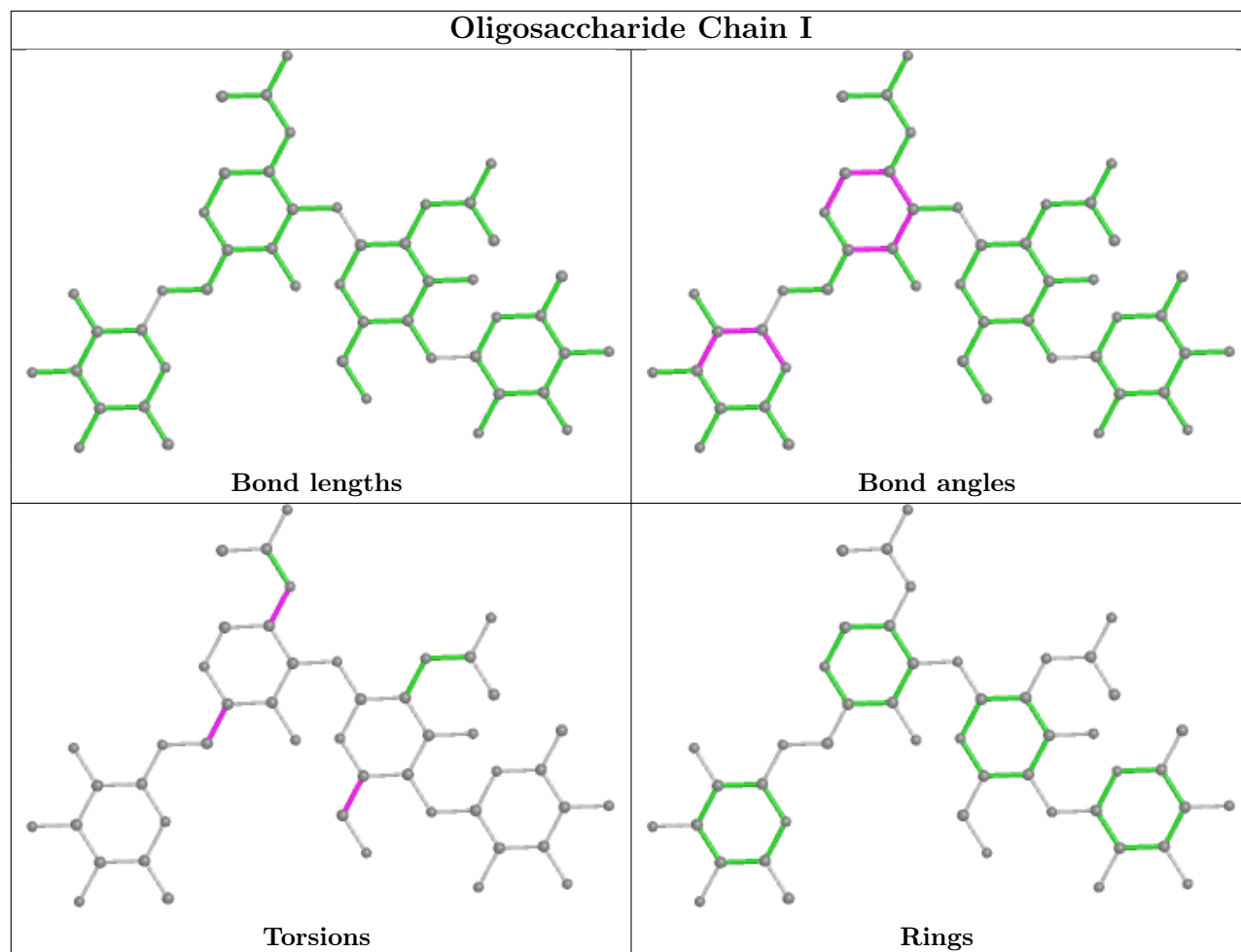


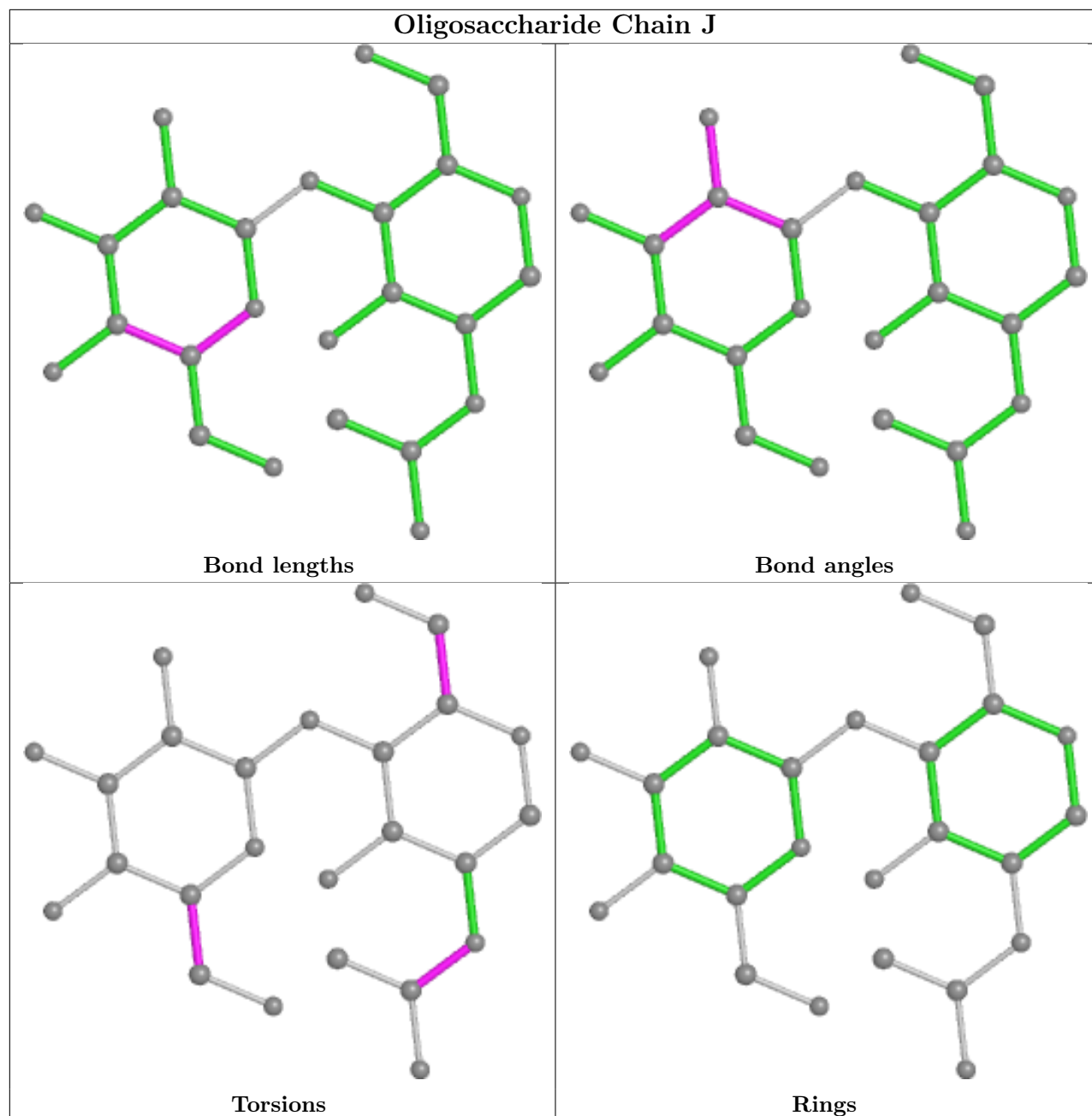
Torsions

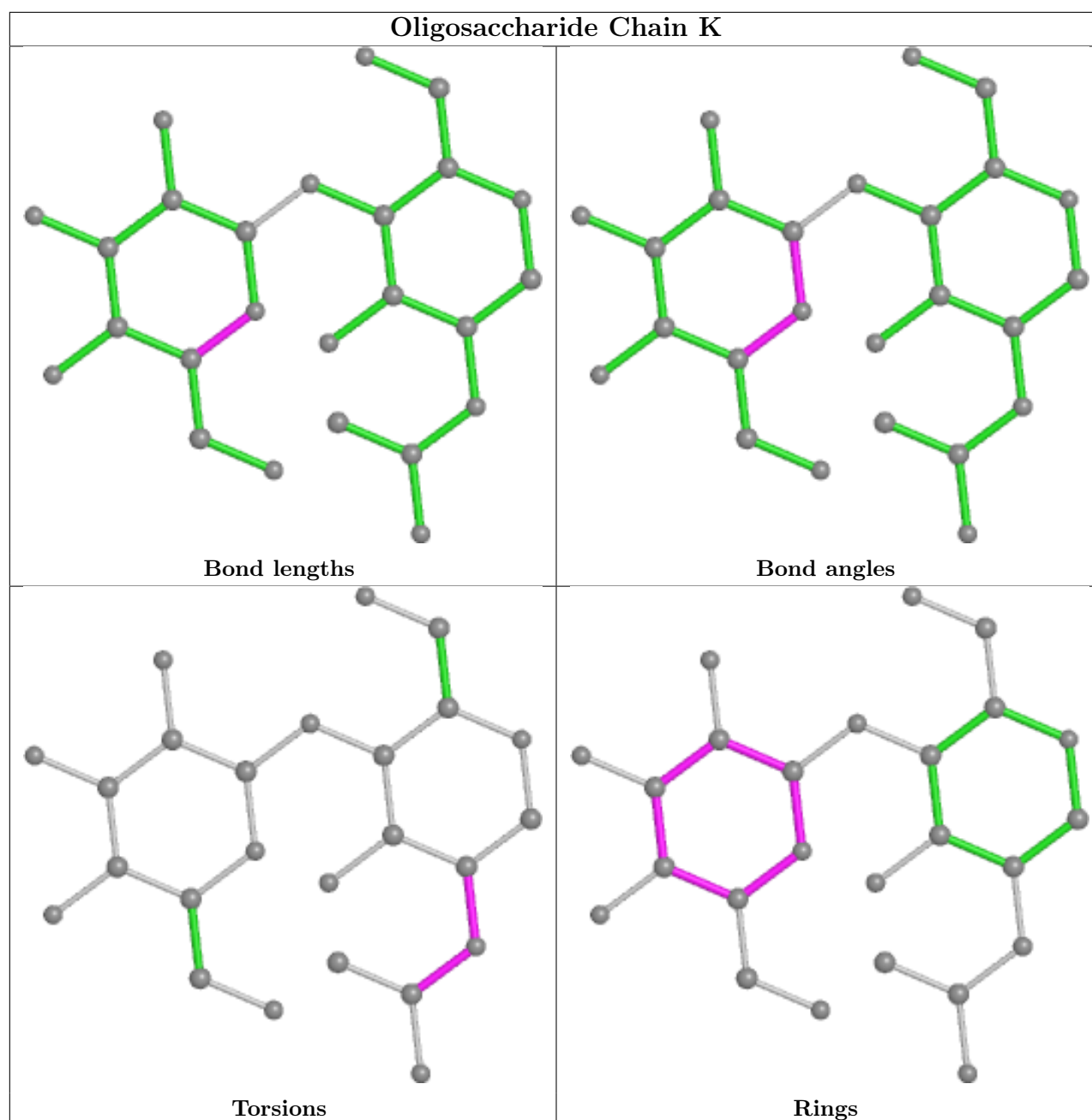


Rings









5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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
11	LDP	C	503	-	10,11,11	0.40	0	13,14,14	0.51	0
11	LDP	A	505	9	10,11,11	0.37	0	13,14,14	0.46	0
11	LDP	B	504	9	10,11,11	0.37	0	13,14,14	0.46	0
10	ACY	D	503	-	3,3,3	1.00	0	3,3,3	0.81	0
10	ACY	B	503	-	3,3,3	0.96	0	3,3,3	0.78	0
10	ACY	A	504	-	3,3,3	1.10	0	3,3,3	0.75	0
10	ACY	A	503	-	3,3,3	0.99	0	3,3,3	0.75	0
11	LDP	D	505	9	10,11,11	0.46	0	13,14,14	0.48	0
10	ACY	D	504	-	3,3,3	1.03	0	3,3,3	0.79	0
12	NDG	D	501	1	14,14,15	0.54	0	17,19,21	0.90	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LDP	C	503	-	-	3/3/3/3	0/1/1/1
11	LDP	A	505	9	-	3/3/3/3	0/1/1/1
11	LDP	B	504	9	-	1/3/3/3	0/1/1/1
11	LDP	D	505	9	-	3/3/3/3	0/1/1/1
12	NDG	D	501	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	501	NDG	O5-C1-C2	2.53	115.29	111.29

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

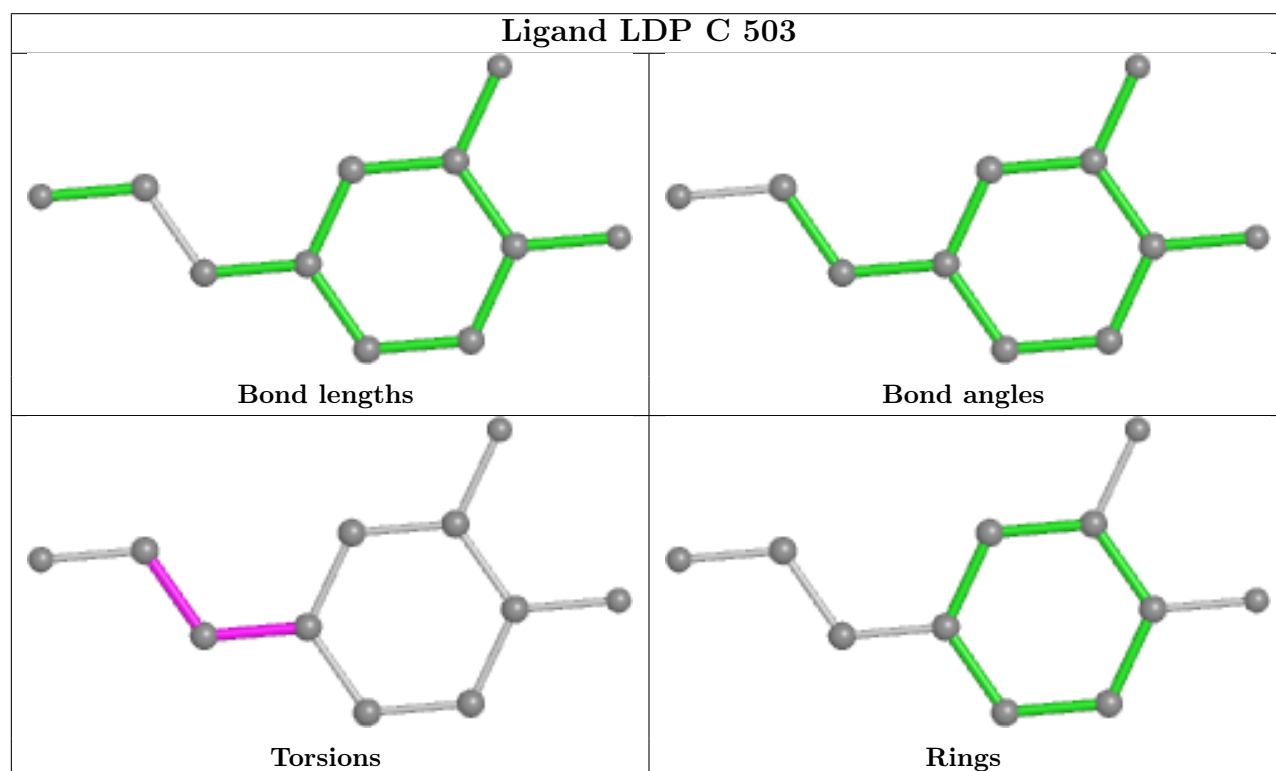
Mol	Chain	Res	Type	Atoms
11	B	504	LDP	C1-C7-C8-N1
11	C	503	LDP	C1-C7-C8-N1
11	D	505	LDP	C1-C7-C8-N1
12	D	501	NDG	C3-C2-N2-C7
12	D	501	NDG	C8-C7-N2-C2

There are no ring outliers.

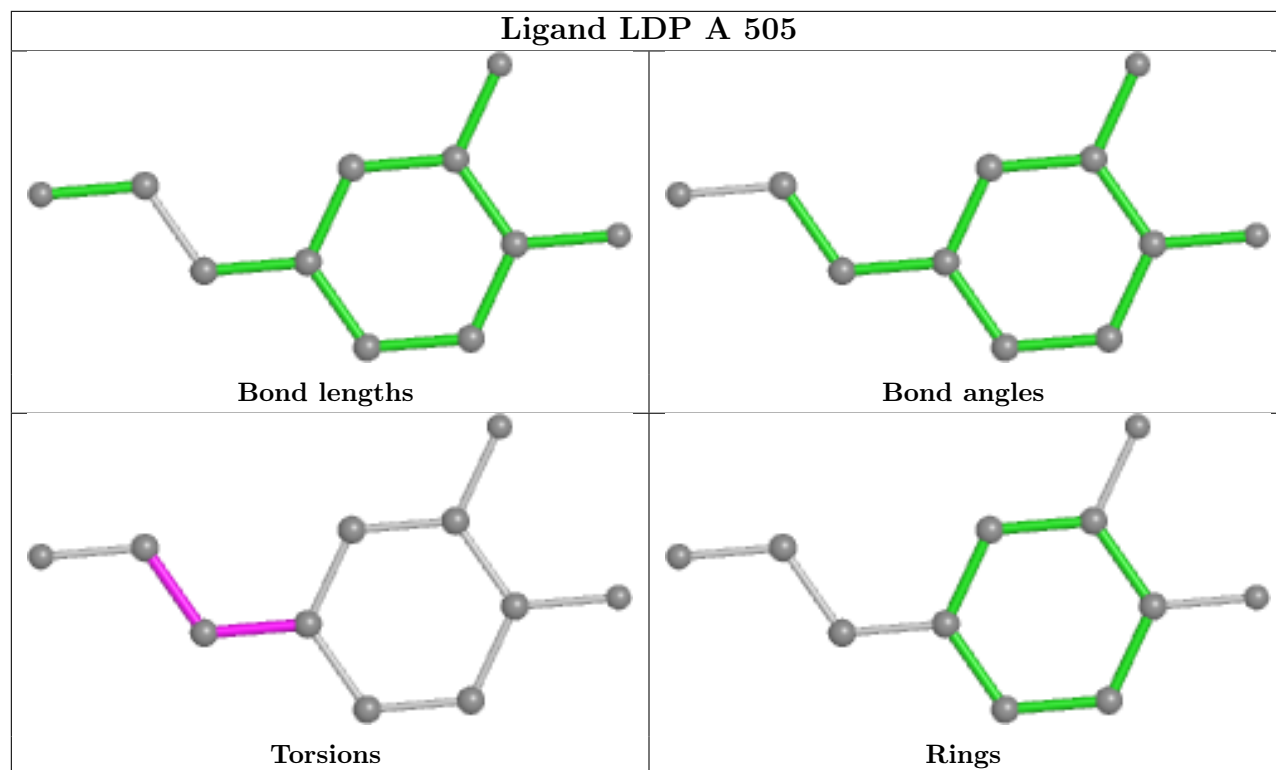
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	503	LDP	1	0
11	A	505	LDP	1	0
11	B	504	LDP	1	0
11	D	505	LDP	2	0

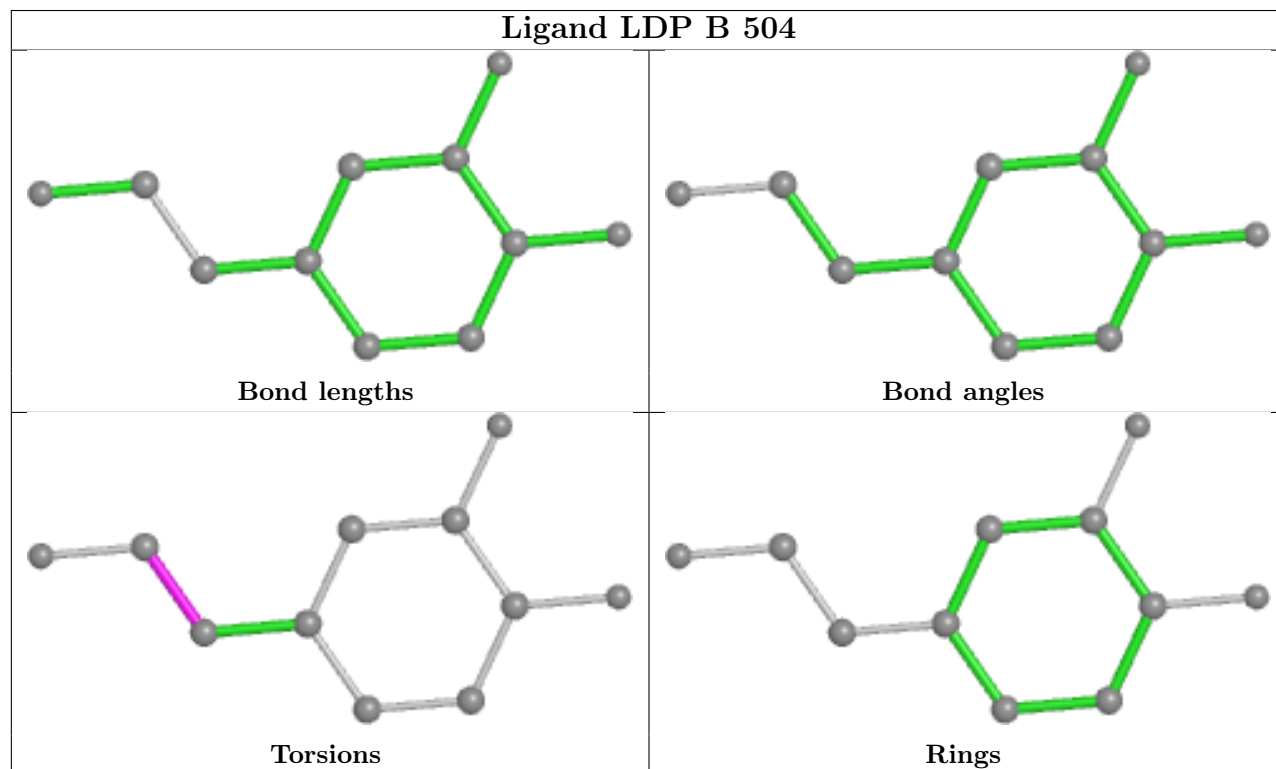
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

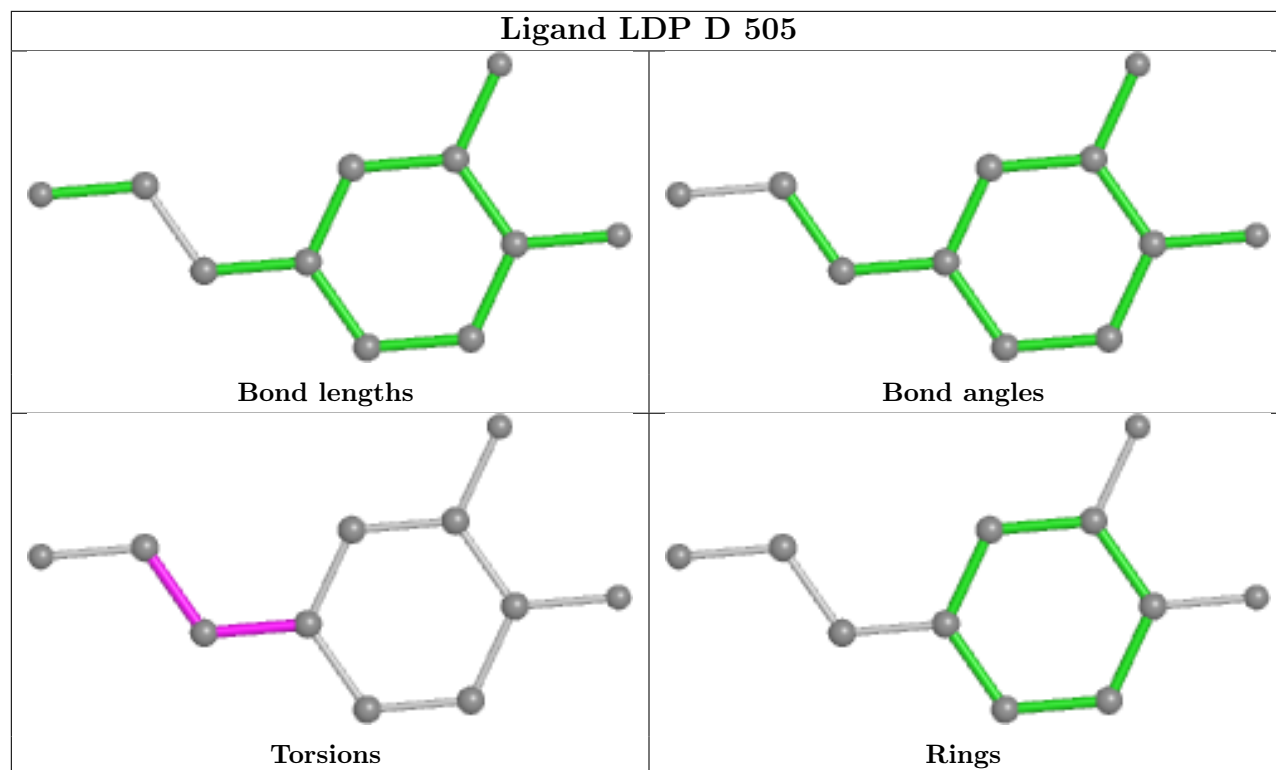


Ligand LDP A 505



Ligand LDP B 504





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	395/463 (85%)	-0.43	0 100 100	36, 64, 97, 141	0
1	B	398/463 (85%)	-0.36	0 100 100	38, 66, 105, 148	0
1	C	395/463 (85%)	-0.35	0 100 100	45, 75, 105, 144	0
1	D	396/463 (85%)	-0.57	0 100 100	34, 54, 78, 114	0
All	All	1584/1852 (85%)	-0.43	0 100 100	34, 65, 101, 148	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
6	FUC	I	4	10/11	0.19	0.16	115,124,130,131	0
6	FUC	I	3	10/11	0.48	0.12	116,129,134,134	0
4	FUC	G	3	10/11	0.59	0.15	161,170,173,179	0
5	FUC	H	6	10/11	0.66	0.17	60,79,87,87	0
2	NAG	E	1	14/15	0.67	0.11	127,135,147,153	0
6	NAG	I	2	14/15	0.67	0.12	70,105,120,127	0
3	FUC	F	3	10/11	0.72	0.15	118,125,128,131	0
6	NAG	I	1	14/15	0.76	0.10	67,99,122,130	0
7	NAG	J	1	14/15	0.86	0.09	74,84,113,128	0

6.3 Carbohydrates ⓘ

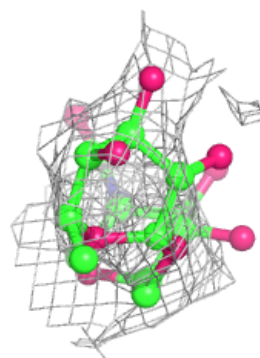
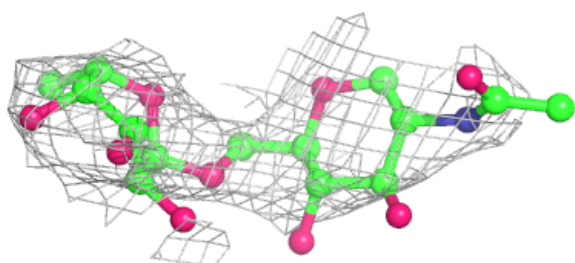
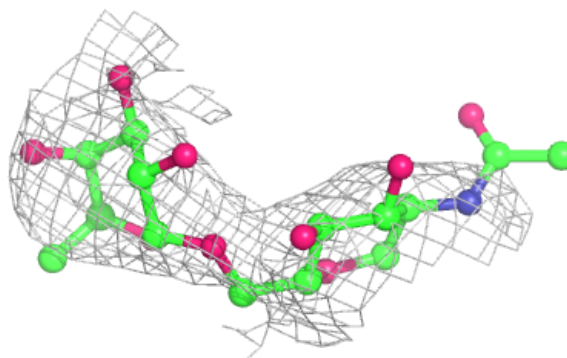
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	FUC	I	4	10/11	0.19	0.16	115,124,130,131	0
4	MAN	G	2	11/12	0.25	0.11	131,152,166,184	0
6	FUC	I	3	10/11	0.48	0.12	116,129,134,134	0
8	MAN	K	2	11/12	0.49	0.10	108,123,130,145	0
3	NDG	F	1	14/15	0.55	0.13	130,141,146,150	0
3	MAN	F	2	11/12	0.58	0.13	93,106,118,128	0
4	FUC	G	3	10/11	0.59	0.15	161,170,173,179	0
5	FUC	H	6	10/11	0.66	0.17	60,79,87,87	0
5	BMA	H	2	11/12	0.67	0.13	54,80,95,108	0
2	NAG	E	1	14/15	0.67	0.11	127,135,147,153	0
6	NAG	I	2	14/15	0.67	0.12	70,105,120,127	0
7	MAN	J	2	11/12	0.68	0.10	78,93,106,113	0
5	BMA	H	4	11/12	0.70	0.12	94,105,109,120	0
3	FUC	F	3	10/11	0.72	0.15	118,125,128,131	0
6	NAG	I	1	14/15	0.76	0.10	67,99,122,130	0
5	MAN	H	3	11/12	0.77	0.10	58,77,85,97	0
5	ARB	H	5	9/10	0.79	0.17	72,80,89,117	0
4	NDG	G	1	14/15	0.80	0.10	132,145,168,177	0
2	FUC	E	2	10/11	0.81	0.09	110,129,152,154	0
5	NDG	H	1	14/15	0.85	0.11	74,80,89,103	0
8	NDG	K	1	14/15	0.86	0.08	95,111,122,123	0
7	NAG	J	1	14/15	0.86	0.09	74,84,113,128	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.

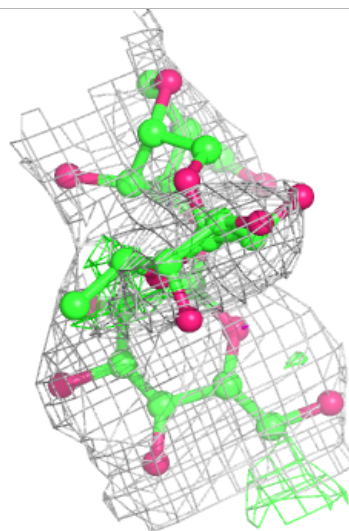
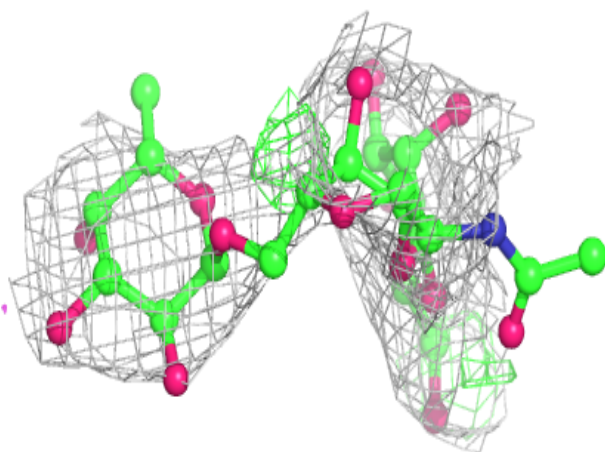
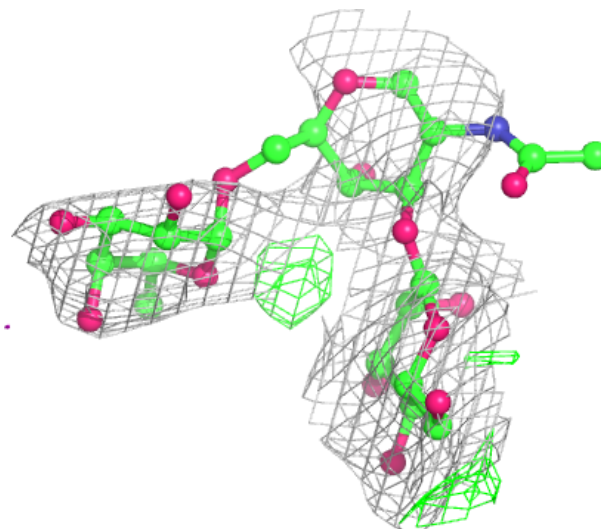
Electron density around Chain E:

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



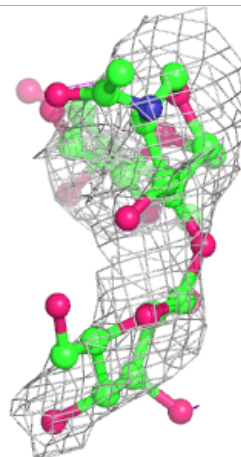
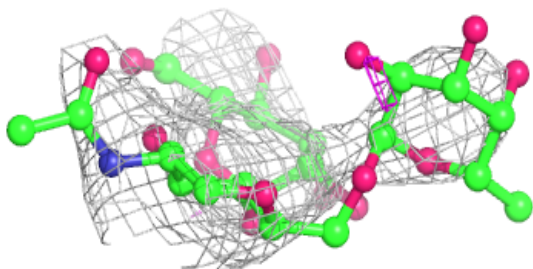
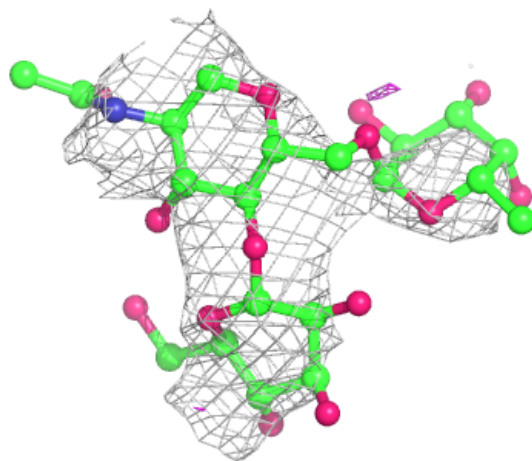
Electron density around Chain F:

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and green (positive)



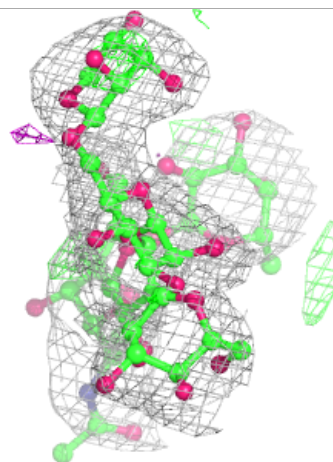
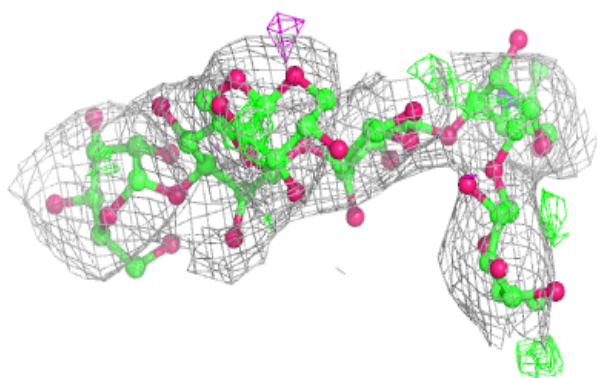
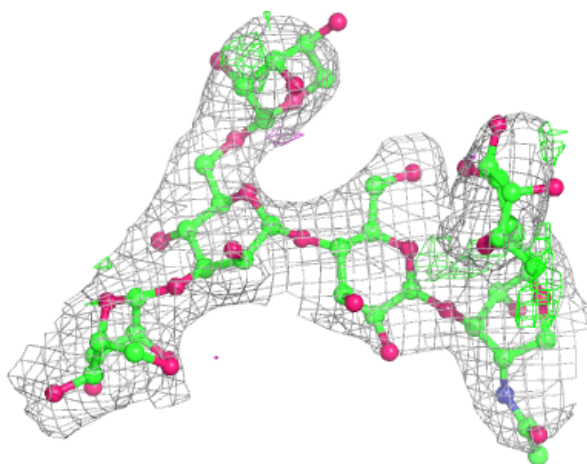
Electron density around Chain G:

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



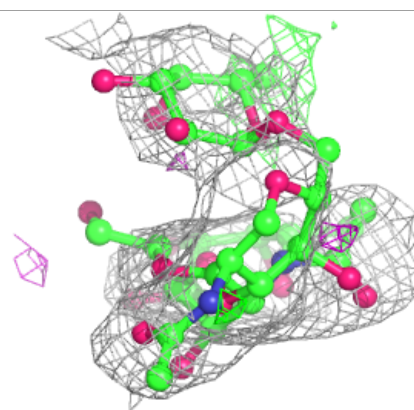
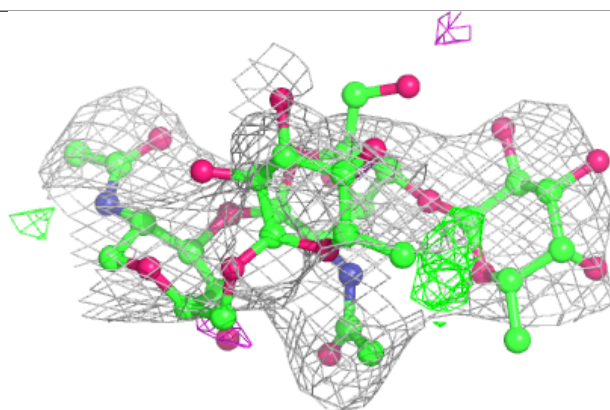
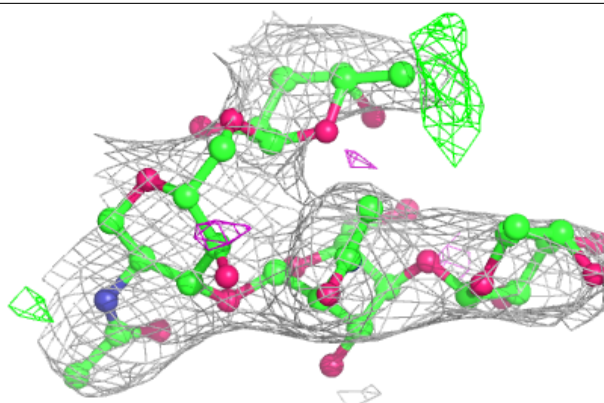
Electron density around Chain H:

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

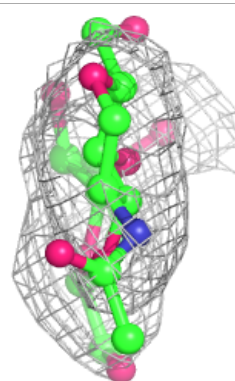
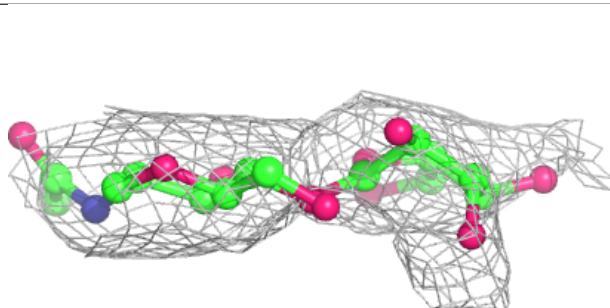
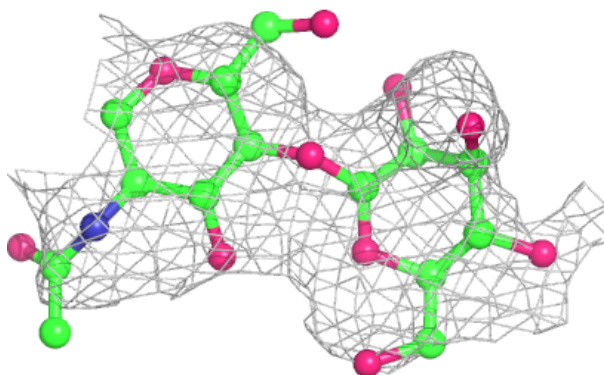


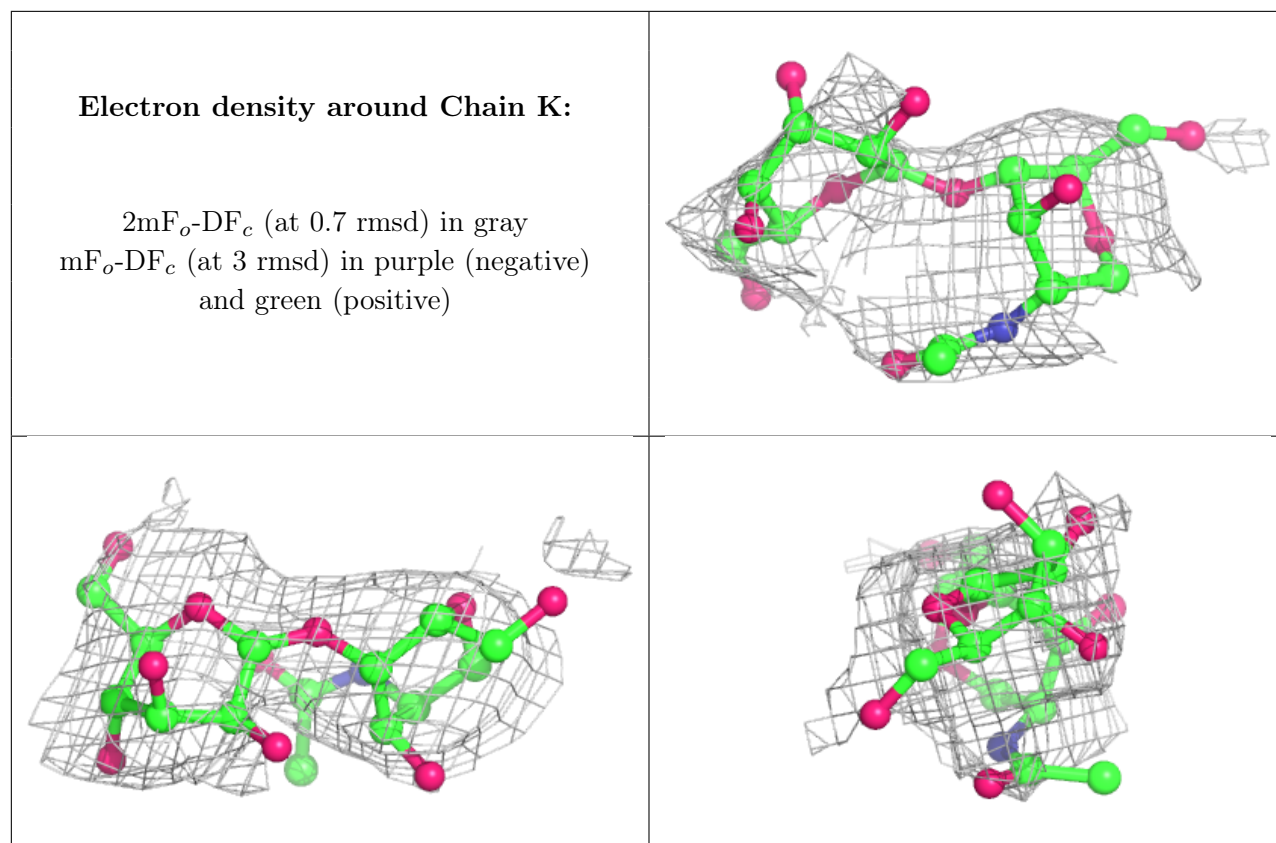
Electron density around Chain I:

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

**Electron density around Chain J:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	ACY	A	503	4/4	0.46	0.19	72,73,78,82	0
10	ACY	D	503	4/4	0.56	0.15	84,86,89,90	0
10	ACY	D	504	4/4	0.66	0.16	70,76,79,80	0
10	ACY	B	503	4/4	0.73	0.15	58,60,61,68	0
11	LDP	C	503	11/11	0.74	0.18	65,69,81,82	0
11	LDP	B	504	11/11	0.76	0.16	56,72,85,100	0
11	LDP	A	505	11/11	0.77	0.20	55,63,66,68	0
11	LDP	D	505	11/11	0.81	0.15	46,53,66,67	0
12	NDG	D	501	14/15	0.81	0.09	85,112,126,135	0
10	ACY	A	504	4/4	0.84	0.13	78,78,78,81	0
9	CA	A	502	1/1	0.95	0.07	68,68,68,68	0
9	CA	B	502	1/1	0.96	0.05	64,64,64,64	0
9	CA	C	501	1/1	0.98	0.07	45,45,45,45	0
9	CA	C	502	1/1	0.98	0.03	78,78,78,78	0

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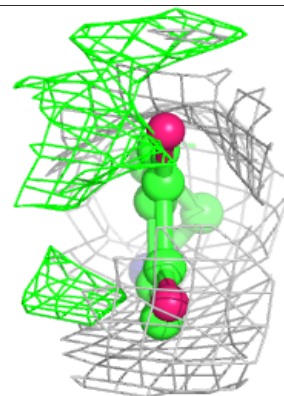
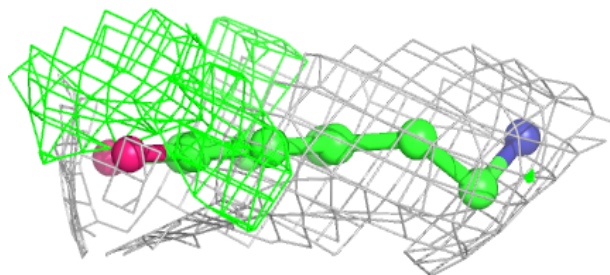
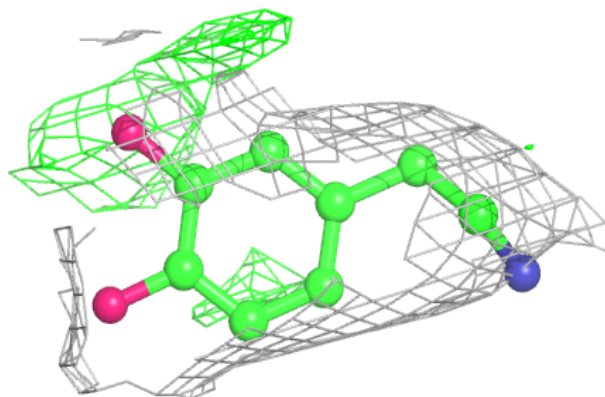
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	CA	A	501	1/1	0.99	0.07	42,42,42,42	0
9	CA	D	502	1/1	0.99	0.09	41,41,41,41	0
9	CA	B	501	1/1	0.99	0.07	43,43,43,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

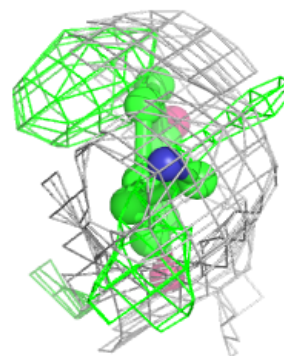
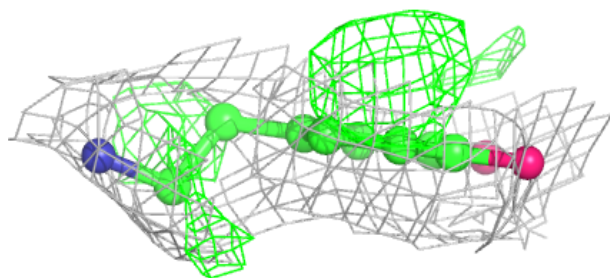
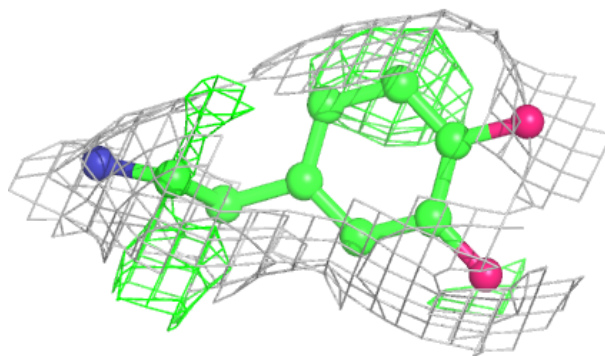
Electron density around LDP C 503:

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

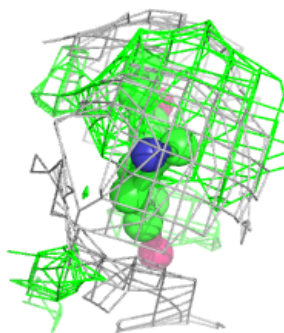
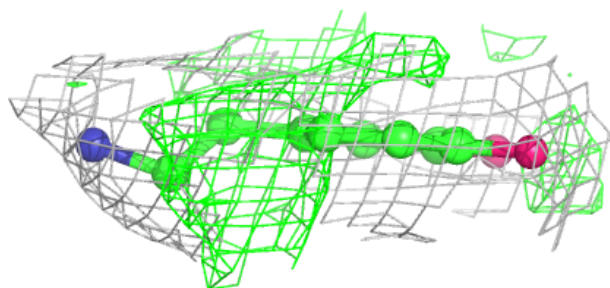
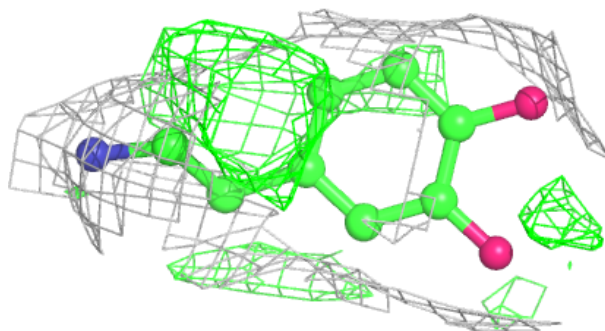


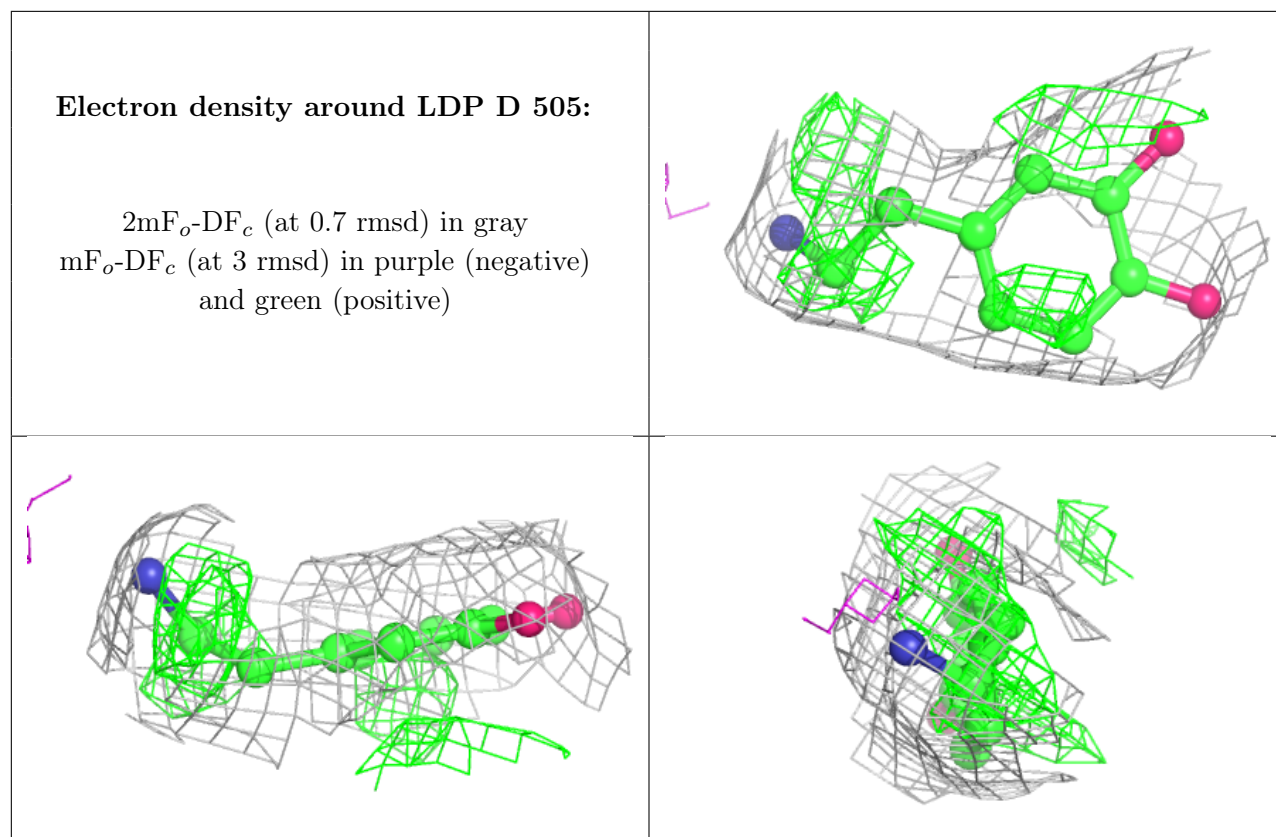
Electron density around LDP B 504:

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

**Electron density around LDP A 505:**

$2mF_o-DF_c$ (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.