



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:33 AM UTC

PDB ID : 5UPH / pdb_00005uph
Title : Lipids bound lysosomal integral membrane protein 2
Authors : Conrad, K.S.; Liu, S.
Deposited on : 2017-02-03
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

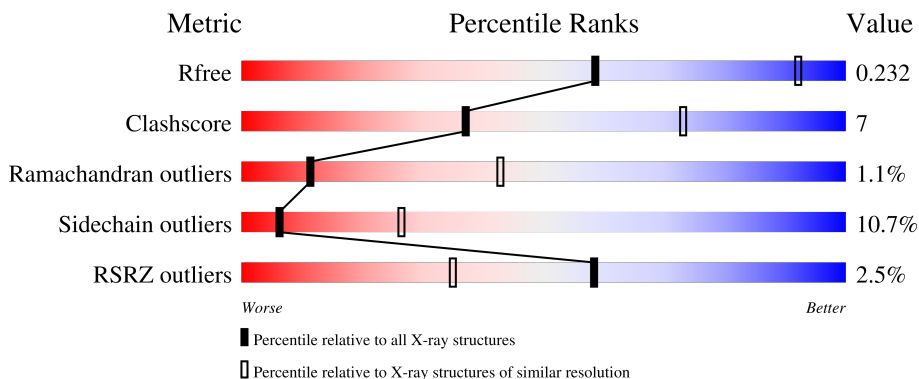
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





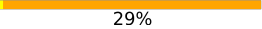
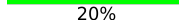
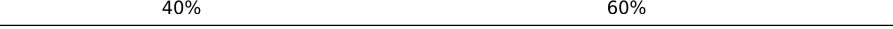
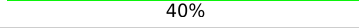
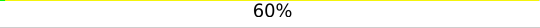
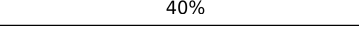
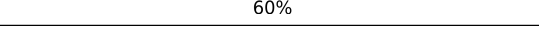
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	410	 2% 56% 18% 23%
1	B	410	 59% 16% 21%
2	C	4	 50% 50%
2	I	4	 25% 50% 25%
3	D	2	 100%

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Mol	Chain	Length	Quality of chain
3	H	2	 100%
4	E	7	 71%  29%
5	F	5	 20%  80%
5	G	5	 40%  60%
5	J	5	 40%  60%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6066 atoms, of which 271 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 Lysosome membrane protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	Total	C	N	O	S	0	0	0
			2566	1672	415	472	7			
1	B	324	Total	C	N	O	S	0	0	0
			2628	1708	427	485	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	HIS	-	expression tag	UNP Q14108
A	433	HIS	-	expression tag	UNP Q14108
A	434	HIS	-	expression tag	UNP Q14108
A	435	HIS	-	expression tag	UNP Q14108
A	436	HIS	-	expression tag	UNP Q14108
A	437	HIS	-	expression tag	UNP Q14108
B	432	HIS	-	expression tag	UNP Q14108
B	433	HIS	-	expression tag	UNP Q14108
B	434	HIS	-	expression tag	UNP Q14108
B	435	HIS	-	expression tag	UNP Q14108
B	436	HIS	-	expression tag	UNP Q14108
B	437	HIS	-	expression tag	UNP Q14108

- 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.



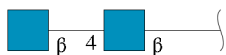
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

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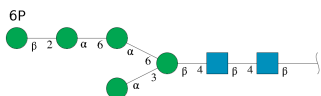
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	4	50	28	2	20	0	0	0

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



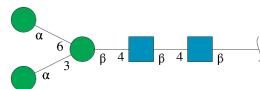
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	28	16	2	10	0	0	0
3	H	2	28	16	2	10	0	0	0

- Molecule 4 is an oligosaccharide called 6-O-phosphono-beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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
			Total	C	N	O	P			
4	E	7	87	46	2	38	1	0	0	0

- 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.



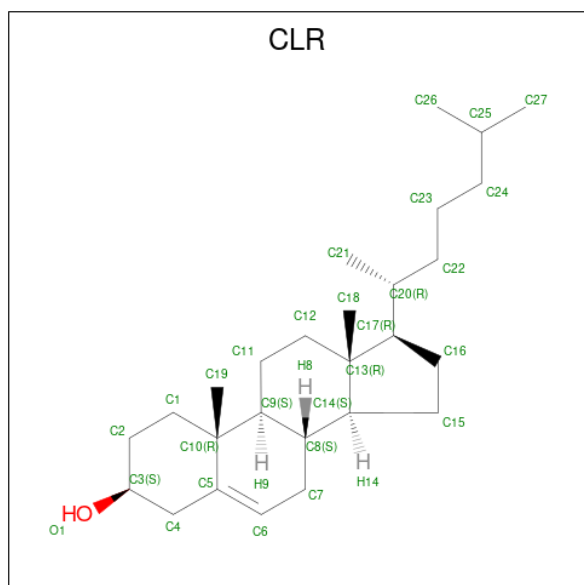
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	F	5	61	34	2	25	0	0	0

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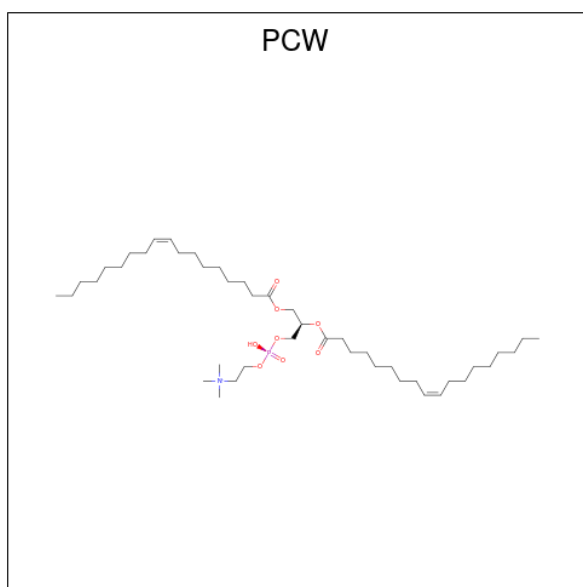
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
5	G	5	Total	C	H	N	O	0	0	0
			72	34	11	2	25			
5	J	5	Total	C	N	O	0	0	0	
			61	34	2	25				

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			74	27	46	1		
6	B	1	Total	C	H	O	0	0
			74	27	46	1		

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	A	1	Total	C	H	N	O	P	0	0
			138	44	84	1	8	1		
7	B	1	Total	C	H	N	O	P	0	0
			138	44	84	1	8	1		
7	B	1	Total	C					0	0
				11	11					

Chain C:  50% 50%



- 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 I:  25% 50% 25%



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

Chain D:  100%

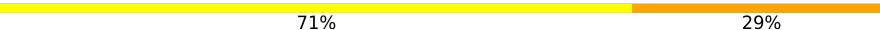


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%




- Molecule 4: 6-O-phosphono-beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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 E:  71% 29%



- 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 F:  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 G:  40% 60%



- 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 J:  40% 60%



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.04Å 139.04Å 178.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.61 – 3.00 40.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.61-3.00) 95.6 (40.61-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.01Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.193 , 0.228 (Not available) , 0.232	Depositor DCC
R_{free} test set	1689 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	103.9	Xtrriage
Anisotropy	0.302	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 116.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6066	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, BMA, MAN, PCW, NAG, M6D

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	0.95	0/2633	1.35	12/3578 (0.3%)
1	B	0.94	1/2696 (0.0%)	1.40	20/3662 (0.5%)
All	All	0.94	1/5329 (0.0%)	1.38	32/7240 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	232	ASN	CA-C	5.27	1.59	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	396	VAL	CA-C-N	9.01	137.92	121.70
1	B	396	VAL	C-N-CA	9.01	137.92	121.70
1	B	293	PHE	CA-CB-CG	7.63	121.44	113.80
1	B	230	GLU	CA-C-N	7.32	134.50	123.23
1	B	230	GLU	C-N-CA	7.32	134.50	123.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2566	0	2491	43	0
1	B	2628	0	2548	41	0
2	C	50	0	43	0	0
2	I	50	0	43	1	0
3	D	28	0	25	0	0
3	H	28	0	25	0	0
4	E	87	0	69	2	0
5	F	61	0	52	0	0
5	G	61	11	52	0	0
5	J	61	0	52	0	0
6	A	28	46	46	7	0
6	B	28	46	46	6	0
7	A	54	84	84	1	0
7	B	65	84	100	0	0
All	All	5795	271	5676	81	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 7.

The worst 5 of 81 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:268:VAL:HG11	6:B:517:CLR:H151	1.47	0.92
1:B:392:LEU:HD11	1:B:396:VAL:HG23	1.56	0.86
1:B:268:VAL:HG11	6:B:517:CLR:C15	2.10	0.81
1:A:381:LYS:HB2	6:A:518:CLR:H122	1.65	0.79
1:B:396:VAL:HA	1:B:397:GLU:HB2	1.72	0.71

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	306/410 (75%)	287 (94%)	15 (5%)	4 (1%)	9	38
1	B	314/410 (77%)	291 (93%)	20 (6%)	3 (1%)	12	45
All	All	620/820 (76%)	578 (93%)	35 (6%)	7 (1%)	11	43

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	GLU
1	A	259	LEU
1	B	52	SER
1	A	52	SER
1	B	53	TRP

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	281/370 (76%)	250 (89%)	31 (11%)	6	25
1	B	288/370 (78%)	258 (90%)	30 (10%)	7	28
All	All	569/740 (77%)	508 (89%)	61 (11%)	6	26

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	391	LYS
1	B	393	ASP
1	B	125	VAL
1	B	385	ILE
1	B	409	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	GLN

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Mol	Chain	Res	Type
1	B	114	ASN
1	B	288	GLN
1	A	148	GLN
1	A	63	GLN

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](#)

34 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	2,1	14,14,15	0.36	0	17,19,21	0.91	1 (5%)
2	NAG	C	2	2	14,14,15	0.27	0	17,19,21	0.64	0
2	BMA	C	3	2	11,11,12	0.32	0	15,15,17	0.77	0
2	MAN	C	4	2	11,11,12	0.33	0	15,15,17	1.00	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.32	0	17,19,21	0.64	0
3	NAG	D	2	3	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	E	1	4,1	14,14,15	0.35	0	17,19,21	1.02	1 (5%)
4	NAG	E	2	4	14,14,15	0.31	0	17,19,21	1.33	2 (11%)
4	BMA	E	3	4	11,11,12	0.45	0	15,15,17	1.56	1 (6%)
4	MAN	E	4	4	11,11,12	0.45	0	15,15,17	0.88	1 (6%)
4	MAN	E	5	4	11,11,12	0.50	0	15,15,17	1.41	1 (6%)
4	M6D	E	6	4	15,15,16	0.74	0	21,22,24	1.08	2 (9%)
4	MAN	E	7	4	11,11,12	0.42	0	15,15,17	0.77	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	F	1	5,1	14,14,15	0.37	0	17,19,21	2.96	5 (29%)
5	NAG	F	2	5	14,14,15	0.35	0	17,19,21	0.54	0
5	BMA	F	3	5	11,11,12	0.30	0	15,15,17	0.80	1 (6%)
5	MAN	F	4	5	11,11,12	0.33	0	15,15,17	0.89	1 (6%)
5	MAN	F	5	5	11,11,12	0.51	0	15,15,17	1.06	2 (13%)
5	NAG	G	1	5,1	14,14,15	0.39	0	17,19,21	0.88	1 (5%)
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.79	0
5	BMA	G	3	5	11,11,12	0.33	0	15,15,17	0.73	0
5	MAN	G	4	5	11,11,12	0.33	0	15,15,17	0.92	1 (6%)
5	MAN	G	5	5	11,11,12	0.40	0	15,15,17	1.06	1 (6%)
3	NAG	H	1	3,1	14,14,15	0.32	0	17,19,21	0.57	0
3	NAG	H	2	3	14,14,15	0.31	0	17,19,21	0.53	0
2	NAG	I	1	2,1	14,14,15	0.45	0	17,19,21	1.27	1 (5%)
2	NAG	I	2	2	14,14,15	0.34	0	17,19,21	1.51	2 (11%)
2	BMA	I	3	2	11,11,12	0.40	0	15,15,17	0.64	0
2	MAN	I	4	2	11,11,12	0.48	0	15,15,17	0.98	1 (6%)
5	NAG	J	1	5,1	14,14,15	0.35	0	17,19,21	3.03	5 (29%)
5	NAG	J	2	5	14,14,15	0.34	0	17,19,21	0.61	0
5	BMA	J	3	5	11,11,12	0.30	0	15,15,17	0.70	0
5	MAN	J	4	5	11,11,12	0.38	0	15,15,17	0.87	1 (6%)
5	MAN	J	5	5	11,11,12	0.50	0	15,15,17	0.97	2 (13%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
4	M6D	E	6	4	-	6/6/23/26	0/1/1/1
4	MAN	E	7	4	-	0/2/19/22	1/1/1/1
5	NAG	F	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	MAN	F	4	5	-	2/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	0/6/23/26	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	-	0/2/19/22	1/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	MAN	I	4	2	-	1/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1
5	MAN	J	4	5	-	2/2/19/22	0/1/1/1
5	MAN	J	5	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1	NAG	C1-O5-C5	7.43	122.15	112.19
5	F	1	NAG	C1-O5-C5	7.28	121.95	112.19
5	J	1	NAG	O5-C1-C2	-7.12	100.27	111.29
5	F	1	NAG	C1-C2-N2	6.13	120.09	110.43
5	F	1	NAG	O5-C1-C2	-5.52	102.75	111.29

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	6	M6D	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	E	6	M6D	O5-C5-C6-O6
4	E	6	M6D	C6-O6-P-O1P
4	E	6	M6D	C6-O6-P-O2P
4	E	6	M6D	C6-O6-P-O3P

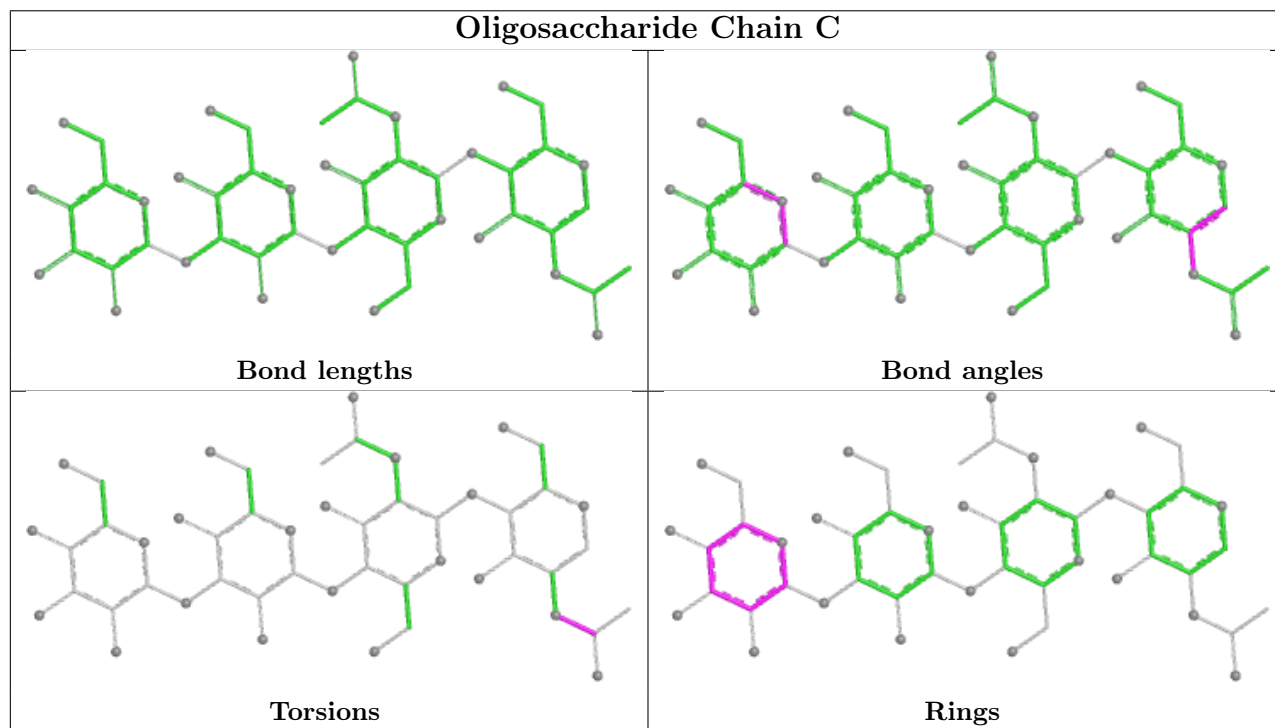
All (4) ring outliers are listed below:

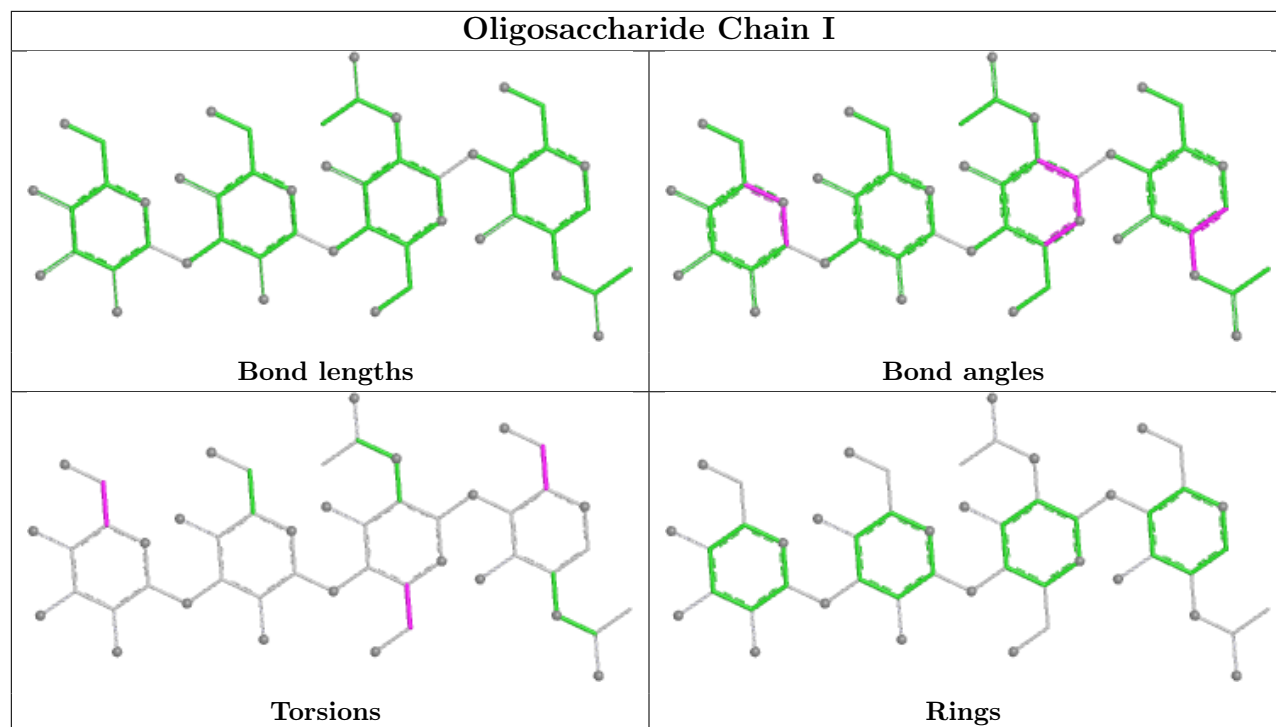
Mol	Chain	Res	Type	Atoms
4	E	3	BMA	C1-C2-C3-C4-C5-O5
4	E	7	MAN	C1-C2-C3-C4-C5-O5
2	C	4	MAN	C1-C2-C3-C4-C5-O5
5	G	4	MAN	C1-C2-C3-C4-C5-O5

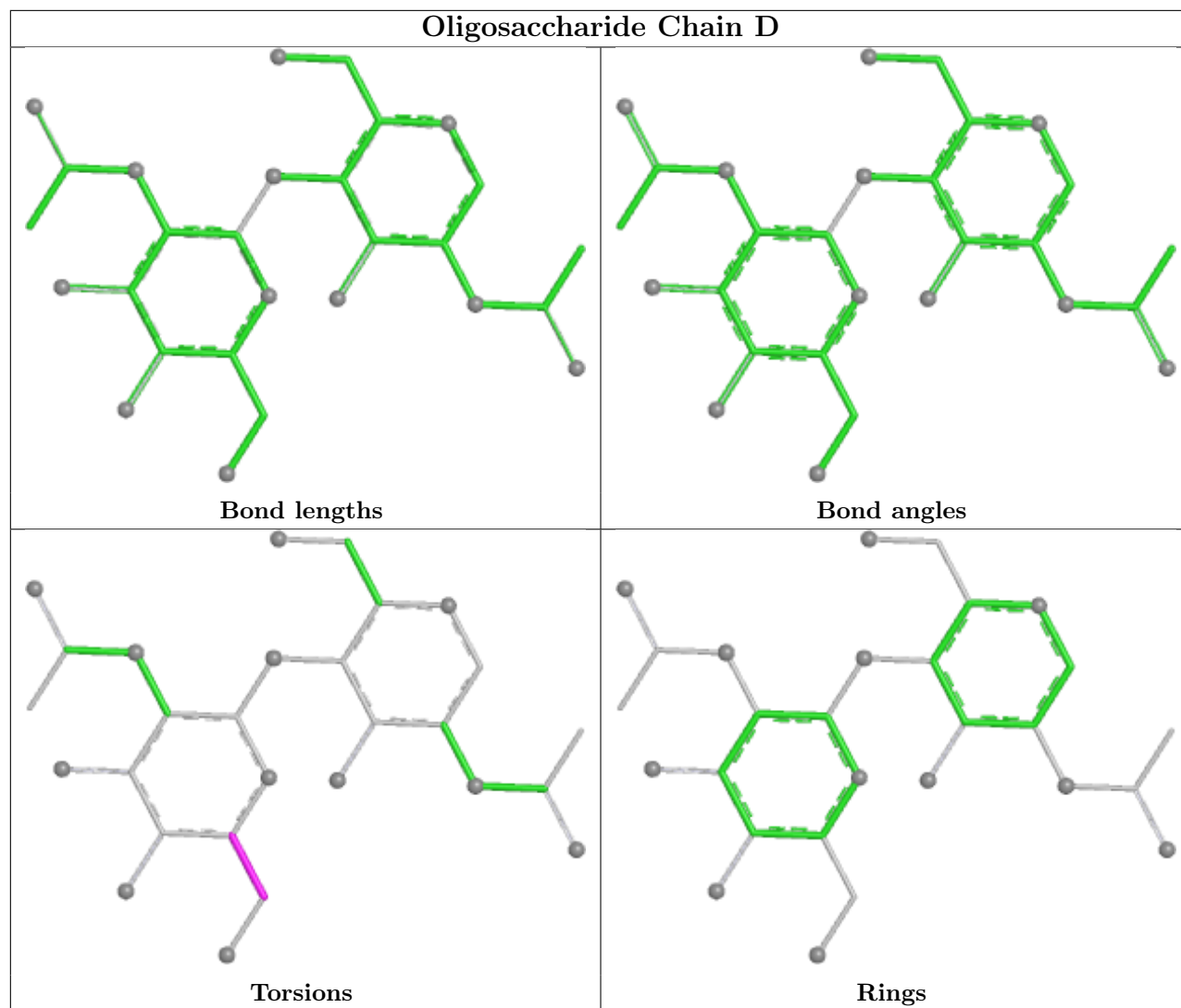
3 monomers are involved in 2 short contacts:

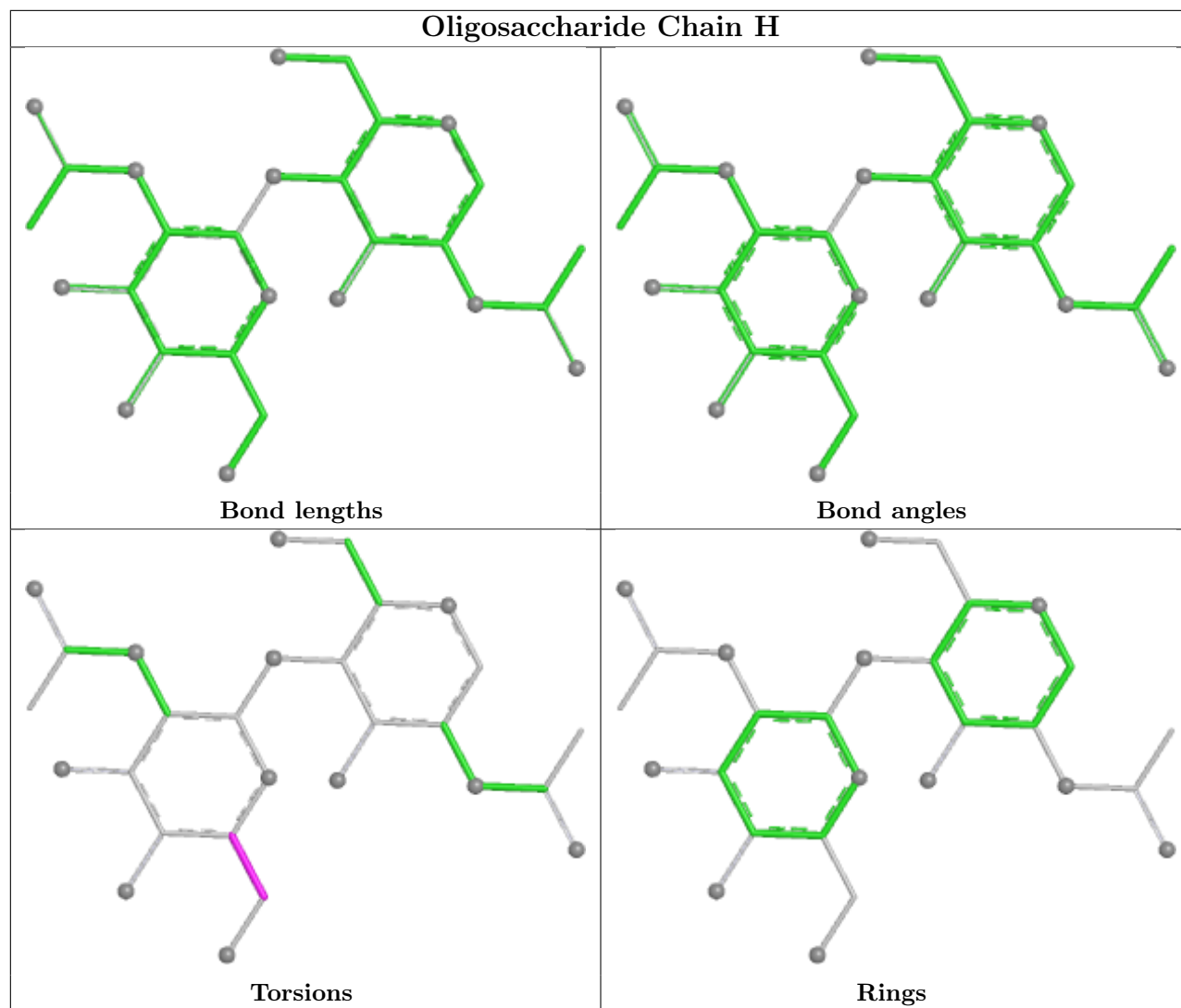
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	1	0
2	I	2	NAG	1	0
4	E	1	NAG	1	0

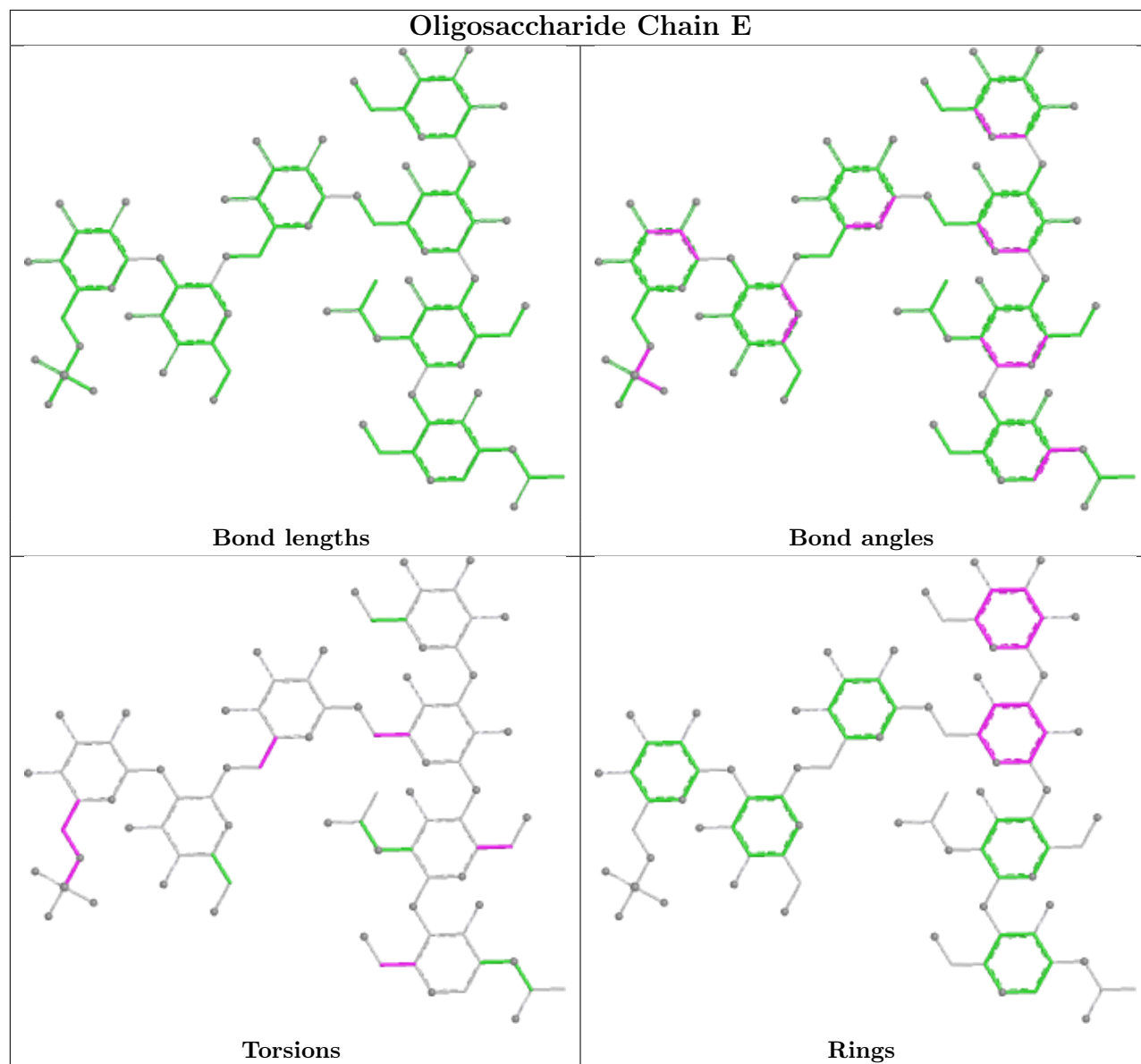
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

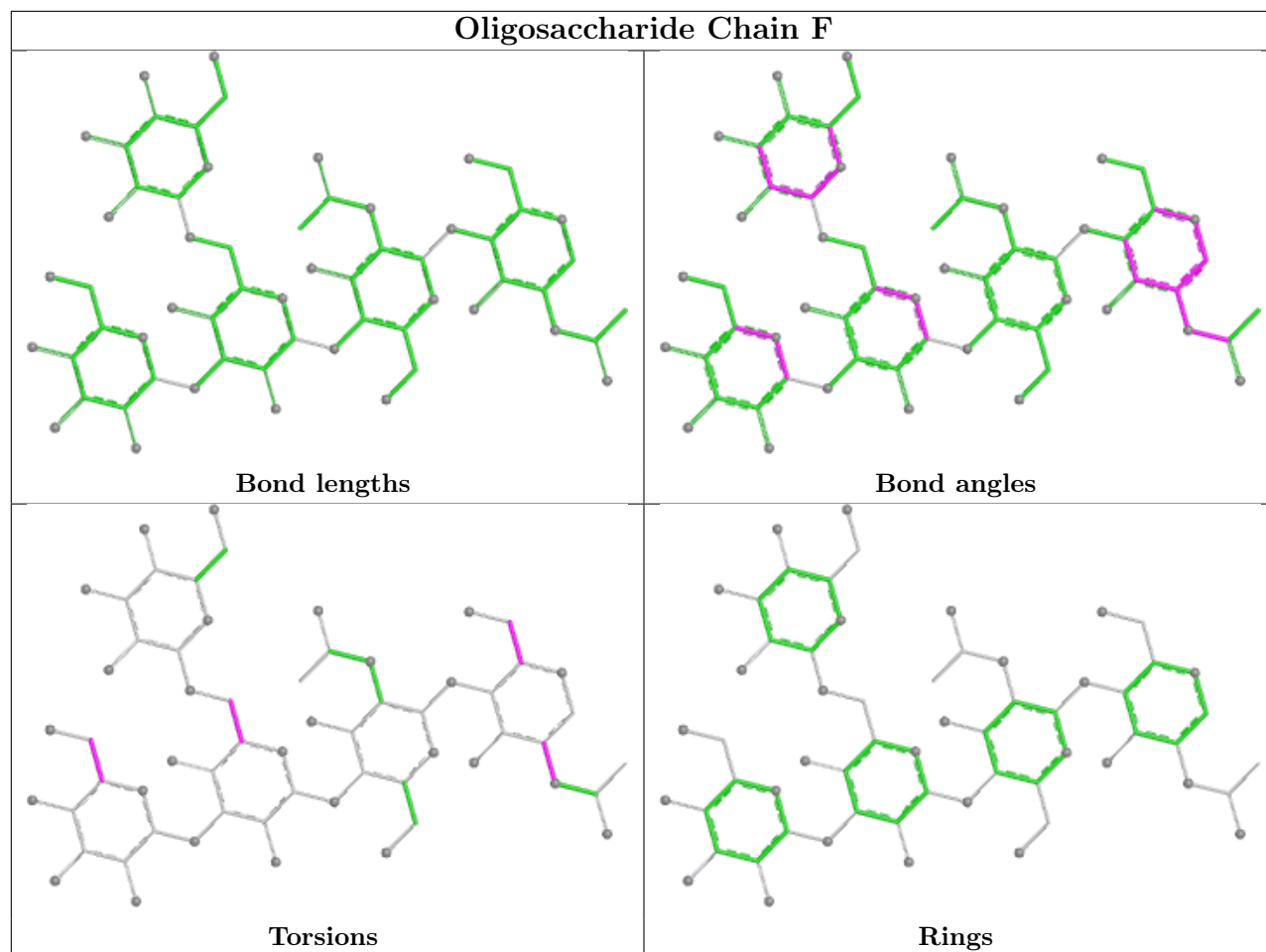


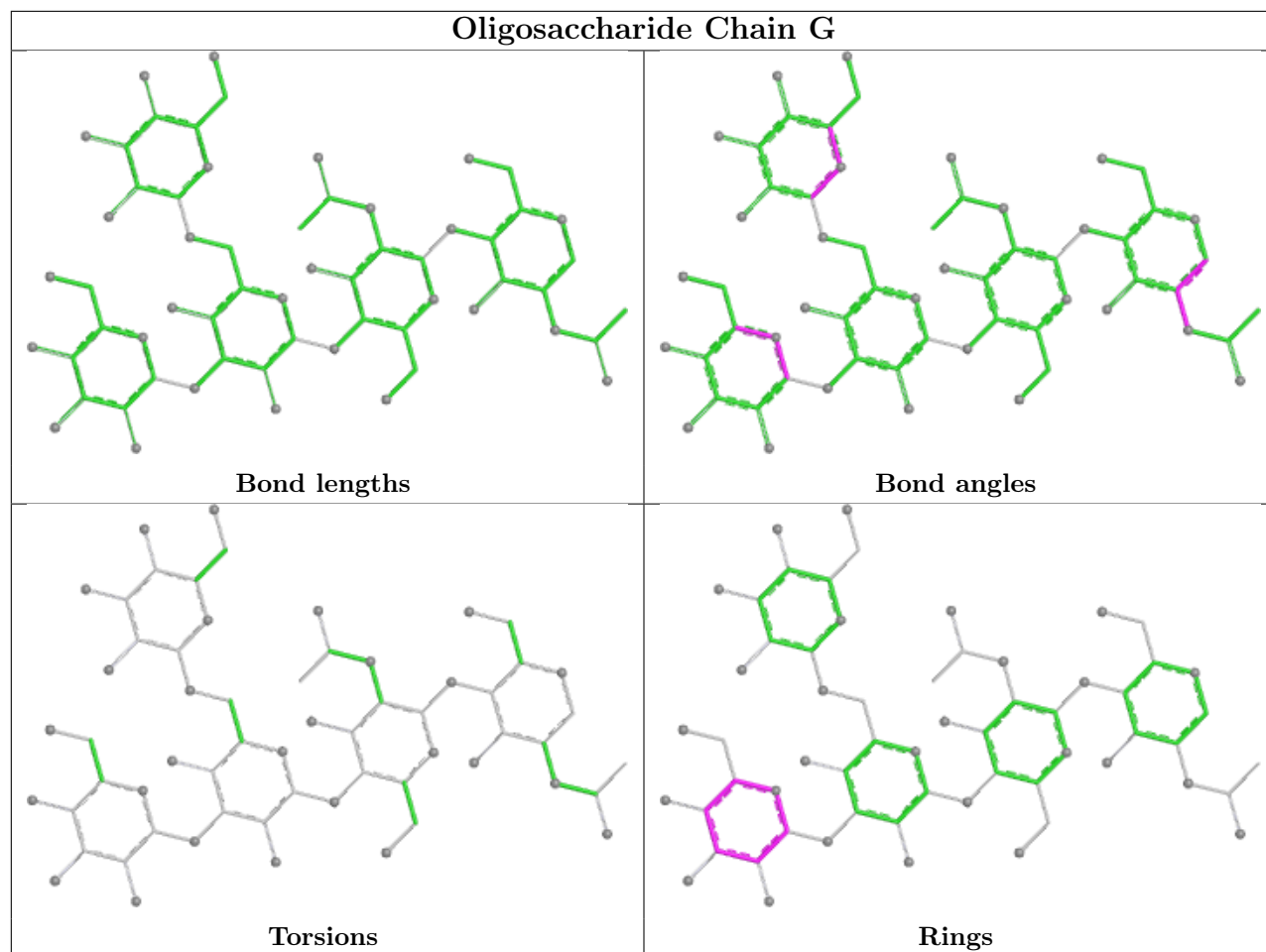


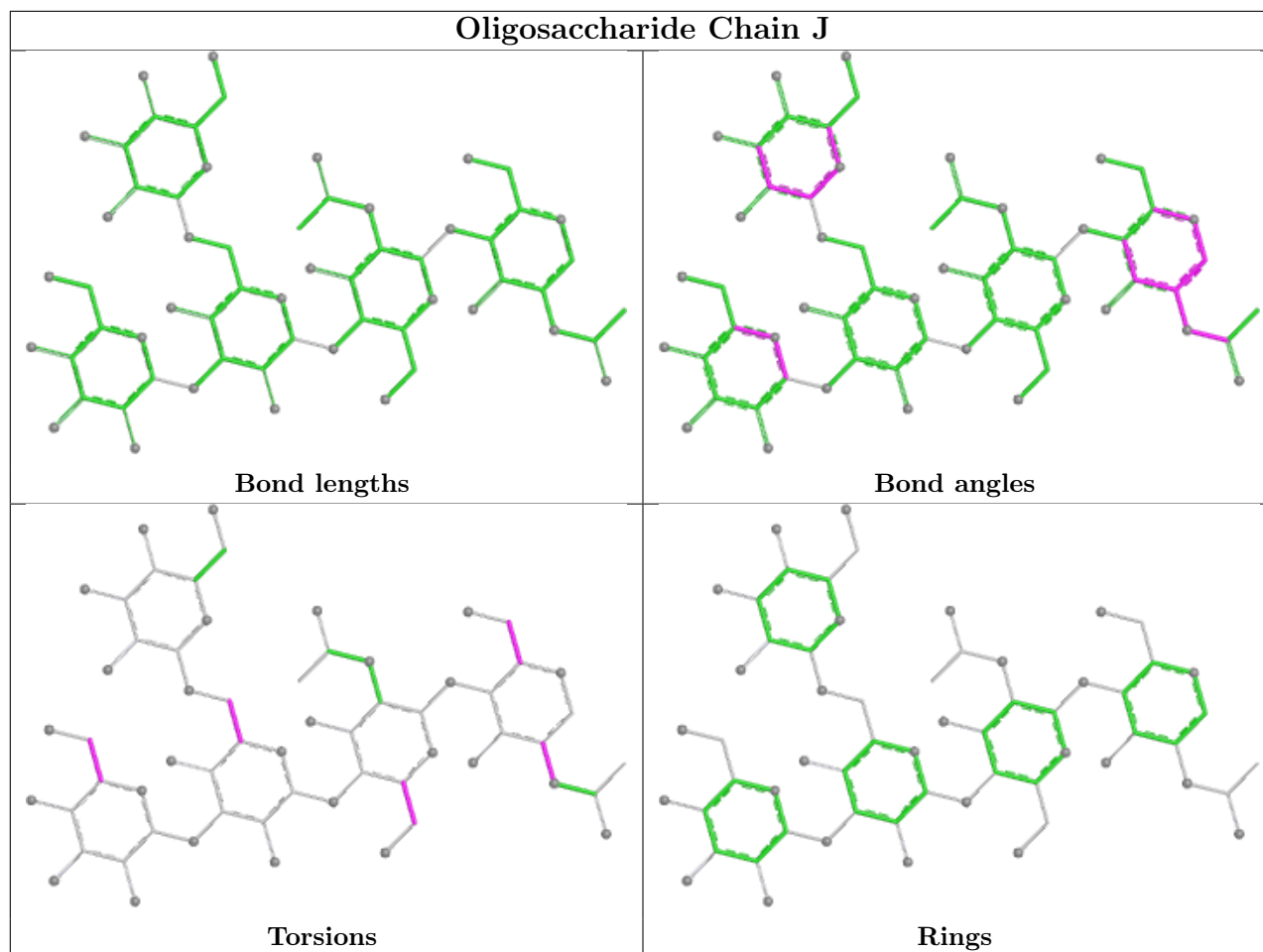












5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	PCW	B	519	-	10,10,53	0.40	0	9,9,61	0.26	0
7	PCW	A	519	-	53,53,53	0.47	1 (1%)	59,61,61	0.53	0
6	CLR	A	518	-	31,31,31	0.47	0	48,48,48	1.00	5 (10%)
7	PCW	B	518	-	53,53,53	0.45	0	59,61,61	0.55	0
6	CLR	B	517	-	31,31,31	0.52	0	48,48,48	1.13	6 (12%)

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
7	PCW	B	519	-	-	1/8/8/57	-
7	PCW	A	519	-	-	22/57/57/57	-
6	CLR	A	518	-	-	4/10/68/68	0/4/4/4
7	PCW	B	518	-	-	22/57/57/57	-
6	CLR	B	517	-	-	4/10/68/68	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	519	PCW	C5-N	2.01	1.57	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	517	CLR	C11-C12-C13	3.16	118.07	112.74
6	B	517	CLR	C17-C13-C14	-2.94	96.73	100.10
6	A	518	CLR	C11-C9-C8	-2.61	108.14	111.78
6	B	517	CLR	C11-C9-C8	-2.58	108.17	111.78
6	A	518	CLR	C17-C13-C14	-2.44	97.29	100.10

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

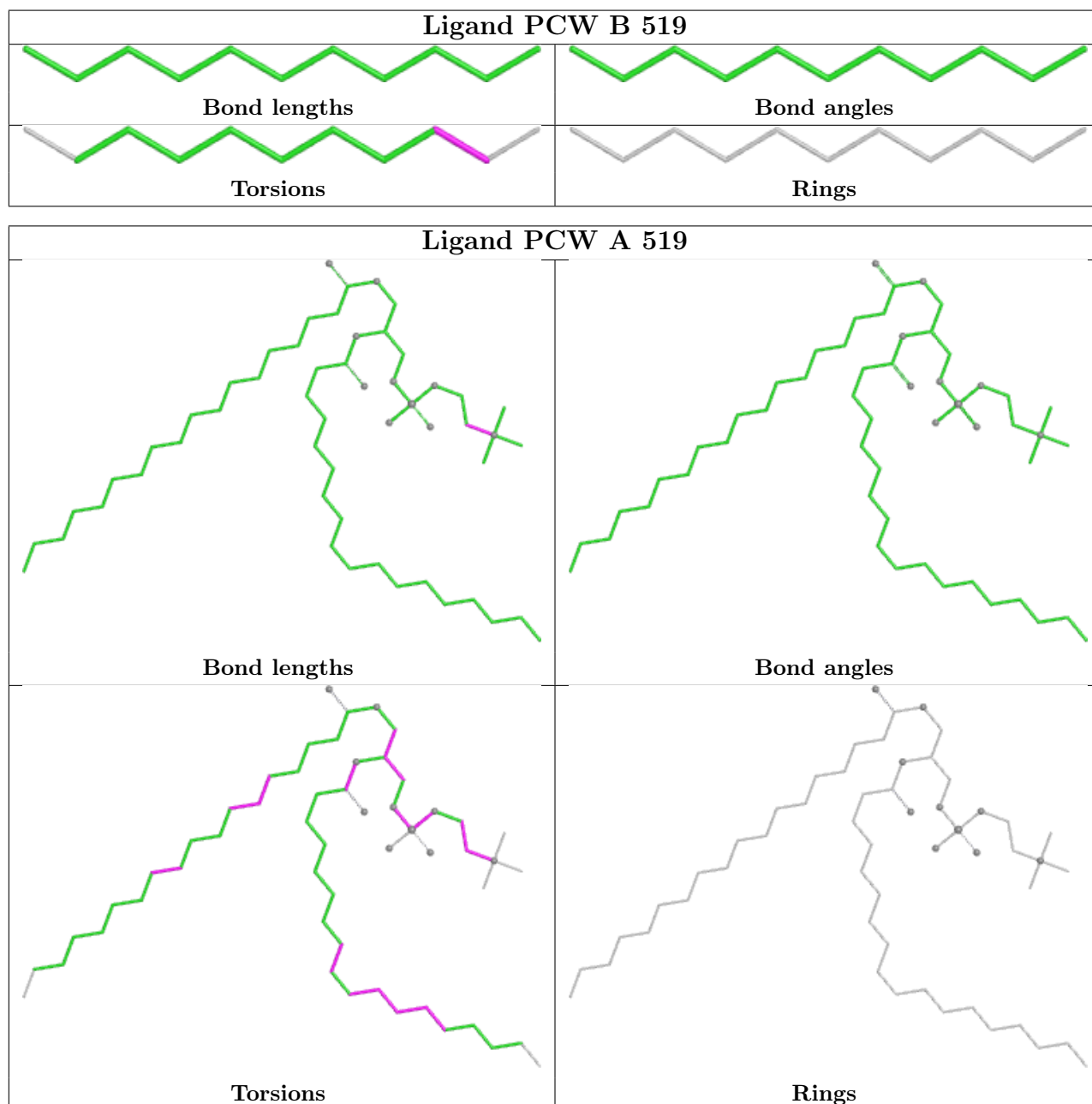
Mol	Chain	Res	Type	Atoms
7	A	519	PCW	O4P-C4-C5-N
7	A	519	PCW	C1-O3P-P-O2P
7	A	519	PCW	C1-O3P-P-O4P
7	A	519	PCW	C4-O4P-P-O1P
7	A	519	PCW	C4-O4P-P-O3P

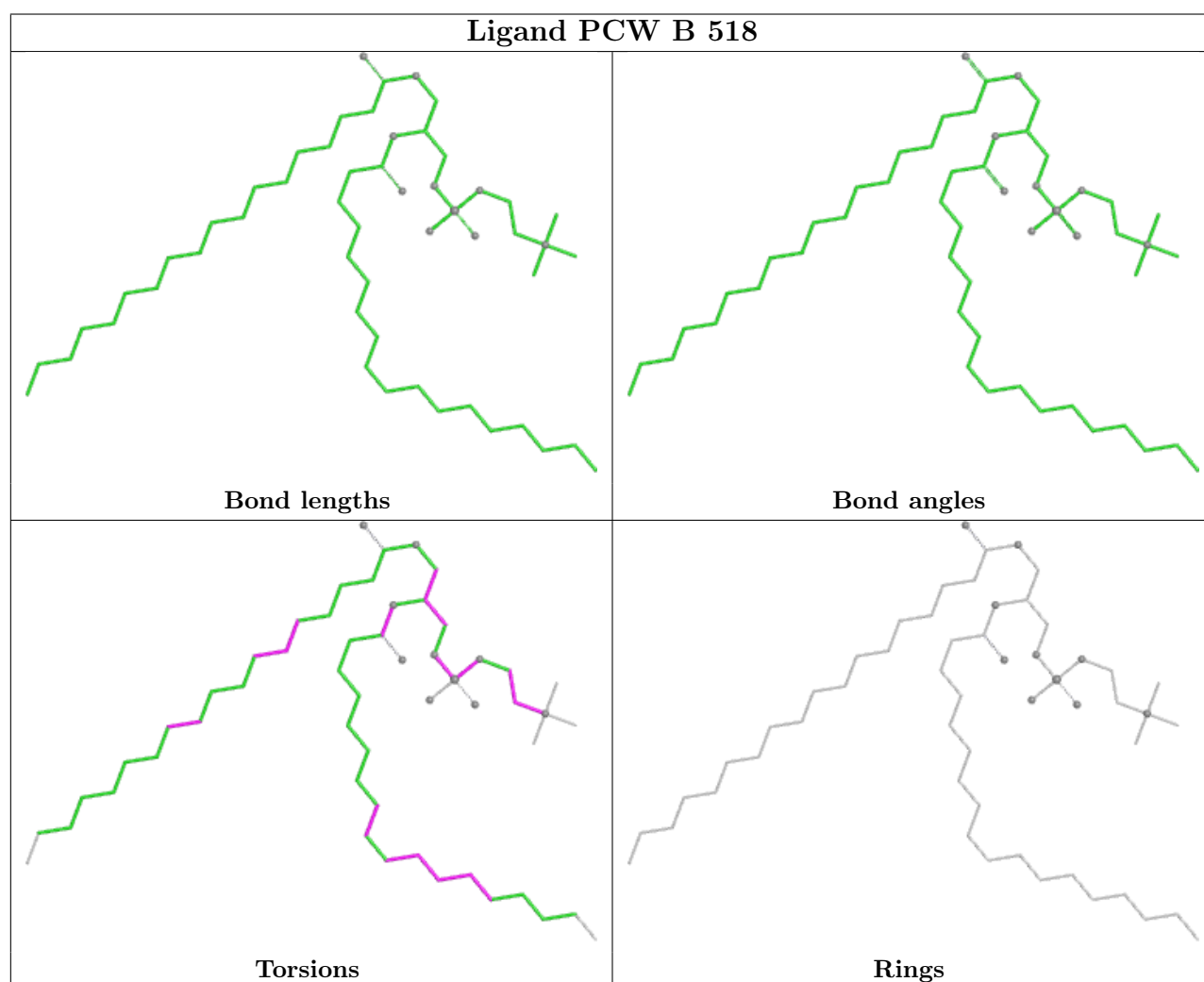
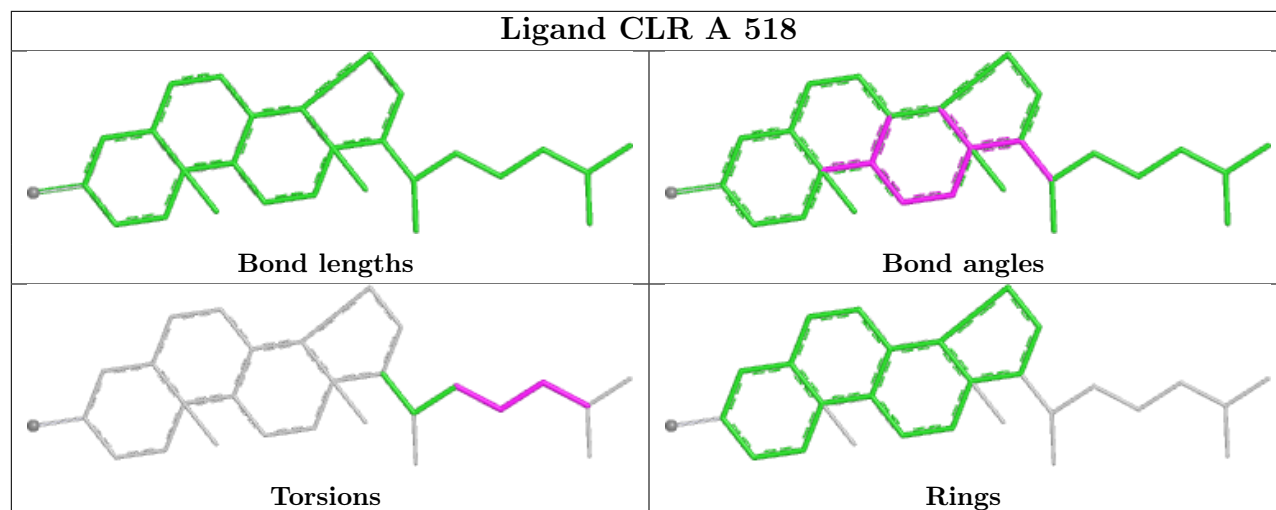
There are no ring outliers.

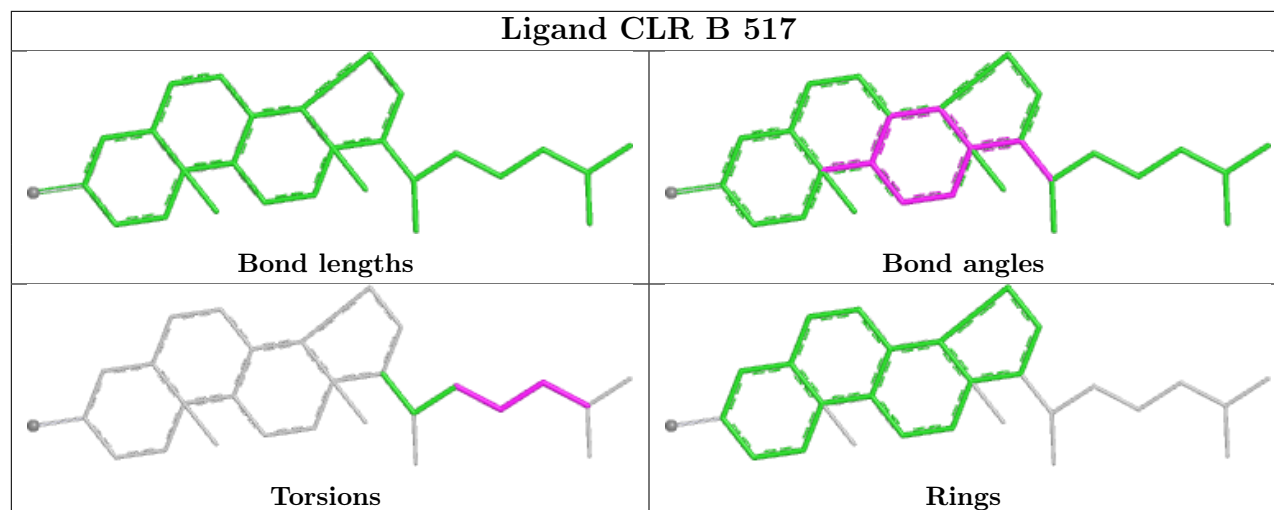
3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	519	PCW	1	0
6	A	518	CLR	7	0
6	B	517	CLR	6	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	316/410 (77%)	0.08	10 (3%) 50 29	91, 119, 174, 204	0
1	B	324/410 (79%)	0.06	6 (1%) 66 43	91, 118, 168, 201	0
All	All	640/820 (78%)	0.07	16 (2%) 58 35	91, 119, 171, 204	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	PRO	6.5
1	A	301	ILE	6.1
1	B	301	ILE	5.8
1	A	259	LEU	5.8
1	A	429	ILE	5.1

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	E	5	11/12	0.24	0.14	220,223,225,225	0
5	MAN	G	5	11/12	0.28	0.15	204,205,207,211	0
4	MAN	E	4	11/12	0.35	0.12	208,213,215,217	0
2	BMA	C	3	11/12	0.39	0.13	163,172,181,186	0
4	MAN	E	7	11/12	0.42	0.17	196,199,204,204	0

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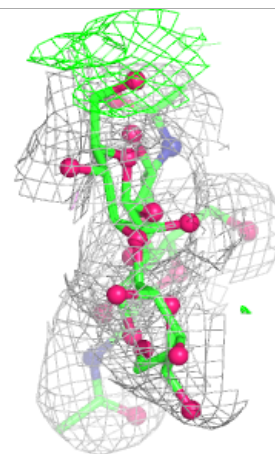
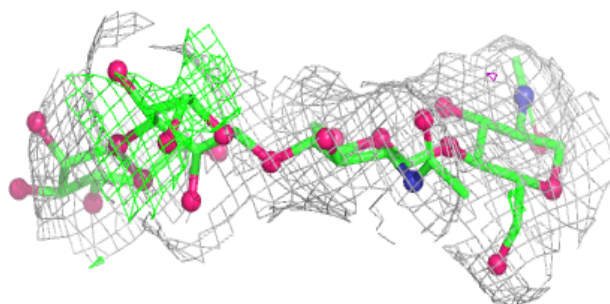
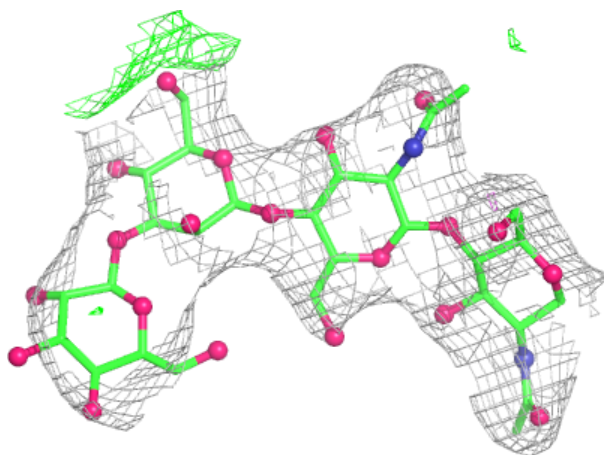
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	I	4	11/12	0.50	0.12	176,188,193,194	0
5	MAN	F	5	11/12	0.52	0.12	181,184,189,190	0
5	MAN	J	5	11/12	0.52	0.13	171,177,181,181	0
2	MAN	C	4	11/12	0.63	0.13	187,191,195,197	0
3	NAG	D	2	14/15	0.66	0.14	164,175,185,188	0
5	MAN	F	4	11/12	0.67	0.12	159,163,174,178	0
2	BMA	I	3	11/12	0.69	0.20	183,190,193,193	0
5	MAN	G	4	11/12	0.69	0.11	171,182,187,189	0
5	MAN	J	4	11/12	0.71	0.09	165,167,168,169	0
4	BMA	E	3	11/12	0.73	0.12	175,188,197,204	0
3	NAG	H	2	14/15	0.75	0.13	156,168,174,176	0
5	BMA	G	3	11/12	0.76	0.09	163,175,185,196	0
4	M6D	E	6	15/16	0.78	0.16	216,219,224,226	0
5	BMA	F	3	11/12	0.84	0.08	154,162,174,178	0
2	NAG	I	2	14/15	0.84	0.17	159,167,174,175	0
4	NAG	E	2	14/15	0.86	0.17	137,146,153,162	0
5	NAG	J	1	14/15	0.89	0.14	110,119,129,133	0
5	NAG	F	1	14/15	0.90	0.11	104,120,127,130	0
5	BMA	J	3	11/12	0.90	0.05	155,164,169,172	0
5	NAG	G	2	14/15	0.92	0.11	132,136,146,156	0
2	NAG	C	2	14/15	0.92	0.09	136,143,148,154	0
3	NAG	H	1	14/15	0.92	0.08	144,150,154,157	0
5	NAG	F	2	14/15	0.92	0.09	115,134,142,145	0
2	NAG	I	1	14/15	0.93	0.12	120,136,145,153	0
5	NAG	J	2	14/15	0.94	0.10	115,130,140,144	0
5	NAG	G	1	14/15	0.95	0.15	113,118,123,124	0
4	NAG	E	1	14/15	0.95	0.10	111,118,123,130	0
3	NAG	D	1	14/15	0.96	0.07	135,146,156,163	0
2	NAG	C	1	14/15	0.96	0.09	115,119,125,129	0

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

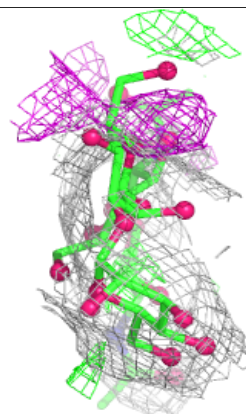
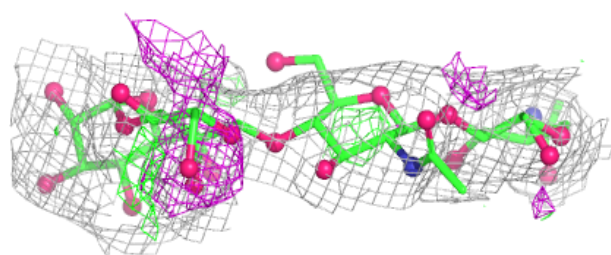
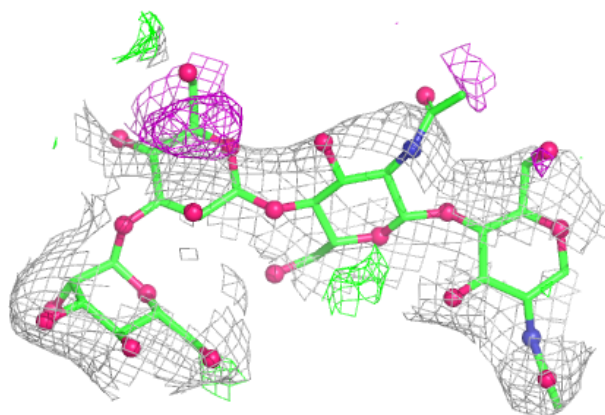
Electron density around Chain C:

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

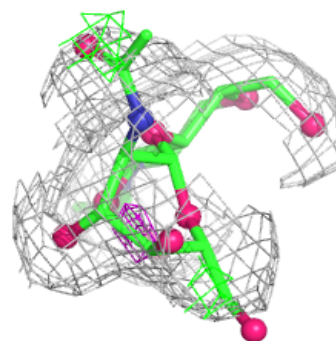
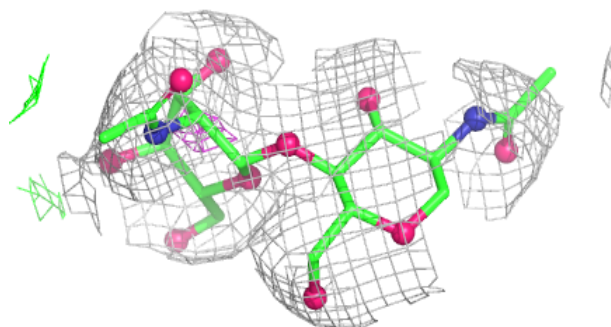
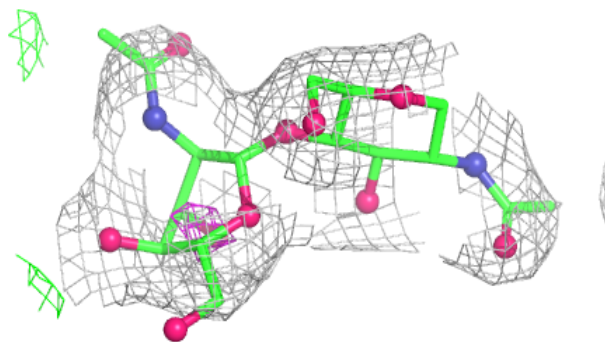


Electron density around Chain I:

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

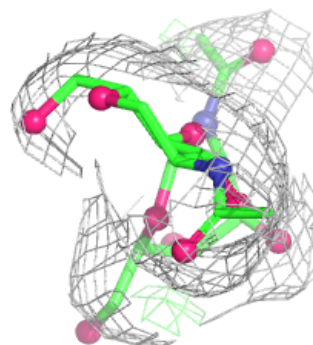
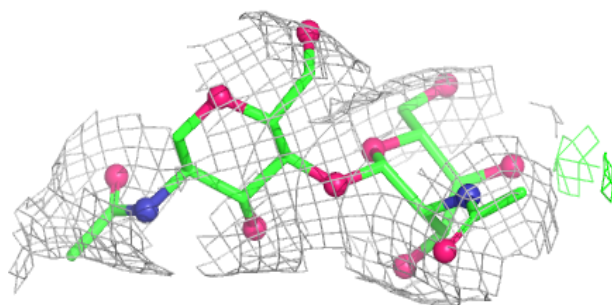
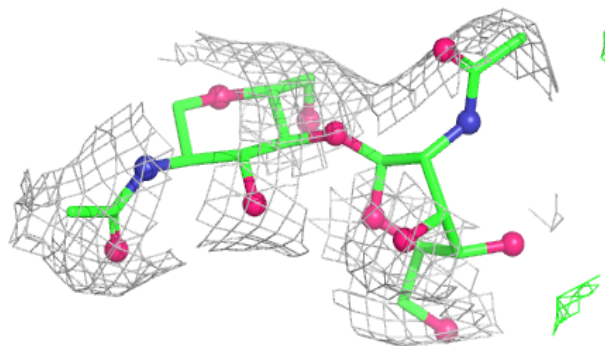
**Electron density around Chain D:**

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

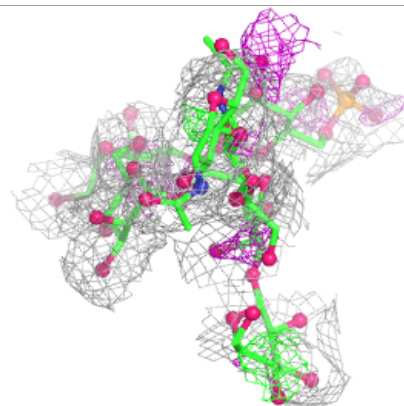
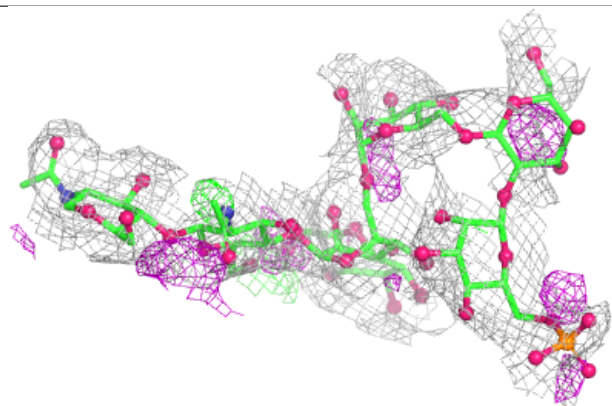
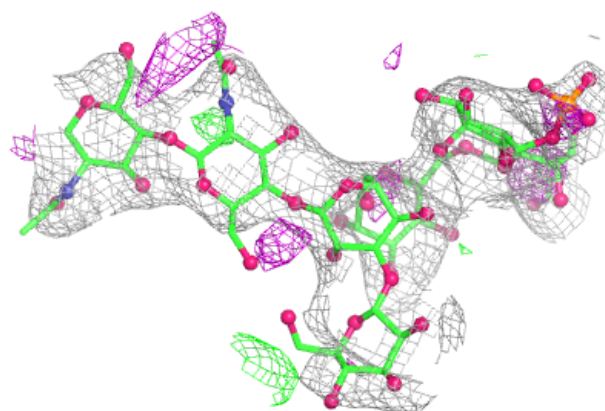


Electron density around Chain H:

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

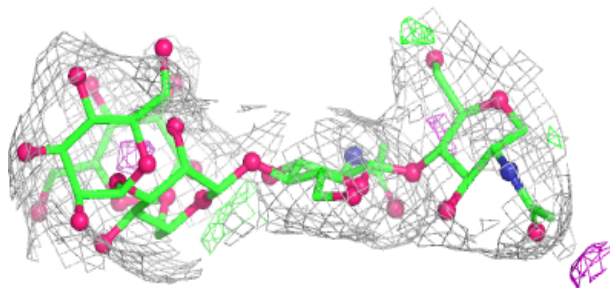
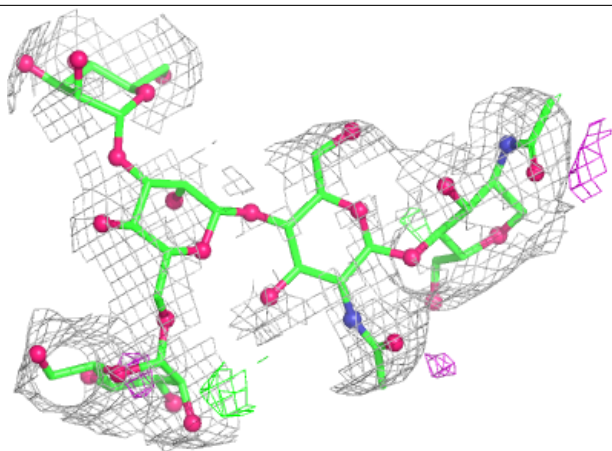
**Electron density around Chain E:**

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



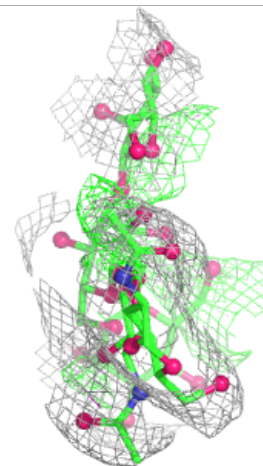
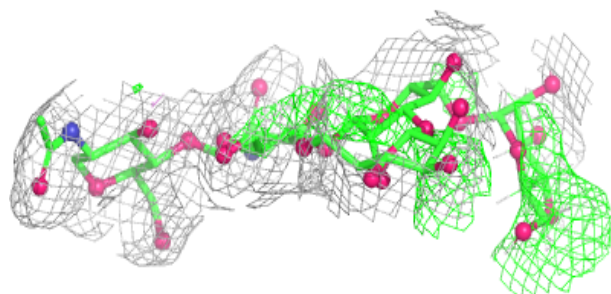
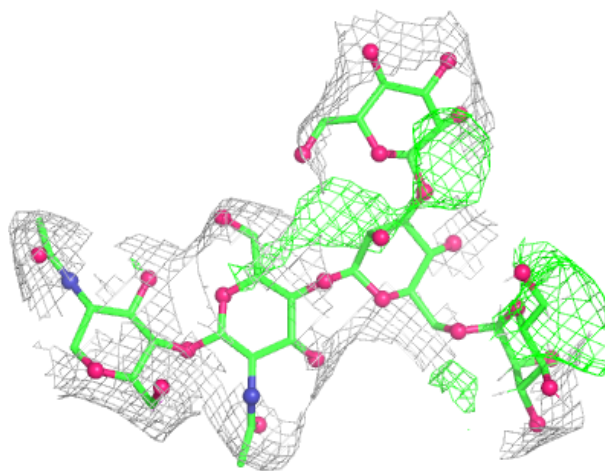
Electron density around Chain F:

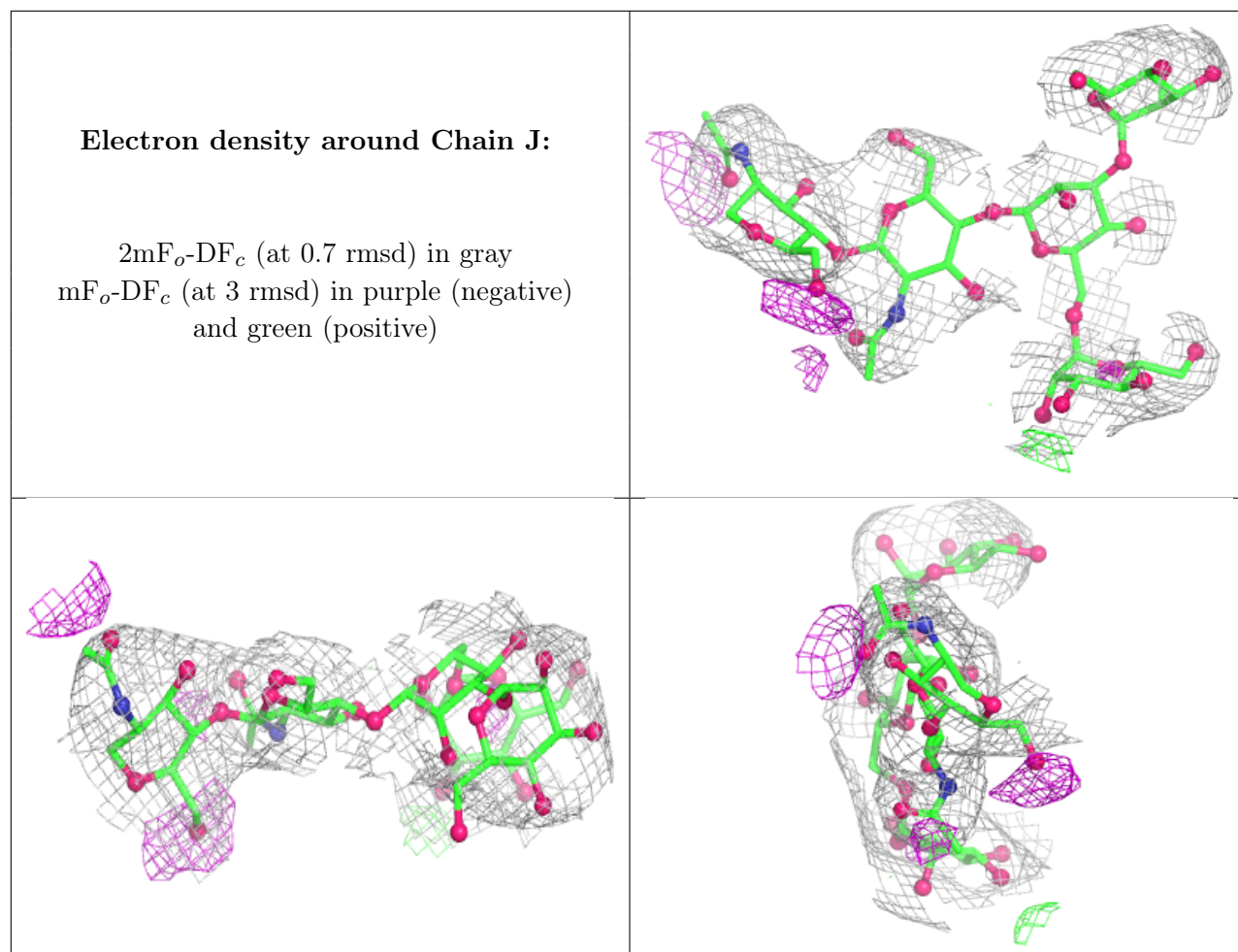
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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 [i](#)

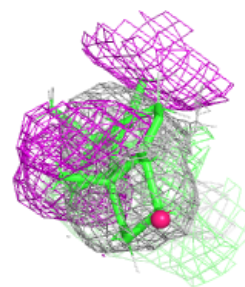
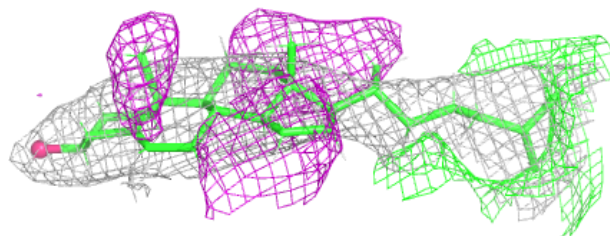
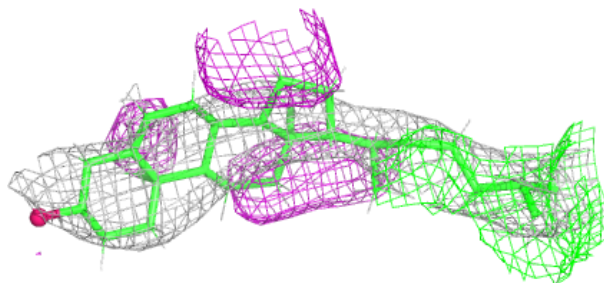
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	CLR	A	518	28/28	0.72	0.31	123,165,176,177	0
6	CLR	B	517	28/28	0.75	0.31	128,171,176,177	0
7	PCW	B	518	54/54	0.84	0.26	115,173,221,225	0
7	PCW	A	519	54/54	0.85	0.26	122,163,241,248	0
7	PCW	B	519	11/54	0.92	0.27	119,130,153,155	0

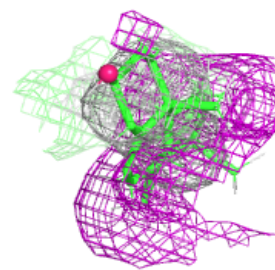
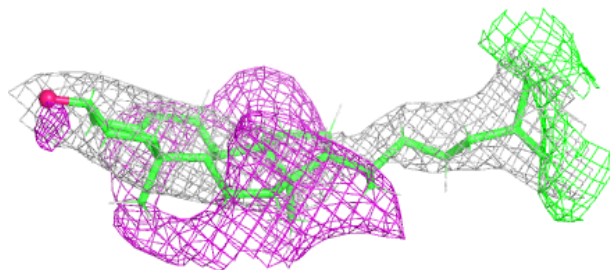
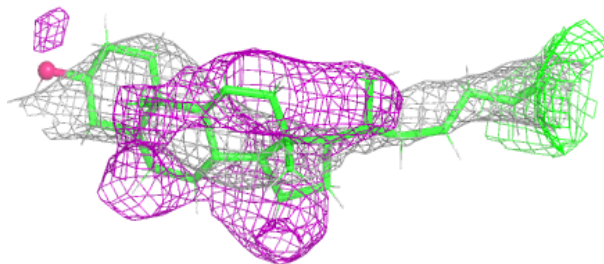
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLR A 518:

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

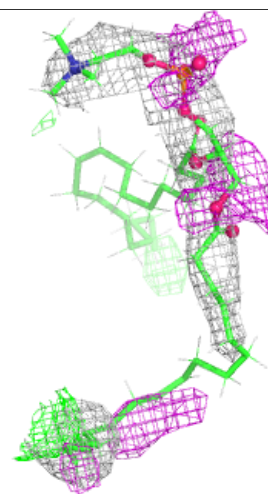
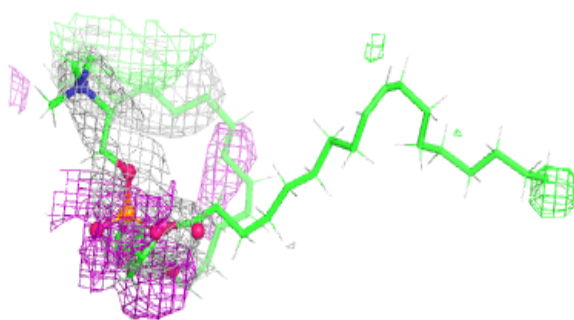
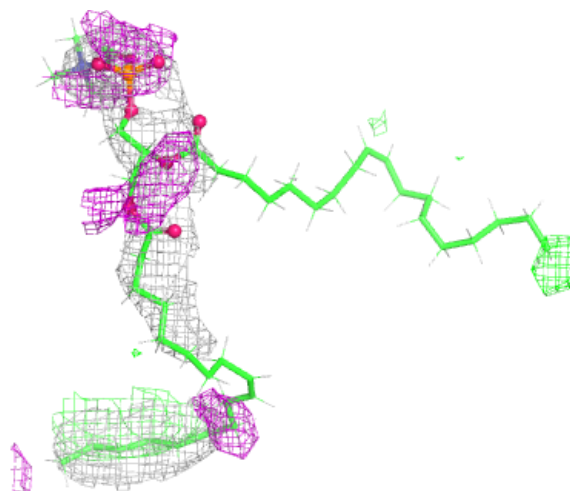
**Electron density around CLR B 517:**

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



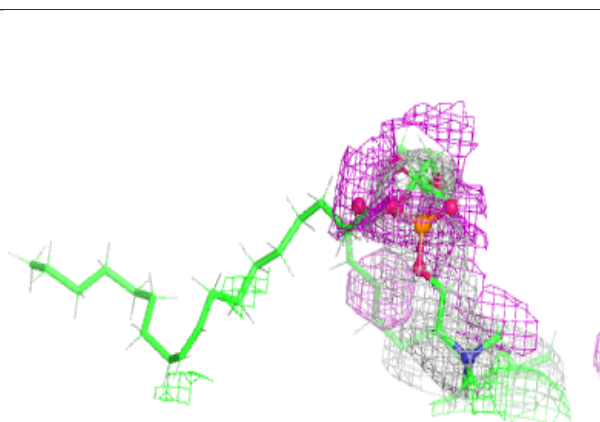
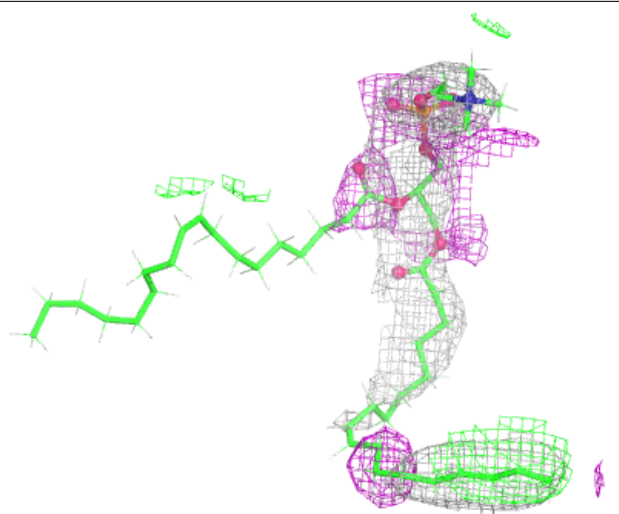
Electron density around PCW B 518:

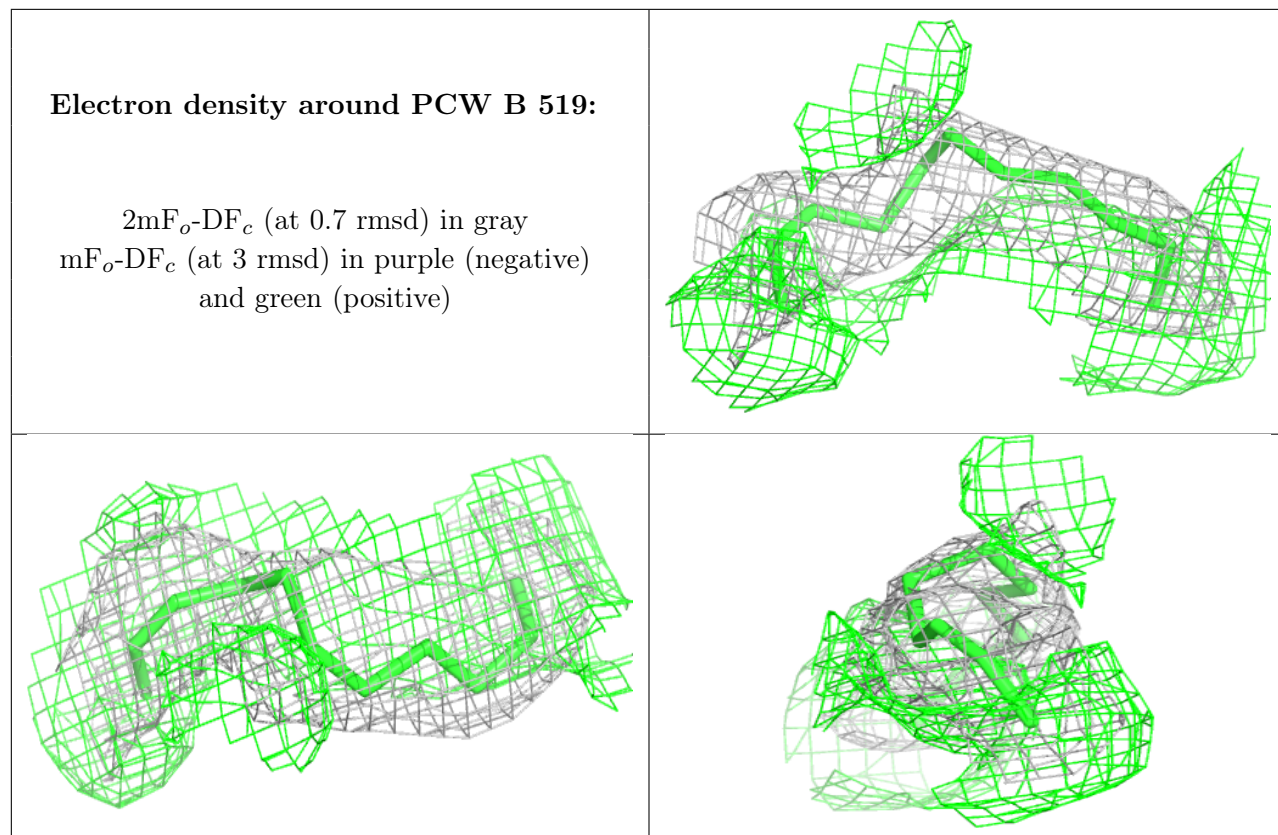
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PCW A 519:

$2mF_o-DF_c$ (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.