



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:49 PM UTC

PDB ID : 8JBL / pdb_00008jbl
Title : Crystal structure of Na⁺,K⁺-ATPase in the E1.Mg²⁺ state
Authors : Kanai, R.; Vilsen, B.; Cornelius, F.; Toyoshima, C.
Deposited on : 2023-05-09
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)
Xtriage (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

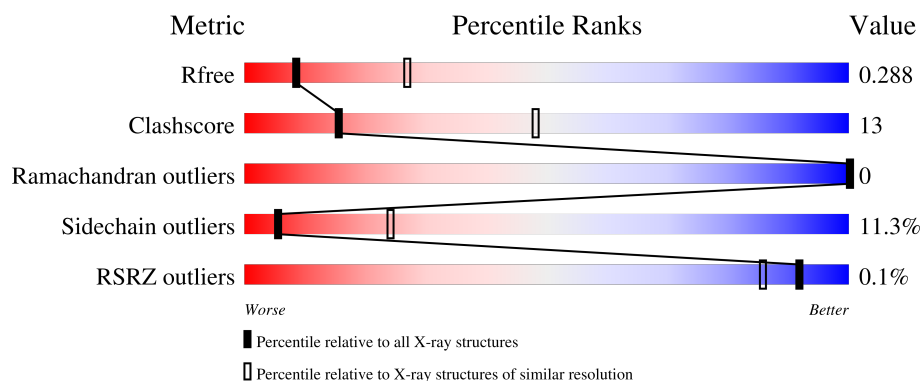
1 Overall quality at a glance

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.



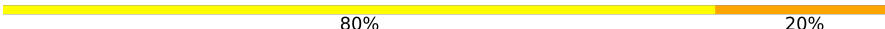
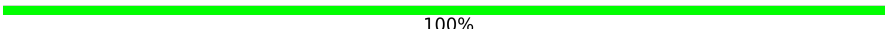
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1021	 63% 30% 5% 2%
1	C	1021	 64% 29% 5% 2%
2	B	303	 57% 34% 5% 4%
2	D	303	 62% 31% 5% 2%
3	E	65	 37% 14% 49%

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Mol	Chain	Length	Quality of chain
3	G	65	 38% 15% 46%
4	F	6	 50% 50%
5	H	5	 80% 20%
6	I	2	 100%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 21682 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 Sodium/potassium-transporting ATPase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	995	Total	C	N	O	S	0	0	0
			7723	4923	1301	1452	47			
1	C	995	Total	C	N	O	S	0	0	0
			7723	4923	1301	1452	47			

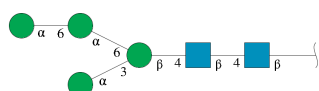
- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	0	0
			2386	1546	390	437	13			
2	D	291	Total	C	N	O	S	0	0	0
			2386	1546	390	437	13			

- Molecule 3 is a protein called FXYD domain-containing ion transport regulator.

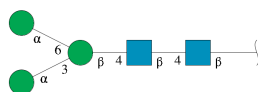
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	35	Total	C	N	O	0	0	0
			285	192	46	47			
3	E	33	Total	C	N	O	0	0	0
			262	179	38	45			

- Molecule 4 is an oligosaccharide called 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
4	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

- 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	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

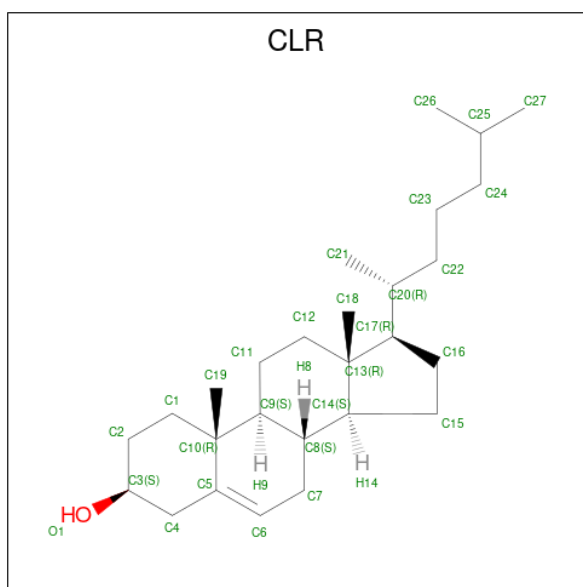


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

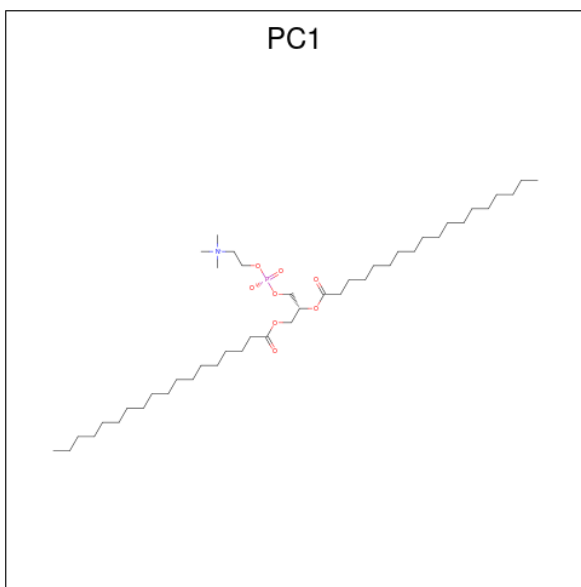
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Mg	0	0
			3	3		
7	C	3	Total	Mg	0	0
			3	3		

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



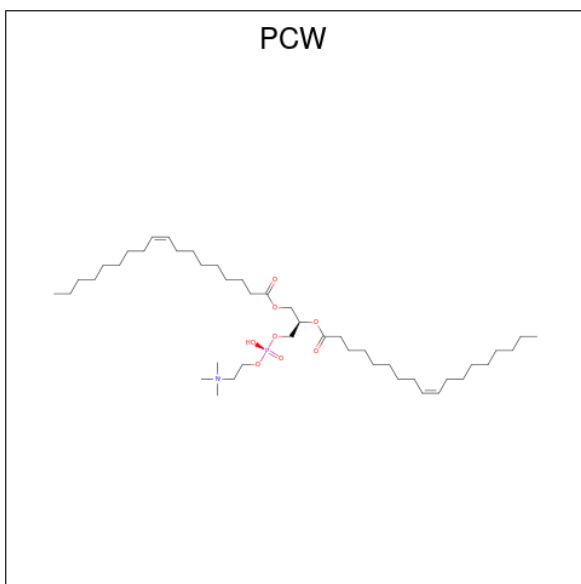
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			28	27	1		
8	A	1	Total	C	O	0	0
			28	27	1		
8	A	1	Total	C	O	0	0
			28	27	1		
8	C	1	Total	C	O	0	0
			28	27	1		
8	C	1	Total	C	O	0	0
			28	27	1		
8	E	1	Total	C	O	0	0
			28	27	1		

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



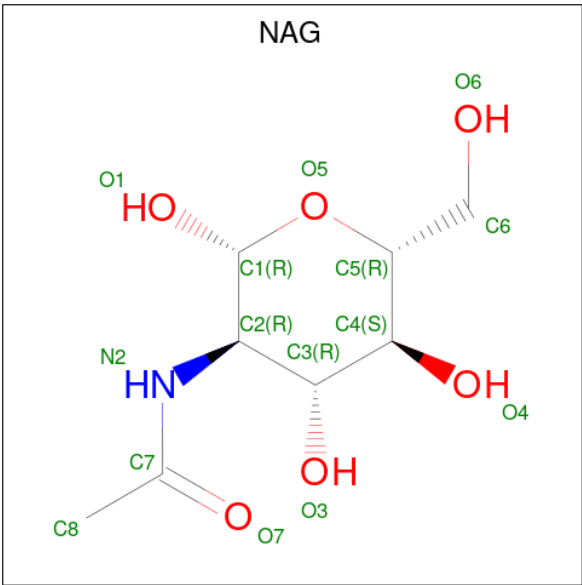
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 10 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



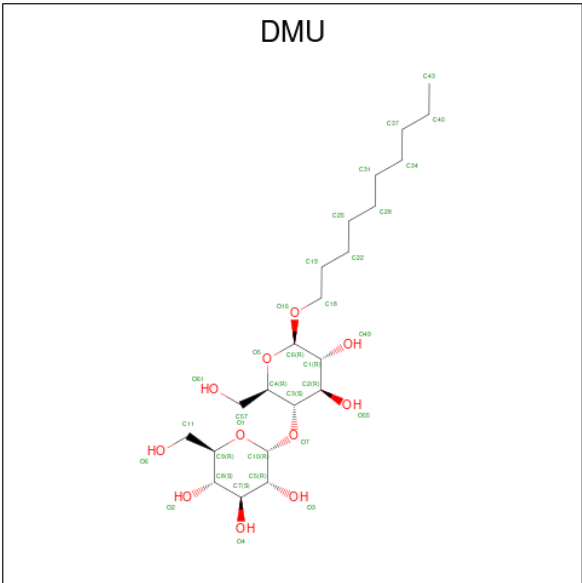
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			22	12	1	8	1		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 12 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	E	1	Total	C	O	0	0
			33	22	11		

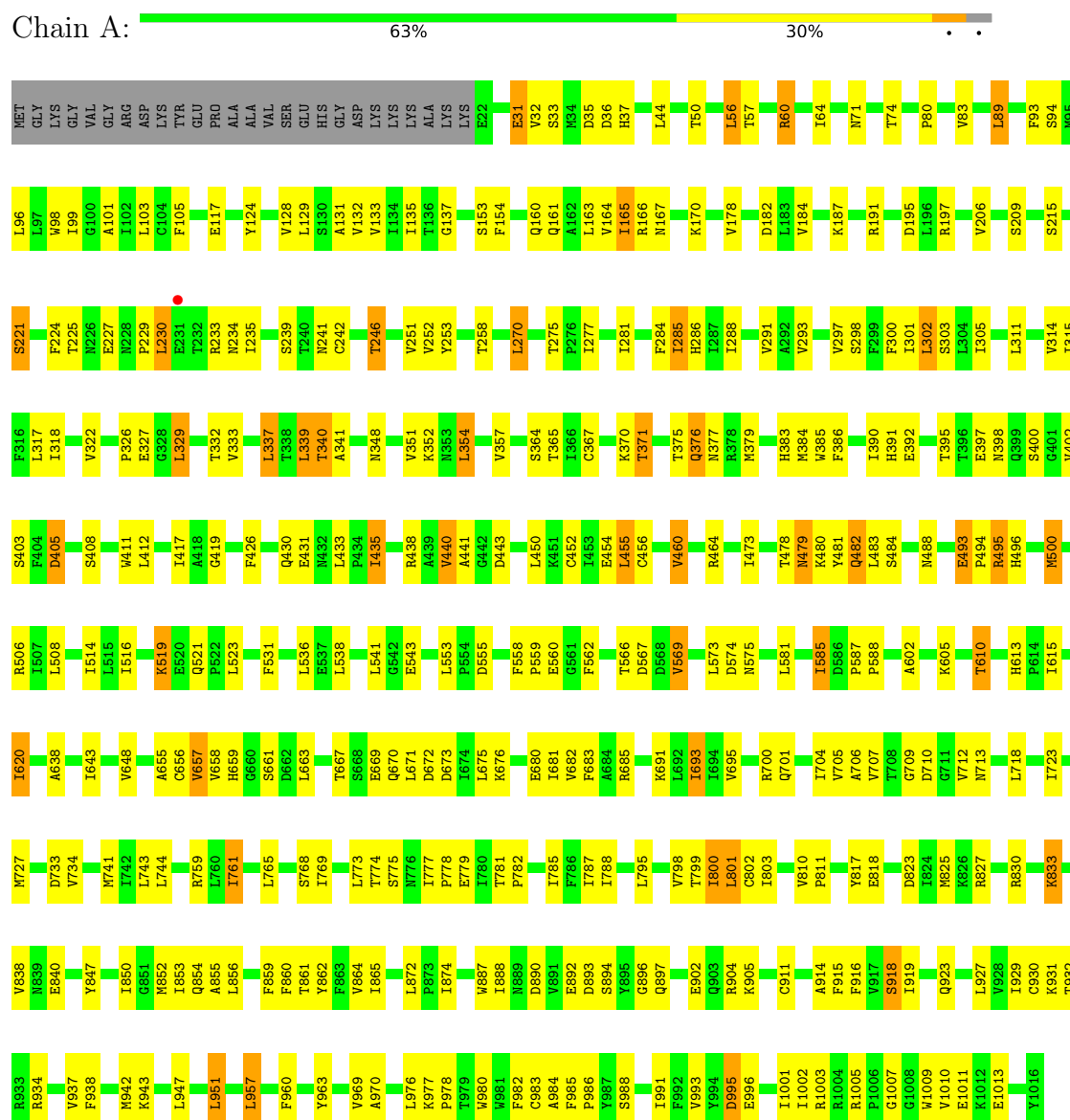
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	19	Total 19	O 19	0	0
13	C	12	Total 12	O 12	0	0
13	D	2	Total 2	O 2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha



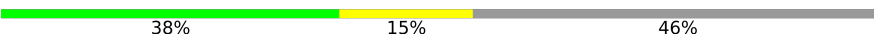
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha

- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain D:  62% 31%



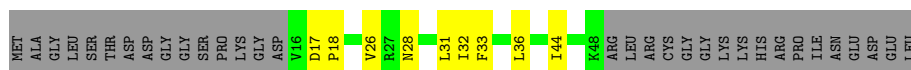
- Molecule 3: FXYP domain-containing ion transport regulator

Chain G:  38% 15% 46%



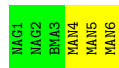
- Molecule 3: FXYP domain-containing ion transport regulator

Chain E:  37% 14% 49%



- Molecule 4: 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 F:  50% 50%



- 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 H:  80% 20%



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

Chain I:

100%

3AG1
3AG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	196.80Å 74.32Å 163.55Å 90.00° 116.29° 90.00°	Depositor
Resolution (Å)	11.99 – 3.00 11.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	53.0 (11.99-3.00) 52.1 (11.99-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.233 , 0.282 0.238 , 0.288	Depositor DCC
R_{free} test set	2311 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.028 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21682	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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: BMA, PC1, MAN, NAG, PCW, DMU, CLR, MG

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	0.17	0/7873	0.43	0/10683
1	C	0.18	0/7873	0.43	0/10683
2	B	0.15	0/2449	0.42	0/3301
2	D	0.16	0/2449	0.43	0/3301
3	E	0.17	0/268	0.35	0/364
3	G	0.15	0/291	0.39	0/393
All	All	0.17	0/21203	0.43	0/28725

There are no bond length outliers.

There are no bond angle outliers.

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	7723	0	7775	215	0
1	C	7723	0	7775	217	0
2	B	2386	0	2362	69	0
2	D	2386	0	2362	61	0
3	E	262	0	268	9	0
3	G	285	0	296	12	0
4	F	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	61	0	52	1	0
6	I	28	0	25	0	0
7	A	3	0	0	0	0
7	C	3	0	0	0	0
8	A	84	0	138	7	0
8	C	56	0	92	5	0
8	E	28	0	46	2	0
9	A	162	0	264	23	0
10	A	186	0	192	11	0
10	C	154	0	126	4	0
11	D	14	0	13	0	0
12	E	33	0	42	7	0
13	A	19	0	0	0	0
13	C	12	0	0	0	0
13	D	2	0	0	0	0
All	All	21682	0	21889	582	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 13.

The worst 5 of 582 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:1009:TRP:HE1	2:D:34:LYS:HD3	1.37	0.87
1:A:340:THR:HG21	1:A:761:ILE:HG12	1.62	0.80
1:C:565:ASP:HB2	1:C:570:ASN:HD22	1.44	0.80
9:A:1108:PC1:H372	8:C:1104:CLR:H71	1.64	0.80
9:A:1108:PC1:H2E2	9:A:1108:PC1:H392	1.65	0.79

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	993/1021 (97%)	963 (97%)	30 (3%)	0	100	100
1	C	993/1021 (97%)	942 (95%)	51 (5%)	0	100	100
2	B	289/303 (95%)	276 (96%)	13 (4%)	0	100	100
2	D	289/303 (95%)	269 (93%)	20 (7%)	0	100	100
3	E	31/65 (48%)	29 (94%)	2 (6%)	0	100	100
3	G	33/65 (51%)	31 (94%)	2 (6%)	0	100	100
All	All	2628/2778 (95%)	2510 (96%)	118 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	845/864 (98%)	746 (88%)	99 (12%)	5	23
1	C	845/864 (98%)	749 (89%)	96 (11%)	5	24
2	B	261/269 (97%)	227 (87%)	34 (13%)	4	19
2	D	261/269 (97%)	234 (90%)	27 (10%)	7	28
3	E	27/52 (52%)	26 (96%)	1 (4%)	30	64
3	G	29/52 (56%)	29 (100%)	0	100	100
All	All	2268/2370 (96%)	2011 (89%)	257 (11%)	5	24

5 of 257 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	36	LEU
2	D	93	ASN
1	A	988	SER
1	A	951	LEU
2	D	159	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	482	GLN
1	C	776	ASN
1	C	521	GLN
1	C	570	ASN
1	C	869	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 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	$\# Z > 2$
4	NAG	F	1	2,4	14,14,15	0.31	0	17,19,21	0.57	0
4	NAG	F	2	4	14,14,15	0.50	0	17,19,21	0.61	0
4	BMA	F	3	4	11,11,12	0.78	0	15,15,17	0.78	0
4	MAN	F	4	4	11,11,12	0.88	0	15,15,17	1.11	1 (6%)
4	MAN	F	5	4	11,11,12	1.35	3 (27%)	15,15,17	1.81	2 (13%)
4	MAN	F	6	4	11,11,12	0.85	1 (9%)	15,15,17	1.16	2 (13%)
5	NAG	H	1	5,2	14,14,15	0.31	0	17,19,21	0.51	0
5	NAG	H	2	5	14,14,15	0.76	1 (7%)	17,19,21	0.74	0
5	BMA	H	3	5	11,11,12	1.57	2 (18%)	15,15,17	0.97	0
5	MAN	H	4	5	11,11,12	1.02	2 (18%)	15,15,17	1.07	1 (6%)
5	MAN	H	5	5	11,11,12	1.00	1 (9%)	15,15,17	1.02	1 (6%)
6	NAG	I	1	2,6	14,14,15	0.44	0	17,19,21	0.55	0
6	NAG	I	2	6	14,14,15	0.35	0	17,19,21	0.79	0

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

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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	BMA	C1-C2	3.07	1.59	1.52
5	H	3	BMA	C4-C5	2.98	1.59	1.53
4	F	5	MAN	O5-C5	2.74	1.48	1.43
4	F	5	MAN	O5-C1	2.50	1.47	1.43
4	F	5	MAN	C1-C2	2.45	1.58	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5	MAN	C1-O5-C5	5.88	120.07	112.19
4	F	4	MAN	C1-O5-C5	3.23	116.52	112.19
4	F	6	MAN	C1-O5-C5	3.09	116.33	112.19
5	H	4	MAN	C1-O5-C5	2.62	115.70	112.19
5	H	5	MAN	C1-O5-C5	2.29	115.26	112.19

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

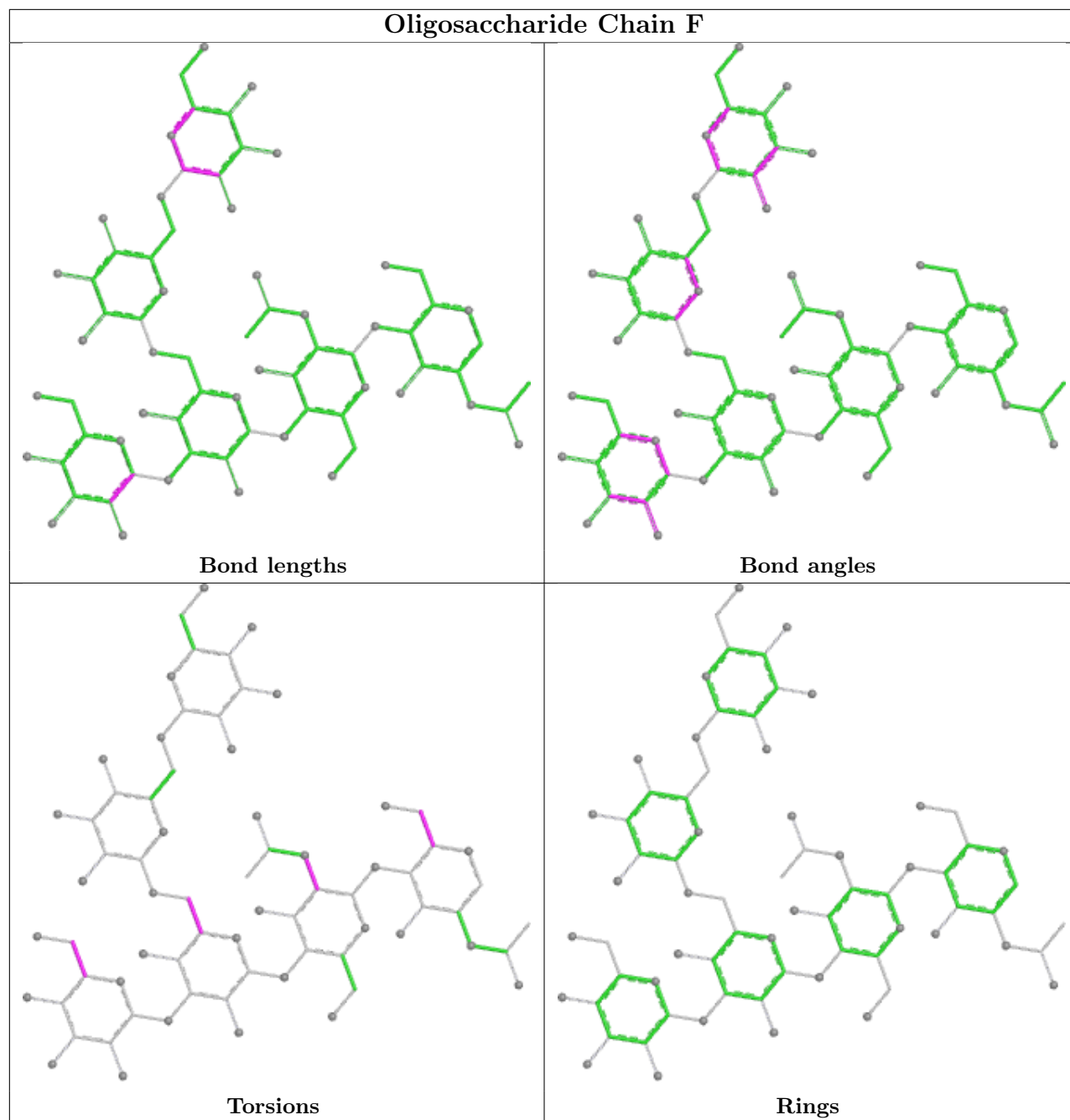
Mol	Chain	Res	Type	Atoms
5	H	3	BMA	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

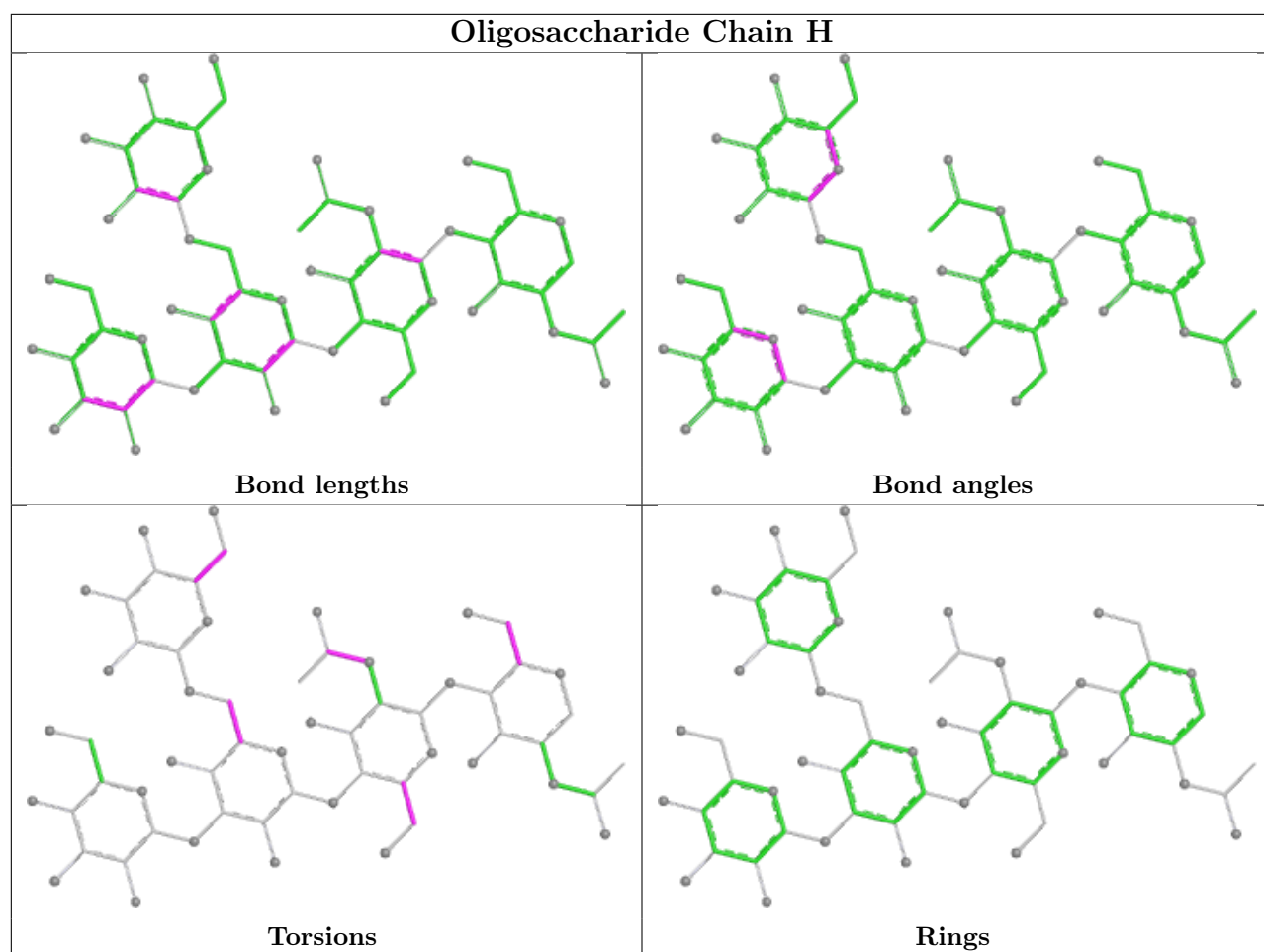
There are no ring outliers.

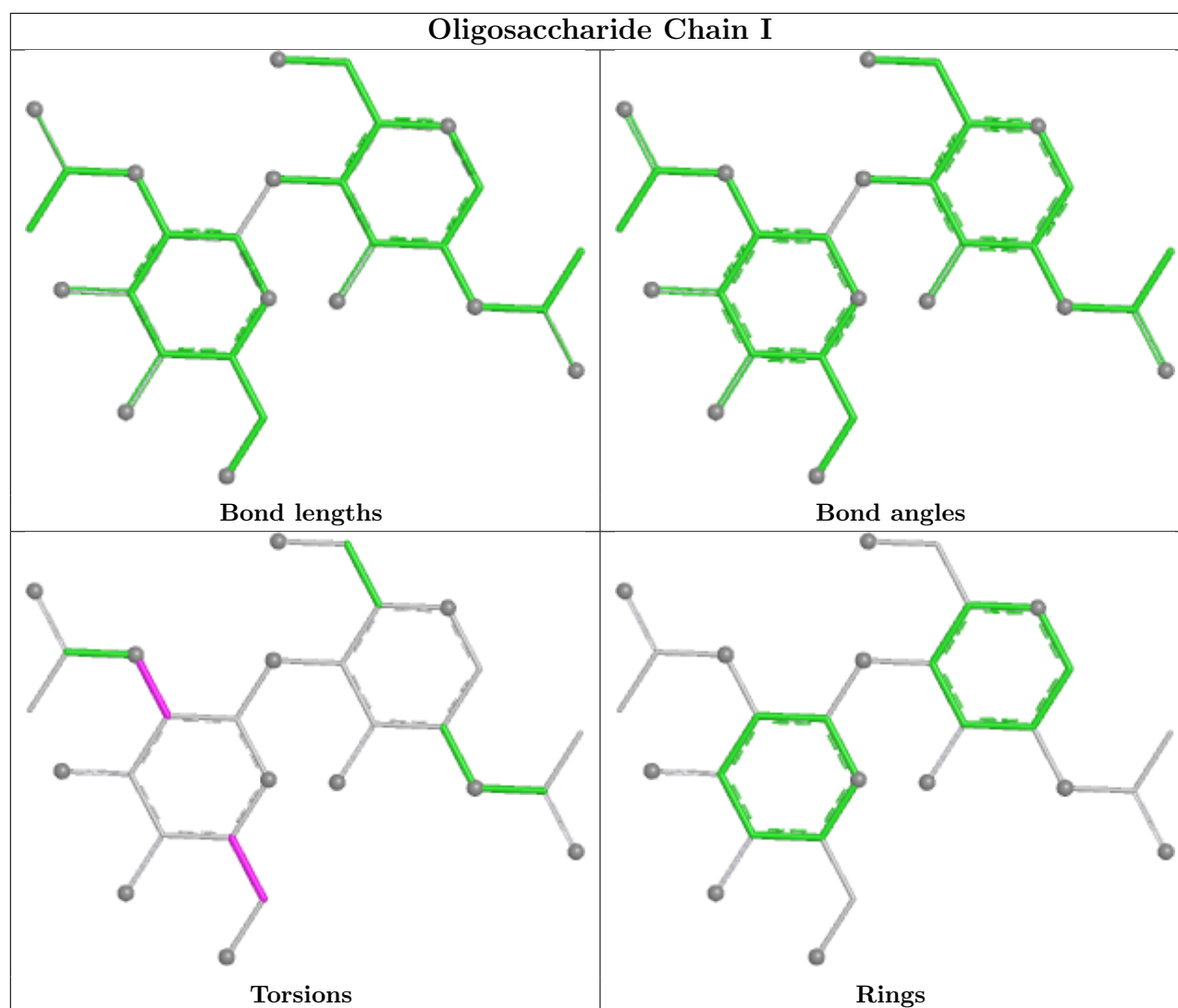
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	1	0
5	H	2	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](#)

Of 31 ligands modelled in this entry, 6 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	PCW	A	1115	-	21,21,53	1.00	0	27,29,61	0.79	1 (3%)
12	DMU	E	102	-	34,34,34	0.69	1 (2%)	45,45,45	1.10	4 (8%)
10	PCW	C	1111	-	21,21,53	0.92	0	27,29,61	1.32	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PC1	A	1108	-	53,53,53	0.62	0	59,61,61	1.09	2 (3%)
10	PCW	A	1109	-	21,21,53	0.96	0	27,29,61	1.04	3 (11%)
10	PCW	A	1113	-	21,21,53	0.91	0	27,29,61	1.03	2 (7%)
8	CLR	C	1104	-	31,31,31	1.19	2 (6%)	48,48,48	1.44	9 (18%)
8	CLR	A	1104	-	31,31,31	1.22	2 (6%)	48,48,48	1.45	9 (18%)
9	PC1	A	1111	-	53,53,53	0.70	0	59,61,61	0.87	1 (1%)
10	PCW	A	1116	-	53,53,53	1.03	2 (3%)	59,61,61	0.76	0
8	CLR	E	101	-	31,31,31	1.20	2 (6%)	48,48,48	1.40	6 (12%)
11	NAG	D	401	2	14,14,15	0.43	0	17,19,21	0.39	0
8	CLR	A	1105	-	31,31,31	1.17	1 (3%)	48,48,48	1.41	9 (18%)
10	PCW	C	1105	-	21,21,53	0.90	0	27,29,61	1.07	2 (7%)
8	CLR	A	1110	-	31,31,31	1.23	2 (6%)	48,48,48	1.37	7 (14%)
10	PCW	C	1110	-	21,21,53	0.91	0	27,29,61	0.98	3 (11%)
10	PCW	C	1108	-	21,21,53	0.96	0	27,29,61	1.03	2 (7%)
8	CLR	C	1107	-	31,31,31	1.22	3 (9%)	48,48,48	1.38	7 (14%)
10	PCW	A	1107	-	21,21,53	0.92	0	27,29,61	1.14	3 (11%)
9	PC1	A	1106	-	53,53,53	0.63	0	59,61,61	0.85	1 (1%)
10	PCW	C	1109	-	21,21,53	0.88	0	27,29,61	1.34	3 (11%)
10	PCW	C	1112	-	21,21,53	0.89	0	27,29,61	1.01	3 (11%)
10	PCW	A	1114	-	21,21,53	0.88	0	27,29,61	1.20	3 (11%)
10	PCW	A	1112	-	21,21,53	0.92	0	27,29,61	1.05	2 (7%)
10	PCW	C	1106	-	21,21,53	1.00	0	27,29,61	0.90	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PCW	A	1115	-	-	9/23/23/57	-
12	DMU	E	102	-	-	4/19/59/59	0/2/2/2
10	PCW	C	1111	-	-	7/23/23/57	-
9	PC1	A	1108	-	-	14/57/57/57	-
10	PCW	A	1109	-	-	8/23/23/57	-
10	PCW	A	1113	-	-	5/23/23/57	-
8	CLR	C	1104	-	-	3/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLR	A	1104	-	-	3/10/68/68	0/4/4/4
9	PC1	A	1111	-	-	10/57/57/57	-
10	PCW	A	1116	-	-	19/57/57/57	-
8	CLR	E	101	-	-	1/10/68/68	0/4/4/4
11	NAG	D	401	2	-	0/6/23/26	0/1/1/1
8	CLR	A	1105	-	-	2/10/68/68	0/4/4/4
10	PCW	C	1105	-	-	5/23/23/57	-
8	CLR	A	1110	-	-	3/10/68/68	0/4/4/4
10	PCW	C	1110	-	-	3/23/23/57	-
10	PCW	C	1108	-	-	9/23/23/57	-
8	CLR	C	1107	-	-	4/10/68/68	0/4/4/4
10	PCW	A	1107	-	-	3/23/23/57	-
9	PC1	A	1106	-	-	5/57/57/57	-
10	PCW	C	1109	-	-	5/23/23/57	-
10	PCW	C	1112	-	-	8/23/23/57	-
10	PCW	A	1114	-	-	7/23/23/57	-
10	PCW	A	1112	-	-	9/23/23/57	-
10	PCW	C	1106	-	-	8/23/23/57	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1116	PCW	C20-C19	3.92	1.54	1.31
10	A	1116	PCW	C40-C39	3.88	1.53	1.31
8	A	1104	CLR	C16-C17	3.05	1.60	1.54
8	A	1110	CLR	C16-C17	3.03	1.60	1.54
8	C	1104	CLR	C16-C17	3.01	1.60	1.54

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1109	PCW	C2-O2-C31	-5.21	108.64	117.85
10	C	1111	PCW	C2-O2-C31	-4.77	109.41	117.85
9	A	1108	PC1	C3-O31-C31	-3.83	103.10	117.12
10	A	1107	PCW	C2-O2-C31	-3.74	111.23	117.85
10	A	1113	PCW	C2-O2-C31	-3.41	111.83	117.85

There are no chirality outliers.

5 of 154 torsion outliers are listed below:

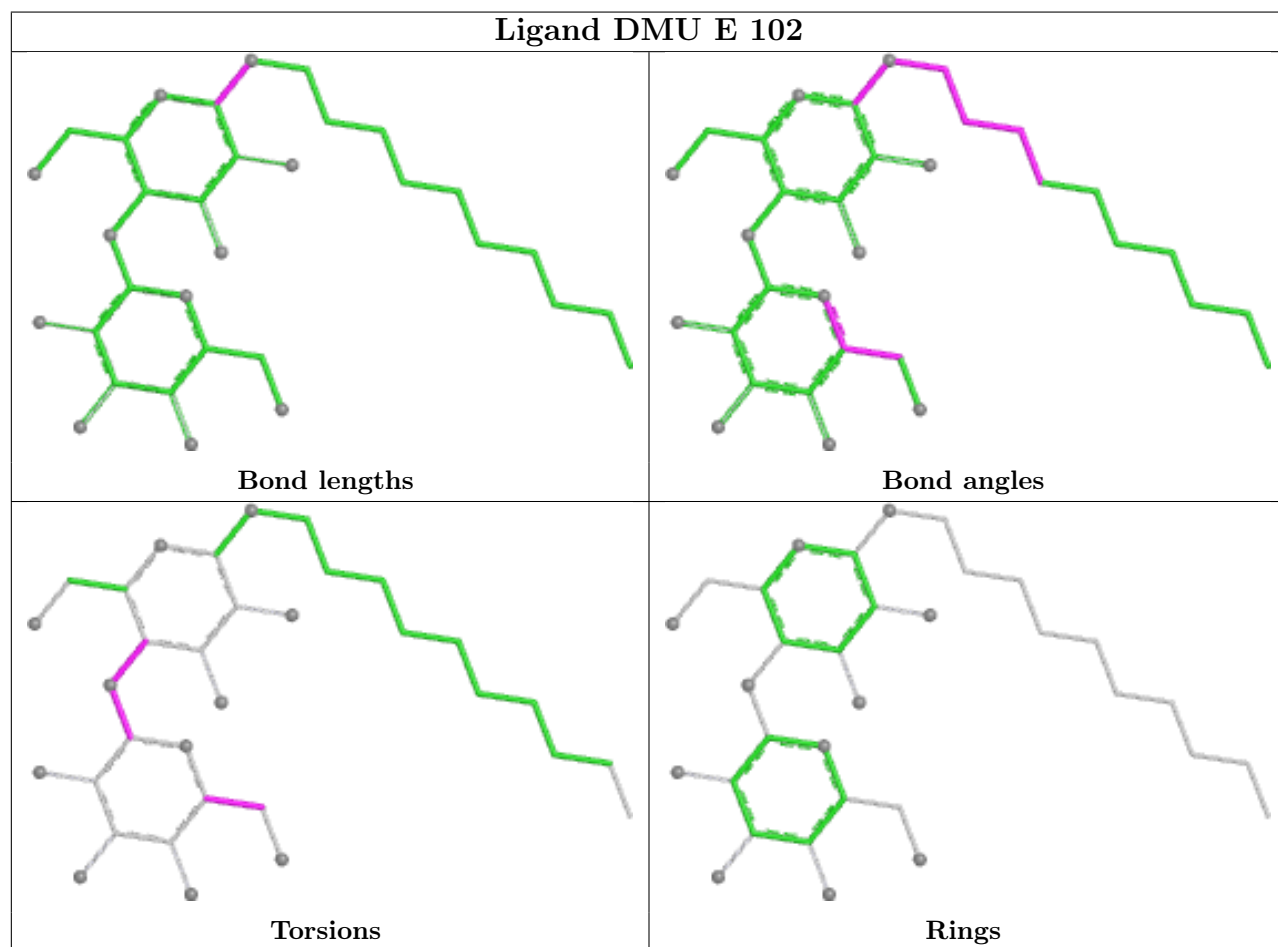
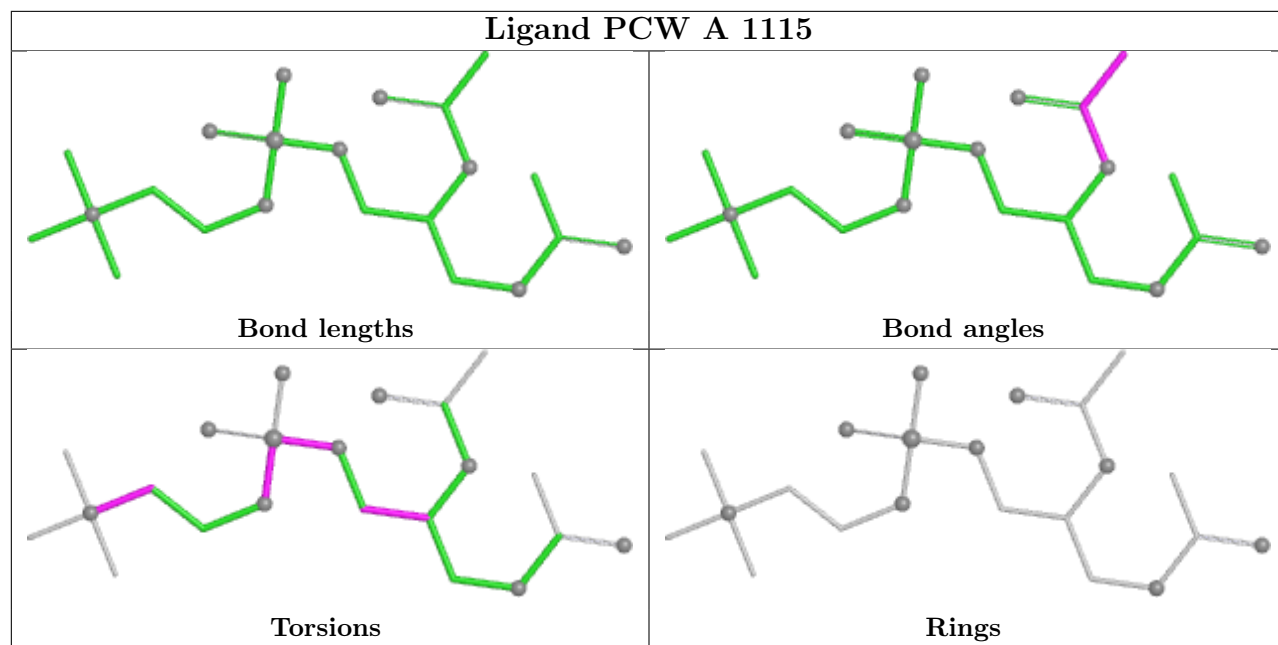
Mol	Chain	Res	Type	Atoms
9	A	1108	PC1	C11-O13-P-O14
9	A	1108	PC1	C1-O11-P-O12
9	A	1111	PC1	C11-O13-P-O14
10	A	1109	PCW	C4-O4P-P-O1P
10	A	1109	PCW	C4-O4P-P-O3P

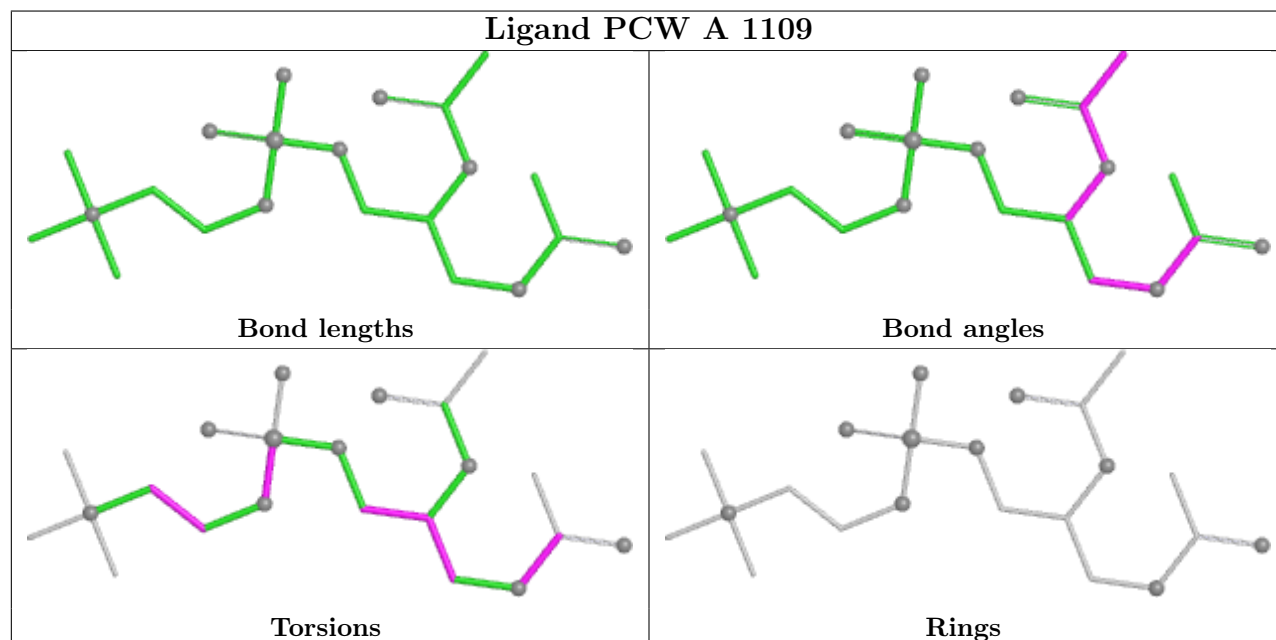
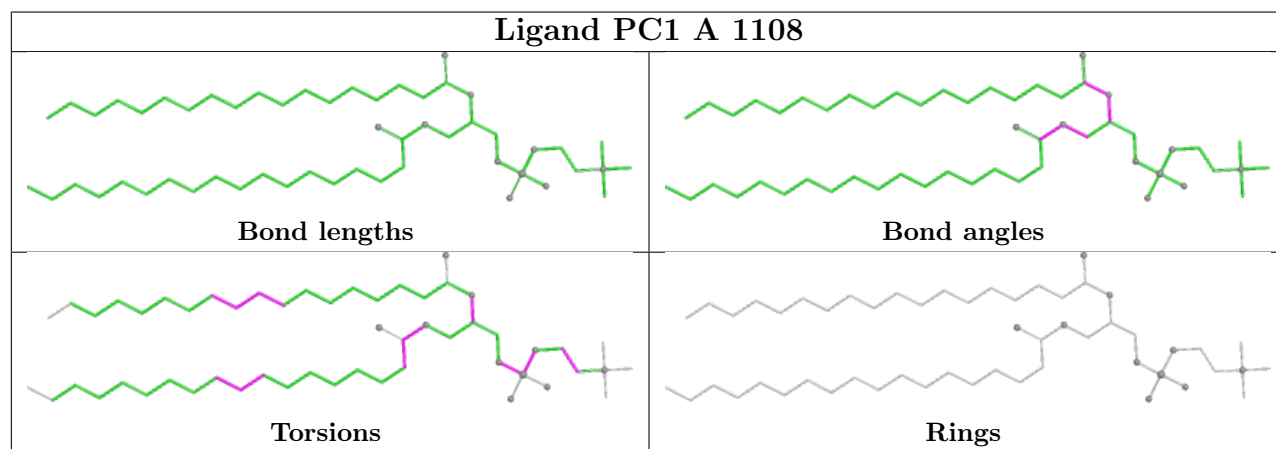
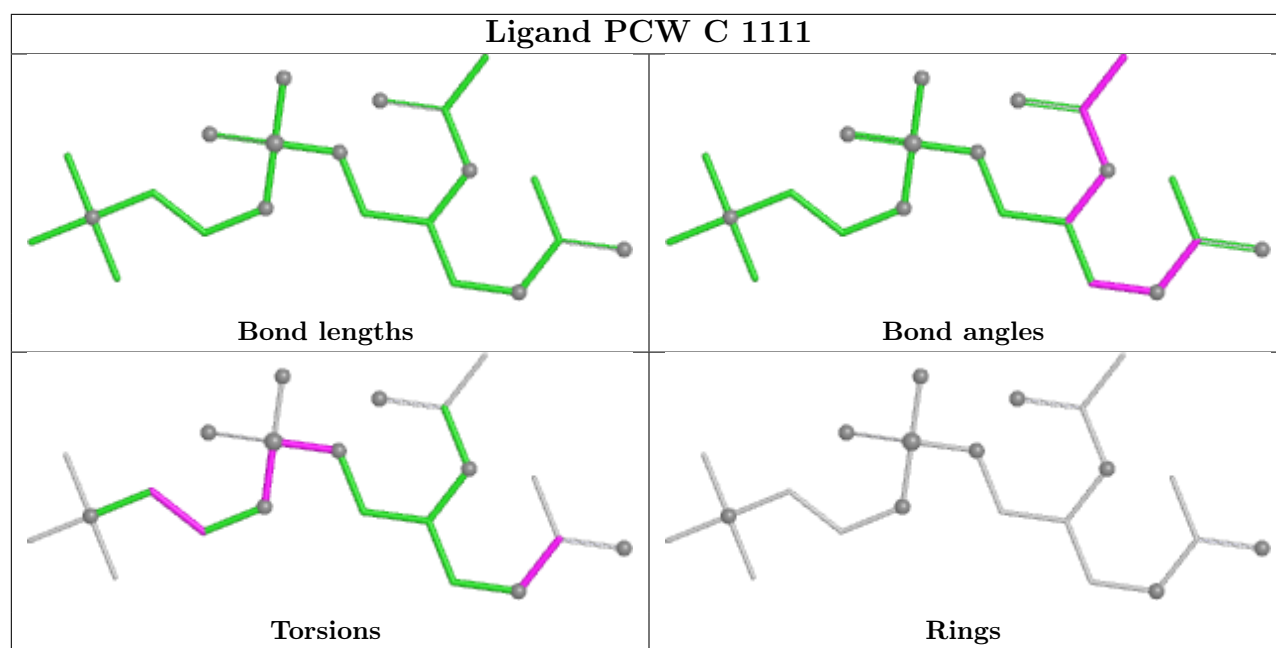
There are no ring outliers.

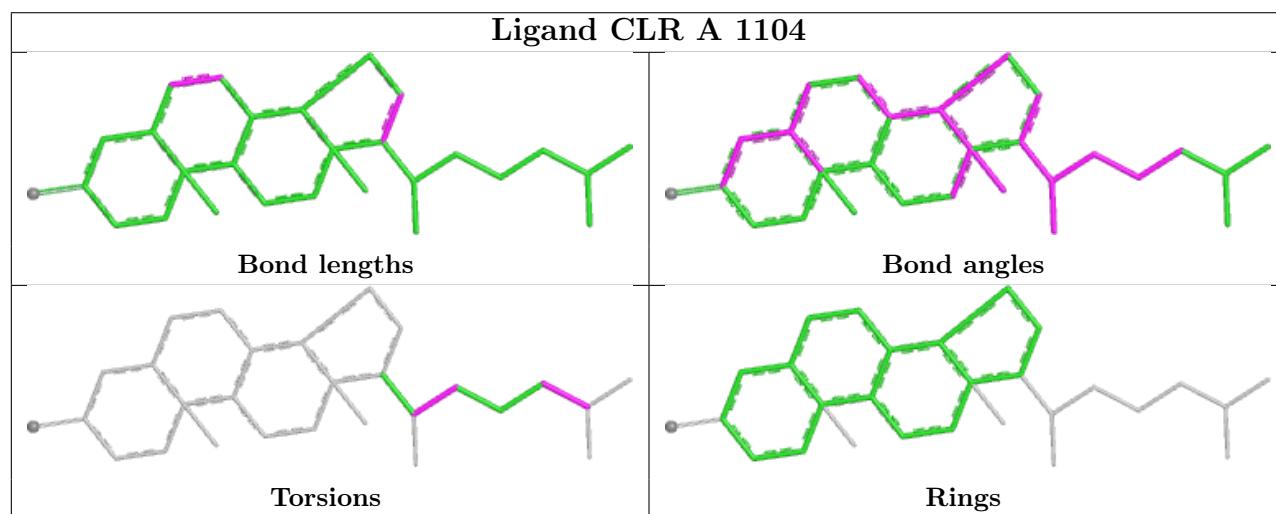
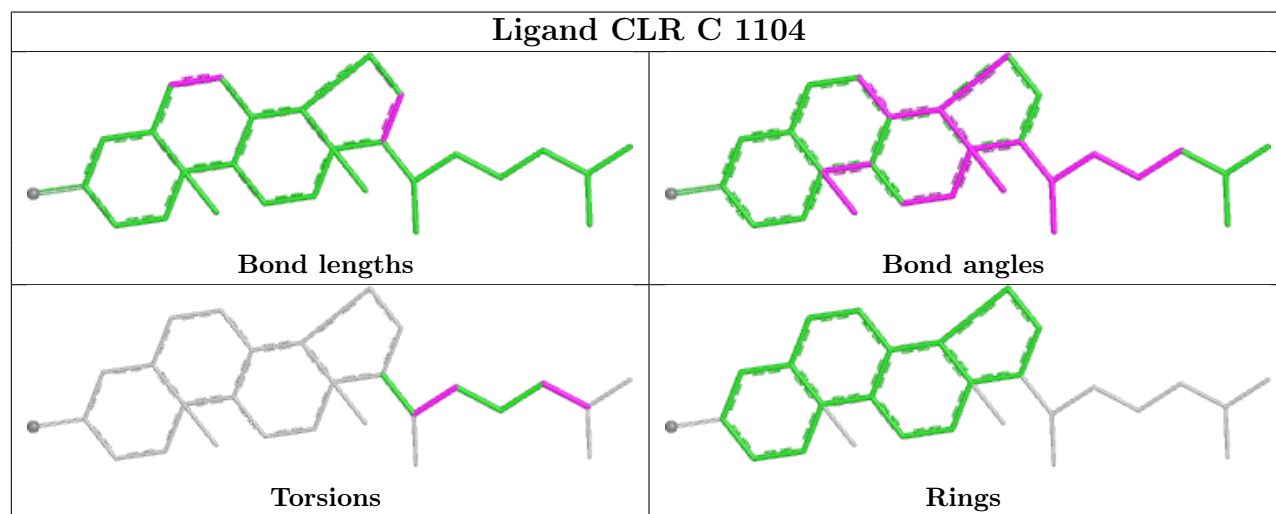
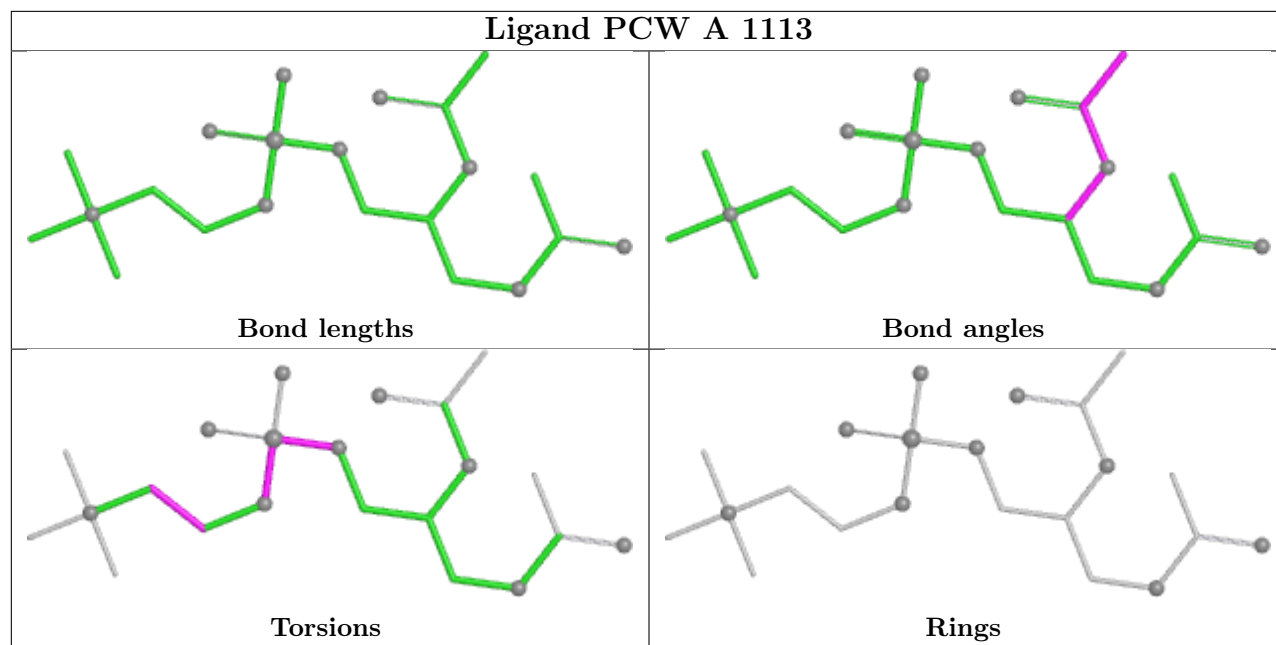
17 monomers are involved in 53 short contacts:

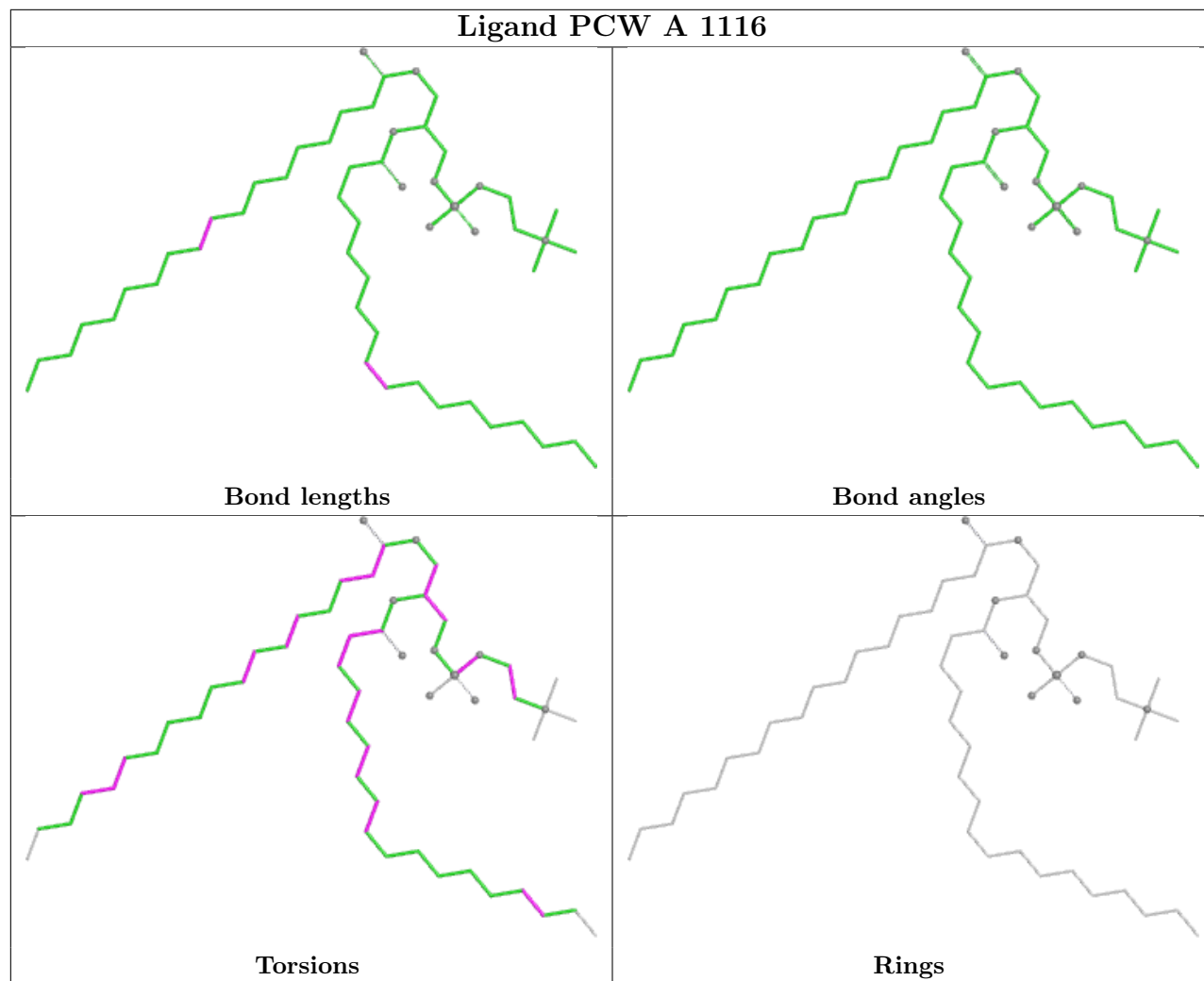
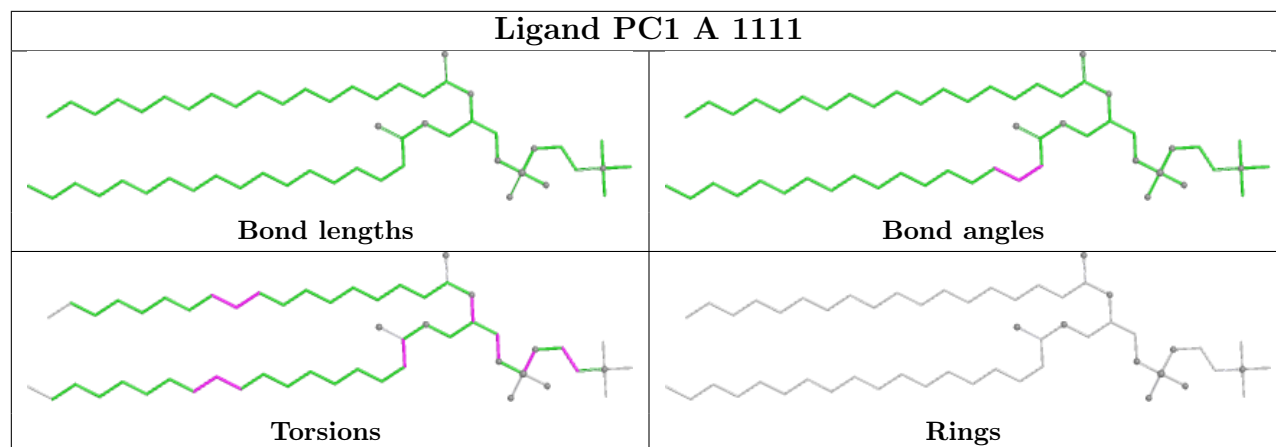
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	102	DMU	7	0
10	C	1111	PCW	1	0
9	A	1108	PC1	11	0
10	A	1113	PCW	2	0
8	C	1104	CLR	3	0
8	A	1104	CLR	1	0
9	A	1111	PC1	9	0
10	A	1116	PCW	5	0
8	E	101	CLR	2	0
8	A	1105	CLR	6	0
10	C	1110	PCW	2	0
8	C	1107	CLR	2	0
10	A	1107	PCW	1	0
9	A	1106	PC1	3	0
10	C	1109	PCW	1	0
10	A	1114	PCW	1	0
10	A	1112	PCW	2	0

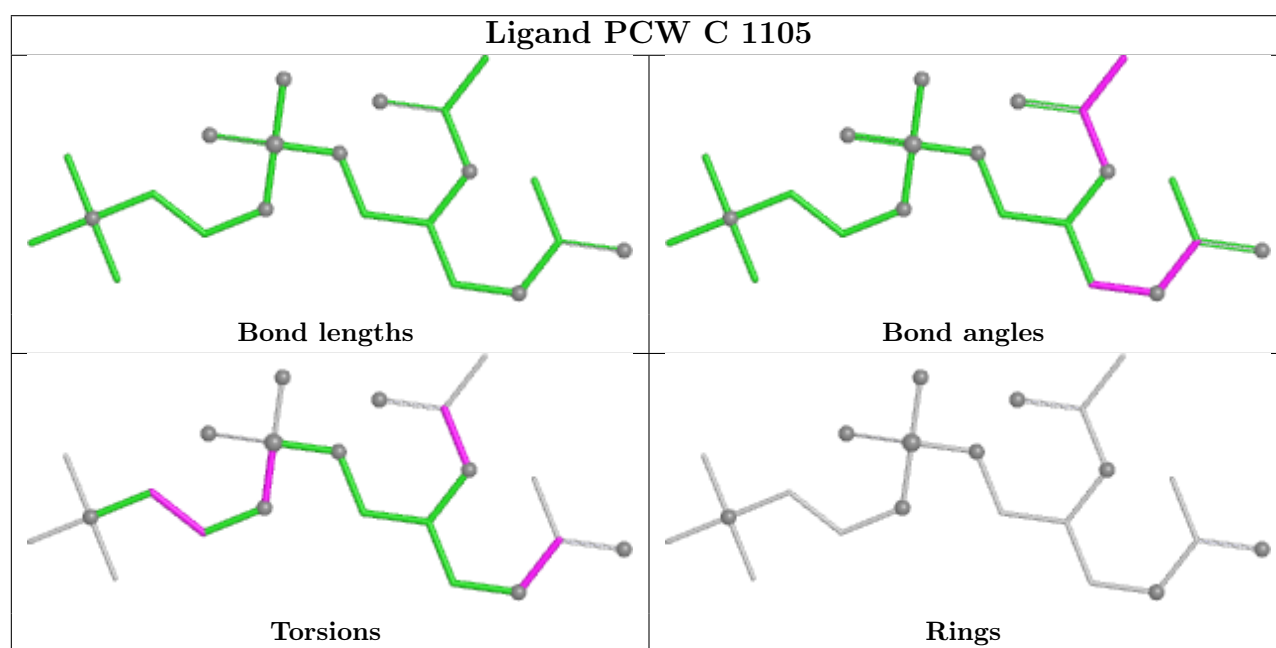
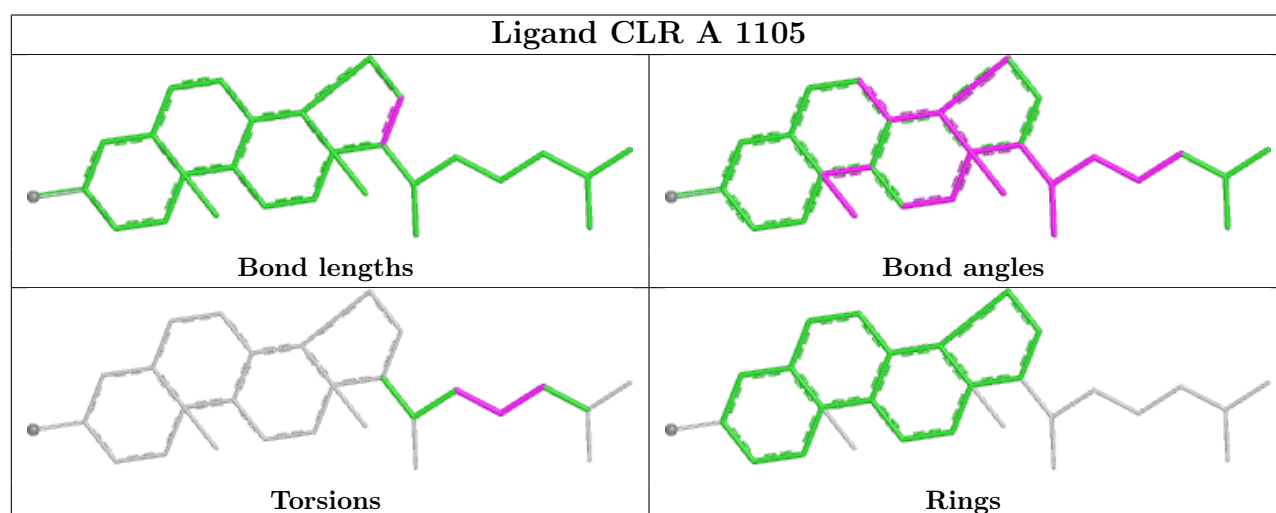
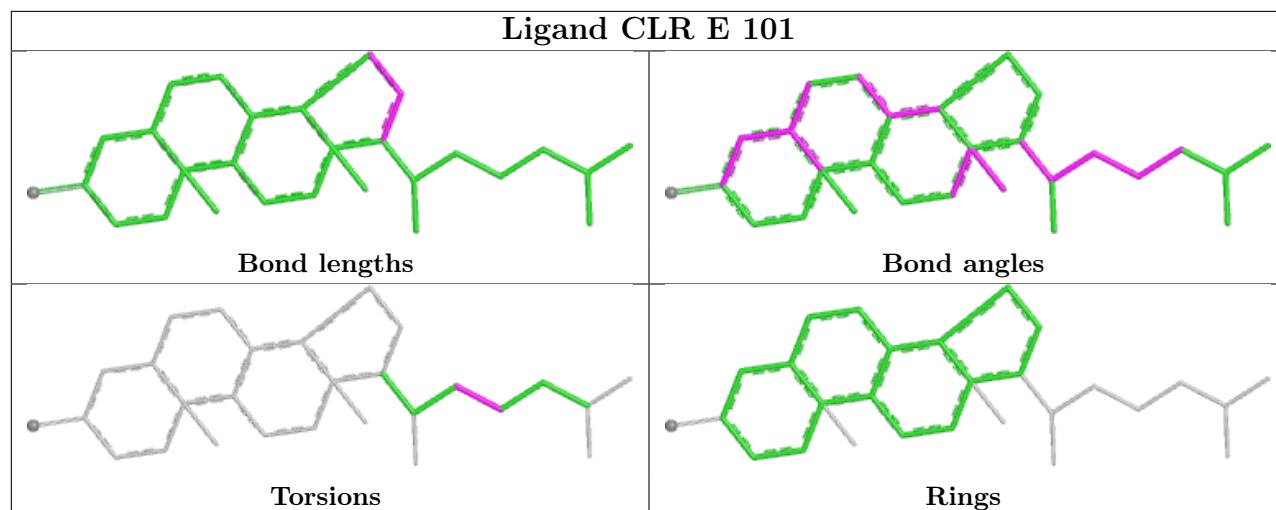
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

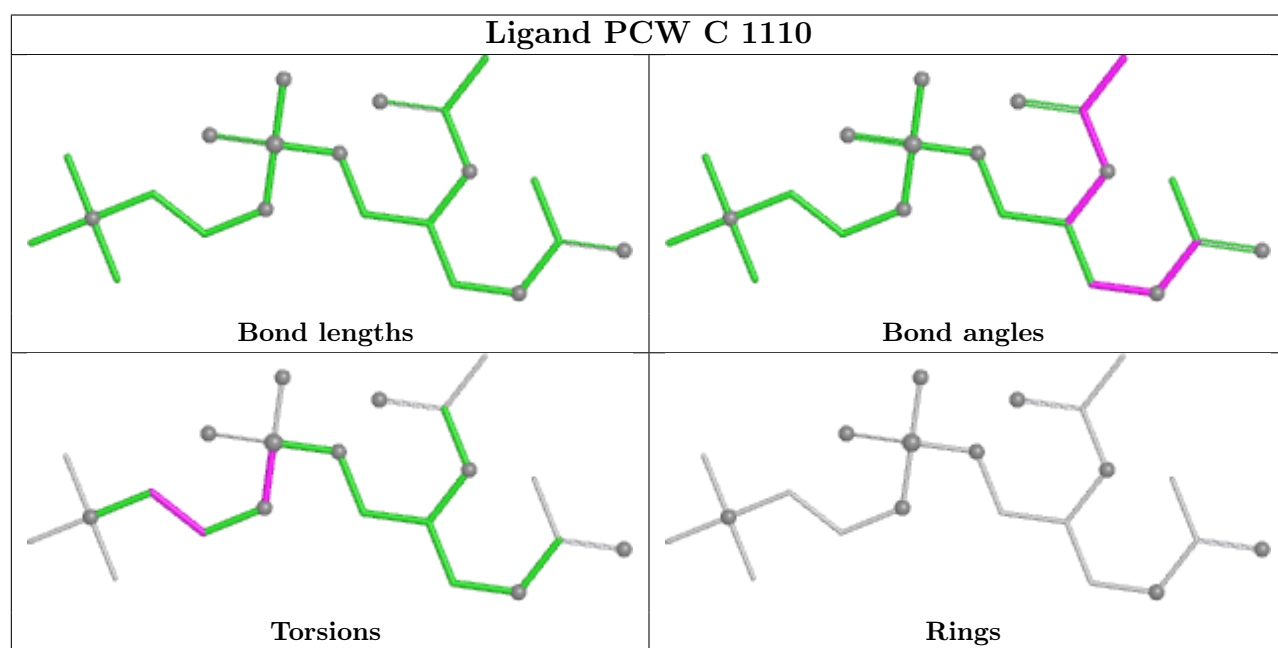
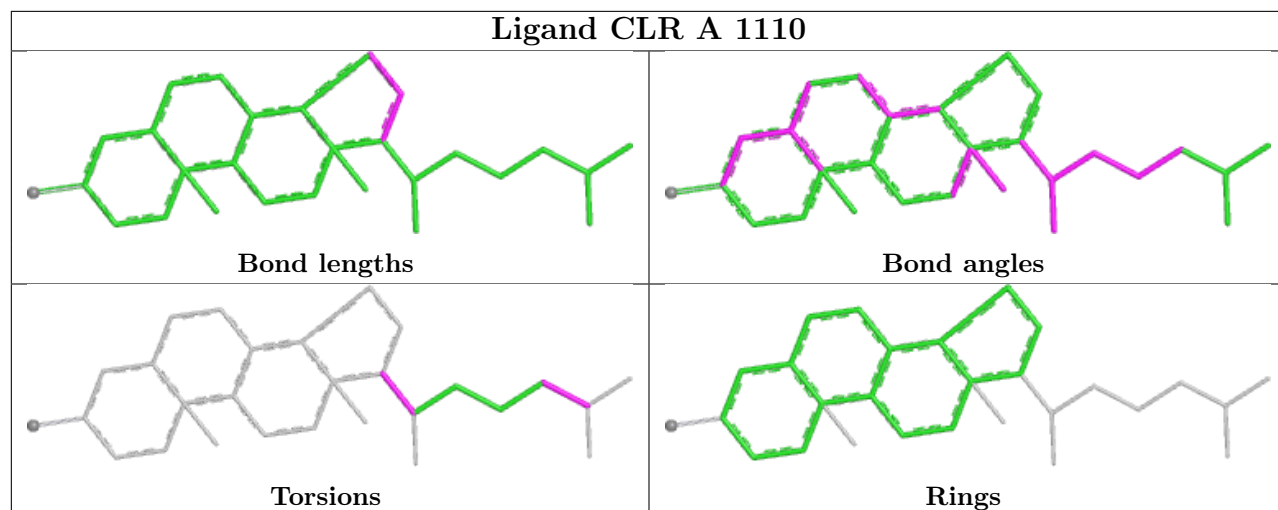


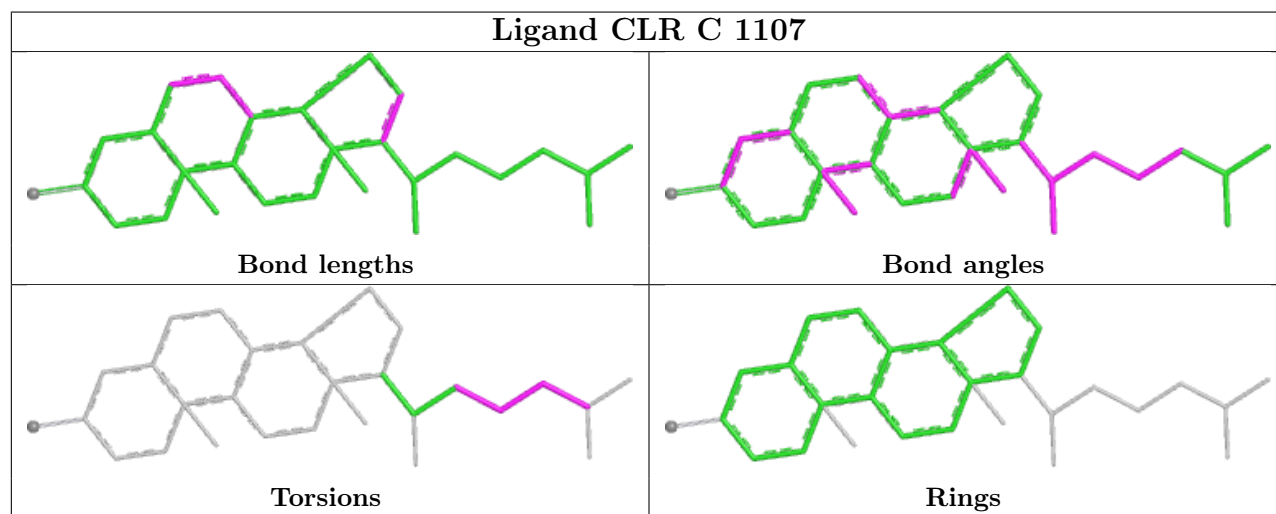
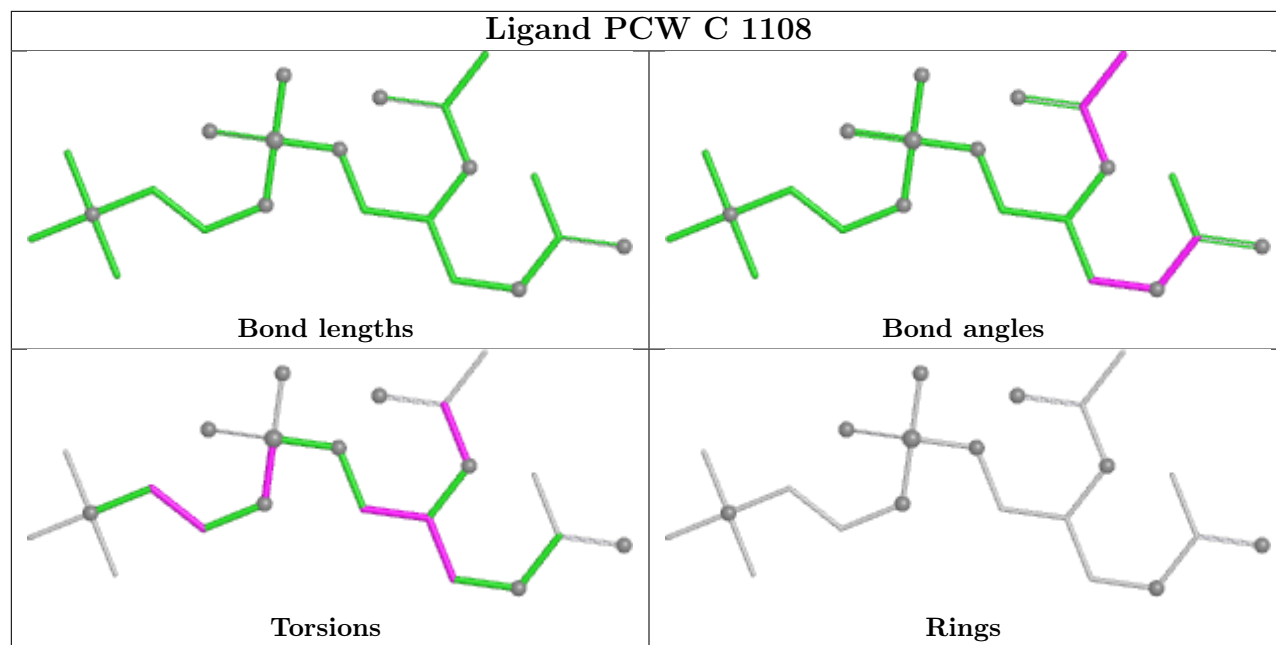


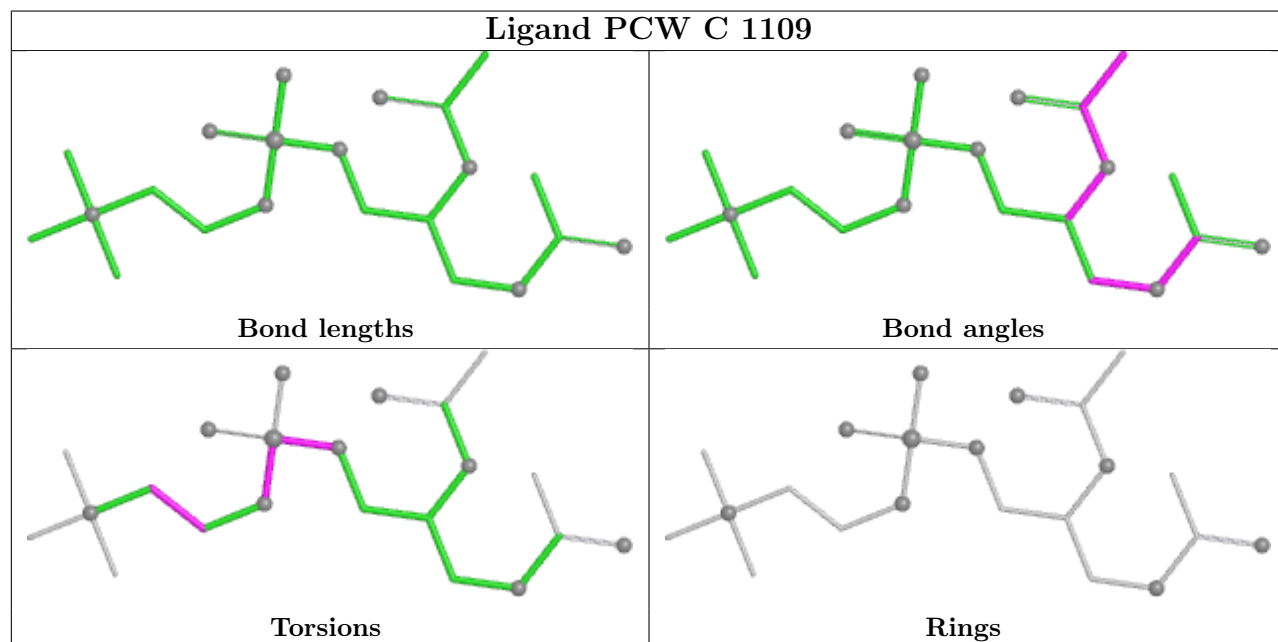
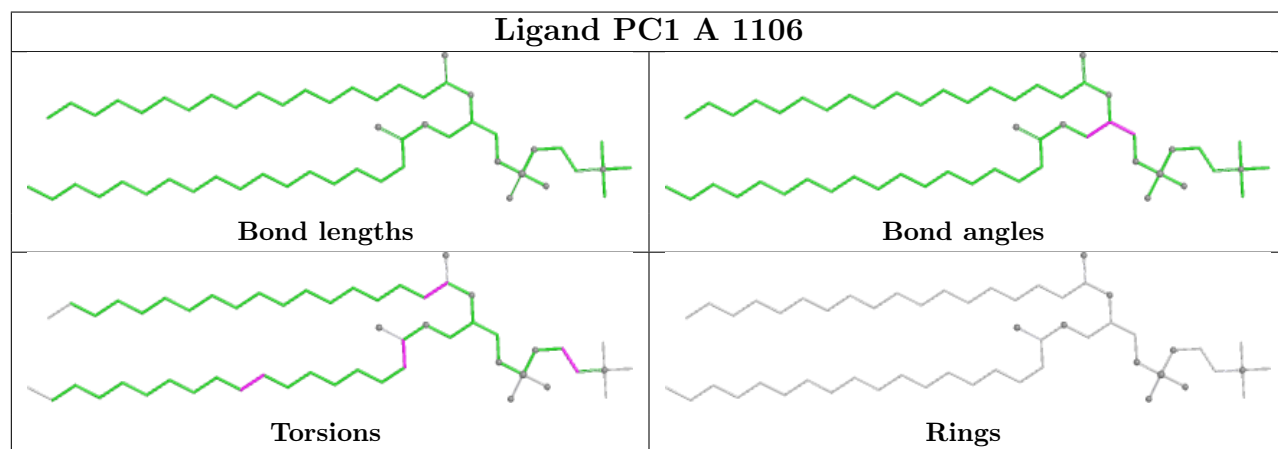
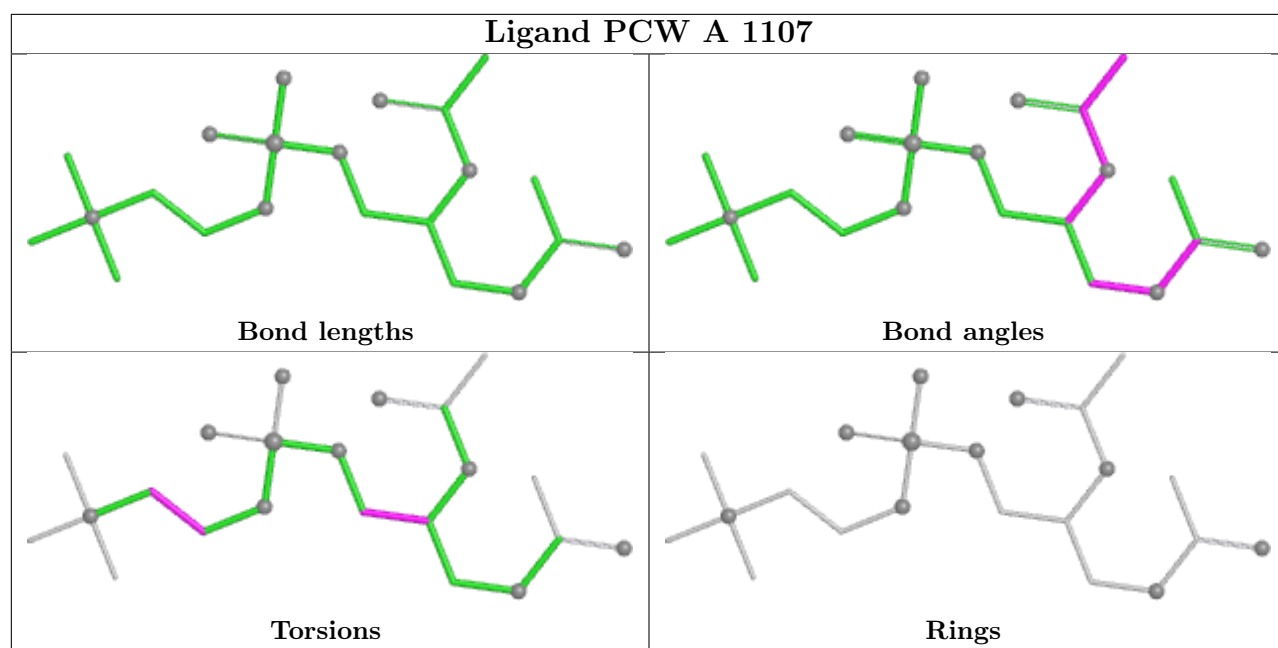




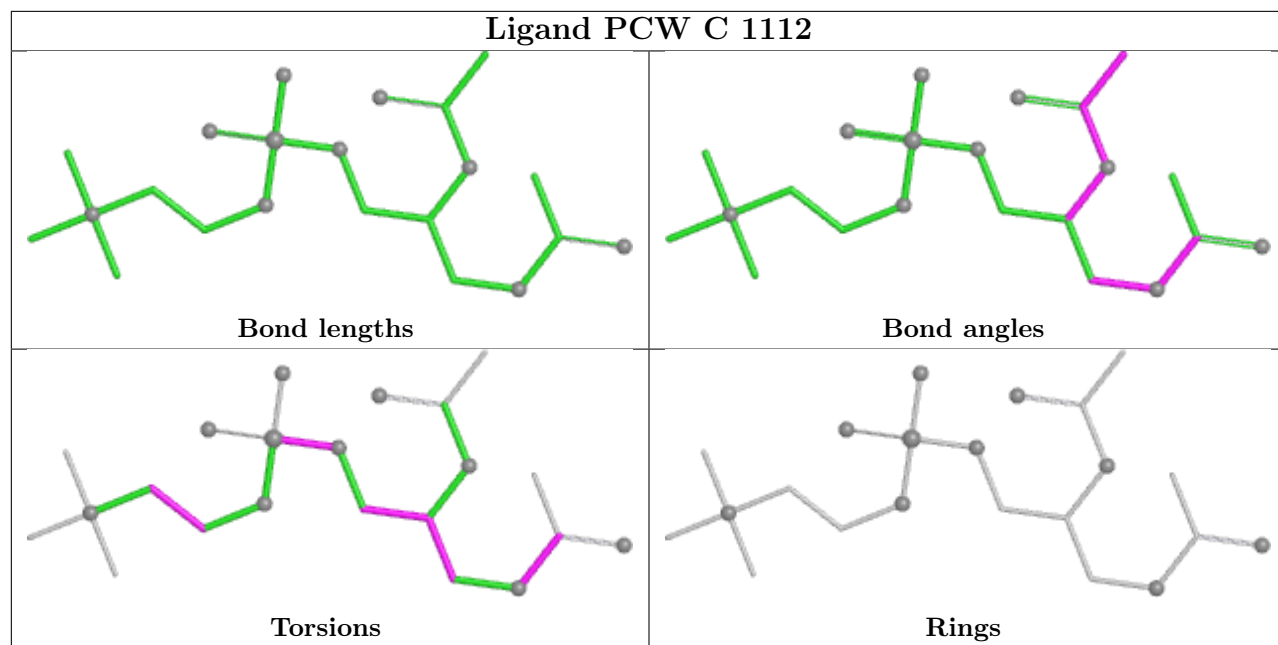




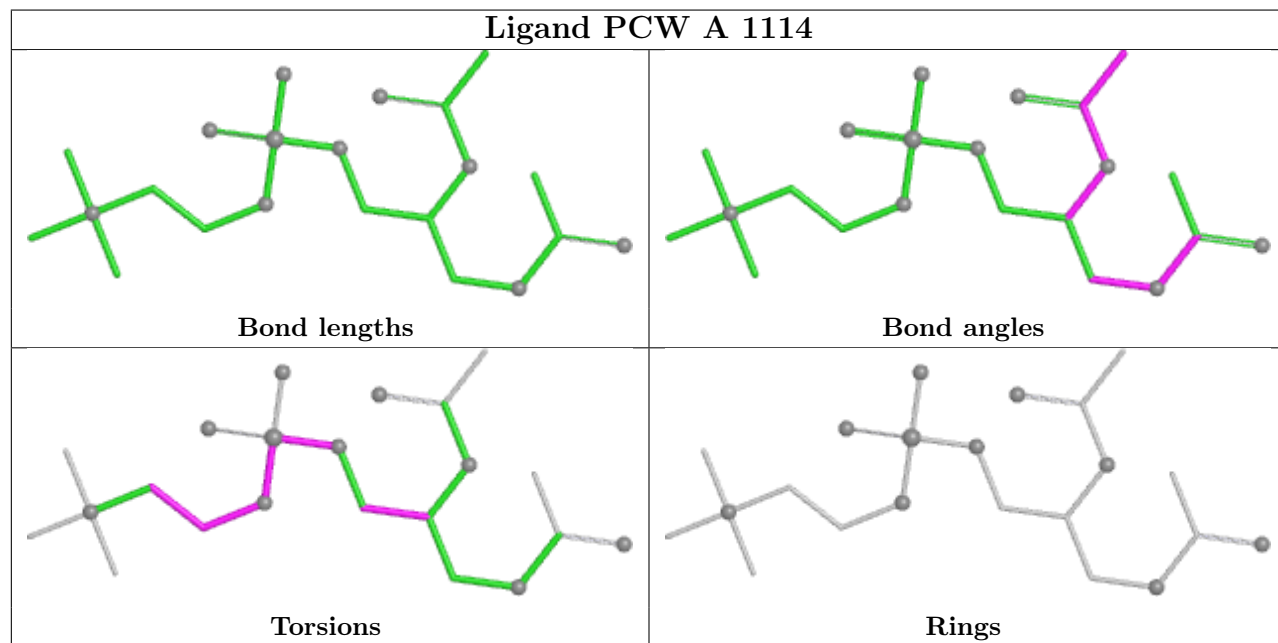


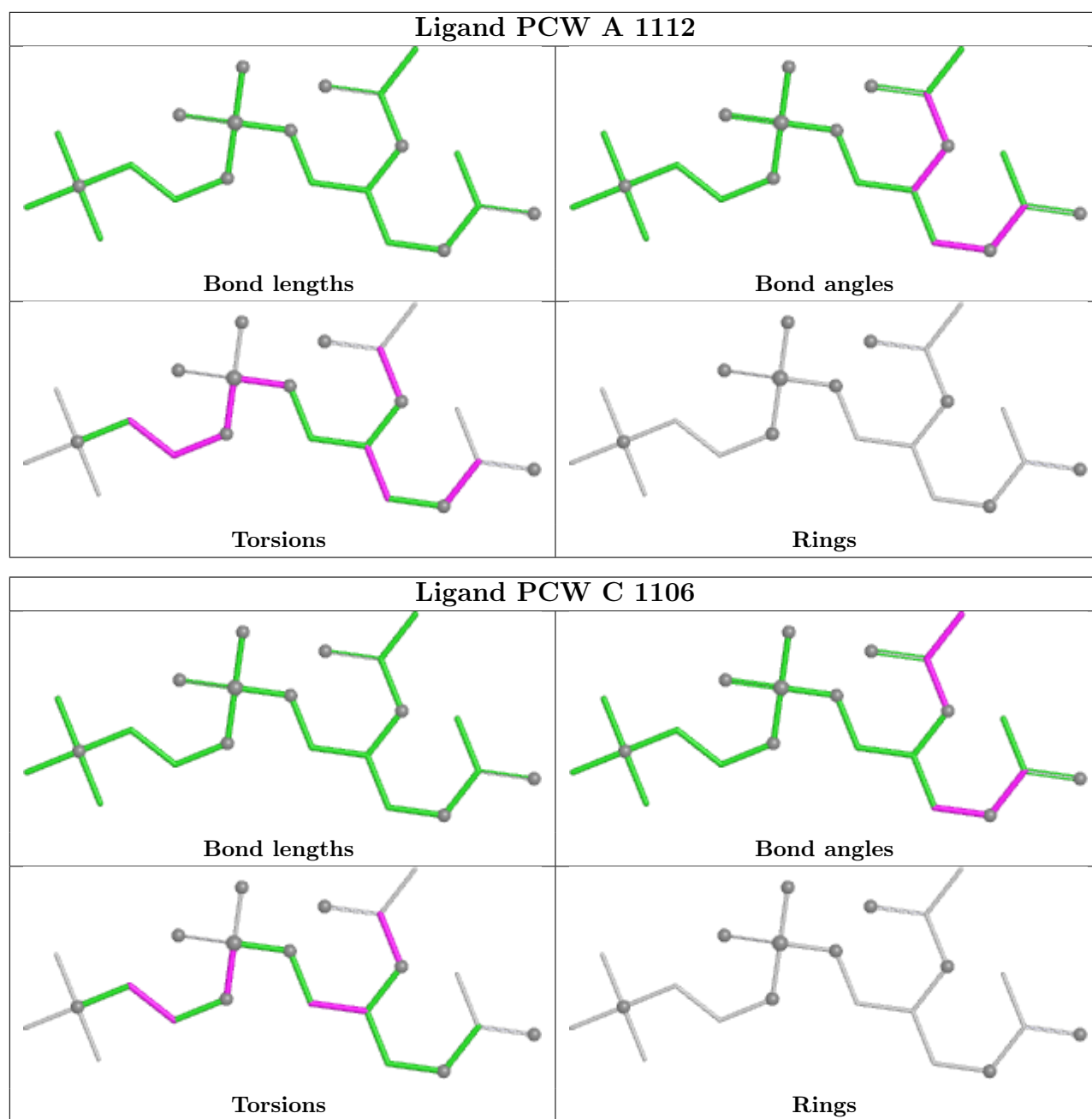


Ligand PCW C 1112



Ligand PCW A 1114





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	995/1021 (97%)	-0.49	1 (0%) 92 86	25, 70, 147, 184	0
1	C	995/1021 (97%)	-0.49	1 (0%) 92 86	37, 80, 138, 197	0
2	B	291/303 (96%)	-0.41	1 (0%) 90 79	54, 94, 146, 183	0
2	D	291/303 (96%)	-0.27	0 100 100	58, 134, 171, 212	0
3	E	33/65 (50%)	-0.53	0 100 100	41, 57, 116, 130	0
3	G	35/65 (53%)	-0.44	0 100 100	44, 60, 98, 116	0
All	All	2640/2778 (95%)	-0.46	3 (0%) 92 86	25, 81, 153, 212	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	26	GLY	2.1
1	A	231	GLU	2.0
1	C	401	GLY	2.0

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	NAG	F	1	14/15	-	-	119,135,146,148	0

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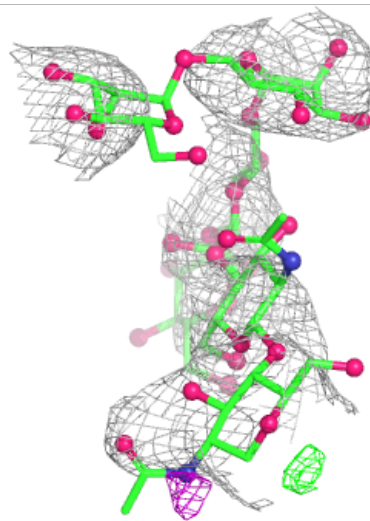
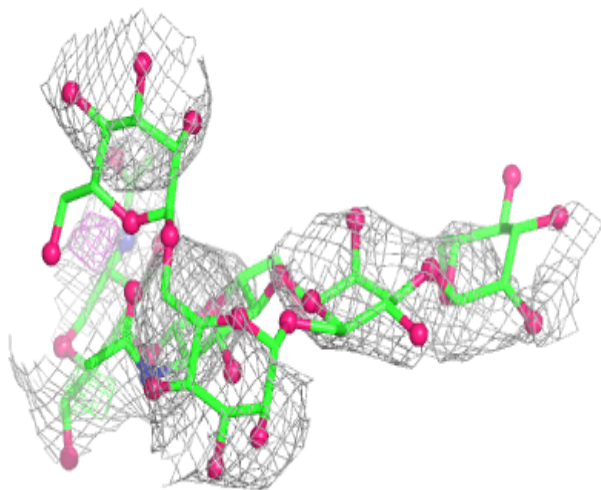
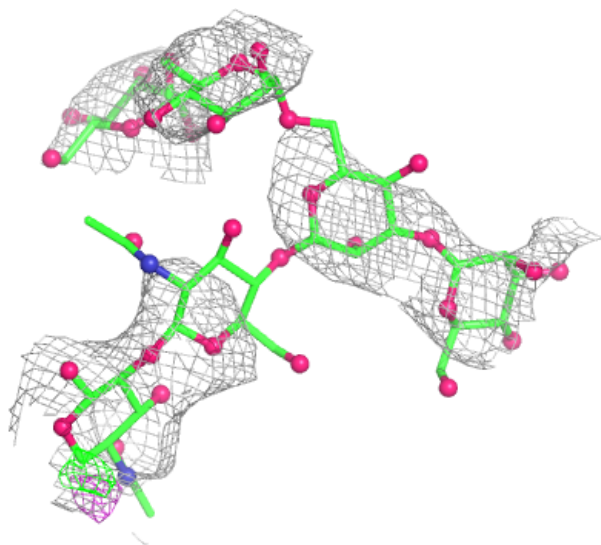
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	F	2	14/15	-	-	132,151,163,169	0
4	BMA	F	3	11/12	-	-	127,140,149,155	0
4	MAN	F	4	11/12	-	-	127,139,145,149	0
4	MAN	F	5	11/12	-	-	124,139,150,159	0
4	MAN	F	6	11/12	-	-	155,157,164,165	0
6	NAG	I	1	14/15	0.13	0.13	143,156,178,186	0
5	MAN	H	4	11/12	0.40	0.15	164,183,197,201	0
6	NAG	I	2	14/15	0.53	0.13	127,150,160,164	0
5	NAG	H	2	14/15	0.57	0.19	149,186,195,199	0
5	BMA	H	3	11/12	0.60	0.11	168,171,186,195	0
5	MAN	H	5	11/12	0.60	0.11	143,162,174,178	0
5	NAG	H	1	14/15	0.72	0.10	127,137,163,184	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.

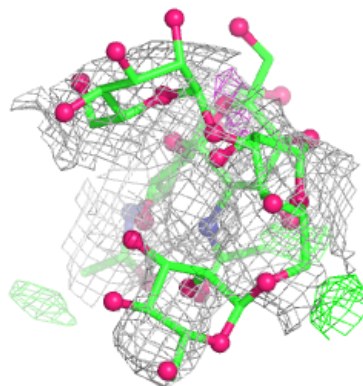
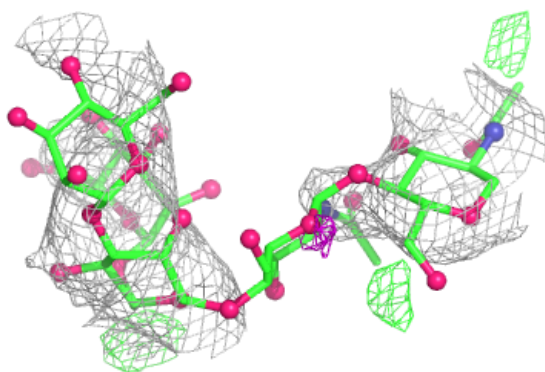
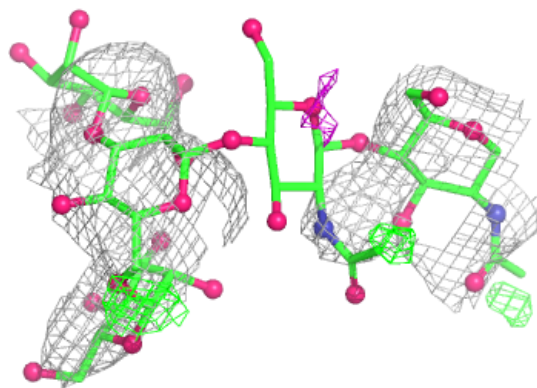
Electron density around Chain F:

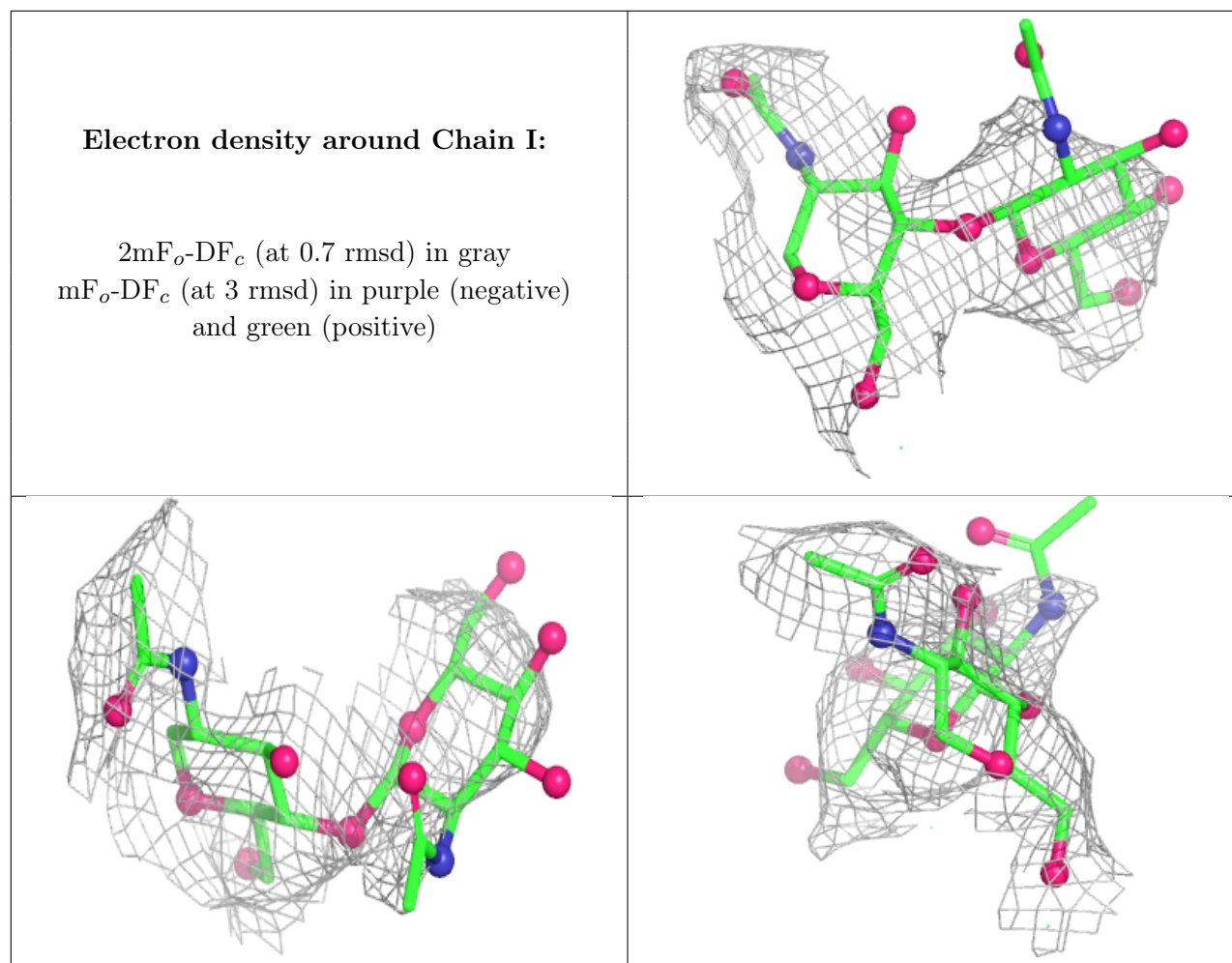
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
10	PCW	C	1109	22/54	0.53	0.12	90,125,155,158	0
10	PCW	A	1109	22/54	0.59	0.14	99,133,167,168	0
11	NAG	D	401	14/15	0.63	0.12	152,167,170,172	0
10	PCW	A	1113	22/54	0.64	0.12	99,143,149,156	0
10	PCW	C	1108	22/54	0.65	0.13	86,115,141,152	0
10	PCW	A	1107	22/54	0.68	0.12	102,121,151,156	0
10	PCW	C	1110	22/54	0.70	0.11	102,140,160,161	0
10	PCW	A	1115	22/54	0.70	0.12	94,128,152,155	0
10	PCW	C	1105	22/54	0.71	0.13	84,117,184,198	0
9	PC1	A	1106	54/54	0.73	0.09	77,109,142,152	0

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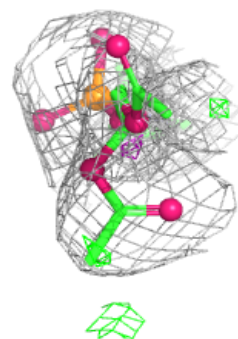
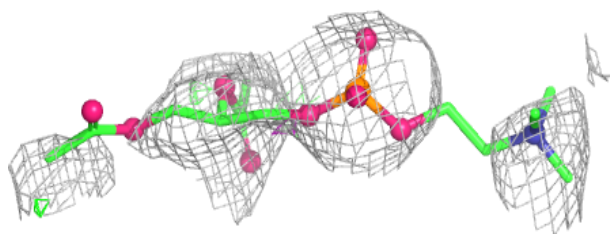
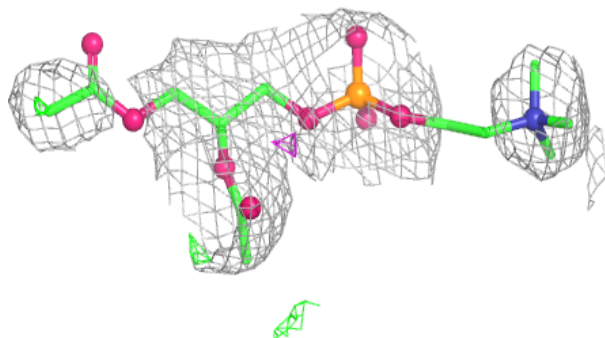
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	PCW	A	1116	54/54	0.75	0.12	60,88,136,146	0
10	PCW	C	1111	22/54	0.77	0.10	78,111,130,136	0
10	PCW	A	1114	22/54	0.80	0.13	88,125,139,145	0
10	PCW	C	1106	22/54	0.81	0.10	85,127,136,141	0
10	PCW	A	1112	22/54	0.81	0.10	68,119,130,139	0
8	CLR	A	1104	28/28	0.81	0.12	72,97,107,111	0
10	PCW	C	1112	22/54	0.82	0.10	78,124,156,168	0
8	CLR	A	1110	28/28	0.84	0.08	103,117,133,137	0
8	CLR	C	1107	28/28	0.85	0.10	92,110,124,125	0
12	DMU	E	102	33/33	0.85	0.11	42,67,85,110	0
9	PC1	A	1111	54/54	0.86	0.11	44,83,119,128	0
9	PC1	A	1108	54/54	0.87	0.10	52,87,109,122	0
7	MG	C	1101	1/1	0.92	0.07	95,95,95,95	0
7	MG	C	1102	1/1	0.92	0.06	64,64,64,64	0
8	CLR	A	1105	28/28	0.93	0.10	33,53,90,93	0
7	MG	A	1102	1/1	0.93	0.07	89,89,89,89	0
8	CLR	C	1104	28/28	0.94	0.09	39,46,84,104	0
8	CLR	E	101	28/28	0.95	0.08	31,40,61,83	0
7	MG	A	1103	1/1	0.95	0.06	34,34,34,34	0
7	MG	A	1101	1/1	0.96	0.10	66,66,66,66	0
7	MG	C	1103	1/1	0.98	0.03	44,44,44,44	0

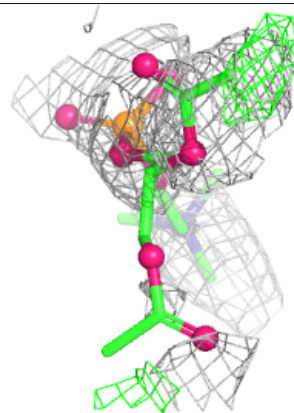
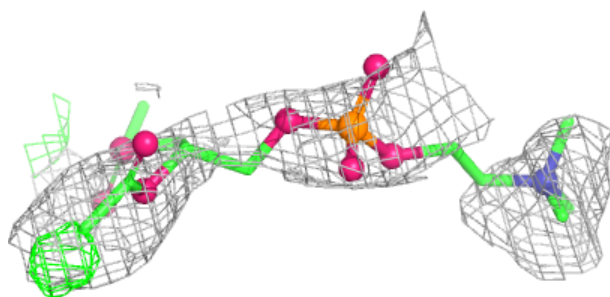
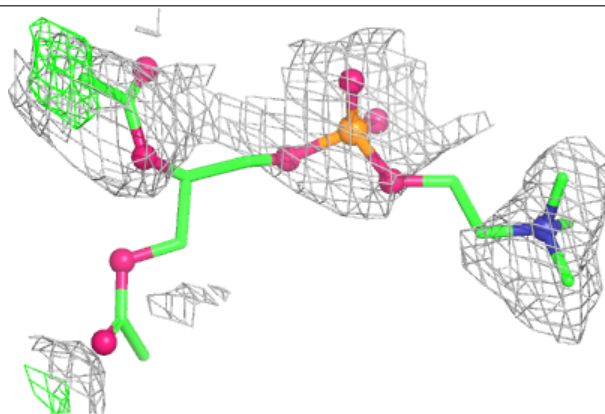
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PCW C 1109:

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

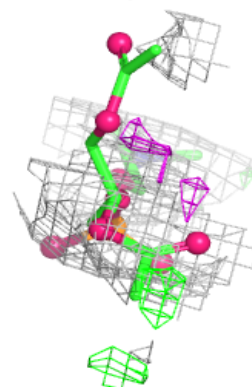
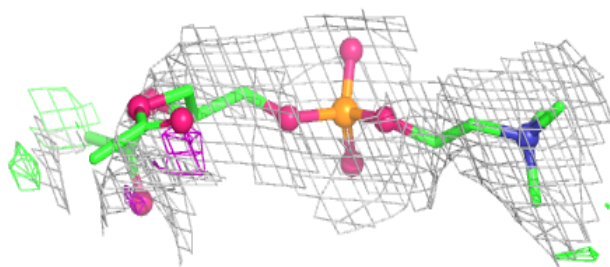
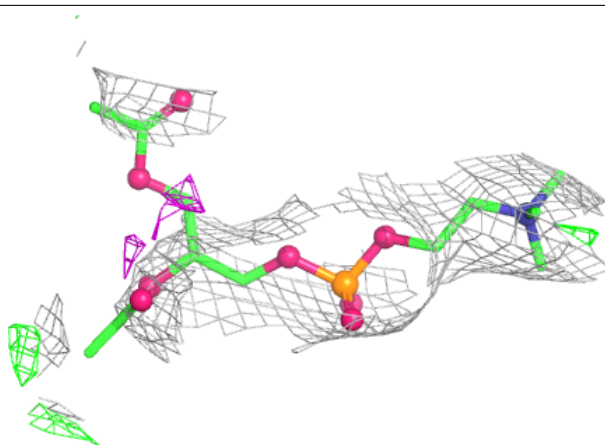
**Electron density around PCW A 1109:**

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

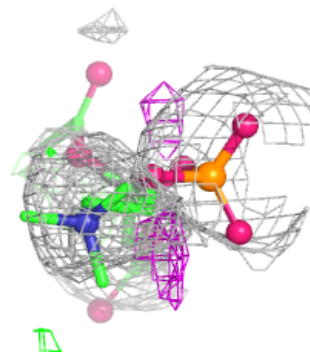
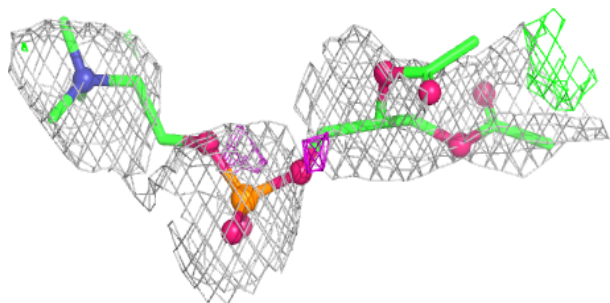
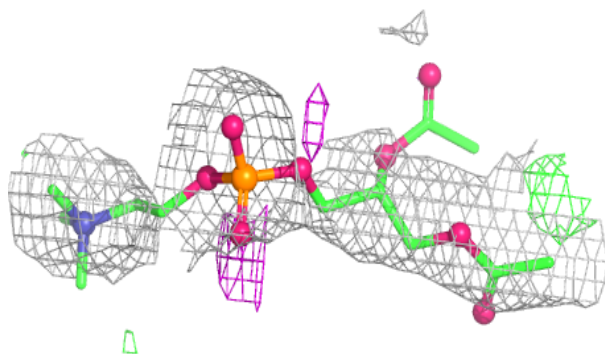


Electron density around PCW A 1113:

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

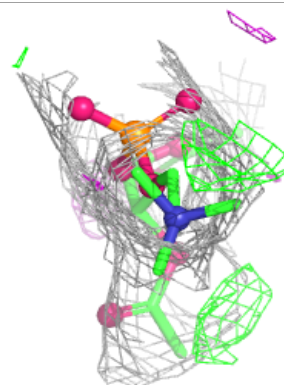
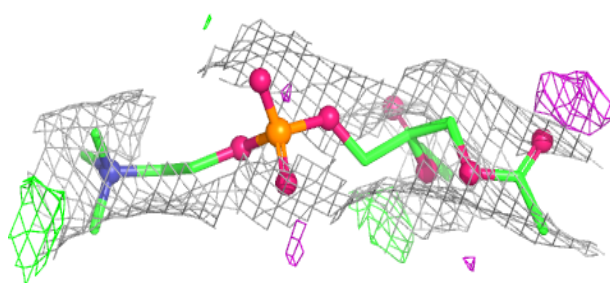
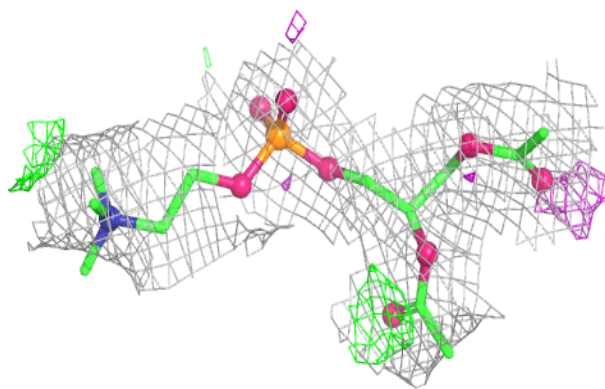
**Electron density around PCW C 1108:**

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



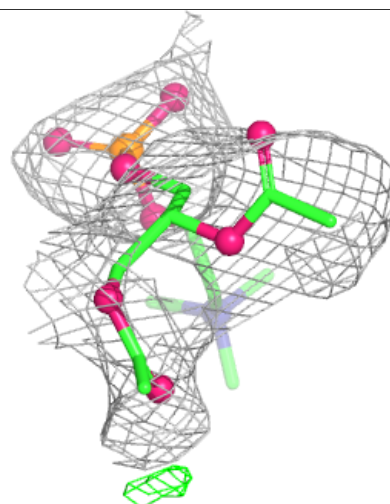
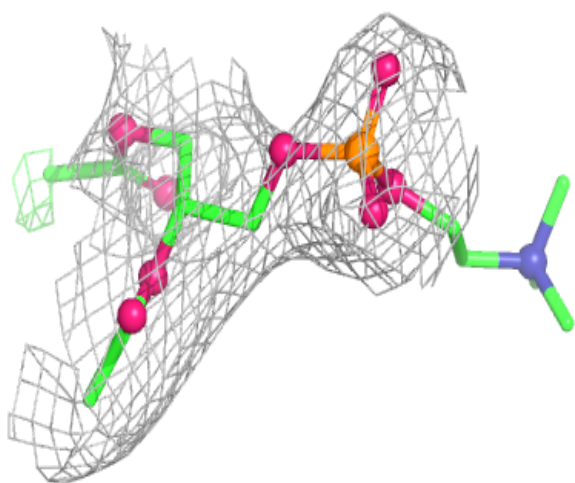
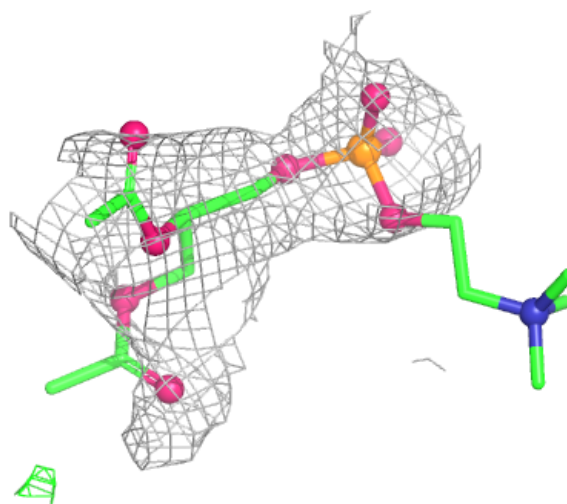
Electron density around PCW A 1107:

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



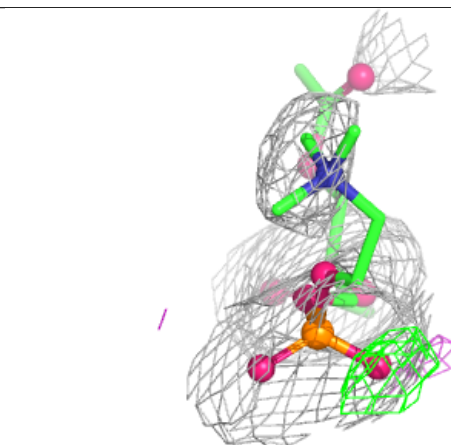
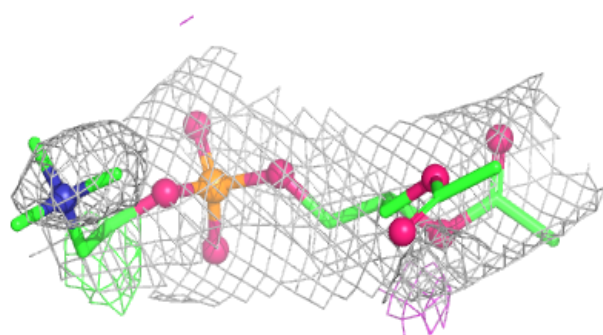
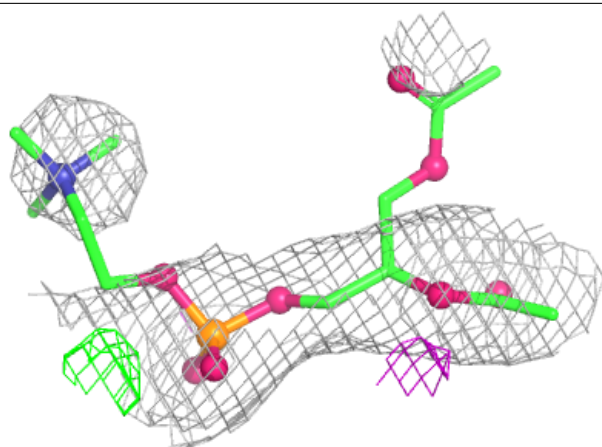
Electron density around PCW C 1110:

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and green (positive)

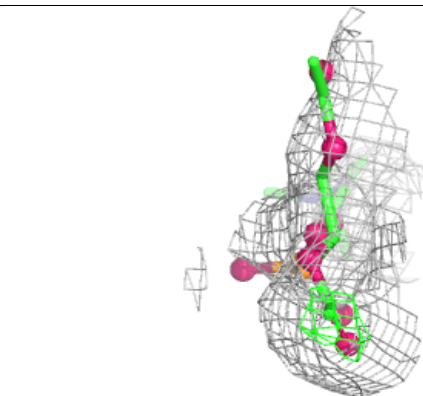
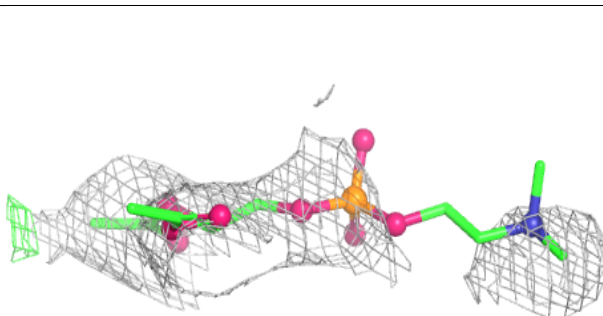
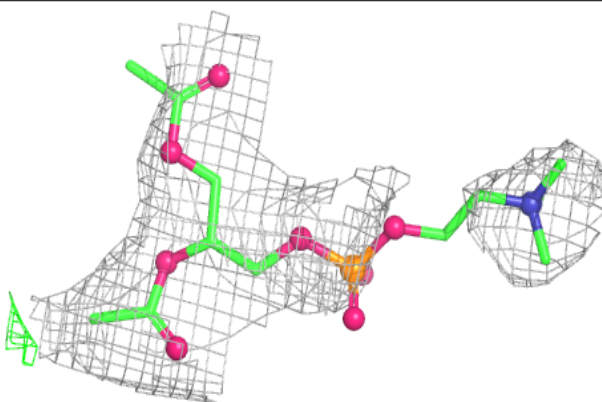


Electron density around PCW A 1115:

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

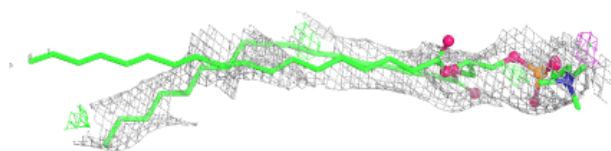
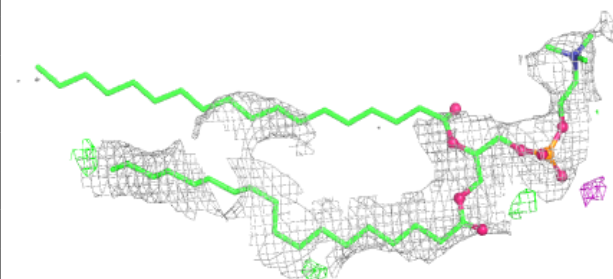
**Electron density around PCW C 1105:**

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

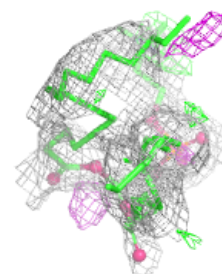
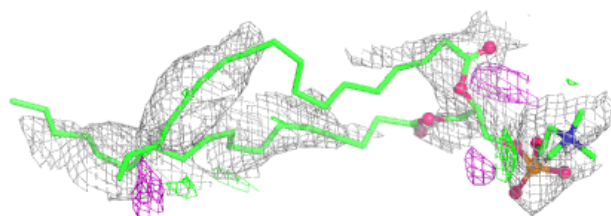
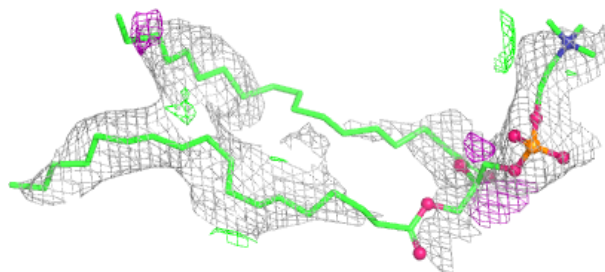


Electron density around PC1 A 1106:

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

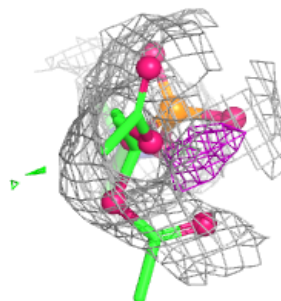
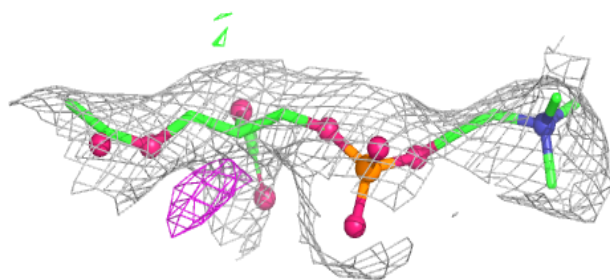
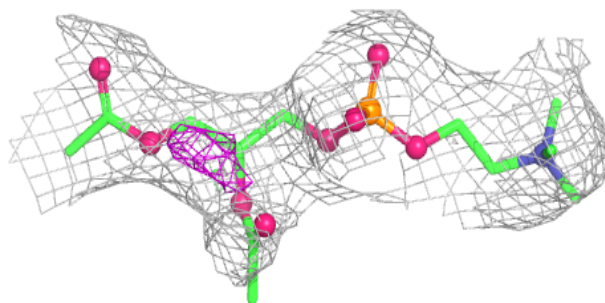
**Electron density around PCW A 1116:**

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



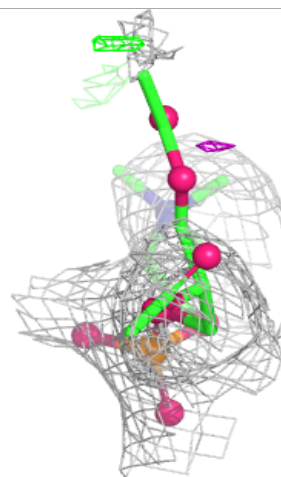
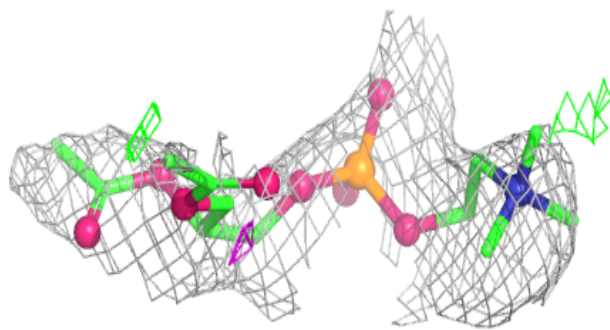
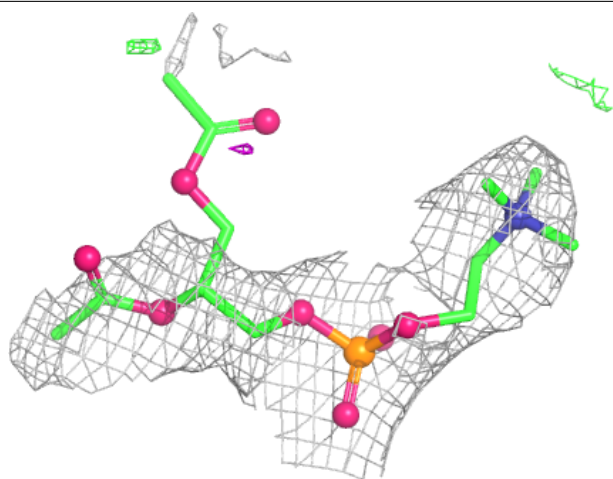
Electron density around PCW C 1111:

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and green (positive)



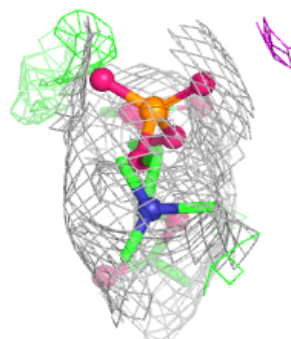
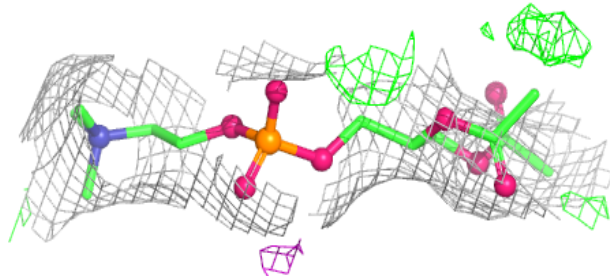
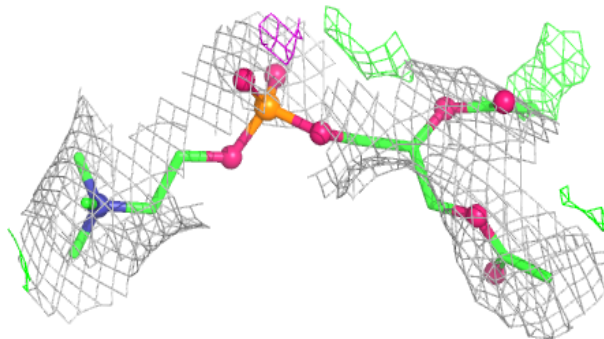
Electron density around PCW A 1114:

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

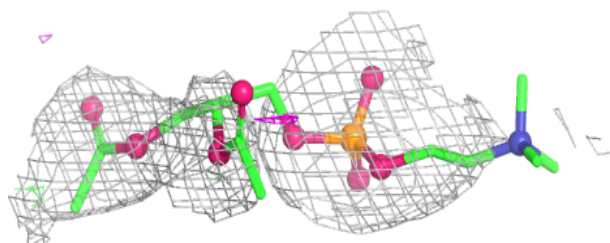
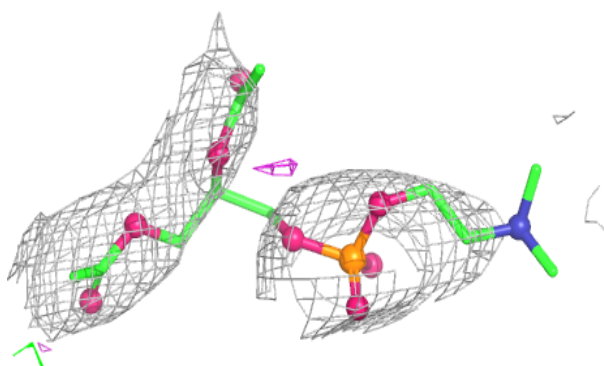


Electron density around PCW C 1106:

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

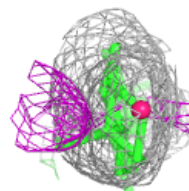
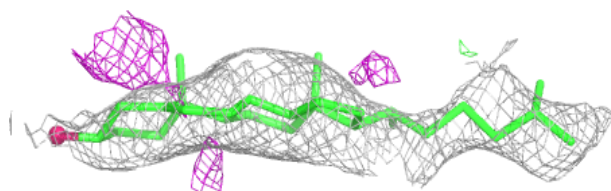
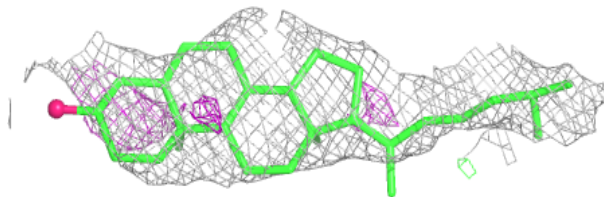
**Electron density around PCW A 1112:**

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and green (positive)

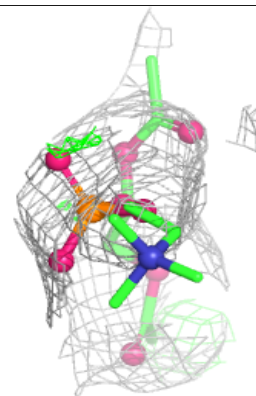
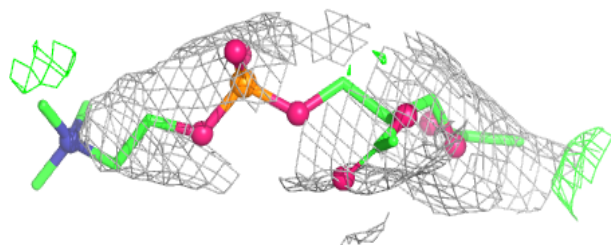
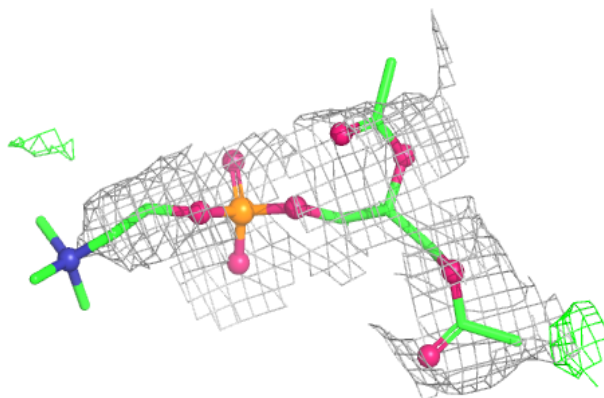


Electron density around CLR A 1104:

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and green (positive)

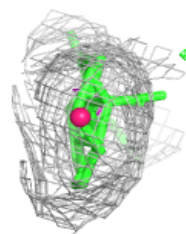
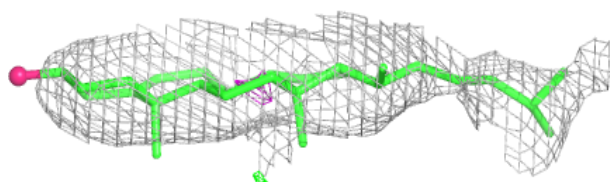
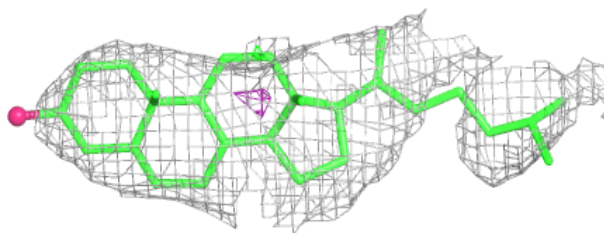
**Electron density around PCW C 1112:**

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and green (positive)

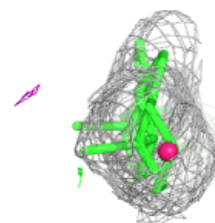
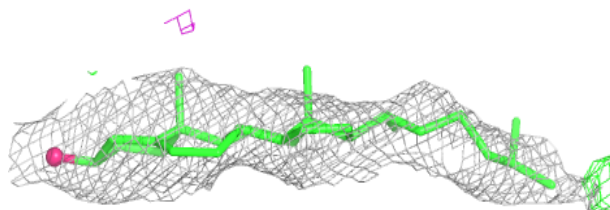
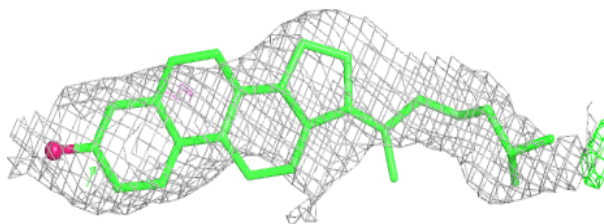


Electron density around CLR A 1110:

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and green (positive)

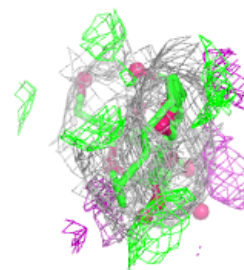
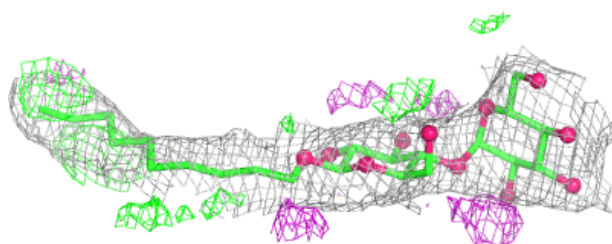
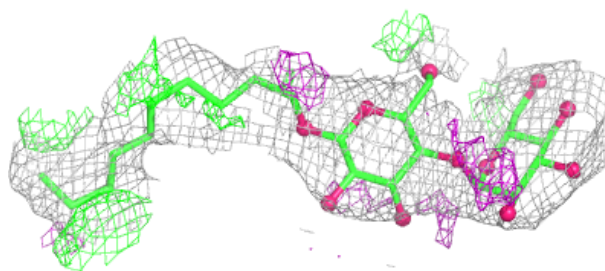
**Electron density around CLR C 1107:**

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and green (positive)

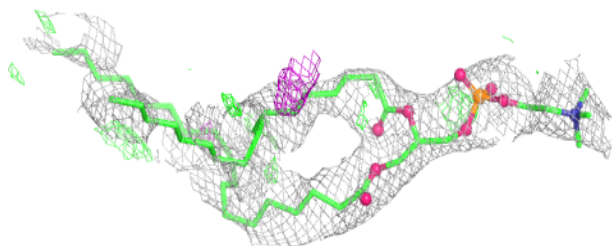
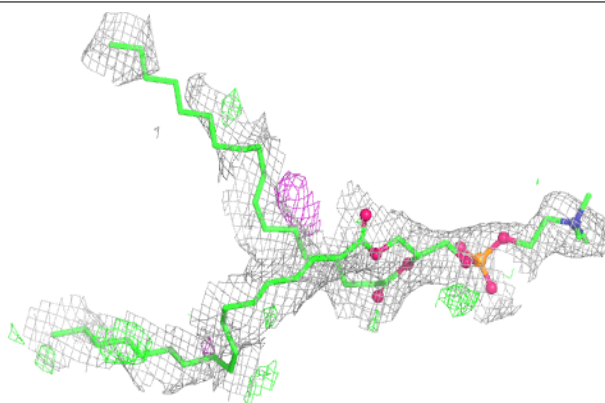


Electron density around DMU E 102:

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and green (positive)

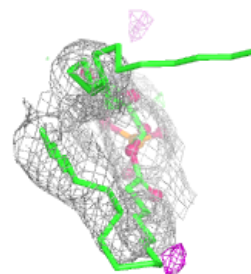
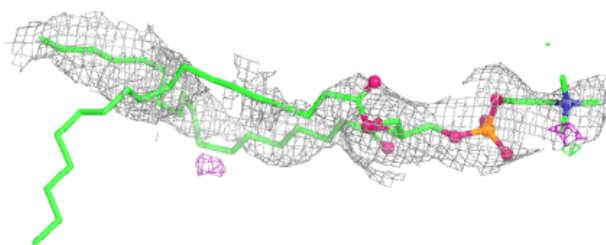
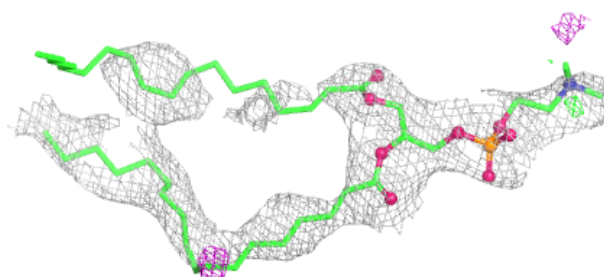
**Electron density around PC1 A 1111:**

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and green (positive)



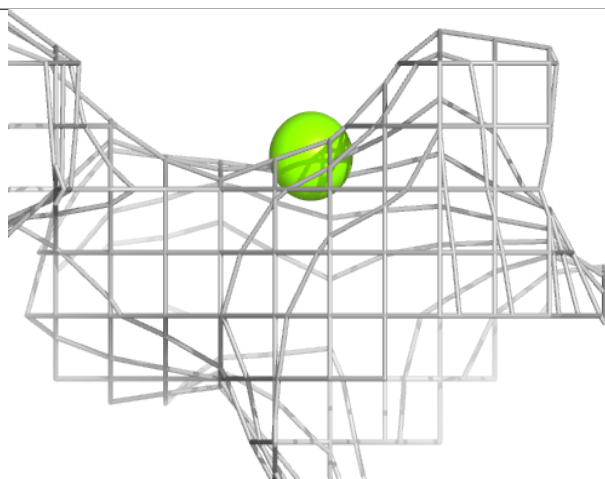
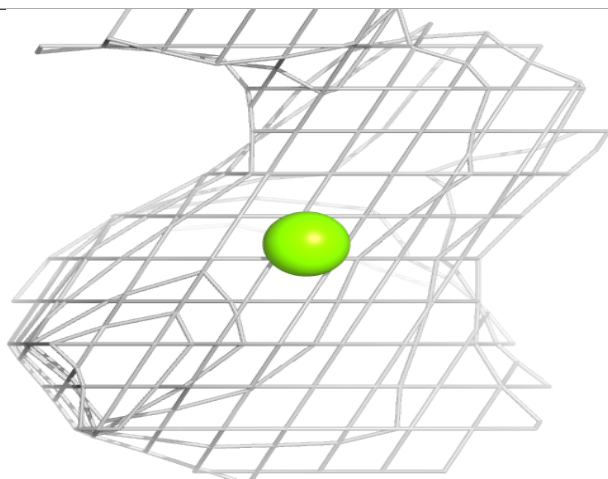
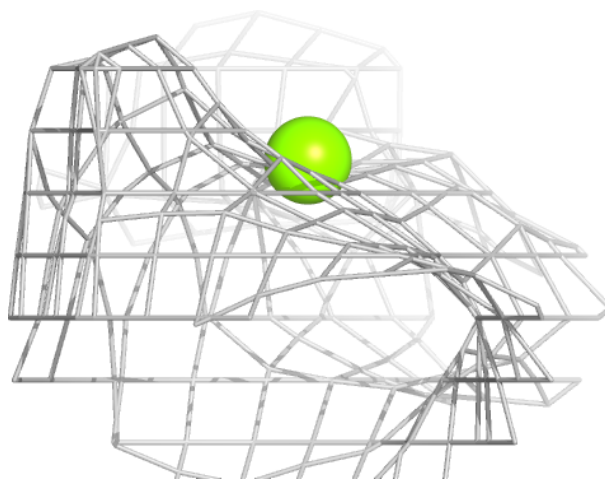
Electron density around PC1 A 1108:

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



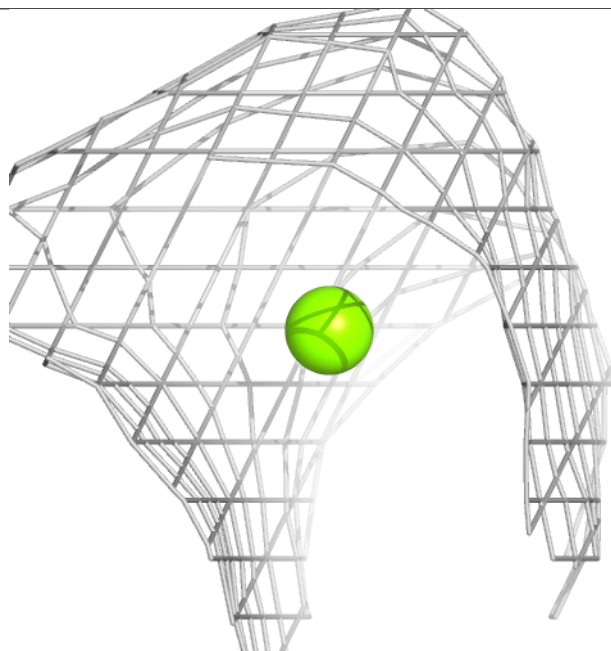
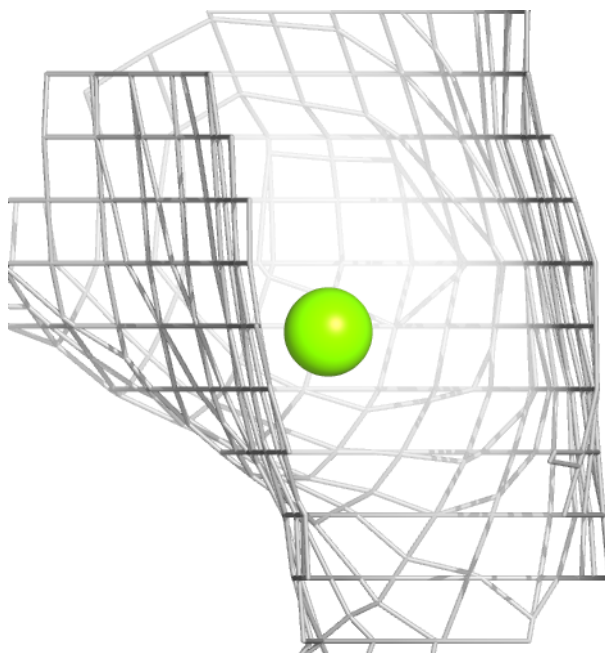
Electron density around MG C 1101:

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



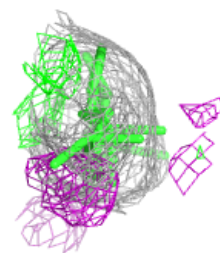
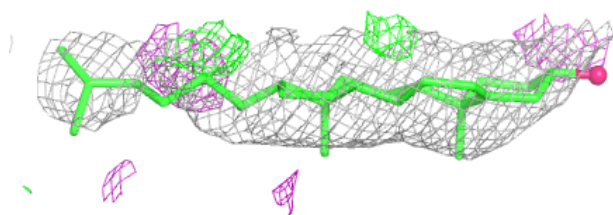
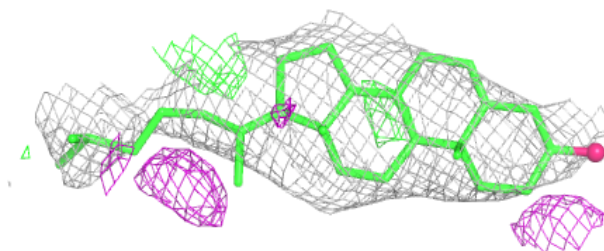
Electron density around MG C 1102:

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



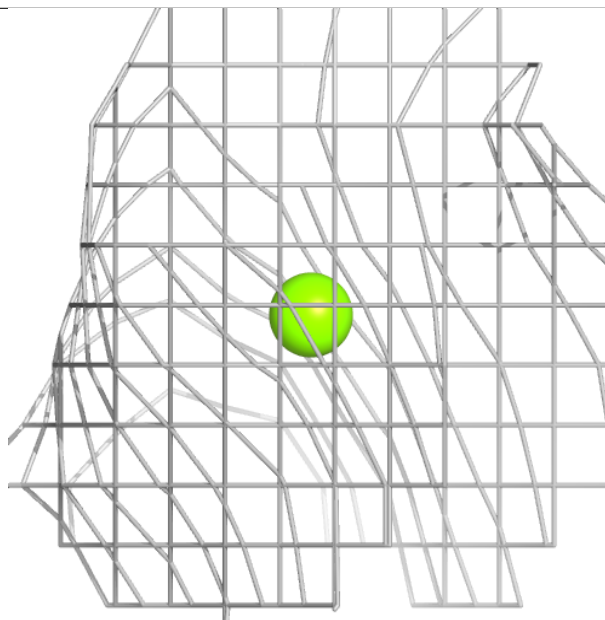
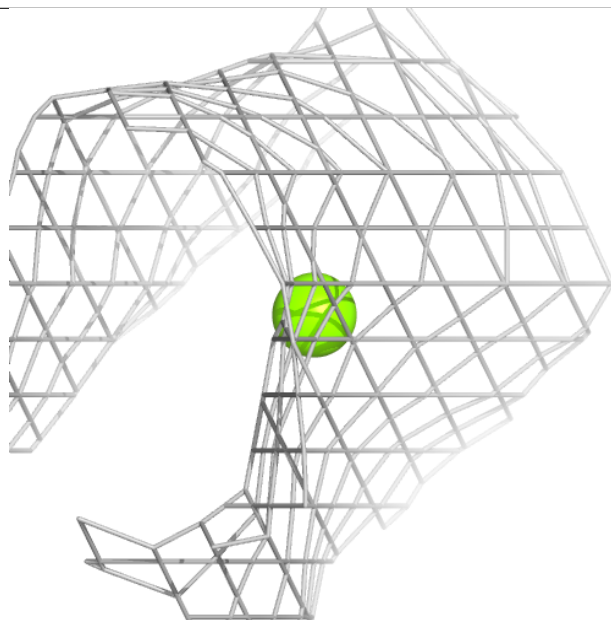
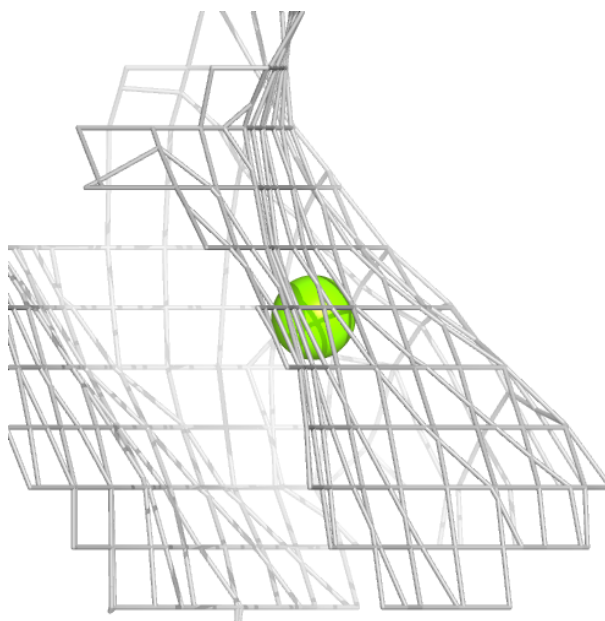
Electron density around CLR A 1105:

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



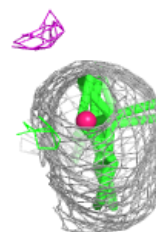
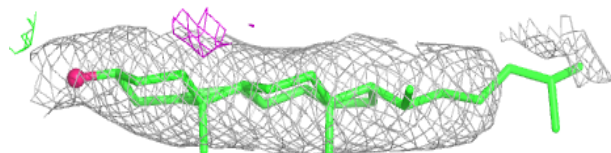
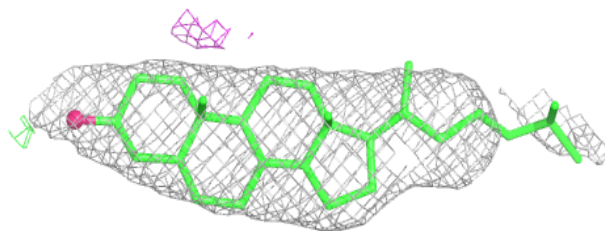
Electron density around MG A 1102:

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

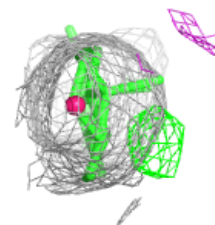
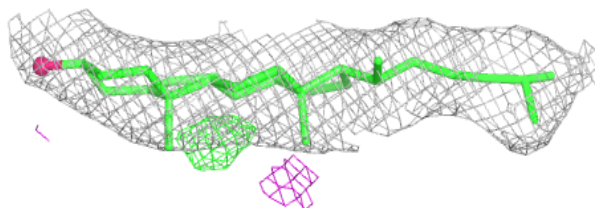
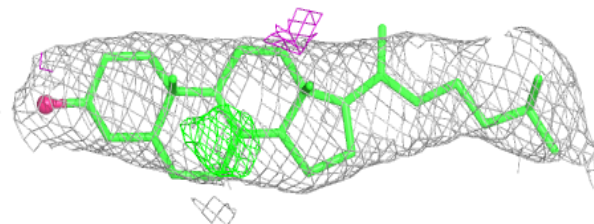


Electron density around CLR C 1104:

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

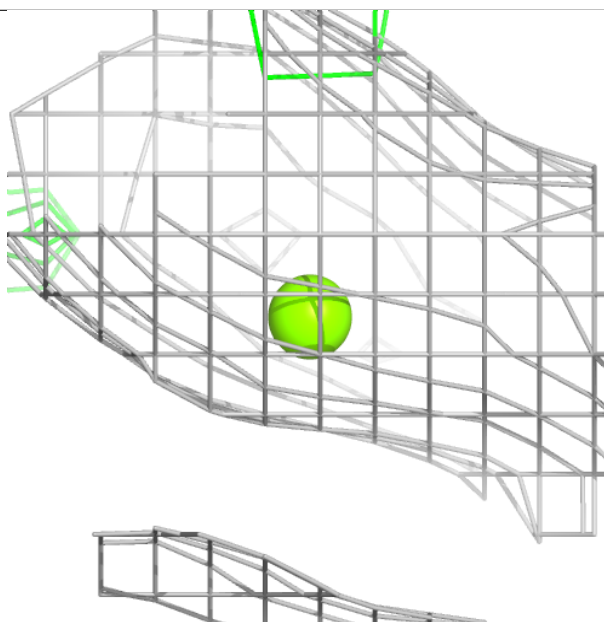
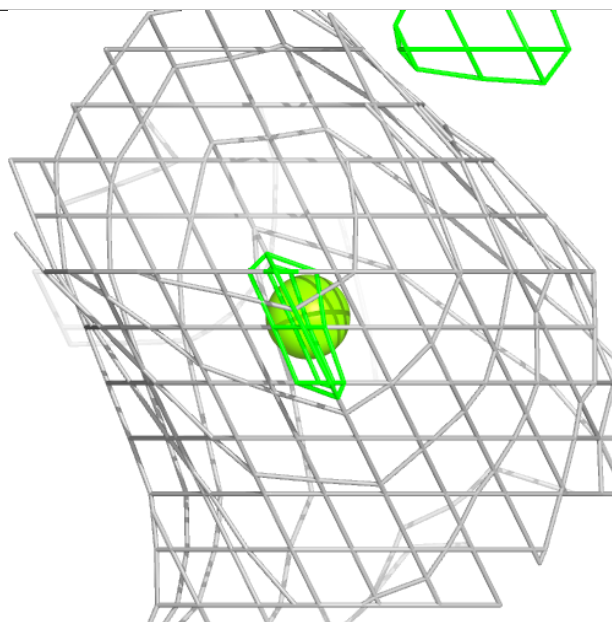
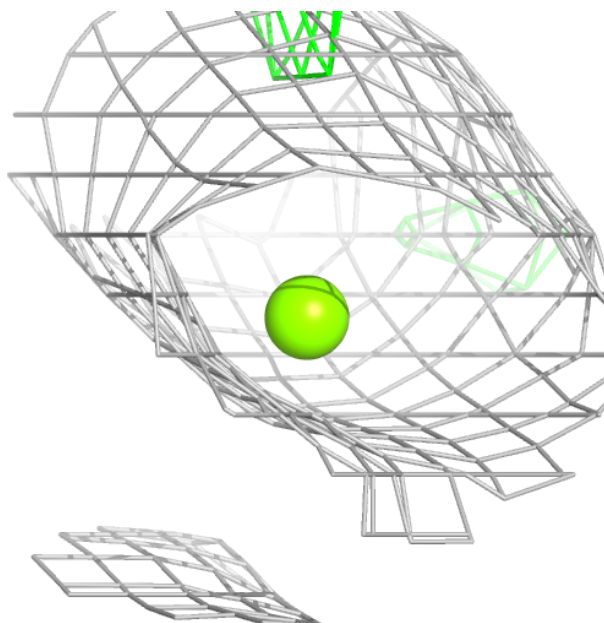
**Electron density around CLR E 101:**

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



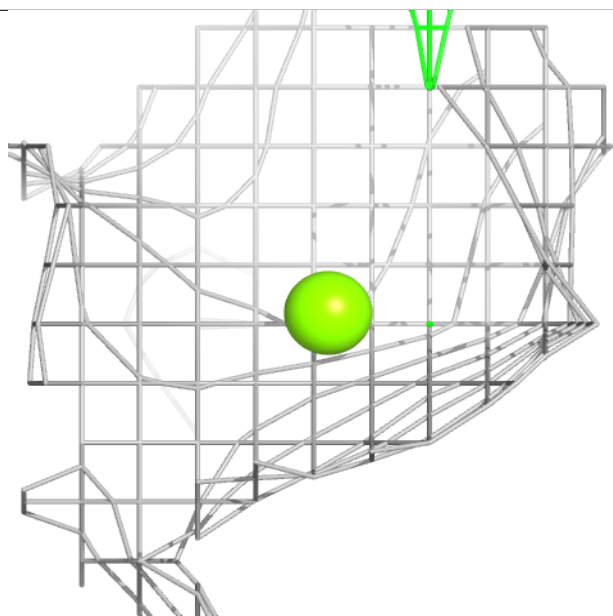
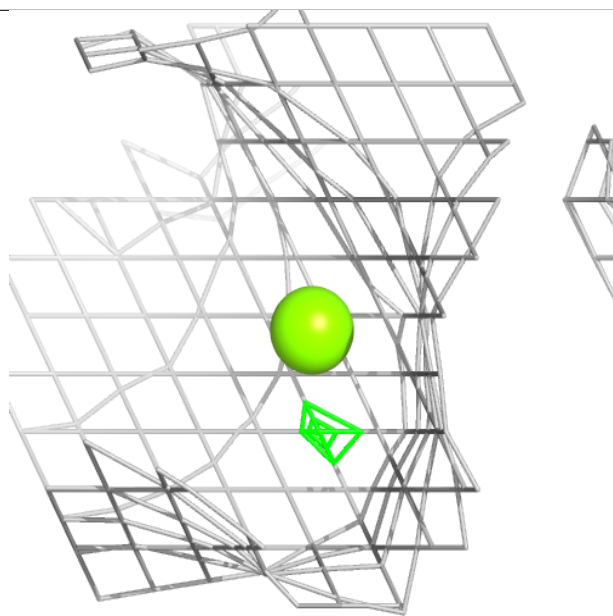
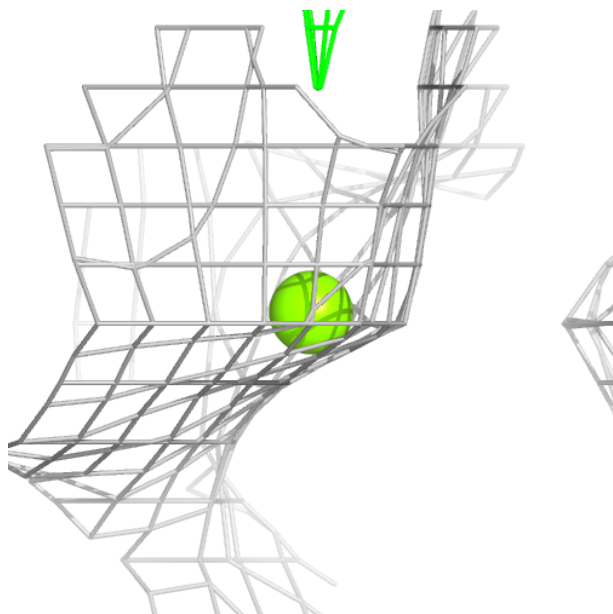
Electron density around MG A 1103:

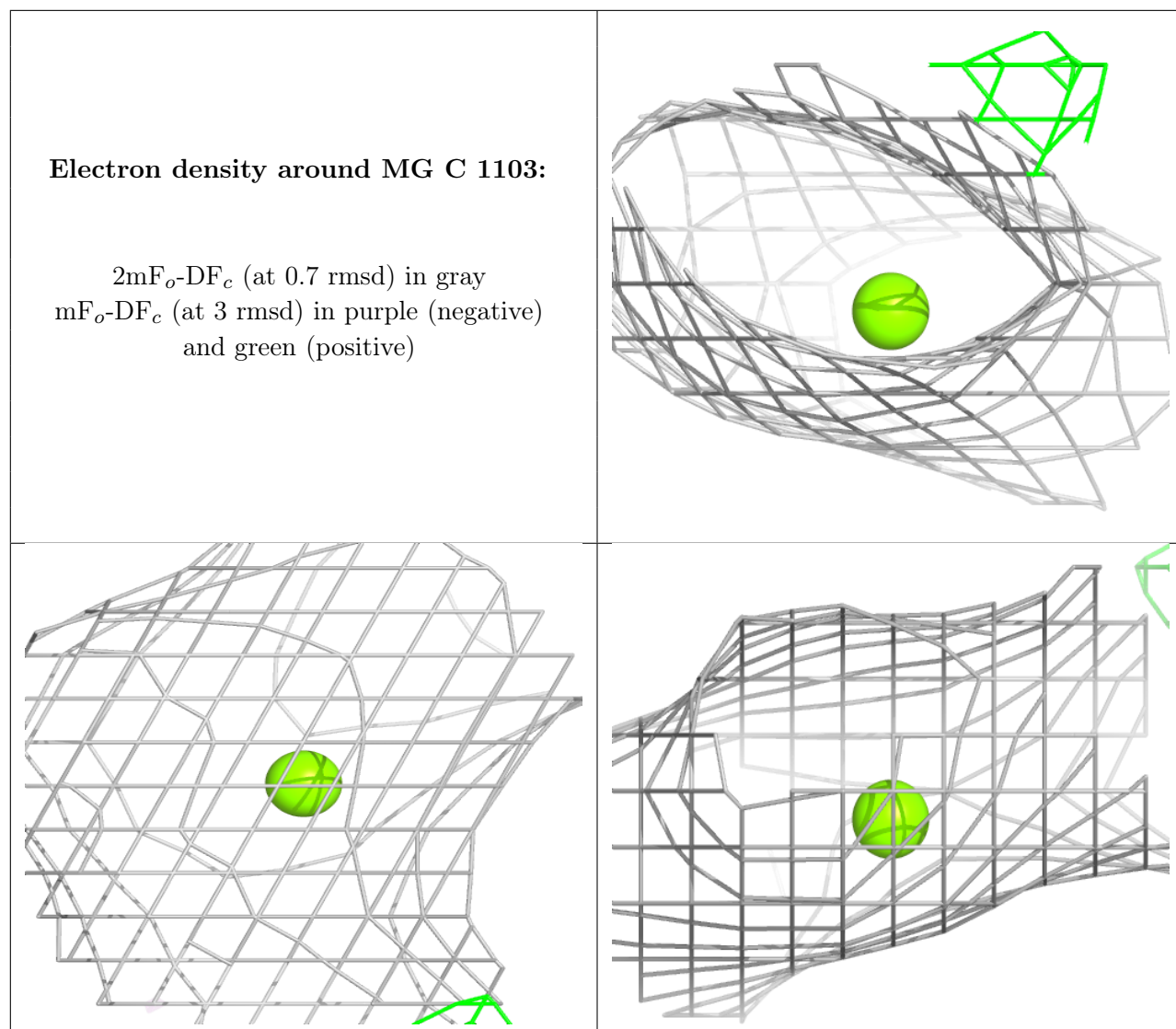
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 1101:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.