



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2023 – 12:24 PM JST

PDB ID : 8JBK
Title : Crystal structure of Na⁺,K⁺-ATPase in the E1.3Na⁺ state
Authors : Kanai, R.; Vilsen, B.; Cornelius, F.; Toyoshima, C.
Deposited on : 2023-05-09
Resolution : 2.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

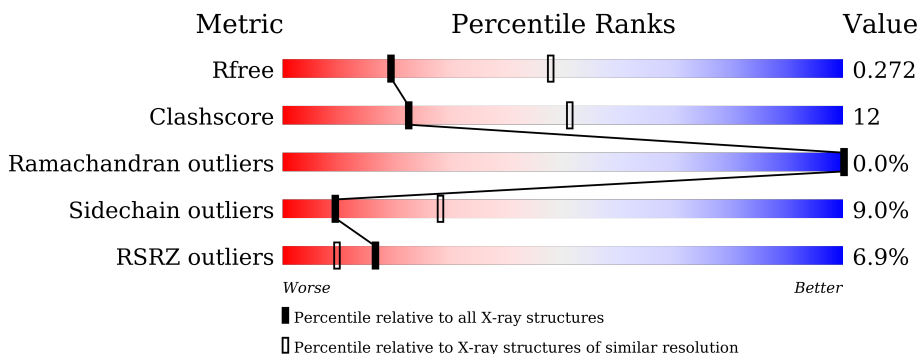
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	
1	C	1021	
2	B	303	
2	D	303	
3	E	65	
3	G	65	

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Mol	Chain	Length	Quality of chain
4	F	6	
5	H	5	
6	I	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PCW	A	1115	-	-	-	X
11	PCW	A	1116	-	-	-	X
11	PCW	C	1110	-	-	-	X
11	PCW	C	1113	-	-	-	X
12	NAG	D	402	-	-	-	X
4	NAG	F	1	-	-	-	X
4	BMA	F	3	-	-	-	X
4	MAN	F	6	-	-	-	X
5	BMA	H	3	-	-	-	X
5	MAN	H	4	-	-	-	X
5	MAN	H	5	-	-	-	X

2 Entry composition [i](#)

There are 14 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
			Total	C	N	O	S			
1	A	995	7723	4923	1301	1452	47	0	0	0
1	C	995	7723	4923	1301	1452	47	0	0	0

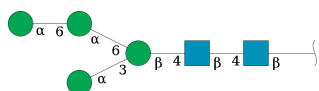
- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

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

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

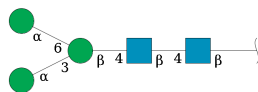
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	G	36	292	197	47	48	0	0	0
3	E	33	262	179	38	45	0	0	0

- 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
			Total	C	N	O			
4	F	6	72	40	2	30	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	H	5	61	34	2	25	0	0	0

- 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
			Total	C	N	O			
6	I	2	28	16	2	10	0	0	0

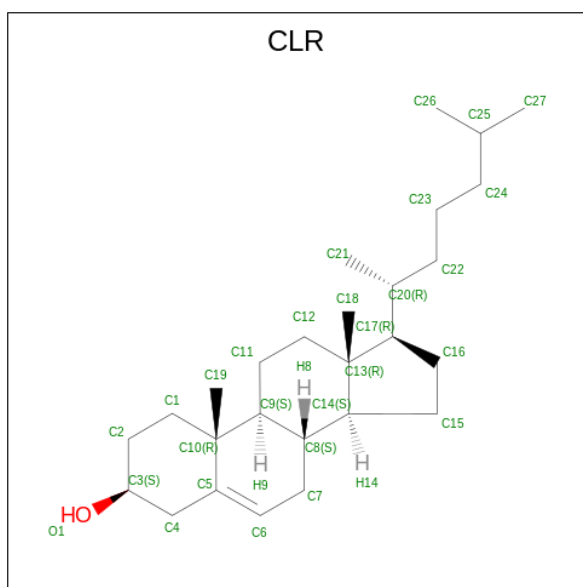
- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
7	A	1	1	1	0	0
7	C	1	1	1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

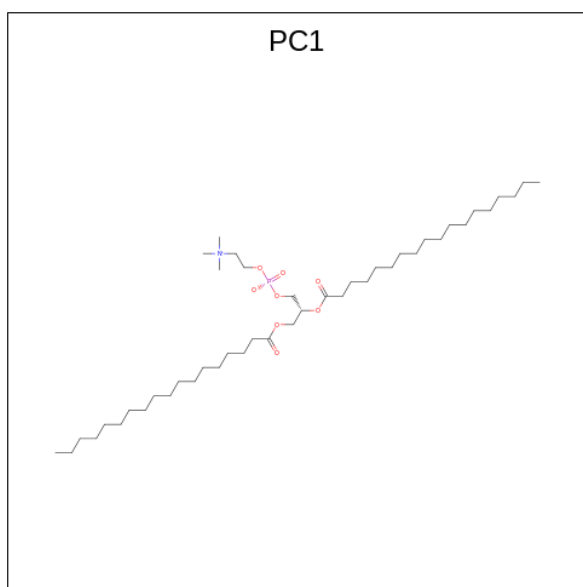
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
8	A	4	4	4	0	0
8	C	4	4	4	0	0

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



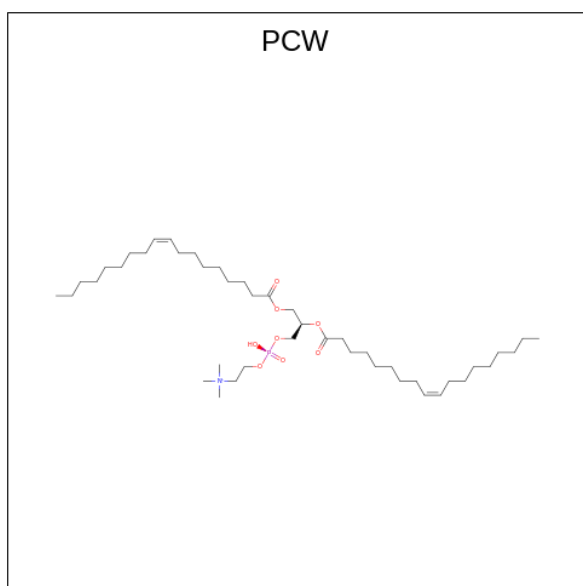
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	C O	0	0
			28	27 1		
9	A	1	Total	C O	0	0
			28	27 1		
9	B	1	Total	C O	0	0
			28	27 1		
9	C	1	Total	C O	0	0
			28	27 1		
9	D	1	Total	C O	0	0
			28	27 1		
9	E	1	Total	C O	0	0
			28	27 1		

- Molecule 10 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



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

- Molecule 11 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



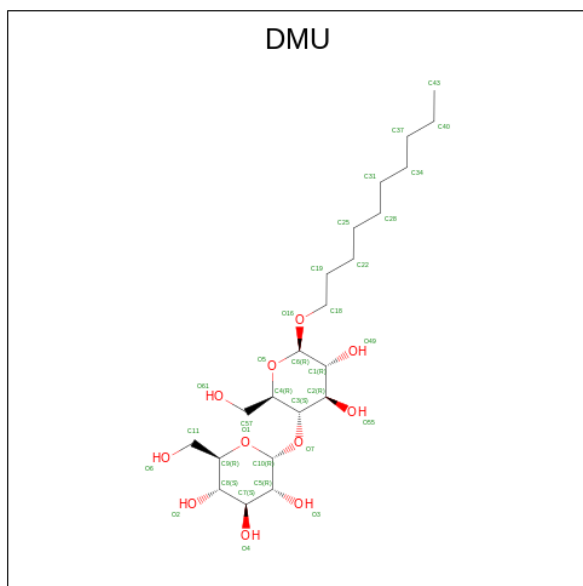
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	A	1	22	12	1	8	1	0	0
11	A	1	22	12	1	8	1	0	0
11	A	1	22	12	1	8	1	0	0
11	A	1	22	12	1	8	1	0	0
11	A	1	22	12	1	8	1	0	0
11	A	1	22	12	1	8	1	0	0
11	B	1	22	12	1	8	1	0	0
11	C	1	22	12	1	8	1	0	0
11	C	1	22	12	1	8	1	0	0
11	C	1	22	12	1	8	1	0	0
11	C	1	22	12	1	8	1	0	0
11	C	1	22	12	1	8	1	0	0
11	C	1	22	12	1	8	1	0	0
11	C	1	22	12	1	8	1	0	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 13 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

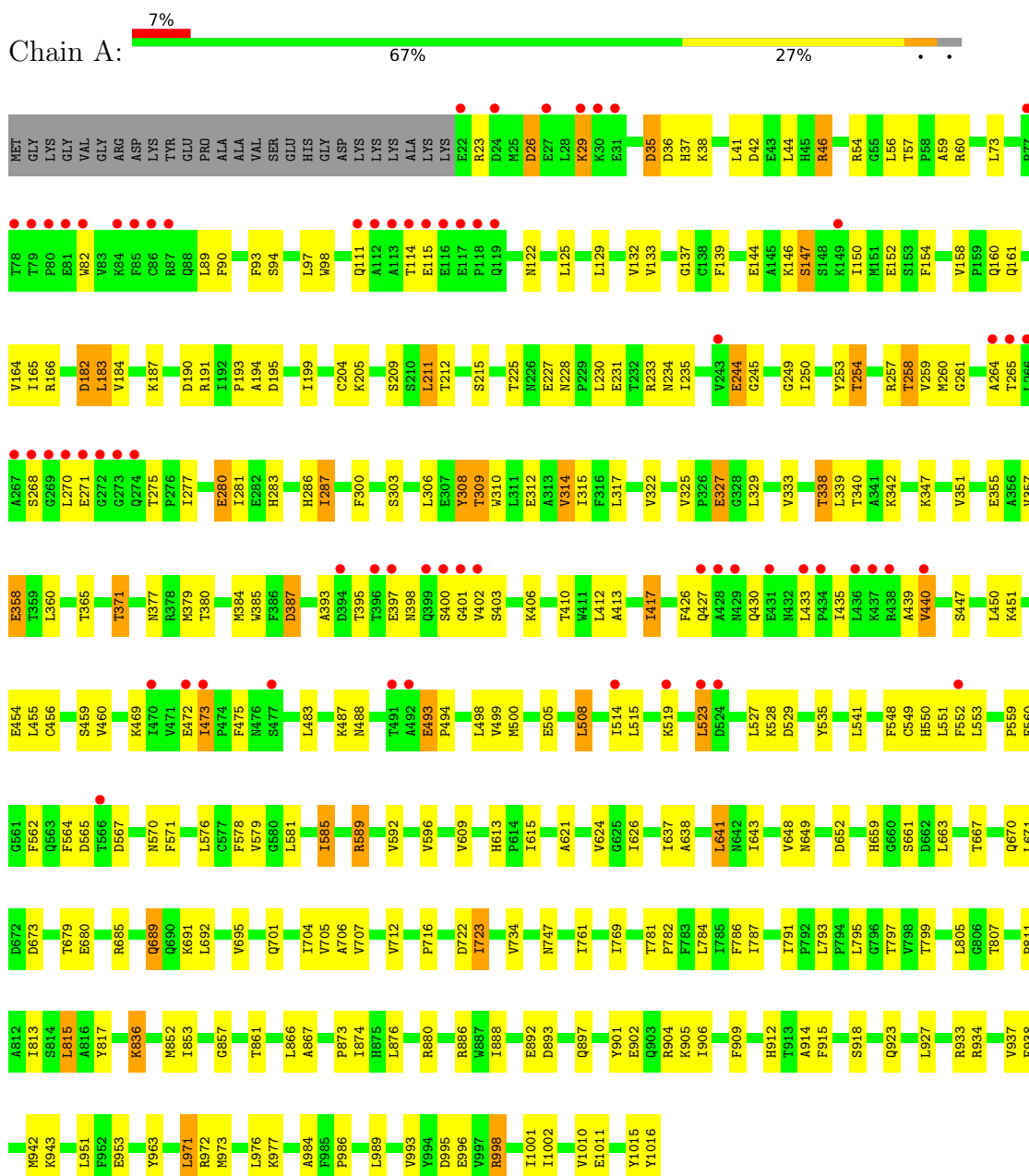
- Molecule 14 is water.

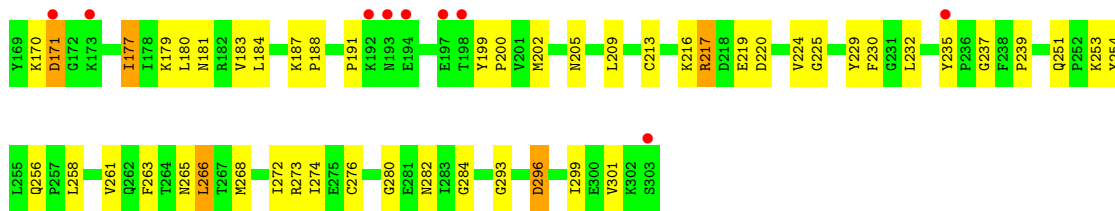
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	15	Total O 15 15	0	0
14	C	14	Total O 14 14	0	0
14	D	3	Total O 3 3	0	0

3 Residue-property plots i

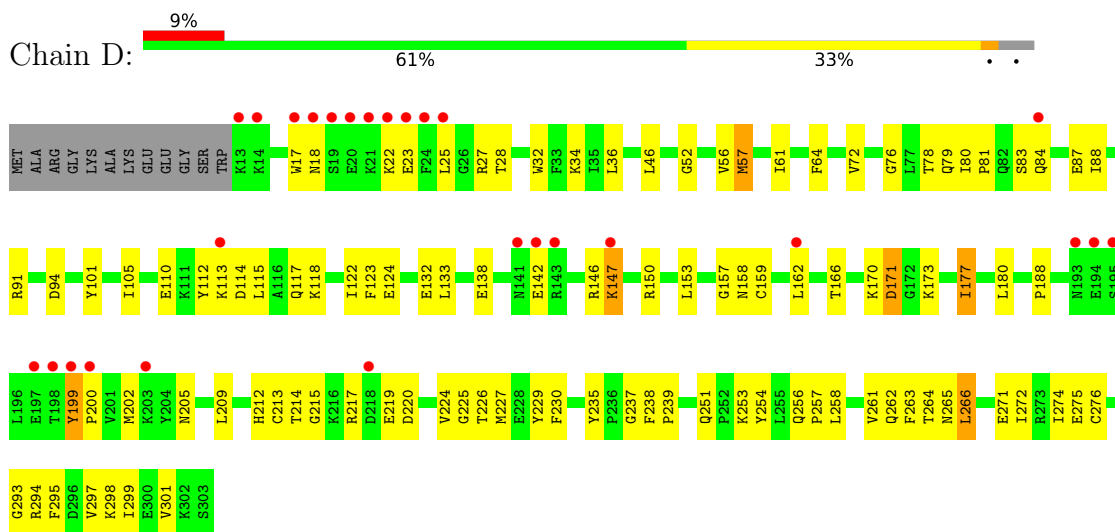
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

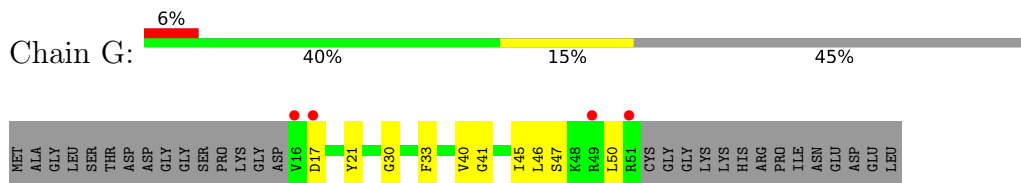




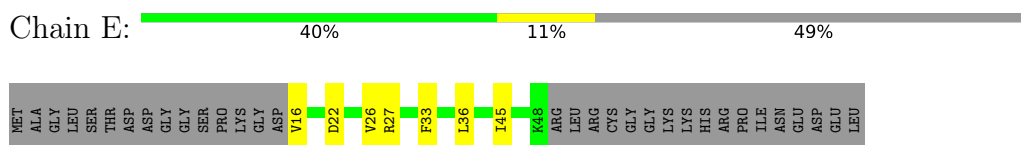
- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



- Molecule 3: FXYP domain-containing ion transport regulator



- Molecule 3: FXYP domain-containing ion transport regulator



- 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



- 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:  40% 60%

MAG1
MAG2
BGA3
MAN4
MAN5

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

Chain I:  50% 50%

MAG1
MAG2

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	193.74Å 74.49Å 162.56Å 90.00° 115.72° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 29.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	64.6 (15.00-2.80) 64.8 (29.98-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.80Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.229 , 0.270 0.233 , 0.272	Depositor DCC
R_{free} test set	3358 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.015 for -h-1,-k,l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21682	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, PCW, BMA, MAN, MN, DMU, NAG, CLR, NA

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	0.28	0/7873	0.51	0/10683
1	C	0.28	0/7873	0.51	0/10683
2	B	0.27	0/2449	0.51	0/3301
2	D	0.27	0/2449	0.51	0/3301
3	E	0.29	0/268	0.43	0/364
3	G	0.27	0/298	0.49	0/403
All	All	0.28	0/21210	0.51	0/28735

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

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	7774	185	0
1	C	7723	0	7774	164	0
2	B	2386	0	2362	74	0
2	D	2386	0	2362	60	0
3	E	262	0	268	6	0
3	G	292	0	305	9	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	2	0
6	I	28	0	25	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	4	0	0	0	0
8	C	4	0	0	0	0
9	A	56	0	92	7	0
9	B	28	0	46	4	0
9	C	28	0	46	4	0
9	D	28	0	46	2	0
9	E	28	0	46	1	0
10	A	162	0	264	16	0
11	A	132	0	108	2	0
11	B	22	0	18	2	0
11	C	176	0	144	7	0
12	D	14	0	13	0	0
13	E	33	0	42	3	0
14	A	15	0	0	0	0
14	C	14	0	0	0	0
14	D	3	0	0	0	0
All	All	21682	0	21848	503	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 12.

The worst 5 of 503 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:494:PRO:HG2	1:C:552:PHE:HB3	1.55	0.87
1:A:417:ILE:HD11	1:A:548:PHE:HB3	1.56	0.86
1:A:993:VAL:HG23	10:A:1110:PC1:H291	1.60	0.82
2:B:88:ILE:HB	2:B:299:ILE:HG22	1.61	0.81
10:A:1110:PC1:H372	9:C:1106:CLR:H71	1.64	0.80

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%)	951 (96%)	41 (4%)	1 (0%)	51	81
1	C	993/1021 (97%)	959 (97%)	34 (3%)	0	100	100
2	B	289/303 (95%)	276 (96%)	13 (4%)	0	100	100
2	D	289/303 (95%)	273 (94%)	16 (6%)	0	100	100
3	E	31/65 (48%)	30 (97%)	1 (3%)	0	100	100
3	G	34/65 (52%)	32 (94%)	2 (6%)	0	100	100
All	All	2629/2778 (95%)	2521 (96%)	107 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASP

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	845/864 (98%)	765 (90%)	80 (10%)	8	25
1	C	845/864 (98%)	770 (91%)	75 (9%)	9	28
2	B	261/269 (97%)	236 (90%)	25 (10%)	8	24
2	D	261/269 (97%)	240 (92%)	21 (8%)	12	34
3	E	27/52 (52%)	25 (93%)	2 (7%)	13	37
3	G	30/52 (58%)	29 (97%)	1 (3%)	38	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2269/2370 (96%)	2065 (91%)	204 (9%)	9 28

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	182	ASP
1	C	425	VAL
2	D	219	GLU
1	C	250	ILE
1	C	310	TRP

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	161	GLN
1	C	550	HIS
1	C	324	ASN
1	C	399	GLN
1	C	649	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	0.59	0	17,19,21	0.63	0
4	NAG	F	2	4	14,14,15	0.45	0	17,19,21	1.24	2 (11%)
4	BMA	F	3	4	11,11,12	1.23	1 (9%)	15,15,17	1.47	1 (6%)
4	MAN	F	4	4	11,11,12	0.94	0	15,15,17	0.93	1 (6%)
4	MAN	F	5	4	11,11,12	0.74	0	15,15,17	1.02	2 (13%)
4	MAN	F	6	4	11,11,12	0.94	0	15,15,17	0.92	0
5	NAG	H	1	5,2	14,14,15	1.15	1 (7%)	17,19,21	1.35	3 (17%)
5	NAG	H	2	5	14,14,15	0.83	1 (7%)	17,19,21	1.04	1 (5%)
5	BMA	H	3	5	11,11,12	1.52	2 (18%)	15,15,17	1.14	2 (13%)
5	MAN	H	4	5	11,11,12	1.17	1 (9%)	15,15,17	1.40	2 (13%)
5	MAN	H	5	5	11,11,12	1.28	1 (9%)	15,15,17	1.61	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.45	0	17,19,21	0.69	0
6	NAG	I	2	6	14,14,15	0.35	0	17,19,21	0.76	1 (5%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1	NAG	O5-C1	-3.99	1.37	1.43
5	H	5	MAN	C1-C2	3.28	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	BMA	C1-C2	3.17	1.59	1.52
4	F	3	BMA	C1-C2	3.03	1.59	1.52
5	H	4	MAN	C1-C2	2.94	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	5	MAN	C1-O5-C5	4.43	118.19	112.19
4	F	2	NAG	C1-O5-C5	3.45	116.86	112.19
5	H	4	MAN	C1-O5-C5	3.27	116.62	112.19
5	H	2	NAG	C1-O5-C5	3.11	116.41	112.19
5	H	1	NAG	C1-O5-C5	3.05	116.32	112.19

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

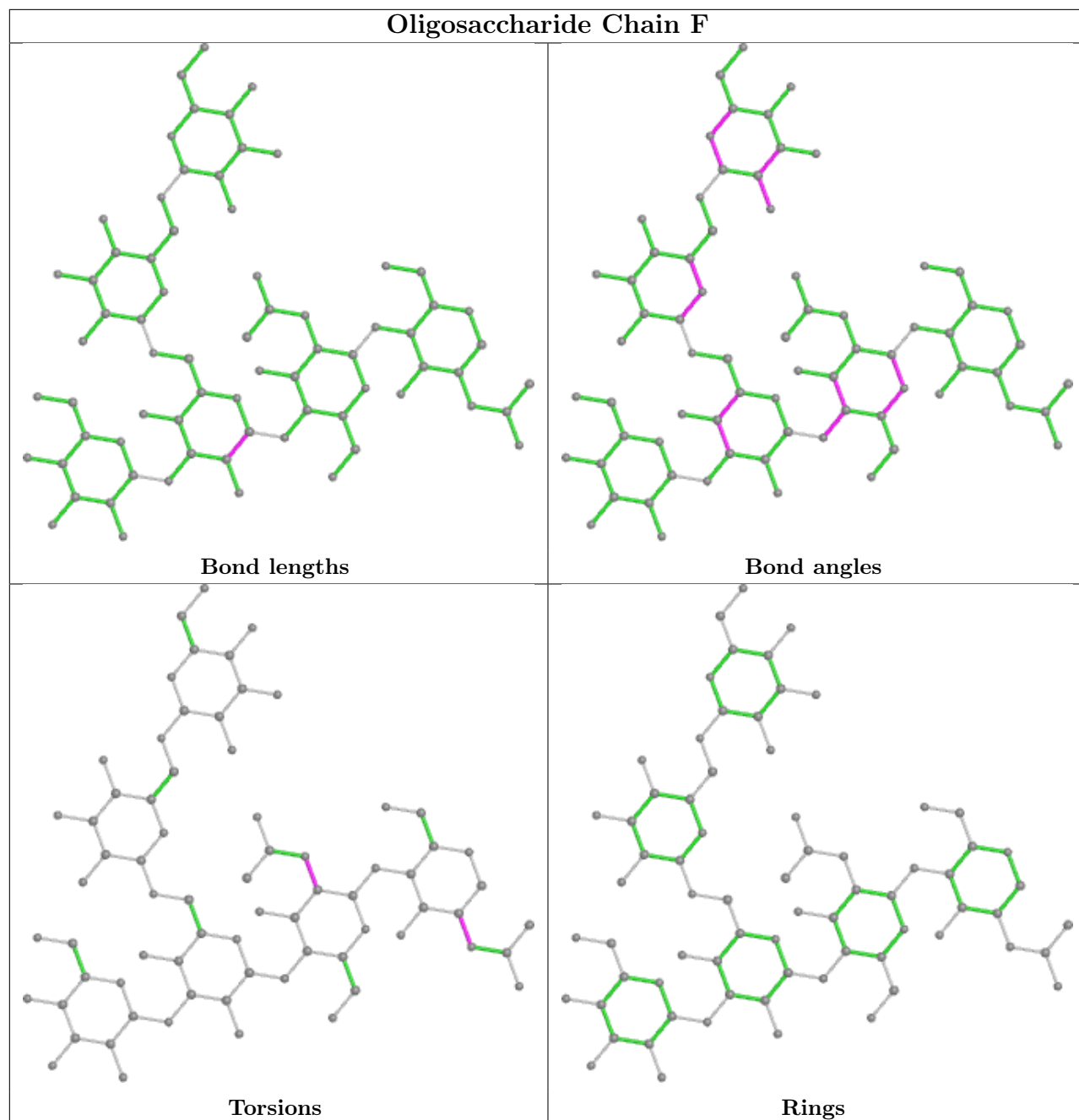
Mol	Chain	Res	Type	Atoms
5	H	3	BMA	C4-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
5	H	4	MAN	C4-C5-C6-O6
5	H	2	NAG	C8-C7-N2-C2

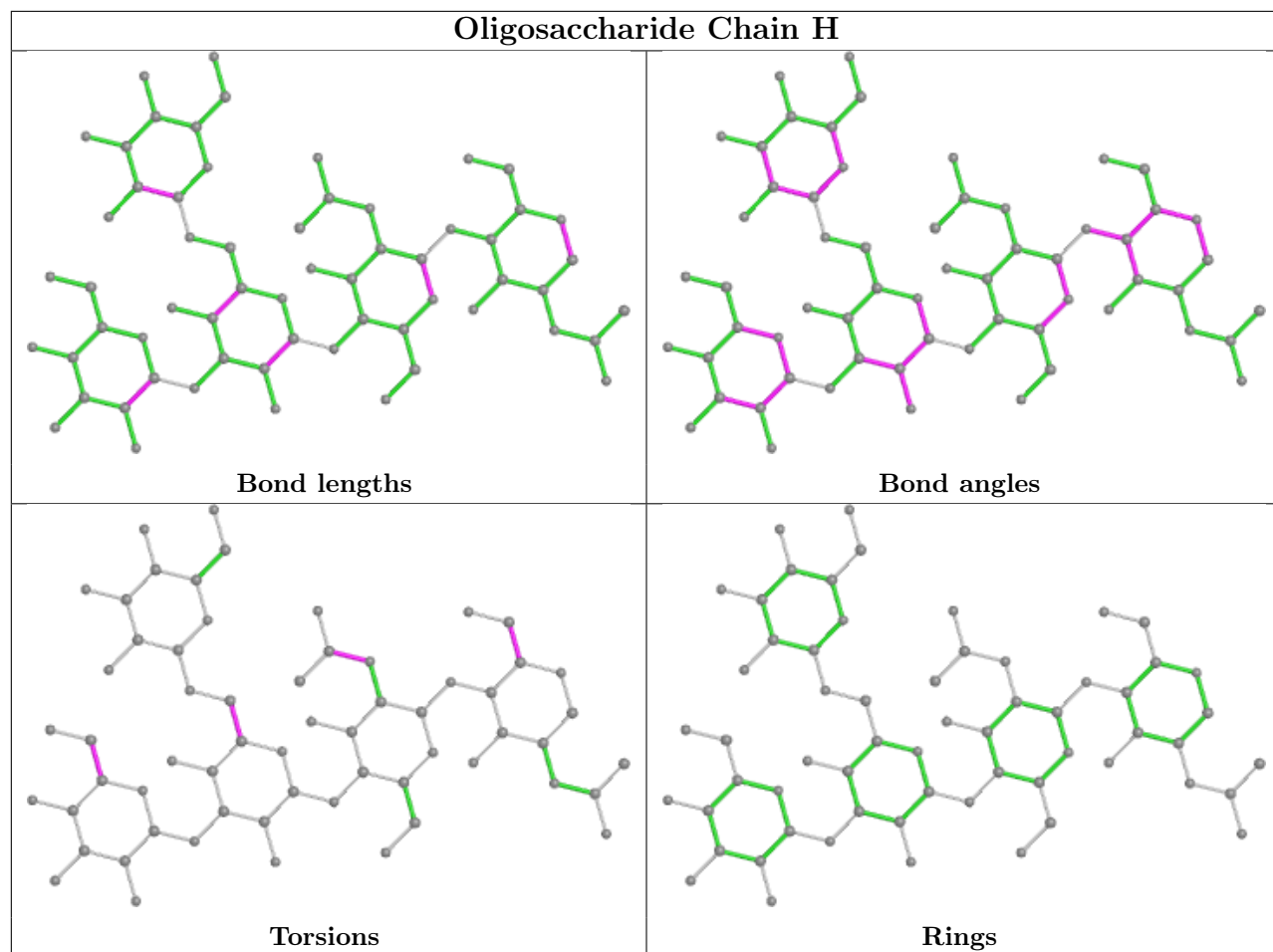
There are no ring outliers.

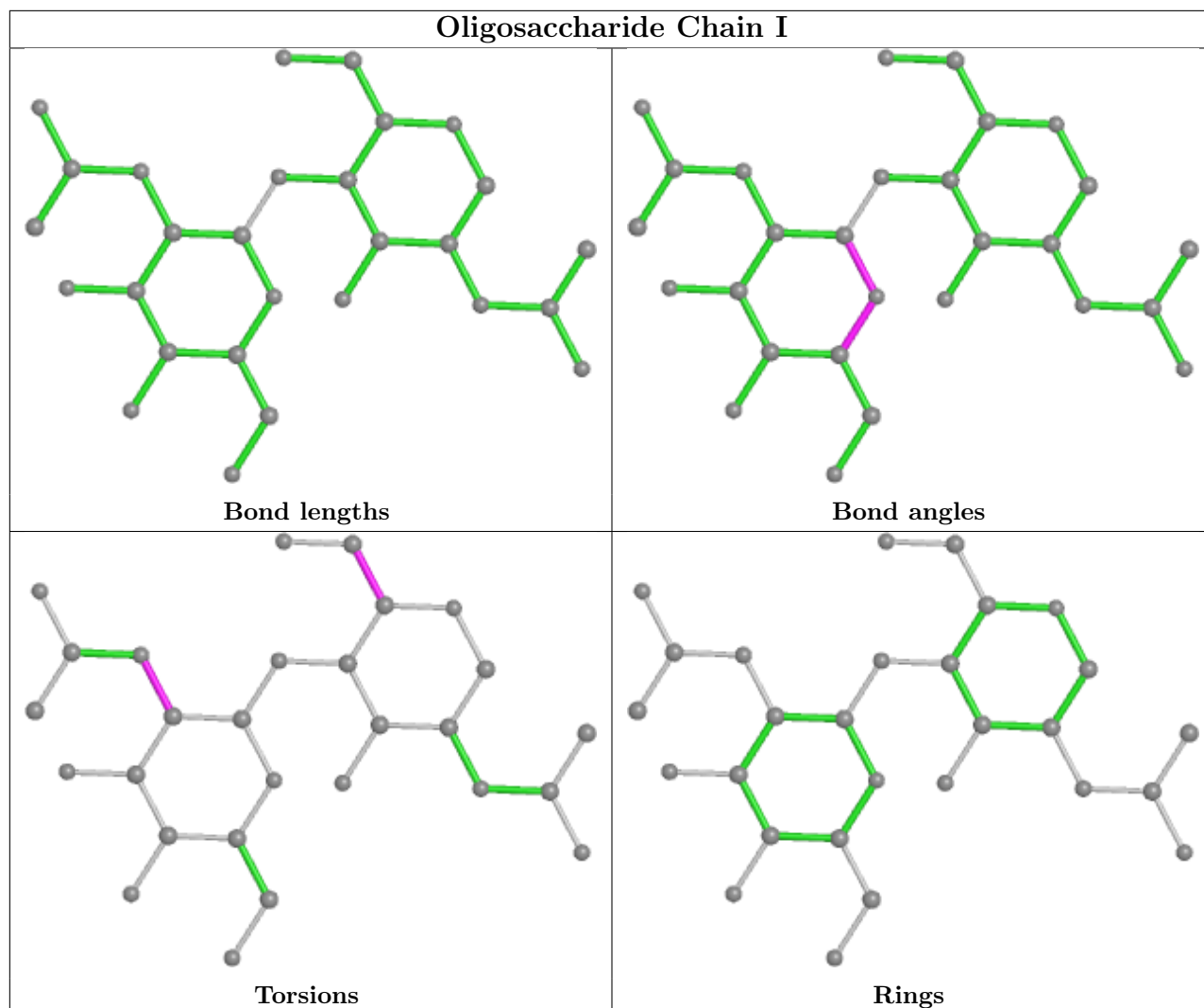
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	NAG	2	0
5	H	1	NAG	1	0
5	H	3	BMA	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 36 ligands modelled in this entry, 10 are monoatomic - leaving 26 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	$\# Z > 2$
9	CLR	E	101	-	31,31,31	1.50	6 (19%)	48,48,48	1.45	11 (22%)
11	PCW	C	1112	-	21,21,53	0.84	0	27,29,61	1.08	2 (7%)
11	PCW	C	1109	-	21,21,53	0.84	0	27,29,61	0.99	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	DMU	E	102	-	34,34,34	0.88	1 (2%)	45,45,45	1.36	5 (11%)
11	PCW	A	1115	-	21,21,53	0.83	0	27,29,61	1.13	3 (11%)
11	PCW	C	1110	-	21,21,53	0.85	0	27,29,61	0.87	1 (3%)
11	PCW	C	1113	-	21,21,53	0.85	0	27,29,61	0.86	1 (3%)
11	PCW	A	1109	-	21,21,53	0.84	0	27,29,61	1.15	2 (7%)
11	PCW	A	1113	-	21,21,53	0.84	0	27,29,61	1.02	2 (7%)
11	PCW	C	1111	-	21,21,53	0.84	0	27,29,61	0.96	2 (7%)
10	PC1	A	1108	-	53,53,53	0.63	0	59,61,61	0.94	1 (1%)
10	PC1	A	1110	-	53,53,53	0.74	0	59,61,61	1.17	5 (8%)
12	NAG	D	402	2	14,14,15	0.33	0	17,19,21	0.47	0
11	PCW	B	401	-	21,21,53	0.84	0	27,29,61	1.05	2 (7%)
11	PCW	C	1108	-	21,21,53	0.84	0	27,29,61	0.90	1 (3%)
11	PCW	C	1114	-	21,21,53	0.84	0	27,29,61	0.91	1 (3%)
9	CLR	D	401	-	31,31,31	1.53	6 (19%)	48,48,48	1.42	10 (20%)
10	PC1	A	1111	-	53,53,53	0.70	0	59,61,61	0.86	1 (1%)
9	CLR	C	1106	-	31,31,31	1.44	6 (19%)	48,48,48	1.42	11 (22%)
9	CLR	B	402	-	31,31,31	1.47	5 (16%)	48,48,48	1.40	10 (20%)
9	CLR	A	1106	-	31,31,31	1.48	6 (19%)	48,48,48	1.42	11 (22%)
11	PCW	A	1114	-	21,21,53	0.84	0	27,29,61	1.00	2 (7%)
11	PCW	C	1107	-	21,21,53	0.83	0	27,29,61	1.00	2 (7%)
11	PCW	A	1112	-	21,21,53	0.84	0	27,29,61	1.06	2 (7%)
11	PCW	A	1116	-	21,21,53	0.83	0	27,29,61	1.02	2 (7%)
9	CLR	A	1107	-	31,31,31	1.50	6 (19%)	48,48,48	1.42	10 (20%)

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
9	CLR	E	101	-	-	1/10/68/68	0/4/4/4
11	PCW	C	1112	-	-	5/23/23/57	-
11	PCW	C	1109	-	-	7/23/23/57	-
13	DMU	E	102	-	-	2/19/59/59	0/2/2/2
11	PCW	A	1115	-	-	7/23/23/57	-
11	PCW	C	1110	-	-	8/23/23/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PCW	C	1113	-	-	8/23/23/57	-
11	PCW	A	1109	-	-	2/23/23/57	-
11	PCW	A	1113	-	-	5/23/23/57	-
11	PCW	C	1111	-	-	7/23/23/57	-
10	PC1	A	1108	-	-	9/57/57/57	-
10	PC1	A	1110	-	-	15/57/57/57	-
12	NAG	D	402	2	-	2/6/23/26	0/1/1/1
11	PCW	B	401	-	-	1/23/23/57	-
11	PCW	C	1108	-	-	6/23/23/57	-
11	PCW	C	1114	-	-	5/23/23/57	-
9	CLR	D	401	-	-	4/10/68/68	0/4/4/4
10	PC1	A	1111	-	-	15/57/57/57	-
9	CLR	C	1106	-	-	1/10/68/68	0/4/4/4
9	CLR	B	402	-	-	7/10/68/68	0/4/4/4
9	CLR	A	1106	-	-	3/10/68/68	0/4/4/4
11	PCW	A	1114	-	-	7/23/23/57	-
11	PCW	C	1107	-	-	7/23/23/57	-
11	PCW	A	1112	-	-	7/23/23/57	-
11	PCW	A	1116	-	-	7/23/23/57	-
9	CLR	A	1107	-	-	5/10/68/68	0/4/4/4

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	401	CLR	C4-C3	3.46	1.58	1.52
9	E	101	CLR	C4-C3	3.27	1.57	1.52
9	A	1107	CLR	C4-C3	3.26	1.57	1.52
9	A	1106	CLR	C4-C3	3.17	1.57	1.52
9	C	1106	CLR	C4-C3	3.05	1.57	1.52

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1110	PC1	C2-O21-C21	4.28	128.32	117.79
13	E	102	DMU	O16-C18-C19	4.00	123.58	109.56
11	A	1109	PCW	C2-O2-C31	-3.77	110.87	117.90
11	C	1112	PCW	C2-O2-C31	-3.53	111.31	117.90
9	C	1106	CLR	C22-C20-C17	-3.29	103.49	110.28

There are no chirality outliers.

5 of 153 torsion outliers are listed below:

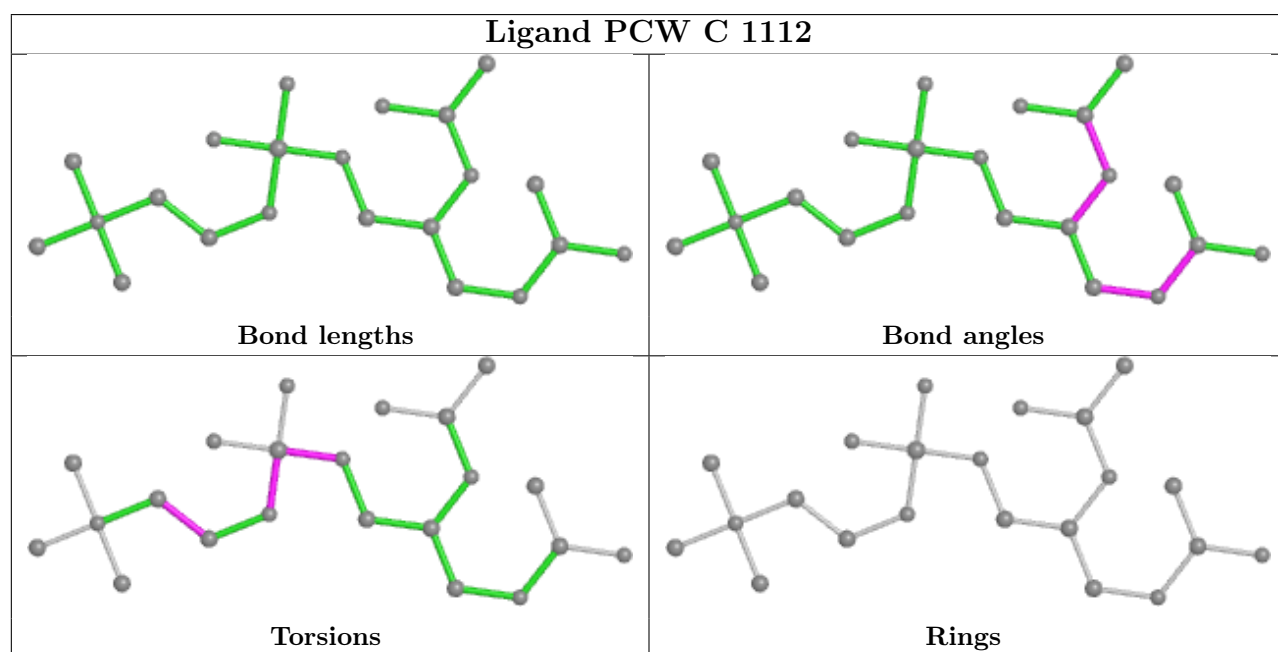
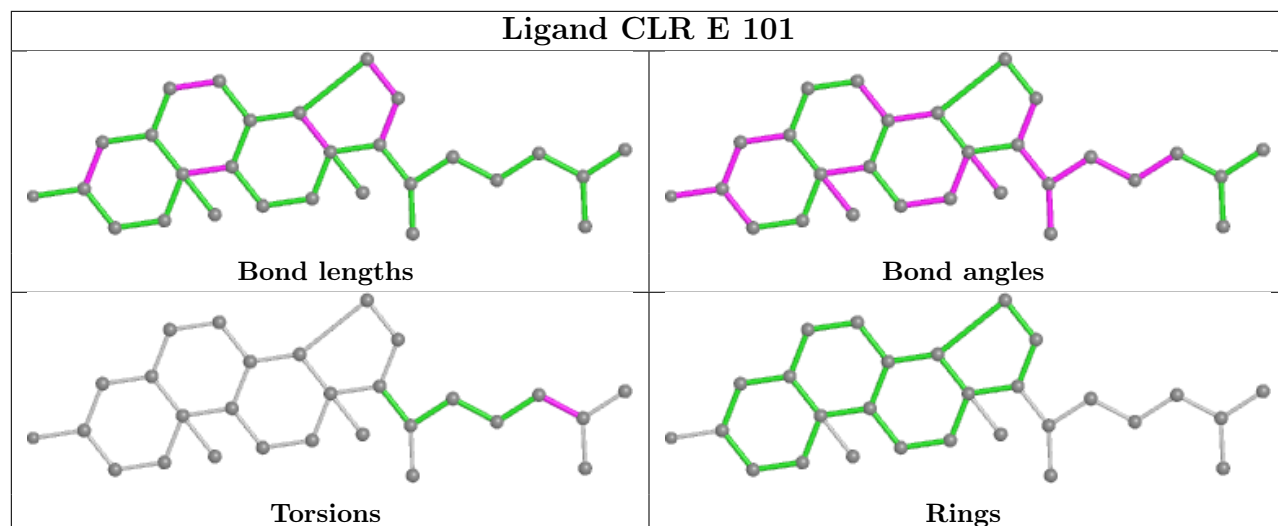
Mol	Chain	Res	Type	Atoms
10	A	1108	PC1	C11-O13-P-O14
10	A	1110	PC1	C11-O13-P-O12
10	A	1110	PC1	C11-O13-P-O14
10	A	1110	PC1	C1-O11-P-O12
10	A	1111	PC1	C11-O13-P-O14

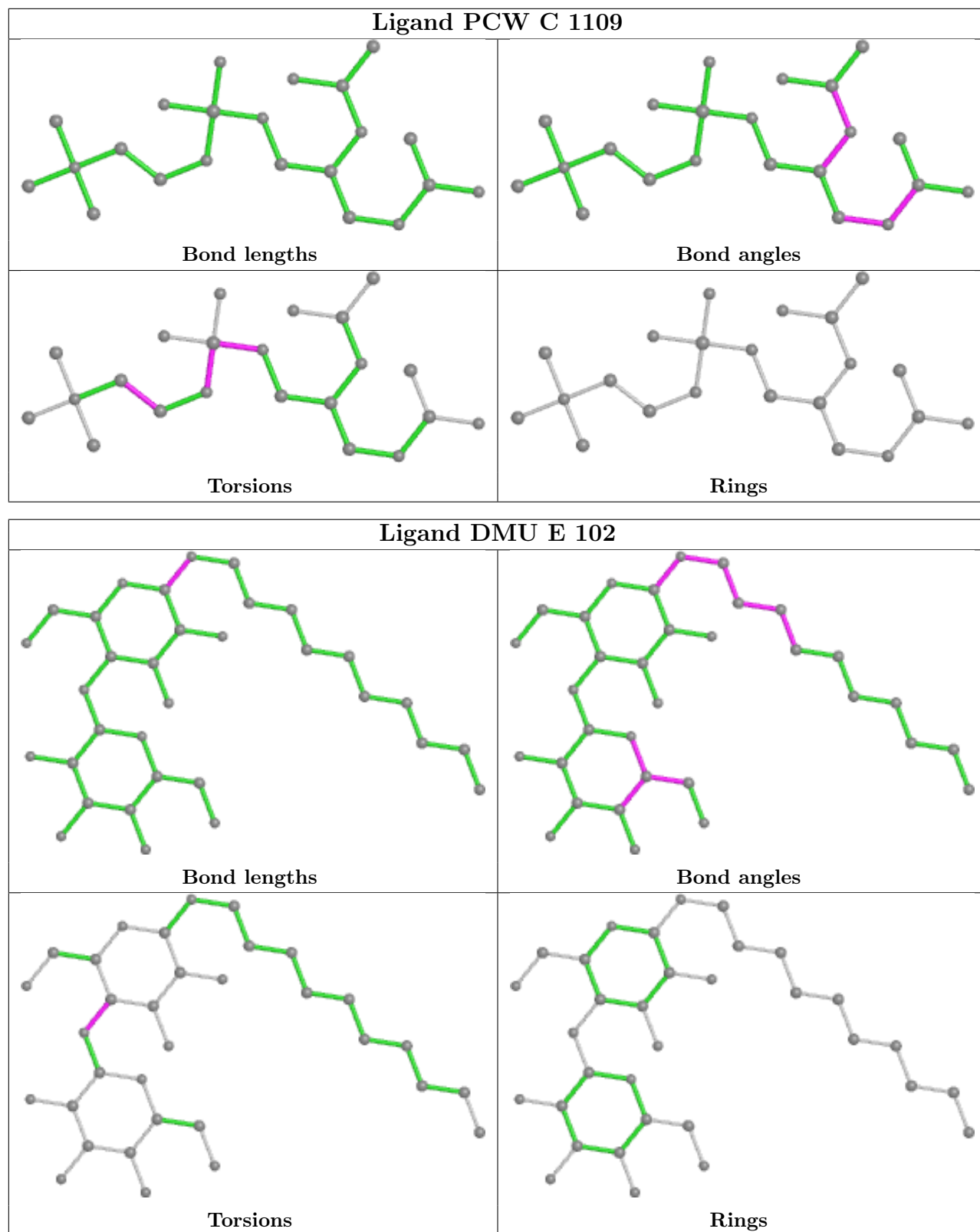
There are no ring outliers.

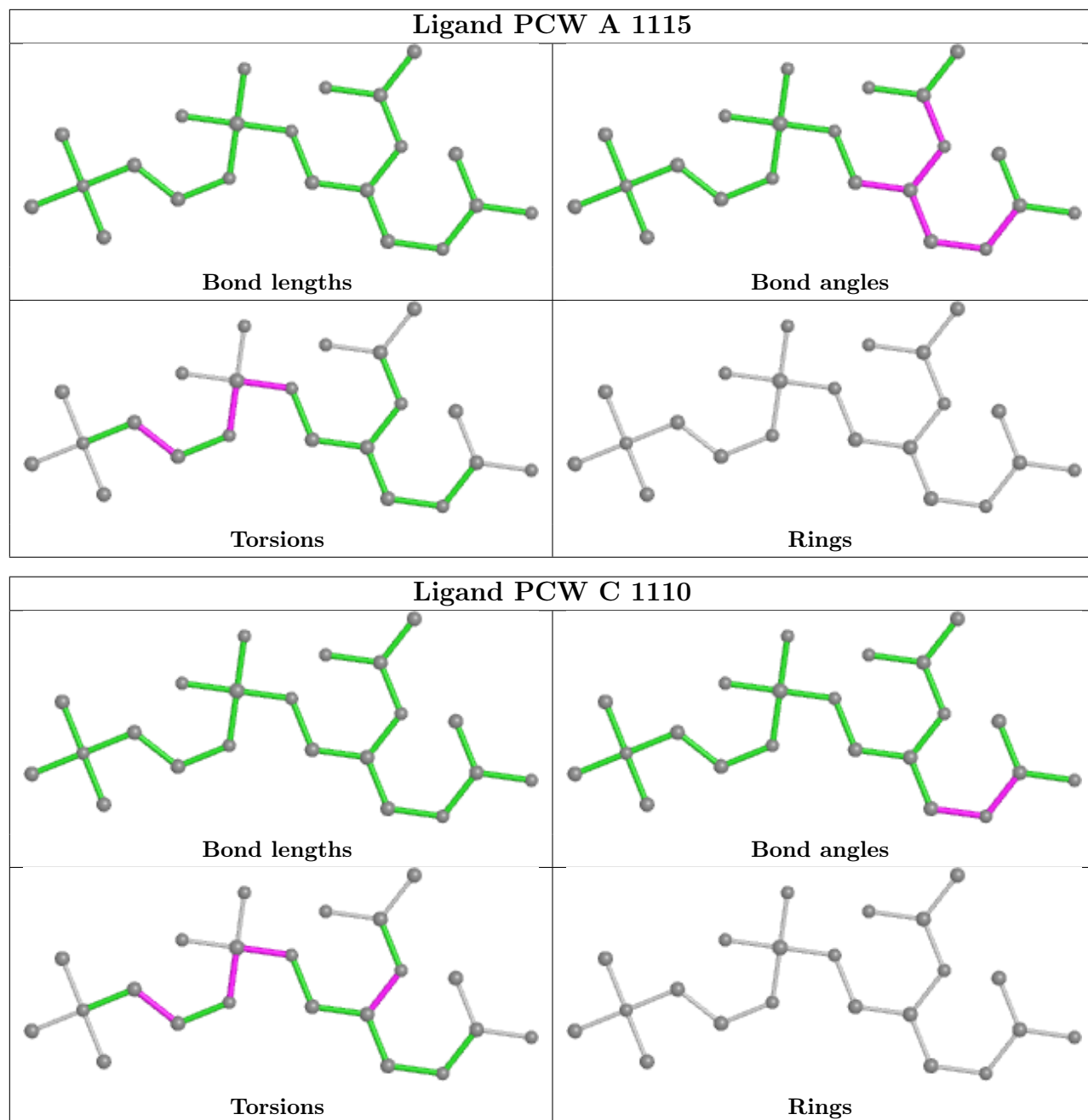
16 monomers are involved in 41 short contacts:

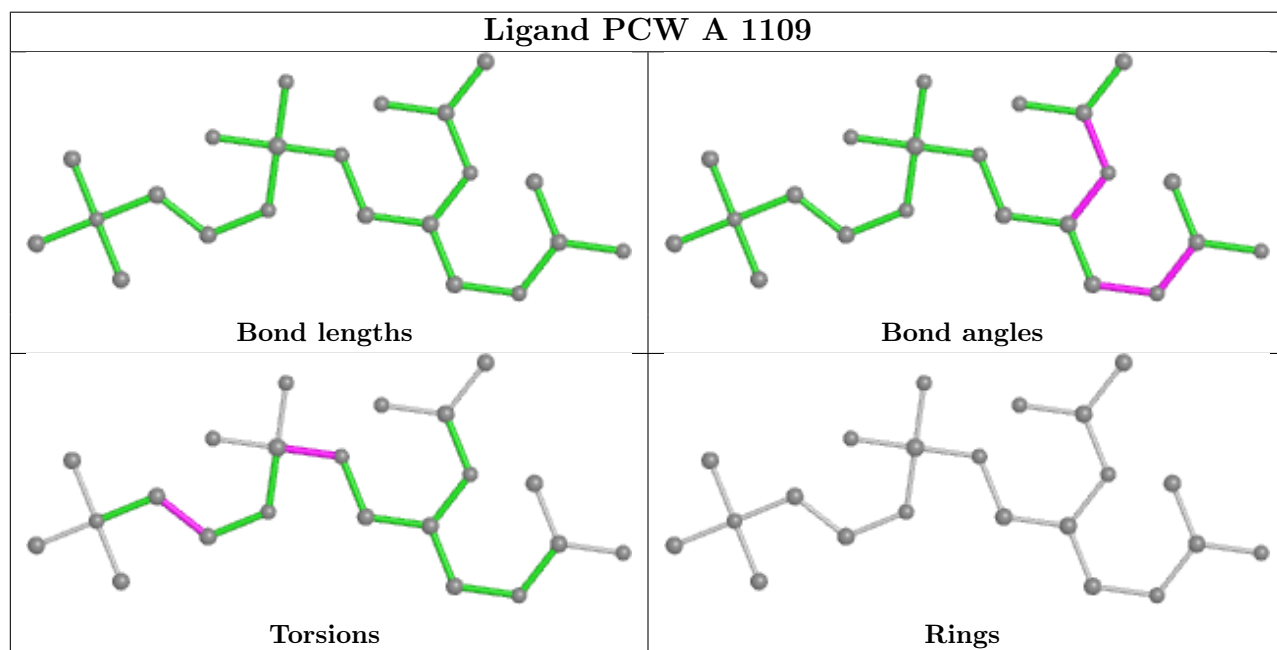
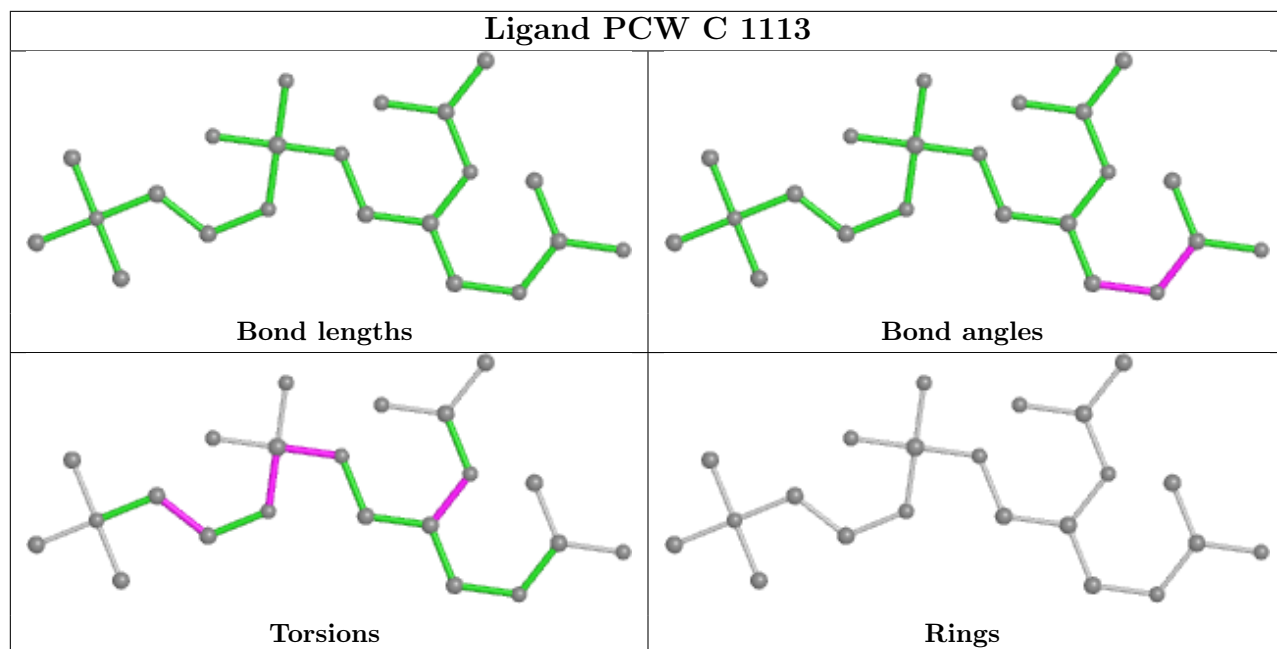
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	101	CLR	1	0
11	C	1109	PCW	2	0
13	E	102	DMU	3	0
11	C	1110	PCW	1	0
11	A	1109	PCW	2	0
10	A	1108	PC1	3	0
10	A	1110	PC1	5	0
11	B	401	PCW	2	0
11	C	1108	PCW	2	0
9	D	401	CLR	2	0
10	A	1111	PC1	9	0
9	C	1106	CLR	4	0
9	B	402	CLR	4	0
9	A	1106	CLR	3	0
11	C	1107	PCW	3	0
9	A	1107	CLR	4	0

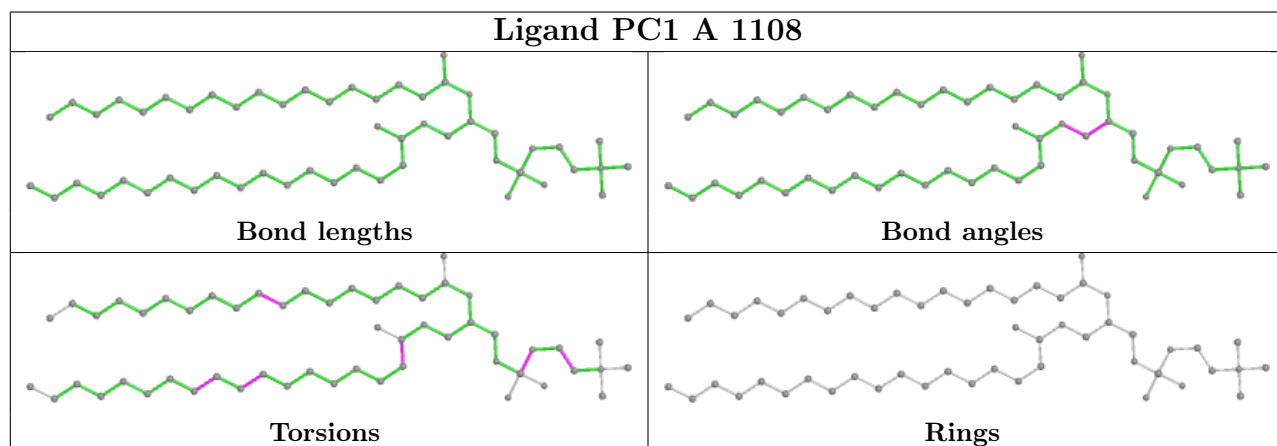
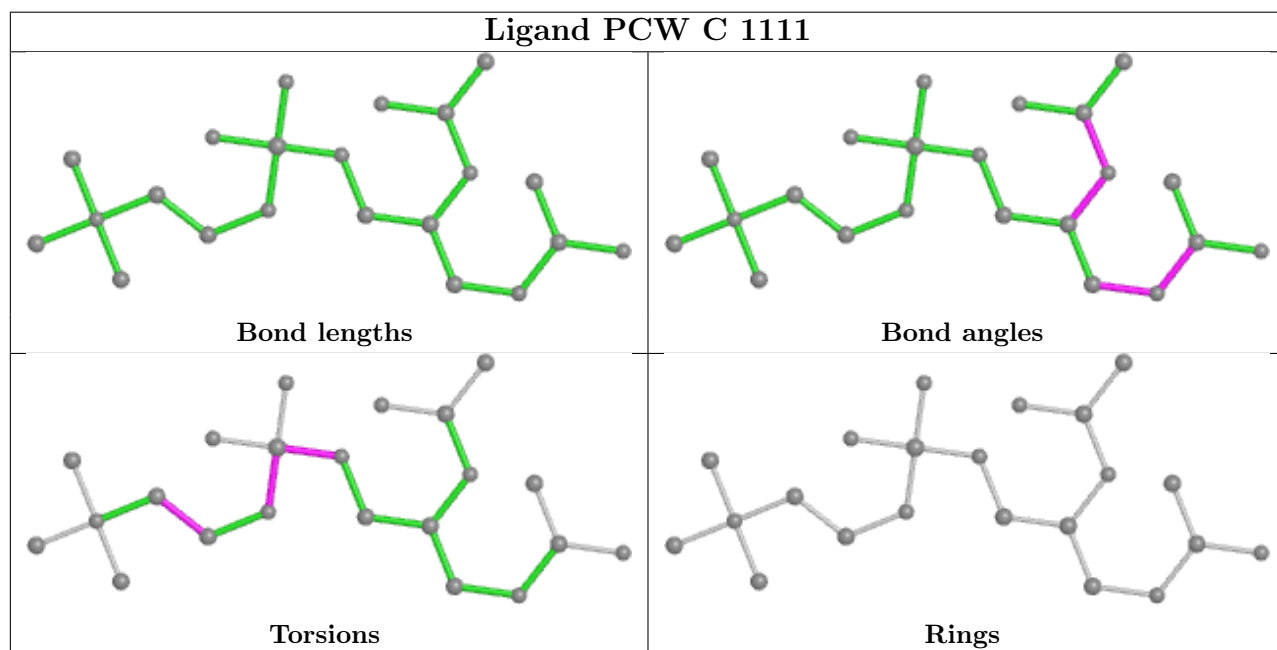
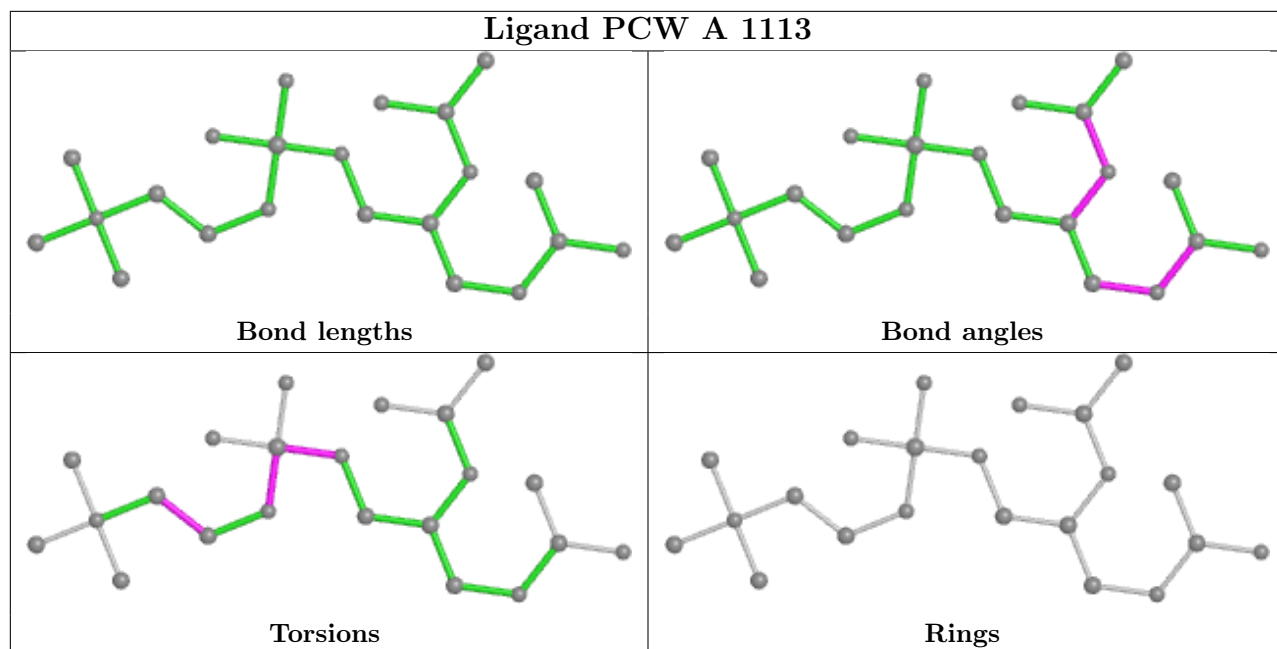
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

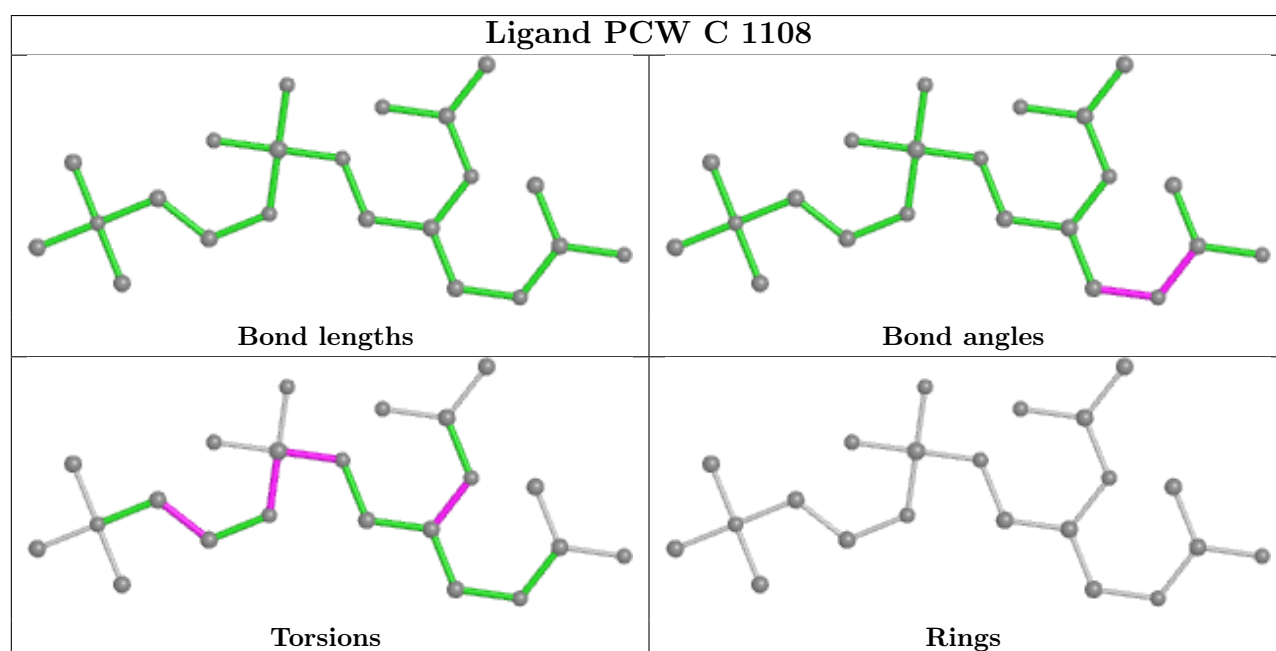
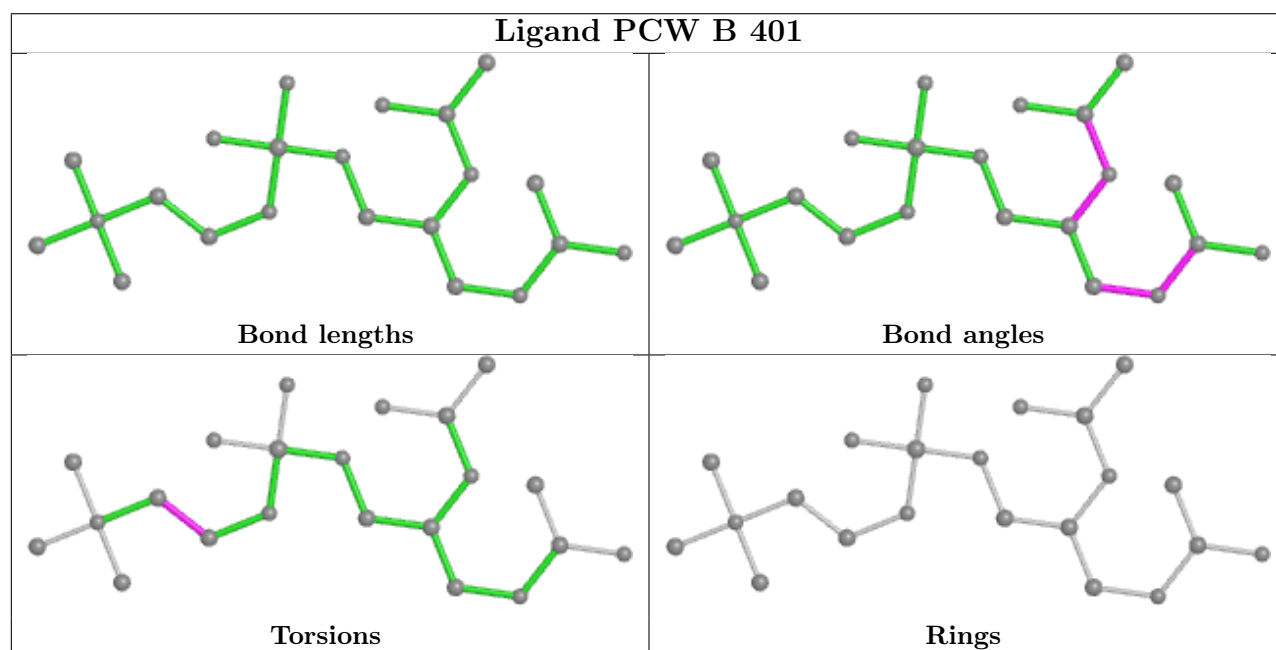
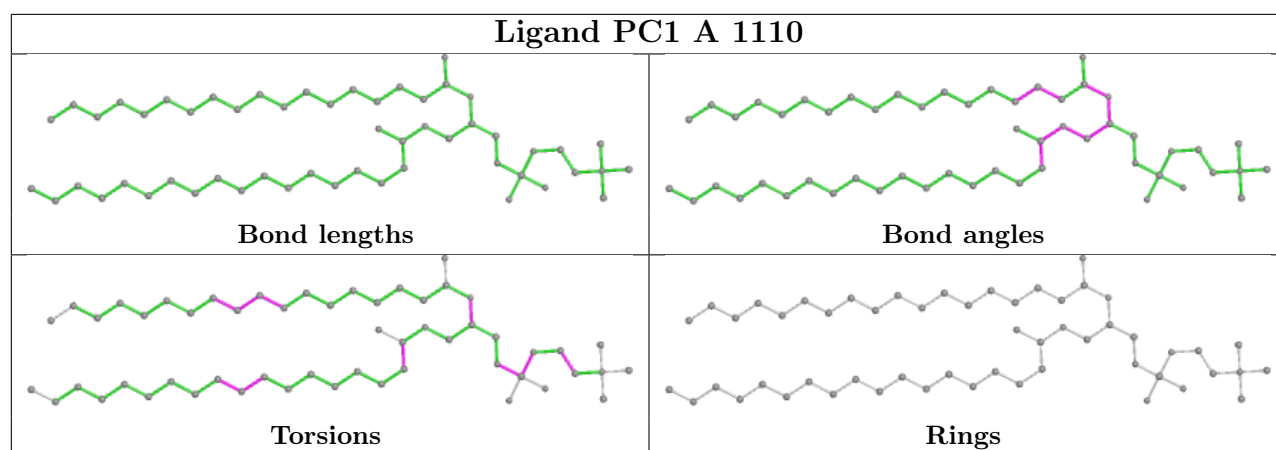


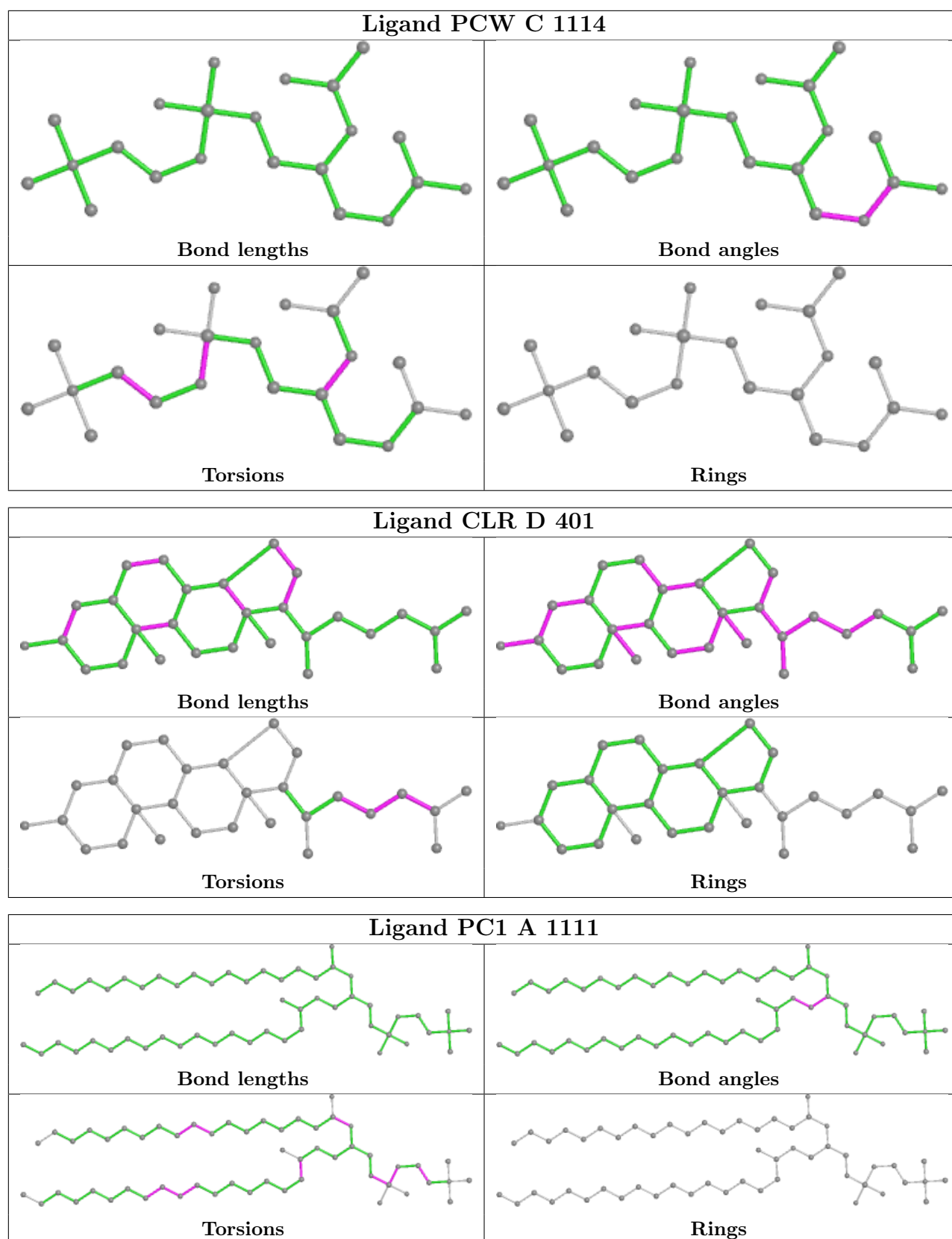


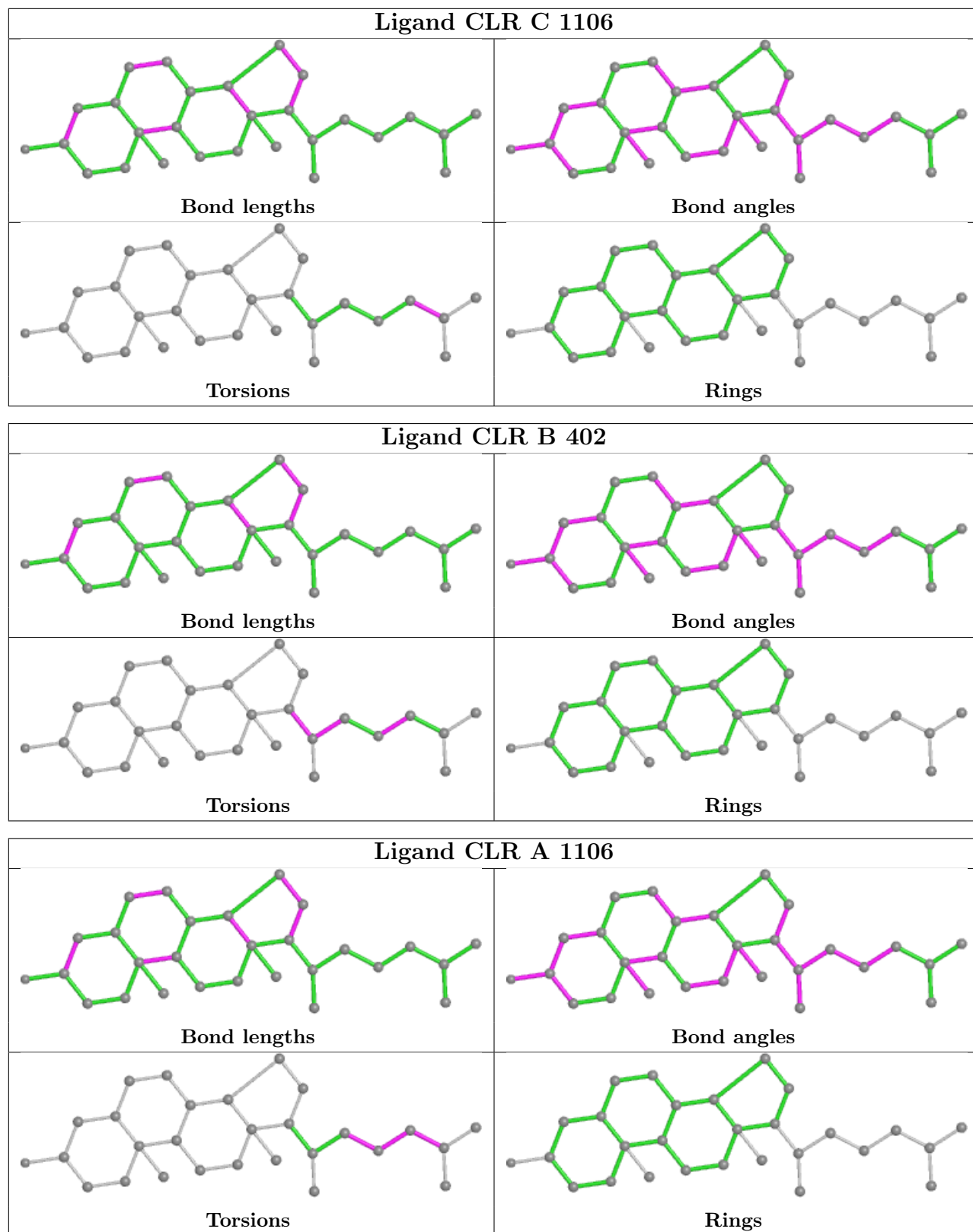


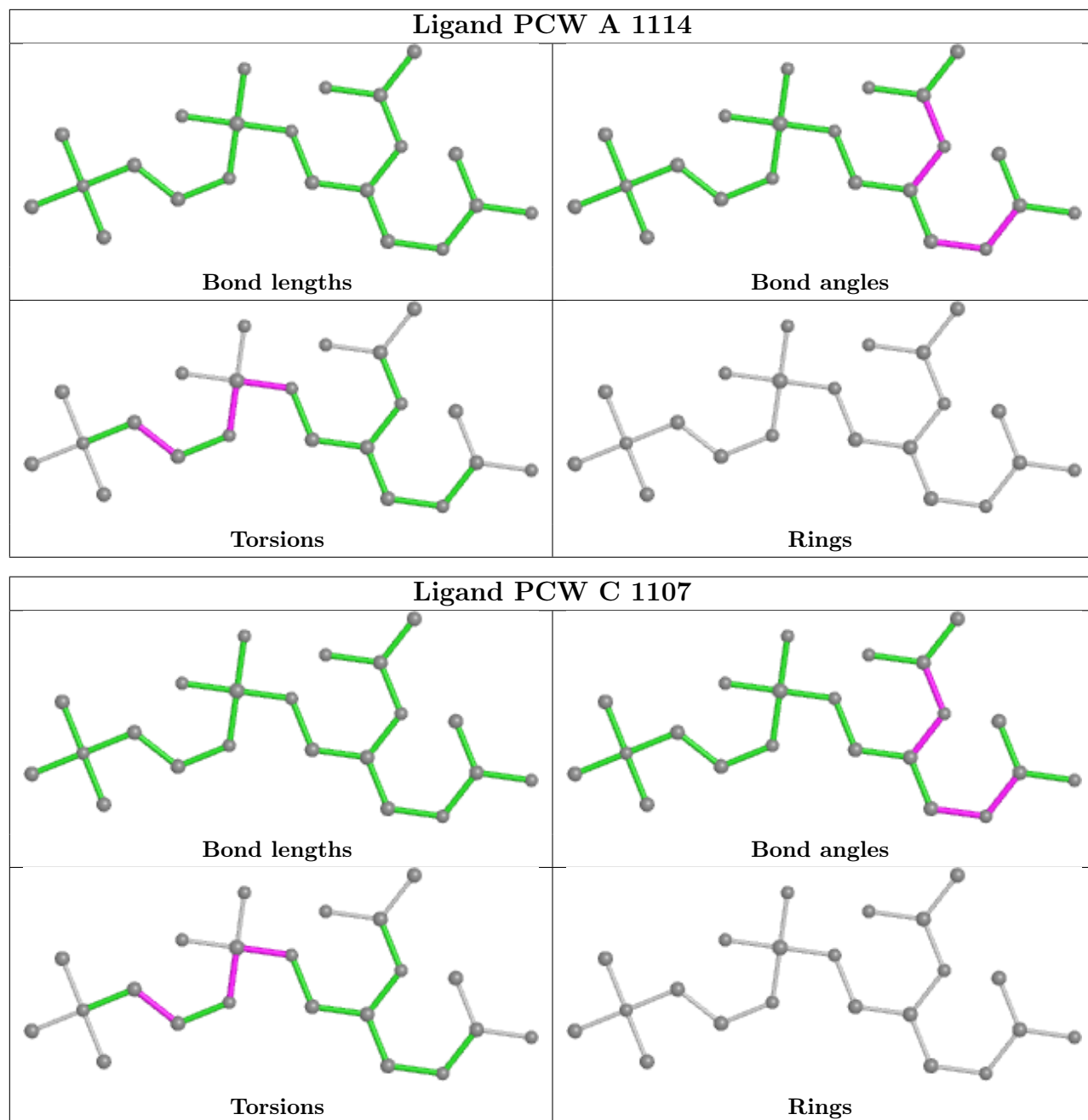


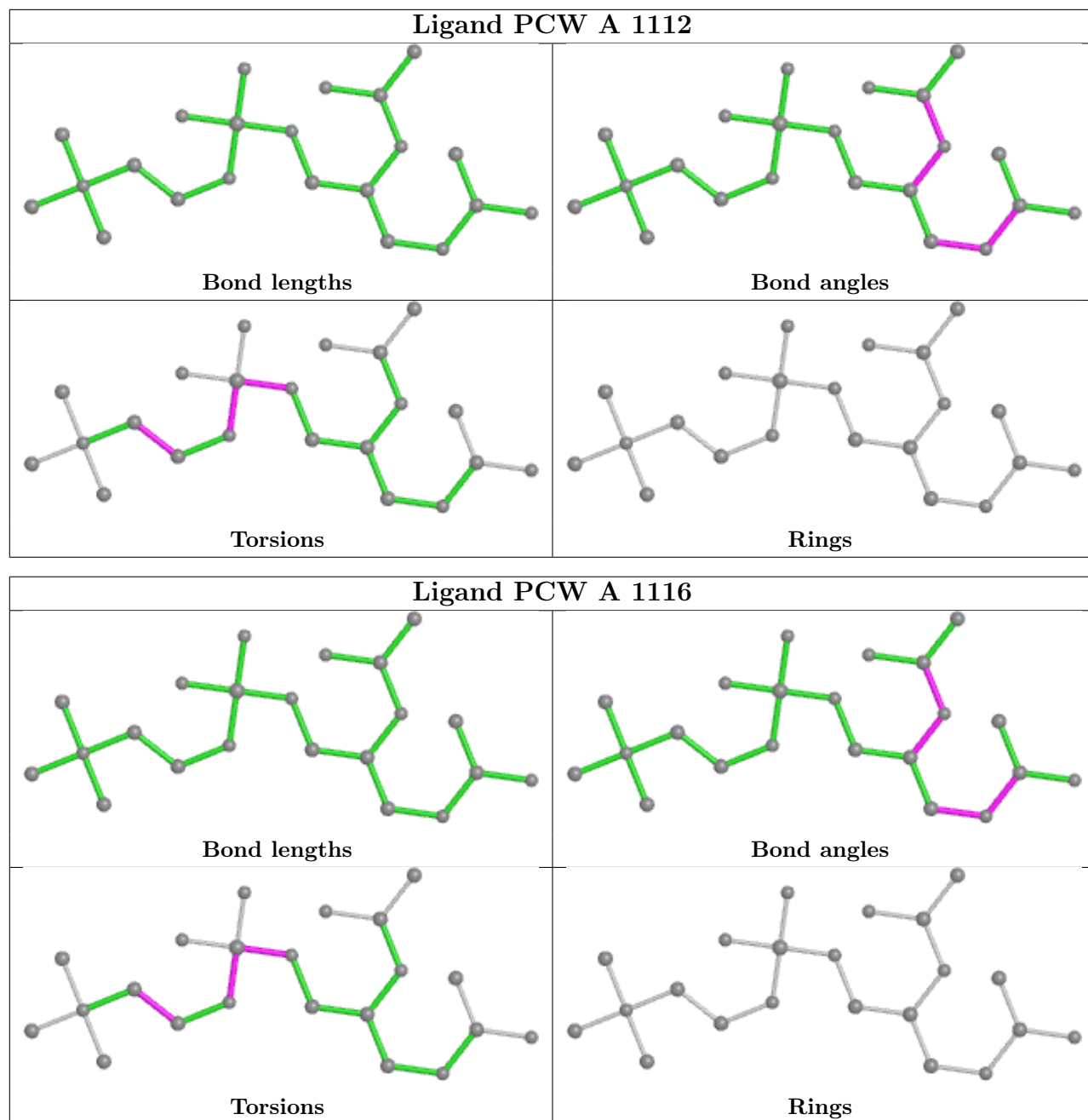


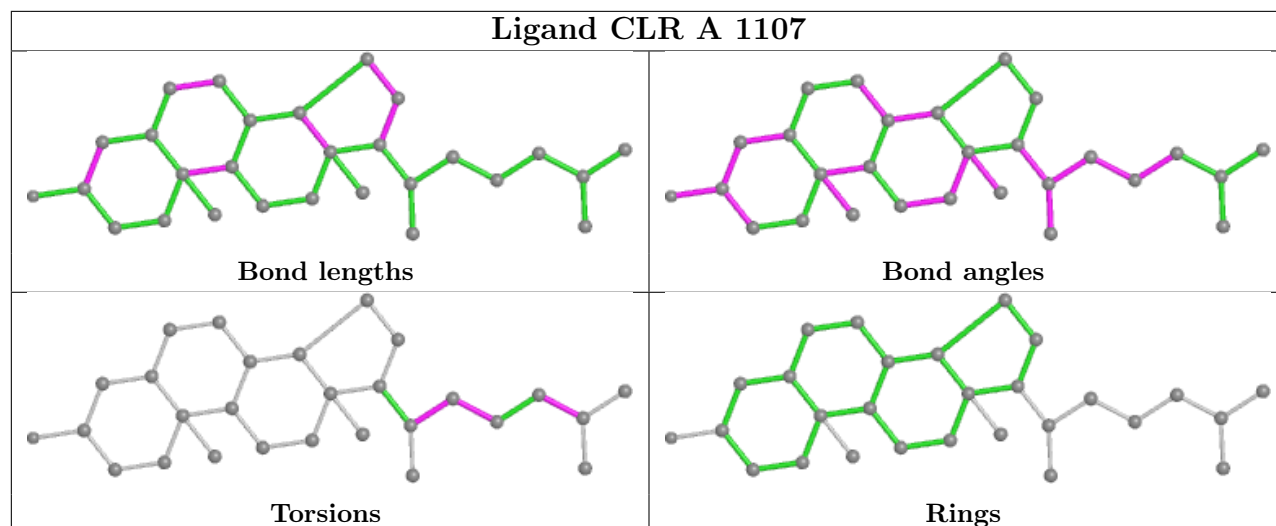












5.7 Other polymers [i](#)

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	995/1021 (97%)	0.09	67 (6%) 17 10	18, 59, 151, 249	0
1	C	995/1021 (97%)	0.11	58 (5%) 23 15	28, 67, 158, 303	0
2	B	291/303 (96%)	0.35	25 (8%) 10 5	52, 95, 162, 212	0
2	D	291/303 (96%)	0.45	27 (9%) 8 4	52, 105, 172, 228	0
3	E	33/65 (50%)	-0.37	0 100 100	36, 50, 100, 101	0
3	G	36/65 (55%)	0.03	4 (11%) 5 3	34, 58, 113, 140	0
All	All	2641/2778 (95%)	0.16	181 (6%) 16 10	18, 73, 158, 303	0

The worst 5 of 181 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	115	GLU	11.4
1	C	23	ARG	9.5
1	C	396	THR	9.4
1	C	265	THR	9.1
2	B	13	LYS	8.4

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

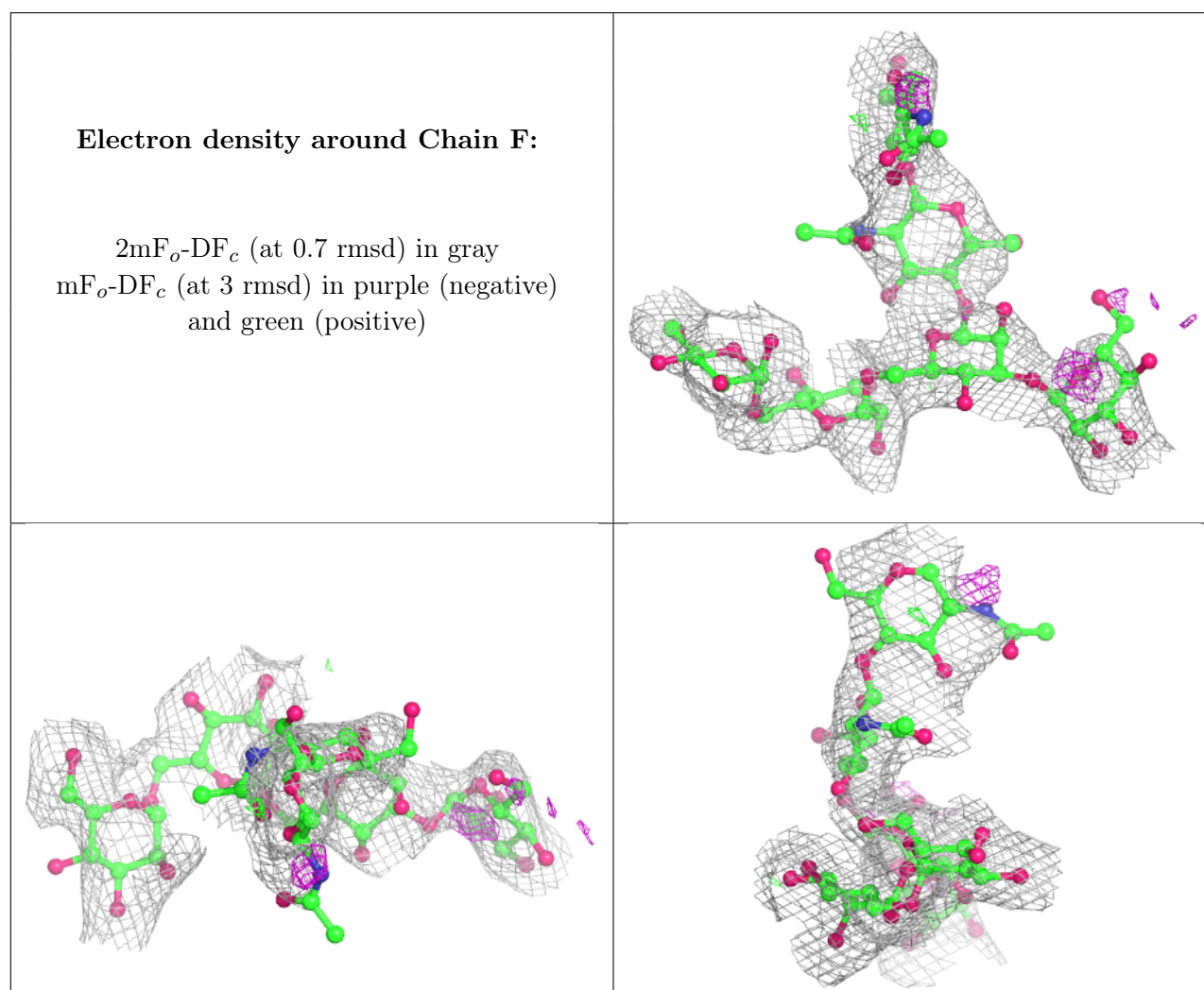
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

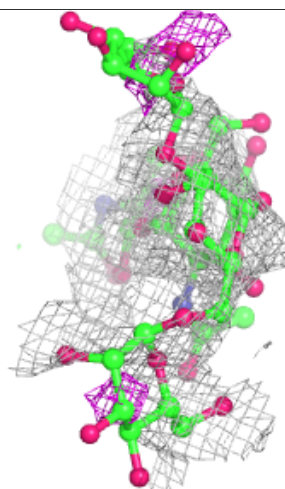
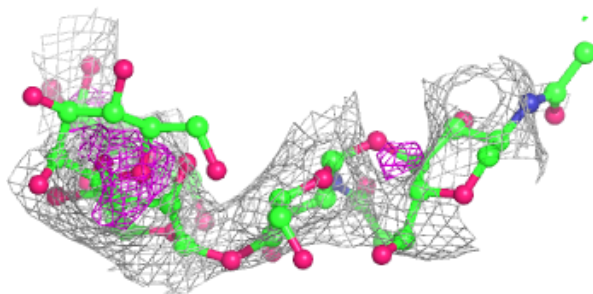
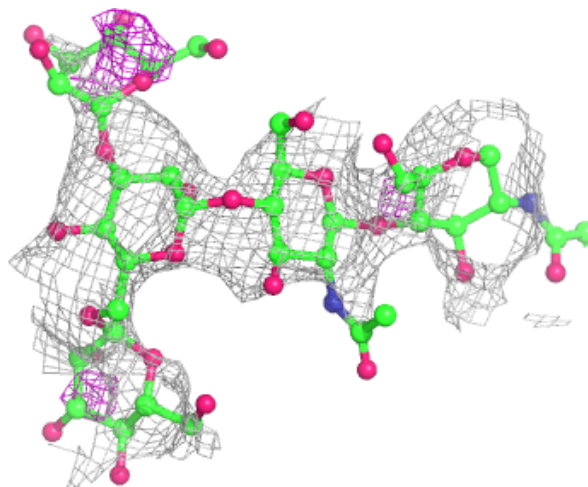
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	H	5	11/12	0.44	0.65	149,152,155,155	0
5	BMA	H	3	11/12	0.60	0.41	148,150,153,153	0
4	MAN	F	4	11/12	0.61	0.32	123,132,136,136	0
5	NAG	H	1	14/15	0.61	0.34	122,134,143,151	0
5	MAN	H	4	11/12	0.64	0.88	129,142,147,147	0
4	MAN	F	6	11/12	0.69	0.63	119,128,130,131	0
4	BMA	F	3	11/12	0.78	0.52	127,131,138,140	0
4	NAG	F	1	14/15	0.79	0.41	91,109,118,123	0
4	MAN	F	5	11/12	0.80	0.31	98,113,126,130	0
5	NAG	H	2	14/15	0.81	0.56	138,152,154,155	0
4	NAG	F	2	14/15	0.82	0.57	125,132,138,140	0
6	NAG	I	2	14/15	0.83	0.42	119,132,138,141	0
6	NAG	I	1	14/15	0.87	0.35	109,128,131,132	0

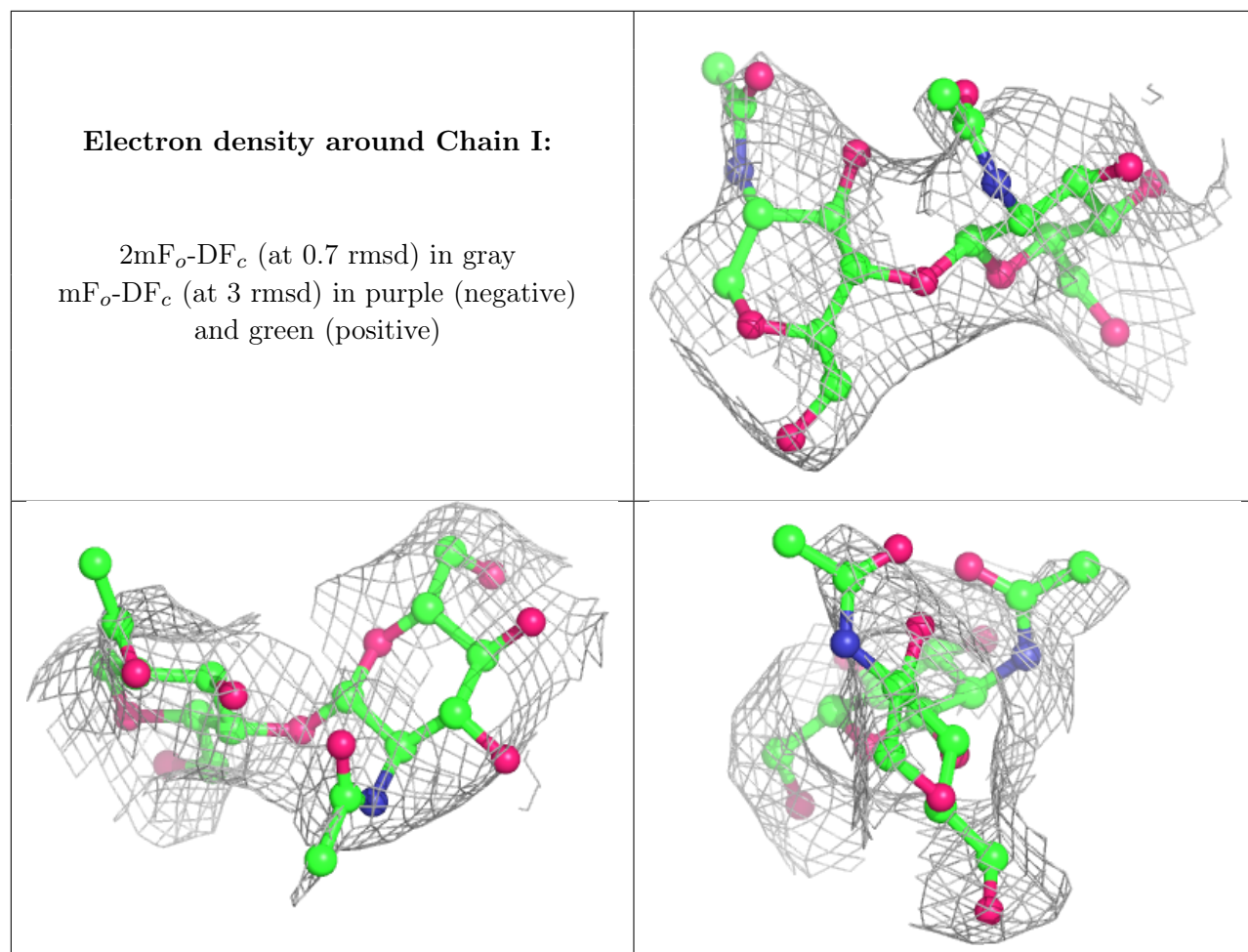
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain 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(Å ²)	Q<0.9
11	PCW	A	1116	22/54	0.59	0.46	119,151,157,160	0
11	PCW	B	401	22/54	0.68	0.33	117,127,163,165	0
11	PCW	C	1107	22/54	0.70	0.36	84,111,146,149	0
11	PCW	C	1113	22/54	0.71	0.54	98,136,160,164	0
8	NA	C	1102	1/1	0.72	0.14	76,76,76,76	0
11	PCW	A	1109	22/54	0.74	0.32	115,135,151,154	0
11	PCW	C	1110	22/54	0.75	0.58	111,143,151,152	0
11	PCW	A	1115	22/54	0.75	0.48	112,135,148,153	0
12	NAG	D	402	14/15	0.75	0.62	125,134,147,152	0
11	PCW	C	1114	22/54	0.76	0.38	95,130,146,151	0
11	PCW	C	1112	22/54	0.76	0.34	84,120,138,145	0

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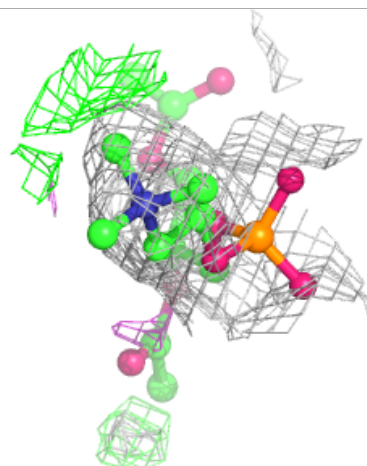
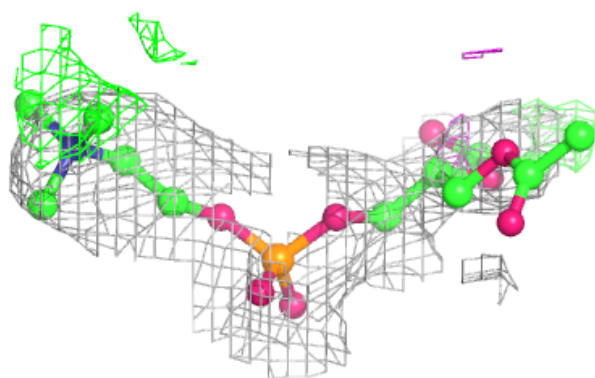
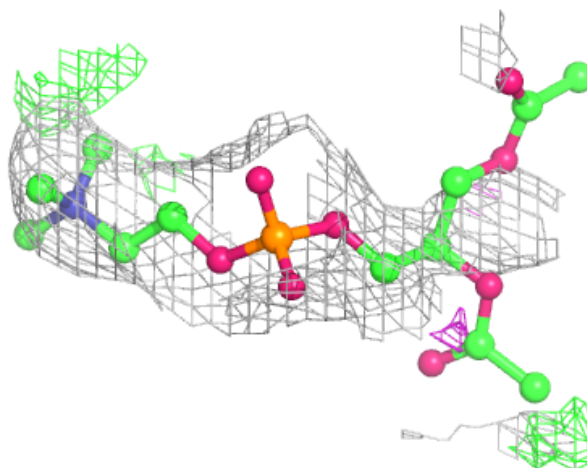
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	PCW	C	1108	22/54	0.77	0.33	106,122,130,138	0
11	PCW	C	1111	22/54	0.77	0.30	74,127,149,150	0
10	PC1	A	1108	54/54	0.78	0.35	72,96,122,127	0
11	PCW	C	1109	22/54	0.81	0.41	99,124,153,154	0
11	PCW	A	1114	22/54	0.82	0.26	109,129,141,146	0
11	PCW	A	1113	22/54	0.83	0.51	114,129,150,152	0
10	PC1	A	1110	54/54	0.84	0.32	58,71,109,115	0
9	CLR	B	402	28/28	0.84	0.26	87,99,107,112	0
9	CLR	D	401	28/28	0.84	0.31	71,87,93,97	0
8	NA	A	1102	1/1	0.84	0.16	61,61,61,61	0
8	NA	C	1105	1/1	0.86	0.15	62,62,62,62	0
9	CLR	A	1106	28/28	0.87	0.22	65,77,87,95	0
11	PCW	A	1112	22/54	0.87	0.32	72,117,123,126	0
8	NA	C	1103	1/1	0.88	0.22	88,88,88,88	0
8	NA	A	1103	1/1	0.89	0.28	73,73,73,73	0
10	PC1	A	1111	54/54	0.89	0.32	42,79,107,113	0
9	CLR	C	1106	28/28	0.91	0.24	25,33,84,91	0
8	NA	C	1104	1/1	0.92	0.23	67,67,67,67	0
13	DMU	E	102	33/33	0.93	0.21	28,55,78,85	0
9	CLR	A	1107	28/28	0.95	0.20	25,46,57,64	0
9	CLR	E	101	28/28	0.95	0.19	22,40,52,62	0
7	MN	C	1101	1/1	0.96	0.11	69,69,69,69	0
8	NA	A	1104	1/1	0.96	0.25	49,49,49,49	0
8	NA	A	1105	1/1	0.96	0.10	47,47,47,47	0
7	MN	A	1101	1/1	0.98	0.06	58,58,58,58	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.

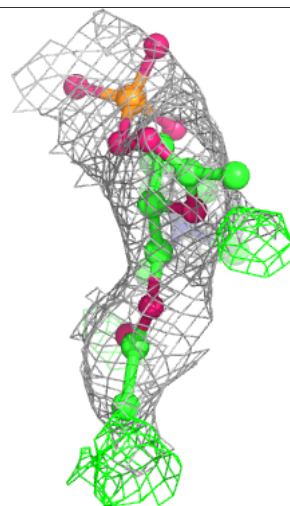
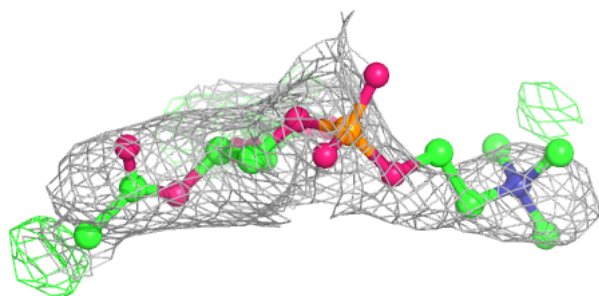
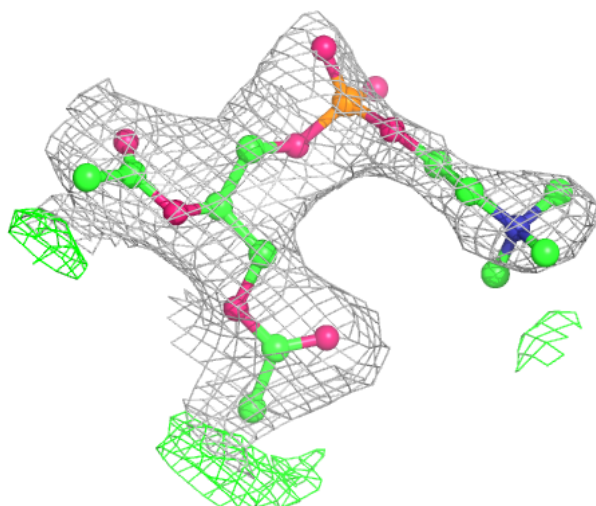
Electron density around PCW A 1116:

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



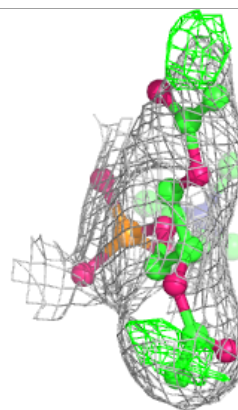
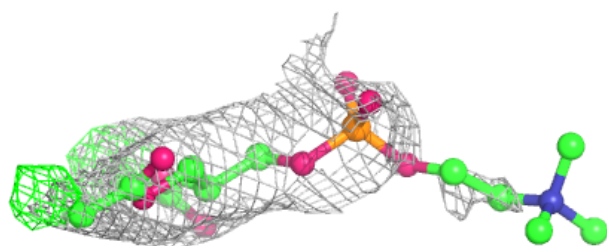
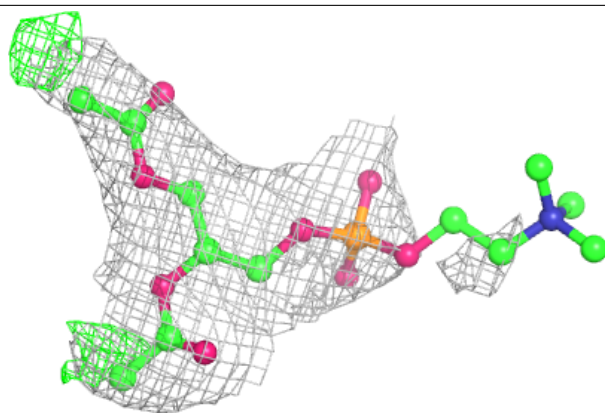
Electron density around PCW B 401:

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

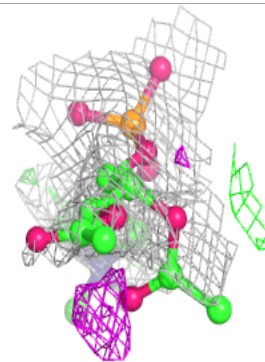
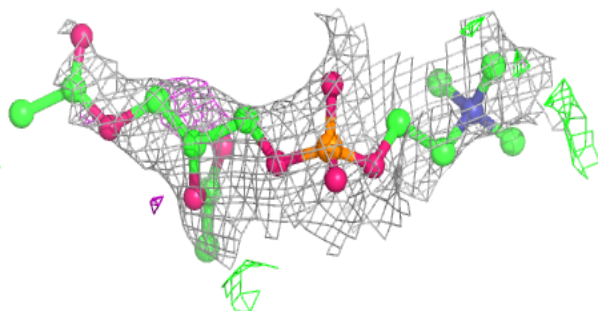
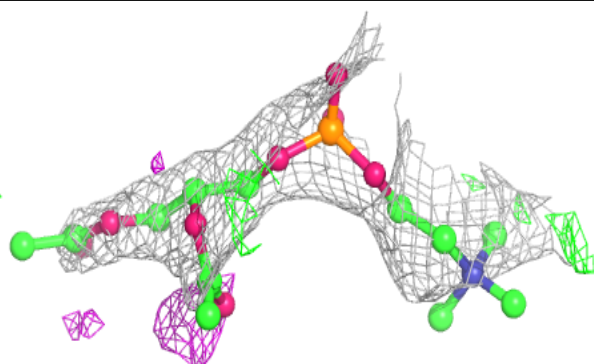


Electron density around PCW C 1107:

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

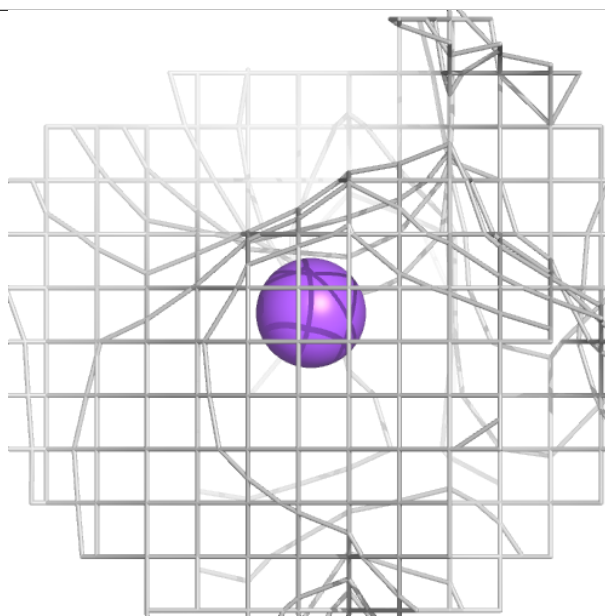
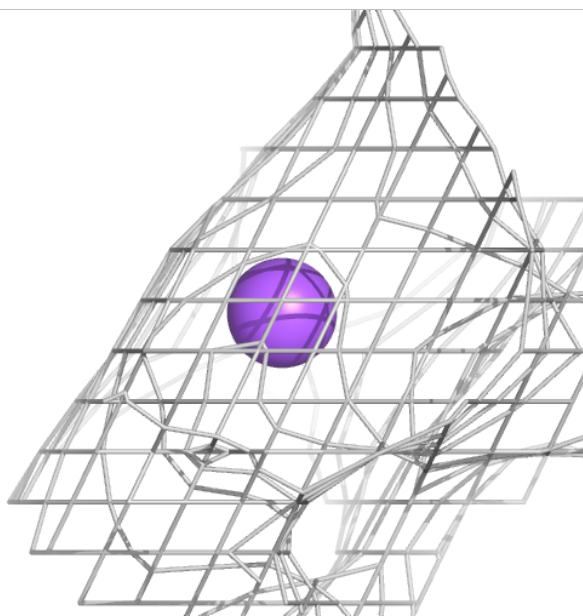
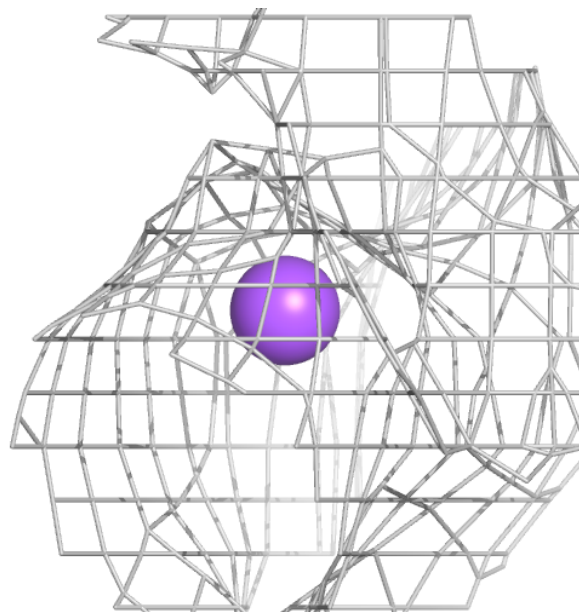
**Electron density around PCW C 1113:**

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



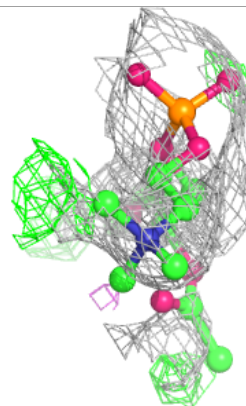
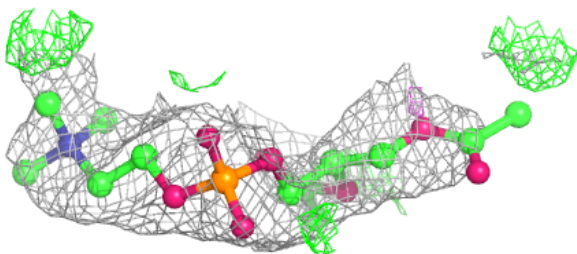
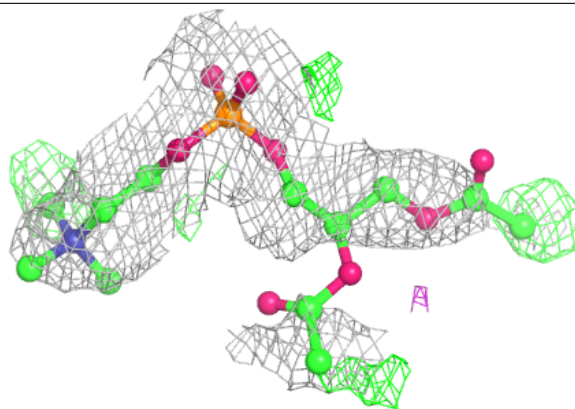
Electron density around NA C 1102:

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

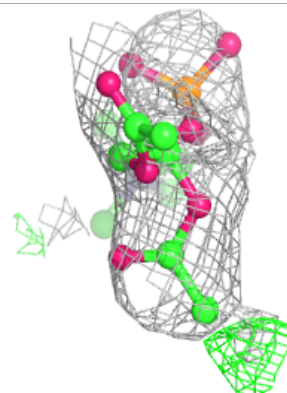
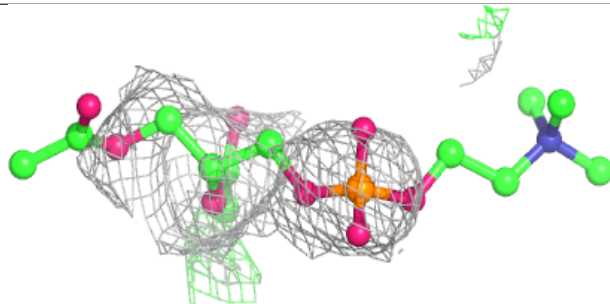
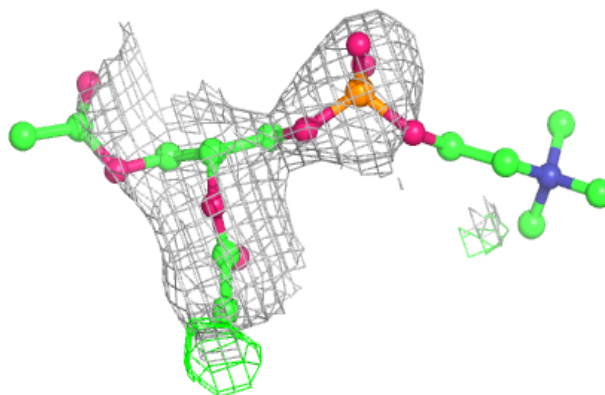


Electron density around PCW A 1109:

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

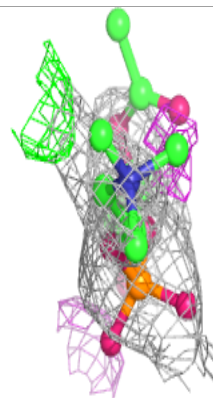
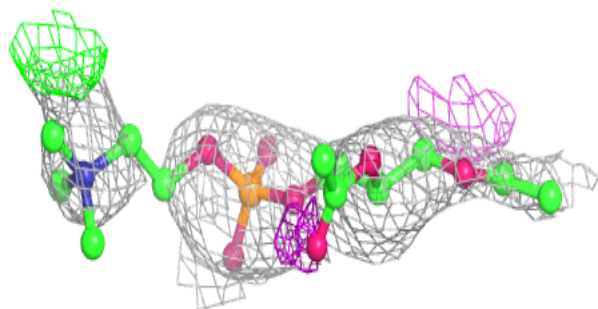
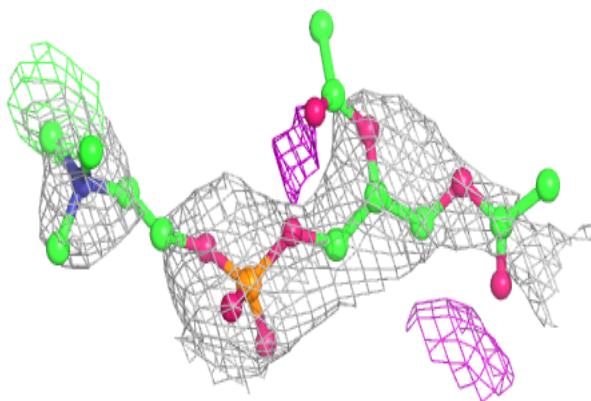
**Electron density around PCW C 1110:**

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

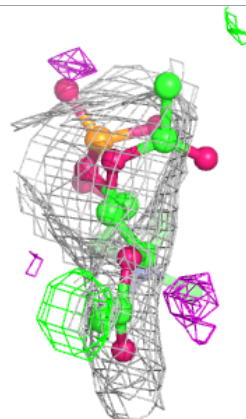
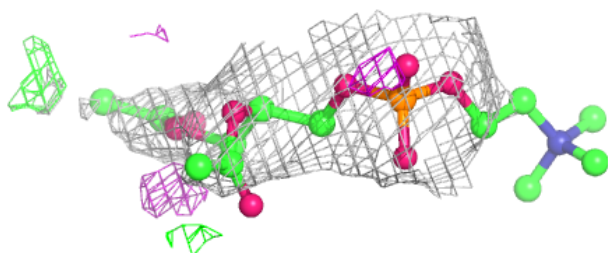
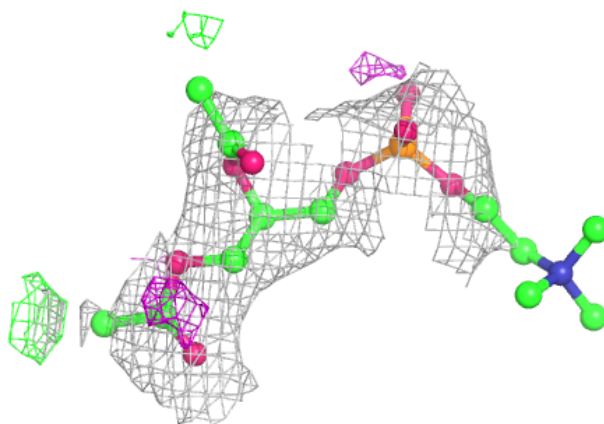


Electron density around PCW A 1115:

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

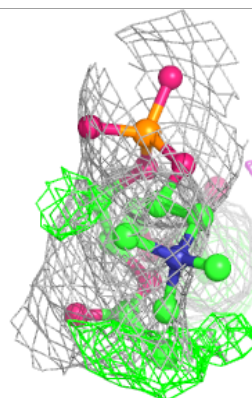
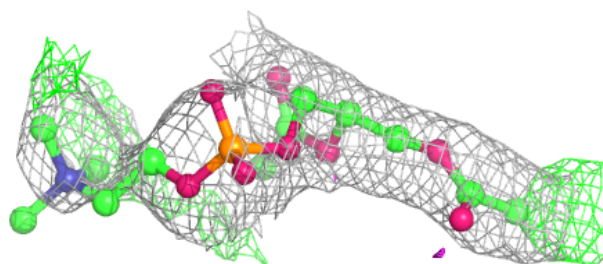
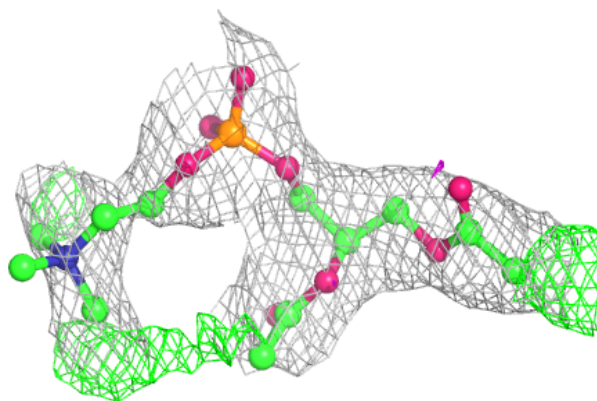
**Electron density around PCW C 1114:**

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

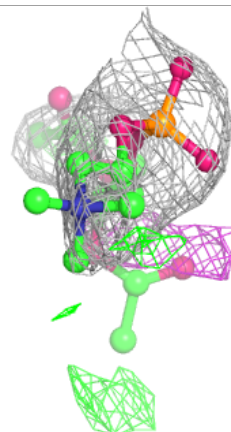
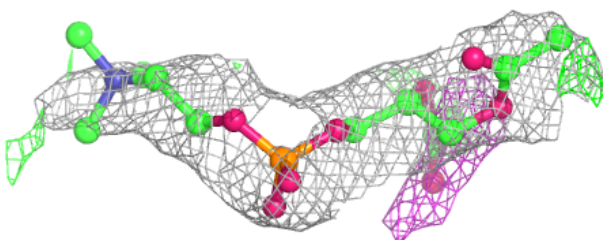
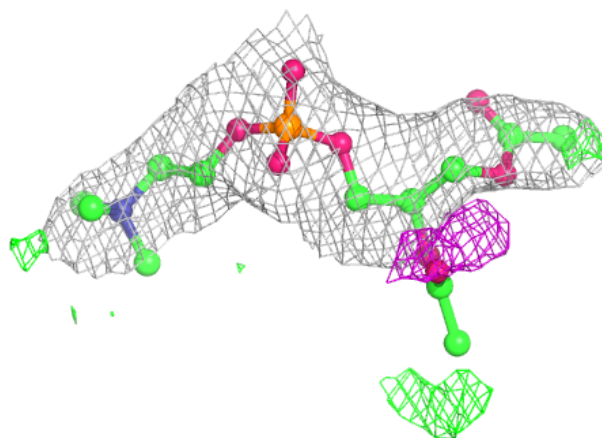


Electron density around PCW C 1112:

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

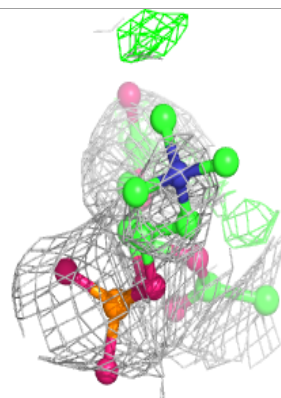
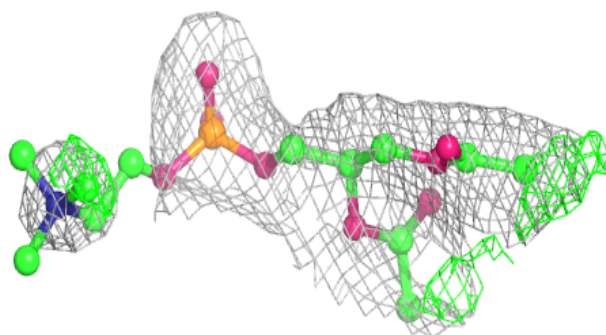
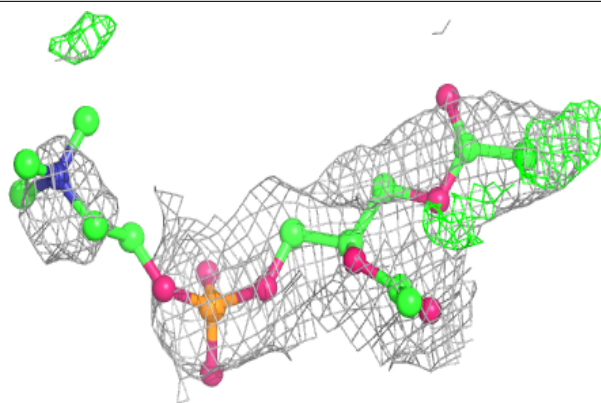
**Electron density around PCW C 1108:**

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

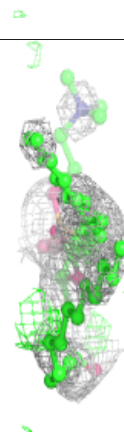
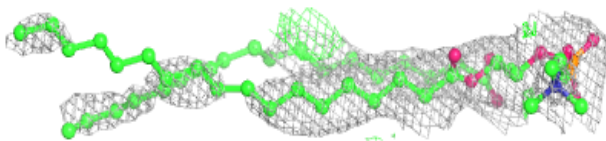
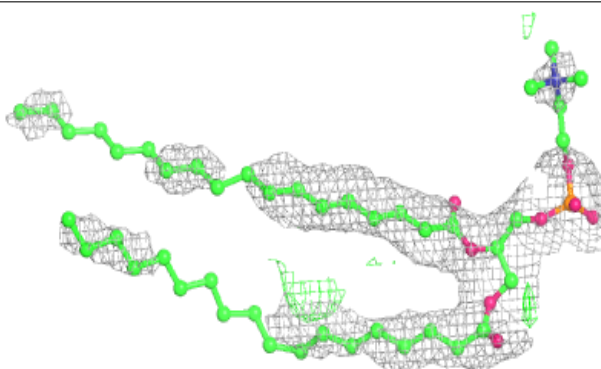


Electron density around PCW C 1111:

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

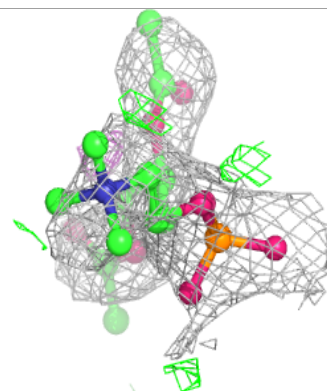
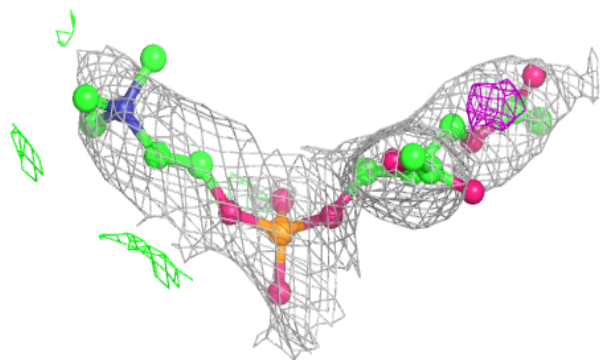
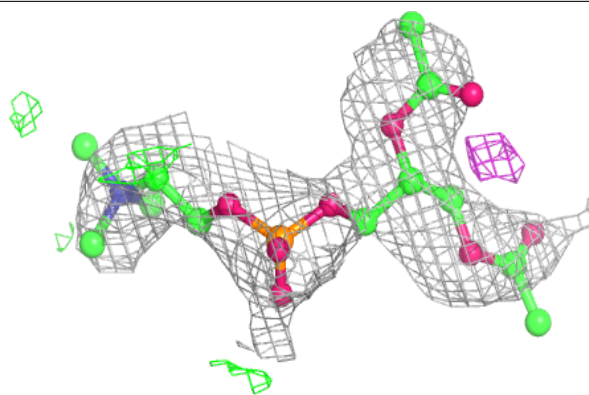
**Electron density around PC1 A 1108:**

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

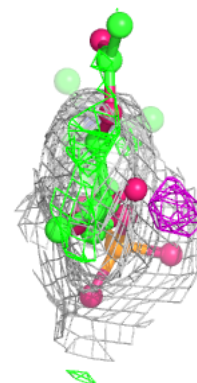
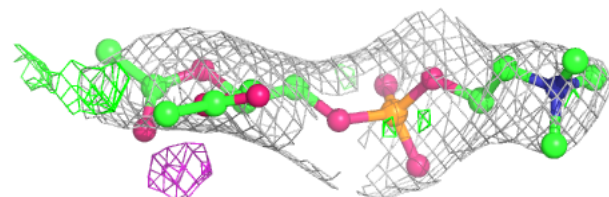
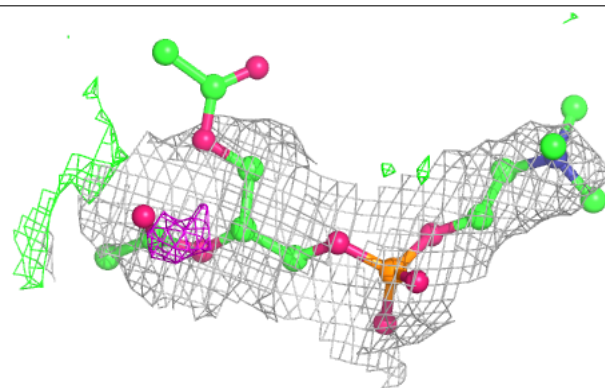


Electron density around PCW C 1109:

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

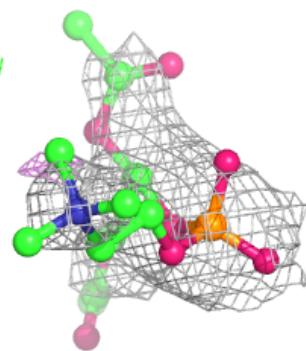
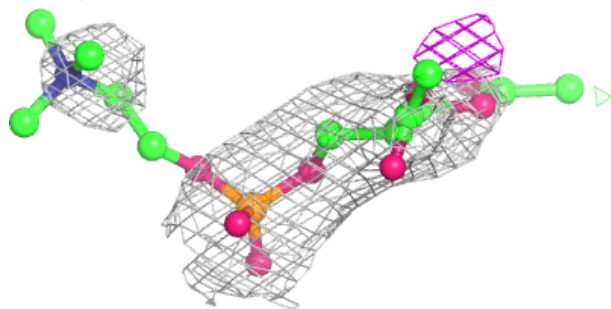
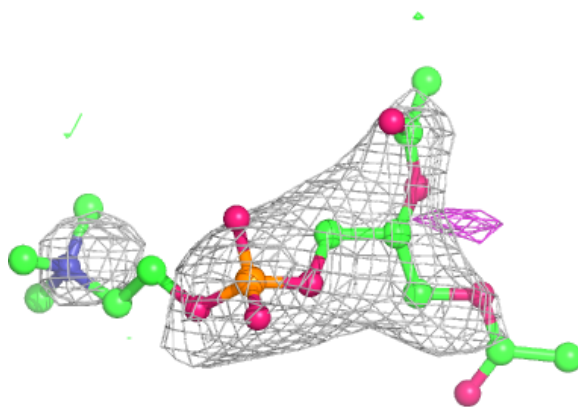
**Electron density around PCW A 1114:**

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



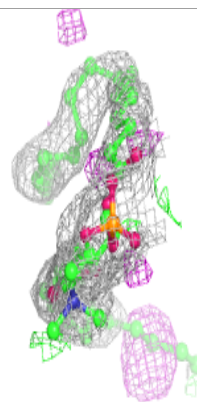
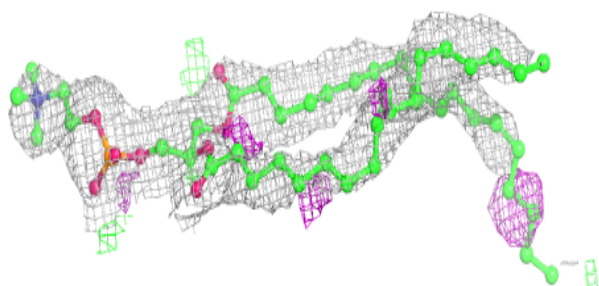
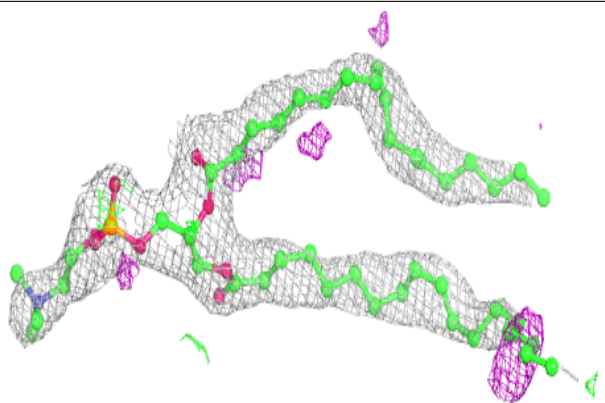
Electron density around PCW A 1113:

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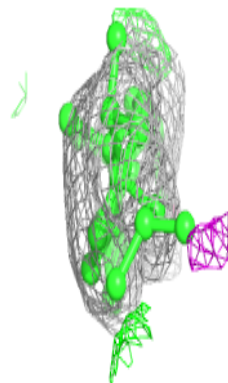
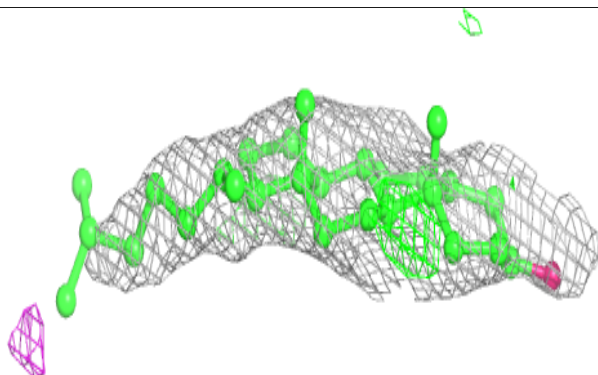
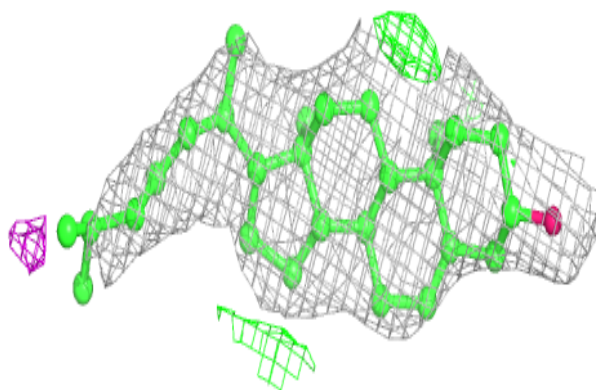


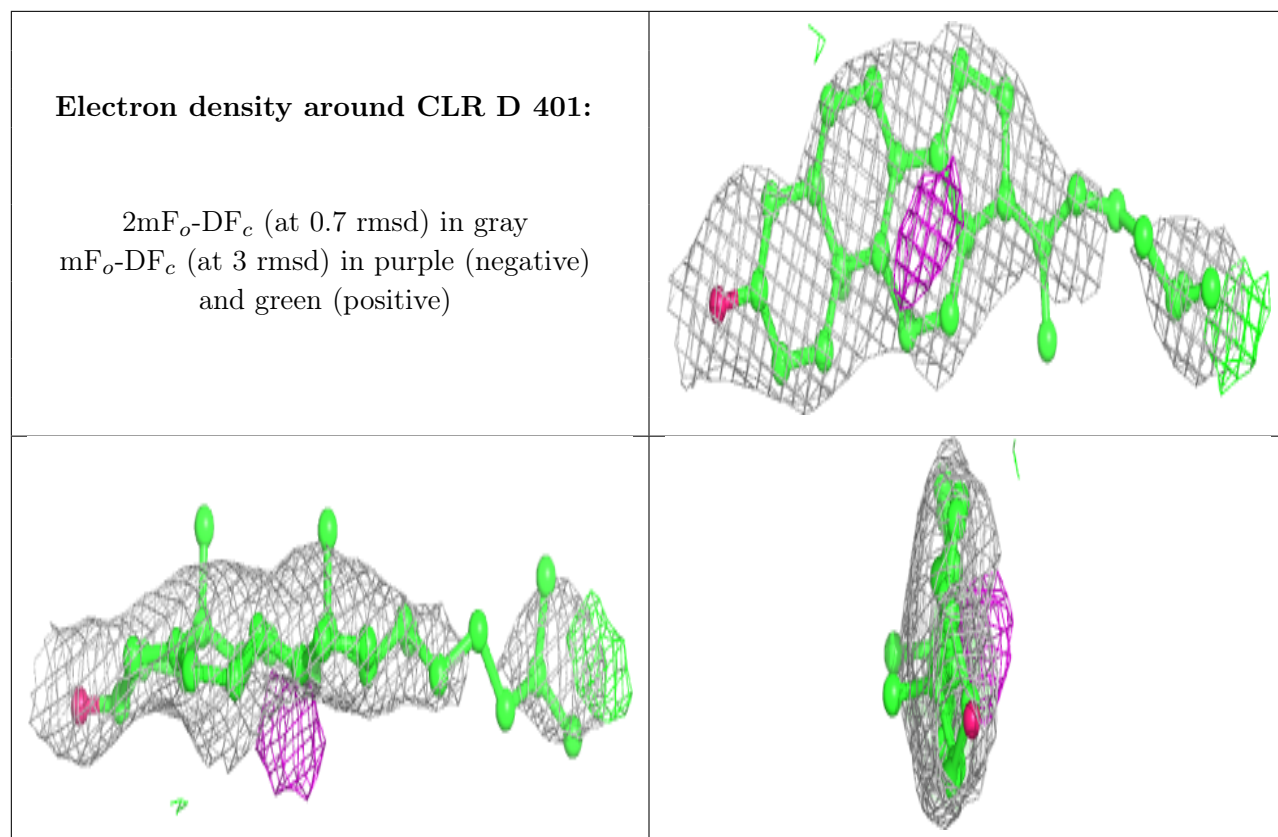
Electron density around PC1 A 1110:

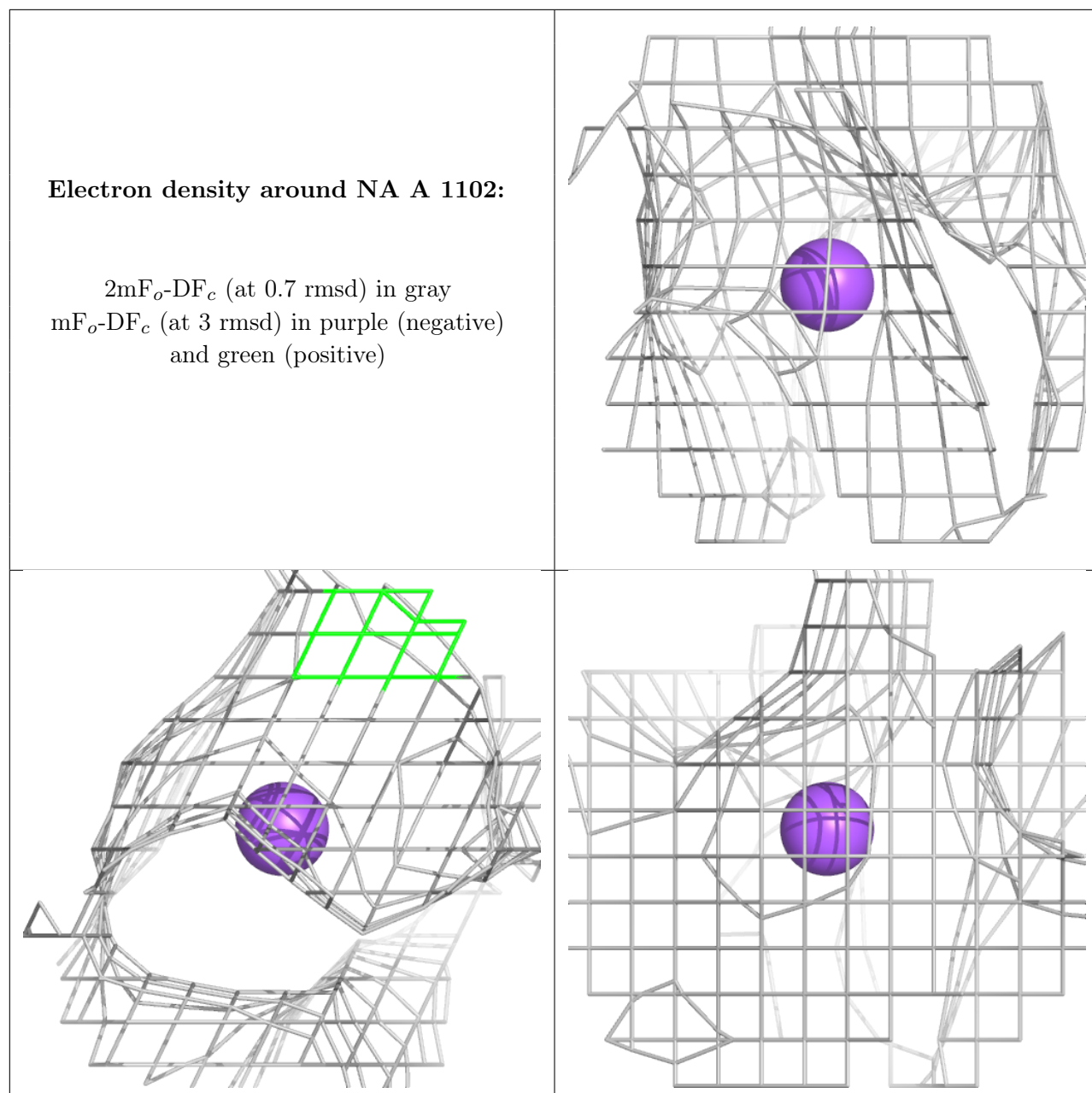
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLR B 402:**

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

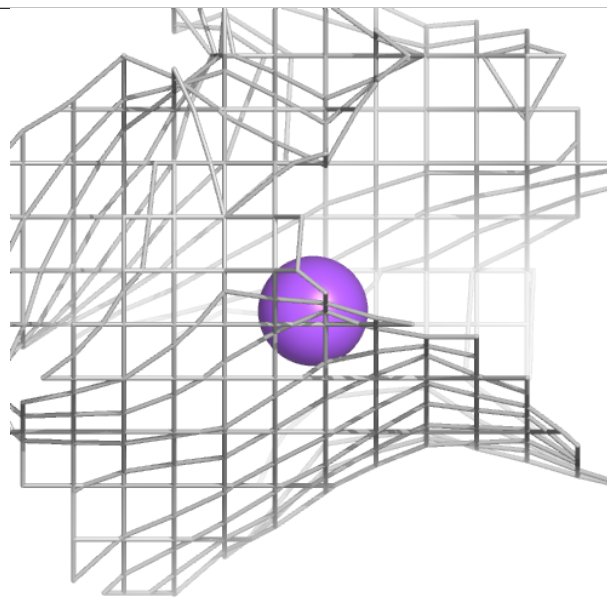
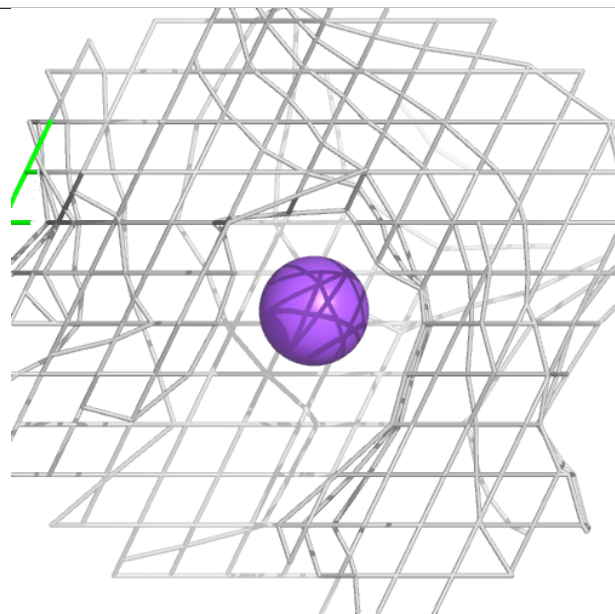
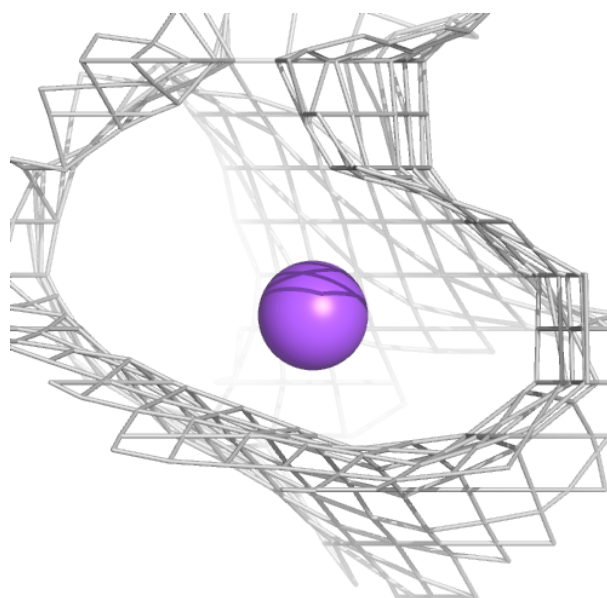






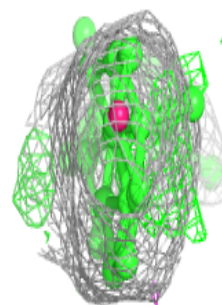
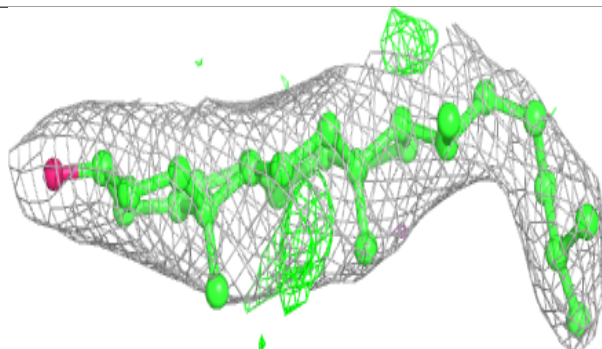
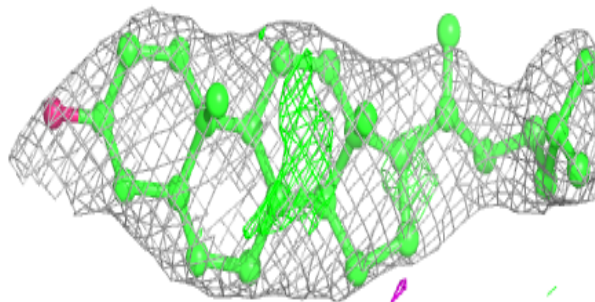
Electron density around NA C 1105:

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and green (positive)

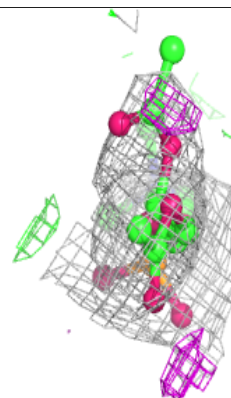
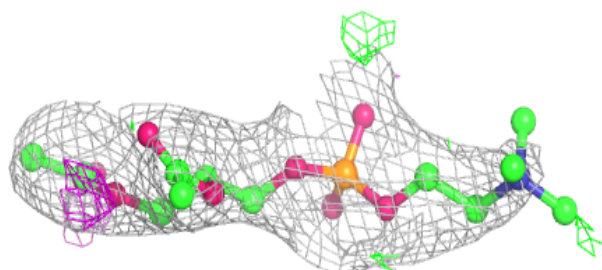
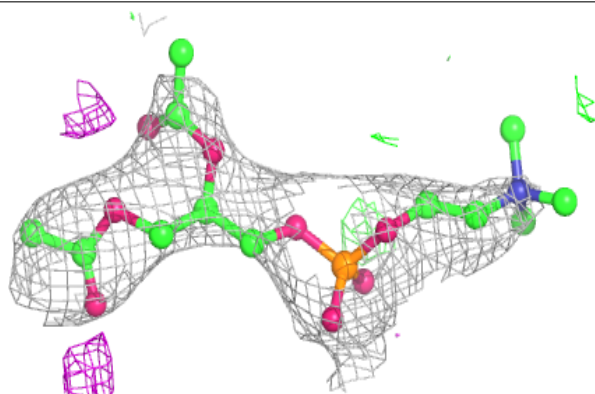


Electron density around CLR A 1106:

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

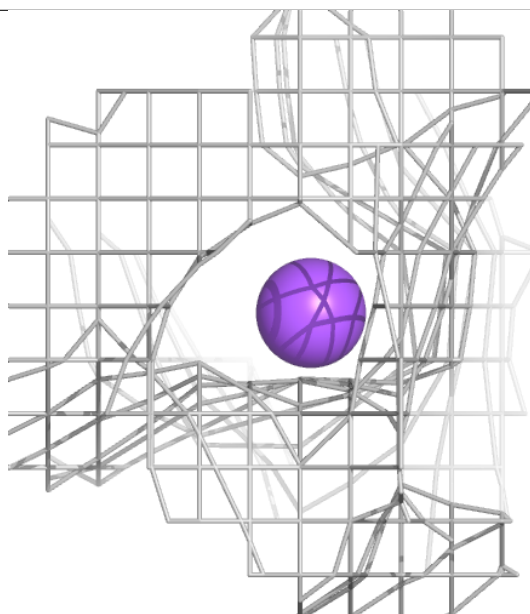
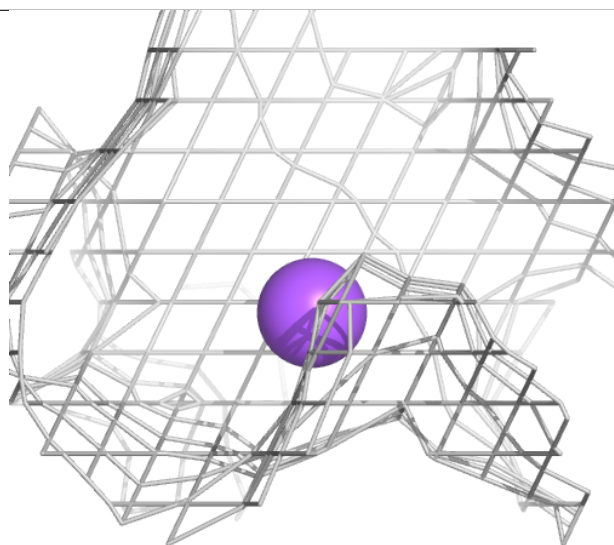
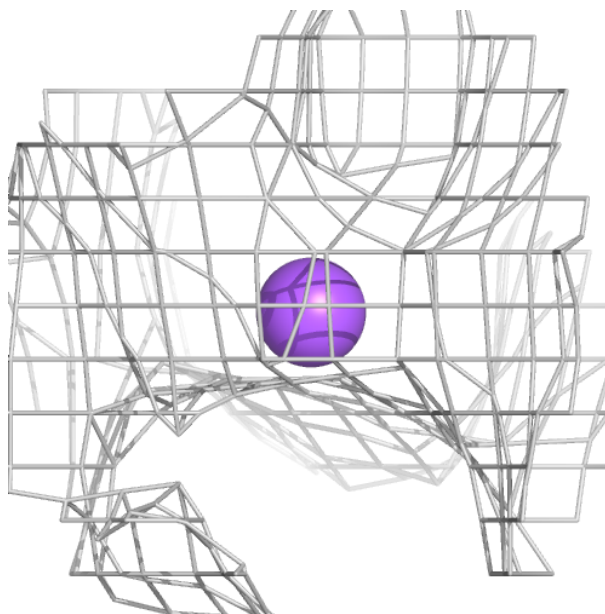
**Electron density around PCW A 1112:**

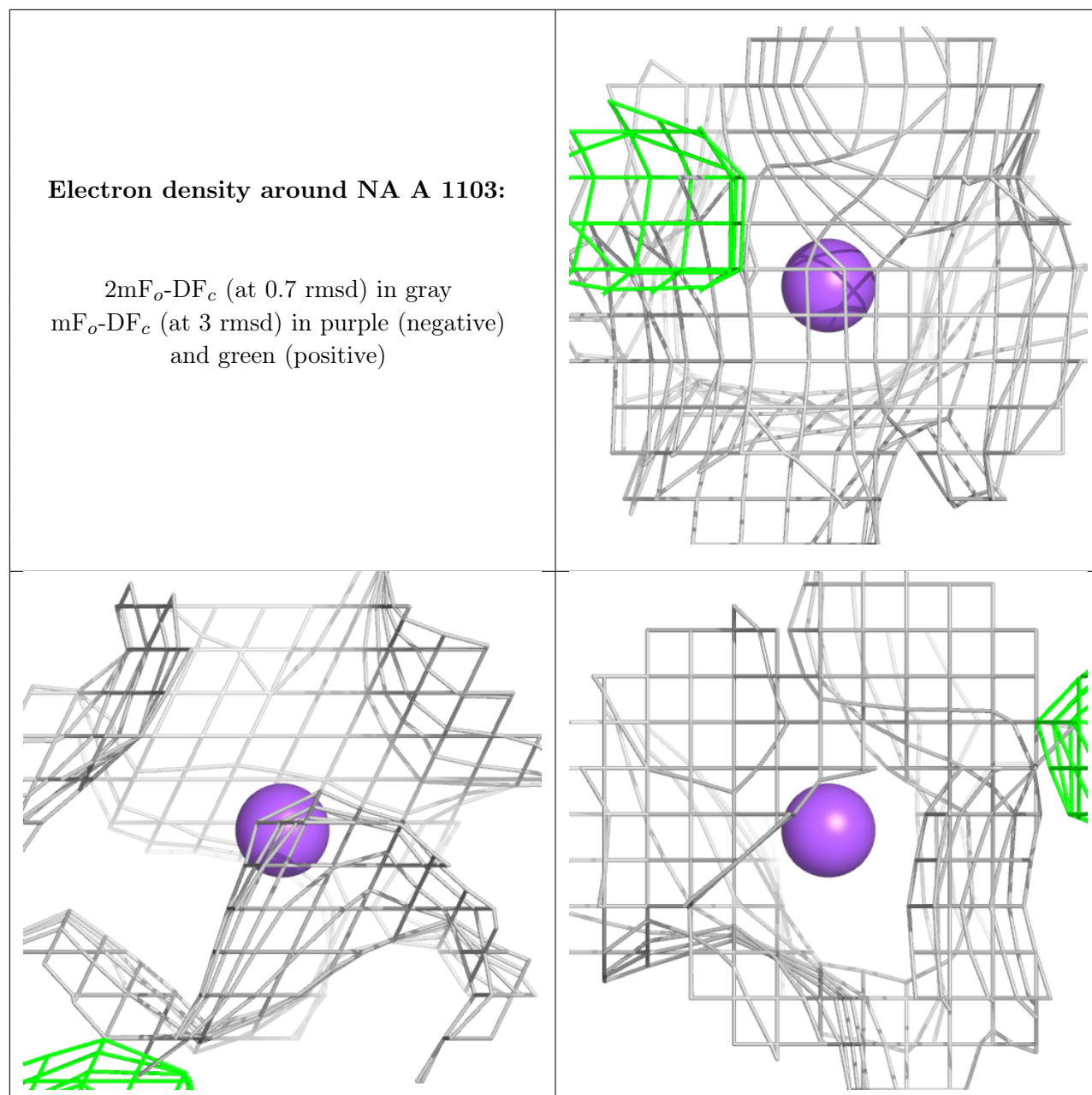
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NA C 1103:

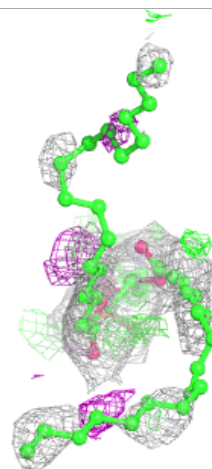
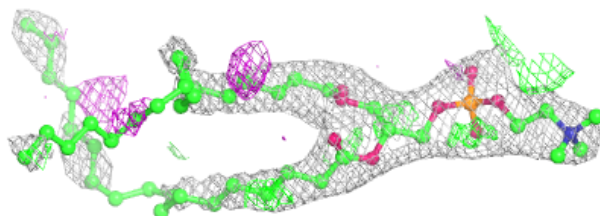
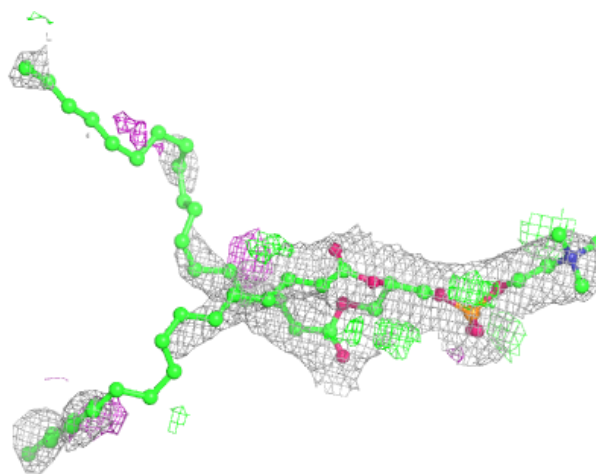
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

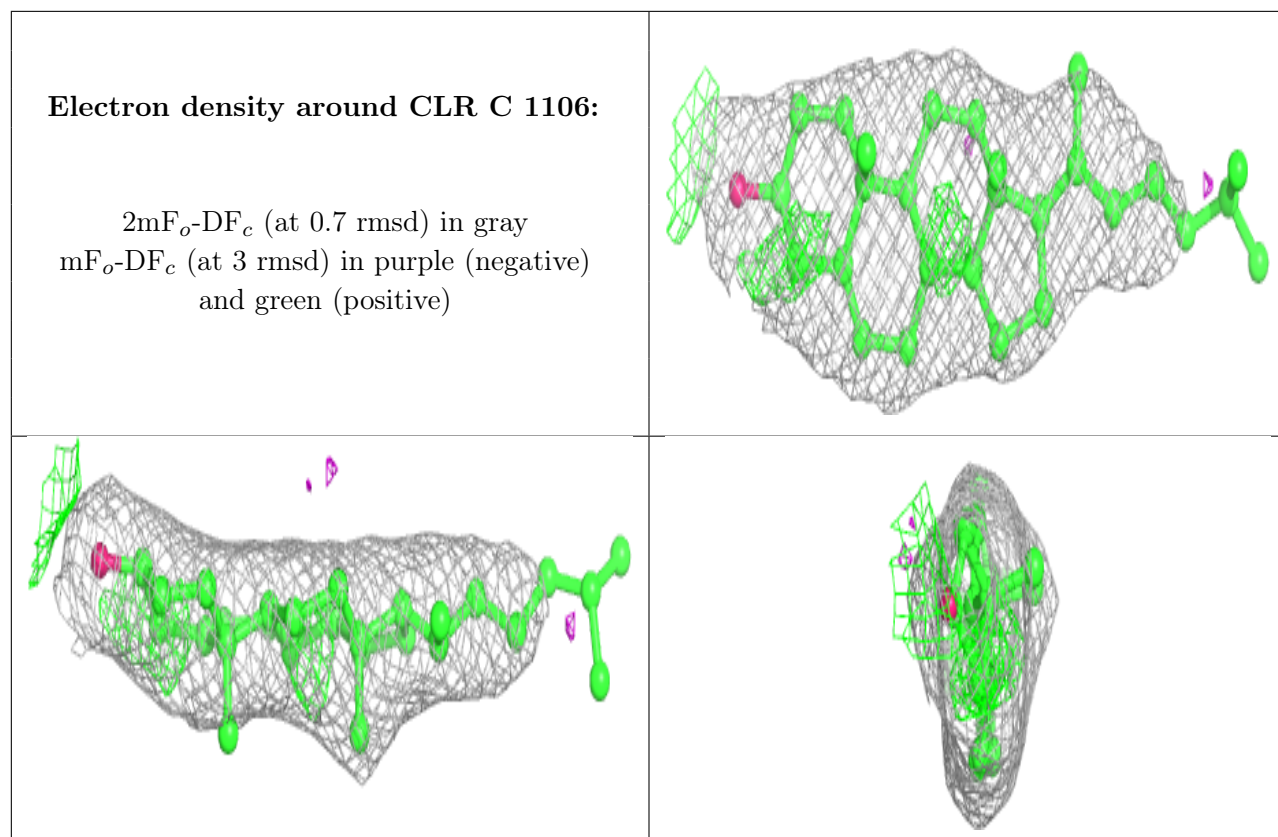




Electron density around PC1 A 1111:

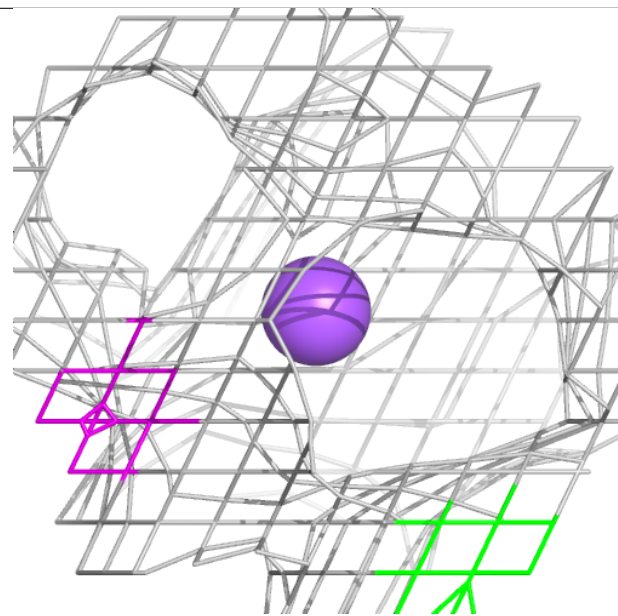
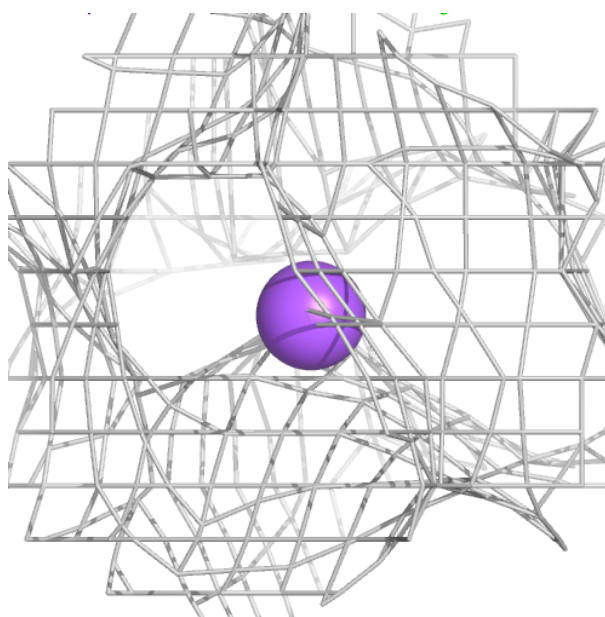
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





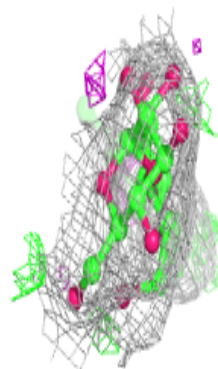
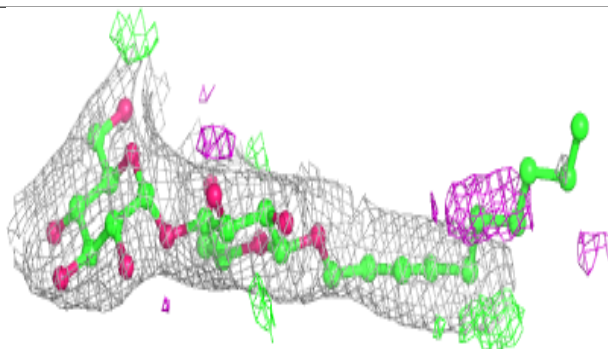
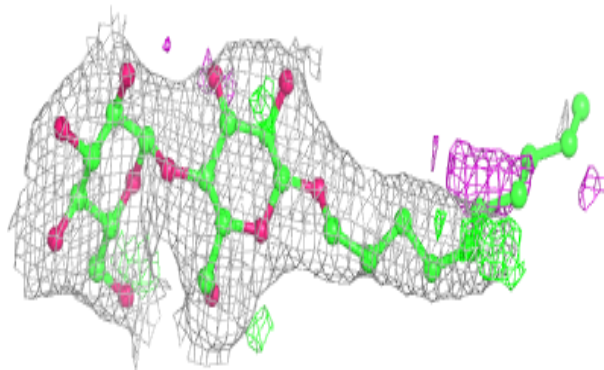
Electron density around NA C 1104:

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

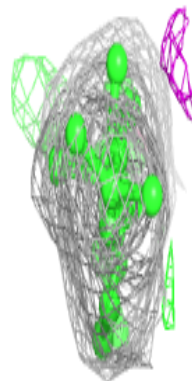
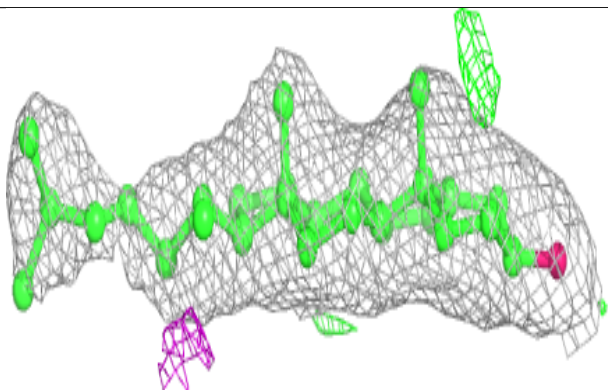
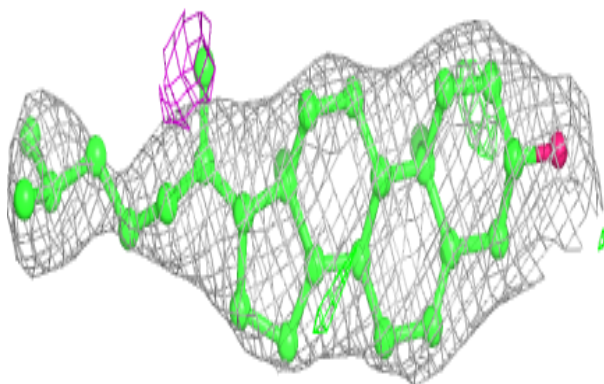


Electron density around DMU E 102:

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

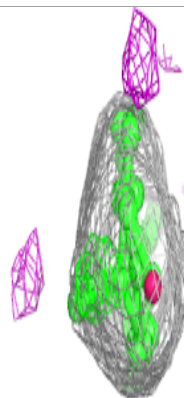
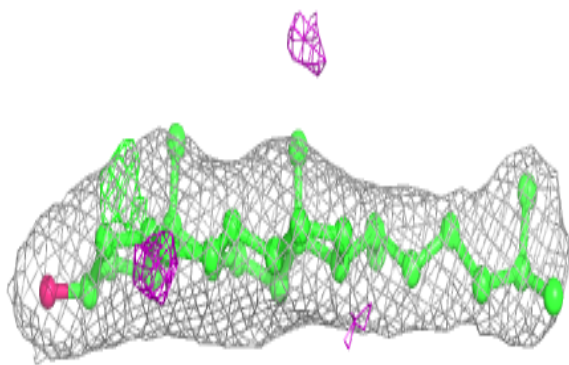
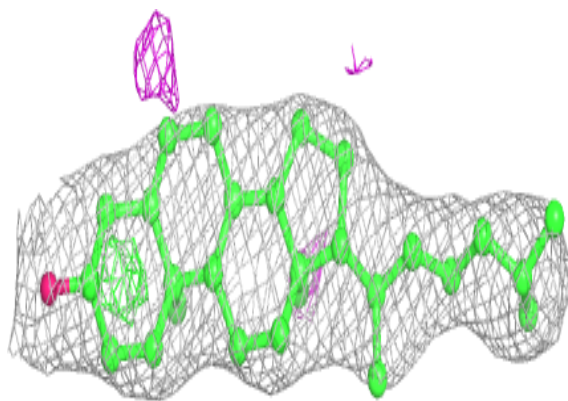
**Electron density around CLR A 1107:**

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



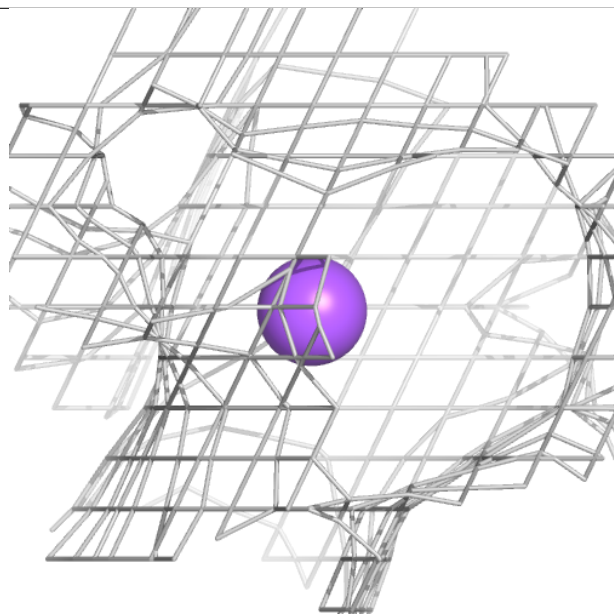
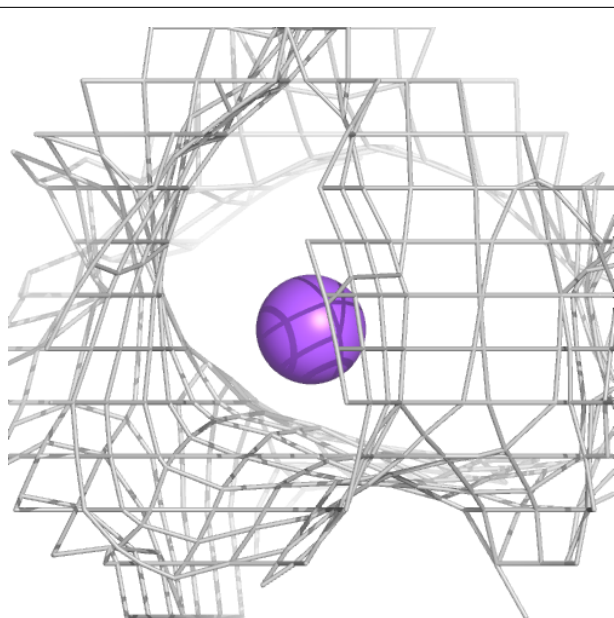
Electron density around CLR E 101:

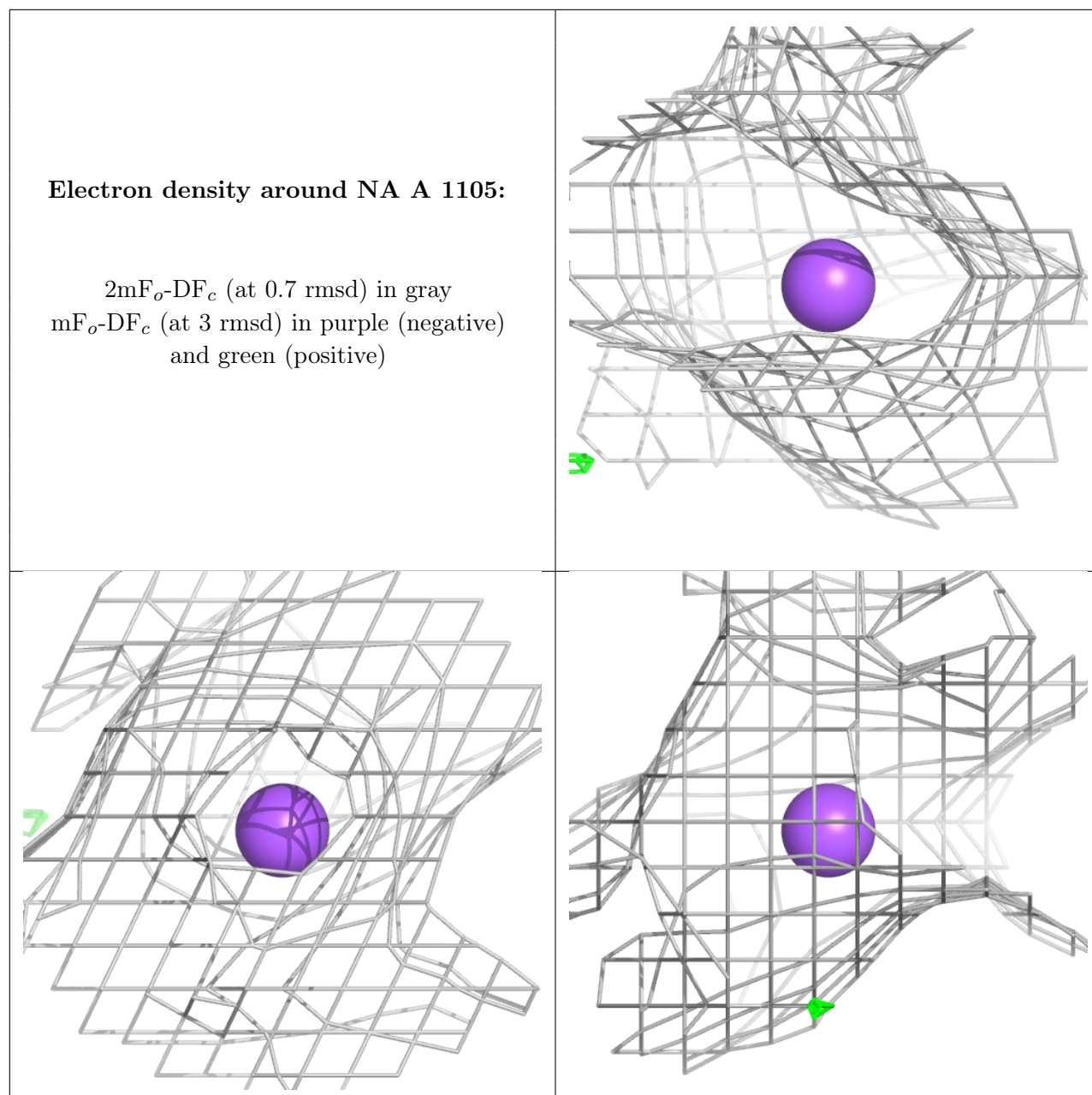
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NA A 1104:

$2mF_o-DF_c$ (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.