



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 09:11 PM UTC

PDB ID : 8JBK / pdb_00008jbk
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	:	4-5-2 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

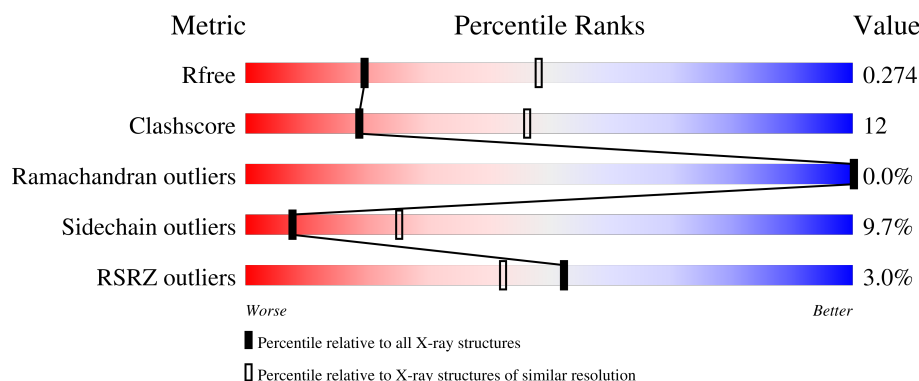
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



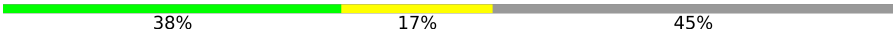
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	3% 67% 27% • •
1	C	1021	3% 68% 26% • •
2	B	303	5% 60% 33% • •
2	D	303	4% 61% 32% • •
3	E	65	40% 11% 49%

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Mol	Chain	Length	Quality of chain
3	G	65	 38% 17% 45%
4	F	6	 33% 67%
5	H	5	 40% 60%
6	I	2	 50% 50%

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
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			

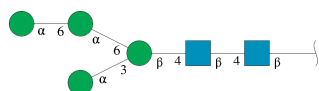
- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

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.

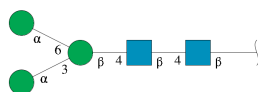
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	36	Total	C	N	O	0	0	0
			292	197	47	48			
3	E	33	Total	C	N	O	0	0	0
			262	179	38	45			

- 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			

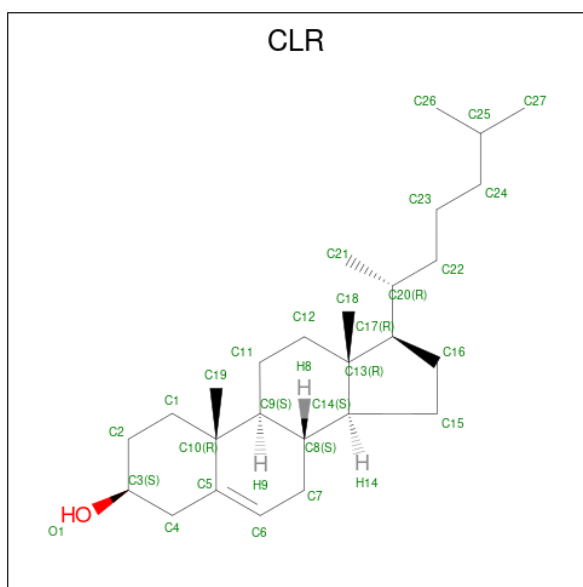
- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

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

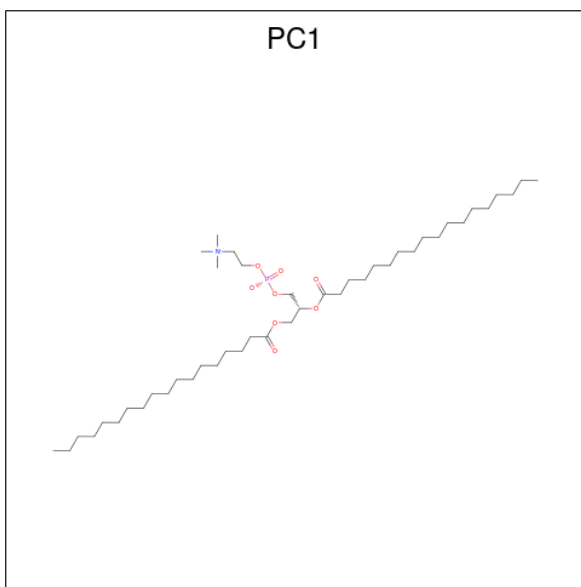
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	Na	0	0
			4	4		
8	C	4	Total	Na	0	0
			4	4		

- Molecule 9 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



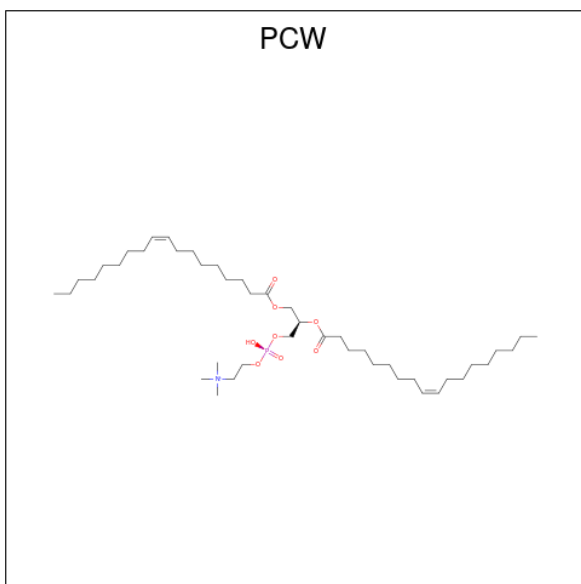
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			28	27	1		
9	A	1	Total	C	O	0	0
			28	27	1		
9	B	1	Total	C	O	0	0
			28	27	1		
9	C	1	Total	C	O	0	0
			28	27	1		
9	D	1	Total	C	O	0	0
			28	27	1		
9	E	1	Total	C	O	0	0
			28	27	1		

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



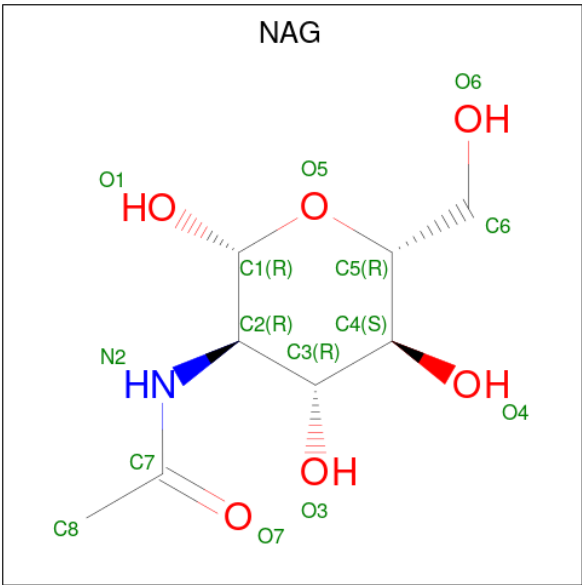
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

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



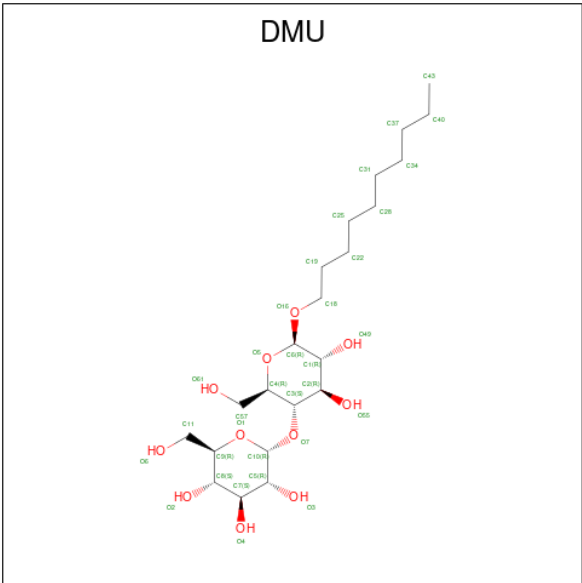
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
11	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
11	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
11	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
11	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
11	B	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
11	C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

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



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

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



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

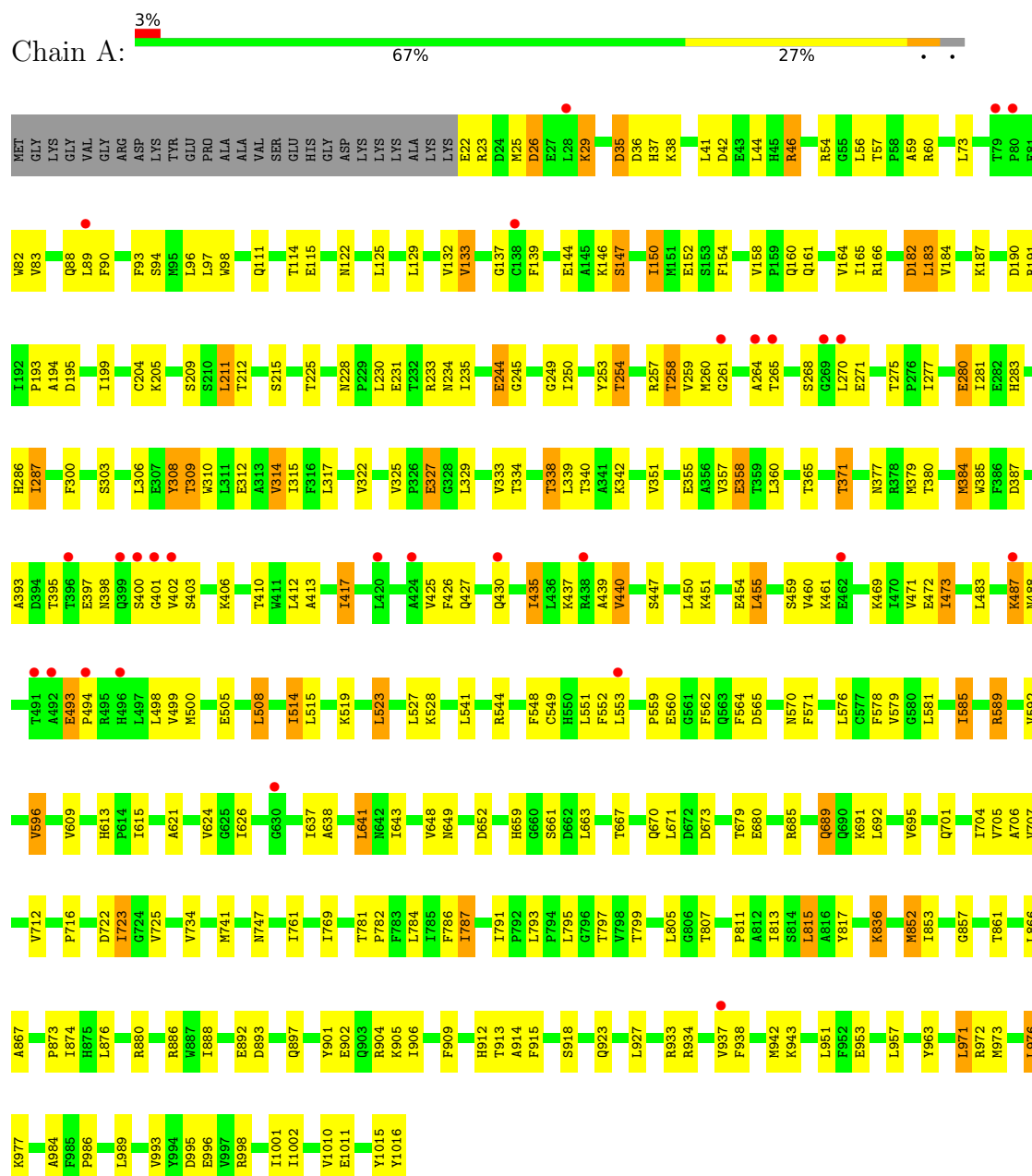
- Molecule 14 is water.

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

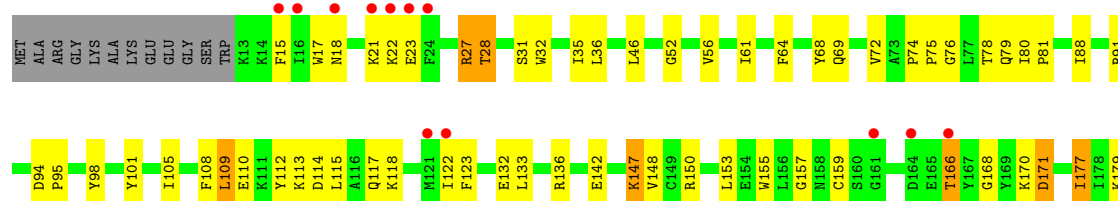
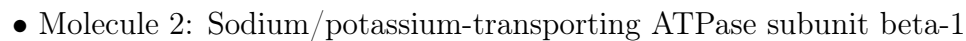
3 Residue-property plots

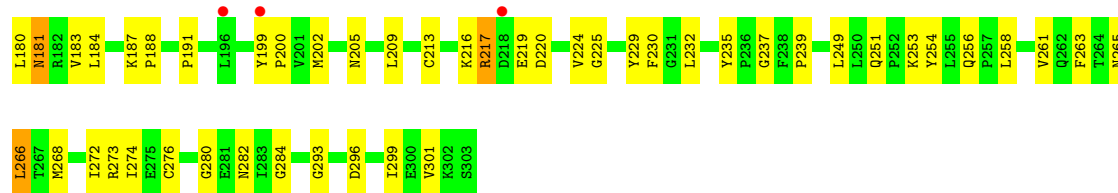
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

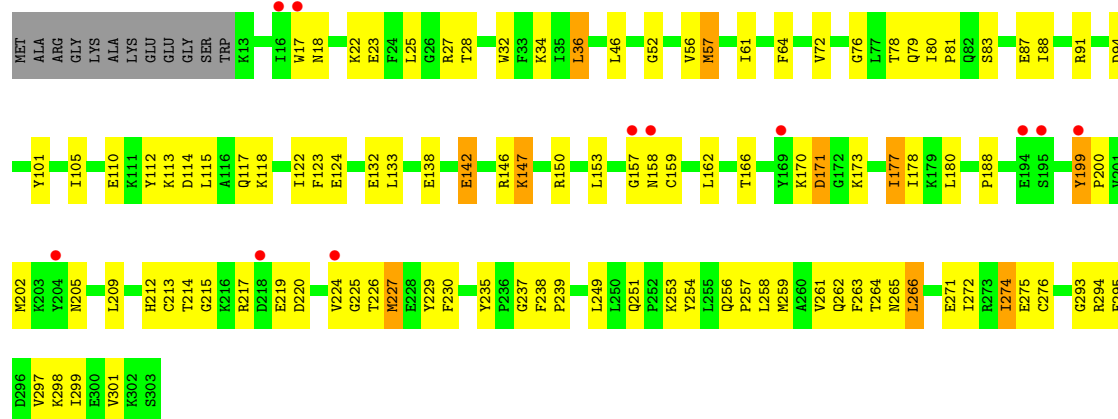


Chain C: 3% 68% 26%





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



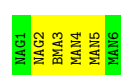
• Molecule 3: FXYD domain-containing ion transport regulator



• Molecule 3: FXYD 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

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 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	64.6 (15.00-2.80) 64.1 (15.00-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.229 , 0.270 0.235 , 0.274	Depositor DCC
R_{free} test set	3358 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21682	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage'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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/7873	0.38	0/10683
1	C	0.16	0/7873	0.37	0/10683
2	B	0.14	0/2449	0.38	0/3301
2	D	0.15	0/2449	0.35	0/3301
3	E	0.15	0/268	0.31	0/364
3	G	0.14	0/298	0.28	0/403
All	All	0.16	0/21210	0.37	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 [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	7774	194	0
1	C	7723	0	7774	168	0
2	B	2386	0	2362	73	0
2	D	2386	0	2362	62	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	517	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 517 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

5.3.1 Protein backbone

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%)	48	77
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

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%)	758 (90%)	87 (10%)	7	23
1	C	845/864 (98%)	764 (90%)	81 (10%)	8	26
2	B	261/269 (97%)	237 (91%)	24 (9%)	8	27
2	D	261/269 (97%)	237 (91%)	24 (9%)	8	27
3	E	27/52 (52%)	25 (93%)	2 (7%)	13	37
3	G	30/52 (58%)	28 (93%)	2 (7%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2269/2370 (96%)	2049 (90%)	220 (10%)	8 25

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	35	ASP
1	C	310	TRP
3	E	26	VAL
2	D	64	PHE
1	C	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	119	GLN
2	D	262	GLN
1	C	399	GLN
2	D	140	ASN
2	D	18	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	0.58	0	17,19,21	0.63	0
4	NAG	F	2	4	14,14,15	0.47	0	17,19,21	1.26	2 (11%)
4	BMA	F	3	4	11,11,12	1.19	1 (9%)	15,15,17	1.33	1 (6%)
4	MAN	F	4	4	11,11,12	0.92	0	15,15,17	0.89	1 (6%)
4	MAN	F	5	4	11,11,12	0.73	0	15,15,17	0.99	2 (13%)
4	MAN	F	6	4	11,11,12	0.91	0	15,15,17	0.89	0
5	NAG	H	1	2,5	14,14,15	1.10	1 (7%)	17,19,21	1.34	3 (17%)
5	NAG	H	2	5	14,14,15	0.82	1 (7%)	17,19,21	1.05	1 (5%)
5	BMA	H	3	5	11,11,12	1.49	2 (18%)	15,15,17	0.95	1 (6%)
5	MAN	H	4	5	11,11,12	1.13	1 (9%)	15,15,17	1.29	2 (13%)
5	MAN	H	5	5	11,11,12	1.24	1 (9%)	15,15,17	1.52	2 (13%)
6	NAG	I	1	2,6	14,14,15	0.47	0	17,19,21	0.69	0
6	NAG	I	2	6	14,14,15	0.37	0	17,19,21	0.79	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	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	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	2,5	-	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	2,6	-	1/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	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	-3.78	1.37	1.43
5	H	5	MAN	C1-C2	3.12	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	BMA	C1-C2	3.02	1.59	1.52
4	F	3	BMA	C1-C2	2.89	1.59	1.52
5	H	4	MAN	C1-C2	2.81	1.58	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	5	MAN	C1-O5-C5	4.49	118.20	112.19
4	F	2	NAG	C1-O5-C5	3.49	116.86	112.19
5	H	4	MAN	C1-O5-C5	3.31	116.63	112.19
5	H	2	NAG	C1-O5-C5	3.15	116.40	112.19
5	H	1	NAG	C1-O5-C5	3.08	116.32	112.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

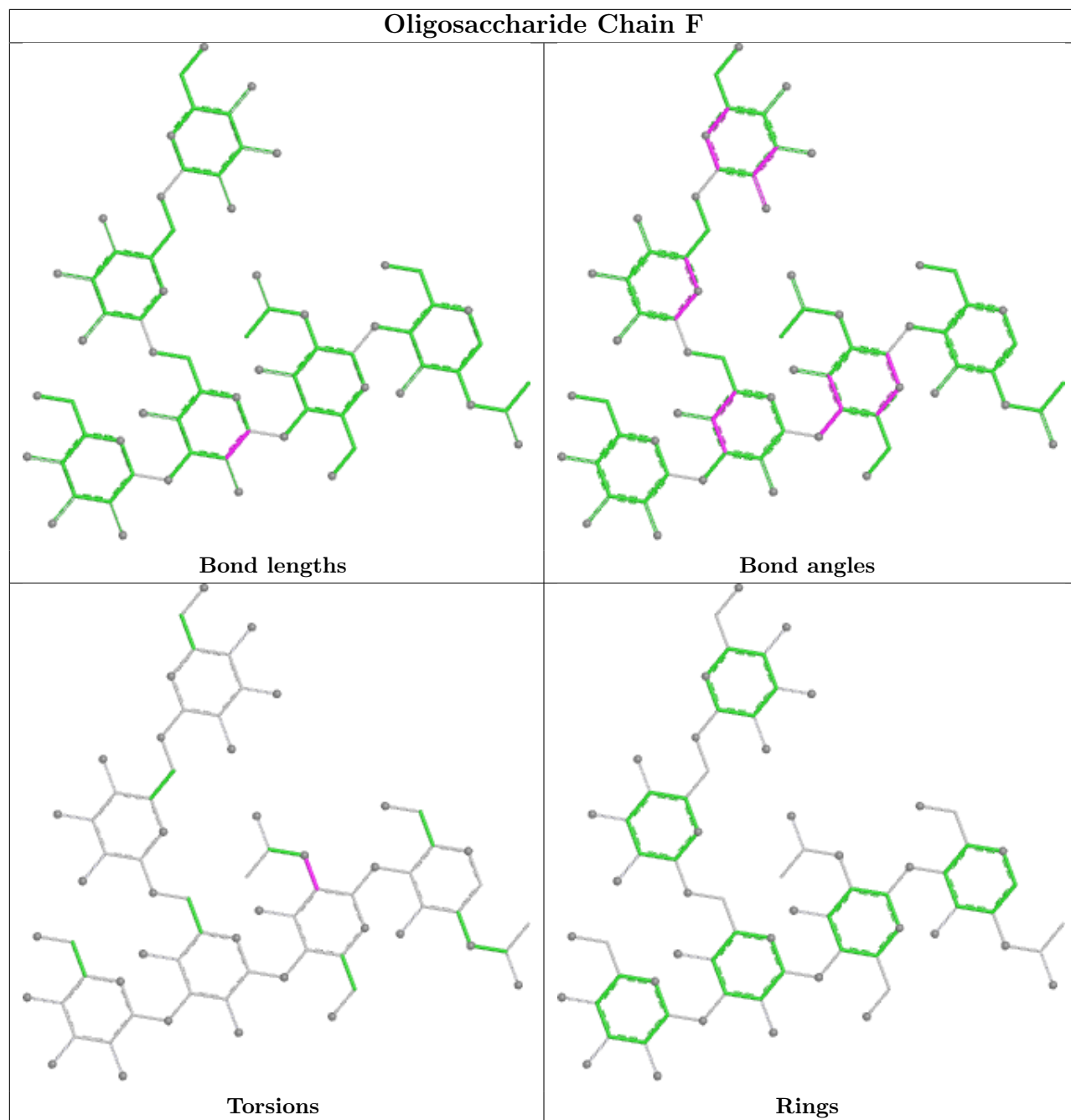
Mol	Chain	Res	Type	Atoms
5	H	3	BMA	C4-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
5	H	4	MAN	C4-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
5	H	2	NAG	C8-C7-N2-C2

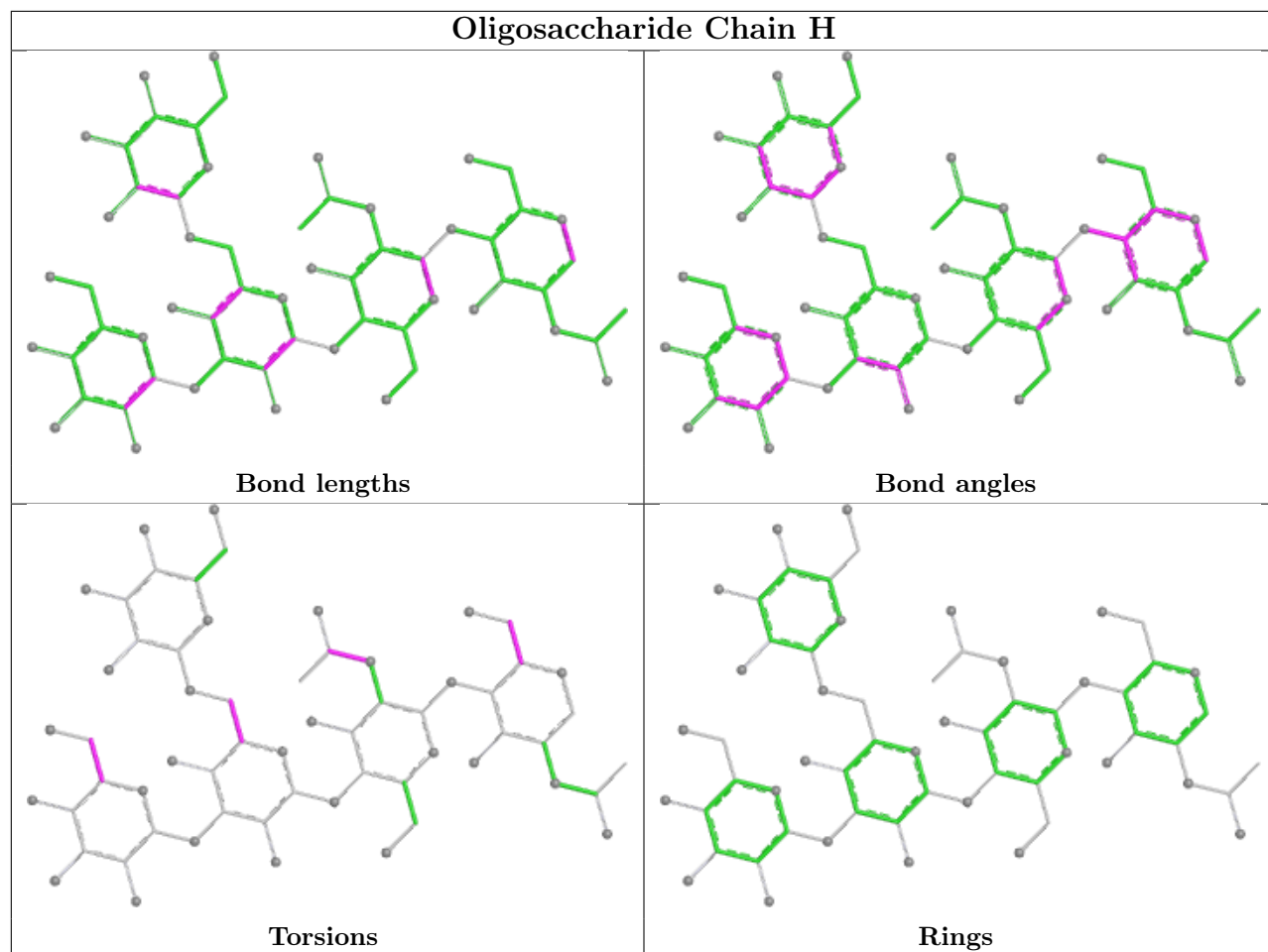
There are no ring outliers.

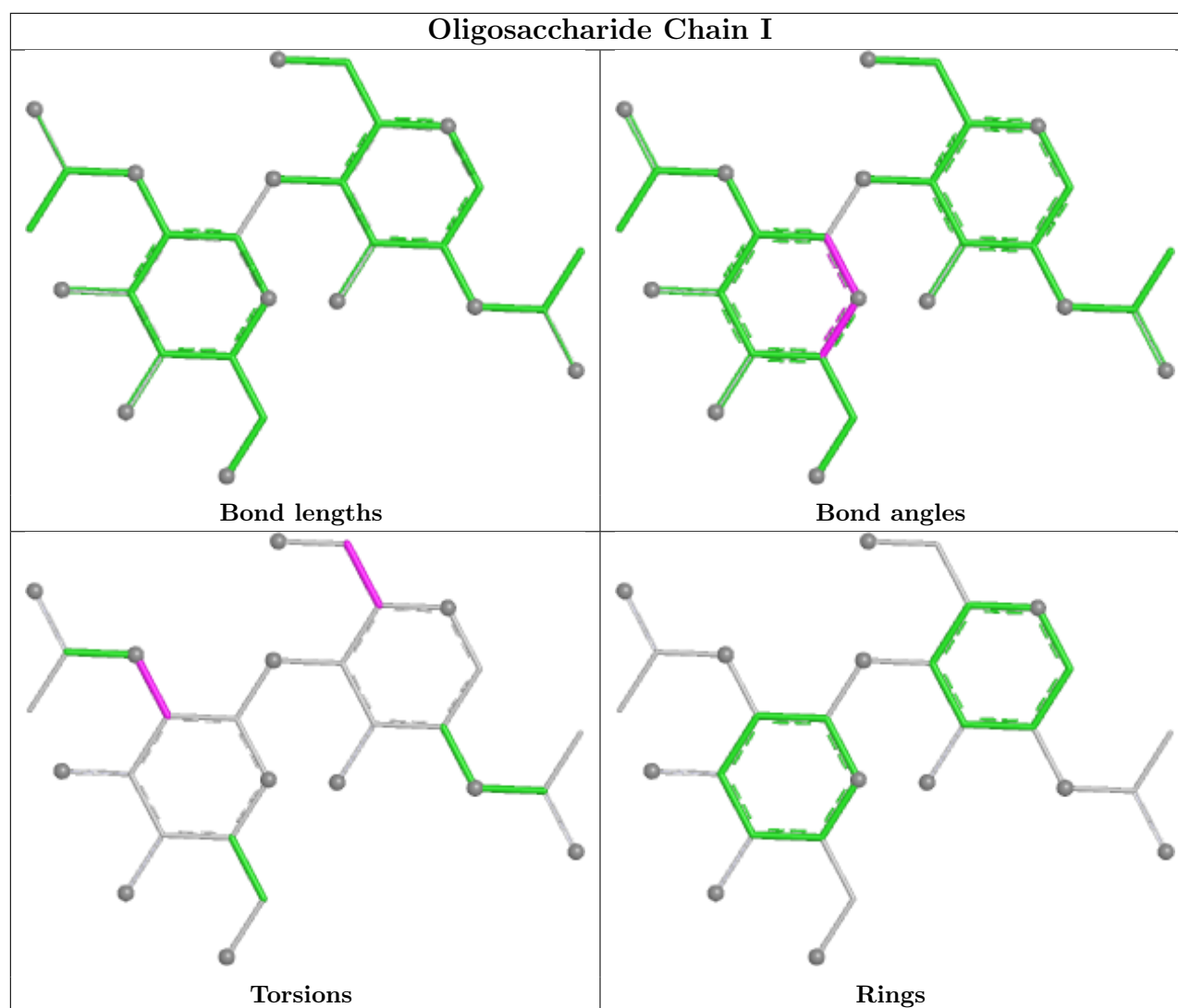
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	1	0
5	H	3	BMA	1	0
5	H	2	NAG	2	0

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







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	$\# Z > 2$
11	PCW	C	1114	-	21,21,53	0.86	0	27,29,61	0.93	1 (3%)
9	CLR	D	401	-	31,31,31	1.57	7 (22%)	48,48,48	1.45	10 (20%)
11	PCW	C	1112	-	21,21,53	0.86	0	27,29,61	1.12	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PC1	A	1110	-	53,53,53	0.76	0	59,61,61	1.19	5 (8%)
11	PCW	A	1116	-	21,21,53	0.85	0	27,29,61	1.04	2 (7%)
11	PCW	C	1107	-	21,21,53	0.85	0	27,29,61	1.03	2 (7%)
11	PCW	C	1113	-	21,21,53	0.86	0	27,29,61	0.89	1 (3%)
9	CLR	E	101	-	31,31,31	1.54	7 (22%)	48,48,48	1.49	10 (20%)
9	CLR	B	402	-	31,31,31	1.52	7 (22%)	48,48,48	1.43	10 (20%)
9	CLR	A	1107	-	31,31,31	1.55	7 (22%)	48,48,48	1.46	11 (22%)
11	PCW	A	1115	-	21,21,53	0.85	0	27,29,61	1.16	3 (11%)
9	CLR	C	1106	-	31,31,31	1.49	6 (19%)	48,48,48	1.45	11 (22%)
11	PCW	B	401	-	21,21,53	0.86	0	27,29,61	1.08	3 (11%)
13	DMU	E	102	-	34,34,34	0.88	2 (5%)	45,45,45	1.38	5 (11%)
11	PCW	A	1113	-	21,21,53	0.86	0	27,29,61	1.05	2 (7%)
11	PCW	C	1109	-	21,21,53	0.86	0	27,29,61	1.02	2 (7%)
11	PCW	C	1108	-	21,21,53	0.86	0	27,29,61	0.92	1 (3%)
11	PCW	C	1110	-	21,21,53	0.87	0	27,29,61	0.90	1 (3%)
11	PCW	A	1112	-	21,21,53	0.85	0	27,29,61	1.09	2 (7%)
11	PCW	A	1114	-	21,21,53	0.85	0	27,29,61	1.03	3 (11%)
11	PCW	C	1111	-	21,21,53	0.85	0	27,29,61	1.00	2 (7%)
10	PC1	A	1108	-	53,53,53	0.64	0	59,61,61	0.94	1 (1%)
11	PCW	A	1109	-	21,21,53	0.86	0	27,29,61	1.19	3 (11%)
9	CLR	A	1106	-	31,31,31	1.52	6 (19%)	48,48,48	1.46	12 (25%)
12	NAG	D	402	2	14,14,15	0.33	0	17,19,21	0.49	0
10	PC1	A	1111	-	53,53,53	0.71	0	59,61,61	0.87	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PCW	C	1114	-	-	5/23/23/57	-
9	CLR	D	401	-	-	4/10/68/68	0/4/4/4
11	PCW	C	1112	-	-	4/23/23/57	-
10	PC1	A	1110	-	-	15/57/57/57	-
11	PCW	A	1116	-	-	7/23/23/57	-
11	PCW	C	1107	-	-	7/23/23/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PCW	C	1113	-	-	8/23/23/57	-
9	CLR	E	101	-	-	1/10/68/68	0/4/4/4
9	CLR	B	402	-	-	8/10/68/68	0/4/4/4
9	CLR	A	1107	-	-	5/10/68/68	0/4/4/4
11	PCW	A	1115	-	-	7/23/23/57	-
9	CLR	C	1106	-	-	1/10/68/68	0/4/4/4
11	PCW	B	401	-	-	1/23/23/57	-
13	DMU	E	102	-	-	2/19/59/59	0/2/2/2
11	PCW	A	1113	-	-	4/23/23/57	-
11	PCW	C	1109	-	-	7/23/23/57	-
11	PCW	C	1108	-	-	5/23/23/57	-
11	PCW	C	1110	-	-	8/23/23/57	-
11	PCW	A	1112	-	-	7/23/23/57	-
11	PCW	A	1114	-	-	7/23/23/57	-
11	PCW	C	1111	-	-	7/23/23/57	-
10	PC1	A	1108	-	-	9/57/57/57	-
11	PCW	A	1109	-	-	2/23/23/57	-
9	CLR	A	1106	-	-	3/10/68/68	0/4/4/4
12	NAG	D	402	2	-	2/6/23/26	0/1/1/1
10	PC1	A	1111	-	-	15/57/57/57	-

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	401	CLR	C4-C3	3.42	1.58	1.52
9	E	101	CLR	C4-C3	3.23	1.57	1.52
9	A	1107	CLR	C4-C3	3.22	1.57	1.52
9	A	1106	CLR	C4-C3	3.13	1.57	1.52
13	E	102	DMU	O16-C6	3.10	1.45	1.40

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1110	PC1	C2-O21-C21	4.40	128.32	117.80
13	E	102	DMU	O16-C18-C19	4.19	123.58	109.37
11	A	1109	PCW	C2-O2-C31	-3.95	110.87	117.85
11	C	1112	PCW	C2-O2-C31	-3.70	111.31	117.85
9	C	1106	CLR	C22-C20-C17	-3.30	103.49	110.33

There are no chirality outliers.

5 of 151 torsion outliers are listed below:

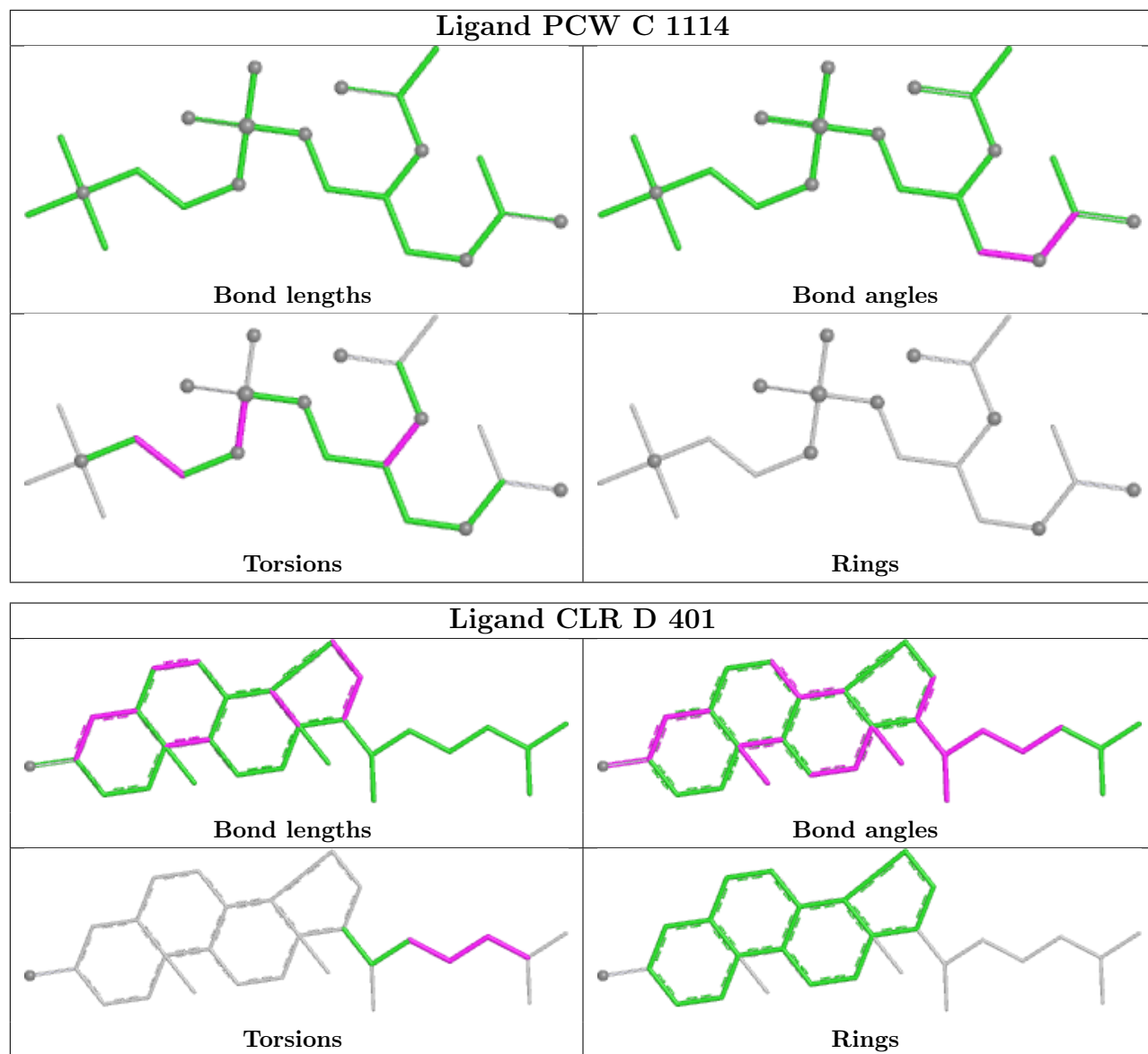
Mol	Chain	Res	Type	Atoms
10	A	1108	PC1	C11-O13-P-O14
10	A	1110	PC1	C11-O13-P-O12
10	A	1110	PC1	C11-O13-P-O14
10	A	1110	PC1	C11-O13-P-O11
10	A	1110	PC1	C1-O11-P-O12

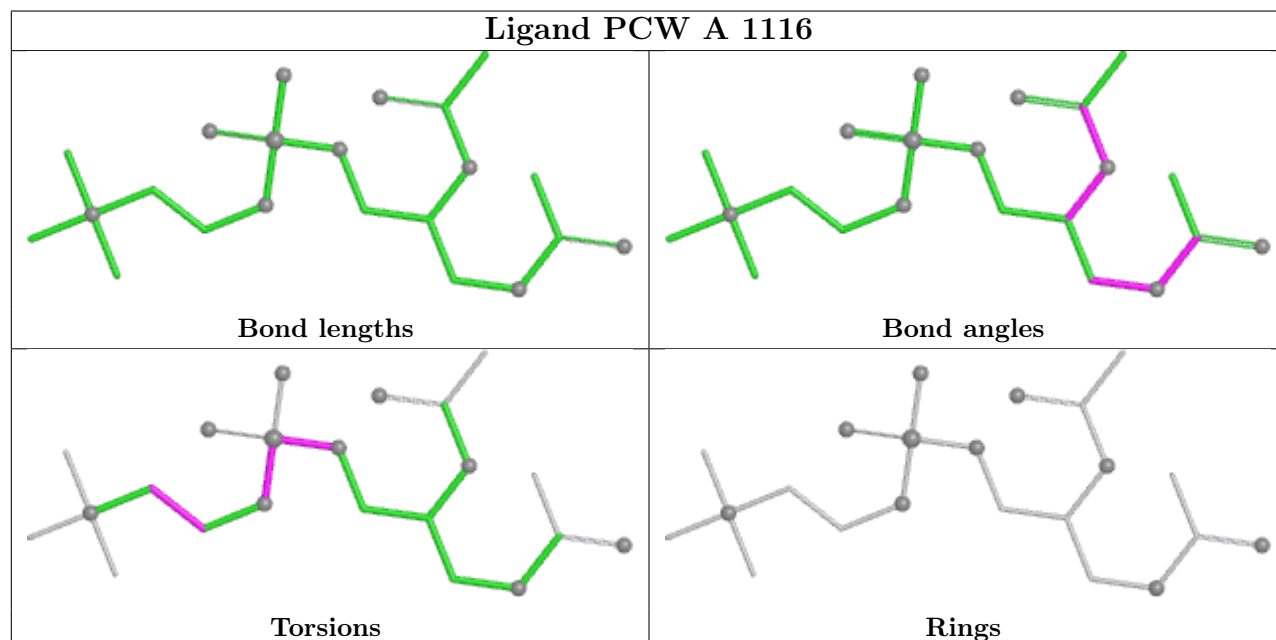
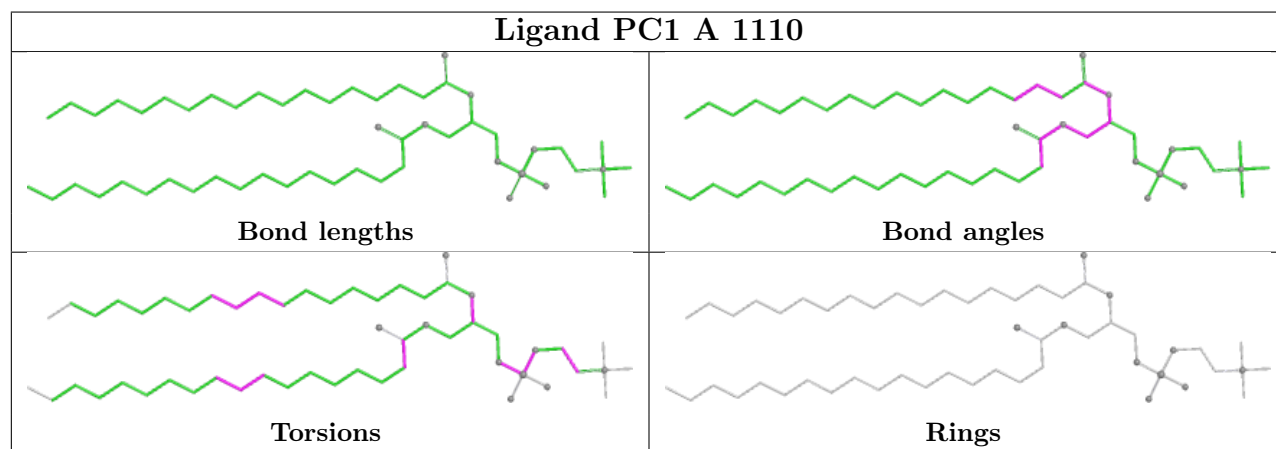
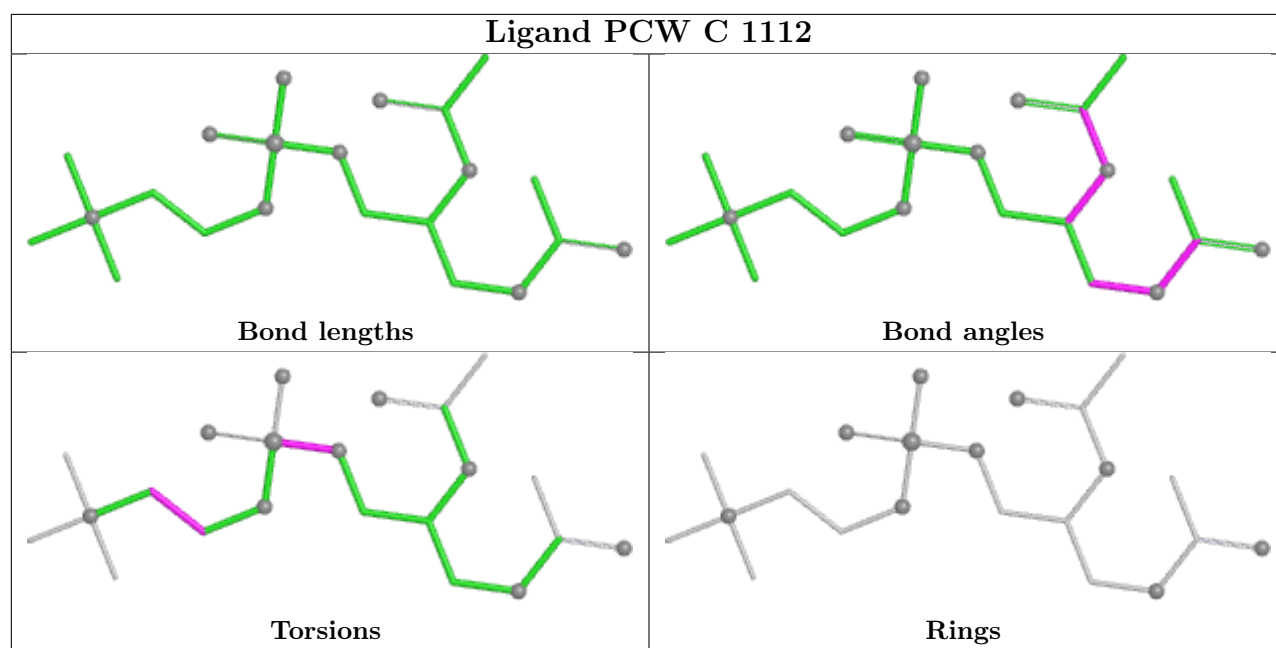
There are no ring outliers.

16 monomers are involved in 41 short contacts:

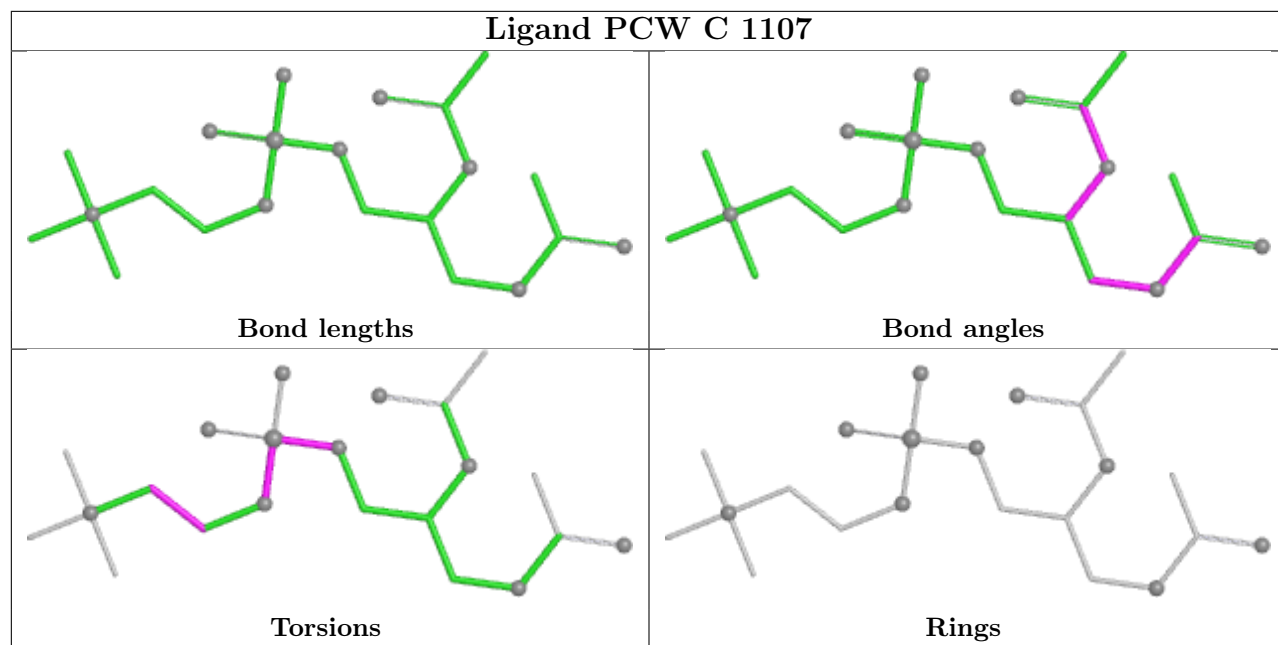
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	401	CLR	2	0
10	A	1110	PC1	5	0
11	C	1107	PCW	3	0
9	E	101	CLR	1	0
9	B	402	CLR	4	0
9	A	1107	CLR	4	0
9	C	1106	CLR	4	0
11	B	401	PCW	2	0
13	E	102	DMU	3	0
11	C	1109	PCW	2	0
11	C	1108	PCW	2	0
11	C	1110	PCW	1	0
10	A	1108	PC1	3	0
11	A	1109	PCW	2	0
9	A	1106	CLR	3	0
10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

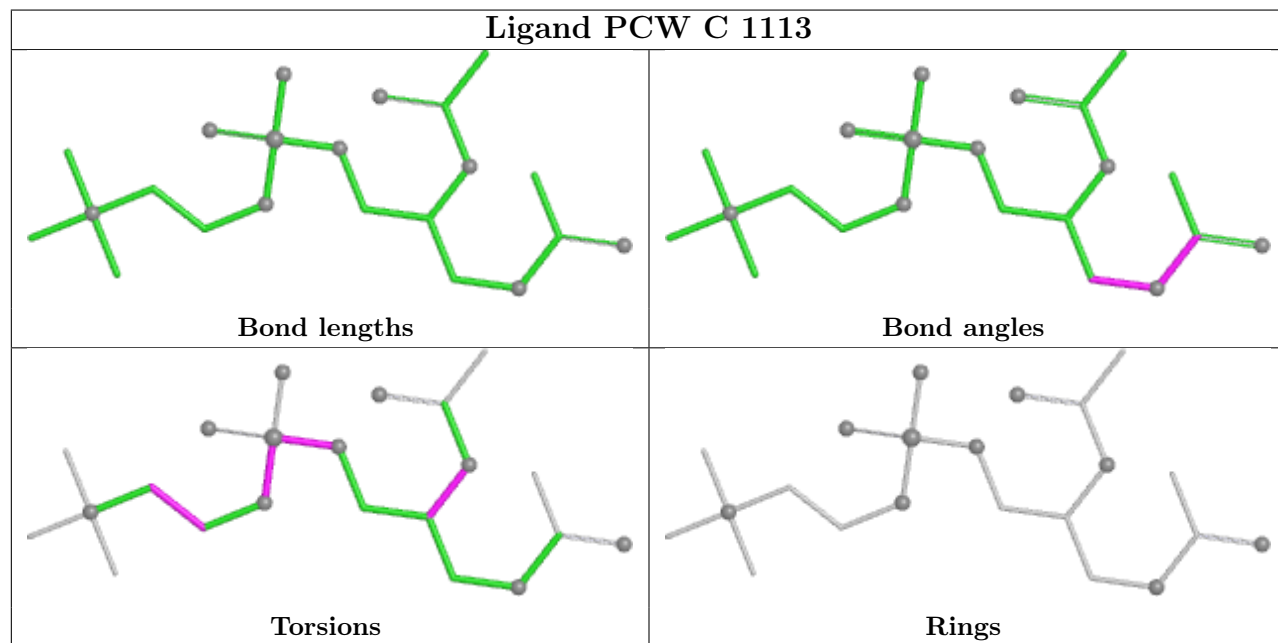




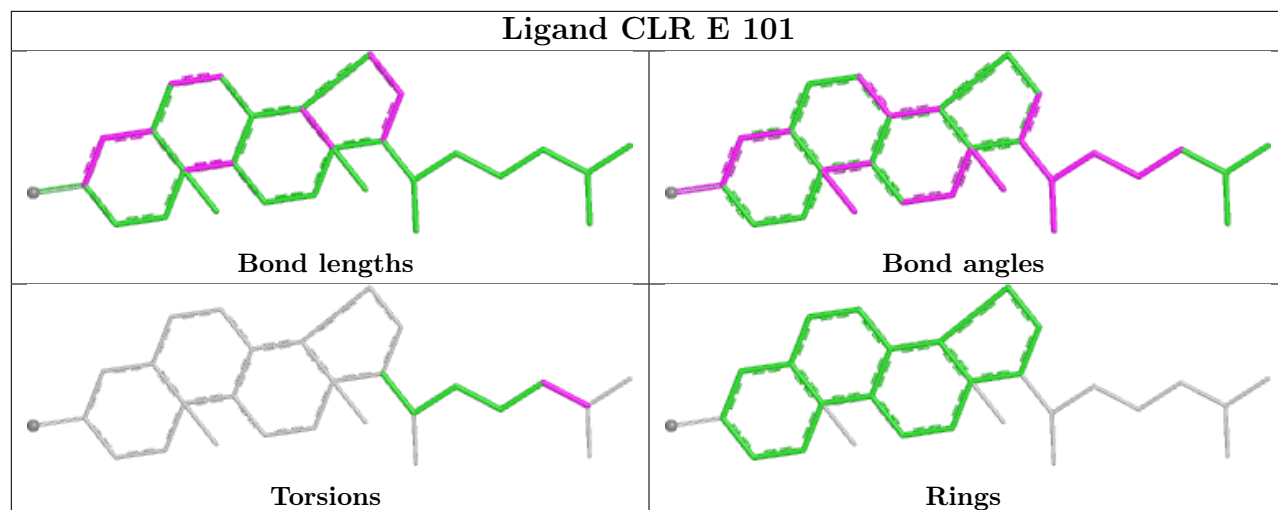
Ligand PCW C 1107



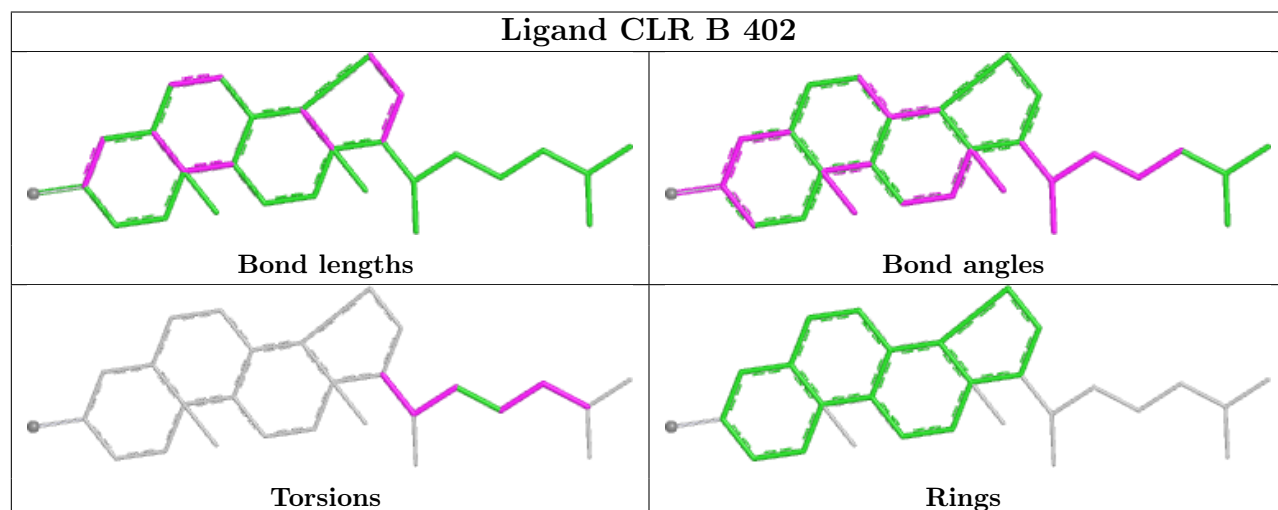
Ligand PCW C 1113



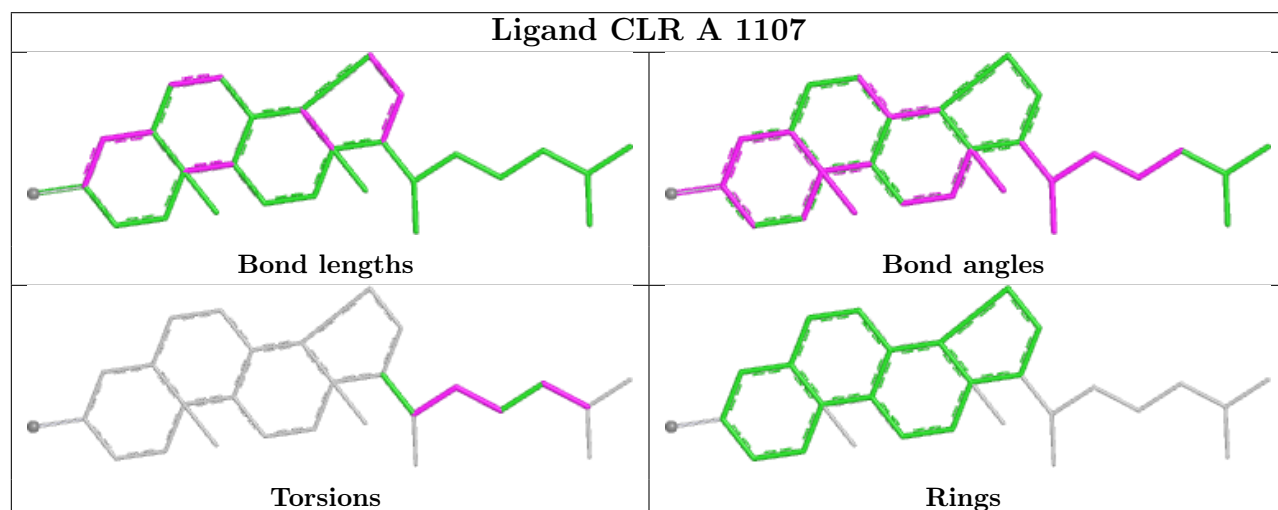
Ligand CLR E 101

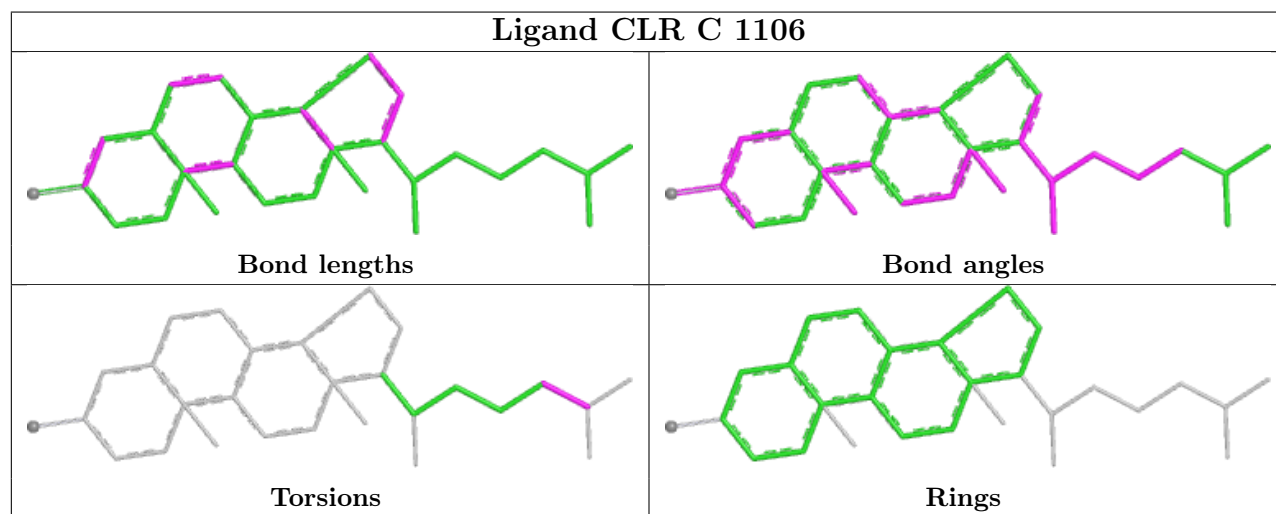
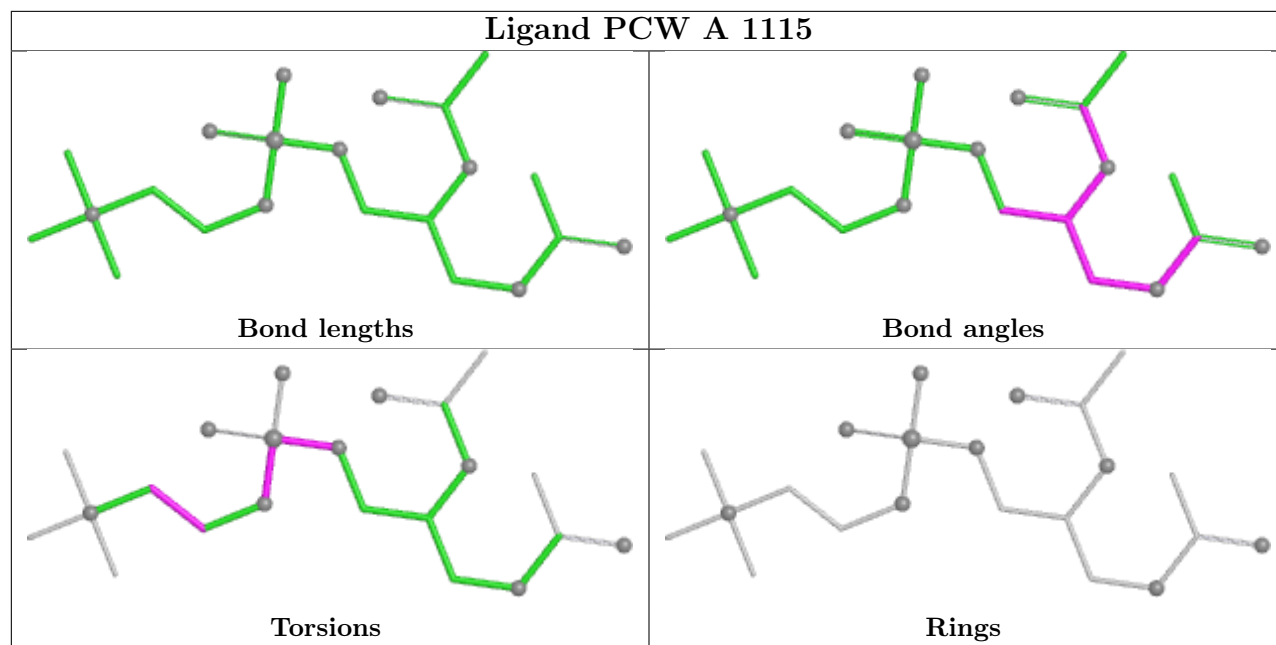


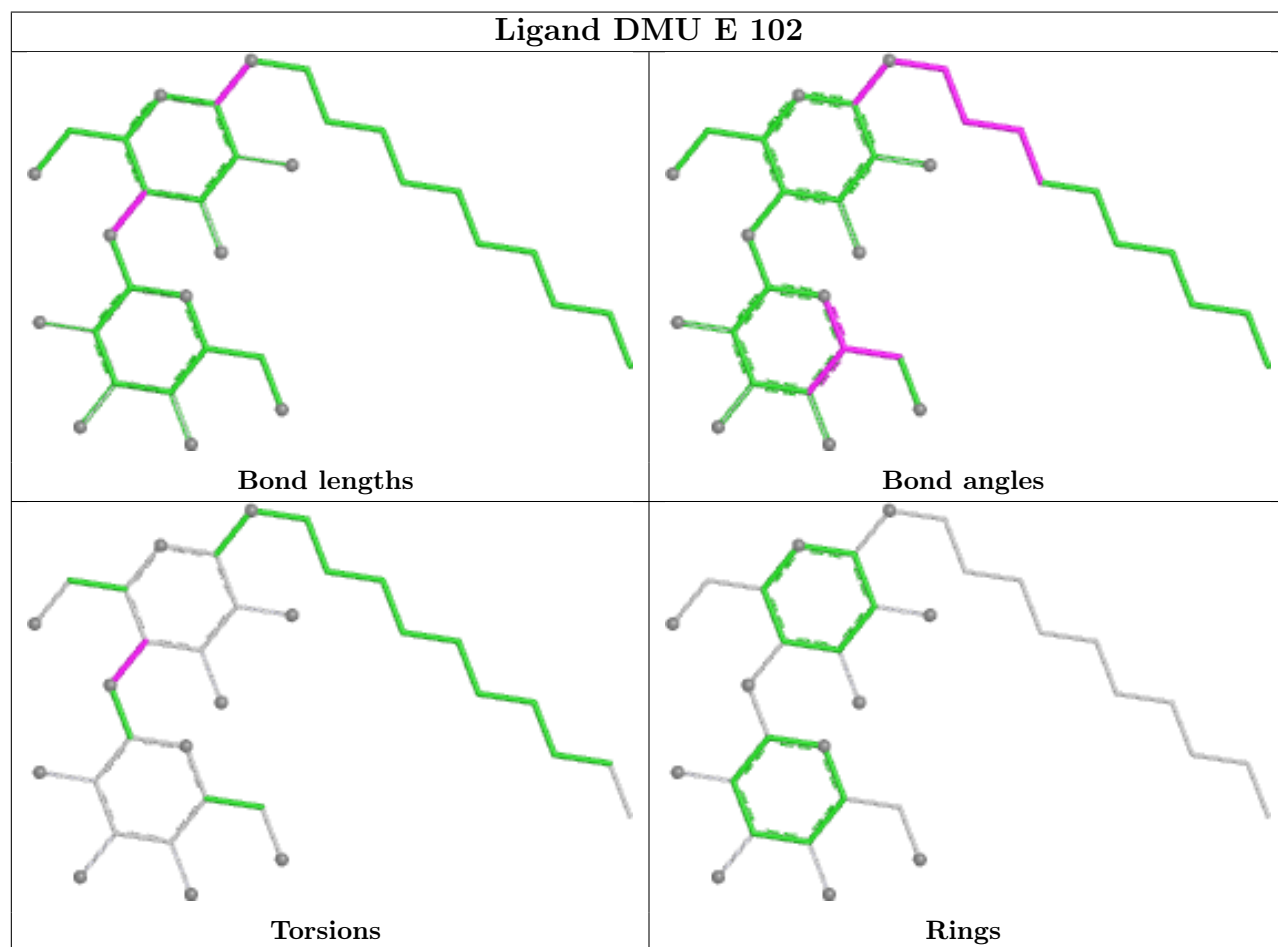
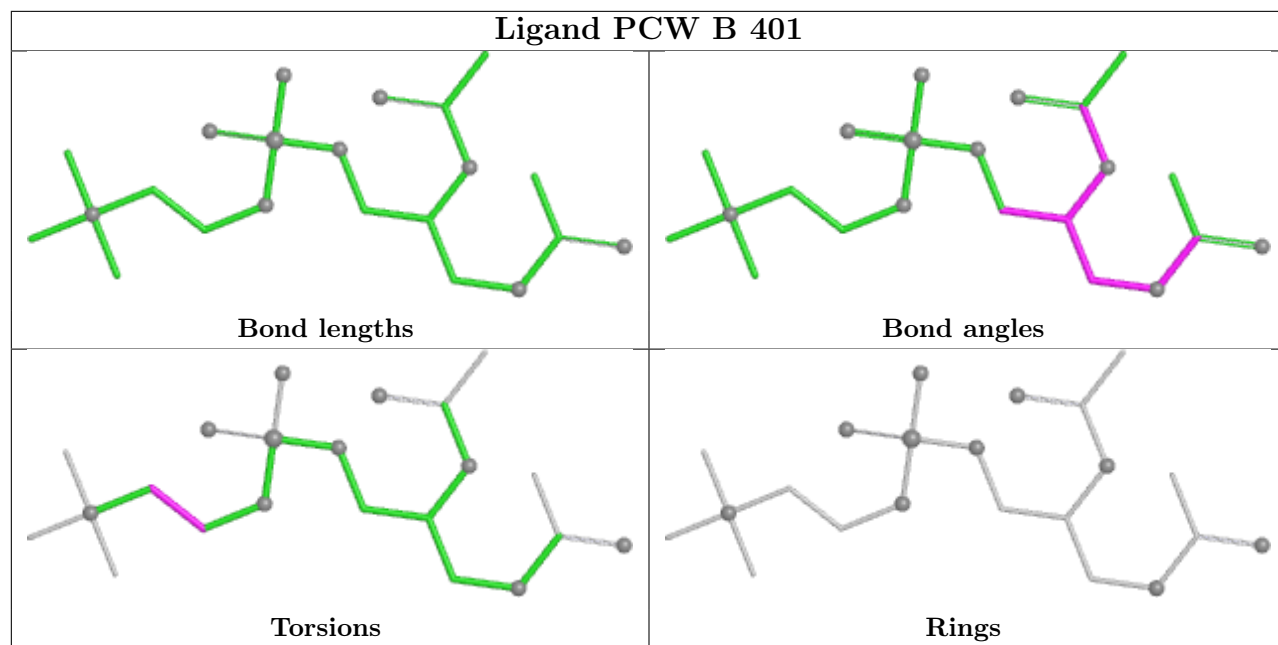
Ligand CLR B 402



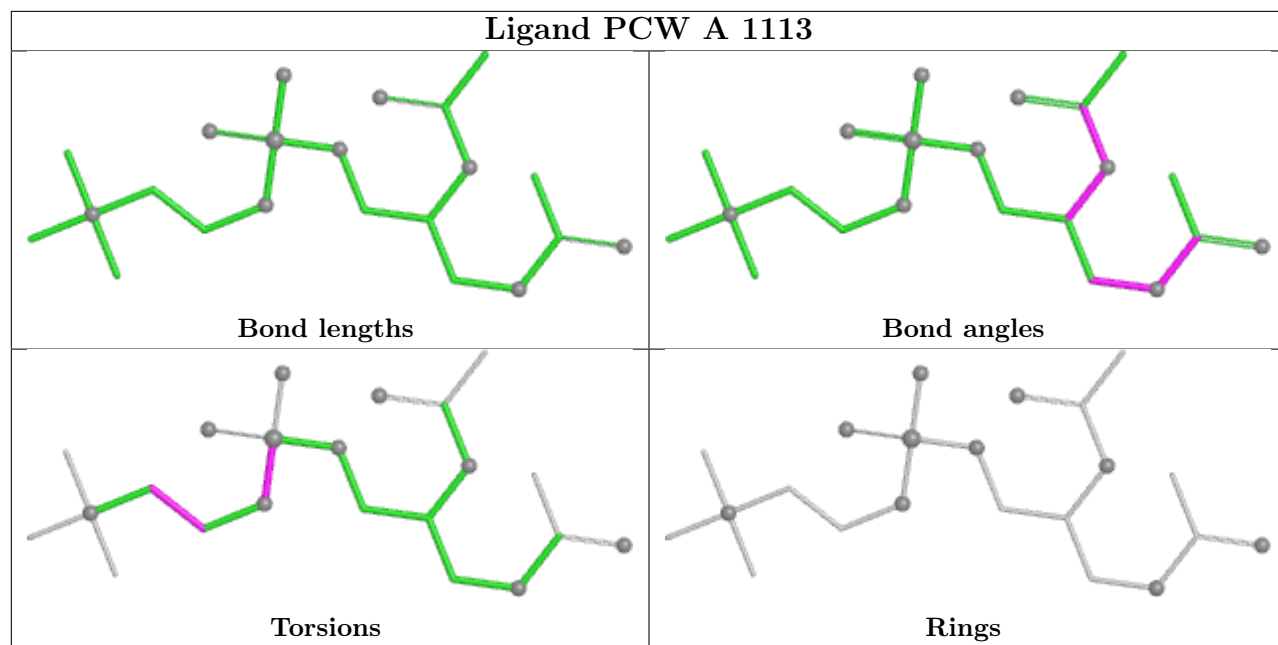
Ligand CLR A 1107



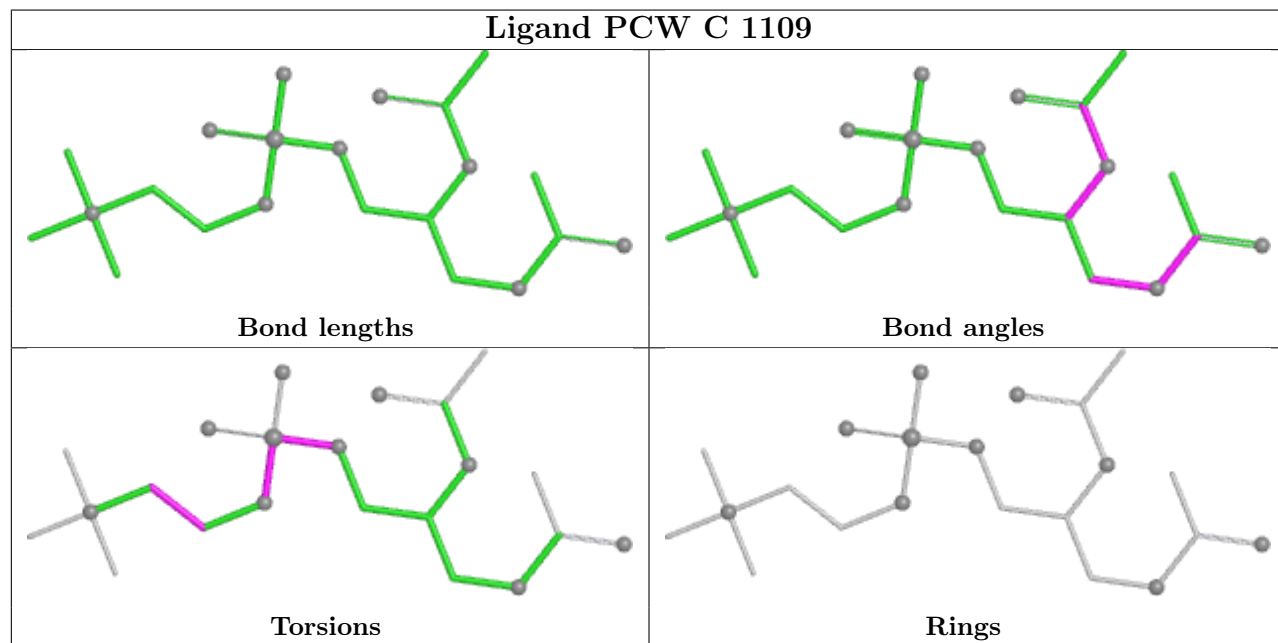




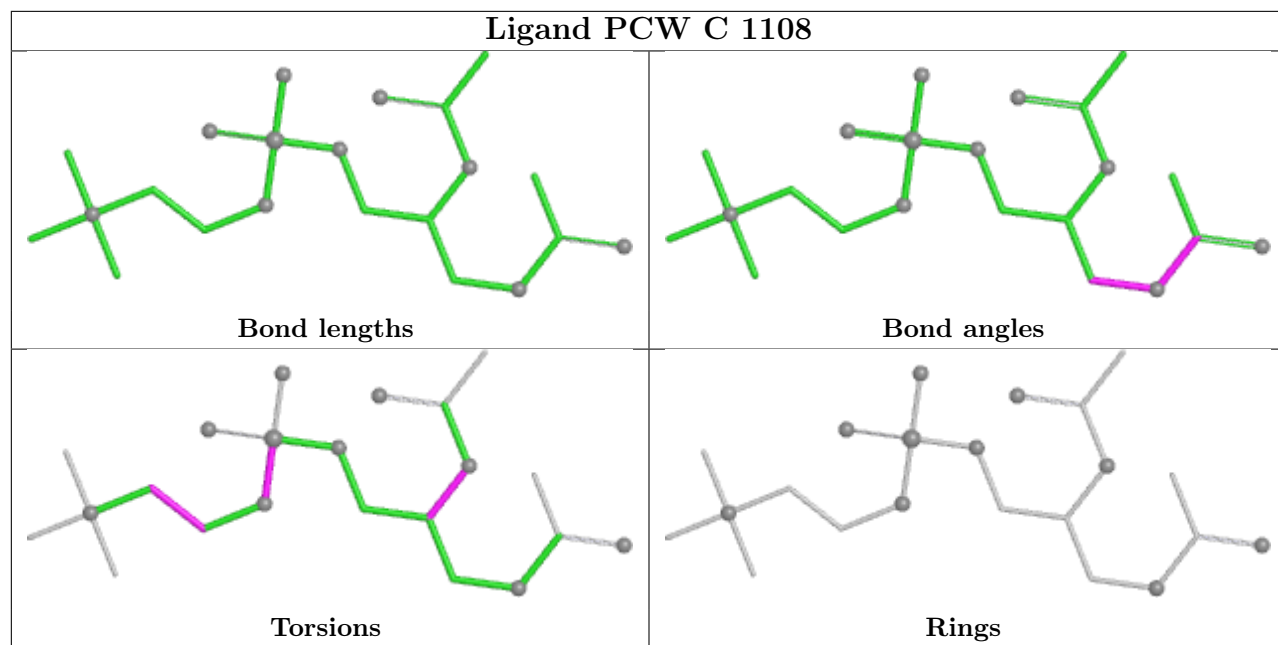
Ligand PCW A 1113



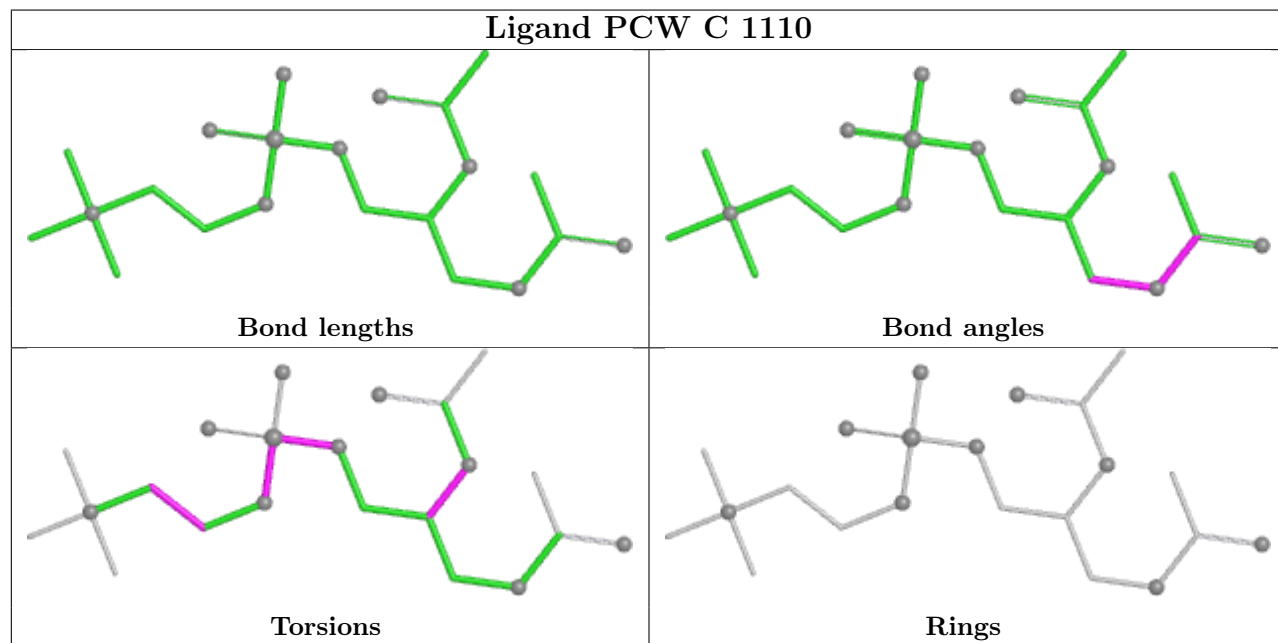
Ligand PCW C 1109



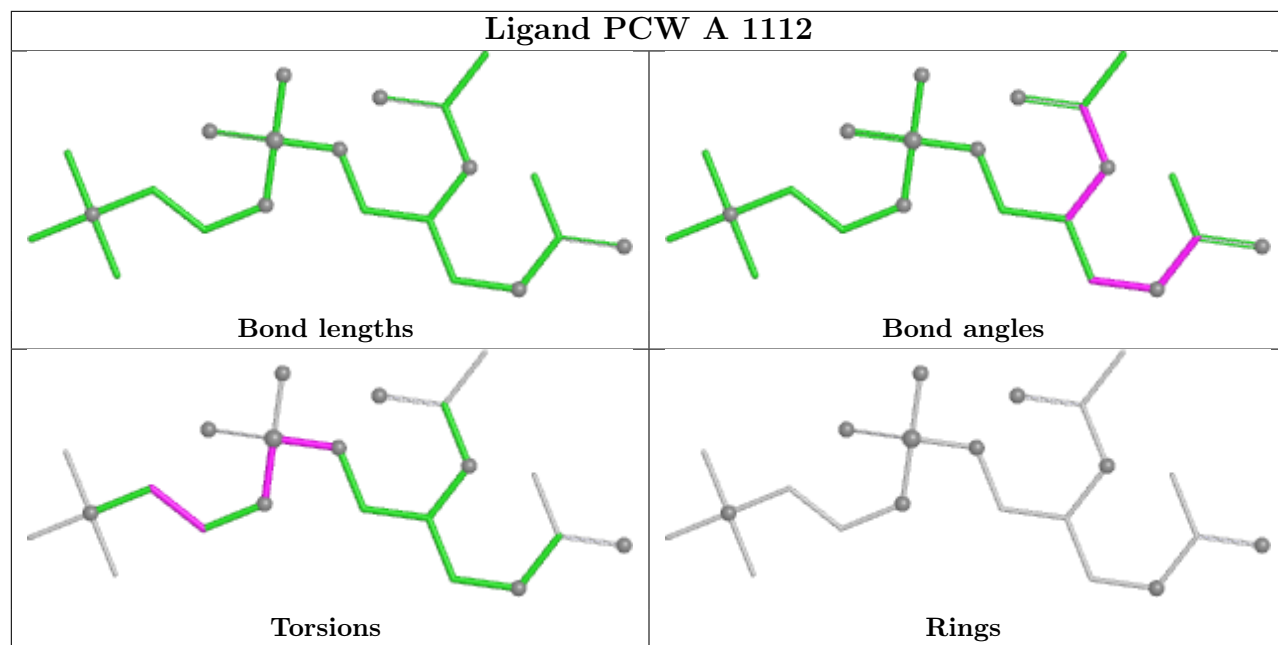
Ligand PCW C 1108



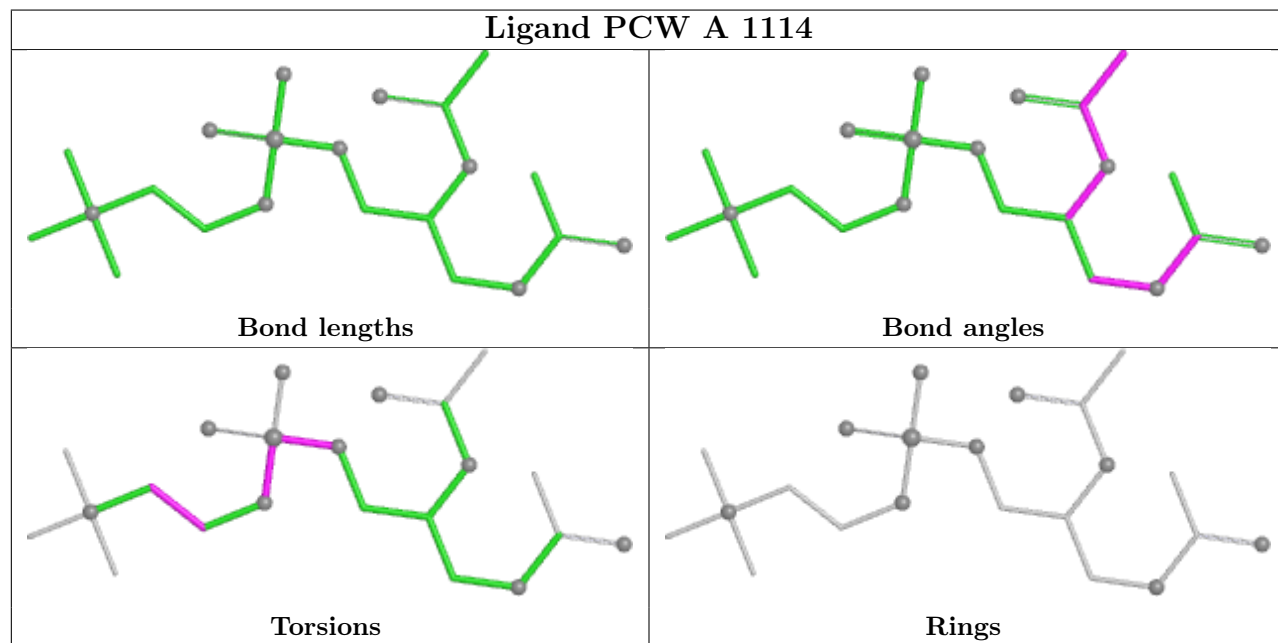
Ligand PCW C 1110

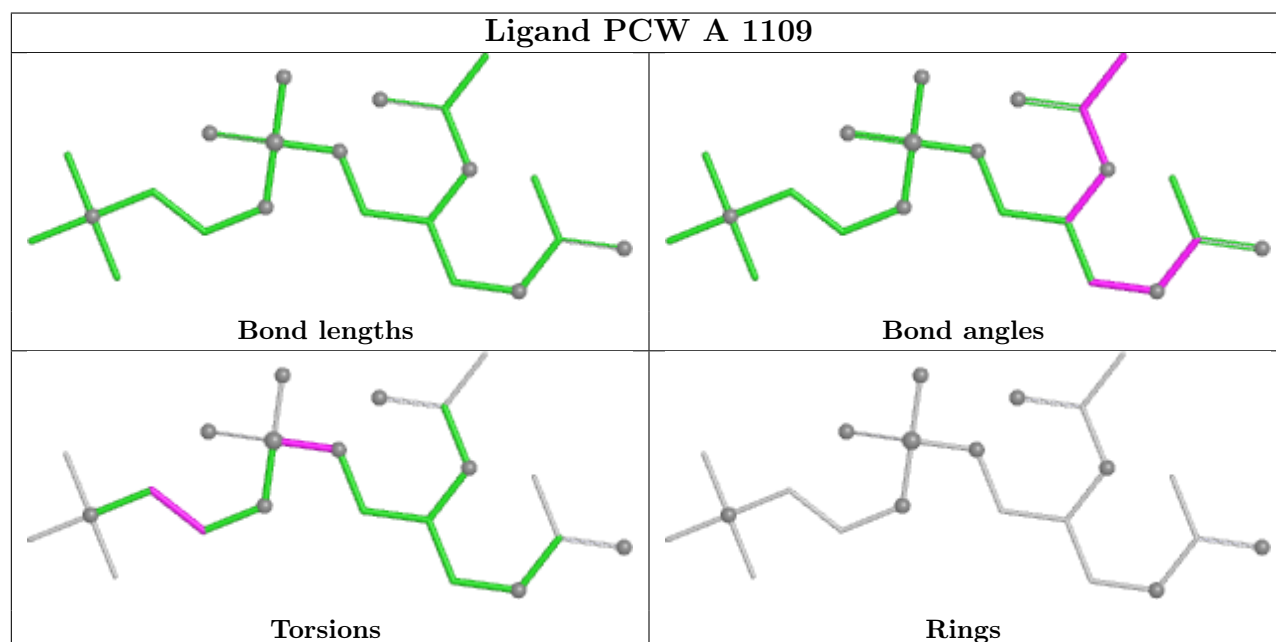
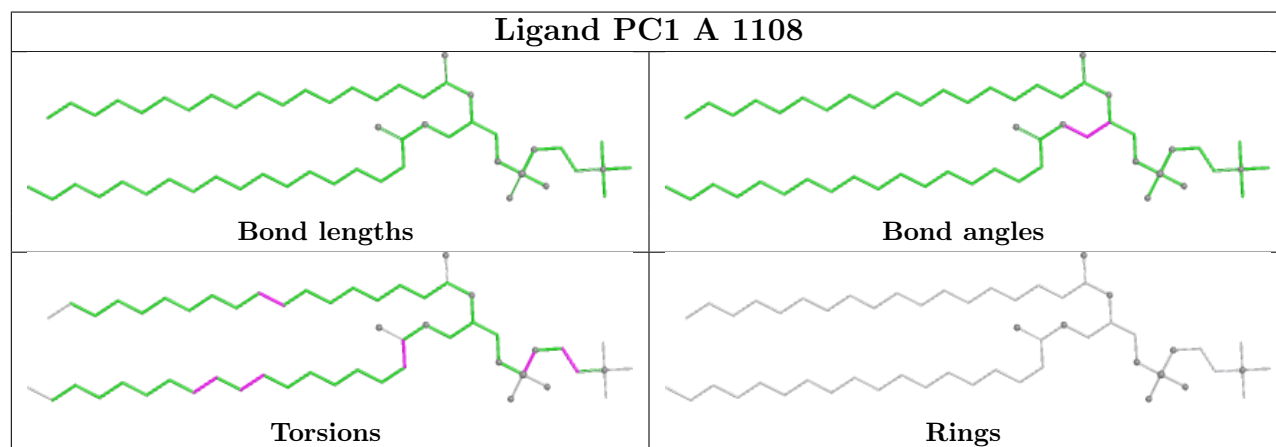
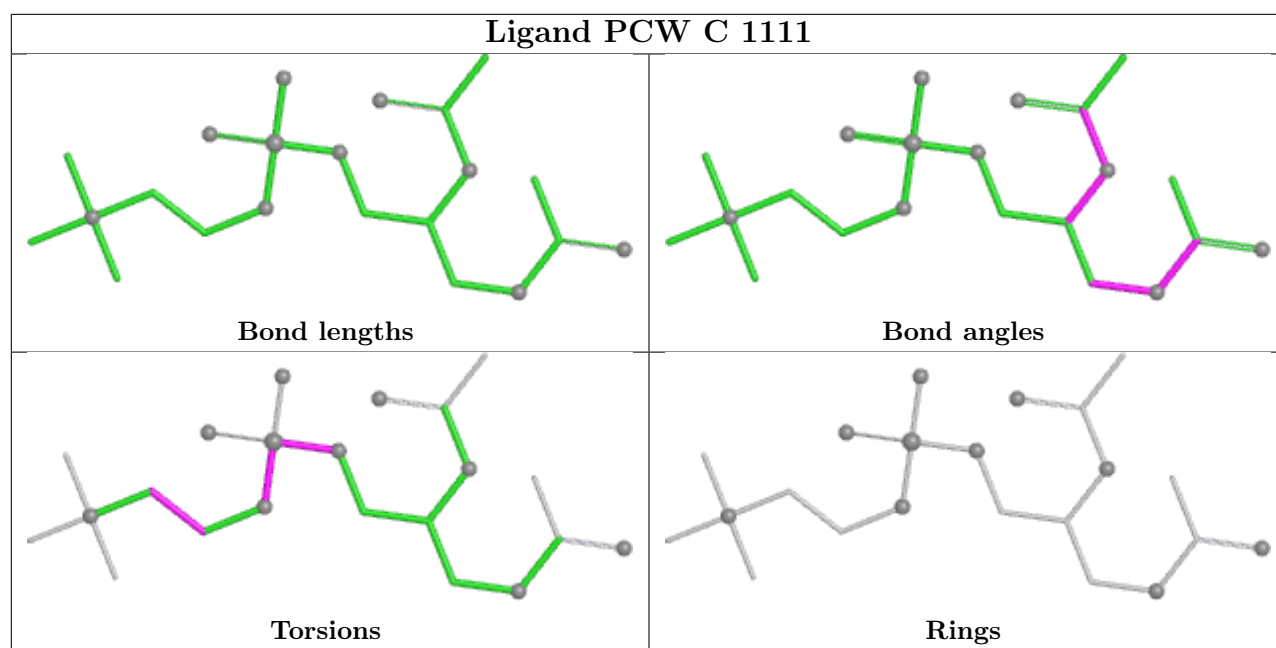


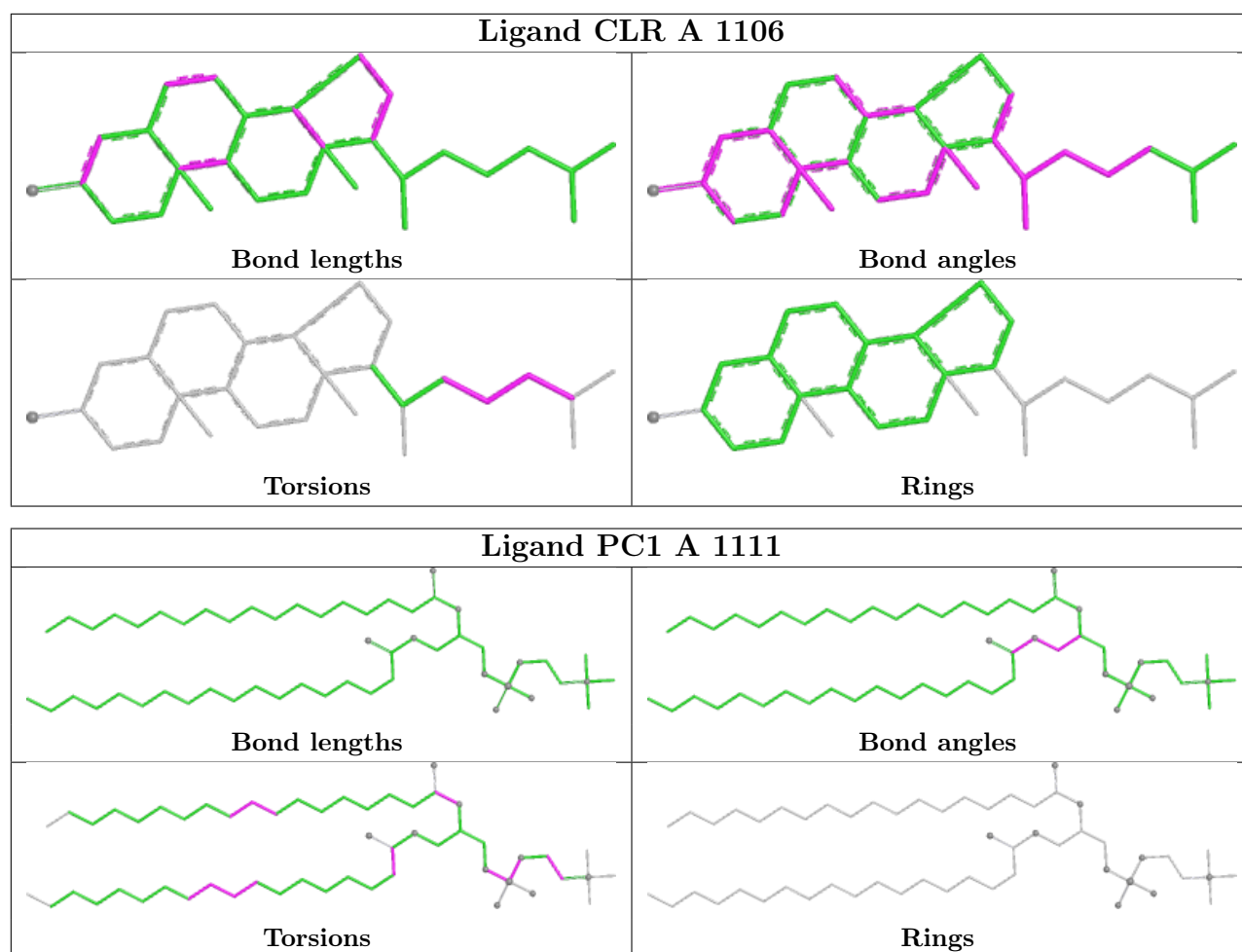
Ligand PCW A 1112



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%)	-0.10	28 (2%) 55 45	18, 59, 151, 249	0
1	C	995/1021 (97%)	-0.02	26 (2%) 57 47	28, 67, 158, 303	0
2	B	291/303 (96%)	0.35	15 (5%) 33 25	52, 95, 162, 212	0
2	D	291/303 (96%)	0.40	11 (3%) 44 35	52, 105, 172, 228	0
3	E	33/65 (50%)	-0.33	0 100 100	36, 50, 100, 101	0
3	G	36/65 (55%)	-0.15	0 100 100	34, 58, 113, 140	0
All	All	2641/2778 (95%)	0.03	80 (3%) 52 42	18, 73, 158, 303	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	265	THR	4.5
1	A	401	GLY	4.1
2	B	122	ILE	3.6
1	A	138	CYS	3.6
1	A	487	LYS	3.5

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

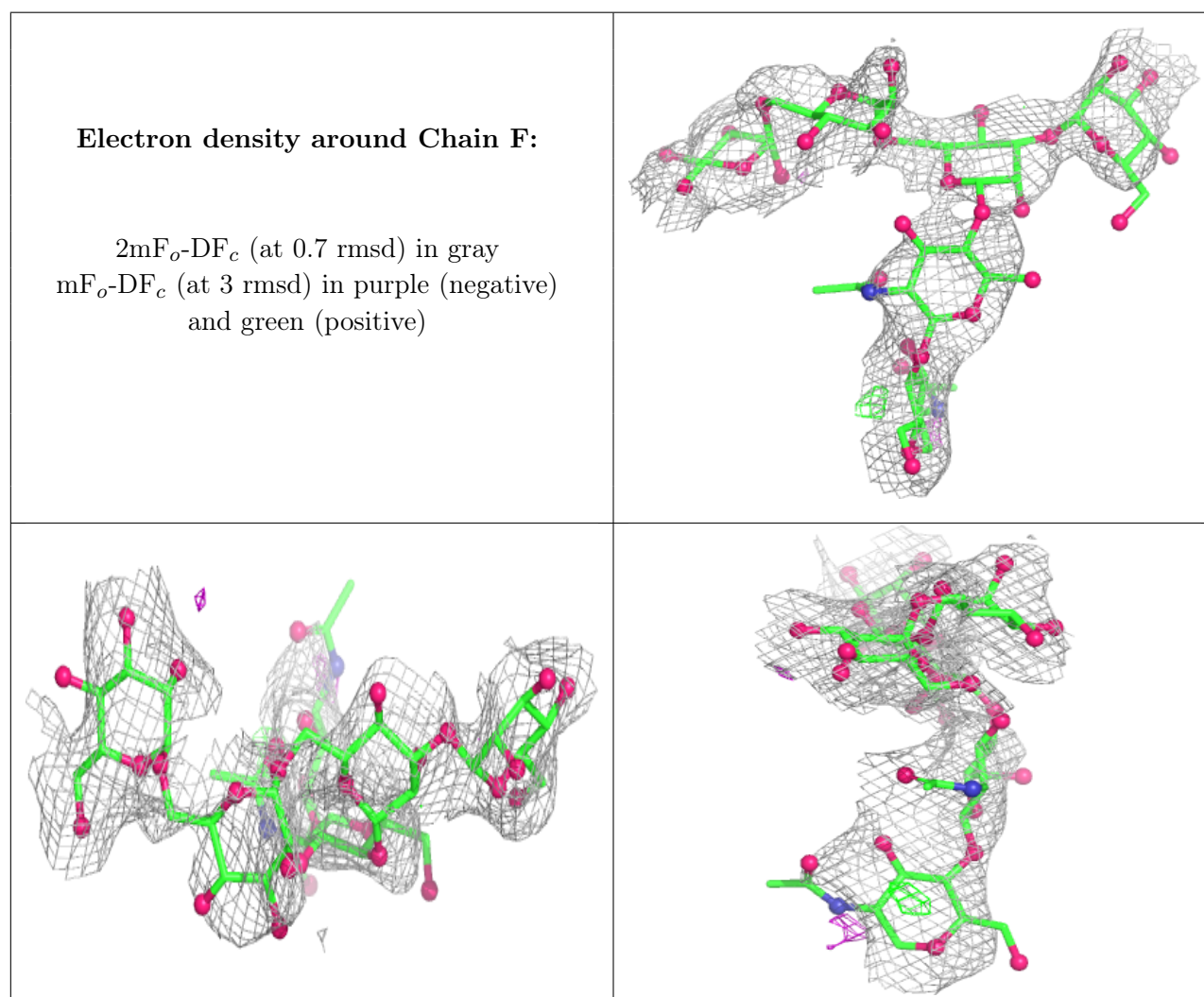
There are no non-standard protein/DNA/RNA residues in this entry.

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.

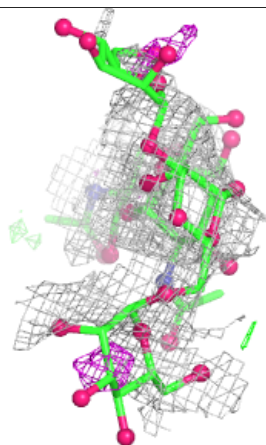
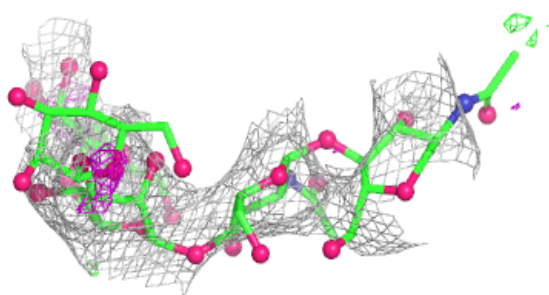
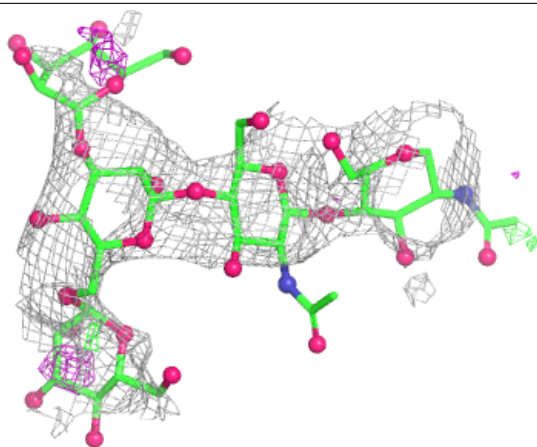
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	F	1	14/15	-	-	91,109,118,123	0
4	NAG	F	2	14/15	-	-	125,132,138,140	0
4	BMA	F	3	11/12	-	-	127,131,138,140	0
4	MAN	F	4	11/12	-	-	123,132,136,136	0
4	MAN	F	5	11/12	-	-	98,113,126,130	0
4	MAN	F	6	11/12	-	-	119,128,130,131	0
6	NAG	I	2	14/15	0.24	0.14	119,132,138,141	0
5	MAN	H	5	11/12	0.29	0.17	149,152,155,155	0
5	NAG	H	1	14/15	0.30	0.18	122,134,143,151	0
5	MAN	H	4	11/12	0.36	0.15	129,142,147,147	0
5	BMA	H	3	11/12	0.38	0.13	148,150,153,153	0
5	NAG	H	2	14/15	0.65	0.12	138,152,154,155	0
6	NAG	I	1	14/15	0.71	0.14	109,128,131,132	0

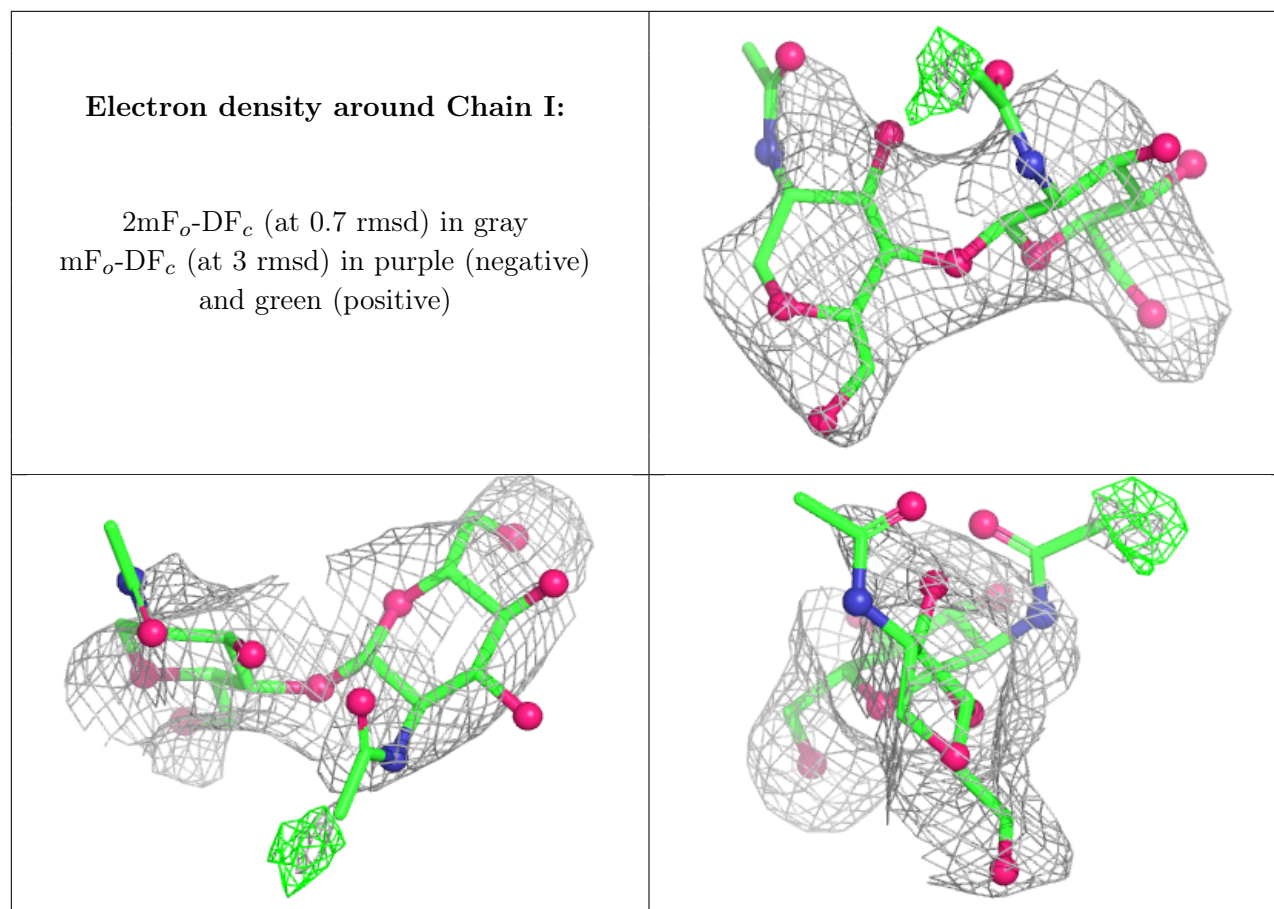
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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($\text{\AA}^2$)	Q<0.9
11	PCW	C	1113	22/54	0.37	0.18	98,136,160,164	0
11	PCW	B	401	22/54	0.39	0.16	117,127,163,165	0
12	NAG	D	402	14/15	0.48	0.14	125,134,147,152	0
11	PCW	A	1116	22/54	0.50	0.19	119,151,157,160	0
11	PCW	C	1110	22/54	0.51	0.18	111,143,151,152	0
11	PCW	A	1115	22/54	0.53	0.19	112,135,148,153	0
11	PCW	C	1111	22/54	0.53	0.17	74,127,149,150	0
11	PCW	C	1112	22/54	0.59	0.21	84,120,138,145	0
11	PCW	A	1113	22/54	0.60	0.16	114,129,150,152	0
11	PCW	A	1109	22/54	0.61	0.18	115,135,151,154	0
11	PCW	C	1109	22/54	0.64	0.18	99,124,153,154	0
11	PCW	C	1107	22/54	0.66	0.18	84,111,146,149	0
11	PCW	C	1108	22/54	0.66	0.19	106,122,130,138	0

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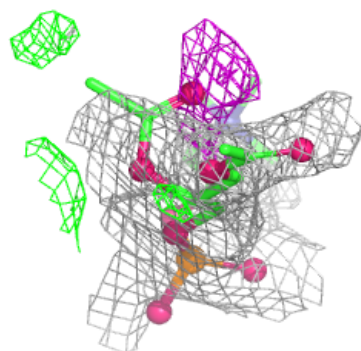
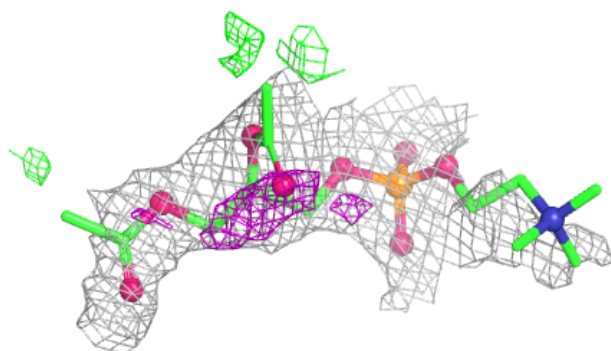
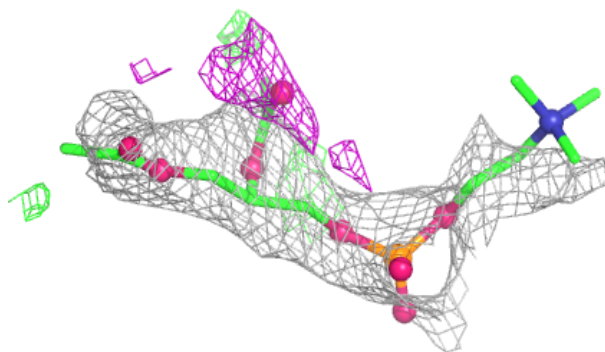
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	PCW	C	1114	22/54	0.67	0.17	95,130,146,151	0
11	PCW	A	1114	22/54	0.72	0.17	109,129,141,146	0
9	CLR	D	401	28/28	0.74	0.15	71,87,93,97	0
10	PC1	A	1108	54/54	0.76	0.13	72,96,122,127	0
10	PC1	A	1110	54/54	0.81	0.15	58,71,109,115	0
9	CLR	B	402	28/28	0.81	0.14	87,99,107,112	0
11	PCW	A	1112	22/54	0.83	0.16	72,117,123,126	0
8	NA	C	1103	1/1	0.84	0.12	88,88,88,88	0
8	NA	A	1103	1/1	0.86	0.10	73,73,73,73	0
10	PC1	A	1111	54/54	0.86	0.15	42,79,107,113	0
9	CLR	A	1106	28/28	0.88	0.12	65,77,87,95	0
13	DMU	E	102	33/33	0.88	0.13	28,55,78,85	0
8	NA	C	1102	1/1	0.89	0.09	76,76,76,76	0
8	NA	A	1102	1/1	0.90	0.06	61,61,61,61	0
9	CLR	A	1107	28/28	0.93	0.09	25,46,57,64	0
8	NA	C	1104	1/1	0.94	0.07	67,67,67,67	0
9	CLR	E	101	28/28	0.94	0.09	22,40,52,62	0
8	NA	C	1105	1/1	0.95	0.09	62,62,62,62	0
9	CLR	C	1106	28/28	0.95	0.10	25,33,84,91	0
7	MN	C	1101	1/1	0.97	0.04	69,69,69,69	0
8	NA	A	1105	1/1	0.97	0.07	47,47,47,47	0
7	MN	A	1101	1/1	0.98	0.02	58,58,58,58	0
8	NA	A	1104	1/1	0.99	0.04	49,49,49,49	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.

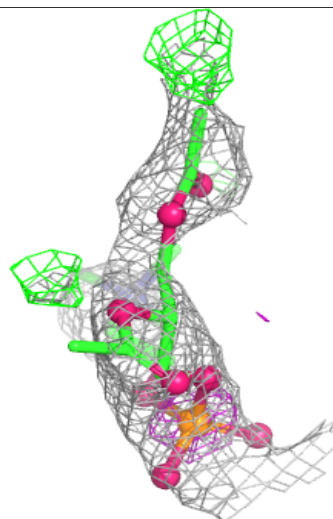
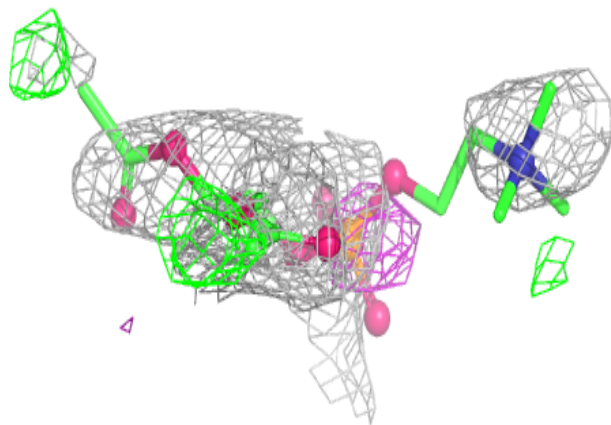
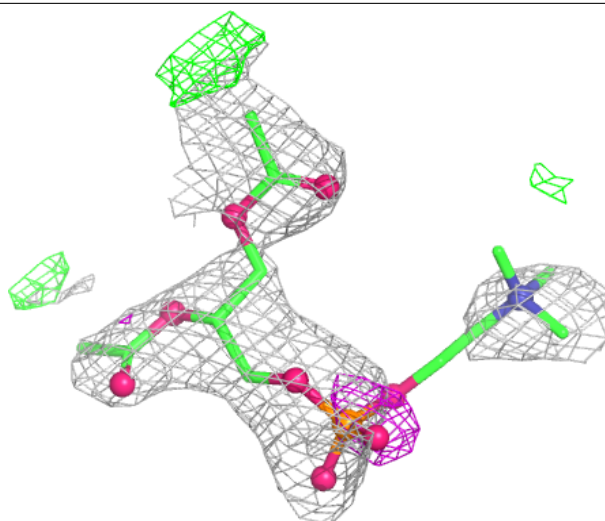
Electron density around PCW C 1113:

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



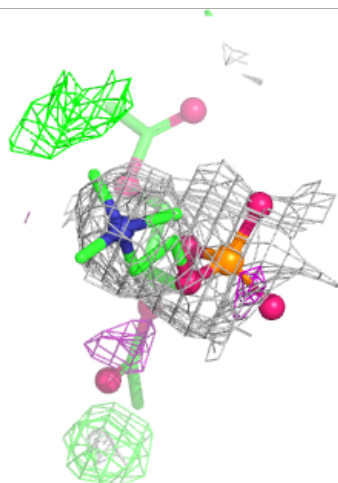
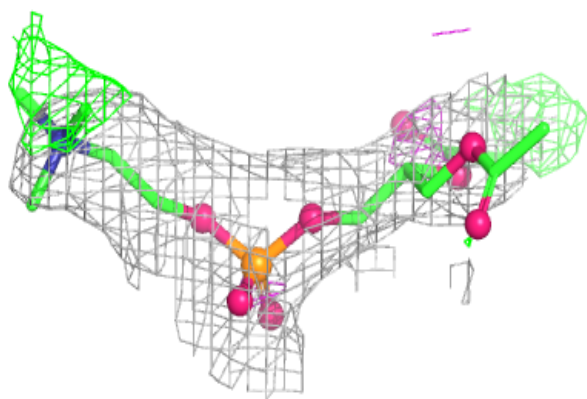
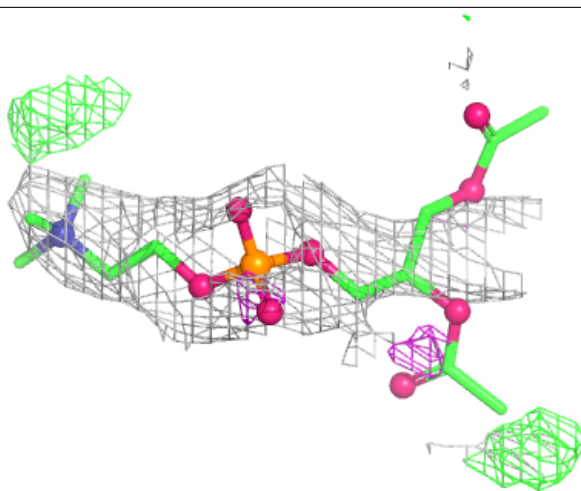
Electron density around PCW B 401:

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



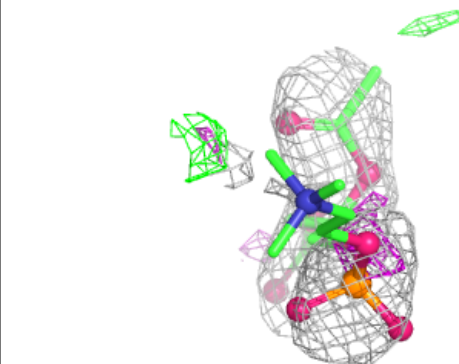
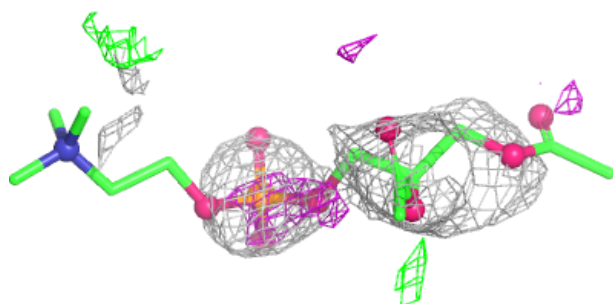
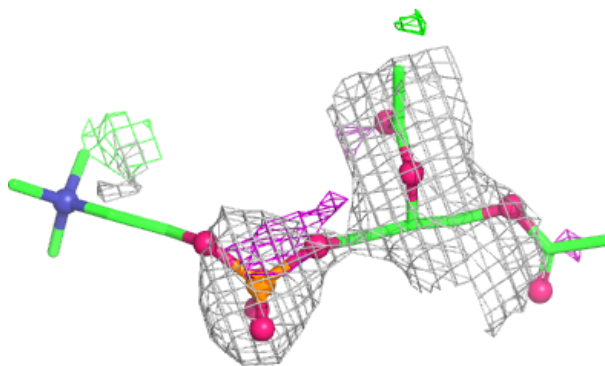
Electron density around PCW A 1116:

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

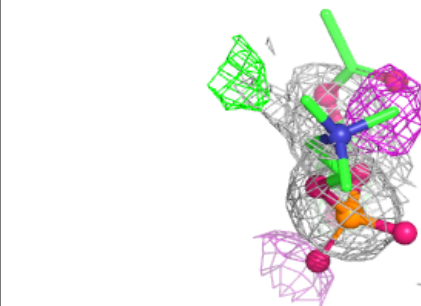
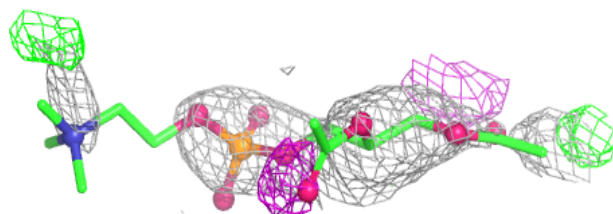
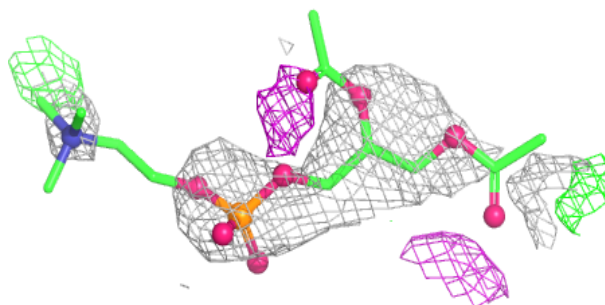


Electron density around PCW C 1110:

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

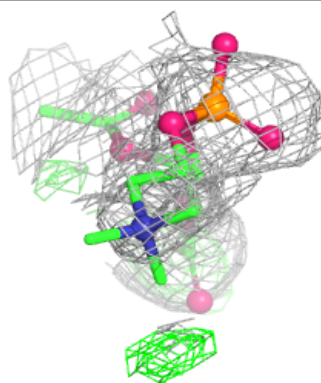
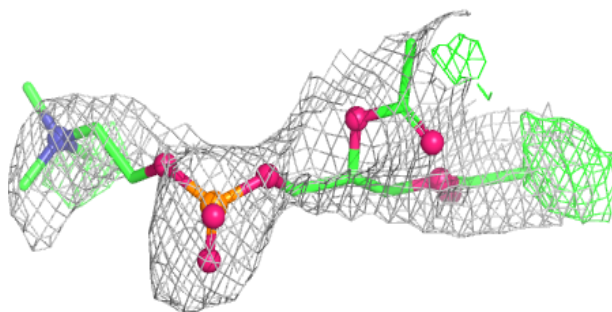
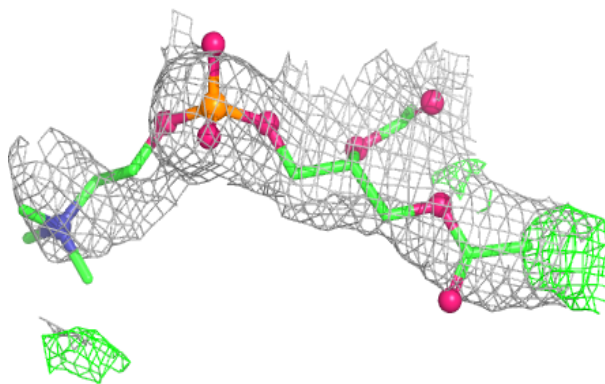
**Electron density around PCW A 1115:**

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

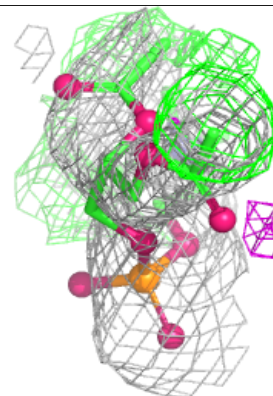
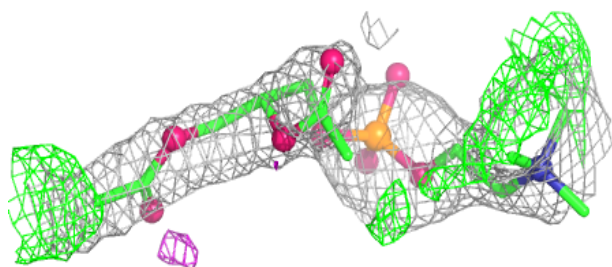
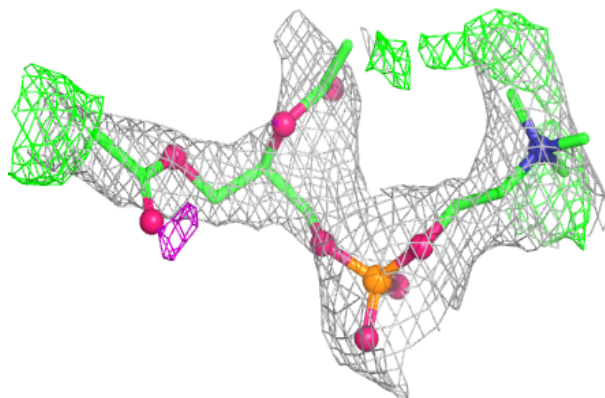


Electron density around PCW C 1111:

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

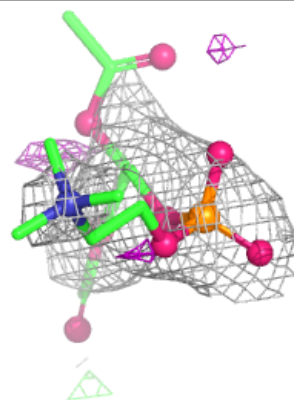
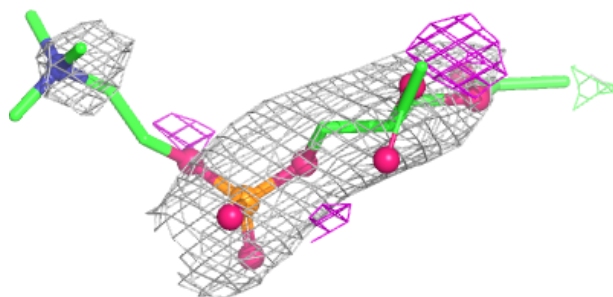
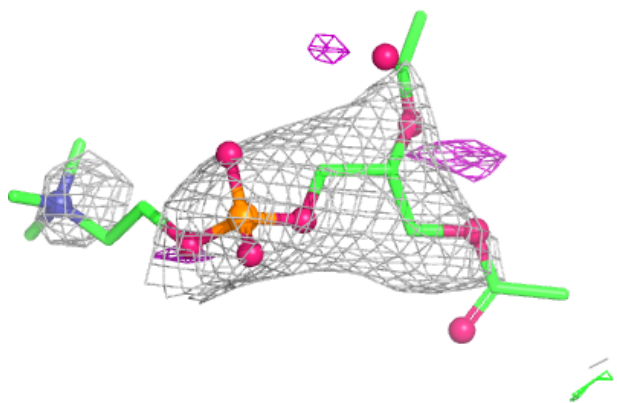
**Electron density around PCW C 1112:**

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

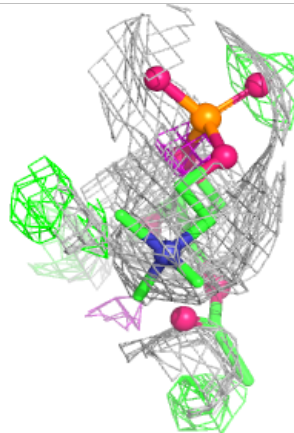
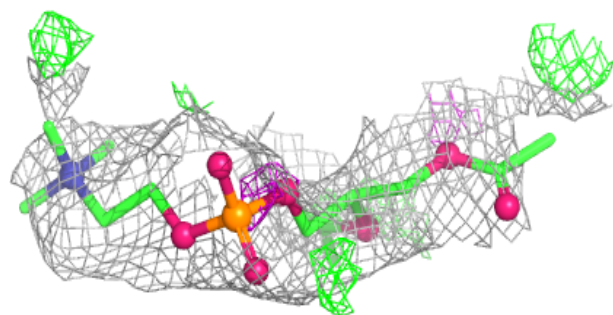
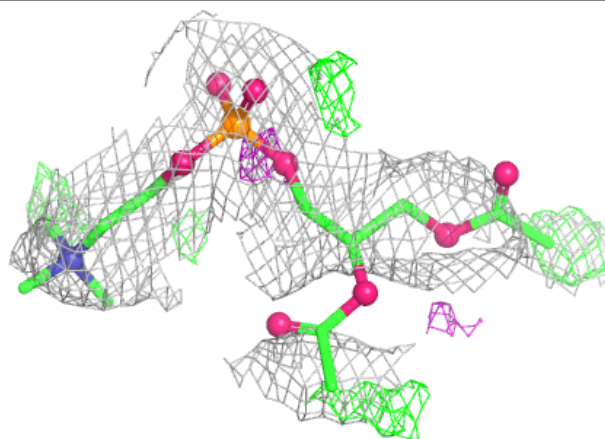


Electron density around PCW A 1113:

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and green (positive)

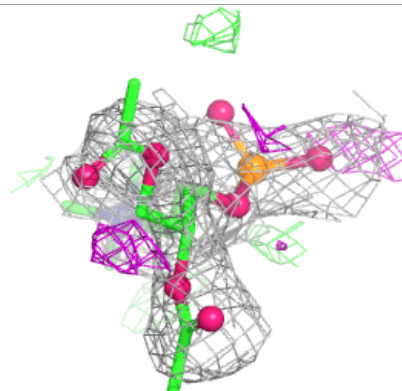
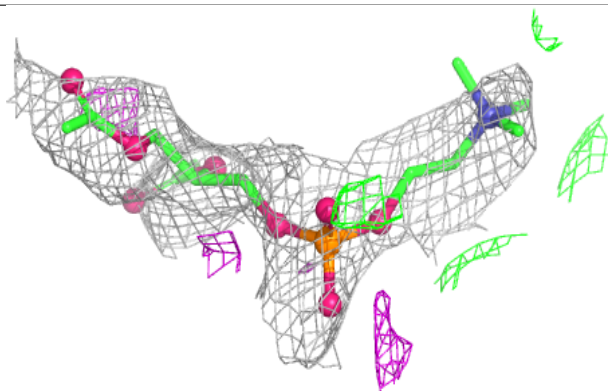
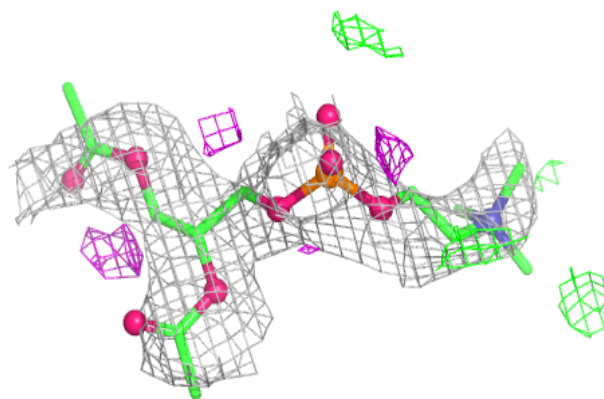
**Electron density around PCW A 1109:**

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

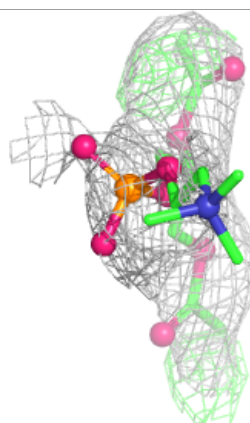
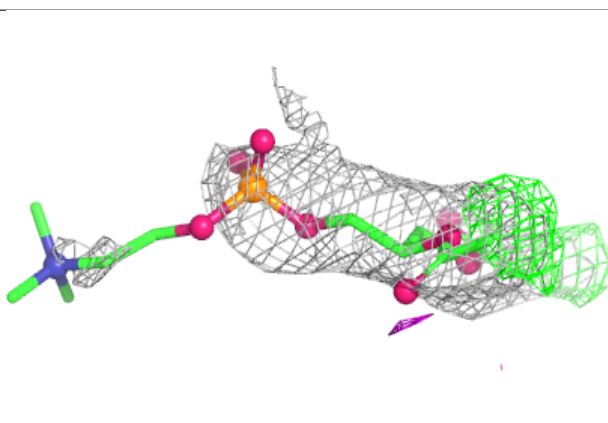
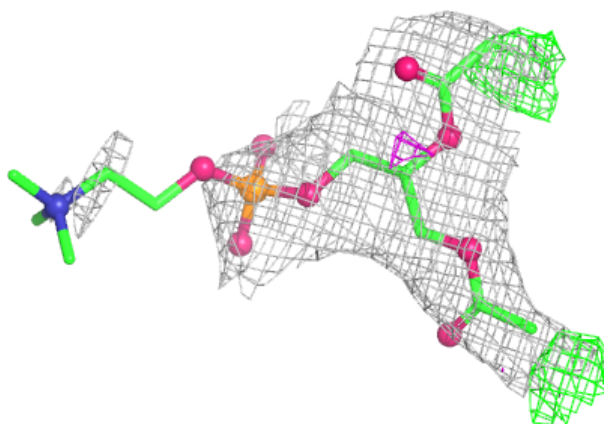


Electron density around PCW C 1109:

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and green (positive)

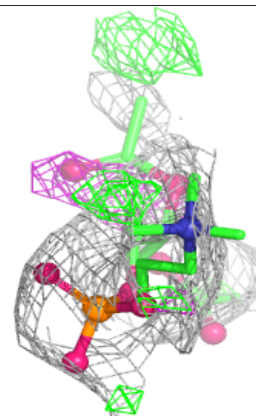
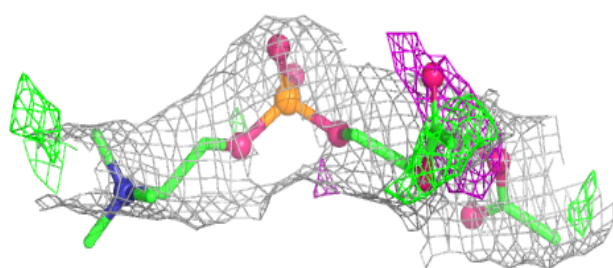
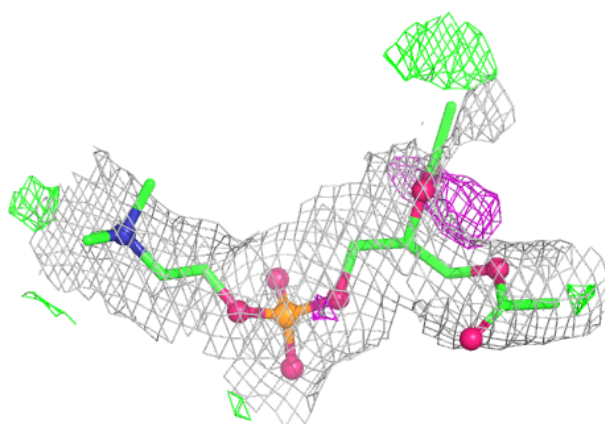
**Electron density around PCW C 1107:**

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

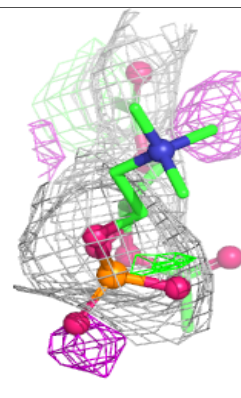
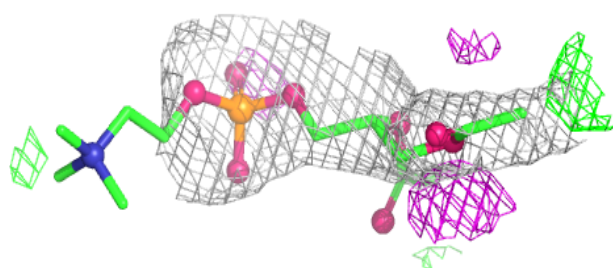
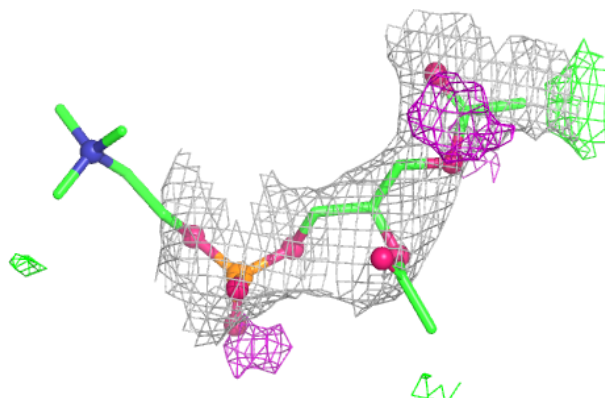


Electron density around PCW C 1108:

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and green (positive)

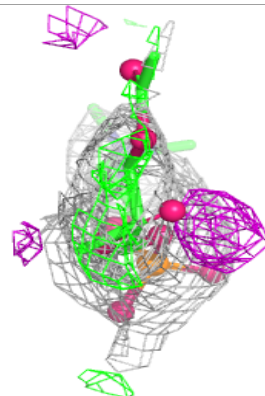
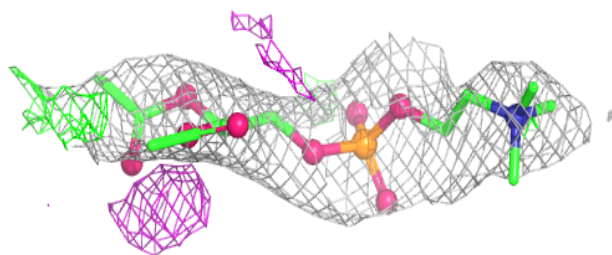
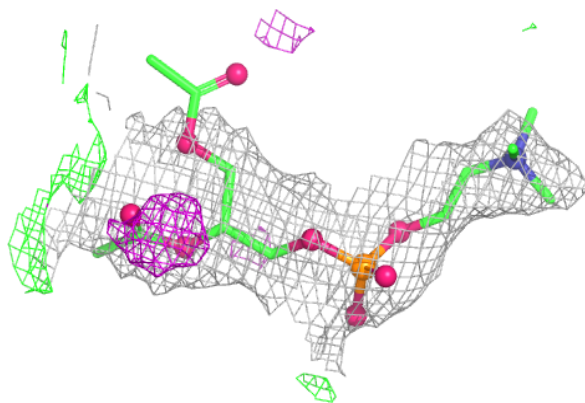
**Electron density around PCW C 1114:**

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and green (positive)

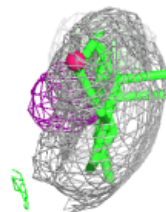
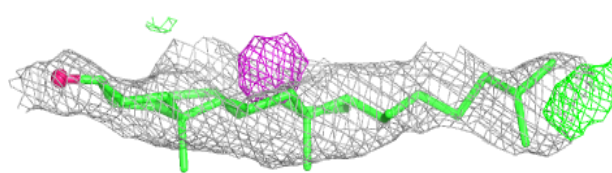
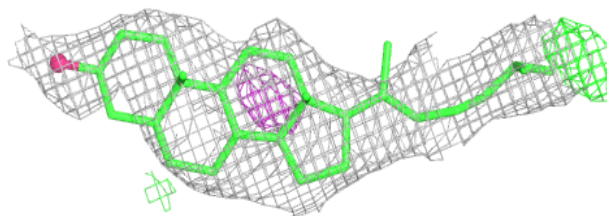


Electron density around PCW A 1114:

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and green (positive)

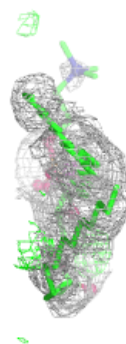
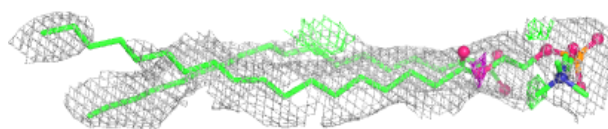
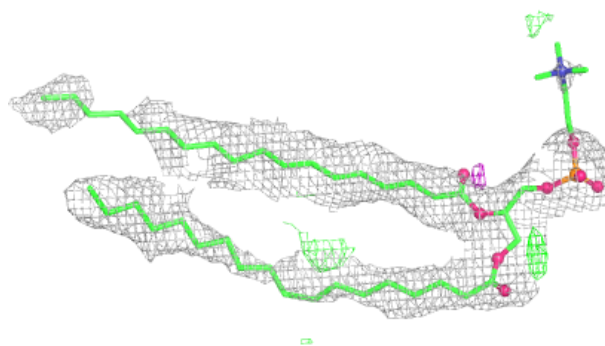
**Electron density around CLR D 401:**

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

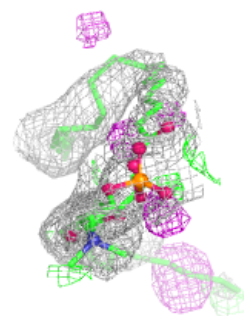
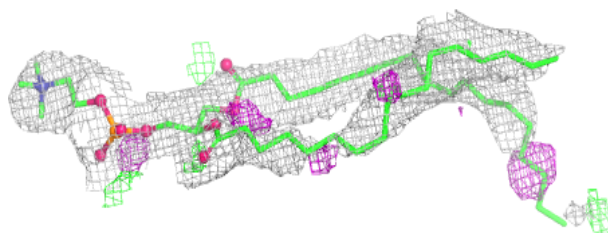
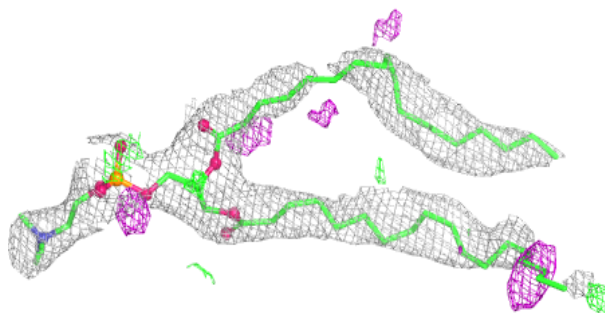


Electron density around PC1 A 1108:

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

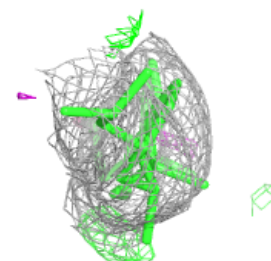
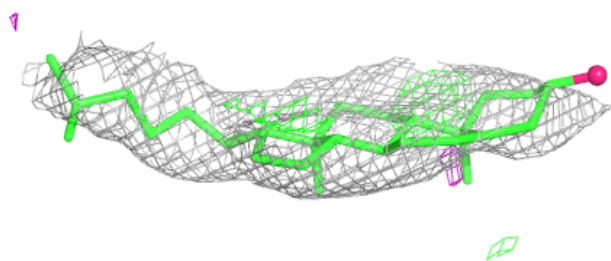
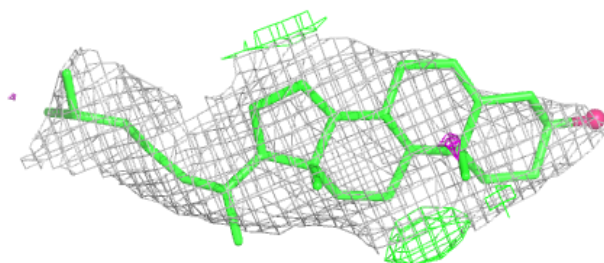
**Electron density around PC1 A 1110:**

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and green (positive)

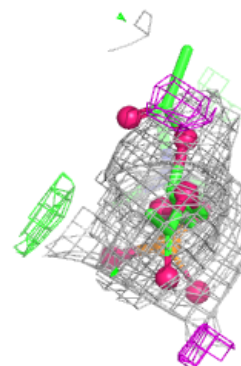
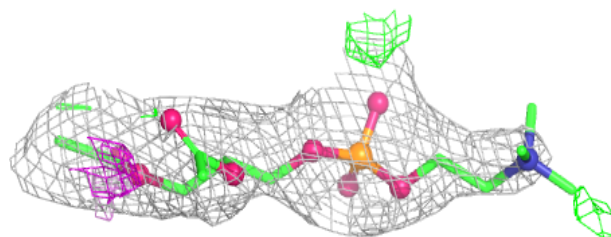
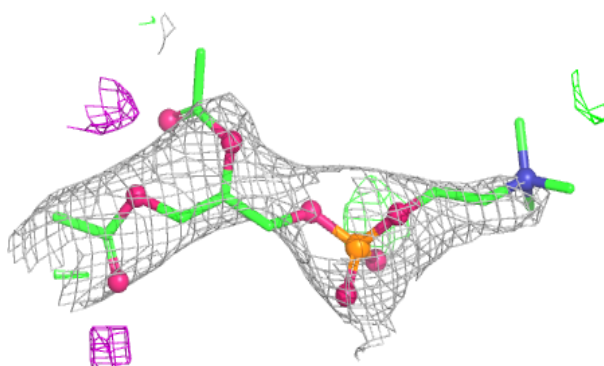


Electron density around CLR B 402:

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

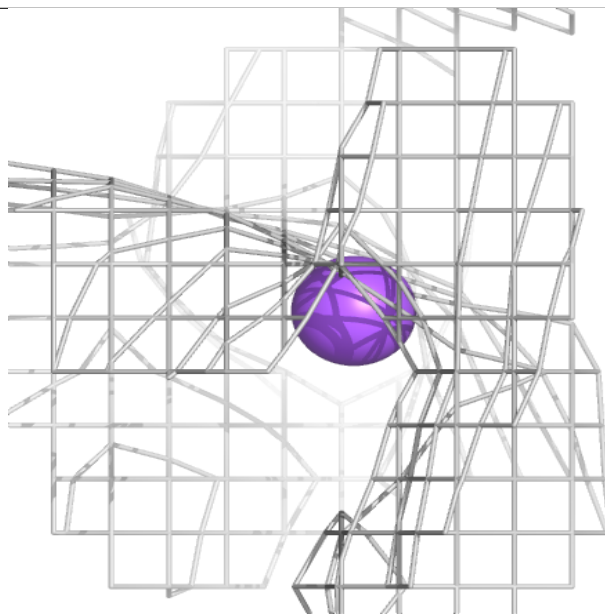
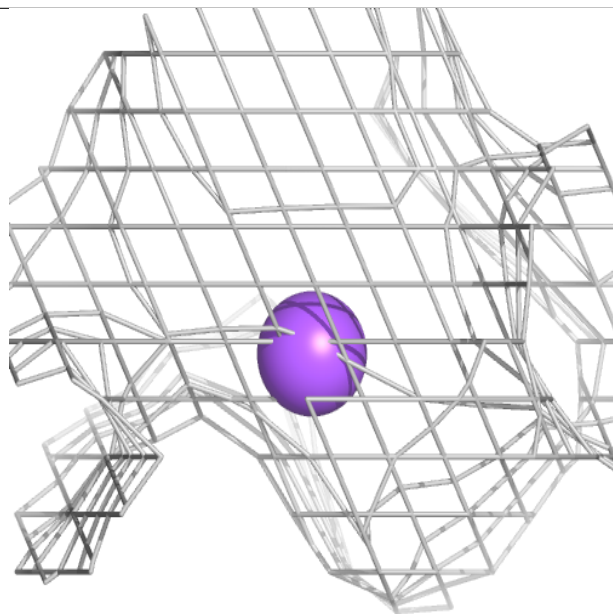
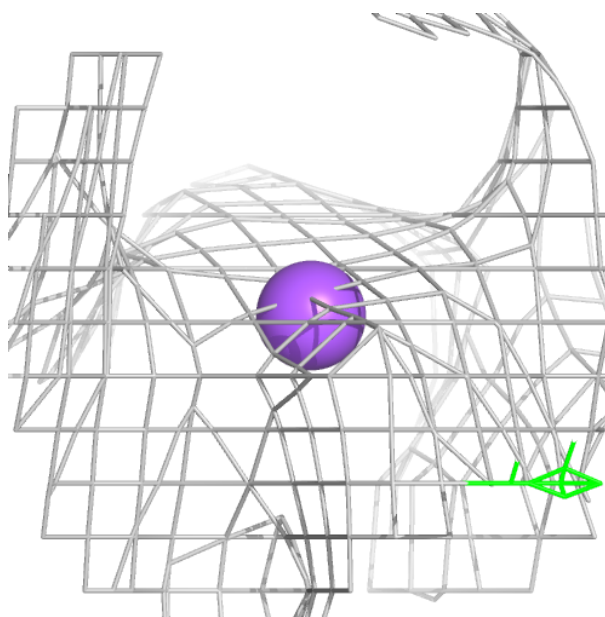
**Electron density around PCW A 1112:**

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



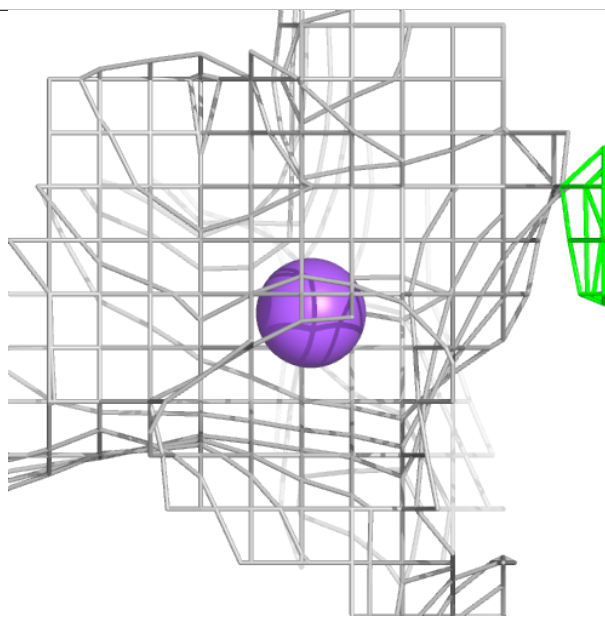
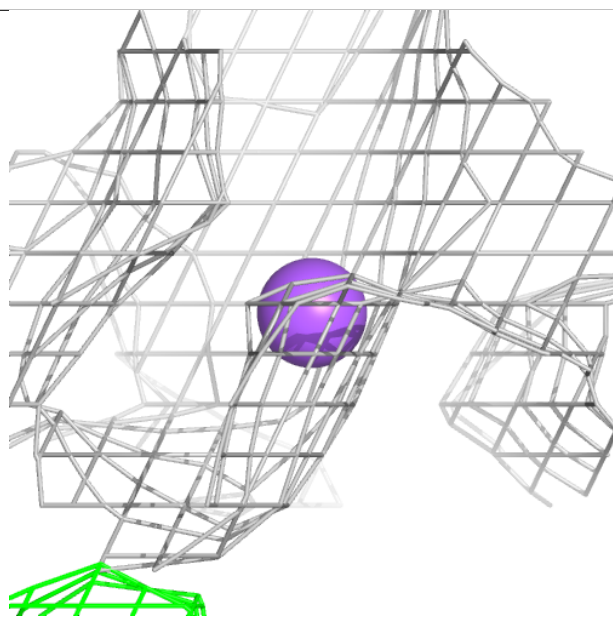
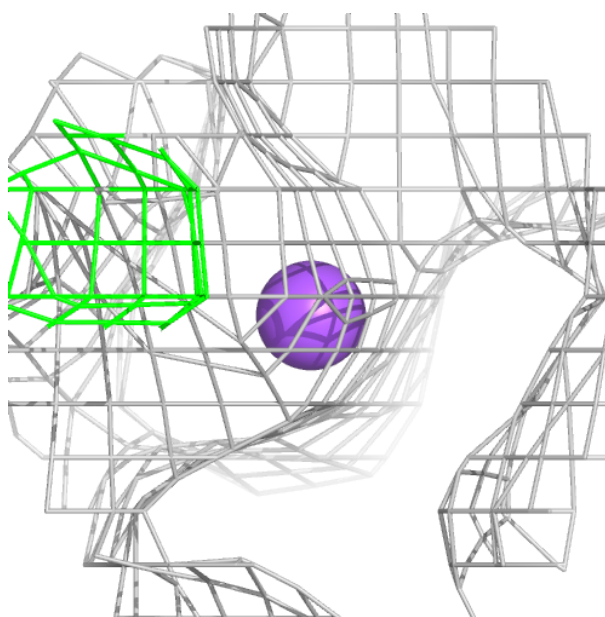
Electron density around NA C 1103:

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



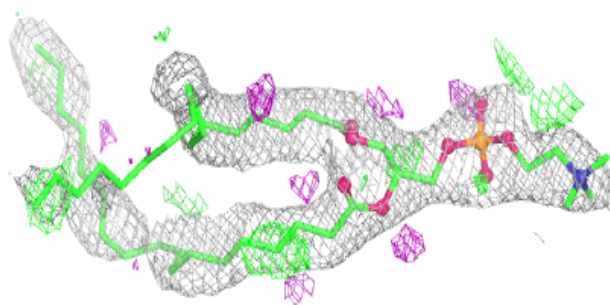
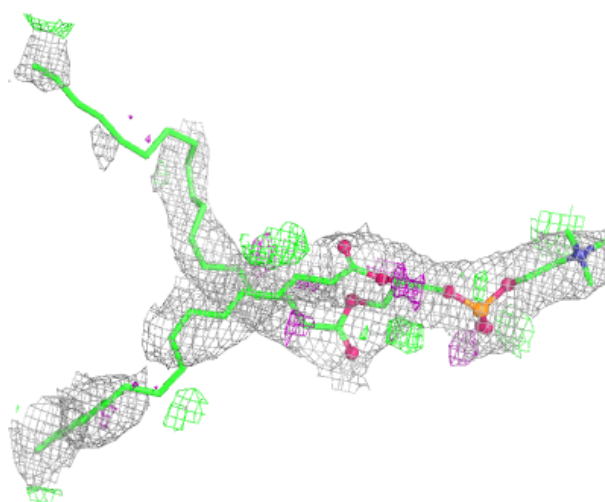
Electron density around NA A 1103:

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



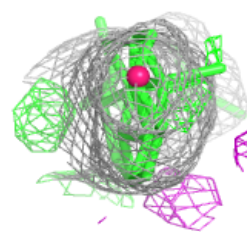
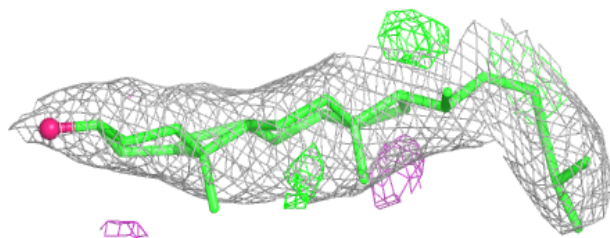
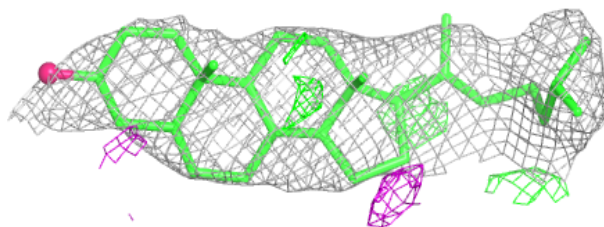
Electron density around PC1 A 1111:

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

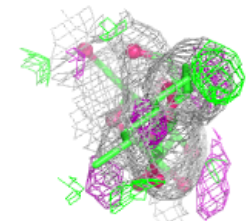
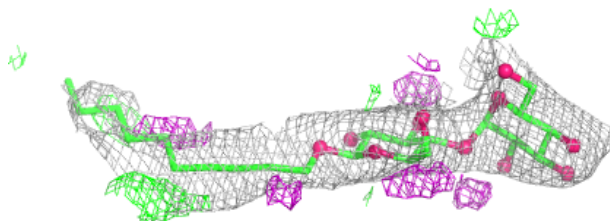
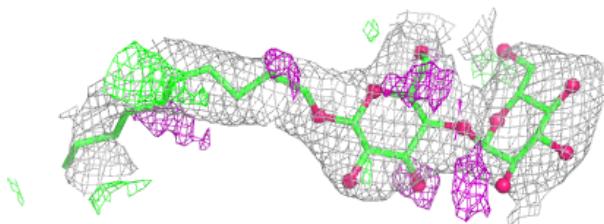


Electron density around CLR A 1106:

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

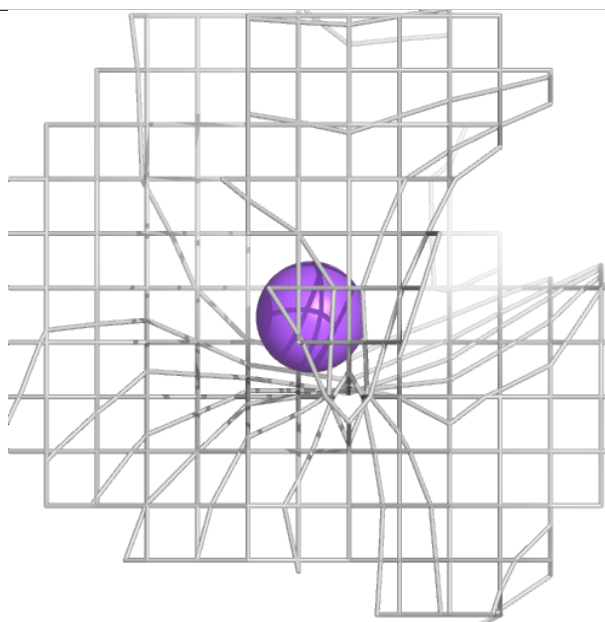
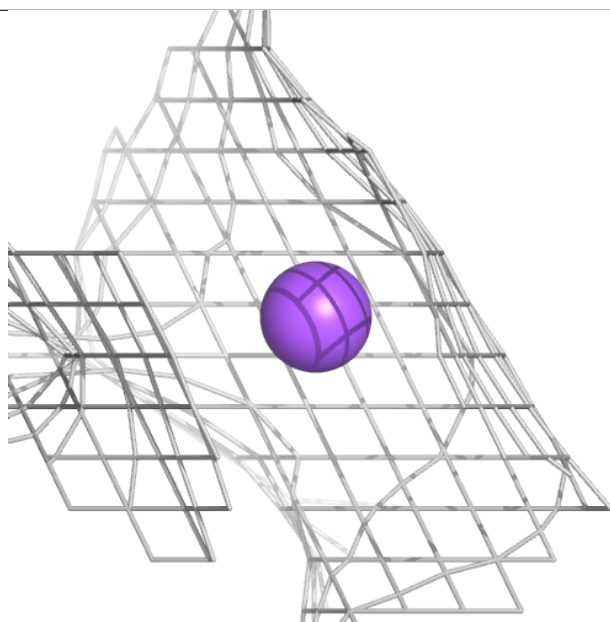
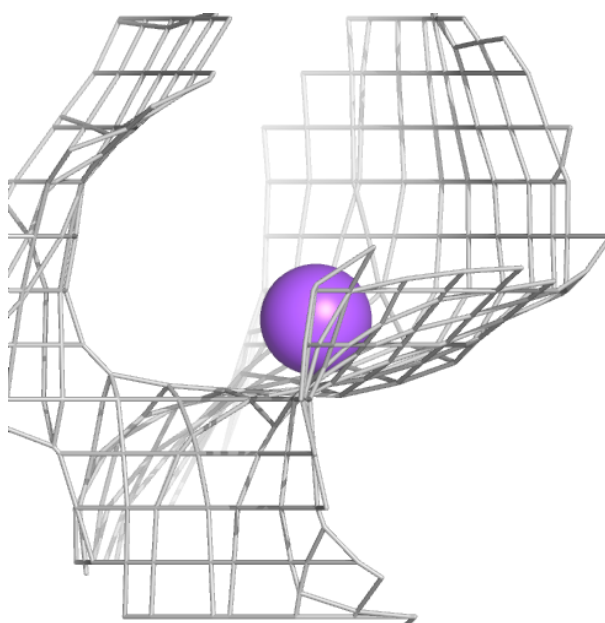
**Electron density around DMU E 102:**

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



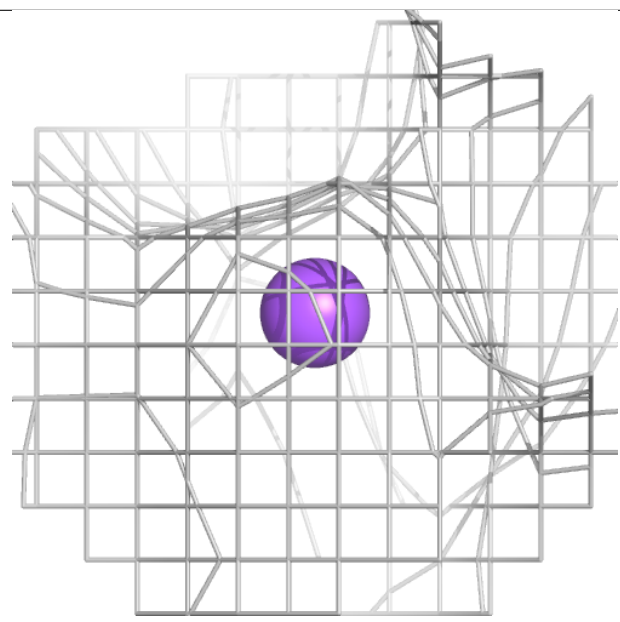
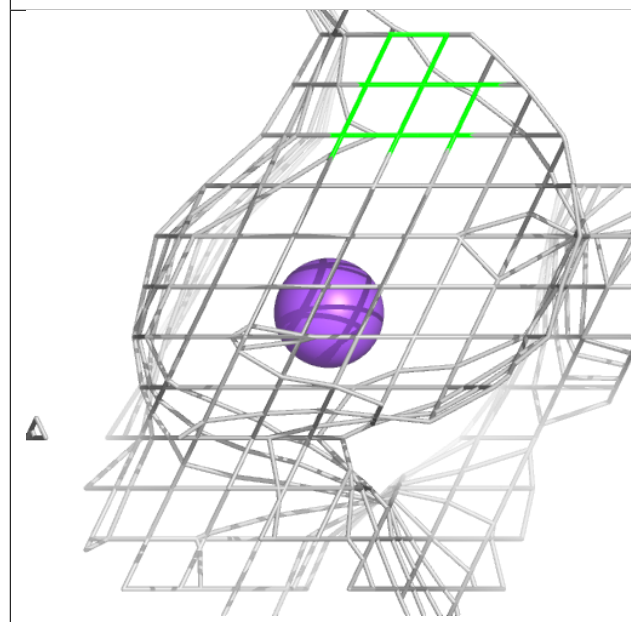
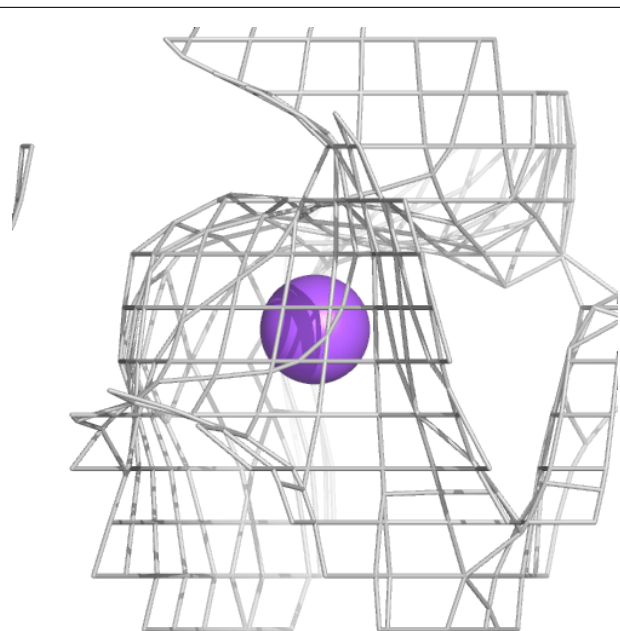
Electron density around NA C 1102:

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



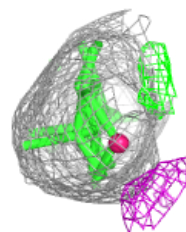
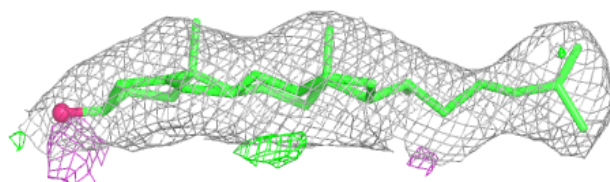
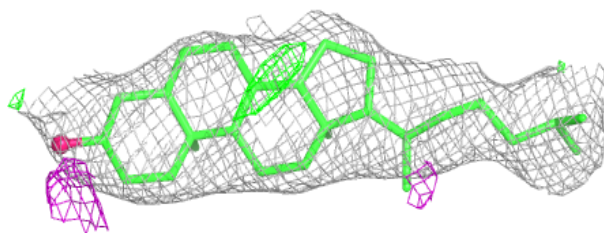
Electron density around NA A 1102:

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



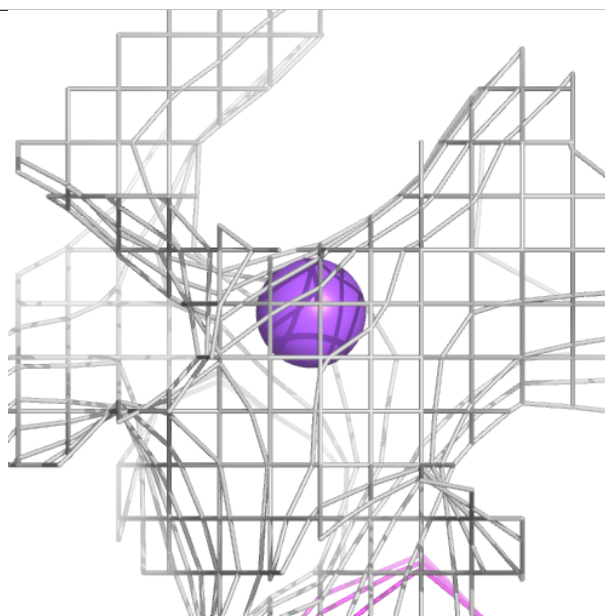
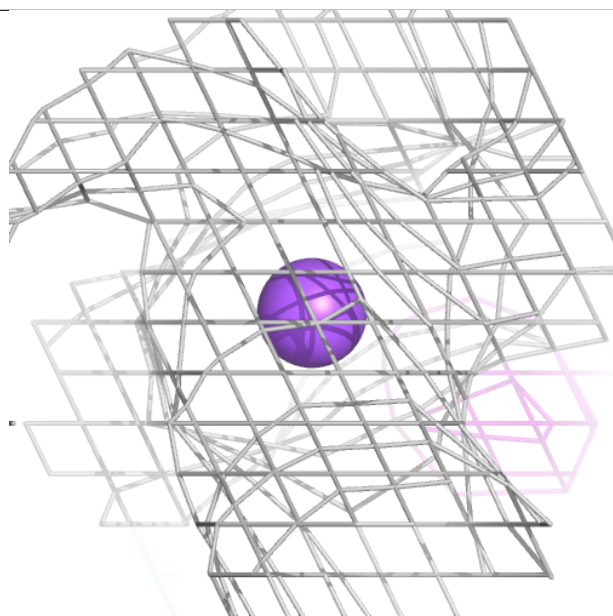
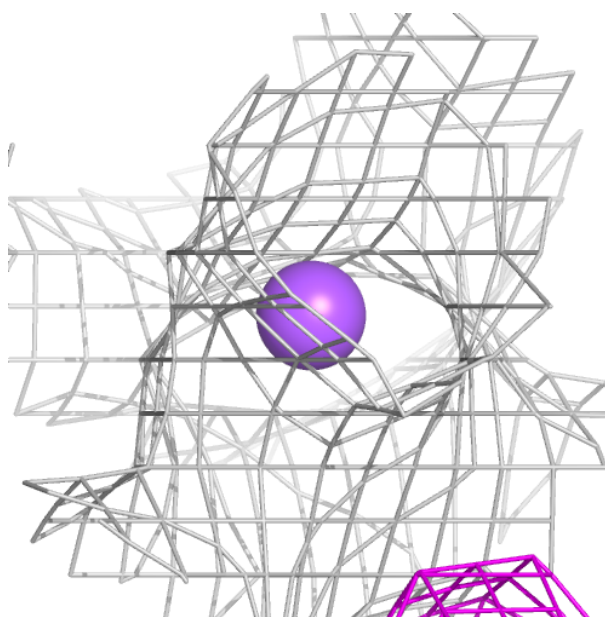
Electron density around CLR A 1107:

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



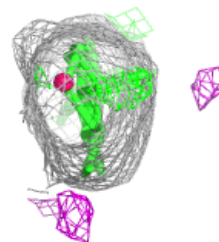
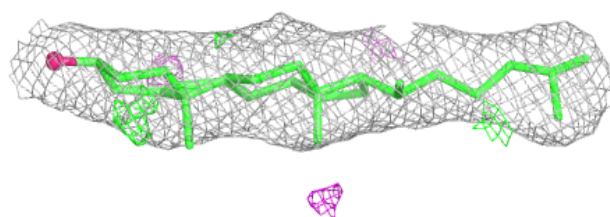
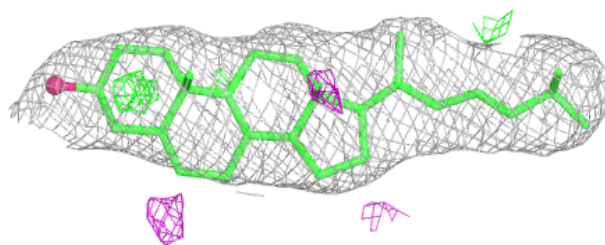
Electron density around NA C 1104:

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



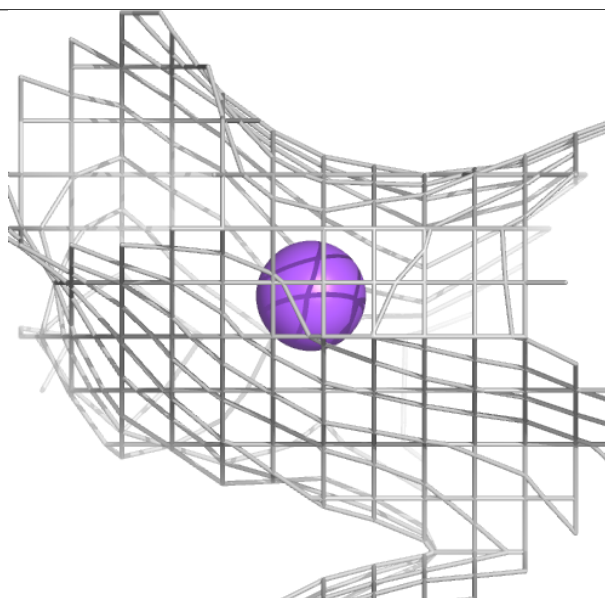
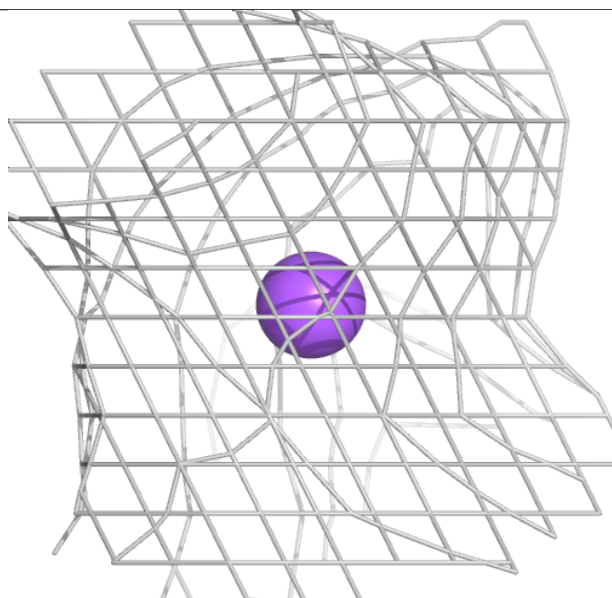
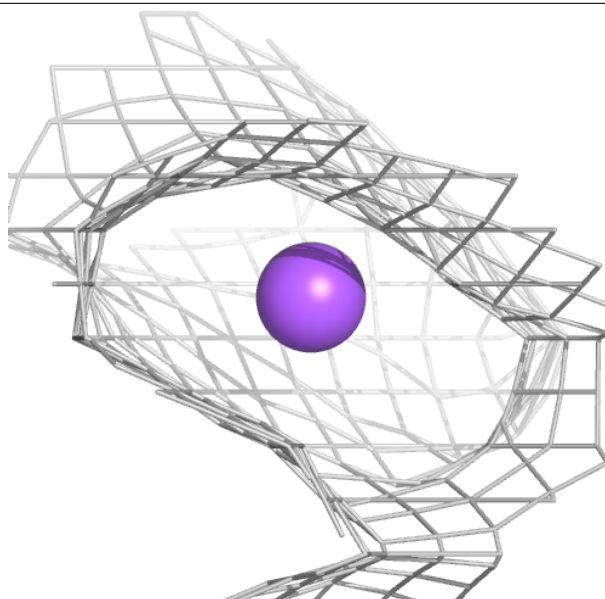
Electron density around CLR E 101:

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



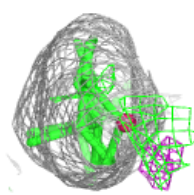
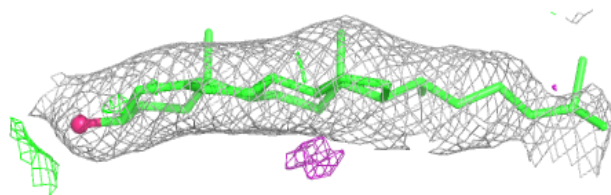
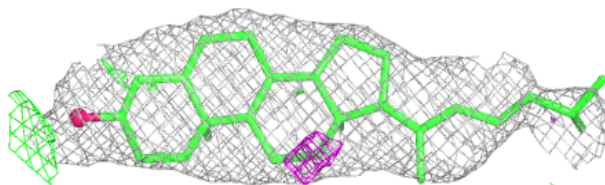
Electron density around NA C 1105:

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



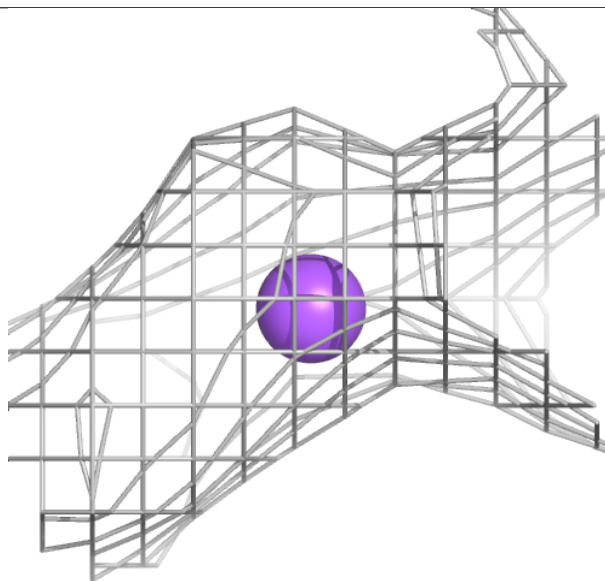
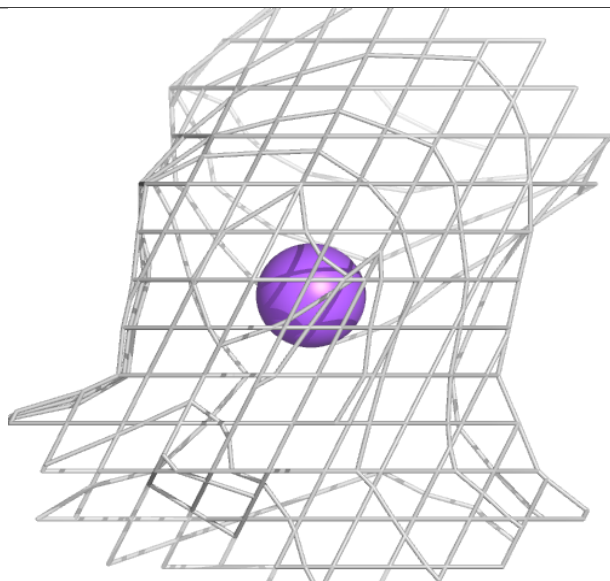
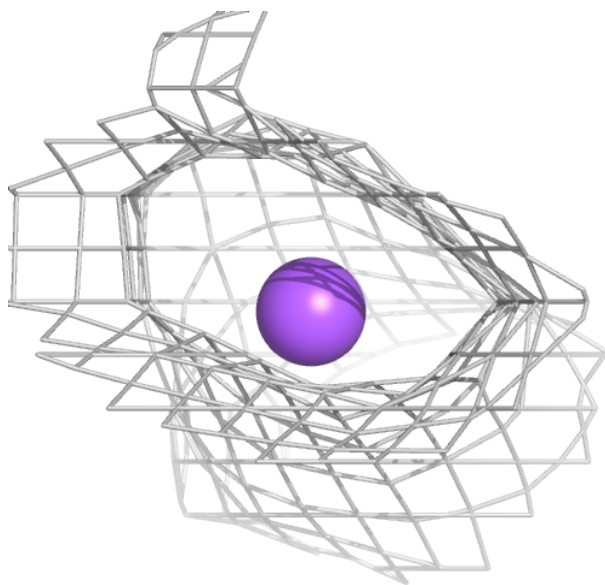
Electron density around CLR C 1106:

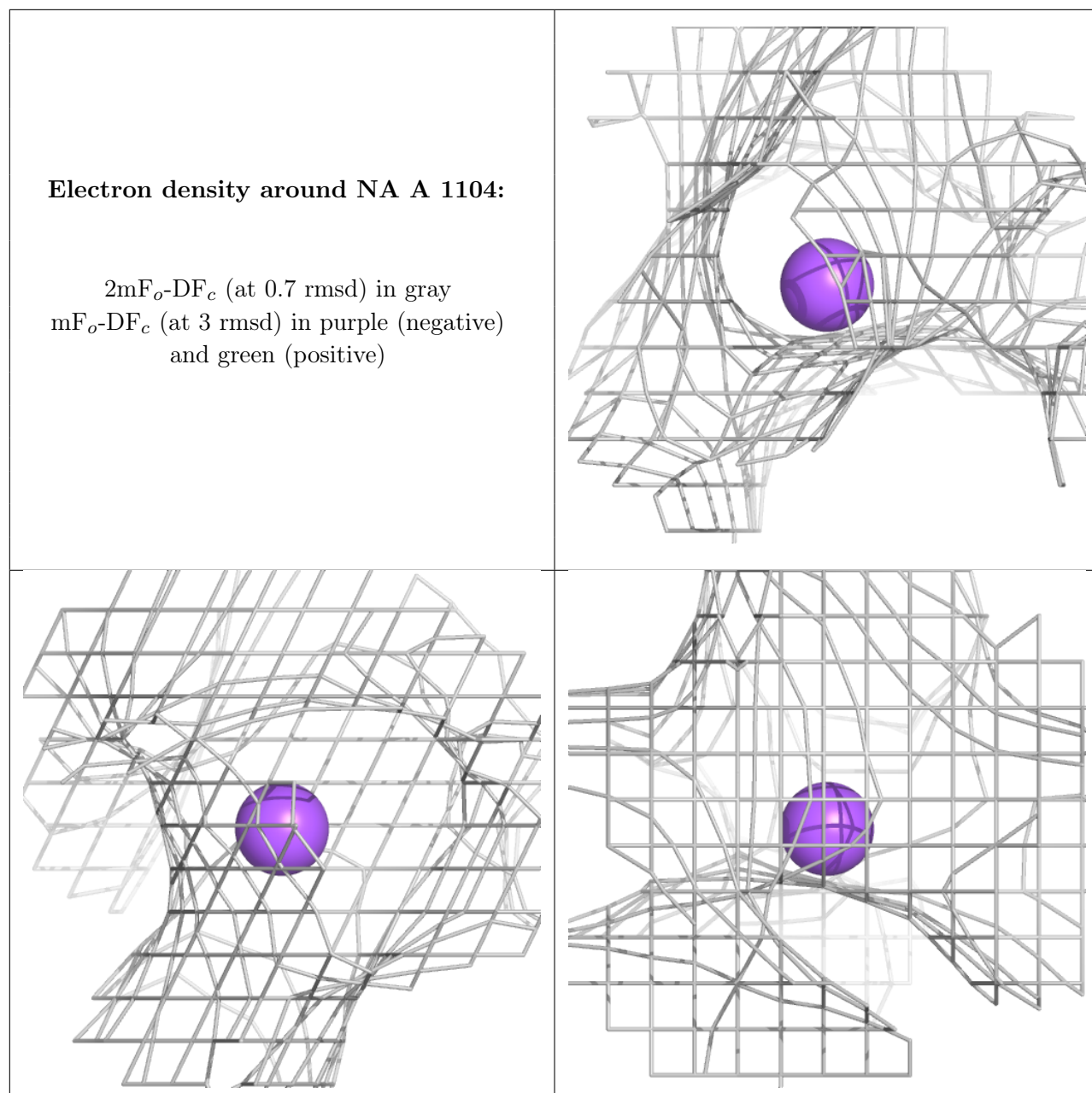
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.