wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2023 – 12:18 PM JST

PDB ID	:	8JBM
Title	:	Crystal structure of Na+,K+-ATPase in the E1.Mn2+ state
Authors	:	Kanai, R.; Vilsen, B.; Cornelius, F.; Toyoshima, C.
Deposited on	:	2023-05-09
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

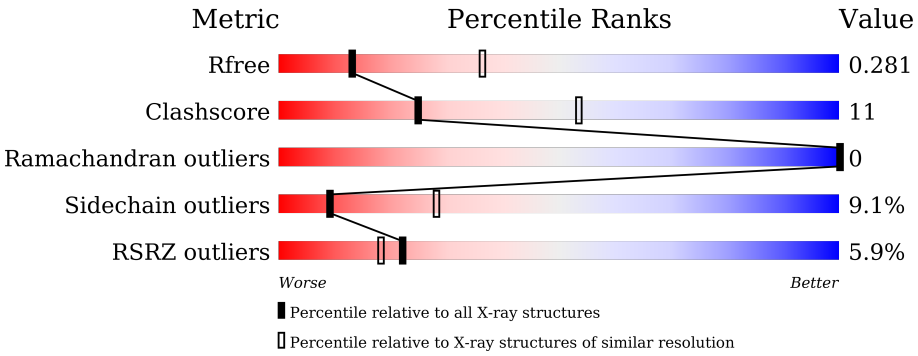
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	6% 72% 22%
1	C	1021	4% 70% 25%
2	B	303	7% 63% 30%
2	D	303	11% 64% 27%
3	E	65	2% 37% 14% 49%
3	G	65	5% 35% 18% 46%

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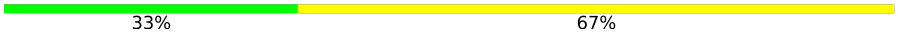
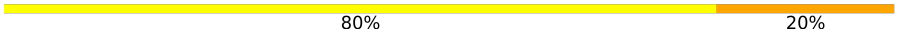
Mol	Chain	Length	Quality of chain
4	F	6	
5	H	5	
6	I	2	

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
10	PCW	A	1112	-	-	-	X
10	PCW	A	1113	-	-	-	X
10	PCW	C	1106	-	-	-	X
10	PCW	C	1108	-	-	-	X
10	PCW	C	1109	-	-	-	X
4	MAN	F	4	-	-	-	X
4	MAN	F	5	-	-	-	X
4	MAN	F	6	-	-	-	X
5	NAG	H	2	-	-	-	X
5	MAN	H	4	-	-	-	X
6	NAG	I	1	-	-	-	X
6	NAG	I	2	-	-	-	X
9	PC1	A	1105	-	-	-	X

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 21682 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

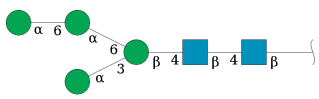
- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

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

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

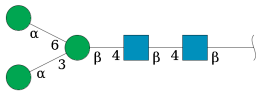
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	35	Total	C	N	O	0	0	0
			285	192	46	47			
3	E	33	Total	C	N	O	0	0	0
			262	179	38	45			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



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

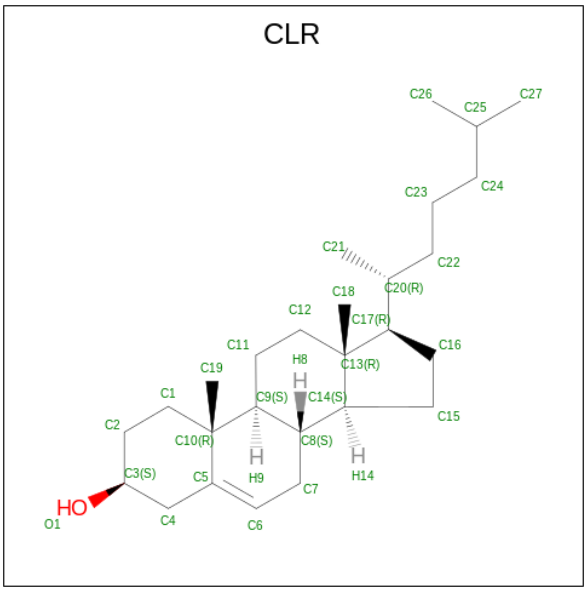
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

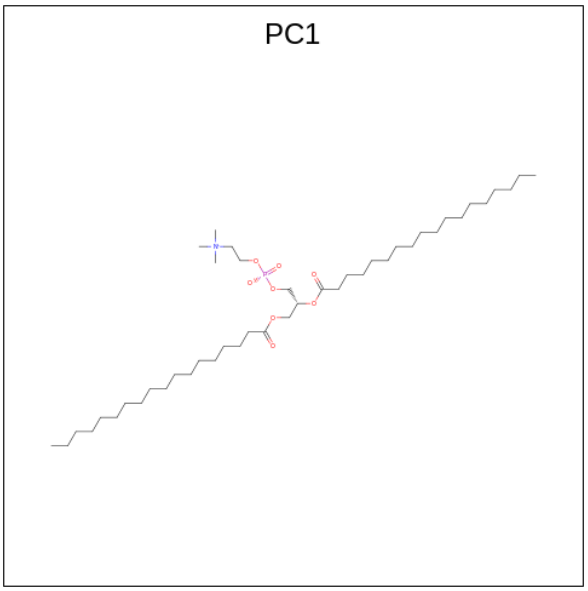
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Mn	0	0
			3	3		
7	C	3	Total	Mn	0	0
			3	3		

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



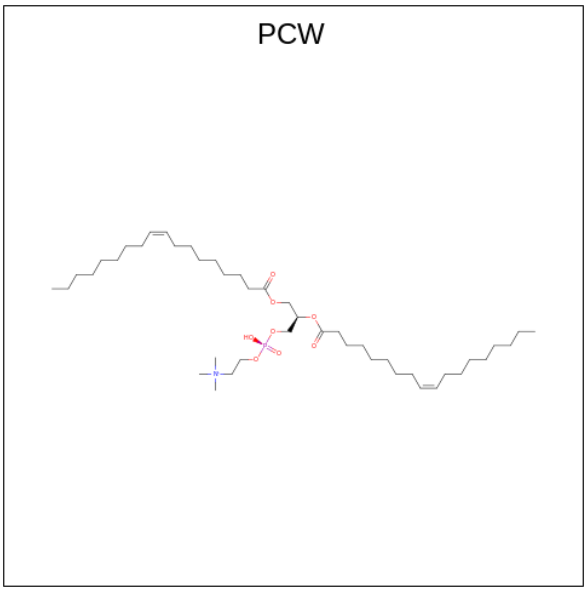
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 28 27 1	0	0
8	A	1	Total C O 28 27 1	0	0
8	G	1	Total C O 28 27 1	0	0
8	C	1	Total C O 28 27 1	0	0
8	D	1	Total C O 28 27 1	0	0
8	E	1	Total C O 28 27 1	0	0

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



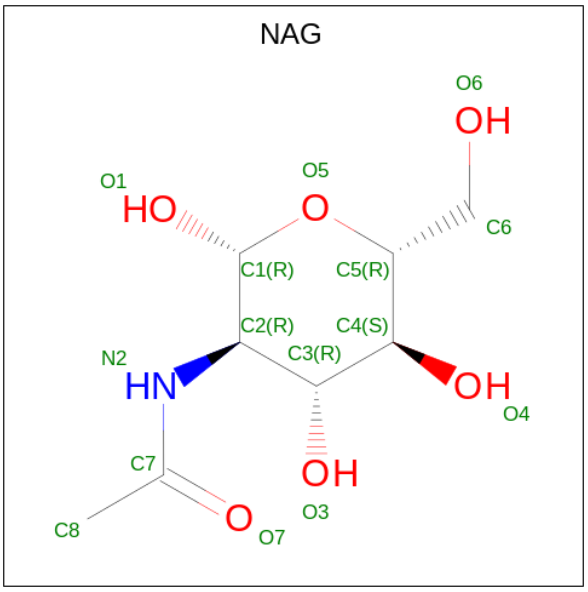
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

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



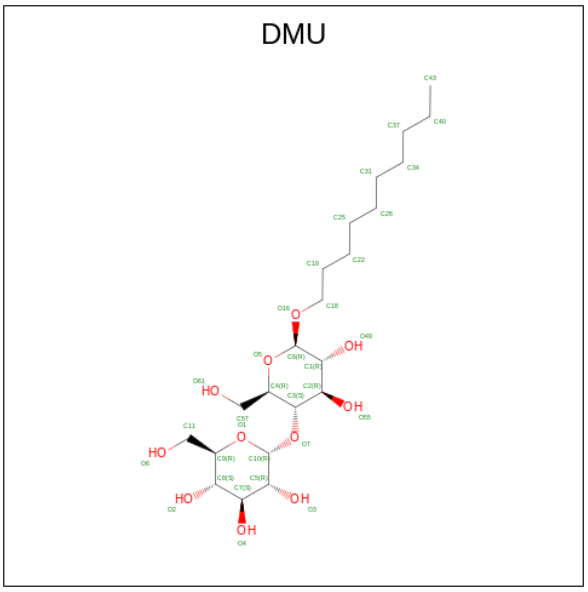
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total 22	C 12	N 1	O 8	P 1	0	0
10	A	1	Total 22	C 12	N 1	O 8	P 1	0	0
10	A	1	Total 22	C 12	N 1	O 8	P 1	0	0
10	A	1	Total 22	C 12	N 1	O 8	P 1	0	0
10	A	1	Total 22	C 12	N 1	O 8	P 1	0	0
10	A	1	Total 54	C 44	N 1	O 8	P 1	0	0
10	B	1	Total 22	C 12	N 1	O 8	P 1	0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

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



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

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



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

- Molecule 13 is water.

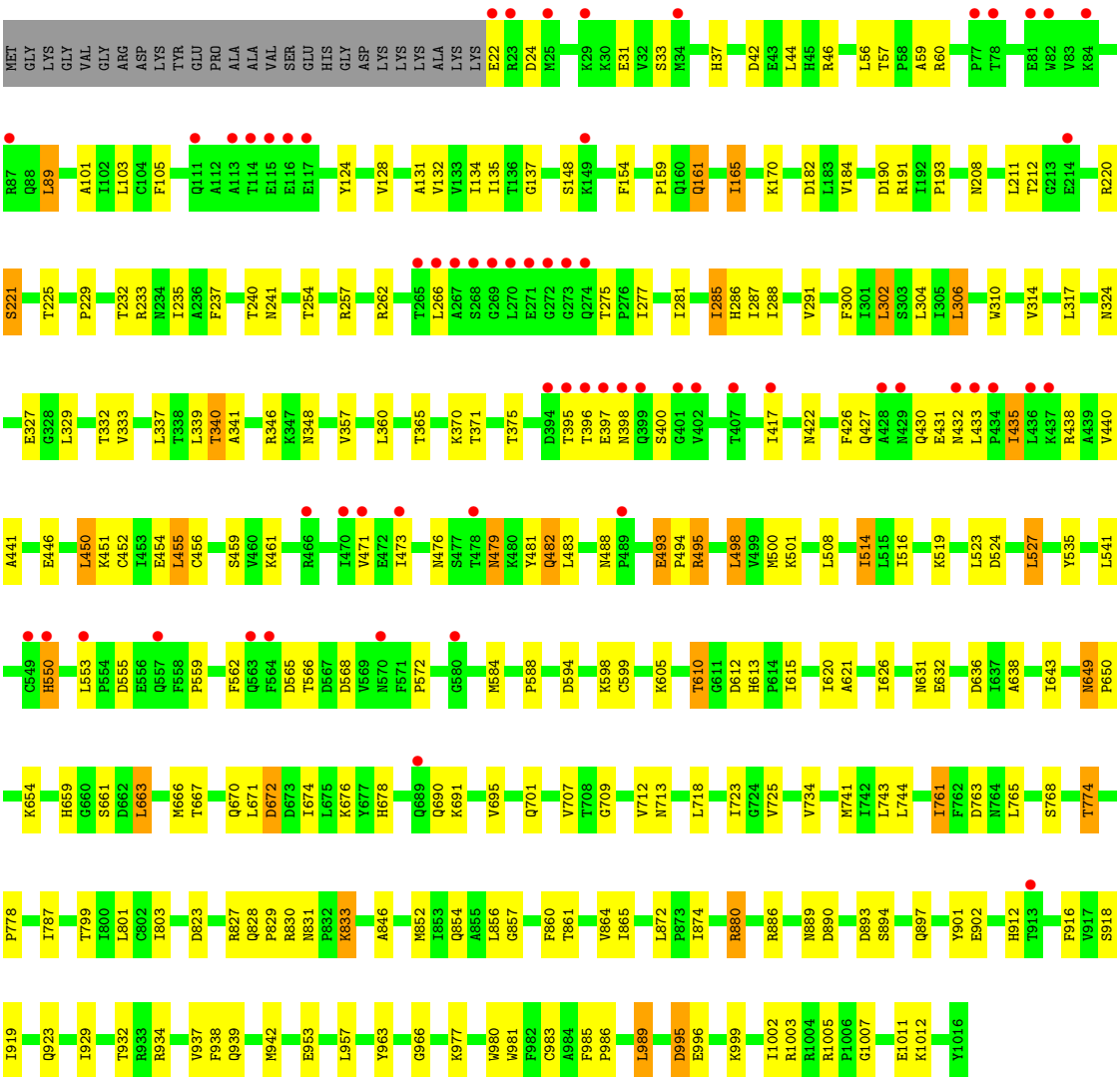
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	19	Total O 19 19	0	0
13	C	12	Total O 12 12	0	0
13	D	2	Total O 2 2	0	0

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.

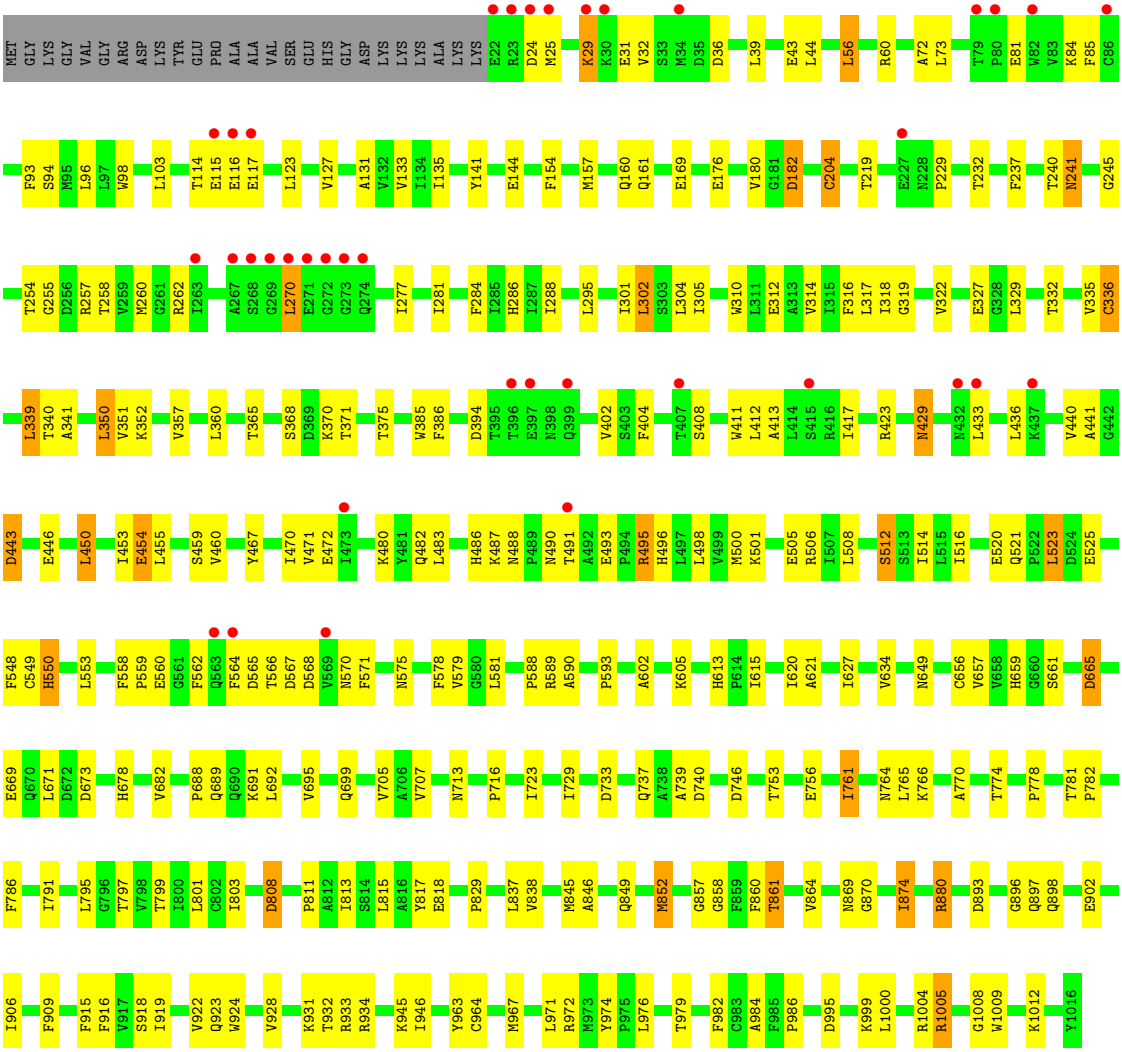
• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha

Chain A:



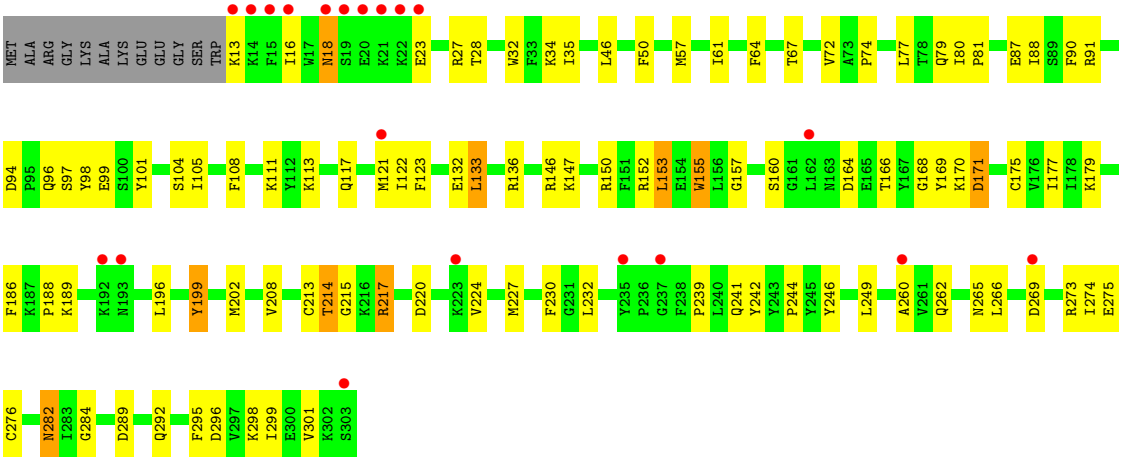
• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha

Chain C:



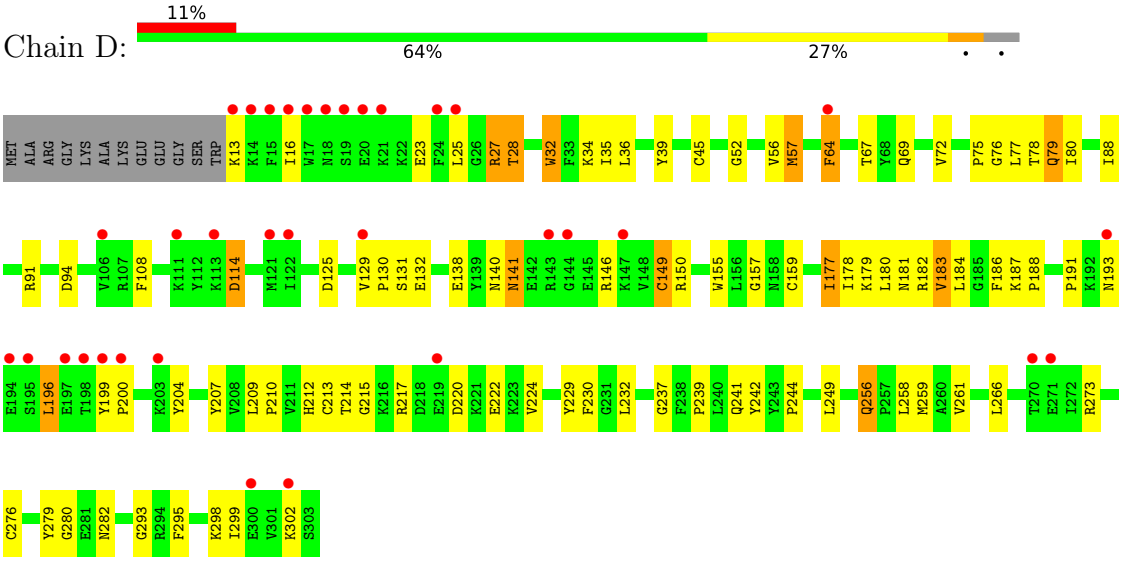
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain B:



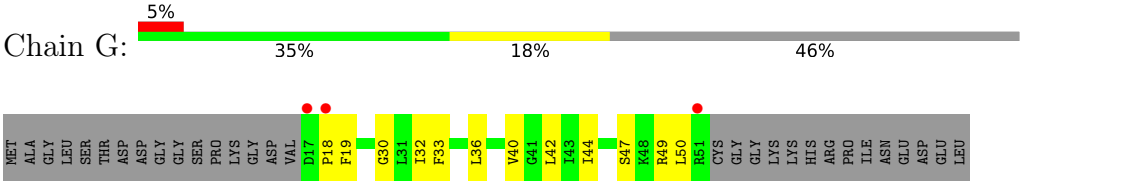
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain D:



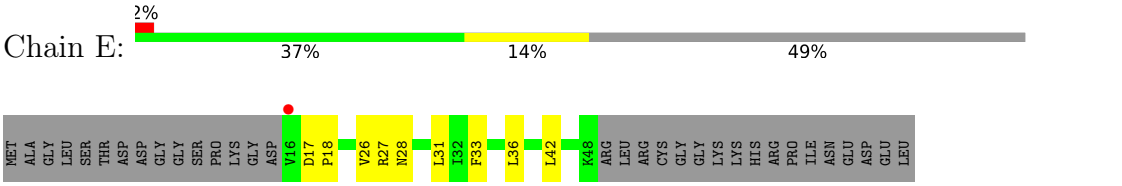
• Molecule 3: FXYD domain-containing ion transport regulator

Chain G:



• Molecule 3: FXYD domain-containing ion transport regulator

Chain E:

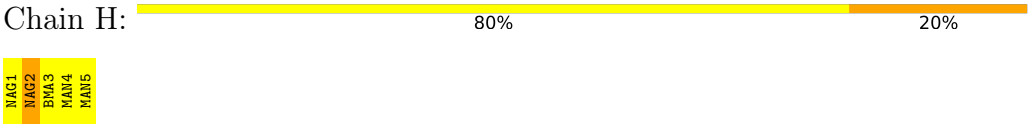


• Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• 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:



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

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	196.98Å 74.43Å 162.98Å 90.00° 116.33° 90.00°	Depositor
Resolution (Å)	12.00 – 2.90 29.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	57.4 (12.00-2.90) 58.0 (29.96-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.224 , 0.278 0.227 , 0.281	Depositor DCC
R_{free} test set	2745 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	83.9	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.026 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)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MN, CLR, NAG, PCW, BMA, PC1, MAN, DMU

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	0.33	0/7873	0.54	0/10683
1	C	0.33	0/7873	0.53	0/10683
2	B	0.31	0/2449	0.53	0/3301
2	D	0.30	0/2449	0.53	0/3301
3	E	0.36	0/268	0.46	0/364
3	G	0.32	0/291	0.53	0/393
All	All	0.32	0/21203	0.53	0/28725

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7723	0	7775	158	0
1	C	7723	0	7775	165	0
2	B	2386	0	2362	63	0
2	D	2386	0	2362	59	0
3	E	262	0	268	7	0
3	G	285	0	296	11	0
4	F	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	61	0	52	1	0
6	I	28	0	25	0	0
7	A	3	0	0	0	0
7	C	3	0	0	0	0
8	A	56	0	92	2	0
8	C	28	0	46	2	0
8	D	28	0	46	3	0
8	E	28	0	46	3	0
8	G	28	0	46	3	0
9	A	162	0	264	21	0
10	A	164	0	174	8	0
10	B	22	0	18	2	0
10	C	154	0	126	6	0
11	D	14	0	13	0	0
12	E	33	0	42	3	0
13	A	19	0	0	0	0
13	C	12	0	0	0	0
13	D	2	0	0	0	0
All	All	21682	0	21889	469	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 11.

The worst 5 of 469 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:A:986:PRO:HG2	8:A:1104:CLR:H181	1.52	0.91
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.57	0.86
9:A:1107:PC1:H372	8:C:1104:CLR:H71	1.61	0.82
1:C:114:THR:HG22	1:C:115:GLU:H	1.46	0.78
1:A:340:THR:HG21	1:A:761:ILE:HG12	1.66	0.78

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%)	948 (96%)	45 (4%)	0	100	100
1	C	993/1021 (97%)	947 (95%)	46 (5%)	0	100	100
2	B	289/303 (95%)	276 (96%)	13 (4%)	0	100	100
2	D	289/303 (95%)	274 (95%)	15 (5%)	0	100	100
3	E	31/65 (48%)	30 (97%)	1 (3%)	0	100	100
3	G	33/65 (51%)	31 (94%)	2 (6%)	0	100	100
All	All	2628/2778 (95%)	2506 (95%)	122 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	845/864 (98%)	771 (91%)	74 (9%)	10	30
1	C	845/864 (98%)	770 (91%)	75 (9%)	9	29
2	B	261/269 (97%)	234 (90%)	27 (10%)	7	22
2	D	261/269 (97%)	235 (90%)	26 (10%)	7	23
3	E	27/52 (52%)	25 (93%)	2 (7%)	13	38
3	G	29/52 (56%)	27 (93%)	2 (7%)	15	41
All	All	2268/2370 (96%)	2062 (91%)	206 (9%)	9	28

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	204	CYS
1	C	498	LEU
2	D	196	LEU
1	C	262	ARG
1	C	351	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	262	GLN
1	C	659	HIS
1	C	119	GLN
1	C	550	HIS
1	C	776	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	0.73	1 (7%)	17,19,21	0.77	0
4	NAG	F	2	4	14,14,15	0.28	0	17,19,21	0.55	0
4	BMA	F	3	4	11,11,12	0.83	0	15,15,17	0.80	0
4	MAN	F	4	4	11,11,12	1.20	1 (9%)	15,15,17	1.26	2 (13%)
4	MAN	F	5	4	11,11,12	1.33	2 (18%)	15,15,17	1.65	3 (20%)
4	MAN	F	6	4	11,11,12	0.90	1 (9%)	15,15,17	1.03	1 (6%)
5	NAG	H	1	2,5	14,14,15	0.32	0	17,19,21	0.69	0
5	NAG	H	2	5	14,14,15	0.79	1 (7%)	17,19,21	0.78	1 (5%)
5	BMA	H	3	5	11,11,12	1.55	2 (18%)	15,15,17	1.15	3 (20%)
5	MAN	H	4	5	11,11,12	1.21	2 (18%)	15,15,17	1.27	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	H	5	5	11,11,12	1.01	1 (9%)	15,15,17	1.31	2 (13%)
6	NAG	I	1	2,6	14,14,15	0.65	1 (7%)	17,19,21	0.70	0
6	NAG	I	2	6	14,14,15	0.44	0	17,19,21	0.71	0

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

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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5	MAN	C1-C2	3.11	1.59	1.52
5	H	3	BMA	C1-C2	2.93	1.58	1.52
5	H	5	MAN	C1-C2	2.87	1.58	1.52
5	H	4	MAN	C2-C3	2.72	1.56	1.52
5	H	4	MAN	C1-C2	2.63	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	5	MAN	C1-O5-C5	4.66	118.51	112.19
4	F	4	MAN	C1-O5-C5	3.69	117.19	112.19
5	H	5	MAN	C1-O5-C5	3.30	116.66	112.19
5	H	4	MAN	C1-C2-C3	2.57	112.83	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	6	MAN	O2-C2-C3	-2.37	105.39	110.14

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	3	BMA	C4-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6

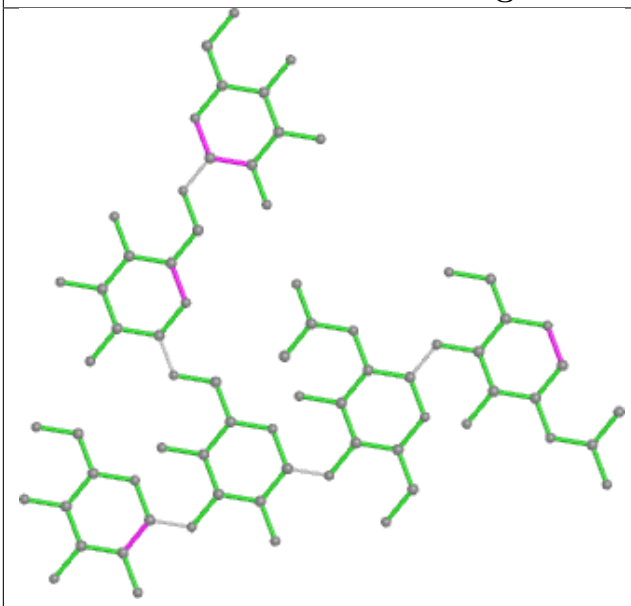
There are no ring outliers.

2 monomers are involved in 1 short contact:

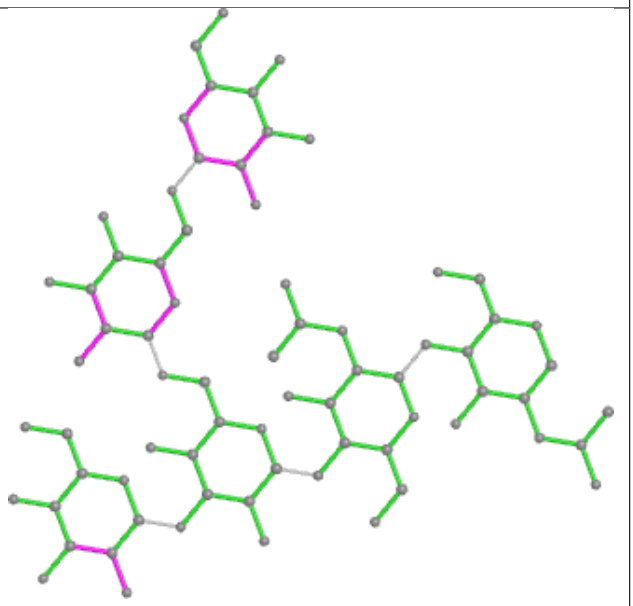
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	NAG	1	0
5	H	1	NAG	1	0

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

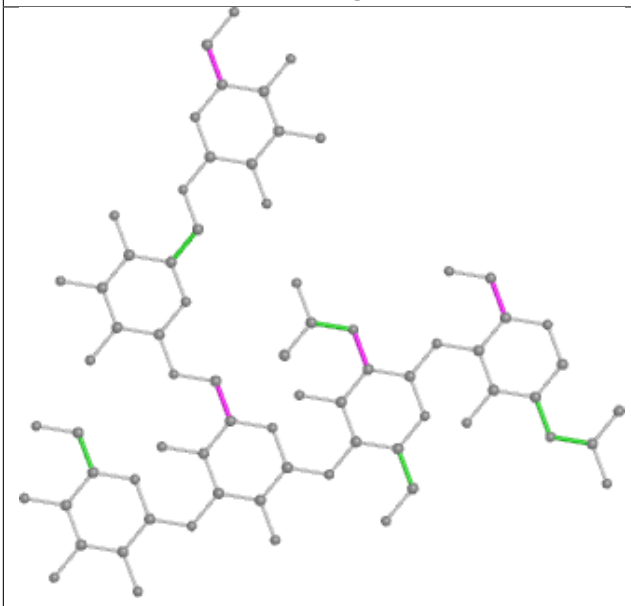
Oligosaccharide Chain F



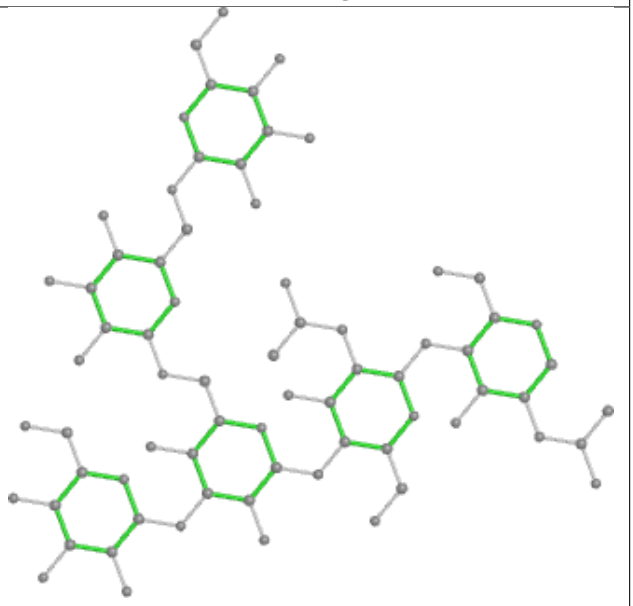
Bond lengths



Bond angles

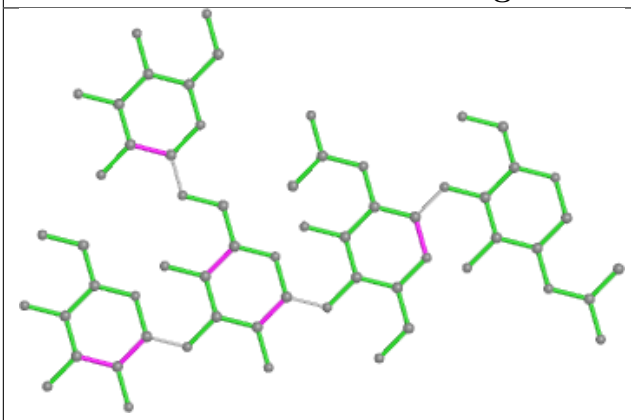


Torsions

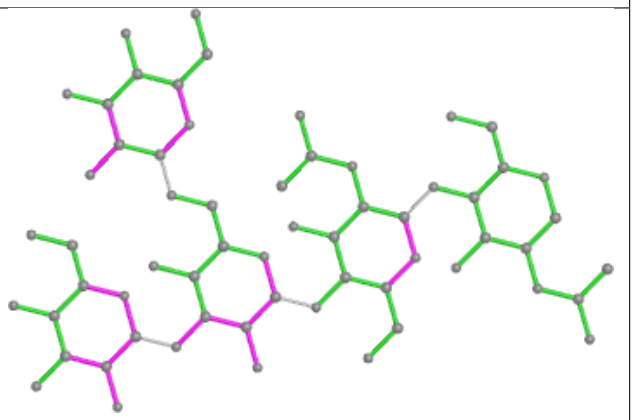


Rings

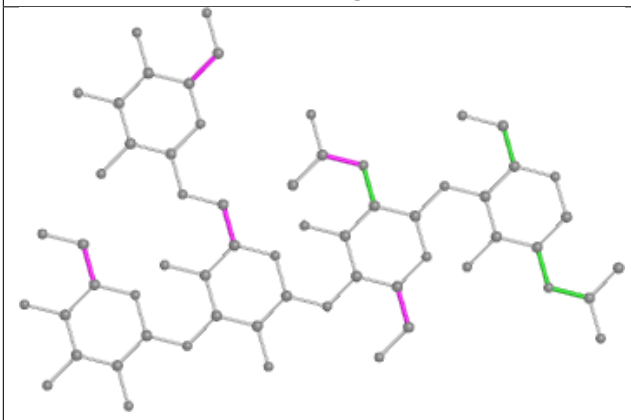
Oligosaccharide Chain H



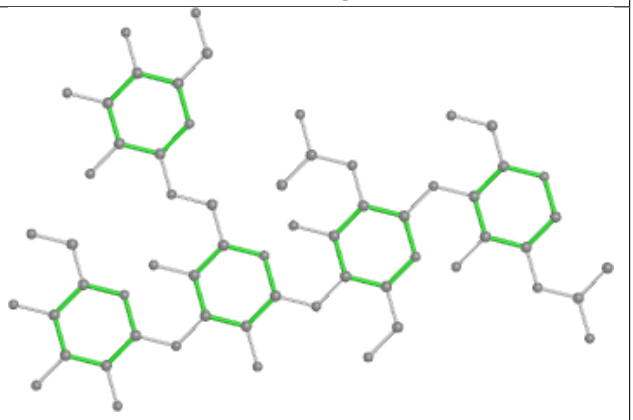
Bond lengths



Bond angles

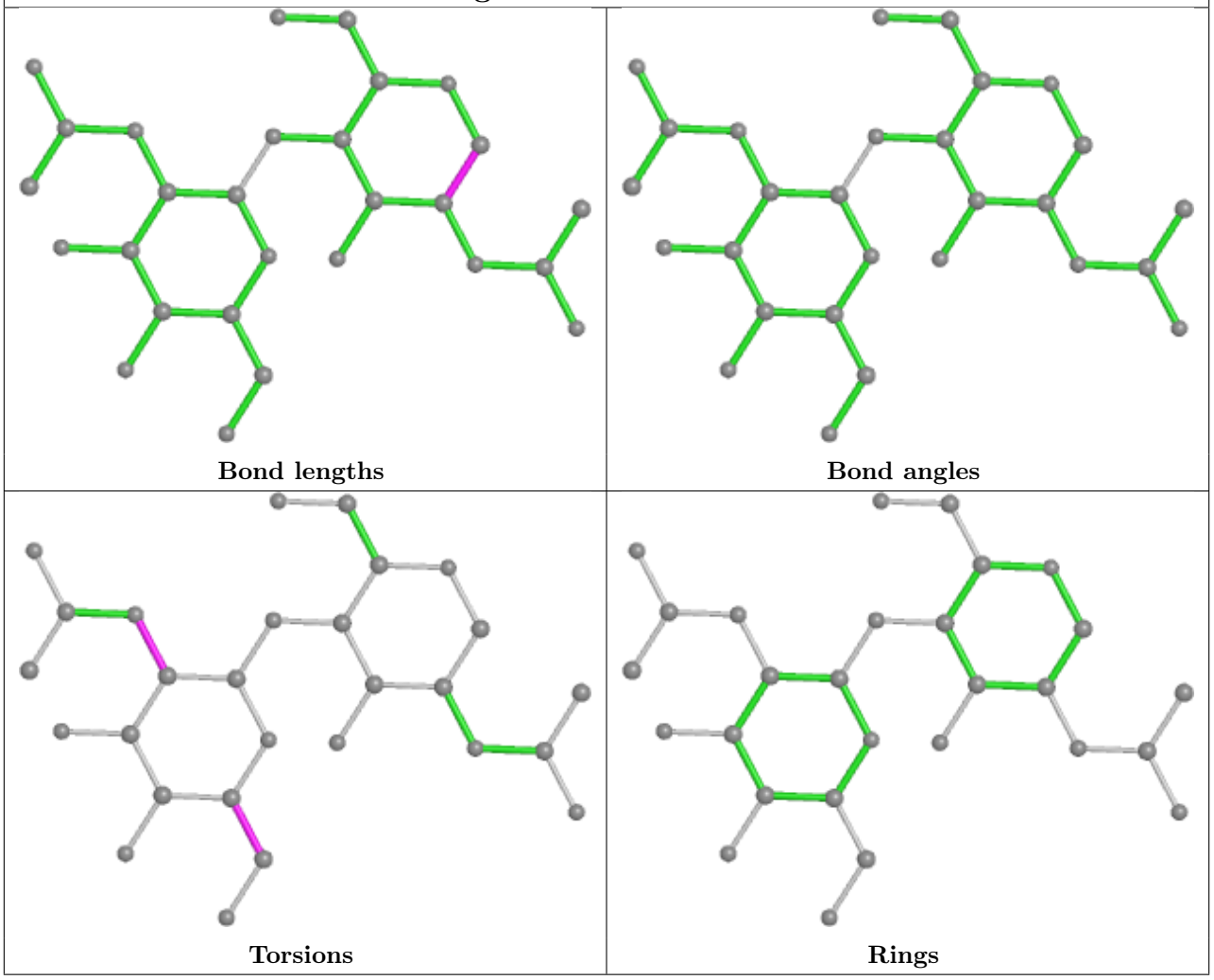


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	PCW	A	1114	-	53,53,53	1.00	2 (3%)	59,61,61	0.85	0
10	PCW	C	1106	-	21,21,53	0.96	0	27,29,61	0.82	1 (3%)
10	PCW	C	1109	-	21,21,53	0.89	0	27,29,61	0.87	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	PCW	C	1105	-	21,21,53	0.92	0	27,29,61	1.05	2 (7%)
10	PCW	B	401	-	21,21,53	0.98	0	27,29,61	0.92	1 (3%)
10	PCW	A	1108	-	21,21,53	0.93	0	27,29,61	0.88	1 (3%)
10	PCW	C	1108	-	21,21,53	0.94	0	27,29,61	0.89	1 (3%)
10	PCW	A	1106	-	21,21,53	0.91	0	27,29,61	1.17	3 (11%)
9	PC1	A	1110	-	53,53,53	0.63	0	59,61,61	1.00	3 (5%)
12	DMU	E	102	-	34,34,34	0.65	0	45,45,45	1.22	4 (8%)
8	CLR	C	1104	-	31,31,31	1.13	1 (3%)	48,48,48	1.37	7 (14%)
10	PCW	A	1113	-	21,21,53	1.00	0	27,29,61	0.94	2 (7%)
11	NAG	D	402	2	14,14,15	0.45	0	17,19,21	0.42	0
8	CLR	D	401	-	31,31,31	1.21	1 (3%)	48,48,48	1.37	7 (14%)
8	CLR	A	1109	-	31,31,31	1.18	2 (6%)	48,48,48	1.35	6 (12%)
10	PCW	C	1111	-	21,21,53	0.95	0	27,29,61	0.96	1 (3%)
10	PCW	A	1111	-	21,21,53	0.93	0	27,29,61	0.98	2 (7%)
10	PCW	C	1110	-	21,21,53	0.89	0	27,29,61	1.07	2 (7%)
10	PCW	A	1112	-	21,21,53	0.91	0	27,29,61	1.03	2 (7%)
8	CLR	E	101	-	31,31,31	1.12	2 (6%)	48,48,48	1.38	6 (12%)
10	PCW	C	1107	-	21,21,53	0.91	0	27,29,61	1.12	3 (11%)
8	CLR	G	101	-	31,31,31	1.16	2 (6%)	48,48,48	1.34	6 (12%)
9	PC1	A	1107	-	53,53,53	0.66	0	59,61,61	1.03	3 (5%)
9	PC1	A	1105	-	53,53,53	0.64	0	59,61,61	0.85	1 (1%)
8	CLR	A	1104	-	31,31,31	1.23	3 (9%)	48,48,48	1.43	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PCW	A	1114	-	-	23/57/57/57	-
10	PCW	C	1106	-	-	10/23/23/57	-
10	PCW	C	1109	-	-	4/23/23/57	-
10	PCW	C	1105	-	-	6/23/23/57	-
10	PCW	B	401	-	-	10/23/23/57	-
10	PCW	A	1108	-	-	9/23/23/57	-
10	PCW	C	1108	-	-	5/23/23/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PCW	A	1106	-	-	8/23/23/57	-
9	PC1	A	1110	-	-	11/57/57/57	-
12	DMU	E	102	-	-	3/19/59/59	0/2/2/2
8	CLR	C	1104	-	-	3/10/68/68	0/4/4/4
10	PCW	A	1113	-	-	10/23/23/57	-
11	NAG	D	402	2	-	0/6/23/26	0/1/1/1
8	CLR	D	401	-	-	2/10/68/68	0/4/4/4
8	CLR	A	1109	-	-	6/10/68/68	0/4/4/4
10	PCW	C	1111	-	-	6/23/23/57	-
10	PCW	A	1111	-	-	11/23/23/57	-
10	PCW	C	1110	-	-	9/23/23/57	-
10	PCW	A	1112	-	-	9/23/23/57	-
8	CLR	E	101	-	-	7/10/68/68	0/4/4/4
10	PCW	C	1107	-	-	8/23/23/57	-
8	CLR	G	101	-	-	6/10/68/68	0/4/4/4
9	PC1	A	1107	-	-	12/57/57/57	-
9	PC1	A	1105	-	-	6/57/57/57	-
8	CLR	A	1104	-	-	0/10/68/68	0/4/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1114	PCW	C20-C19	3.96	1.54	1.31
10	A	1114	PCW	C40-C39	3.82	1.53	1.31
8	A	1104	CLR	C16-C17	3.03	1.60	1.54
8	D	401	CLR	C16-C17	3.02	1.60	1.54
8	G	101	CLR	C16-C17	2.93	1.60	1.54

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1106	PCW	C2-O2-C31	-3.73	110.94	117.90
10	A	1112	PCW	C2-O2-C31	-3.44	111.49	117.90
9	A	1107	PC1	C3-O31-C31	-3.35	104.72	117.12
12	E	102	DMU	O1-C9-C11	3.27	114.55	106.44
10	C	1107	PCW	C3-O3-C11	-3.15	109.19	117.10

There are no chirality outliers.

5 of 184 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	101	CLR	C13-C17-C20-C21
9	A	1105	PC1	C11-O13-P-O14
9	A	1107	PC1	C1-O11-P-O12
10	A	1106	PCW	O4P-C4-C5-N
10	A	1106	PCW	C1-O3P-P-O2P

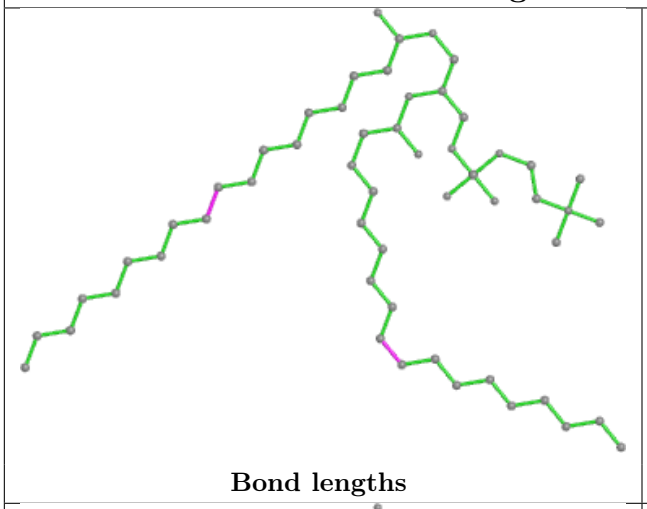
There are no ring outliers.

18 monomers are involved in 49 short contacts:

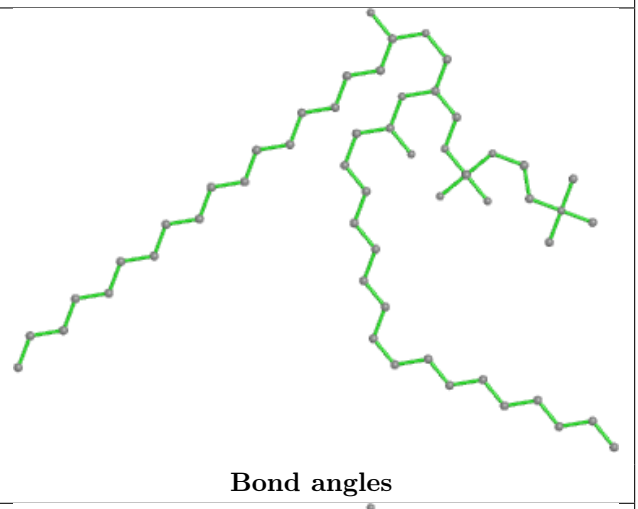
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1114	PCW	4	0
10	C	1109	PCW	2	0
10	C	1105	PCW	1	0
10	B	401	PCW	2	0
9	A	1110	PC1	8	0
12	E	102	DMU	3	0
8	C	1104	CLR	2	0
8	D	401	CLR	3	0
8	A	1109	CLR	1	0
10	C	1111	PCW	1	0
10	A	1111	PCW	2	0
10	A	1112	PCW	2	0
8	E	101	CLR	3	0
10	C	1107	PCW	2	0
8	G	101	CLR	3	0
9	A	1107	PC1	13	0
9	A	1105	PC1	1	0
8	A	1104	CLR	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 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 then 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.

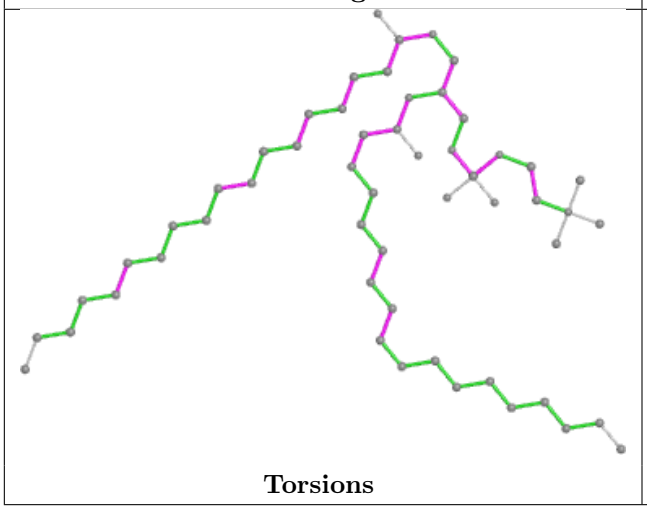
Ligand PCW A 1114



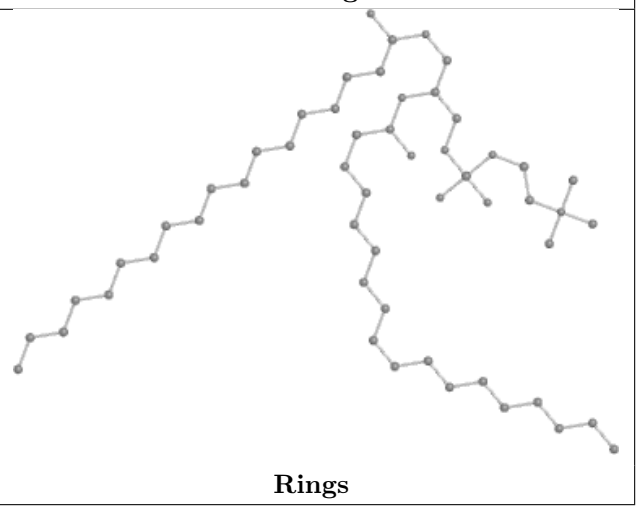
Bond lengths



Bond angles

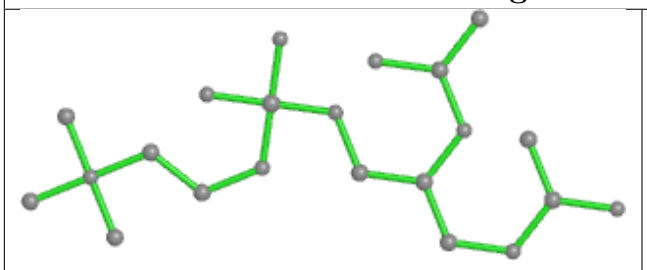


Torsions

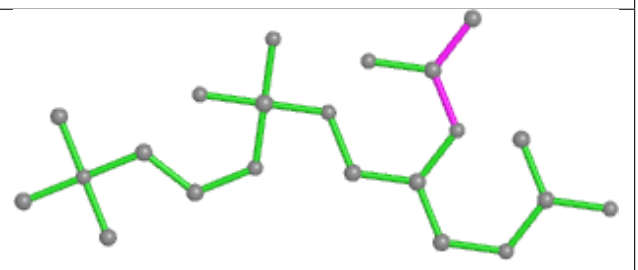


Rings

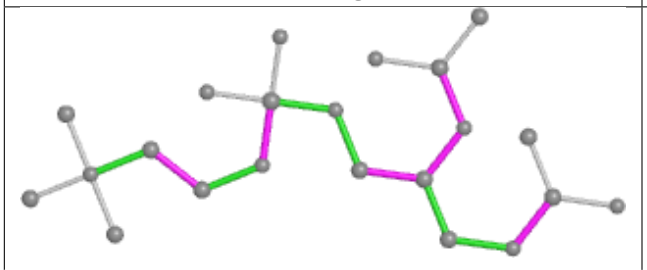
Ligand PCW C 1106



Bond lengths



Bond angles



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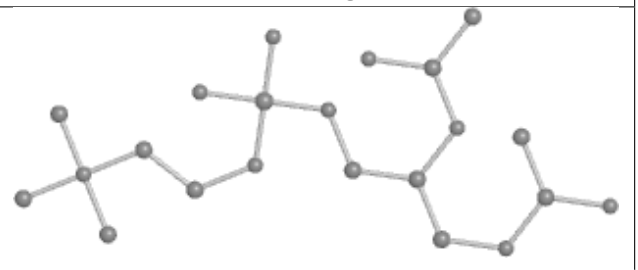
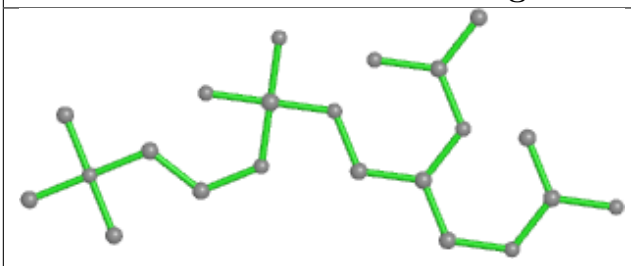
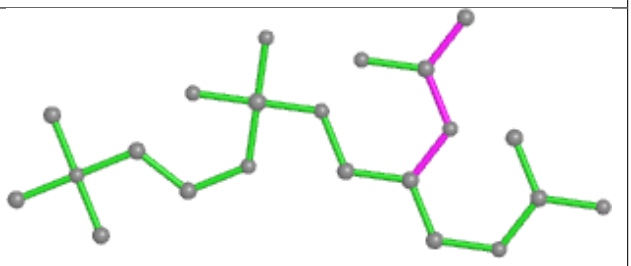


Rings

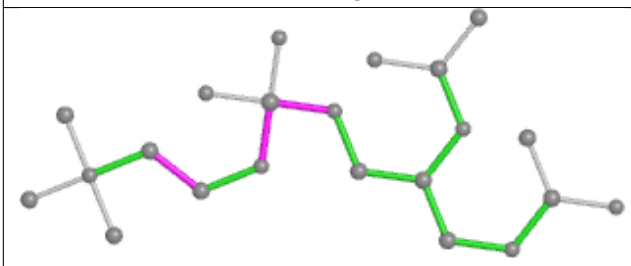
Ligand PCW C 1109



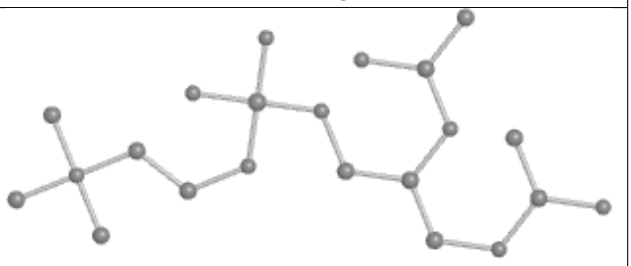
Bond lengths



Bond angles

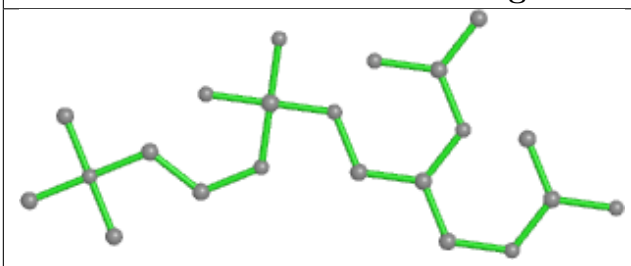


Torsions

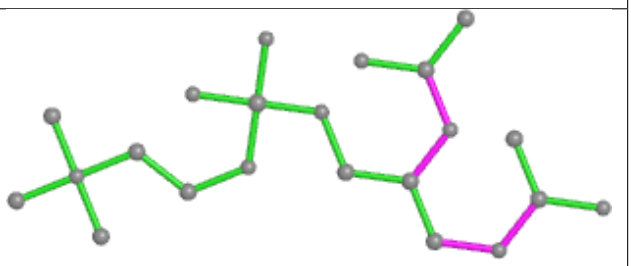


Rings

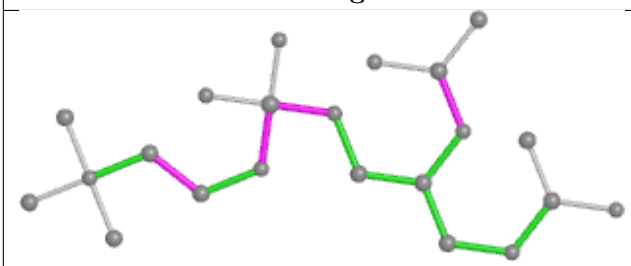
Ligand PCW C 1105



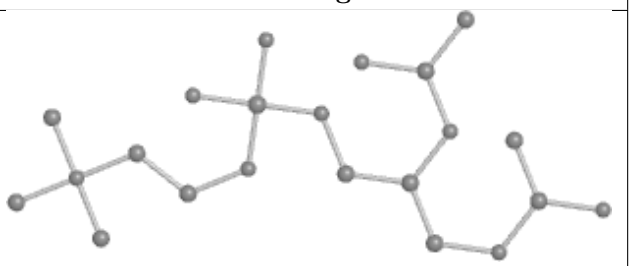
Bond lengths



Bond angles

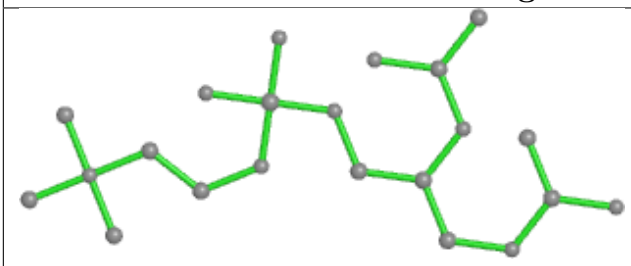


Torsions

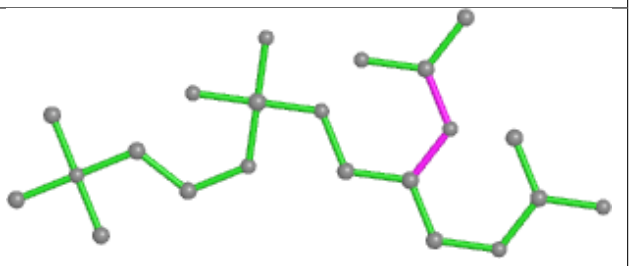


Rings

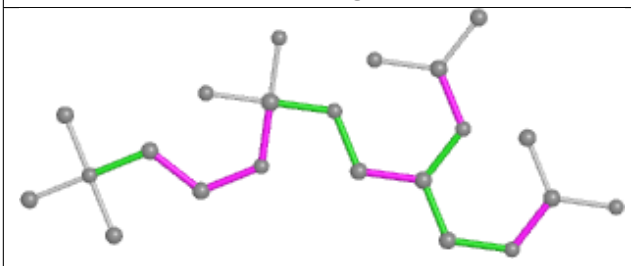
Ligand PCW B 401



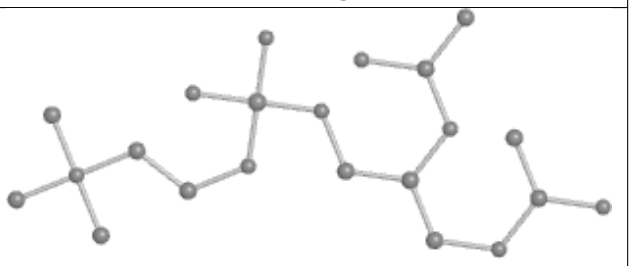
Bond lengths



Bond angles

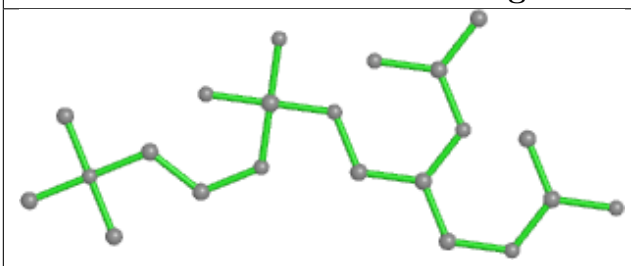


Torsions



Rings

Ligand PCW A 1108



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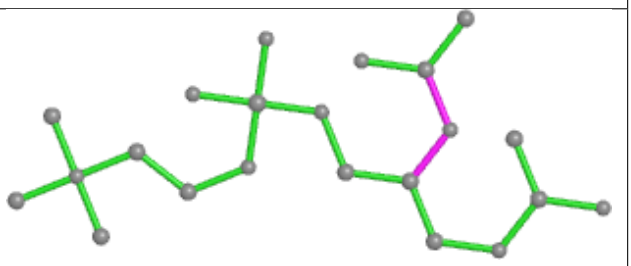
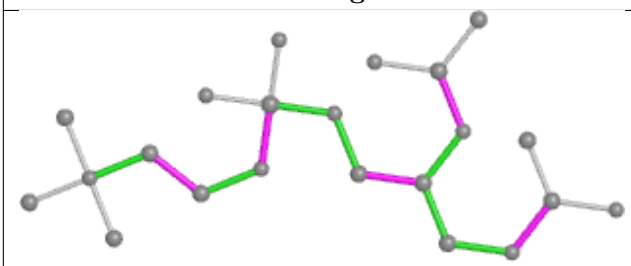


Bond angles



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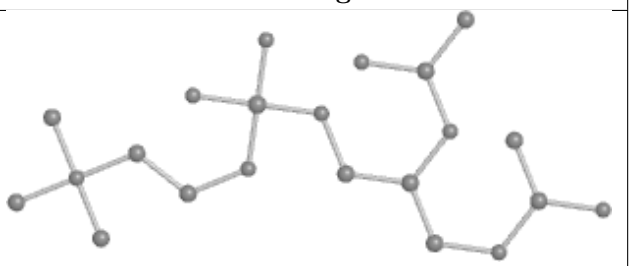
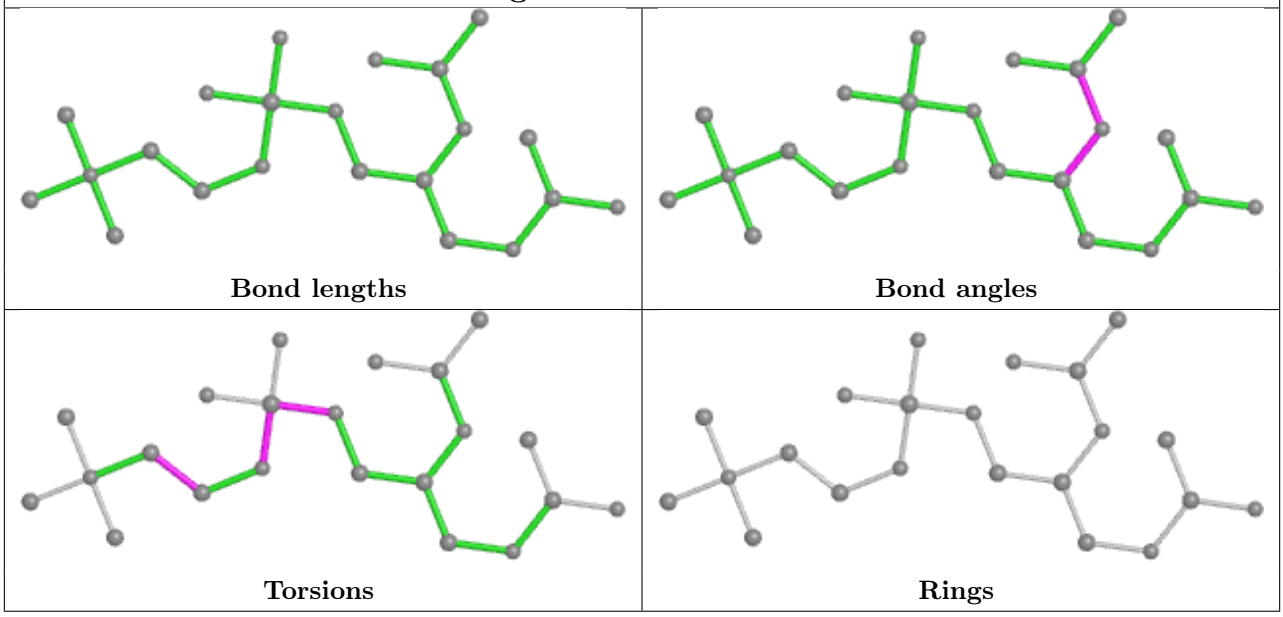
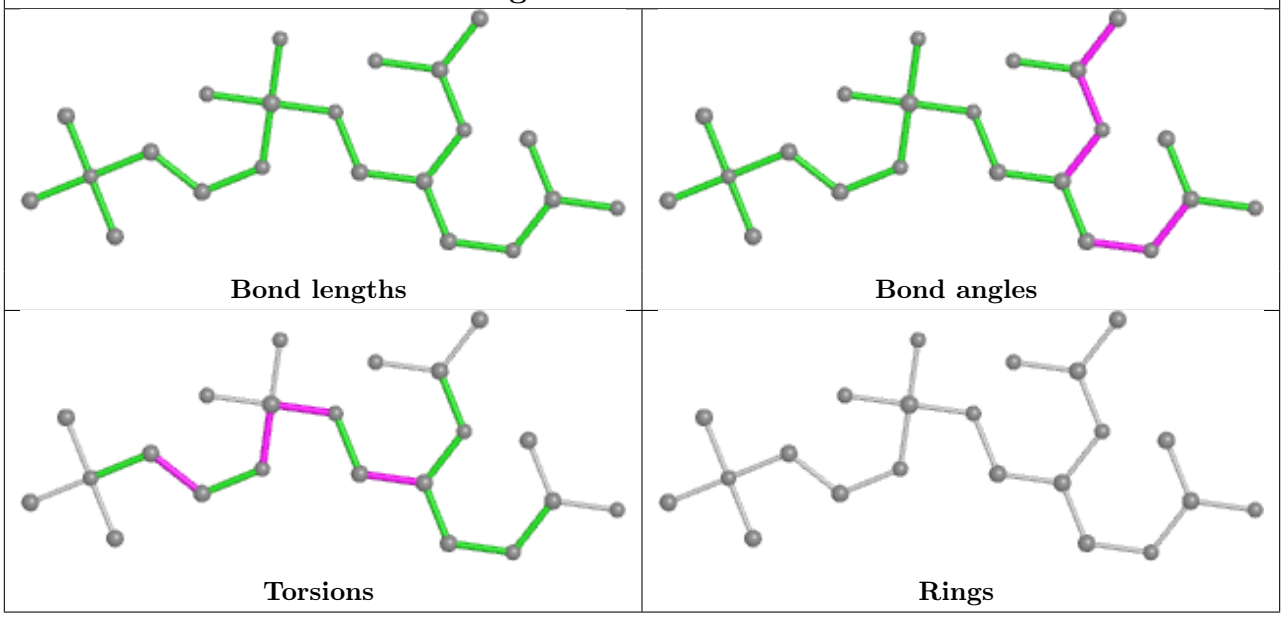


Rings

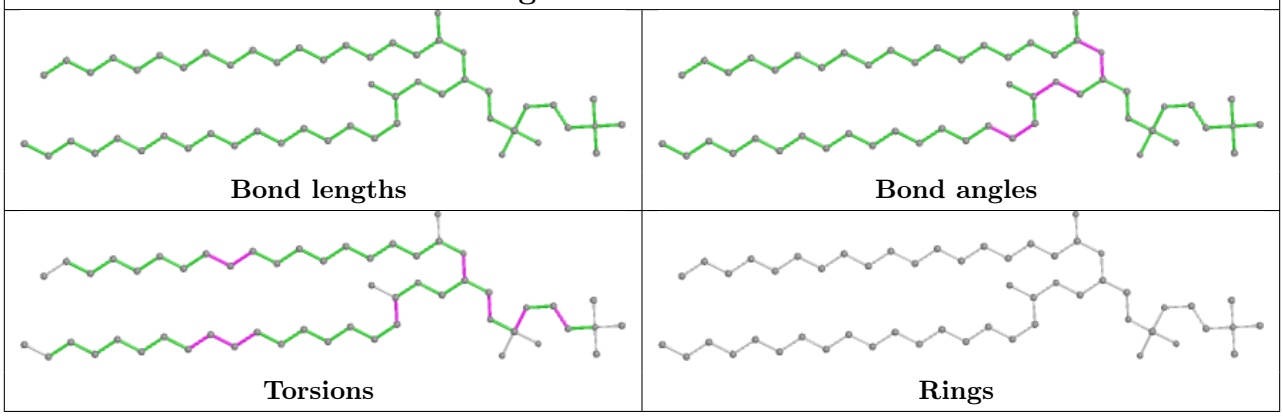
Ligand PCW C 1108



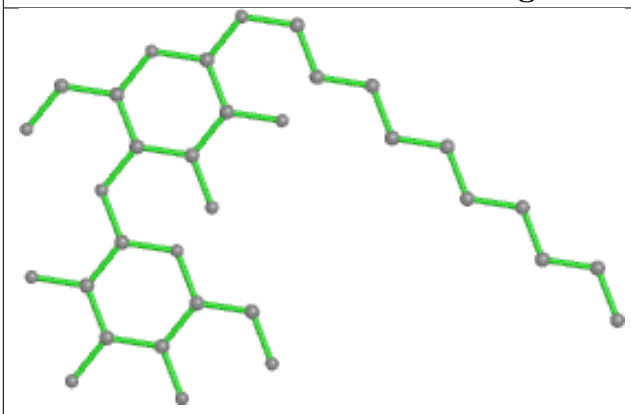
Ligand PCW A 1106



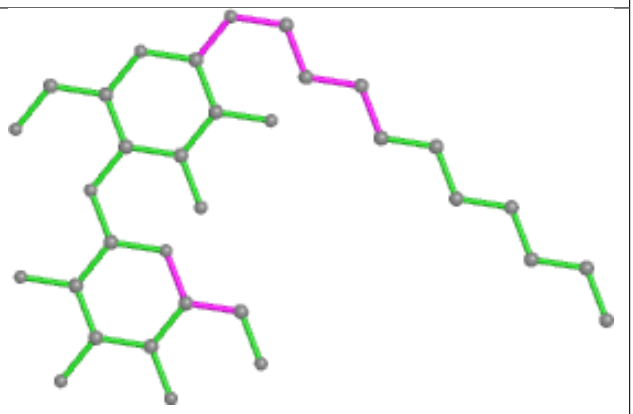
Ligand PC1 A 1110



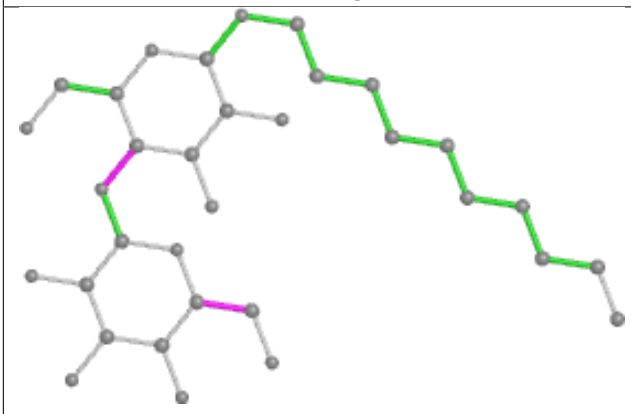
Ligand DMU E 102



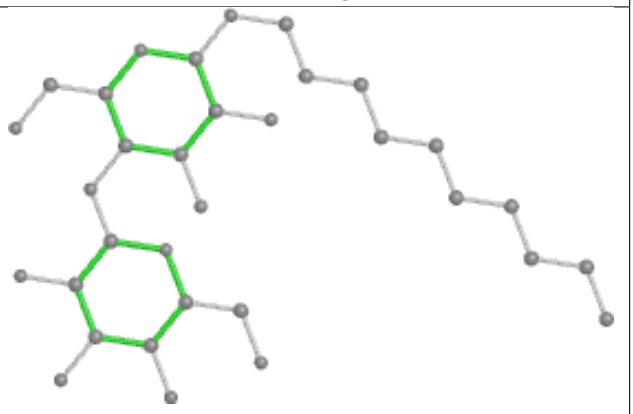
Bond lengths



Bond angles

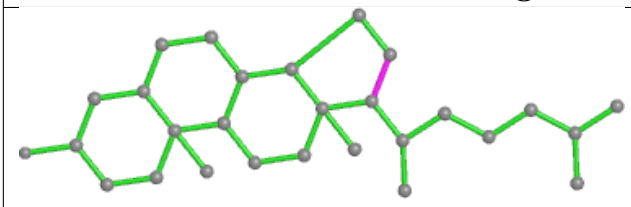


Torsions

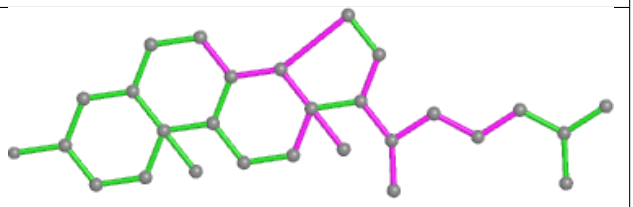


Rings

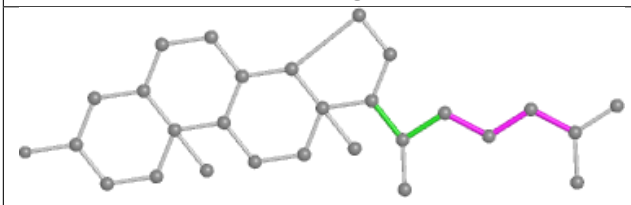
Ligand CLR C 1104



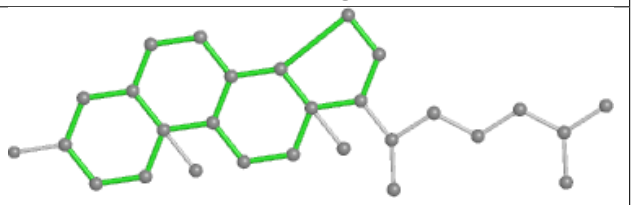
Bond lengths



Bond angles

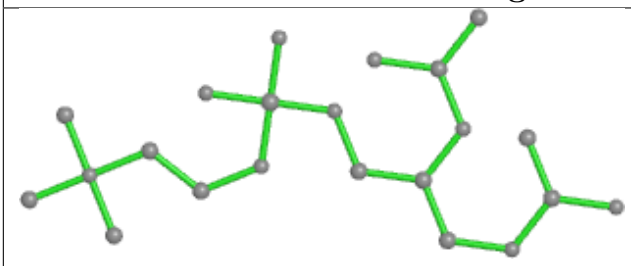


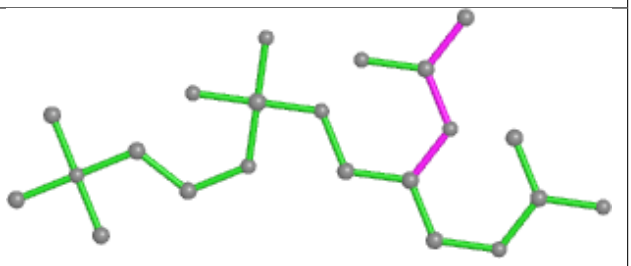
Torsions

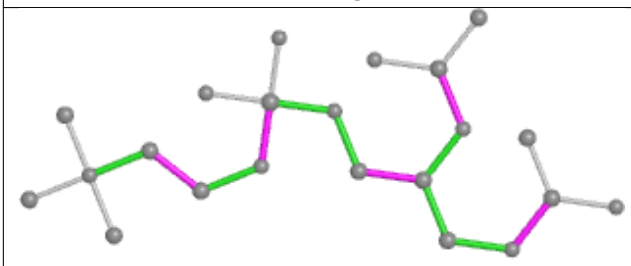


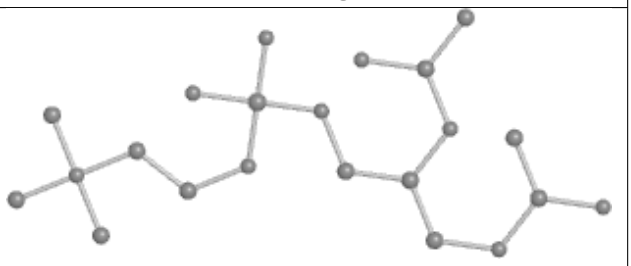
Rings

Ligand PCW A 1113

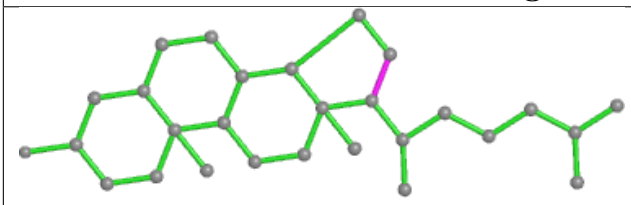

Bond lengths


Bond angles


Torsions


Rings

Ligand CLR D 401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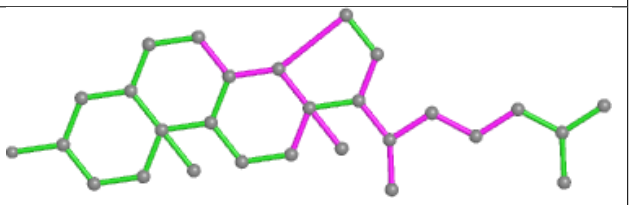
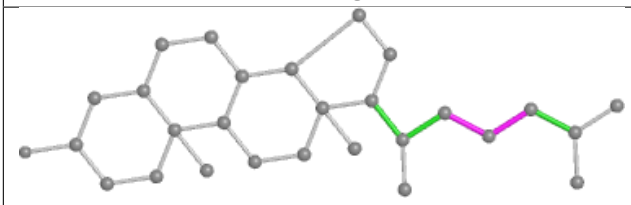
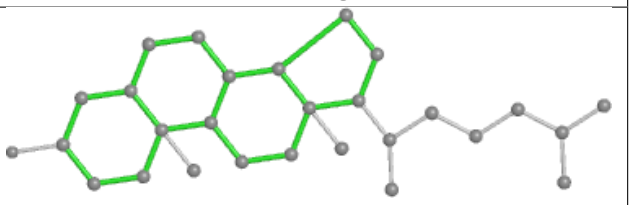
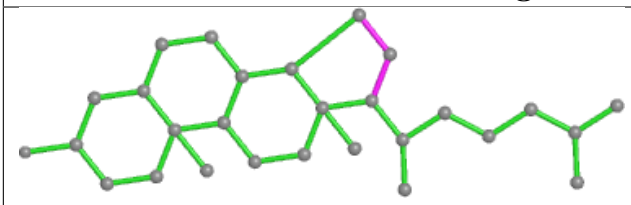
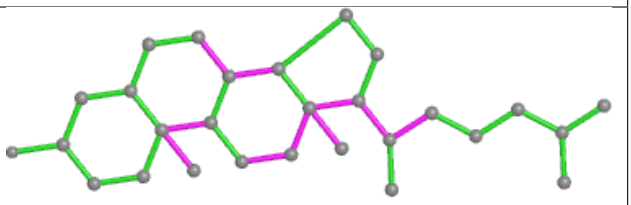

Bond angles

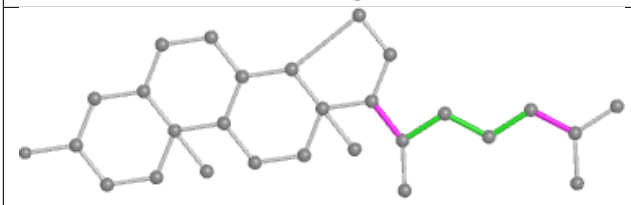

Torsions

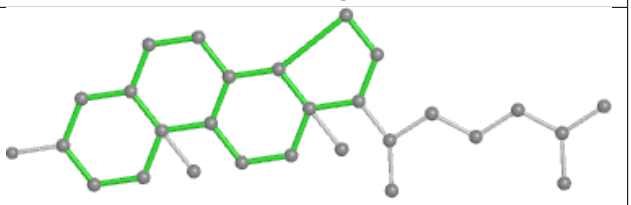

Rings

Ligand CLR A 1109

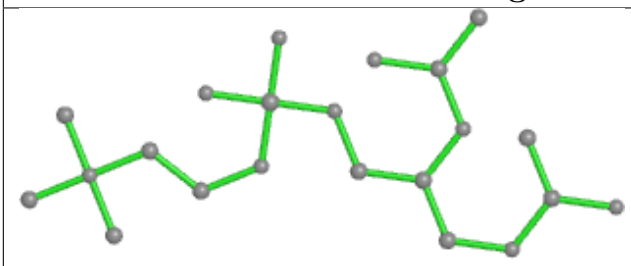

Bond lengths


Bond angles

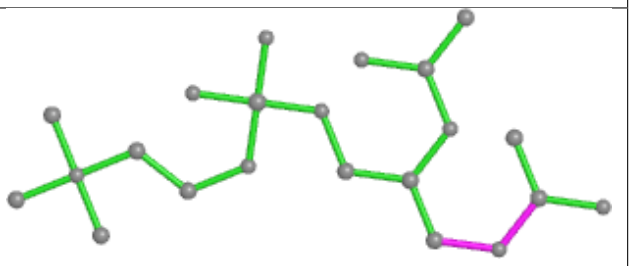

Torsions


Rings

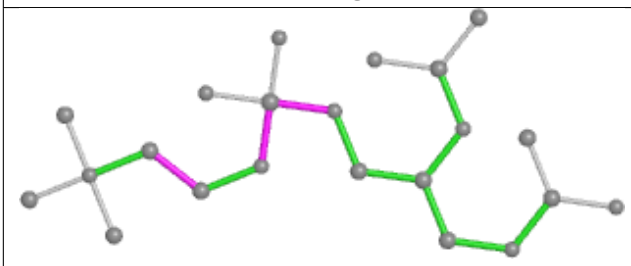
Ligand PCW C 1111



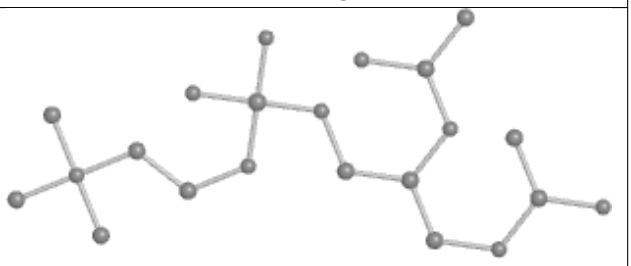
Bond lengths



Bond angles

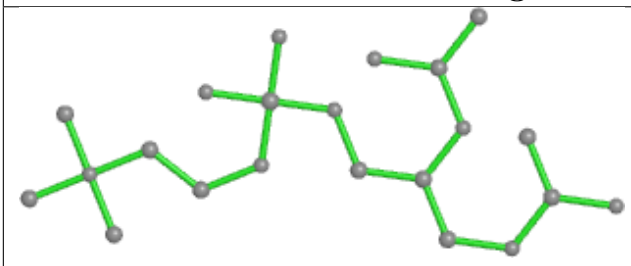


Torsions



Rings

Ligand PCW A 1111



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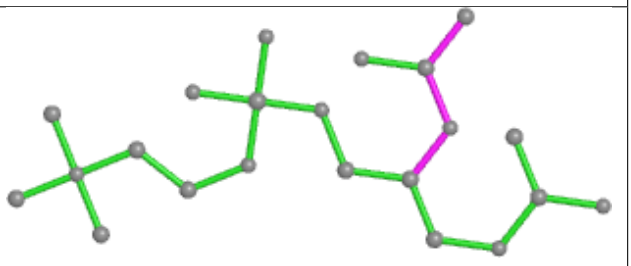
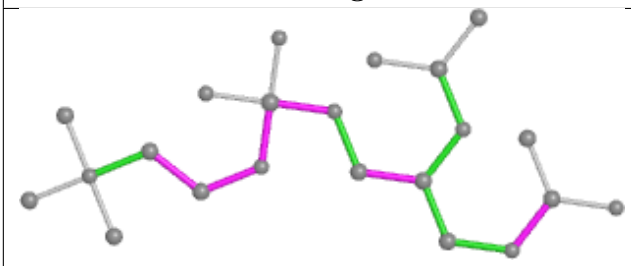
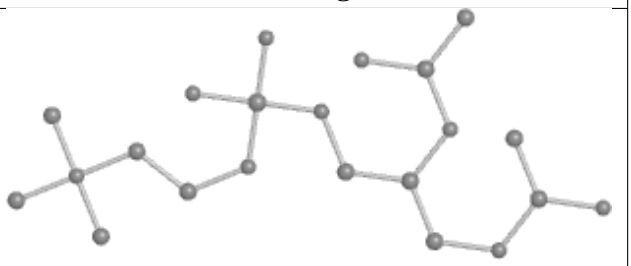


Bond angles

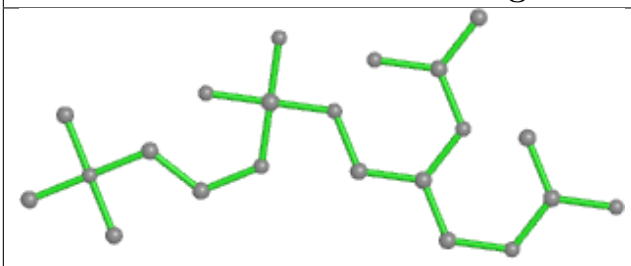


Torsions

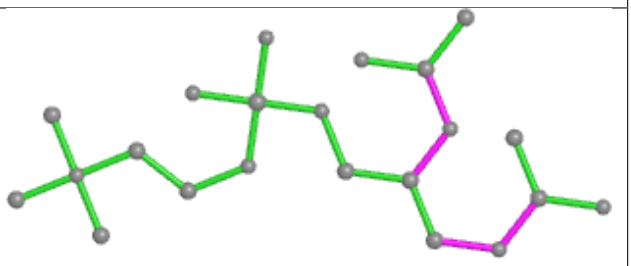


Rings

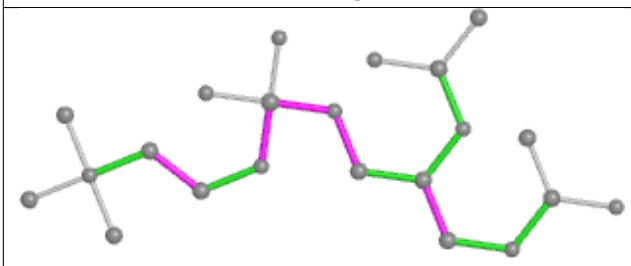
Ligand PCW C 1110



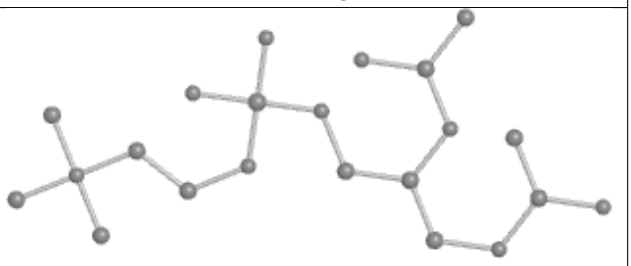
Bond lengths



Bond angles

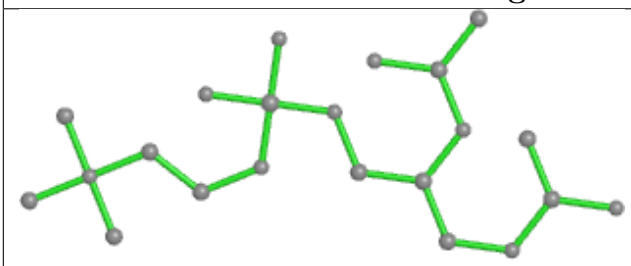


Torsions

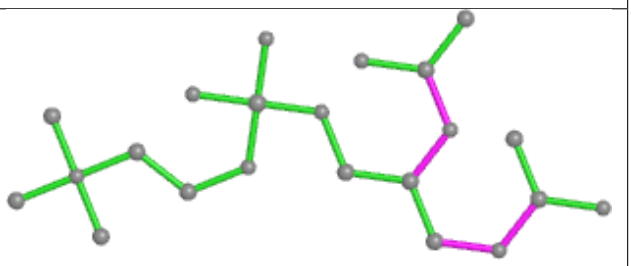


Rings

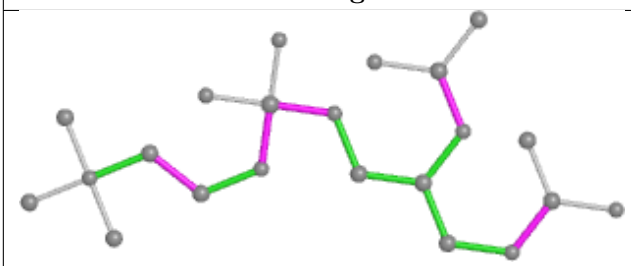
Ligand PCW A 1112



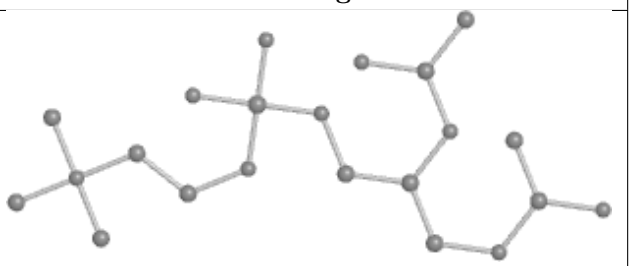
Bond lengths



Bond angles

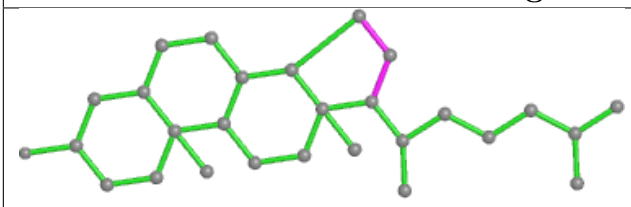


Torsions

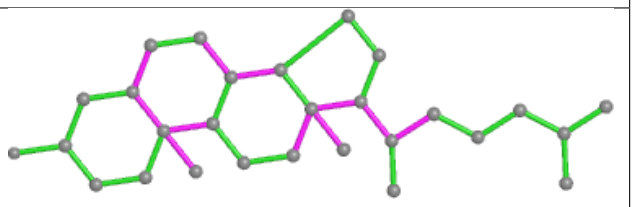


Rings

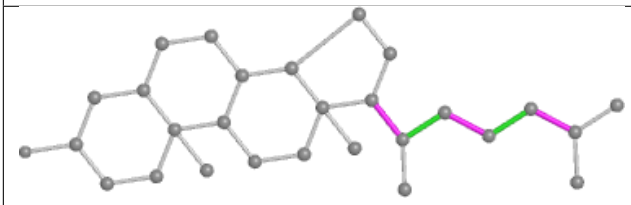
Ligand CLR E 101



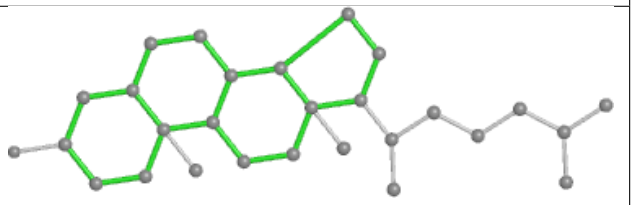
Bond lengths



Bond angles

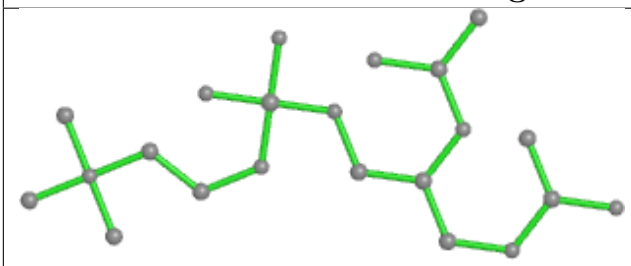


Torsions

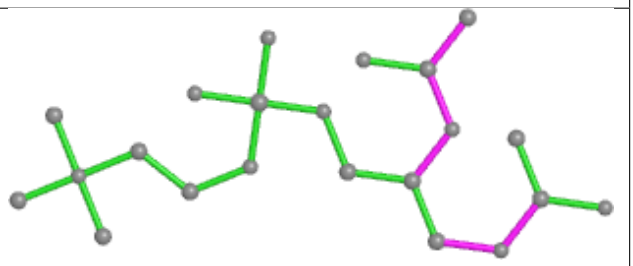


Rings

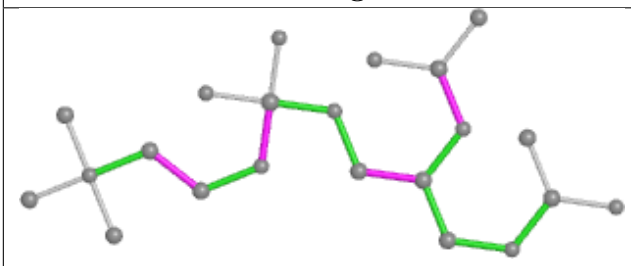
Ligand PCW C 1107



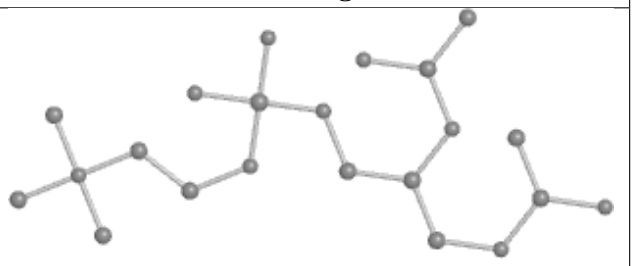
Bond lengths



Bond angles

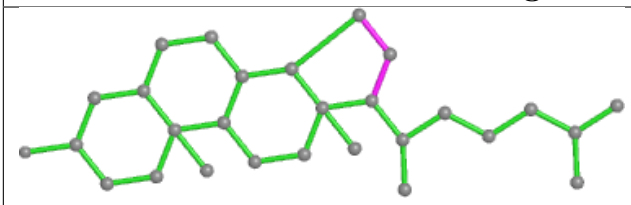


Torsions

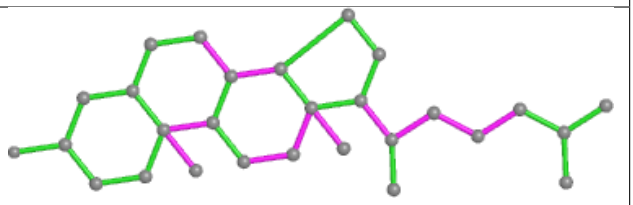


Rings

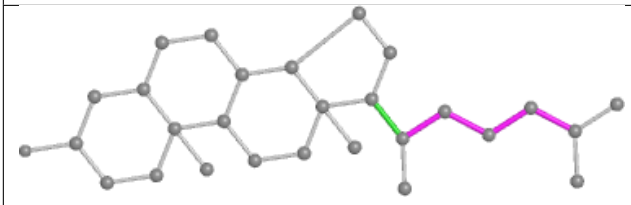
Ligand CLR G 101



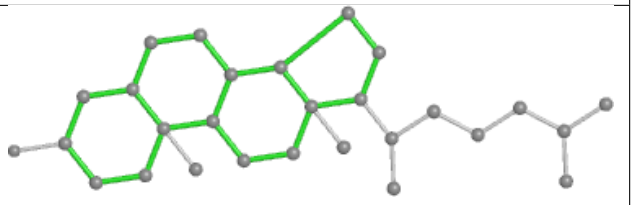
Bond lengths



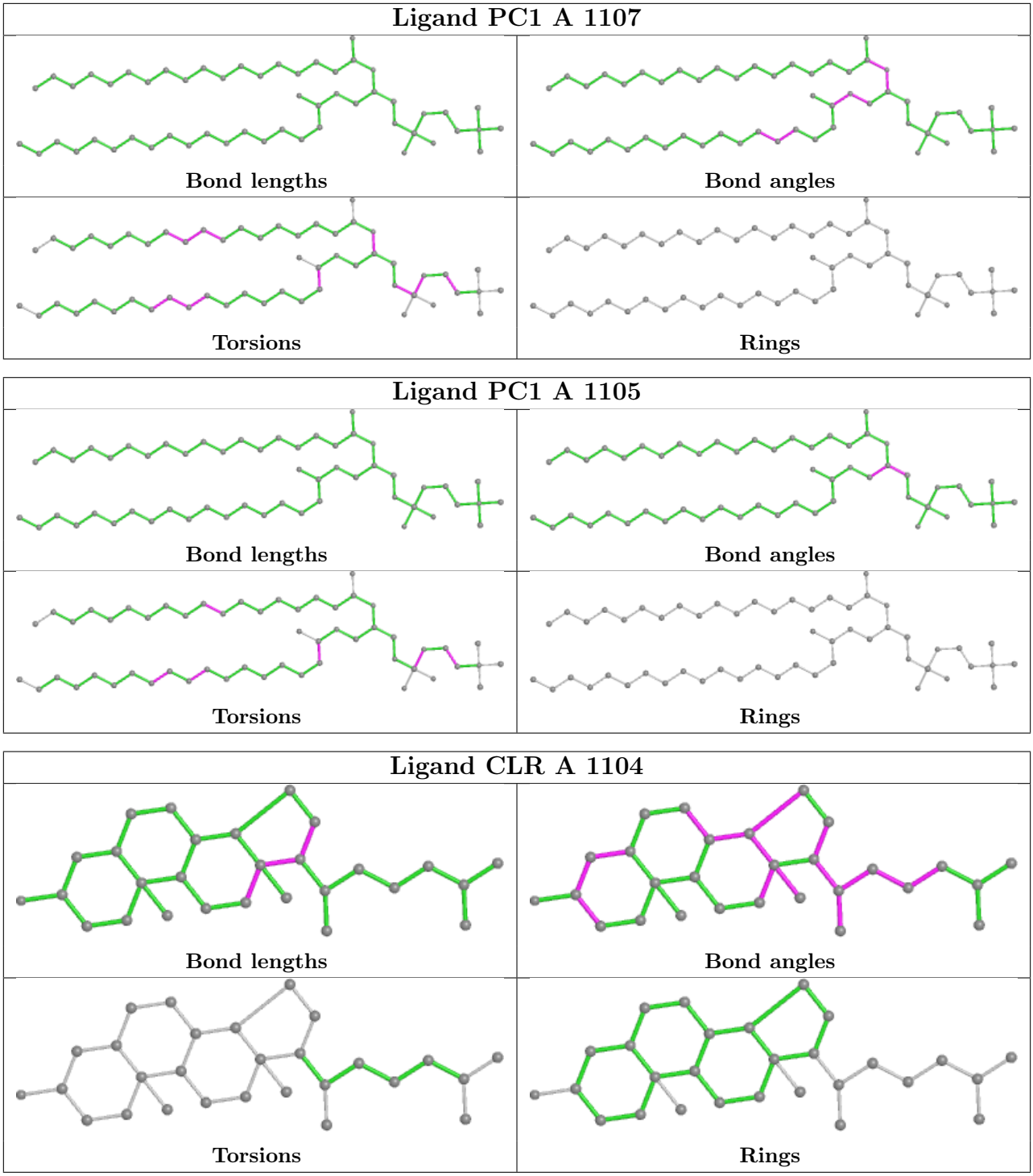
Bond angles



Torsions



Rings



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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	0.12	62 (6%) 20 16	25, 68, 144, 191	0
1	C	995/1021 (97%)	0.05	37 (3%) 41 37	34, 76, 134, 190	0
2	B	291/303 (96%)	0.17	20 (6%) 16 13	59, 93, 143, 172	0
2	D	291/303 (96%)	0.52	34 (11%) 4 3	67, 128, 168, 212	0
3	E	33/65 (50%)	-0.19	1 (3%) 50 45	44, 56, 108, 138	0
3	G	35/65 (53%)	-0.15	3 (8%) 10 8	37, 59, 105, 106	0
All	All	2640/2778 (95%)	0.14	157 (5%) 22 18	25, 78, 150, 212	0

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	269	GLY	7.4
1	C	432	ASN	7.4
1	C	23	ARG	7.2
1	A	29	LYS	7.1
1	A	268	SER	6.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

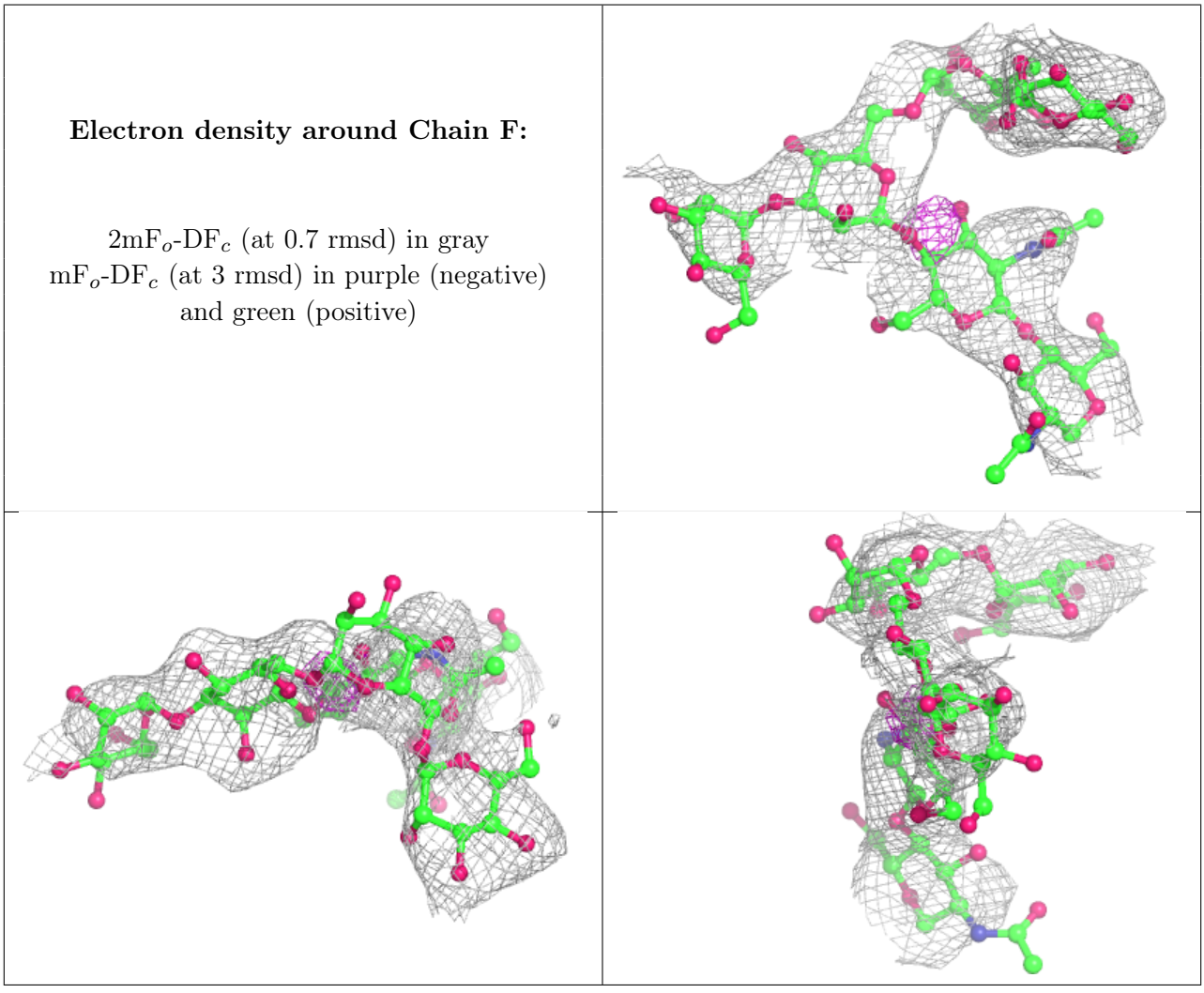
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	MAN	H	4	11/12	0.63	0.66	164,185,190,193	0
5	BMA	H	3	11/12	0.64	0.26	186,189,193,195	0
5	NAG	H	2	14/15	0.64	0.57	168,200,209,210	0
4	MAN	F	4	11/12	0.72	0.45	118,149,154,155	0
4	MAN	F	5	11/12	0.74	0.42	113,133,144,147	0
5	NAG	H	1	14/15	0.76	0.21	161,178,195,206	0
5	MAN	H	5	11/12	0.76	0.36	167,180,190,192	0
4	MAN	F	6	11/12	0.77	0.61	137,145,153,153	0
6	NAG	I	1	14/15	0.77	0.41	137,148,170,174	0
6	NAG	I	2	14/15	0.77	0.49	132,155,166,168	0
4	NAG	F	2	14/15	0.83	0.54	107,136,148,151	0
4	NAG	F	1	14/15	0.84	0.46	114,140,147,148	0
4	BMA	F	3	11/12	0.86	0.39	108,121,134,137	0

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

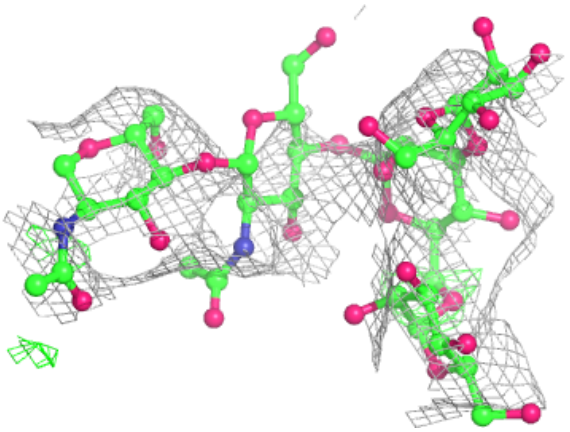
Electron density around Chain F:

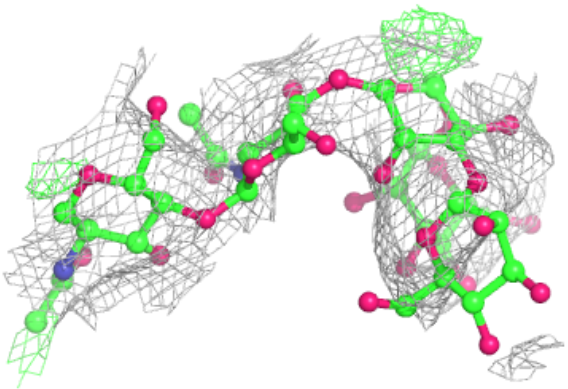
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

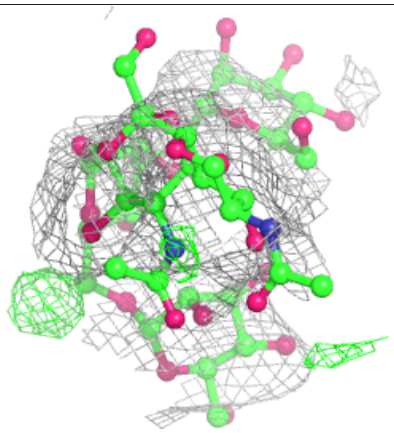


Electron density around Chain H:

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

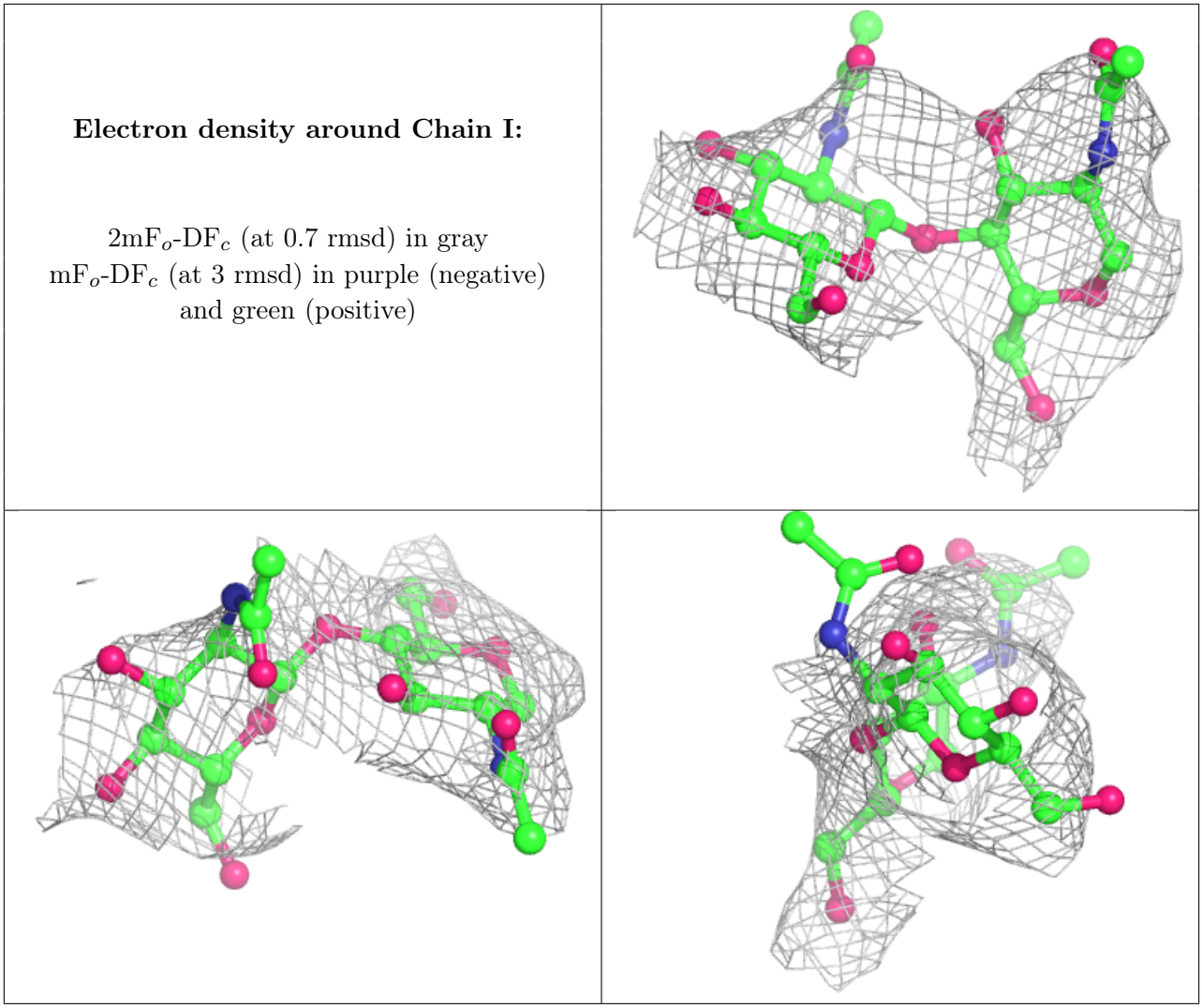






Electron density around Chain I:

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



6.4 Ligands

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	PCW	C	1111	22/54	0.57	0.36	87,118,153,159	0
9	PC1	A	1105	54/54	0.59	0.51	69,115,161,175	0
10	PCW	C	1108	22/54	0.68	0.41	86,124,177,183	0
10	PCW	A	1108	22/54	0.68	0.32	80,125,155,161	0
10	PCW	A	1113	22/54	0.70	0.70	102,130,158,164	0
10	PCW	C	1105	22/54	0.72	0.35	92,113,161,172	0
10	PCW	A	1112	22/54	0.74	0.51	88,128,140,144	0
10	PCW	C	1107	22/54	0.75	0.27	90,122,165,173	0

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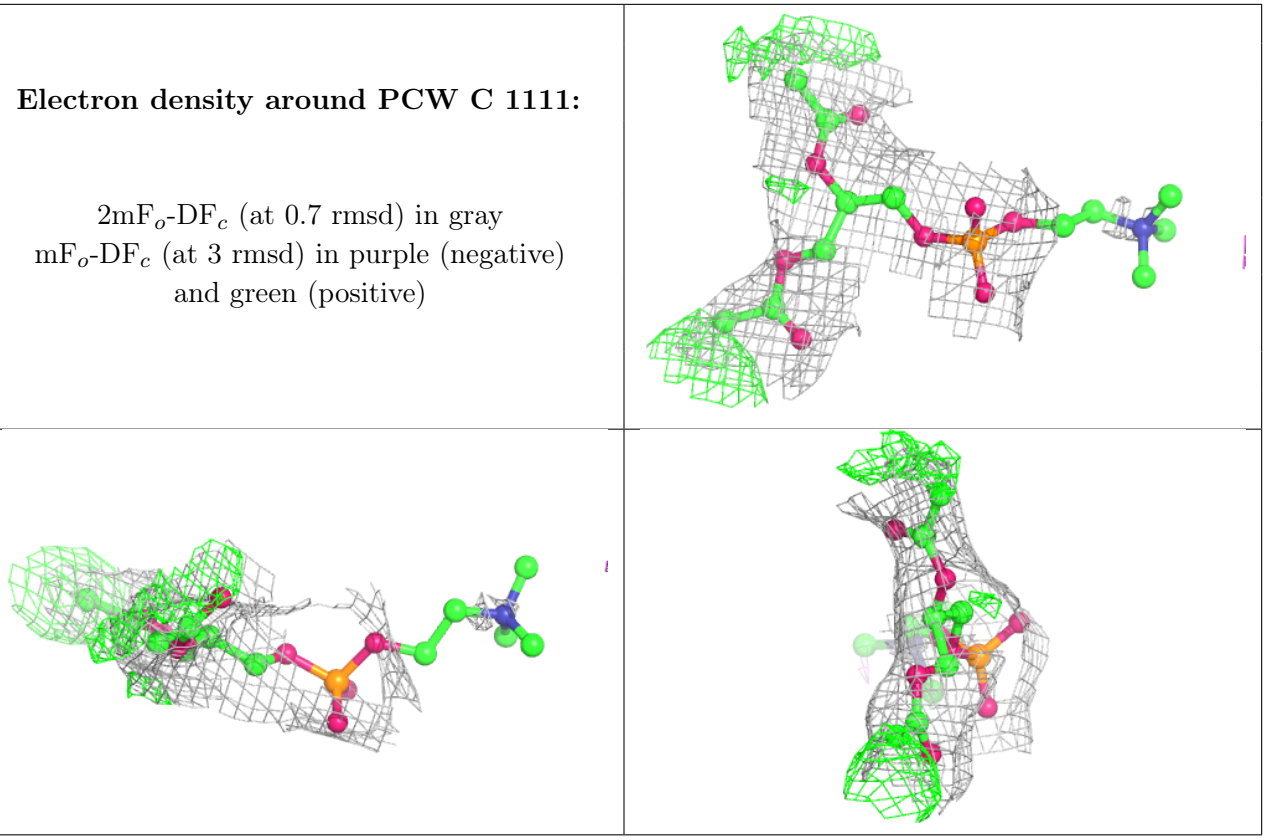
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	PCW	C	1109	22/54	0.76	0.60	119,153,167,170	0
8	CLR	A	1109	28/28	0.77	0.37	94,115,130,134	0
10	PCW	C	1106	22/54	0.77	0.54	101,134,145,148	0
11	NAG	D	402	14/15	0.79	0.37	156,170,184,184	0
10	PCW	B	401	22/54	0.80	0.24	76,114,145,152	0
8	CLR	D	401	28/28	0.81	0.34	81,107,112,117	0
10	PCW	A	1106	22/54	0.82	0.31	90,121,142,146	0
10	PCW	C	1110	22/54	0.84	0.46	105,126,137,144	0
10	PCW	A	1114	54/54	0.85	0.60	64,87,156,173	0
9	PC1	A	1107	54/54	0.85	0.37	50,91,122,137	0
8	CLR	A	1104	28/28	0.89	0.25	59,91,107,110	0
9	PC1	A	1110	54/54	0.89	0.36	48,88,132,137	0
10	PCW	A	1111	22/54	0.89	0.26	67,109,117,126	0
12	DMU	E	102	33/33	0.89	0.25	37,71,89,94	0
7	MN	A	1101	1/1	0.92	0.13	77,77,77,77	0
8	CLR	C	1104	28/28	0.92	0.26	37,43,102,111	0
8	CLR	G	101	28/28	0.94	0.29	33,50,107,113	0
8	CLR	E	101	28/28	0.95	0.21	31,45,67,74	0
7	MN	C	1102	1/1	0.96	0.17	68,68,68,68	0
7	MN	C	1101	1/1	0.97	0.10	80,80,80,80	0
7	MN	A	1103	1/1	0.98	0.18	54,54,54,54	0
7	MN	A	1102	1/1	0.98	0.18	69,69,69,69	0
7	MN	C	1103	1/1	0.99	0.14	72,72,72,72	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.

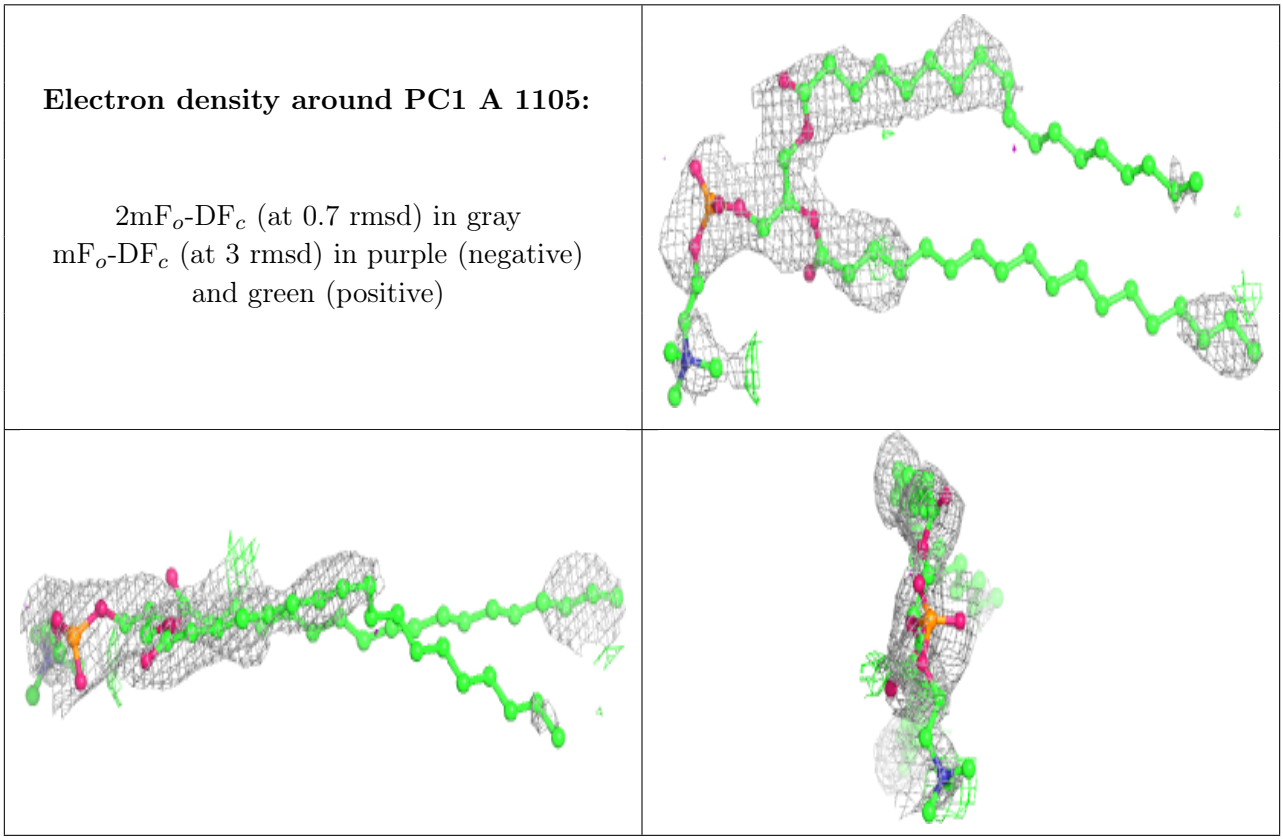
Electron density around PCW C 1111:

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



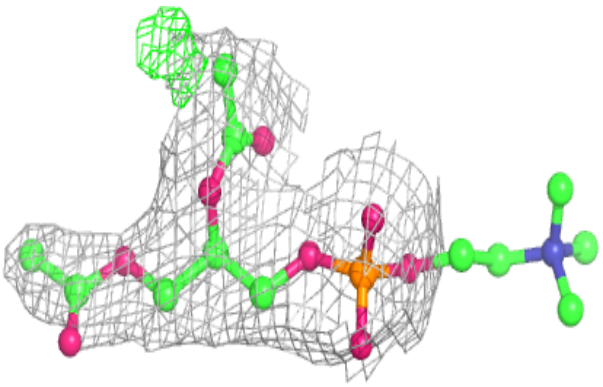
Electron density around PC1 A 1105:

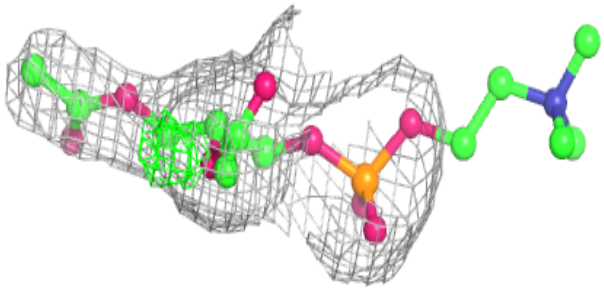
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

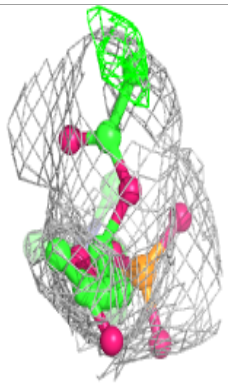


Electron density around PCW C 1108:

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

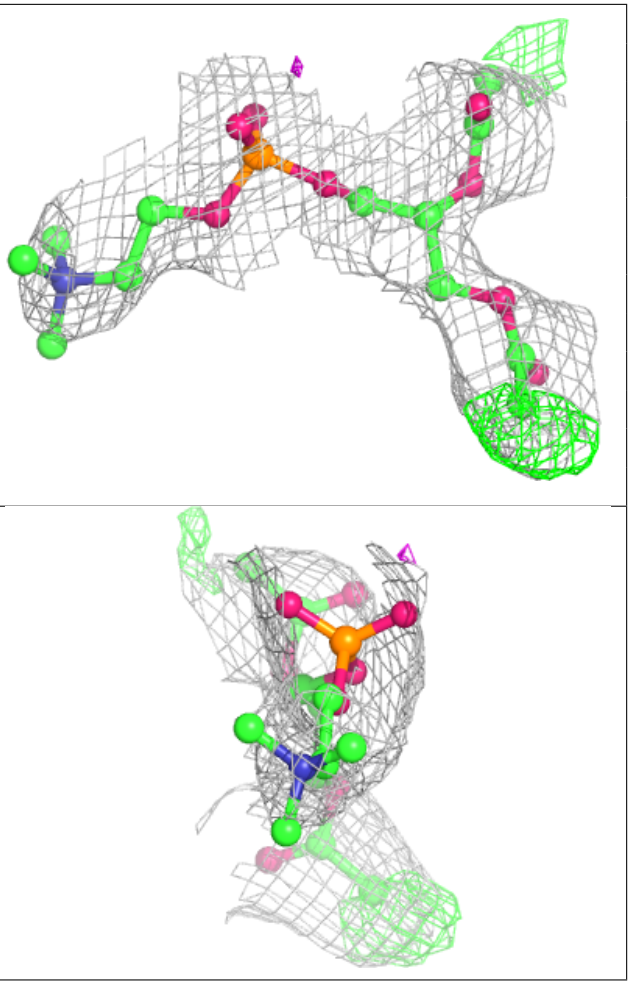


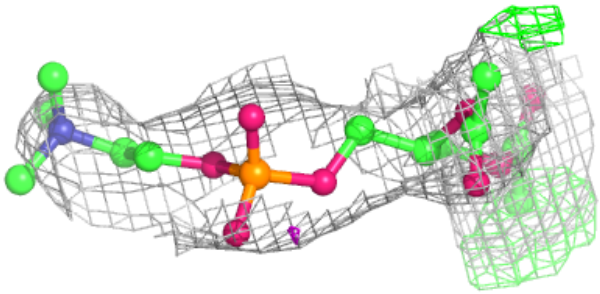




Electron density around PCW A 1108:

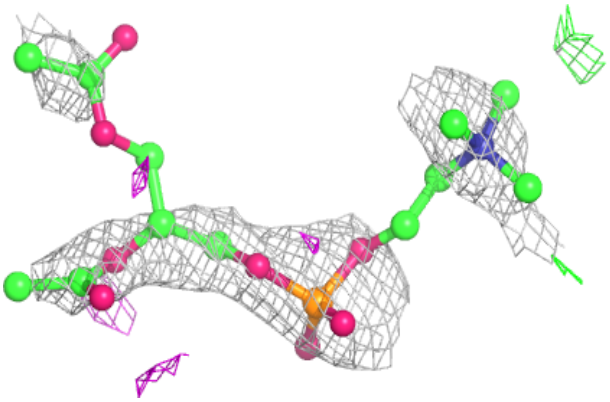
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

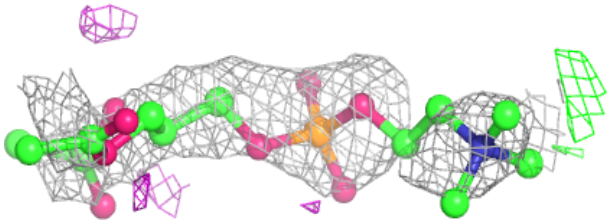


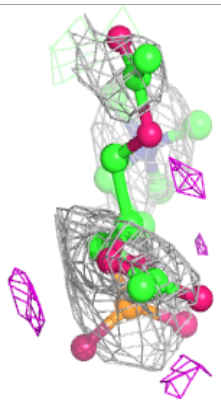


Electron density around PCW A 1113:

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

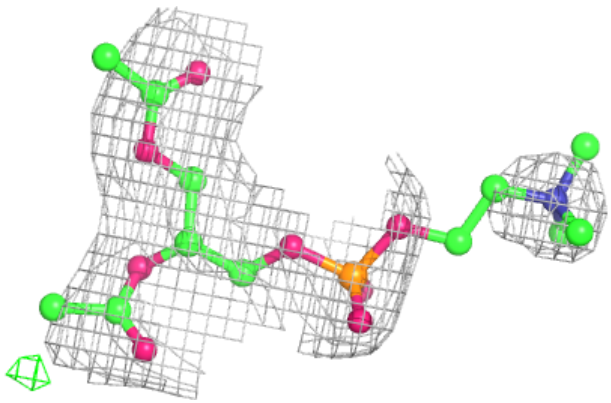


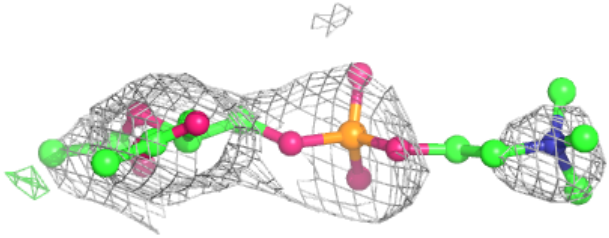


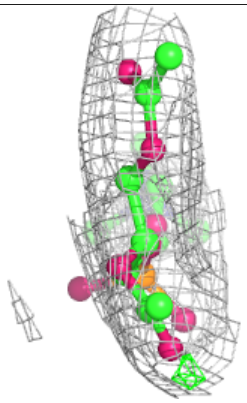


Electron density around PCW C 1105:

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

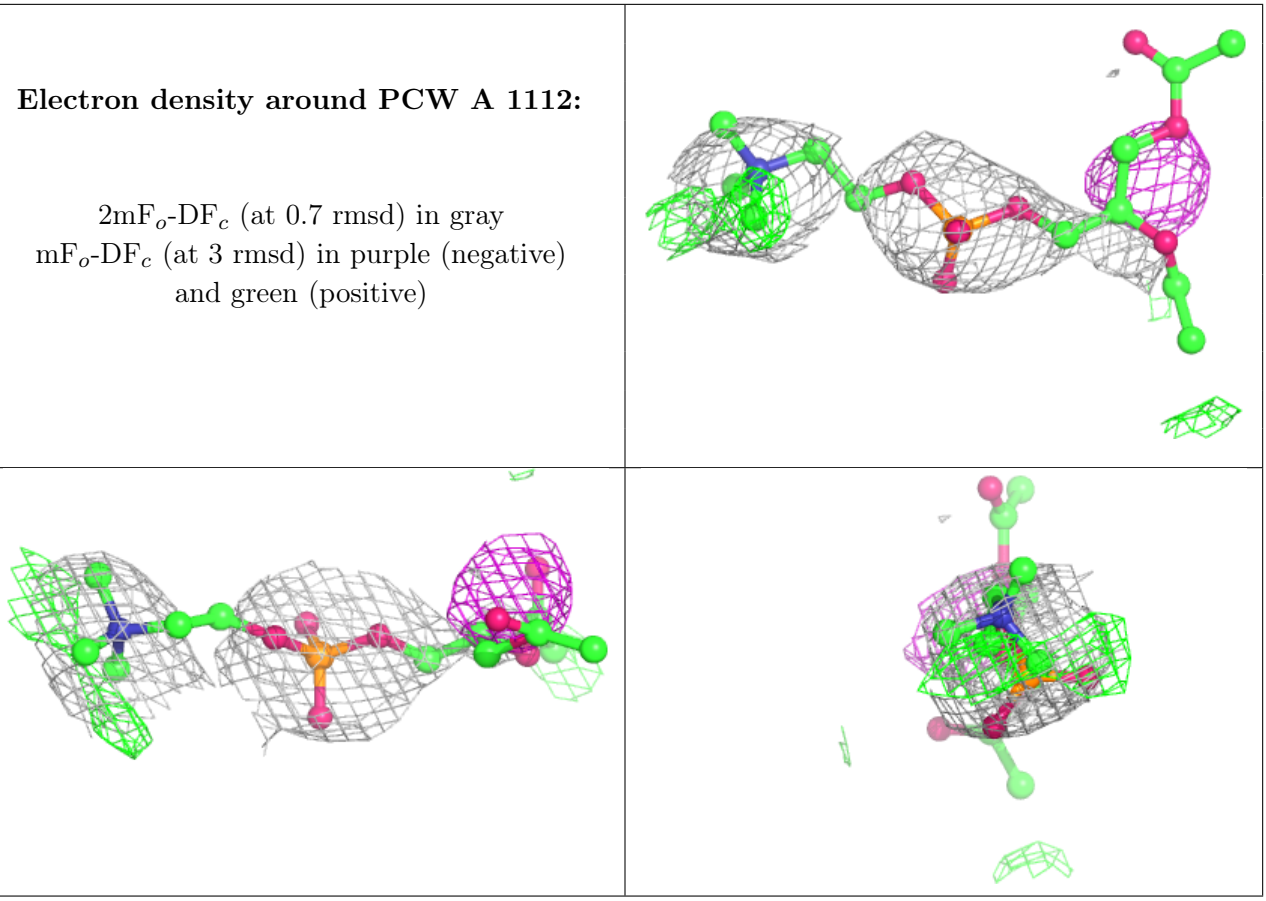






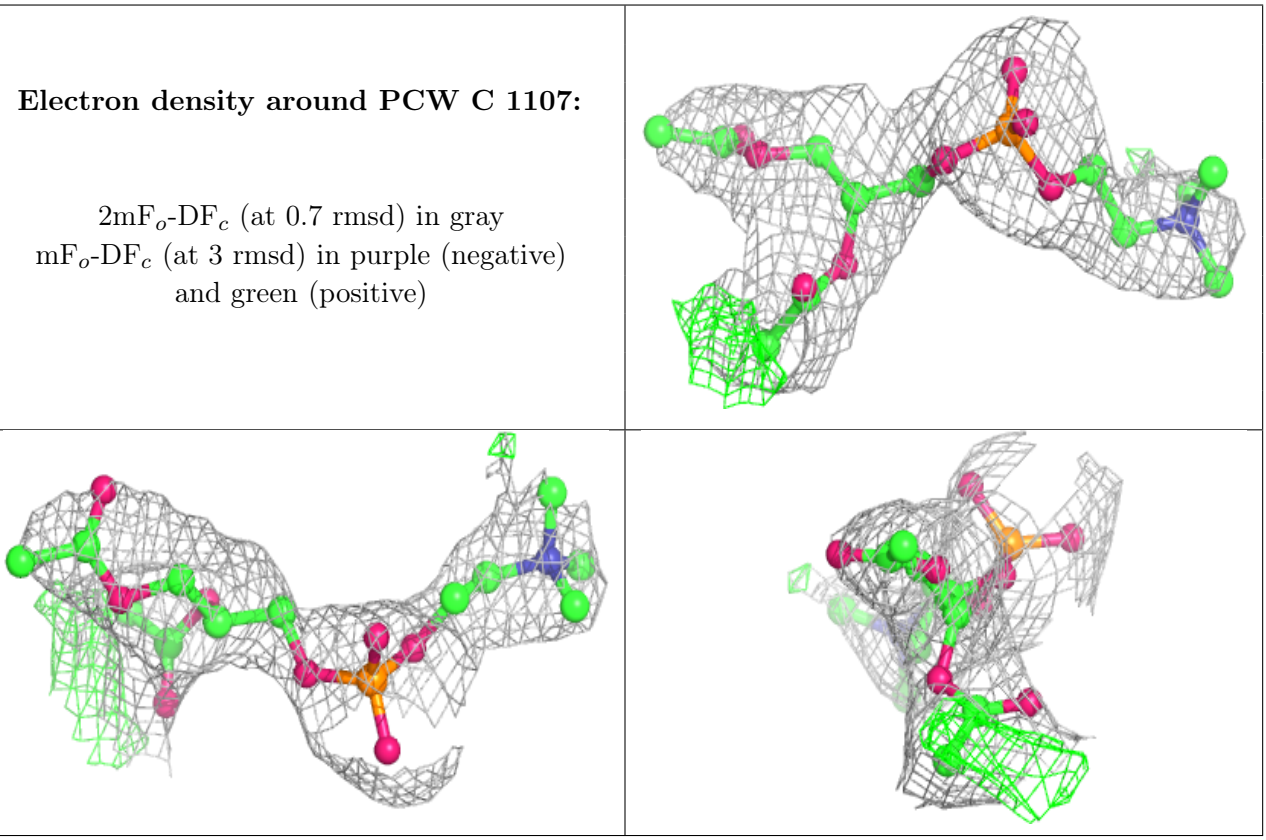
Electron density around PCW A 1112:

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



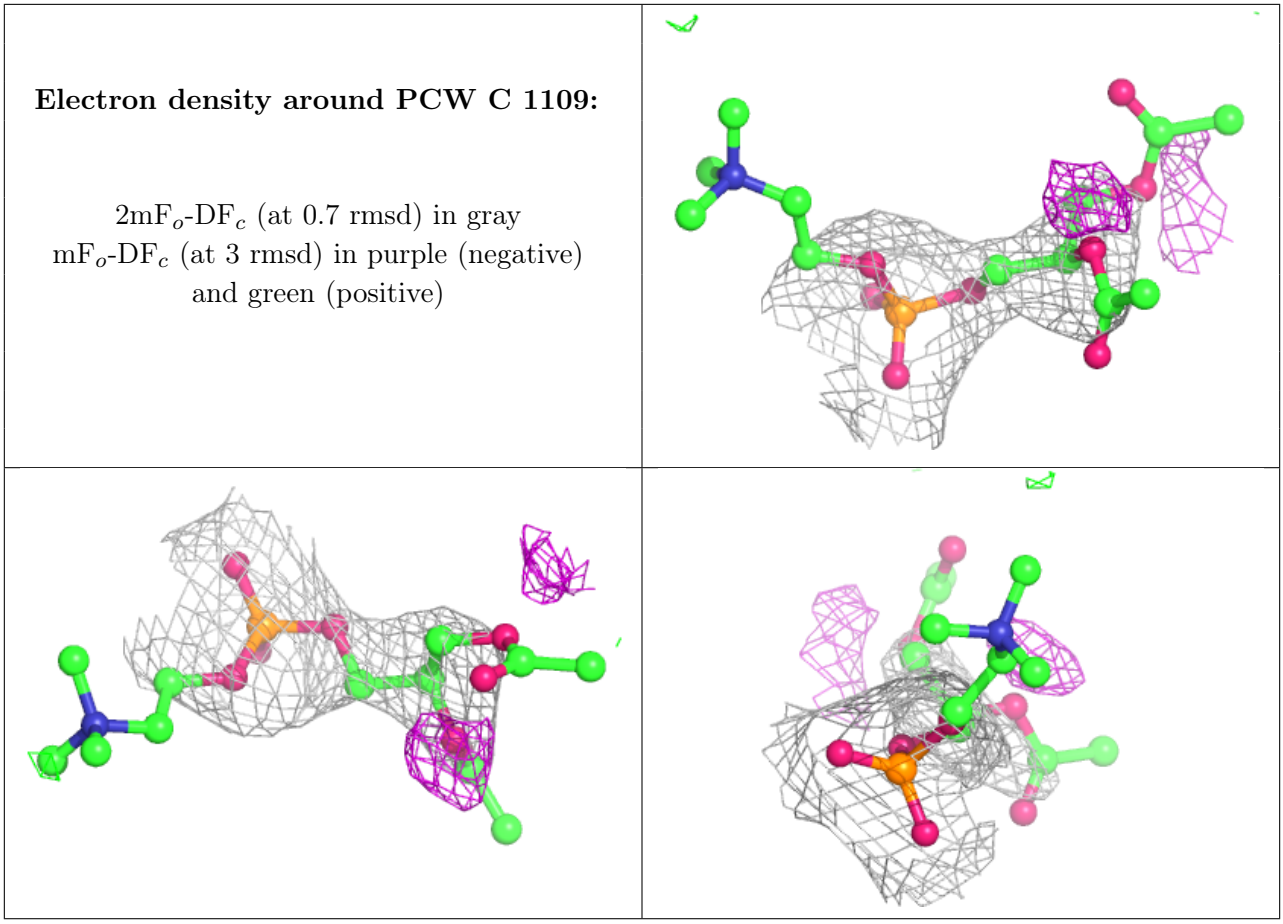
Electron density around PCW C 1107:

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



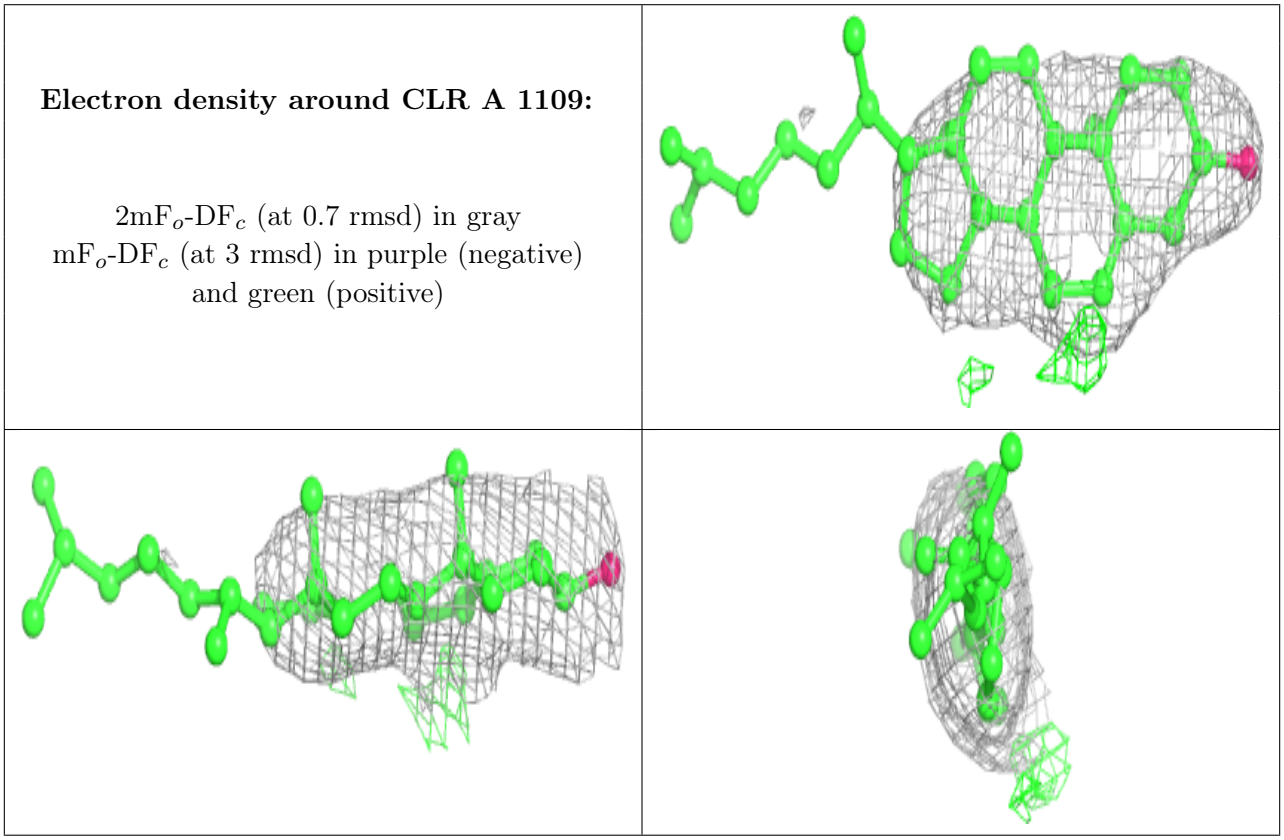
Electron density around PCW C 1109:

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



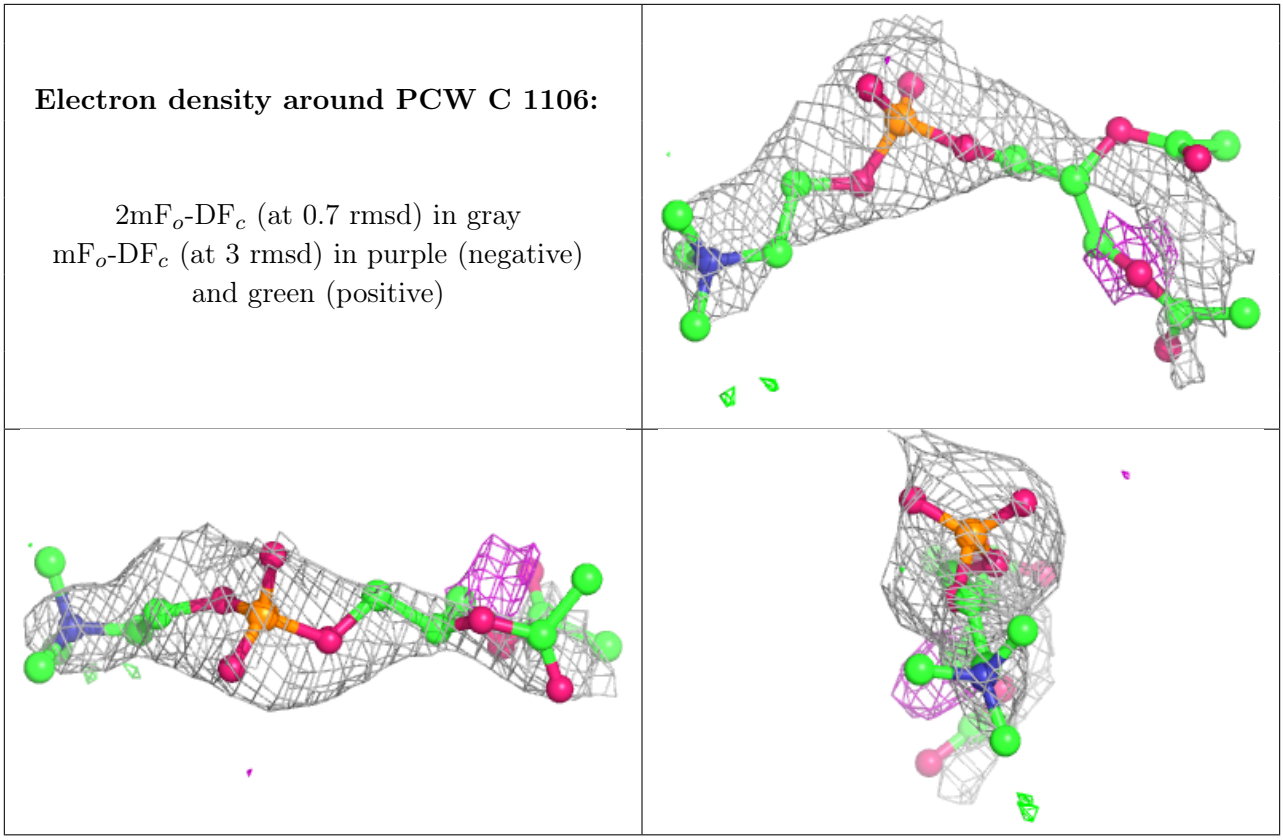
Electron density around CLR A 1109:

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



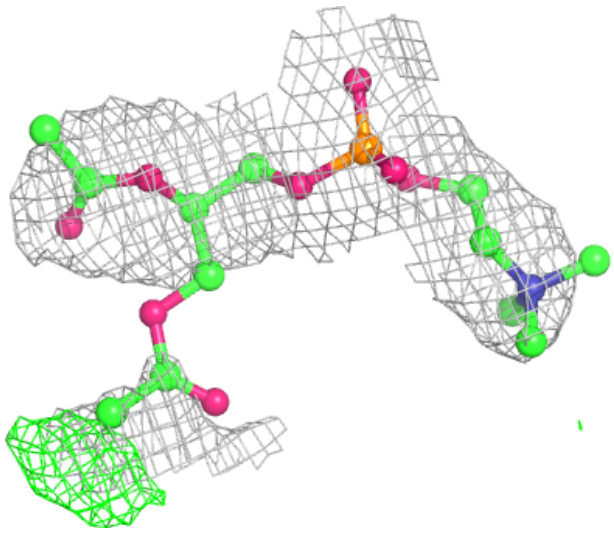
Electron density around PCW C 1106:

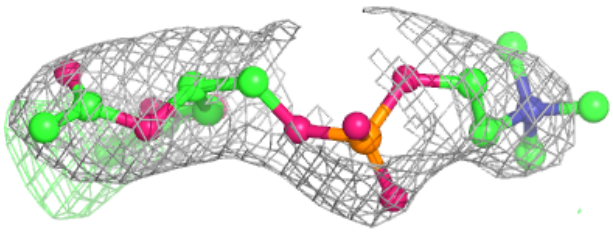
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

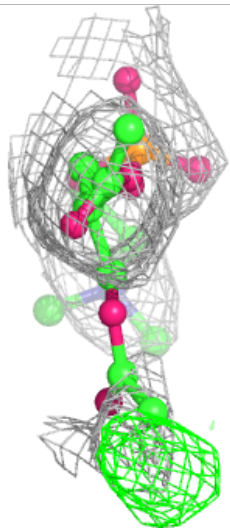


Electron density around PCW B 401:

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

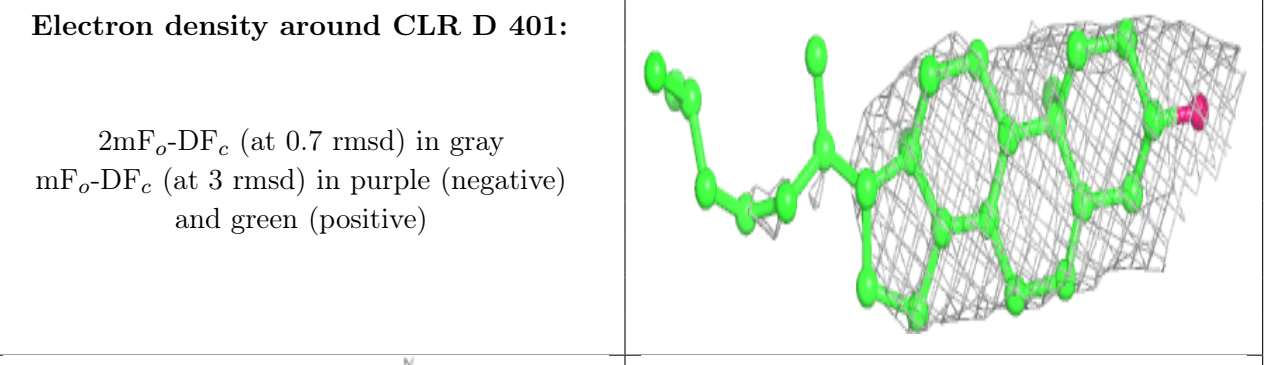






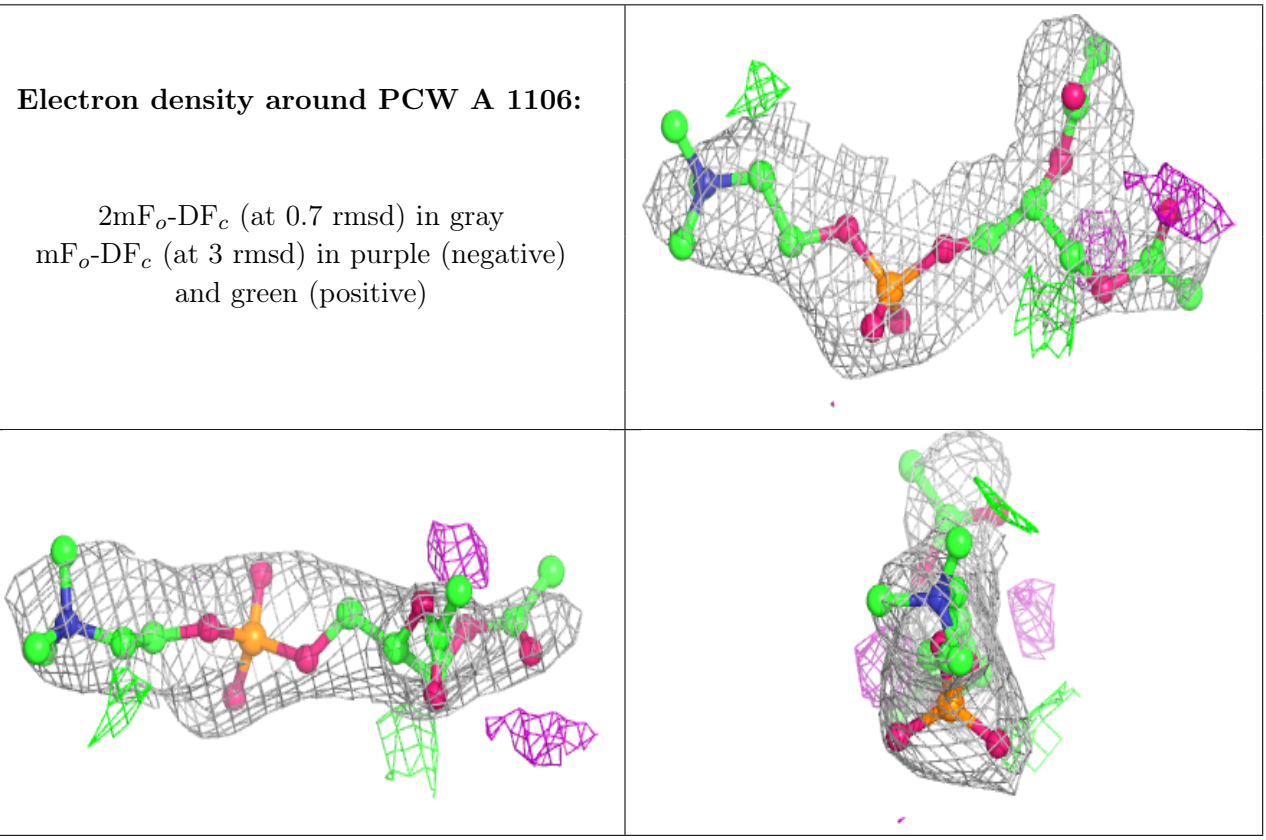
Electron density around CLR D 401:

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



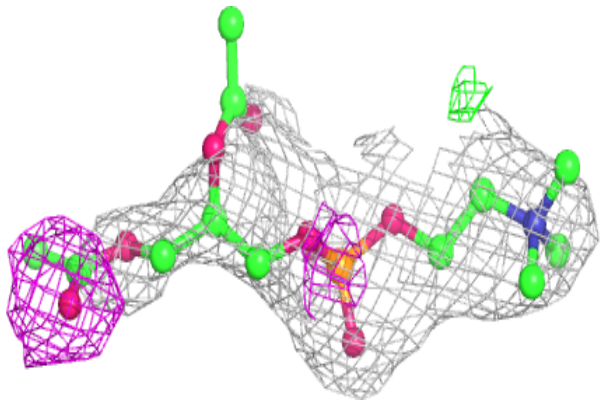
Electron density around PCW A 1106:

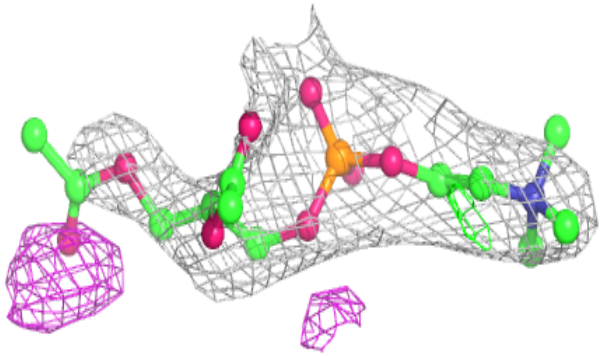
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

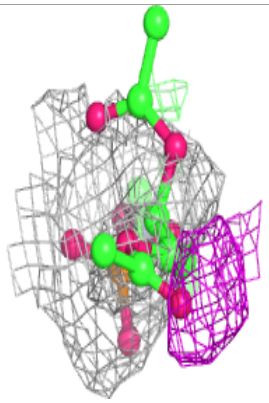


Electron density around PCW C 1110:

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

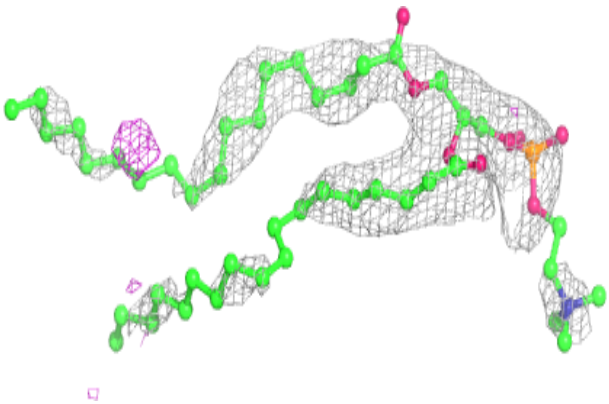


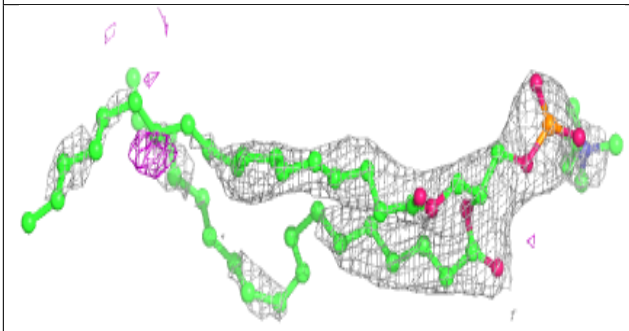


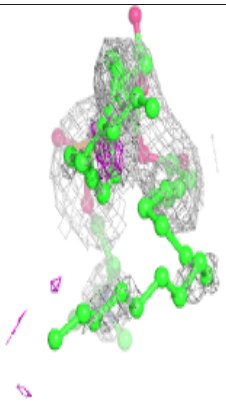


Electron density around PCW A 1114:

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

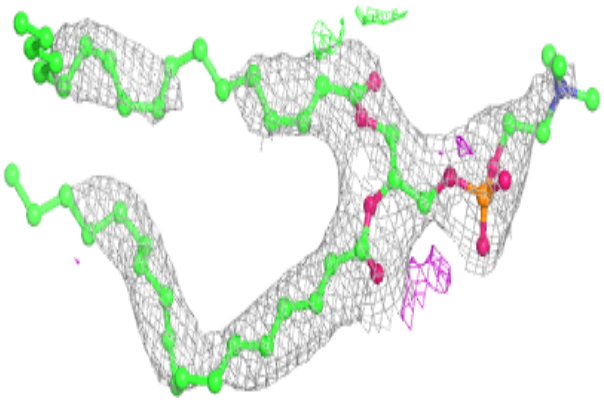


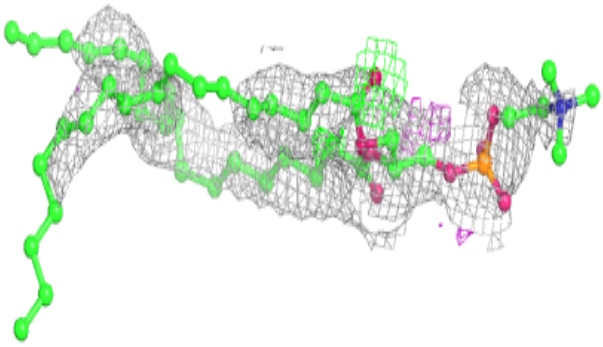


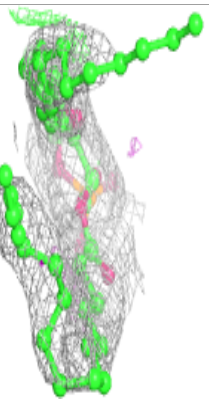


Electron density around PC1 A 1107:

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

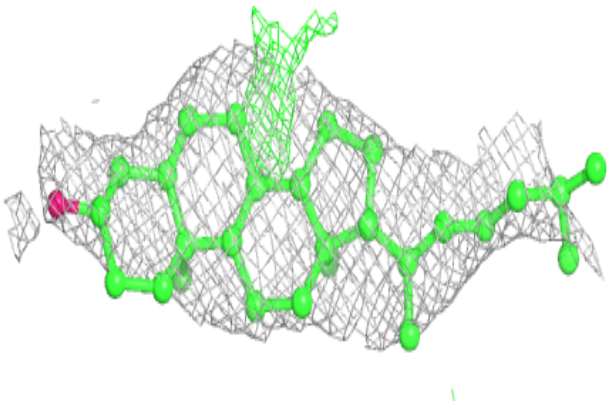


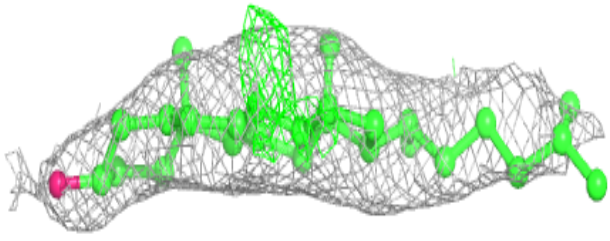


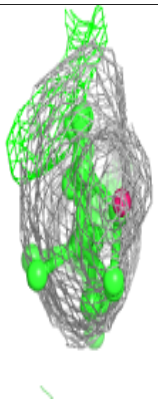


Electron density around CLR A 1104:

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

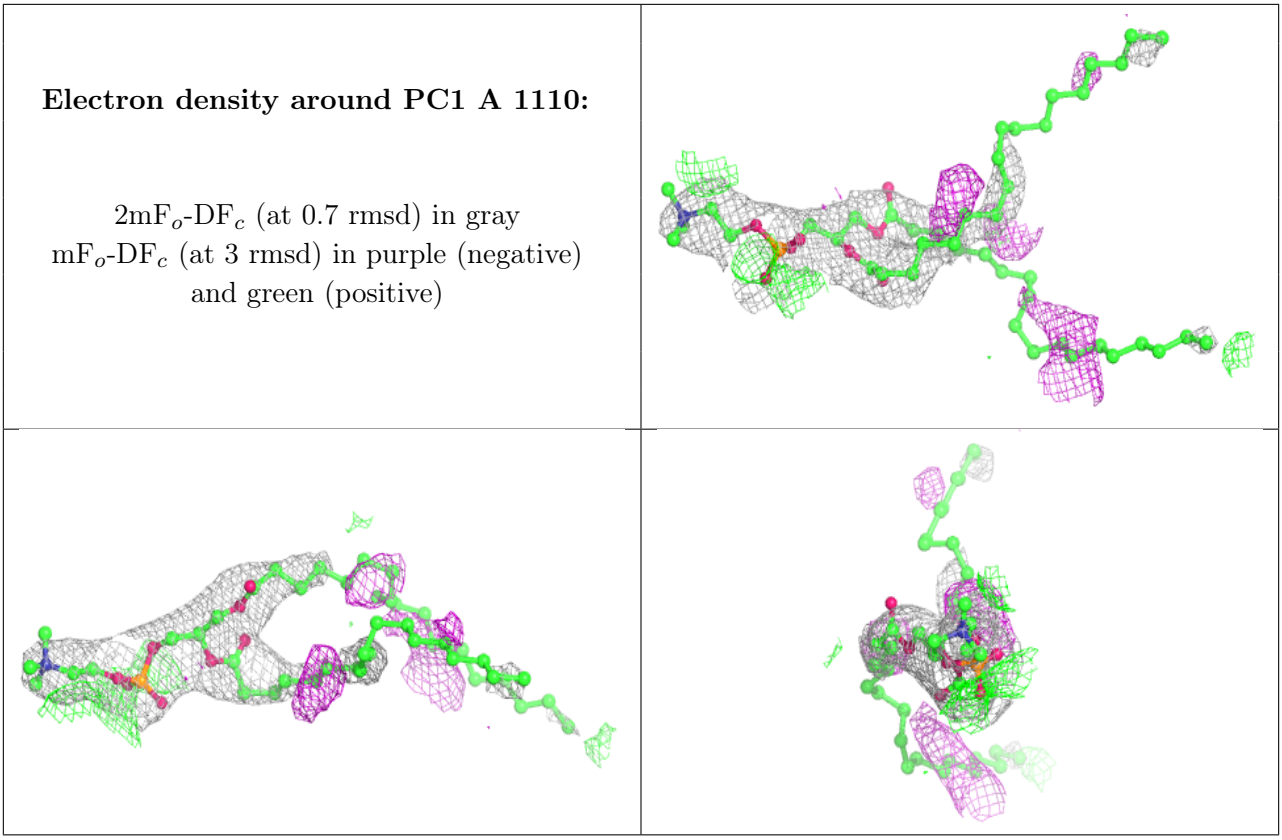






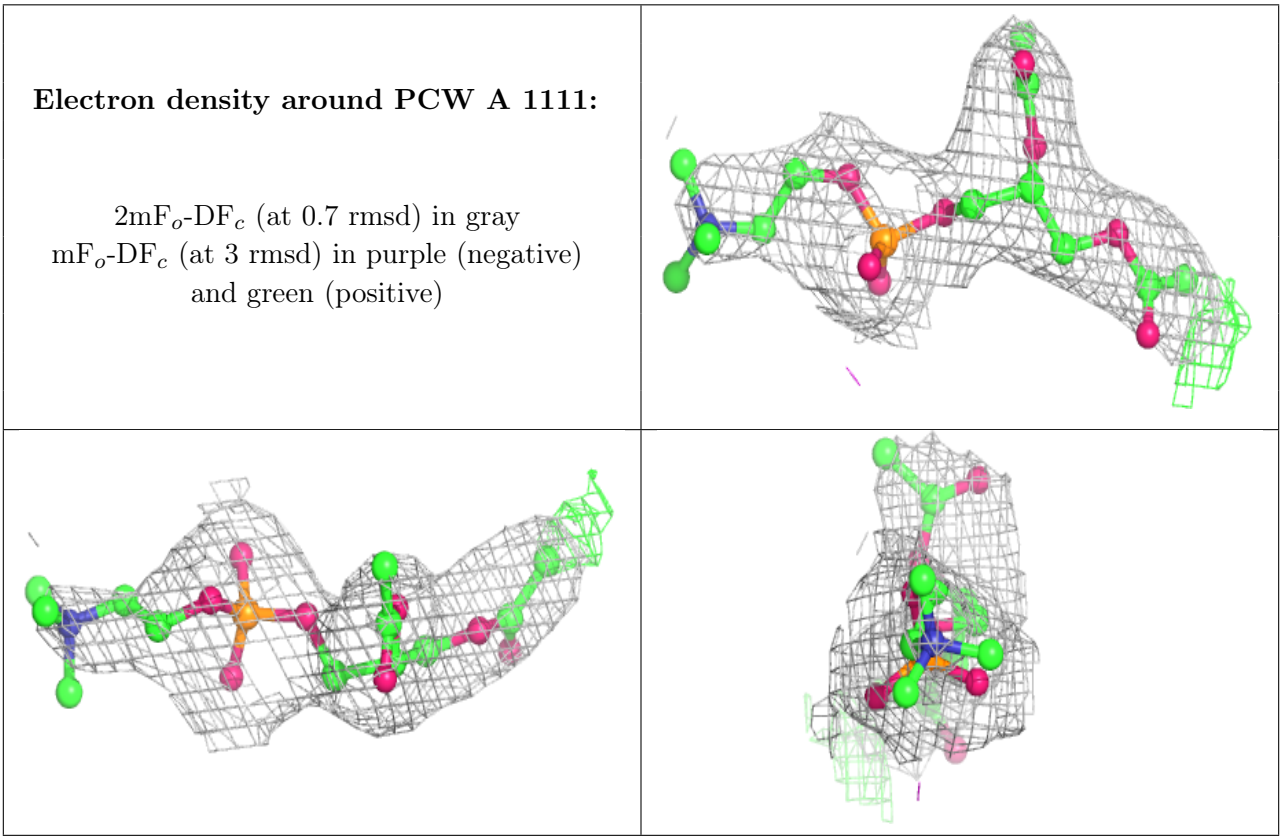
Electron density around PC1 A 1110:

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



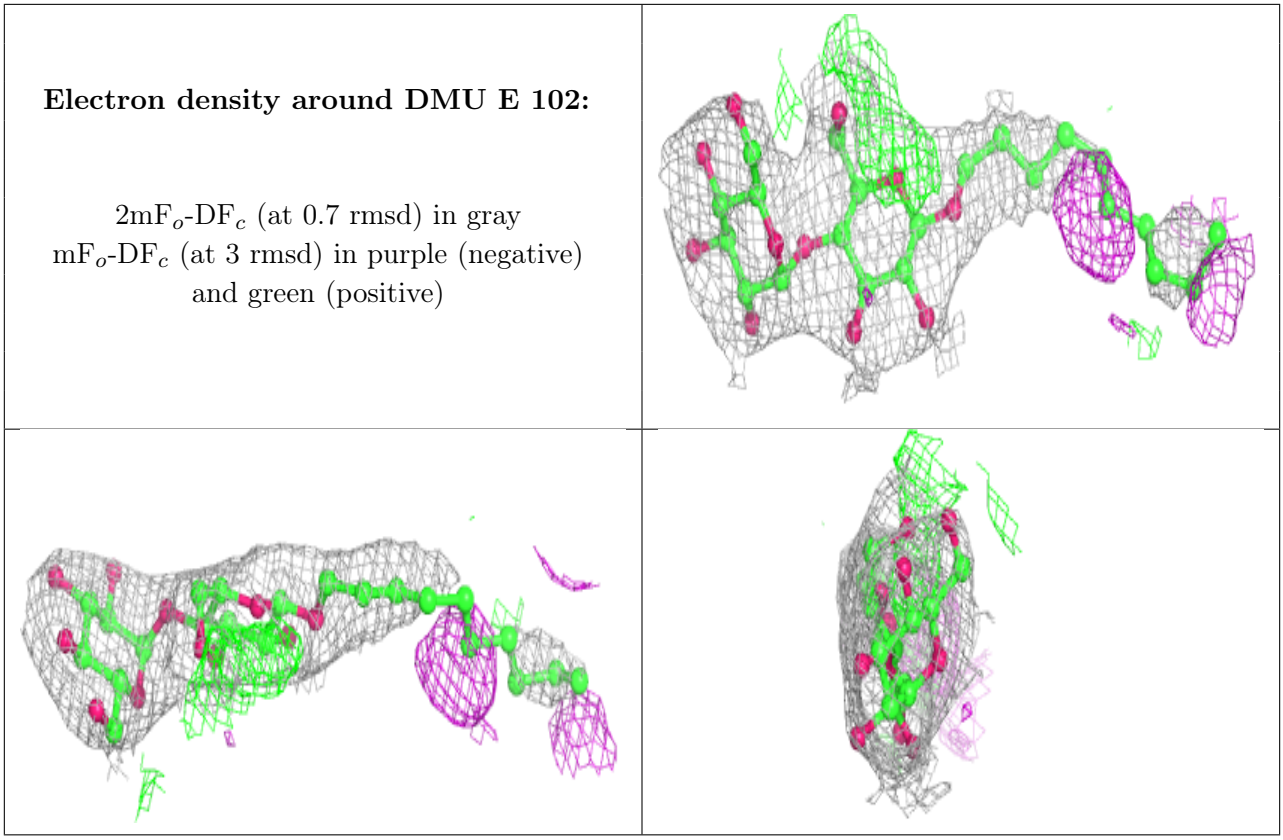
Electron density around PCW A 1111:

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



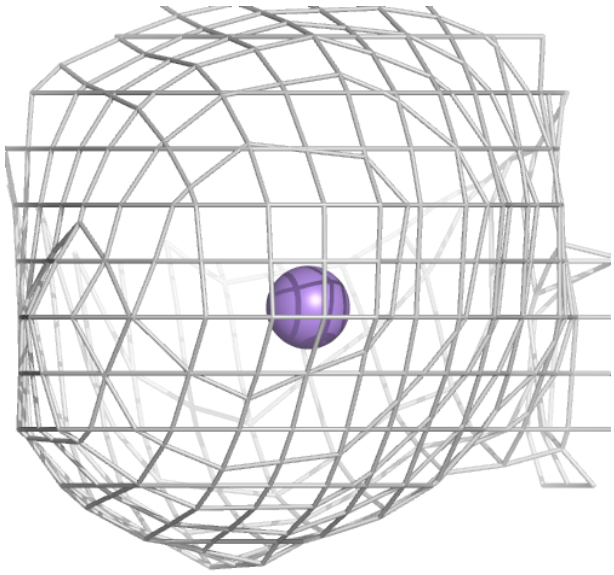
Electron density around DMU E 102:

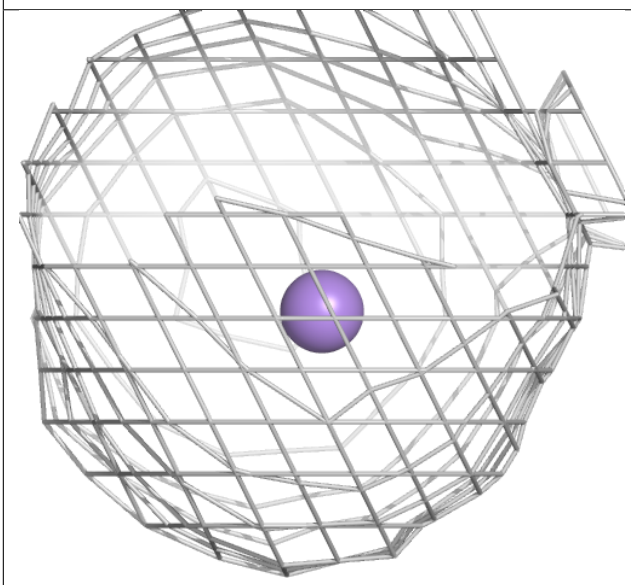
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

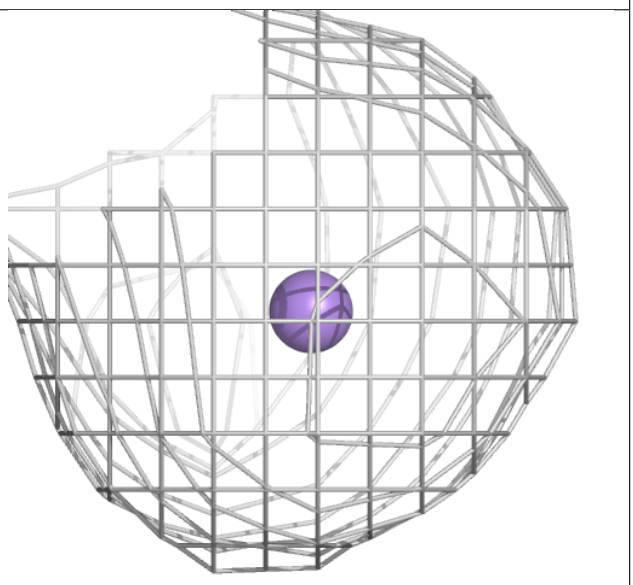


Electron density around MN A 1101:

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

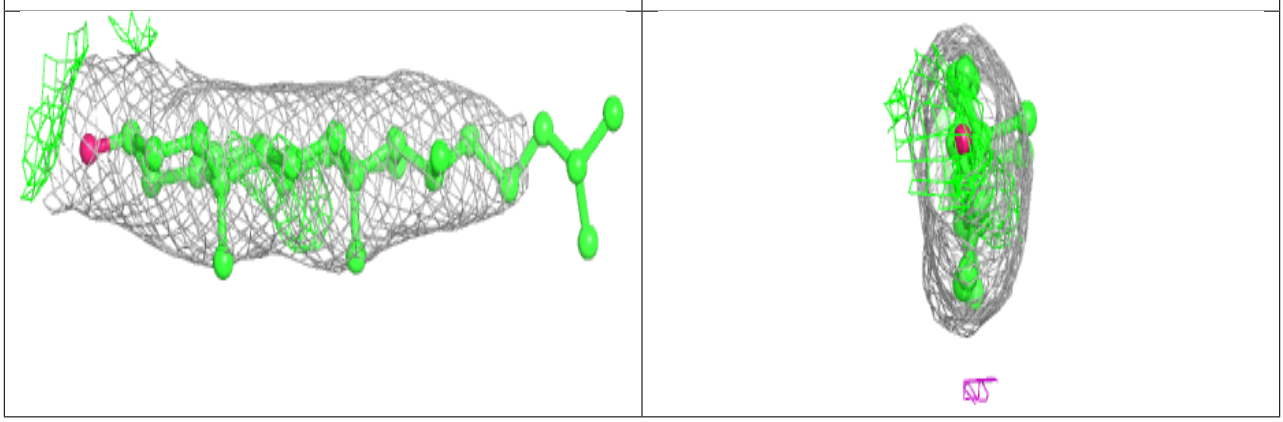






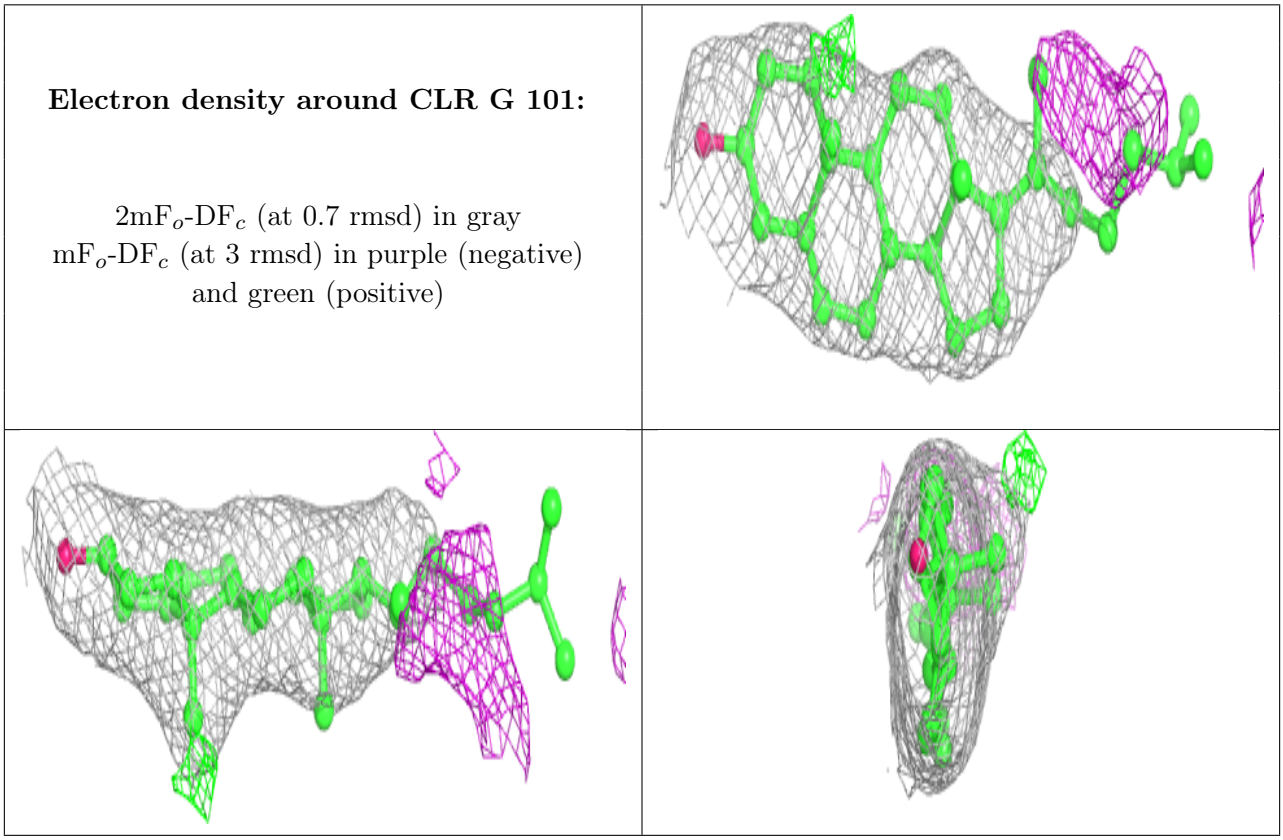
Electron density around CLR C 1104:

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



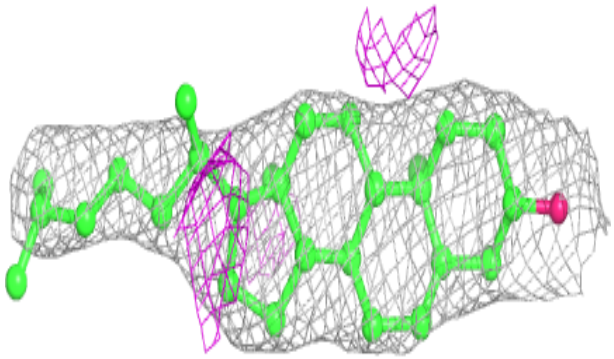
Electron density around CLR G 101:

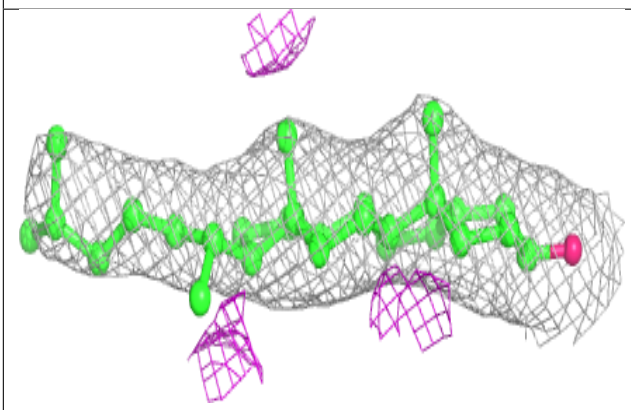
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

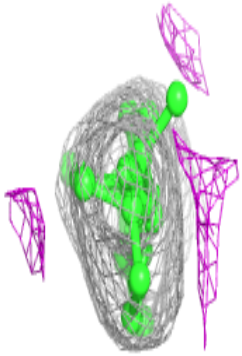


Electron density around CLR E 101:

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

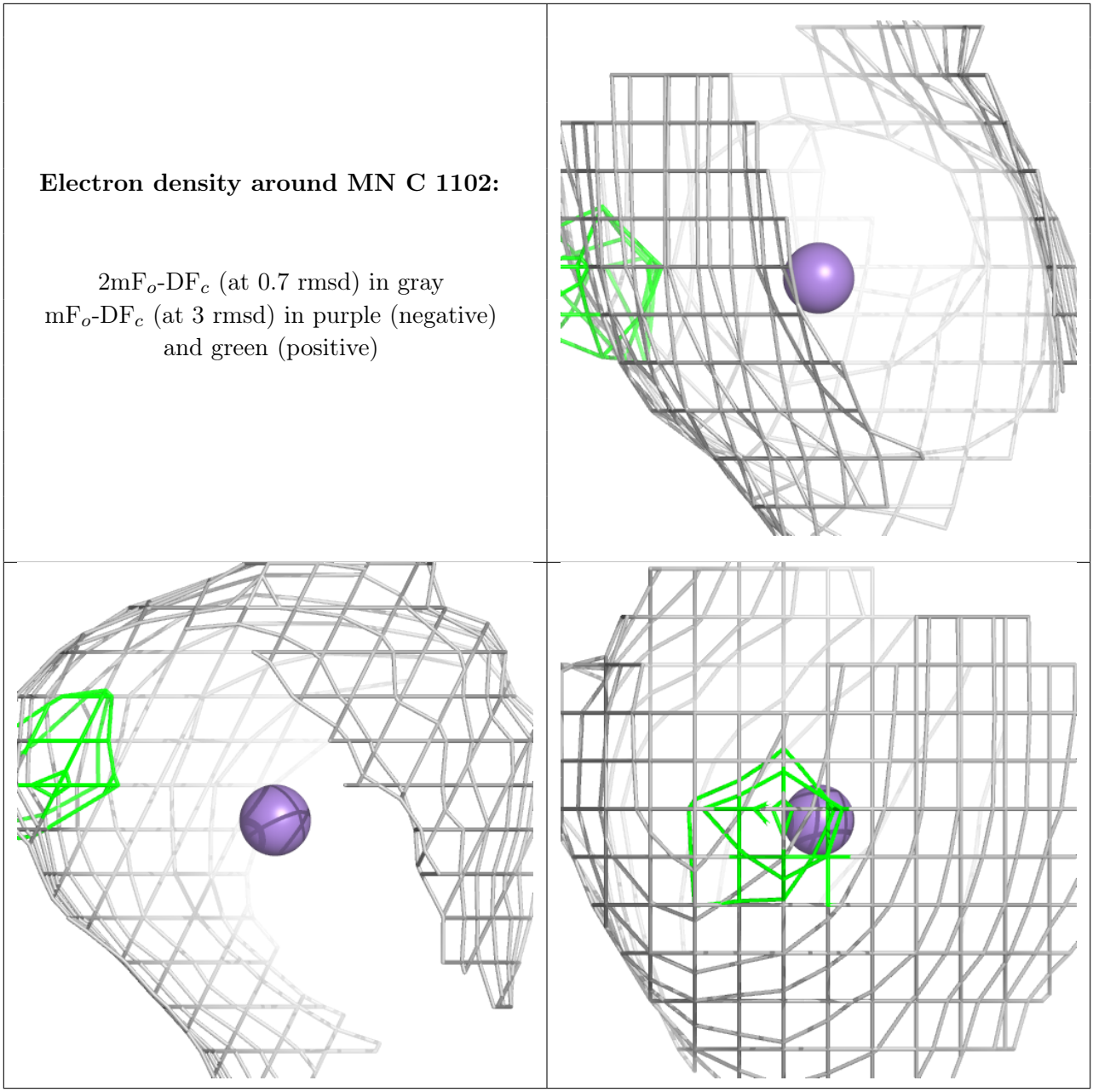






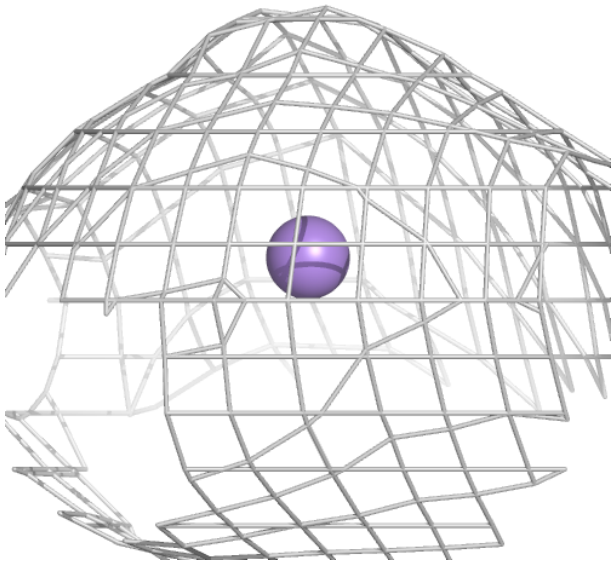
Electron density around MN C 1102:

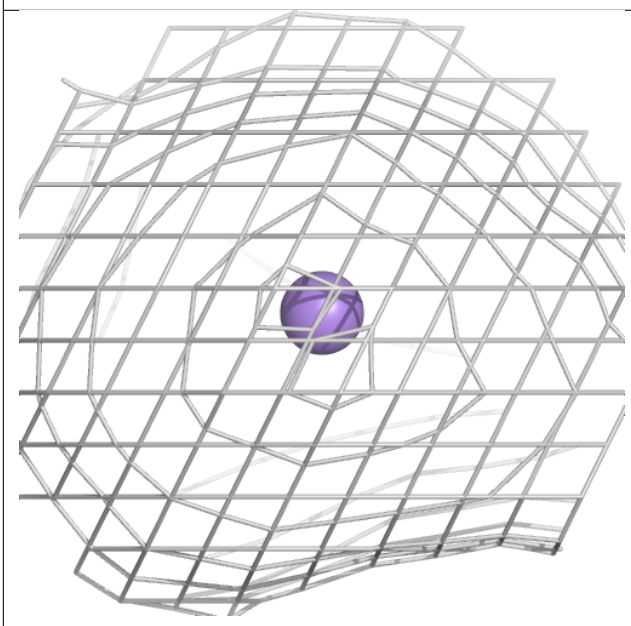
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

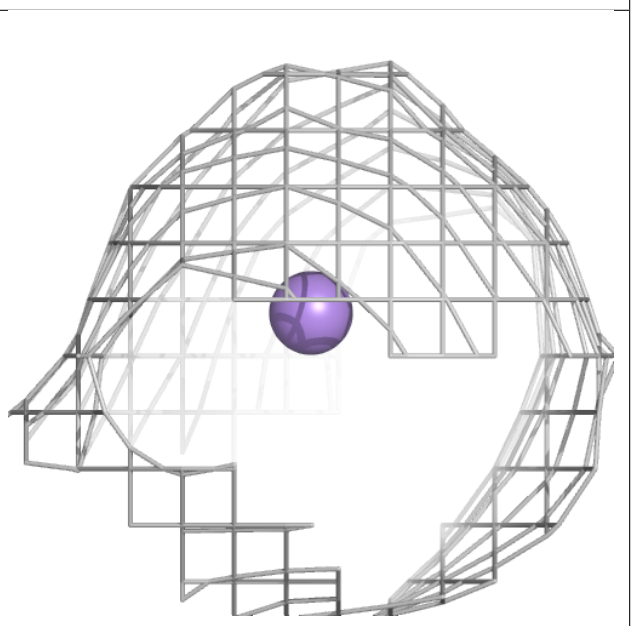


Electron density around MN C 1101:

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

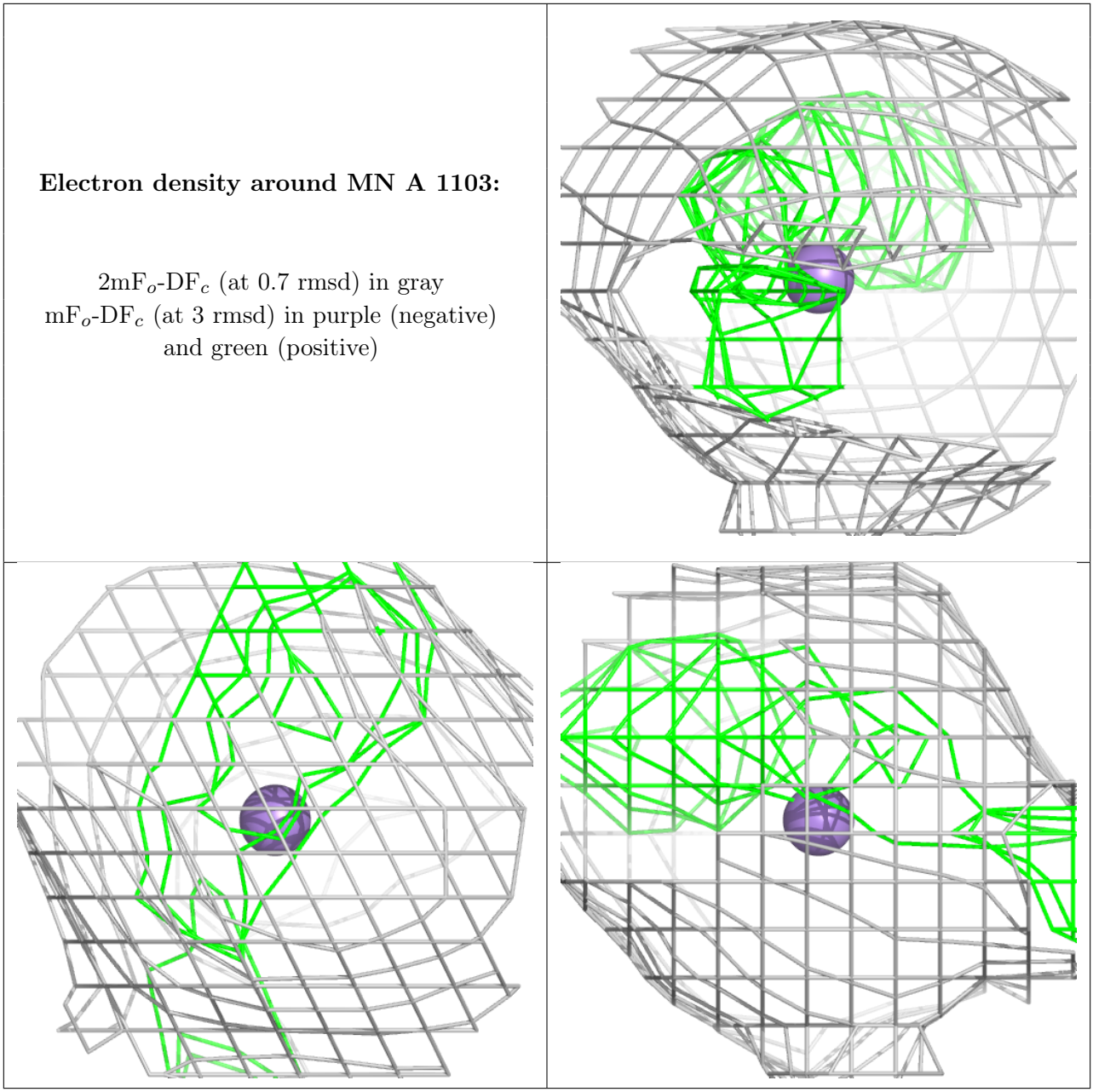






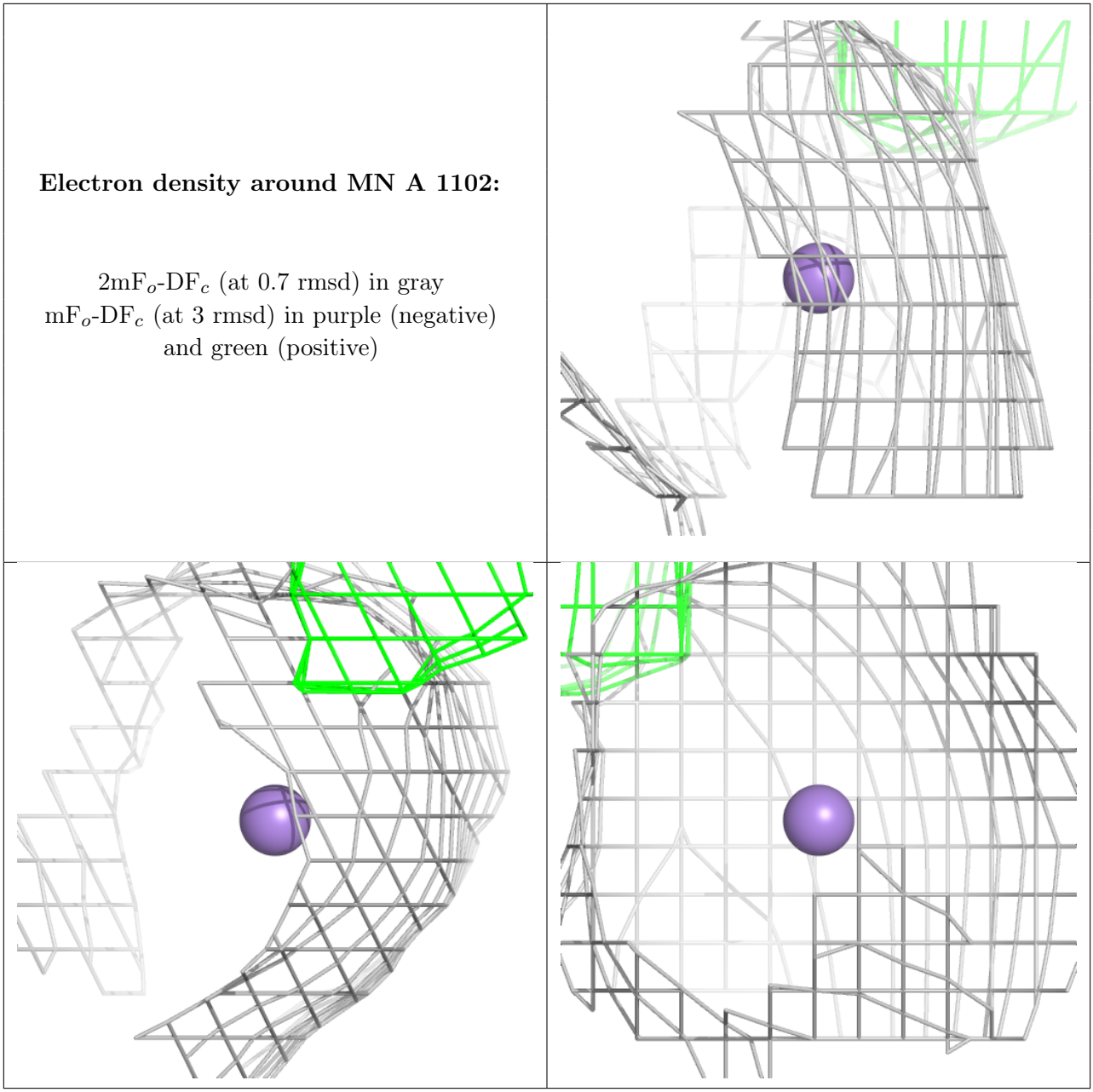
Electron density around MN A 1103:

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



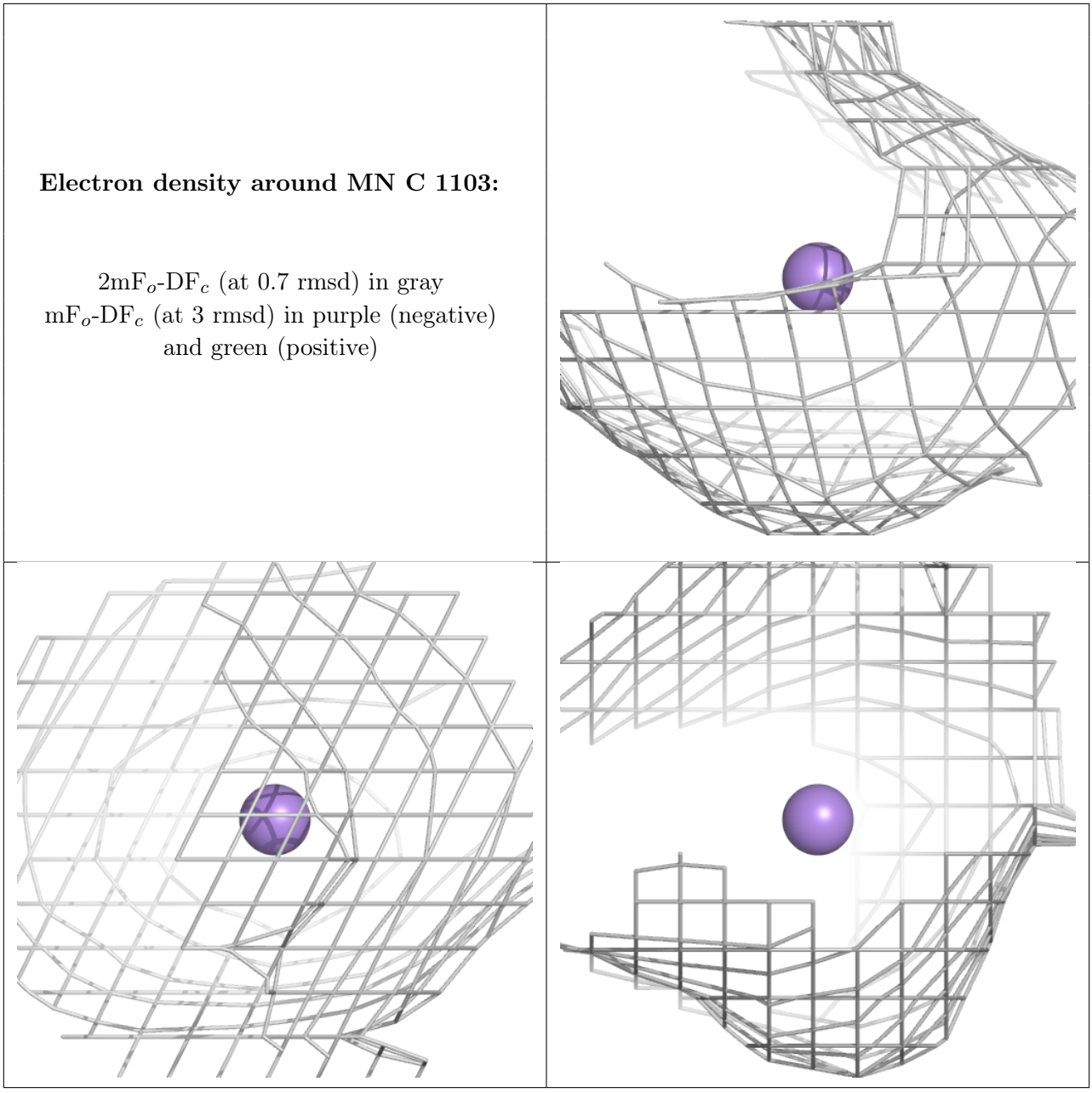
Electron density around MN A 1102:

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



Electron density around MN 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)



6.5 Other polymers (i)

There are no such residues in this entry.