wwPDB X-ray Structure Validation Summary Report (i)

Nov 20, 2023 – 07:54 PM JST

PDB ID	:	7DDK
Title	:	Crystal structures of Na+,K+-ATPase in complex with rostafuroxin
Authors	:	Ogawa, H.; Cornelius, F.; Kanai, R.; Motoyama, K.; Vilsen, B.; Toyoshima, C.
Deposited on	:	2020-10-29
Resolution	:	3.50 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:

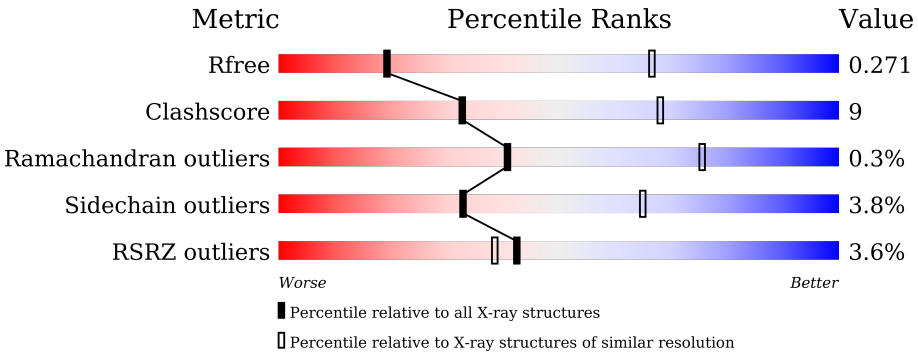
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	1016	5% 75% 22%
1	C	1016	3% 77% 21%
2	B	303	4% 70% 24%
2	D	303	2% 65% 27% 6%
3	E	65	45% 51%
3	G	65	35% 14% 51%

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Mol	Chain	Length	Quality of chain
4	F	2	100%
4	H	2	50% 50%
4	I	2	50% 50%
4	J	2	50% 50%

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
4	NAG	F	2	-	-	-	X
4	NAG	H	1	-	-	-	X
4	NAG	H	2	-	-	-	X
4	NAG	J	1	-	-	-	X
4	NAG	J	2	-	-	-	X
7	PCW	A	1105	-	-	-	X
7	PCW	A	1106	-	-	-	X
7	PCW	A	1108	-	-	-	X
7	PCW	A	1110	-	-	-	X
7	PCW	C	1106	-	-	-	X
7	PCW	C	1108	-	-	-	X
7	PCW	C	1109	-	-	-	X
7	PCW	C	1110	-	-	-	X
7	PCW	C	1111	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 21354 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-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			
1	C	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	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	285	Total	C	N	O	S	0	0	0
			2334	1514	383	424	13			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	32	Total	C	N	O	0	0	0
			255	174	37	44			
3	E	32	Total	C	N	O	0	0	0
			255	174	37	44			

- Molecule 4 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
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

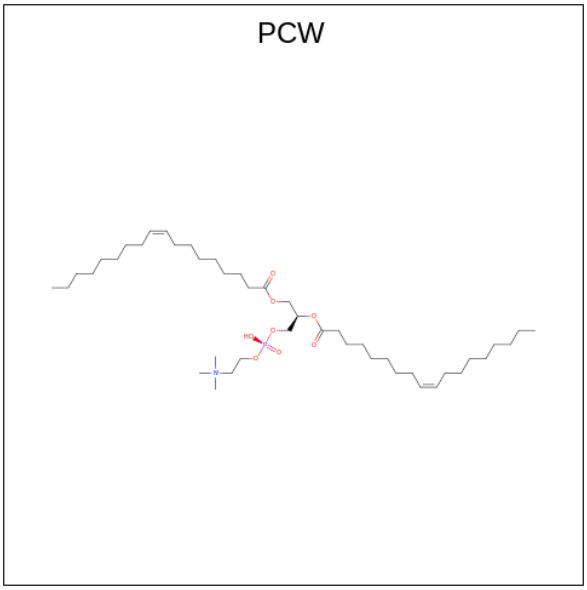
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0
5	C	2	Total Mg 2 2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

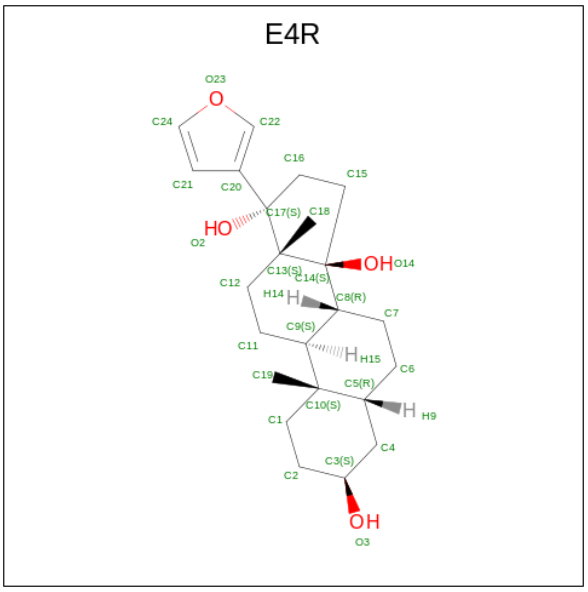
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0
6	C	1	Total Na 1 1	0	0

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



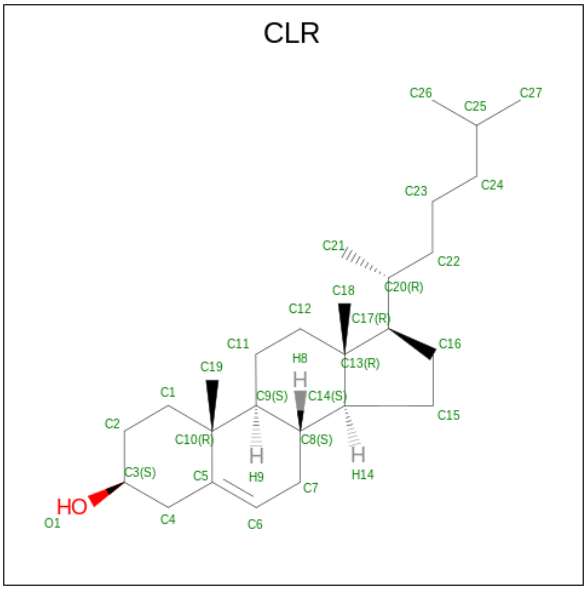
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O P 22 12 1 8 1	0	0
7	A	1	Total C N O P 22 12 1 8 1	0	0
7	A	1	Total C N O P 22 12 1 8 1	0	0
7	A	1	Total C N O P 22 12 1 8 1	0	0
7	A	1	Total C N O P 22 12 1 8 1	0	0
7	A	1	Total C N O P 22 12 1 8 1	0	0
7	C	1	Total C N O P 22 12 1 8 1	0	0
7	C	1	Total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

- Molecule 8 is (3S,5R,8R,9S,10S,13S,14S,17S)-17-(furan-3-yl)-10,13-dimethyl-2,3,4,5,6,7,8 ,9,11,12,15,16-dodecahydro-1H-cyclopenta[a]phenanthrene-3,14,17-triol (three-letter code: E4R) (formula: $C_{23}H_{34}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 27 23 4	0	0
8	C	1	Total C O 27 23 4	0	0

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

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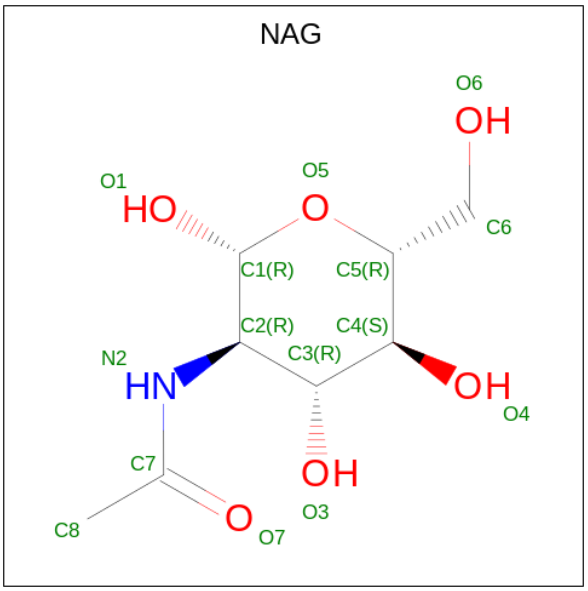
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	1	Total C O 28 27 1	0	0
9	C	1	Total C O 28 27 1	0	0
9	D	1	Total C O 28 27 1	0	0
9	E	1	Total C O 28 27 1	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is water.

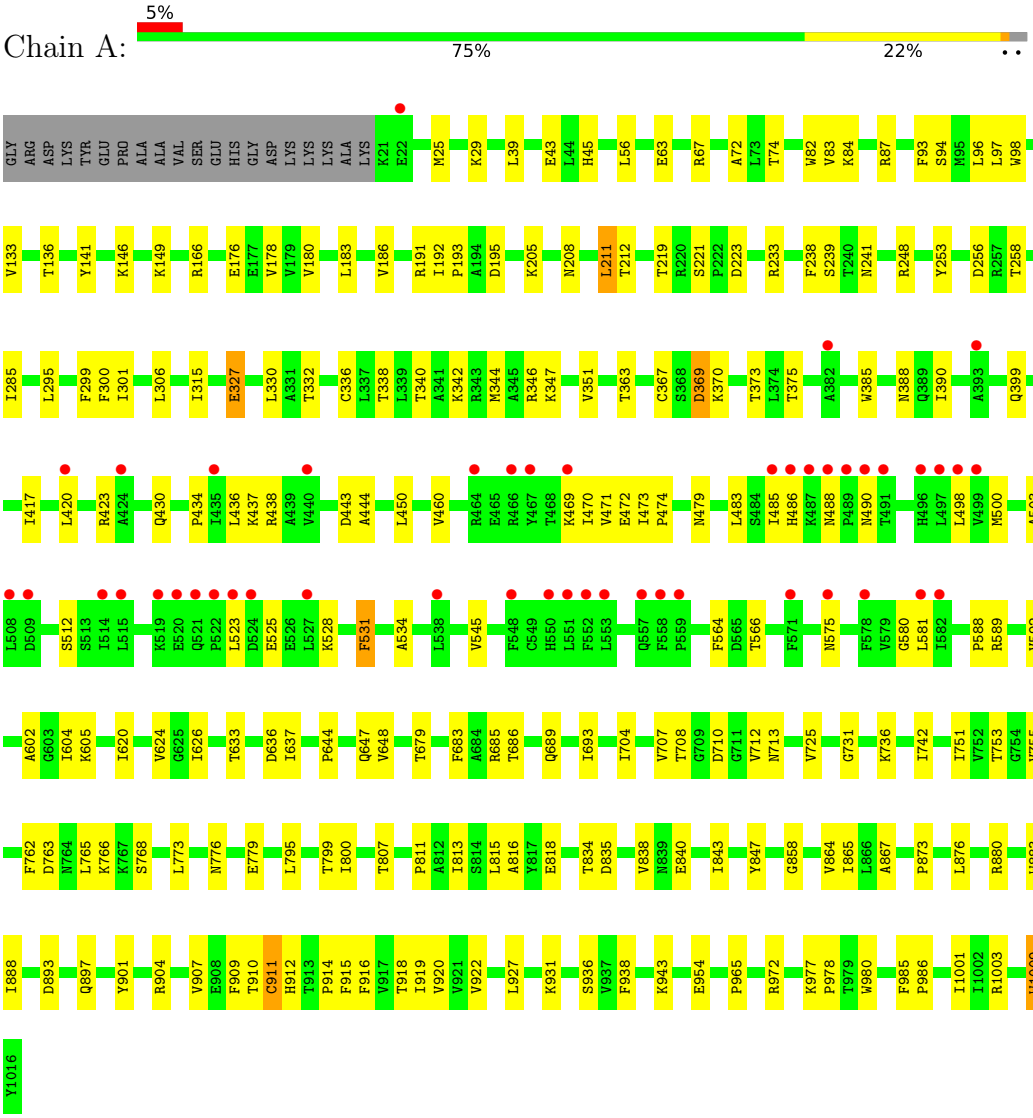
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	5	Total O 5 5	0	0
11	C	5	Total O 5 5	0	0

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.

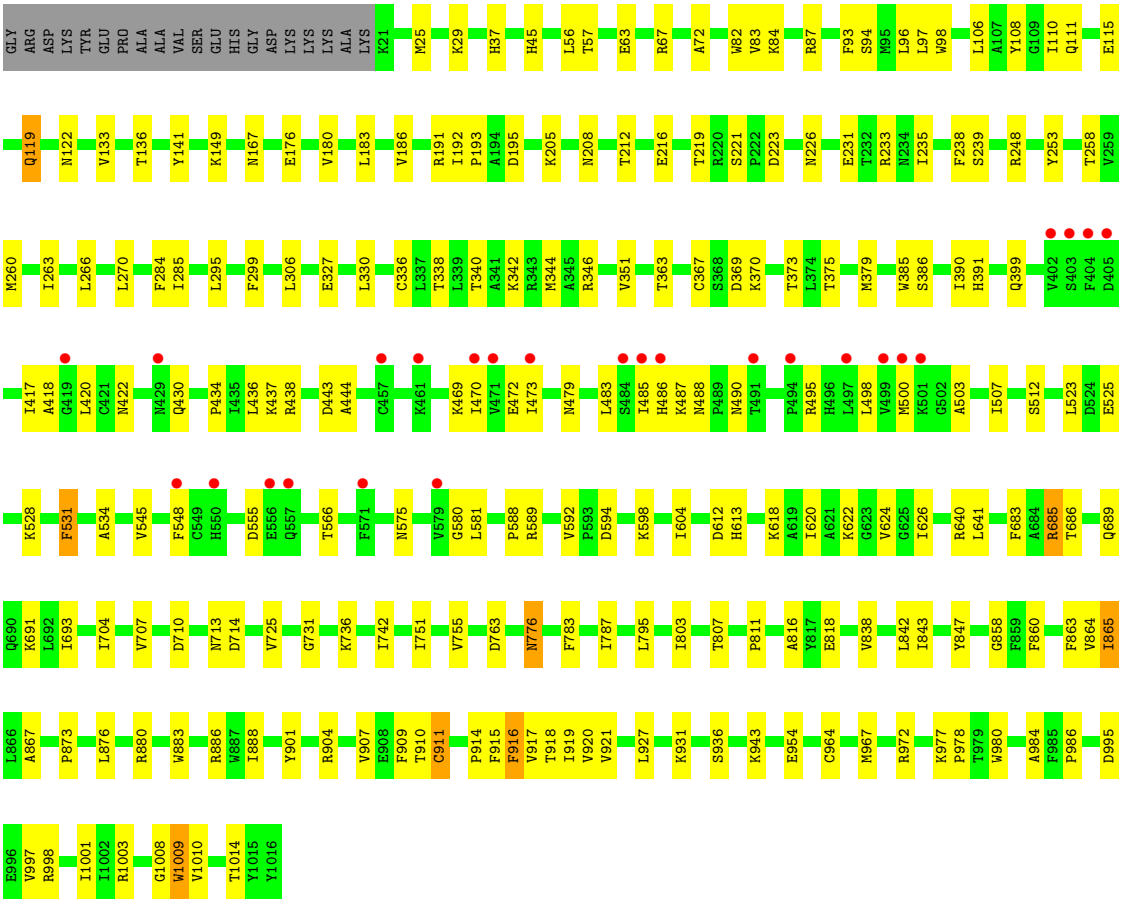
• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain A:

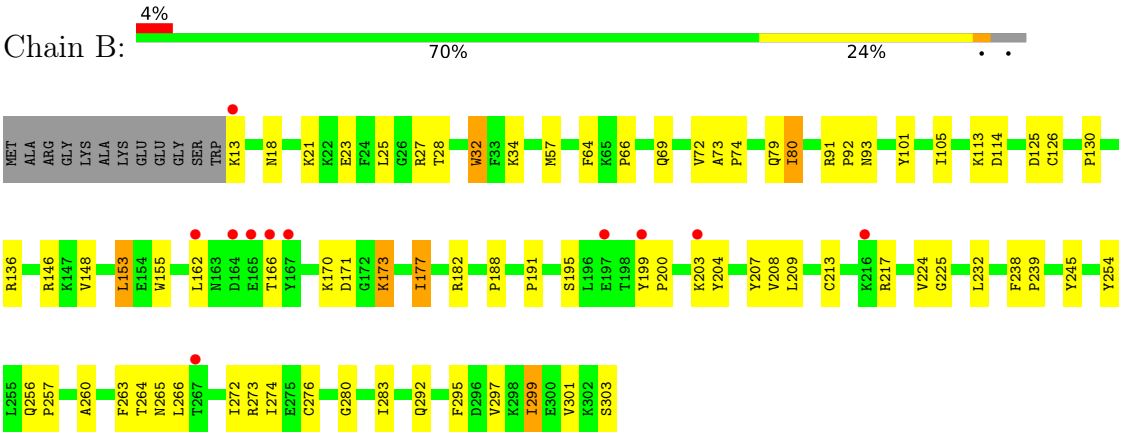


• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

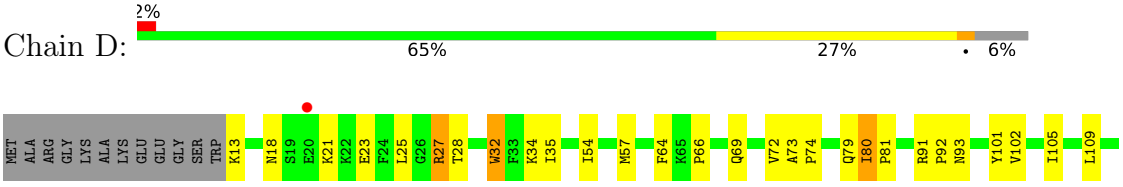
Chain C:

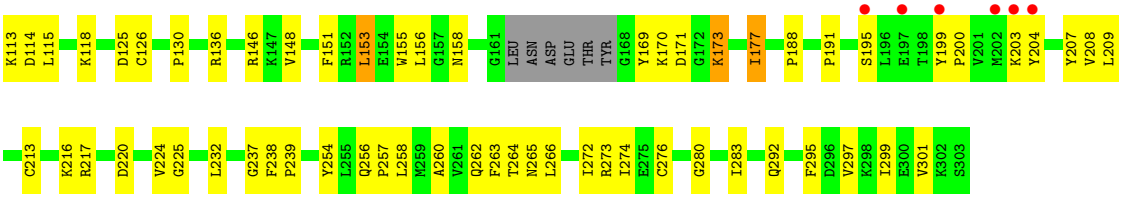


• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



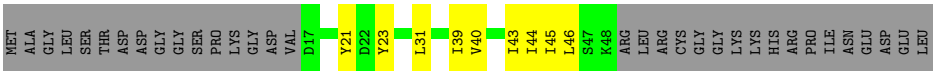
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1





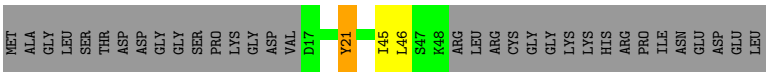
• Molecule 3: FXYD domain-containing ion transport regulator

Chain G:



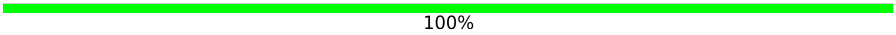
• Molecule 3: FXYD domain-containing ion transport regulator

Chain E:



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

Chain F:



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

Chain H:

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

Chain I:

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

Chain J:


NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.36Å 118.18Å 494.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.00 – 3.50 49.84 – 3.50	Depositor EDS
% Data completeness (in resolution range)	57.9 (16.00-3.50) 58.4 (49.84-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.220 , 0.269 0.232 , 0.271	Depositor DCC
R_{free} test set	2476 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	89.5	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 81.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.049 for k,h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	21354	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: PCW, NAG, MG, E4R, CLR, PHD, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/7867	0.51	0/10674
1	C	0.29	0/7867	0.51	1/10674 (0.0%)
2	B	0.29	0/2449	0.54	0/3301
2	D	0.30	0/2395	0.56	0/3225
3	E	0.32	0/261	0.50	0/354
3	G	0.30	0/261	0.46	0/354
All	All	0.29	0/21100	0.52	1/28582 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1008	GLY	N-CA-C	5.04	125.70	113.10

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	7730	0	7777	135	0
1	C	7730	0	7777	134	0
2	B	2386	0	2361	44	0
2	D	2334	0	2317	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	255	0	259	3	0
3	G	255	0	259	6	0
4	F	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	1	0
4	J	28	0	25	0	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	132	0	108	9	0
7	C	154	0	126	5	0
8	A	27	0	0	0	0
8	C	27	0	0	0	0
9	A	28	0	46	1	0
9	B	28	0	46	0	0
9	C	28	0	46	3	0
9	D	28	0	46	1	0
9	E	28	0	46	2	0
9	G	28	0	46	2	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
11	A	5	0	0	0	0
11	C	5	0	0	0	0
All	All	21354	0	21386	373	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 9.

The worst 5 of 373 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)
2:D:80:ILE:HG12	2:D:177:ILE:HG12	1.63	0.81
1:A:978:PRO:HB3	9:G:101:CLR:H192	1.64	0.80
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.64	0.79
2:B:80:ILE:HG12	2:B:177:ILE:HG12	1.65	0.79
1:A:430:GLN:HG3	1:A:438:ARG:HB2	1.65	0.79

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	993/1016 (98%)	927 (93%)	64 (6%)	2 (0%)	47 81
1	C	993/1016 (98%)	930 (94%)	61 (6%)	2 (0%)	47 81
2	B	289/303 (95%)	261 (90%)	26 (9%)	2 (1%)	22 61
2	D	281/303 (93%)	254 (90%)	25 (9%)	2 (1%)	22 61
3	E	30/65 (46%)	28 (93%)	2 (7%)	0	100 100
3	G	30/65 (46%)	27 (90%)	3 (10%)	0	100 100
All	All	2616/2768 (94%)	2427 (93%)	181 (7%)	8 (0%)	41 75

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	200	PRO
1	A	193	PRO
1	C	193	PRO
1	C	306	LEU
2	D	200	PRO

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	846/861 (98%)	825 (98%)	21 (2%)	47 75
1	C	846/861 (98%)	825 (98%)	21 (2%)	47 75
2	B	261/269 (97%)	239 (92%)	22 (8%)	11 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	255/269 (95%)	234 (92%)	21 (8%)	11	40
3	E	26/52 (50%)	25 (96%)	1 (4%)	33	65
3	G	26/52 (50%)	25 (96%)	1 (4%)	33	65
All	All	2260/2364 (96%)	2173 (96%)	87 (4%)	33	65

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	566	THR
2	D	72	VAL
1	C	763	ASP
2	D	13	LYS
2	D	126	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	613	HIS
2	D	262	GLN
1	C	111	GLN
1	C	119	GLN
1	C	122	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	PHD	A	369	1,5	9,11,12	0.93	0	10,15,17	1.47	2 (20%)
1	PHD	C	369	1,5	9,11,12	0.93	0	10,15,17	1.08	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
1	PHD	A	369	1,5	-	0/8/11/13	-
1	PHD	C	369	1,5	-	1/8/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	369	PHD	CA-CB-CG	2.99	119.12	112.86
1	A	369	PHD	OD1-CG-CB	2.64	118.38	111.11

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	369	PHD	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	369	PHD	1	0
1	C	369	PHD	1	0

5.5 Carbohydrates (i)

8 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	4,2	14,14,15	0.34	0	17,19,21	0.46	0
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.51	0
4	NAG	H	1	4,2	14,14,15	0.63	1 (7%)	17,19,21	0.70	0
4	NAG	H	2	4	14,14,15	0.36	0	17,19,21	0.36	0
4	NAG	I	1	4,2	14,14,15	0.37	0	17,19,21	0.47	0
4	NAG	I	2	4	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	J	1	4,2	14,14,15	0.61	1 (7%)	17,19,21	0.67	0
4	NAG	J	2	4	14,14,15	0.33	0	17,19,21	0.36	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	4,2	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	O5-C1	-2.20	1.40	1.43
4	J	1	NAG	O5-C1	-2.11	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C4-C5-C6-O6

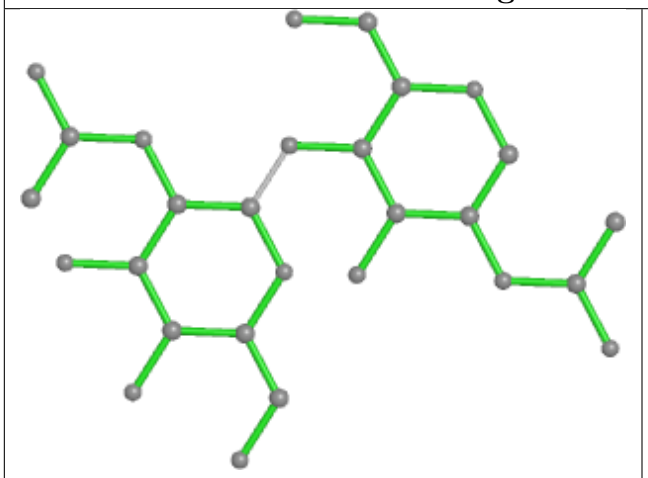
There are no ring outliers.

1 monomer is involved in 1 short contact:

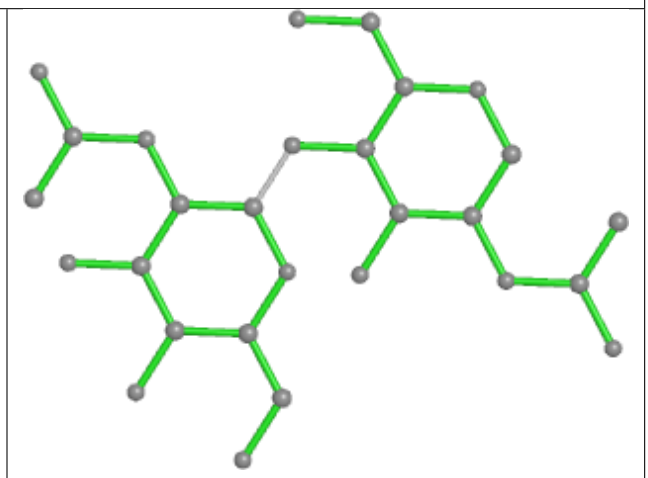
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0

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

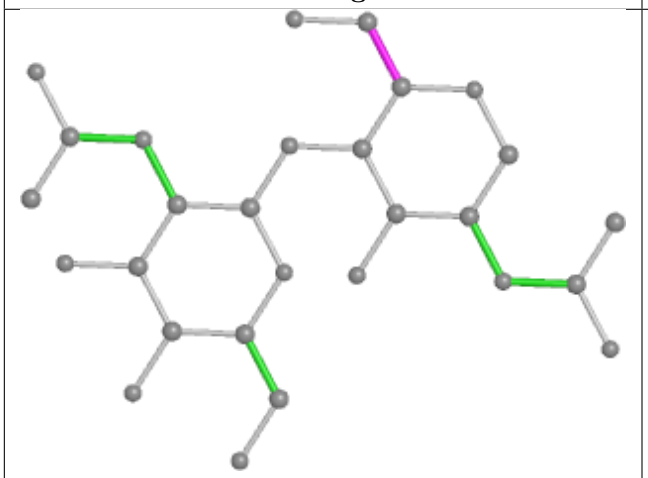
Oligosaccharide Chain F



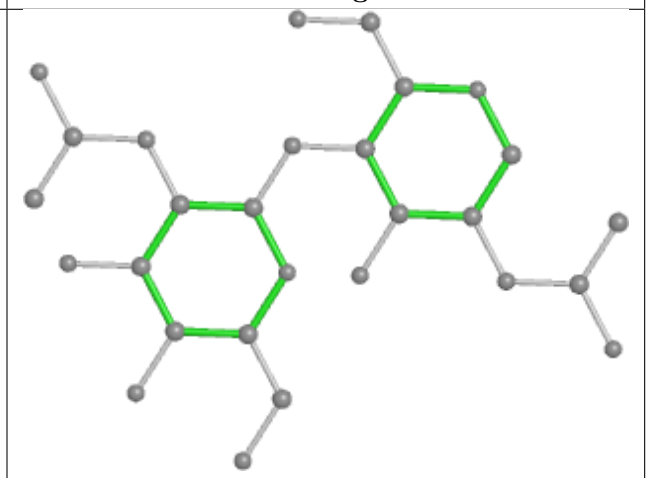
Bond lengths



Bond angles

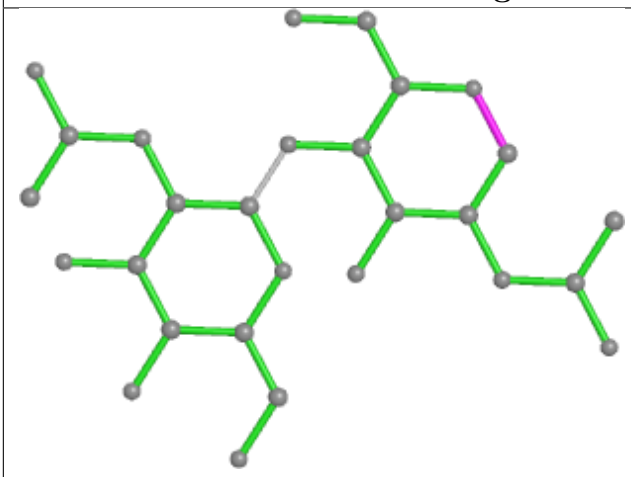


Torsions

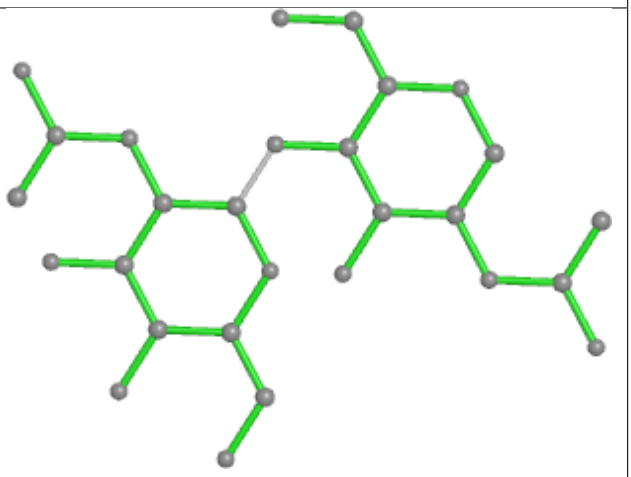


Rings

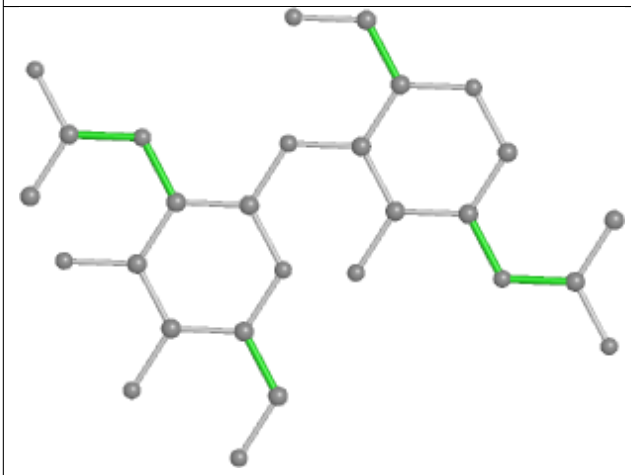
Oligosaccharide Chain H



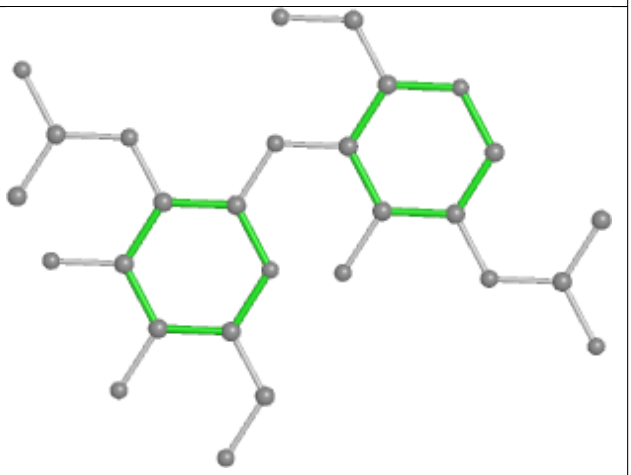
Bond lengths



Bond angles

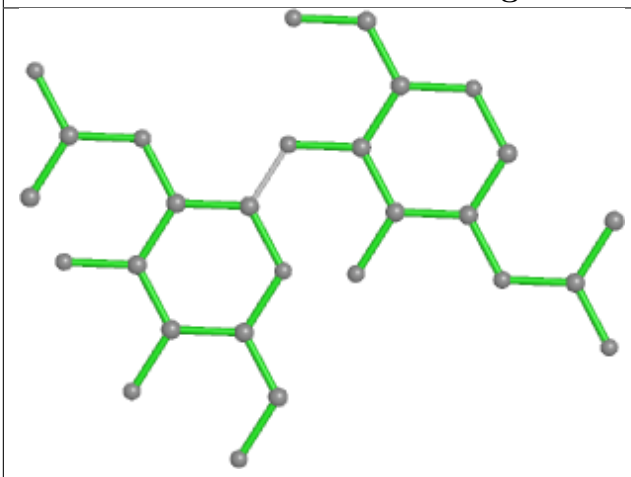


Torsions

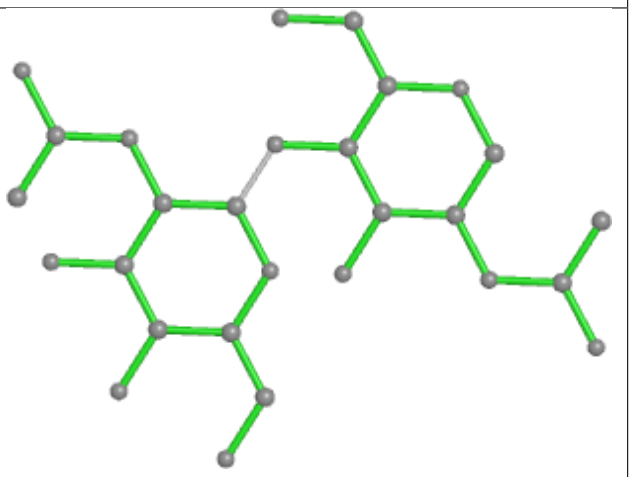


Rings

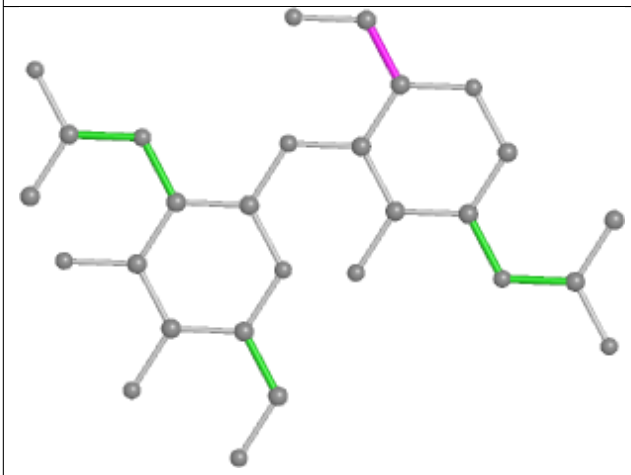
Oligosaccharide Chain I



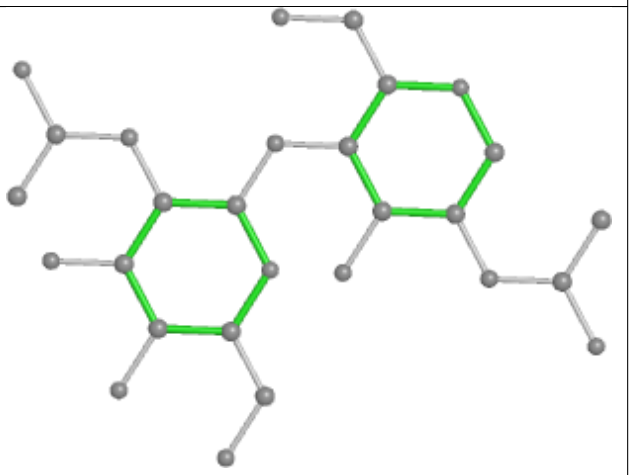
Bond lengths



Bond angles

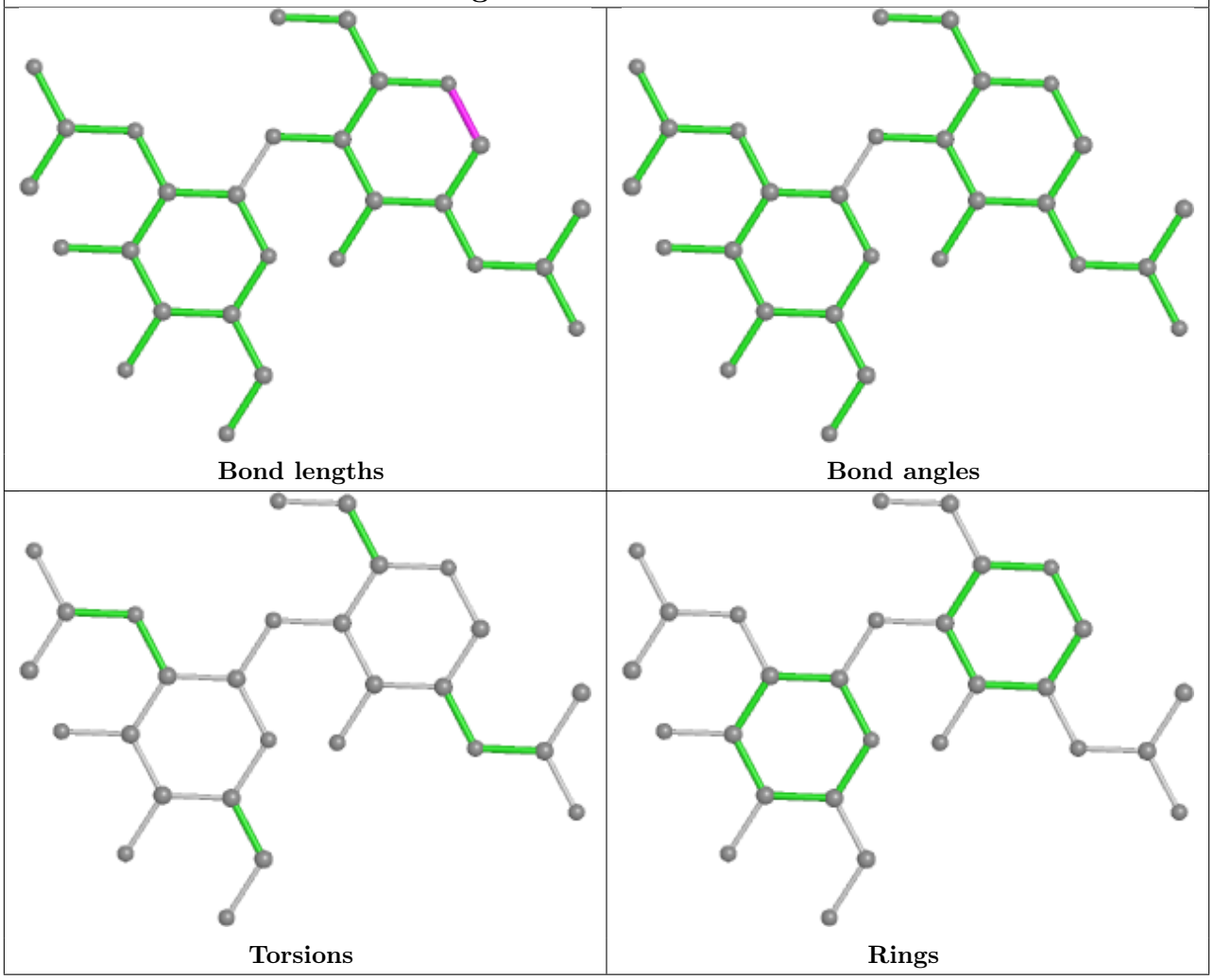


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 6 are monoatomic - leaving 23 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	$\#\|Z\| > 2$
7	PCW	C	1112	-	21,21,53	1.68	4 (19%)	27,29,61	1.40	3 (11%)
7	PCW	C	1109	-	21,21,53	1.75	4 (19%)	27,29,61	1.27	1 (3%)
8	E4R	C	1121	-	26,31,31	1.32	2 (7%)	41,52,52	1.84	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	PCW	A	1105	-	21,21,53	1.68	4 (19%)	27,29,61	1.16	1 (3%)
7	PCW	C	1110	-	21,21,53	1.69	5 (23%)	27,29,61	1.21	1 (3%)
7	PCW	C	1108	-	21,21,53	1.70	5 (23%)	27,29,61	1.18	1 (3%)
9	CLR	D	501	-	31,31,31	1.87	11 (35%)	48,48,48	1.49	12 (25%)
10	NAG	D	401	2	14,14,15	0.34	0	17,19,21	0.56	0
7	PCW	A	1106	-	21,21,53	1.70	6 (28%)	27,29,61	1.19	1 (3%)
7	PCW	A	1110	-	21,21,53	1.72	6 (28%)	27,29,61	1.26	1 (3%)
7	PCW	A	1108	-	21,21,53	1.69	6 (28%)	27,29,61	1.17	1 (3%)
7	PCW	C	1111	-	21,21,53	1.72	5 (23%)	27,29,61	1.18	1 (3%)
9	CLR	A	1104	-	31,31,31	1.80	12 (38%)	48,48,48	1.57	12 (25%)
9	CLR	E	101	-	31,31,31	1.86	11 (35%)	48,48,48	1.63	12 (25%)
9	CLR	G	101	-	31,31,31	1.87	12 (38%)	48,48,48	1.70	14 (29%)
10	NAG	B	401	2	14,14,15	0.26	0	17,19,21	0.44	0
7	PCW	C	1106	-	21,21,53	1.73	5 (23%)	27,29,61	1.26	1 (3%)
8	E4R	A	1121	-	26,31,31	1.47	4 (15%)	41,52,52	1.81	6 (14%)
7	PCW	A	1107	-	21,21,53	1.67	6 (28%)	27,29,61	1.25	1 (3%)
9	CLR	C	1104	-	31,31,31	1.71	9 (29%)	48,48,48	1.63	12 (25%)
9	CLR	B	501	-	31,31,31	2.00	12 (38%)	48,48,48	1.61	13 (27%)
7	PCW	C	1107	-	21,21,53	1.69	6 (28%)	27,29,61	1.23	2 (7%)
7	PCW	A	1109	-	21,21,53	1.70	6 (28%)	27,29,61	1.44	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PCW	C	1112	-	-	11/23/23/57	-
7	PCW	C	1109	-	-	9/23/23/57	-
8	E4R	C	1121	-	-	0/0/74/74	0/5/5/5
7	PCW	A	1105	-	-	16/23/23/57	-
7	PCW	C	1110	-	-	13/23/23/57	-
7	PCW	C	1108	-	-	10/23/23/57	-
9	CLR	D	501	-	-	1/10/68/68	0/4/4/4
10	NAG	D	401	2	-	4/6/23/26	0/1/1/1
7	PCW	A	1106	-	-	11/23/23/57	-
7	PCW	A	1110	-	-	9/23/23/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PCW	A	1108	-	-	10/23/23/57	-
7	PCW	C	1111	-	-	10/23/23/57	-
9	CLR	A	1104	-	-	4/10/68/68	0/4/4/4
9	CLR	E	101	-	-	3/10/68/68	0/4/4/4
9	CLR	G	101	-	-	6/10/68/68	0/4/4/4
10	NAG	B	401	2	-	1/6/23/26	0/1/1/1
7	PCW	C	1106	-	-	11/23/23/57	-
8	E4R	A	1121	-	-	0/0/74/74	0/5/5/5
7	PCW	A	1107	-	-	7/23/23/57	-
9	CLR	C	1104	-	-	5/10/68/68	0/4/4/4
9	CLR	B	501	-	-	2/10/68/68	0/4/4/4
7	PCW	C	1107	-	-	12/23/23/57	-
7	PCW	A	1109	-	-	11/23/23/57	-

The worst 5 of 141 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	CLR	C10-C9	5.24	1.64	1.56
9	G	101	CLR	C10-C9	4.37	1.63	1.56
9	E	101	CLR	C10-C9	4.24	1.63	1.56
7	C	1109	PCW	O2-C31	4.21	1.44	1.35
9	A	1104	CLR	C10-C9	4.12	1.62	1.56

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1121	E4R	C12-C13-C17	-7.98	106.49	116.87
8	A	1121	E4R	C12-C13-C17	-7.61	106.96	116.87
7	C	1112	PCW	O2-C31-C32	5.24	120.72	111.09
7	C	1106	PCW	O2-C31-C32	5.21	120.68	111.09
7	A	1110	PCW	O2-C31-C32	5.14	120.54	111.09

There are no chirality outliers.

5 of 166 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1106	PCW	O2-C2-C3-O3
7	A	1106	PCW	C4-O4P-P-O2P
7	A	1107	PCW	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
7	A	1107	PCW	O31-C31-O2-C2
7	A	1108	PCW	C4-O4P-P-O1P

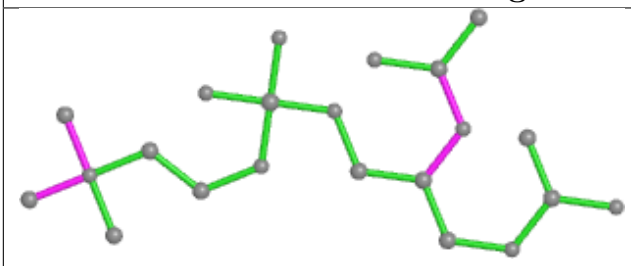
There are no ring outliers.

12 monomers are involved in 23 short contacts:

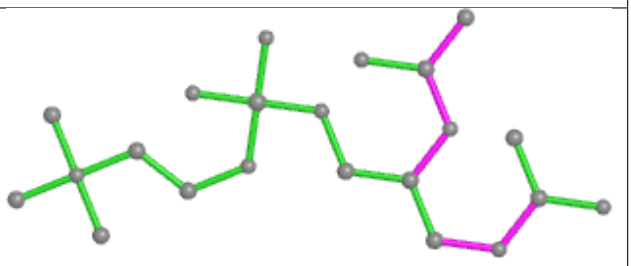
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1112	PCW	2	0
7	A	1105	PCW	3	0
9	D	501	CLR	1	0
7	A	1110	PCW	2	0
7	A	1108	PCW	2	0
7	C	1111	PCW	2	0
9	A	1104	CLR	1	0
9	E	101	CLR	2	0
9	G	101	CLR	2	0
9	C	1104	CLR	3	0
7	C	1107	PCW	1	0
7	A	1109	PCW	2	0

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

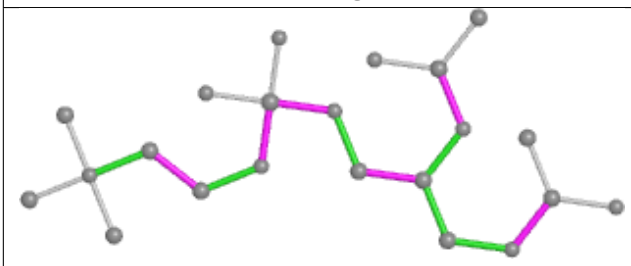
Ligand PCW C 1112



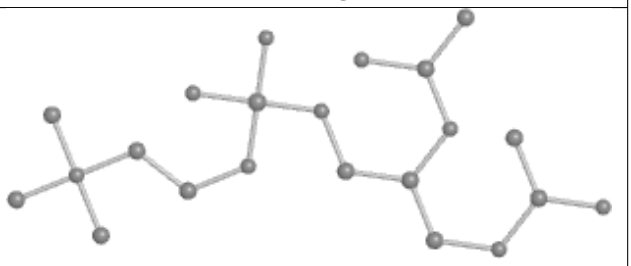
Bond lengths



Bond angles

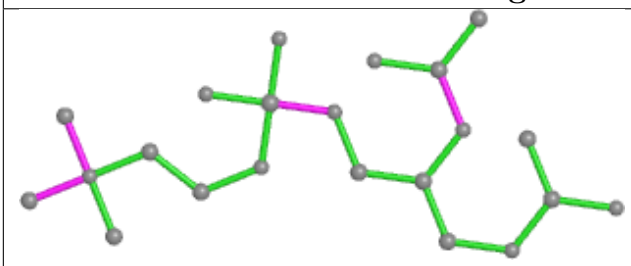


Torsions

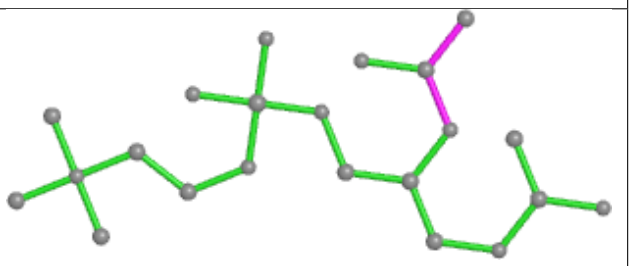


Rings

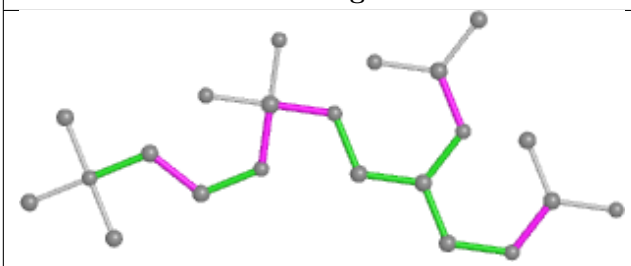
Ligand PCW C 1109



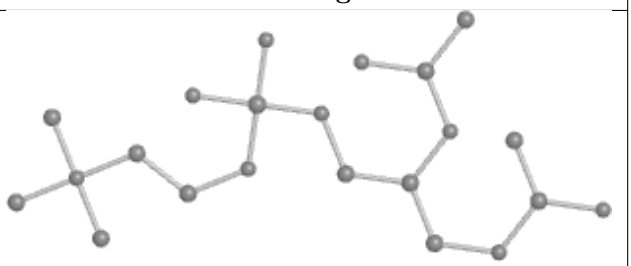
Bond lengths



Bond angles

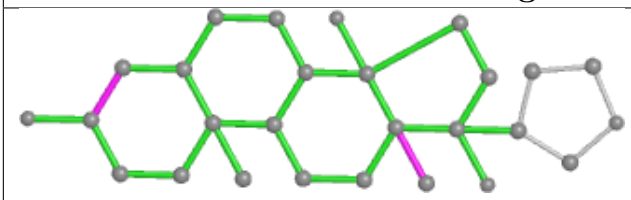


Torsions

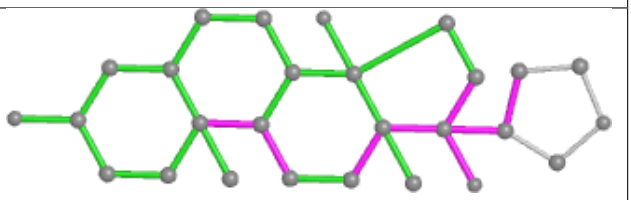


Rings

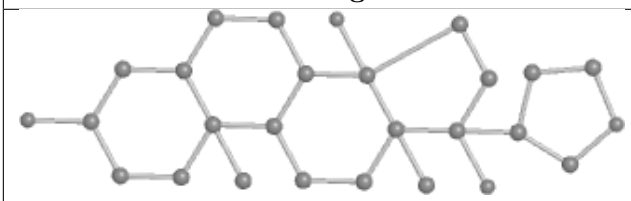
Ligand E4R C 1121



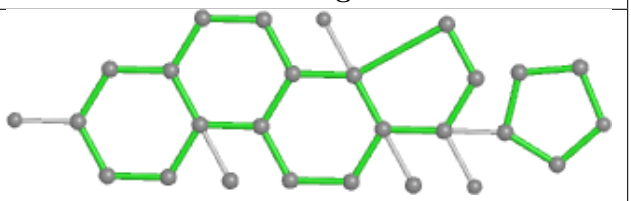
Bond lengths



Bond angles

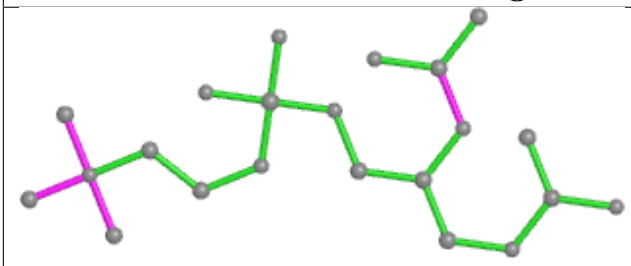


Torsions

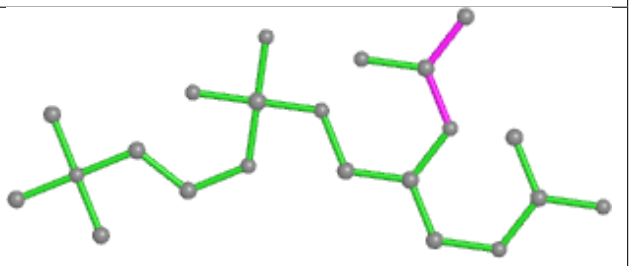


Rings

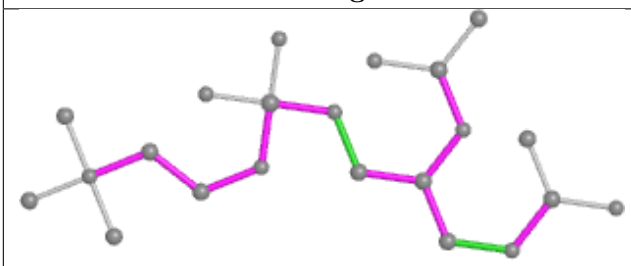
Ligand PCW A 1105



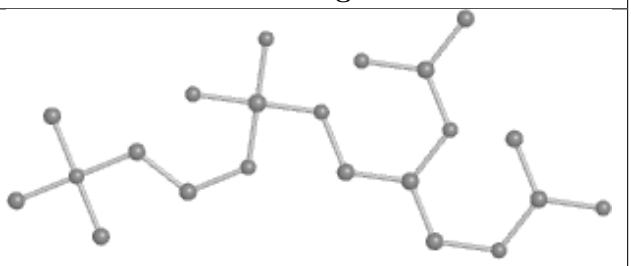
Bond lengths



Bond angles

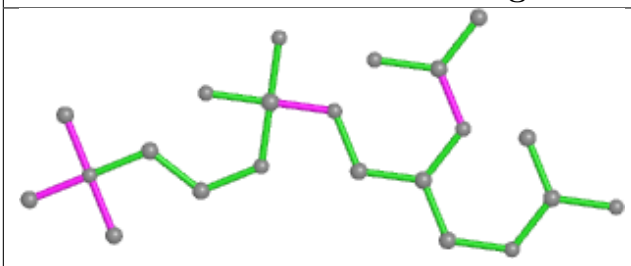


Torsions



Rings

Ligand PCW C 1110



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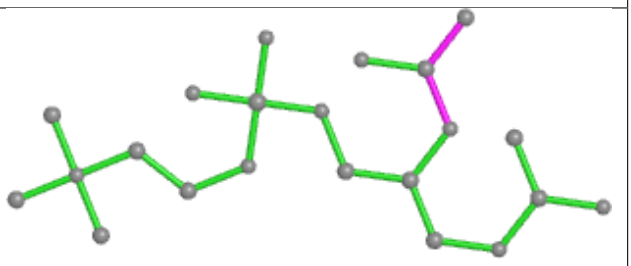
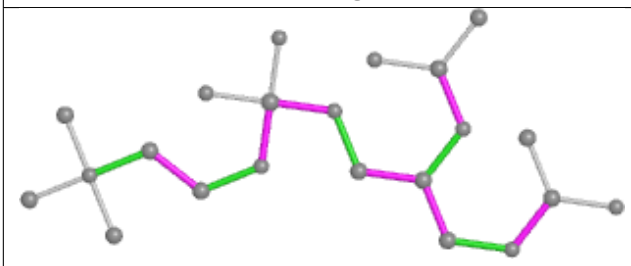
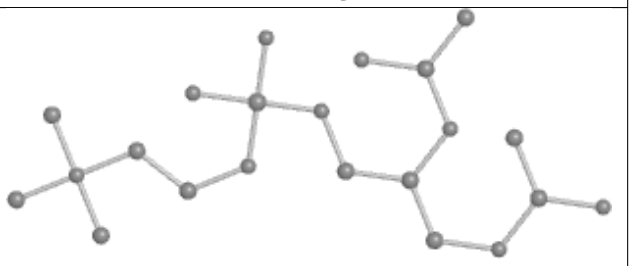


Bond angles

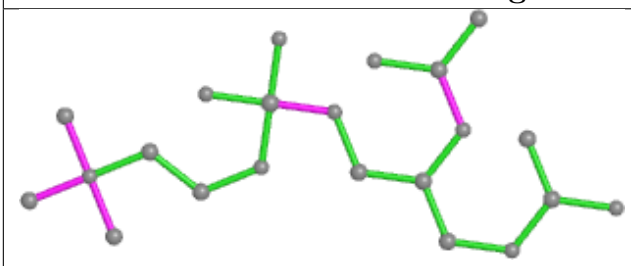


Torsions



Rings

Ligand PCW C 1108



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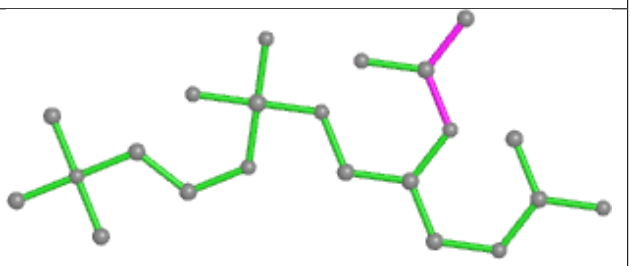
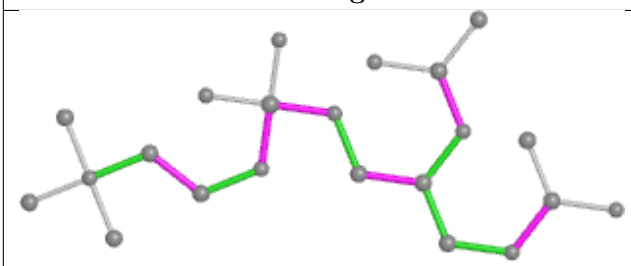
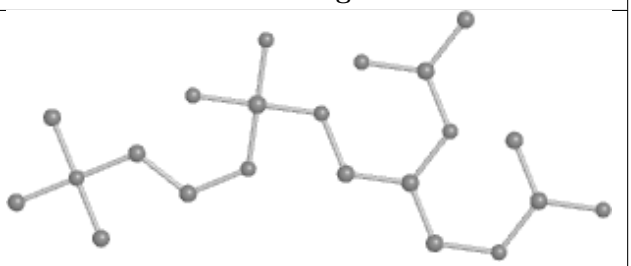


Bond angles

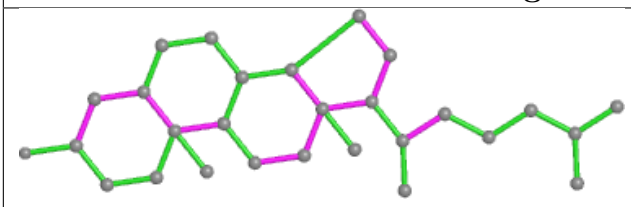


Torsions



Rings

Ligand CLR D 501



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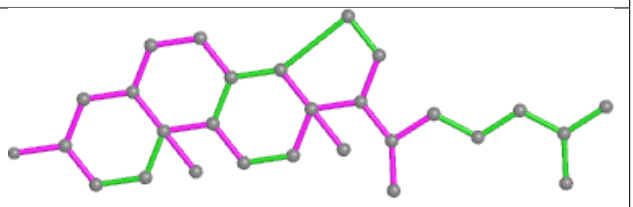
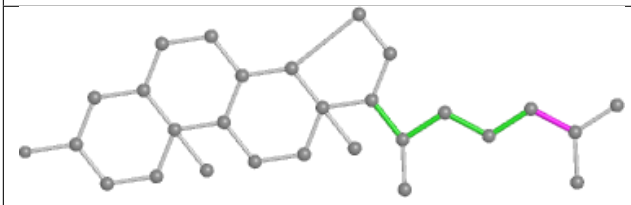
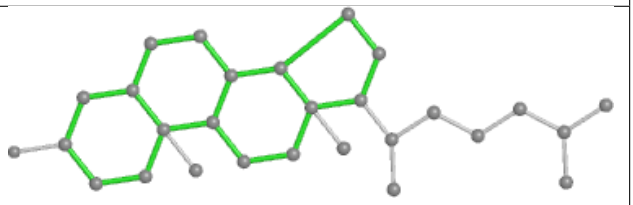


Bond angles

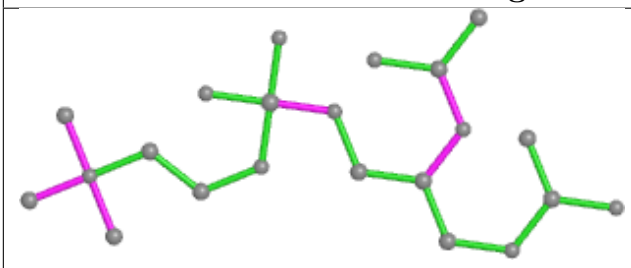


Torsions



Rings

Ligand PCW A 1106



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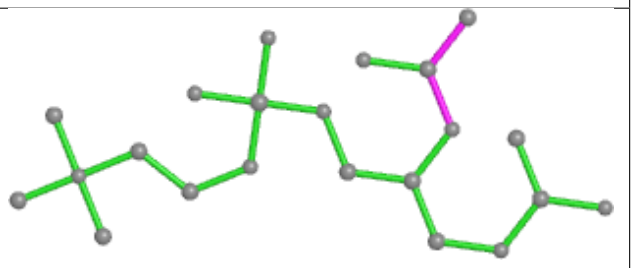
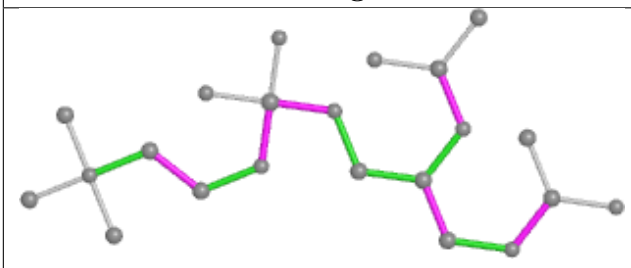


Bond angles



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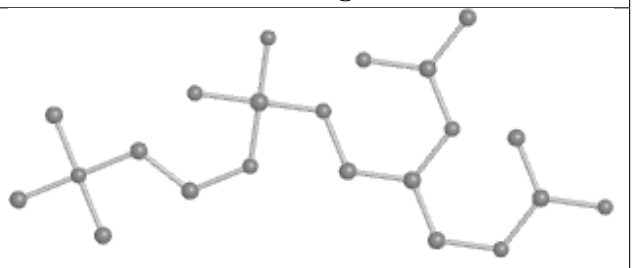
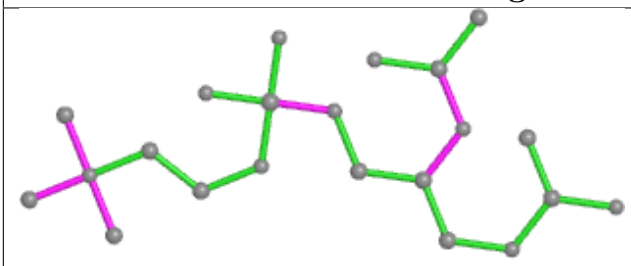


Rings

Ligand PCW A 1110



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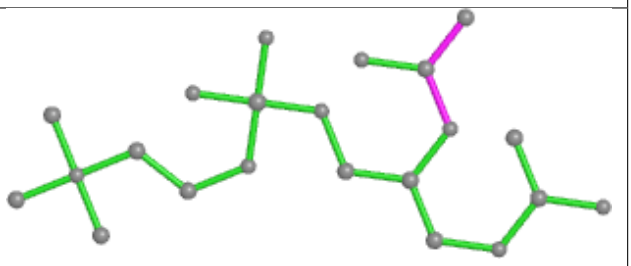
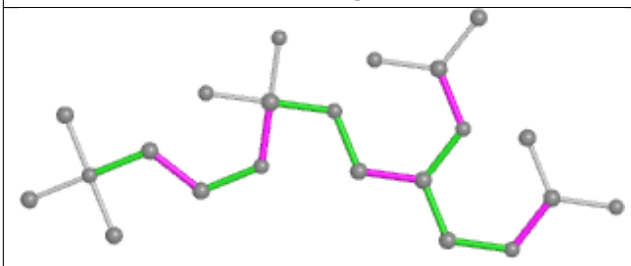


Bond angles



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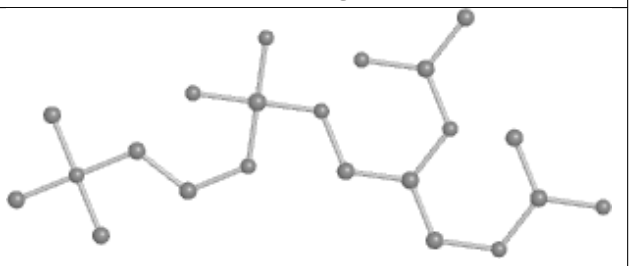
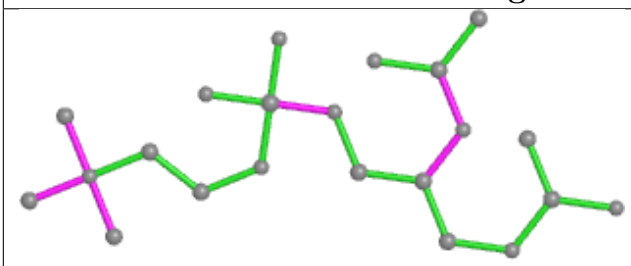


Rings

Ligand PCW A 1108



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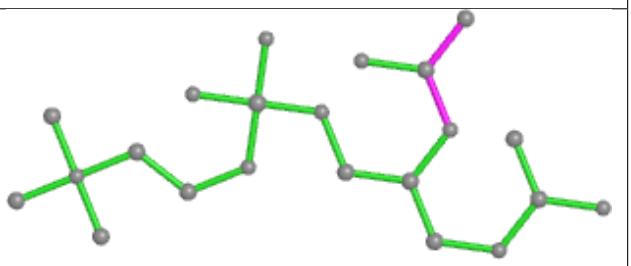
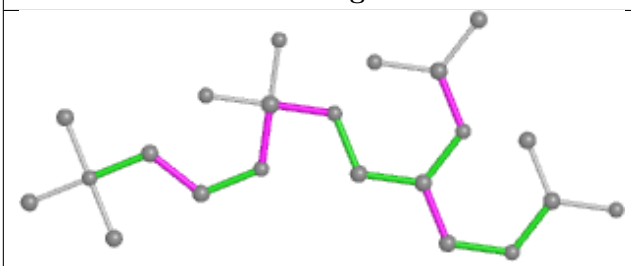


Bond angles



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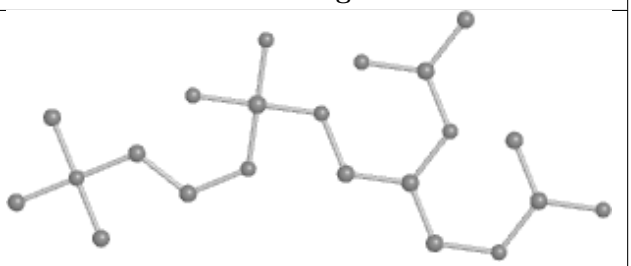
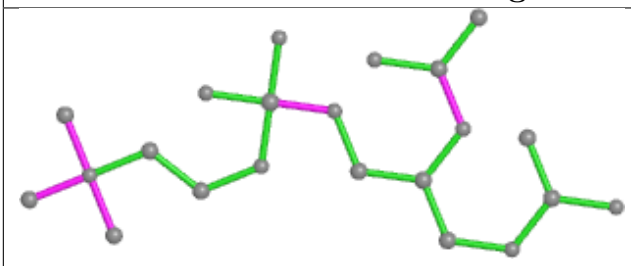


Rings

Ligand PCW C 1111



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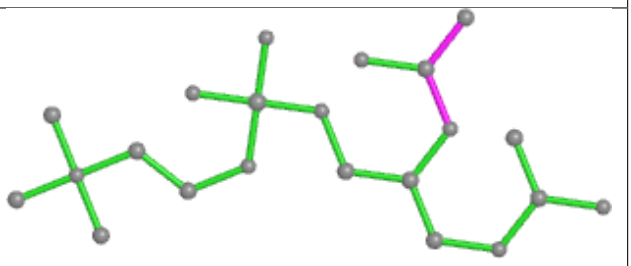
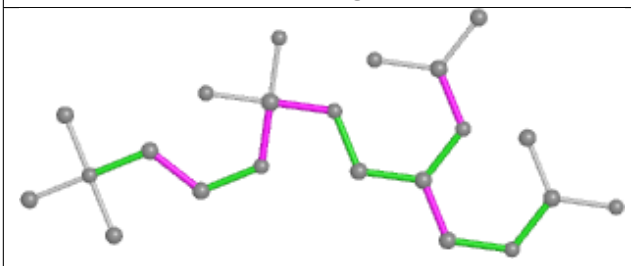


Bond angles



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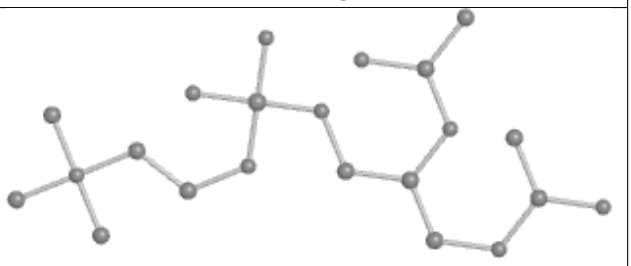
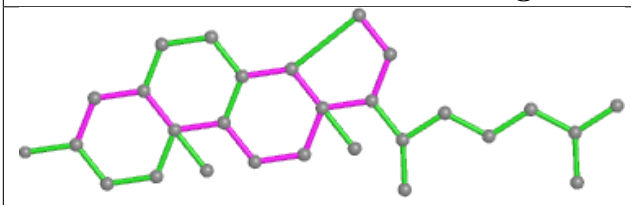
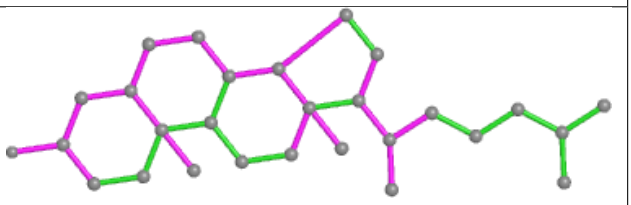


Rings

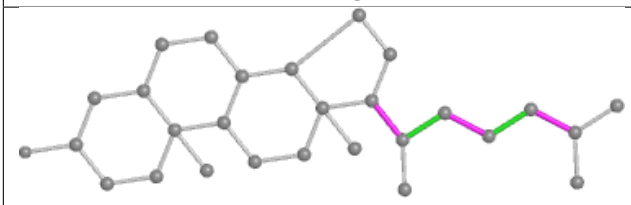
Ligand CLR A 1104



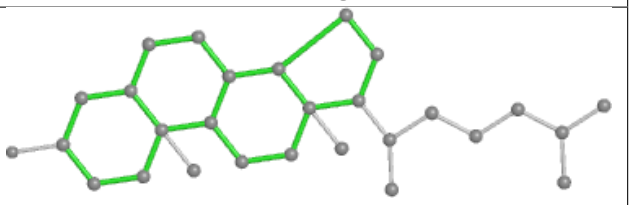
Bond lengths



Bond angles

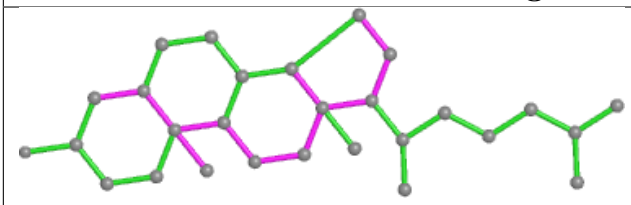


Torsions

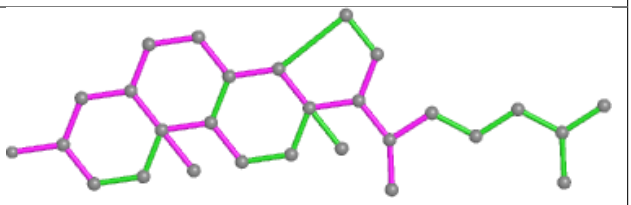


Rings

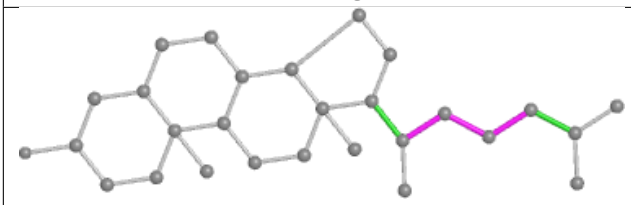
Ligand CLR E 101



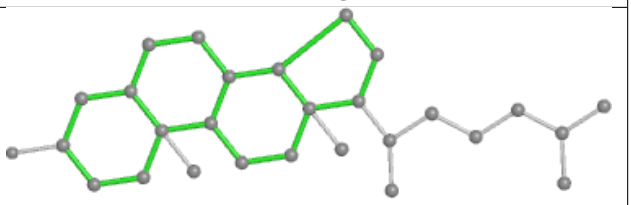
Bond lengths



Bond angles

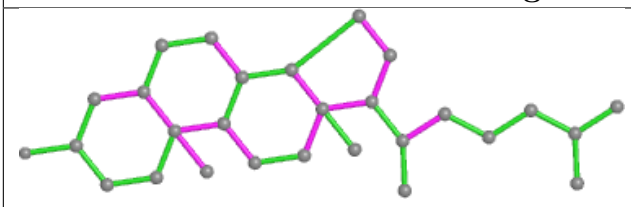


Torsions

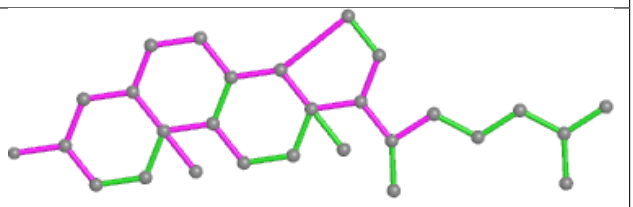


Rings

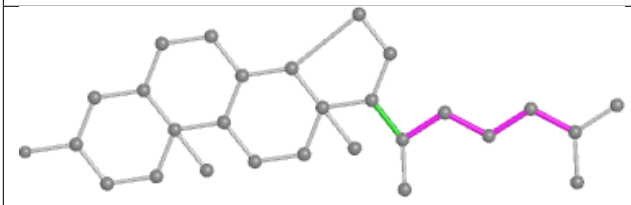
Ligand CLR G 101



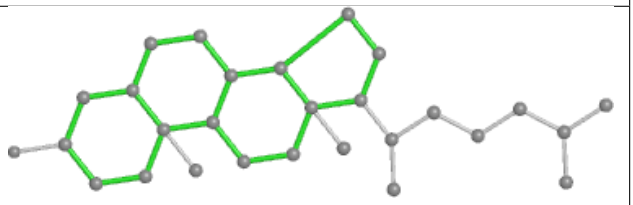
Bond lengths



Bond angles

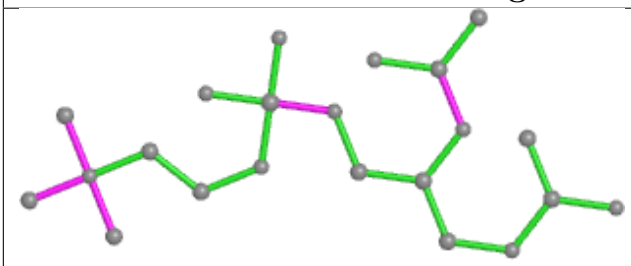


Torsions



Rings

Ligand PCW C 1106



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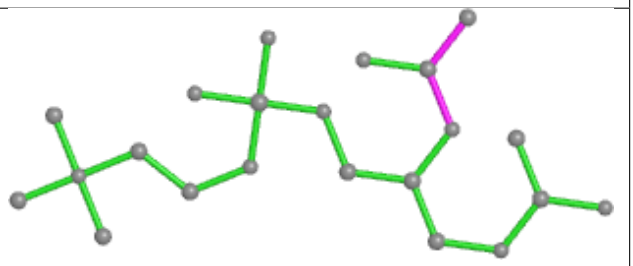
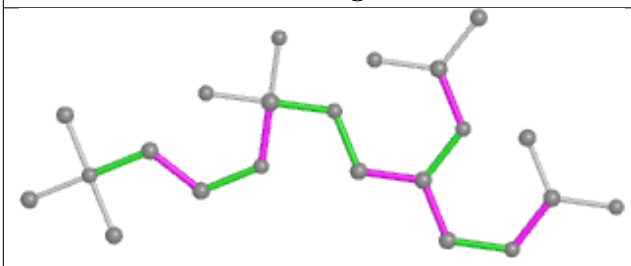


Bond angles



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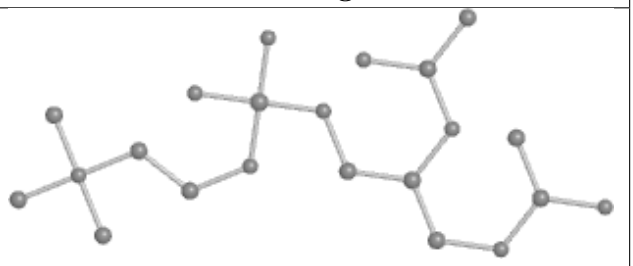
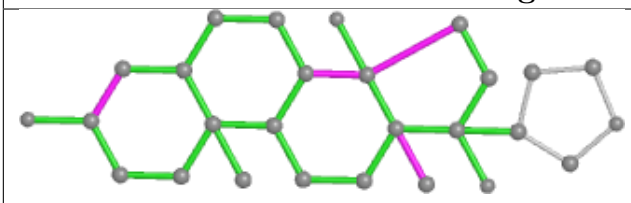
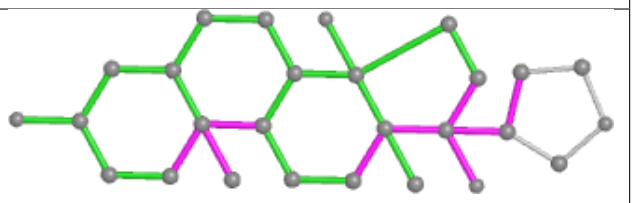


Rings

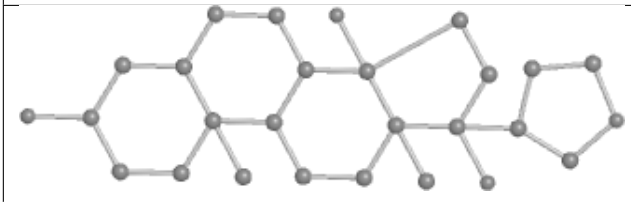
Ligand E4R A 1121



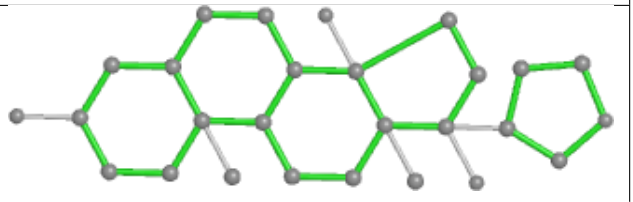
Bond lengths



Bond angles

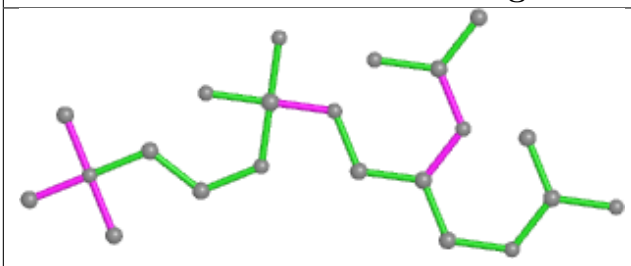


Torsions

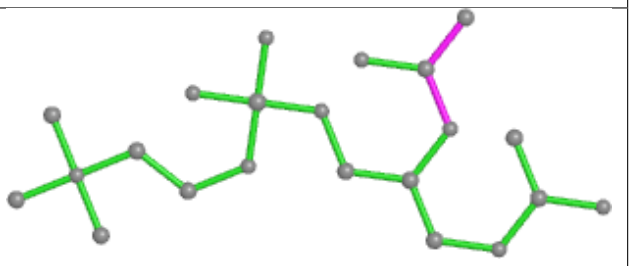


Rings

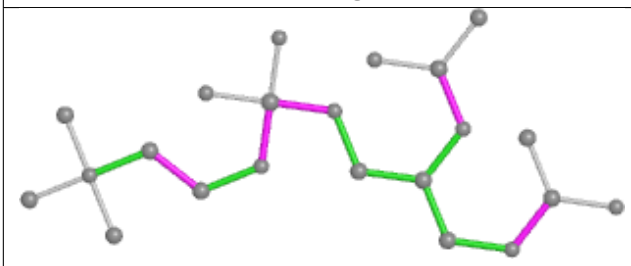
Ligand PCW A 1107



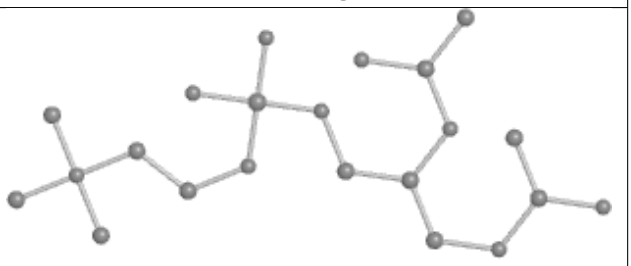
Bond lengths



Bond angles

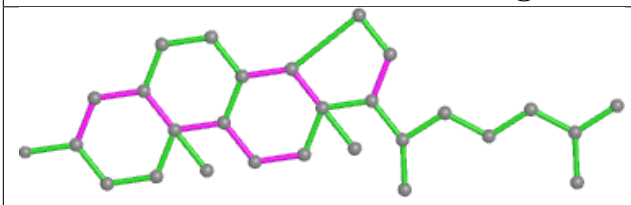


Torsions

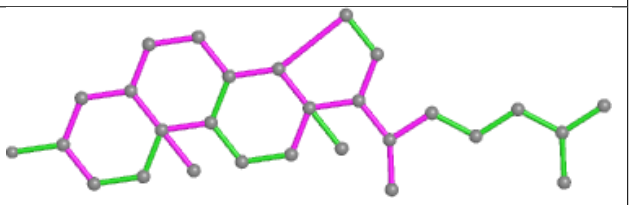


Rings

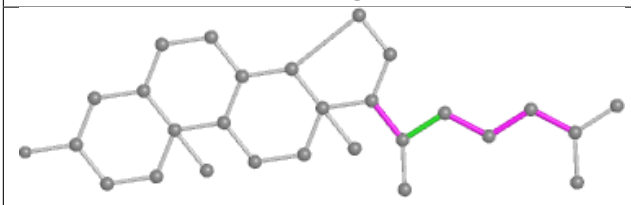
Ligand CLR C 1104



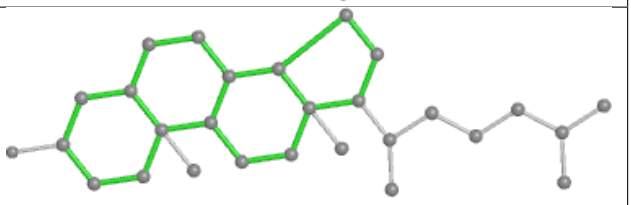
Bond lengths



Bond angles

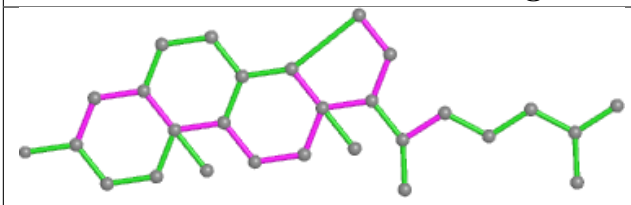


Torsions

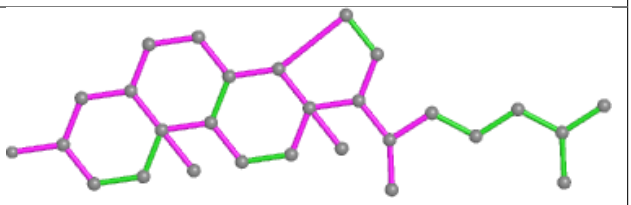


Rings

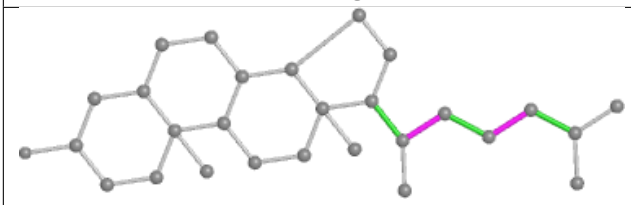
Ligand CLR B 501



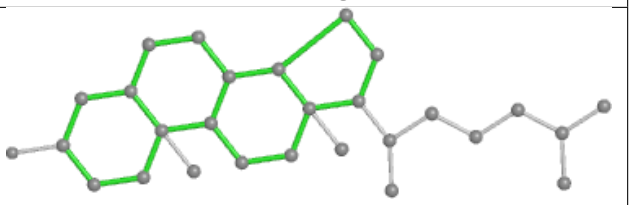
Bond lengths



Bond angles

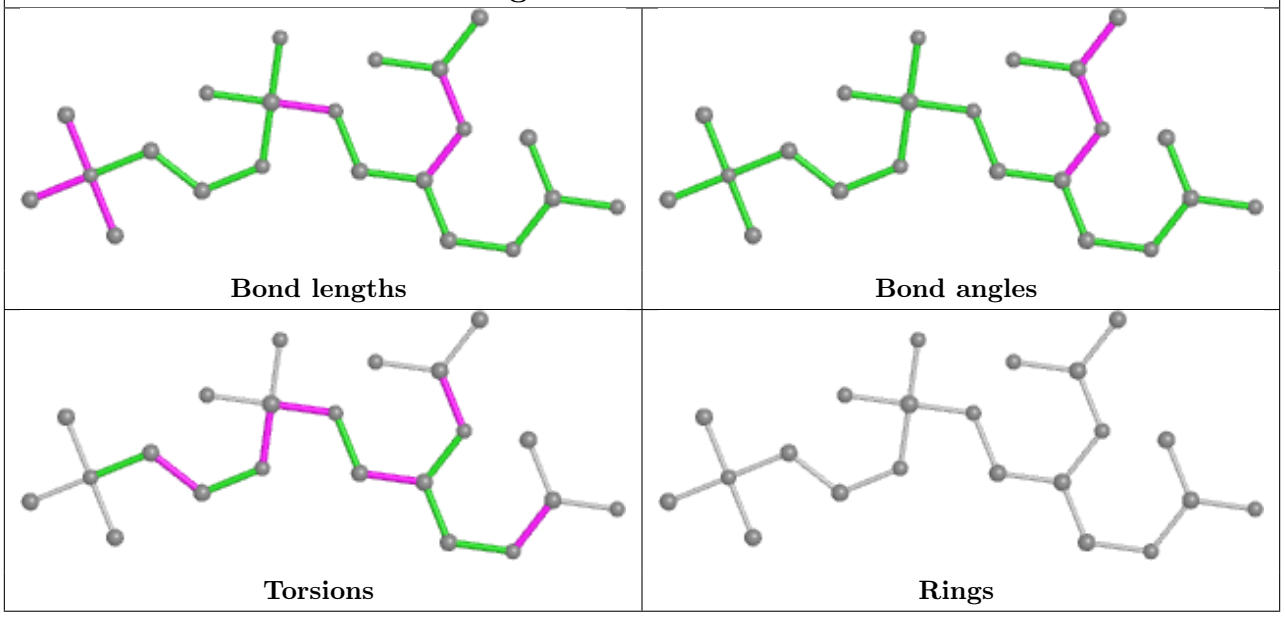


Torsions

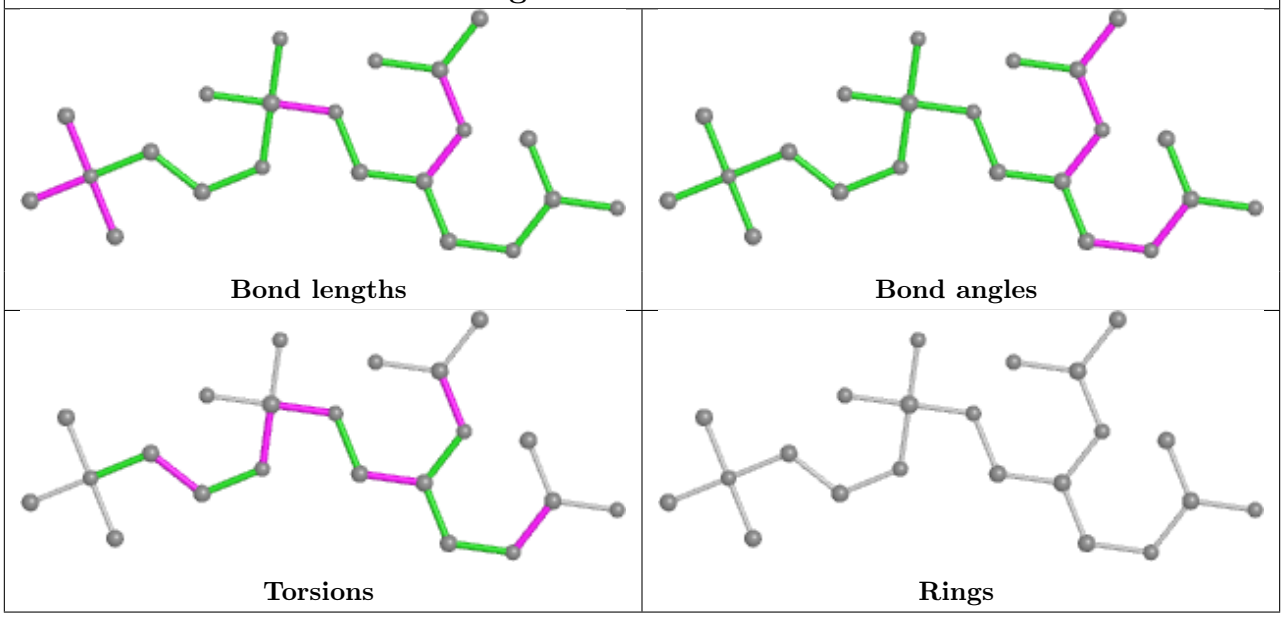


Rings

Ligand PCW C 1107



Ligand PCW A 1109



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	995/1016 (97%)	-0.14	50 (5%) 28 25	28, 89, 228, 316	0
1	C	995/1016 (97%)	-0.24	26 (2%) 56 49	25, 89, 197, 229	0
2	B	291/303 (96%)	-0.03	11 (3%) 40 36	50, 124, 205, 251	0
2	D	285/303 (94%)	-0.25	7 (2%) 57 51	27, 104, 179, 230	0
3	E	32/65 (49%)	-0.49	0 100 100	36, 68, 123, 127	0
3	G	32/65 (49%)	-0.74	0 100 100	24, 62, 121, 146	0
All	All	2630/2768 (95%)	-0.19	94 (3%) 42 38	24, 95, 210, 316	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	489	PRO	7.1
2	B	165	GLU	6.2
1	A	578	PHE	6.2
2	B	166	THR	6.1
1	A	467	TYR	5.5

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

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
1	PHD	A	369	12/13	0.99	0.24	32,62,76,80	0
1	PHD	C	369	12/13	0.99	0.20	40,59,80,83	0

6.3 Carbohydrates (i)

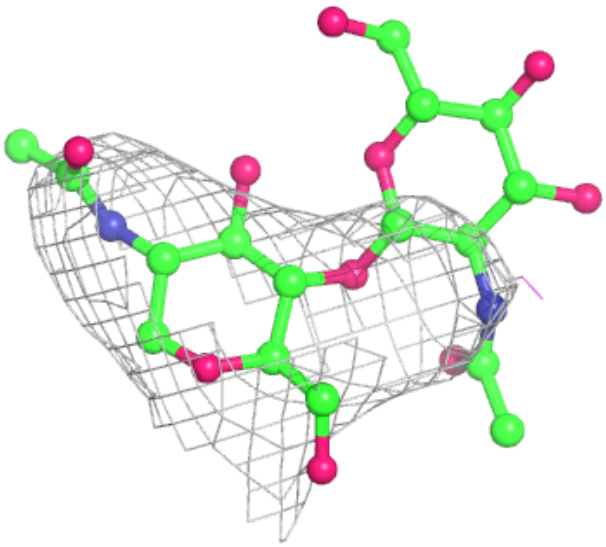
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

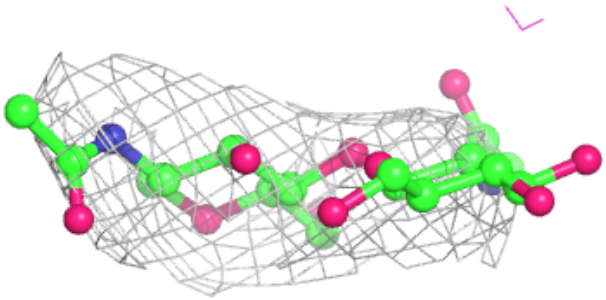
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	H	2	14/15	0.34	0.99	228,244,259,259	0
4	NAG	F	2	14/15	0.66	0.89	200,227,236,242	0
4	NAG	F	1	14/15	0.70	0.31	131,188,209,225	0
4	NAG	H	1	14/15	0.72	0.62	180,209,228,245	0
4	NAG	J	2	14/15	0.72	0.84	199,222,239,244	0
4	NAG	J	1	14/15	0.75	0.55	163,198,209,220	0
4	NAG	I	1	14/15	0.88	0.19	126,143,154,167	0
4	NAG	I	2	14/15	0.89	0.17	103,166,190,223	0

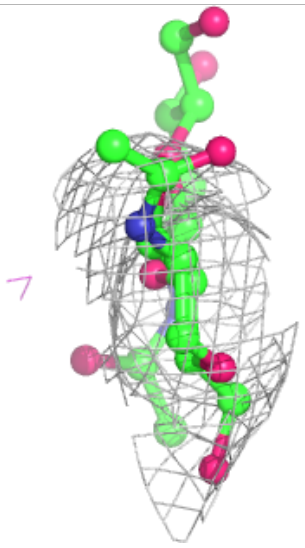
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

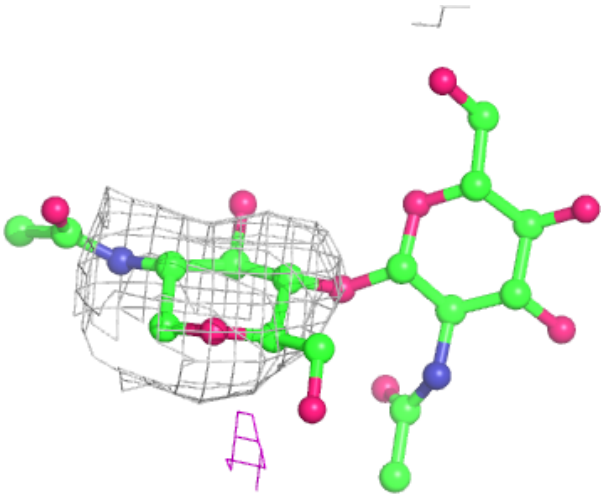


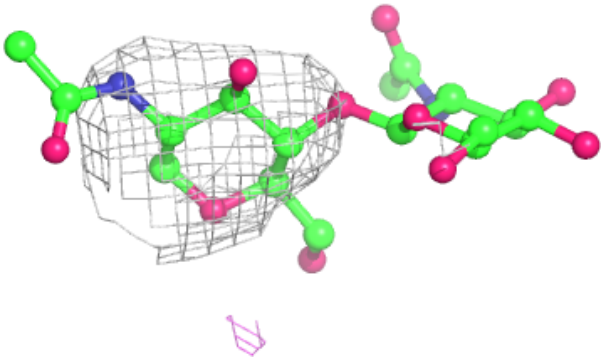


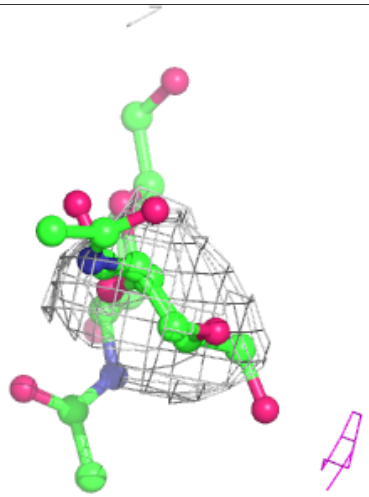


Electron density around Chain H:

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

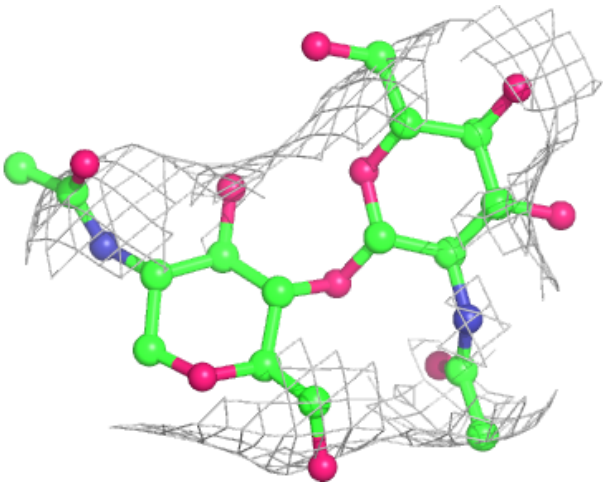


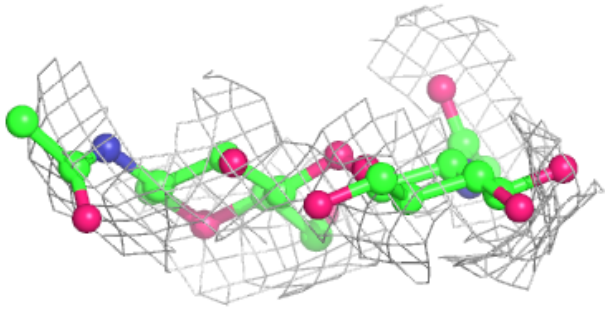


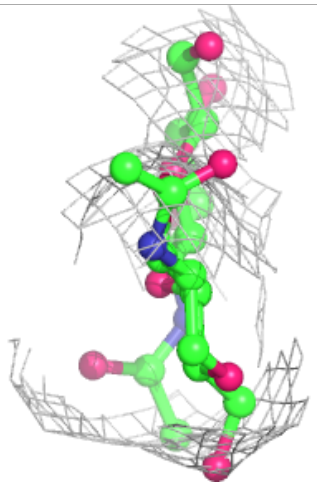


Electron density around Chain I:

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

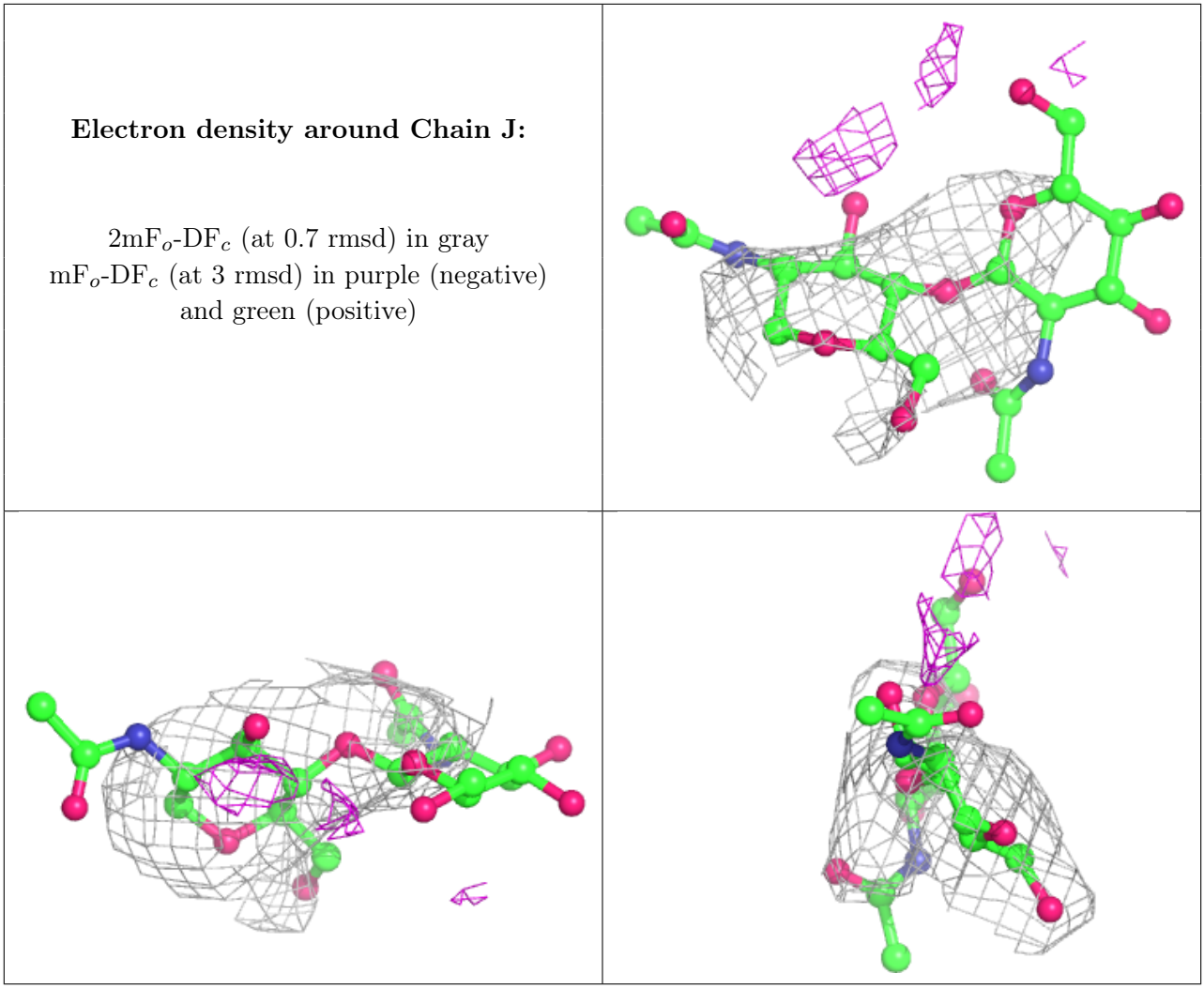






Electron density around Chain J:

$2mF_o$-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
7	PCW	C	1109	22/54	0.50	0.77	148,173,221,228	0
7	PCW	A	1108	22/54	0.62	0.87	135,172,205,211	0
7	PCW	C	1108	22/54	0.69	0.41	138,183,205,208	0
7	PCW	A	1106	22/54	0.72	0.52	128,166,191,201	0
10	NAG	D	401	14/15	0.72	0.27	125,171,184,187	0
7	PCW	C	1110	22/54	0.74	0.47	155,186,192,193	0
7	PCW	A	1105	22/54	0.74	0.48	155,173,197,214	0
10	NAG	B	401	14/15	0.75	0.31	129,183,195,196	0
7	PCW	C	1106	22/54	0.78	0.56	129,161,166,173	0

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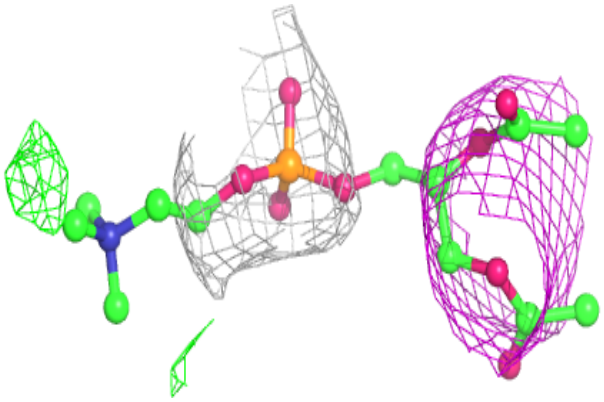
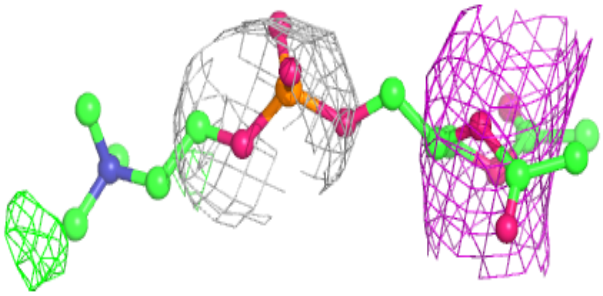
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PCW	A	1110	22/54	0.79	0.45	127,149,169,170	0
7	PCW	C	1111	22/54	0.79	0.57	113,178,200,206	0
9	CLR	D	501	28/28	0.82	0.53	129,147,159,161	0
9	CLR	B	501	28/28	0.83	0.48	116,148,158,161	0
7	PCW	A	1107	22/54	0.83	0.34	146,185,203,209	0
9	CLR	A	1104	28/28	0.84	0.39	104,132,147,150	0
7	PCW	C	1112	22/54	0.89	0.29	78,116,153,158	0
7	PCW	A	1109	22/54	0.89	0.32	73,107,124,132	0
7	PCW	C	1107	22/54	0.90	0.23	103,130,147,154	0
9	CLR	C	1104	28/28	0.91	0.32	66,102,130,139	0
8	E4R	A	1121	27/27	0.94	0.23	69,106,122,139	0
5	MG	A	1101	1/1	0.95	0.21	84,84,84,84	0
8	E4R	C	1121	27/27	0.96	0.24	40,77,101,108	0
9	CLR	G	101	28/28	0.96	0.23	22,48,80,101	0
6	NA	A	1102	1/1	0.97	0.32	37,37,37,37	0
9	CLR	E	101	28/28	0.97	0.23	20,46,76,85	0
6	NA	C	1102	1/1	0.99	0.37	13,13,13,13	0
5	MG	C	1101	1/1	0.99	0.13	61,61,61,61	0
5	MG	C	1103	1/1	0.99	0.22	26,26,26,26	0
5	MG	A	1103	1/1	0.99	0.27	78,78,78,78	0

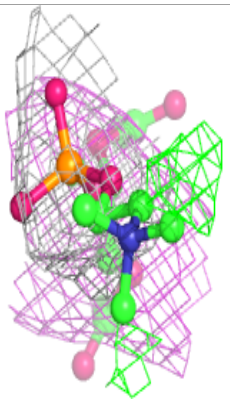
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PCW C 1109:

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

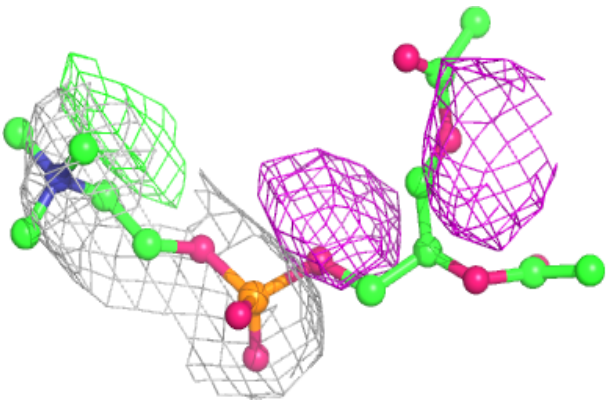


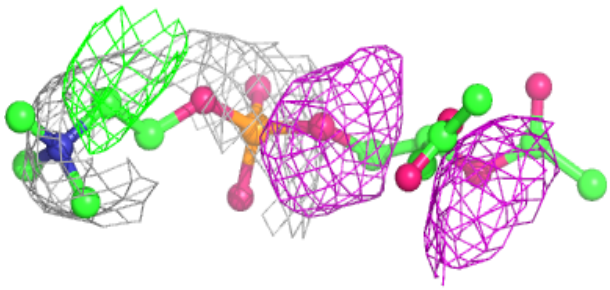


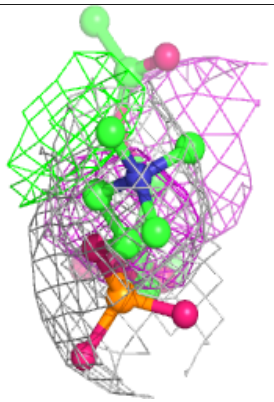


Electron density around PCW A 1108:

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

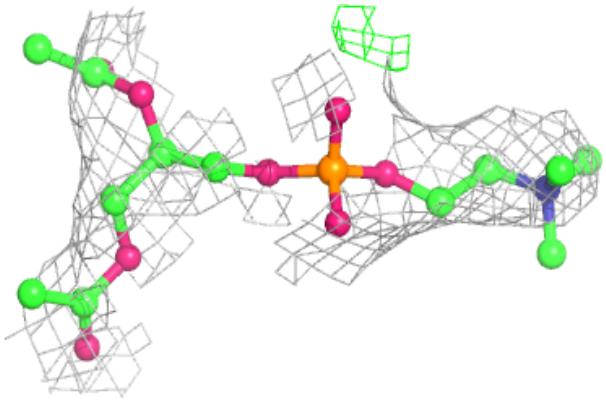


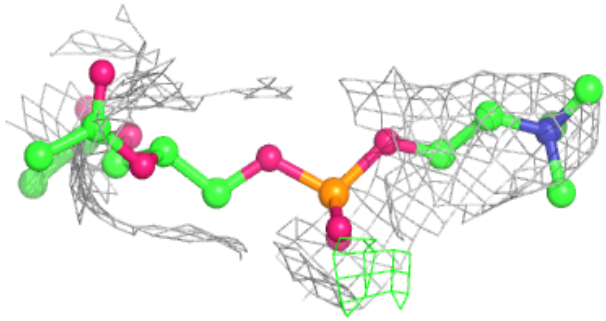


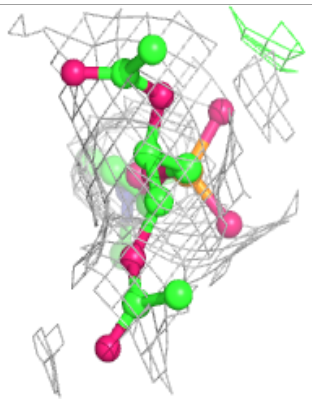


Electron density around PCW C 1108:

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

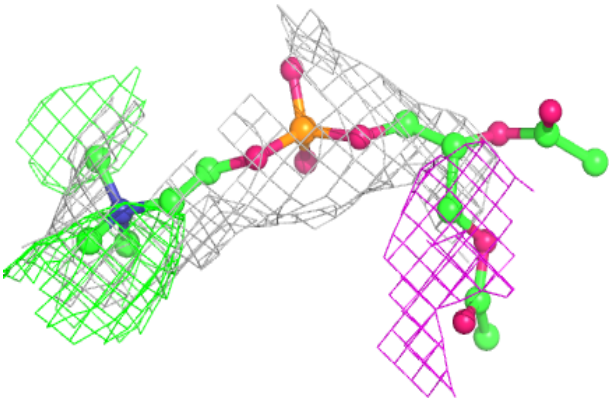


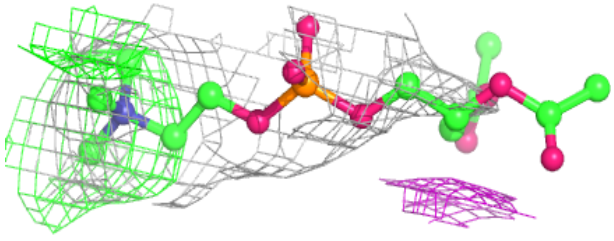


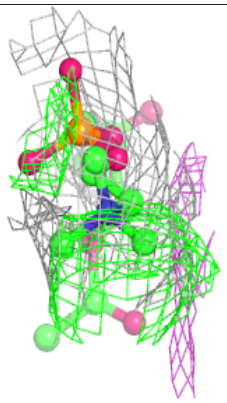


Electron density around PCW A 1106:

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

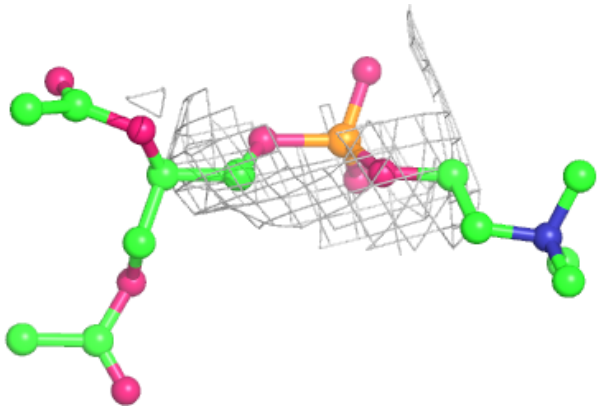


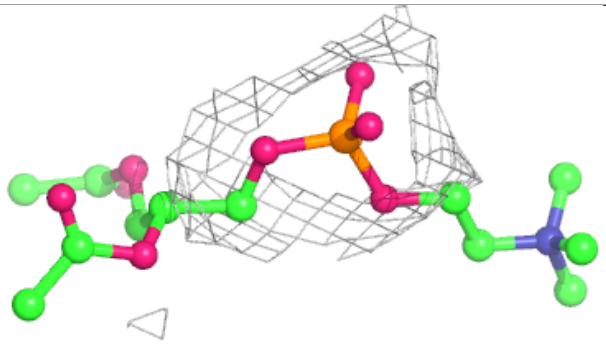


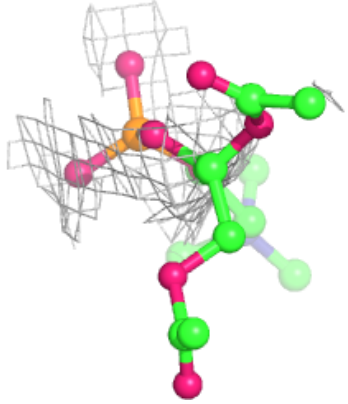


Electron density around PCW C 1110:

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

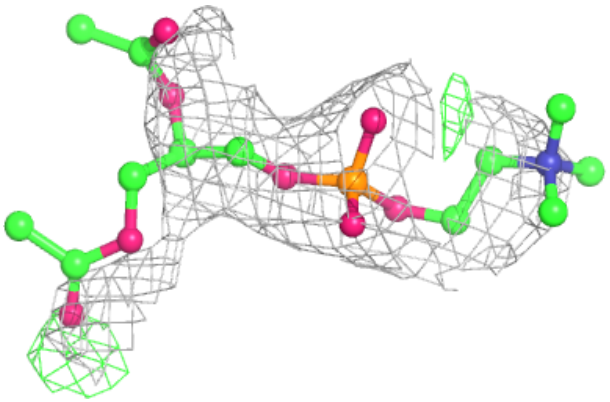


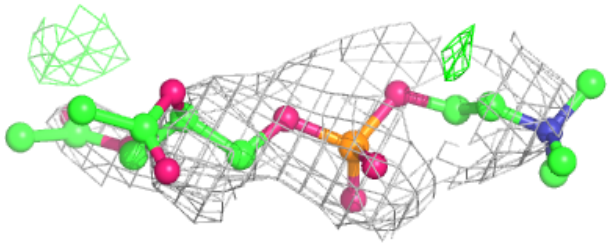


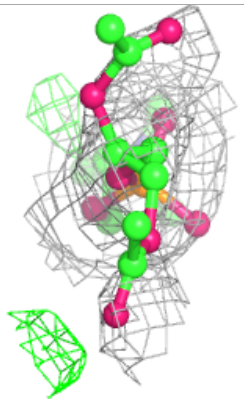


Electron density around PCW A 1105:

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

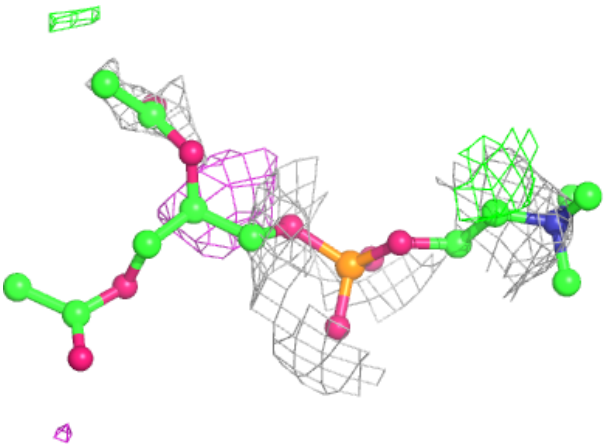


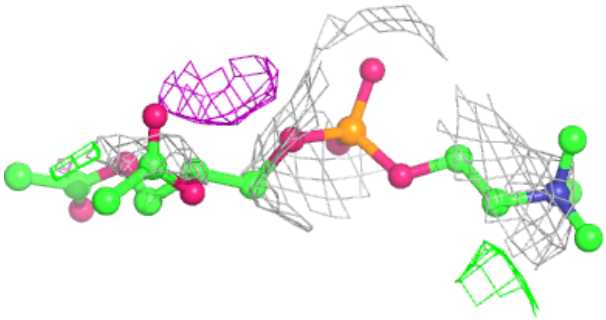


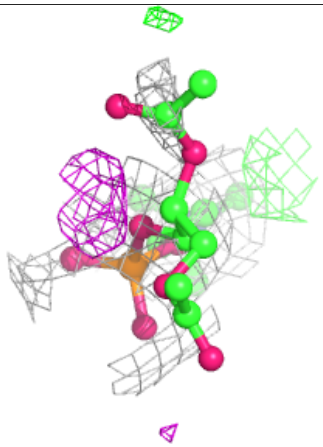


Electron density around PCW C 1106:

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

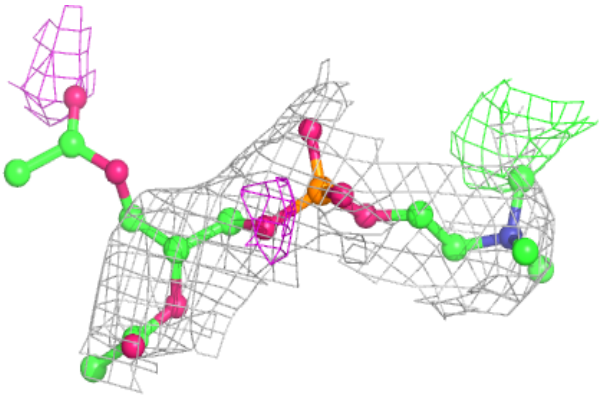


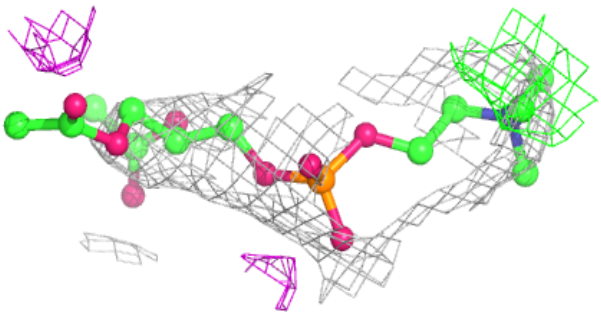


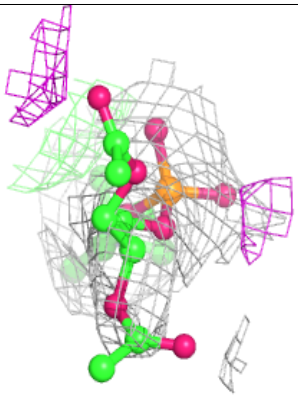


Electron density around PCW A 1110:

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

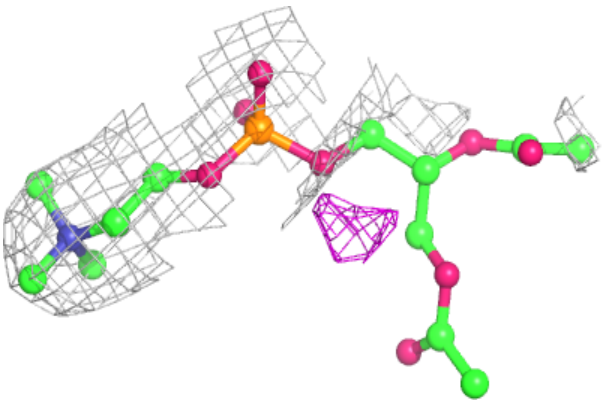


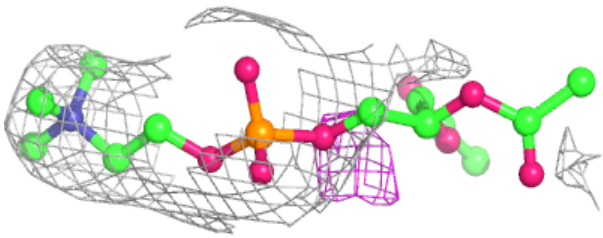


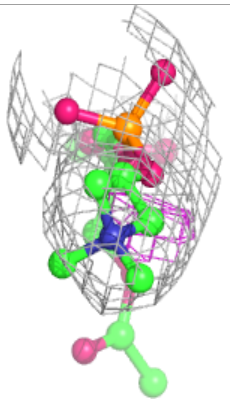


Electron density around PCW C 1111:

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

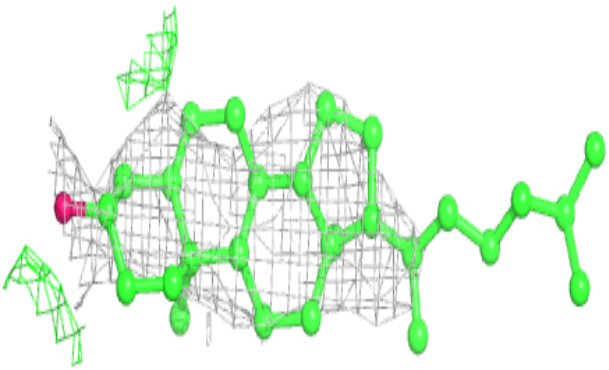


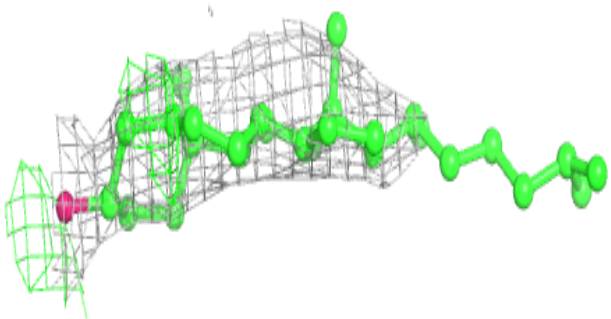


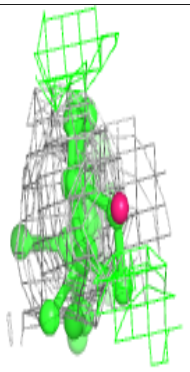


Electron density around CLR D 501:

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

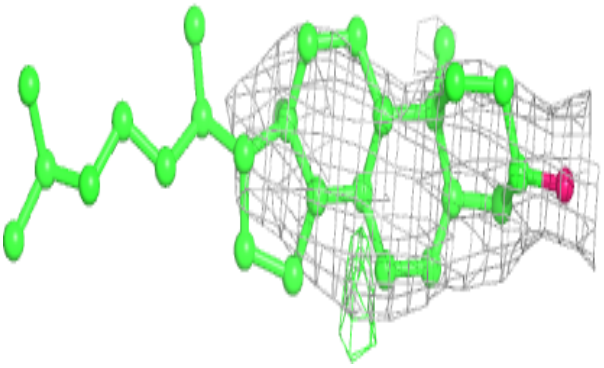


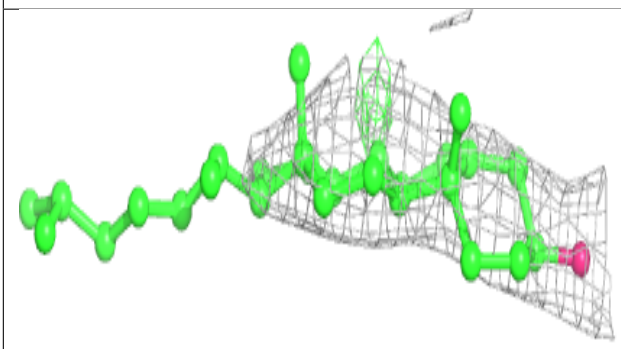


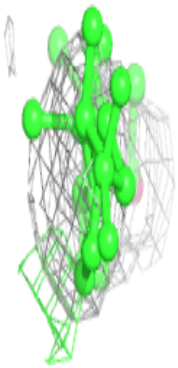


Electron density around CLR B 501:

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

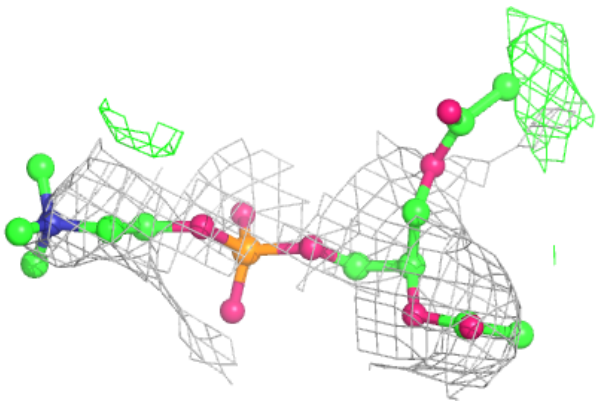


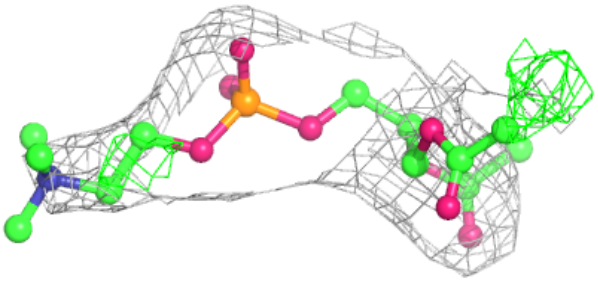


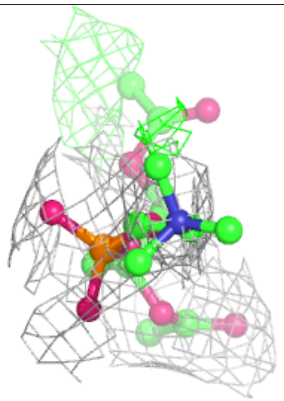


Electron density around PCW A 1107:

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

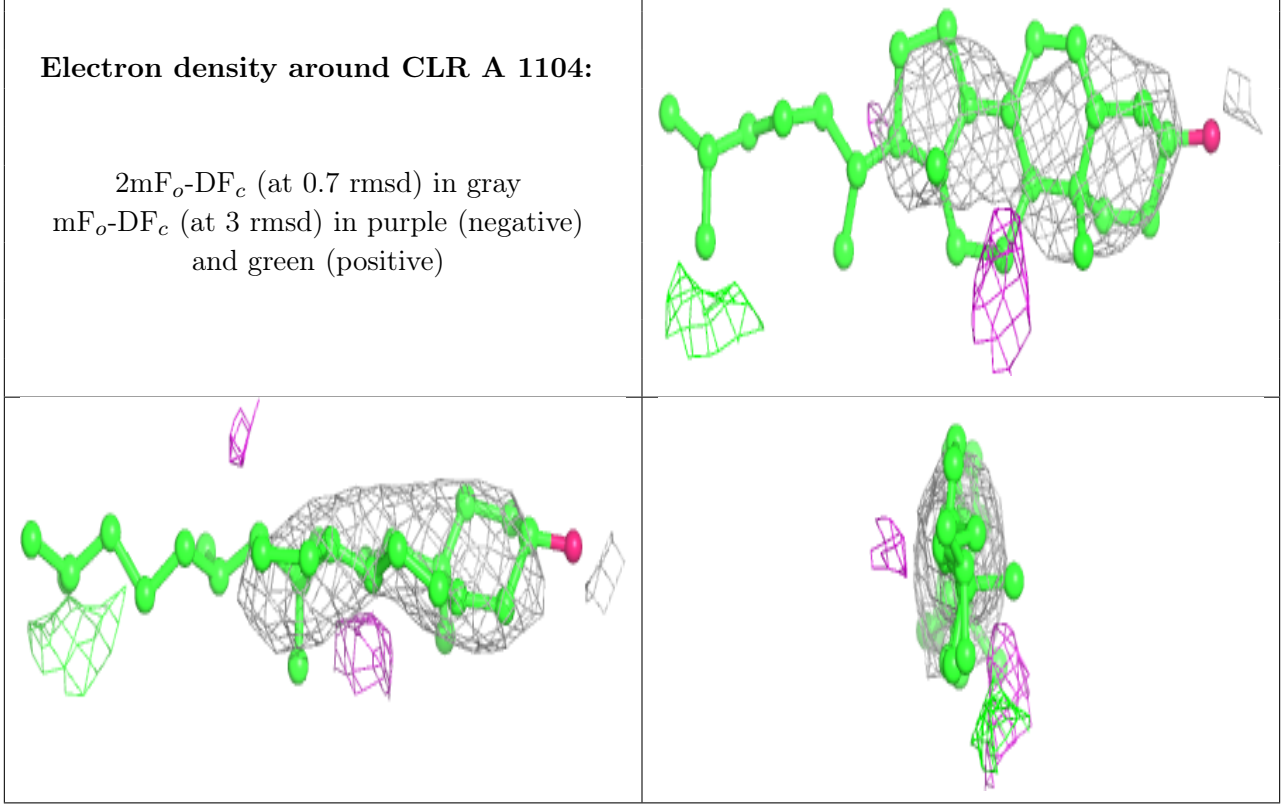






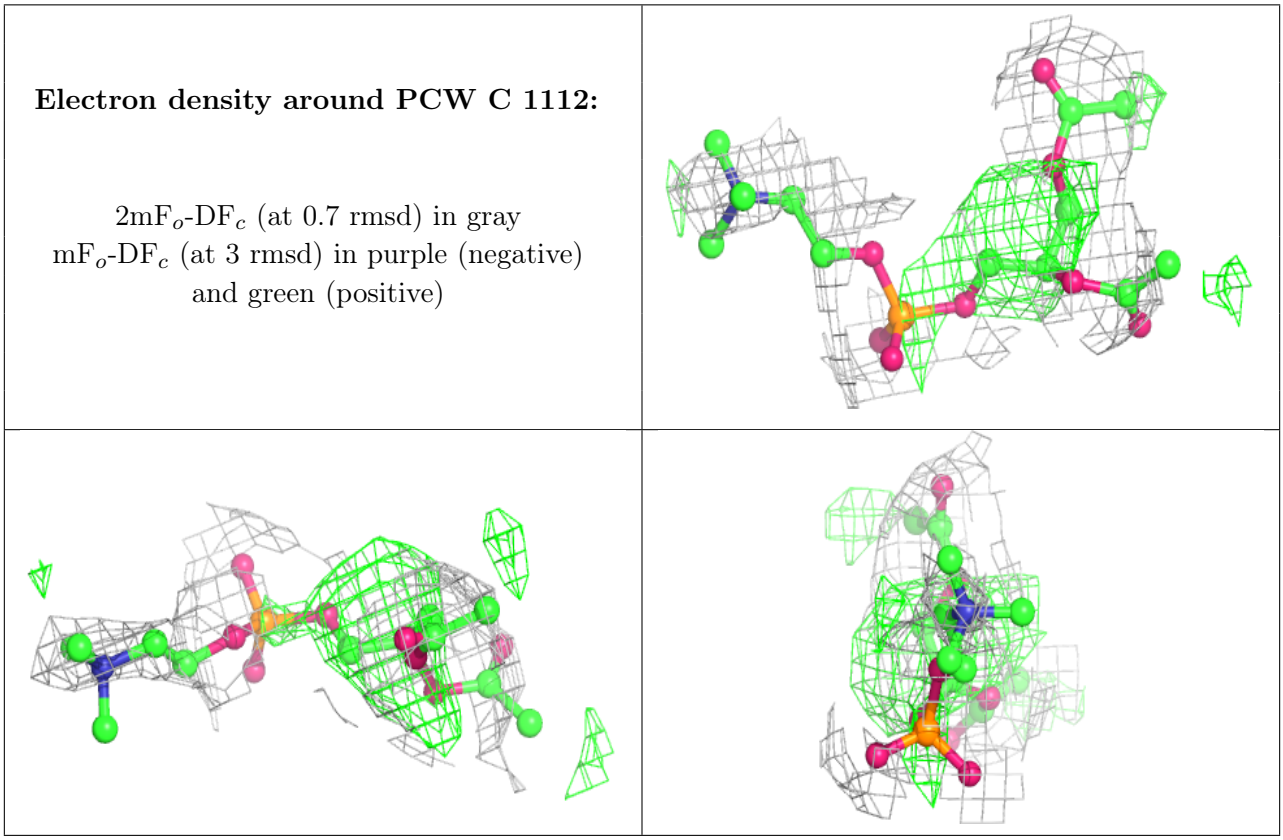
Electron density around CLR A 1104:

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



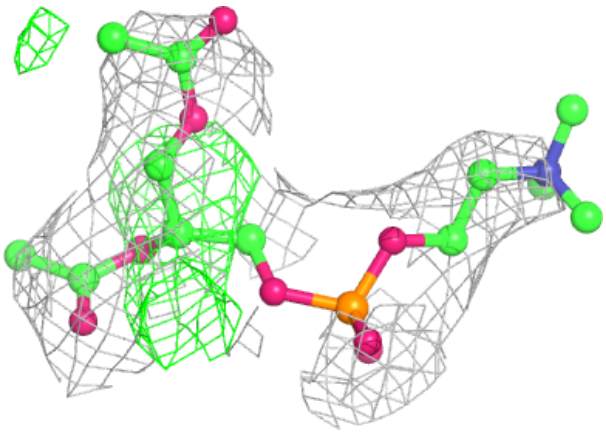
Electron density around PCW C 1112:

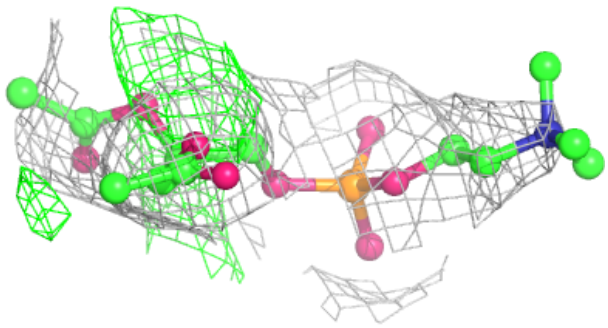
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

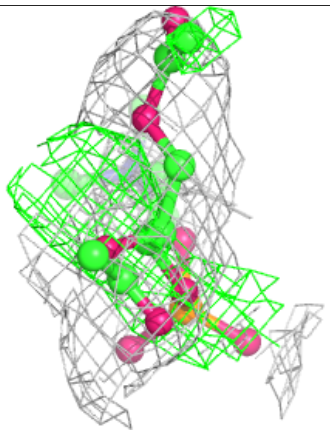


Electron density around PCW A 1109:

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

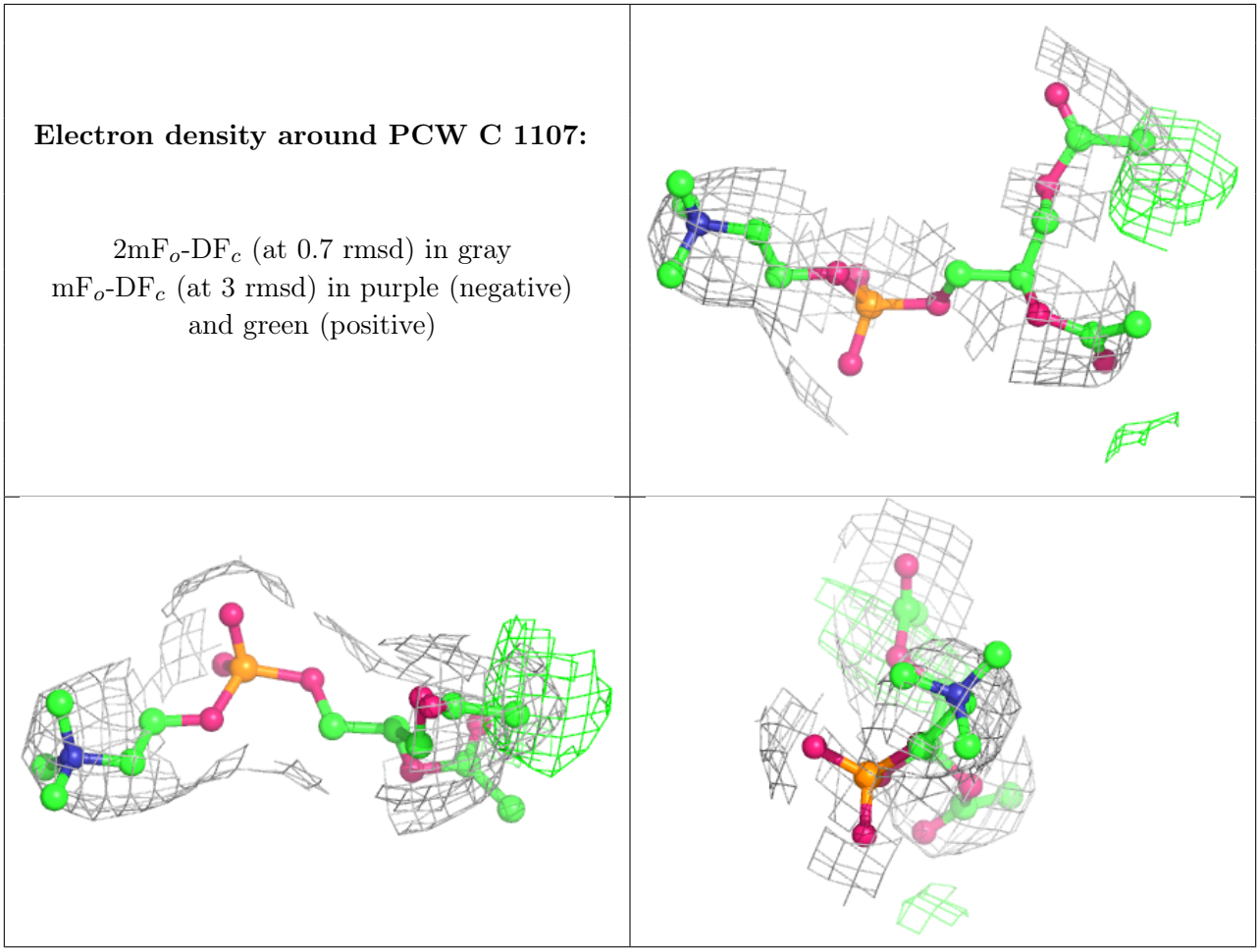






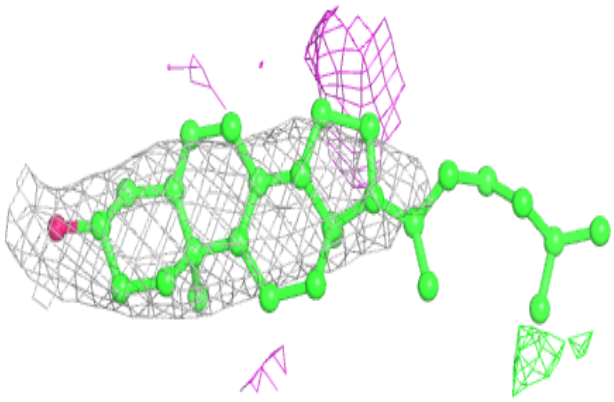
Electron density around PCW C 1107:

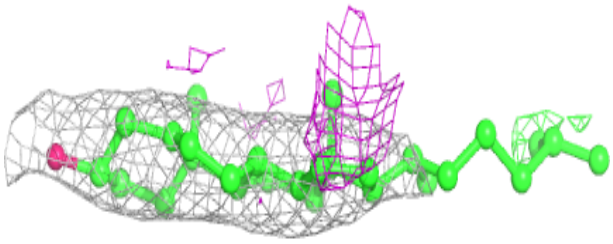
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

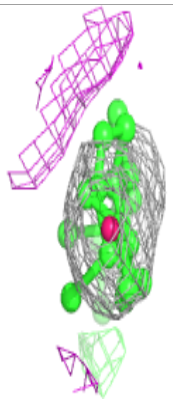


Electron density around CLR C 1104:

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

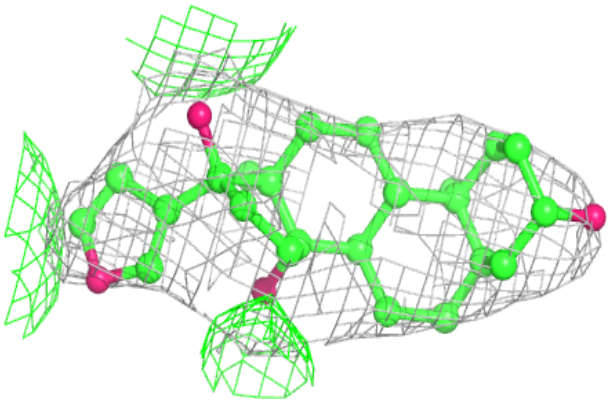


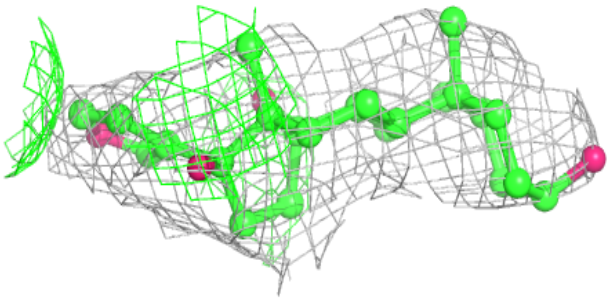


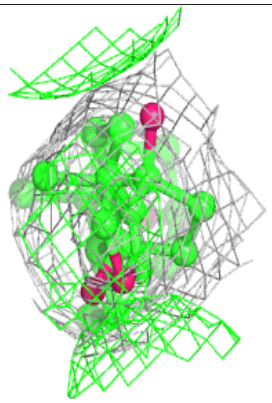


Electron density around E4R A 1121:

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

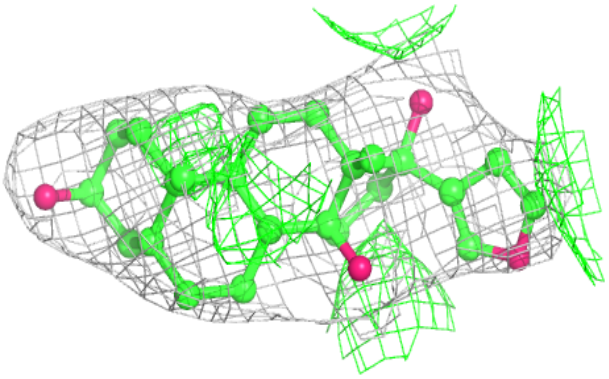


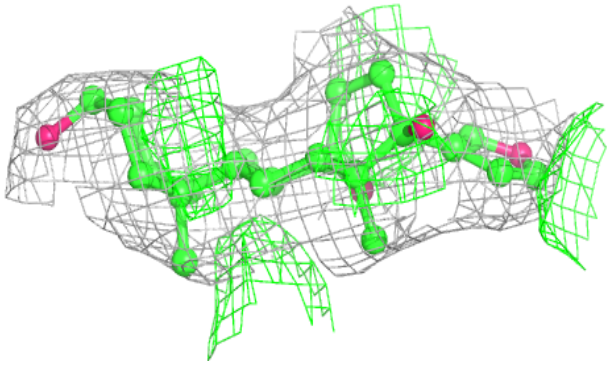


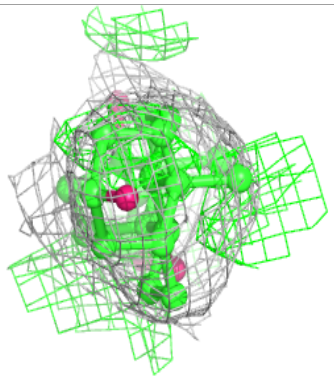


Electron density around E4R C 1121:

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

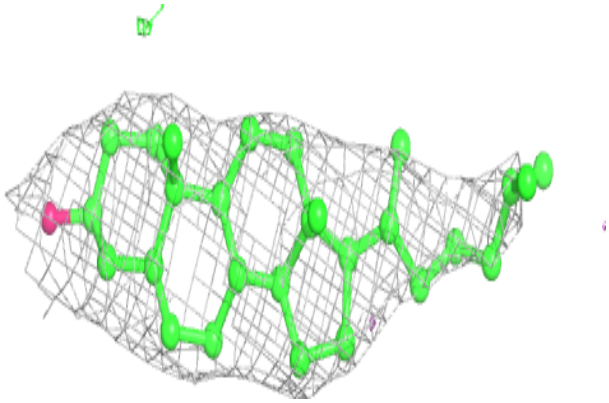


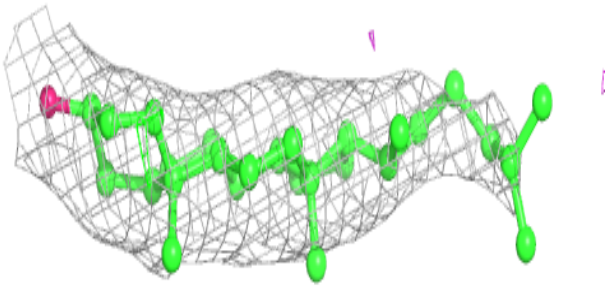


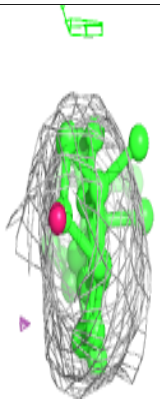


Electron density around CLR G 101:

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

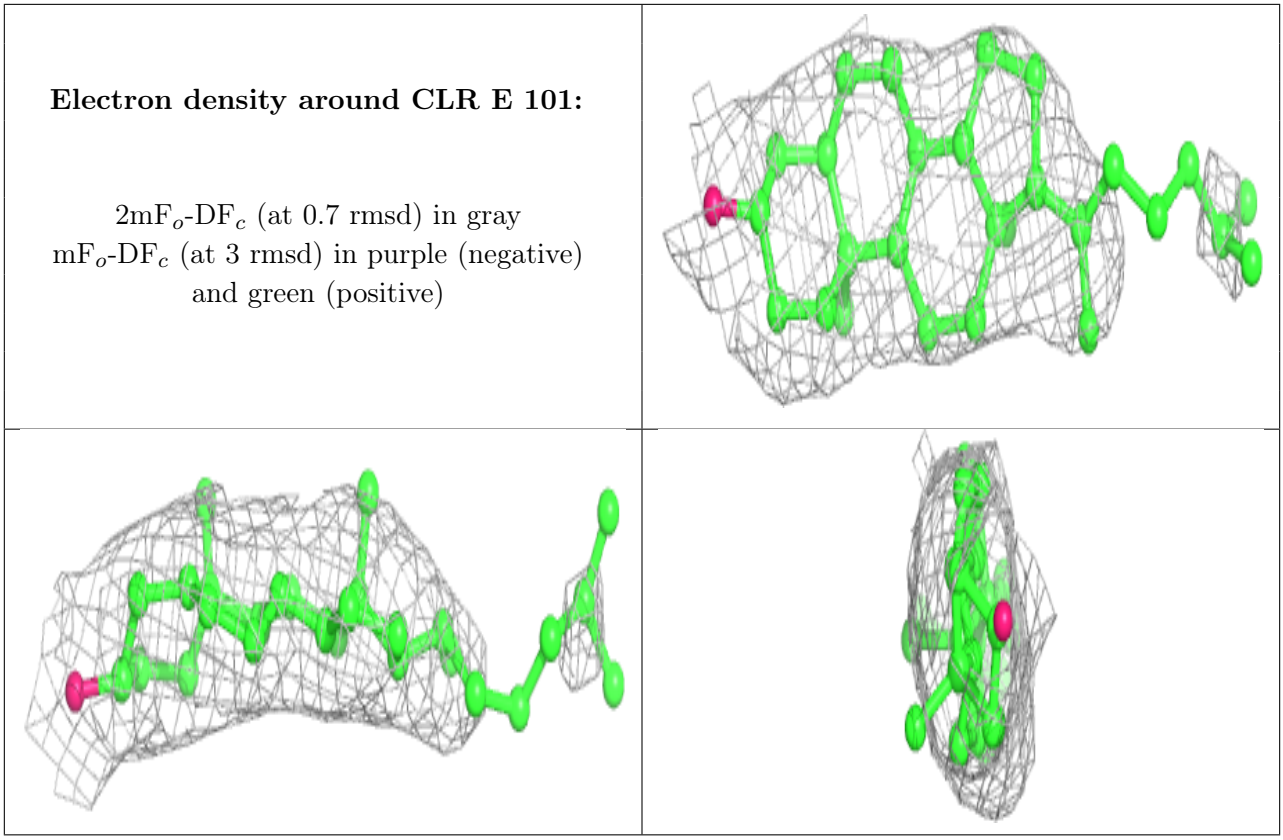






Electron density around CLR E 101:

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



6.5 Other polymers (i)

There are no such residues in this entry.