wwPDB X-ray Structure Validation Summary Report (i)

Nov 20, 2023 – 07:31 PM JST

PDB ID	:	7DDF
Title	:	Crystal structures of Na+,K+-ATPase in complex with beryllium fluoride
Authors	:	Ogawa, H.; Cornelius, F.; Kanai, R.; Motoyama, K.; Vilsen, B.; Toyoshima, C.
Deposited on	:	2020-10-29
Resolution	:	4.62 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:

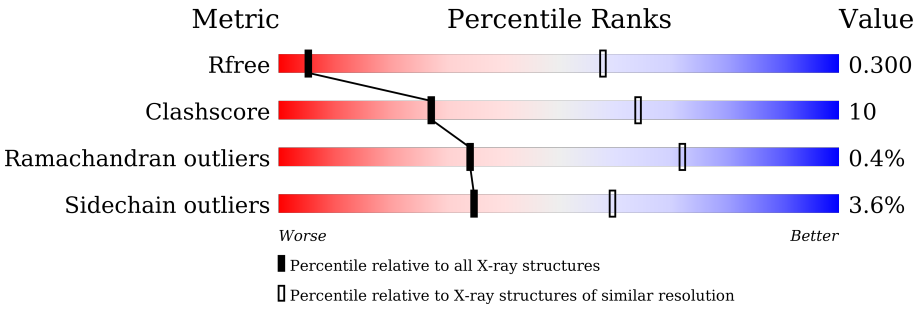
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 4.62 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	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1016	74% 23%
1	C	1016	73% 24%
2	B	303	65% 29%
2	D	303	68% 24% 6%
3	E	65	37% 11% 51%
3	G	65	42% 8% 51%
4	F	2	100%

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

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 21190 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	Be	C	F	N	O	S	0	0	0
			7730	1	4922	3	1301	1456	47			
1	C	996	Total	Be	C	F	N	O	S	0	0	0
			7730	1	4922	3	1301	1456	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

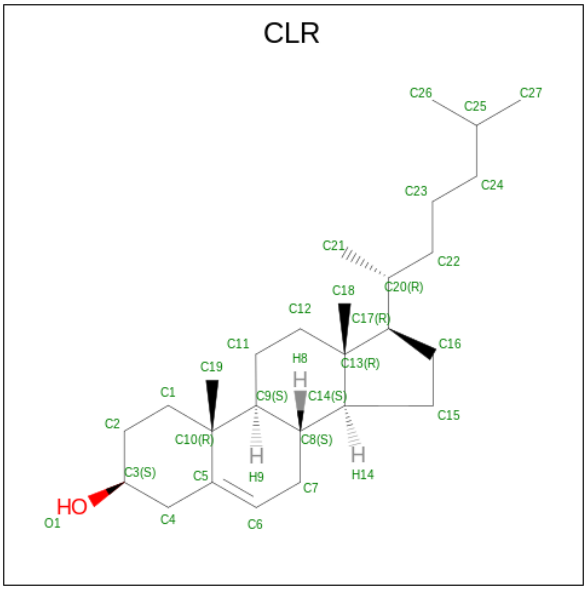
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

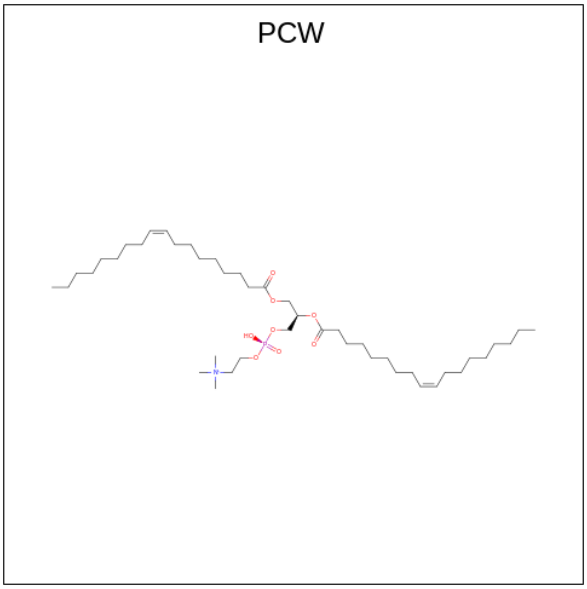
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0
6	C	1	Total Na 1 1	0	0

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 8 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
8	A	1	Total C N O P 22 12 1 8 1	0	0
8	A	1	Total C N O P 22 12 1 8 1	0	0
8	A	1	Total C N O P 22 12 1 8 1	0	0
8	A	1	Total C N O P 22 12 1 8 1	0	0
8	A	1	Total C N O P 22 12 1 8 1	0	0

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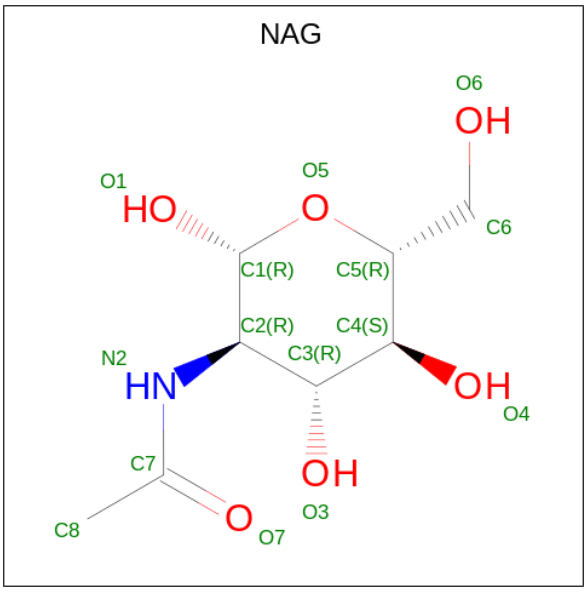
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C N O P 22 12 1 8 1	0	0
8	C	1	Total C N O P 22 12 1 8 1	0	0
8	C	1	Total C N O P 22 12 1 8 1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is water.

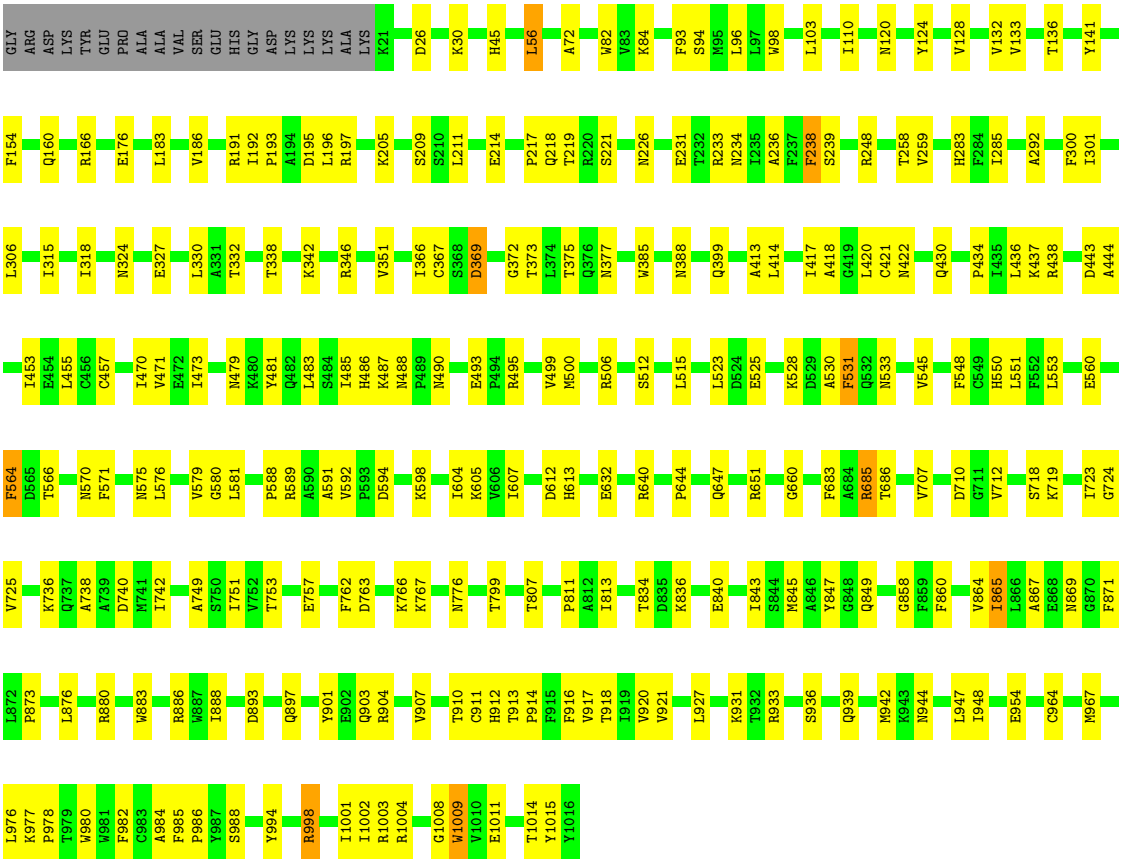
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	5	Total O 5 5	0	0
10	C	5	Total O 5 5	0	0

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. 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. 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.

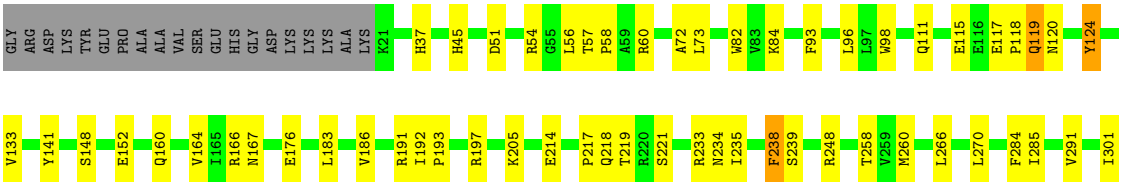
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

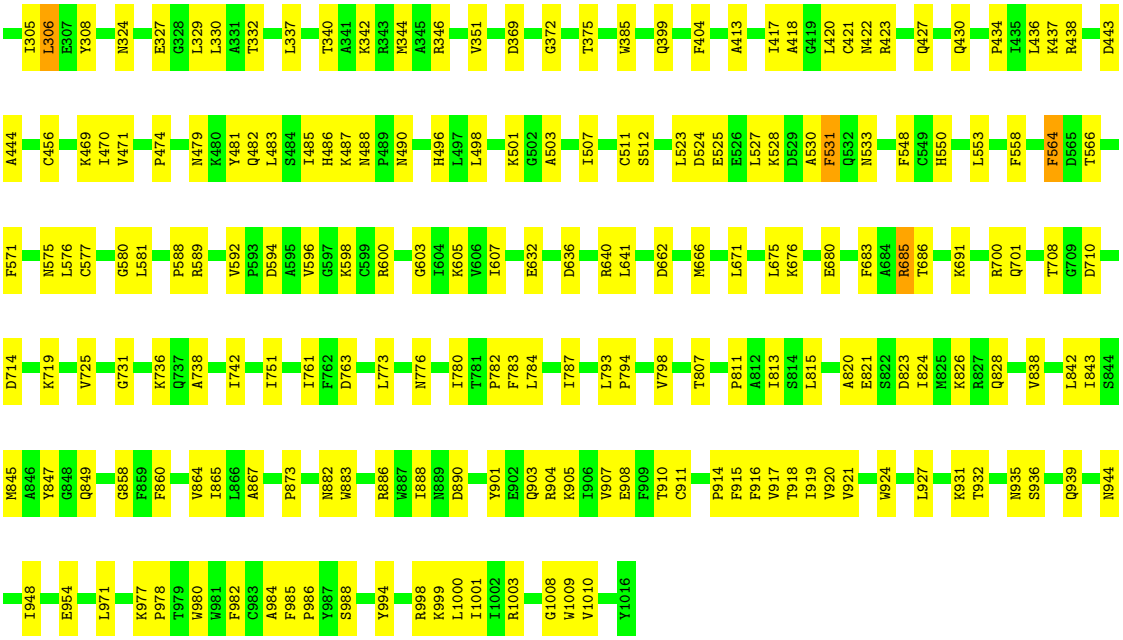
Chain A:



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

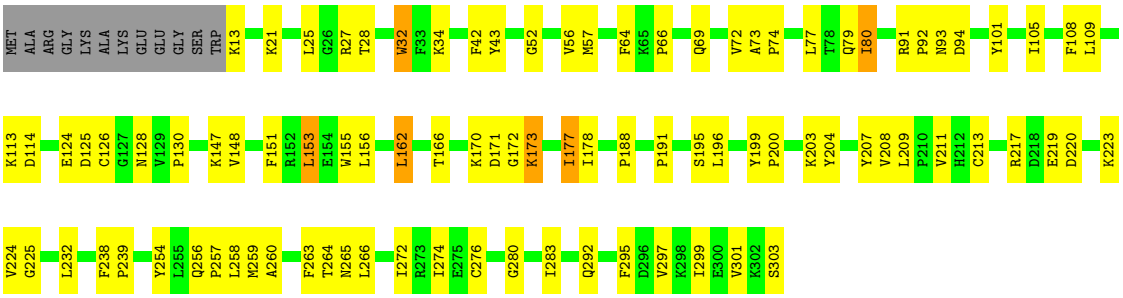
Chain C:





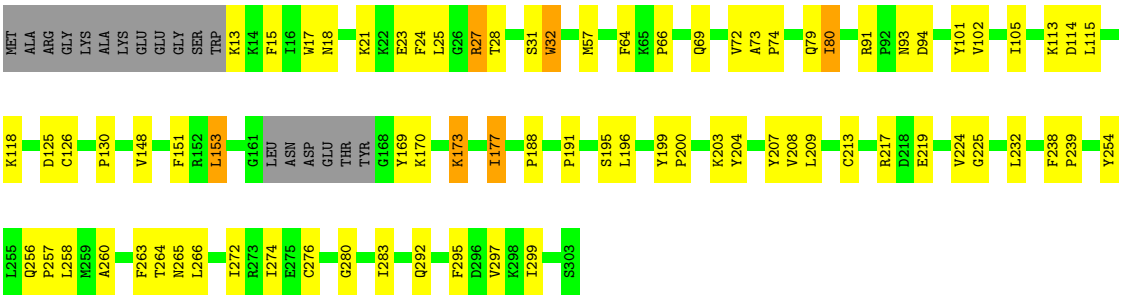
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain B:



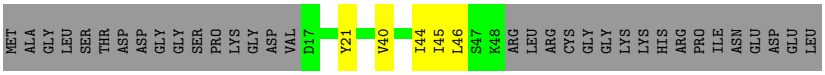
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain D:



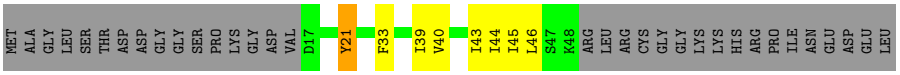
• Molecule 3: FXYD domain-containing ion transport regulator

Chain G:



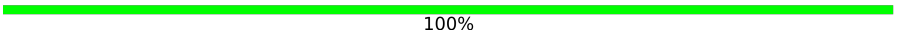
• Molecule 3: FXYD domain-containing ion transport regulator

Chain E:



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

Chain F:

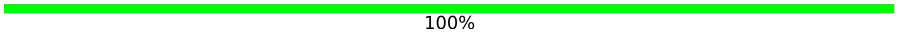


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.48Å 118.37Å 495.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.99 – 4.62 49.56 – 4.62	Depositor EDS
% Data completeness (in resolution range)	28.2 (15.99-4.62) 29.5 (49.56-4.62)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 4.64Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.194 , 0.241 0.233 , 0.300	Depositor DCC
R_{free} test set	527 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å^2)	88.5	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , -26.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.078 for k,h,-l	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	21190	wwPDB-VP
Average B, all atoms (Å^2)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.30% 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: MG, NAG, NA, PCW, CLR, BFD

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	0.34	0/7867	0.55	0/10674
1	C	0.33	0/7867	0.56	0/10674
2	B	0.36	0/2449	0.61	0/3301
2	D	0.37	0/2395	0.59	0/3225
3	E	0.34	0/261	0.52	0/354
3	G	0.34	0/261	0.52	0/354
All	All	0.34	0/21100	0.56	0/28582

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	7730	0	7777	157	0
1	C	7730	0	7777	160	0
2	B	2386	0	2361	54	0
2	D	2334	0	2317	46	0
3	E	255	0	259	6	0
3	G	255	0	259	3	0
4	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	28	0	25	0	0
4	I	28	0	25	0	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	28	0	46	2	0
7	B	28	0	46	0	0
7	C	28	0	46	2	0
7	D	28	0	46	0	0
7	E	28	0	46	4	0
7	G	28	0	46	2	0
8	A	110	0	90	7	0
8	C	66	0	54	1	0
9	B	14	0	13	0	0
9	D	14	0	13	0	0
10	A	5	0	0	0	0
10	C	5	0	0	0	0
All	All	21190	0	21296	427	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 10.

The worst 5 of 427 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:221:SER:H	1:A:233:ARG:HB3	1.46	0.80
2:B:80:ILE:HG12	2:B:177:ILE:HG12	1.63	0.78
1:C:375:THR:HA	1:C:588:PRO:HA	1.66	0.77
1:A:375:THR:HA	1:A:588:PRO:HA	1.66	0.76
2:D:80:ILE:HG12	2:D:177:ILE:HG12	1.69	0.74

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%)	63 (6%)	3 (0%)	41 76
1	C	993/1016 (98%)	925 (93%)	65 (6%)	3 (0%)	41 76
2	B	289/303 (95%)	258 (89%)	29 (10%)	2 (1%)	22 62
2	D	281/303 (93%)	254 (90%)	25 (9%)	2 (1%)	22 62
3	E	30/65 (46%)	28 (93%)	2 (7%)	0	100 100
3	G	30/65 (46%)	28 (93%)	2 (7%)	0	100 100
All	All	2616/2768 (94%)	2420 (92%)	186 (7%)	10 (0%)	34 72

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	200	PRO
1	C	306	LEU
1	A	306	LEU
2	D	200	PRO
2	B	199	TYR

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%)	827 (98%)	19 (2%)	52 71
1	C	846/861 (98%)	829 (98%)	17 (2%)	55 73
2	B	261/269 (97%)	238 (91%)	23 (9%)	10 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	255/269 (95%)	234 (92%)	21 (8%)	11 36
3	E	26/52 (50%)	25 (96%)	1 (4%)	33 58
3	G	26/52 (50%)	25 (96%)	1 (4%)	33 58
All	All	2260/2364 (96%)	2178 (96%)	82 (4%)	35 59

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	776	ASN
2	D	153	LEU
1	C	1009	TRP
2	D	64	PHE
2	D	195	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	898	GLN
1	C	897	GLN
1	C	119	GLN
1	C	488	ASN
1	C	111	GLN

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	BFD	A	369	1,5	8,11,12	0.94	0	3,15,17	1.36	1 (33%)
1	BFD	C	369	1,5	8,11,12	0.95	0	3,15,17	1.35	1 (33%)

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	BFD	A	369	1,5	-	0/5/11/13	-
1	BFD	C	369	1,5	-	0/5/11/13	-

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	BFD	OD2-CG-CB	-2.34	119.56	124.73
1	C	369	BFD	OD2-CG-CB	-2.25	119.76	124.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	369	BFD	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	2,4	14,14,15	0.37	0	17,19,21	0.49	0
4	NAG	F	2	4	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	H	1	2,4	14,14,15	0.67	1 (7%)	17,19,21	0.72	0
4	NAG	H	2	4	14,14,15	0.39	0	17,19,21	0.37	0
4	NAG	I	1	2,4	14,14,15	0.33	0	17,19,21	0.56	0
4	NAG	I	2	4	14,14,15	0.39	0	17,19,21	0.53	0
4	NAG	J	1	2,4	14,14,15	0.70	1 (7%)	17,19,21	0.62	0
4	NAG	J	2	4	14,14,15	0.44	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	2,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	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	2,4	-	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	2,4	-	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	J	1	NAG	O5-C1	-2.50	1.39	1.43
4	H	1	NAG	O5-C1	-2.40	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

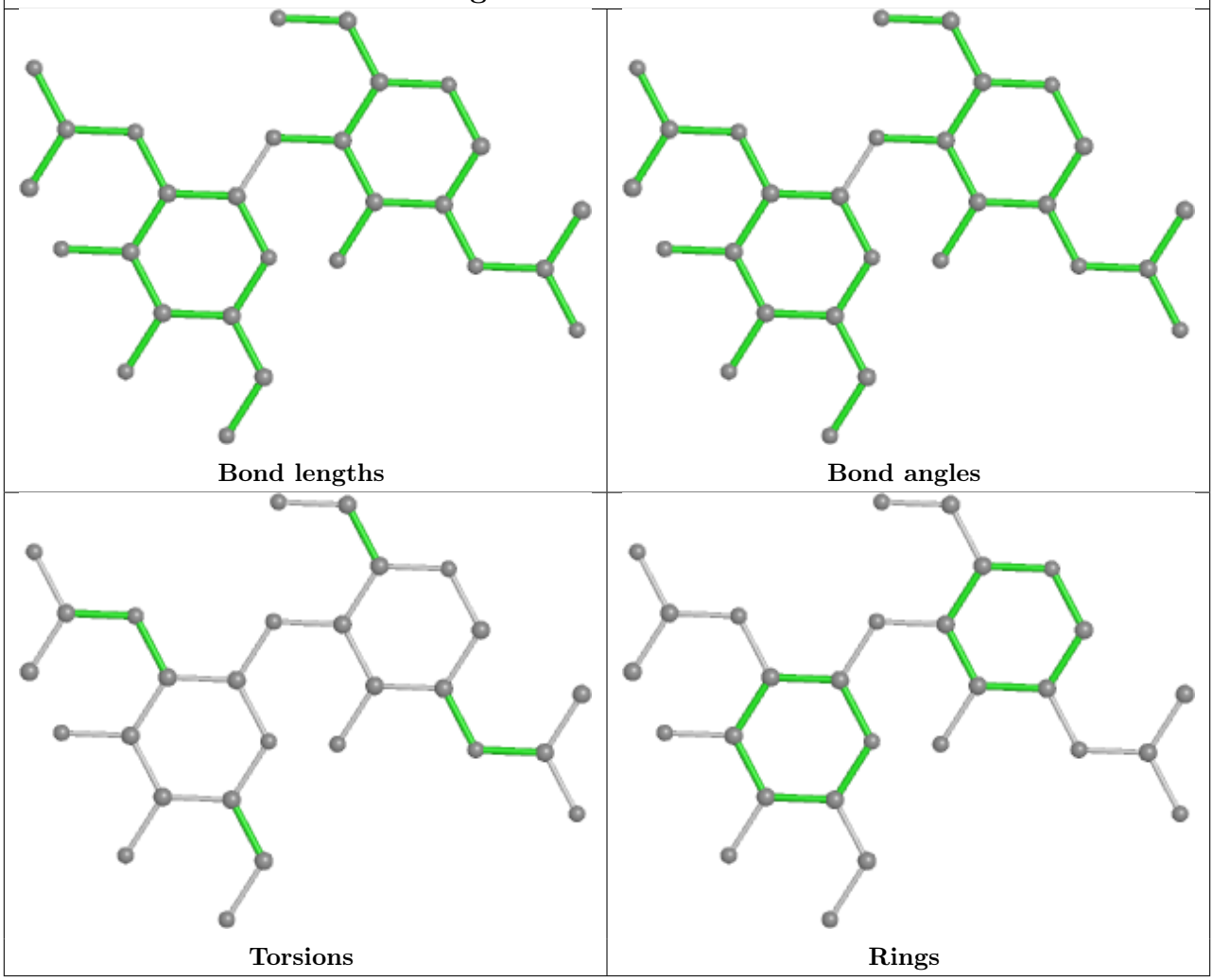
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6

There are no ring outliers.

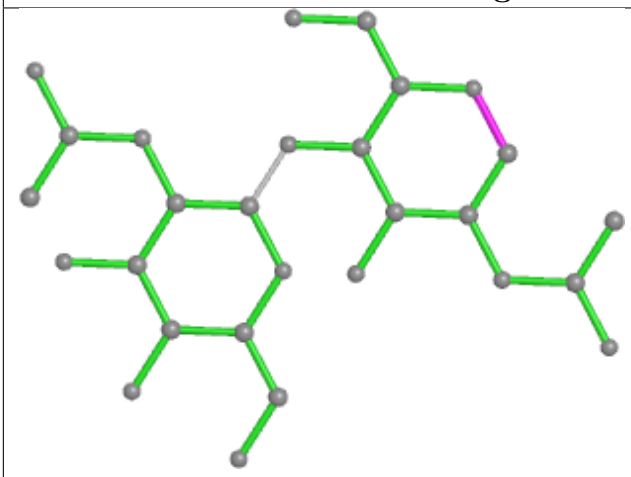
No monomer is involved in short contacts.

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

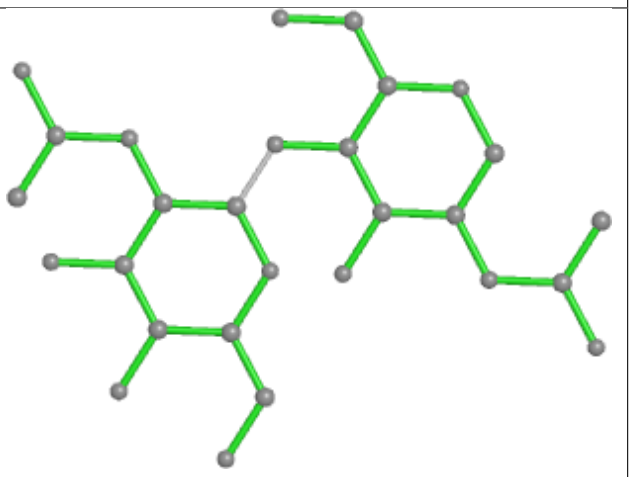
Oligosaccharide Chain F



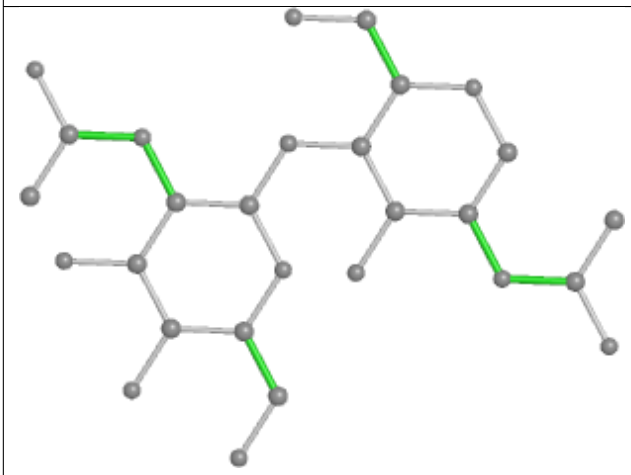
Oligosaccharide Chain H



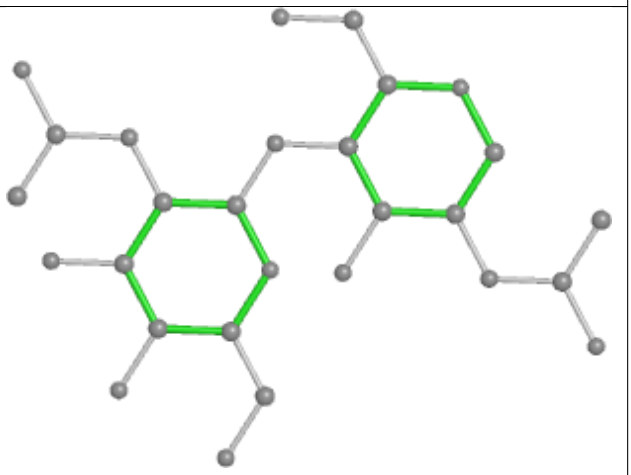
Bond lengths



Bond angles

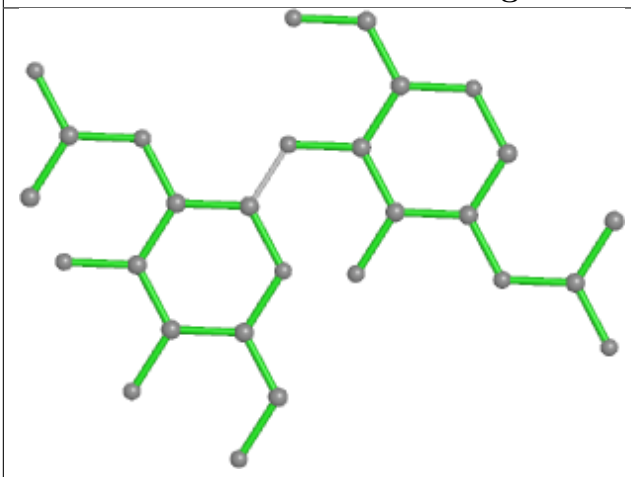


Torsions

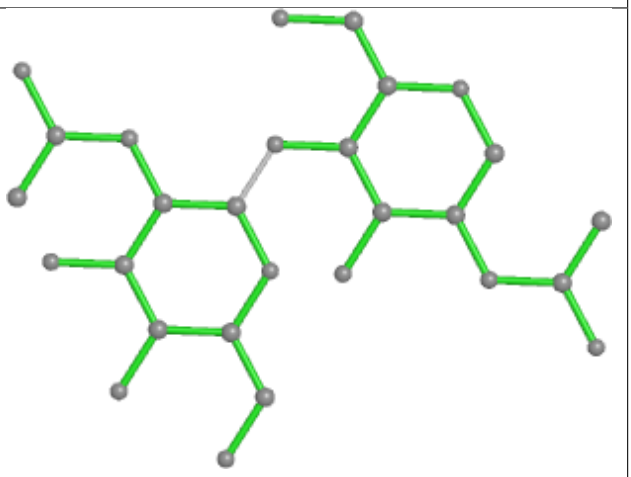


Rings

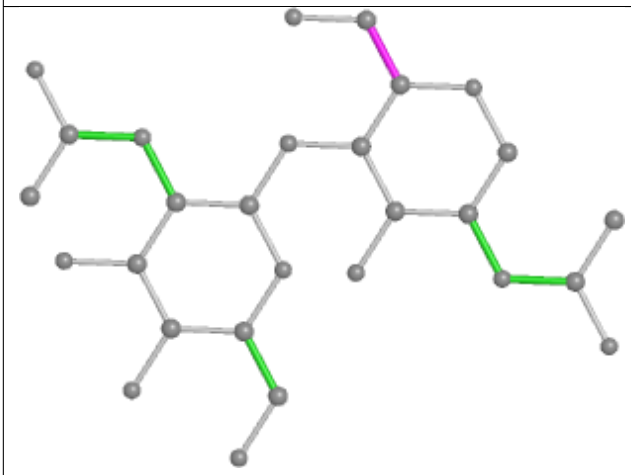
Oligosaccharide Chain I



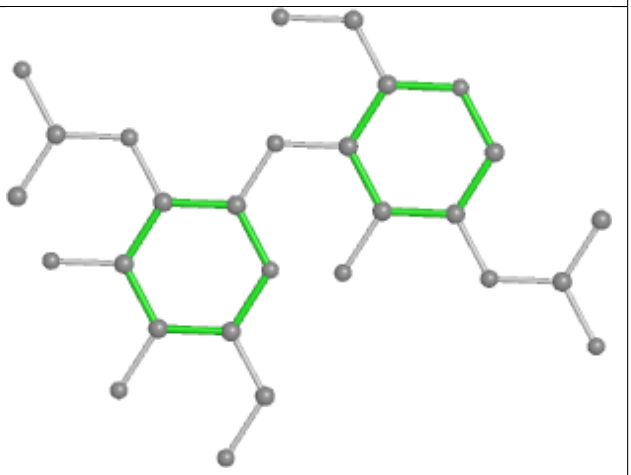
Bond lengths



Bond angles

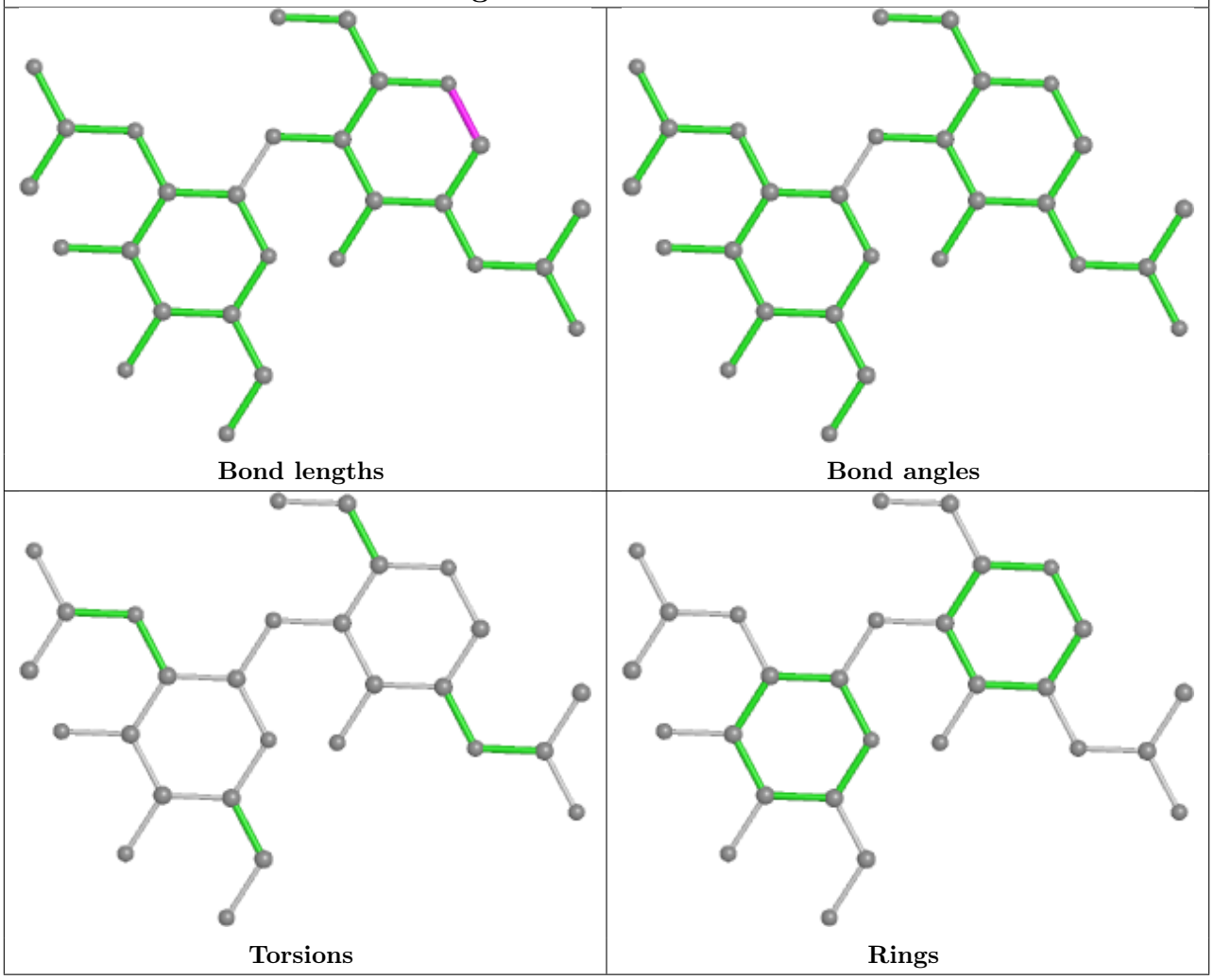


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
8	PCW	A	1106	-	21,21,53	1.76	6 (28%)	27,29,61	1.37	2 (7%)
8	PCW	A	1107	-	21,21,53	1.72	5 (23%)	27,29,61	1.19	1 (3%)
7	CLR	E	101	-	31,31,31	2.84	14 (45%)	48,48,48	2.05	16 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	CLR	D	501	-	31,31,31	2.78	17 (54%)	48,48,48	1.78	9 (18%)
7	CLR	B	501	-	31,31,31	3.21	17 (54%)	48,48,48	1.95	12 (25%)
7	CLR	G	101	-	31,31,31	2.64	11 (35%)	48,48,48	2.00	15 (31%)
8	PCW	C	1106	-	21,21,53	1.74	5 (23%)	27,29,61	1.21	2 (7%)
9	NAG	D	401	2	14,14,15	0.32	0	17,19,21	0.56	0
8	PCW	C	1105	-	21,21,53	1.78	6 (28%)	27,29,61	1.39	1 (3%)
8	PCW	A	1109	-	21,21,53	1.67	5 (23%)	27,29,61	1.36	2 (7%)
8	PCW	A	1105	-	21,21,53	1.78	5 (23%)	27,29,61	1.34	1 (3%)
7	CLR	A	1104	-	31,31,31	2.78	12 (38%)	48,48,48	1.87	13 (27%)
8	PCW	A	1108	-	21,21,53	1.74	5 (23%)	27,29,61	1.12	1 (3%)
9	NAG	B	401	2	14,14,15	0.21	0	17,19,21	0.47	0
7	CLR	C	1104	-	31,31,31	2.73	12 (38%)	48,48,48	1.90	15 (31%)
8	PCW	C	1107	-	21,21,53	1.69	4 (19%)	27,29,61	1.31	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PCW	A	1106	-	-	15/23/23/57	-
8	PCW	A	1107	-	-	9/23/23/57	-
7	CLR	E	101	-	-	4/10/68/68	0/4/4/4
7	CLR	D	501	-	-	2/10/68/68	0/4/4/4
7	CLR	B	501	-	-	1/10/68/68	0/4/4/4
7	CLR	G	101	-	-	3/10/68/68	0/4/4/4
8	PCW	C	1106	-	-	12/23/23/57	-
9	NAG	D	401	2	-	4/6/23/26	0/1/1/1
8	PCW	C	1105	-	-	8/23/23/57	-
8	PCW	A	1109	-	-	13/23/23/57	-
8	PCW	A	1105	-	-	9/23/23/57	-
7	CLR	A	1104	-	-	5/10/68/68	0/4/4/4
8	PCW	A	1108	-	-	11/23/23/57	-
9	NAG	B	401	2	-	1/6/23/26	0/1/1/1
7	CLR	C	1104	-	-	5/10/68/68	0/4/4/4
8	PCW	C	1107	-	-	9/23/23/57	-

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	101	CLR	C10-C5	8.24	1.69	1.52
7	G	101	CLR	C10-C5	7.99	1.68	1.52
7	B	501	CLR	C10-C9	7.50	1.68	1.56
7	B	501	CLR	C10-C5	7.47	1.67	1.52
7	A	1104	CLR	C10-C5	7.46	1.67	1.52

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	101	CLR	C7-C6-C5	-5.70	114.54	125.06
8	C	1105	PCW	O2-C31-C32	5.63	121.44	111.09
8	A	1105	PCW	O2-C31-C32	5.56	121.32	111.09
7	B	501	CLR	C7-C6-C5	-5.52	114.88	125.06
8	A	1106	PCW	O2-C31-C32	5.51	121.23	111.09

There are no chirality outliers.

5 of 111 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1106	PCW	O4P-C4-C5-N
8	A	1108	PCW	C1-O3P-P-O1P
8	A	1108	PCW	C4-O4P-P-O1P
8	A	1108	PCW	C4-O4P-P-O3P
8	A	1109	PCW	C4-O4P-P-O1P

There are no ring outliers.

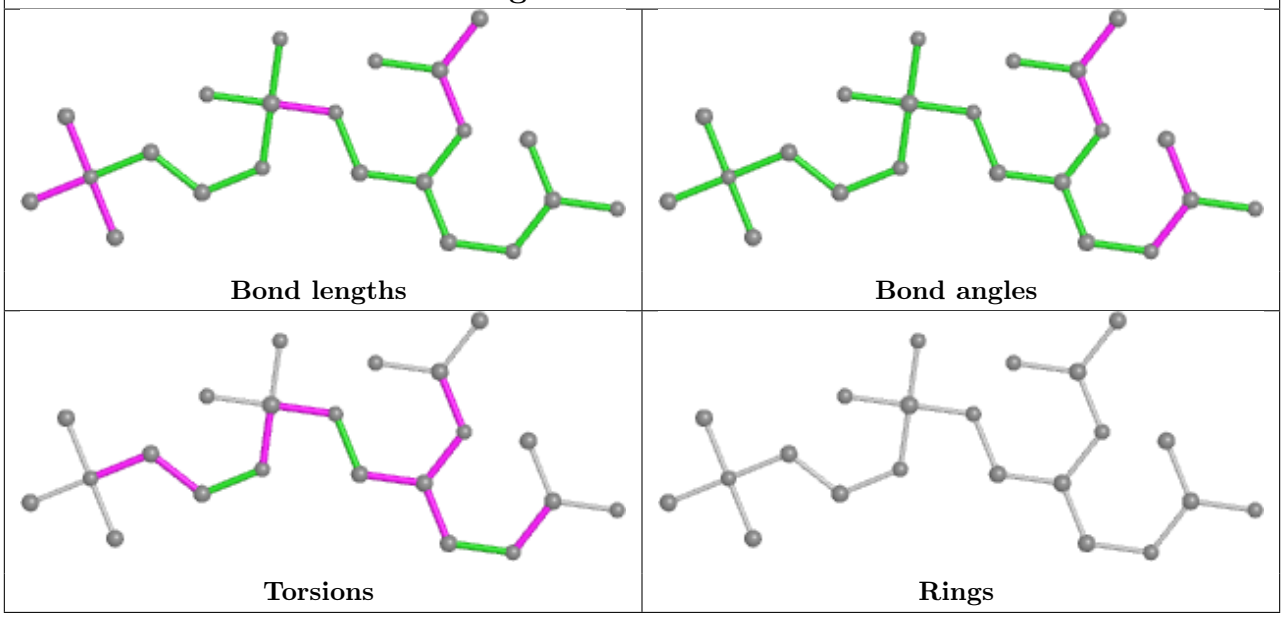
8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1106	PCW	4	0
7	E	101	CLR	4	0
7	G	101	CLR	2	0
8	C	1105	PCW	1	0
8	A	1109	PCW	2	0
7	A	1104	CLR	2	0
8	A	1108	PCW	1	0
7	C	1104	CLR	2	0

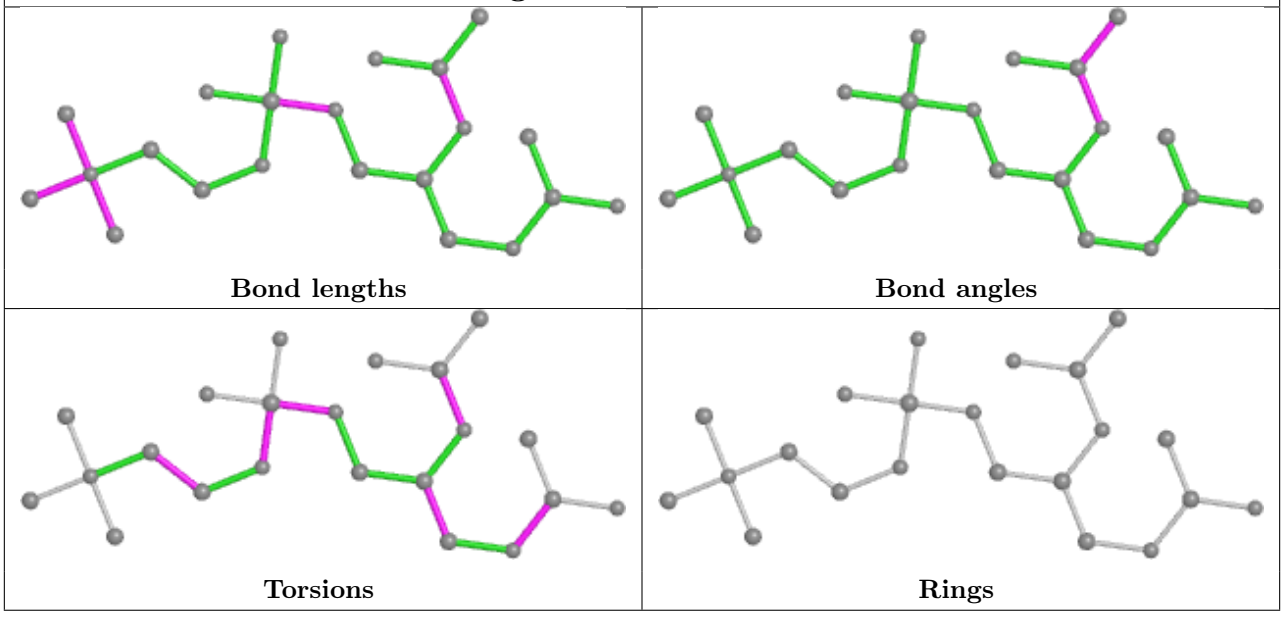
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

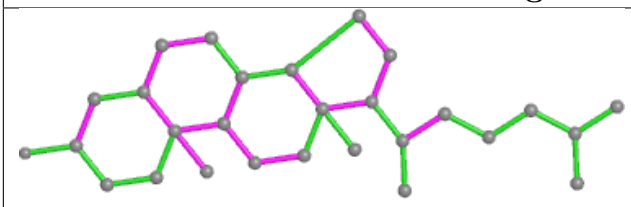
Ligand PCW A 1106



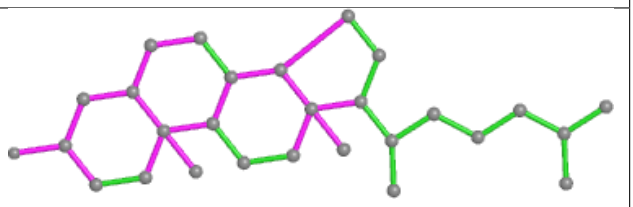
Ligand PCW A 1107



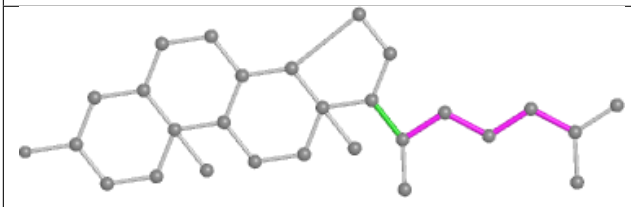
Ligand CLR E 101



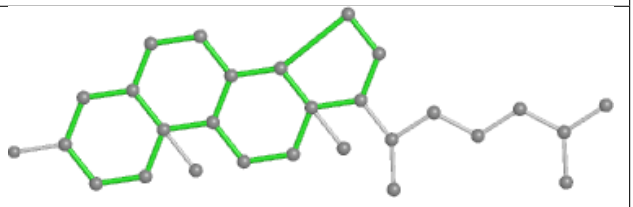
Bond lengths



Bond angles

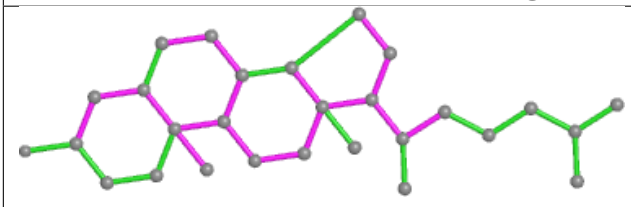


Torsions

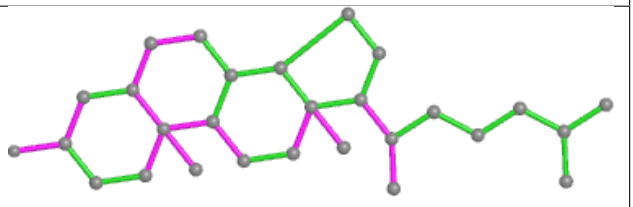


Rings

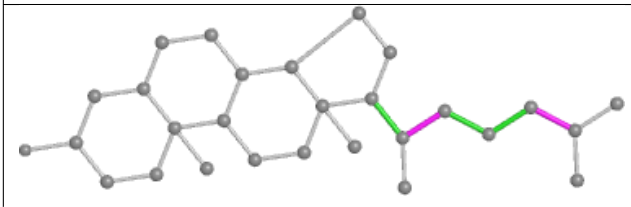
Ligand CLR D 501



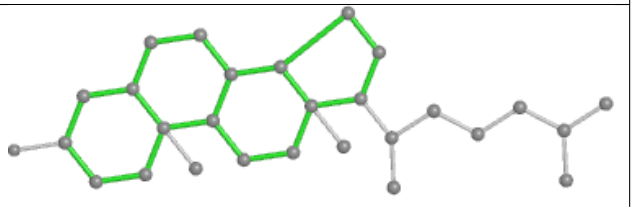
Bond lengths



Bond angles

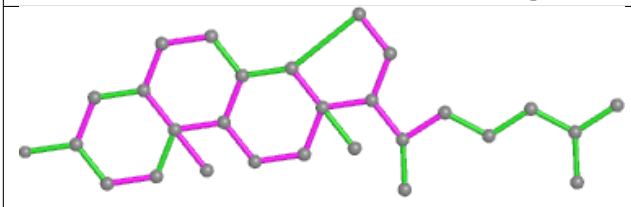


Torsions

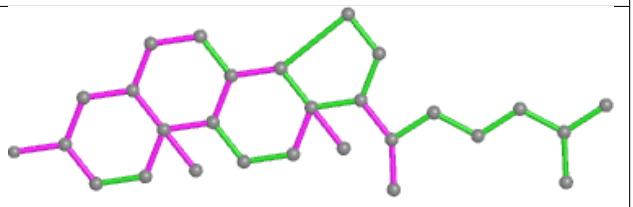


Rings

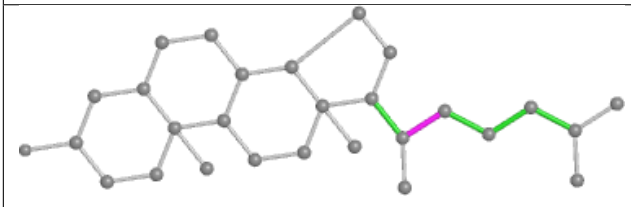
Ligand CLR B 501



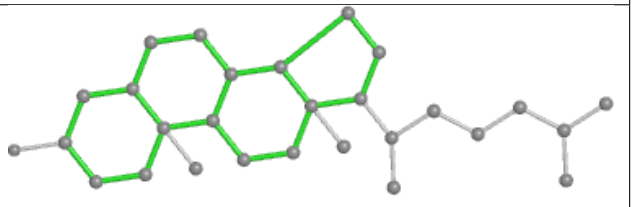
Bond lengths



Bond angles

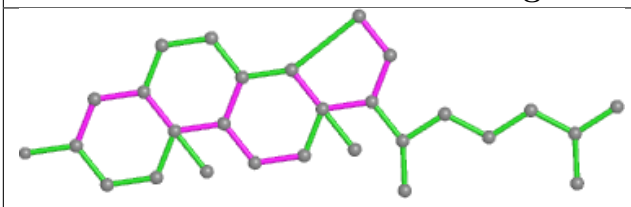


Torsions

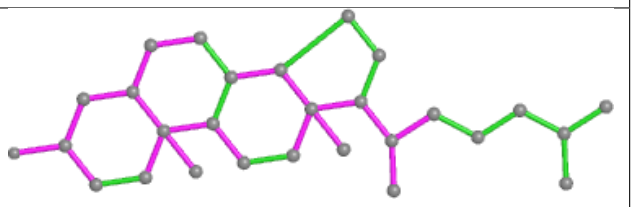


Rings

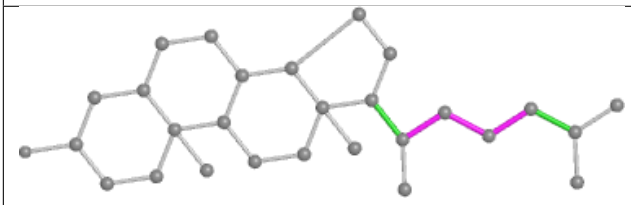
Ligand CLR G 101



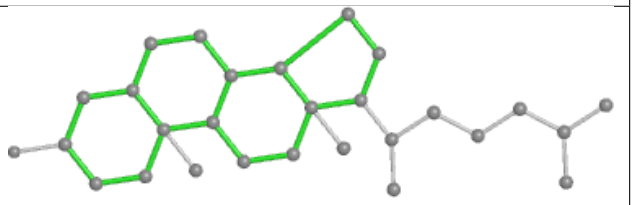
Bond lengths



Bond angles

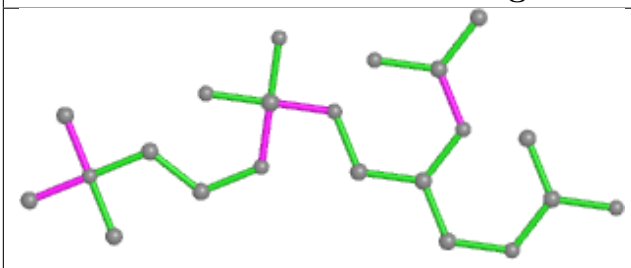


Torsions

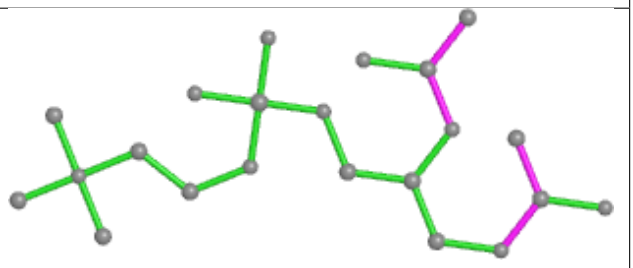


Rings

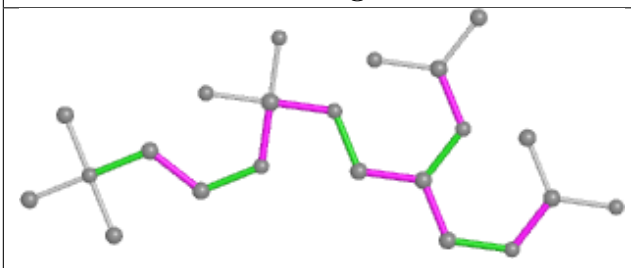
Ligand PCW C 1106



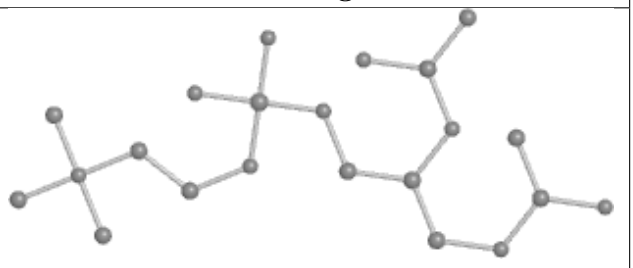
Bond lengths



Bond angles

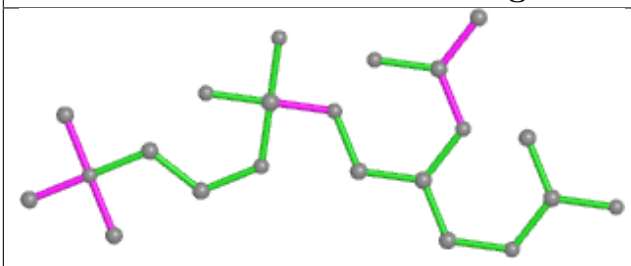


Torsions

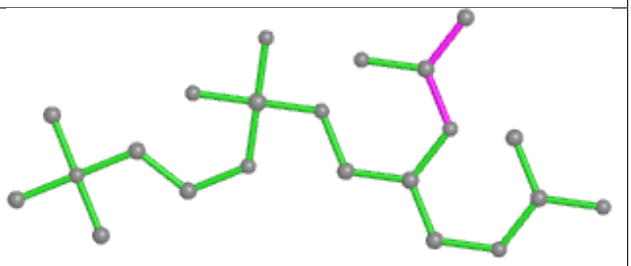


Rings

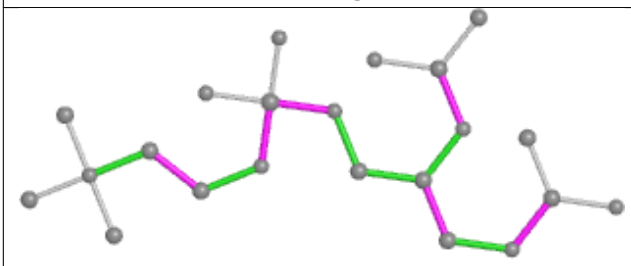
Ligand PCW C 1105



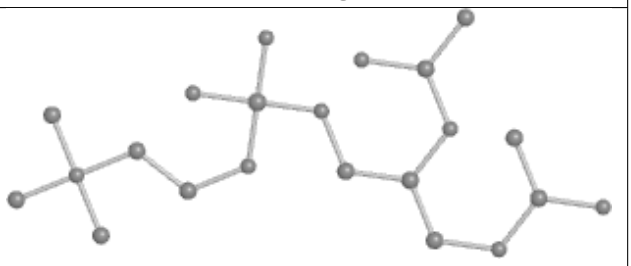
Bond lengths



Bond angles

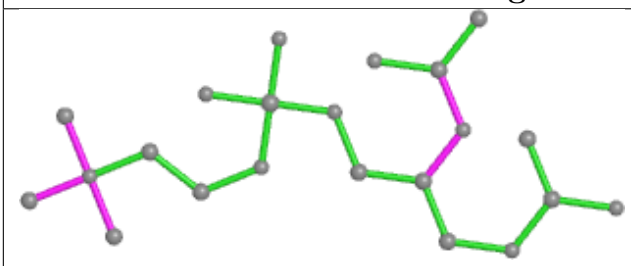


Torsions

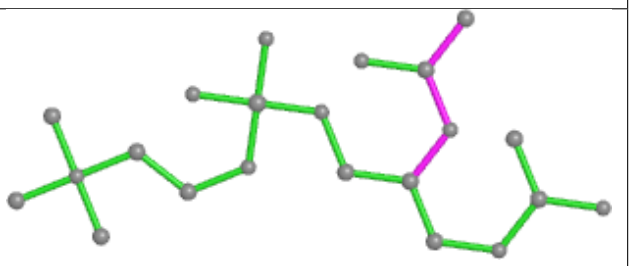


Rings

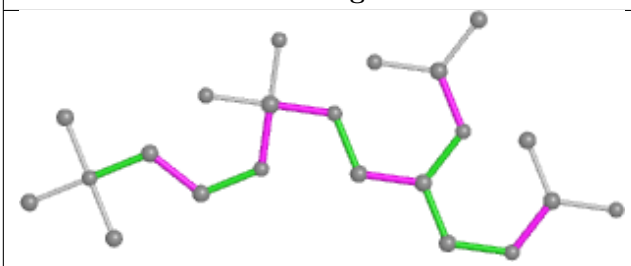
Ligand PCW A 1109



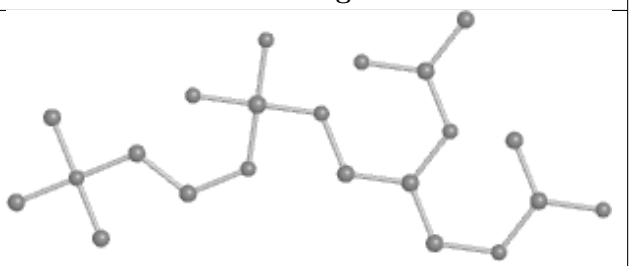
Bond lengths



Bond angles

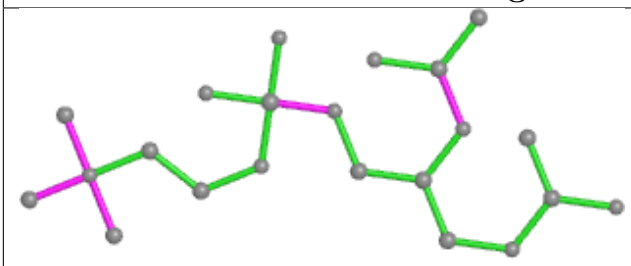


Torsions

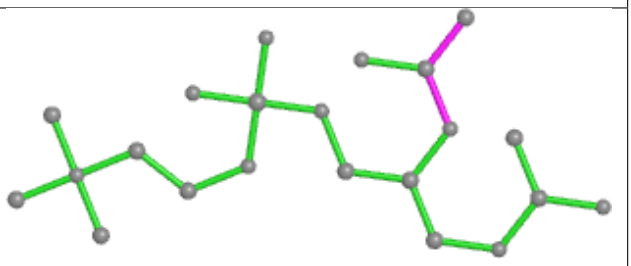


Rings

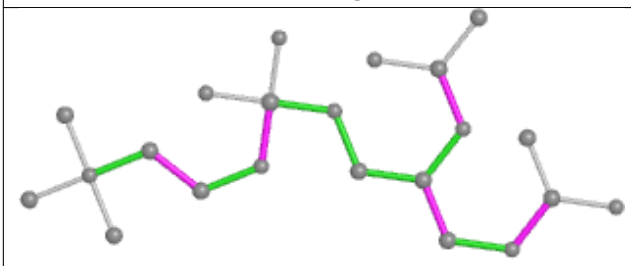
Ligand PCW A 1105



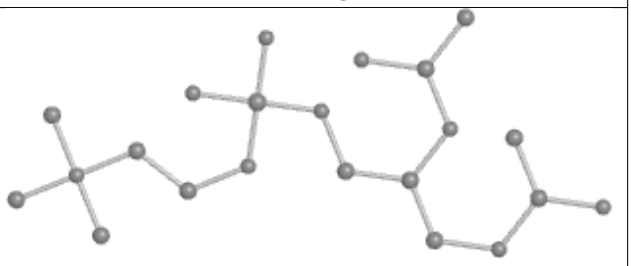
Bond lengths



Bond angles

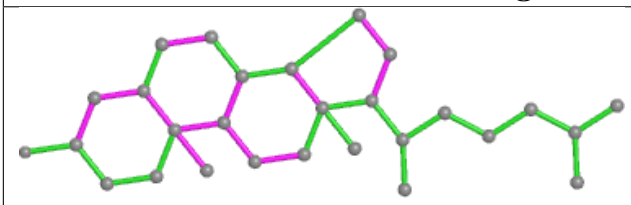


Torsions

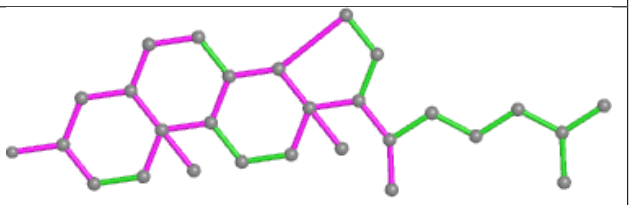


Rings

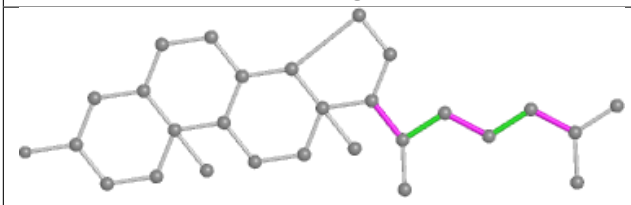
Ligand CLR A 1104



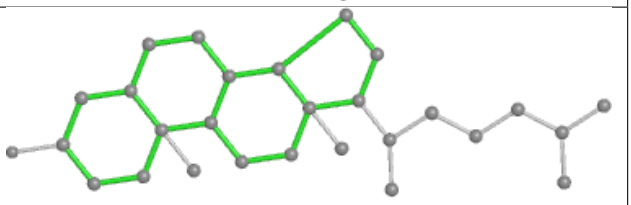
Bond lengths



Bond angles

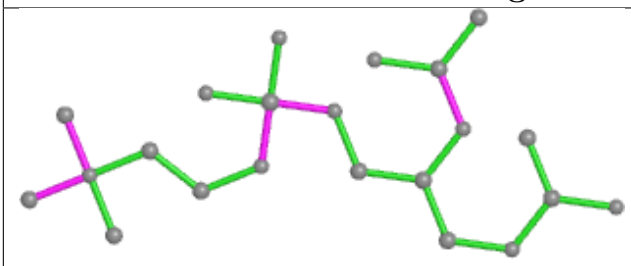


Torsions

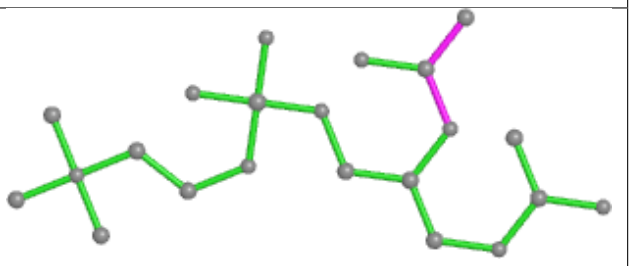


Rings

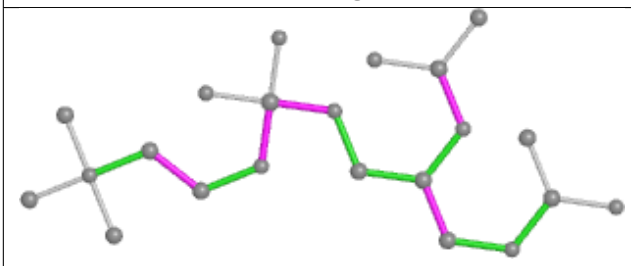
Ligand PCW A 1108



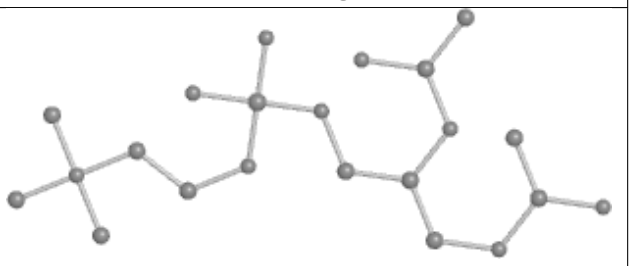
Bond lengths



Bond angles

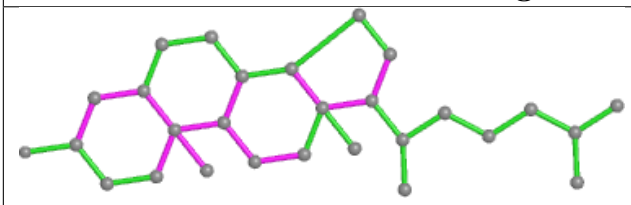


Torsions

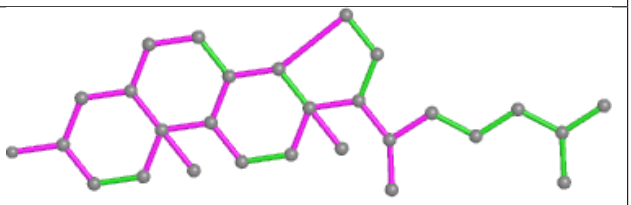


Rings

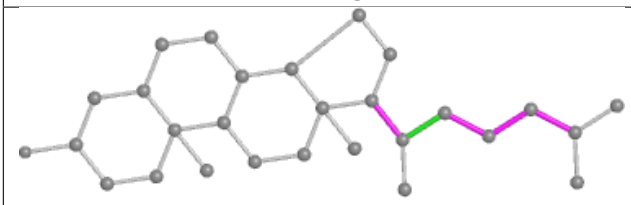
Ligand CLR C 1104



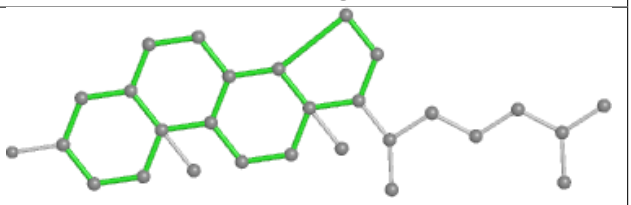
Bond lengths



Bond angles

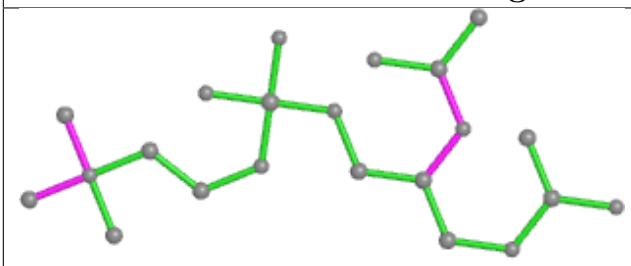


Torsions

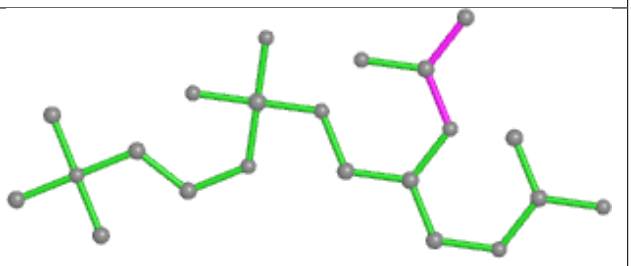


Rings

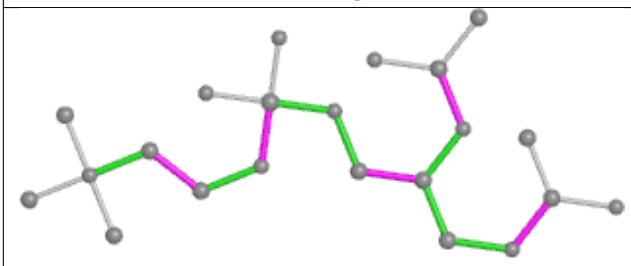
Ligand PCW C 1107



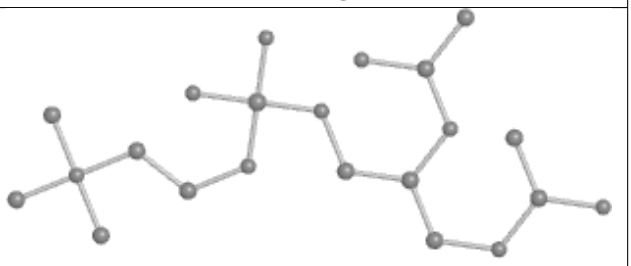
Bond lengths



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

Unable to reproduce the depositors R factor - this section is therefore empty.

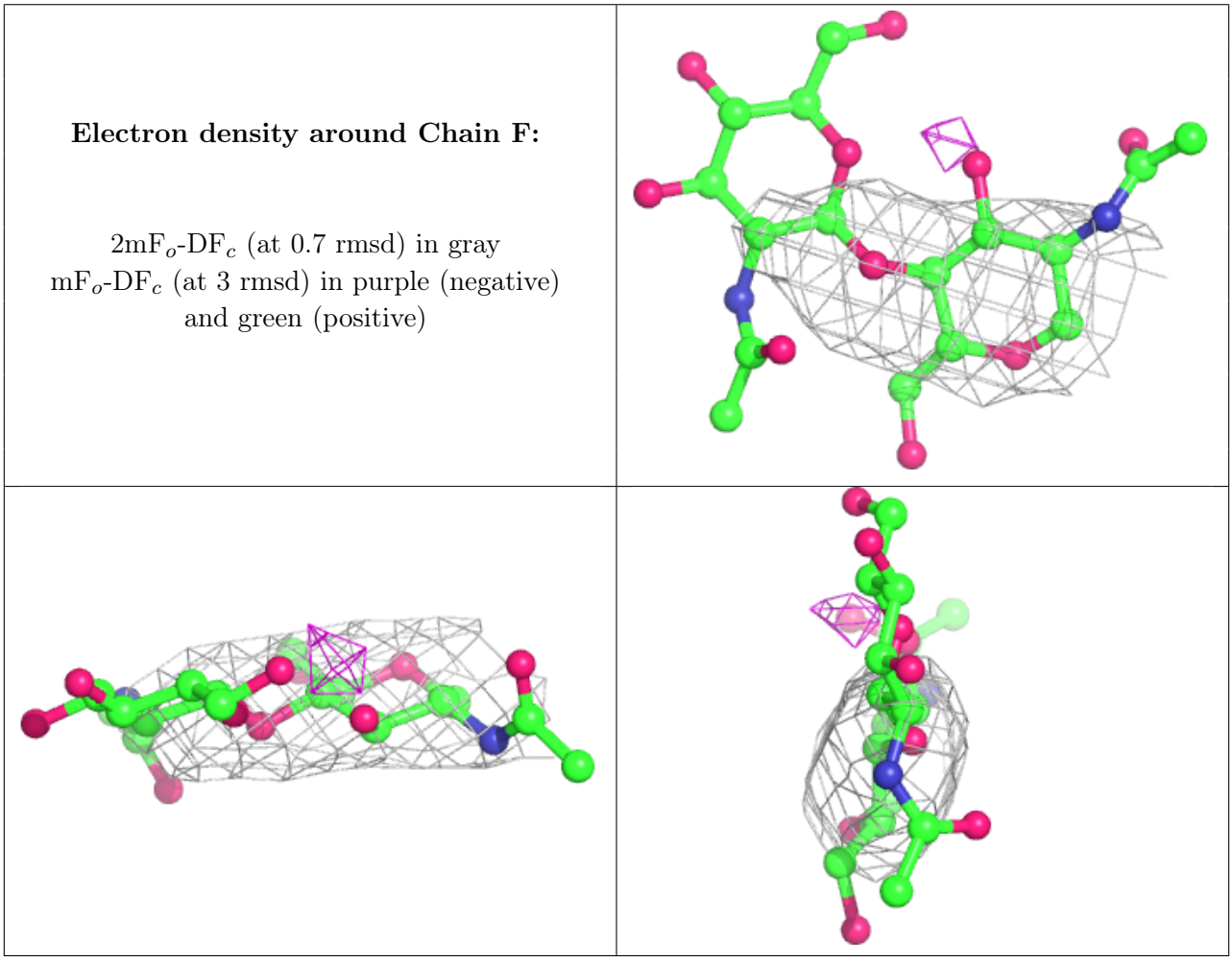
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

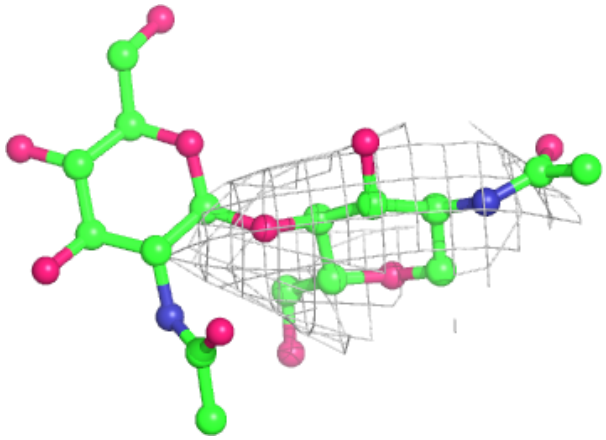
Unable to reproduce the depositors R factor - this section is therefore empty.

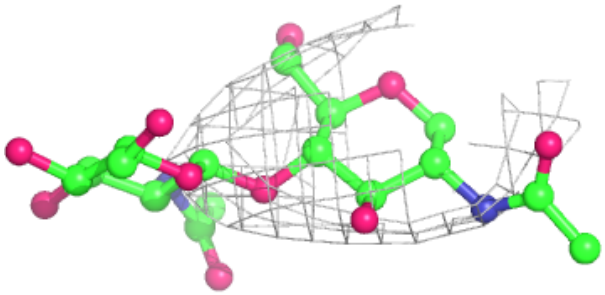
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

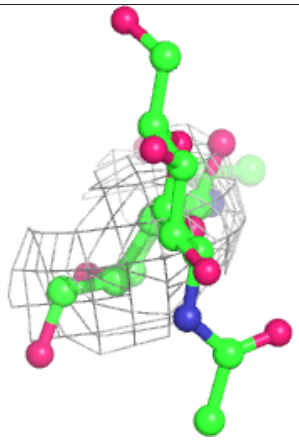


Electron density around Chain H:

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

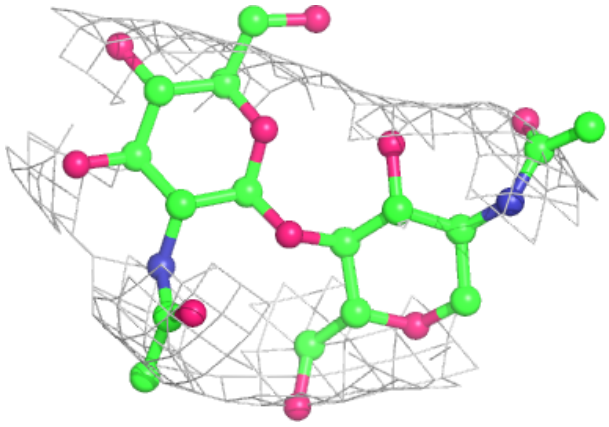


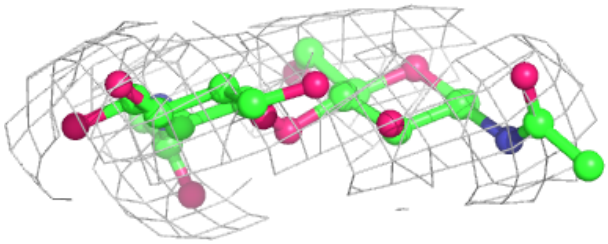


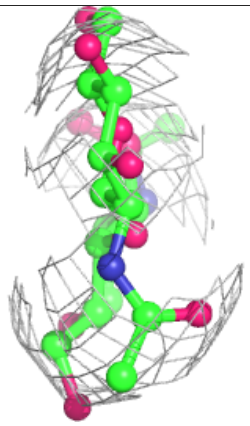


Electron density around Chain I:

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

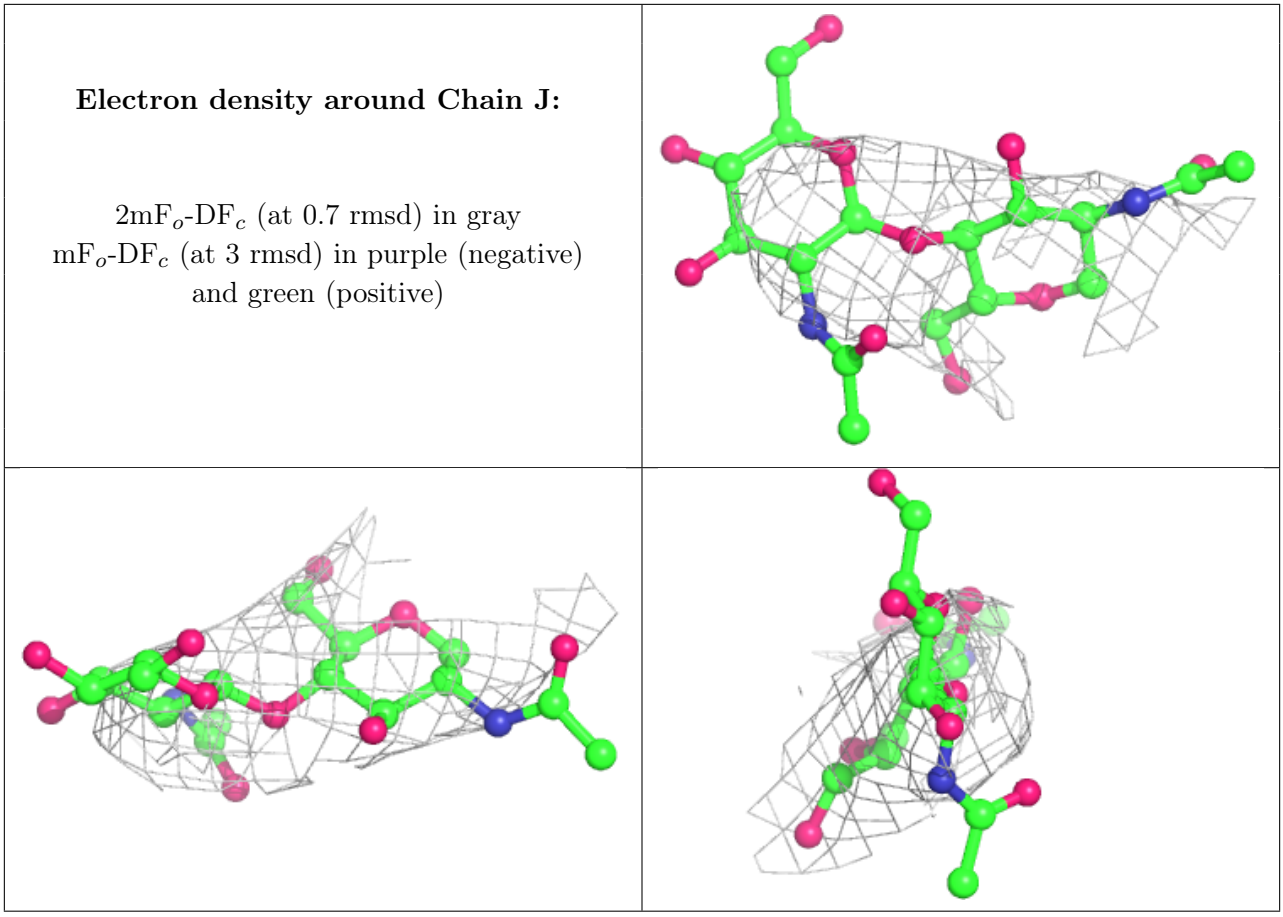






Electron density around Chain J:

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



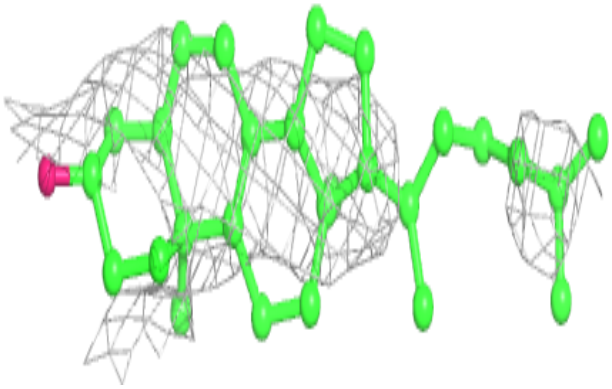
6.4 Ligands

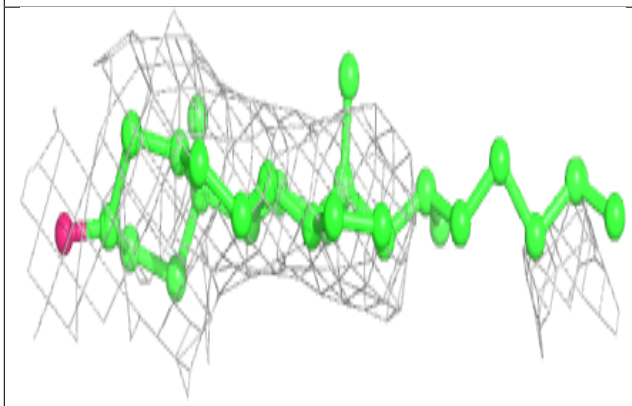
Unable to reproduce the depositors R factor - this section is therefore empty.

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 CLR A 1104:

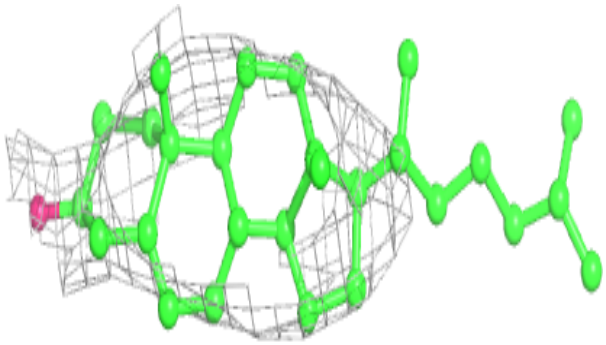
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

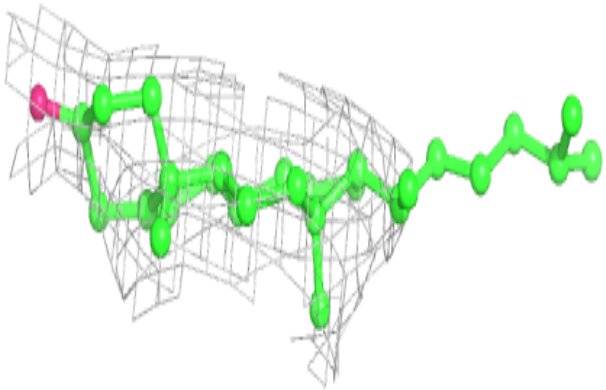


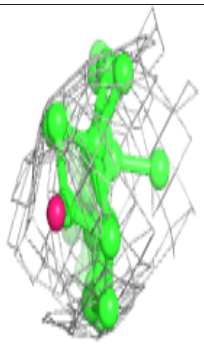


Electron density around CLR B 501:

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

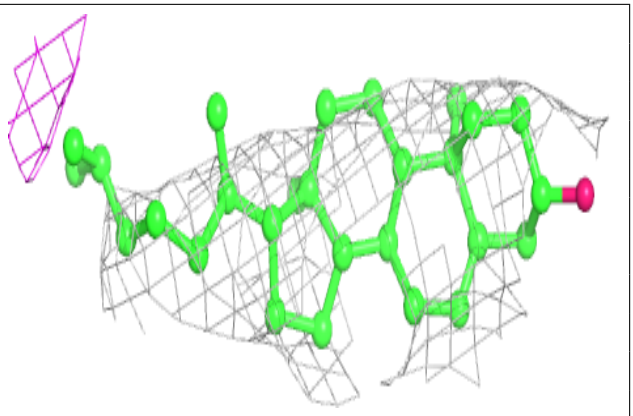


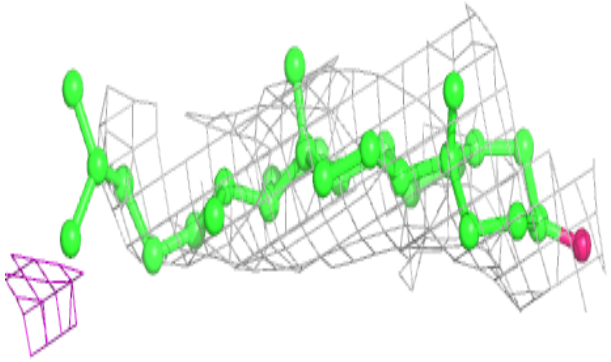


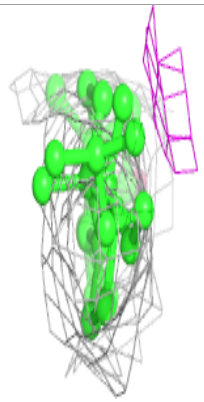


Electron density around CLR G 101:

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

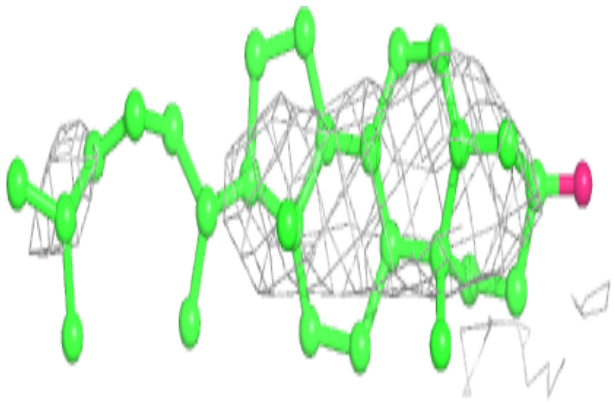


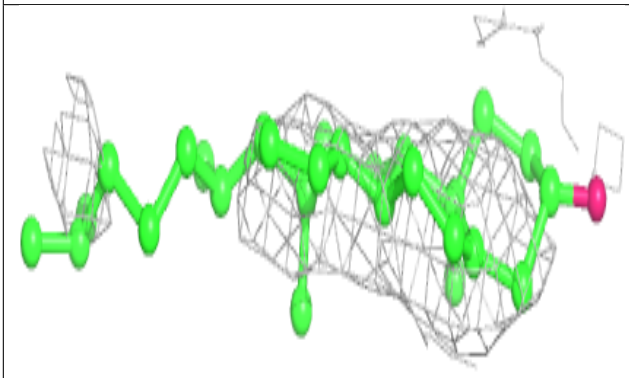


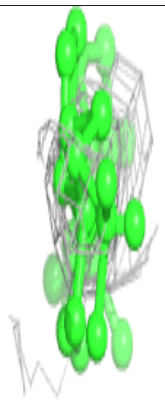


Electron density around CLR C 1104:

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

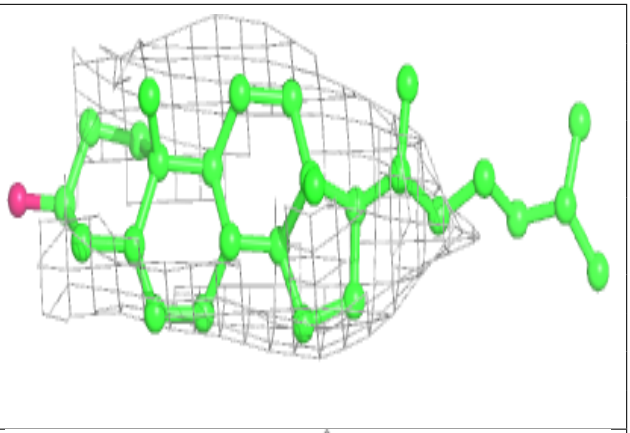


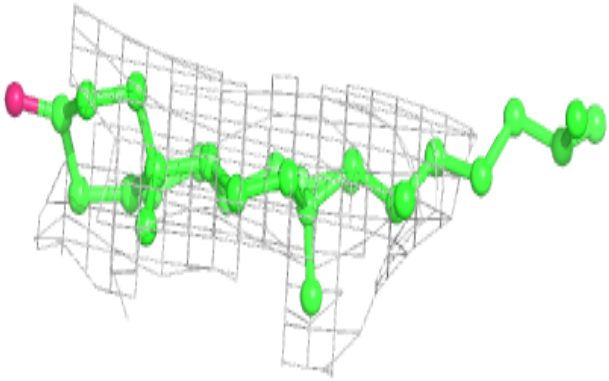


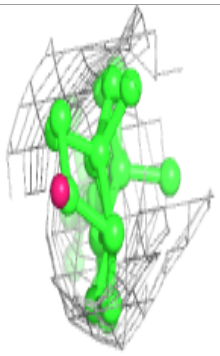


Electron density around CLR D 501:

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

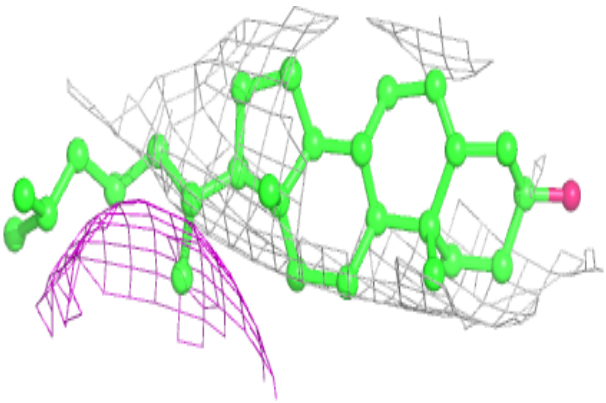


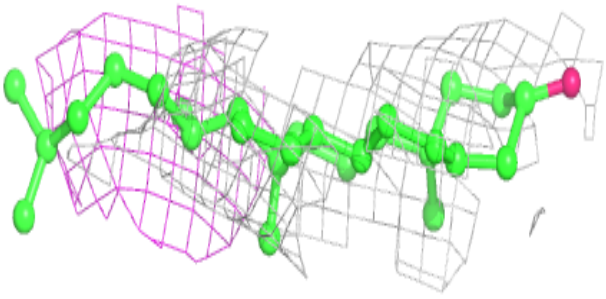


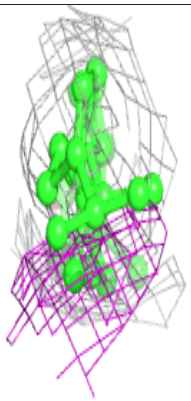


Electron density around CLR E 101:

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

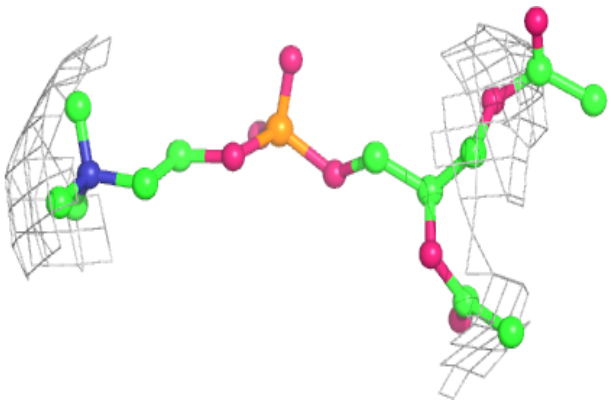


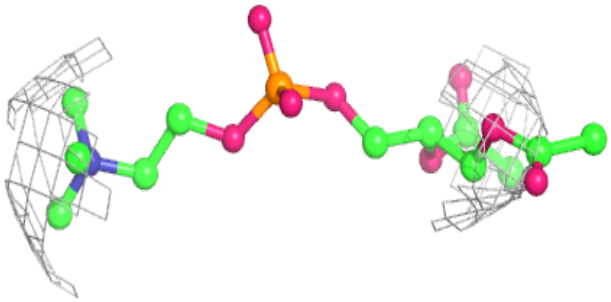


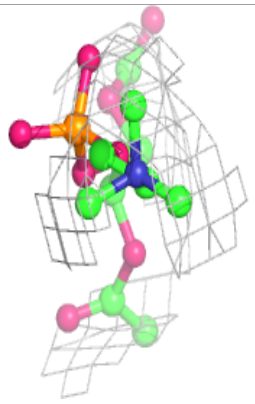


Electron density around PCW A 1105:

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

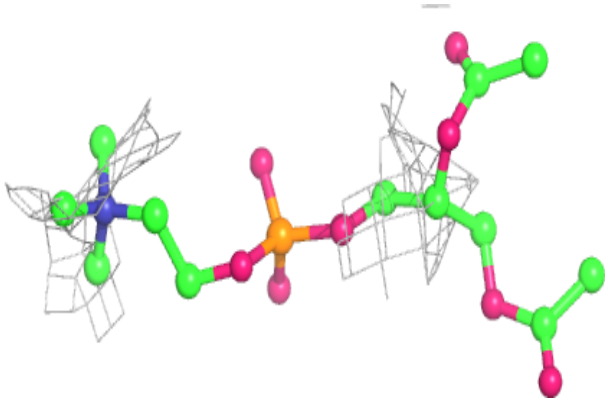


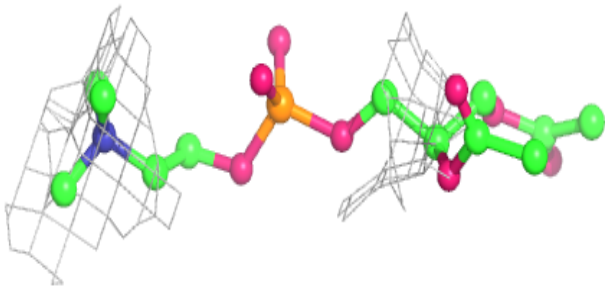


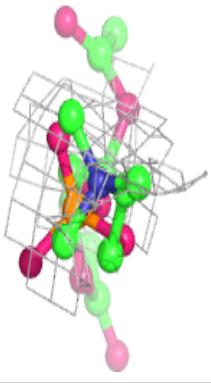


Electron density around PCW A 1106:

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

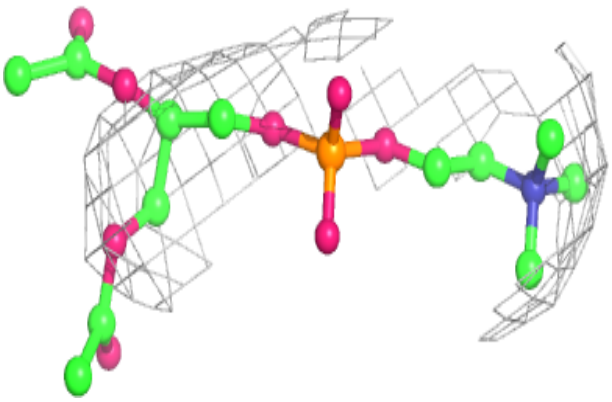


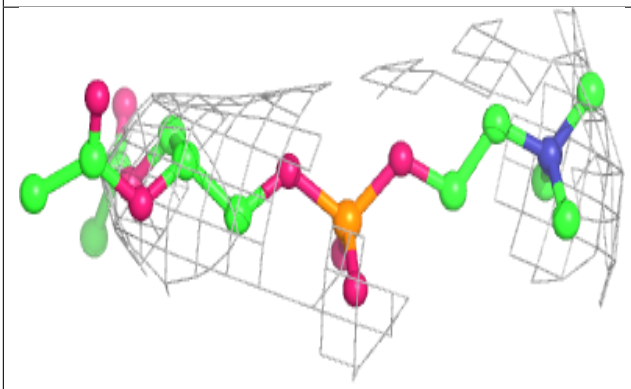


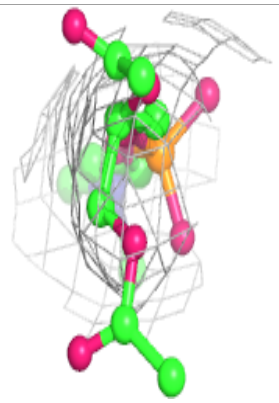


Electron density around PCW A 1107:

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

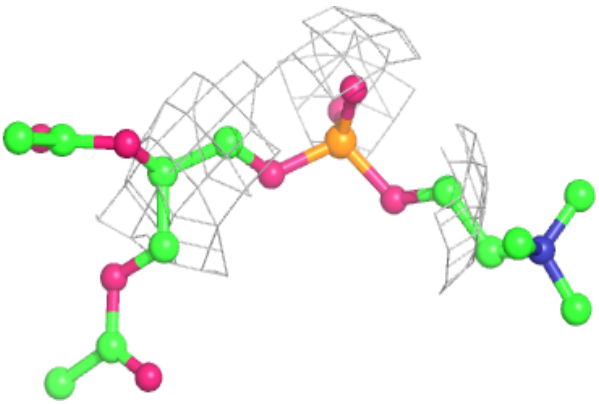


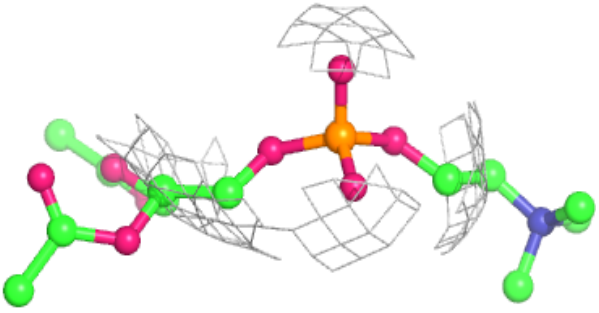




Electron density around PCW A 1108:

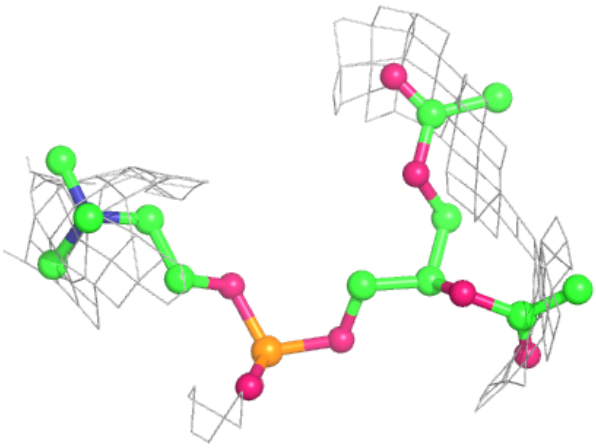
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

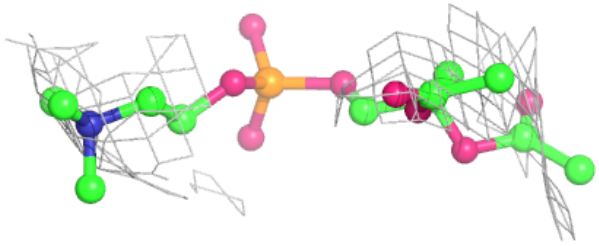


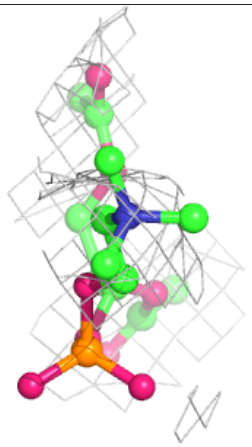


Electron density around PCW A 1109:

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

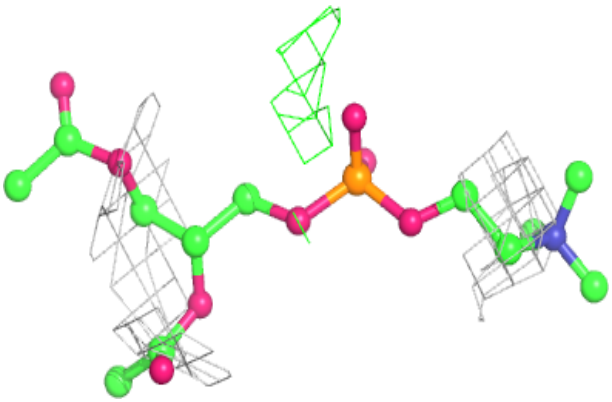


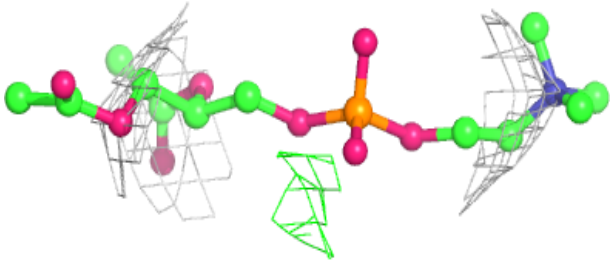


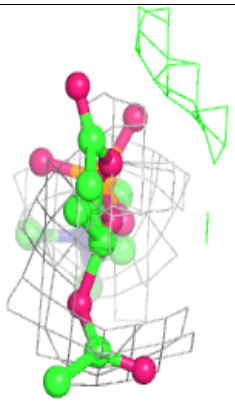


Electron density around PCW C 1105:

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

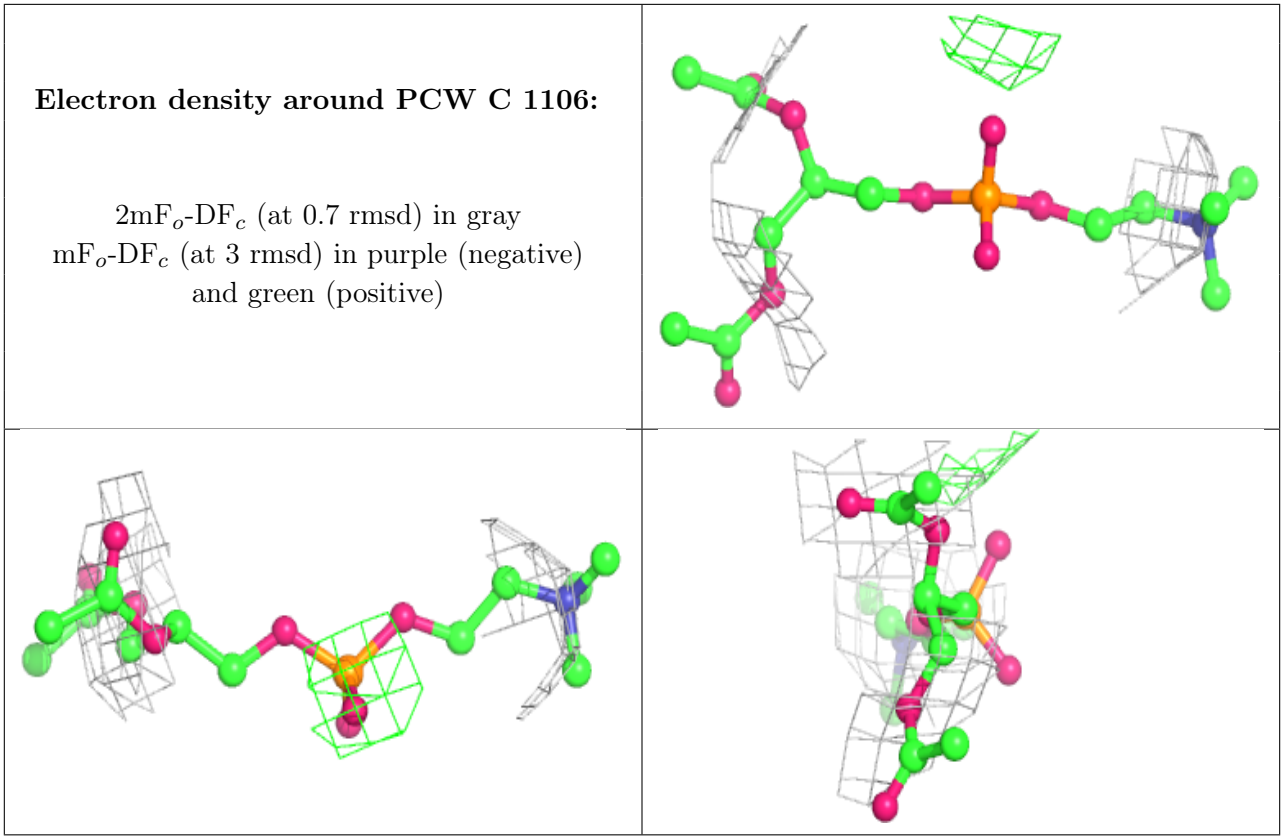






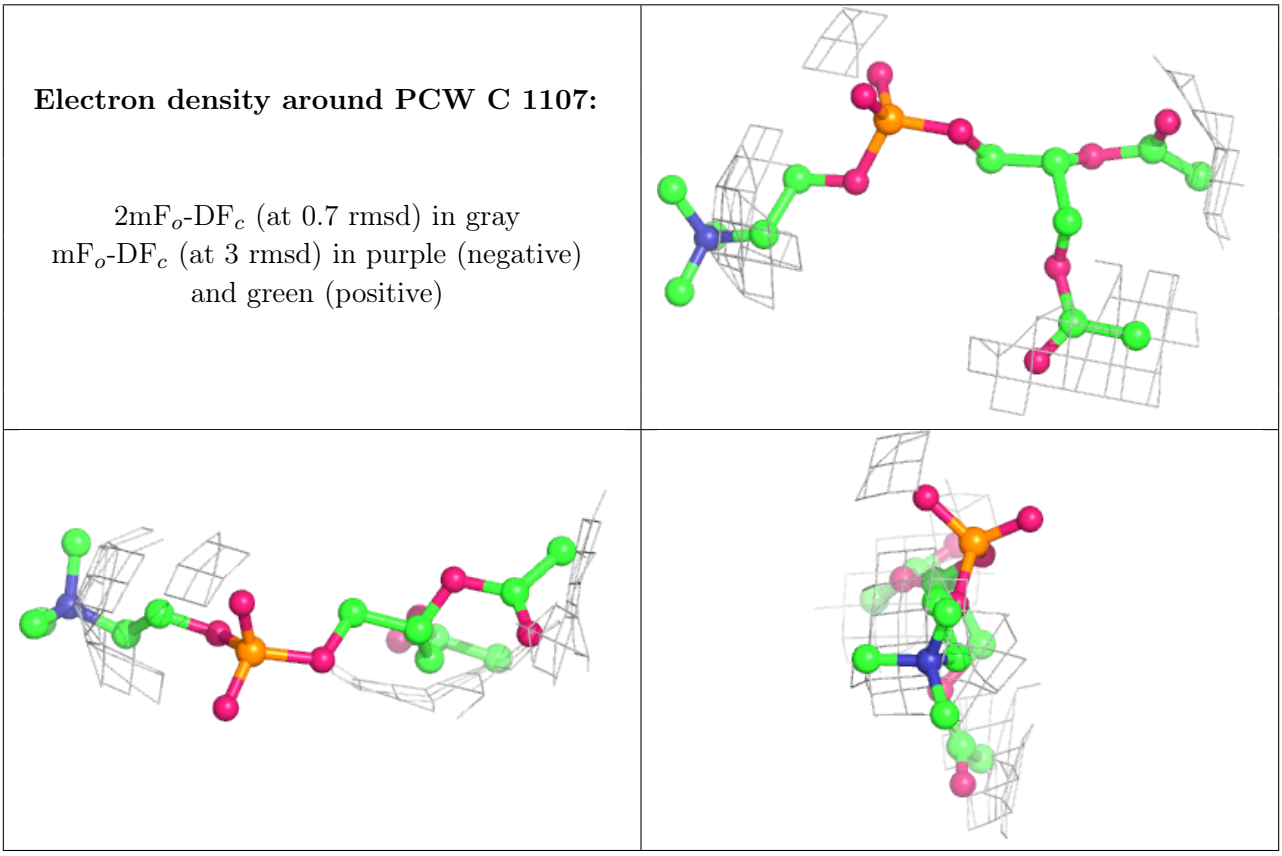
Electron density around PCW C 1106:

$2mF_o$-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 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)



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.