wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2022 – 03:20 pm GMT

PDB ID	:	7QTV
Title	:	Beryllium fluoride form of the Na+,K+-ATPase (E2-BeFx)
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Deposited on	:	2022-01-16
Resolution	:	4.05 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:

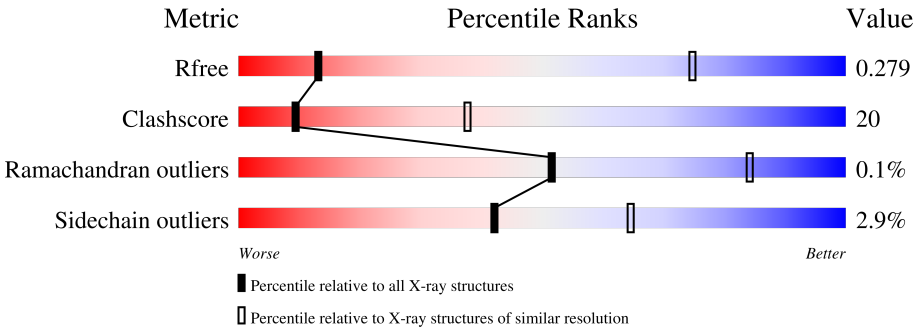
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.05 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	1127 (4.42-3.70)
Clashscore	141614	1033 (4.40-3.72)
Ramachandran outliers	138981	1145 (4.42-3.70)
Sidechain outliers	138945	1133 (4.42-3.70)

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	1021	63% 33%
1	C	1021	61% 36%
2	B	303	50% 44%
2	D	303	59% 36%
3	E	65	37% 11% 51%
3	G	65	37% 12% 51%
4	F	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
5	BEF	C	1101	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 21017 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	S	0	0	0
			7726	4922	1301	1456	47			
1	C	996	Total	C	N	O	S	0	0	0
			7726	4922	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	291	Total	C	N	O	S	0	0	0
			2386	1546	390	437	13			

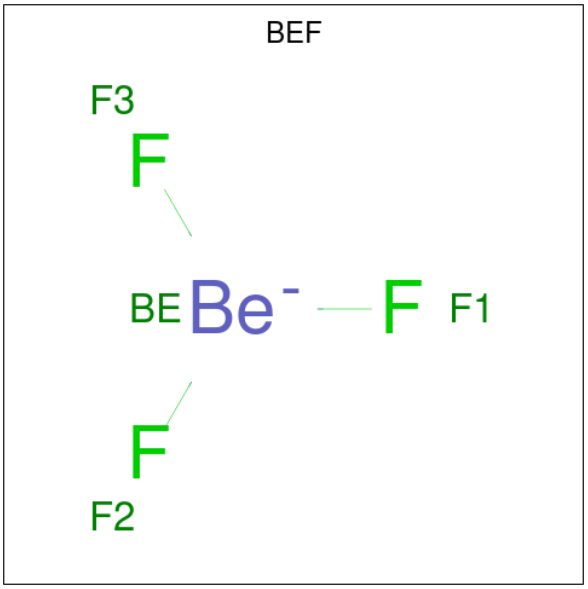
- Molecule 3 is a protein called FXYD domain-containing ion transport regulator.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	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.

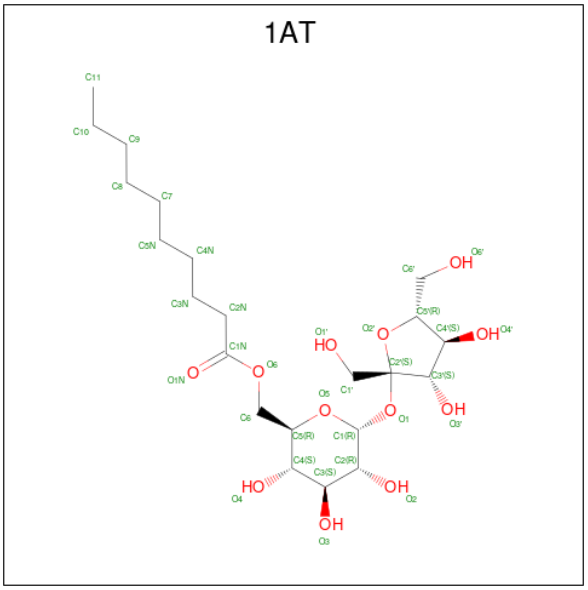
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			30	16	2	12			

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



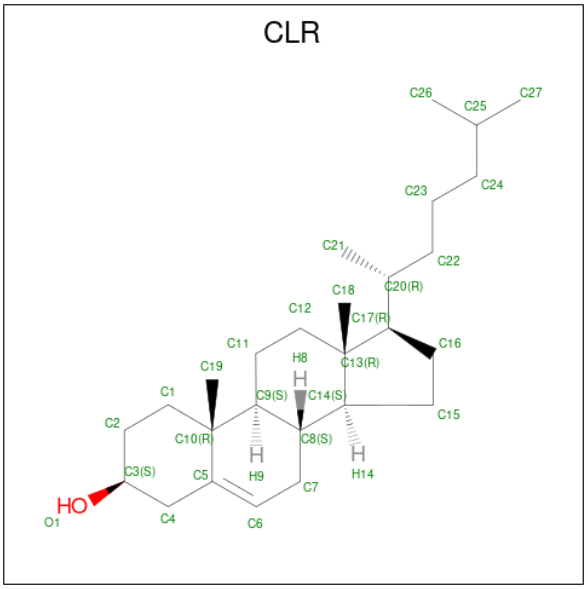
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Be F 4 1 3	0	0
5	C	1	Total Be F 4 1 3	0	0

- Molecule 6 is beta-D-fructofuranosyl 6-O-decanoyl-alpha-D-glucopyranoside (three-letter code: 1AT) (formula: $C_{22}H_{40}O_{12}$).



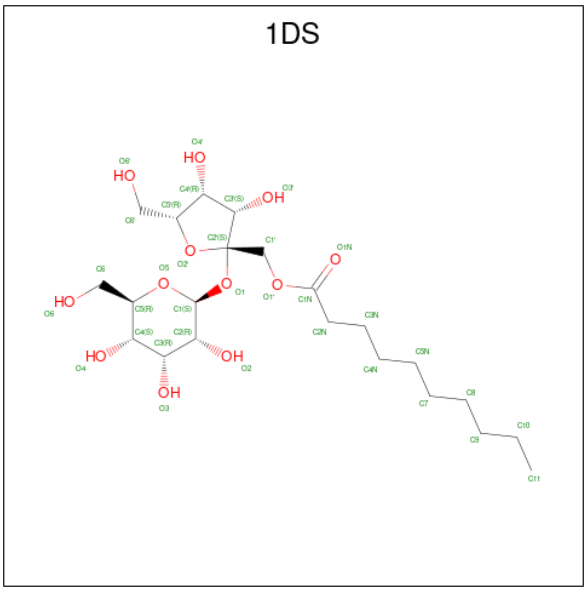
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 29 17 12	0	0

- 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	G	1	Total C O 28 27 1	0	0
7	C	1	Total C O 28 27 1	0	0
7	E	1	Total C O 28 27 1	0	0

- Molecule 8 is 1-O-decanoyl-beta-D-tagatofuranosyl beta-D-allopyranoside (three-letter code: 1DS) (formula: $C_{22}H_{40}O_{12}$).

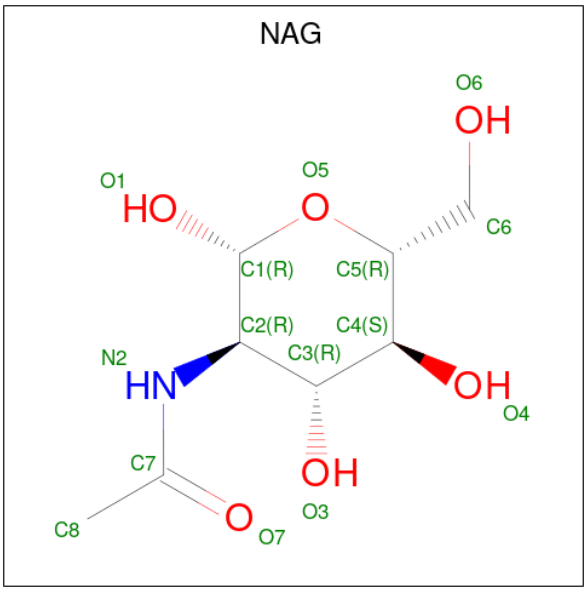


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 29 17 12	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total Mg 3 3	0	0
9	C	3	Total Mg 3 3	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 15 8 1 6	0	0
10	B	1	Total C N O 15 8 1 6	0	0
10	D	1	Total C N O 15 8 1 6	0	0
10	D	1	Total C N O 15 8 1 6	0	0

- Molecule 11 is water.

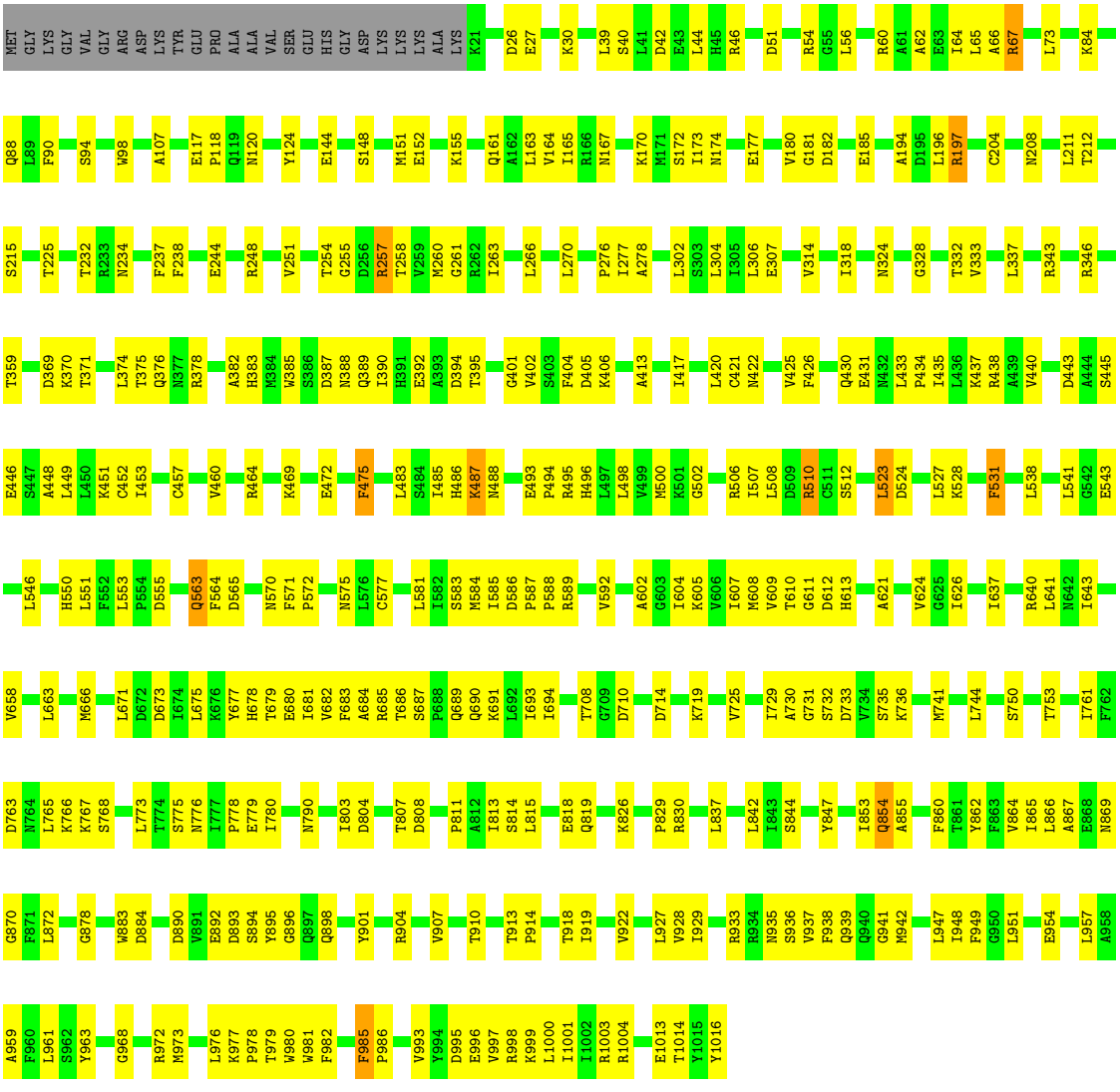
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	5	Total O 5 5	0	0
11	C	4	Total O 4 4	0	0

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.

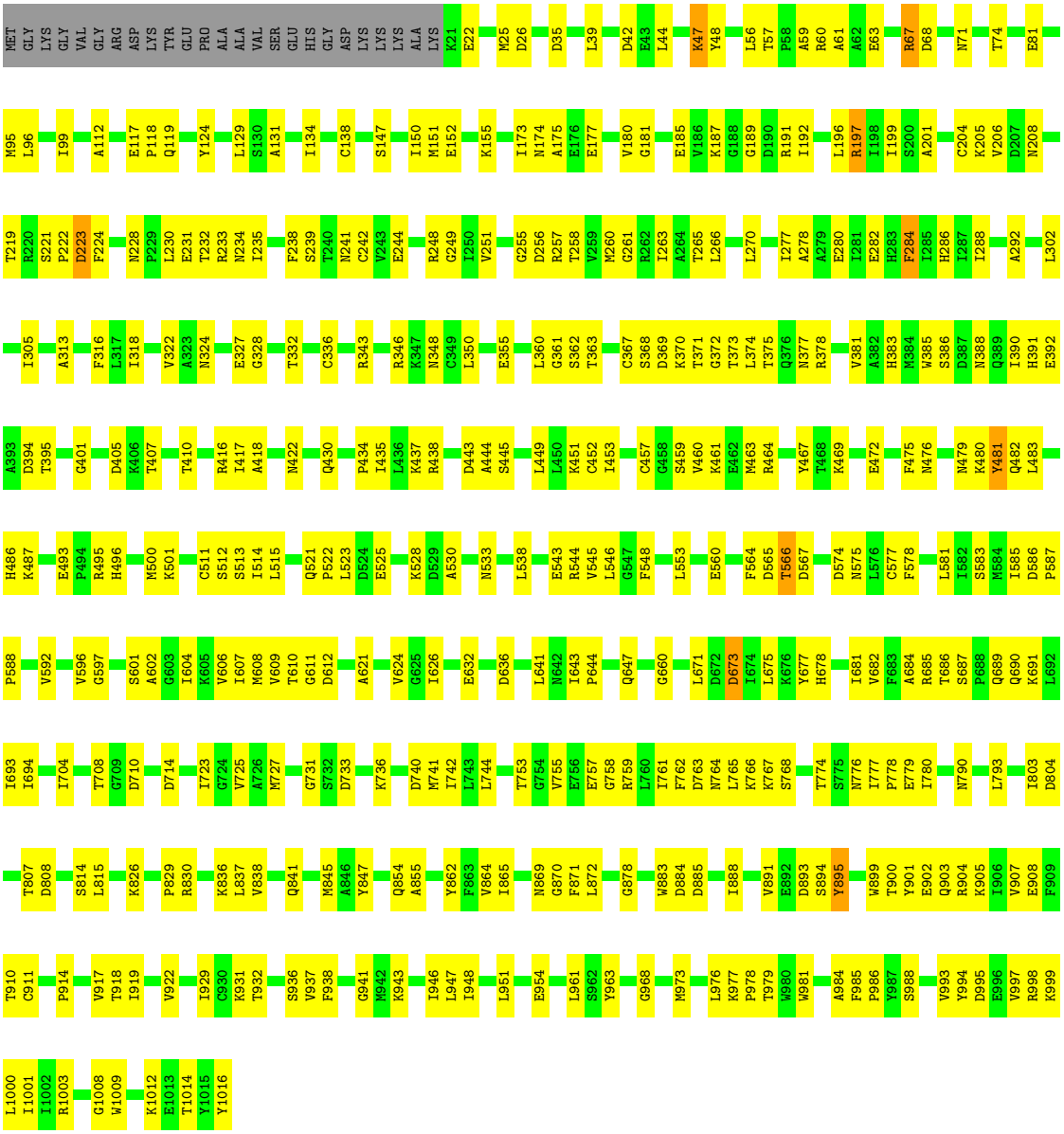
• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain A:



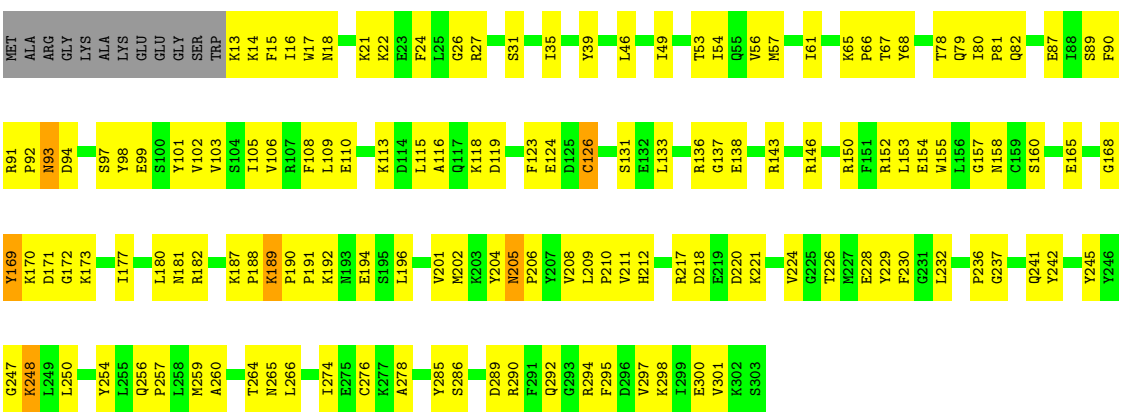
• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain C:



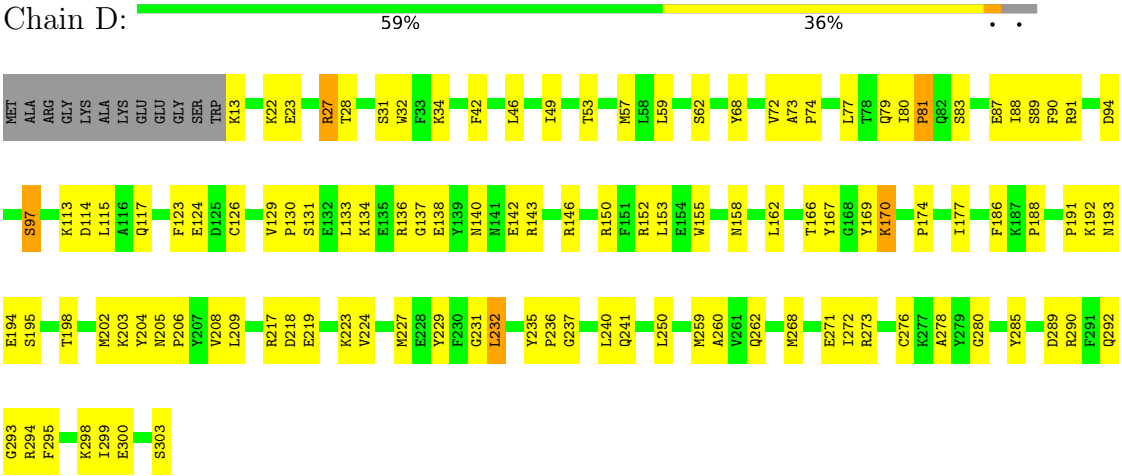
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain B:



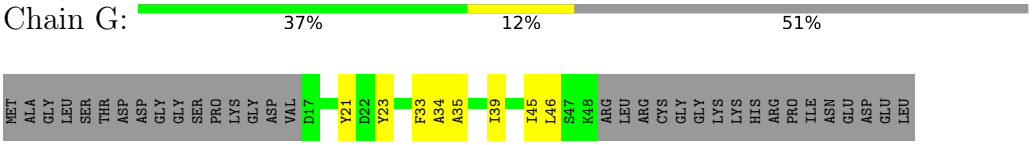
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain D:



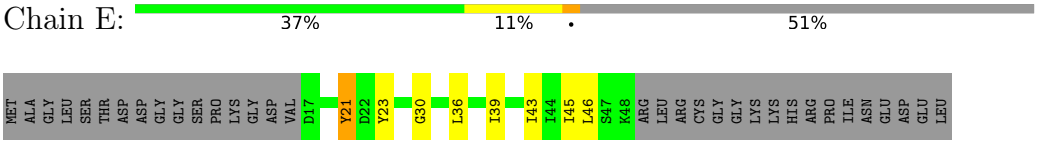
• Molecule 3: FXYD domain-containing ion transport regulator

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:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.47Å 118.08Å 494.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 4.05 29.67 – 4.05	Depositor EDS
% Data completeness (in resolution range)	68.9 (29.67-4.05) 68.9 (29.67-4.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 4.11Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.246 , 0.281 0.247 , 0.279	Depositor DCC
R_{free} test set	1928 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	147.7	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.065 for k,h,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	21017	wwPDB-VP
Average B, all atoms (Å^2)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: NAG, 1DS, MG, 1AT, CLR, BEF

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	0.31	0/7876	0.56	2/10688 (0.0%)
1	C	0.32	1/7876 (0.0%)	0.59	5/10688 (0.0%)
2	B	0.34	0/2449	0.63	0/3301
2	D	0.34	0/2449	0.63	2/3301 (0.1%)
3	E	0.26	0/261	0.48	0/354
3	G	0.32	0/261	0.47	0/354
All	All	0.32	1/21172 (0.0%)	0.59	9/28686 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	564	PHE	CE1-CZ	5.77	1.48	1.37

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	565	ASP	CB-CG-OD1	6.90	124.51	118.30
1	C	566	THR	OG1-CB-CG2	-6.32	95.46	110.00
1	A	487	LYS	CA-CB-CG	5.46	125.42	113.40
1	C	565	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	59	ALA	N-CA-CB	5.39	117.65	110.10

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	7726	0	7776	303	1
1	C	7726	0	7776	285	0
2	B	2386	0	2360	138	0
2	D	2386	0	2363	108	0
3	E	255	0	259	7	0
3	G	255	0	259	8	0
4	F	30	0	29	1	0
5	A	4	0	0	1	0
5	C	4	0	0	4	0
6	A	29	0	25	6	0
7	A	28	0	46	8	0
7	C	28	0	46	4	0
7	E	28	0	46	4	0
7	G	28	0	46	6	0
8	A	29	0	27	9	0
9	A	3	0	0	0	0
9	C	3	0	0	0	0
10	B	30	0	29	3	0
10	D	30	0	28	4	0
11	A	5	0	0	2	0
11	C	4	0	0	3	0
All	All	21017	0	21115	828	1

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 20.

The worst 5 of 828 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:193:ASN:ND2	10:D:401:NAG:O3	1.87	1.08
1:C:845:MET:SD	1:C:998:ARG:NH1	2.31	1.03
1:A:487:LYS:NZ	1:A:494:PRO:O	1.92	1.01
2:B:208:VAL:HG22	2:B:237:GLY:HA3	1.40	0.99
2:B:80:ILE:HG13	2:B:81:PRO:HD3	1.45	0.98

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:SER:OG	1:A:640:ARG:O[4_445]	1.85	0.35

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	994/1021 (97%)	935 (94%)	59 (6%)	0	100 100
1	C	994/1021 (97%)	936 (94%)	58 (6%)	0	100 100
2	B	289/303 (95%)	267 (92%)	20 (7%)	2 (1%)	22 61
2	D	289/303 (95%)	272 (94%)	17 (6%)	0	100 100
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	2626/2778 (94%)	2465 (94%)	159 (6%)	2 (0%)	51 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	169	TYR
2	B	205	ASN

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	847/865 (98%)	825 (97%)	22 (3%)	46 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	847/865 (98%)	824 (97%)	23 (3%)	44 66
2	B	261/269 (97%)	255 (98%)	6 (2%)	50 70
2	D	261/269 (97%)	249 (95%)	12 (5%)	27 54
3	E	26/52 (50%)	24 (92%)	2 (8%)	13 40
3	G	26/52 (50%)	26 (100%)	0	100 100
All	All	2268/2372 (96%)	2203 (97%)	65 (3%)	42 64

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	158	ASN
2	D	186	PHE
2	B	126	CYS
2	B	93	ASN
2	D	218	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	193	ASN
2	D	205	ASN
2	B	79	GLN
2	B	212	HIS
1	C	488	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 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	15,15,15	1.34	2 (13%)	21,21,21	1.58	4 (19%)
4	NAG	F	2	4	15,15,15	1.08	1 (6%)	21,21,21	0.94	3 (14%)

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	-	0/6/26/26	0/1/1/1
4	NAG	F	2	4	-	1/6/26/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	-4.71	1.31	1.42
4	F	2	NAG	C1-C2	-3.57	1.48	1.52
4	F	1	NAG	C1-C2	-2.02	1.50	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1	NAG	O1-C1-O5	-4.57	96.67	110.38
4	F	1	NAG	C4-C3-C2	2.99	114.72	110.34
4	F	1	NAG	O1-C1-C2	-2.63	103.76	109.22
4	F	2	NAG	C1-C2-C3	-2.50	107.14	110.54
4	F	1	NAG	C3-C4-C5	2.45	114.61	110.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

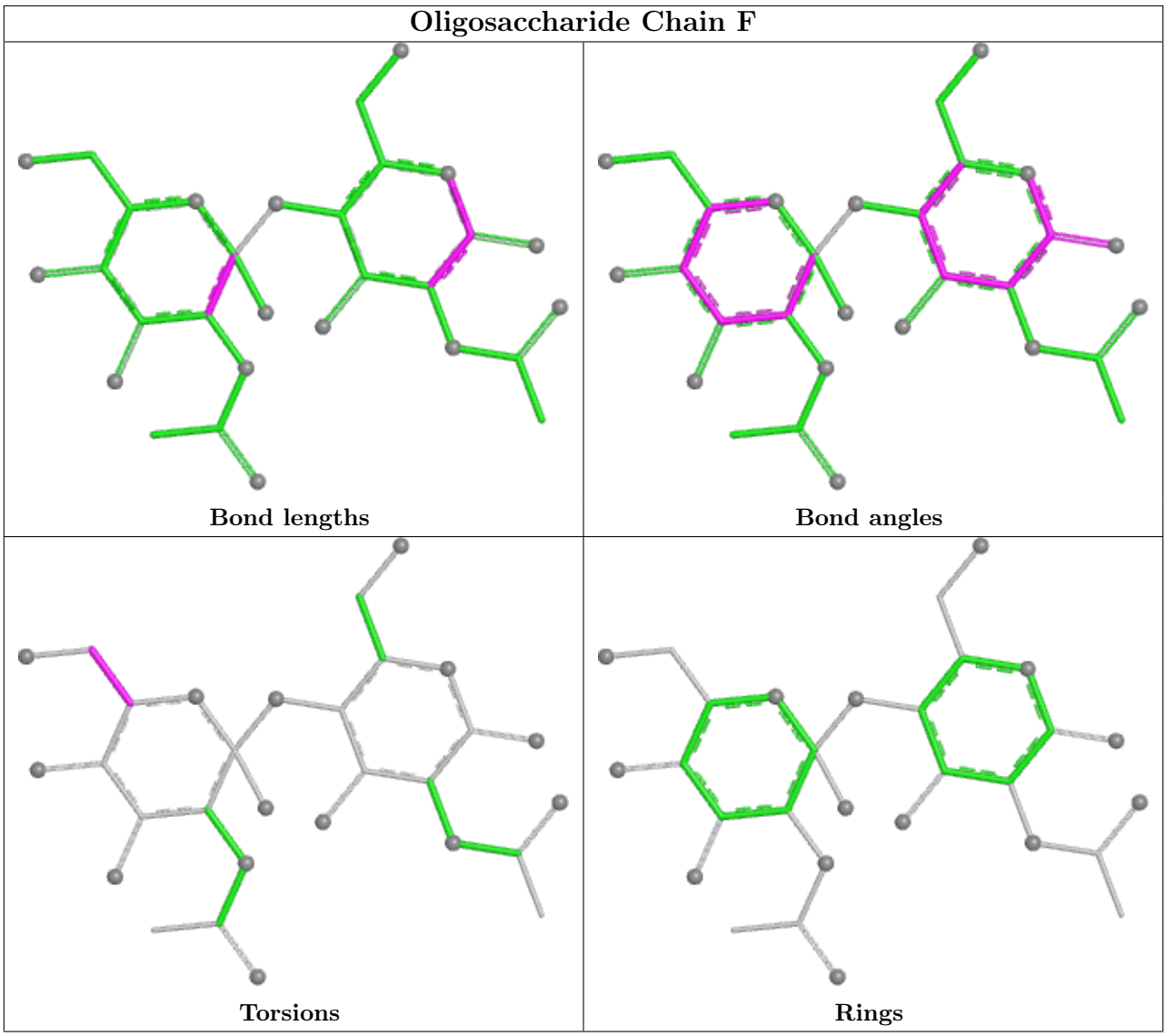
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	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.



5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	NAG	D	401	-	15,15,15	0.24	0	21,21,21	0.49	0
7	CLR	E	101	-	31,31,31	0.74	1 (3%)	48,48,48	1.21	6 (12%)
5	BEF	A	1101	1	0,3,3	-	-	-		
7	CLR	G	101	-	31,31,31	0.70	1 (3%)	48,48,48	1.28	9 (18%)
7	CLR	C	1102	-	31,31,31	0.72	1 (3%)	48,48,48	1.37	7 (14%)
6	1AT	A	1102	-	30,30,35	1.49	3 (10%)	43,43,48	2.47	15 (34%)
7	CLR	A	1103	-	31,31,31	0.68	0	48,48,48	1.58	8 (16%)
8	1DS	A	1104	-	30,30,35	1.33	5 (16%)	42,43,48	2.88	18 (42%)
10	NAG	D	402	2	15,15,15	0.90	1 (6%)	21,21,21	0.71	0
10	NAG	B	401	2	15,15,15	0.42	0	21,21,21	0.60	1 (4%)
10	NAG	B	402	2	15,15,15	0.86	1 (6%)	21,21,21	1.46	2 (9%)
5	BEF	C	1101	-	0,3,3	-	-	-		

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
10	NAG	D	401	-	-	2/6/26/26	0/1/1/1
7	CLR	E	101	-	-	5/10/68/68	0/4/4/4
7	CLR	G	101	-	-	2/10/68/68	0/4/4/4
7	CLR	C	1102	-	-	4/10/68/68	0/4/4/4
6	1AT	A	1102	-	-	10/19/58/63	0/2/2/2
7	CLR	A	1103	-	-	9/10/68/68	0/4/4/4
8	1DS	A	1104	-	-	7/19/58/63	0/2/2/2
10	NAG	B	401	2	-	2/6/26/26	0/1/1/1
10	NAG	B	402	2	-	0/6/26/26	0/1/1/1
10	NAG	D	402	2	-	2/6/26/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1102	1AT	O6-C1N	4.65	1.46	1.33
8	A	1104	1DS	O1'-C1N	3.01	1.42	1.33
10	B	402	NAG	O5-C1	-2.86	1.35	1.42
10	D	402	NAG	C1-C2	2.85	1.56	1.52
6	A	1102	1AT	C4'-C5'	-2.73	1.46	1.53

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1102	1AT	O2-C2-C3	-6.92	94.36	110.35
8	A	1104	1DS	C1'-O1'-C1N	6.92	128.87	116.88
8	A	1104	1DS	O2-C2-C3	6.22	124.72	110.35
6	A	1102	1AT	O1-C1-C2	5.94	125.76	108.29
8	A	1104	1DS	O1-C2'-C3'	5.86	126.47	108.08

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1102	1AT	O1'-C1'-C2'-O1
6	A	1102	1AT	O1'-C1'-C2'-C3'
8	A	1104	1DS	O1'-C1'-C2'-O1
8	A	1104	1DS	O1'-C1'-C2'-C3'
8	A	1104	1DS	O1'-C1'-C2'-O2'

There are no ring outliers.

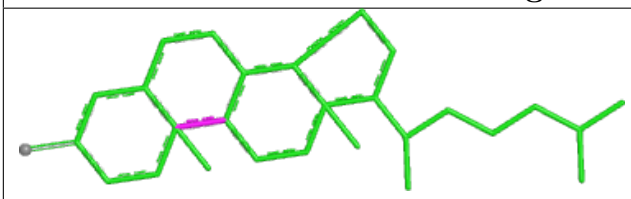
11 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	401	NAG	4	0
7	E	101	CLR	4	0
5	A	1101	BEF	1	0
7	G	101	CLR	6	0
7	C	1102	CLR	4	0
6	A	1102	1AT	6	0
7	A	1103	CLR	8	0
8	A	1104	1DS	9	0
10	B	401	NAG	2	0
10	B	402	NAG	1	0
5	C	1101	BEF	4	0

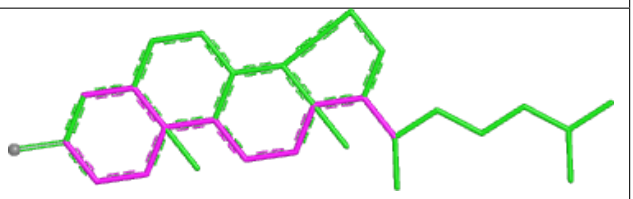
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

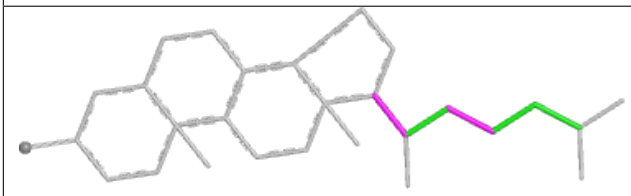
Ligand CLR E 101



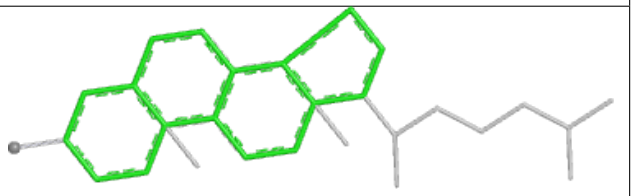
Bond lengths



Bond angles

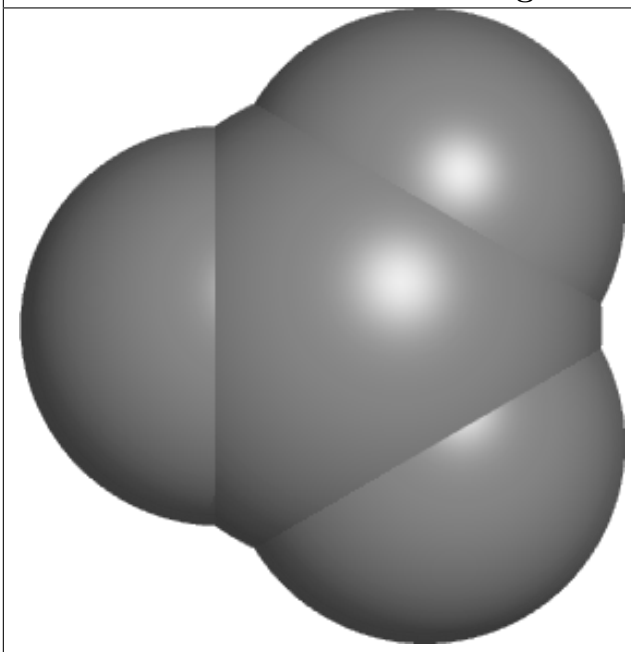


Torsions

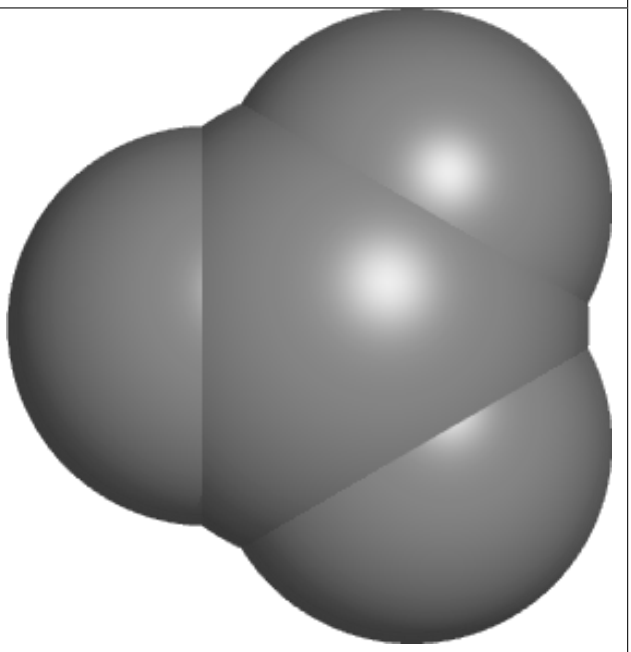


Rings

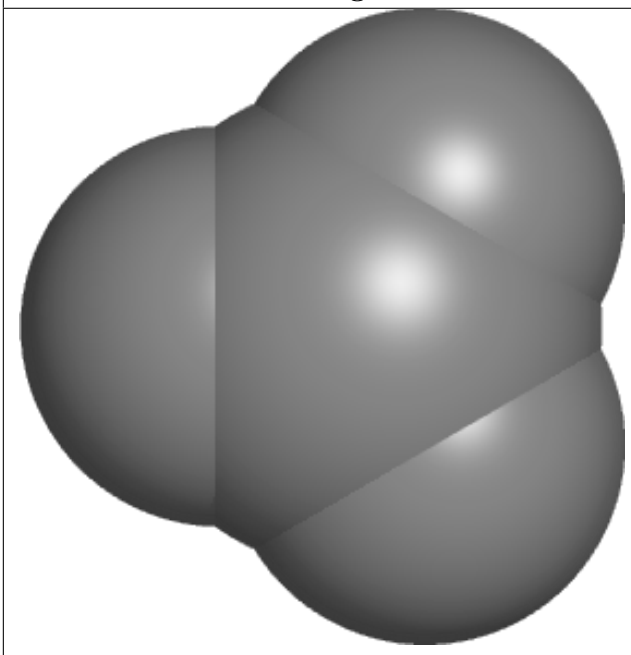
Ligand BEF A 1101



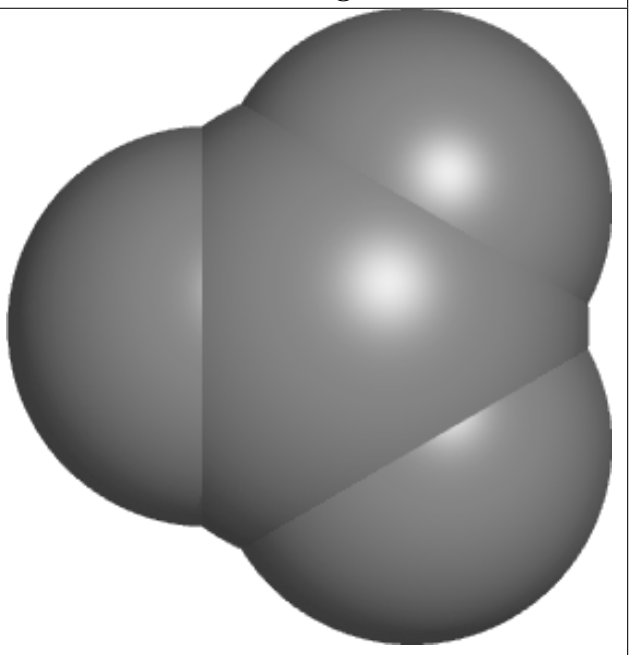
Bond lengths



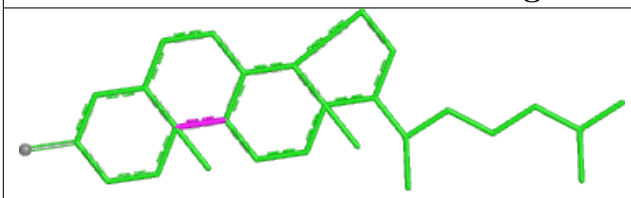
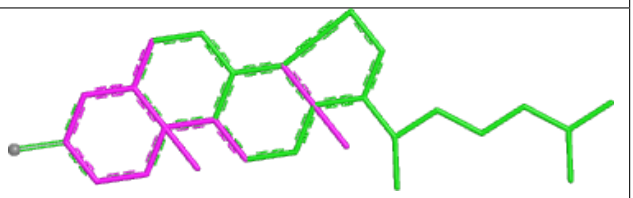
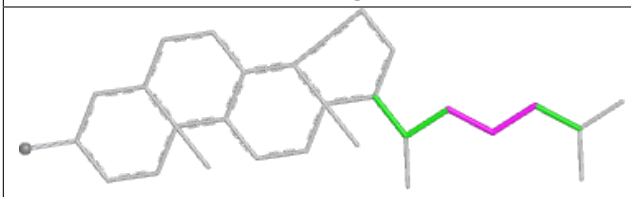
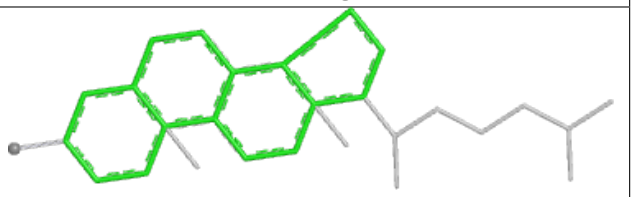
Bond angles

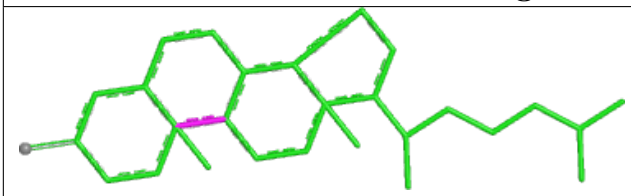
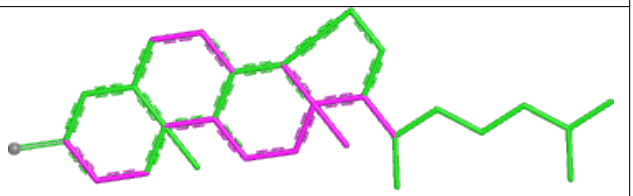
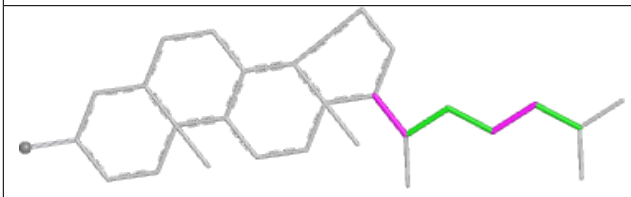
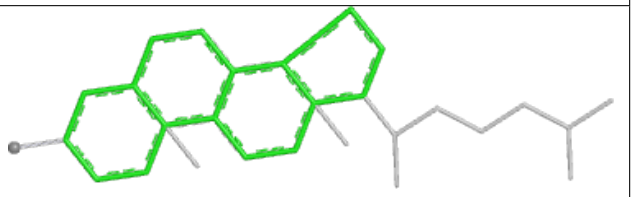


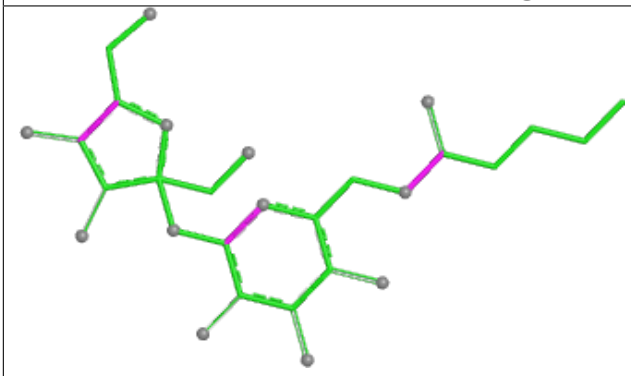
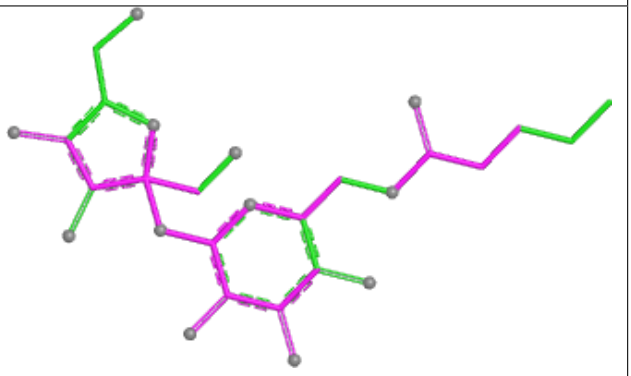
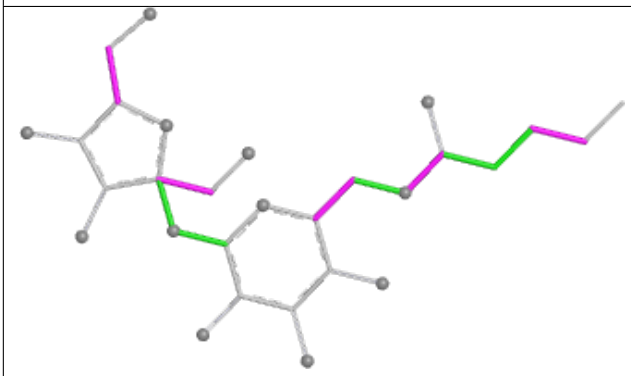
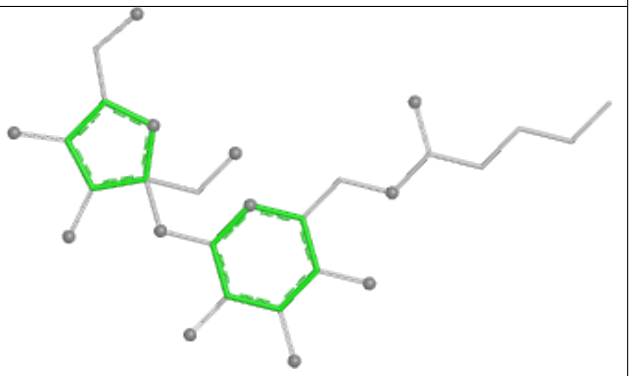
Torsions

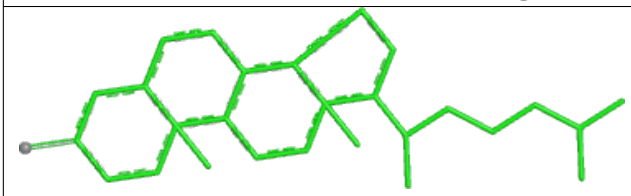
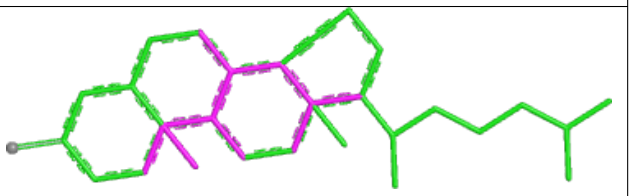
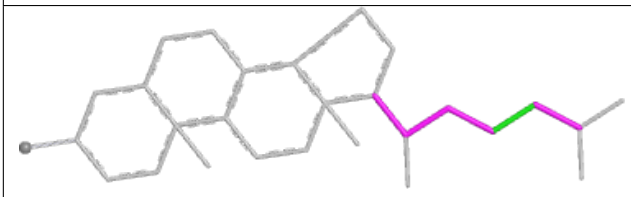
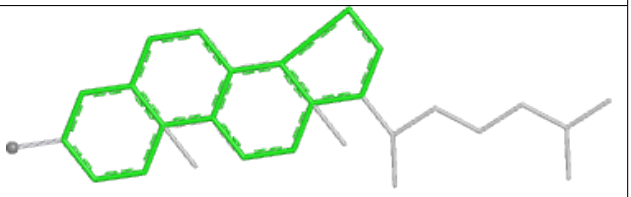


Rings

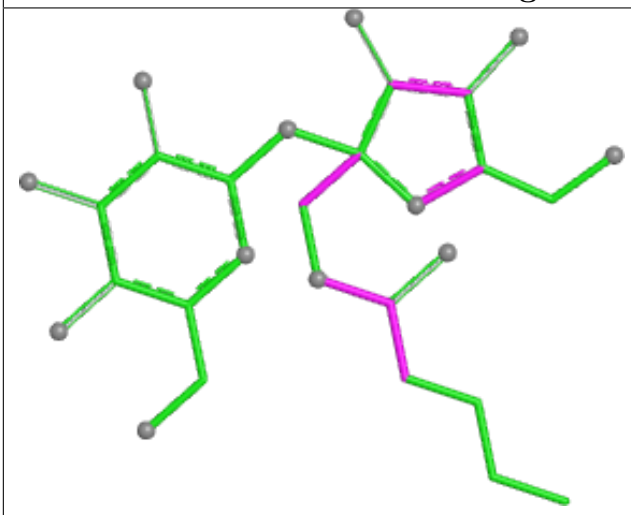
Ligand CLR G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLR C 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

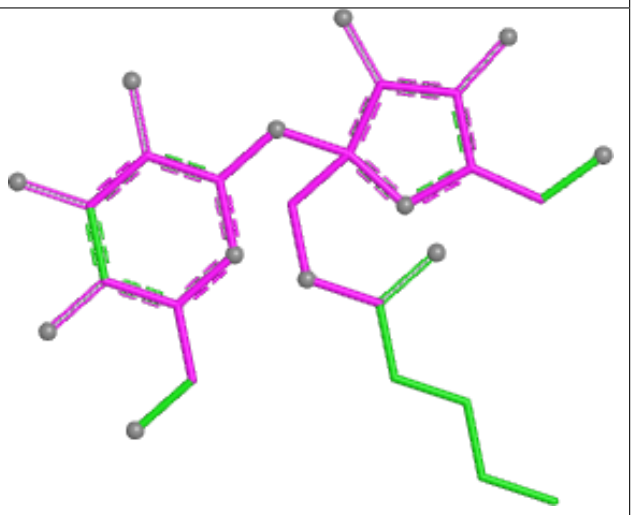
Ligand 1AT A 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLR A 1103	
 Bond lengths	 Bond angles
 Torsions	 Rings

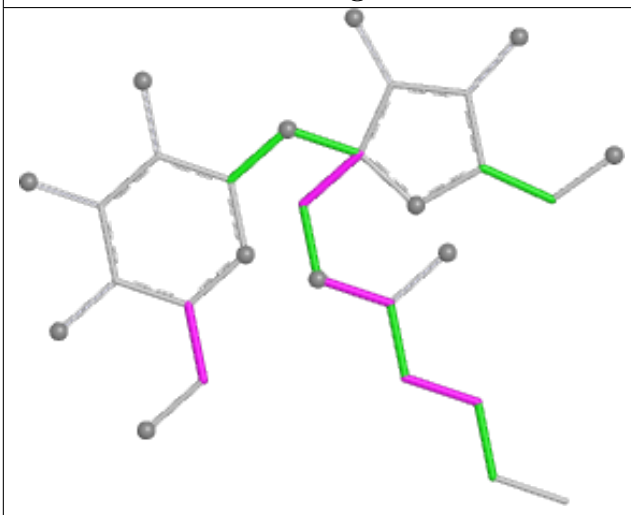
Ligand 1DS A 1104



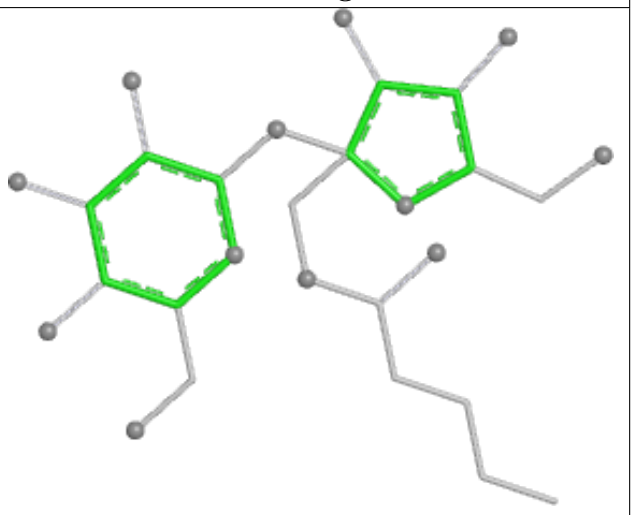
Bond lengths



Bond angles

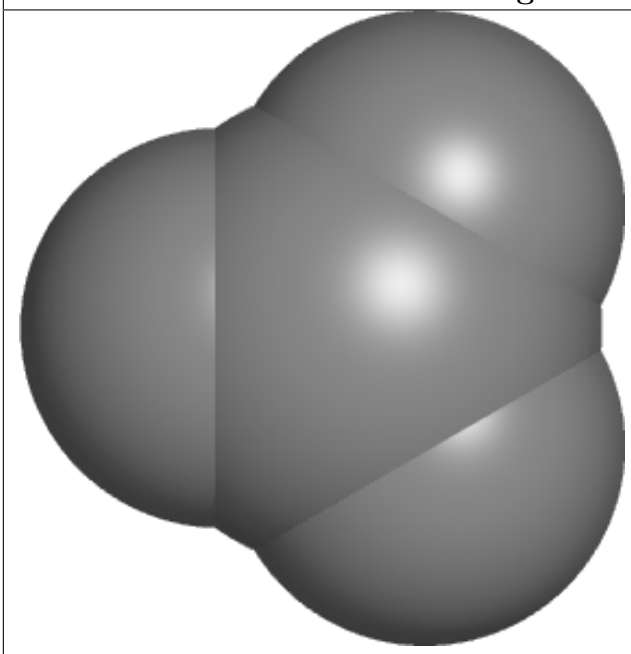


Torsions

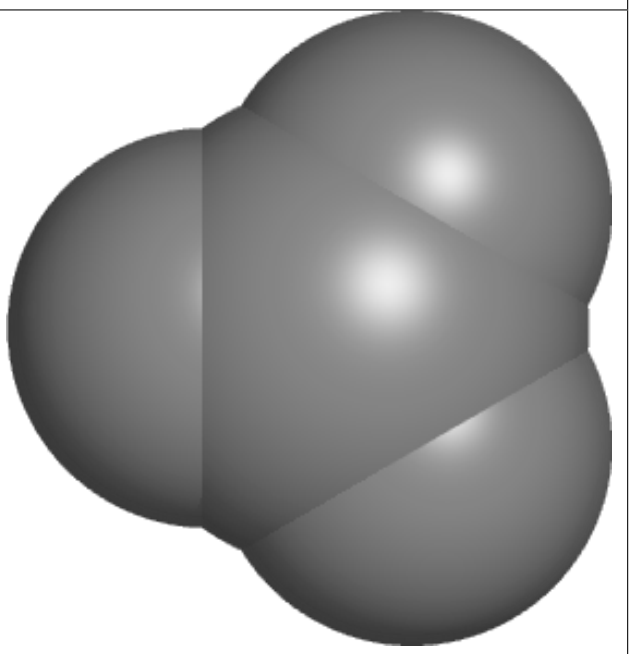


Rings

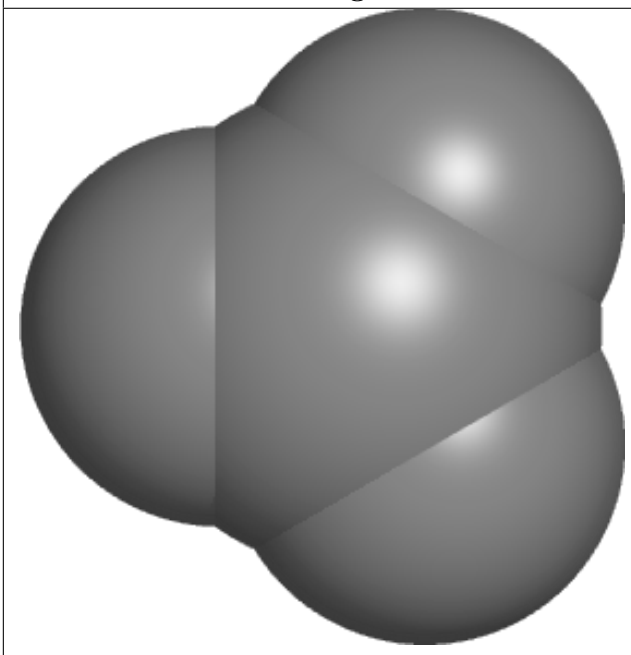
Ligand BEF C 1101



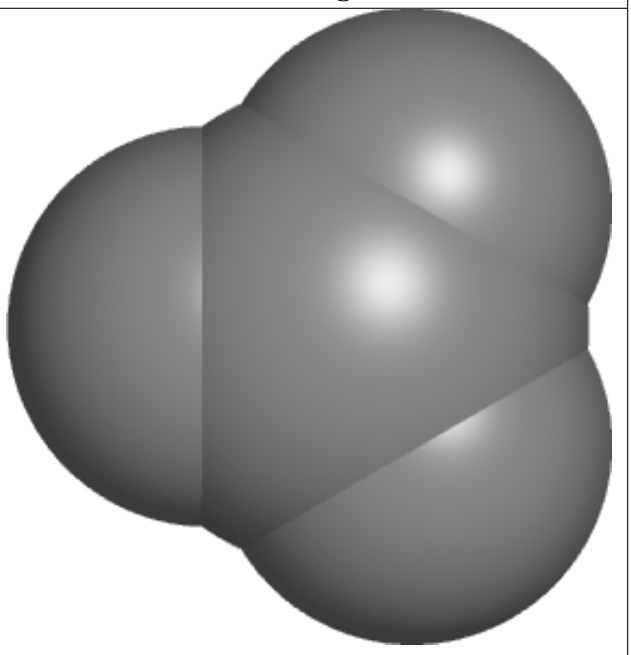
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.

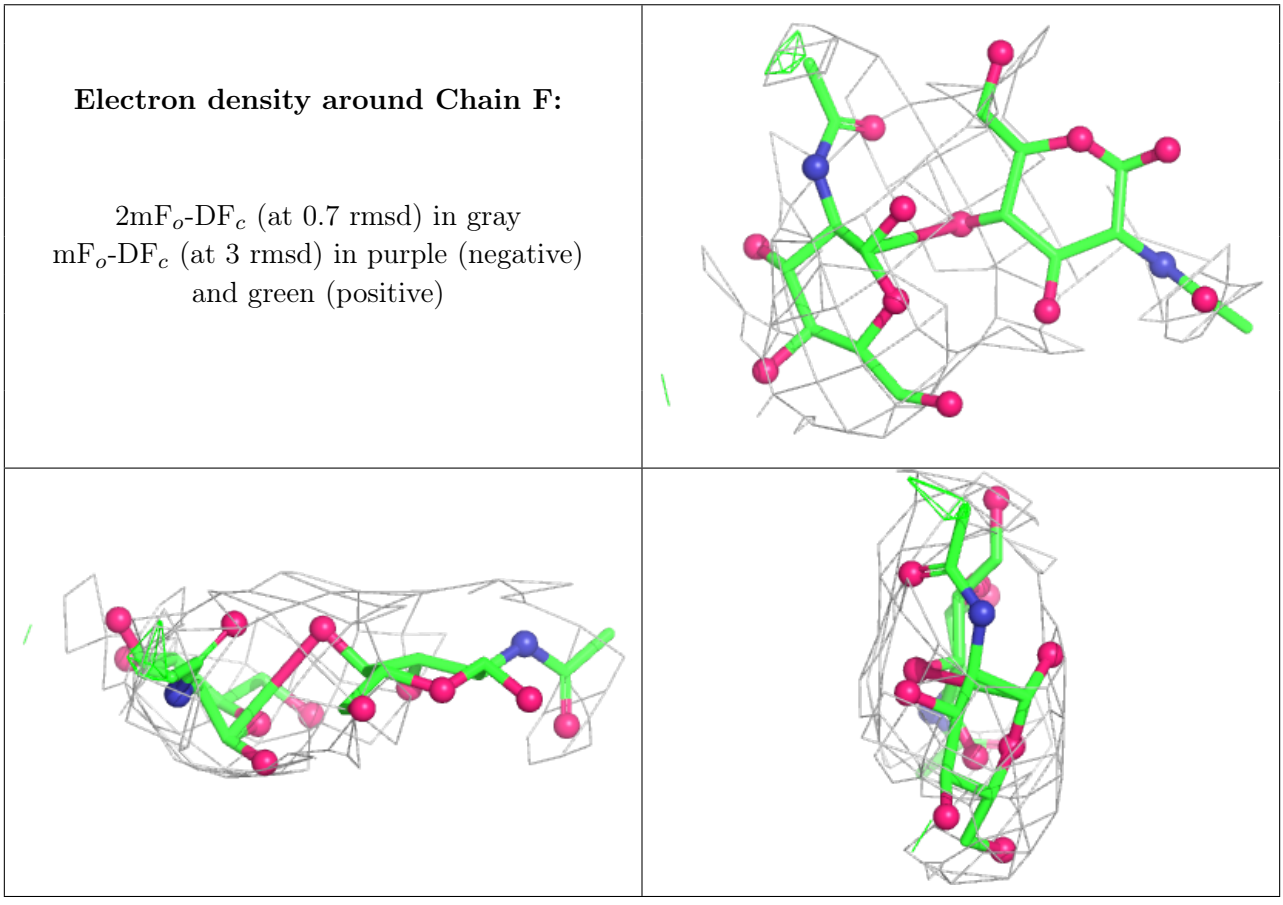
6.2 Non-standard residues in protein, DNA, RNA chains

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.



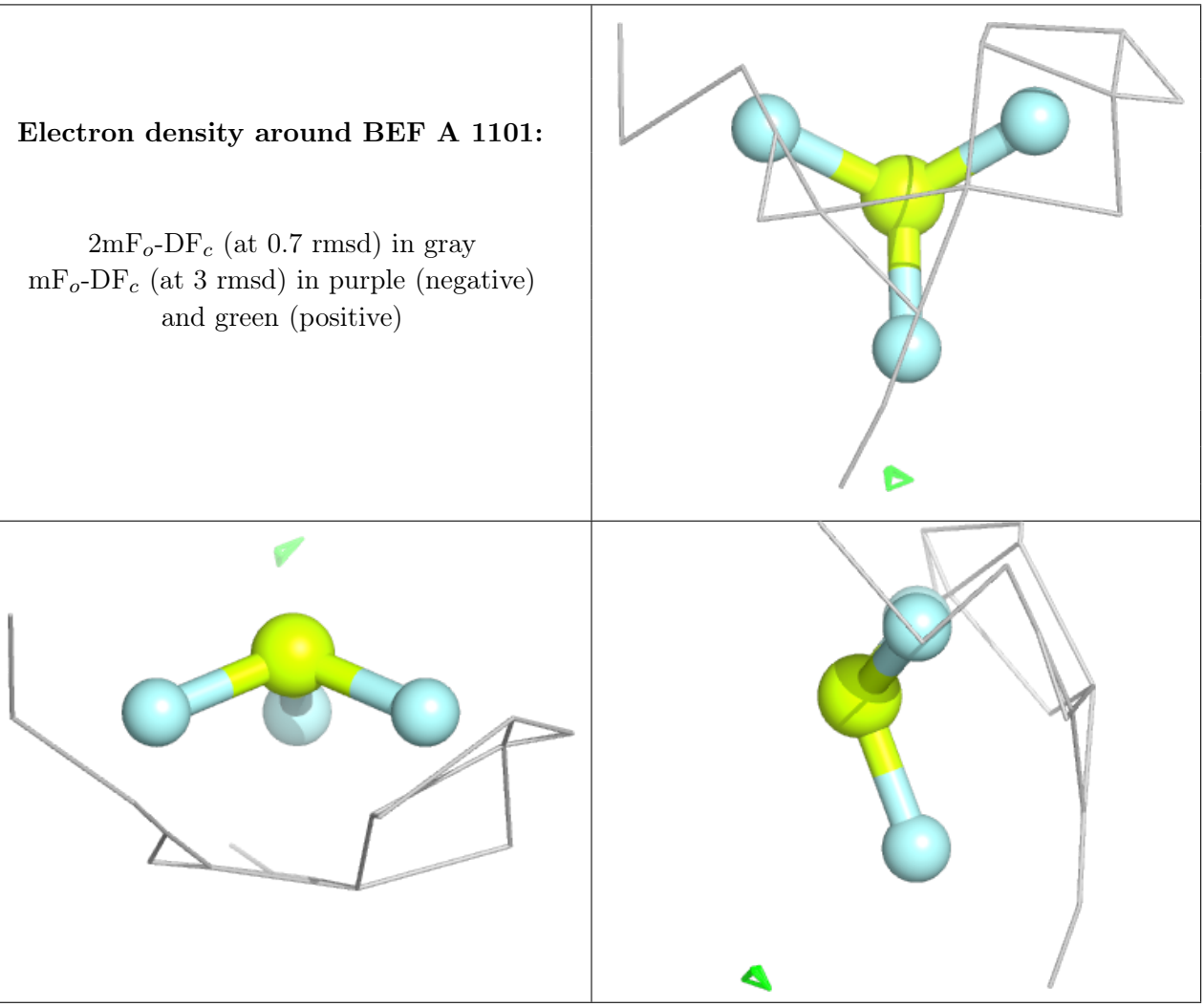
6.4 Ligands

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.

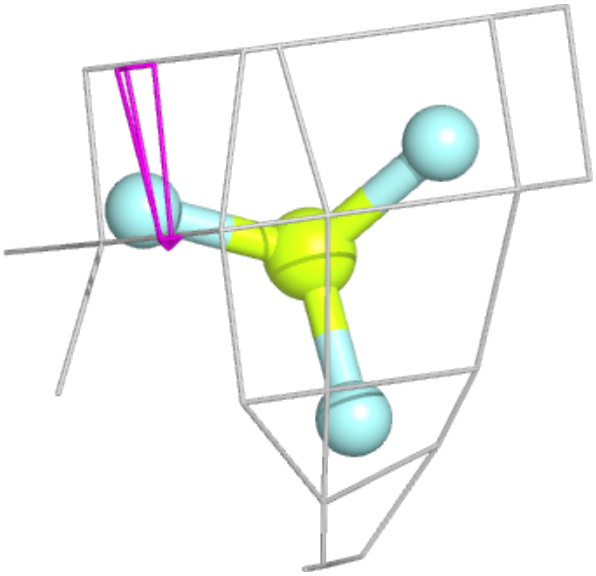
Electron density around BEF A 1101:

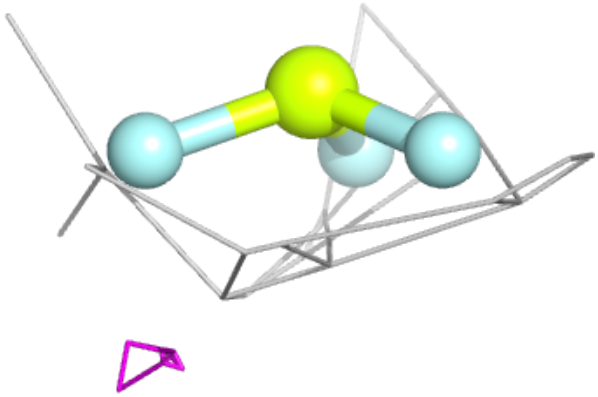
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

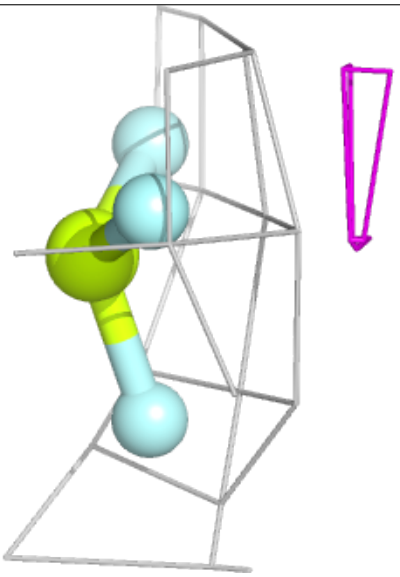


Electron density around BEF C 1101:

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







Electron density around 1AT A 1102:

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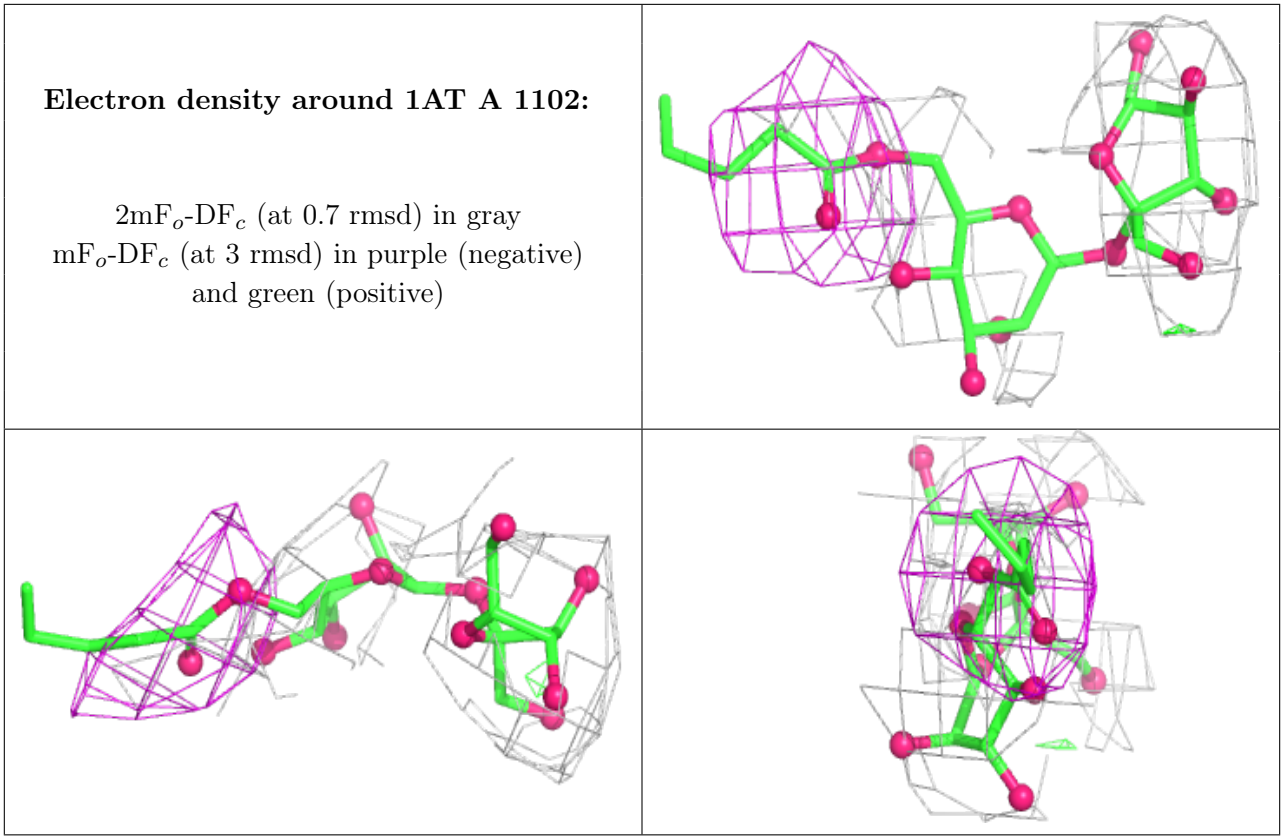
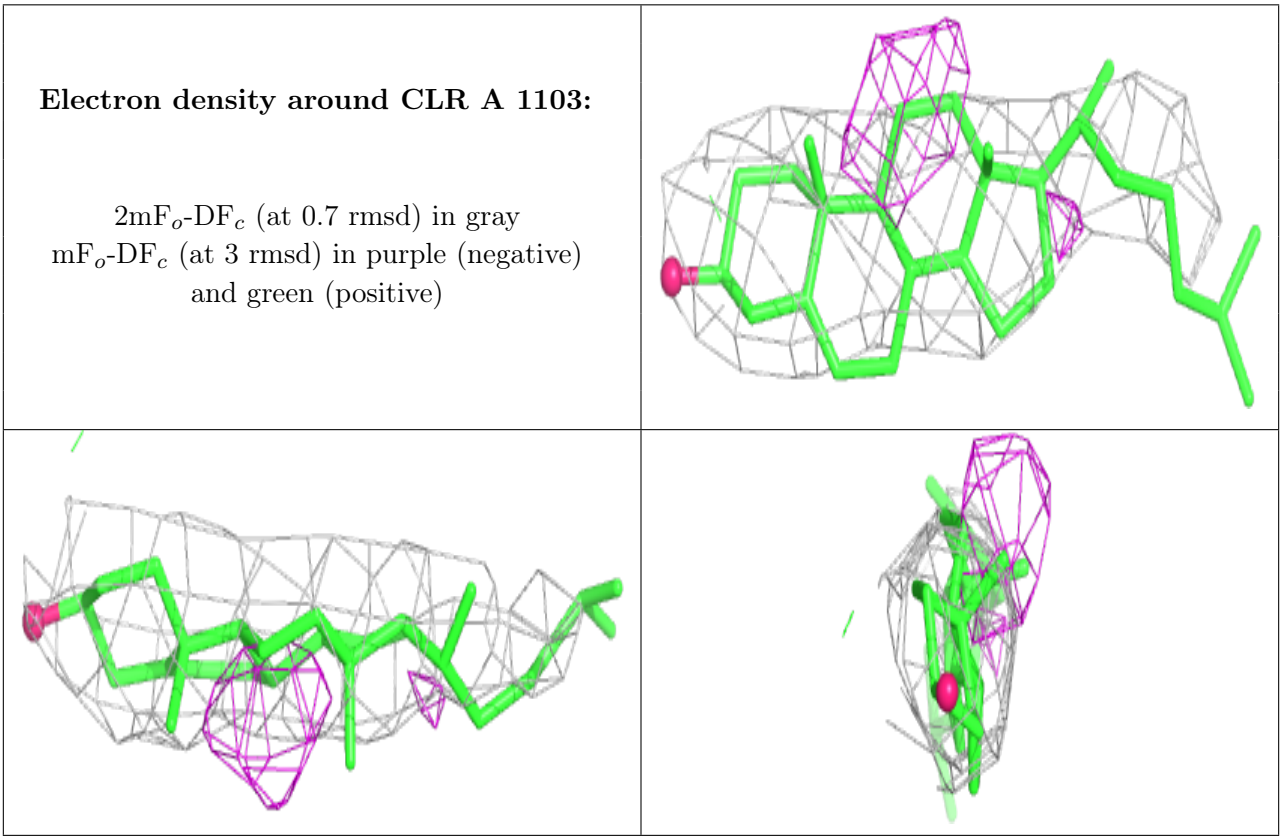


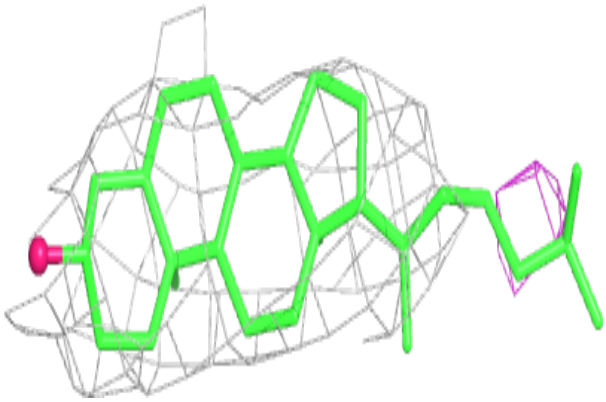
Electron density around CLR A 1103:

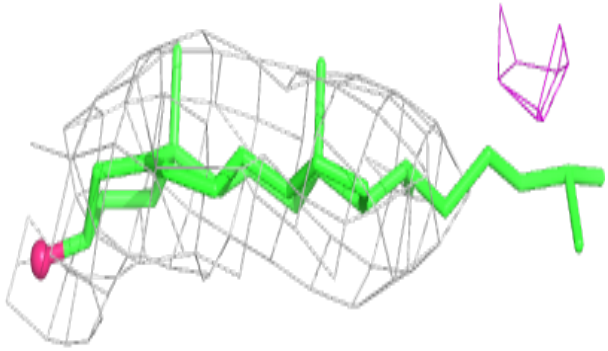
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLR G 101:

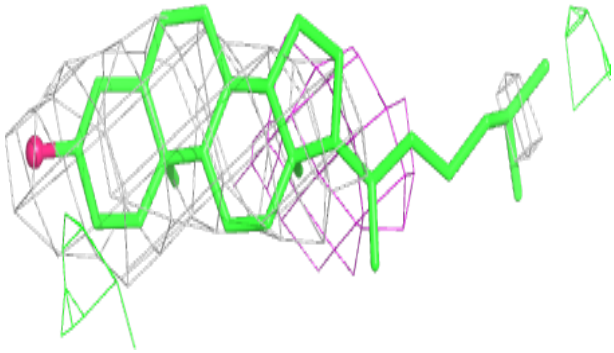
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

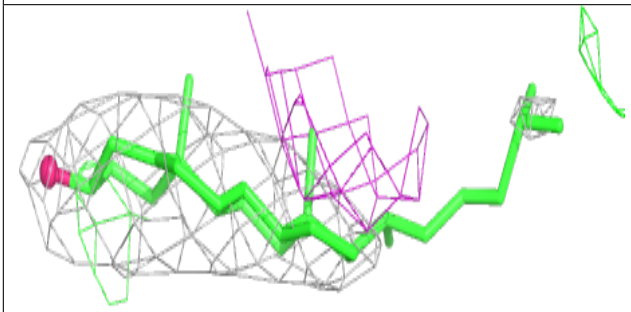


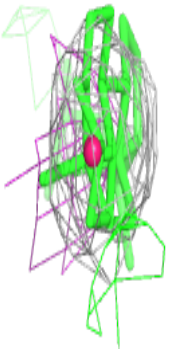


Electron density around CLR C 1102:

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

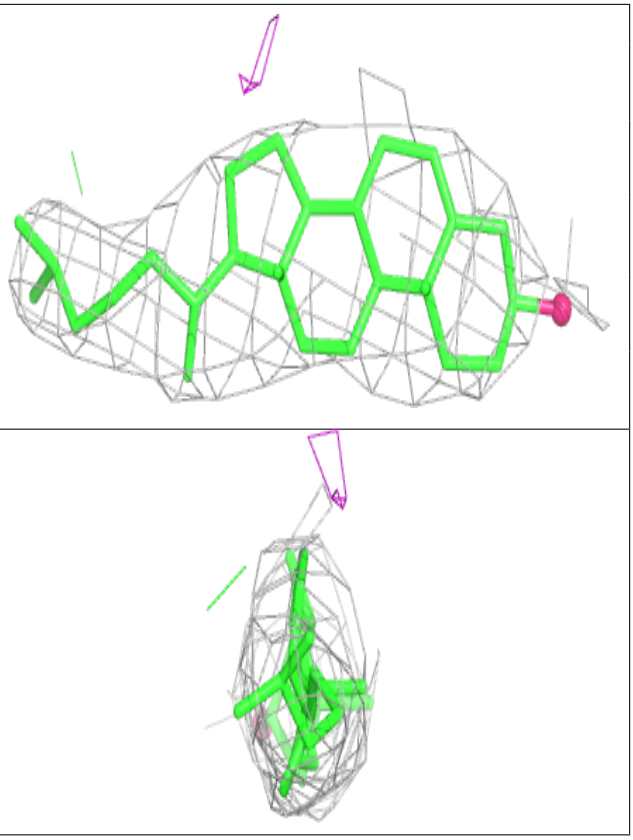


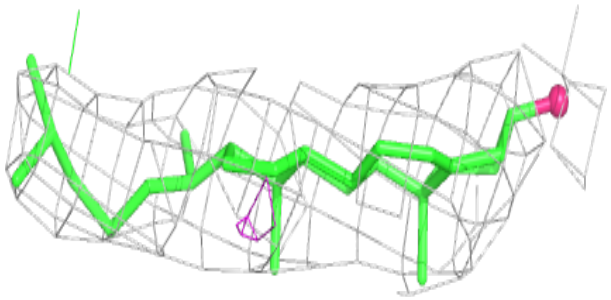




Electron density around CLR E 101:

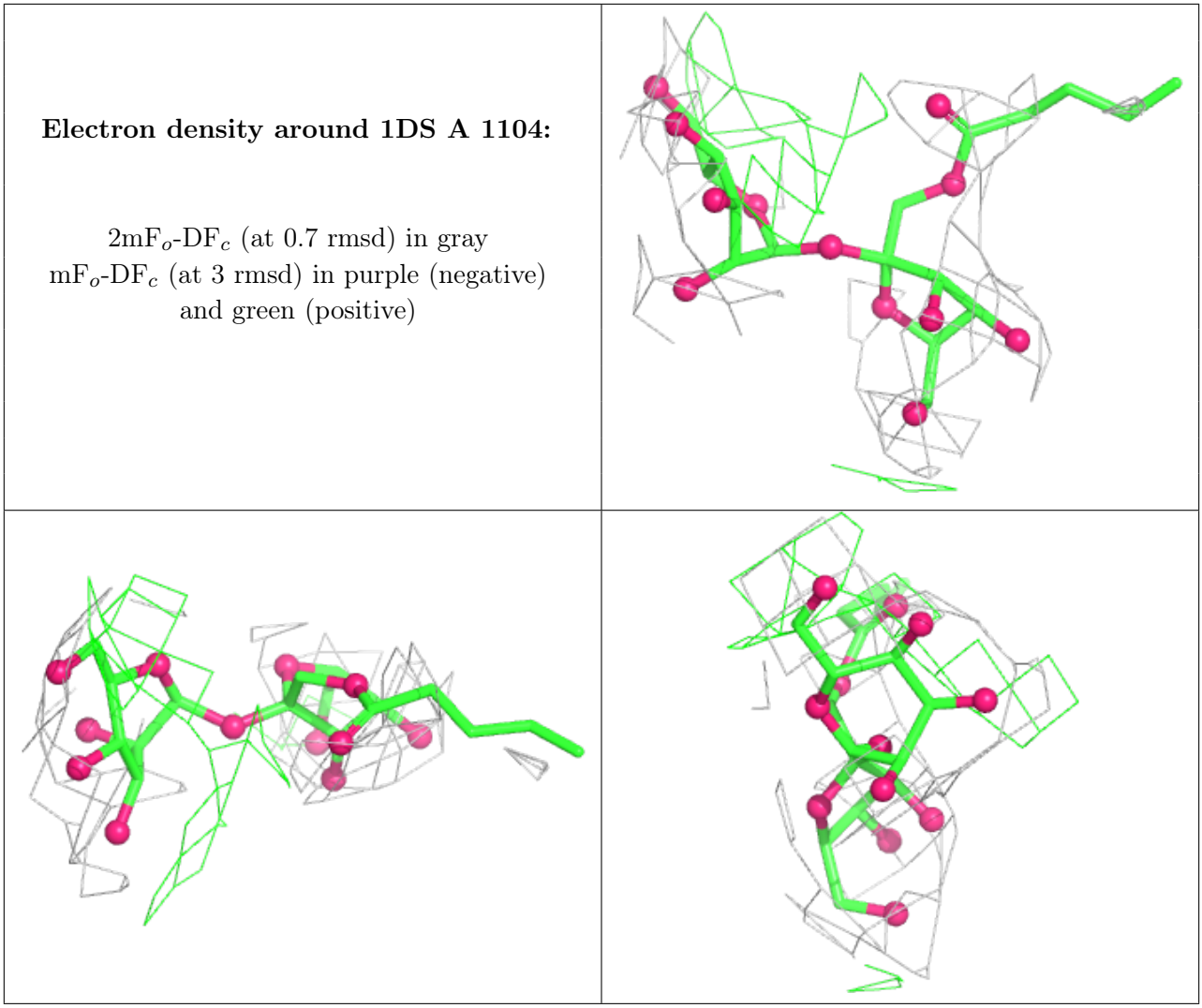
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around 1DS A 1104:

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



6.5 Other polymers (i)

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