



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 11:56 PM BST

PDB ID : 4HYT
Title : Na,K-ATPase in the E2P state with bound ouabain and Mg²⁺ in the cation-binding site
Authors : Laursen, M.; Yatime, L.; Nissen, P.; Fedosova, N.U.
Deposited on : 2012-11-14
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

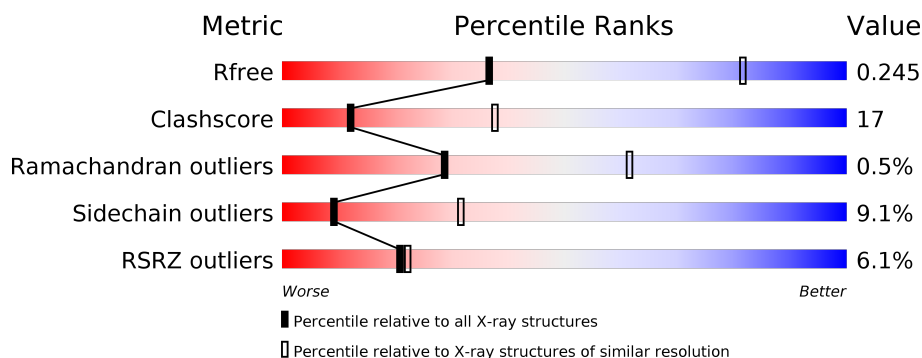
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1021	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>• •</div> </div> </div>
1	C	1021	<div> <div>8%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>• •</div> </div> </div>
2	B	303	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>37%</div> <div>7% 5%</div> </div> </div>
2	D	303	<div> <div>7%</div> <div> <div></div> <div>50%</div> <div>38%</div> <div>6% • 5%</div> </div> </div>
3	E	65	<div> <div></div> <div> <div></div> <div>32%</div> <div>15%</div> <div>•</div> <div>51%</div> </div> </div>
3	G	65	<div> <div>2%</div> <div> <div></div> <div>29%</div> <div>17%</div> <div>•</div> <div>51%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	2	 100%

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
12	NAG	B	1004	-	-	-	X
4	NAG	F	2	-	-	-	X

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 21220 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			
1	C	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	289	Total	C	N	O	S	0	0	0
			2368	1534	386	435	13			
2	D	287	Total	C	N	O	S	0	0	0
			2349	1519	384	433	13			

- Molecule 3 is a protein called Na⁺/K⁺ ATPase gamma subunit transcript variant a.

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.

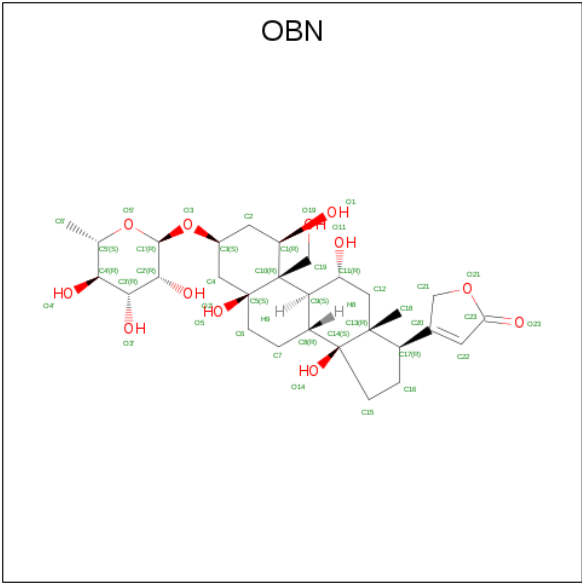


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

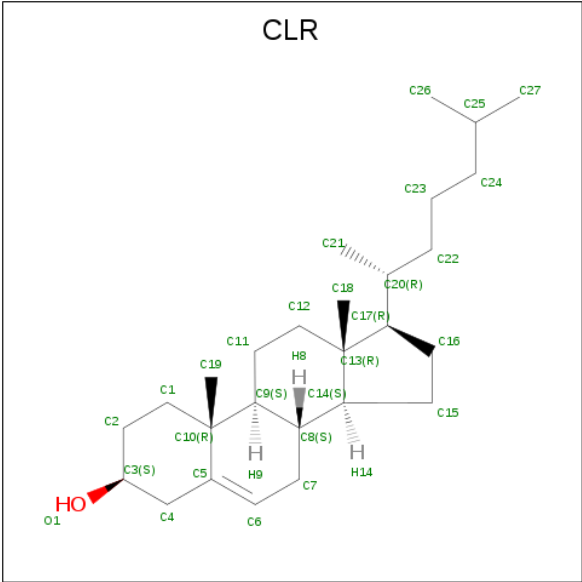
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Mg	0	0
			3	3		
5	C	3	Total	Mg	0	0
			3	3		

- Molecule 6 is OUABAIN (three-letter code: OBN) (formula: C₂₉H₄₄O₁₂).



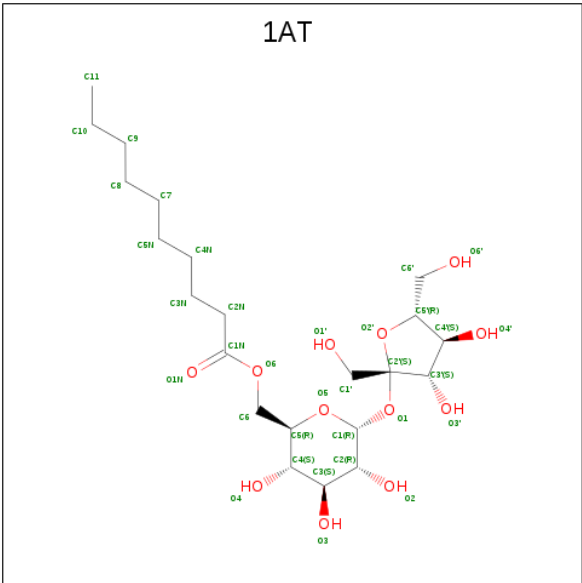
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			41	29	12		
6	C	1	Total	C	O	0	0
			41	29	12		

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



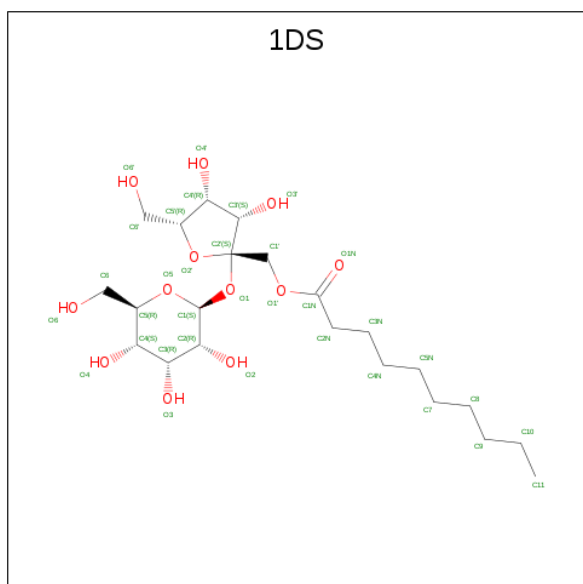
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			28	27	1		
7	G	1	Total	C	O	0	0
			28	27	1		
7	C	1	Total	C	O	0	0
			28	27	1		
7	E	1	Total	C	O	0	0
			28	27	1		

- Molecule 8 is beta-D-fructofuranosyl 6-O-decanoyl-alpha-D-glucopyranoside (three-letter code: 1AT) (formula: C₂₂H₄₀O₁₂).



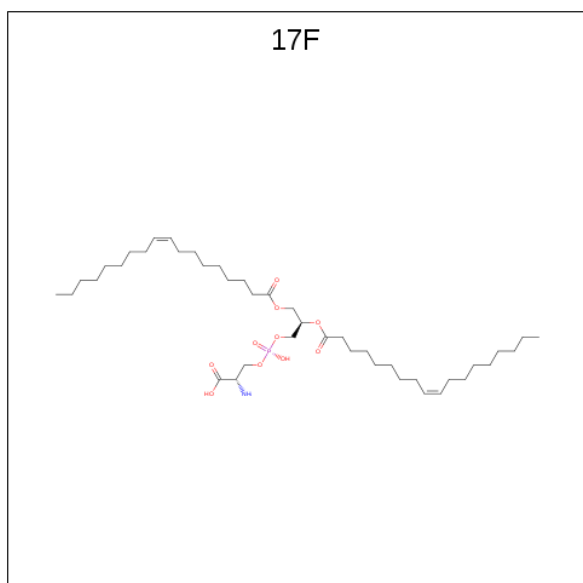
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			29	17	12		

- Molecule 9 is 1-O-decanoyl-beta-D-tagatofuranosyl beta-D-allopyranoside (three-letter code: 1DS) (formula: $C_{22}H_{40}O_{12}$).



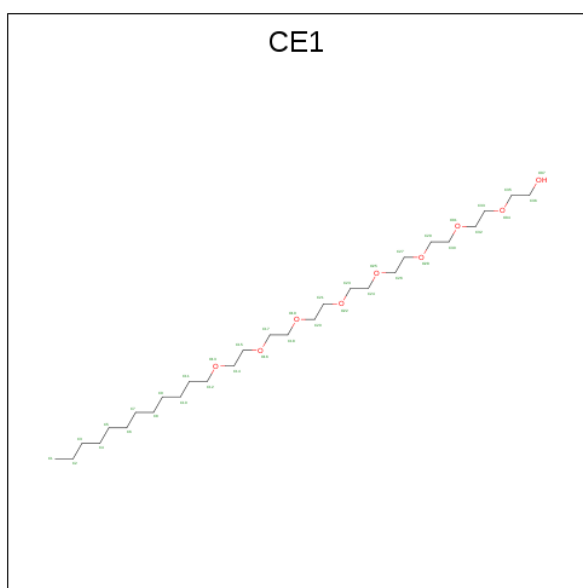
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			29	17	12		

- Molecule 10 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (three-letter code: 17F) (formula: $C_{42}H_{78}NO_{10}P$).



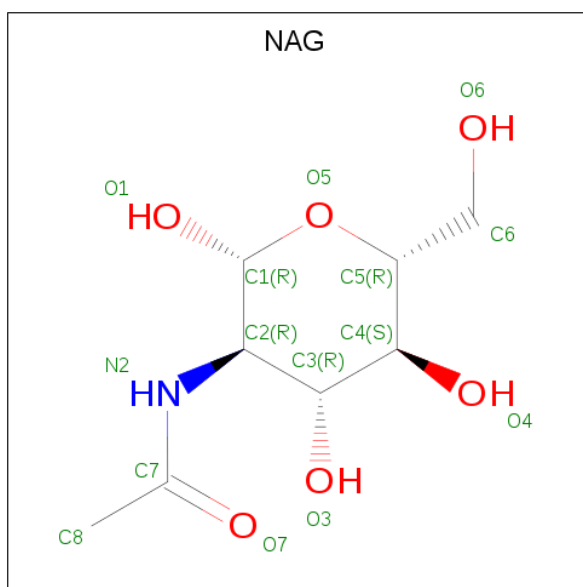
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	P	0	0
			18	8	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			18	8	1	8	1		
10	B	1	Total	C	N	O	P	0	0
			24	14	1	8	1		
10	G	1	Total	C	N	O	P	0	0
			27	15	1	10	1		
10	D	1	Total	C	N	O	P	0	0
			28	16	1	10	1		

- Molecule 11 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: $C_{28}H_{58}O_9$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	C O	0	0
			34 26 8			
11	E	1	Total	C O	0	0
			22 18 4			

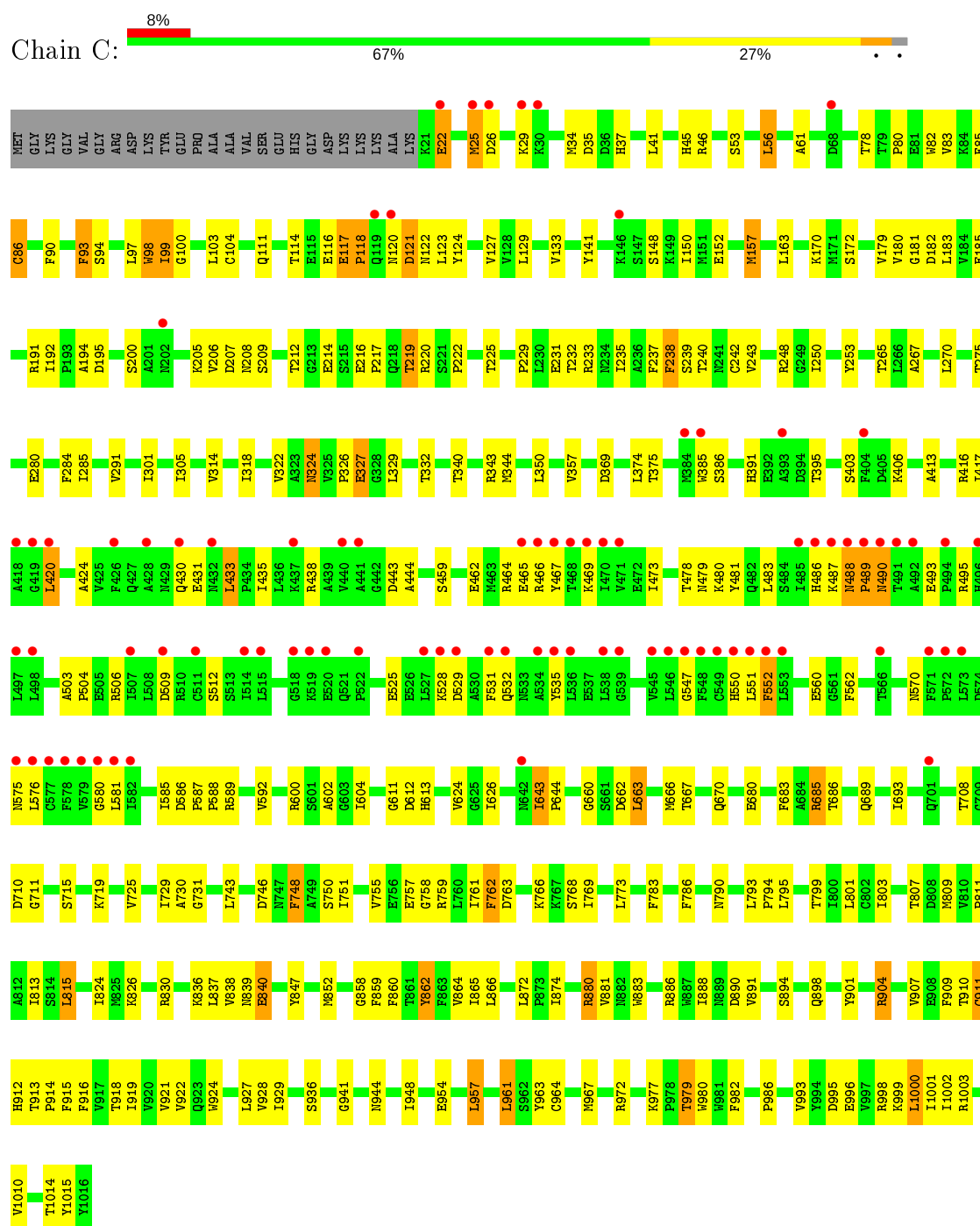
- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



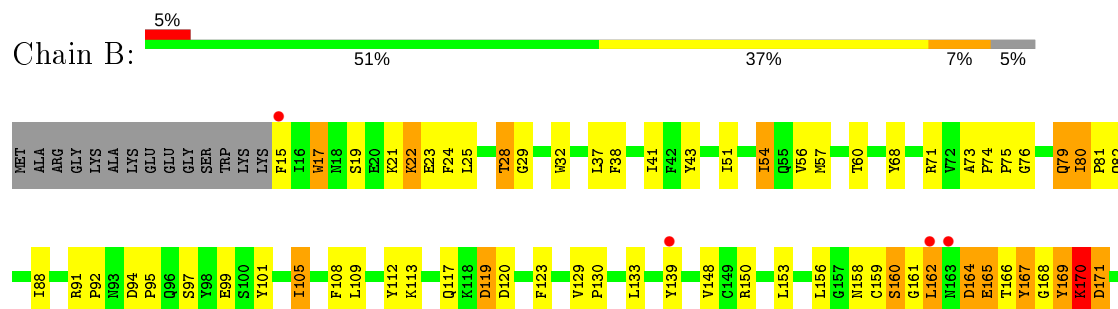
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			14	8	1	5		
12	B	1	Total	C	N	O	0	0
			14	8	1	5		
12	D	1	Total	C	N	O	0	0
			14	8	1	5		
12	D	1	Total	C	N	O	0	0
			14	8	1	5		
12	D	1	Total	C	N	O	0	0
			14	8	1	5		

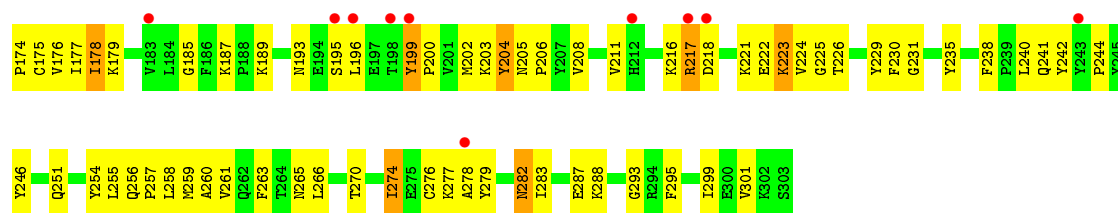
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	3	Total	O	0	0
			3	3		
13	C	3	Total	O	0	0
			3	3		

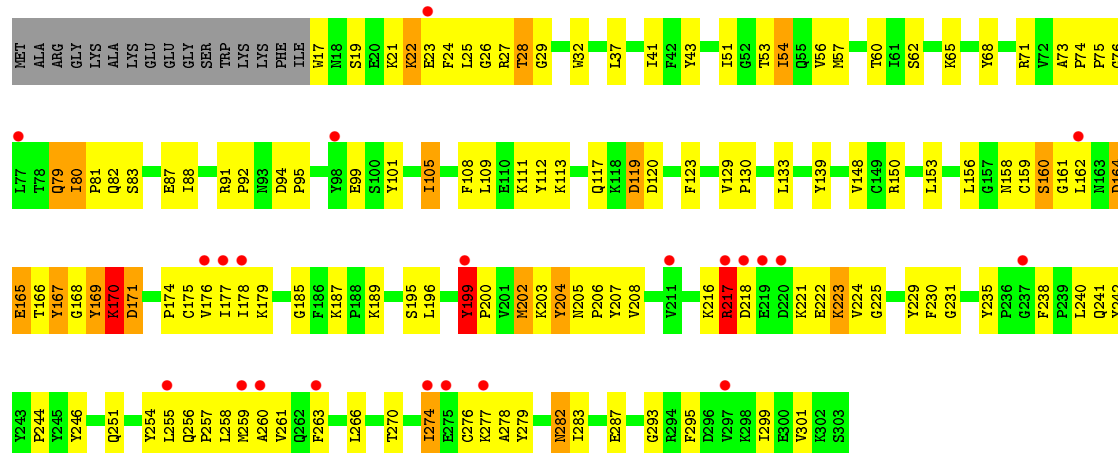


- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

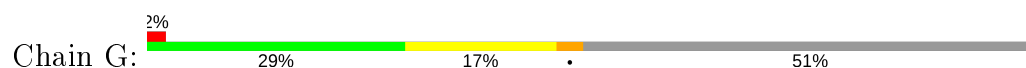




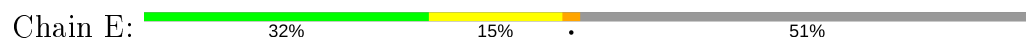
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



• Molecule 3: Na⁺/K⁺ ATPase gamma subunit transcript variant a



• Molecule 3: Na⁺/K⁺ ATPase gamma subunit transcript variant a



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



4 Data and refinement statistics

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)	49.83 – 3.40 53.88 – 3.40	Depositor EDS
% Data completeness (in resolution range)	75.7 (49.83-3.40) 75.7 (53.88-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, R_{free}	0.226 , 0.244 0.226 , 0.245	Depositor DCC
R_{free} test set	3603 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	111.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 70.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21220	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OBN, 1AT, MG, NAG, 17F, PHD, 1DS, CE1, CLR

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	0/7867	0.53	0/10674
1	C	0.30	0/7867	0.53	0/10674
2	B	0.32	0/2431	0.59	0/3279
2	D	0.34	0/2411	0.59	2/3252 (0.1%)
3	E	0.38	0/261	0.54	0/354
3	G	0.39	0/261	0.55	0/354
All	All	0.31	0/21098	0.54	2/28587 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	217	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	D	199	TYR	CB-CG-CD2	-5.15	117.91	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	160	SER	Peptide
2	B	165	GLU	Peptide
2	D	160	SER	Peptide
2	D	165	GLU	Peptide

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	243	0
1	C	7730	0	7777	226	0
2	B	2368	0	2335	116	0
2	D	2349	0	2315	119	0
3	E	255	0	259	7	0
3	G	255	0	259	9	0
4	F	28	0	25	0	0
5	A	3	0	0	0	0
5	C	3	0	0	0	0
6	A	41	0	44	10	0
6	C	41	0	44	6	0
7	A	28	0	46	5	0
7	C	28	0	46	2	0
7	E	28	0	46	4	0
7	G	28	0	46	4	0
8	A	29	0	27	6	0
9	A	29	0	27	6	0
10	A	36	0	16	7	0
10	B	24	0	20	2	0
10	D	28	0	22	0	0
10	G	27	0	20	4	0
11	A	34	0	53	18	0
11	E	22	0	37	1	0
12	B	28	0	26	0	0
12	D	42	0	39	0	0
13	A	3	0	0	1	0
13	C	3	0	0	0	0
All	All	21220	0	21306	726	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 17.

The worst 5 of 726 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:68:ASP:OD1	1:A:69:GLY:N	1.78	1.15
1:A:794:PRO:HG3	1:A:862:TYR:HE2	1.15	1.07
1:C:794:PRO:HG3	1:C:862:TYR:HE2	1.17	1.07
1:C:794:PRO:HG3	1:C:862:TYR:CE2	1.95	1.00
1:A:794:PRO:HG3	1:A:862:TYR:CE2	1.95	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	993/1021 (97%)	940 (95%)	51 (5%)	2 (0%)	47	78
1	C	993/1021 (97%)	947 (95%)	44 (4%)	2 (0%)	47	78
2	B	287/303 (95%)	255 (89%)	28 (10%)	4 (1%)	11	37
2	D	285/303 (94%)	255 (90%)	26 (9%)	4 (1%)	11	37
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	2618/2778 (94%)	2453 (94%)	153 (6%)	12 (0%)	29	61

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	199	TYR
2	D	199	TYR
2	B	161	GLY
2	D	161	GLY
2	B	170	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	846/864 (98%)	777 (92%)	69 (8%)	11	37
1	C	846/864 (98%)	780 (92%)	66 (8%)	12	39
2	B	259/269 (96%)	225 (87%)	34 (13%)	4	15
2	D	257/269 (96%)	226 (88%)	31 (12%)	5	18
3	E	26/52 (50%)	23 (88%)	3 (12%)	5	20
3	G	26/52 (50%)	23 (88%)	3 (12%)	5	20
All	All	2260/2370 (95%)	2054 (91%)	206 (9%)	9	32

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

Mol	Chain	Res	Type
2	B	203	LYS
1	C	85	PHE
2	D	178	ILE
2	B	217	ARG
3	G	45	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	HIS
2	B	241	GLN
1	C	486	HIS
2	D	241	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PHD	C	369	1,5	9,11,12	1.33	2 (22%)	10,15,17	1.54	2 (20%)
1	PHD	A	369	1,5	9,11,12	1.41	2 (22%)	10,15,17	1.58	3 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PHD	C	369	1,5	-	0/8/11/13	-
1	PHD	A	369	1,5	-	0/8/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	PHD	P-OD1	-2.66	1.55	1.59
1	C	369	PHD	P-OD1	-2.25	1.55	1.59
1	C	369	PHD	CB-CA	-2.13	1.49	1.53
1	A	369	PHD	CB-CA	-2.01	1.49	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	PHD	OD2-CG-CB	-2.96	118.19	124.73
1	C	369	PHD	OD1-CG-CB	2.87	118.99	111.11
1	A	369	PHD	OD1-CG-CB	2.83	118.89	111.11
1	C	369	PHD	OD2-CG-CB	-2.70	118.77	124.73
1	A	369	PHD	CA-CB-CG	2.03	117.11	112.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

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	14,14,15	0.35	0	17,19,21	0.48	0
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 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
12	NAG	D	2003	2	14,14,15	0.56	0	17,19,21	0.54	0
10	17F	D	2004	-	24,27,53	1.15	4 (16%)	26,34,60	1.93	7 (26%)
7	CLR	G	1001	-	31,31,31	2.45	8 (25%)	48,48,48	2.80	17 (35%)
10	17F	A	1109	-	14,17,53	1.27	2 (14%)	15,23,60	3.60	6 (40%)
10	17F	G	1002	-	23,26,53	1.14	2 (8%)	25,33,60	2.58	7 (28%)
11	CE1	A	1110	-	33,33,36	0.57	0	32,32,35	0.94	1 (3%)
9	1DS	A	1107	-	30,30,35	1.32	5 (16%)	42,43,48	2.30	14 (33%)
7	CLR	C	2005	-	31,31,31	2.46	8 (25%)	48,48,48	2.84	17 (35%)
12	NAG	D	2001	2	14,14,15	0.35	0	17,19,21	0.45	0
11	CE1	E	2002	-	21,21,36	0.72	0	20,20,35	1.13	2 (10%)
12	NAG	B	1003	2	14,14,15	0.33	0	17,19,21	0.51	0
7	CLR	A	1105	-	31,31,31	2.49	8 (25%)	48,48,48	2.92	17 (35%)
12	NAG	D	2002	2	14,14,15	0.58	0	17,19,21	0.56	0
8	1AT	A	1106	-	30,30,35	1.46	3 (10%)	43,43,48	2.43	14 (32%)
7	CLR	E	2001	-	31,31,31	2.44	8 (25%)	48,48,48	2.80	19 (39%)
10	17F	A	1108	-	14,17,53	1.42	2 (14%)	15,23,60	3.22	5 (33%)
10	17F	B	1005	-	20,23,53	1.29	2 (10%)	21,29,60	2.93	8 (38%)
12	NAG	B	1004	2	14,14,15	0.46	0	17,19,21	0.40	0
6	OBN	A	1104	-	44,46,46	0.83	1 (2%)	66,76,76	1.82	18 (27%)
6	OBN	C	2004	-	44,46,46	0.78	1 (2%)	66,76,76	1.71	17 (25%)

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
12	NAG	D	2003	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	17F	D	2004	-	-	13/29/33/59	-
7	CLR	G	1001	-	-	4/10/68/68	0/4/4/4
10	17F	A	1109	-	-	14/16/20/59	-
10	17F	G	1002	-	-	8/27/31/59	-
11	CE1	A	1110	-	-	16/31/31/34	-
9	1DS	A	1107	-	-	7/19/58/63	0/2/2/2
7	CLR	C	2005	-	-	7/10/68/68	0/4/4/4
12	NAG	D	2001	2	-	2/6/23/26	0/1/1/1
11	CE1	E	2002	-	-	14/19/19/34	-
12	NAG	B	1003	2	-	0/6/23/26	0/1/1/1
7	CLR	A	1105	-	-	9/10/68/68	0/4/4/4
12	NAG	D	2002	2	-	4/6/23/26	0/1/1/1
8	1AT	A	1106	-	-	8/19/58/63	0/2/2/2
7	CLR	E	2001	-	-	4/10/68/68	0/4/4/4
10	17F	A	1108	-	-	9/16/20/59	-
10	17F	B	1005	-	-	18/23/27/59	-
12	NAG	B	1004	2	-	4/6/23/26	0/1/1/1
6	OBN	A	1104	-	-	4/11/116/116	0/6/6/6
6	OBN	C	2004	-	-	4/11/116/116	0/6/6/6

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	2005	CLR	C6-C5	9.42	1.53	1.33
7	A	1105	CLR	C6-C5	9.38	1.53	1.33
7	G	1001	CLR	C6-C5	9.22	1.53	1.33
7	E	2001	CLR	C6-C5	9.17	1.53	1.33
7	A	1105	CLR	C11-C9	5.26	1.62	1.53

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1005	17F	C5-O9-C17	9.54	130.15	117.88
10	A	1109	17F	C5-O9-C17	8.38	132.78	118.31
7	A	1105	CLR	C4-C5-C6	-8.30	108.65	120.61
10	G	1002	17F	O3-C1-C2	7.70	114.78	108.06
10	A	1109	17F	O3-C1-C2	7.66	114.73	108.06

There are no chirality outliers.

5 of 153 torsion outliers are listed below:

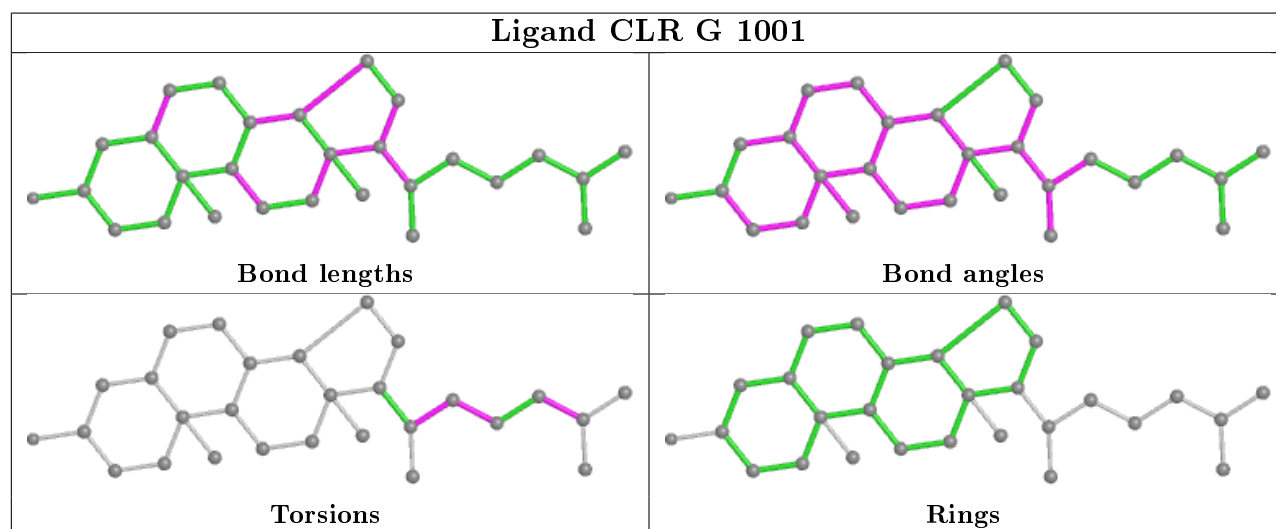
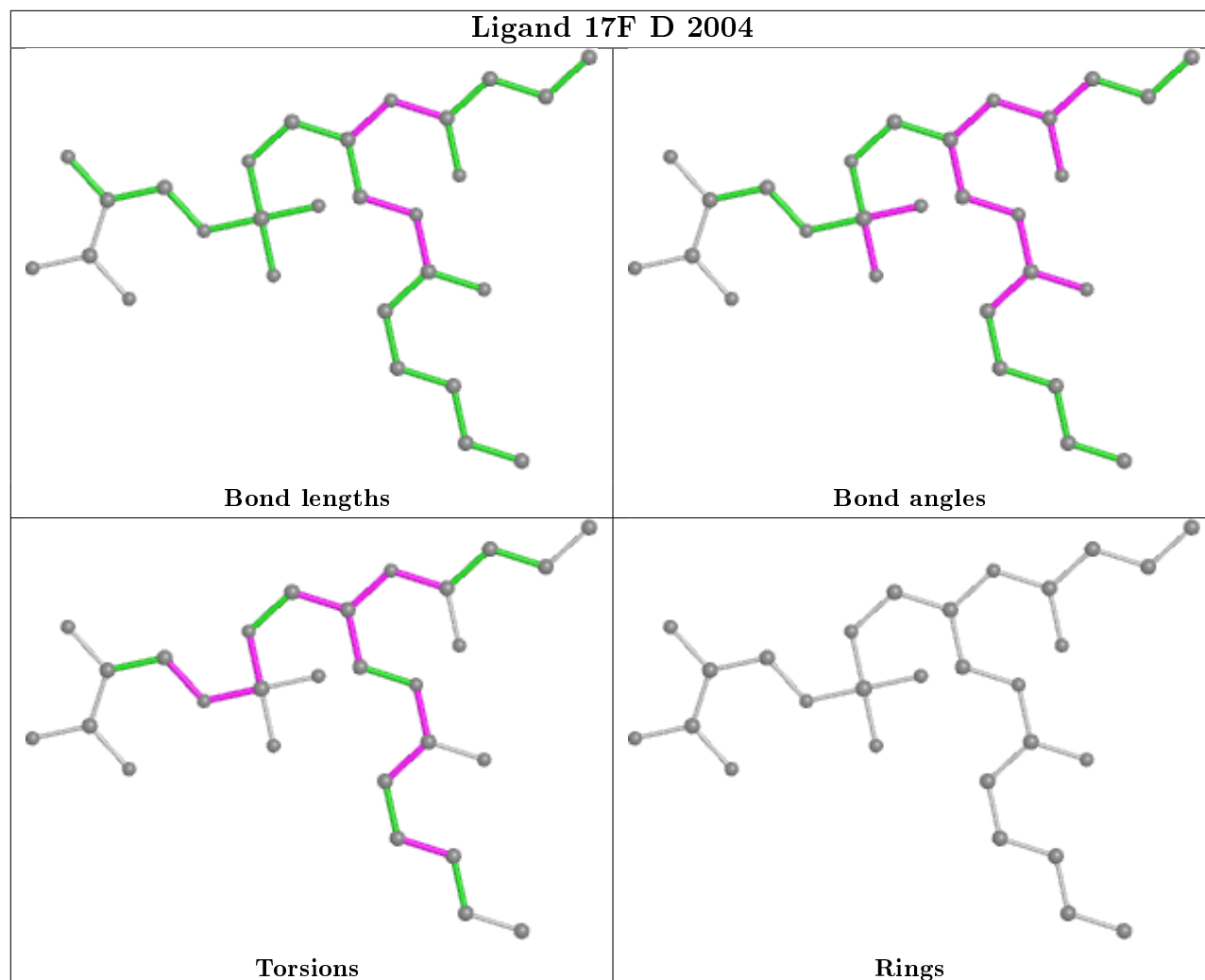
Mol	Chain	Res	Type	Atoms
10	B	1005	17F	O3-C1-C2-N1
10	B	1005	17F	O3-C1-C2-C3
10	B	1005	17F	C1-O3-P1-O1
10	B	1005	17F	C1-O3-P1-O2
10	B	1005	17F	C1-O3-P1-O6

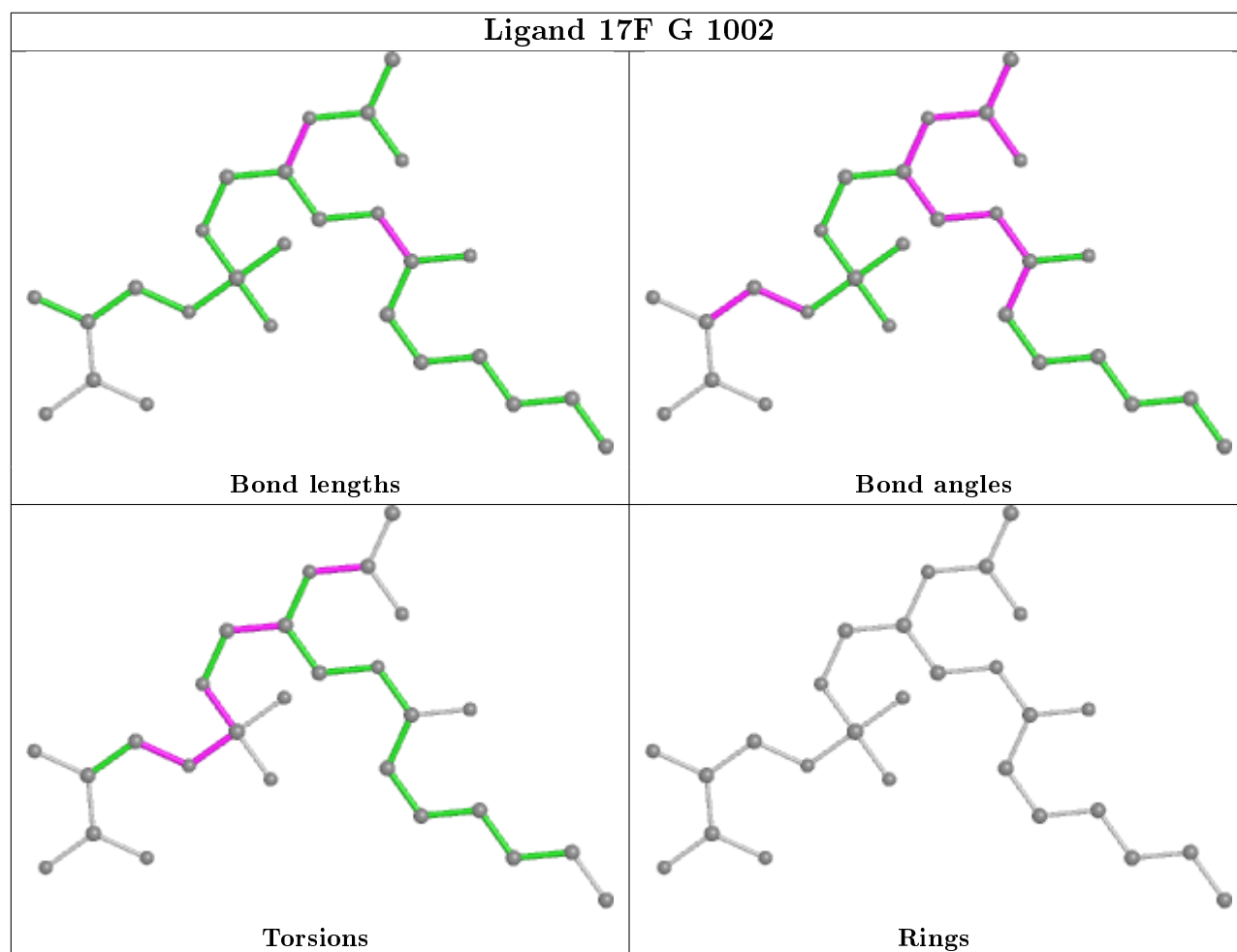
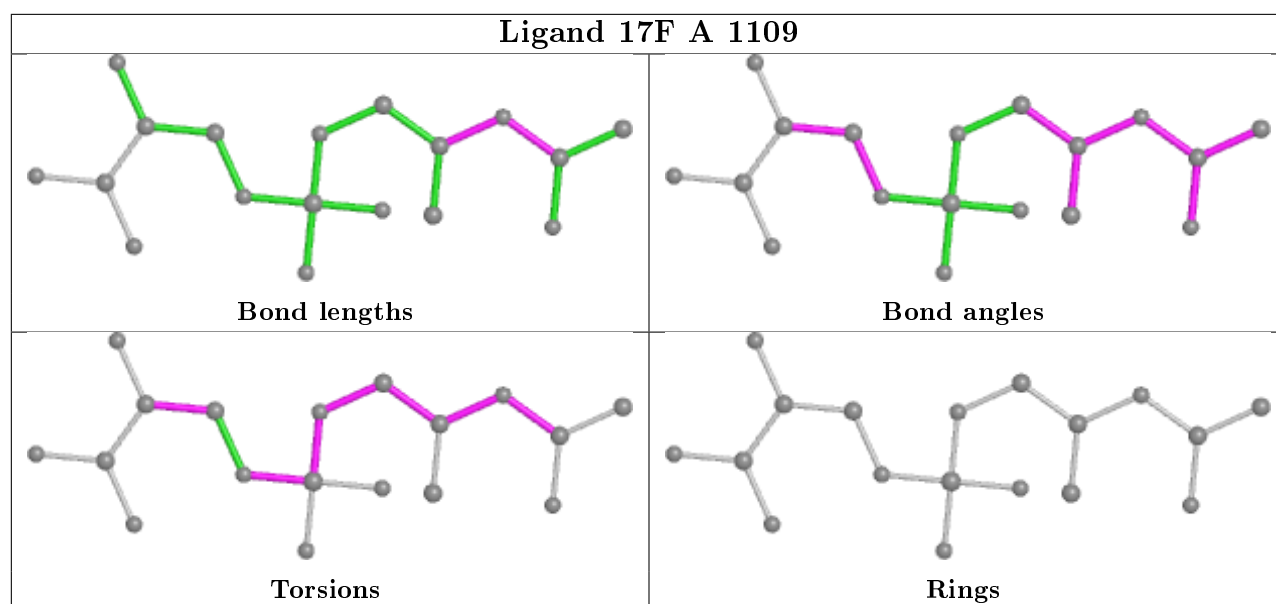
There are no ring outliers.

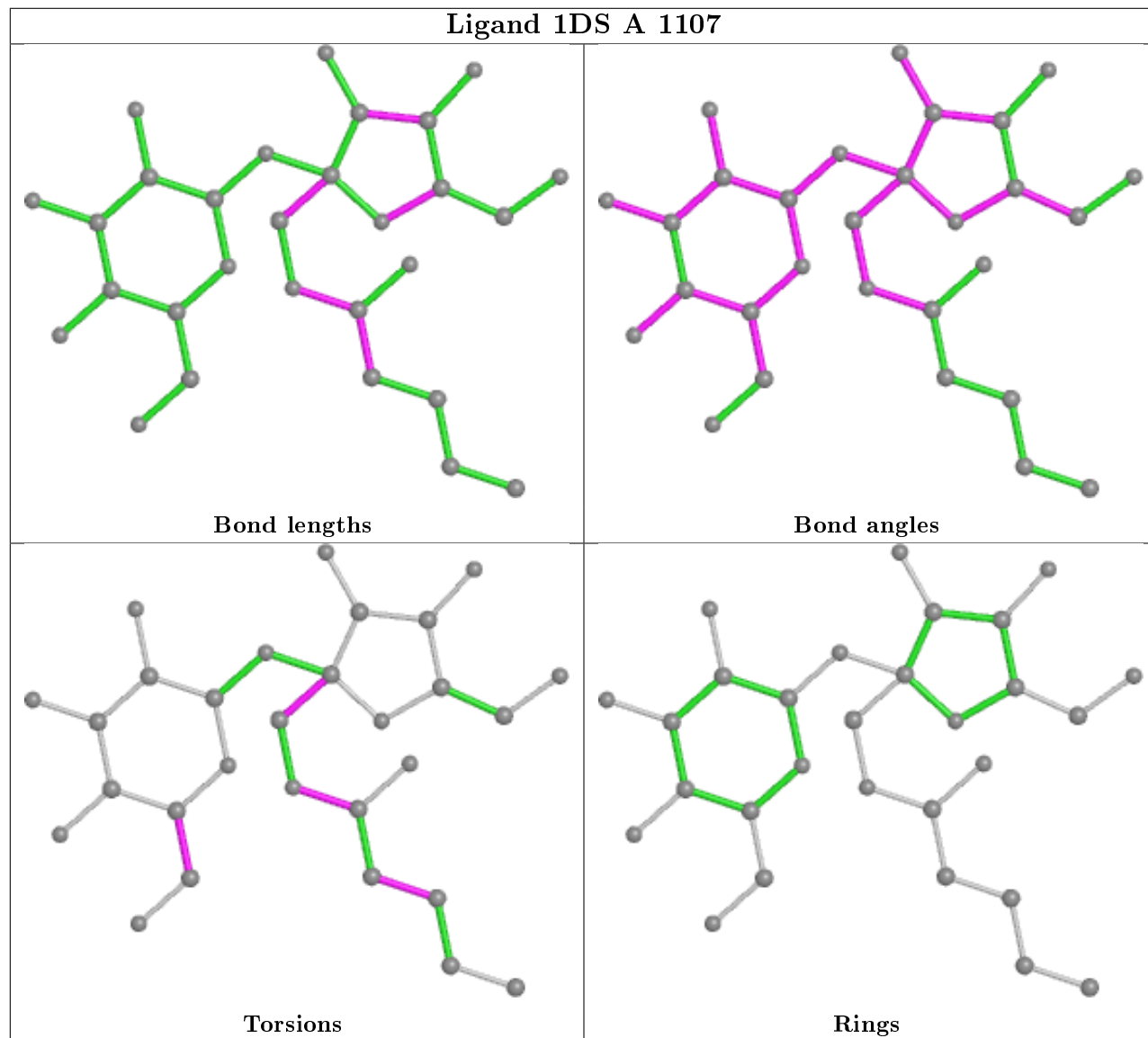
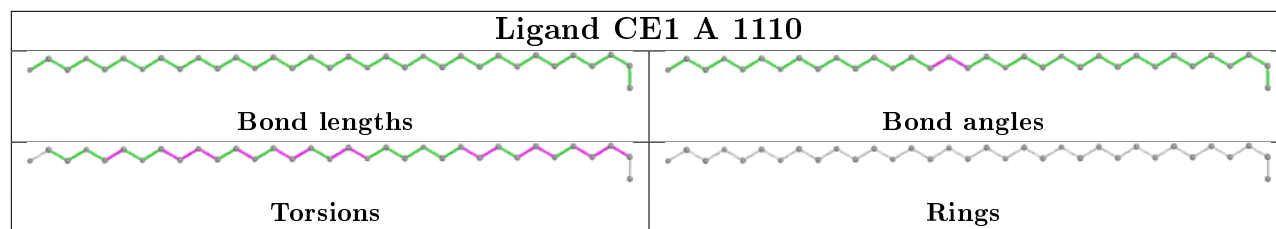
14 monomers are involved in 75 short contacts:

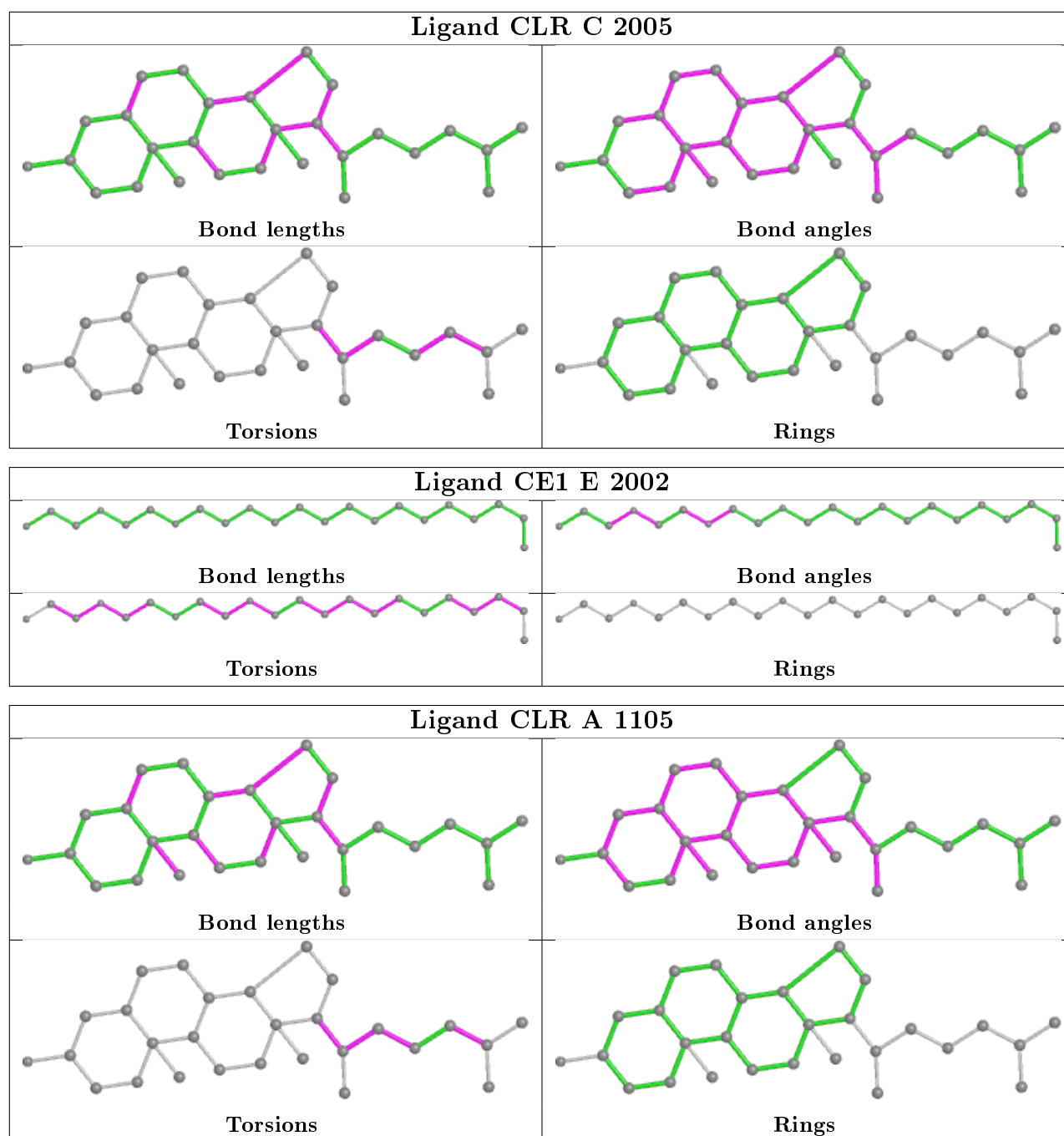
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	1001	CLR	4	0
10	A	1109	17F	2	0
10	G	1002	17F	4	0
11	A	1110	CE1	18	0
9	A	1107	1DS	6	0
7	C	2005	CLR	2	0
11	E	2002	CE1	1	0
7	A	1105	CLR	5	0
8	A	1106	1AT	6	0
7	E	2001	CLR	4	0
10	A	1108	17F	6	0
10	B	1005	17F	2	0
6	A	1104	OBN	10	0
6	C	2004	OBN	6	0

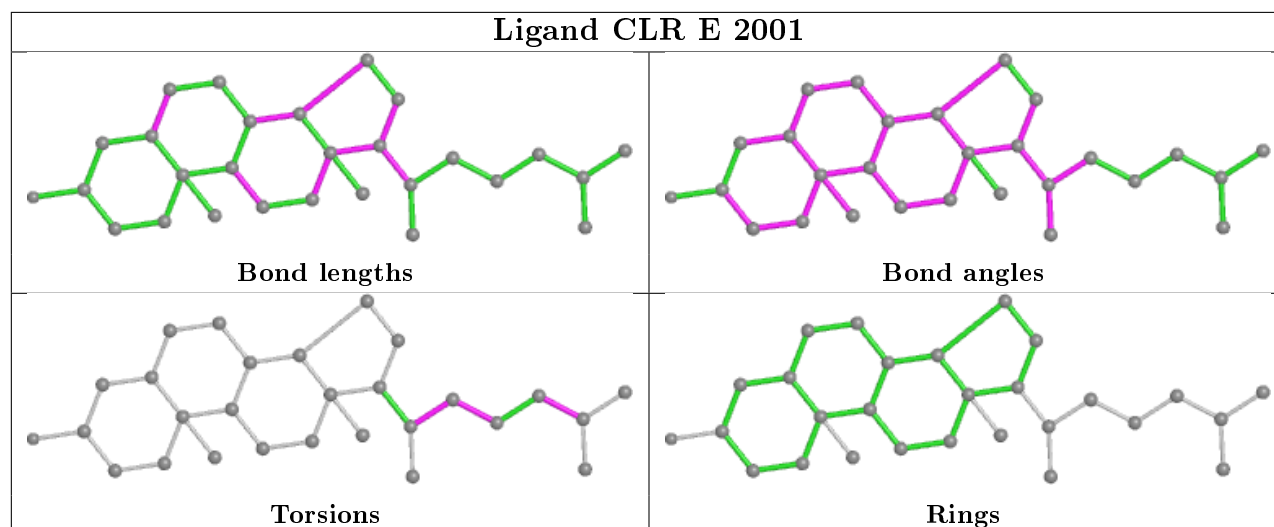
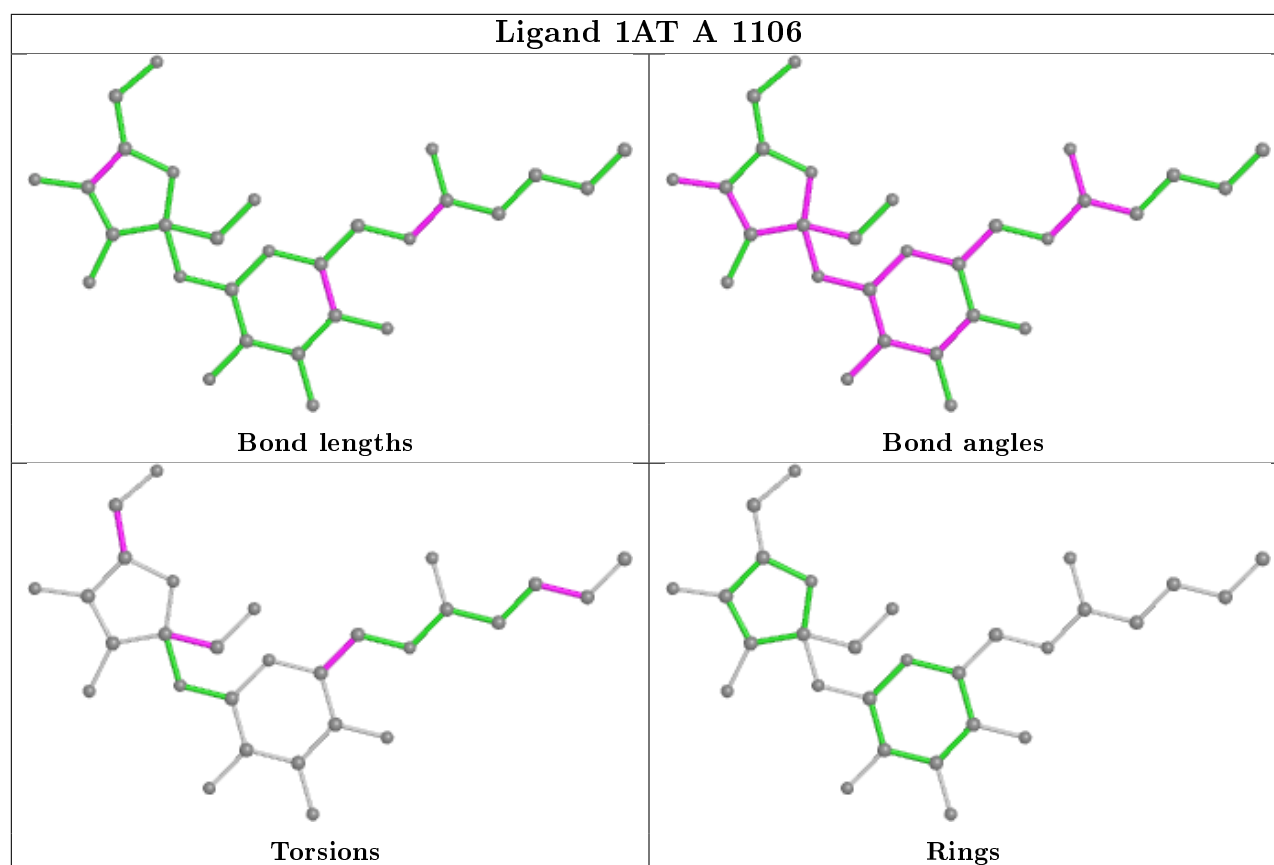
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

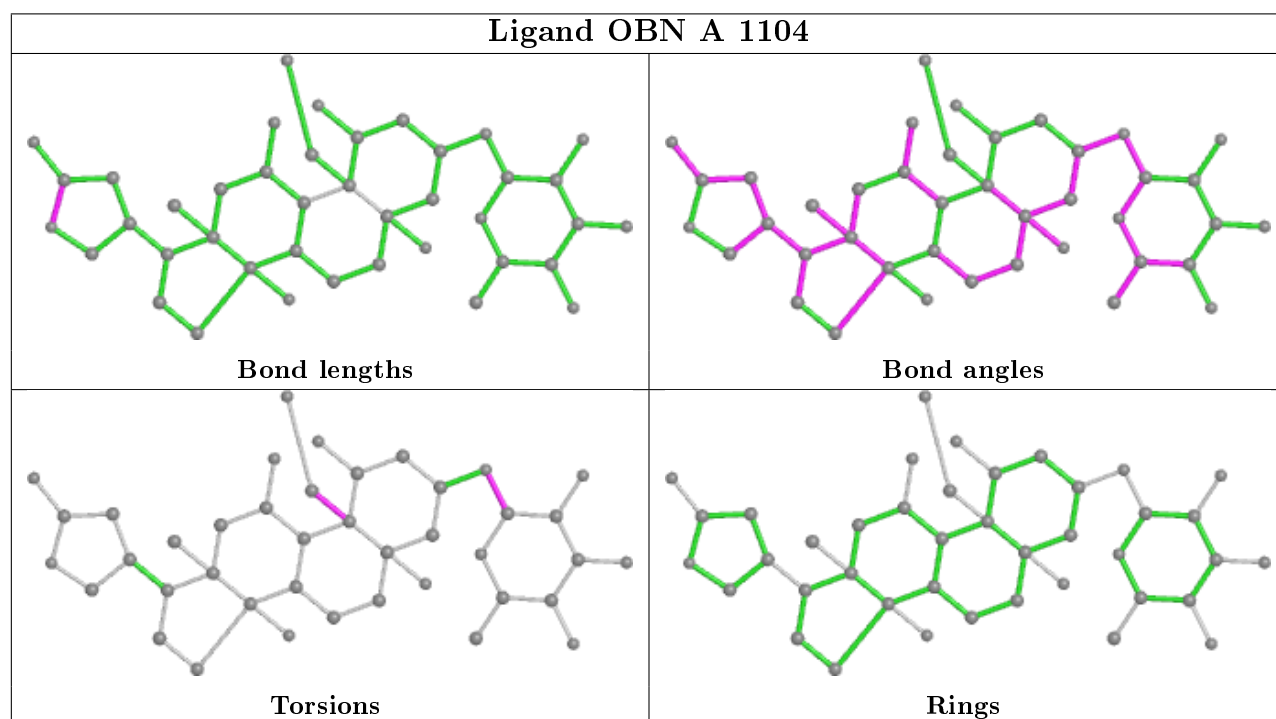
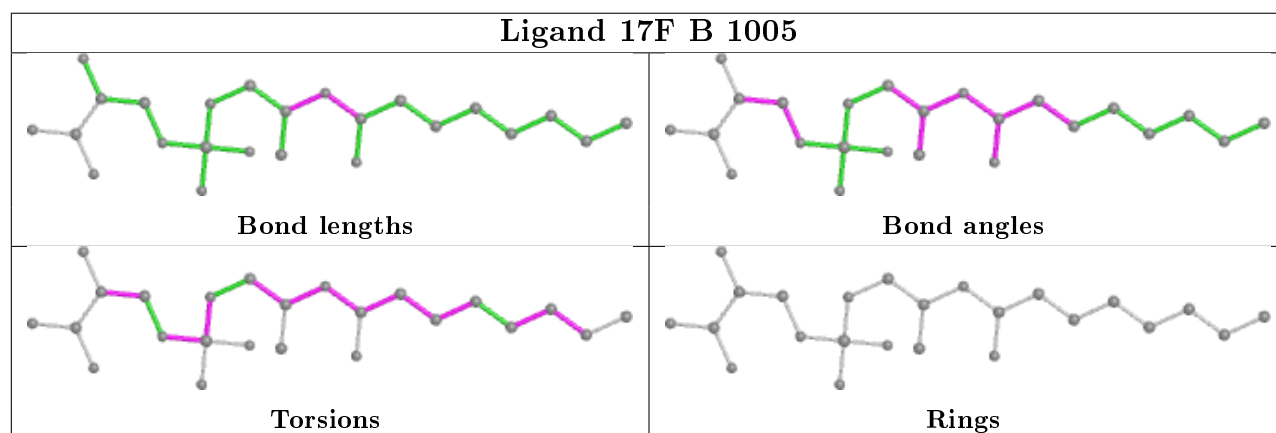
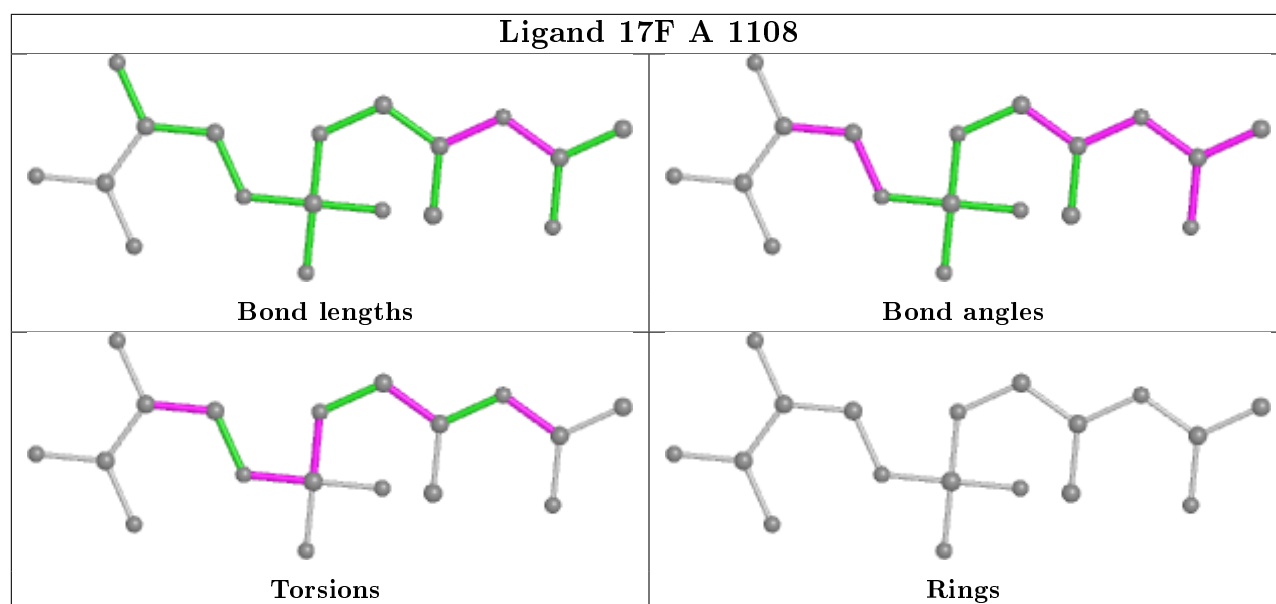


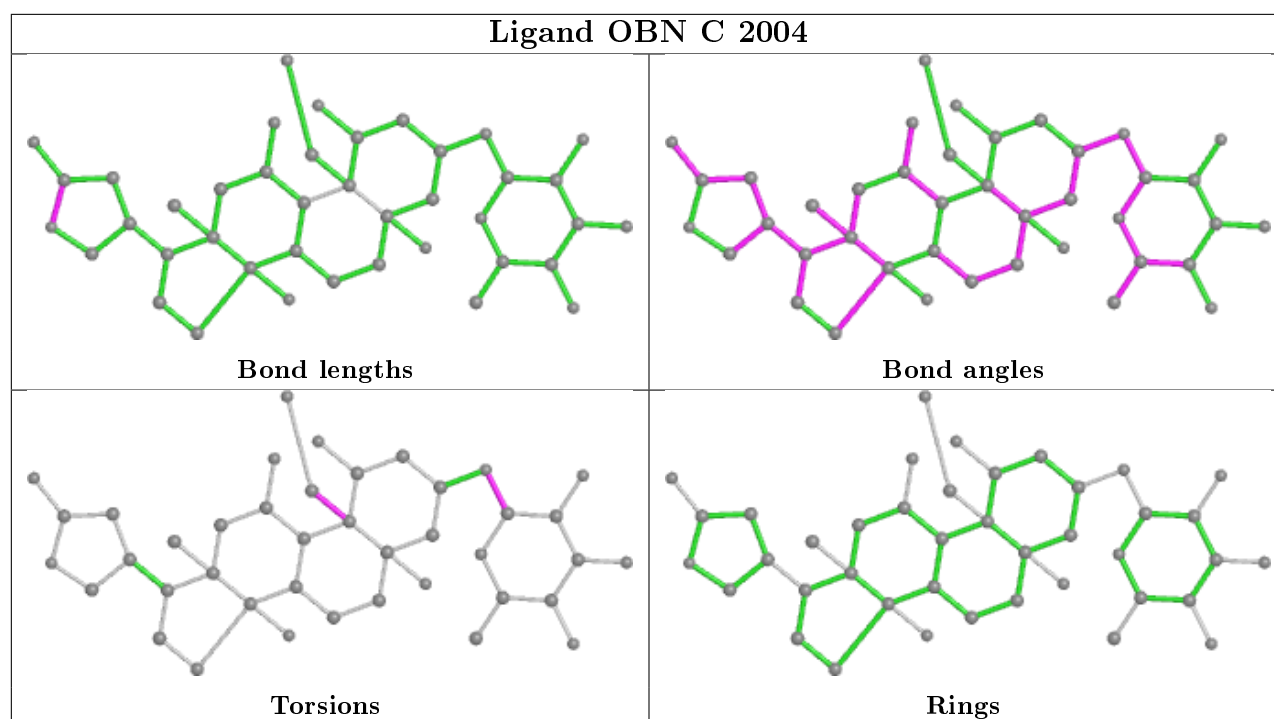












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	995/1021 (97%)	0.01	39 (3%) 39 38	51, 91, 218, 288	0
1	C	995/1021 (97%)	0.24	85 (8%) 10 12	58, 126, 273, 342	0
2	B	289/303 (95%)	0.09	14 (4%) 30 31	67, 151, 221, 258	0
2	D	287/303 (94%)	0.31	22 (7%) 13 15	63, 136, 210, 241	0
3	E	32/65 (49%)	-0.48	0 100 100	72, 81, 120, 147	0
3	G	32/65 (49%)	-0.13	1 (3%) 49 48	64, 83, 134, 141	0
All	All	2630/2778 (94%)	0.13	161 (6%) 21 22	51, 116, 242, 342	0

The worst 5 of 161 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	217	ARG	14.6
2	D	218	ASP	10.6
1	C	491	THR	8.3
1	C	545	VAL	8.0
1	A	471	VAL	7.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PHD	C	369	12/13	0.98	0.18	107,112,123,124	0
1	PHD	A	369	12/13	0.98	0.17	66,71,74,75	0

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	F	2	14/15	0.72	0.41	205,218,224,229	0
4	NAG	F	1	14/15	0.82	0.18	179,192,203,207	0

6.4 Ligands [i](#)

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

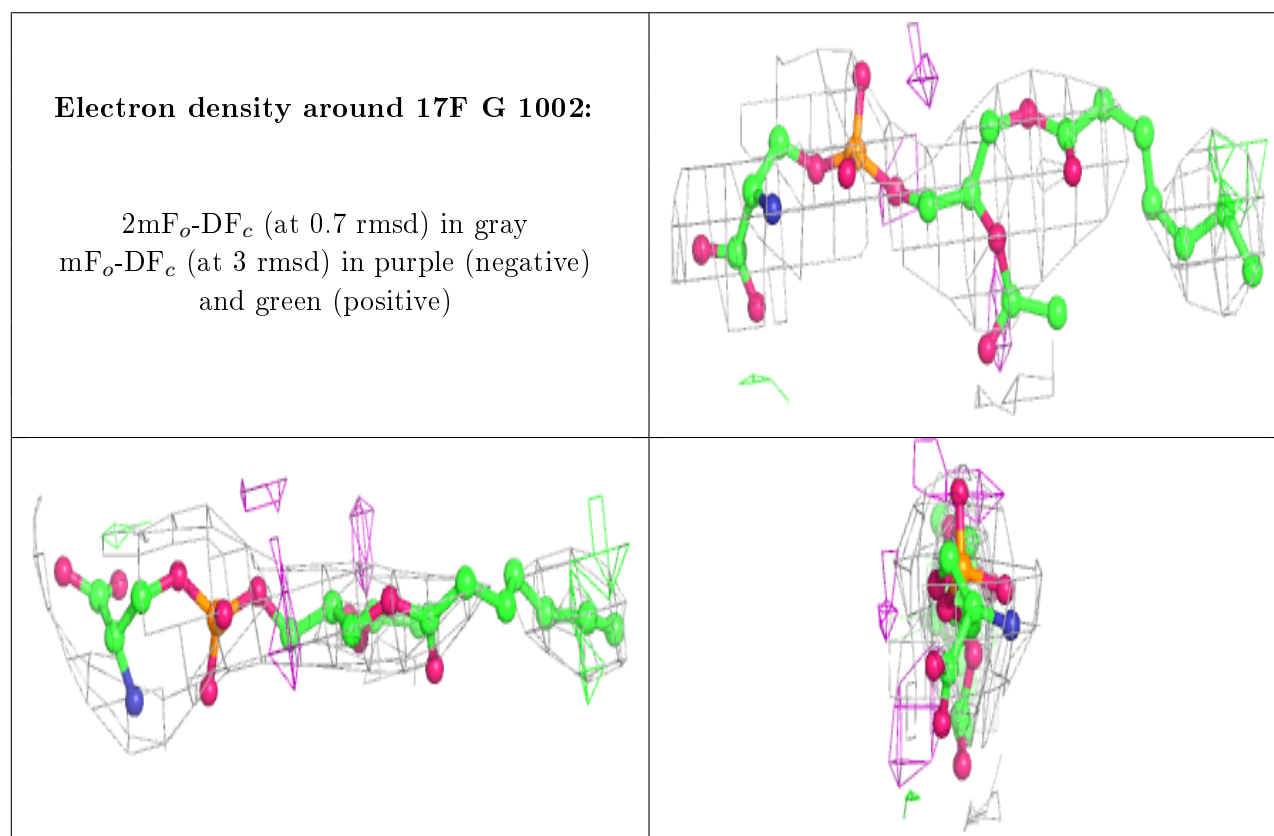
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	17F	G	1002	27/54	0.71	0.40	83,124,256,258	0
12	NAG	B	1003	14/15	0.71	0.22	197,209,221,225	0
12	NAG	B	1004	14/15	0.74	0.45	199,203,212,213	0
10	17F	B	1005	24/54	0.78	0.28	74,128,199,208	0
12	NAG	D	2002	14/15	0.79	0.14	142,150,163,169	0
12	NAG	D	2003	14/15	0.81	0.31	191,198,211,218	0
10	17F	D	2004	28/54	0.82	0.47	154,172,243,246	0
7	CLR	C	2005	28/28	0.84	0.49	93,104,113,231	0
10	17F	A	1109	18/54	0.84	0.32	96,114,166,169	0
10	17F	A	1108	18/54	0.84	0.32	80,155,188,197	0
12	NAG	D	2001	14/15	0.85	0.22	138,159,173,175	0
11	CE1	E	2002	22/37	0.86	0.36	67,109,155,157	0
11	CE1	A	1110	34/37	0.87	0.30	79,110,144,146	0
5	MG	C	2003	1/1	0.92	0.19	81,81,81,81	0
9	1DS	A	1107	29/34	0.93	0.20	56,123,141,170	0
7	CLR	A	1105	28/28	0.93	0.26	74,112,143,159	0
6	OBN	C	2004	41/41	0.94	0.19	84,92,99,104	0
8	1AT	A	1106	29/34	0.94	0.19	85,99,116,118	0
5	MG	A	1103	1/1	0.95	0.22	58,58,58,58	0
6	OBN	A	1104	41/41	0.95	0.19	72,81,85,88	0
5	MG	A	1101	1/1	0.96	0.18	113,113,113,113	0
7	CLR	E	2001	28/28	0.96	0.25	64,71,73,73	0
7	CLR	G	1001	28/28	0.97	0.20	57,66,79,83	0
5	MG	C	2002	1/1	0.97	0.34	124,124,124,124	0
5	MG	A	1102	1/1	0.97	0.41	82,82,82,82	0

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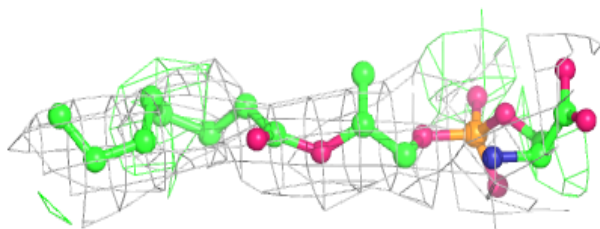
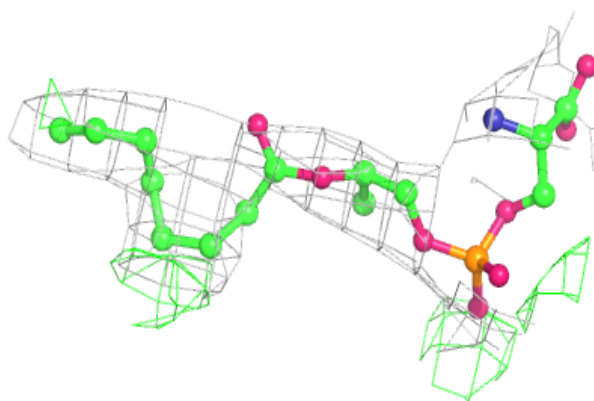
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	C	2001	1/1	0.98	0.20	147,147,147,147	0

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

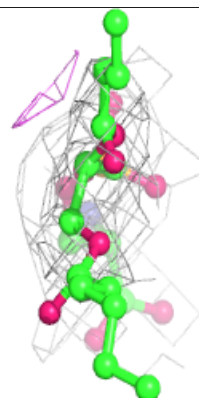
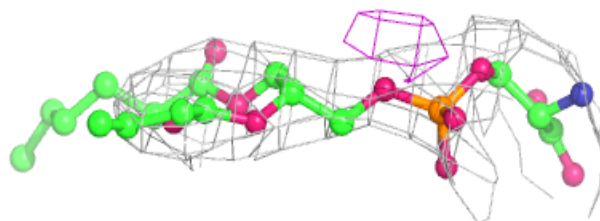
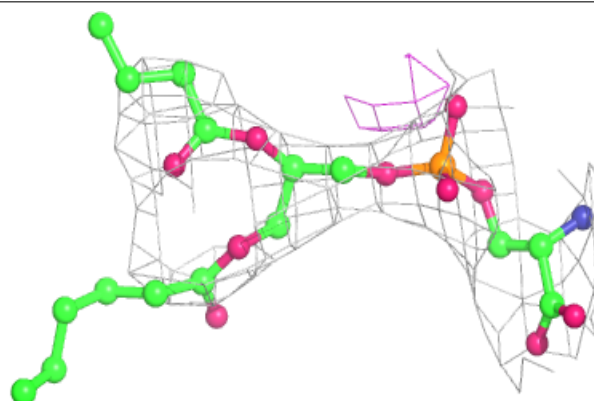


Electron density around 17F B 1005:

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

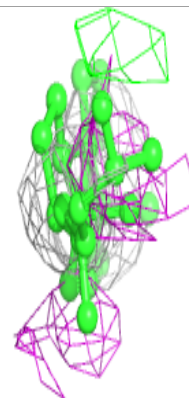
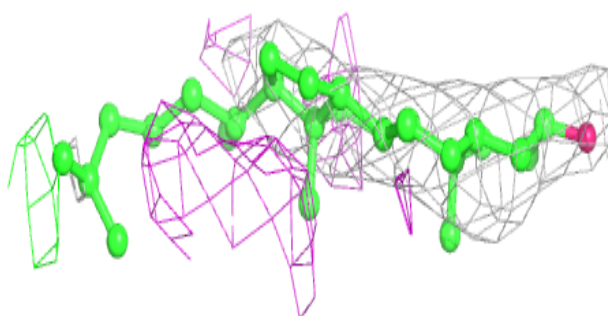
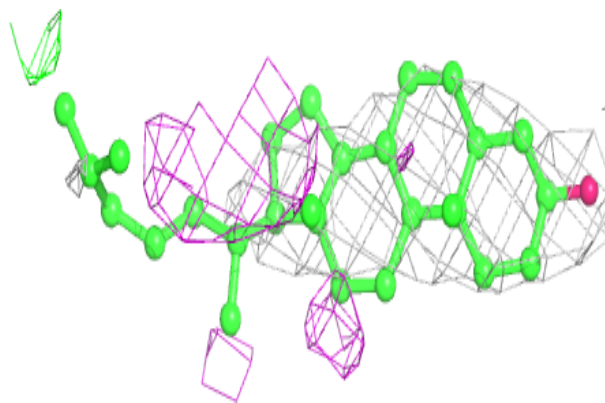
**Electron density around 17F D 2004:**

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

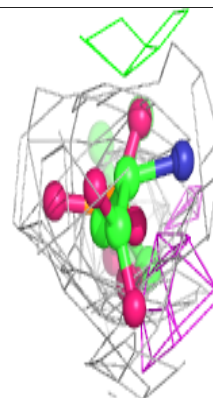
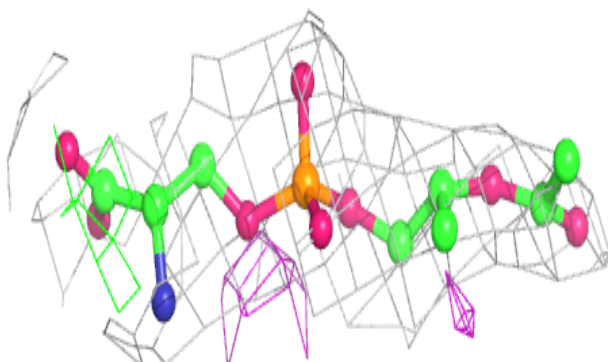
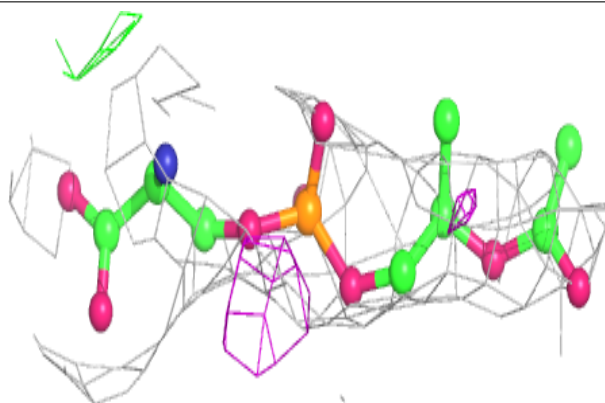


Electron density around CLR C 2005:

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

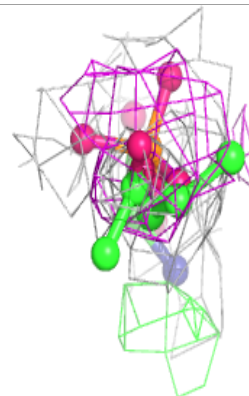
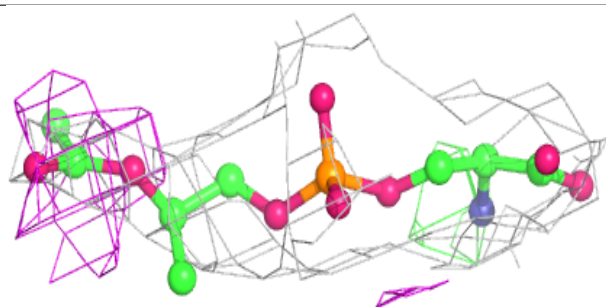
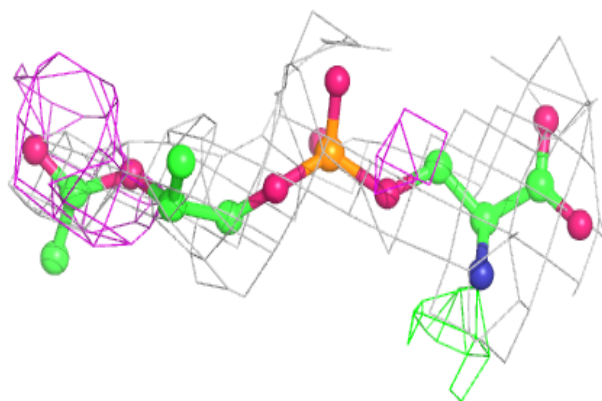
**Electron density around 17F A 1109:**

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and green (positive)

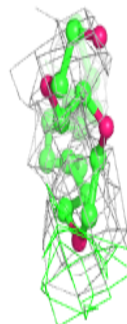
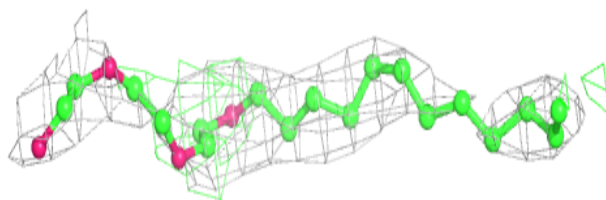
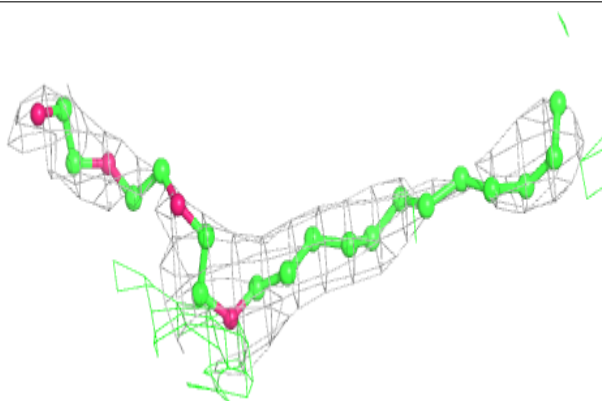


Electron density around 17F A 1108:

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

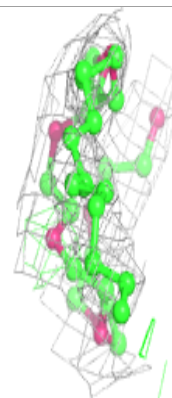
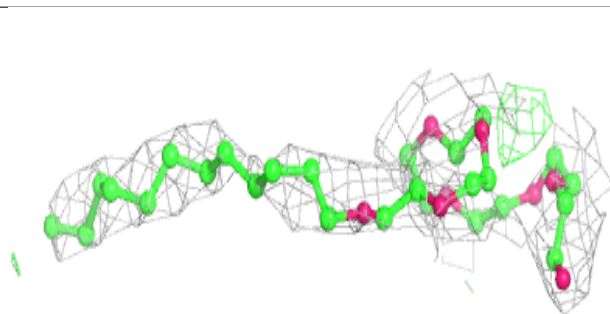
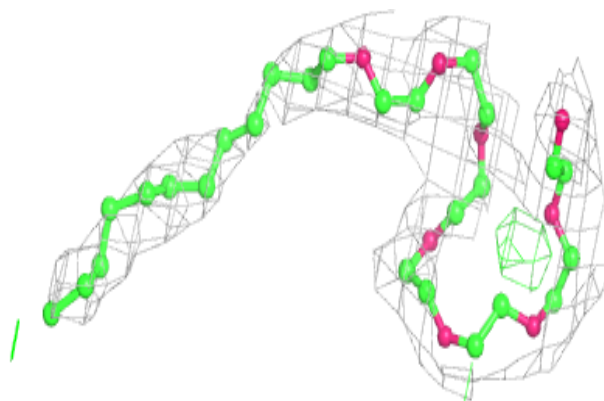
**Electron density around CE1 E 2002:**

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

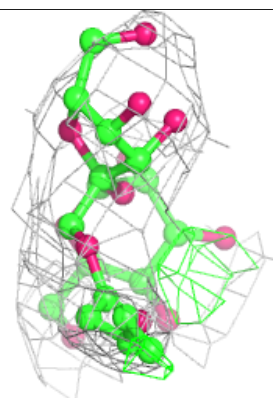
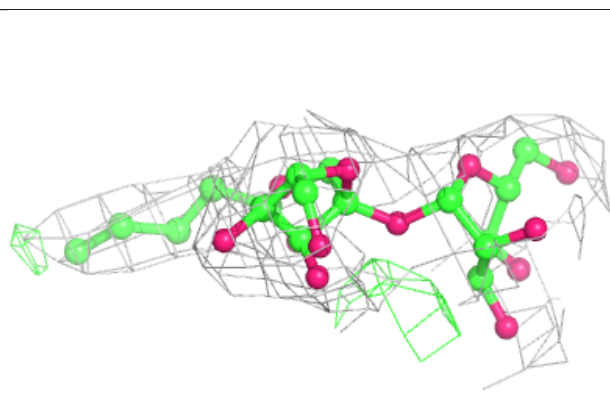
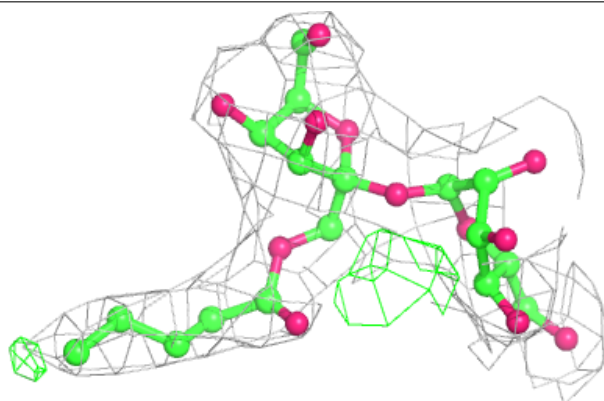


Electron density around CE1 A 1110:

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

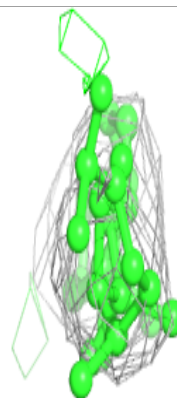
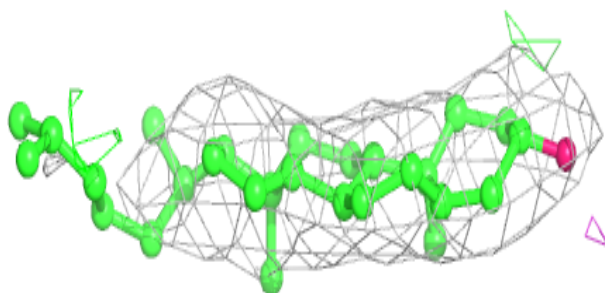
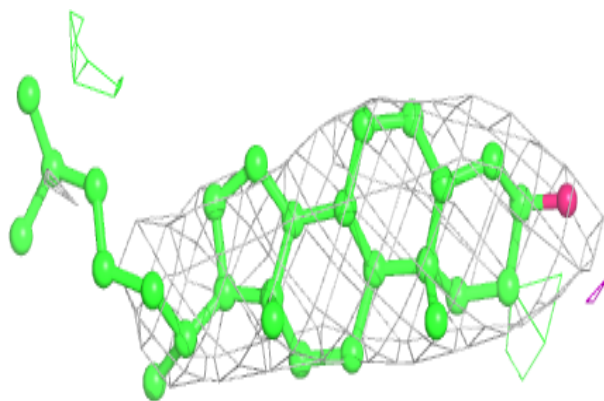
**Electron density around 1DS A 1107:**

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

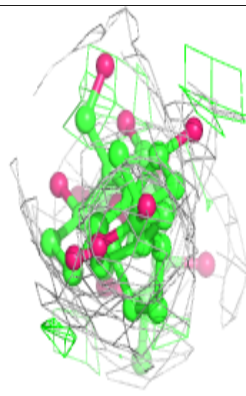
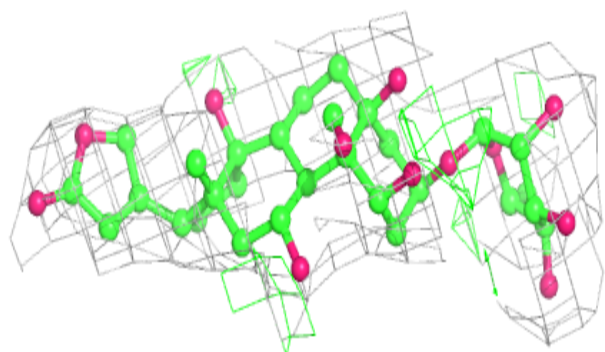
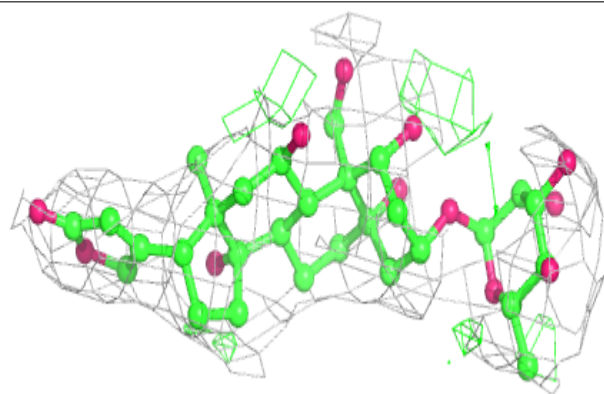


Electron density around CLR A 1105:

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

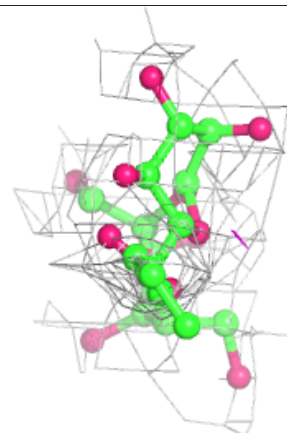
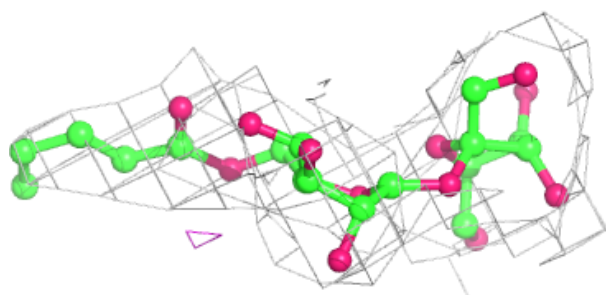
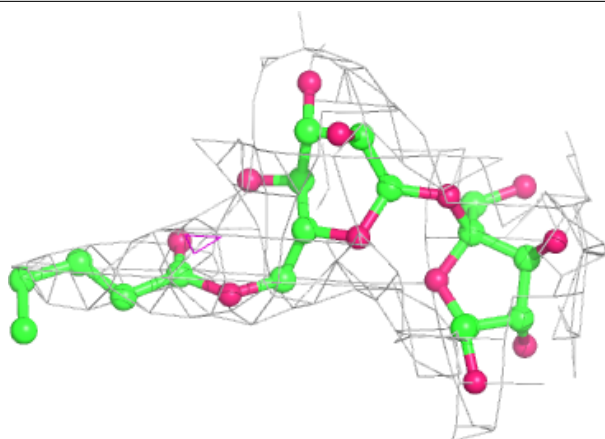
**Electron density around OBN C 2004:**

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

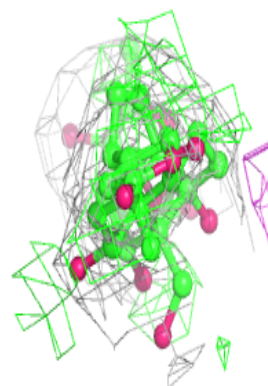
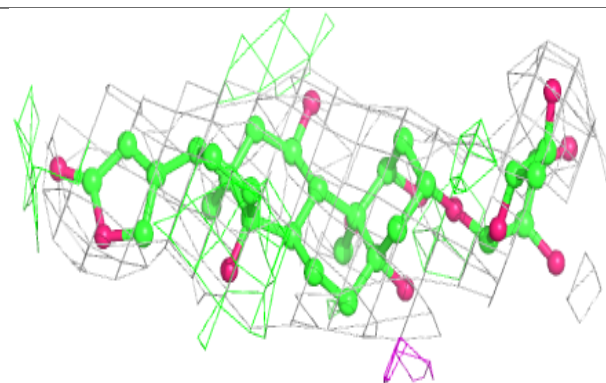
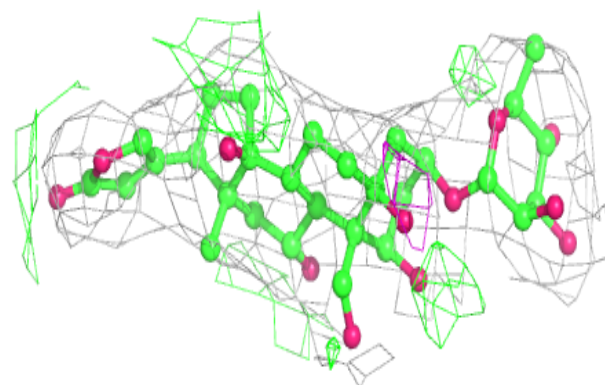


Electron density around 1AT A 1106:

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

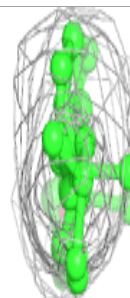
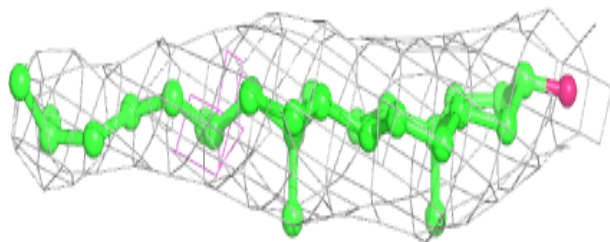
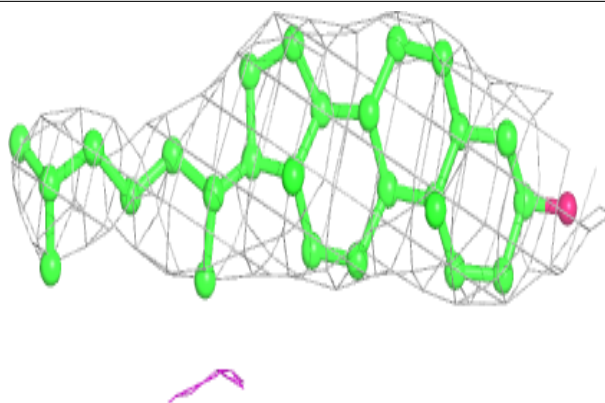
**Electron density around OBN A 1104:**

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

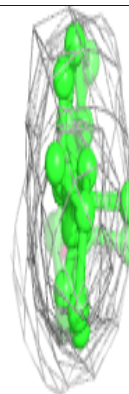
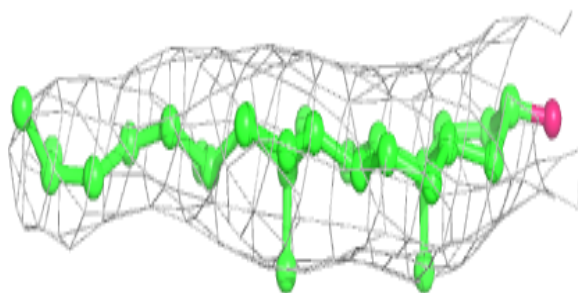
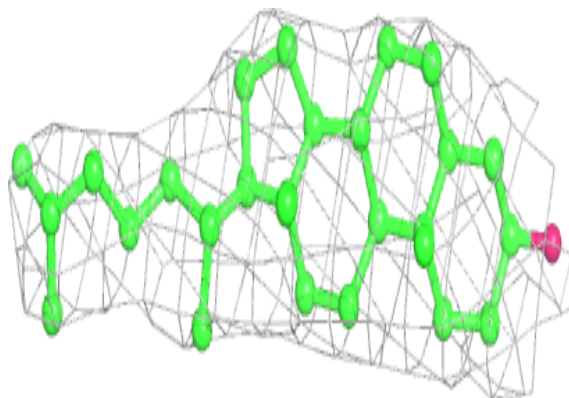


Electron density around CLR E 2001:

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

**Electron density around CLR G 1001:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.