



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 10:04 PM BST

PDB ID : 3WGV  
Title : Crystal structure of a Na<sup>+</sup>-bound Na<sup>+</sup>,K<sup>+</sup>-ATPase preceding the E1P state with oligomycin  
Authors : Kanai, R.; Ogawa, H.; Vilsen, B.; Cornelius, F.; Toyoshima, C.  
Deposited on : 2013-08-09  
Resolution : 2.80 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](mailto: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.

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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

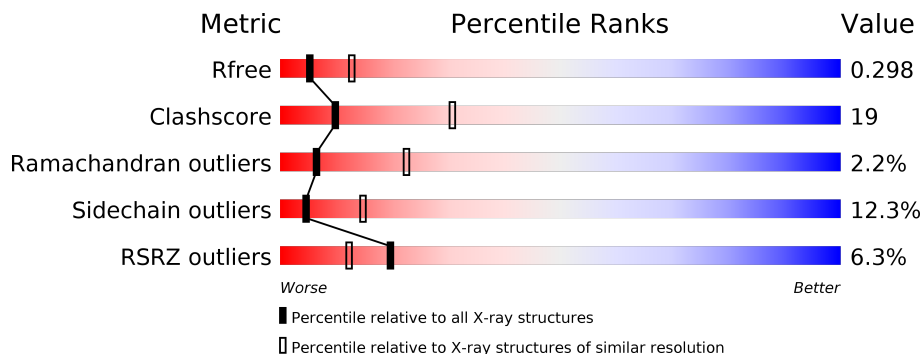
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1016	
1	C	1016	
2	B	303	
2	D	303	
3	E	65	
3	G	65	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
10	EFO	C	2013	-	-	-	X
5	ALF	C	2002	-	-	X	-
7	NA	C	2006	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21909 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
			Total	C	N	O	S			
1	A	994	7714	4918	1300	1449	47	0	0	0
1	C	994	7714	4918	1300	1449	47	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	303	2479	1603	408	454	14	0	0	0
2	D	303	2479	1603	408	454	14	0	0	0

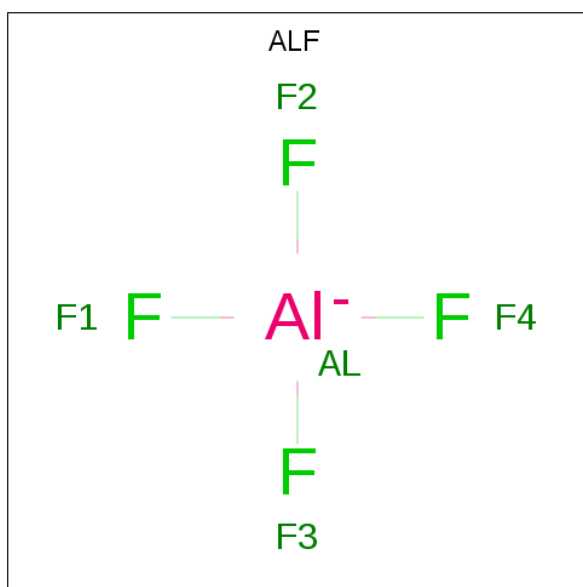
- Molecule 3 is a protein called Na<sup>+</sup>/K<sup>+</sup> ATPase gamma subunit transcript variant a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	G	34	270	183	39	48	0	0	0
3	E	35	281	189	43	49	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

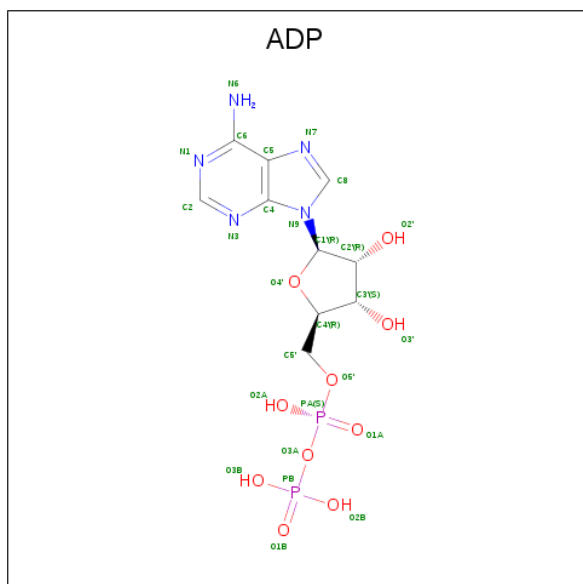
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	2	2	2	0	0
4	C	2	2	2	0	0

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF<sub>4</sub>).



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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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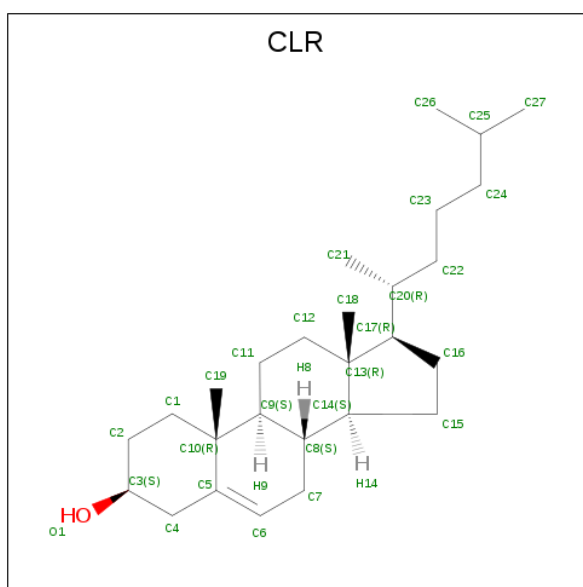
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	C	1	27	10	5	10	2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

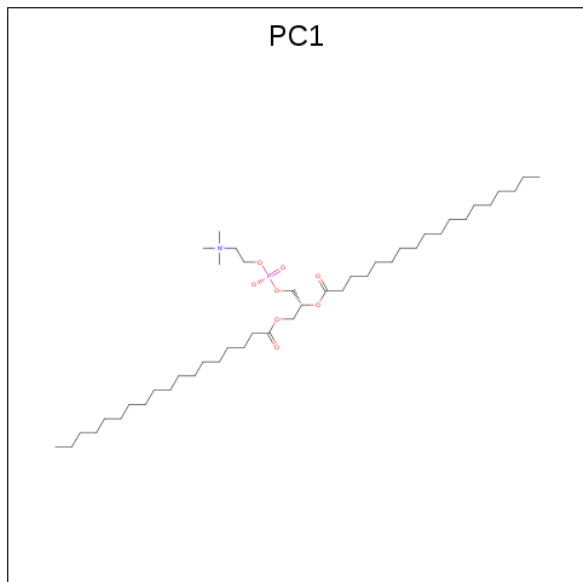
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Na	0	0
			4	4		
7	C	4	Total	Na	0	0
			4	4		

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



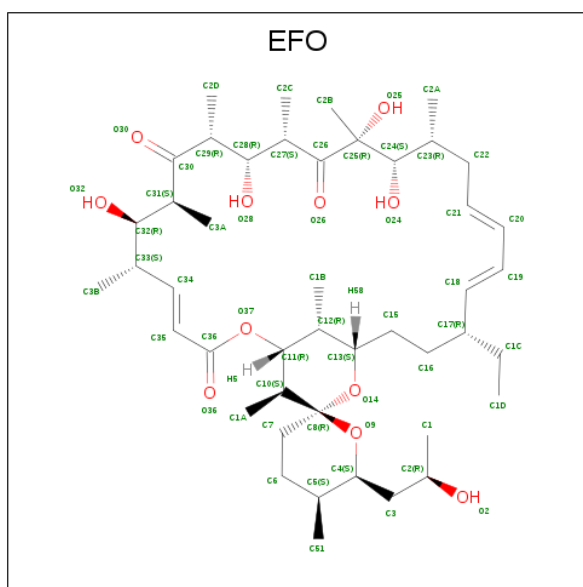
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			28	27	1		
8	A	1	Total	C	O	0	0
			28	27	1		
8	G	1	Total	C	O	0	0
			28	27	1		
8	D	1	Total	C	O	0	0
			28	27	1		
8	D	1	Total	C	O	0	0
			28	27	1		
8	E	1	Total	C	O	0	0
			28	27	1		

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



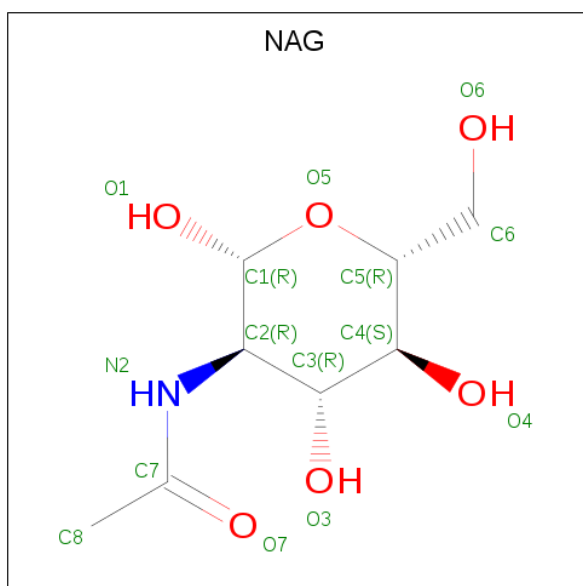
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44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

- Molecule 10 is Oligomycin A (three-letter code: EFO) (formula:  $C_{45}H_{74}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			56	45	11		
10	C	1	Total	C	O	0	0
			56	45	11		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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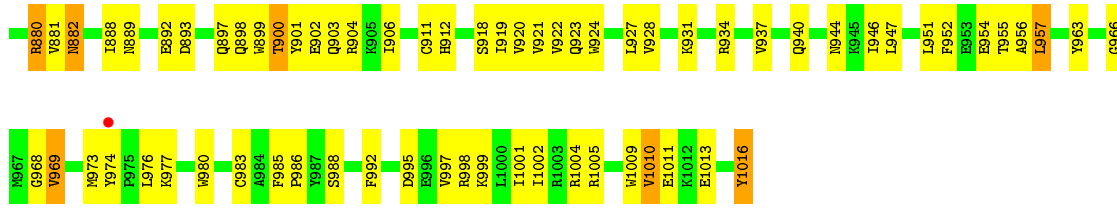
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	D	1	14	8	1	5	0	0

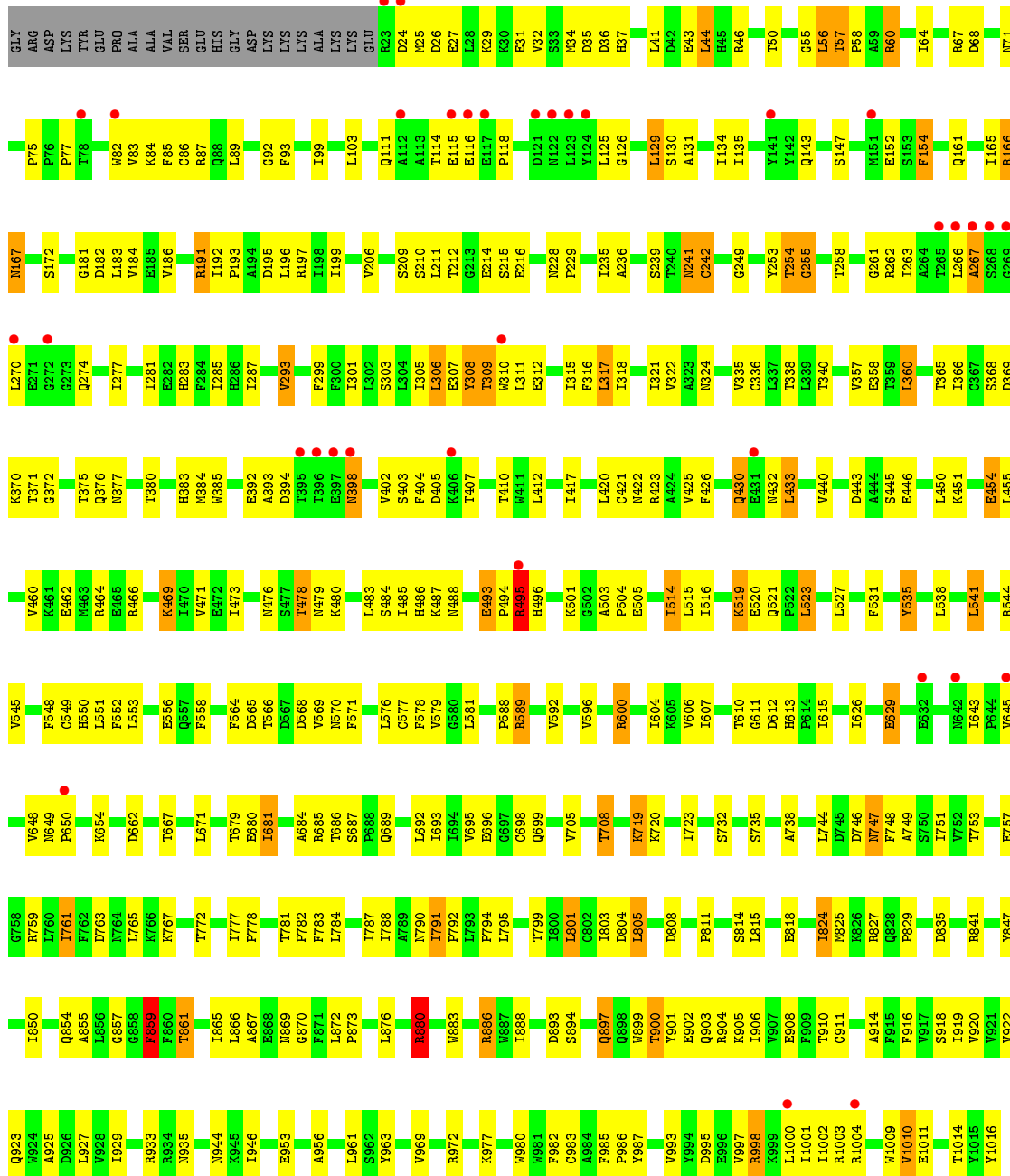
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	24	Total	O	0	0
			24	24		
12	B	2	Total	O	0	0
			2	2		
12	C	20	Total	O	0	0
			20	20		
12	D	2	Total	O	0	0
			2	2		

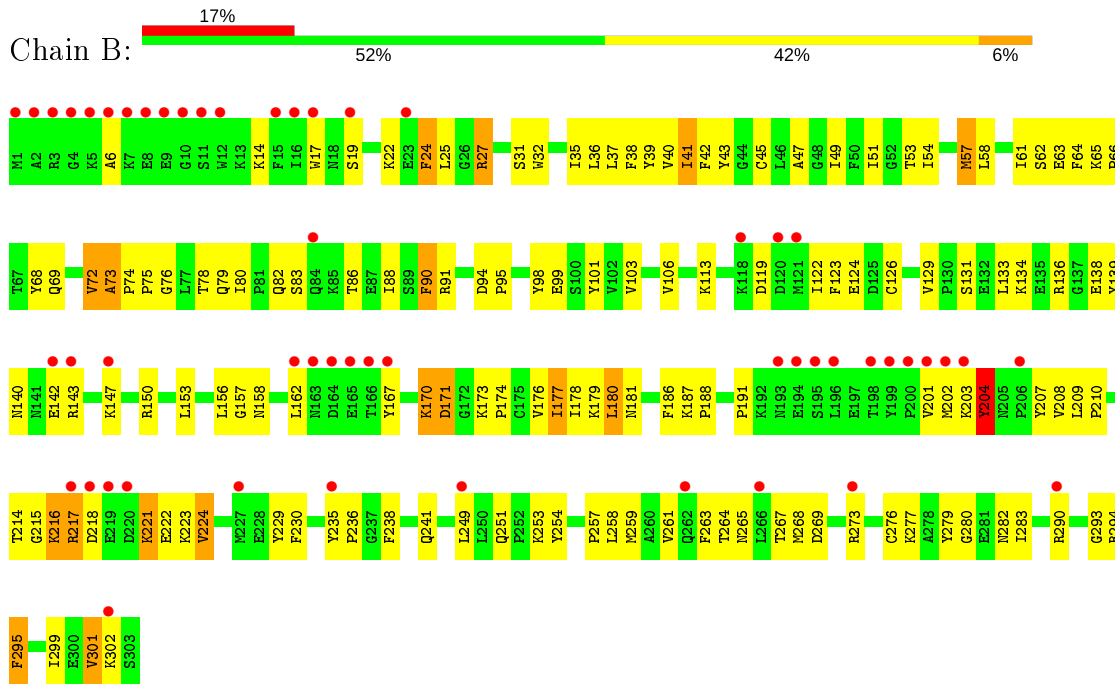




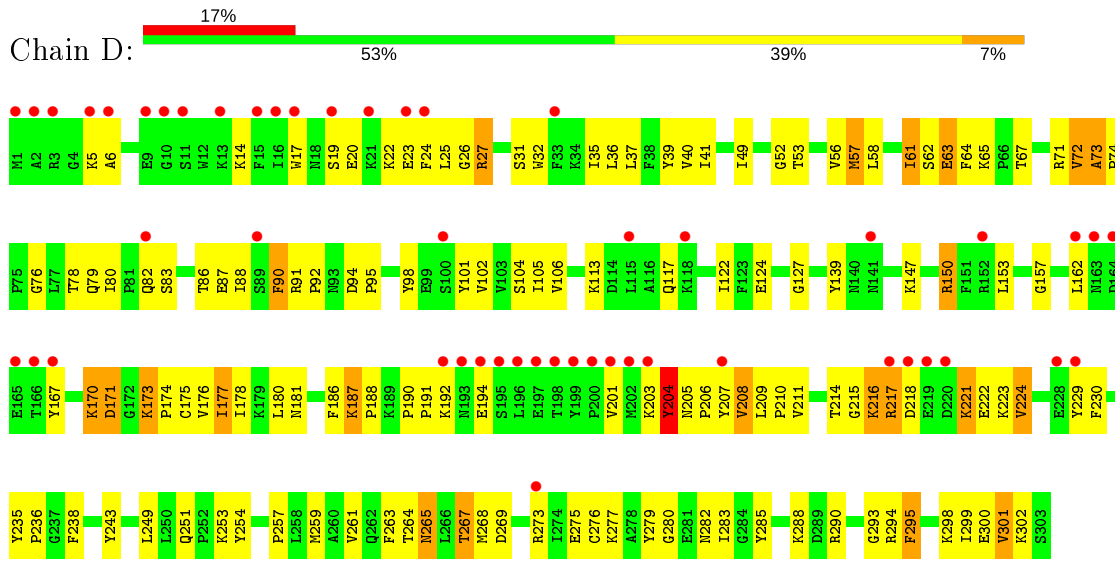
• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1



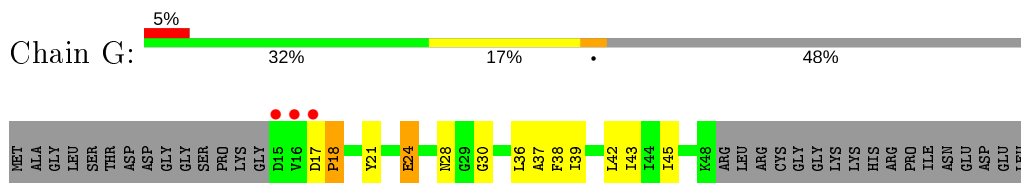
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



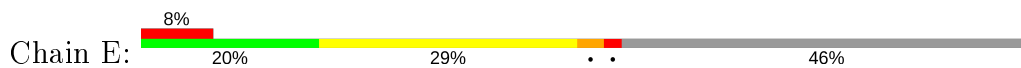
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

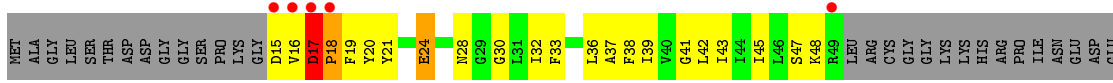


• Molecule 3: Na<sup>+</sup>/K<sup>+</sup> ATPase gamma subunit transcript variant a



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





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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.28Å 210.18Å 256.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.99 – 2.80 15.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (15.99-2.80) 94.4 (15.99-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.82Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.270 , 0.298 0.270 , 0.298	Depositor DCC
$R_{free}$ test set	3965 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtrriage
Anisotropy	0.394	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.10 , -10.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	21909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAG, ADP, ALF, NA, PC1, EFO, 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	0.46	1/7864 (0.0%)	0.66	7/10671 (0.1%)
1	C	0.39	0/7864	0.58	2/10671 (0.0%)
2	B	0.34	0/2544	0.53	1/3426 (0.0%)
2	D	0.34	0/2544	0.53	0/3426
3	E	0.35	0/287	0.56	0/389
3	G	0.38	0/276	0.54	0/375
All	All	0.41	1/21379 (0.0%)	0.60	10/28958 (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
3	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	656	CYS	CB-SG	-5.07	1.73	1.81

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	ARG	CB-CA-C	-9.36	91.69	110.40
1	A	600	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	A	600	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	239	SER	CB-CA-C	-6.59	97.57	110.10
1	C	239	SER	CB-CA-C	-6.45	97.85	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	17	ASP	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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	7714	0	7770	303	0
1	C	7714	0	7769	264	0
2	B	2479	0	2458	103	0
2	D	2479	0	2458	98	0
3	E	281	0	285	14	0
3	G	270	0	272	12	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	A	5	0	0	1	0
5	C	5	0	0	2	0
6	A	27	0	12	3	0
6	C	27	0	12	6	0
7	A	4	0	0	0	0
7	C	4	0	0	0	0
8	A	56	0	92	27	0
8	D	56	0	92	29	0
8	E	28	0	45	13	0
8	G	28	0	45	9	0
9	A	216	0	352	14	0
9	B	54	0	88	2	0
9	C	216	0	352	15	0
9	D	54	0	88	2	0
10	A	56	0	74	0	0
10	C	56	0	74	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	A	24	0	0	0	0
12	B	2	0	0	0	0
12	C	20	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	2	0	0	0	0
All	All	21909	0	22364	851	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 19.

The worst 5 of 851 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)
8:A:2009:CLR:C11	8:A:2009:CLR:C9	1.77	1.62
8:D:3002:CLR:C11	8:D:3002:CLR:C12	1.74	1.60
8:A:2010:CLR:C9	8:A:2010:CLR:C11	1.76	1.59
8:D:3001:CLR:C9	8:D:3001:CLR:C11	1.78	1.57
8:E:101:CLR:C11	8:E:101:CLR:C9	1.78	1.56

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	992/1016 (98%)	859 (87%)	114 (12%)	19 (2%)	8	26
1	C	992/1016 (98%)	884 (89%)	91 (9%)	17 (2%)	9	29
2	B	301/303 (99%)	238 (79%)	55 (18%)	8 (3%)	5	17
2	D	301/303 (99%)	231 (77%)	59 (20%)	11 (4%)	3	11
3	E	33/65 (51%)	31 (94%)	1 (3%)	1 (3%)	4	15
3	G	32/65 (49%)	27 (84%)	4 (12%)	1 (3%)	4	14
All	All	2651/2768 (96%)	2270 (86%)	324 (12%)	57 (2%)	6	22

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	A	402	VAL
2	B	82	GLN
2	B	139	TYR
3	G	18	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	844/861 (98%)	725 (86%)	119 (14%)	3	10
1	C	844/861 (98%)	755 (90%)	89 (10%)	7	20
2	B	269/269 (100%)	235 (87%)	34 (13%)	4	14
2	D	269/269 (100%)	237 (88%)	32 (12%)	5	16
3	E	29/52 (56%)	24 (83%)	5 (17%)	2	6
3	G	28/52 (54%)	26 (93%)	2 (7%)	14	39
All	All	2283/2364 (97%)	2002 (88%)	281 (12%)	4	15

5 of 281 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	63	GLU
1	C	41	LEU
2	D	177	ILE
2	B	90	PHE
2	B	217	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	262	GLN
1	C	120	ASN
2	D	158	ASN
3	G	28	ASN

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Mol	Chain	Res	Type
1	C	143	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	CLR	A	2010	-	31,31,31	4.42	11 (35%)	48,48,48	2.23	14 (29%)
8	CLR	D	3001	-	31,31,31	4.46	12 (38%)	48,48,48	2.15	15 (31%)
10	EFO	C	2013	-	57,58,58	2.26	21 (36%)	73,85,85	5.17	25 (34%)
9	PC1	C	2010	-	53,53,53	0.89	3 (5%)	59,61,61	1.37	5 (8%)
9	PC1	C	2011	-	53,53,53	0.93	5 (9%)	59,61,61	1.31	5 (8%)
9	PC1	A	2014	-	53,53,53	0.90	3 (5%)	59,61,61	1.33	4 (6%)
10	EFO	A	2015	-	57,58,58	2.18	20 (35%)	73,85,85	5.27	26 (35%)
5	ALF	C	2002	-	0,4,4	0.00	-	-	-	-
9	PC1	C	2012	-	53,53,53	0.90	3 (5%)	59,61,61	1.27	4 (6%)
11	NAG	D	3004	-	14,14,15	0.24	0	17,19,21	0.49	0
5	ALF	A	2002	-	0,4,4	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	PC1	A	2012	-	53,53,53	0.92	2 (3%)	59,61,61	1.41	7 (11%)
9	PC1	A	2013	-	53,53,53	0.88	3 (5%)	59,61,61	1.18	4 (6%)
6	ADP	A	2004	4	24,29,29	1.12	3 (12%)	29,45,45	1.50	3 (10%)
6	ADP	C	2004	-	24,29,29	0.88	0	29,45,45	1.24	3 (10%)
8	CLR	A	2009	-	31,31,31	4.44	11 (35%)	48,48,48	2.16	15 (31%)
9	PC1	A	2011	-	53,53,53	0.90	4 (7%)	59,61,61	1.31	6 (10%)
11	NAG	B	402	-	14,14,15	0.22	0	17,19,21	0.42	0
8	CLR	D	3002	-	31,31,31	4.51	12 (38%)	48,48,48	1.93	15 (31%)
9	PC1	C	2009	-	53,53,53	0.91	4 (7%)	59,61,61	1.28	5 (8%)
9	PC1	B	401	-	53,53,53	0.89	4 (7%)	59,61,61	1.30	5 (8%)
8	CLR	E	101	-	31,31,31	4.62	13 (41%)	48,48,48	2.42	14 (29%)
9	PC1	D	3003	-	53,53,53	0.90	4 (7%)	59,61,61	1.20	4 (6%)
8	CLR	G	101	-	31,31,31	4.63	13 (41%)	48,48,48	2.66	13 (27%)

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	CLR	A	2010	-	-	1/10/68/68	0/4/4/4
8	CLR	D	3001	-	-	0/10/68/68	0/4/4/4
10	EFO	C	2013	-	-	10/72/110/110	0/2/3/3
9	PC1	C	2010	-	-	35/57/57/57	-
9	PC1	C	2011	-	-	33/57/57/57	-
9	PC1	A	2014	-	-	30/57/57/57	-
10	EFO	A	2015	-	-	9/72/110/110	0/2/3/3
9	PC1	C	2012	-	-	26/57/57/57	-
11	NAG	D	3004	-	-	1/6/23/26	0/1/1/1
9	PC1	A	2012	-	-	30/57/57/57	-
9	PC1	A	2013	-	-	30/57/57/57	-
6	ADP	A	2004	4	-	6/12/32/32	0/3/3/3
6	ADP	C	2004	-	-	1/12/32/32	0/3/3/3
8	CLR	A	2009	-	-	0/10/68/68	0/4/4/4
9	PC1	A	2011	-	-	24/57/57/57	-
11	NAG	B	402	-	-	0/6/23/26	0/1/1/1
8	CLR	D	3002	-	-	1/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PC1	C	2009	-	-	27/57/57/57	-
9	PC1	B	401	-	-	32/57/57/57	-
8	CLR	E	101	-	-	0/10/68/68	0/4/4/4
9	PC1	D	3003	-	-	29/57/57/57	-
8	CLR	G	101	-	-	1/10/68/68	0/4/4/4

The worst 5 of 151 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	101	CLR	C11-C9	15.42	1.79	1.53
8	D	3002	CLR	C11-C9	14.84	1.78	1.53
8	E	101	CLR	C11-C9	14.69	1.78	1.53
8	D	3001	CLR	C11-C9	14.57	1.78	1.53
8	A	2009	CLR	C11-C9	14.11	1.77	1.53

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2015	EFO	O9-C8-C10	-31.61	83.23	106.28
10	C	2013	EFO	O9-C8-C10	-30.78	83.85	106.28
10	A	2015	EFO	O9-C8-O14	20.84	161.70	109.68
10	C	2013	EFO	O9-C8-O14	20.26	160.24	109.68
10	A	2015	EFO	O14-C8-C7	-12.43	63.03	107.43

There are no chirality outliers.

5 of 326 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	2013	EFO	C12-C13-C15-C16
10	C	2013	EFO	C1-C2-C3-C4
10	C	2013	EFO	O2-C2-C3-C4
9	C	2010	PC1	O13-C11-C12-N
9	C	2011	PC1	C11-O13-P-O14

There are no ring outliers.

19 monomers are involved in 116 short contacts:

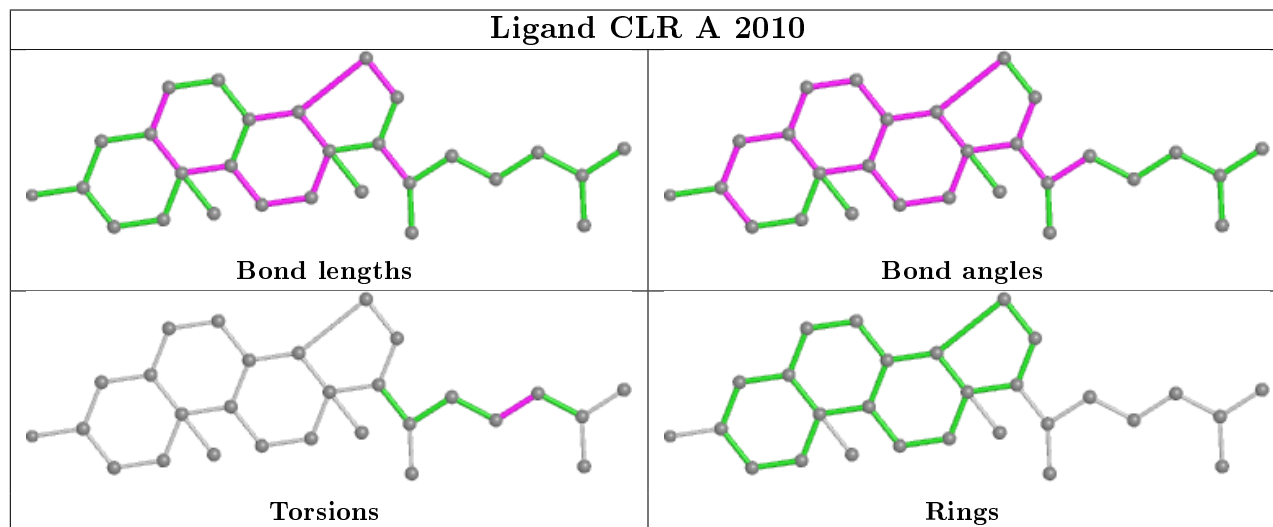
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2010	CLR	15	0
8	D	3001	CLR	12	0

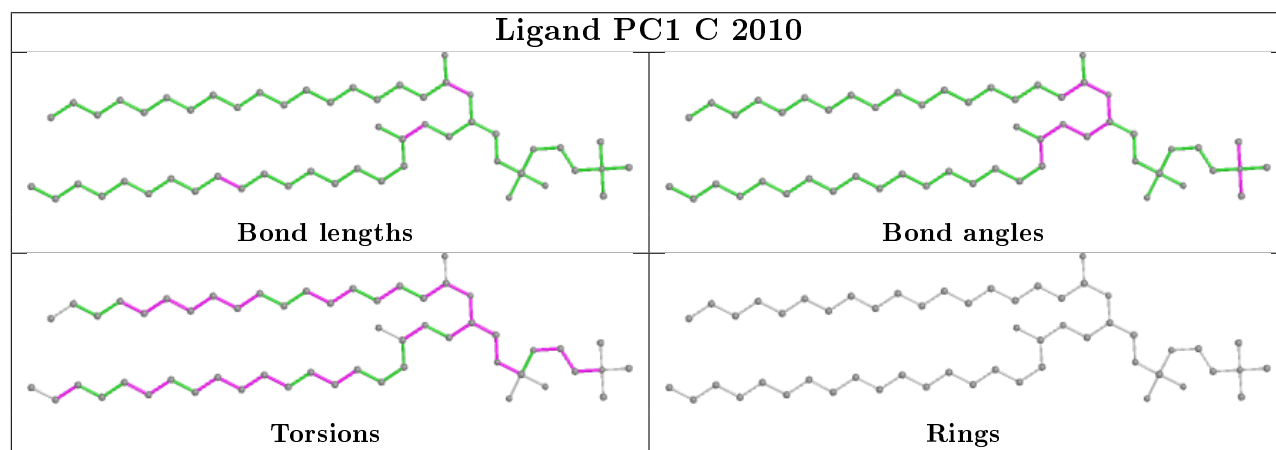
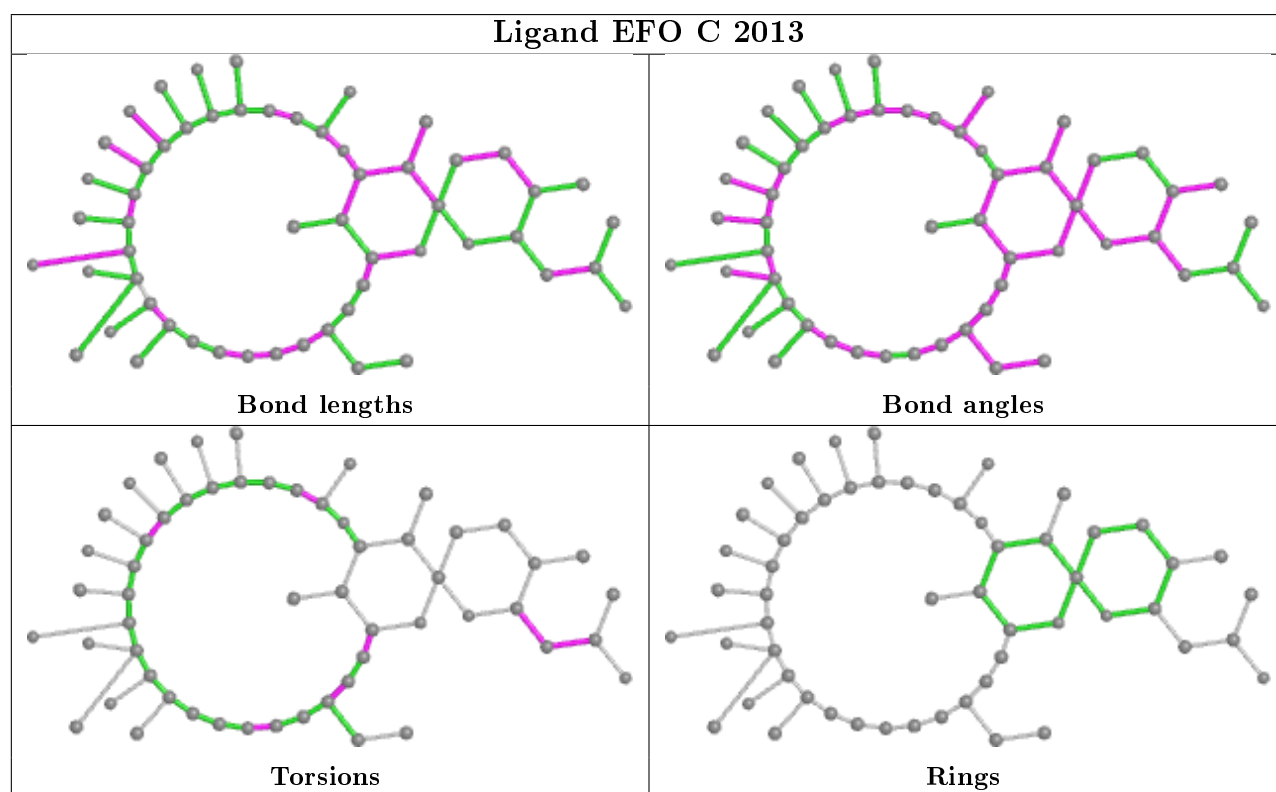
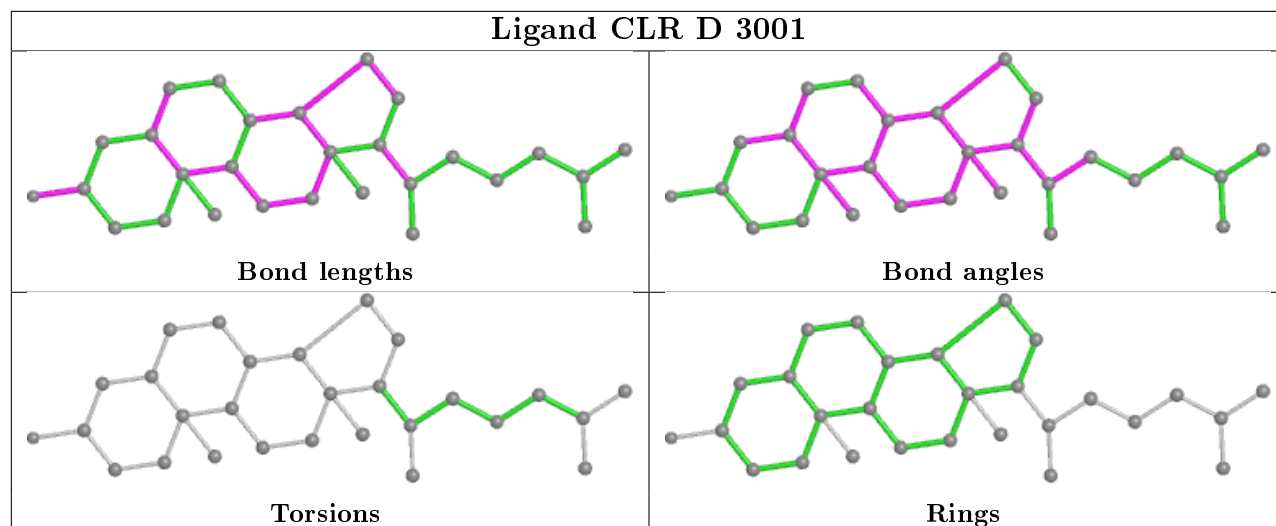
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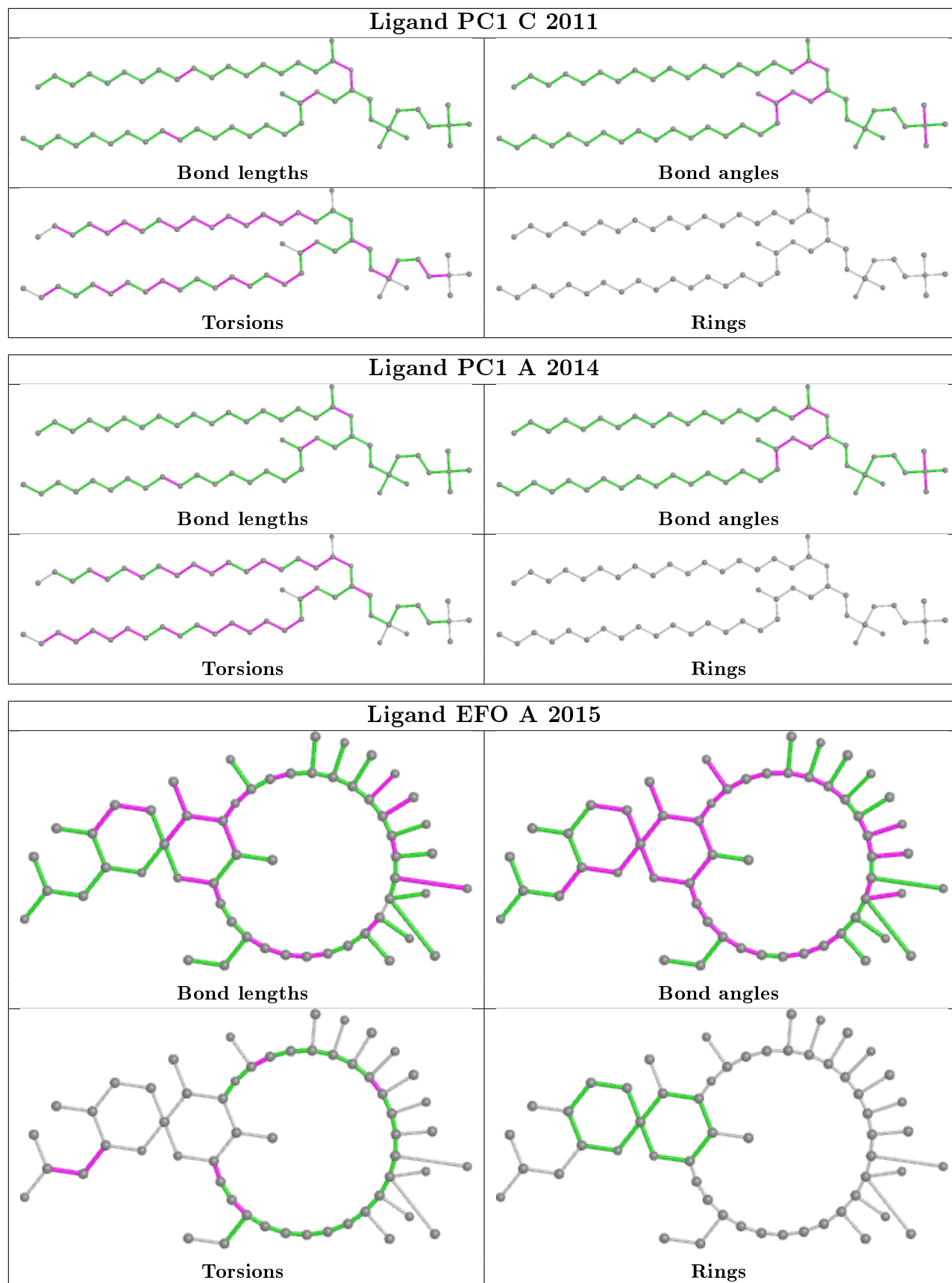
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	2011	PC1	3	0
9	A	2014	PC1	4	0
5	C	2002	ALF	2	0
9	C	2012	PC1	6	0
5	A	2002	ALF	1	0
9	A	2012	PC1	2	0
9	A	2013	PC1	7	0
6	A	2004	ADP	3	0
6	C	2004	ADP	6	0
8	A	2009	CLR	12	0
9	A	2011	PC1	1	0
8	D	3002	CLR	17	0
9	C	2009	PC1	8	0
9	B	401	PC1	2	0
8	E	101	CLR	13	0
9	D	3003	PC1	2	0
8	G	101	CLR	9	0

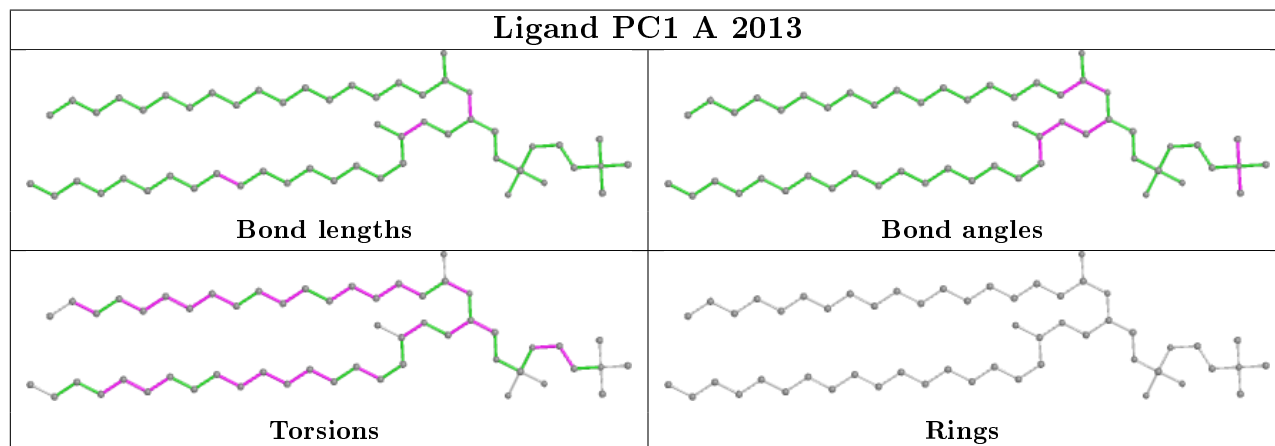
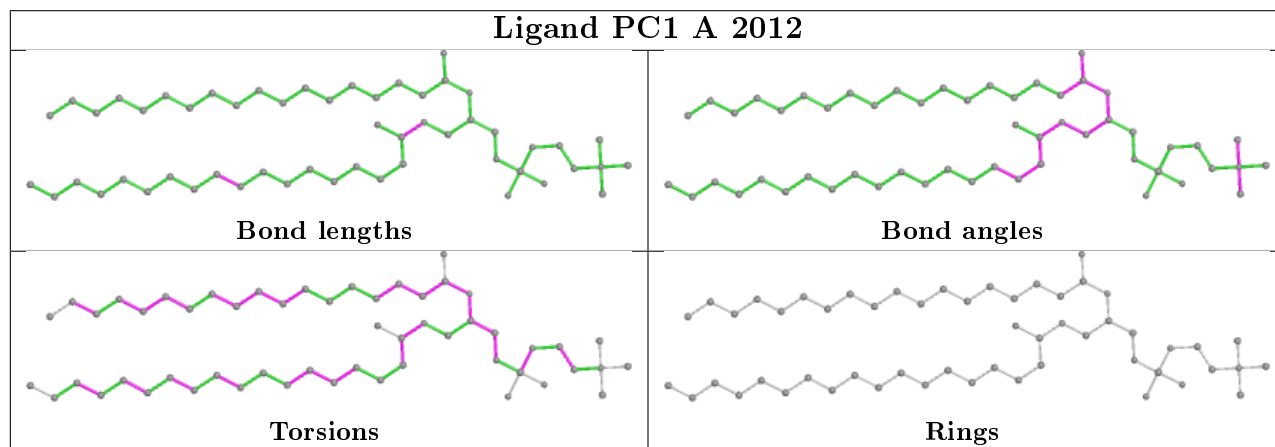
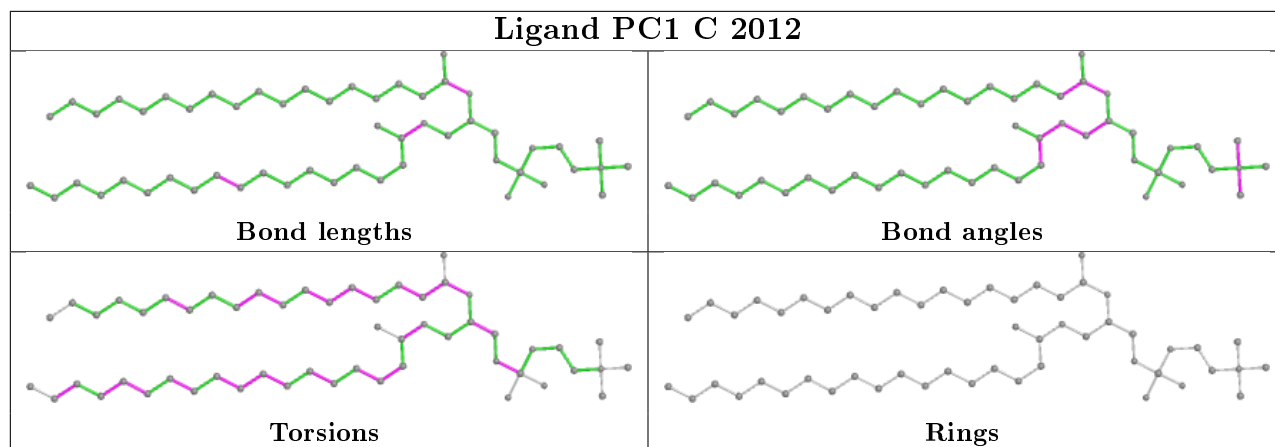
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

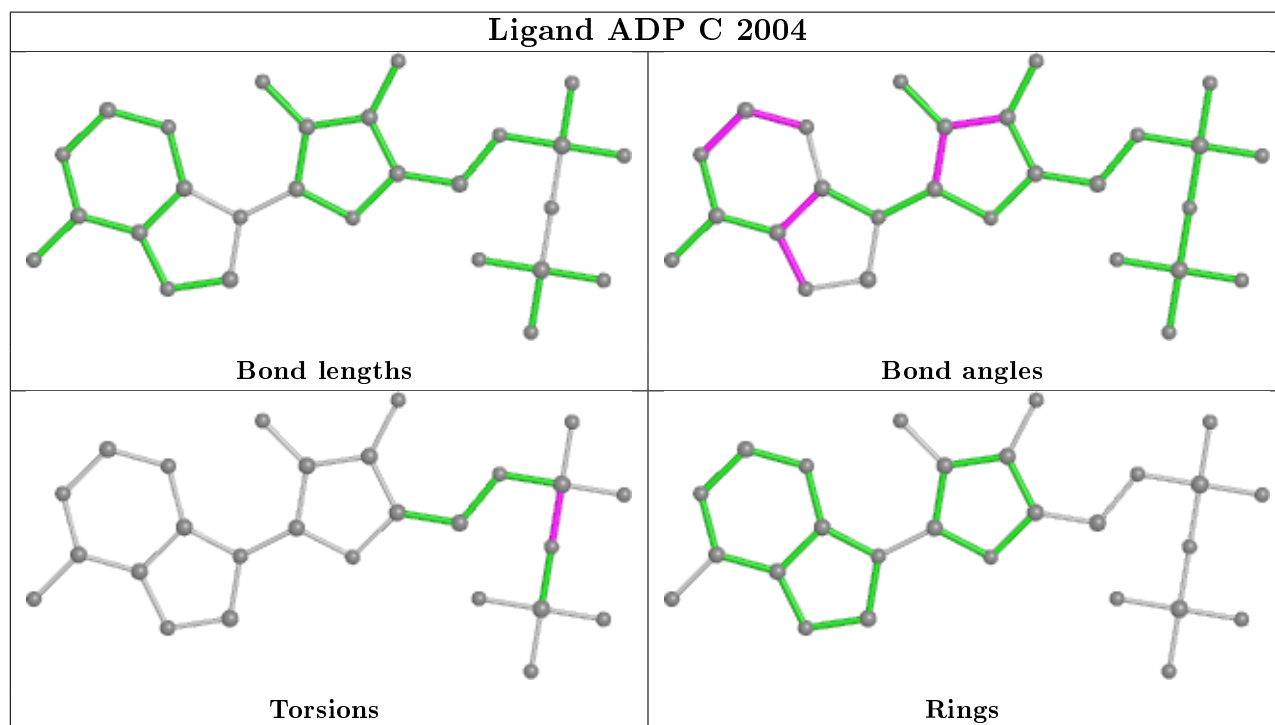
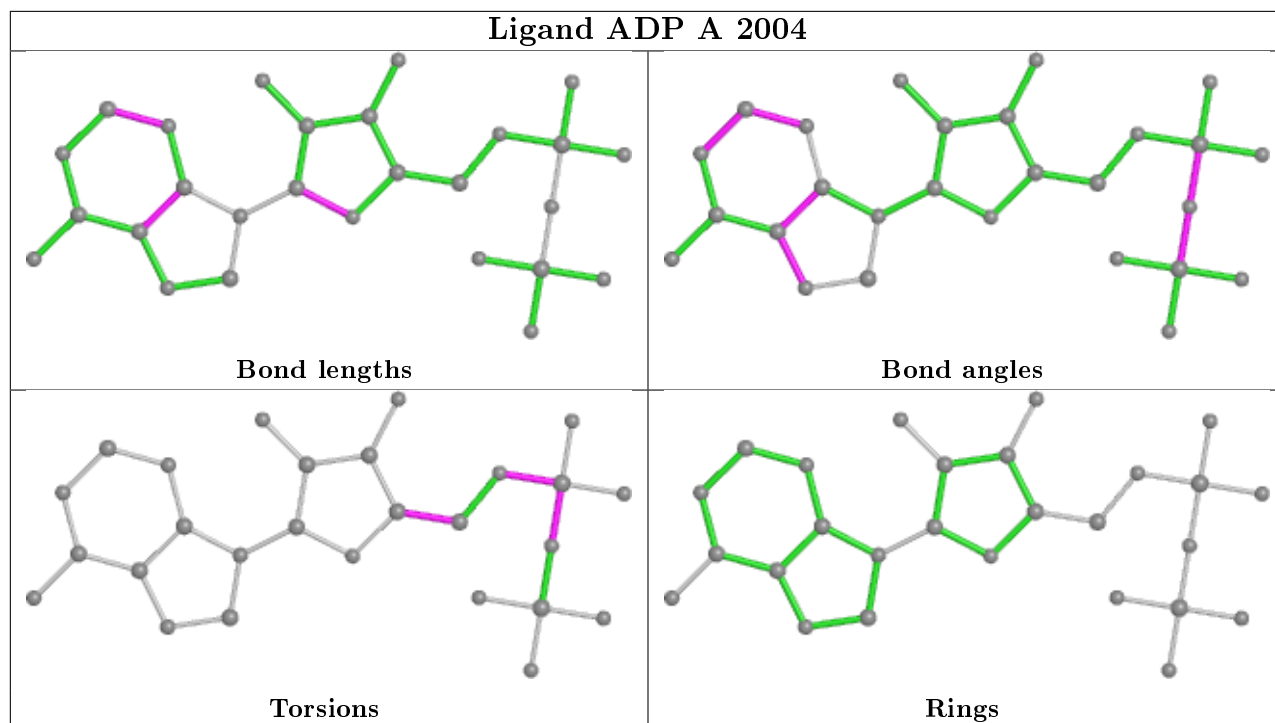


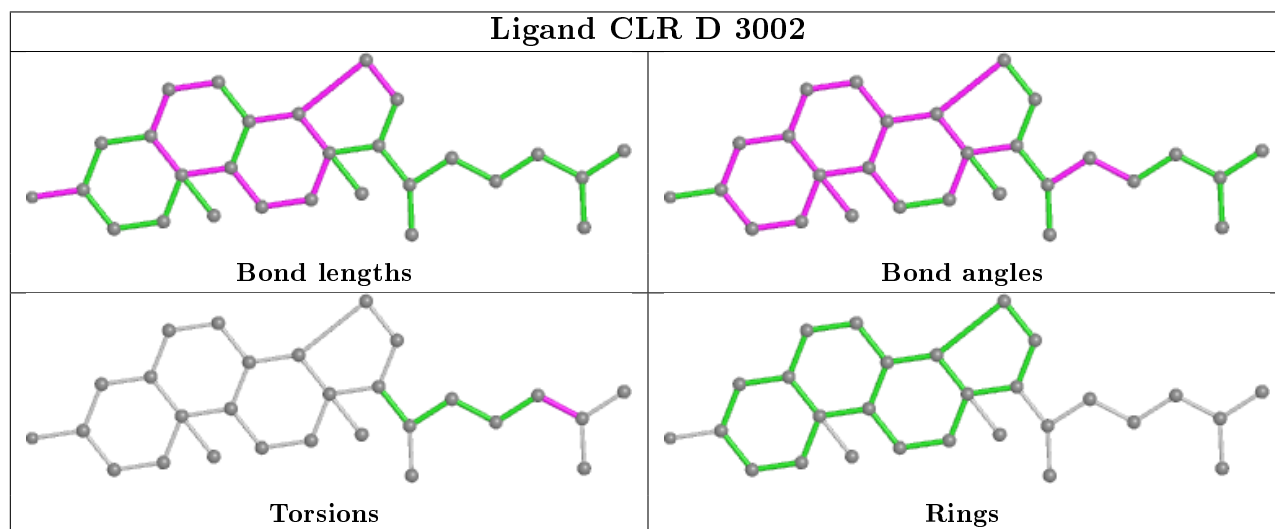
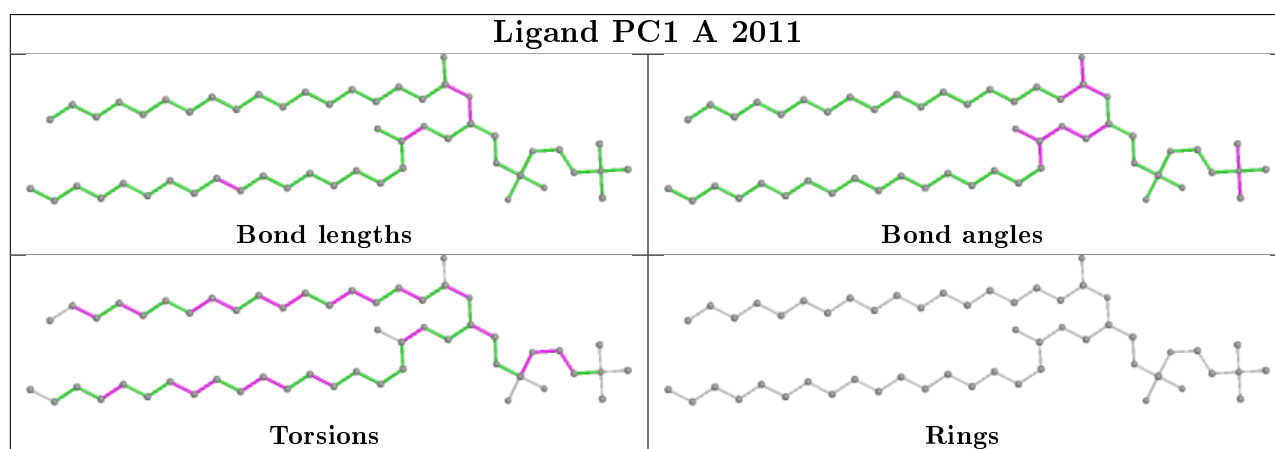
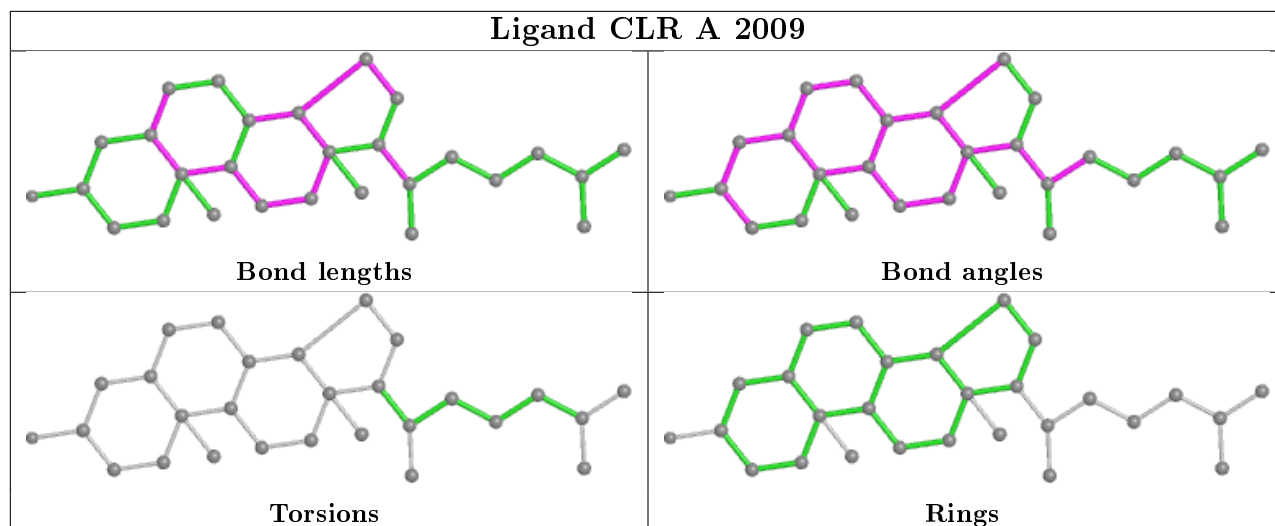


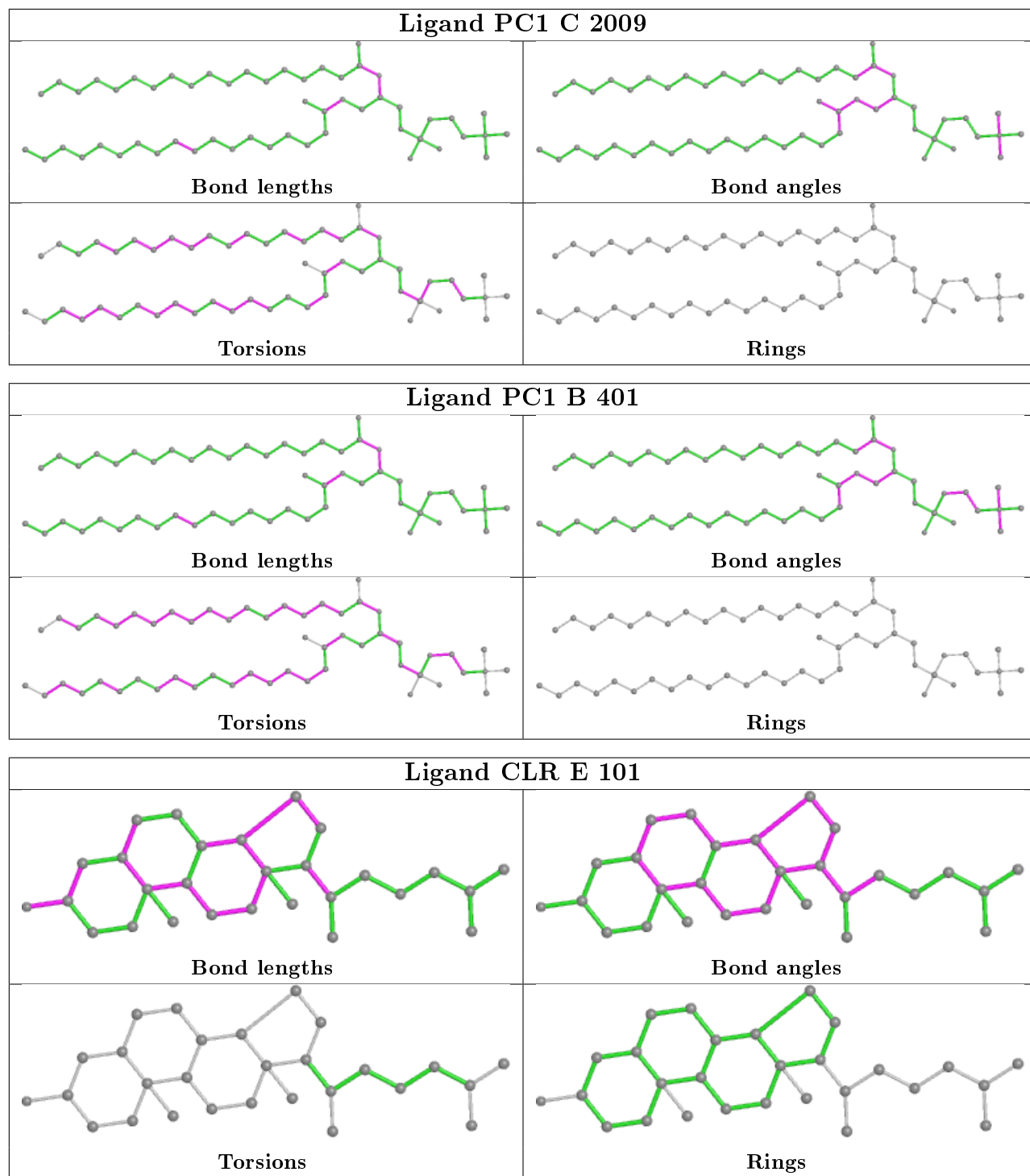


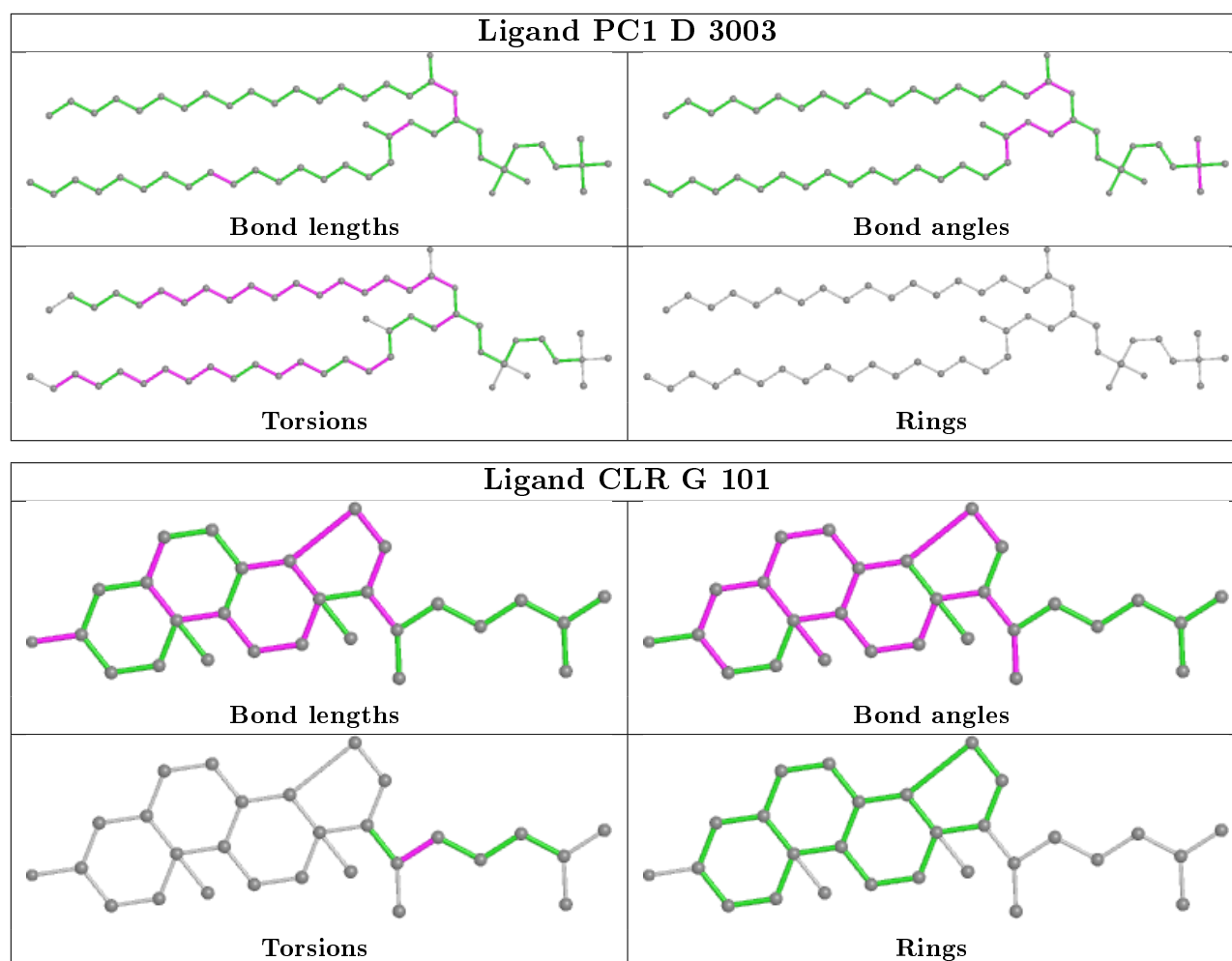












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	994/1016 (97%)	-0.29	21 (2%) 63 54	17, 57, 117, 181	0
1	C	994/1016 (97%)	0.01	35 (3%) 44 34	34, 74, 143, 199	0
2	B	303/303 (100%)	0.88	53 (17%) 1 1	59, 130, 199, 229	0
2	D	303/303 (100%)	0.90	50 (16%) 1 1	68, 127, 205, 239	0
3	E	35/65 (53%)	0.80	5 (14%) 2 1	70, 88, 165, 168	0
3	G	34/65 (52%)	0.50	3 (8%) 10 5	75, 91, 164, 175	0
All	All	2663/2768 (96%)	0.11	167 (6%) 20 12	17, 77, 161, 239	0

The worst 5 of 167 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	218	ASP	18.2
2	D	219	GLU	14.7
2	B	1	MET	9.8
3	E	16	VAL	9.6
3	E	15	ASP	9.3

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

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

### 6.3 Carbohydrates [i](#)

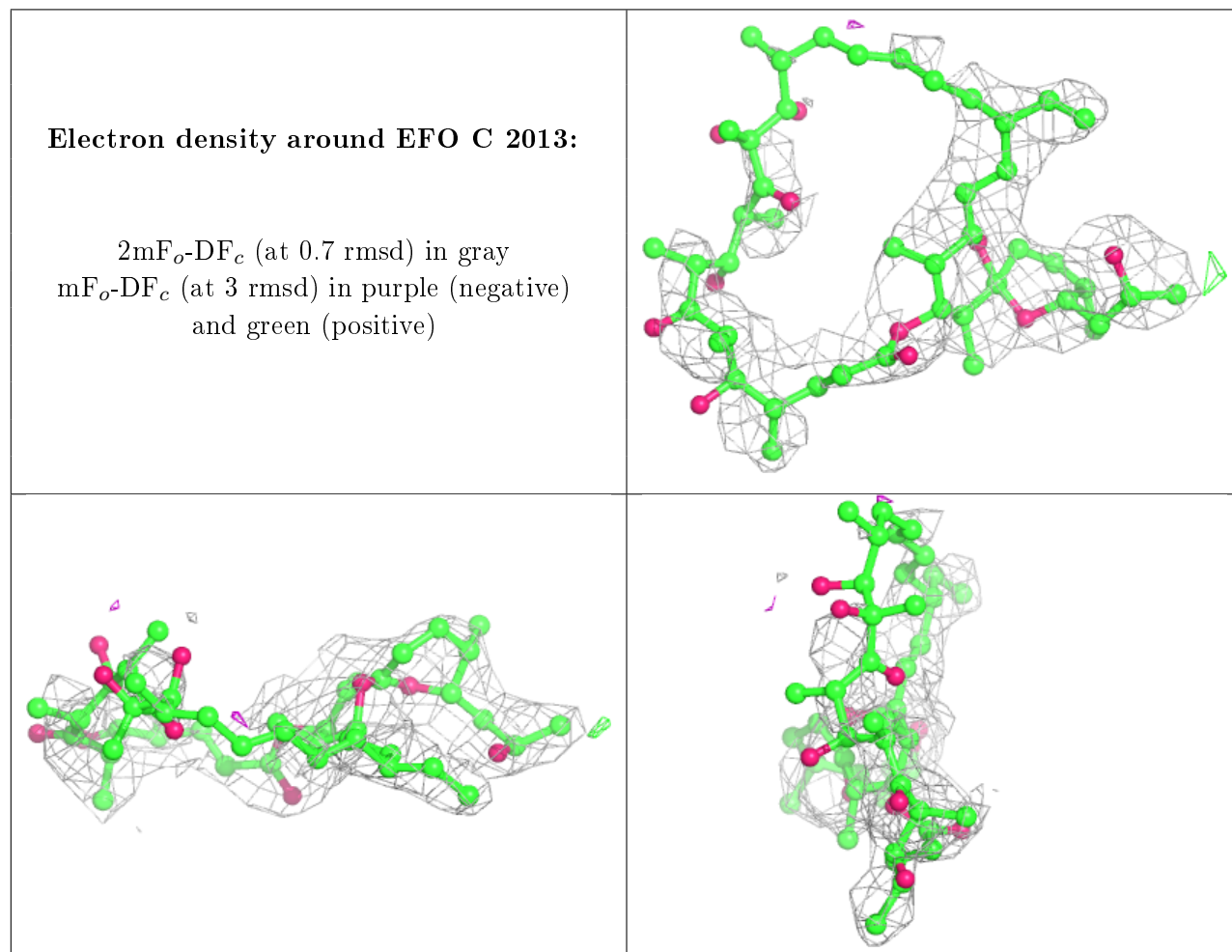
There are no monosaccharides in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	NA	C	2006	1/1	0.18	0.44	83,83,83,83	0
7	NA	A	2008	1/1	0.71	0.18	59,59,59,59	0
10	EFO	C	2013	56/56	0.77	0.41	49,150,194,195	0
9	PC1	C	2012	54/54	0.77	0.35	79,133,162,185	0
9	PC1	A	2012	54/54	0.80	0.36	61,117,163,176	0
9	PC1	A	2014	54/54	0.81	0.36	86,123,160,189	0
9	PC1	C	2010	54/54	0.82	0.31	68,101,143,205	0
10	EFO	A	2015	56/56	0.82	0.33	91,134,150,160	0
9	PC1	B	401	54/54	0.82	0.26	61,90,146,170	0
9	PC1	C	2011	54/54	0.83	0.42	77,117,163,173	0
4	MG	C	2001	1/1	0.83	0.23	54,54,54,54	0
11	NAG	B	402	14/15	0.84	0.34	126,137,144,146	0
11	NAG	D	3004	14/15	0.84	0.31	96,123,132,133	0
8	CLR	D	3002	28/28	0.87	0.29	13,97,131,141	0
7	NA	C	2005	1/1	0.87	0.31	103,103,103,103	0
7	NA	A	2007	1/1	0.88	0.31	98,98,98,98	0
9	PC1	C	2009	54/54	0.88	0.26	59,107,140,145	0
9	PC1	A	2013	54/54	0.88	0.28	71,103,124,174	0
9	PC1	D	3003	54/54	0.88	0.23	44,80,121,142	0
8	CLR	A	2010	28/28	0.89	0.33	60,98,131,138	0
8	CLR	A	2009	28/28	0.89	0.22	62,93,107,147	0
9	PC1	A	2011	54/54	0.90	0.26	57,97,128,130	0
8	CLR	D	3001	28/28	0.91	0.18	35,83,89,92	0
8	CLR	G	101	28/28	0.91	0.18	54,91,100,131	0
7	NA	A	2005	1/1	0.92	0.19	95,95,95,95	0
8	CLR	E	101	28/28	0.92	0.16	37,77,109,172	0
7	NA	A	2006	1/1	0.93	0.16	65,65,65,65	0
4	MG	A	2001	1/1	0.94	0.38	61,61,61,61	0
7	NA	C	2007	1/1	0.95	0.26	77,77,77,77	0
7	NA	C	2008	1/1	0.95	0.16	46,46,46,46	0
6	ADP	C	2004	27/27	0.96	0.14	31,47,57,60	0
4	MG	C	2003	1/1	0.97	0.12	51,51,51,51	0
6	ADP	A	2004	27/27	0.97	0.11	10,23,38,47	0
5	ALF	A	2002	5/5	0.98	0.17	14,14,28,29	0
5	ALF	C	2002	5/5	0.99	0.16	20,24,71,106	0
4	MG	A	2003	1/1	1.00	0.11	15,15,15,15	0

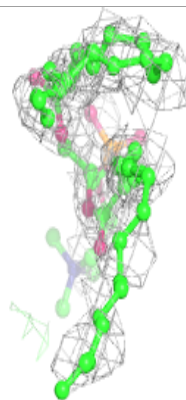
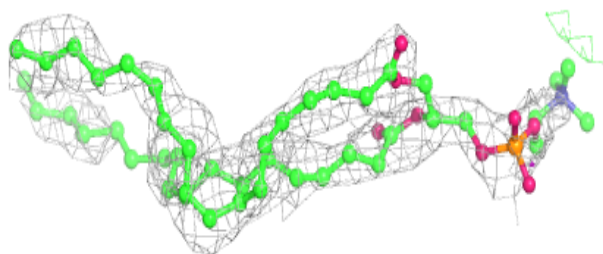
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



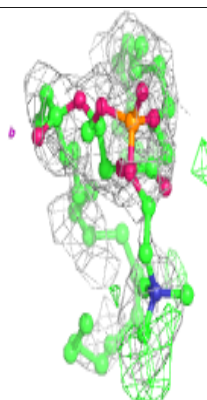
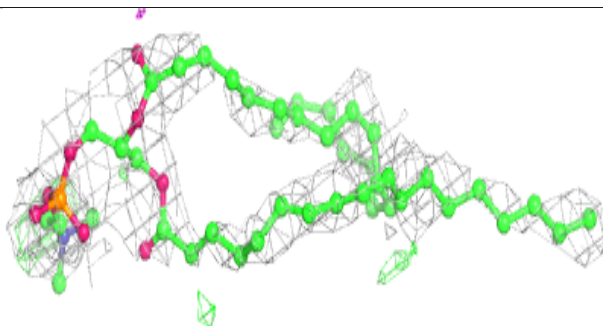
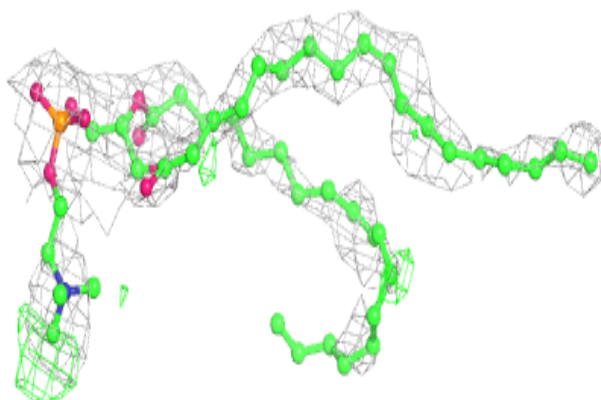


**Electron density around PC1 C 2012:**

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

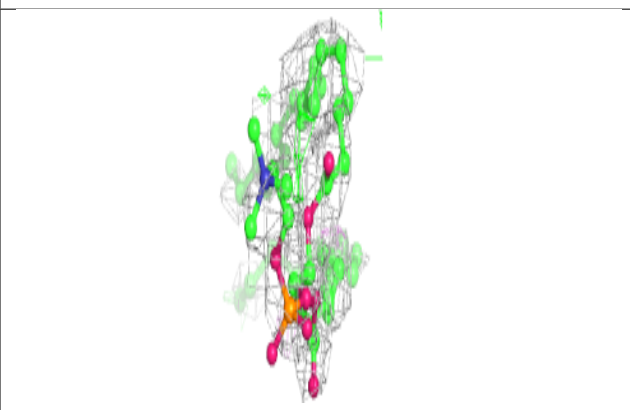
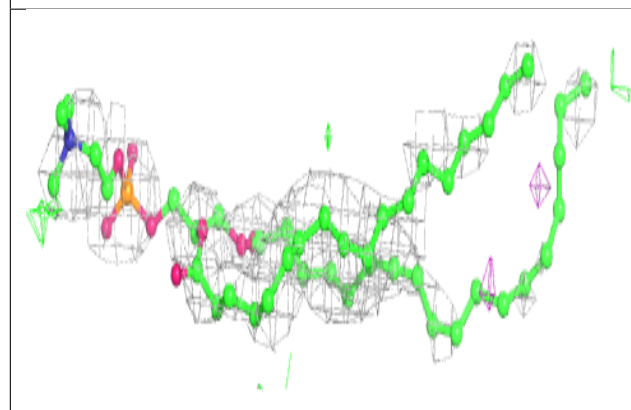
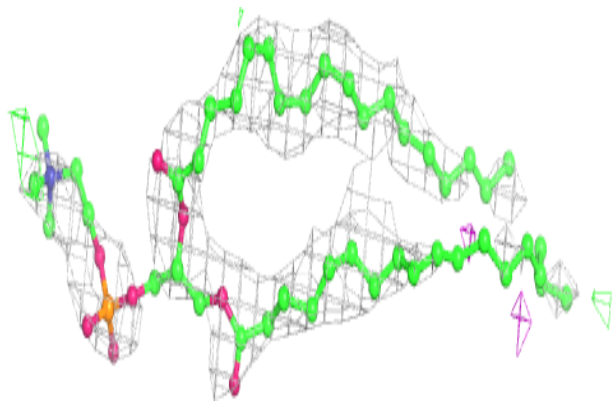
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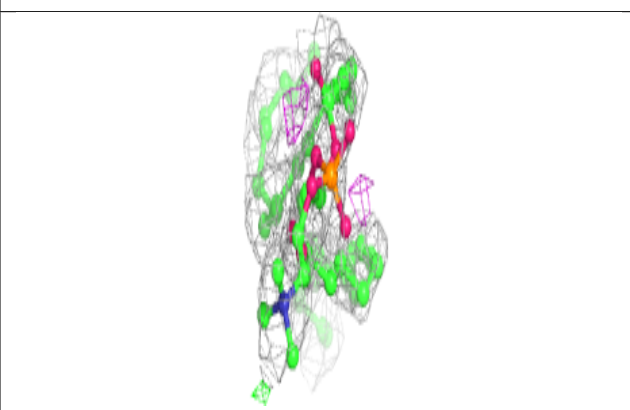
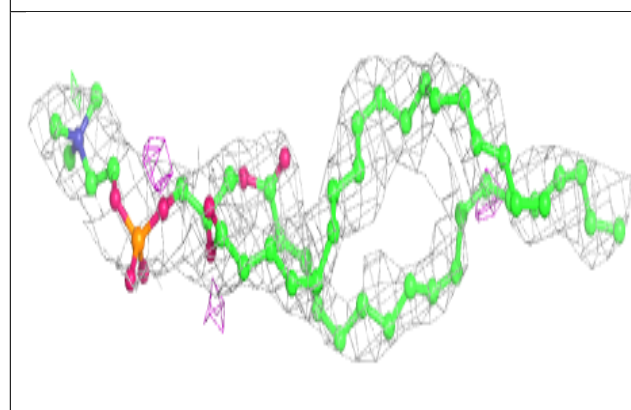
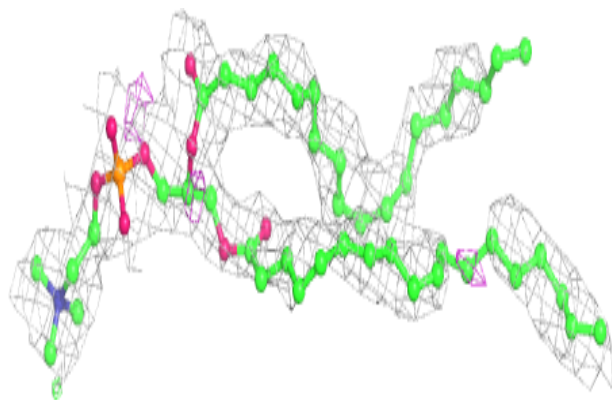


**Electron density around PC1 A 2014:**

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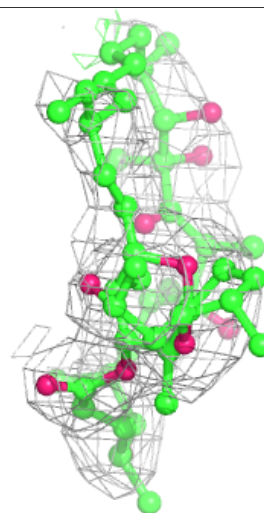
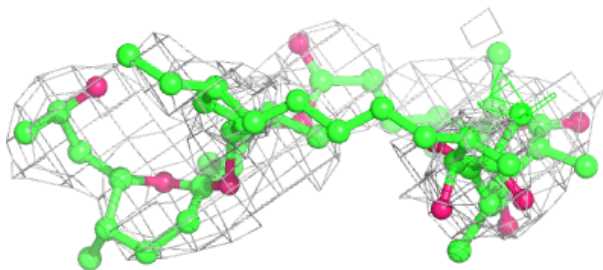
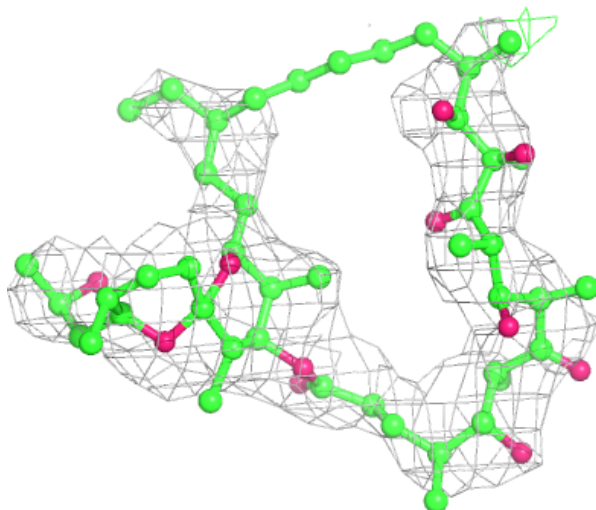
**Electron density around PC1 C 2010:**

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and green (positive)



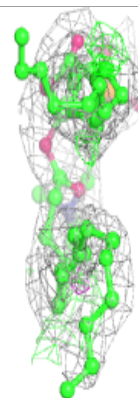
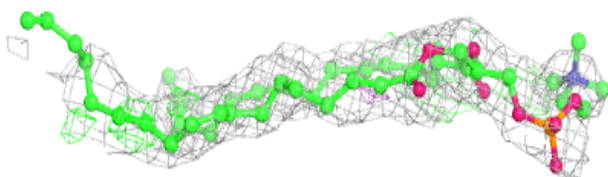
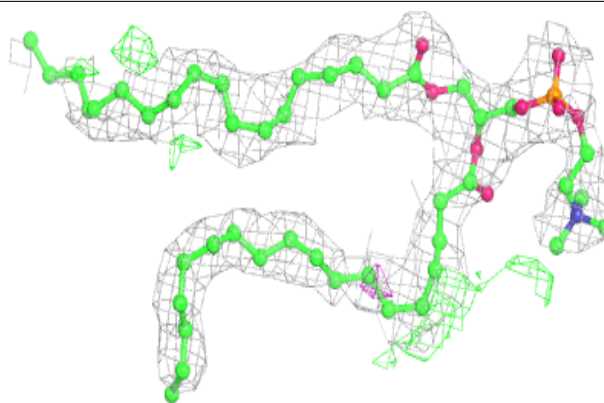
**Electron density around EFO A 2015:**

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and green (positive)

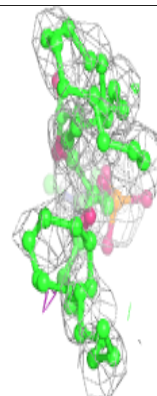
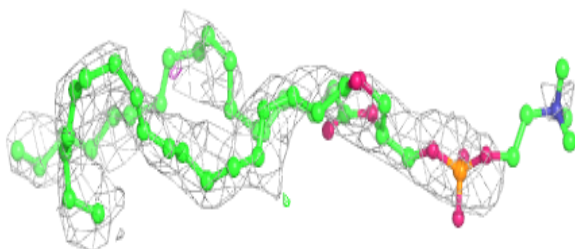
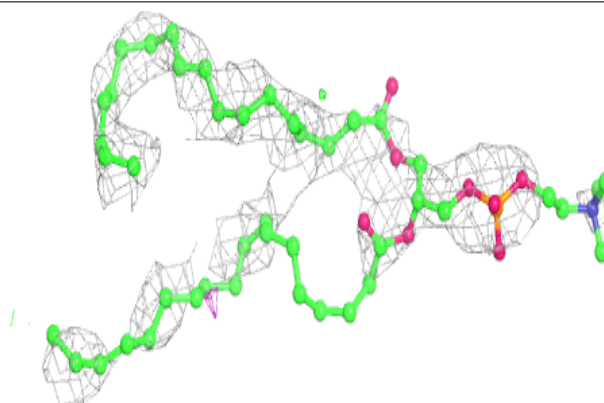


**Electron density around PC1 B 401:**

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and green (positive)

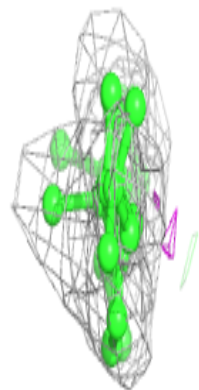
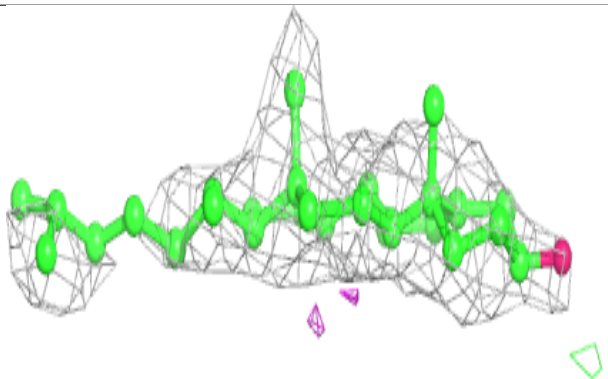
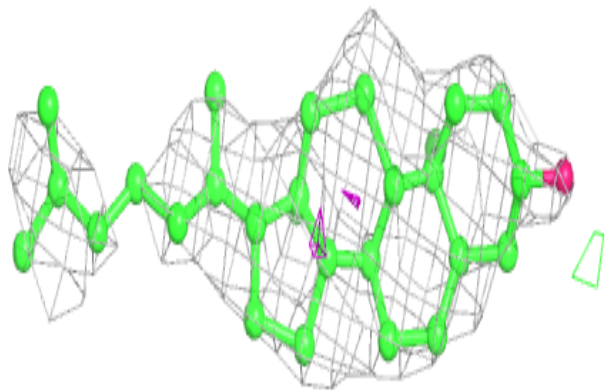
**Electron density around PC1 C 2011:**

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

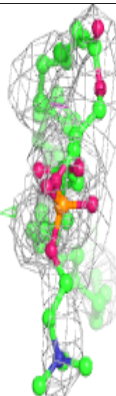
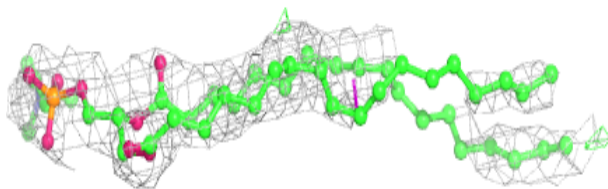
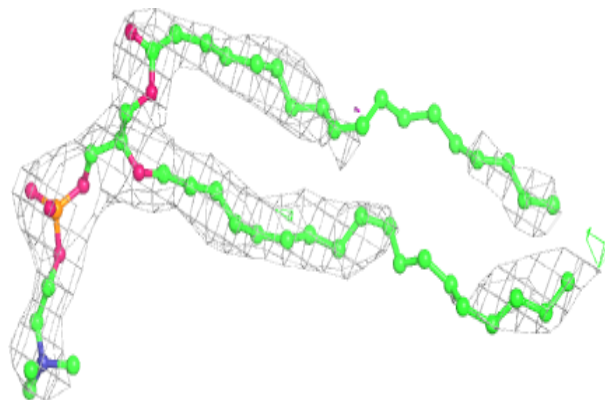


**Electron density around CLR D 3002:**

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

**Electron density around PC1 C 2009:**

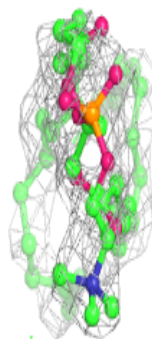
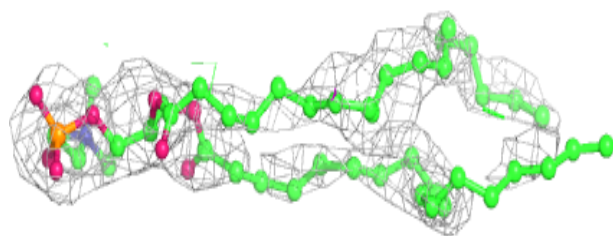
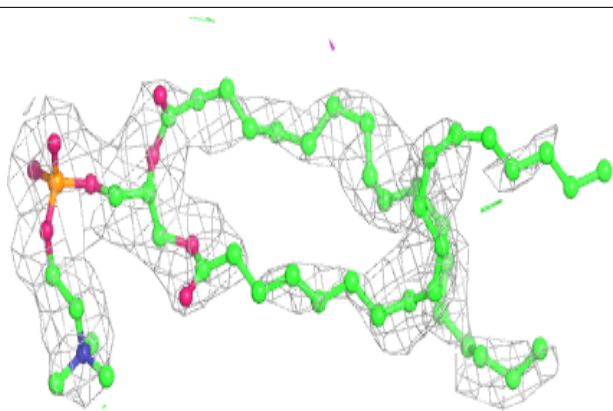
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



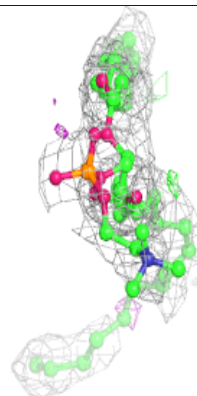
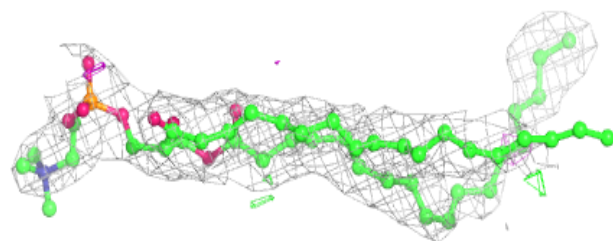
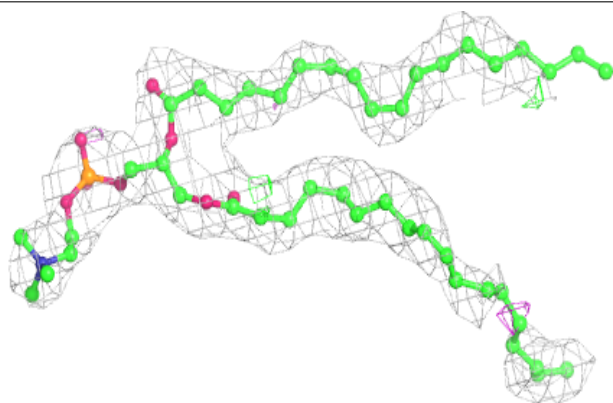


**Electron density around PC1 A 2013:**

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

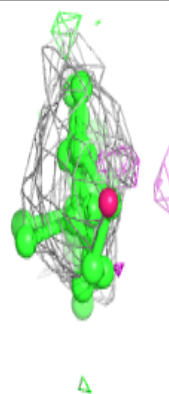
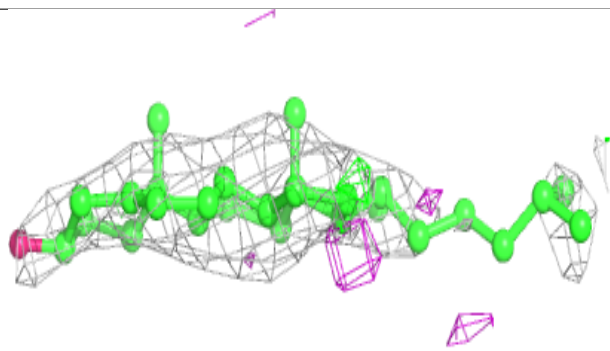
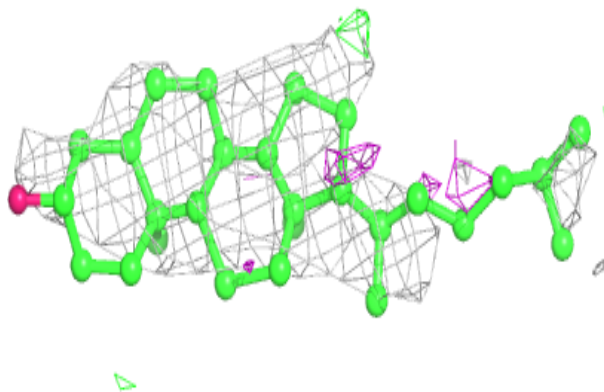
**Electron density around PC1 D 3003:**

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

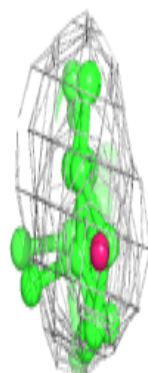
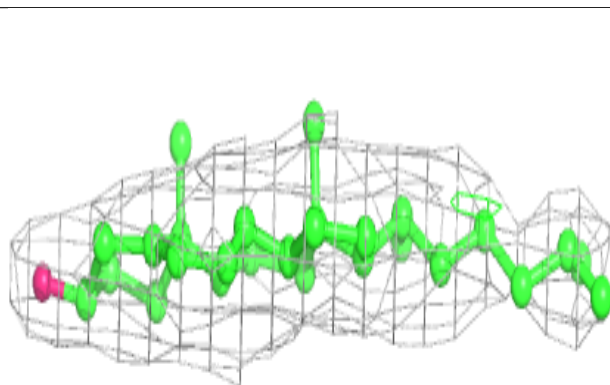
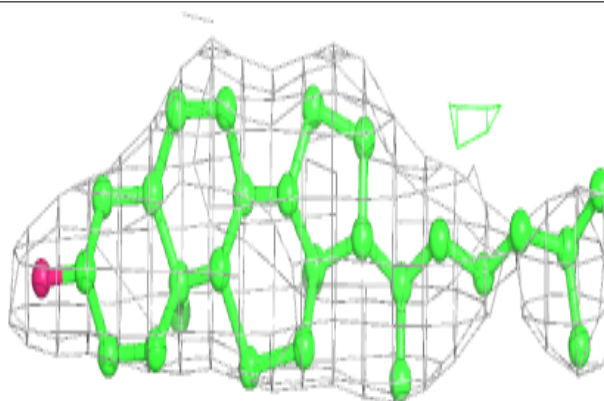


**Electron density around CLR A 2010:**

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

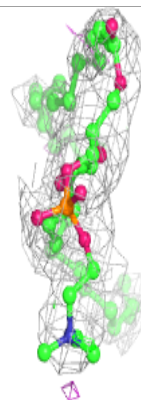
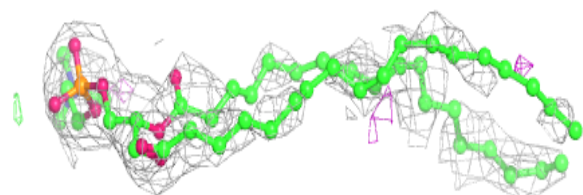
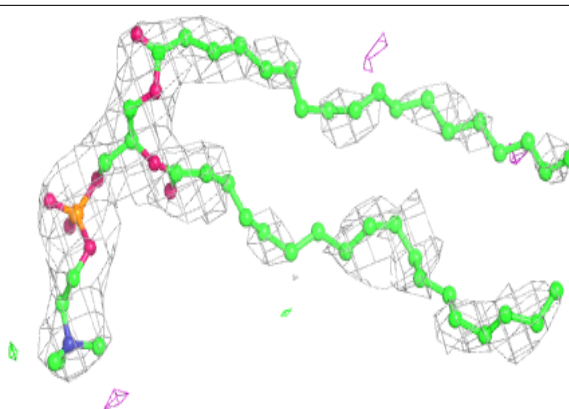
**Electron density around CLR A 2009:**

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

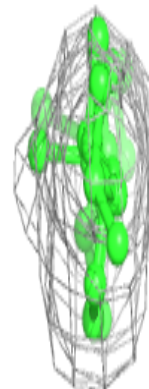
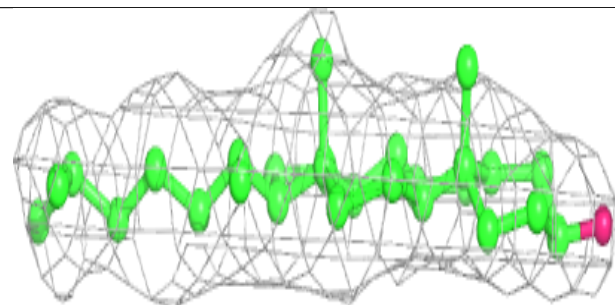
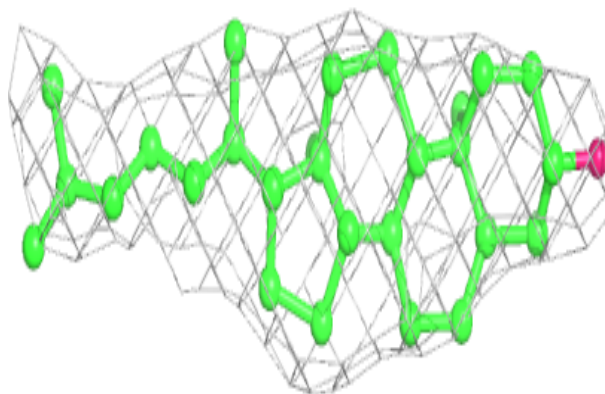


**Electron density around PC1 A 2011:**

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

**Electron density around CLR D 3001:**

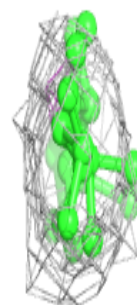
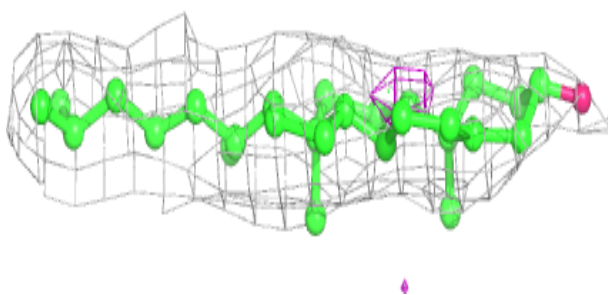
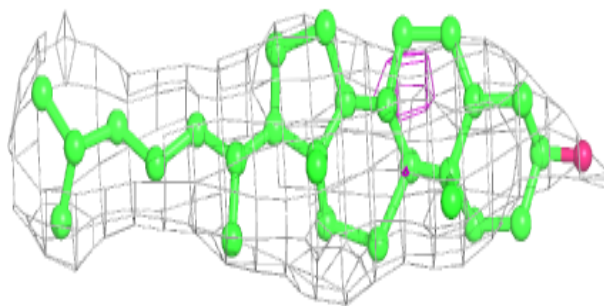
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



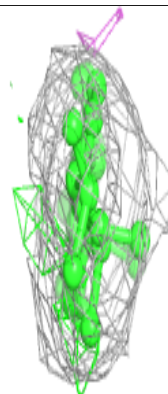
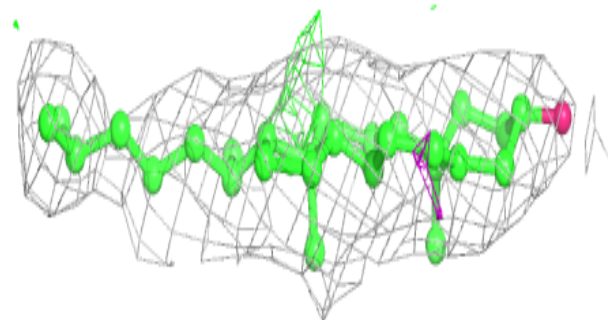
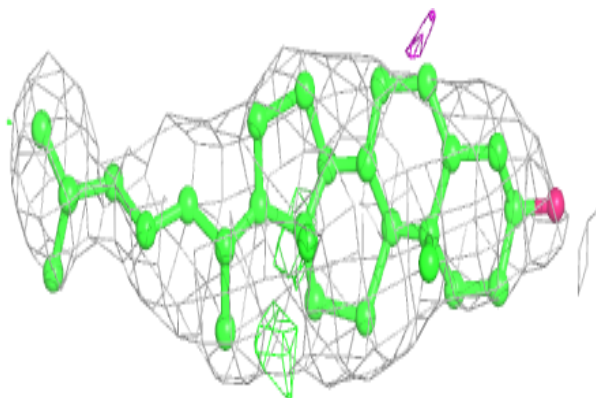


**Electron density around CLR G 101:**

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

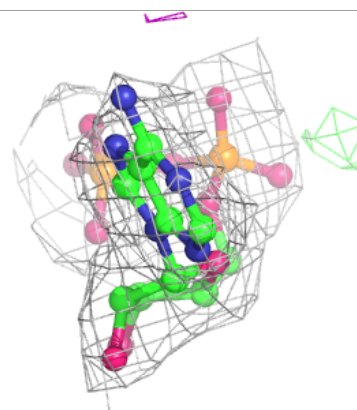
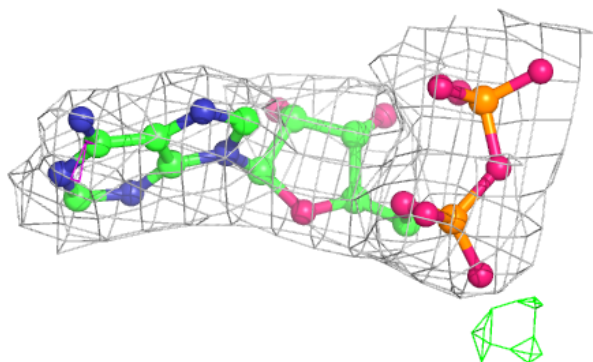
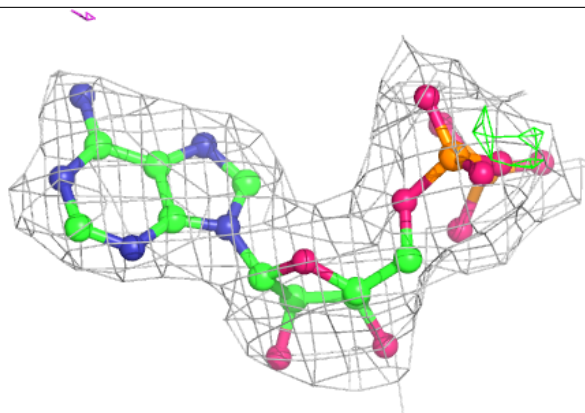
**Electron density around CLR E 101:**

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

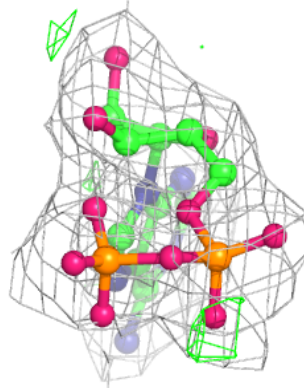
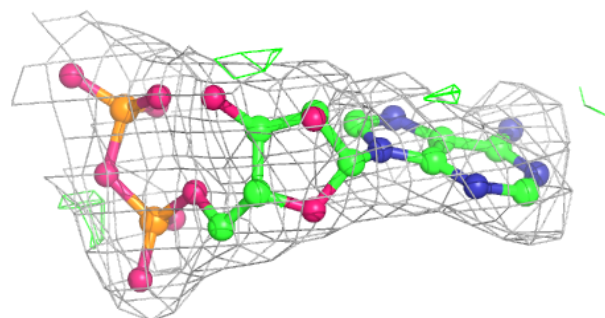
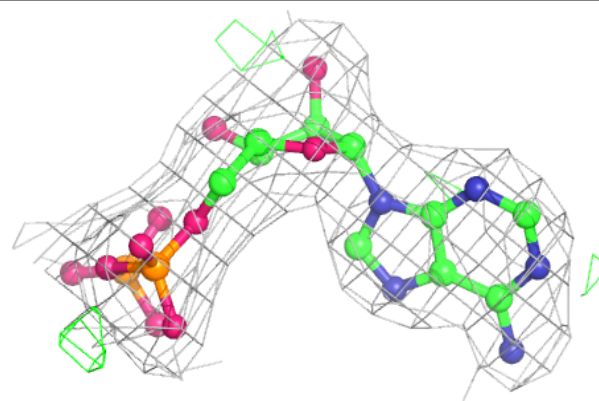


**Electron density around ADP C 2004:**

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

**Electron density around ADP A 2004:**

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



## 6.5 Other polymers

There are no such residues in this entry.