wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 02:21 PM EDT

PDB ID	:	3WGU
Title	:	Crystal structure of a Na+-bound Na+,K+-ATPase preceding the E1P state without 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

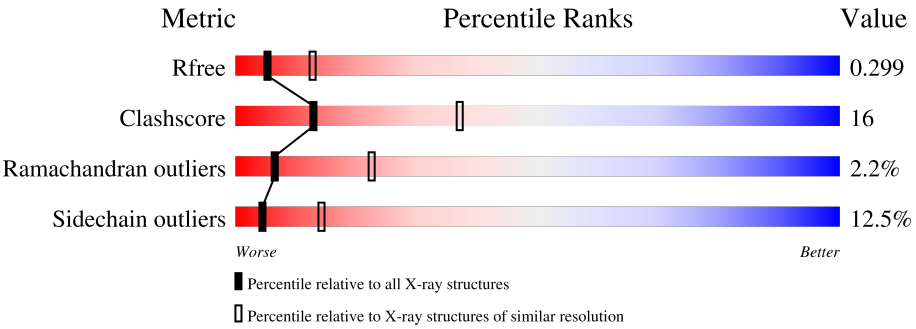
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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)

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

Mol	Chain	Length	Quality of chain
1	A	1016	58% 34% 6% •
1	C	1016	60% 34% • •
2	B	303	51% 42% 6% •
2	D	303	56% 37% 6% •
3	E	65	28% 23% • 46%
3	G	65	32% 17% • 48%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ALF	C	2002	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 21807 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	994	Total	C	N	O	S	0	0	0
			7714	4918	1300	1449	47			
1	C	994	Total	C	N	O	S	0	0	0
			7714	4918	1300	1449	47			

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

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

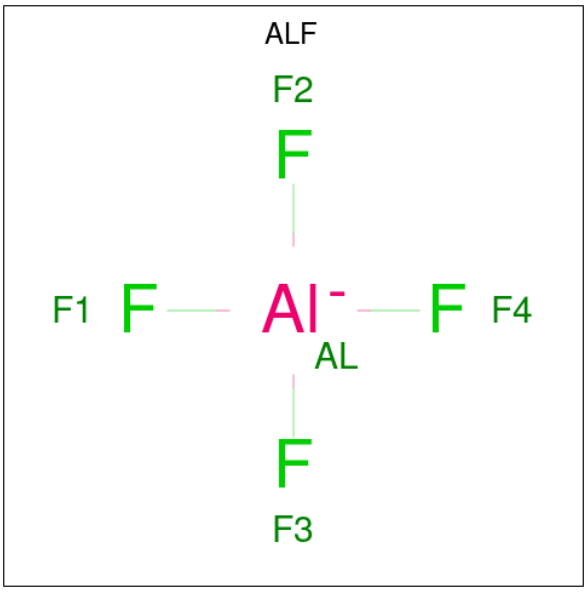
- Molecule 3 is a protein called Na+/K+ ATPase gamma subunit transcript variant a.

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

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

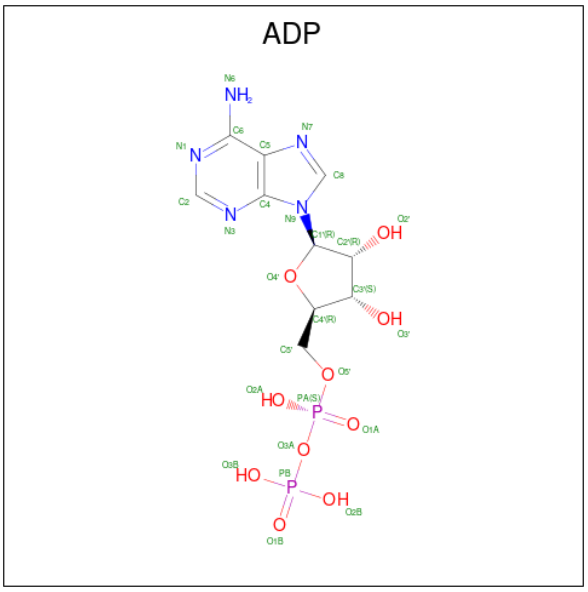
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



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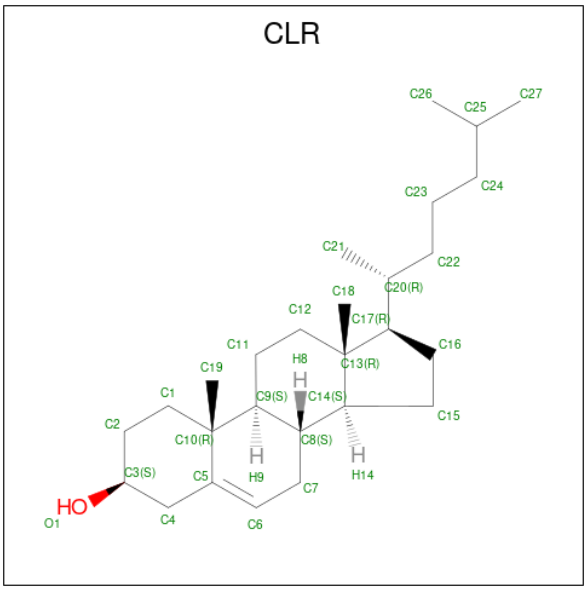
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O P 27 10 5 10 2	0	0

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

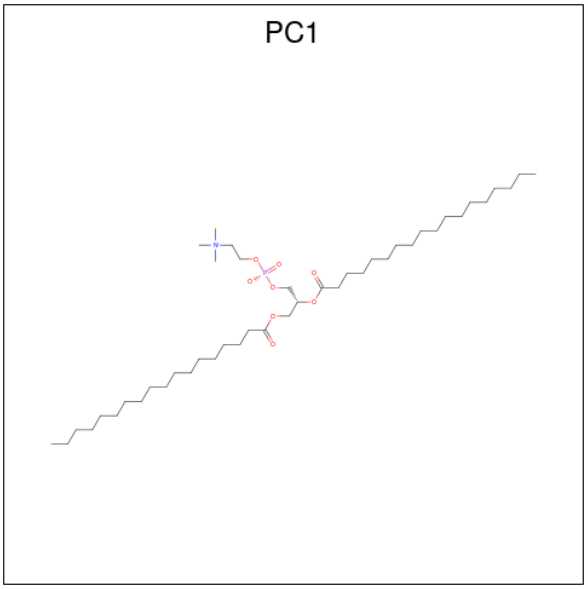
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	4	Total Na 4 4	0	0
7	C	4	Total Na 4 4	0	0

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



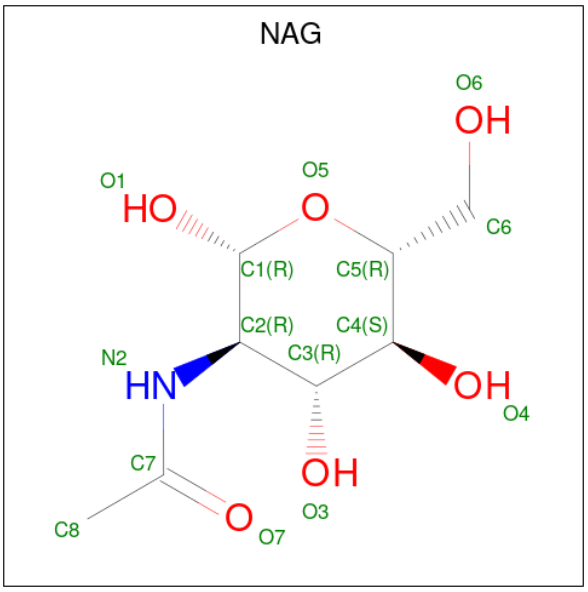
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 28 27 1	0	0
8	A	1	Total C O 28 27 1	0	0
8	B	1	Total C O 28 27 1	0	0
8	C	1	Total C O 28 27 1	0	0
8	C	1	Total C O 28 27 1	0	0
8	C	1	Total C O 28 27 1	0	0

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



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

- Molecule 11 is water.

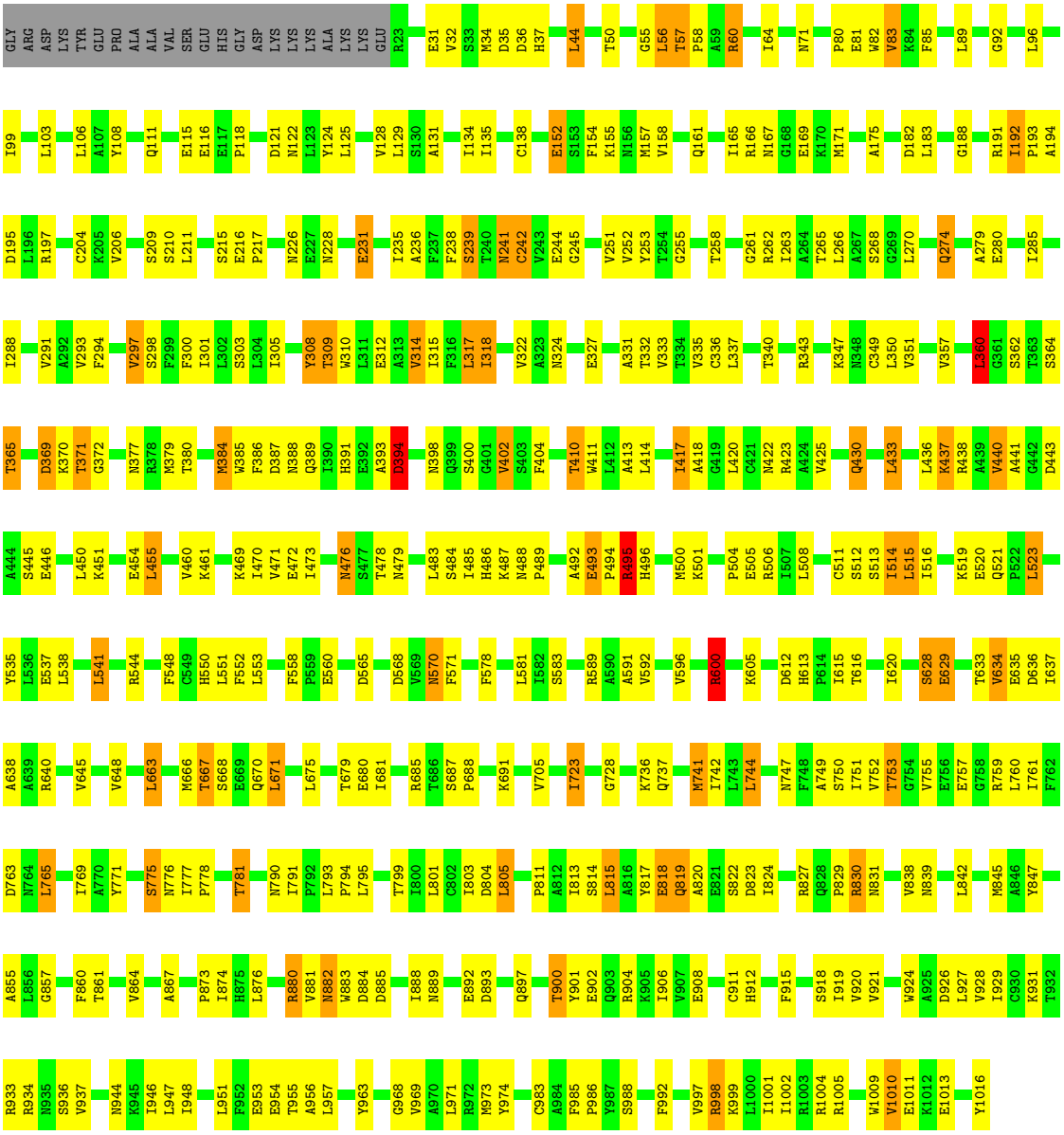
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	30	Total O 30 30	0	0
11	B	2	Total O 2 2	0	0
11	C	23	Total O 23 23	0	0
11	D	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

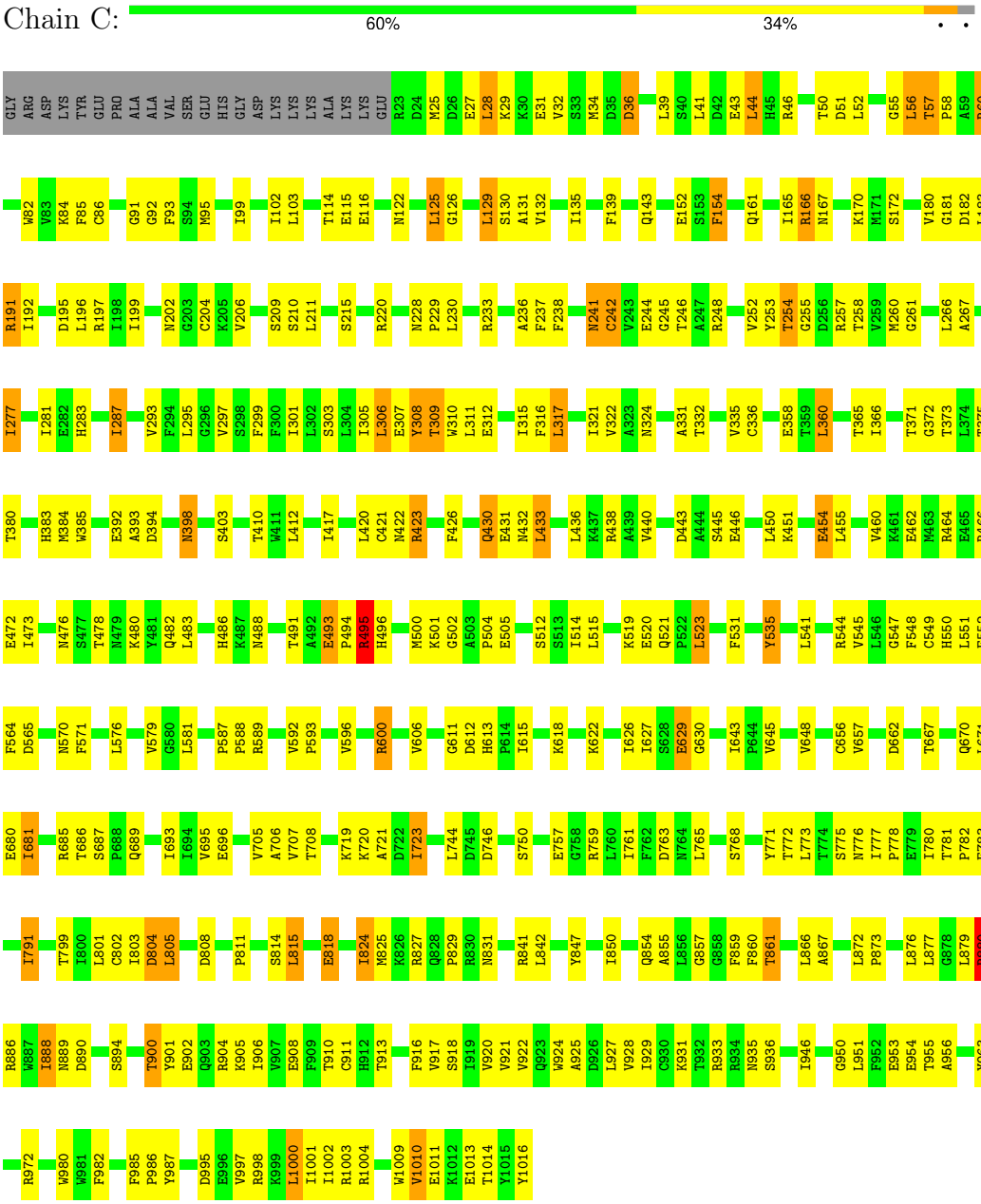
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain A:



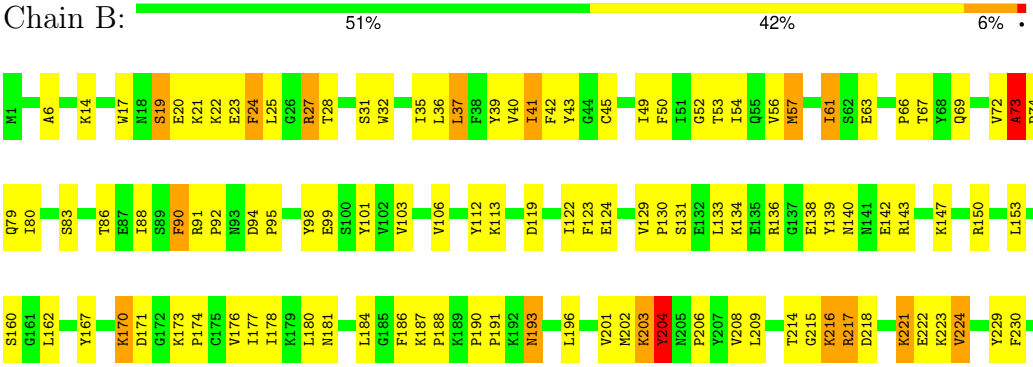
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain C:



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

Chain B:



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

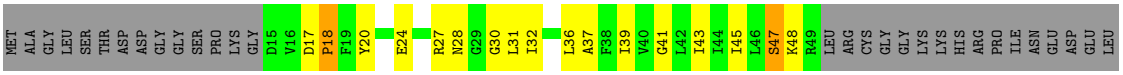
Chain D:

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

Chain G:

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

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.38Å 211.60Å 257.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.99 – 2.80 15.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (15.99-2.80) 88.9 (15.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.265 , 0.299 0.267 , 0.299	Depositor DCC
R_{free} test set	6460 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.13 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	21807	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CLR, NAG, NA, PC1, MG, ALF

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	0.48	1/7864 (0.0%)	0.65	5/10671 (0.0%)
1	C	0.41	0/7864	0.58	1/10671 (0.0%)
2	B	0.33	0/2544	0.53	1/3426 (0.0%)
2	D	0.34	0/2544	0.51	0/3426
3	E	0.59	1/287 (0.3%)	0.87	3/389 (0.8%)
3	G	0.43	0/276	0.57	0/375
All	All	0.43	2/21379 (0.0%)	0.60	10/28958 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	18	PRO	N-CD	7.79	1.58	1.47
1	A	511	CYS	CB-SG	-5.39	1.73	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	17	ASP	C-N-CD	-10.59	97.31	120.60
1	C	495	ARG	CB-CA-C	-8.16	94.09	110.40
1	A	495	ARG	CB-CA-C	-7.90	94.59	110.40
1	A	600	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	369	ASP	CB-CG-OD2	6.80	124.42	118.30

There are no chirality outliers.

There are no planarity outliers.

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	7769	262	0
1	C	7714	0	7768	248	0
2	B	2479	0	2458	92	0
2	D	2479	0	2458	80	0
3	E	281	0	285	9	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	5	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	87	12	0
8	B	28	0	44	4	0
8	C	84	0	131	23	0
9	A	216	0	352	14	0
9	B	54	0	88	0	0
9	C	216	0	352	21	0
9	D	54	0	88	3	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
11	A	30	0	0	0	0
11	B	2	0	0	0	0
11	C	23	0	0	3	0
11	D	3	0	0	1	0
All	All	21807	0	22202	724	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 16.

The worst 5 of 724 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:C:495:ARG:HG3	1:C:495:ARG:O	1.61	0.97
1:C:57:THR:HG23	1:C:60:ARG:HB2	1.52	0.90
2:B:221:LYS:HE3	2:B:223:LYS:HB2	1.54	0.90
8:C:2010:CLR:H272	9:C:2014:PC1:H2I2	1.54	0.88
1:A:494:PRO:HG2	1:A:552:PHE:HB3	1.56	0.87

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%)	882 (89%)	97 (10%)	13 (1%)	12 36
1	C	992/1016 (98%)	890 (90%)	88 (9%)	14 (1%)	11 34
2	B	301/303 (99%)	234 (78%)	55 (18%)	12 (4%)	3 9
2	D	301/303 (99%)	231 (77%)	55 (18%)	15 (5%)	2 6
3	E	33/65 (51%)	32 (97%)	0	1 (3%)	4 15
3	G	32/65 (49%)	27 (84%)	3 (9%)	2 (6%)	1 3
All	All	2651/2768 (96%)	2296 (87%)	298 (11%)	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	139	TYR
3	G	17	ASP
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%)	723 (86%)	121 (14%)	3 10
1	C	844/861 (98%)	751 (89%)	93 (11%)	6 19
2	B	269/269 (100%)	234 (87%)	35 (13%)	4 13
2	D	269/269 (100%)	238 (88%)	31 (12%)	5 17
3	E	29/52 (56%)	24 (83%)	5 (17%)	2 6
3	G	28/52 (54%)	27 (96%)	1 (4%)	35 69
All	All	2283/2364 (97%)	1997 (88%)	286 (12%)	4 14

5 of 286 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	791	ILE
1	C	880	ARG
2	D	119	ASP
1	A	775	SER
1	A	753	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	430	GLN
1	C	897	GLN
1	C	550	HIS
1	C	790	ASN
1	C	923	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 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	NAG	B	3003	-	14,14,15	0.41	0	17,19,21	0.74	0
6	ADP	C	2004	-	24,29,29	1.20	2 (8%)	29,45,45	1.31	4 (13%)
9	PC1	A	2014	-	53,53,53	0.93	4 (7%)	59,61,61	1.31	4 (6%)
10	NAG	D	402	-	14,14,15	0.46	0	17,19,21	0.68	0
8	CLR	A	2009	-	31,31,31	4.86	16 (51%)	48,48,48	2.66	19 (39%)
9	PC1	A	2013	-	53,53,53	0.93	4 (7%)	59,61,61	1.19	5 (8%)
6	ADP	A	2004	4	24,29,29	1.39	3 (12%)	29,45,45	1.50	5 (17%)
8	CLR	C	2009	-	31,31,31	4.78	18 (58%)	48,48,48	2.61	19 (39%)
8	CLR	A	2010	-	31,31,31	4.90	15 (48%)	48,48,48	3.22	25 (52%)
5	ALF	A	2002	-	4,4,4	1.38	0	-		
9	PC1	A	2011	-	53,53,53	0.92	4 (7%)	59,61,61	1.21	5 (8%)
8	CLR	C	2010	-	31,31,31	4.87	16 (51%)	48,48,48	2.67	21 (43%)
9	PC1	D	401	-	53,53,53	0.95	5 (9%)	59,61,61	1.24	6 (10%)
5	ALF	C	2002	-	4,4,4	1.32	0	-		
9	PC1	C	2015	-	53,53,53	0.92	5 (9%)	59,61,61	1.28	5 (8%)
9	PC1	C	2012	-	53,53,53	0.93	5 (9%)	59,61,61	1.27	5 (8%)
8	CLR	C	2011	-	31,31,31	4.98	14 (45%)	48,48,48	2.72	22 (45%)
9	PC1	C	2013	-	53,53,53	0.94	4 (7%)	59,61,61	1.32	6 (10%)
9	PC1	C	2014	-	53,53,53	0.98	4 (7%)	59,61,61	1.31	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	PC1	A	2012	-	53,53,53	0.94	4 (7%)	59,61,61	1.32	6 (10%)
9	PC1	B	3002	-	53,53,53	0.91	3 (5%)	59,61,61	1.20	5 (8%)
8	CLR	B	3001	-	31,31,31	4.86	17 (54%)	48,48,48	2.57	19 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	B	3003	-	-	1/6/23/26	0/1/1/1
6	ADP	C	2004	-	-	1/12/32/32	0/3/3/3
9	PC1	A	2014	-	-	30/57/57/57	-
10	NAG	D	402	-	-	1/6/23/26	0/1/1/1
8	CLR	A	2009	-	-	0/10/68/68	0/4/4/4
9	PC1	A	2013	-	-	32/57/57/57	-
6	ADP	A	2004	4	-	5/12/32/32	0/3/3/3
8	CLR	C	2009	-	-	0/10/68/68	0/4/4/4
8	CLR	A	2010	-	-	2/10/68/68	0/4/4/4
9	PC1	A	2011	-	-	25/57/57/57	-
8	CLR	C	2010	-	-	1/10/68/68	0/4/4/4
9	PC1	D	401	-	-	33/57/57/57	-
9	PC1	C	2015	-	-	24/57/57/57	-
9	PC1	C	2012	-	-	27/57/57/57	-
8	CLR	C	2011	-	-	0/10/68/68	0/4/4/4
9	PC1	C	2013	-	-	32/57/57/57	-
9	PC1	C	2014	-	-	36/57/57/57	-
9	PC1	A	2012	-	-	32/57/57/57	-
9	PC1	B	3002	-	-	32/57/57/57	-
8	CLR	B	3001	-	-	0/10/68/68	0/4/4/4

The worst 5 of 143 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2011	CLR	C10-C9	-14.19	1.33	1.56
8	A	2010	CLR	C10-C9	-14.09	1.33	1.56
8	A	2009	CLR	C10-C9	-13.85	1.34	1.56
8	C	2010	CLR	C10-C9	-13.57	1.34	1.56
8	B	3001	CLR	C10-C9	-13.55	1.34	1.56

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	2010	CLR	C21-C20-C22	-10.84	93.56	110.34
8	A	2010	CLR	C21-C20-C17	-8.54	100.07	112.88
8	C	2009	CLR	C17-C13-C14	7.28	108.45	100.10
8	C	2010	CLR	C17-C13-C14	7.19	108.35	100.10
8	A	2009	CLR	C17-C13-C14	7.02	108.16	100.10

There are no chirality outliers.

5 of 314 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2004	ADP	C5'-O5'-PA-O2A
6	A	2004	ADP	C5'-O5'-PA-O3A
9	A	2011	PC1	C11-O13-P-O11
9	A	2011	PC1	C12-C11-O13-P
9	A	2011	PC1	O13-C11-C12-N

There are no ring outliers.

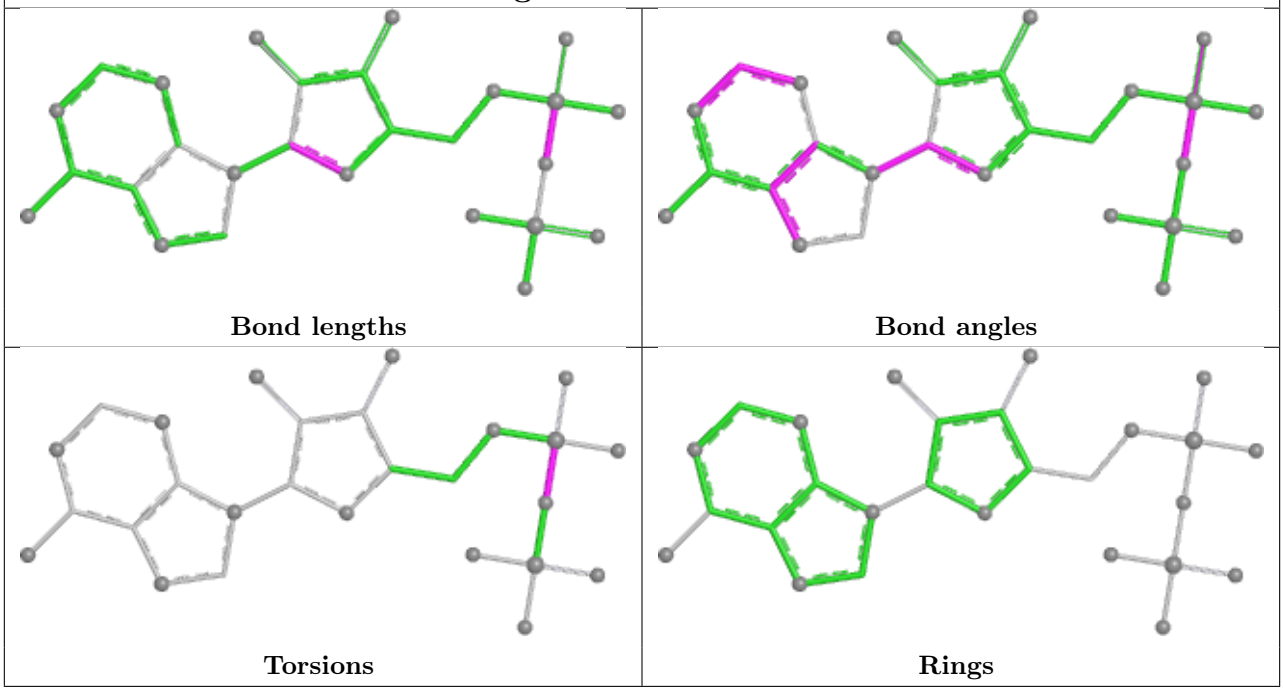
19 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2004	ADP	6	0
9	A	2014	PC1	4	0
8	A	2009	CLR	4	0
9	A	2013	PC1	3	0
6	A	2004	ADP	5	0
8	C	2009	CLR	4	0
8	A	2010	CLR	8	0
5	A	2002	ALF	1	0
9	A	2011	PC1	4	0
8	C	2010	CLR	12	0
9	D	401	PC1	3	0
5	C	2002	ALF	2	0
9	C	2015	PC1	6	0
9	C	2012	PC1	3	0
8	C	2011	CLR	7	0
9	C	2013	PC1	3	0
9	C	2014	PC1	11	0
9	A	2012	PC1	4	0
8	B	3001	CLR	4	0

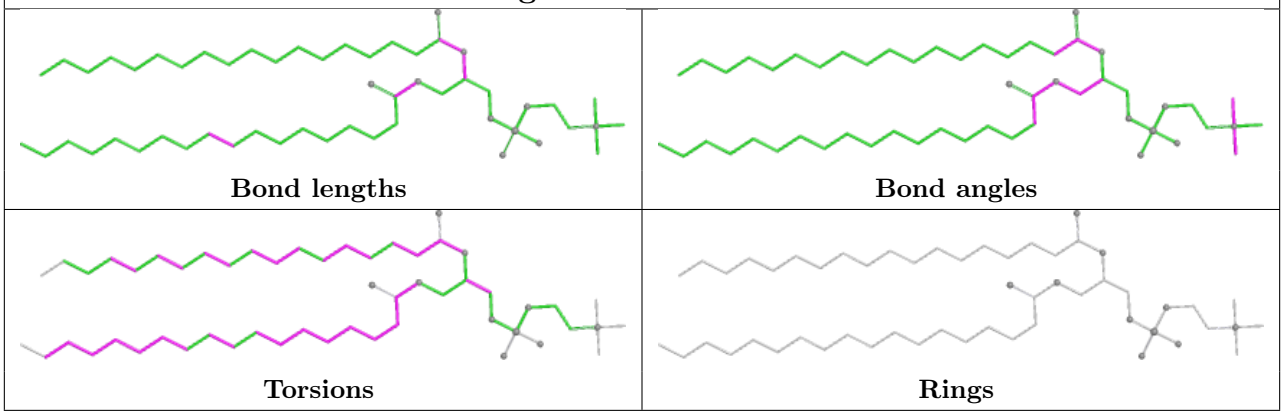
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

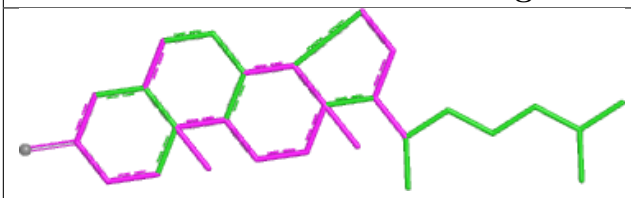
Ligand ADP C 2004



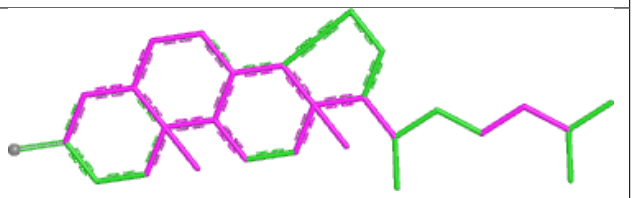
Ligand PC1 A 2014



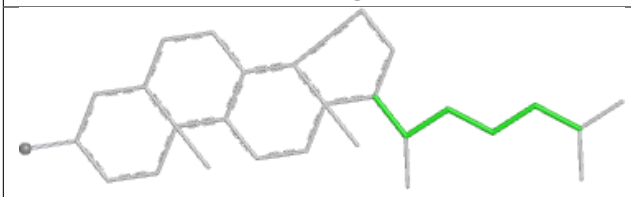
Ligand CLR A 2009



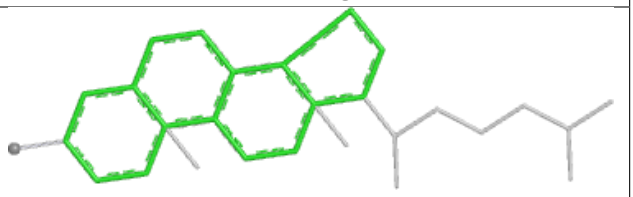
Bond lengths



Bond angles

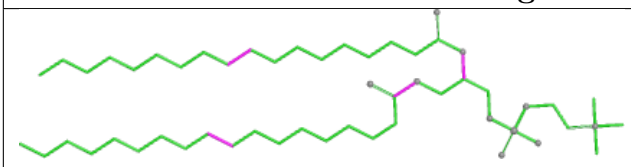


Torsions

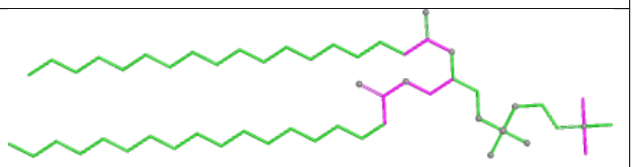


Rings

Ligand PC1 A 2013



Bond lengths



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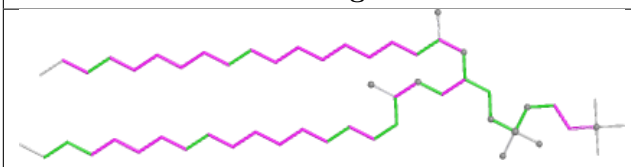

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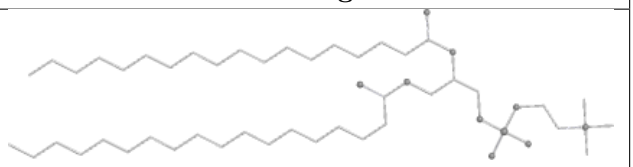

Rings

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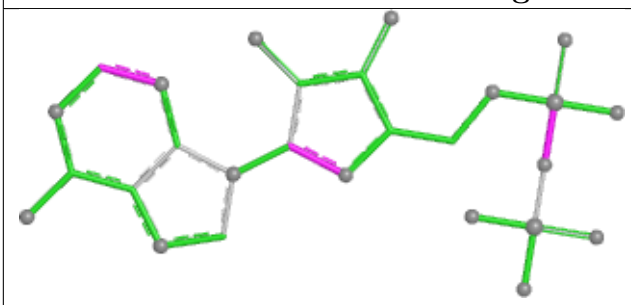

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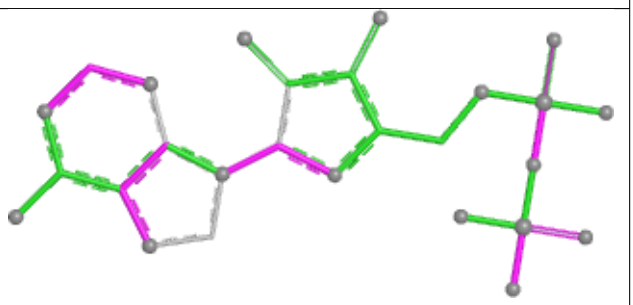
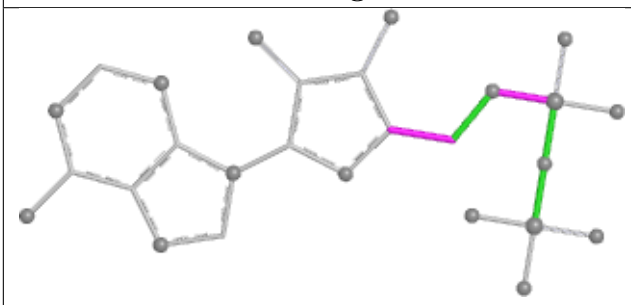


Bond angles



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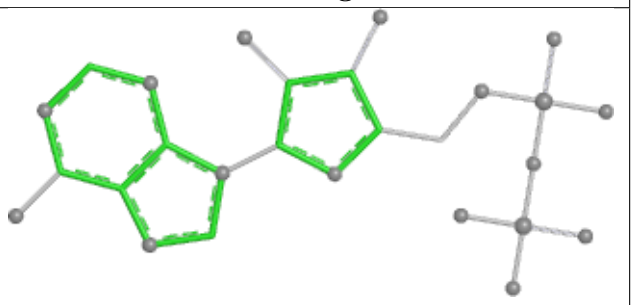
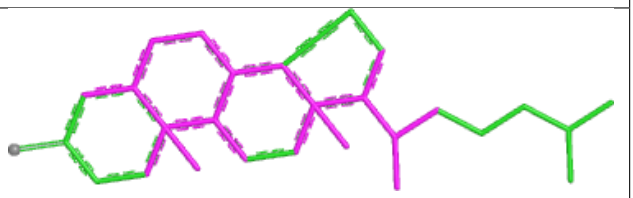


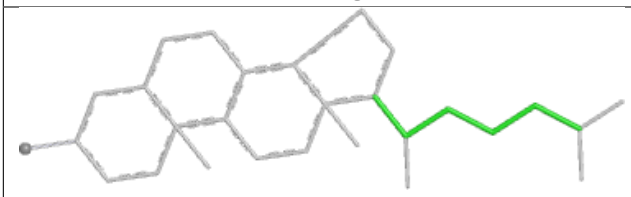
Rings

Ligand CLR C 2009

Bond lengths



Bond angles



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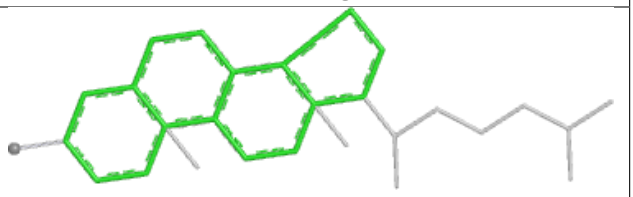
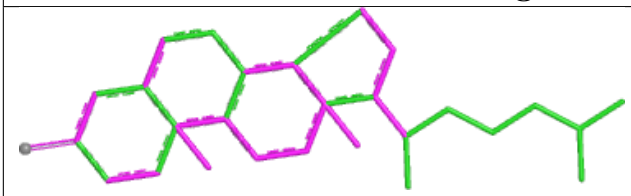


Rings

Ligand CLR A 2010



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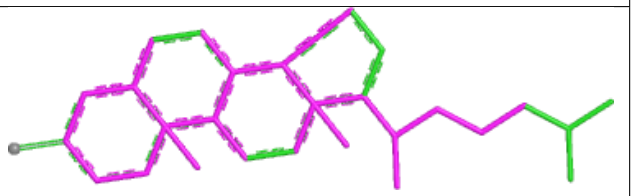

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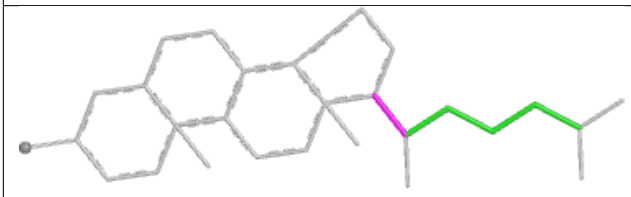

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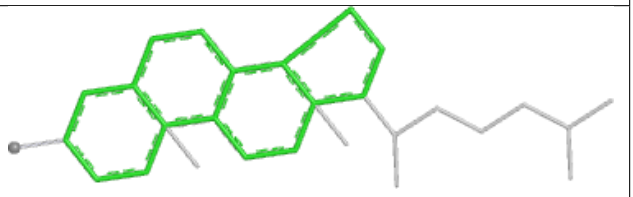
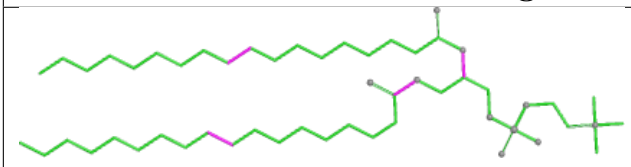


Rings

Ligand PC1 A 2011



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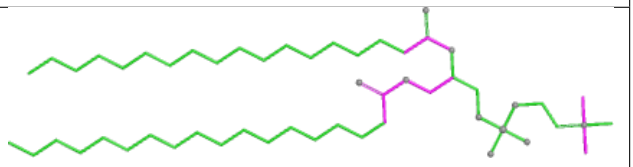

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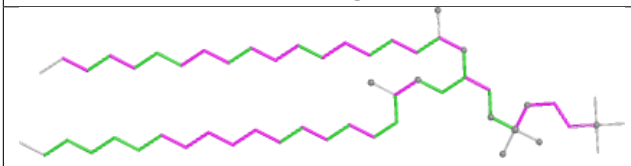

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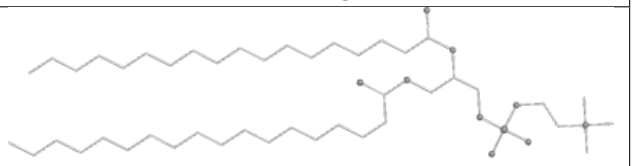
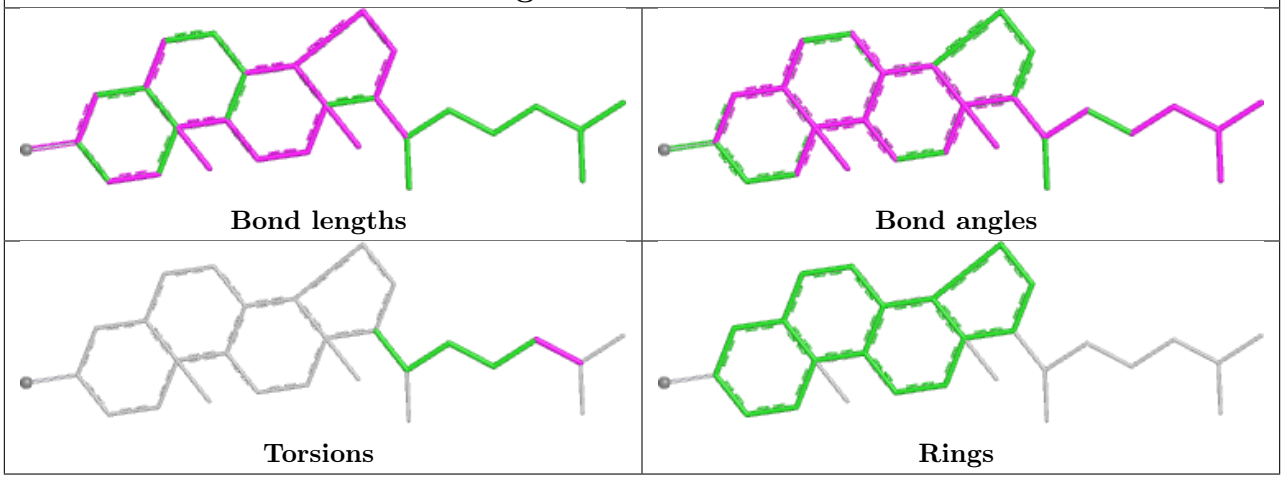
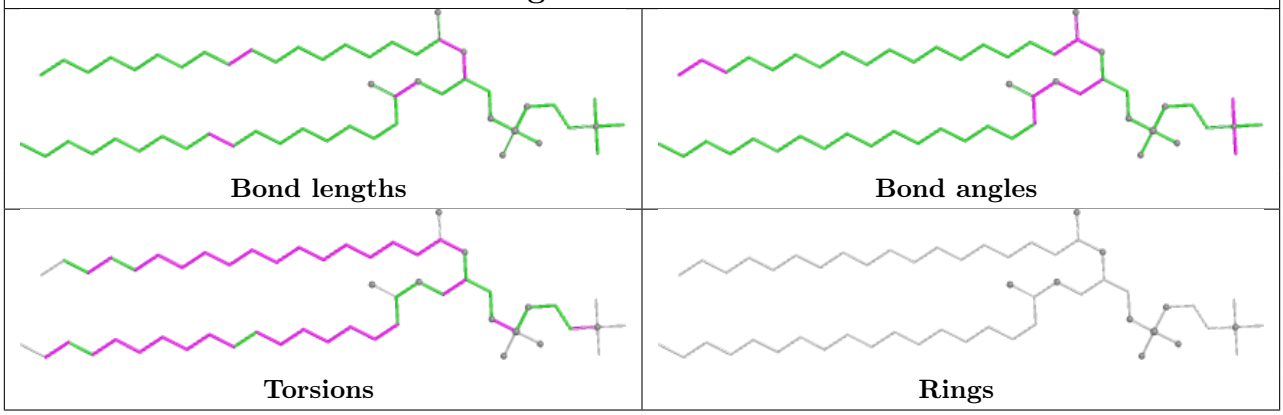


Rings

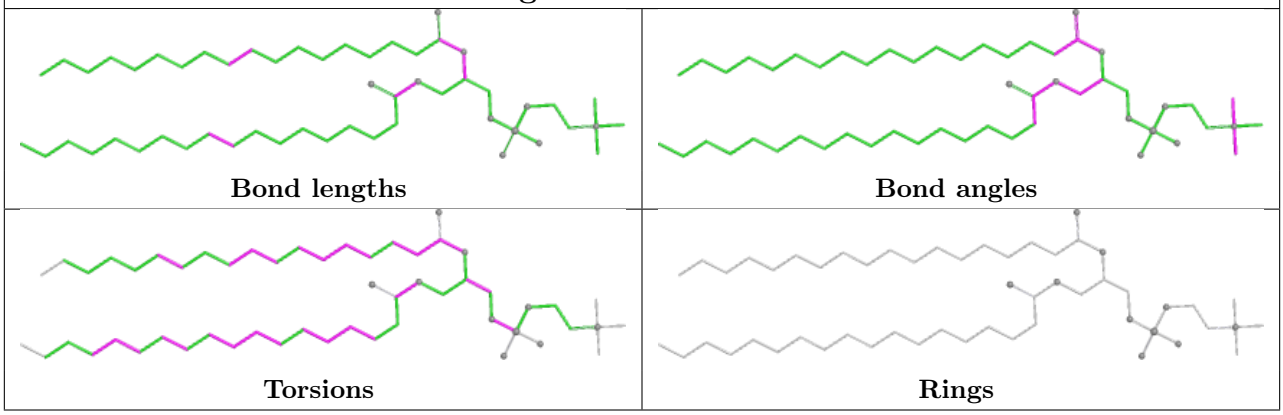
Ligand CLR C 2010



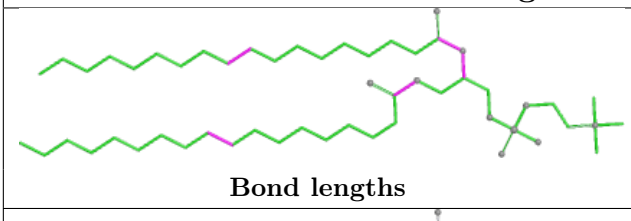
Ligand PC1 D 401



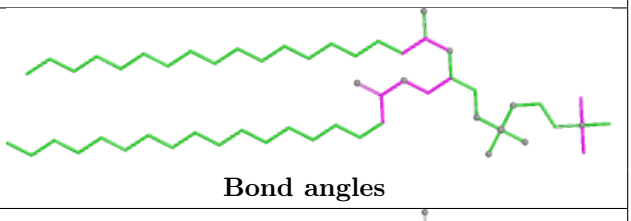
Ligand PC1 C 2015



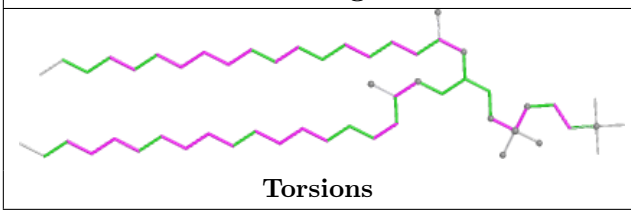
Ligand PC1 C 2012



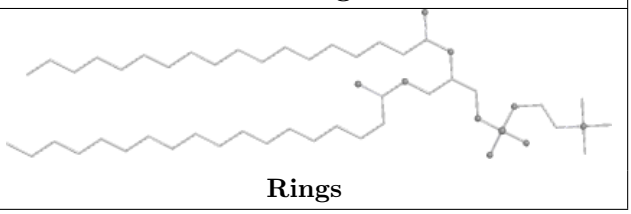
Bond lengths



Bond angles

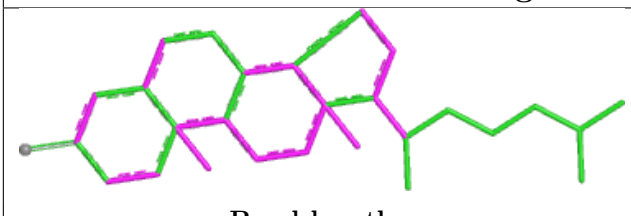


Torsions

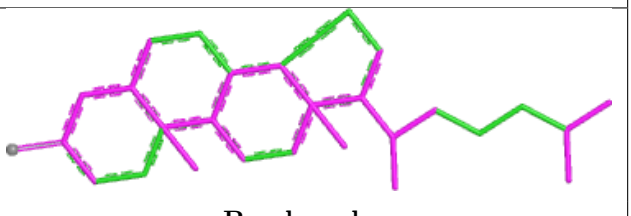


Rings

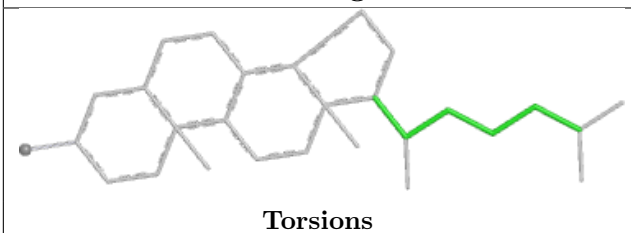
Ligand CLR C 2011



Bond lengths



Bond angles



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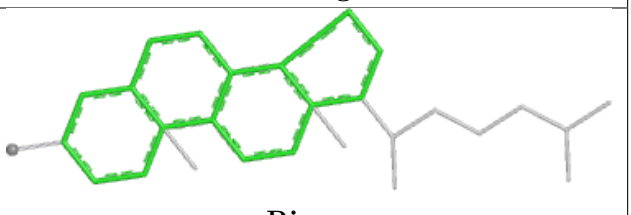
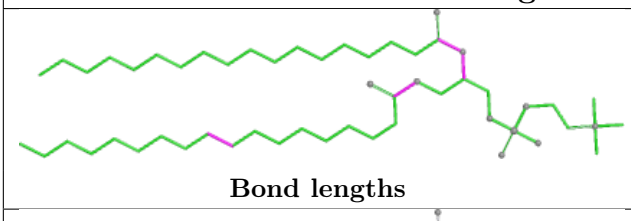


Rings

Ligand PC1 C 2013



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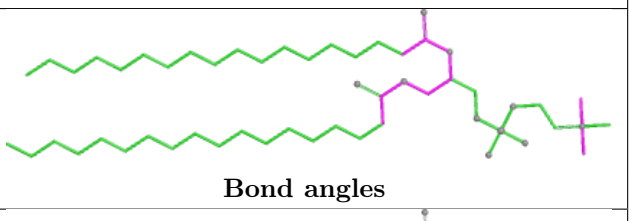
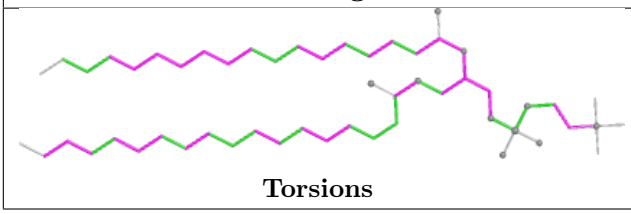
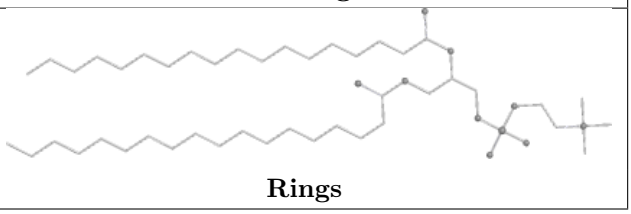


Bond angles

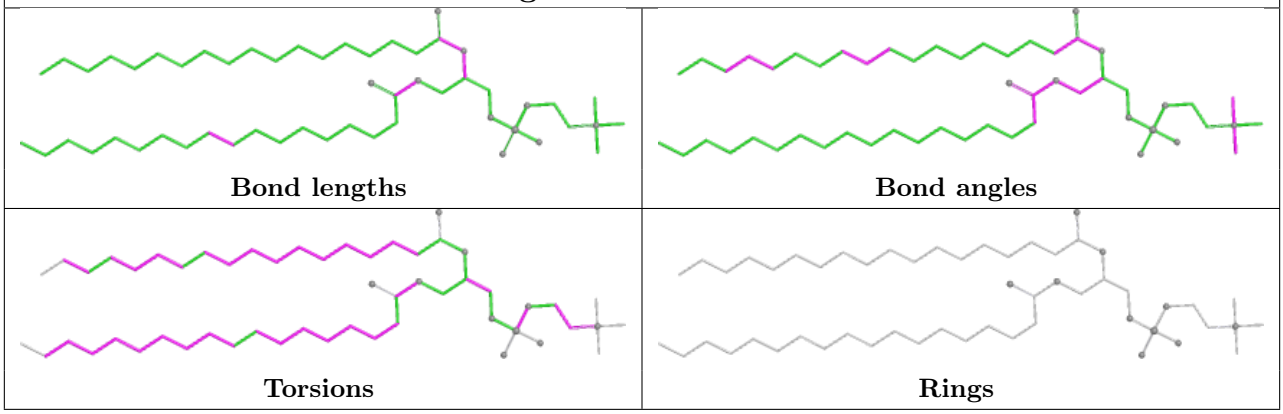


Torsions

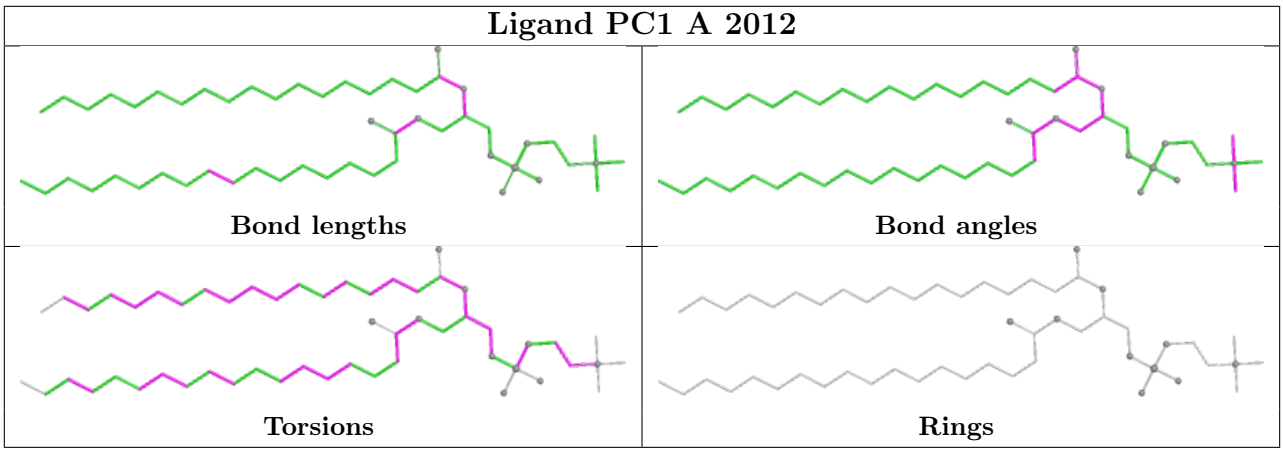


Rings

Ligand PC1 C 2014



Ligand PC1 A 2012



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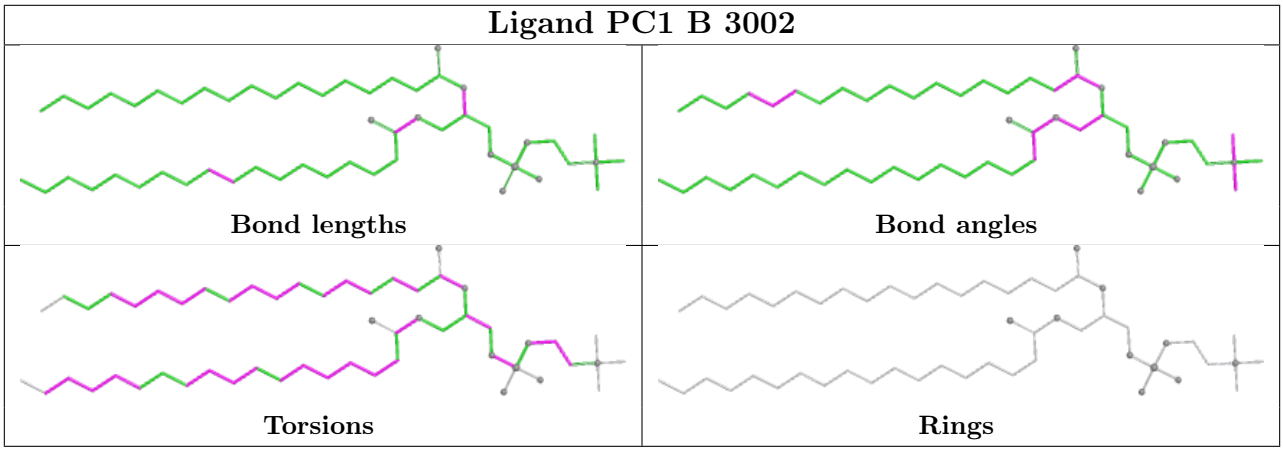

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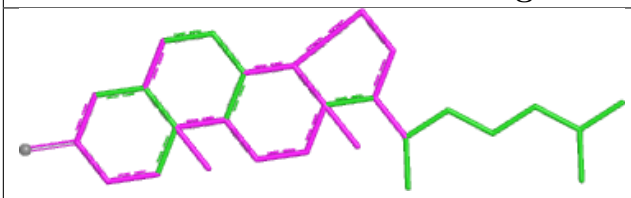
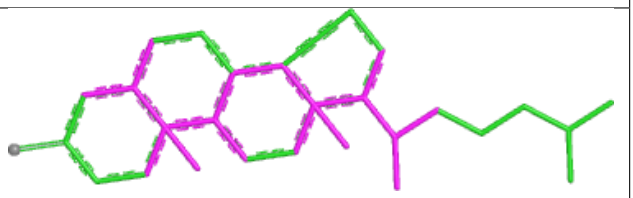
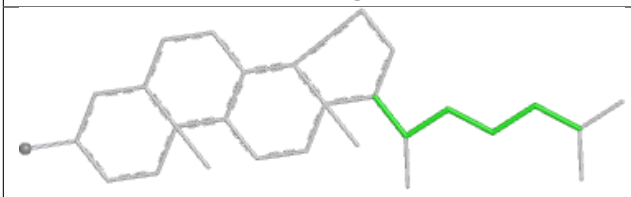


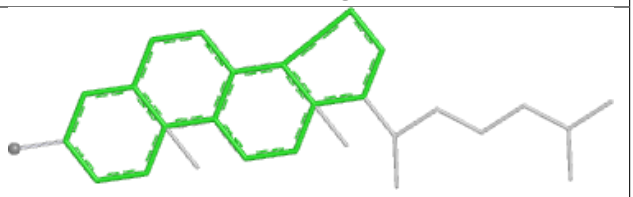
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

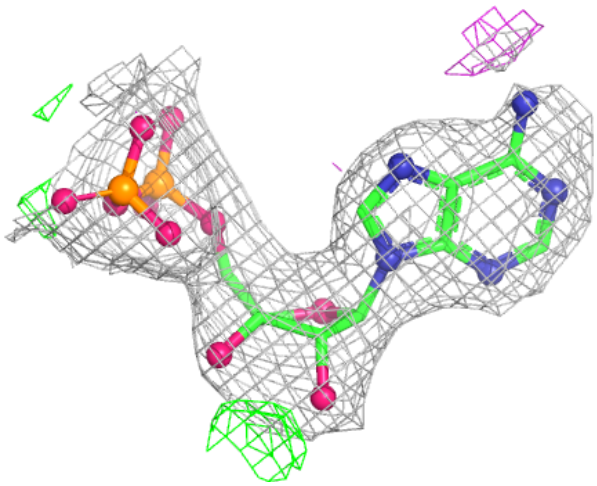
6.4 Ligands

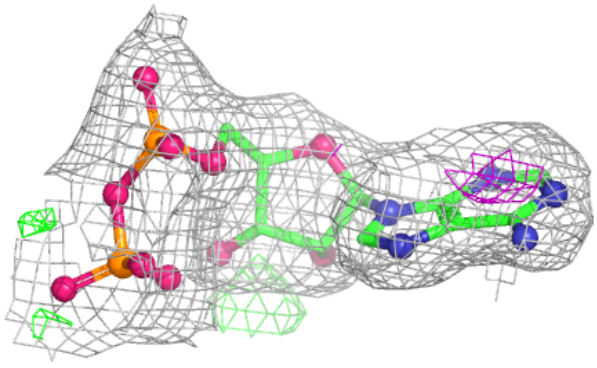
Unable to reproduce the depositors R factor - this section is therefore empty.

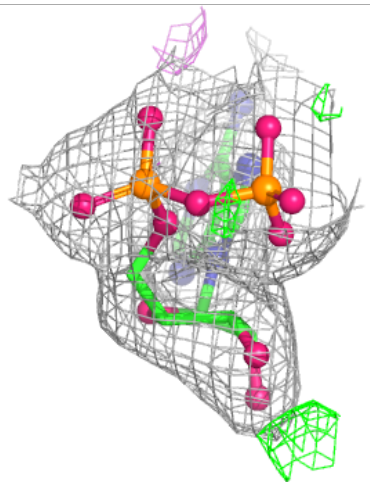
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

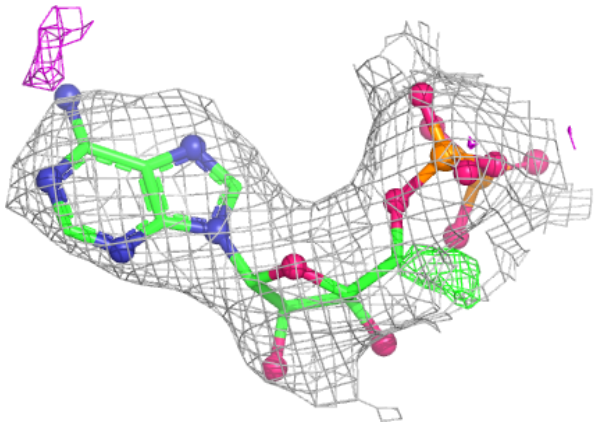


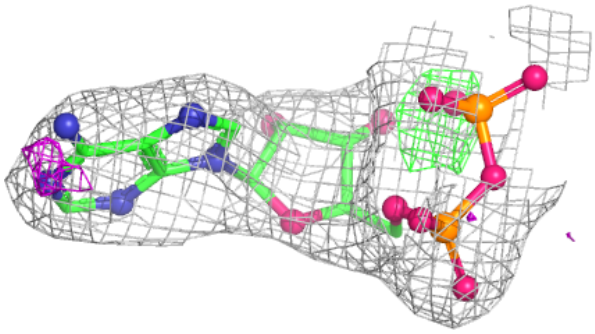


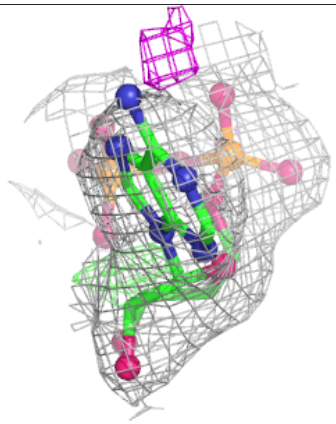


Electron density around ADP C 2004:

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

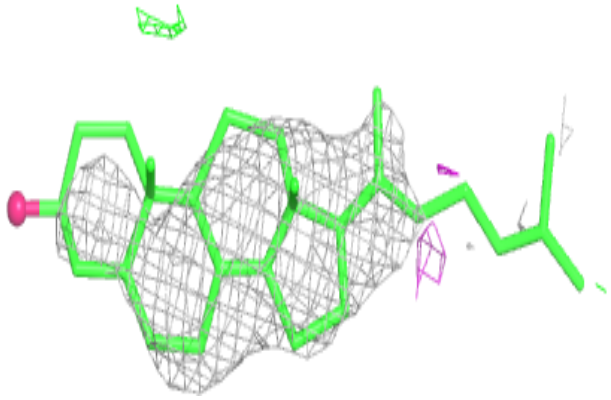


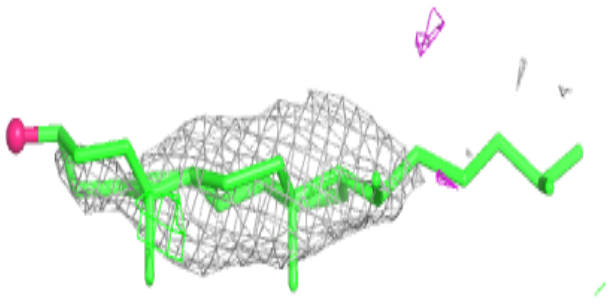


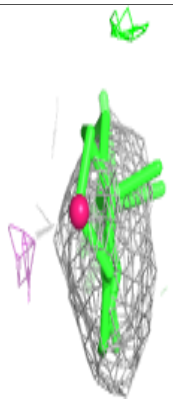


Electron density around CLR A 2009:

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

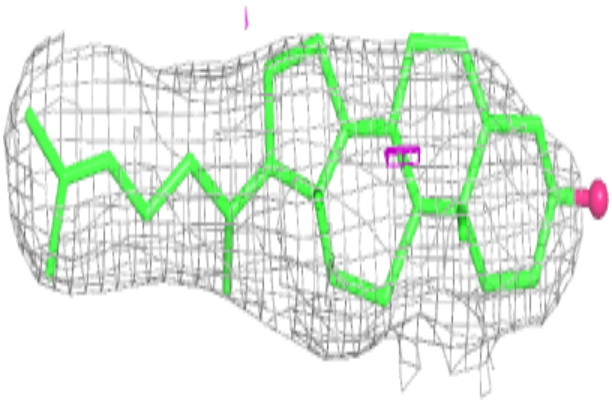


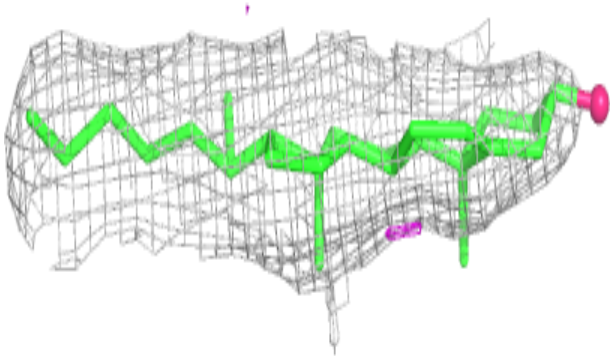


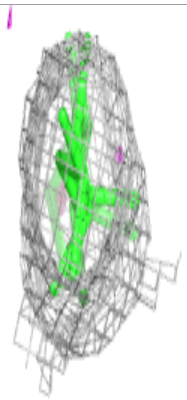


Electron density around CLR A 2010:

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

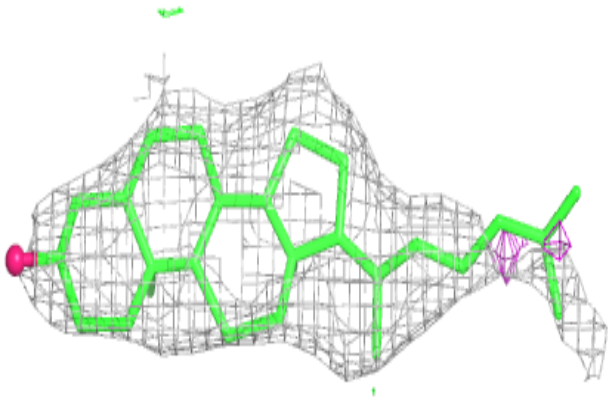


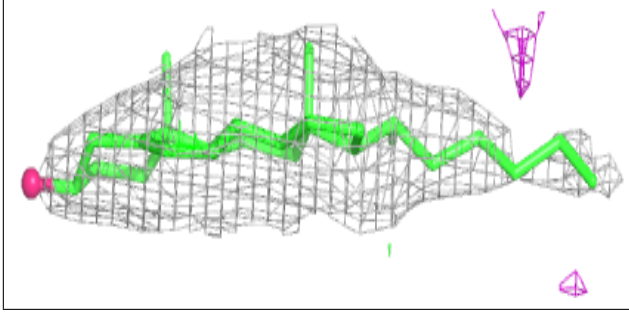


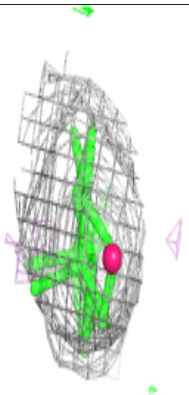


Electron density around CLR B 3001:

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

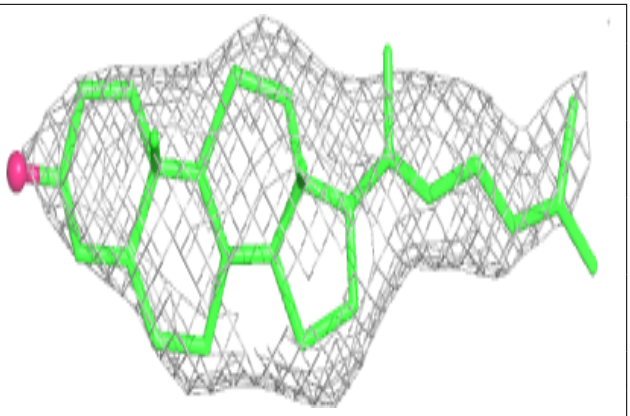


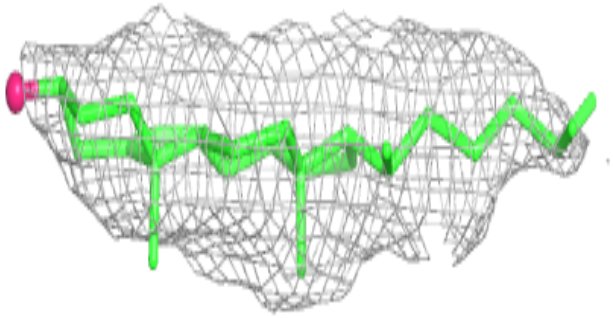


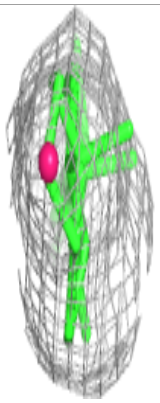


Electron density around CLR C 2009:

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

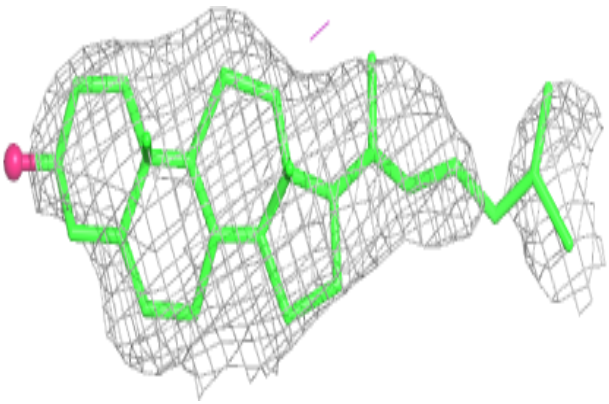


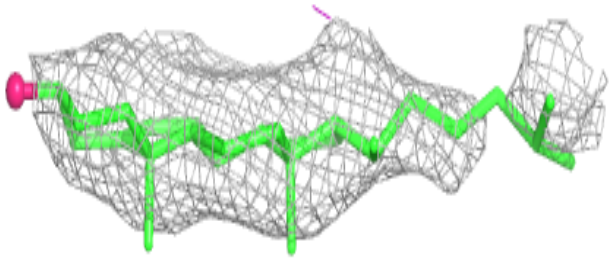


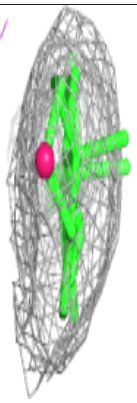


Electron density around CLR C 2010:

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

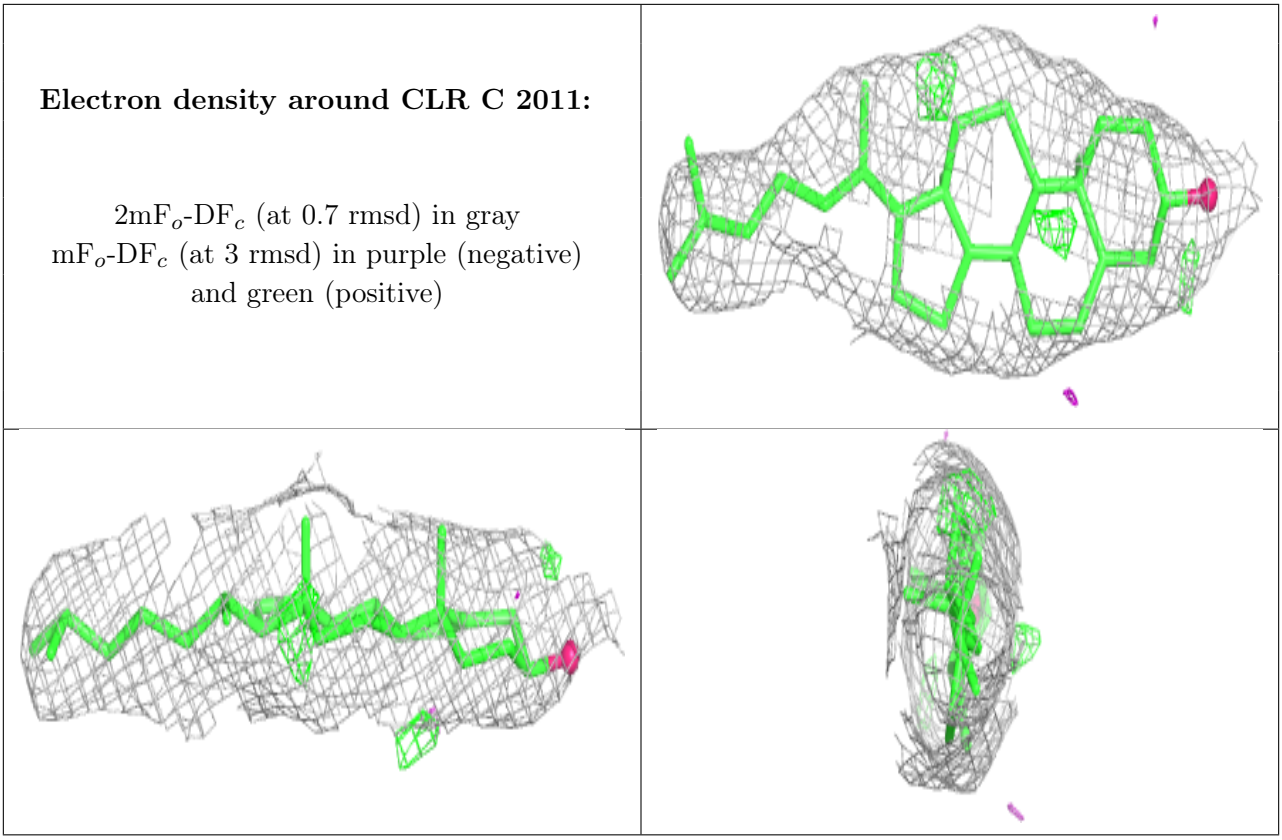






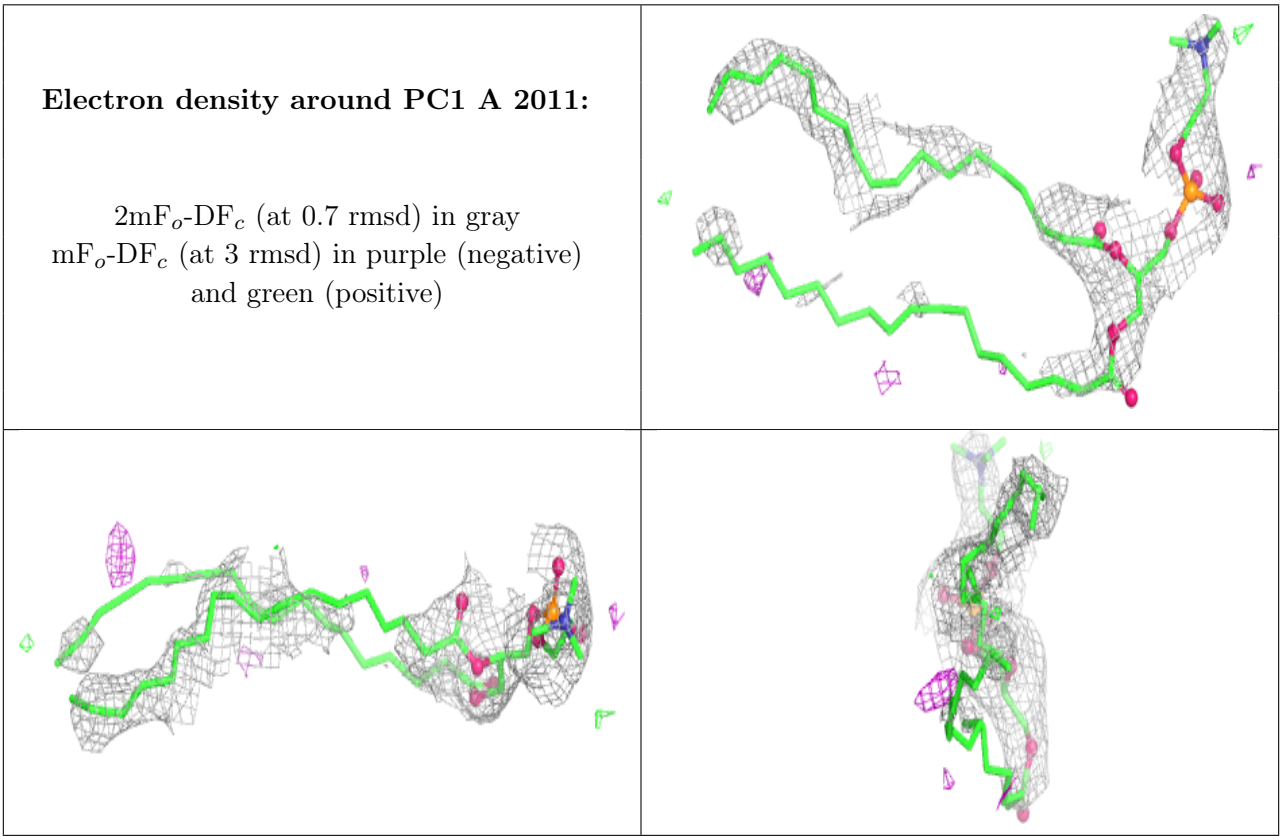
Electron density around CLR C 2011:

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



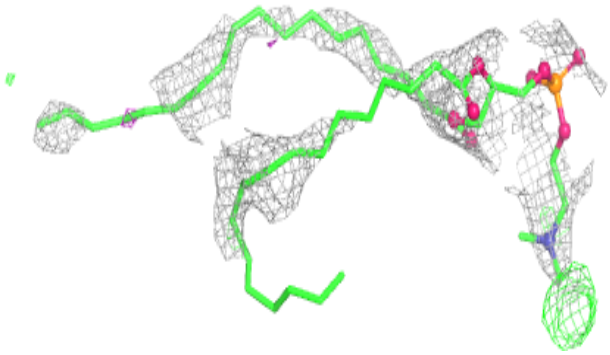
Electron density around PC1 A 2011:

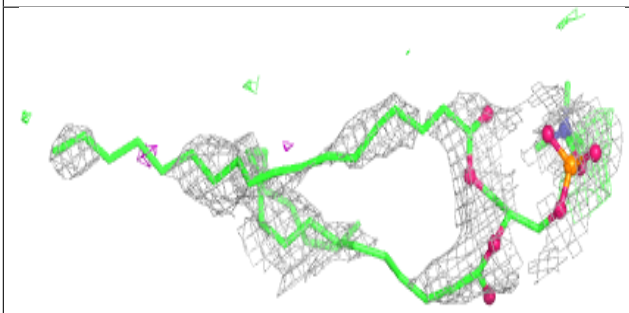
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

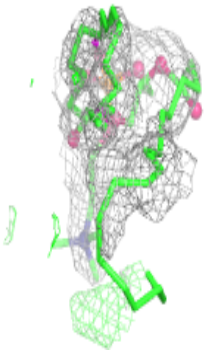


Electron density around PC1 A 2012:

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

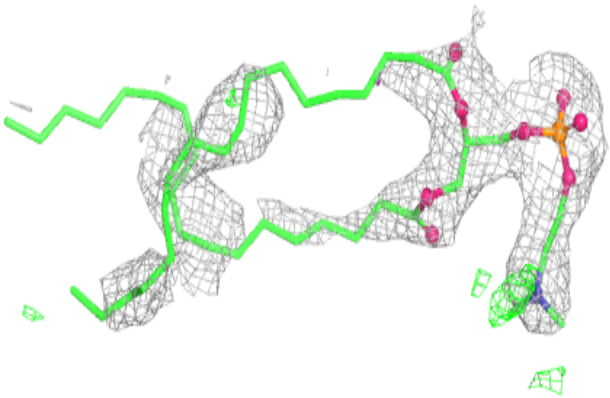


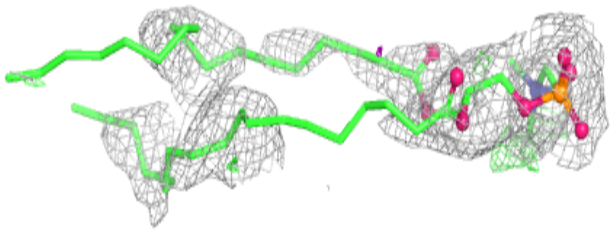


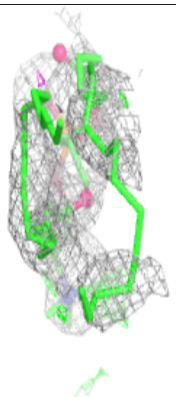


Electron density around PC1 A 2013:

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

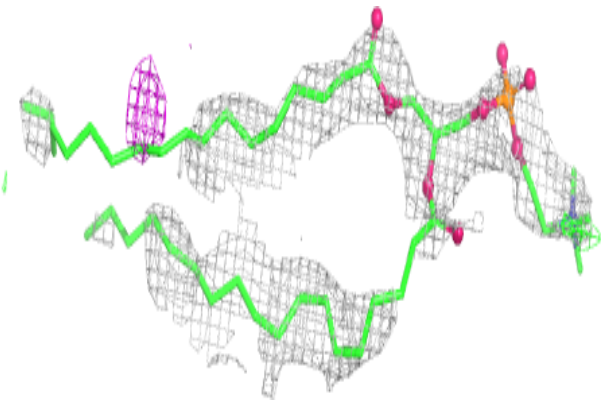


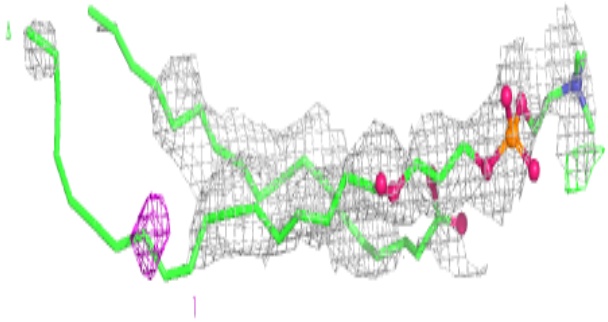


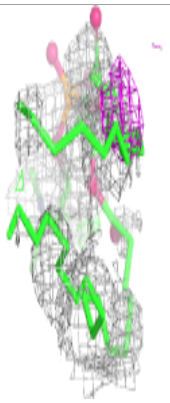


Electron density around PC1 A 2014:

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

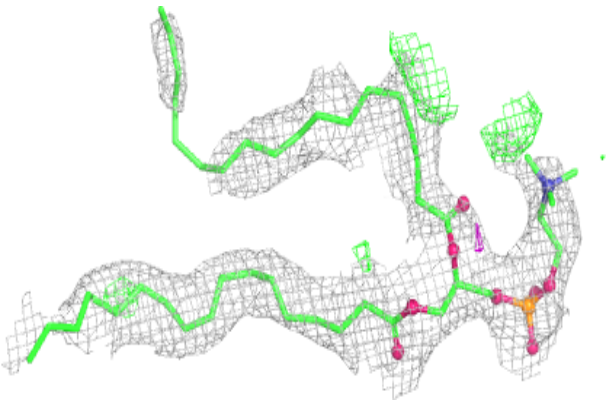


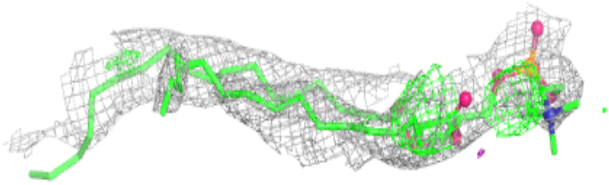


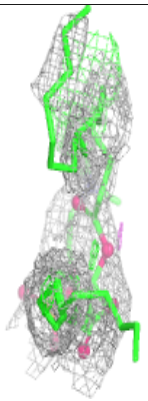


Electron density around PC1 B 3002:

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

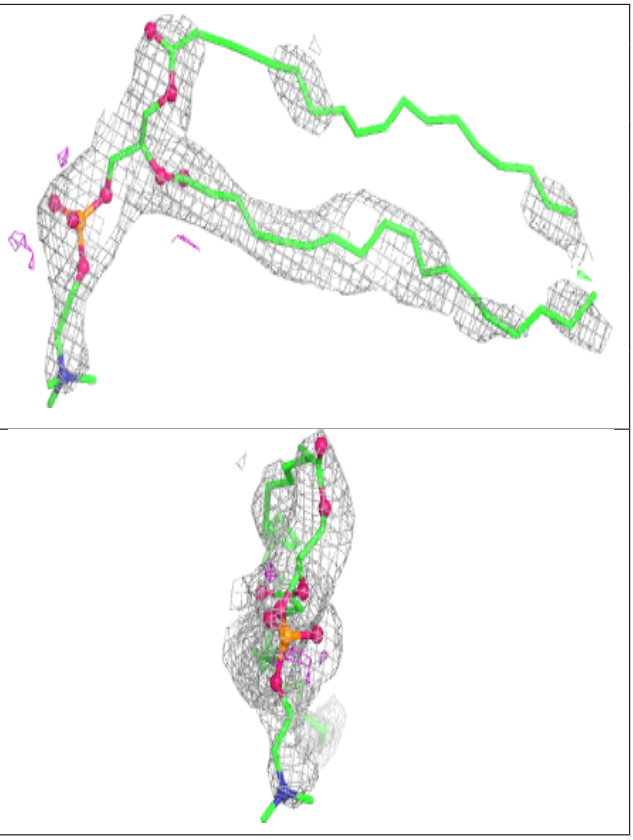






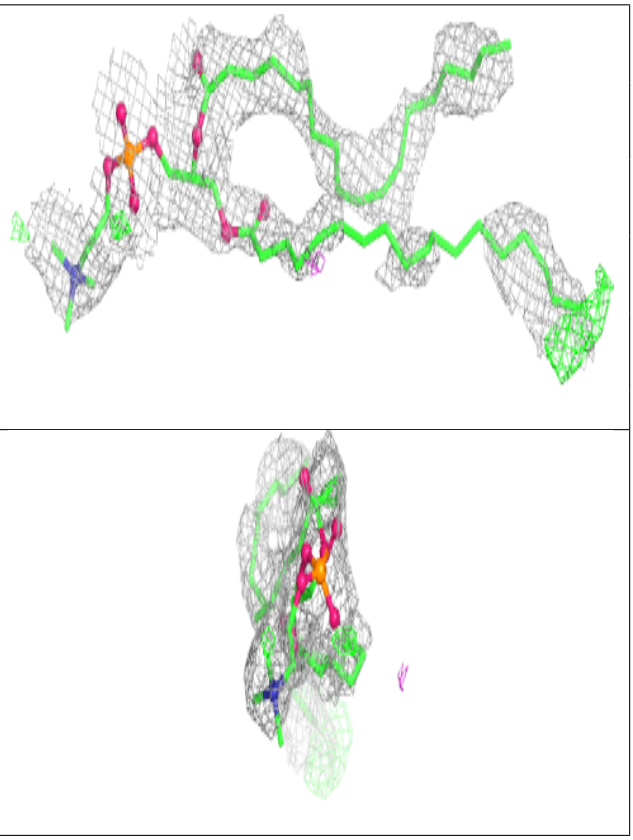
Electron density around PC1 C 2012:

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



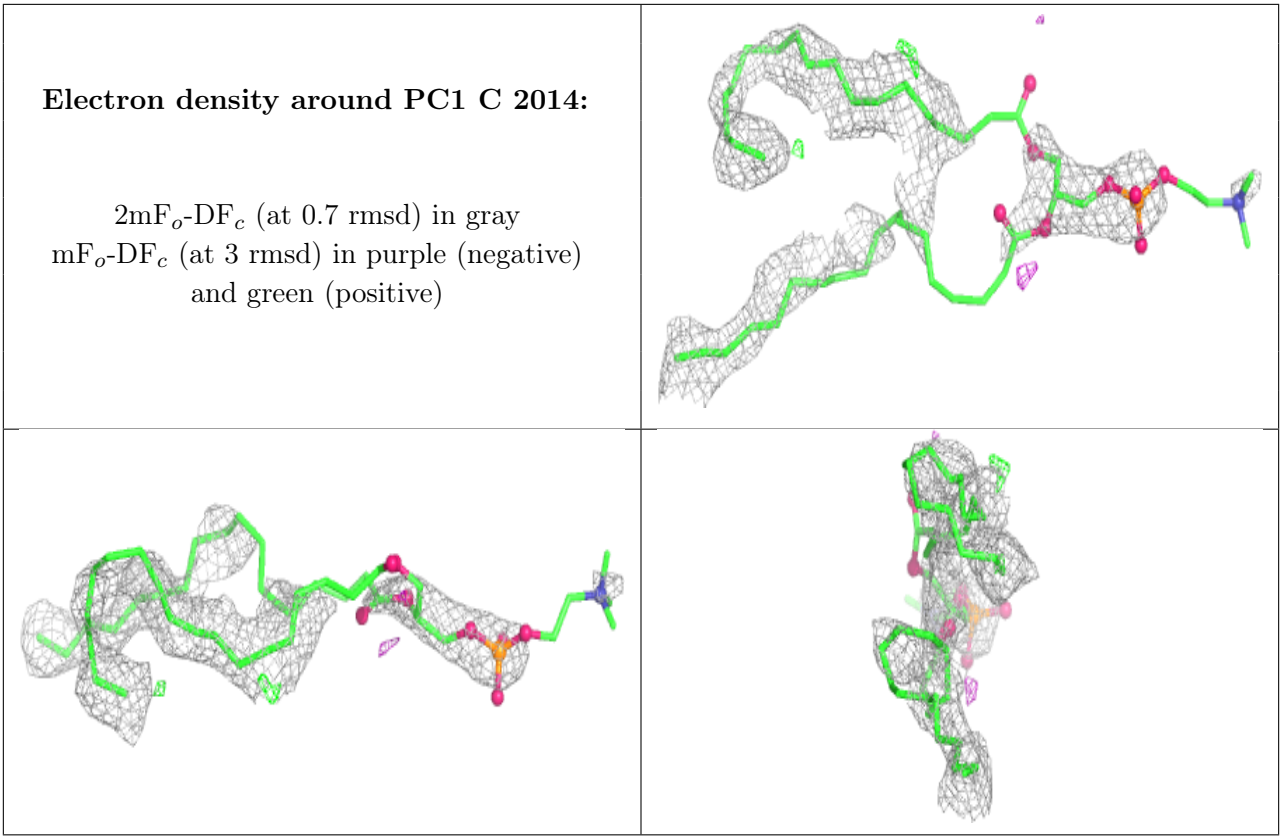
Electron density around PC1 C 2013:

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



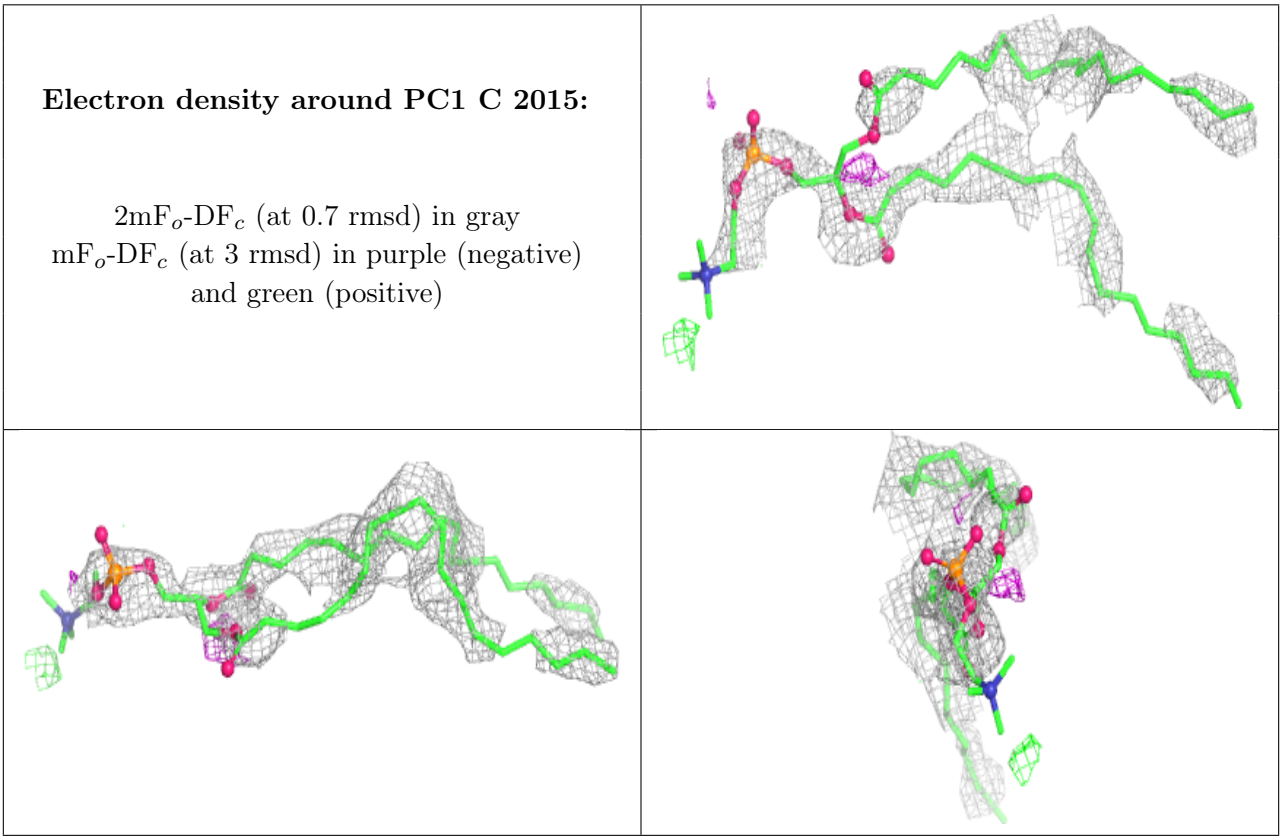
Electron density around PC1 C 2014:

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



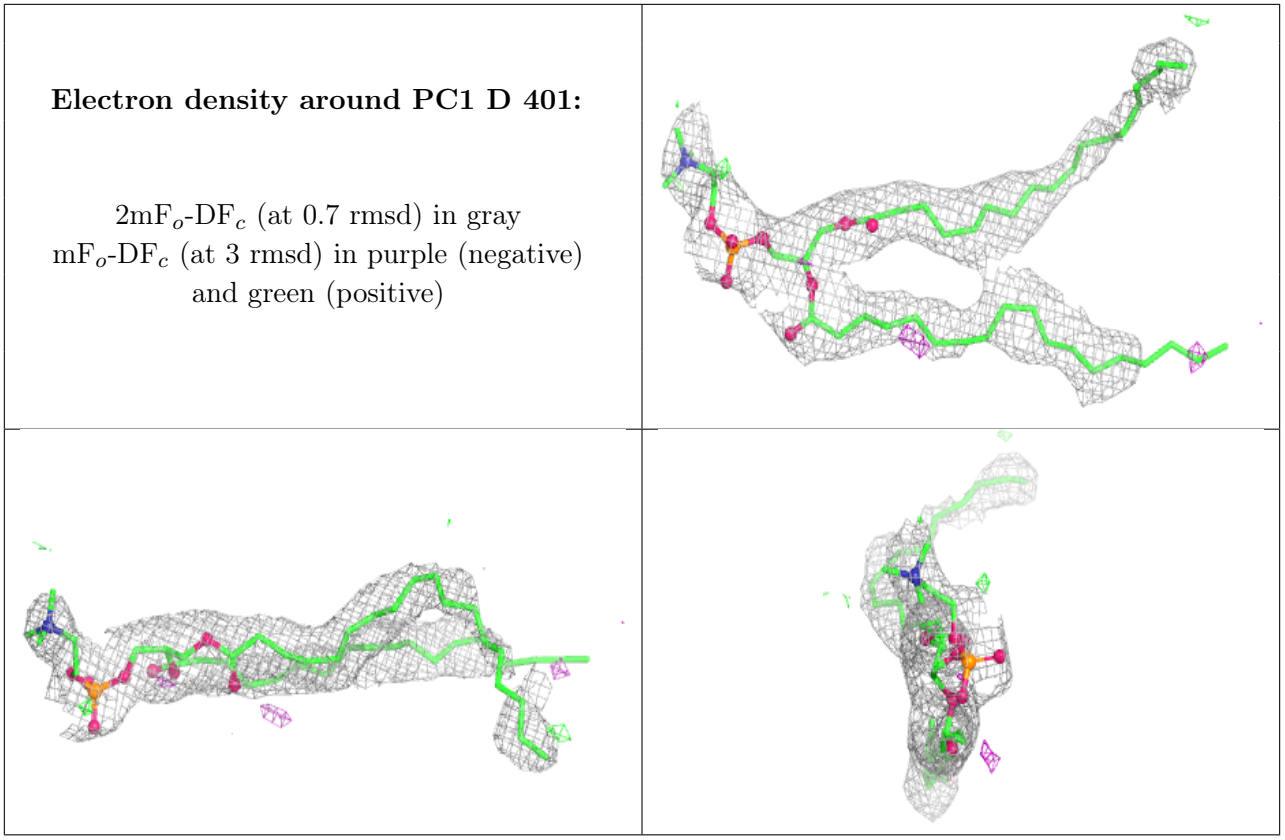
Electron density around PC1 C 2015:

$2mF_o$-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 401:

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



6.5 Other polymers (i)

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