



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:09 am BST

PDB ID : 4C9Q  
Title : Structure of yeast mitochondrial ADP/ATP carrier isoform 3 inhibited by carboxyatractyloside (P21 crystal form)  
Authors : Ruprecht, J.J.; Hellawell, A.M.; Harding, M.; Crichton, P.G.; McCoy, A.J.; Kunji, E.R.S.  
Deposited on : 2013-10-02  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.11  
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) : 2.11

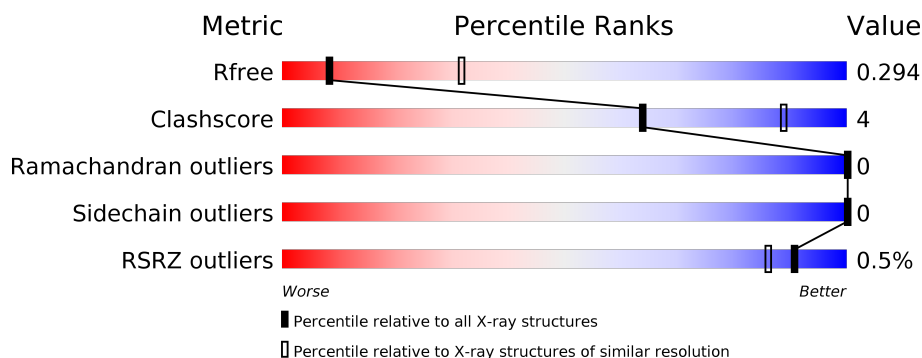
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	322	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>80%</span> <span>8%</span> <span>11%</span> </div> </div>
1	B	322	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>81%</span> <span>9%</span> <span>10%</span> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4576 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 ADP, ATP CARRIER PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2122	1364	363	381	14			
1	B	290	Total	C	N	O	S	0	0	0
			2137	1374	365	384	14			

There are 34 discrepancies between the modelled and reference sequences:

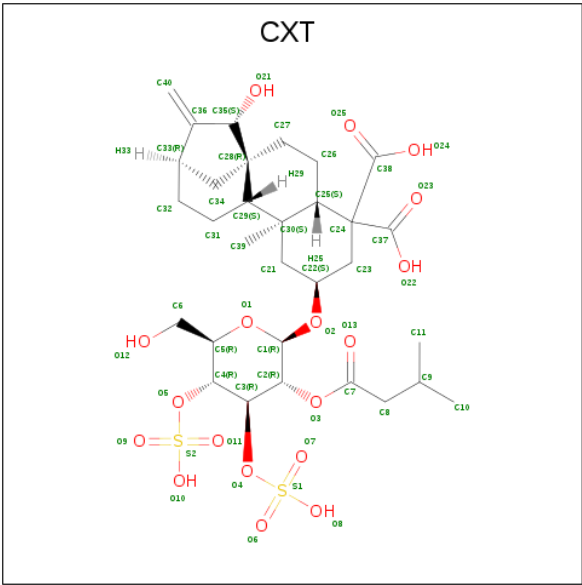
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	expression tag	UNP P18238
A	-13	HIS	-	expression tag	UNP P18238
A	-12	HIS	-	expression tag	UNP P18238
A	-11	HIS	-	expression tag	UNP P18238
A	-10	HIS	-	expression tag	UNP P18238
A	-9	HIS	-	expression tag	UNP P18238
A	-8	HIS	-	expression tag	UNP P18238
A	-7	HIS	-	expression tag	UNP P18238
A	-6	HIS	-	expression tag	UNP P18238
A	-5	HIS	-	expression tag	UNP P18238
A	-4	ILE	-	expression tag	UNP P18238
A	-3	GLU	-	expression tag	UNP P18238
A	-2	GLY	-	expression tag	UNP P18238
A	-1	ARG	-	expression tag	UNP P18238
A	0	SER	-	expression tag	UNP P18238
A	1	MET	-	expression tag	UNP P18238
A	2	ALA	-	expression tag	UNP P18238
B	-14	MET	-	expression tag	UNP P18238
B	-13	HIS	-	expression tag	UNP P18238
B	-12	HIS	-	expression tag	UNP P18238
B	-11	HIS	-	expression tag	UNP P18238
B	-10	HIS	-	expression tag	UNP P18238
B	-9	HIS	-	expression tag	UNP P18238
B	-8	HIS	-	expression tag	UNP P18238
B	-7	HIS	-	expression tag	UNP P18238

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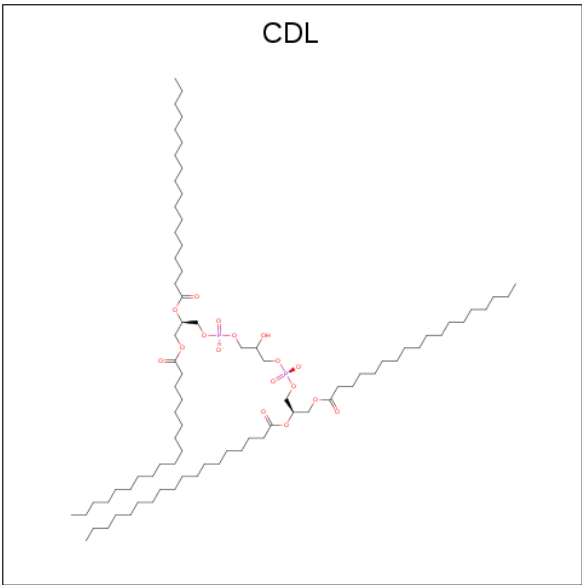
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP P18238
B	-5	HIS	-	expression tag	UNP P18238
B	-4	ILE	-	expression tag	UNP P18238
B	-3	GLU	-	expression tag	UNP P18238
B	-2	GLY	-	expression tag	UNP P18238
B	-1	ARG	-	expression tag	UNP P18238
B	0	SER	-	expression tag	UNP P18238
B	1	MET	-	expression tag	UNP P18238
B	2	ALA	-	expression tag	UNP P18238

- Molecule 2 is Carboxyatractyloside (three-letter code: CXT) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>18</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			51	31	18	2		
2	B	1	Total	C	O	S	0	0
			51	31	18	2		

- Molecule 3 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			28	13	13	2		
3	A	1	Total	C	O	P	0	0
			35	19	14	2		
3	A	1	Total	C	O	P	0	0
			38	19	17	2		
3	B	1	Total	C	O	P	0	0
			37	19	16	2		
3	B	1	Total	C	O	P	0	0
			38	23	13	2		
3	B	1	Total	C	O	P	0	0
			39	20	17	2		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.70Å 107.88Å 57.00Å 90.00° 93.62° 90.00°	Depositor
Resolution (Å)	41.45 – 3.20 41.45 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.6 (41.45-3.20) 97.6 (41.45-3.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 3.18Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.258 , 0.295 0.258 , 0.294	Depositor DCC
$R_{free}$ test set	526 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.731	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8567e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, CXT

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	0.21	0/2157	0.35	0/2906
1	B	0.22	0/2174	0.36	0/2933
All	All	0.22	0/4331	0.35	0/5839

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2122	0	2105	18	0
1	B	2137	0	2095	18	0
2	A	51	0	44	0	0
2	B	51	0	44	1	0
3	A	101	0	61	8	0
3	B	114	0	81	5	0
All	All	4576	0	4430	38	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 4.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLY:HA2	3:A:802:CDL:HA21	1.75	0.68
1:A:278:GLY:H	3:A:801:CDL:HB31	1.57	0.68
1:B:278:GLY:H	3:B:801:CDL:HB31	1.58	0.67
1:A:27:LYS:HD3	1:A:82:ASN:HB3	1.81	0.62
1:A:44:ASP:HB2	1:A:243:ARG:HH12	1.66	0.60
1:B:162:LEU:H	3:B:800:CDL:HB22	1.65	0.60
1:A:92:LEU:HD23	1:A:130:SER:HA	1.84	0.59
1:B:44:ASP:HB2	1:B:243:ARG:HH12	1.70	0.57
1:A:247:THR:HB	1:A:253:LYS:HG2	1.86	0.57
1:B:247:THR:HB	1:B:253:LYS:HG2	1.88	0.56
3:A:802:CDL:HB62	1:B:258:ILE:HD12	1.89	0.54
1:B:92:LEU:HD23	1:B:130:SER:HA	1.90	0.54
1:A:258:ILE:HD12	3:B:802:CDL:HB62	1.91	0.52
1:B:258:ILE:HG13	3:B:802:CDL:HA32	1.93	0.50
1:B:32:PRO:HB3	1:B:75:PHE:HB3	1.95	0.49
1:B:27:LYS:HD3	1:B:82:ASN:HB3	1.94	0.49
1:B:158:GLN:O	1:B:168:LYS:NZ	2.36	0.48
1:A:173:ASP:OD2	1:A:249:GLY:N	2.45	0.48
1:A:135:TYR:OH	1:A:180:ARG:O	2.23	0.48
1:A:35:ARG:HG3	1:A:145:ALA:HB1	1.95	0.47
1:A:162:LEU:HB2	3:A:800:CDL:H1	1.97	0.47
1:B:173:ASP:OD2	1:B:249:GLY:N	2.45	0.47
1:A:78:GLY:N	3:A:800:CDL:OA4	2.27	0.46
3:A:802:CDL:O1	3:B:802:CDL:OA4	2.24	0.46
1:B:143:ARG:NH1	1:B:248:SER:OG	2.48	0.46
1:A:58:GLY:HA3	3:A:801:CDL:HA22	1.99	0.45
1:A:143:ARG:NH1	1:A:248:SER:OG	2.51	0.43
1:A:33:ILE:HD12	1:A:33:ILE:H	1.84	0.43
1:A:179:TYR:O	3:A:802:CDL:HB32	2.18	0.43
1:B:141:ARG:NH1	1:B:145:ALA:HB2	2.34	0.42
1:B:135:TYR:OH	1:B:180:ARG:O	2.22	0.42
1:B:35:ARG:NH1	1:B:74:SER:O	2.53	0.42
2:B:401:CXT:H34	2:B:401:CXT:H39	2.02	0.42
1:A:31:SER:N	1:A:32:PRO:HD2	2.34	0.42
1:B:31:SER:N	1:B:32:PRO:HD2	2.35	0.41
1:B:144:LEU:HD11	1:B:162:LEU:HA	2.03	0.41
1:A:32:PRO:HB3	1:A:75:PHE:HB3	2.01	0.41
1:B:86:TYR:CZ	1:B:90:GLN:HG3	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	278/322 (86%)	277 (100%)	1 (0%)	0	100	100
1	B	284/322 (88%)	281 (99%)	3 (1%)	0	100	100
All	All	562/644 (87%)	558 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/255 (81%)	207 (100%)	0	100	100
1	B	205/255 (80%)	205 (100%)	0	100	100
All	All	412/510 (81%)	412 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	250	GLN
1	B	250	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CXT	A	401	-	51,55,55	1.05	2 (3%)	63,89,89	1.25	6 (9%)
3	CDL	A	802	-	37,37,99	1.50	4 (10%)	43,49,111	1.60	5 (11%)
3	CDL	B	802	-	38,38,99	1.48	4 (10%)	44,50,111	1.53	5 (11%)
3	CDL	A	800	-	27,27,99	1.09	2 (7%)	31,36,111	1.23	2 (6%)
2	CXT	B	401	-	51,55,55	1.05	2 (3%)	63,89,89	1.19	5 (7%)
3	CDL	B	801	-	37,37,99	1.09	2 (5%)	41,46,111	1.10	3 (7%)
3	CDL	B	800	-	36,36,99	1.20	3 (8%)	41,47,111	1.25	3 (7%)
3	CDL	A	801	-	33,34,99	1.15	2 (6%)	37,44,111	1.20	3 (8%)

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
2	CXT	A	401	-	-	0/24/120/120	0/6/5/5
3	CDL	A	802	-	-	20/45/45/110	-
3	CDL	B	802	-	-	19/46/46/110	-
3	CDL	A	800	-	-	12/33/33/110	-
2	CXT	B	401	-	-	0/24/120/120	0/6/5/5
3	CDL	B	801	-	-	11/44/44/110	-
3	CDL	B	800	-	-	17/45/45/110	-
3	CDL	A	801	-	-	11/41/41/110	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	CDL	OB6-CB5	4.87	1.46	1.35
3	B	802	CDL	OB6-CB5	4.84	1.46	1.35
3	A	802	CDL	OA6-CA5	4.76	1.46	1.35
3	B	802	CDL	OA6-CA5	4.74	1.45	1.35
3	B	801	CDL	OB8-CB7	4.30	1.45	1.33
3	A	801	CDL	OB8-CB7	4.29	1.45	1.33
3	B	802	CDL	OB8-CB7	4.24	1.45	1.33
3	A	802	CDL	OB8-CB7	4.23	1.45	1.33
3	A	800	CDL	OA6-CA5	4.20	1.46	1.34
3	B	800	CDL	OB6-CB5	4.16	1.46	1.34
3	A	801	CDL	OB6-CB5	4.15	1.46	1.34
3	B	801	CDL	OB6-CB5	4.13	1.45	1.34
2	A	401	CXT	O3-C7	4.12	1.45	1.34
3	B	800	CDL	OA6-CA5	4.09	1.45	1.34
2	B	401	CXT	O3-C7	4.08	1.45	1.34
2	B	401	CXT	C23-C24	-3.01	1.52	1.55
2	A	401	CXT	C23-C24	-2.84	1.52	1.55
3	B	800	CDL	OA8-CA7	2.51	1.45	1.33
3	A	800	CDL	OA8-CA7	2.51	1.45	1.33
3	B	802	CDL	OA8-CA7	2.51	1.45	1.33
3	A	802	CDL	OA8-CA7	2.50	1.45	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	CDL	OA6-CA5-C11	5.21	120.67	111.09
3	B	802	CDL	OA6-CA5-C11	5.00	120.29	111.09
3	A	802	CDL	OB6-CB5-C51	4.97	120.23	111.09
3	B	802	CDL	OB6-CB5-C51	4.89	120.09	111.09
2	A	401	CXT	O3-C7-C8	4.66	120.02	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	CXT	O3-C7-C8	4.32	119.39	111.46
3	A	800	CDL	OA6-CA5-C11	4.24	120.64	111.50
3	A	801	CDL	OB6-CB5-C51	4.11	120.36	111.50
3	B	801	CDL	OB6-CB5-C51	4.05	120.24	111.50
3	B	800	CDL	OA6-CA5-C11	4.02	120.17	111.50
3	B	802	CDL	CA4-OA6-CA5	-3.50	111.38	117.90
3	A	801	CDL	OB8-CB7-C71	3.40	120.30	111.38
2	B	401	CXT	C33-C36-C40	-3.37	123.72	127.44
2	A	401	CXT	C33-C36-C40	-3.33	123.76	127.44
3	B	800	CDL	OB6-CB5-C51	3.21	119.77	110.80
3	A	802	CDL	CA4-OA6-CA5	-3.15	112.03	117.90
2	A	401	CXT	C2-O3-C7	-3.11	112.34	117.53
3	A	802	CDL	CB4-OB6-CB5	-3.00	112.30	117.90
2	A	401	CXT	C33-C36-C35	2.94	112.68	107.93
2	B	401	CXT	C33-C36-C35	2.88	112.58	107.93
3	A	800	CDL	CA4-OA6-CA5	-2.87	110.72	117.79
3	B	800	CDL	CA4-OA6-CA5	-2.76	110.99	117.79
2	B	401	CXT	C2-O3-C7	-2.68	113.06	117.53
3	B	801	CDL	OB8-CB7-C71	2.47	119.65	111.91
3	A	802	CDL	OB8-CB7-C71	2.41	119.48	111.91
3	B	801	CDL	CB4-OB6-CB5	-2.38	111.93	117.79
3	A	801	CDL	CB4-OB6-CB5	-2.38	111.94	117.79
3	B	802	CDL	OB8-CB7-C71	2.37	119.35	111.91
3	B	802	CDL	CB4-OB6-CB5	-2.28	113.64	117.90
2	A	401	CXT	C27-C28-C29	2.17	113.88	110.28
2	B	401	CXT	C32-C31-C29	2.14	117.26	112.43
2	A	401	CXT	C32-C31-C29	2.08	117.13	112.43

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	CDL	CA2-OA2-PA1-OA4
3	A	802	CDL	C11-CA5-OA6-CA4
3	A	802	CDL	CB2-OB2-PB2-OB3
3	A	802	CDL	CB2-OB2-PB2-OB4
3	A	802	CDL	CB2-OB2-PB2-OB5
3	A	802	CDL	CB3-OB5-PB2-OB2
3	A	802	CDL	CB3-OB5-PB2-OB3
3	A	802	CDL	CB3-OB5-PB2-OB4
3	B	802	CDL	O1-C1-CB2-OB2
3	B	802	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
3	B	802	CDL	CA2-OA2-PA1-OA4
3	B	802	CDL	CA3-OA5-PA1-OA3
3	B	802	CDL	OA7-CA5-OA6-CA4
3	B	802	CDL	C11-CA5-OA6-CA4
3	B	802	CDL	CB2-OB2-PB2-OB3
3	B	802	CDL	CB2-OB2-PB2-OB4
3	B	802	CDL	CB2-OB2-PB2-OB5
3	B	801	CDL	CA2-OA2-PA1-OA3
3	B	801	CDL	CB2-OB2-PB2-OB4
3	B	801	CDL	CB3-OB5-PB2-OB4
3	B	800	CDL	CA3-OA5-PA1-OA3
3	B	800	CDL	CB3-OB5-PB2-OB3
3	B	800	CDL	CB3-OB5-PB2-OB4
3	A	801	CDL	CA2-OA2-PA1-OA3
3	A	801	CDL	CA2-OA2-PA1-OA5
3	A	802	CDL	OA7-CA5-OA6-CA4
3	A	800	CDL	O1-C1-CA2-OA2
3	A	800	CDL	C11-CA5-OA6-CA4
3	B	800	CDL	O1-C1-CA2-OA2
3	A	800	CDL	OA7-CA5-OA6-CA4
3	A	802	CDL	CA2-OA2-PA1-OA5
3	B	801	CDL	CB2-OB2-PB2-OB5
3	B	801	CDL	CB3-OB5-PB2-OB2
3	B	800	CDL	CA2-OA2-PA1-OA5
3	B	800	CDL	CB2-OB2-PB2-OB5
3	B	800	CDL	CB3-OB5-PB2-OB2
3	A	801	CDL	CA3-OA5-PA1-OA2
3	A	801	CDL	CB2-OB2-PB2-OB5
3	A	800	CDL	CB2-C1-CA2-OA2
3	A	802	CDL	O1-C1-CB2-OB2
3	B	801	CDL	CB7-C71-C72-C73
3	B	800	CDL	OA7-CA5-OA6-CA4
3	B	800	CDL	CA5-C11-C12-C13
3	B	800	CDL	C11-CA5-OA6-CA4
3	B	801	CDL	OB5-CB3-CB4-CB6
3	A	802	CDL	CA3-CA4-CA6-OA8
3	B	802	CDL	CB3-CB4-CB6-OB8
3	A	801	CDL	OB5-CB3-CB4-CB6
3	A	802	CDL	CB3-CB4-CB6-OB8
3	A	801	CDL	CB3-CB4-CB6-OB8
3	A	802	CDL	OB6-CB4-CB6-OB8
3	A	801	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
3	B	800	CDL	CB3-CB4-CB6-OB8
3	B	802	CDL	OB5-CB3-CB4-CB6
3	B	802	CDL	CA3-CA4-CA6-OA8
3	B	802	CDL	OB5-CB3-CB4-OB6
3	A	800	CDL	OA5-CA3-CA4-OA6
3	B	801	CDL	OB5-CB3-CB4-OB6
3	A	801	CDL	OB5-CB3-CB4-OB6
3	B	800	CDL	CA3-OA5-PA1-OA2
3	A	801	CDL	CB3-OB5-PB2-OB2
3	A	800	CDL	C1-CA2-OA2-PA1
3	B	800	CDL	CA2-OA2-PA1-OA3
3	B	800	CDL	CB2-OB2-PB2-OB3
3	A	801	CDL	CA3-OA5-PA1-OA3
3	A	801	CDL	CB2-OB2-PB2-OB4
3	B	800	CDL	CB2-C1-CA2-OA2
3	A	802	CDL	OA6-CA4-CA6-OA8
3	B	802	CDL	OA6-CA4-CA6-OA8
3	B	802	CDL	OB6-CB4-CB6-OB8
3	B	802	CDL	C51-CB5-OB6-CB4
3	A	802	CDL	OB5-CB3-CB4-OB6
3	A	802	CDL	CA3-OA5-PA1-OA2
3	B	802	CDL	CA3-OA5-PA1-OA2
3	A	800	CDL	CA2-OA2-PA1-OA5
3	A	800	CDL	CB2-OB2-PB2-OB5
3	B	801	CDL	CA2-OA2-PA1-OA5
3	A	800	CDL	CB3-OB5-PB2-OB3
3	B	802	CDL	OB7-CB5-OB6-CB4
3	B	800	CDL	CA2-C1-CB2-OB2
3	B	800	CDL	OB5-CB3-CB4-CB6
3	B	801	CDL	CA3-OA5-PA1-OA3
3	A	802	CDL	OB5-CB3-CB4-CB6
3	A	800	CDL	OA5-CA3-CA4-CA6
3	A	802	CDL	CA3-OA5-PA1-OA3
3	B	802	CDL	CA2-OA2-PA1-OA3
3	A	800	CDL	CA2-OA2-PA1-OA3
3	A	800	CDL	CB2-OB2-PB2-OB3
3	A	802	CDL	CA2-C1-CB2-OB2
3	B	801	CDL	C72-C71-CB7-OB8

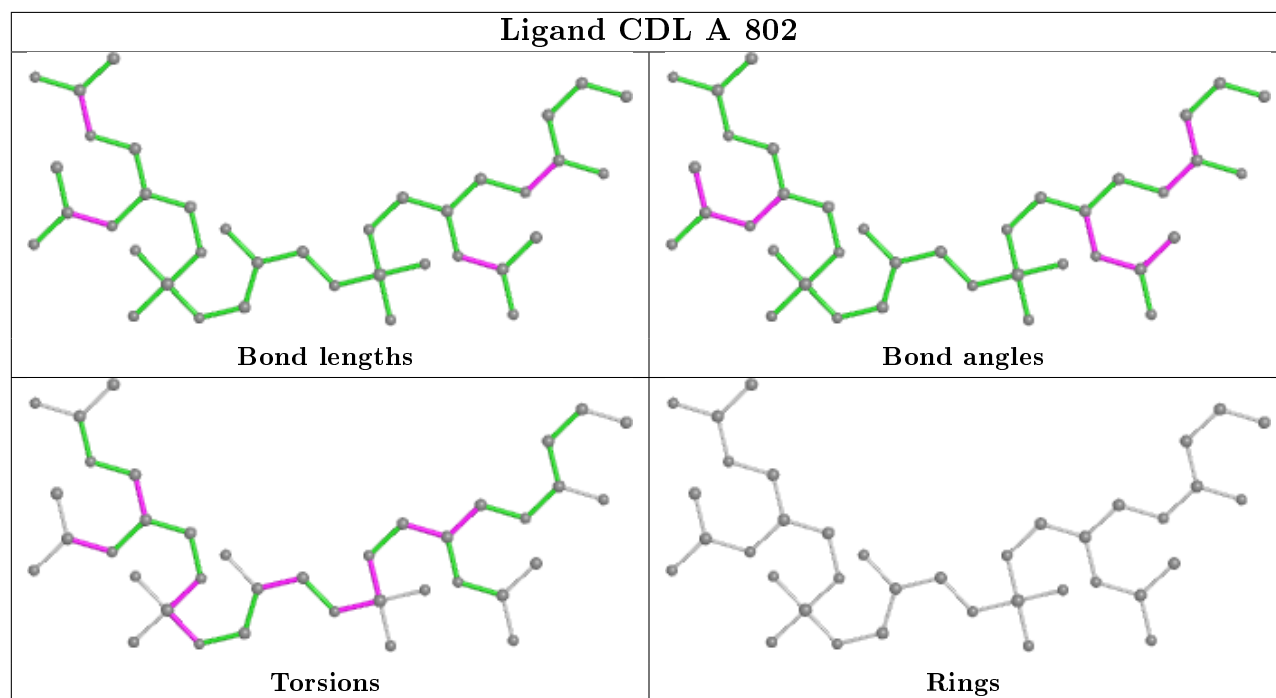
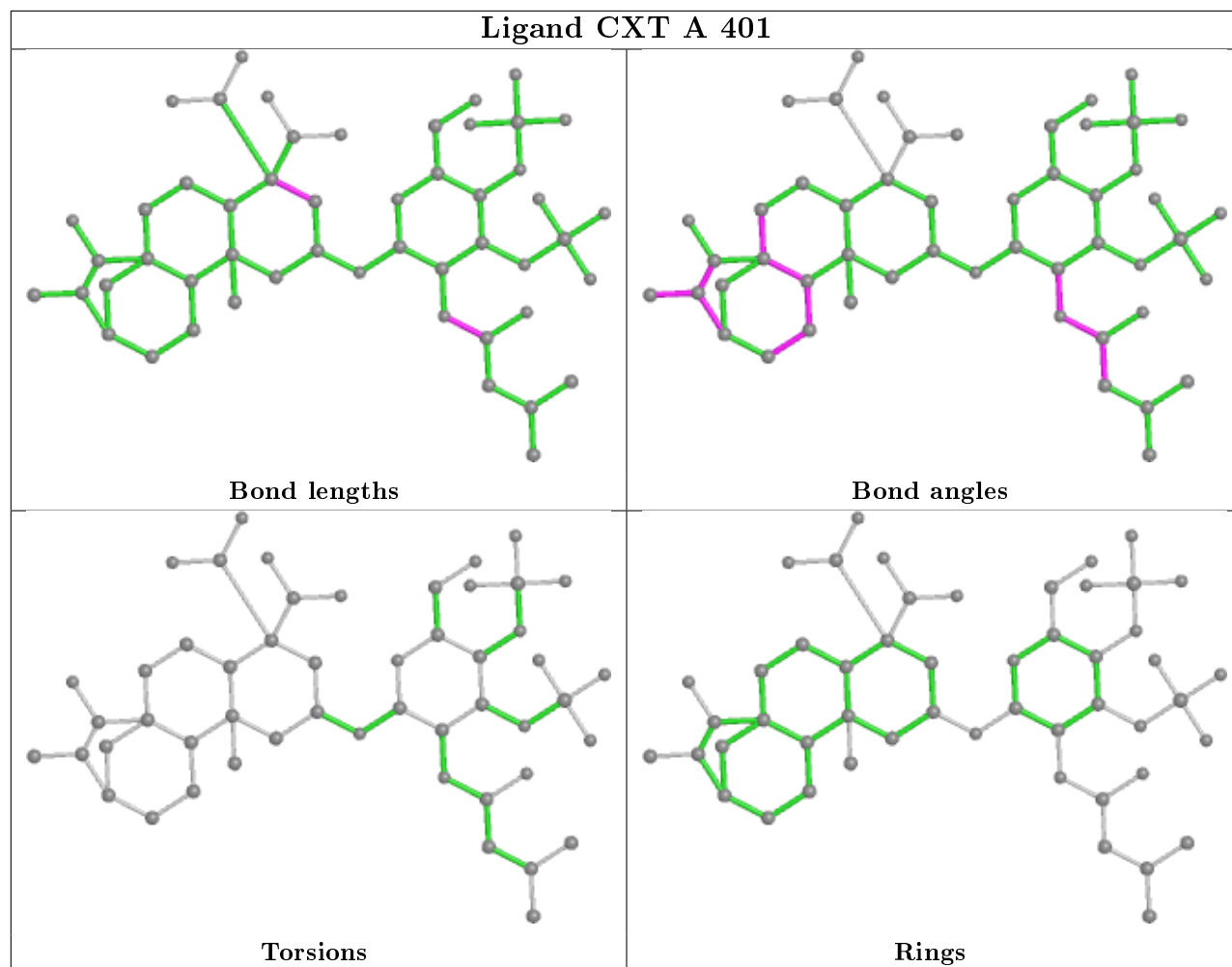
There are no ring outliers.

7 monomers are involved in 13 short contacts:

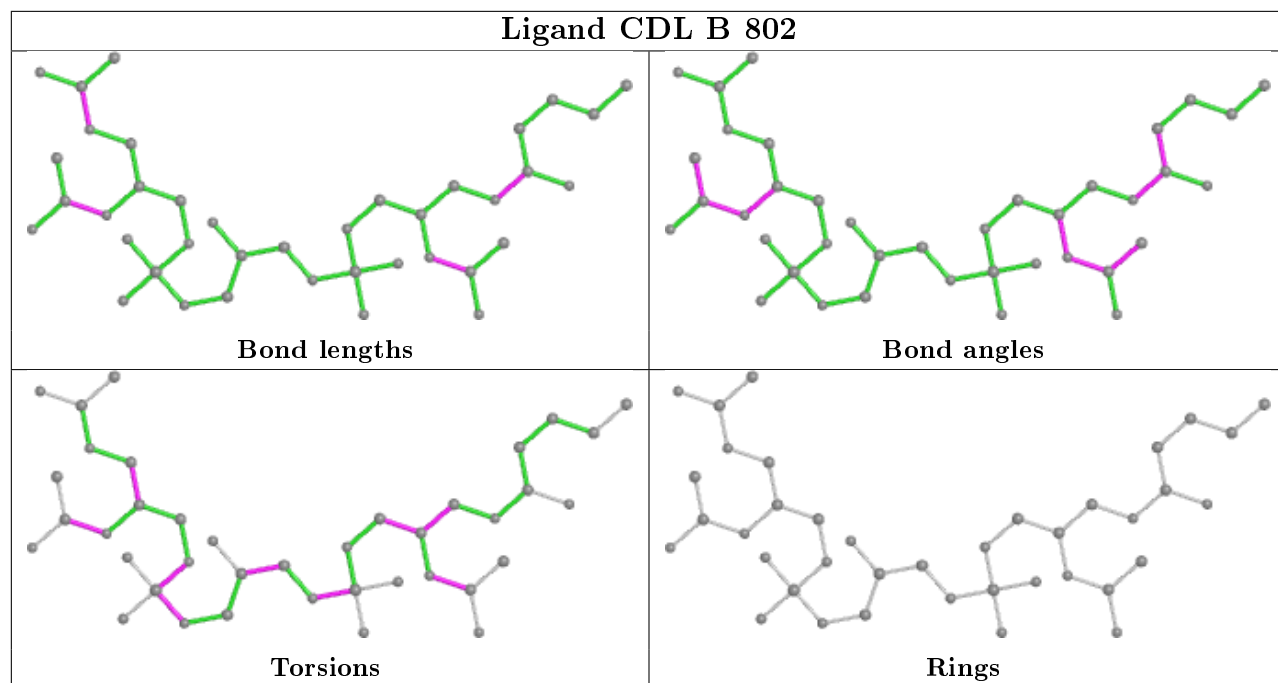
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	CDL	4	0
3	B	802	CDL	3	0
3	A	800	CDL	2	0
2	B	401	CXT	1	0
3	B	801	CDL	1	0
3	B	800	CDL	1	0
3	A	801	CDL	2	0

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

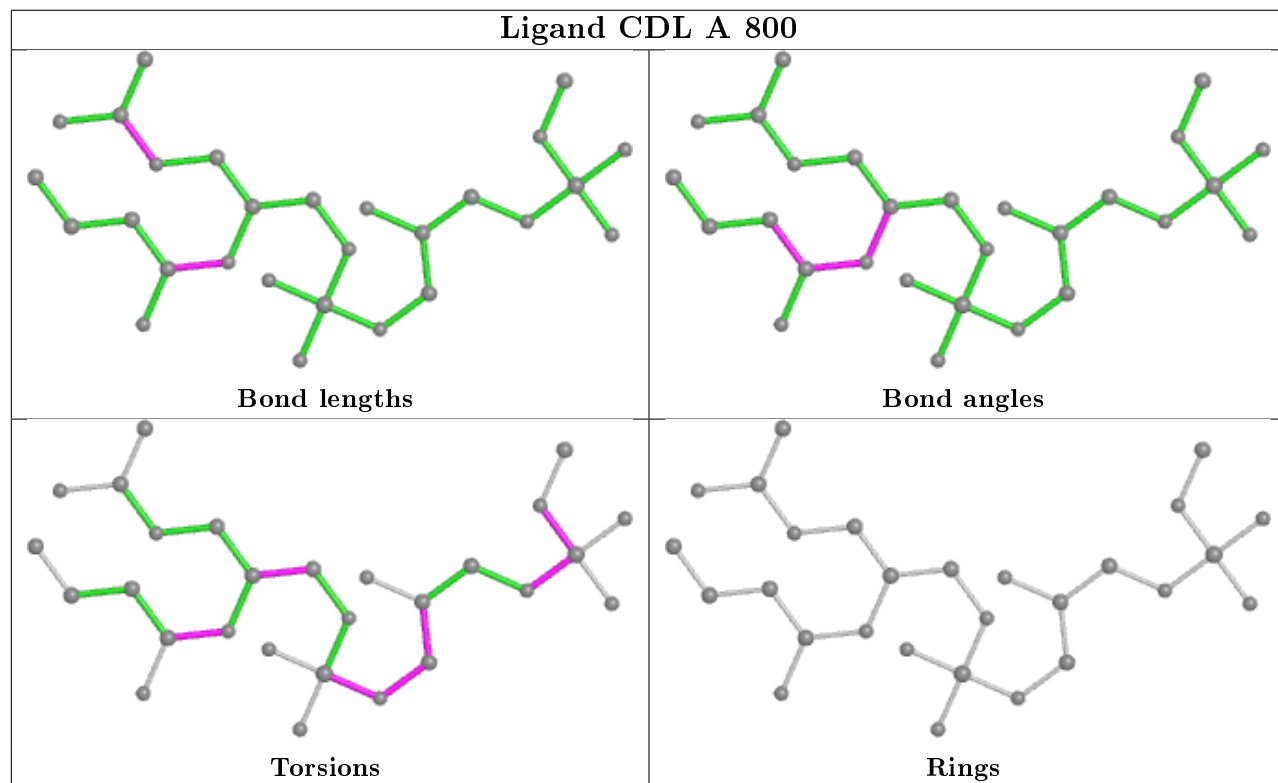




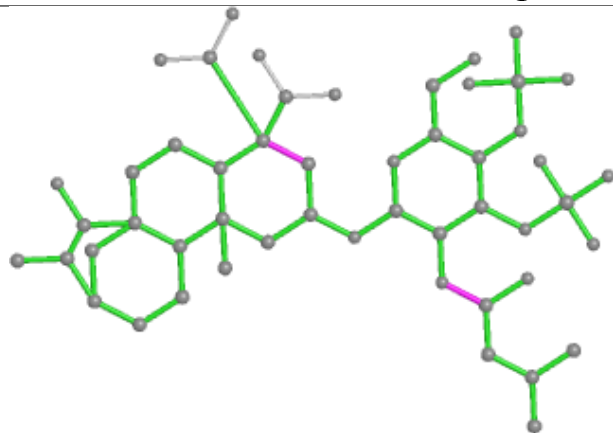
## Ligand CDL B 802



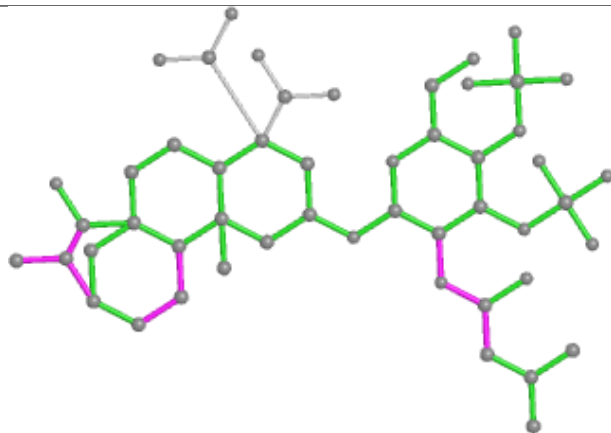
## Ligand CDL A 800



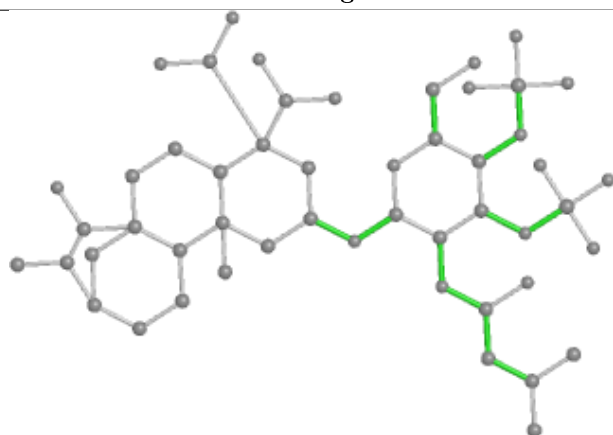
## Ligand CXT B 401



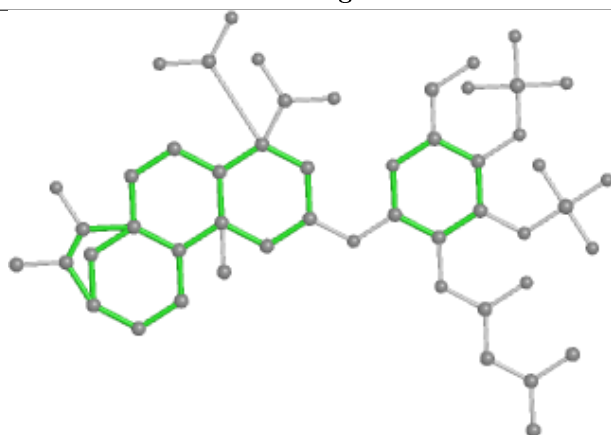
Bond lengths



Bond angles

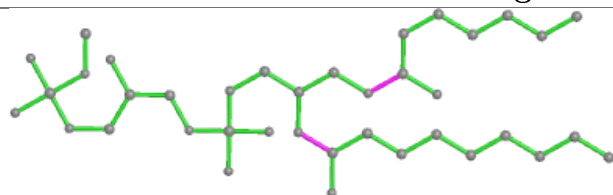


Torsions

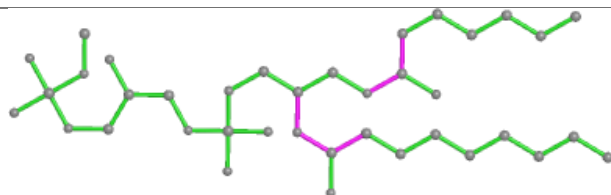


Rings

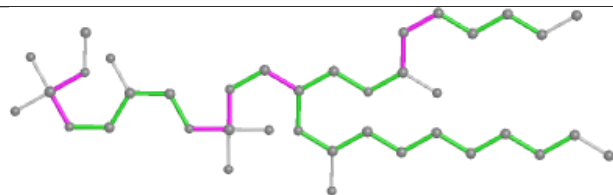
## Ligand CDL B 801



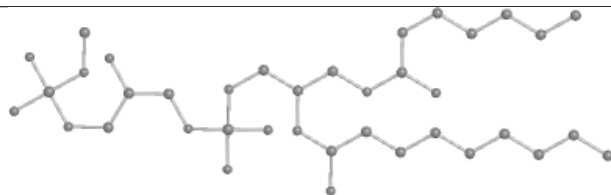
Bond lengths



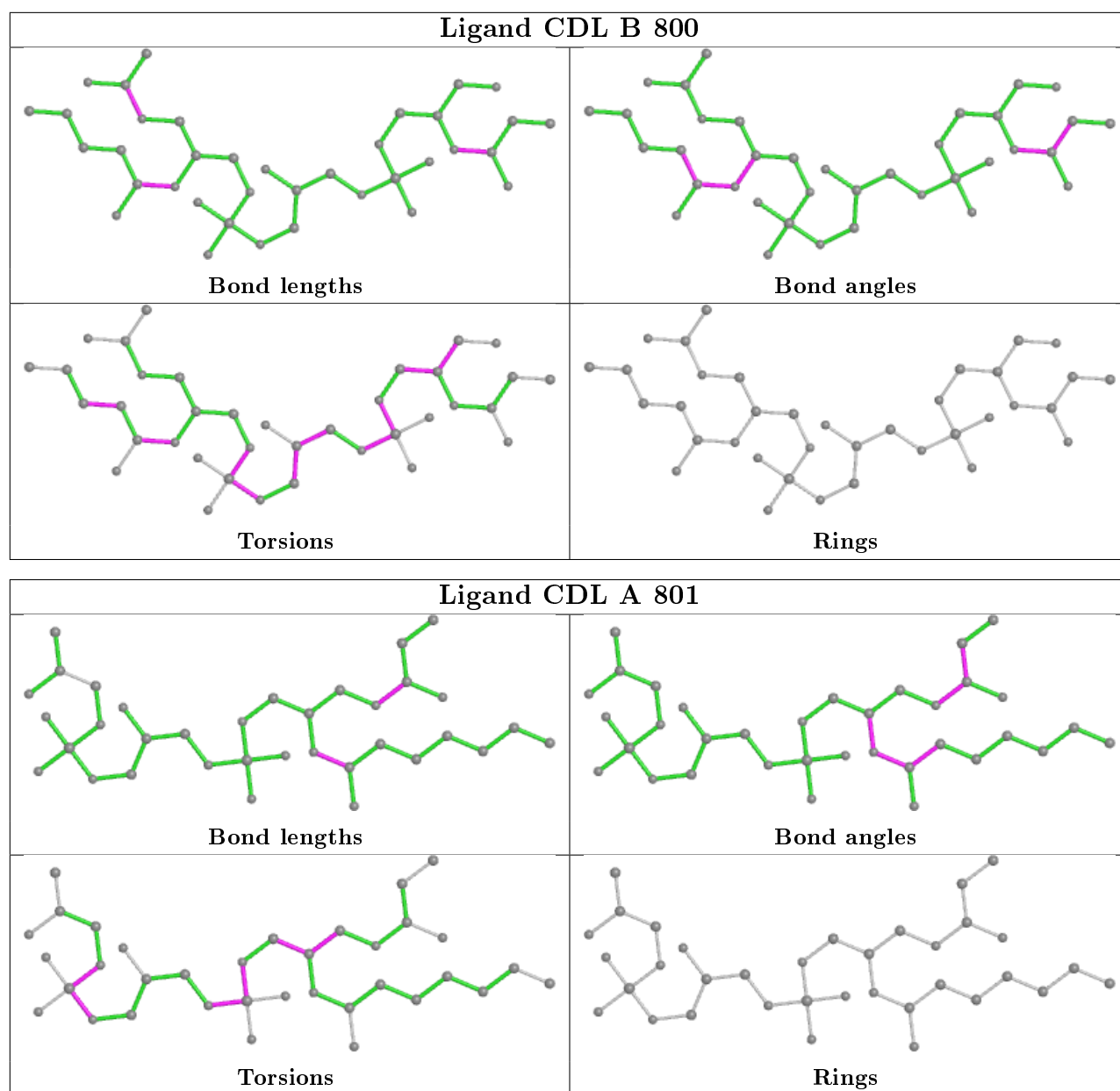
Bond angles



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 [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	286/322 (88%)	-0.24	2 (0%) 87 81	12, 26, 49, 71	0
1	B	290/322 (90%)	-0.25	1 (0%) 94 92	12, 27, 51, 72	0
All	All	576/644 (89%)	-0.25	3 (0%) 91 86	12, 26, 50, 72	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	ALA	3.9
1	B	53	ASP	2.2
1	A	150	SER	2.0

### 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 carbohydrates 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.

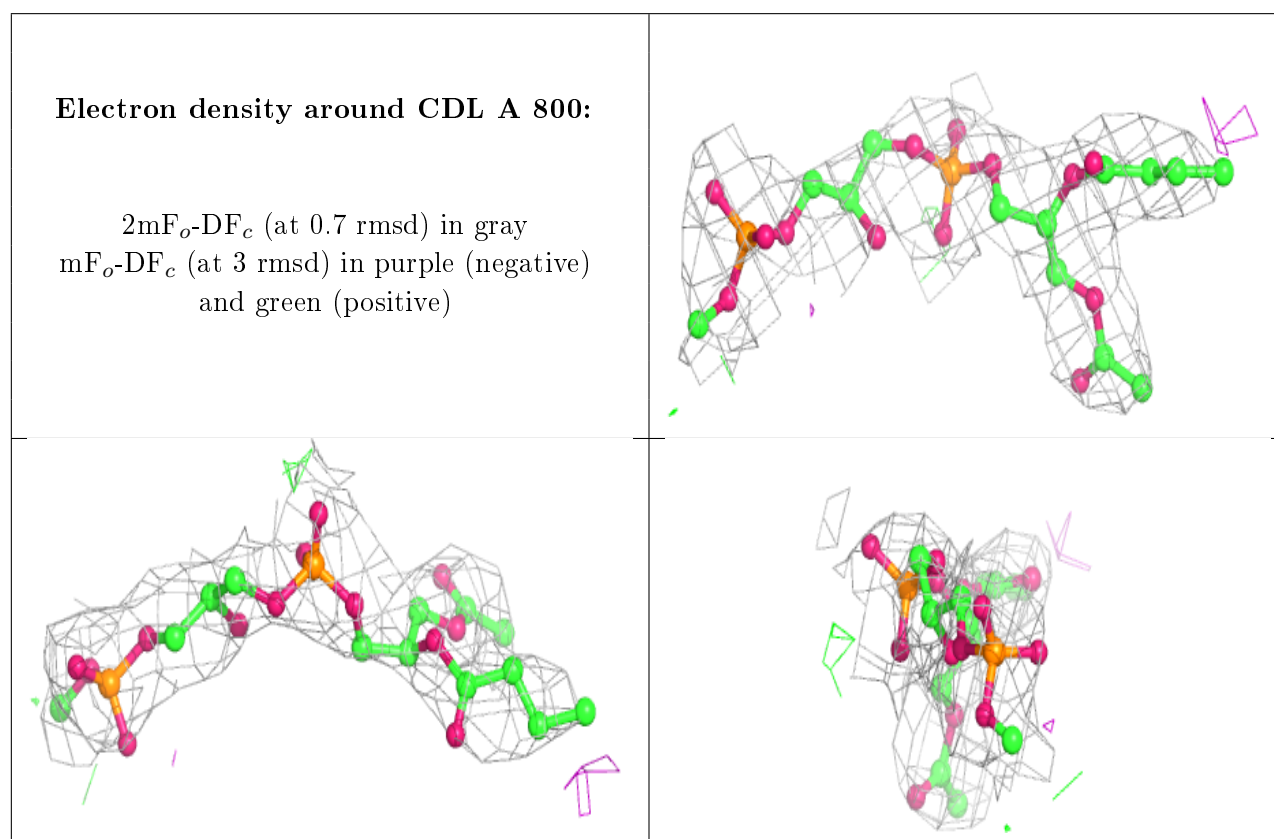
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CDL	A	800	28/100	0.89	0.28	10,34,72,99	0
3	CDL	A	801	35/100	0.89	0.26	9,38,64,66	0

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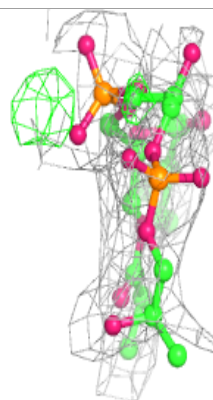
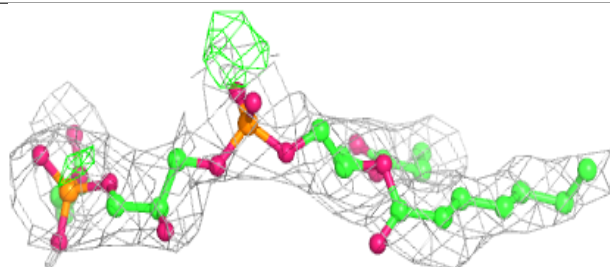
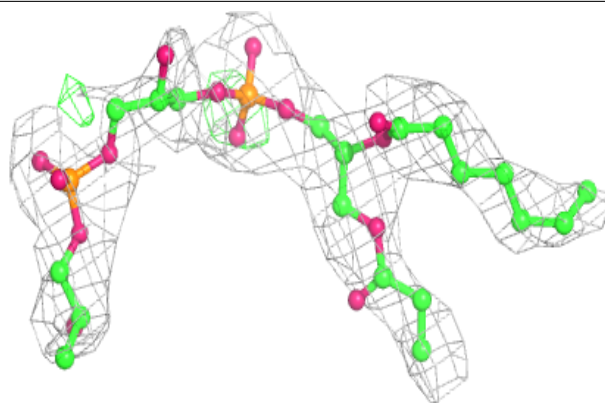
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CDL	B	801	38/100	0.90	0.28	19,38,63,80	0
3	CDL	A	802	38/100	0.90	0.24	18,36,56,75	0
3	CDL	B	800	37/100	0.91	0.28	10,38,74,83	0
3	CDL	B	802	39/100	0.91	0.22	12,36,62,78	0
2	CXT	B	401	51/51	0.92	0.20	6,24,56,79	0
2	CXT	A	401	51/51	0.93	0.17	5,24,50,62	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.

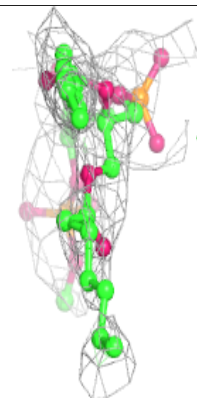
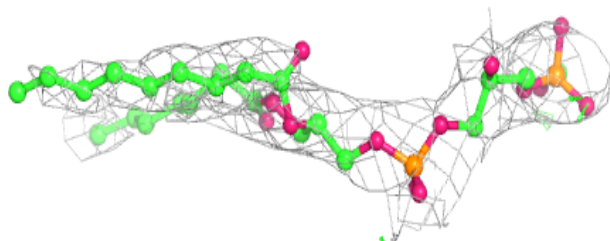
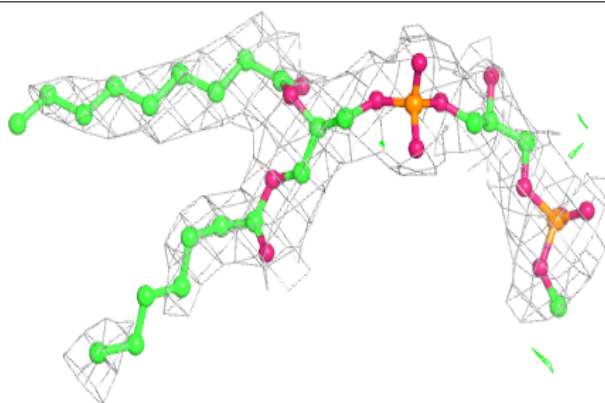


**Electron density around CDL A 801:**

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

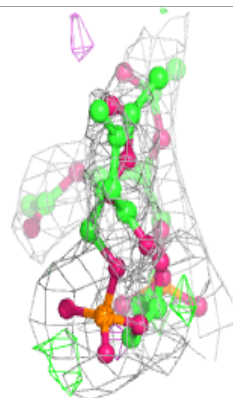
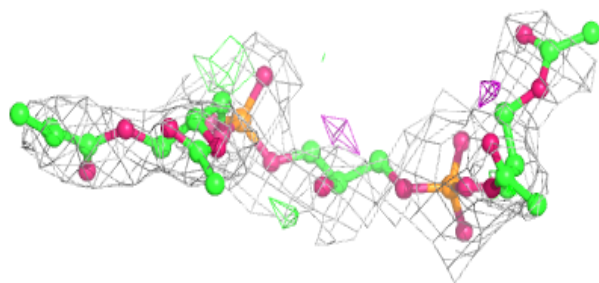
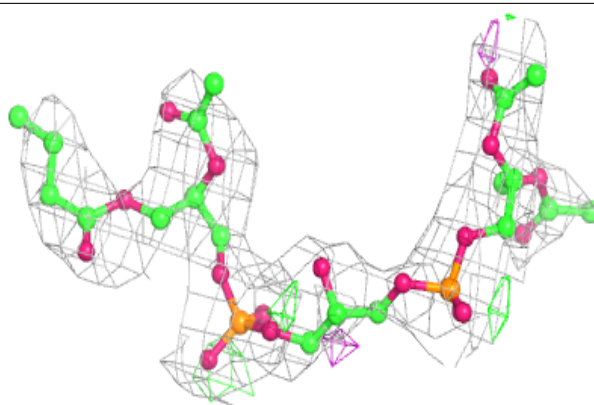
**Electron density around CDL B 801:**

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

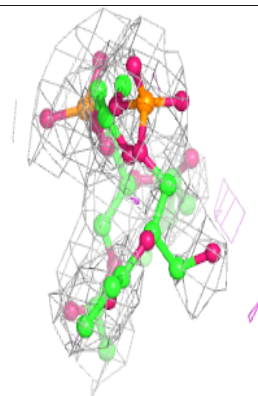
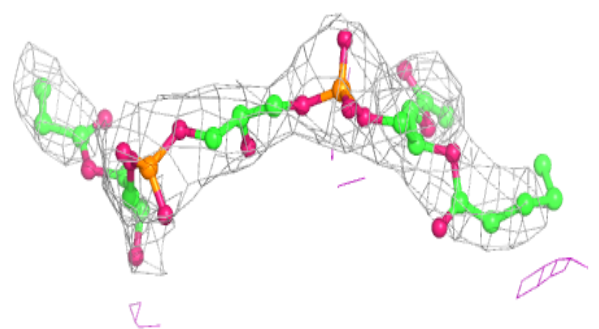
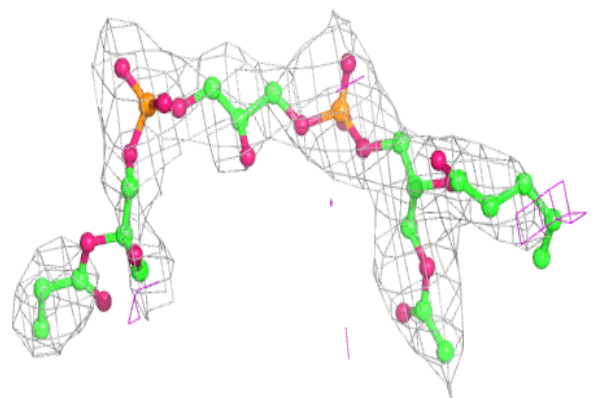


**Electron density around CDL A 802:**

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

**Electron density around CDL B 800:**

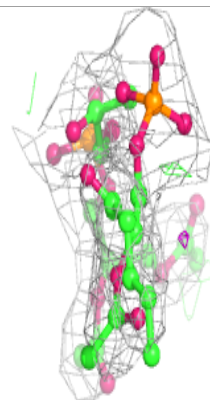
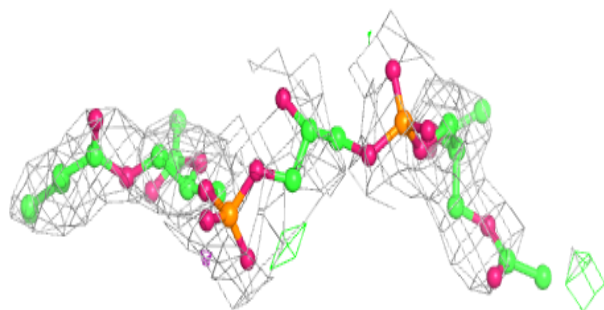
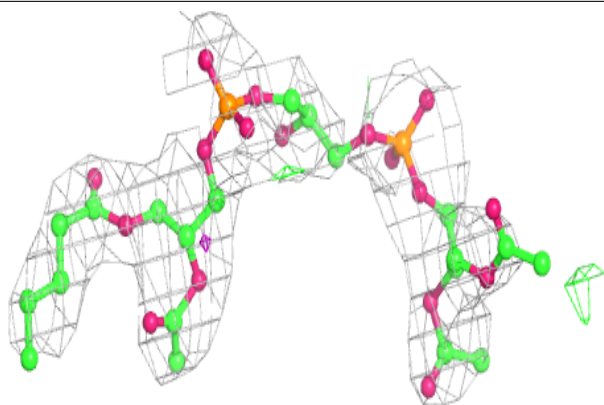
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



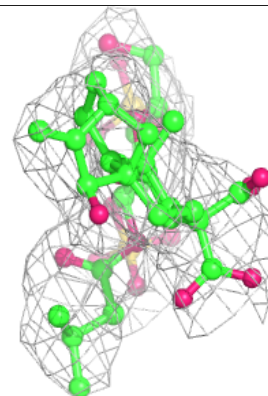
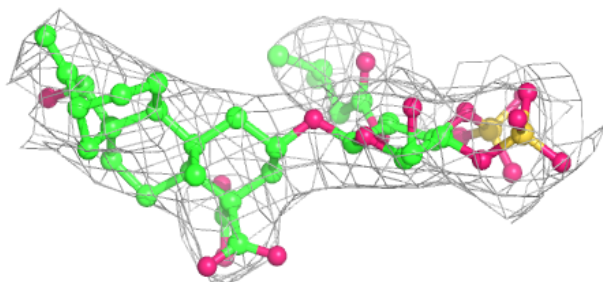
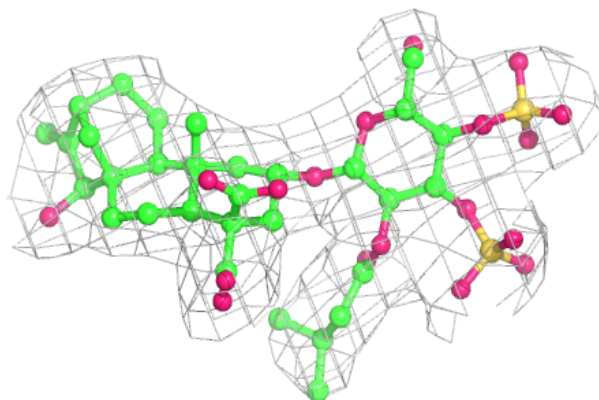


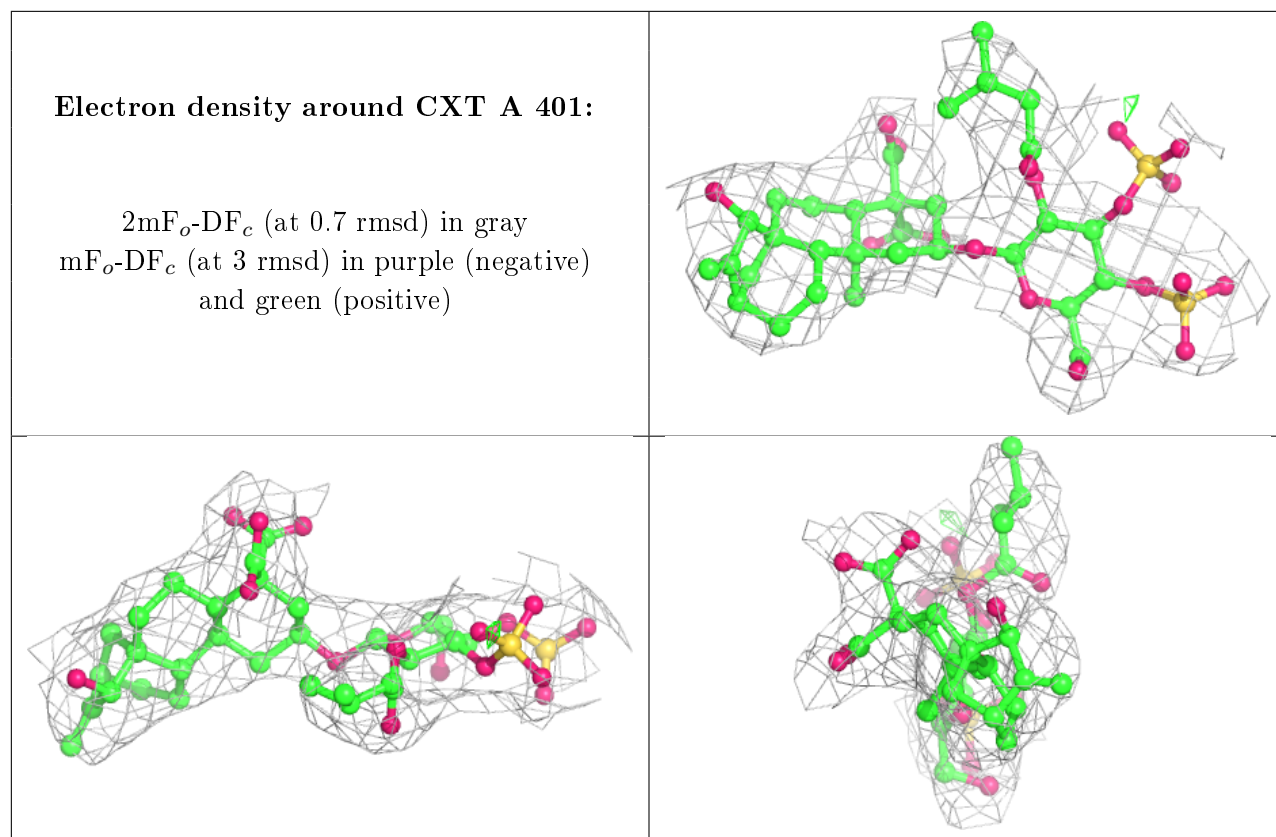
**Electron density around CDL B 802:**

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

**Electron density around CXT B 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](#)

There are no such residues in this entry.