



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2021 – 10:09 AM EDT

PDB ID : 1ET4  
Title : CRYSTAL STRUCTURE OF A VITAMIN B12 BINDING RNA APTAMER  
WITH LIGAND AT 2.3 Å  
Authors : Sussman, D.; Wilson, C.  
Deposited on : 2000-04-12  
Resolution : 2.30 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 : 2.23.1  
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) : 2.23.1

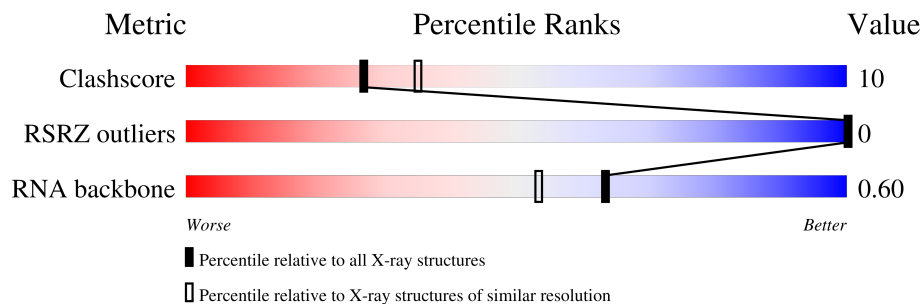
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

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  $\geq 3$ , 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	35	
1	B	35	
1	C	35	
1	D	35	
1	E	35	

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
2	CNC	A	701	X	-	-	-
2	CNC	B	801	X	-	-	-
2	CNC	C	901	X	-	-	-
2	CNC	D	1001	X	-	-	-
2	CNC	E	601	X	-	-	-

## 2 Entry composition [i](#)

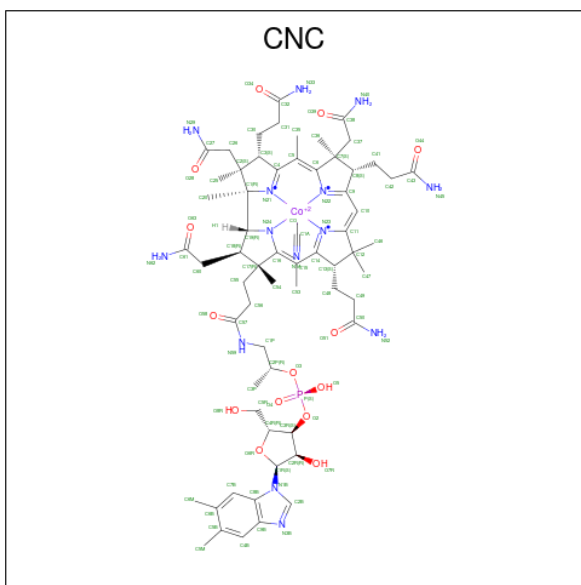
There are 3 unique types of molecules in this entry. The entry contains 4945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RNA chain called RNA APTAMER, 35-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	35	Total 751	C 335	N 141	O 240	P 35	0	0	0
1	B	35	Total 751	C 335	N 141	O 240	P 35	0	0	0
1	C	35	Total 751	C 335	N 141	O 240	P 35	0	0	0
1	D	35	Total 751	C 335	N 141	O 240	P 35	0	0	0
1	E	35	Total 751	C 335	N 141	O 240	P 35	0	0	0

- Molecule 2 is CYANOCOBALAMIN (three-letter code: CNC) (formula:  $C_{63}H_{89}CoN_{14}O_{14}P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
2	A	1	Total 93	C 63	Co 1	N 14	O 14	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	B	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		
2	C	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		
2	D	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		
2	E	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total	O	0	0
			150	150		
3	B	176	Total	O	0	0
			176	176		
3	C	136	Total	O	0	0
			136	136		
3	D	155	Total	O	0	0
			155	155		
3	E	108	Total	O	0	0
			108	108		

### 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

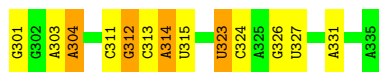
- Molecule 1: RNA APTAMER, 35-MER

Chain A:  57% 37% . .



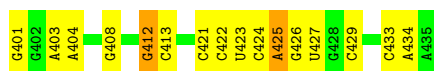
- Molecule 1: RNA APTAMER, 35-MER

Chain B:  63% 26% 11%



- Molecule 1: RNA APTAMER, 35-MER

Chain C:  54% 40% 6%



- Molecule 1: RNA APTAMER, 35-MER

Chain D:  51% 31% 17%



- Molecule 1: RNA APTAMER, 35-MER

Chain E:  69% 26% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.27Å 98.08Å 217.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 19.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 87.6 (19.89-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 2.30Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.199 , 0.232 0.194 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtrriage
Anisotropy	0.212	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4945	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: CNC

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	0.74	1/840 (0.1%)	0.86	1/1306 (0.1%)
1	B	0.75	0/840	0.93	4/1306 (0.3%)
1	C	0.70	1/840 (0.1%)	0.83	1/1306 (0.1%)
1	D	0.73	1/840 (0.1%)	0.84	2/1306 (0.2%)
1	E	0.67	1/840 (0.1%)	0.83	3/1306 (0.2%)
All	All	0.72	4/4200 (0.1%)	0.86	11/6530 (0.2%)

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
1	A	1	2
1	B	2	1
1	C	1	0
1	D	2	0
1	E	1	0
All	All	7	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	501	G	OP3-P	-6.79	1.53	1.61
1	A	201	G	OP3-P	-6.32	1.53	1.61
1	E	101	G	OP3-P	-6.29	1.53	1.61
1	C	401	G	OP3-P	-5.99	1.53	1.61

All (11) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	U	C2'-C3'-O3'	8.81	128.89	109.50
1	E	112	G	C2'-C3'-O3'	8.20	127.54	109.50
1	C	412	G	C2'-C3'-O3'	7.69	126.41	109.50
1	A	212	G	C2'-C3'-O3'	7.58	126.17	109.50
1	D	512	G	C2'-C3'-O3'	7.20	125.33	109.50
1	B	312	G	C2'-C3'-O3'	6.51	124.12	113.70
1	B	323	U	C4'-C3'-O3'	5.89	124.78	113.00
1	E	112	G	N9-C1'-C2'	5.66	121.36	114.00
1	D	512	G	N9-C1'-C2'	5.49	121.14	114.00
1	B	323	U	OP2-P-O3'	5.49	117.28	105.20
1	E	101	G	OP1-P-OP2	-5.04	112.04	119.60

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	212	G	C3'
1	B	312	G	C3'
1	B	323	U	C3'
1	C	412	G	C3'
1	D	512	G	C3'
1	D	523	U	C3'
1	E	112	G	C3'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	A	Sidechain
1	A	226	G	Sidechain
1	B	314	A	Sidechain

## 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	751	0	382	8	0
1	B	751	0	382	6	0
1	C	751	0	382	9	0
1	D	751	0	382	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	751	0	382	6	0
2	A	93	0	85	3	0
2	B	93	0	85	8	0
2	C	93	0	85	5	0
2	D	93	0	85	4	0
2	E	93	0	85	5	0
3	A	150	0	0	5	0
3	B	176	0	0	3	0
3	C	136	0	0	7	0
3	D	155	0	0	5	0
3	E	108	0	0	5	0
All	All	4945	0	2335	66	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 10.

All (66) 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:B:304:A:H2'	3:B:1417:HOH:O	1.87	0.74
2:D:1001:CNC:H362	2:D:1001:CNC:H351	1.71	0.73
2:C:901:CNC:H362	2:C:901:CNC:H351	1.71	0.72
1:B:303:A:H5'	1:B:304:A:OP2	1.91	0.71
2:A:701:CNC:H362	2:A:701:CNC:H351	1.71	0.70
2:B:801:CNC:H362	2:B:801:CNC:H351	1.74	0.68
1:C:429:C:C2	3:C:1236:HOH:O	2.47	0.68
1:C:433:C:OP2	3:C:1309:HOH:O	2.12	0.67
1:D:523:U:O2'	3:D:1302:HOH:O	2.01	0.66
2:E:601:CNC:H362	2:E:601:CNC:H351	1.76	0.66
1:D:501:G:OP2	3:D:1750:HOH:O	2.15	0.64
2:B:801:CNC:H552	2:B:801:CNC:H531	1.79	0.64
2:E:601:CNC:H552	2:E:601:CNC:H531	1.81	0.61
2:C:901:CNC:H531	2:C:901:CNC:H552	1.83	0.61
1:B:301:G:OP2	3:B:1525:HOH:O	2.16	0.60
3:C:1550:HOH:O	1:D:527:U:C4'	2.49	0.59
1:A:205:C:P	3:A:1429:HOH:O	2.61	0.59
1:A:235:A:O3'	3:A:1643:HOH:O	2.17	0.59
1:B:304:A:H3'	3:B:1278:HOH:O	2.02	0.58
1:C:403:A:O2'	1:C:404:A:H5'	2.04	0.56
2:A:701:CNC:H552	2:A:701:CNC:H531	1.89	0.55
2:D:1001:CNC:H552	2:D:1001:CNC:H531	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:A:H4'	1:B:304:A:OP1	2.07	0.54
2:B:801:CNC:H521	2:B:801:CNC:H533	1.72	0.53
2:B:801:CNC:H533	2:B:801:CNC:N52	2.26	0.51
3:C:1550:HOH:O	1:D:527:U:H4'	2.08	0.51
1:A:204:A:H3'	3:A:1347:HOH:O	2.11	0.50
1:E:123:U:H3'	3:E:1392:HOH:O	2.13	0.49
1:A:228:G:C2'	1:A:229:C:H5'	2.43	0.49
1:D:504:A:N3	3:D:1342:HOH:O	2.35	0.49
2:E:601:CNC:H311	3:E:1759:HOH:O	2.12	0.48
2:B:801:CNC:H203	2:B:801:CNC:H301	1.96	0.48
1:C:433:C:H2'	1:C:434:A:O4'	2.15	0.47
1:E:103:A:O2'	1:E:104:A:H5'	2.14	0.47
1:C:421:C:O2'	1:C:422:C:H5'	2.15	0.46
2:E:601:CNC:H3	2:E:601:CNC:O28	2.15	0.46
2:A:701:CNC:H311	3:A:1673:HOH:O	2.15	0.46
1:E:109:U:O3'	3:E:1196:HOH:O	2.20	0.46
1:A:212:G:P	3:A:1345:HOH:O	2.73	0.45
2:B:801:CNC:H531	2:B:801:CNC:C55	2.46	0.45
2:D:1001:CNC:H533	2:D:1001:CNC:H521	1.82	0.45
2:B:801:CNC:H601	2:B:801:CNC:H252	1.99	0.45
3:C:1202:HOH:O	1:D:526:G:H5''	2.17	0.44
1:E:124:C:OP1	3:E:1615:HOH:O	2.21	0.44
1:D:509:U:H2'	3:D:1198:HOH:O	2.17	0.43
1:D:533:C:C2'	1:D:534:A:H5'	2.47	0.43
1:C:423:U:H6	1:C:423:U:O5'	2.02	0.43
1:A:228:G:H2'	1:A:229:C:H5'	2.00	0.43
1:C:403:A:C2'	1:C:404:A:H5'	2.48	0.43
2:D:1001:CNC:H203	2:D:1001:CNC:H301	2.01	0.43
1:D:503:A:O2'	1:D:504:A:H5'	2.19	0.43
1:C:408:G:O2'	1:C:425:A:N1	2.49	0.43
1:E:114:A:N6	1:E:132:G:C2	2.87	0.42
2:C:901:CNC:H351	2:C:901:CNC:C36	2.47	0.42
1:A:203:A:O2'	1:A:204:A:H5'	2.20	0.41
1:B:311:C:C2	1:B:315:U:C5	3.08	0.41
1:D:508:G:O2'	1:D:525:A:N1	2.47	0.41
1:D:530:G:P	3:D:1760:HOH:O	2.79	0.41
1:A:204:A:H2'	1:A:205:C:O5'	2.21	0.41
2:E:601:CNC:H531	2:E:601:CNC:C55	2.49	0.41
1:C:424:C:OP1	3:C:1679:HOH:O	2.21	0.41
2:B:801:CNC:H521	2:B:801:CNC:H482	1.72	0.41
2:C:901:CNC:H531	2:C:901:CNC:C55	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:901:CNC:N29	3:C:1236:HOH:O	2.36	0.40
1:E:123:U:C3'	3:E:1392:HOH:O	2.70	0.40
1:D:523:U:O2'	1:D:523:U:O2	2.40	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

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

There are no protein molecules in this entry.

#### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	34/35 (97%)	6 (17%)	3 (8%)
1	B	34/35 (97%)	8 (23%)	2 (5%)
1	C	34/35 (97%)	5 (14%)	1 (2%)
1	D	34/35 (97%)	9 (26%)	2 (5%)
1	E	34/35 (97%)	4 (11%)	2 (5%)
All	All	170/175 (97%)	32 (18%)	10 (5%)

All (32) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	212	G
1	A	213	C
1	A	224	C
1	A	226	G
1	A	227	U
1	A	230	G
1	B	304	A
1	B	312	G
1	B	313	C
1	B	314	A

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Mol	Chain	Res	Type
1	B	324	C
1	B	326	G
1	B	327	U
1	B	331	A
1	C	412	G
1	C	413	C
1	C	425	A
1	C	426	G
1	C	427	U
1	D	512	G
1	D	513	C
1	D	514	A
1	D	523	U
1	D	524	C
1	D	525	A
1	D	526	G
1	D	527	U
1	D	532	G
1	E	112	G
1	E	113	C
1	E	124	C
1	E	126	G

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	211	C
1	A	212	G
1	A	226	G
1	B	312	G
1	B	323	U
1	C	412	G
1	D	512	G
1	D	523	U
1	E	112	G
1	E	126	G

#### 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](#)

5 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	CNC	B	801	-	77,103,103	1.28	8 (10%)	100,171,171	1.16	9 (9%)
2	CNC	D	1001	-	77,103,103	1.27	7 (9%)	100,171,171	1.18	8 (8%)
2	CNC	E	601	-	77,103,103	1.25	7 (9%)	100,171,171	1.13	7 (7%)
2	CNC	A	701	-	77,103,103	1.23	7 (9%)	100,171,171	1.15	10 (10%)
2	CNC	C	901	-	77,103,103	1.26	7 (9%)	100,171,171	1.13	8 (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	CNC	B	801	-	1/1/36/38	7/51/235/235	0/3/11/11
2	CNC	D	1001	-	1/1/36/38	7/51/235/235	0/3/11/11
2	CNC	E	601	-	1/1/36/38	5/51/235/235	0/3/11/11
2	CNC	A	701	-	1/1/36/38	9/51/235/235	0/3/11/11
2	CNC	C	901	-	1/1/36/38	9/51/235/235	0/3/11/11

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	CNC	C61-N62	-3.74	1.20	1.32
2	C	901	CNC	O63-C61	3.40	1.34	1.24
2	E	601	CNC	C61-N62	-3.38	1.21	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	CNC	O63-C61	3.27	1.33	1.24
2	B	801	CNC	O63-C61	3.25	1.33	1.24
2	D	1001	CNC	C61-N62	-3.23	1.22	1.32
2	E	601	CNC	C17-C18	3.15	1.58	1.54
2	A	701	CNC	C61-N62	-3.10	1.22	1.32
2	C	901	CNC	C17-C18	3.01	1.58	1.54
2	B	801	CNC	C7B-C6B	2.99	1.45	1.37
2	A	701	CNC	C7B-C6B	2.96	1.45	1.37
2	C	901	CNC	C61-N62	-2.95	1.23	1.32
2	B	801	CNC	C4B-C9B	2.88	1.46	1.41
2	E	601	CNC	O63-C61	2.85	1.32	1.24
2	A	701	CNC	O63-C61	2.84	1.32	1.24
2	D	1001	CNC	C17-C18	2.67	1.57	1.54
2	A	701	CNC	O6R-C1R	2.62	1.44	1.41
2	C	901	CNC	C5M-C5B	2.60	1.56	1.51
2	A	701	CNC	O44-C43	2.59	1.31	1.24
2	E	601	CNC	C1-C2	2.58	1.64	1.58
2	B	801	CNC	C1-C2	2.54	1.64	1.58
2	D	1001	CNC	C1-C2	2.53	1.64	1.58
2	C	901	CNC	C1-C2	2.51	1.64	1.58
2	E	601	CNC	C7B-C6B	2.50	1.44	1.37
2	C	901	CNC	C2-C3	-2.48	1.54	1.58
2	A	701	CNC	C5M-C5B	2.38	1.55	1.51
2	C	901	CNC	C7B-C6B	2.31	1.43	1.37
2	A	701	CNC	C16-C15	2.29	1.49	1.41
2	B	801	CNC	O6R-C1R	2.28	1.44	1.41
2	B	801	CNC	O58-C57	2.26	1.27	1.23
2	D	1001	CNC	C16-C15	2.14	1.49	1.41
2	D	1001	CNC	C4B-C9B	2.08	1.45	1.41
2	D	1001	CNC	C11-C10	-2.03	1.37	1.40
2	B	801	CNC	C17-C18	2.01	1.57	1.54
2	E	601	CNC	C16-C15	2.00	1.48	1.41
2	E	601	CNC	C48-C49	2.00	1.59	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	CNC	C7B-C8B-C9B	3.90	124.40	120.54
2	C	901	CNC	C7B-C8B-C9B	3.86	124.36	120.54
2	A	701	CNC	C7B-C8B-C9B	3.77	124.27	120.54
2	E	601	CNC	C7B-C8B-C9B	3.76	124.26	120.54
2	D	1001	CNC	C20-C1-C19	-3.52	105.96	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	CNC	C7B-C8B-C9B	3.45	123.95	120.54
2	B	801	CNC	C4B-C9B-C8B	-3.32	117.70	121.10
2	C	901	CNC	C4B-C9B-C8B	-3.23	117.79	121.10
2	E	601	CNC	C20-C1-C19	-3.22	106.25	109.36
2	D	1001	CNC	C4B-C9B-C8B	-3.16	117.86	121.10
2	B	801	CNC	C20-C1-C19	-3.07	106.39	109.36
2	A	701	CNC	C4B-C9B-C8B	-3.04	117.99	121.10
2	E	601	CNC	C4B-C9B-C8B	-2.97	118.06	121.10
2	C	901	CNC	C20-C1-C19	-2.88	106.58	109.36
2	B	801	CNC	C2R-C3R-C4R	2.81	108.21	103.22
2	D	1001	CNC	C2R-C3R-C4R	2.81	108.20	103.22
2	E	601	CNC	C2R-C3R-C4R	2.76	108.11	103.22
2	A	701	CNC	C55-C17-C16	2.69	118.87	109.92
2	A	701	CNC	O63-C61-C60	-2.60	115.38	120.87
2	A	701	CNC	C2R-C3R-C4R	2.58	107.80	103.22
2	D	1001	CNC	C55-C17-C16	2.55	118.42	109.92
2	C	901	CNC	C2R-C3R-C4R	2.55	107.74	103.22
2	D	1001	CNC	C1-C2-C3	-2.52	98.44	101.59
2	A	701	CNC	C20-C1-C19	-2.42	107.02	109.36
2	C	901	CNC	O63-C61-C60	-2.41	115.79	120.87
2	E	601	CNC	C55-C17-C16	2.39	117.87	109.92
2	C	901	CNC	C55-C17-C16	2.35	117.74	109.92
2	A	701	CNC	C1-C2-C3	-2.18	98.85	101.59
2	B	801	CNC	C3-C4-C5	-2.18	123.78	131.68
2	E	601	CNC	O63-C61-C60	-2.17	116.30	120.87
2	B	801	CNC	C1-C2-C3	-2.16	98.88	101.59
2	E	601	CNC	C3-C4-C5	-2.12	123.98	131.68
2	A	701	CNC	C1-C19-N24	2.12	108.62	106.24
2	B	801	CNC	C37-C7-C6	-2.12	102.87	109.92
2	D	1001	CNC	C1-C19-N24	2.09	108.59	106.24
2	C	901	CNC	C3-C4-C5	-2.07	124.18	131.68
2	A	701	CNC	C3-C4-C5	-2.06	124.20	131.68
2	C	901	CNC	C2-C1-C19	2.06	121.85	118.60
2	B	801	CNC	C19-C1-N21	2.06	104.27	102.16
2	A	701	CNC	C47-C12-C46	-2.06	105.41	109.73
2	B	801	CNC	C1-C19-N24	2.04	108.54	106.24
2	D	1001	CNC	O63-C61-C60	-2.02	116.61	120.87

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	701	CNC	N24

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Mol	Chain	Res	Type	Atom
2	B	801	CNC	N24
2	C	901	CNC	N24
2	D	1001	CNC	N24
2	E	601	CNC	N24

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	CNC	C18-C60-C61-O63
2	A	701	CNC	C18-C60-C61-N62
2	B	801	CNC	C13-C48-C49-C50
2	B	801	CNC	C18-C60-C61-O63
2	B	801	CNC	C18-C60-C61-N62
2	C	901	CNC	C13-C48-C49-C50
2	C	901	CNC	C18-C60-C61-O63
2	C	901	CNC	C18-C60-C61-N62
2	D	1001	CNC	C18-C60-C61-O63
2	D	1001	CNC	C18-C60-C61-N62
2	E	601	CNC	C18-C60-C61-O63
2	E	601	CNC	C18-C60-C61-N62
2	D	1001	CNC	C13-C48-C49-C50
2	E	601	CNC	C13-C48-C49-C50
2	B	801	CNC	O6R-C4R-C5R-O8R
2	B	801	CNC	C3R-C4R-C5R-O8R
2	A	701	CNC	C13-C48-C49-C50
2	C	901	CNC	O6R-C4R-C5R-O8R
2	A	701	CNC	C7-C37-C38-N40
2	C	901	CNC	C2-C3-C30-C31
2	A	701	CNC	C7-C37-C38-O39
2	D	1001	CNC	C48-C49-C50-O51
2	B	801	CNC	C48-C49-C50-N52
2	C	901	CNC	C3R-C4R-C5R-O8R
2	A	701	CNC	C2-C3-C30-C31
2	D	1001	CNC	C48-C49-C50-N52
2	B	801	CNC	C48-C49-C50-O51
2	C	901	CNC	C7-C37-C38-O39
2	C	901	CNC	C7-C37-C38-N40
2	D	1001	CNC	C7-C37-C38-O39
2	A	701	CNC	C17-C18-C60-C61
2	E	601	CNC	C2-C3-C30-C31
2	D	1001	CNC	O6R-C4R-C5R-O8R
2	A	701	CNC	C4-C3-C30-C31

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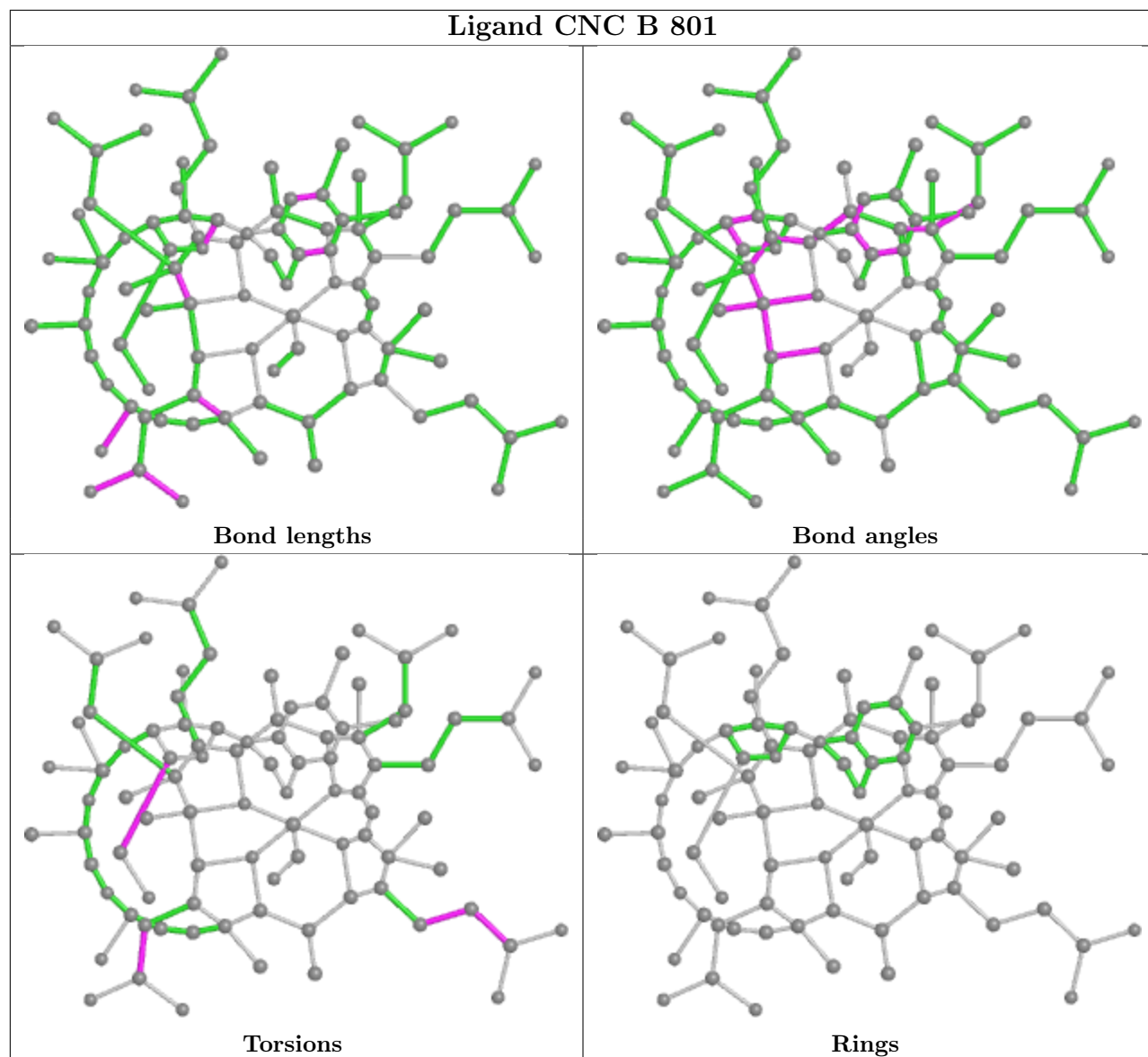
Mol	Chain	Res	Type	Atoms
2	C	901	CNC	C4-C3-C30-C31
2	E	601	CNC	C4-C3-C30-C31
2	A	701	CNC	C19-C18-C60-C61

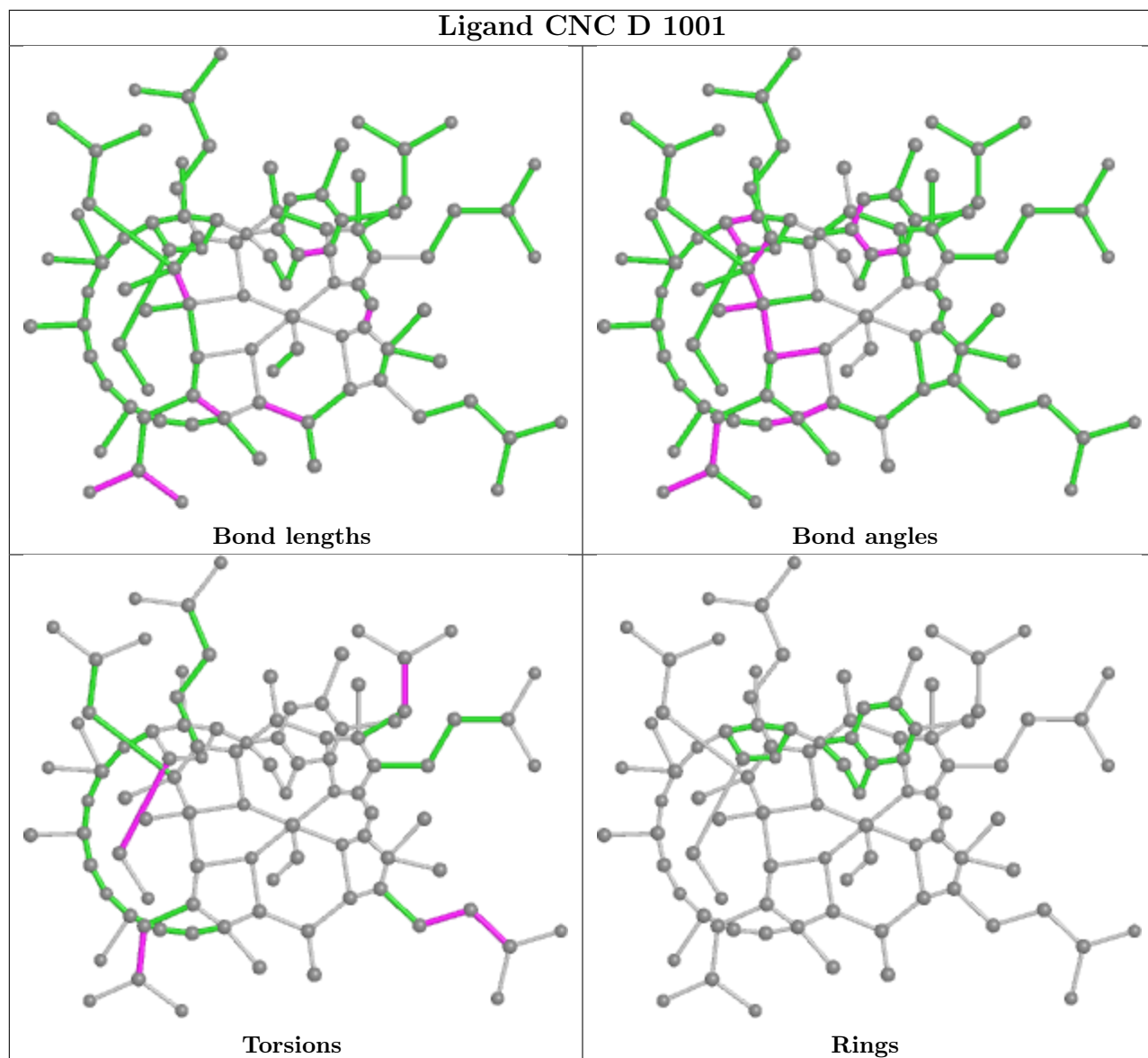
There are no ring outliers.

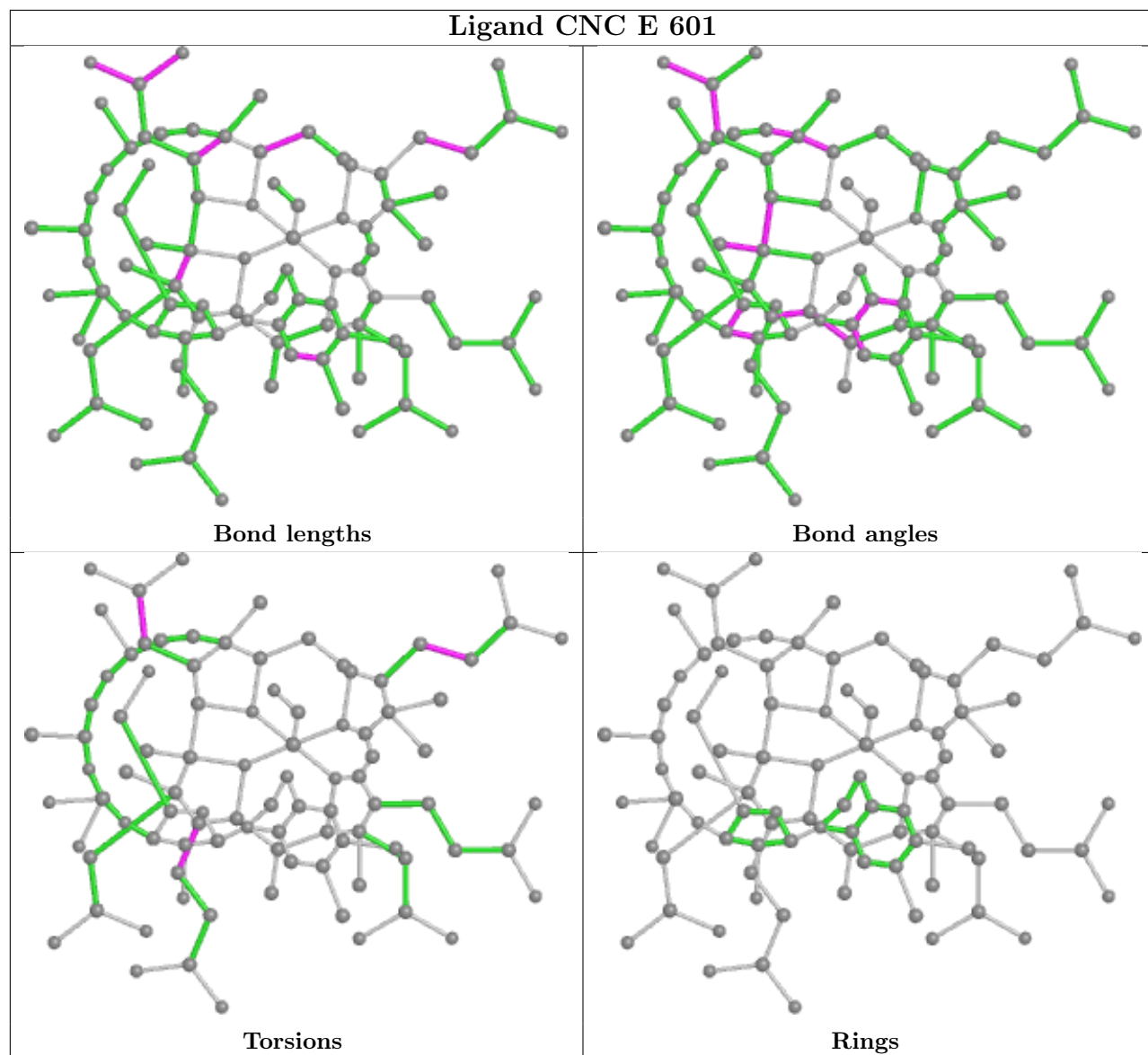
5 monomers are involved in 25 short contacts:

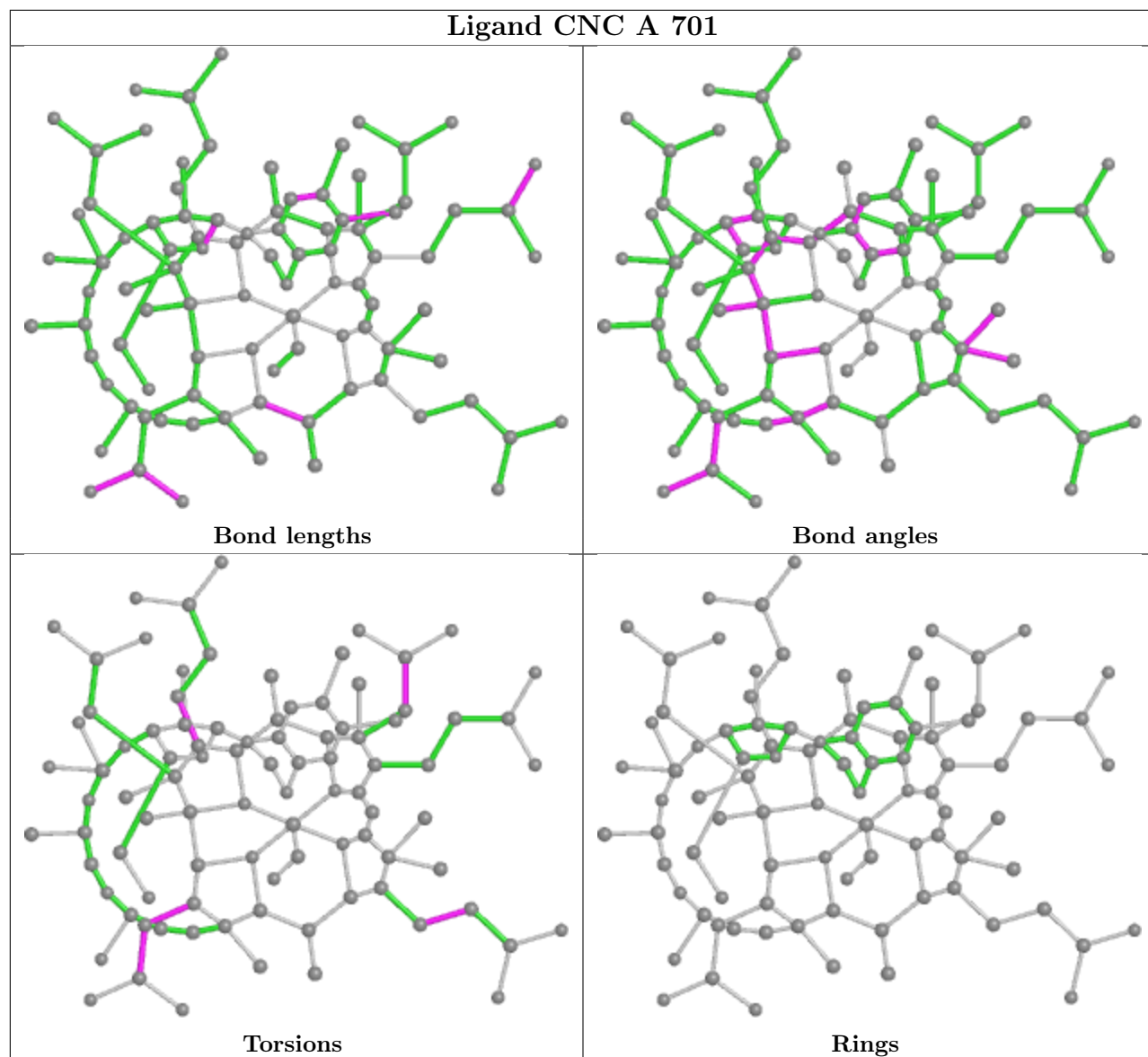
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	CNC	8	0
2	D	1001	CNC	4	0
2	E	601	CNC	5	0
2	A	701	CNC	3	0
2	C	901	CNC	5	0

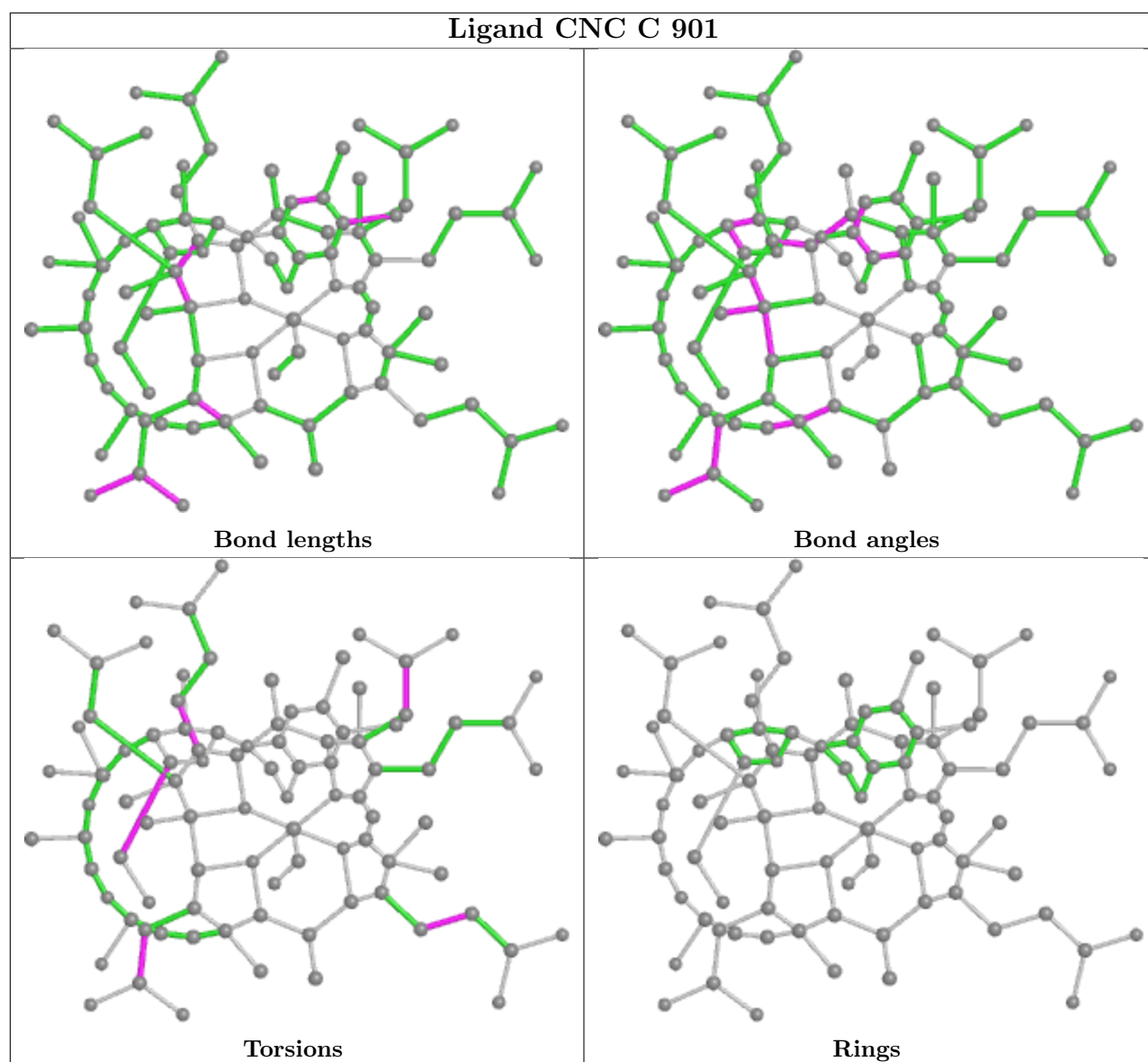
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	35/35 (100%)	-0.23	0 100 100	21, 30, 42, 45	0
1	B	35/35 (100%)	-0.22	0 100 100	19, 27, 45, 50	0
1	C	35/35 (100%)	-0.28	0 100 100	24, 35, 45, 47	0
1	D	35/35 (100%)	-0.21	0 100 100	22, 34, 38, 45	0
1	E	35/35 (100%)	0.09	0 100 100	24, 43, 51, 55	0
All	All	175/175 (100%)	-0.17	0 100 100	19, 34, 47, 55	0

There are no RSRZ outliers to report.

### 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
2	CNC	E	601	93/93	0.84	0.22	48,51,54,54	0
2	CNC	C	901	93/93	0.86	0.20	42,44,47,49	0
2	CNC	A	701	93/93	0.87	0.18	29,34,39,40	0

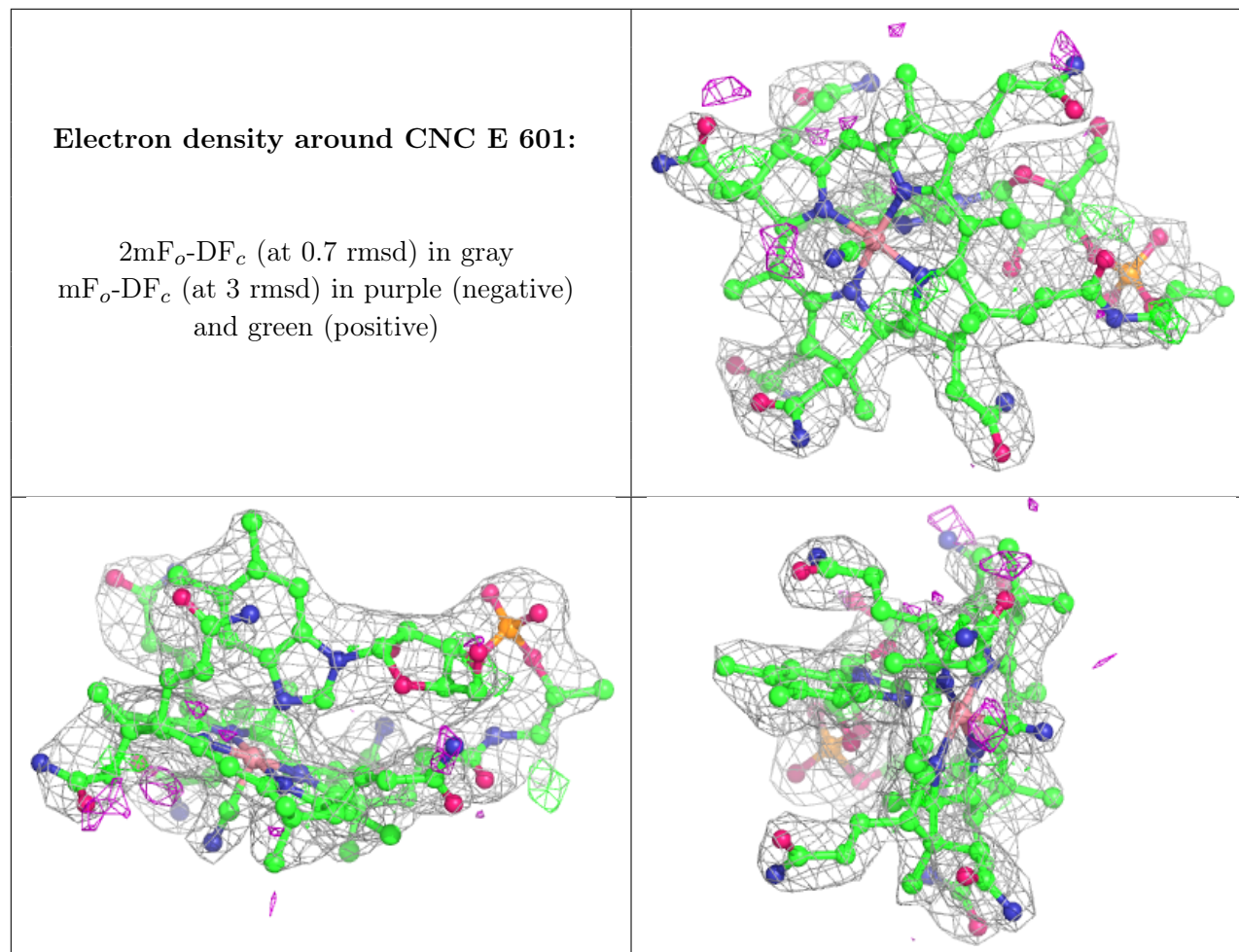
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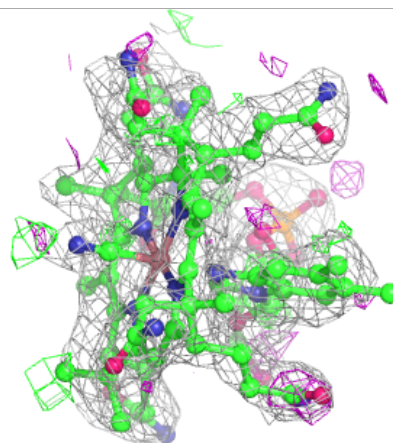
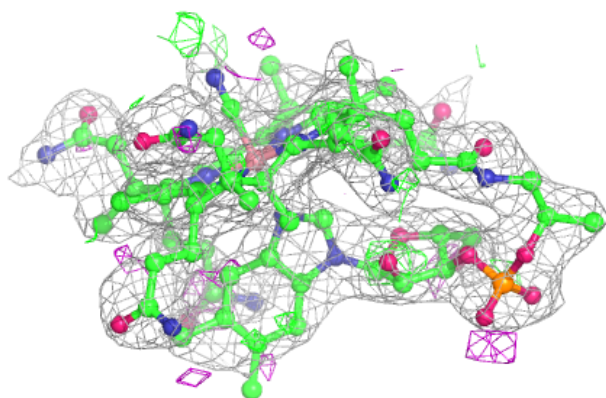
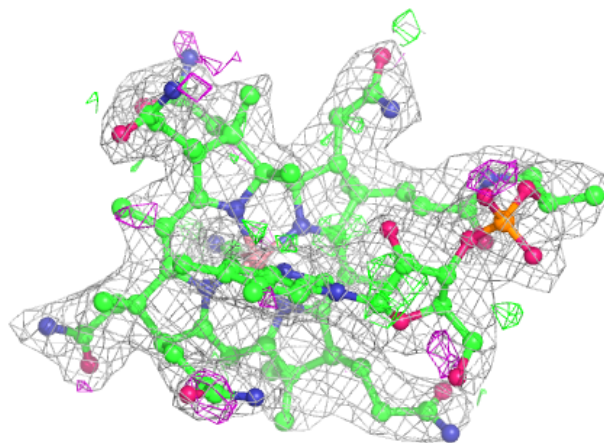
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CNC	D	1001	93/93	0.91	0.17	31,35,39,42	0
2	CNC	B	801	93/93	0.93	0.14	31,33,35,38	0

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.



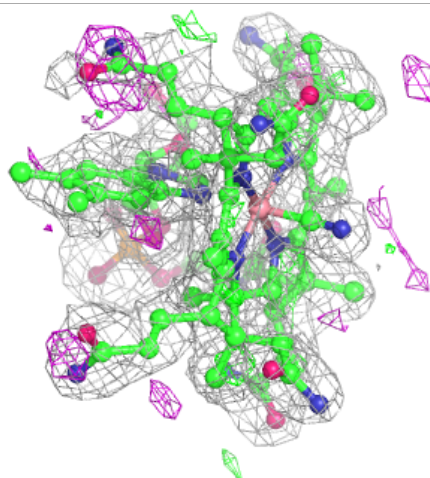
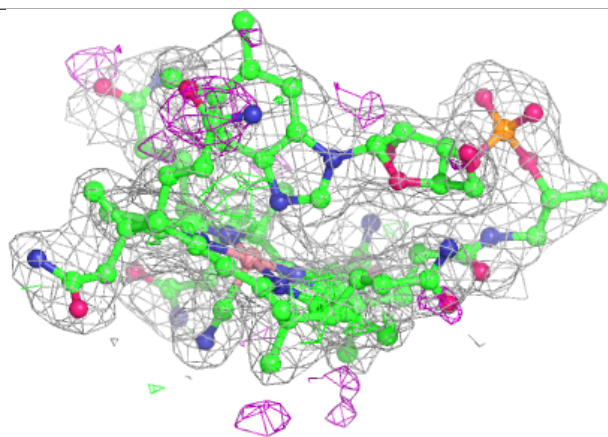
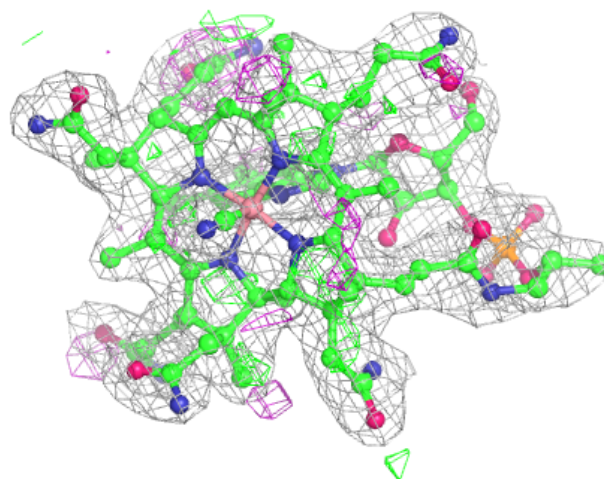
**Electron density around CNC C 901:**

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



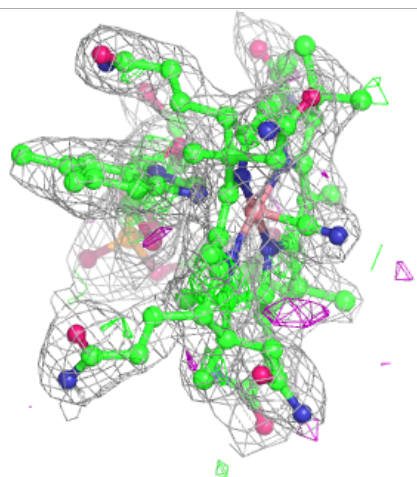
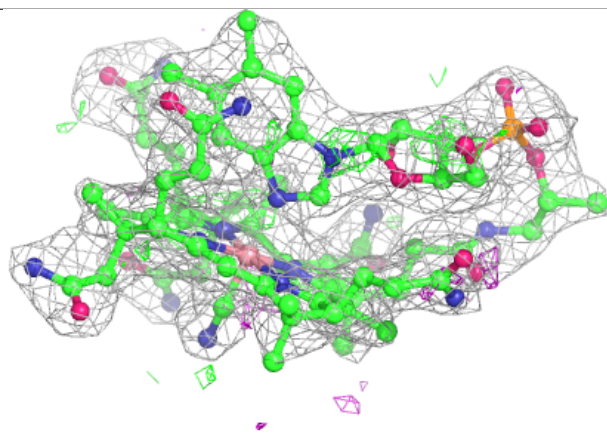
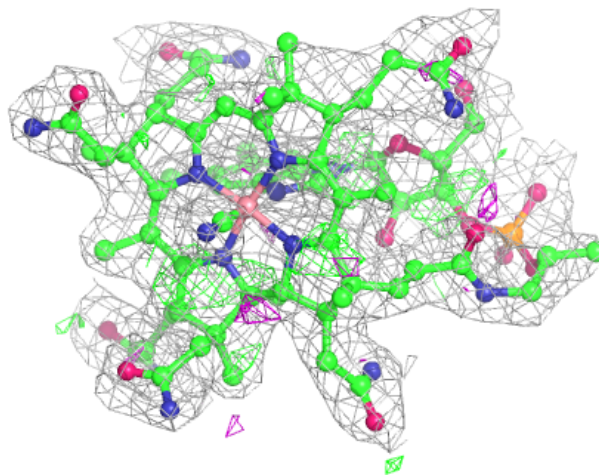
**Electron density around CNC A 701:**

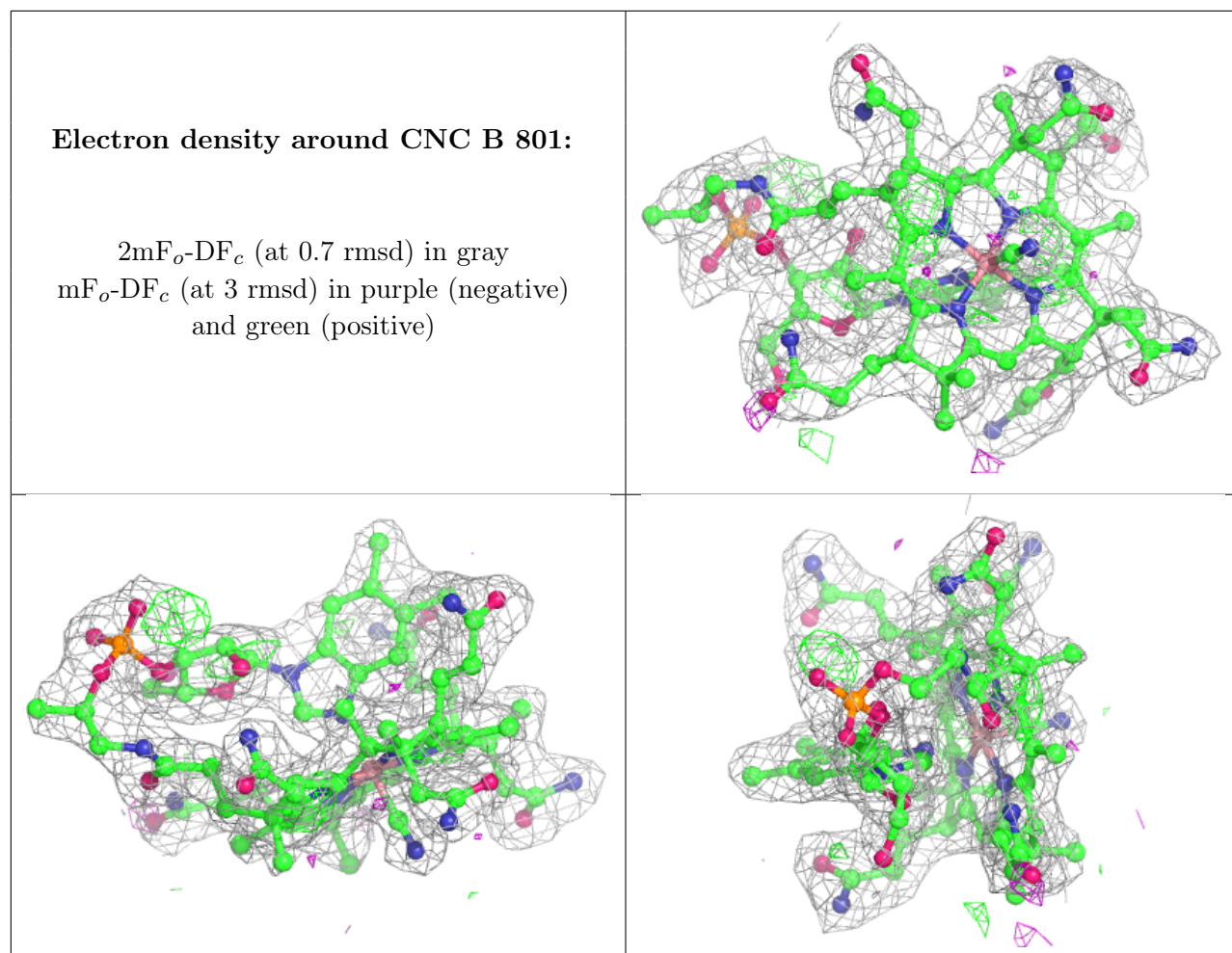
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CNC D 1001:**

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





## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.