



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:07 PM UTC

PDB ID : 9E5H / pdb\_00009e5h  
Title : env2 cobalamin riboswitch aptamer domain in complex with cyanocobalamin  
Authors : Olenginski, L.T.; Batey, R.T.  
Deposited on : 2024-10-28  
Resolution : 2.80 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.

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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

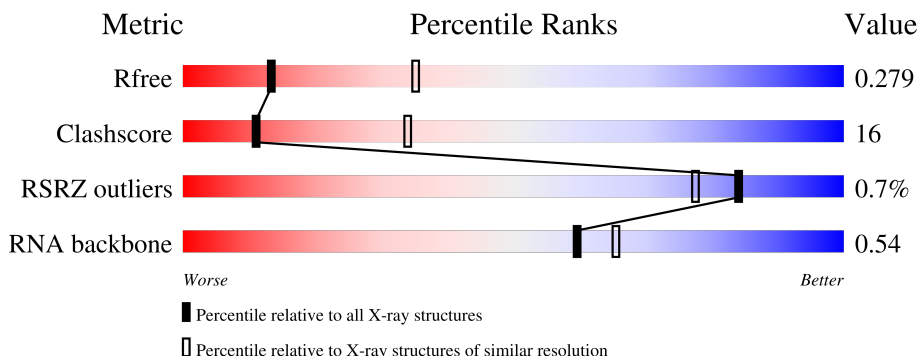
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	76	<div> <div></div> <div>51%</div> <div>42%</div> <div>7%</div> </div>
1	B	76	<div> <div>53%</div> <div>39%</div> <div>8%</div> </div>

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
4	TRS	B	103	-	X	-	-

## 2 Entry composition [i](#)

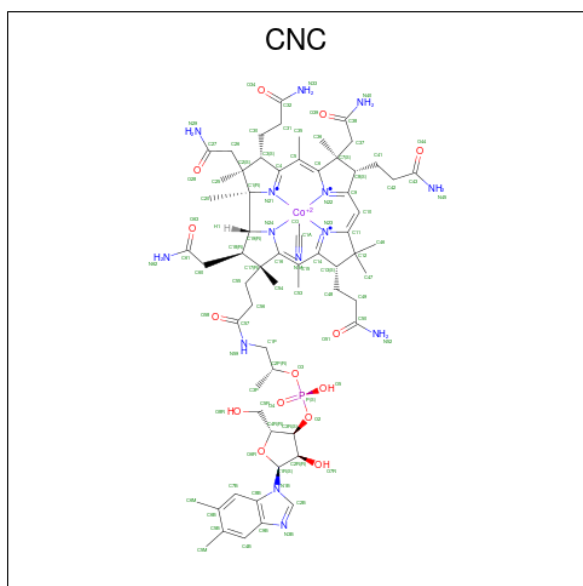
There are 7 unique types of molecules in this entry. The entry contains 3768 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (76-MER).

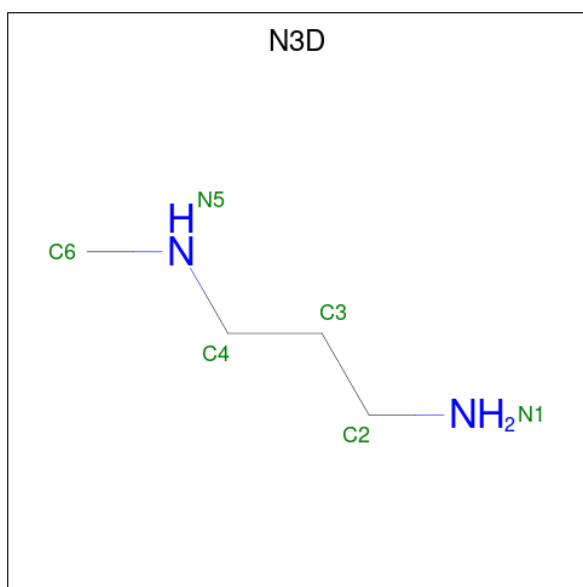
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	76	Total	C	N	O	P	0	0	0
			1640	730	306	526	78			
1	B	76	Total	C	N	O	P	0	0	0
			1640	730	306	526	78			

- Molecule 2 is CYANOCOBALAMIN (CCD ID: CNC) (formula:  $C_{63}H_{89}CoN_{14}O_{14}P$ ) (labeled as "Ligand of Interest" by depositor).



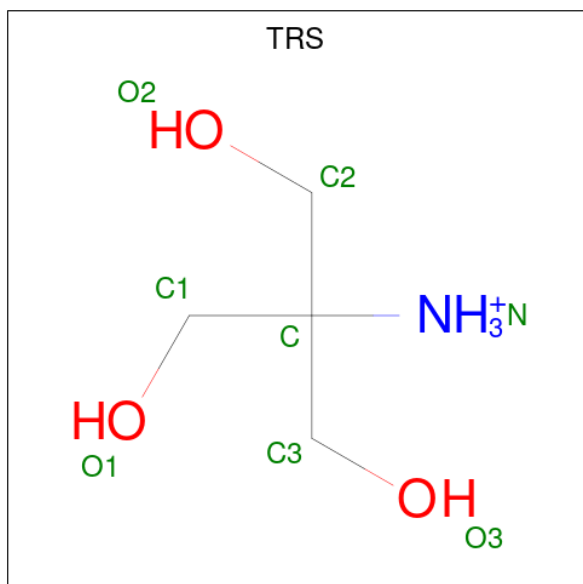
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		

- Molecule 3 is N-methylpropane-1,3-diamine (CCD ID: N3D) (formula:  $C_4H_{12}N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			6	4	2		
3	B	1	Total	C	N	0	0
			6	4	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	Mg	0	0
			9	9		
5	B	9	Total	Mg	0	0
			9	9		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K	0	0
			1	1		
6	B	1	Total	K	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	112	Total	O	0	0
			112	112		
7	B	142	Total	O	0	0
			142	142		

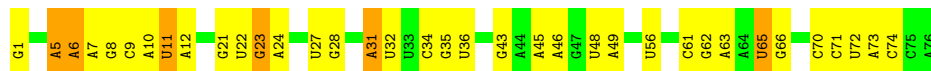
### 3 Residue-property plots [i](#)

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 (76-MER)



- Molecule 1: RNA (76-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.86Å 114.49Å 63.64Å 90.00° 99.28° 90.00°	Depositor
Resolution (Å)	19.66 – 2.80 19.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.66-2.80) 97.6 (19.66-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.06 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.208 , 0.278 0.207 , 0.279	Depositor DCC
$R_{free}$ test set	2000 reflections (7.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	1.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 32.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3768	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.80% 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: GTP, TRS, CNC, K, MG, N3D

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	0.41	0/1802	0.65	0/2807
1	B	0.40	0/1802	0.65	0/2807
All	All	0.40	0/3604	0.65	0/5614

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 [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	1640	0	823	31	0
1	B	1640	0	822	34	0
2	A	93	0	87	11	0
2	B	93	0	87	10	0
3	A	6	0	12	1	0
3	B	6	0	12	0	0
4	A	8	0	9	0	0
4	B	8	0	9	1	0
5	A	9	0	0	0	0
5	B	9	0	0	0	0
6	A	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	112	0	0	5	0
7	B	142	0	0	9	0
All	All	3768	0	1861	86	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.

All (86) 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:5:A:H2'	1:A:6:A:C8	2.04	0.91
1:B:5:A:H2'	1:B:6:A:C8	2.05	0.90
2:B:101:CNC:H362	2:B:101:CNC:H351	1.63	0.81
1:A:48:U:OP1	7:A:201:HOH:O	1.98	0.81
2:A:101:CNC:H351	2:A:101:CNC:H362	1.62	0.80
1:A:29:A:OP2	7:A:202:HOH:O	2.01	0.79
2:A:101:CNC:H552	2:A:101:CNC:H531	1.63	0.79
1:B:46:A:OP1	7:B:201:HOH:O	2.03	0.74
1:A:72:U:H2'	1:A:73:A:H8	1.52	0.73
2:B:101:CNC:H552	2:B:101:CNC:H531	1.69	0.71
1:B:1:GTP:O1A	7:B:202:HOH:O	2.08	0.71
1:B:7:A:OP1	7:B:203:HOH:O	2.09	0.69
1:B:72:U:H2'	1:B:73:A:H8	1.56	0.68
1:B:5:A:H2'	1:B:6:A:H8	1.53	0.68
1:A:72:U:H2'	1:A:73:A:C8	2.29	0.67
1:A:10:A:OP2	7:A:203:HOH:O	2.15	0.65
1:B:72:U:H2'	1:B:73:A:C8	2.33	0.64
1:B:34:C:H2'	1:B:35:G:H8	1.62	0.63
1:A:73:A:H2'	1:A:74:C:C6	2.33	0.62
2:B:101:CNC:H552	2:B:101:CNC:C53	2.30	0.61
1:B:10:A:H2'	1:B:11:U:H5''	1.83	0.61
2:A:101:CNC:H353	2:A:101:CNC:H302	1.82	0.60
2:A:101:CNC:H351	2:A:101:CNC:C36	2.29	0.60
1:B:9:C:OP1	7:B:204:HOH:O	2.16	0.60
1:A:5:A:H2'	1:A:6:A:H8	1.66	0.59
1:B:73:A:H2'	1:B:74:C:C6	2.38	0.59
1:A:62:G:N2	7:A:204:HOH:O	2.18	0.56
1:A:34:C:H2'	1:A:35:G:H8	1.71	0.55
1:A:35:G:H2'	1:A:36:U:H6	1.71	0.55
1:B:34:C:H2'	1:B:35:G:C8	2.41	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:U:O4	3:A:102:N3D:N1	2.39	0.54
1:A:35:G:H2'	1:A:36:U:C6	2.42	0.54
1:A:48:U:H5''	1:A:49:A:H5'	1.90	0.53
1:B:8:G:H22	1:B:11:U:H5'	1.74	0.52
2:B:101:CNC:H203	2:B:101:CNC:H301	1.91	0.52
2:A:101:CNC:H5R2	7:A:257:HOH:O	2.11	0.50
1:B:28:G:N1	1:B:31:A:OP2	2.44	0.50
2:B:101:CNC:C6	2:B:101:CNC:C1A	2.87	0.50
1:B:49:A:OP2	7:B:205:HOH:O	2.20	0.49
1:A:34:C:H2'	1:A:35:G:C8	2.48	0.49
1:B:63:A:H8	7:B:207:HOH:O	1.96	0.49
1:B:63:A:H5''	7:B:207:HOH:O	2.13	0.48
2:B:101:CNC:O28	2:B:101:CNC:H251	2.14	0.48
1:B:70:C:H2'	1:B:71:C:O4'	2.14	0.48
2:B:101:CNC:H10	2:B:101:CNC:H422	1.96	0.48
1:B:35:G:H2'	1:B:36:U:C6	2.49	0.47
1:A:4:A:C6	1:A:12:A:C8	3.03	0.47
1:A:69:A:O2'	1:A:70:C:H5'	2.14	0.47
1:A:43:G:H2'	1:A:45:A:H2	1.81	0.46
1:A:11:U:O4'	1:A:65:U:H1'	2.16	0.46
1:B:7:A:H2'	1:B:8:G:O4'	2.16	0.46
2:A:101:CNC:H2B	2:A:101:CNC:C14	2.45	0.46
1:B:28:G:N2	1:B:31:A:OP2	2.49	0.46
2:B:101:CNC:H351	2:B:101:CNC:C36	2.39	0.46
1:B:48:U:H5''	1:B:49:A:H5'	1.97	0.46
1:A:23:G:H2'	1:A:24:A:H8	1.80	0.45
2:A:101:CNC:H531	2:A:101:CNC:C55	2.39	0.45
2:A:101:CNC:H252	2:A:101:CNC:C61	2.46	0.45
1:A:35:G:C4	1:A:36:U:C5	3.06	0.43
1:A:7:A:H2'	1:A:8:G:O4'	2.19	0.43
1:A:10:A:C2	1:A:65:U:C2	3.06	0.43
1:A:23:G:H2'	1:A:24:A:C8	2.54	0.42
1:B:43:G:H4'	4:B:103:TRS:N	2.34	0.42
1:A:65:U:H4'	1:A:66:G:OP2	2.19	0.42
1:B:5:A:C2'	1:B:6:A:C8	2.91	0.42
1:B:27:U:H2'	1:B:28:G:O4'	2.20	0.42
1:B:61:C:H2'	1:B:62:G:O4'	2.19	0.42
1:A:8:G:H22	1:A:11:U:H5'	1.85	0.42
1:A:70:C:H2'	1:A:71:C:O4'	2.19	0.42
1:B:10:A:C2	1:B:65:U:C2	3.08	0.41
2:B:101:CNC:O5	7:B:206:HOH:O	2.22	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:101:CNC:C48	2:A:101:CNC:H533	2.51	0.41
2:A:101:CNC:C4B	2:A:101:CNC:H421	2.50	0.41
1:A:10:A:C2'	1:A:11:U:H5''	2.49	0.41
1:A:75:C:OP2	1:A:76:A:O2'	2.23	0.41
1:B:45:A:N6	7:B:218:HOH:O	2.46	0.41
1:B:35:G:H2'	1:B:36:U:H6	1.86	0.41
2:B:101:CNC:H562	2:B:101:CNC:H18	1.90	0.41
1:B:23:G:H2'	1:B:24:A:H8	1.86	0.41
1:B:5:A:O2'	1:B:6:A:OP1	2.29	0.40
2:A:101:CNC:H533	2:A:101:CNC:H482	2.02	0.40
1:B:43:G:H2'	1:B:45:A:H2	1.86	0.40
1:A:60:C:H2'	1:A:61:C:C6	2.57	0.40
1:A:61:C:H2'	1:A:62:G:O4'	2.20	0.40
1:B:1:GTP:O5'	1:B:1:GTP:H8	2.04	0.40
1:B:11:U:O4'	1:B:65:U:H1'	2.21	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	74/76 (97%)	11 (14%)	1 (1%)
1	B	74/76 (97%)	12 (16%)	1 (1%)
All	All	148/152 (97%)	23 (15%)	2 (1%)

All (23) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	6	A
1	A	13	G
1	A	21	G
1	A	22	U
1	A	23	G
1	A	32	U
1	A	55	A
1	A	56	U
1	A	65	U
1	A	66	G
1	B	5	A
1	B	6	A
1	B	11	U
1	B	12	A
1	B	21	G
1	B	22	U
1	B	23	G
1	B	31	A
1	B	32	U
1	B	56	U
1	B	65	U
1	B	66	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
1	B	5	A

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 20 are monoatomic - leaving 6 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	$\# Z  > 2$
3	N3D	A	102	-	5,5,5	0.33	0	4,4,4	0.85	0
2	CNC	B	101	-	93,103,103	1.10	1 (1%)	149,171,171	1.40	22 (14%)
4	TRS	B	103	-	7,7,7	2.37	1 (14%)	9,9,9	1.19	0
3	N3D	B	102	-	5,5,5	0.43	0	4,4,4	0.79	0
2	CNC	A	101	-	93,103,103	1.09	1 (1%)	149,171,171	1.07	8 (5%)
4	TRS	A	103	-	7,7,7	2.39	1 (14%)	9,9,9	1.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	N3D	A	102	-	-	1/3/3/3	-
2	CNC	B	101	-	-	11/56/235/235	0/3/11/11
4	TRS	B	103	-	-	9/9/9/9	-
3	N3D	B	102	-	-	1/3/3/3	-
2	CNC	A	101	-	-	9/56/235/235	0/3/11/11
4	TRS	A	103	-	-	8/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	CNC	C1A-N1A	8.82	1.47	1.15
2	B	101	CNC	C1A-N1A	8.74	1.46	1.15
4	A	103	TRS	C-N	-6.18	1.29	1.49
4	B	103	TRS	C-N	-5.92	1.30	1.49

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	CNC	C26-C2-C1	4.52	116.98	110.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	CNC	C55-C56-C57	-4.27	101.72	111.25
2	A	101	CNC	C1-C19-C18	-3.93	115.85	121.75
2	B	101	CNC	C17-C18-C19	-3.87	97.99	102.70
2	B	101	CNC	C9B-C8B-N1B	3.79	106.98	105.30
2	B	101	CNC	C18-C60-C61	3.24	122.29	114.04
2	B	101	CNC	C1P-N59-C57	-3.11	116.02	122.69
2	B	101	CNC	C41-C8-C9	-3.09	105.80	111.19
2	B	101	CNC	O3-C2P-C1P	-3.06	100.87	106.94
2	B	101	CNC	C9-C10-C11	-3.02	121.40	125.84
2	B	101	CNC	C18-C19-N24	-2.94	97.24	101.92
2	A	101	CNC	C41-C8-C9	-2.91	106.11	111.19
2	B	101	CNC	C1-C19-C18	-2.90	117.39	121.75
2	B	101	CNC	C20-C1-C19	-2.83	104.61	110.23
2	A	101	CNC	C18-C19-N24	-2.72	97.60	101.92
2	A	101	CNC	C25-C2-C1	-2.55	109.94	113.75
2	A	101	CNC	C10-C9-N22	-2.54	122.84	125.74
2	B	101	CNC	C12-C13-C14	2.49	105.11	101.86
2	B	101	CNC	C19-N24-C16	-2.38	108.16	111.96
2	B	101	CNC	C9B-N3B-C2B	2.32	107.25	104.40
2	B	101	CNC	C26-C2-C3	-2.28	103.45	107.42
2	A	101	CNC	C1-C2-C3	2.27	104.45	101.60
2	B	101	CNC	C60-C18-C19	-2.25	108.78	114.08
2	A	101	CNC	C55-C56-C57	-2.23	106.27	111.25
2	B	101	CNC	N1B-C2B-N3B	-2.23	110.77	113.94
2	A	101	CNC	C9B-C8B-N1B	2.21	106.28	105.30
2	B	101	CNC	C60-C61-N62	-2.09	111.17	116.19
2	B	101	CNC	C48-C49-C50	-2.09	105.45	112.55
2	B	101	CNC	C20-C1-N21	2.01	113.59	110.26
2	B	101	CNC	O5-P-O4	2.01	121.82	112.44

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	CNC	N59-C1P-C2P-C3P
2	A	101	CNC	N59-C1P-C2P-O3
3	B	102	N3D	C3-C4-N5-C6
4	A	103	TRS	N-C-C1-O1
4	A	103	TRS	C1-C-C3-O3
4	A	103	TRS	C2-C-C3-O3
4	A	103	TRS	N-C-C3-O3
4	B	103	TRS	C2-C-C1-O1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	B	103	TRS	C3-C-C1-O1
4	B	103	TRS	N-C-C1-O1
4	B	103	TRS	C1-C-C2-O2
4	B	103	TRS	C3-C-C2-O2
4	B	103	TRS	N-C-C2-O2
4	B	103	TRS	C2-C-C3-O3
4	B	103	TRS	N-C-C3-O3
2	B	101	CNC	C14-C13-C48-C49
2	B	101	CNC	C18-C17-C55-C56
2	B	101	CNC	C12-C13-C48-C49
2	B	101	CNC	C16-C17-C55-C56
4	A	103	TRS	C3-C-C1-O1
2	A	101	CNC	C14-C13-C48-C49
2	B	101	CNC	N59-C1P-C2P-C3P
2	A	101	CNC	C12-C13-C48-C49
2	B	101	CNC	C48-C49-C50-N52
2	A	101	CNC	C13-C48-C49-C50
4	A	103	TRS	C3-C-C2-O2
4	A	103	TRS	N-C-C2-O2
2	A	101	CNC	C18-C17-C55-C56
4	B	103	TRS	C1-C-C3-O3
3	A	102	N3D	N1-C2-C3-C4
2	B	101	CNC	C41-C42-C43-N45
2	A	101	CNC	C41-C42-C43-O44
2	B	101	CNC	C41-C42-C43-O44
2	B	101	CNC	N59-C1P-C2P-O3
2	A	101	CNC	C41-C42-C43-N45
2	B	101	CNC	C19-C18-C60-C61
2	B	101	CNC	C48-C49-C50-O51
4	A	103	TRS	C1-C-C2-O2
2	A	101	CNC	O6R-C4R-C5R-O8R

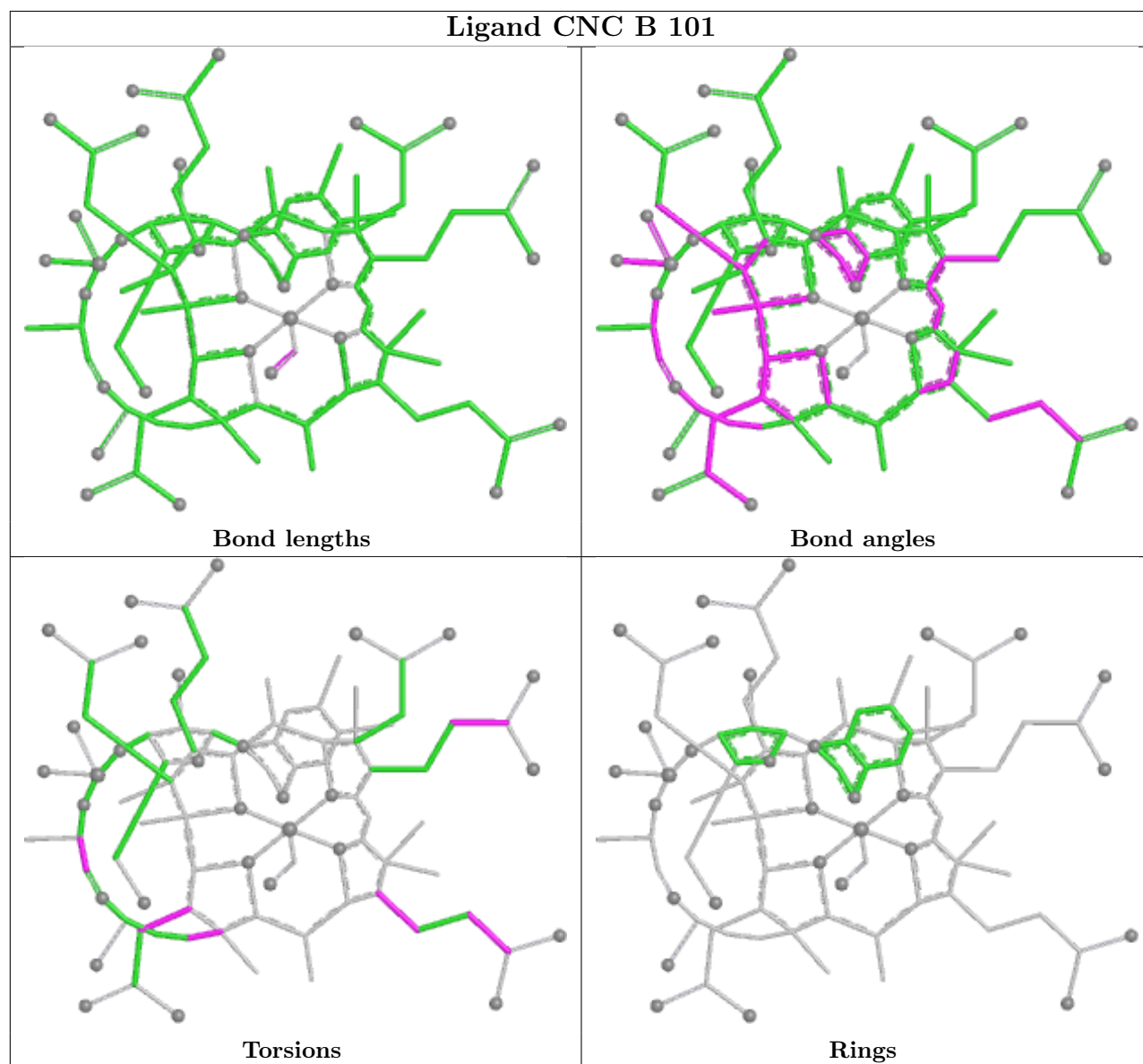
There are no ring outliers.

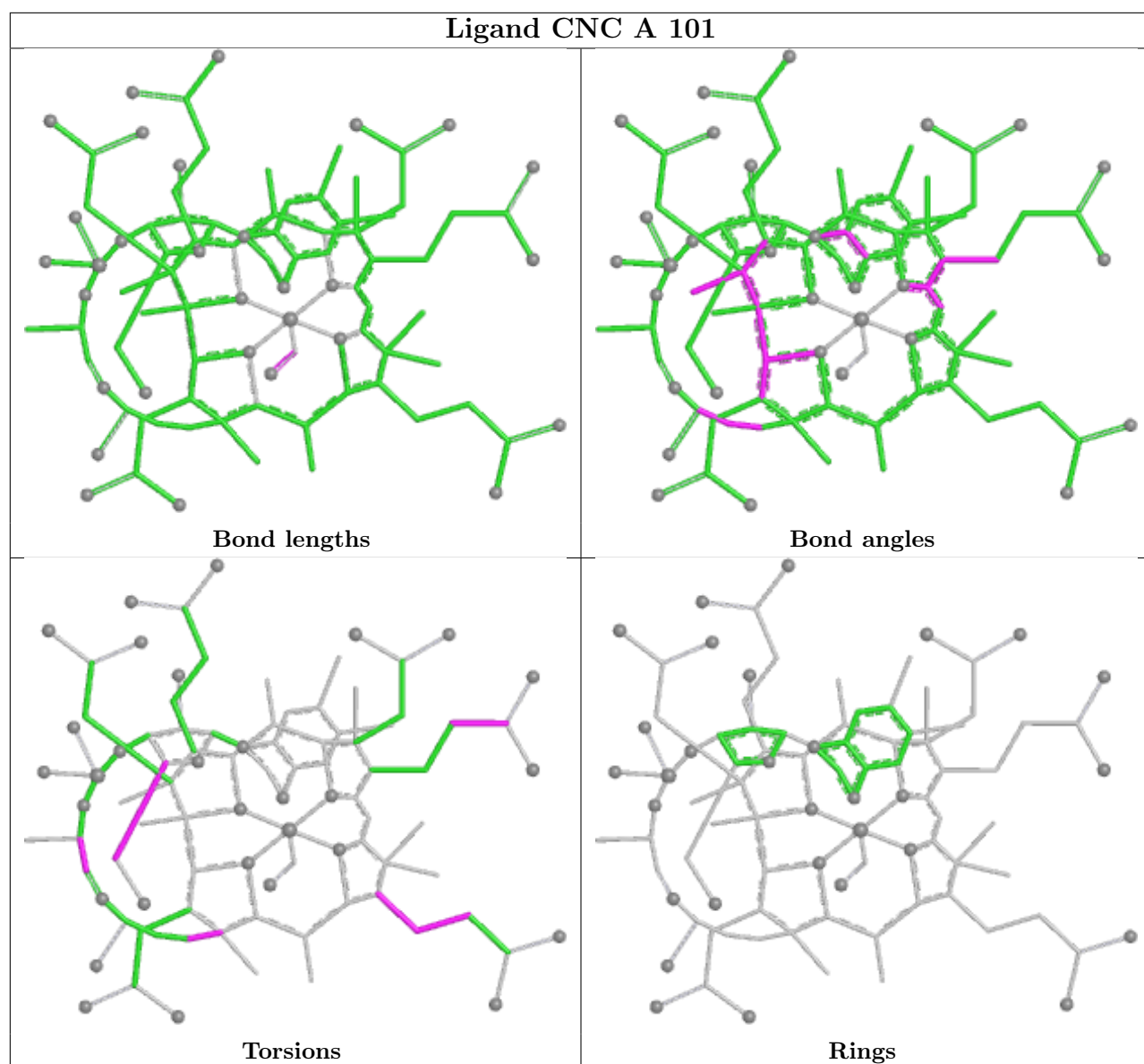
4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	102	N3D	1	0
2	B	101	CNC	10	0
4	B	103	TRS	1	0
2	A	101	CNC	11	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	75/76 (98%)	0.06	1 (1%) 75 66	23, 31, 43, 56	0
1	B	75/76 (98%)	0.04	0 100 100	24, 33, 46, 54	0
All	All	150/152 (98%)	0.05	1 (0%) 84 77	23, 32, 46, 56	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	A	2.1

### 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 oligosaccharides 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
5	MG	A	104	1/1	0.68	0.12	49,49,49,49	0
4	TRS	B	103	8/8	0.73	0.18	28,32,39,47	0
3	N3D	B	102	6/6	0.75	0.15	21,22,24,27	0
5	MG	A	108	1/1	0.76	0.16	28,28,28,28	0

*Continued on next page...*

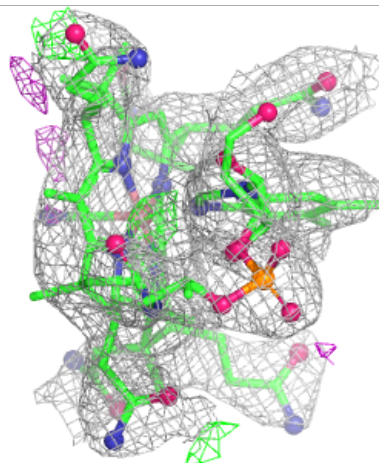
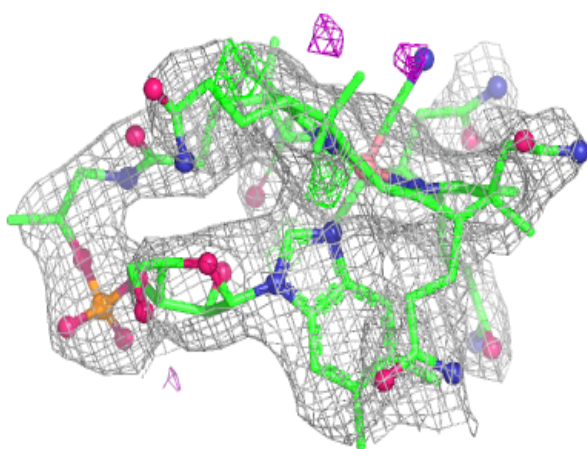
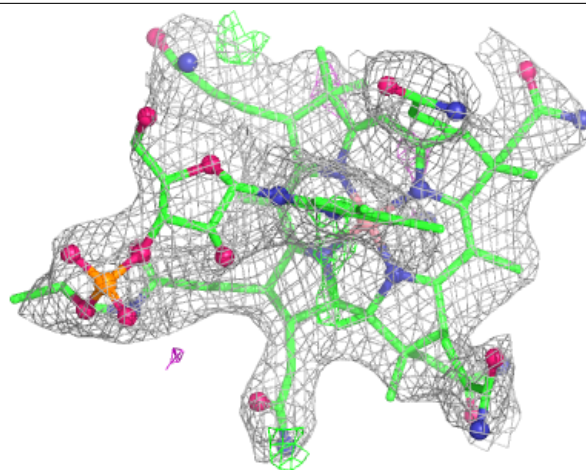
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	K	A	113	1/1	0.77	0.17	48,48,48,48	0
5	MG	B	111	1/1	0.78	0.28	36,36,36,36	0
5	MG	A	111	1/1	0.79	0.39	32,32,32,32	0
5	MG	B	104	1/1	0.79	0.07	48,48,48,48	0
3	N3D	A	102	6/6	0.84	0.12	23,26,28,29	0
5	MG	A	109	1/1	0.84	0.31	32,32,32,32	0
5	MG	B	109	1/1	0.85	0.26	36,36,36,36	0
5	MG	B	110	1/1	0.86	0.22	28,28,28,28	0
6	K	B	113	1/1	0.86	0.10	54,54,54,54	0
5	MG	B	107	1/1	0.88	0.17	28,28,28,28	0
5	MG	A	105	1/1	0.88	0.34	31,31,31,31	0
5	MG	B	105	1/1	0.88	0.29	35,35,35,35	0
5	MG	A	107	1/1	0.89	0.26	33,33,33,33	0
5	MG	A	106	1/1	0.90	0.14	27,27,27,27	0
4	TRS	A	103	8/8	0.91	0.17	23,26,32,34	0
5	MG	A	112	1/1	0.91	0.16	25,25,25,25	0
5	MG	B	112	1/1	0.92	0.14	27,27,27,27	0
5	MG	B	106	1/1	0.93	0.29	42,42,42,42	0
2	CNC	B	101	93/93	0.93	0.11	21,26,33,43	0
2	CNC	A	101	93/93	0.94	0.12	14,23,33,41	0
5	MG	B	108	1/1	0.94	0.15	28,28,28,28	0
5	MG	A	110	1/1	0.97	0.11	28,28,28,28	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.

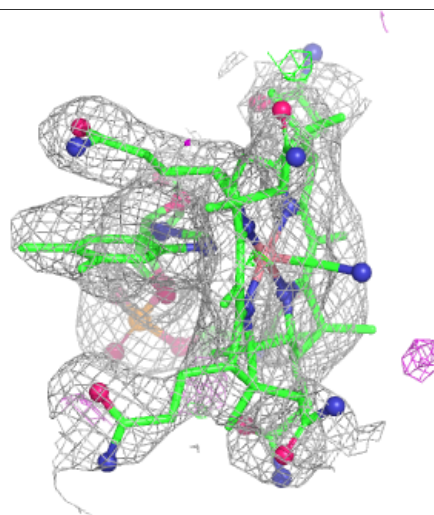
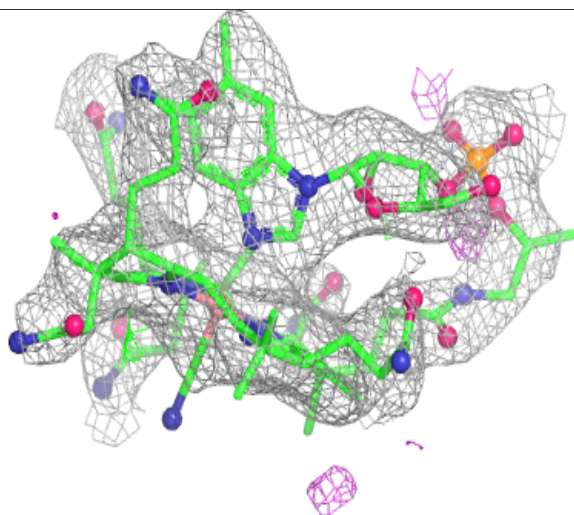
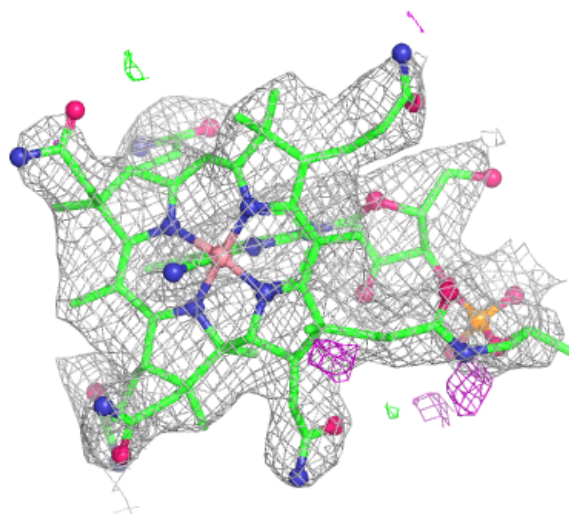
**Electron density around CNC B 101:**

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



**Electron density around CNC A 101:**

$2mF_o-DF_c$  (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.