



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 04:56 AM EDT

PDB ID : 9E5T / pdb\_00009e5t  
Title : env2 cobalamin riboswitch aptamer domain in complex with ethynyl-4-(4-phenyl-2,3,4-triazole)-guanidinium-cobalamin  
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Deposited on : 2024-10-28  
Resolution : 2.19 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>.

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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

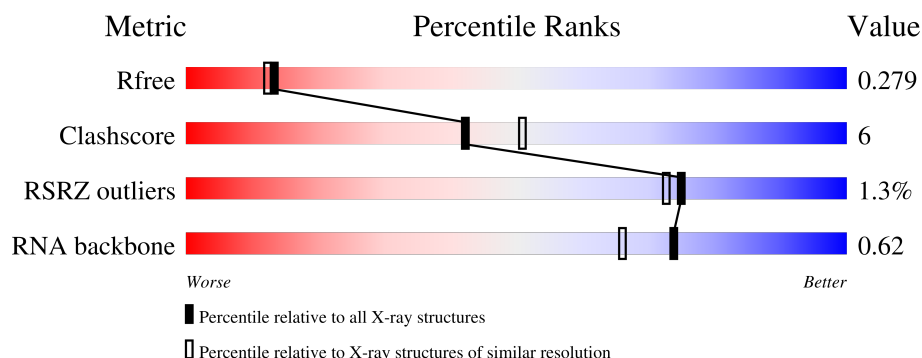
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)
RNA backbone	3983	1052 (2.50-1.90)

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	76	
1	B	76	

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](#)

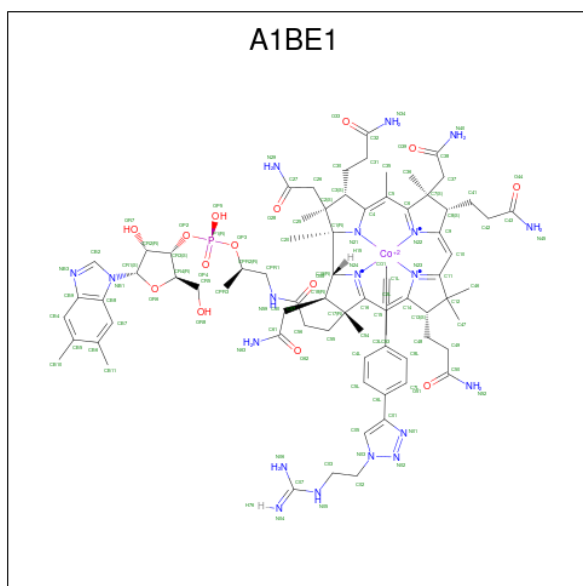
There are 7 unique types of molecules in this entry. The entry contains 3889 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).

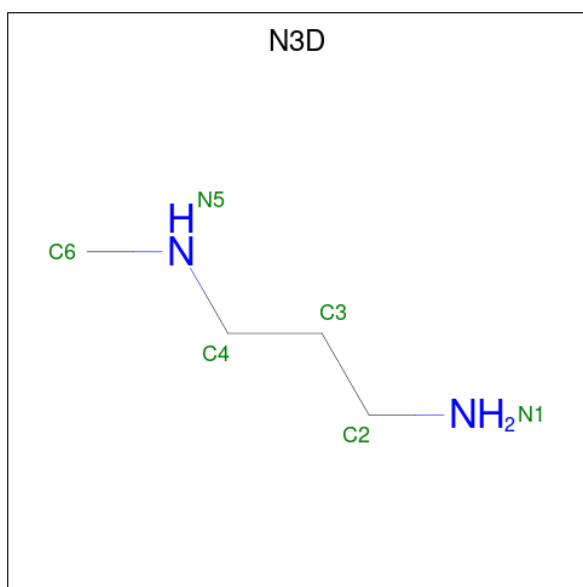
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	76	Total	C	N	O	P	0	0	0
			1640	730	306	526	78			
1	B	76	Total	C	N	O	P	0	0	0
			1640	730	306	526	78			

- Molecule 2 is ethynyl-4-(4-phenyl-2,3,4-triazole)-guanidinium-cobalamin (CCD ID: A1BE1) (formula:  $C_{75}H_{102}CoN_{19}O_{14}P$ ) (labeled as "Ligand of Interest" by depositor).



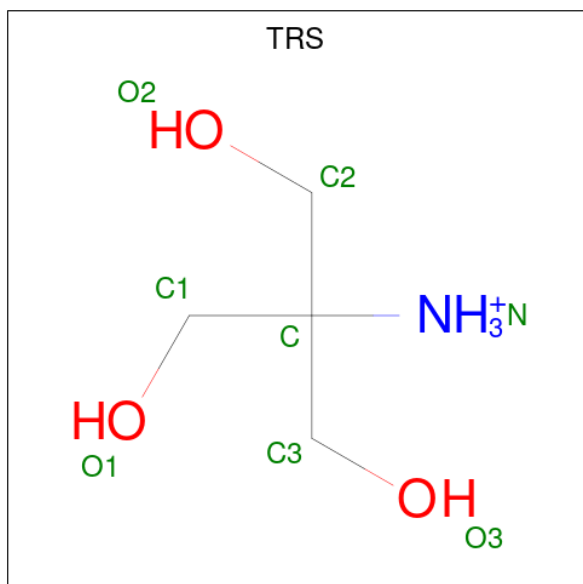
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O P	0	0
			110	75	1	19	14 1		
2	B	1	Total	C	Co	N	O P	0	0
			110	75	1	19	14 1		

- 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		

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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	10	Total	Mg	0	0
			10	10		

- 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		

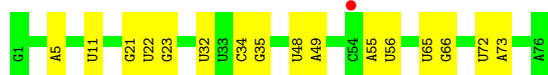
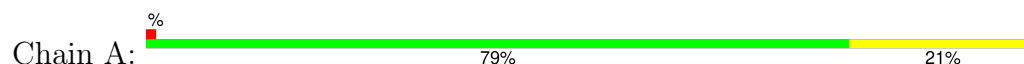
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	218	Total	O	0	0
			218	218		
7	B	122	Total	O	0	0
			122	122		

### 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, $\alpha$ , $\beta$ , $\gamma$	42.21Å 78.20Å 77.10Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	19.73 – 2.19 19.73 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.2 (19.73-2.19) 97.3 (19.73-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.39 (at 2.19Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.225 , 0.279 0.225 , 0.279	Depositor DCC
$R_{free}$ test set	2002 reflections (7.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.012 for -h,-l,-k 0.000 for -h,l,k 0.024 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, K, N3D, TRS, A1BE1

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	0.10	0/1802	0.25	0/2807
1	B	0.12	0/1802	0.32	1/2807 (0.0%)
All	All	0.11	0/3604	0.29	1/5614 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	G	N9-C1'-C2'	-5.25	106.12	114.00

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	822	6	0
1	B	1640	0	823	14	0
2	A	110	0	0	6	0
2	B	110	0	0	8	0
3	A	6	0	12	0	0
3	B	6	0	12	1	0
4	A	8	0	9	0	0
4	B	8	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	9	0	0	0	0
5	B	10	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	218	0	0	0	0
7	B	122	0	0	0	0
All	All	3889	0	1687	33	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 6.

All (33) 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)
2:B:101:A1BE1:CPR2	2:B:101:A1BE1:CPR1	1.52	1.51
2:A:101:A1BE1:CPR2	2:A:101:A1BE1:CPR1	1.52	1.50
2:A:101:A1BE1:CPR2	2:A:101:A1BE1:CPR3	1.51	1.49
2:B:101:A1BE1:CPR2	2:B:101:A1BE1:CPR3	1.51	1.49
2:A:101:A1BE1:CPR1	2:A:101:A1BE1:CPR3	2.50	1.08
2:B:101:A1BE1:CPR1	2:B:101:A1BE1:CPR3	2.50	1.08
2:B:101:A1BE1:CPR1	2:B:101:A1BE1:OP3	2.38	0.81
2:A:101:A1BE1:CPR3	2:A:101:A1BE1:OP3	2.38	0.81
2:B:101:A1BE1:CPR3	2:B:101:A1BE1:OP3	2.39	0.81
2:A:101:A1BE1:CPR1	2:A:101:A1BE1:OP3	2.38	0.80
2:A:101:A1BE1:CPR2	2:A:101:A1BE1:N59	2.52	0.77
2:B:101:A1BE1:CPR2	2:B:101:A1BE1:N59	2.52	0.77
1:A:48:U:H5''	1:A:49:A:H5'	1.80	0.62
1:B:5:A:H2'	1:B:6:A:C8	2.36	0.60
1:B:34:C:H2'	1:B:35:G:H8	1.69	0.56
1:B:11:U:H2'	1:B:11:U:O2	2.07	0.55
1:A:11:U:H2'	1:A:11:U:O2	2.07	0.53
1:A:72:U:H2'	1:A:73:A:C8	2.44	0.52
1:B:48:U:H5''	1:B:49:A:H5'	1.92	0.52
1:A:72:U:H2'	1:A:73:A:H8	1.75	0.51
1:A:34:C:H2'	1:A:35:G:H8	1.74	0.51
1:B:5:A:OP2	1:B:12:A:H4'	2.13	0.49
1:B:5:A:O2'	1:B:6:A:OP1	2.31	0.48
1:B:34:C:H2'	1:B:35:G:C8	2.50	0.47
1:B:66:G:H3'	1:B:67:C:H6	1.80	0.47
1:A:34:C:H2'	1:A:35:G:C8	2.51	0.46
2:B:101:A1BE1:C6	2:B:101:A1BE1:C1L	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:A:OP2	2:B:101:A1BE1:C02	2.65	0.44
1:B:72:U:H2'	1:B:73:A:C8	2.53	0.43
1:B:34:C:OP2	3:B:102:N3D:N5	2.53	0.42
1:B:1:GTP:H2'	1:B:2:G:C8	2.54	0.42
1:B:8:G:N1	1:B:11:U:OP2	2.51	0.42
1:B:66:G:H3'	1:B:67:C:C6	2.55	0.41

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%)	9 (12%)	0
1	B	74/76 (97%)	12 (16%)	2 (2%)
All	All	148/152 (97%)	21 (14%)	2 (1%)

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
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

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Mol	Chain	Res	Type
1	B	6	A
1	B	17	G
1	B	18	A
1	B	21	G
1	B	22	U
1	B	23	G
1	B	32	U
1	B	55	A
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	B	5	A
1	B	17	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 21 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	$\# Z  > 2$
4	TRS	A	103	-	7,7,7	2.32	1 (14%)	9,9,9	1.42	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	N3D	B	102	-	5,5,5	0.36	0	4,4,4	0.85	0
4	TRS	B	103	-	7,7,7	2.32	1 (14%)	9,9,9	1.37	2 (22%)
2	A1BE1	B	101	-	110,122,122	2.00	9 (8%)	164,197,197	1.66	19 (11%)
3	N3D	A	102	-	5,5,5	0.34	0	4,4,4	0.85	0
2	A1BE1	A	101	-	110,122,122	1.99	9 (8%)	164,197,197	1.64	18 (10%)

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
4	TRS	A	103	-	-	6/9/9/9	-
3	N3D	B	102	-	-	0/3/3/3	-
4	TRS	B	103	-	-	7/9/9/9	-
2	A1BE1	B	101	-	-	9/68/248/248	0/5/13/13
3	N3D	A	102	-	-	0/3/3/3	-
2	A1BE1	A	101	-	-	12/68/248/248	0/5/13/13

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	A1BE1	C6L-C01	-9.02	1.34	1.47
2	B	101	A1BE1	C6L-C01	-9.01	1.34	1.47
2	A	101	A1BE1	C05-N03	7.89	1.47	1.34
2	B	101	A1BE1	N01-N02	7.87	1.44	1.32
2	B	101	A1BE1	C05-N03	7.78	1.47	1.34
2	B	101	A1BE1	C05-C01	7.69	1.50	1.37
2	A	101	A1BE1	C05-C01	7.68	1.50	1.37
2	A	101	A1BE1	N01-N02	7.63	1.44	1.32
2	A	101	A1BE1	N03-N02	6.91	1.45	1.34
2	B	101	A1BE1	N03-N02	6.87	1.45	1.34
2	B	101	A1BE1	C07-N05	6.07	1.45	1.33
4	A	103	TRS	C-N	-6.05	1.29	1.49
2	A	101	A1BE1	C07-N05	6.04	1.44	1.33
4	B	103	TRS	C-N	-6.03	1.29	1.49
2	B	101	A1BE1	C01-N01	5.25	1.46	1.36
2	A	101	A1BE1	C01-N01	5.13	1.46	1.36
2	B	101	A1BE1	C07-N04	4.32	1.47	1.32
2	A	101	A1BE1	C07-N04	4.29	1.47	1.32
2	B	101	A1BE1	C07-N06	3.66	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	A1BE1	C07-N06	3.57	1.47	1.34

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	101	A1BE1	C01-C05-N03	-9.69	97.48	105.28
2	B	101	A1BE1	C01-C05-N03	-9.51	97.62	105.28
2	A	101	A1BE1	C05-C01-N01	6.85	114.46	107.85
2	B	101	A1BE1	C05-C01-N01	6.83	114.44	107.85
2	B	101	A1BE1	C05-N03-N02	5.85	116.45	110.75
2	A	101	A1BE1	C05-N03-N02	5.84	116.44	110.75
2	B	101	A1BE1	N06-C07-N05	-5.42	106.95	119.27
2	A	101	A1BE1	N06-C07-N05	-5.36	107.08	119.27
2	B	101	A1BE1	C6L-C01-C05	-5.11	121.85	129.65
2	A	101	A1BE1	C6L-C01-C05	-4.25	123.15	129.65
2	B	101	A1BE1	C02-N03-C05	-4.09	121.20	128.83
2	A	101	A1BE1	C7L-C6L-C5L	3.81	123.42	118.57
2	A	101	A1BE1	C4L-C5L-C6L	-3.80	116.74	120.80
2	A	101	A1BE1	C02-N03-C05	-3.77	121.78	128.83
2	B	101	A1BE1	C7L-C6L-C5L	3.75	123.34	118.57
2	B	101	A1BE1	C4L-C5L-C6L	-3.58	116.98	120.80
2	B	101	A1BE1	C14-N23-C11	3.08	109.64	105.44
2	B	101	A1BE1	C5L-C6L-C01	-3.02	117.48	120.87
2	A	101	A1BE1	C14-N23-C11	3.01	109.53	105.44
2	B	101	A1BE1	C01-N01-N02	-2.85	106.18	109.23
2	A	101	A1BE1	N05-C07-N04	2.75	125.39	120.67
2	A	101	A1BE1	C7L-C6L-C01	-2.72	117.82	120.87
2	A	101	A1BE1	C01-N01-N02	-2.65	106.39	109.23
4	A	103	TRS	C3-C-C2	2.60	117.59	110.66
4	B	103	TRS	C3-C-C2	2.42	117.10	110.66
2	B	101	A1BE1	CB9-CB8-NB1	2.41	106.37	105.30
2	A	101	A1BE1	C41-C8-C9	-2.39	107.02	111.19
2	A	101	A1BE1	CB9-CB8-NB1	2.37	106.36	105.30
2	B	101	A1BE1	C41-C8-C9	-2.36	107.07	111.19
2	A	101	A1BE1	C35-C5-C4	-2.26	113.94	118.42
2	B	101	A1BE1	C35-C5-C4	-2.24	113.97	118.42
2	B	101	A1BE1	N05-C07-N04	2.19	124.44	120.67
2	B	101	A1BE1	C42-C41-C8	2.12	120.67	114.65
2	A	101	A1BE1	C47-C12-C46	-2.11	105.91	109.41
2	A	101	A1BE1	C42-C41-C8	2.11	120.62	114.65
2	B	101	A1BE1	C55-C17-C16	2.06	120.62	116.59
4	B	103	TRS	C3-C-C1	2.04	116.10	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	A1BE1	C56-C55-C17	-2.04	111.65	115.58
2	B	101	A1BE1	CPR2-CPR1-N59	2.02	115.90	112.92
2	A	101	A1BE1	C5-C6-N22	-2.01	122.31	126.52
4	A	103	TRS	C3-C-C1	2.01	116.00	110.66

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	A1BE1	C03-C02-N03-N02
2	A	101	A1BE1	N04-C07-N05-C03
2	A	101	A1BE1	N06-C07-N05-C03
2	B	101	A1BE1	C03-C02-N03-N02
2	B	101	A1BE1	N04-C07-N05-C03
2	B	101	A1BE1	N06-C07-N05-C03
2	B	101	A1BE1	OR6-CR4-CR5-OR8
4	A	103	TRS	N-C-C1-O1
4	A	103	TRS	C1-C-C3-O3
4	B	103	TRS	N-C-C1-O1
4	B	103	TRS	C2-C-C3-O3
4	B	103	TRS	N-C-C3-O3
2	B	101	A1BE1	CR3-CR4-CR5-OR8
2	A	101	A1BE1	C2-C26-C27-N29
2	B	101	A1BE1	C7-C37-C38-O39
2	A	101	A1BE1	C25-C2-C26-C27
2	A	101	A1BE1	C2-C26-C27-O28
2	A	101	A1BE1	C03-C02-N03-C05
2	B	101	A1BE1	C03-C02-N03-C05
4	A	103	TRS	C2-C-C1-O1
4	A	103	TRS	C2-C-C3-O3
4	B	103	TRS	C2-C-C1-O1
4	B	103	TRS	C1-C-C3-O3
2	A	101	A1BE1	C18-C60-C61-O62
2	A	101	A1BE1	C17-C18-C60-C61
2	A	101	A1BE1	C19-C18-C60-C61
4	A	103	TRS	C3-C-C1-O1
4	A	103	TRS	N-C-C3-O3
2	A	101	A1BE1	C1-C2-C26-C27
2	B	101	A1BE1	C7-C37-C38-N40
4	B	103	TRS	C3-C-C1-O1
4	B	103	TRS	C3-C-C2-O2
2	A	101	A1BE1	C3-C2-C26-C27

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Mol	Chain	Res	Type	Atoms
2	B	101	A1BE1	C19-C18-C60-C61

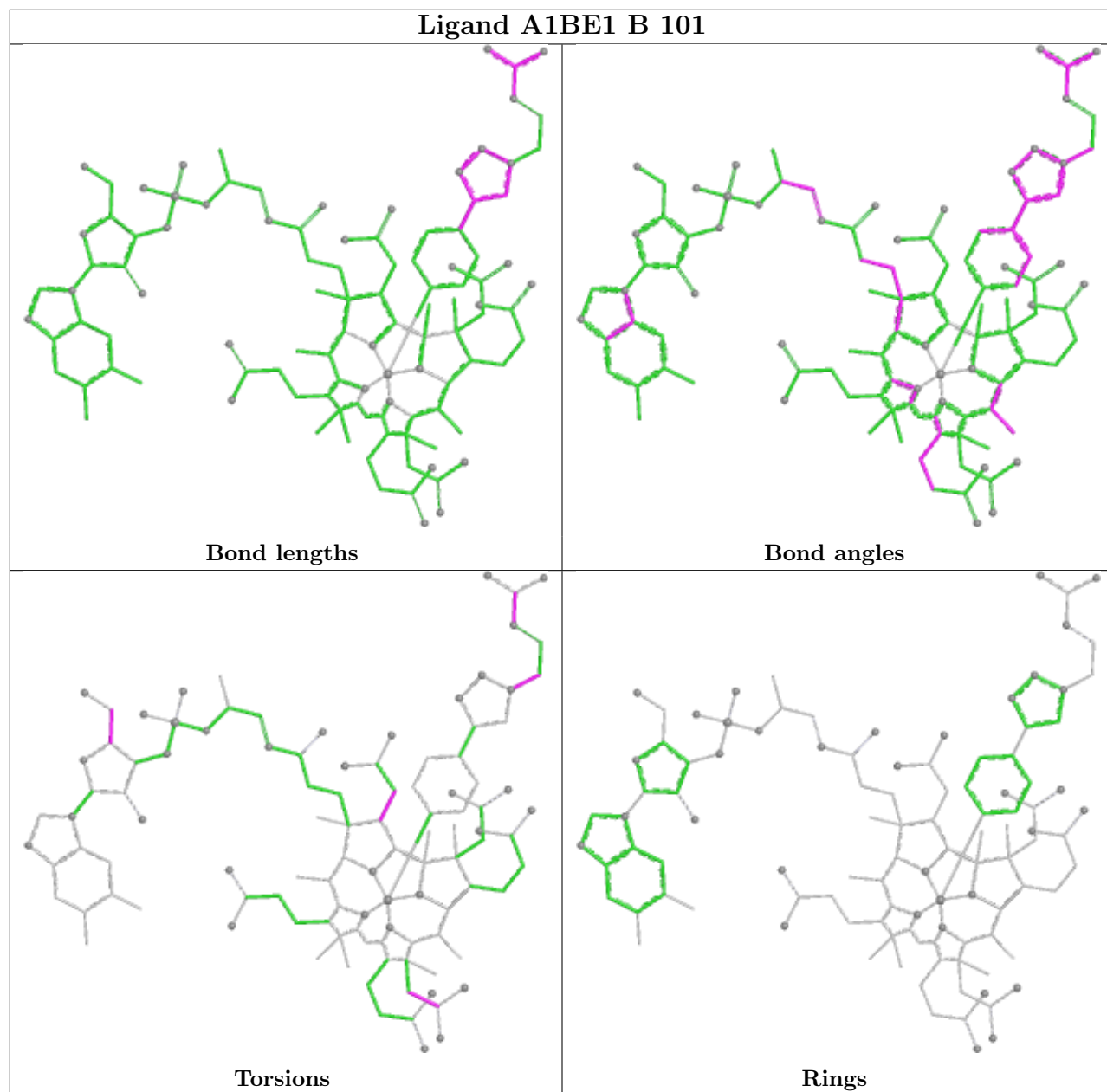
There are no ring outliers.

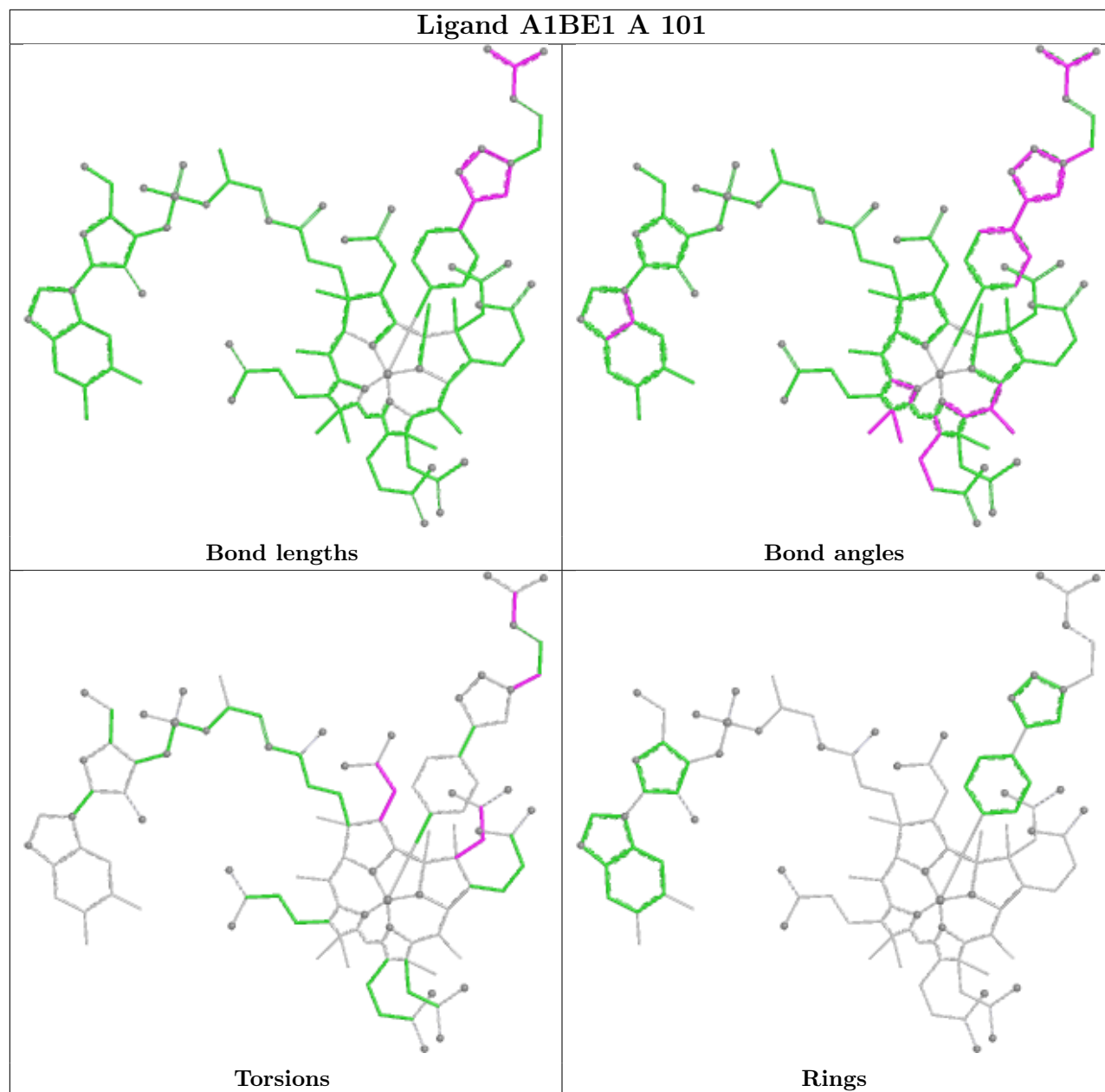
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	102	N3D	1	0
2	B	101	A1BE1	8	0
2	A	101	A1BE1	6	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 A1BE1 B 101





## 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%)	-0.36	1 (1%) 75 73	25, 32, 46, 64	0
1	B	75/76 (98%)	-0.05	1 (1%) 75 73	31, 40, 50, 79	0
All	All	150/152 (98%)	-0.20	2 (1%) 75 73	25, 35, 49, 79	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	C	2.6
1	B	18	A	2.4

### 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	0.41	0.27	88,88,88,88	0
5	MG	B	104	1/1	0.64	0.25	73,73,73,73	0
4	TRS	B	103	8/8	0.70	0.22	44,48,52,52	0

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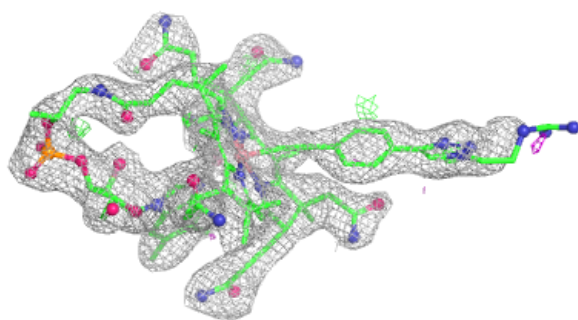
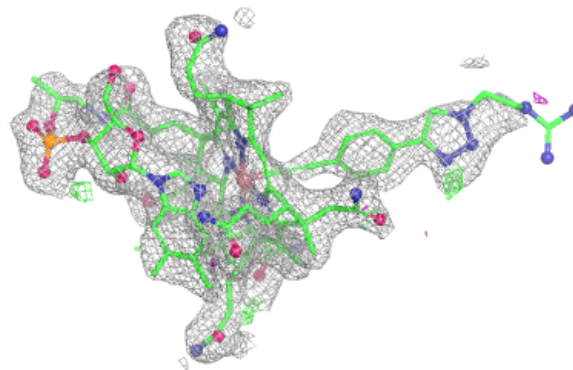
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	N3D	B	102	6/6	0.76	0.16	28,34,34,35	0
4	TRS	A	103	8/8	0.78	0.19	37,43,45,53	0
5	MG	B	106	1/1	0.85	0.09	37,37,37,37	0
6	K	B	114	1/1	0.85	0.16	51,51,51,51	0
5	MG	B	105	1/1	0.87	0.07	54,54,54,54	0
5	MG	B	113	1/1	0.89	0.07	33,33,33,33	0
5	MG	B	110	1/1	0.90	0.07	40,40,40,40	0
5	MG	B	107	1/1	0.90	0.10	42,42,42,42	0
5	MG	B	109	1/1	0.90	0.08	41,41,41,41	0
2	A1BE1	B	101	110/110	0.91	0.12	27,37,50,80	0
3	N3D	A	102	6/6	0.91	0.10	20,24,26,30	0
2	A1BE1	A	101	110/110	0.92	0.10	21,29,40,69	0
5	MG	A	112	1/1	0.92	0.06	24,24,24,24	0
5	MG	A	110	1/1	0.93	0.04	28,28,28,28	0
5	MG	A	108	1/1	0.93	0.11	32,32,32,32	0
5	MG	A	111	1/1	0.94	0.06	31,31,31,31	0
5	MG	B	111	1/1	0.94	0.05	39,39,39,39	0
5	MG	B	108	1/1	0.95	0.07	35,35,35,35	0
6	K	A	113	1/1	0.95	0.06	35,35,35,35	0
5	MG	A	109	1/1	0.95	0.08	30,30,30,30	0
5	MG	A	105	1/1	0.96	0.05	23,23,23,23	0
5	MG	A	106	1/1	0.96	0.05	27,27,27,27	0
5	MG	B	112	1/1	0.97	0.06	34,34,34,34	0
5	MG	A	107	1/1	0.98	0.08	29,29,29,29	0

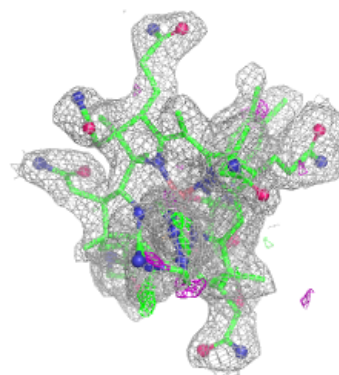
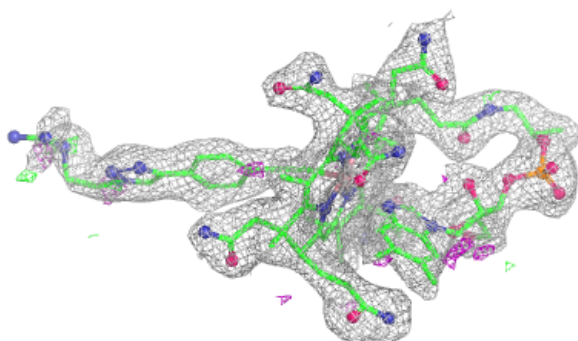
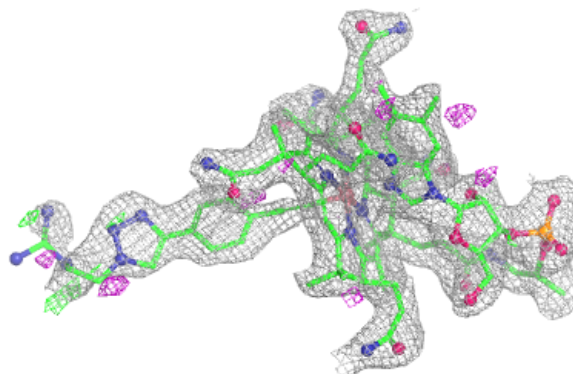
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1BE1 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 A1BE1 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.