



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:13 AM UTC

PDB ID : 9EWA / pdb\_00009ewa  
Title : The sTeLIC pentameric Ligand-Gated Ion Channel (wild-type) in complex with 4-Bromophenethylamine  
Authors : Fourati, Z.; Delarue, M.  
Deposited on : 2024-04-03  
Resolution : 3.01 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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)  
Xtrriage (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

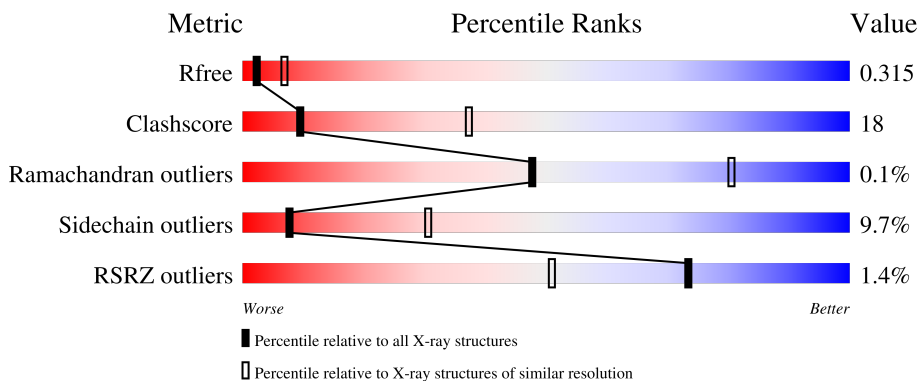
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	AAA	320	
1	BBB	320	
1	CCC	320	
1	DDD	320	
1	EEE	320	

## 2 Entry composition [i](#)

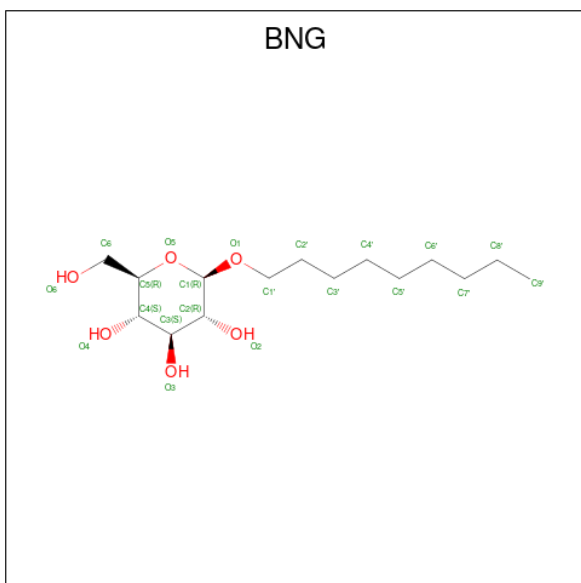
There are 4 unique types of molecules in this entry. The entry contains 13062 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	310	Total 2574	C 1696	N 424	O 449	S 5	0	1	0
1	BBB	310	Total 2566	C 1690	N 423	O 448	S 5	0	0	0
1	CCC	310	Total 2566	C 1690	N 423	O 448	S 5	0	0	0
1	DDD	310	Total 2566	C 1690	N 423	O 448	S 5	0	0	0
1	EEE	312	Total 2576	C 1696	N 425	O 450	S 5	0	0	0

- Molecule 2 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C<sub>15</sub>H<sub>30</sub>O<sub>6</sub>).



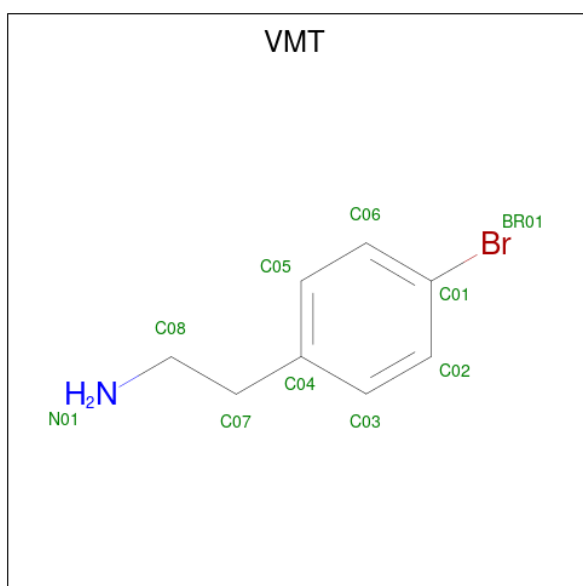
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	AAA	1	Total 21	C 15	O 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	BBB	1	Total	C	O	0	0
			21	15	6		
2	BBB	1	Total	C	O	0	0
			21	15	6		
2	DDD	1	Total	C	O	0	0
			21	15	6		
2	DDD	1	Total	C	O	0	0
			21	15	6		

- Molecule 3 is 2-(4-bromophenyl)ethanamine (CCD ID: VMT) (formula: C<sub>8</sub>H<sub>10</sub>BrN) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	Br	C	N	0	0
			10	1	8	1		
3	BBB	1	Total	Br	C	N	0	0
			10	1	8	1		
3	CCC	1	Total	Br	C	N	0	0
			10	1	8	1		
3	DDD	1	Total	Br	C	N	0	0
			10	1	8	1		
3	EEE	1	Total	Br	C	N	0	0
			10	1	8	1		

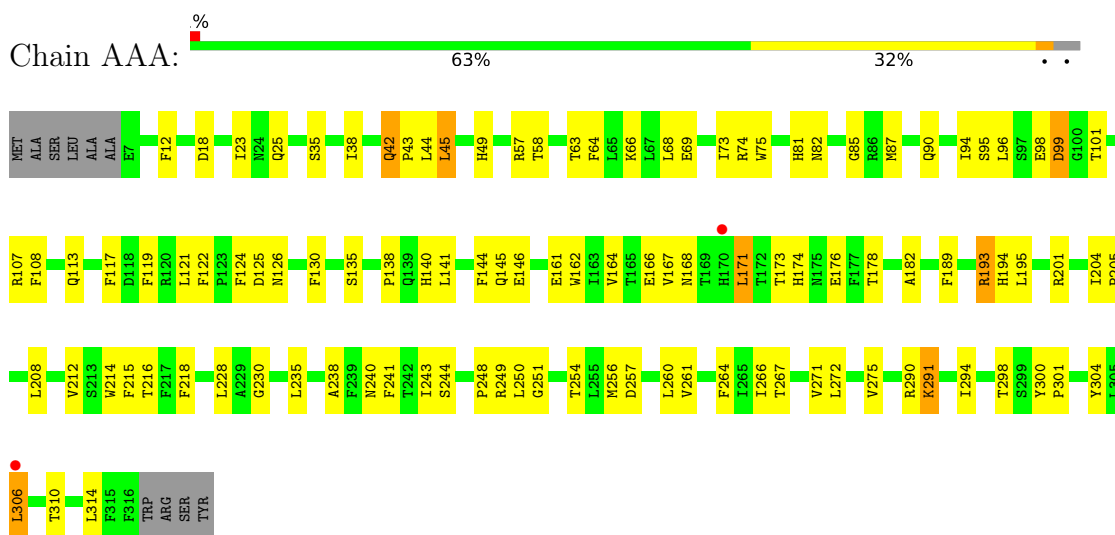
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	AAA	13	Total 13	O 13	0	0
4	BBB	12	Total 12	O 12	0	0
4	CCC	12	Total 12	O 12	0	0
4	DDD	18	Total 18	O 18	0	0
4	EEE	4	Total 4	O 4	0	0

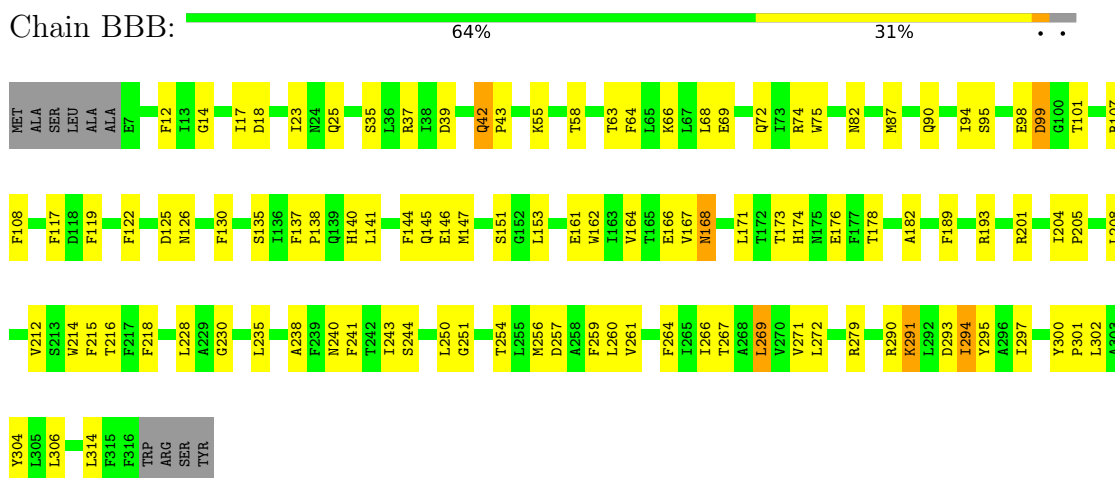
### 3 Residue-property plots

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: Cys-loop ligand-gated ion channel

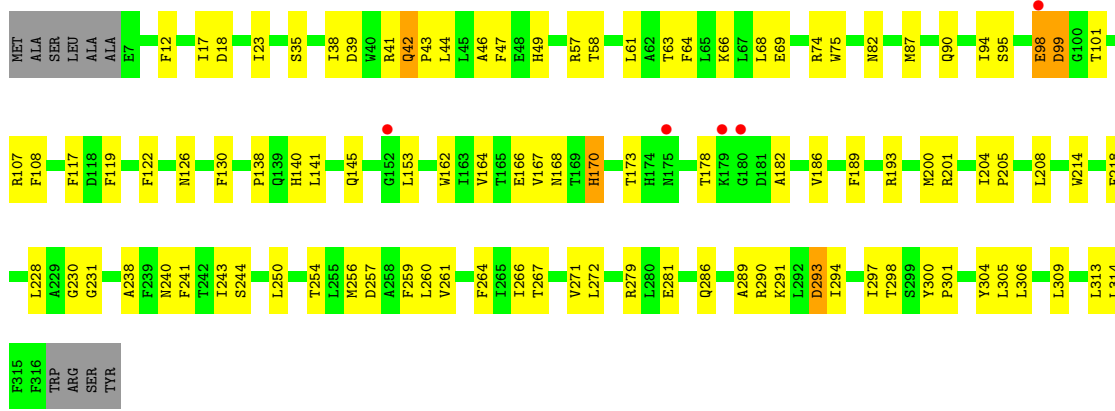


- Molecule 1: Cys-loop ligand-gated ion channel

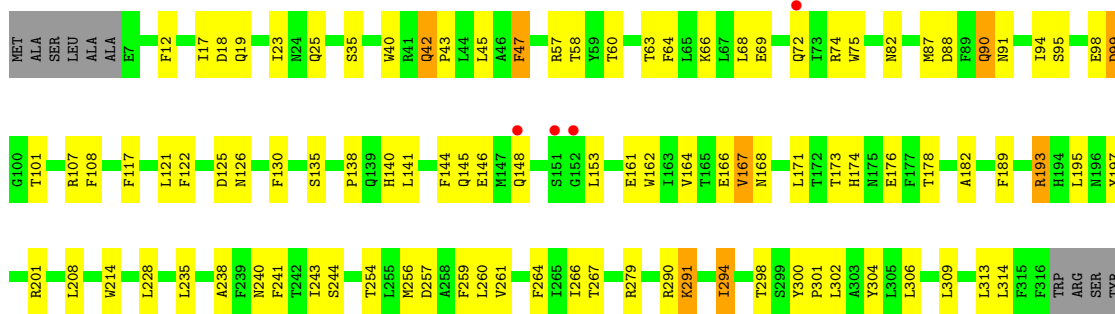
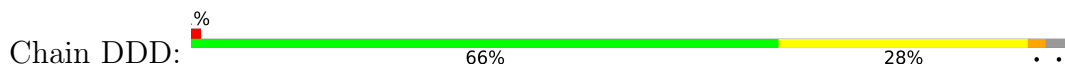


- Molecule 1: Cys-loop ligand-gated ion channel

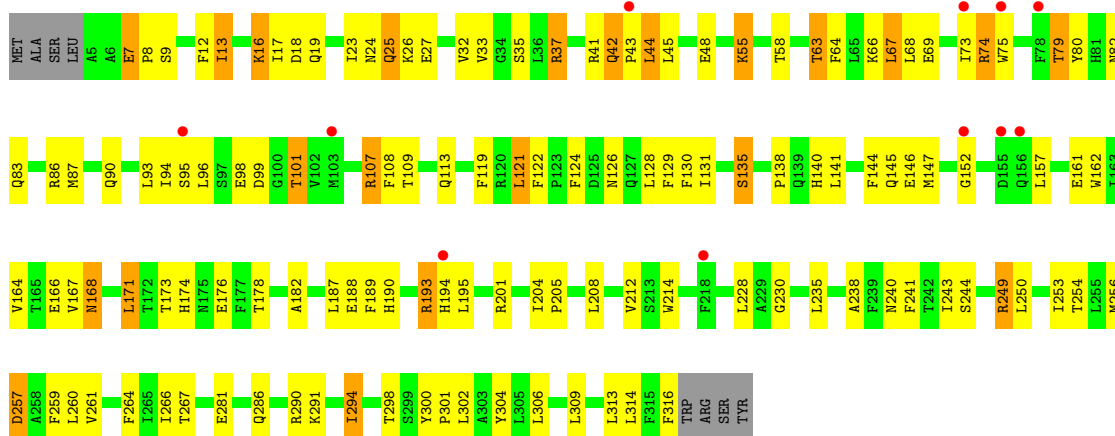




• Molecule 1: Cys-loop ligand-gated ion channel



• Molecule 1: Cys-loop ligand-gated ion channel



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.21Å 112.34Å 210.80Å 90.00° 106.18° 90.00°	Depositor
Resolution (Å)	25.00 – 3.01 25.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.00-3.01) 98.9 (25.00-3.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.99Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.241 , 0.281 0.275 , 0.315	Depositor DCC
$R_{free}$ test set	3175 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.4	Xtrriage
Anisotropy	0.385	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 70.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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: VMT, BNG

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	AAA	0.94	0/2647	1.37	0/3594
1	BBB	0.92	0/2639	1.36	0/3583
1	CCC	0.94	0/2639	1.38	3/3583 (0.1%)
1	DDD	0.94	0/2639	1.36	0/3583
1	EEE	0.98	0/2649	1.38	0/3597
All	All	0.94	0/13213	1.37	3/17940 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	CCC	293	ASP	CA-CB-CG	6.00	118.60	112.60
1	CCC	98	GLU	CA-C-N	5.78	128.60	120.28
1	CCC	98	GLU	C-N-CA	5.78	128.60	120.28

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	AAA	2574	0	2549	119	2
1	BBB	2566	0	2539	88	0
1	CCC	2566	0	2539	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DDD	2566	0	2539	103	0
1	EEE	2576	0	2549	137	0
2	AAA	21	0	30	2	0
2	BBB	42	0	60	11	0
2	DDD	42	0	60	8	0
3	AAA	10	0	0	0	0
3	BBB	10	0	0	0	0
3	CCC	10	0	0	1	0
3	DDD	10	0	0	2	0
3	EEE	10	0	0	0	0
4	AAA	13	0	0	2	0
4	BBB	12	0	0	2	0
4	CCC	12	0	0	2	2
4	DDD	18	0	0	1	0
4	EEE	4	0	0	1	0
All	All	13062	0	12865	462	2

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 18.

The worst 5 of 462 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:AAA:310:THR:O	1:AAA:314:LEU:CD1	1.79	1.30
1:AAA:45:LEU:CD2	1:AAA:73:ILE:HD13	1.75	1.16
1:AAA:310:THR:O	1:AAA:314:LEU:HD12	1.52	1.09
1:BBB:146:GLU:HG3	1:BBB:171:LEU:HD11	1.27	1.08
1:EEE:254:THR:O	1:EEE:257:ASP:OD2	1.68	1.07

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:49:HIS:NE2	4:CCC:501:HOH:O[4_455]	1.78	0.42
1:AAA:98:GLU:OE1	4:CCC:501:HOH:O[4_455]	2.04	0.16

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	309/320 (97%)	295 (96%)	14 (4%)	0	100	100
1	BBB	308/320 (96%)	294 (96%)	14 (4%)	0	100	100
1	CCC	308/320 (96%)	293 (95%)	15 (5%)	0	100	100
1	DDD	308/320 (96%)	291 (94%)	17 (6%)	0	100	100
1	EEE	310/320 (97%)	295 (95%)	14 (4%)	1 (0%)	36	70
All	All	1543/1600 (96%)	1468 (95%)	74 (5%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	EEE	7	GLU

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	276/282 (98%)	253 (92%)	23 (8%)	10	37
1	BBB	275/282 (98%)	252 (92%)	23 (8%)	10	37
1	CCC	275/282 (98%)	254 (92%)	21 (8%)	12	41
1	DDD	275/282 (98%)	250 (91%)	25 (9%)	9	33
1	EEE	275/282 (98%)	232 (84%)	43 (16%)	2	13
All	All	1376/1410 (98%)	1241 (90%)	135 (10%)	8	30

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EEE	107	ARG
1	EEE	141	LEU
1	EEE	290	ARG
1	CCC	66	LYS
1	CCC	42	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

10 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$
3	VMT	DDD	403	-	10,10,10	0.62	0	12,12,12	0.81	0
2	BNG	DDD	401	-	21,21,21	0.71	1 (4%)	26,26,26	0.89	1 (3%)
2	BNG	BBB	402	-	21,21,21	1.01	1 (4%)	26,26,26	1.30	3 (11%)
3	VMT	BBB	403	-	10,10,10	0.33	0	12,12,12	1.07	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	VMT	CCC	401	-	10,10,10	0.73	0	12,12,12	1.40	2 (16%)
2	BNG	BBB	401	-	21,21,21	0.66	0	26,26,26	1.53	5 (19%)
3	VMT	EEE	401	-	10,10,10	0.45	0	12,12,12	1.08	0
3	VMT	AAA	402	-	10,10,10	0.55	0	12,12,12	1.07	1 (8%)
2	BNG	DDD	402	-	21,21,21	0.90	1 (4%)	26,26,26	1.11	3 (11%)
2	BNG	AAA	401	-	21,21,21	0.77	1 (4%)	26,26,26	1.10	2 (7%)

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	VMT	DDD	403	-	-	0/3/3/3	0/1/1/1
2	BNG	DDD	401	-	-	6/12/32/32	0/1/1/1
2	BNG	BBB	402	-	-	10/12/32/32	0/1/1/1
3	VMT	BBB	403	-	-	0/3/3/3	0/1/1/1
3	VMT	CCC	401	-	-	3/3/3/3	0/1/1/1
2	BNG	BBB	401	-	-	8/12/32/32	0/1/1/1
3	VMT	EEE	401	-	-	2/3/3/3	0/1/1/1
3	VMT	AAA	402	-	-	0/3/3/3	0/1/1/1
2	BNG	DDD	402	-	-	10/12/32/32	0/1/1/1
2	BNG	AAA	401	-	-	11/12/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	402	BNG	O1-C1	3.21	1.45	1.40
2	DDD	402	BNG	O1-C1	2.91	1.45	1.40
2	AAA	401	BNG	O1-C1	2.55	1.44	1.40
2	DDD	401	BNG	O1-C1	2.34	1.44	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	401	BNG	C1-C2-C3	-3.28	103.12	110.01
2	BBB	402	BNG	C1-O5-C5	2.97	119.51	113.72
2	BBB	401	BNG	O1-C1'-C2'	2.82	118.94	109.37
3	AAA	402	VMT	C08-C07-C04	-2.60	107.00	112.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	403	VMT	C07-C08-N01	-2.59	105.62	112.71

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

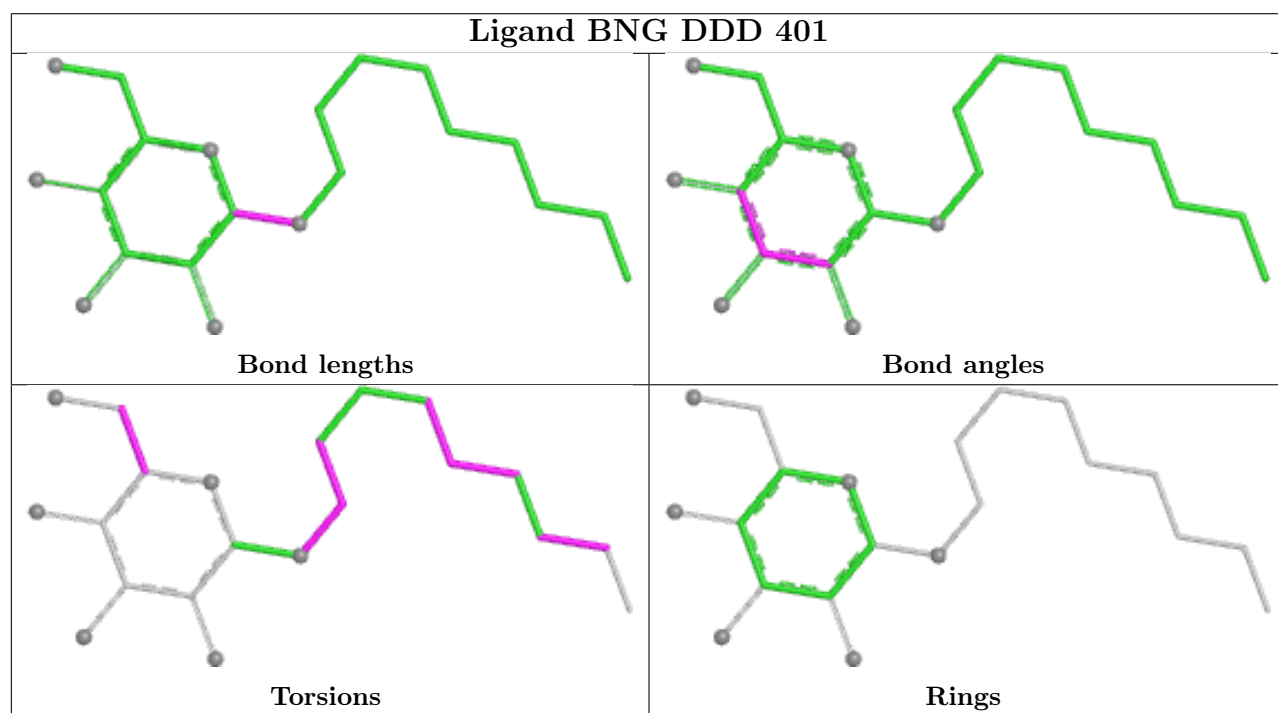
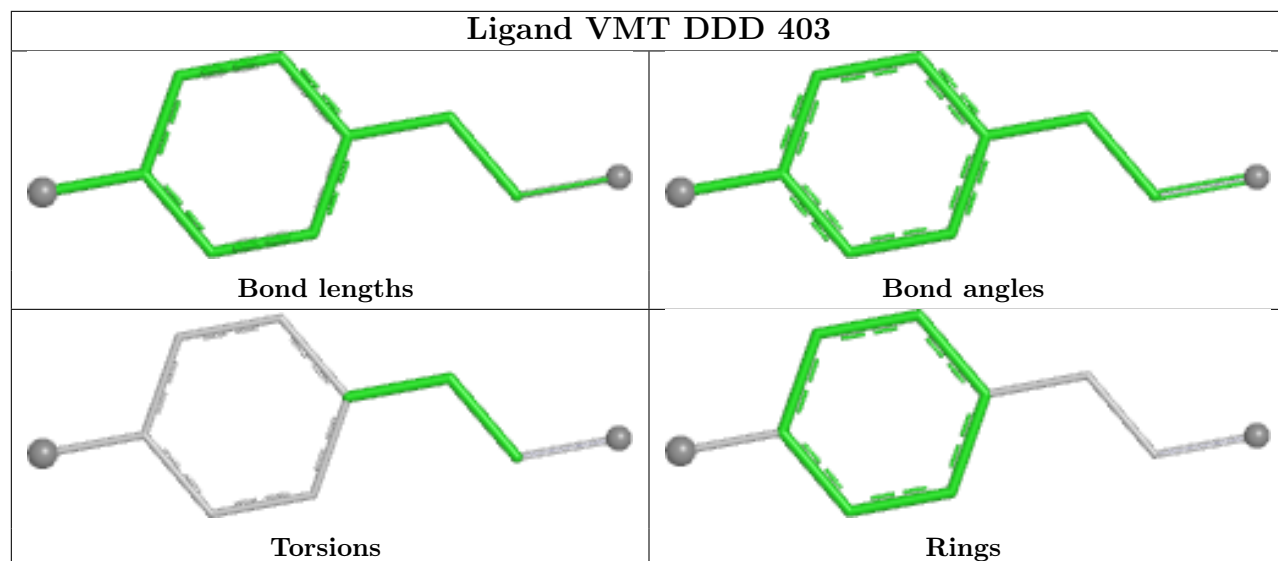
Mol	Chain	Res	Type	Atoms
2	BBB	401	BNG	C2'-C1'-O1-C1
2	DDD	401	BNG	C2'-C1'-O1-C1
2	DDD	402	BNG	C2-C1-O1-C1'
3	CCC	401	VMT	C04-C07-C08-N01
2	DDD	402	BNG	C4-C5-C6-O6

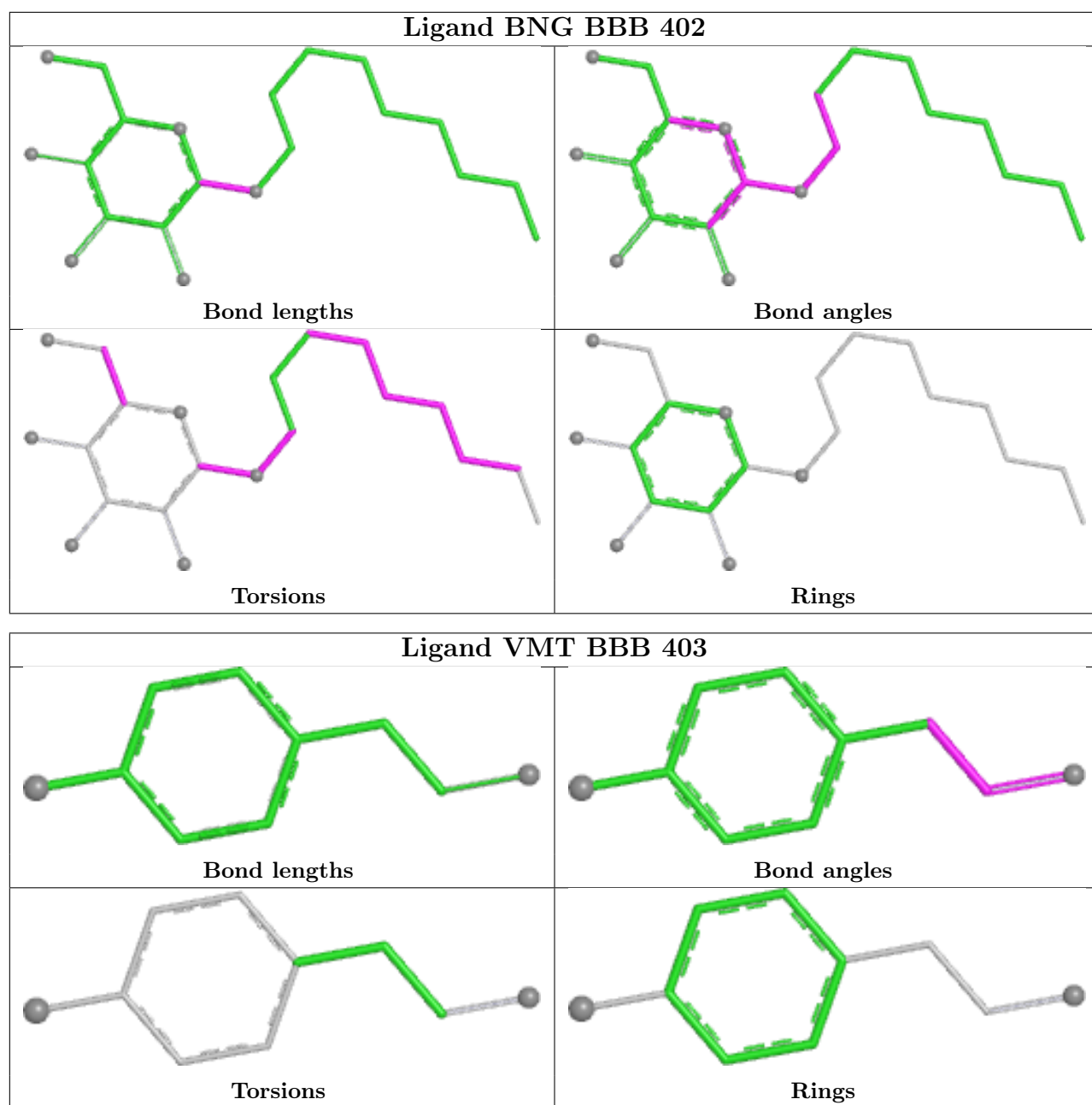
There are no ring outliers.

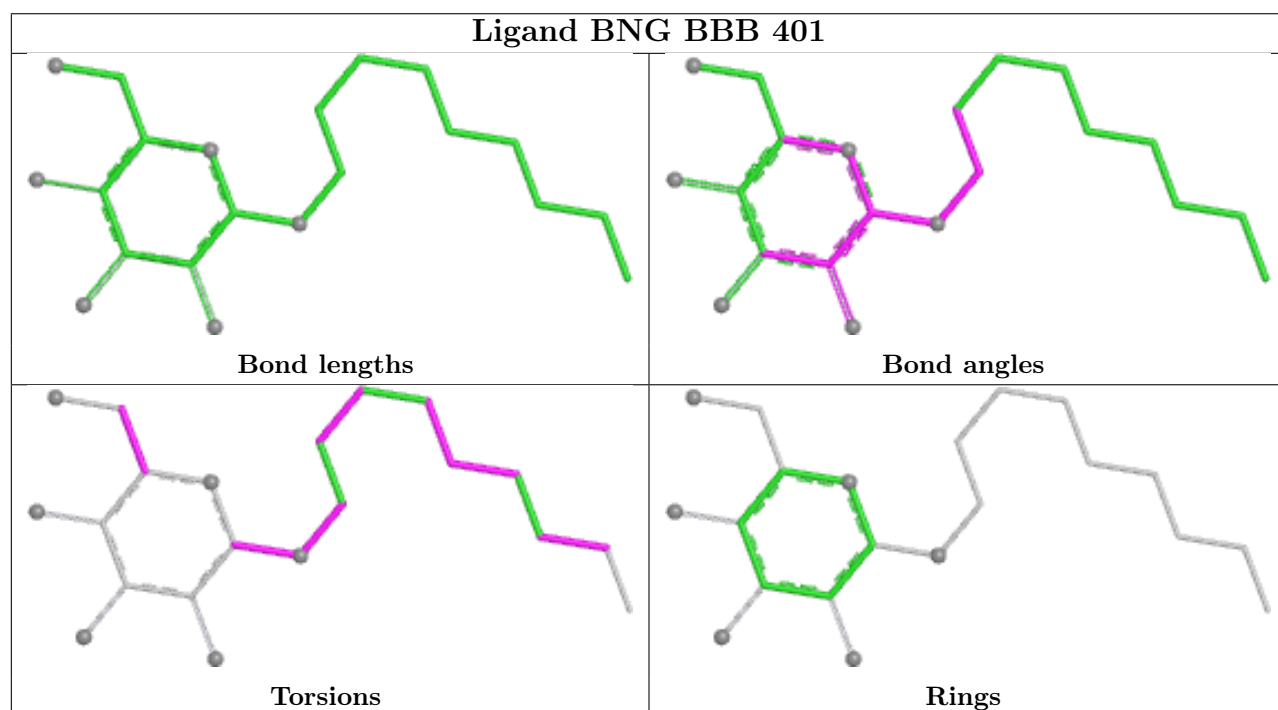
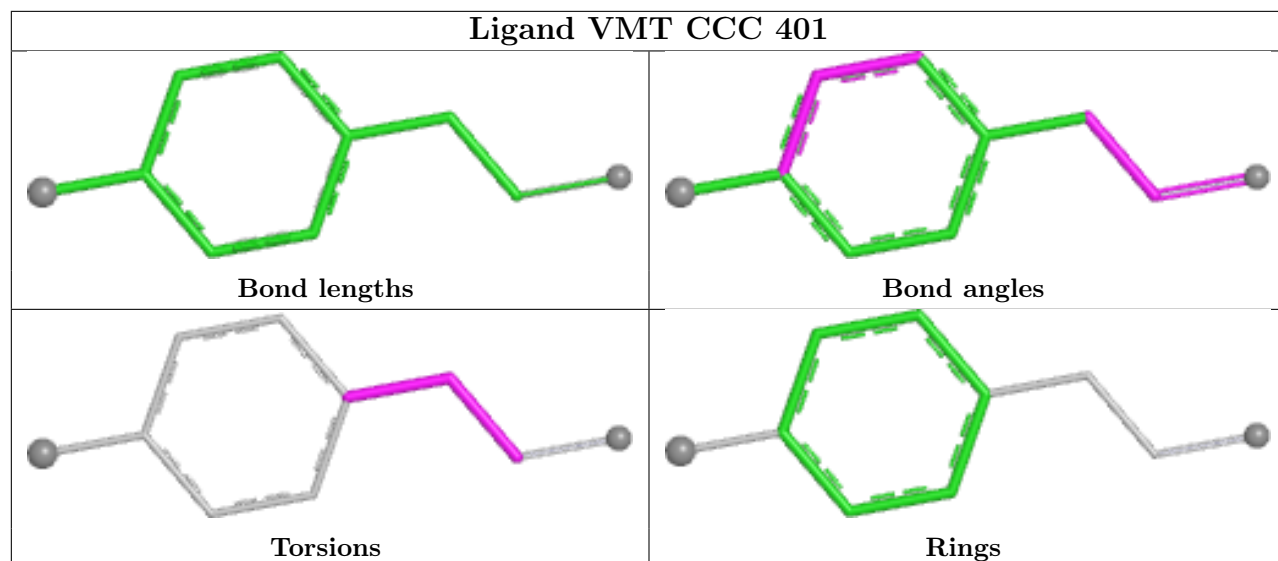
7 monomers are involved in 24 short contacts:

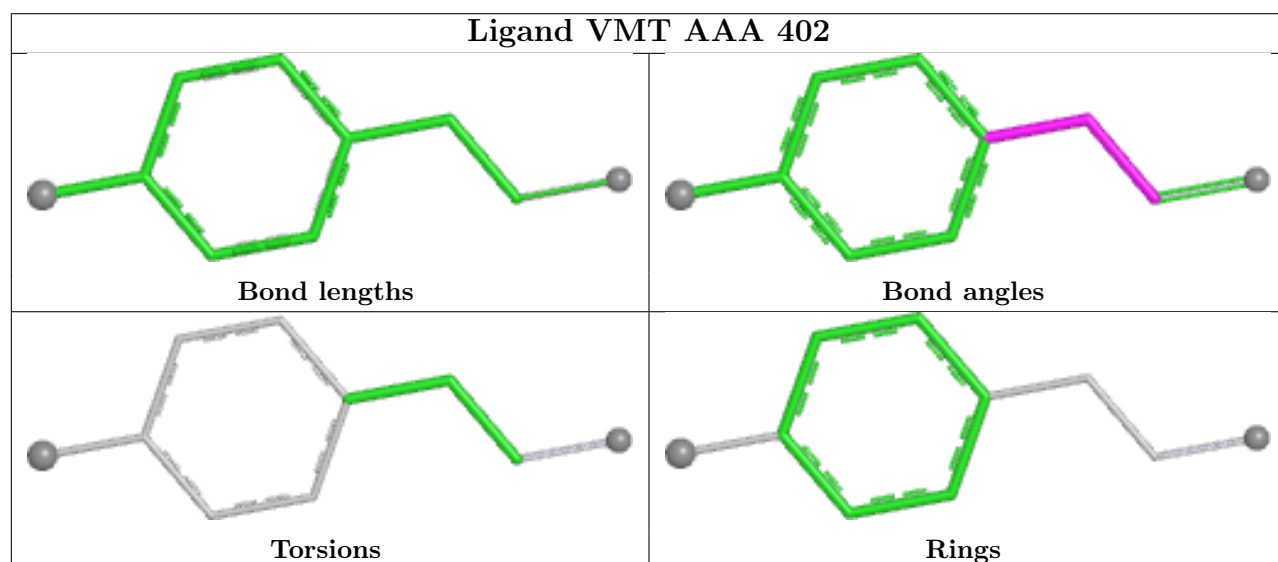
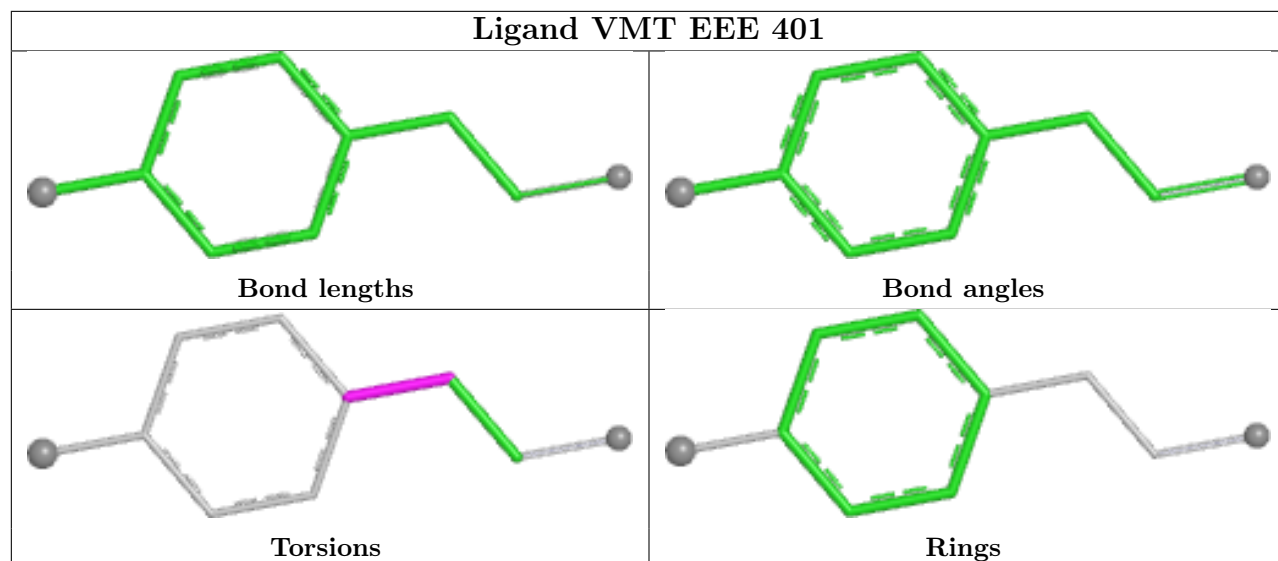
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DDD	403	VMT	2	0
2	DDD	401	BNG	5	0
2	BBB	402	BNG	5	0
3	CCC	401	VMT	1	0
2	BBB	401	BNG	6	0
2	DDD	402	BNG	3	0
2	AAA	401	BNG	2	0

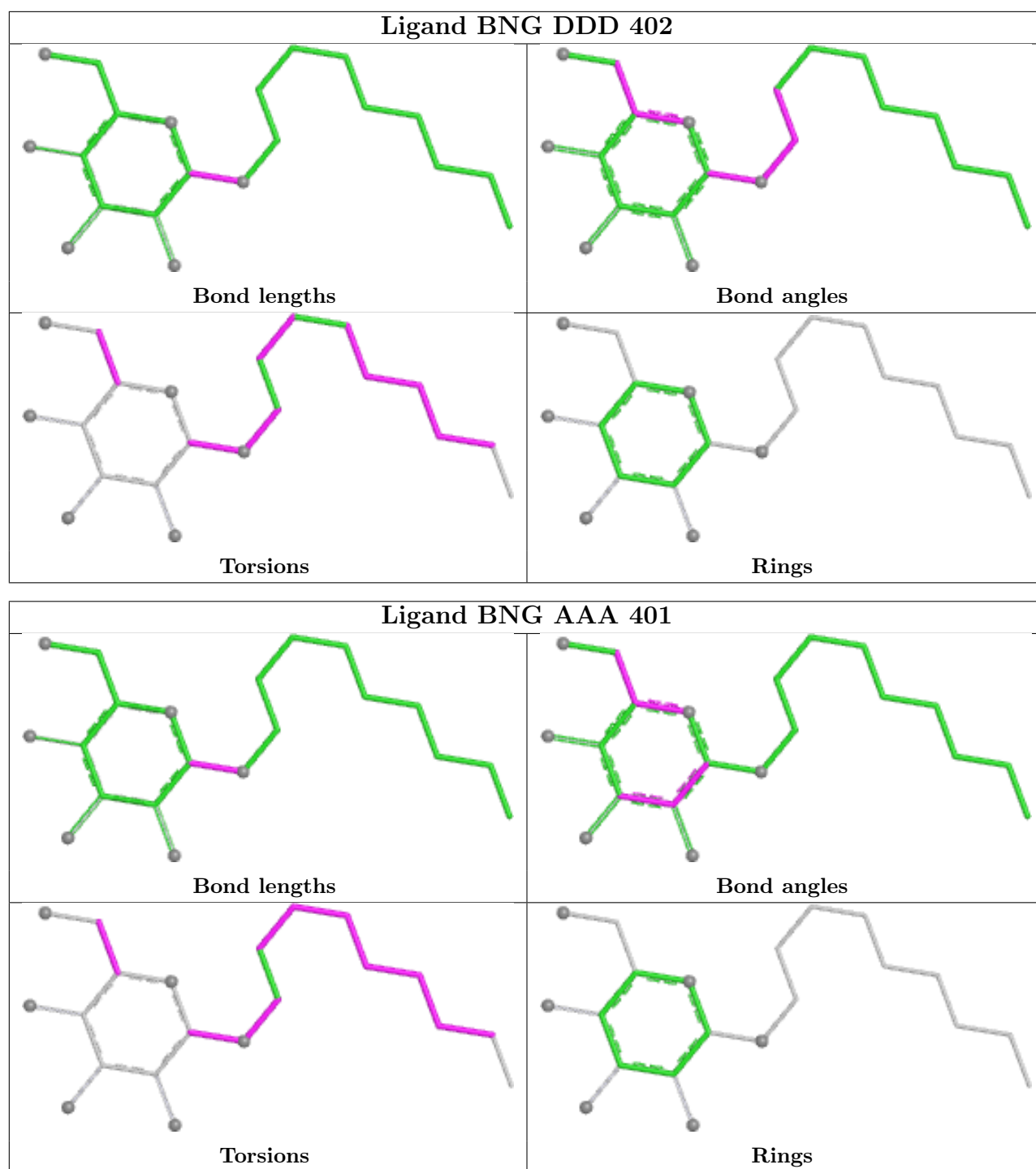
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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	AAA	310/320 (96%)	0.23	2 (0%) 85 69	54, 100, 133, 160	1 (0%)
1	BBB	310/320 (96%)	0.08	0 100 100	66, 98, 131, 214	0
1	CCC	310/320 (96%)	0.17	5 (1%) 70 47	63, 96, 128, 157	0
1	DDD	310/320 (96%)	0.25	4 (1%) 75 53	64, 102, 148, 212	0
1	EEE	312/320 (97%)	0.15	11 (3%) 47 27	74, 113, 156, 202	0
All	All	1552/1600 (97%)	0.18	22 (1%) 73 51	54, 101, 142, 214	1 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	152	GLY	6.6
1	AAA	306[A]	LEU	5.2
1	CCC	152	GLY	4.4
1	EEE	155	ASP	3.1
1	CCC	98	GLU	2.8

### 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.

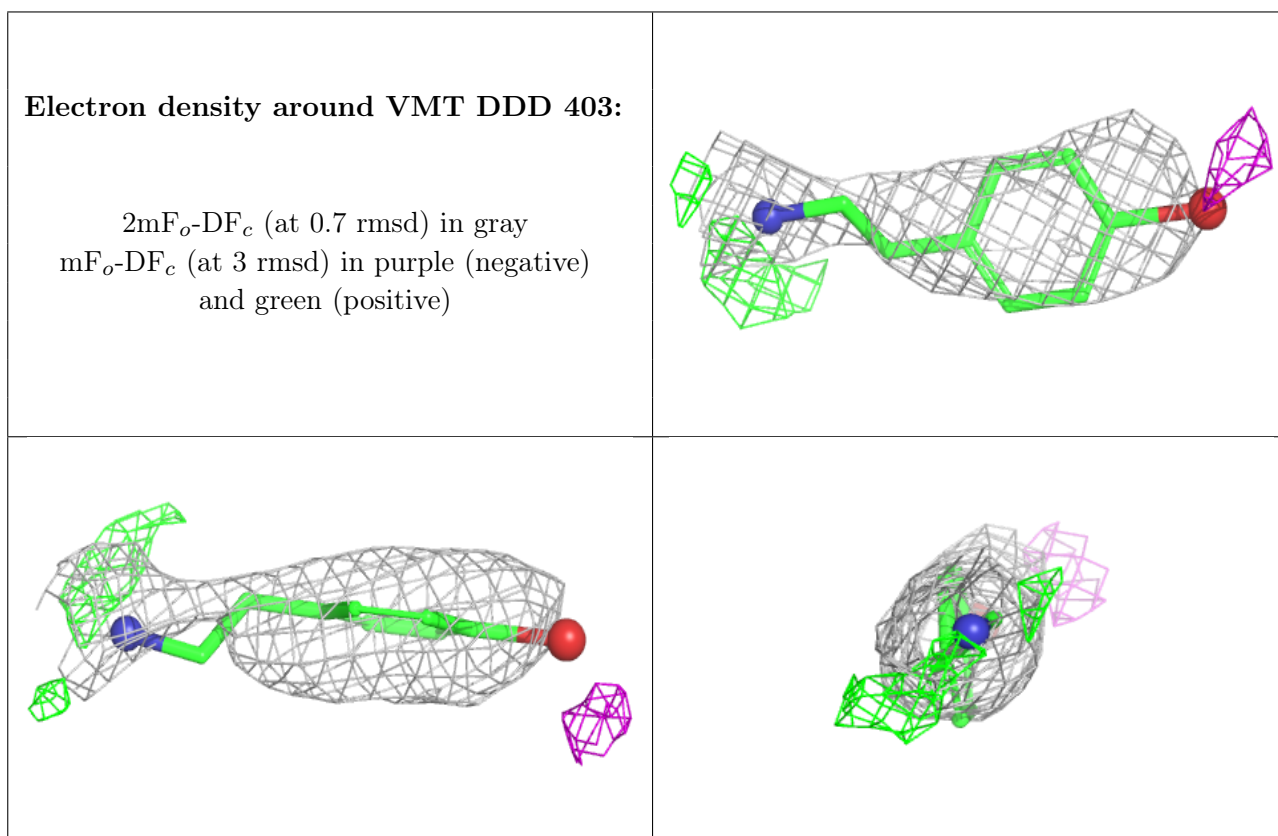
### 6.4 Ligands [i](#)

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.

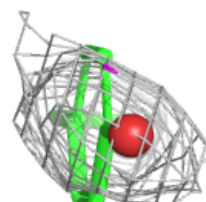
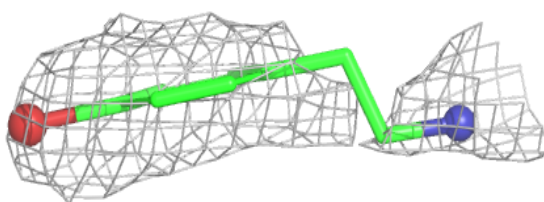
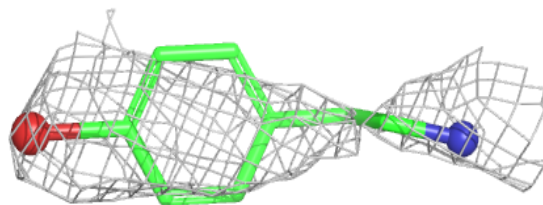
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	VMT	DDD	403	10/10	0.80	0.34	134,144,153,247	0
3	VMT	AAA	402	10/10	0.82	0.29	113,139,156,194	0
3	VMT	CCC	401	10/10	0.83	0.26	116,131,159,159	0
2	BNG	AAA	401	21/21	0.87	0.15	77,125,150,167	0
2	BNG	BBB	402	21/21	0.88	0.13	62,114,134,143	0
3	VMT	EEE	401	10/10	0.88	0.27	113,183,194,196	0
2	BNG	BBB	401	21/21	0.89	0.14	76,129,139,147	0
2	BNG	DDD	401	21/21	0.90	0.14	75,118,158,166	0
2	BNG	DDD	402	21/21	0.90	0.14	78,118,128,130	0
3	VMT	BBB	403	10/10	0.94	0.15	92,117,123,151	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.

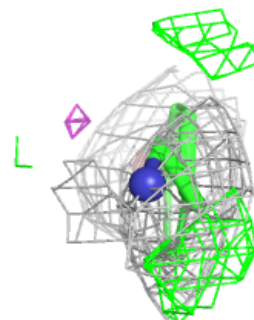
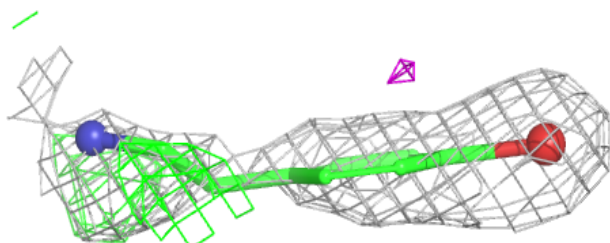
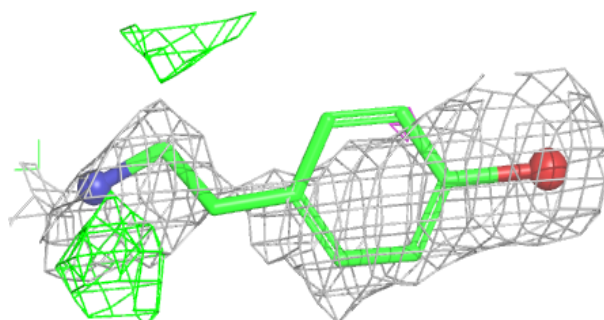


**Electron density around VMT AAA 402:**

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

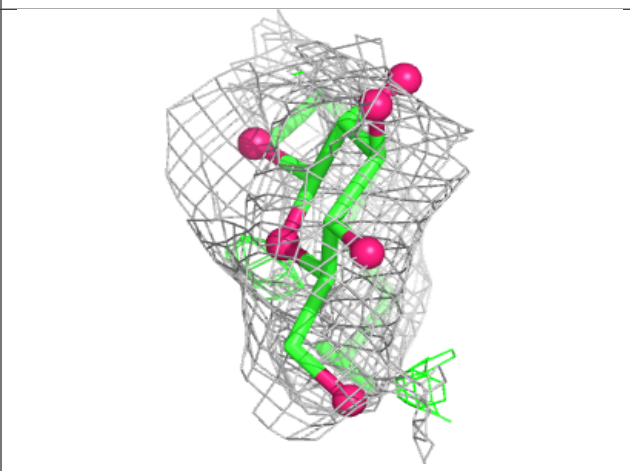
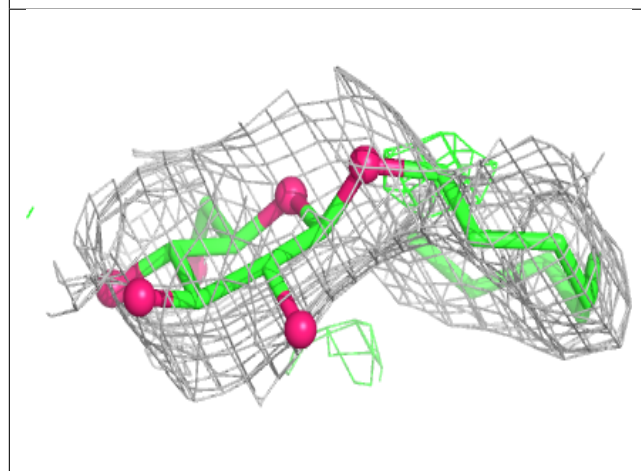
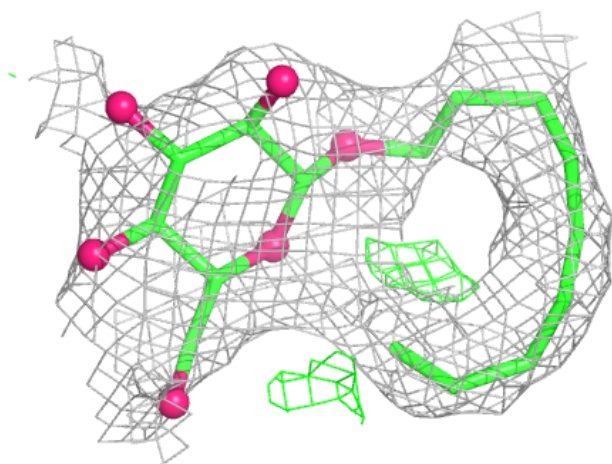
**Electron density around VMT CCC 401:**

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



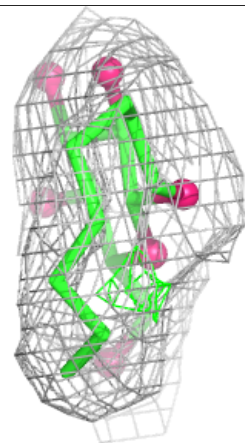
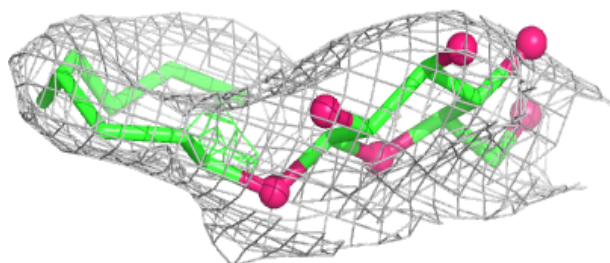
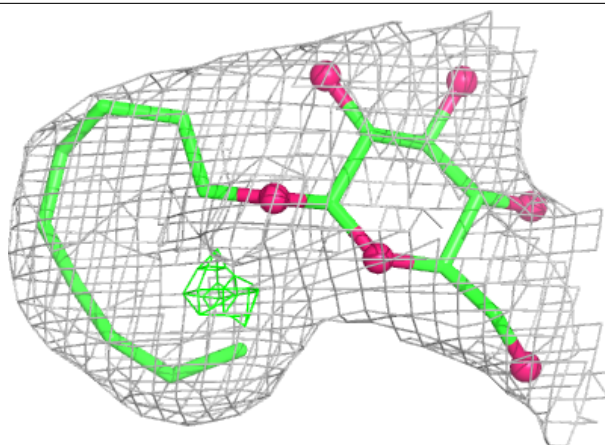
**Electron density around BNG AAA 401:**

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

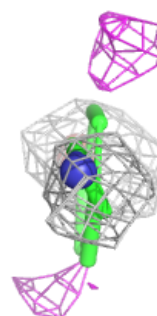
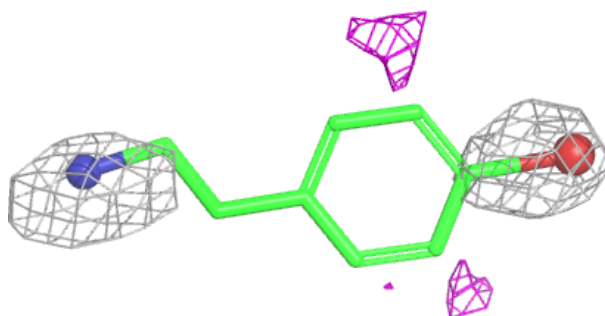


**Electron density around BNG BBB 402:**

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

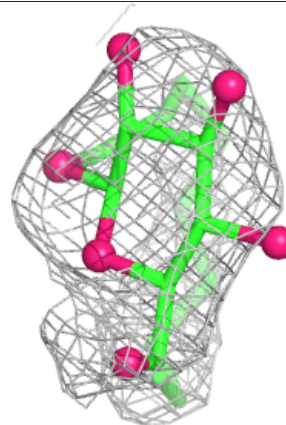
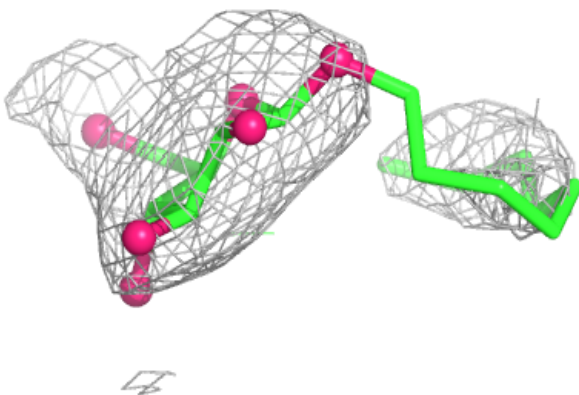
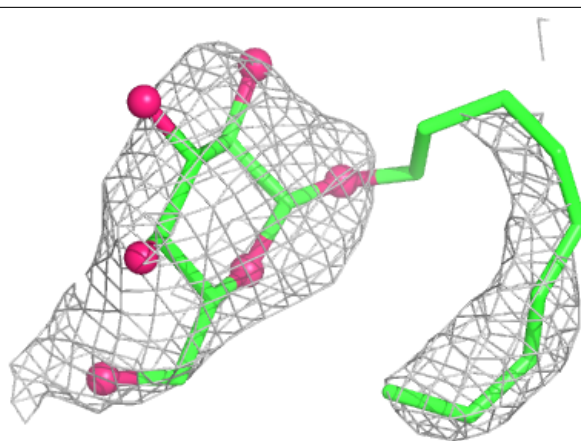
**Electron density around VMT EEE 401:**

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



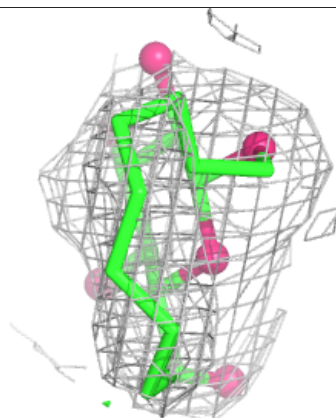
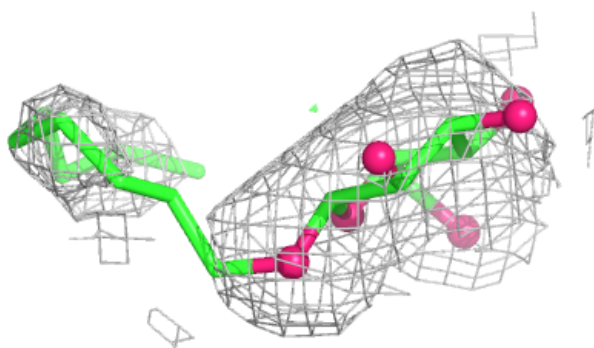
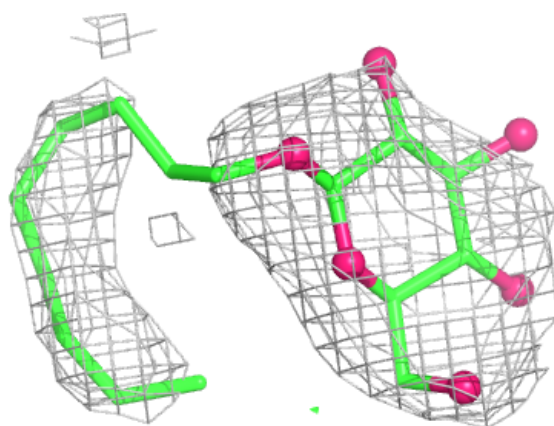
**Electron density around BNG BBB 401:**

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



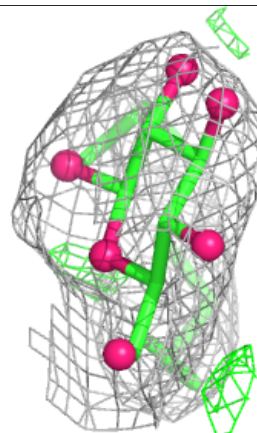
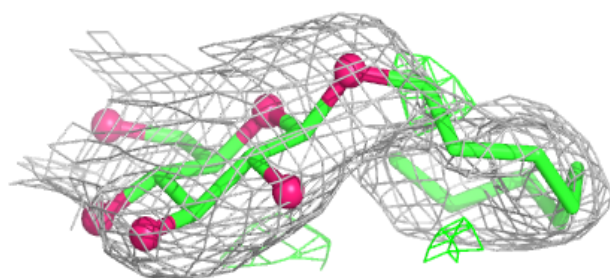
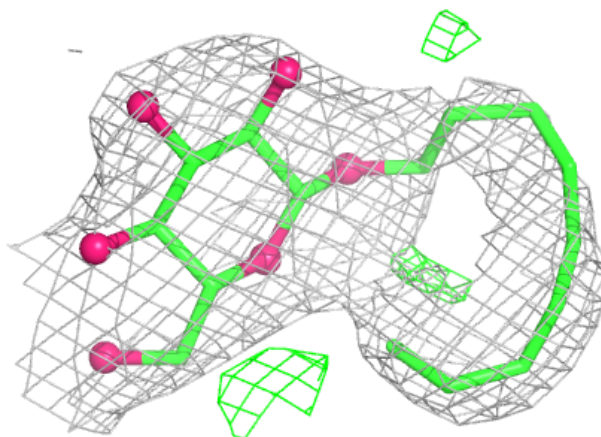
**Electron density around BNG DDD 401:**

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

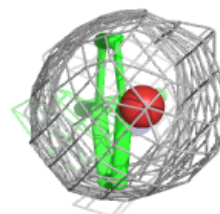
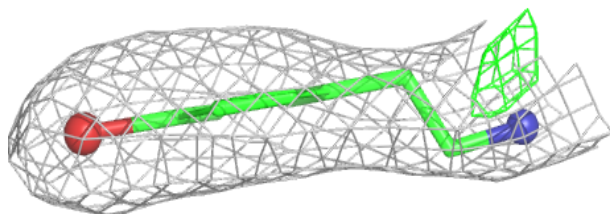
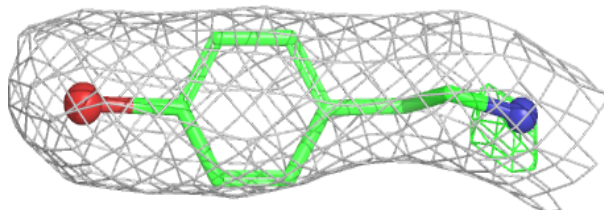


**Electron density around BNG DDD 402:**

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

**Electron density around VMT BBB 403:**

$2mF_o-DF_c$  (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.