



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2021 – 10:23 AM EDT

PDB ID : 6WL5
Title : Crystal structure of EcmrR C-terminal domain
Authors : Yang, Y.; Liu, C.; Liu, B.
Deposited on : 2020-04-18
Resolution : 1.40 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.18
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) : 2.18

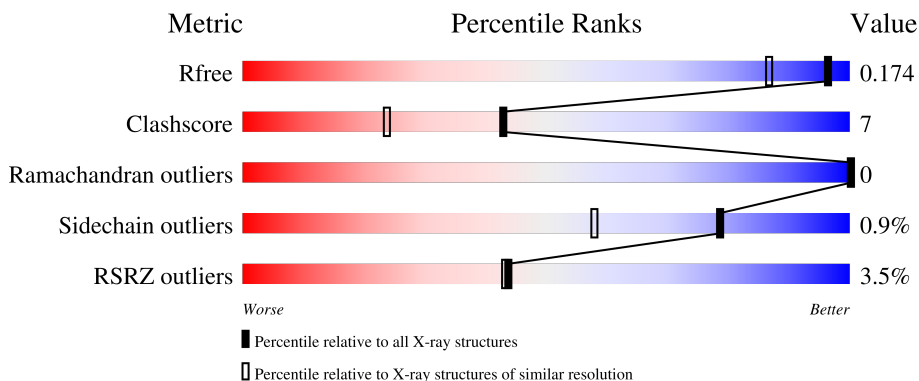
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 ≥ 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	159	<p>4% 91% 8%</p>
1	B	159	<p>3% 90% 9%</p>
1	C	159	<p>5% 86% 13%</p>
1	D	159	<p>2% 91% 8%</p>

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
3	GOL	C	306[A]	-	-	X	-
3	GOL	C	306[B]	-	-	X	-
3	GOL	D	304	-	X	-	-

2 Entry composition i

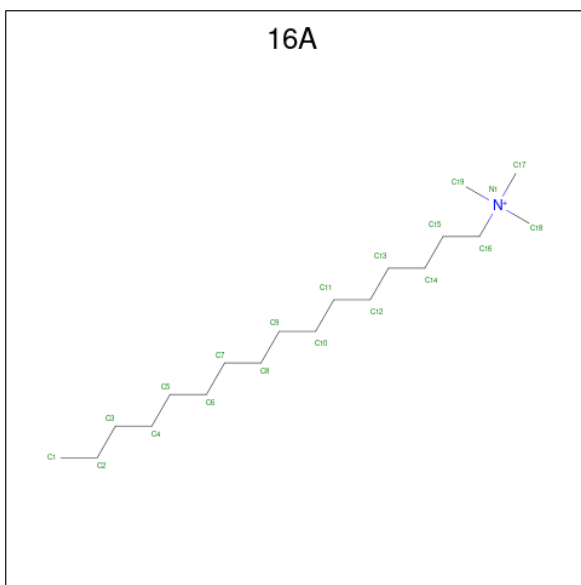
There are 6 unique types of molecules in this entry. The entry contains 12554 atoms, of which 5855 are hydrogens and 0 are deuteriums.

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 EcmrR transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	158	2684	877	1329	210	258	10	0	13	0
1	B	158	2684	877	1329	209	259	10	0	15	0
1	C	158	2761	899	1370	216	265	11	0	21	0
1	D	158	2716	884	1352	213	257	10	0	17	0

- Molecule 2 is CETYL-TRIMETHYL-AMMONIUM (three-letter code: 16A) (formula: $C_{19}H_{42}N$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
2	A	1	62	19	42	1	0	0
2	A	1	62	19	42	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H 34 11 23	0	0
2	B	1	Total C H N 62 19 42 1	0	0
2	B	1	Total C H N 62 19 42 1	0	0
2	C	1	Total C H N 61 19 41 1	0	0
2	C	1	Total C H N 62 19 42 1	0	0
2	C	1	Total C H 37 12 25	0	0
2	D	1	Total C H N 62 19 42 1	0	0
2	D	1	Total C H N 62 19 42 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0

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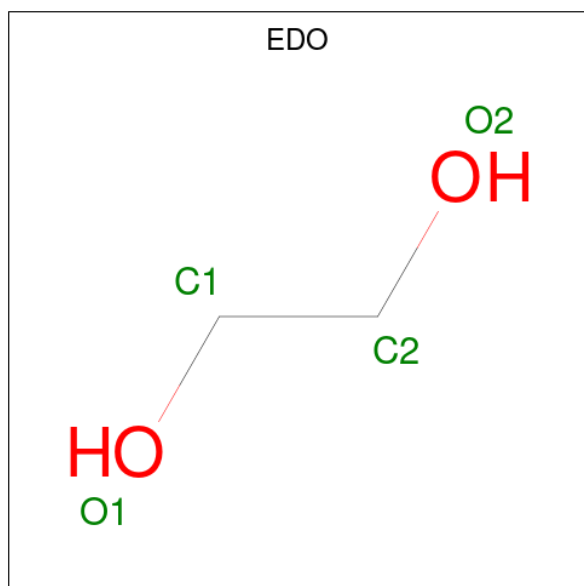
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C H O 13 3 7 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C O 12 6 6	0	1
3	D	1	Total C H O 14 3 8 3	0	0
3	D	1	Total C H O 13 3 7 3	0	0
3	D	1	Total C H O 14 3 8 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 10 2 6 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	213	Total	O	0	0
			213	213		
6	B	220	Total	O	0	0
			220	220		
6	C	260	Total	O	0	0
			260	260		
6	D	276	Total	O	0	0
			276	276		

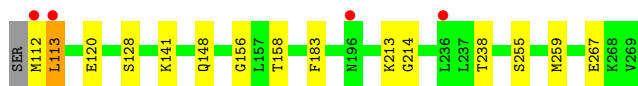
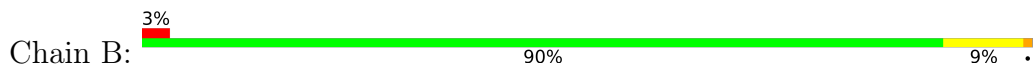
3 Residue-property plots [i](#)

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.

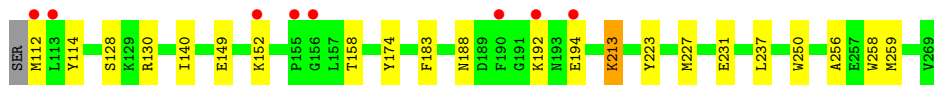
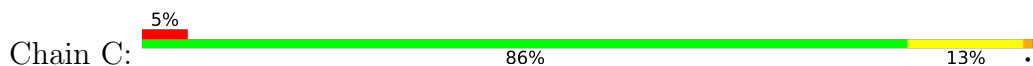
- Molecule 1: EcmrR transcriptional regulator



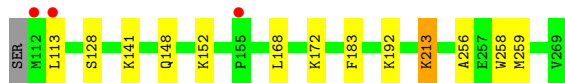
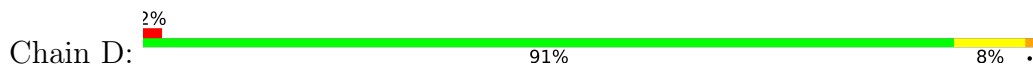
- Molecule 1: EcmrR transcriptional regulator



- Molecule 1: EcmrR transcriptional regulator



- Molecule 1: EcmrR transcriptional regulator



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.39Å 42.42Å 115.80Å 90.00° 117.27° 90.00°	Depositor
Resolution (Å)	102.93 – 1.40 102.93 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (102.93-1.40) 98.4 (102.93-1.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.40Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.142 , 0.173 0.144 , 0.174	Depositor DCC
R_{free} test set	8919 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12554	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5099e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, GOL, 16A, EDO

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	0.59	0/1429	0.72	0/1938
1	B	0.61	0/1455	0.77	0/1976
1	C	0.70	0/1513	0.80	0/2050
1	D	0.75	0/1469	0.83	0/1989
All	All	0.67	0/5866	0.78	0/7953

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	1355	1329	1273	9	0
1	B	1355	1329	1250	14	0
1	C	1391	1370	1274	27	0
1	D	1364	1352	1268	15	0
2	A	51	107	105	3	0
2	B	40	84	84	2	0
2	C	52	108	107	14	0
2	D	40	84	84	0	0
3	A	12	16	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	8	8	0	0
3	C	24	15	29	20	0
3	D	18	23	23	3	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	4	6	6	1	0
5	B	12	18	18	1	0
5	D	4	6	6	0	0
6	A	213	0	0	1	0
6	B	220	0	0	4	0
6	C	260	0	0	1	0
6	D	276	0	0	2	0
All	All	6699	5855	5551	79	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 7.

All (79) 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:C:301:16A:H21	3:C:306[B]:GOL:O3	1.69	0.91
1:D:152:LYS:HA	1:D:152:LYS:HE2	1.65	0.76
1:D:168:LEU:HD13	3:D:303:GOL:H2	1.67	0.76
1:C:213[A]:LYS:HE3	1:C:259[A]:MET:SD	2.30	0.71
1:B:213[A]:LYS:HE3	1:B:259[A]:MET:SD	2.31	0.70
1:C:213[A]:LYS:CE	1:C:259[A]:MET:SD	2.80	0.70
1:C:130:ARG:HH22	3:C:304:GOL:H11	1.59	0.67
1:A:149[B]:GLU:OE2	1:A:152:LYS:NZ	2.28	0.67
1:A:130:ARG:HH22	3:A:304:GOL:H11	1.61	0.65
1:A:213[A]:LYS:HG2	1:A:259[A]:MET:SD	2.37	0.65
1:D:213[A]:LYS:HE3	1:D:259[A]:MET:SD	2.37	0.65
1:C:112:MET:HB2	6:C:403:HOH:O	1.97	0.64
1:B:141:LYS:HZ2	2:C:303:16A:H52	1.66	0.61
2:C:302:16A:H102	2:C:303:16A:H11	1.83	0.61
2:C:302:16A:H172	2:C:303:16A:H41	1.83	0.60
1:C:112:MET:HG2	1:C:114:TYR:CZ	2.37	0.59
1:C:130:ARG:NH2	3:C:304:GOL:H11	2.18	0.59
1:B:213[A]:LYS:HG2	6:B:440:HOH:O	2.02	0.58
1:D:213[A]:LYS:CE	1:D:259[A]:MET:SD	2.93	0.57
2:C:301:16A:H71	3:C:306[A]:GOL:O3	2.04	0.57
2:C:301:16A:H51	3:C:306[A]:GOL:O3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213[A]:LYS:HD3	1:C:258:TRP:O	2.06	0.55
1:B:213[A]:LYS:CE	1:B:259[A]:MET:SD	2.95	0.55
1:C:237:LEU:HD22	3:C:306[B]:GOL:H31	1.88	0.54
1:C:227[B]:MET:HG2	3:C:306[B]:GOL:O2	2.09	0.52
1:B:156:GLY:O	1:B:158[B]:THR:HG23	2.10	0.52
1:C:237:LEU:HB2	3:C:306[B]:GOL:C3	2.40	0.51
1:C:237:LEU:HB2	3:C:306[B]:GOL:H32	1.93	0.51
2:C:301:16A:C6	3:C:306[A]:GOL:O3	2.59	0.51
1:C:174:TYR:CD1	3:C:306[A]:GOL:H2	2.46	0.50
2:C:301:16A:H21	3:C:306[B]:GOL:HO3	1.74	0.49
2:C:302:16A:H172	2:C:303:16A:C4	2.42	0.49
1:D:213[A]:LYS:HD2	1:D:256:ALA:O	2.11	0.49
1:B:113:LEU:HG	1:B:113:LEU:O	2.12	0.48
1:B:214:GLY:HA2	1:B:255:SER:O	2.14	0.48
1:A:172:LYS:HE3	6:A:491:HOH:O	2.14	0.47
1:C:213[A]:LYS:HD2	1:C:256:ALA:O	2.13	0.47
1:D:152:LYS:HE2	1:D:152:LYS:CA	2.41	0.47
1:C:112:MET:HG2	1:C:114:TYR:CE1	2.49	0.47
1:C:158[B]:THR:HG23	1:C:188:ASN:OD1	2.14	0.47
1:A:128:SER:HA	1:A:183:PHE:O	2.15	0.47
1:A:206:THR:HG21	5:A:307:EDO:H22	1.96	0.47
1:D:213[A]:LYS:HD3	1:D:258:TRP:O	2.14	0.46
1:C:130:ARG:HH22	3:C:304:GOL:C1	2.24	0.46
1:A:156:GLY:O	1:A:158[B]:THR:HG23	2.16	0.46
1:D:152:LYS:HA	1:D:152:LYS:CE	2.35	0.46
2:A:303:16A:H71	1:D:141:LYS:HD3	1.99	0.45
5:B:305:EDO:H22	6:B:506:HOH:O	2.16	0.45
1:B:128:SER:HA	1:B:183:PHE:O	2.17	0.45
1:C:227[A]:MET:HB2	3:C:306[A]:GOL:H32	1.99	0.45
1:B:238:THR:HG21	1:B:267[A]:GLU:HG2	1.99	0.45
1:B:259[A]:MET:HE1	6:B:609:HOH:O	2.16	0.45
1:C:237:LEU:CB	3:C:306[B]:GOL:C3	2.95	0.45
1:B:141:LYS:NZ	2:C:303:16A:H52	2.33	0.44
1:D:152:LYS:CA	1:D:152:LYS:CE	2.96	0.44
1:D:172:LYS:HE2	3:D:305:GOL:H2	2.00	0.44
1:C:128:SER:HA	1:C:183:PHE:O	2.18	0.43
1:C:223:TYR:HB3	3:C:306[A]:GOL:H11	2.00	0.43
2:C:301:16A:C5	3:C:306[A]:GOL:O3	2.67	0.43
1:D:148[B]:GLN:O	1:D:152:LYS:HG2	2.19	0.43
1:D:113:LEU:HD13	1:D:113:LEU:HA	1.89	0.42
2:A:302:16A:H192	2:A:302:16A:H151	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LYS:HB3	1:C:152:LYS:HE2	1.84	0.42
1:A:224:ILE:HG21	1:B:120[B]:GLU:HG2	2.02	0.42
2:C:301:16A:C7	3:C:306[A]:GOL:O3	2.68	0.42
3:C:305:GOL:O1	3:C:305:GOL:O3	2.37	0.42
1:D:128:SER:HA	1:D:183:PHE:O	2.19	0.42
2:B:302:16A:H42	1:C:140:ILE:HB	2.02	0.41
1:A:251:ASN:HB3	2:A:303:16A:H92	2.00	0.41
1:C:231:GLU:HG2	3:C:306[B]:GOL:O1	2.20	0.41
1:B:148:GLN:NE2	6:B:402:HOH:O	2.32	0.41
1:C:213[A]:LYS:HE2	1:C:259[A]:MET:SD	2.58	0.41
1:D:152:LYS:HE3	6:D:435:HOH:O	2.19	0.41
1:C:149[A]:GLU:HG2	1:C:194:GLU:HG2	2.02	0.41
2:B:302:16A:H13	2:C:302:16A:H141	2.03	0.41
1:C:250:TRP:CD1	2:C:303:16A:H62	2.56	0.40
1:C:192:LYS:HA	1:C:192:LYS:HD3	1.95	0.40
3:D:305:GOL:H12	6:D:466:HOH:O	2.20	0.40

There are no symmetry-related clashes.

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	A	169/159 (106%)	166 (98%)	3 (2%)	0	100	100
1	B	171/159 (108%)	169 (99%)	2 (1%)	0	100	100
1	C	179/159 (113%)	177 (99%)	2 (1%)	0	100	100
1	D	173/159 (109%)	171 (99%)	2 (1%)	0	100	100
All	All	692/636 (109%)	683 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	A	154/143 (108%)	154 (100%)	0	100	100
1	B	157/143 (110%)	155 (99%)	2 (1%)	69	42
1	C	164/143 (115%)	162 (99%)	2 (1%)	71	47
1	D	159/143 (111%)	156 (98%)	3 (2%)	57	25
All	All	634/572 (111%)	627 (99%)	7 (1%)	78	50

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	112	MET
1	B	113	LEU
1	C	213[A]	LYS
1	C	213[B]	LYS
1	D	192	LYS
1	D	213[A]	LYS
1	D	213[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	196	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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
5	EDO	A	307	-	3,3,3	0.51	0	2,2,2	0.08	0
2	16A	A	301	-	19,19,19	0.48	0	21,21,21	0.83	0
3	GOL	A	305	-	5,5,5	0.94	0	5,5,5	1.40	1 (20%)
2	16A	C	301	-	19,19,19	0.63	0	21,21,21	0.88	1 (4%)
2	16A	C	302	-	19,19,19	0.54	0	21,21,21	1.00	1 (4%)
3	GOL	C	306[B]	-	5,5,5	1.70	1 (20%)	5,5,5	0.98	0
3	GOL	C	305	-	5,5,5	0.97	0	5,5,5	0.99	0
2	16A	B	302	-	19,19,19	0.51	0	21,21,21	0.85	0
2	16A	D	302	-	19,19,19	0.53	0	21,21,21	0.99	0
3	GOL	D	304	-	5,5,5	1.76	2 (40%)	5,5,5	0.89	0
3	GOL	D	305	-	5,5,5	0.76	0	5,5,5	1.33	1 (20%)
3	GOL	B	303	-	5,5,5	0.35	0	5,5,5	0.66	0
3	GOL	D	303	-	5,5,5	1.33	1 (20%)	5,5,5	0.50	0
2	16A	C	303	-	11,11,19	0.32	0	10,10,21	0.37	0
2	16A	A	302	-	19,19,19	0.51	0	21,21,21	1.04	1 (4%)
3	GOL	A	304	-	5,5,5	1.13	0	5,5,5	1.11	0
5	EDO	B	305	-	3,3,3	0.63	0	2,2,2	0.31	0
3	GOL	C	306[A]	-	5,5,5	1.31	0	5,5,5	1.62	1 (20%)
5	EDO	B	304	-	3,3,3	0.53	0	2,2,2	0.22	0
2	16A	B	301	-	19,19,19	0.56	0	21,21,21	1.20	2 (9%)
2	16A	D	301	-	19,19,19	0.45	0	21,21,21	1.10	1 (4%)
3	GOL	C	304	-	5,5,5	1.05	0	5,5,5	0.84	0
2	16A	A	303	-	10,10,19	0.35	0	9,9,21	0.55	0
5	EDO	B	306	-	3,3,3	0.55	0	2,2,2	0.32	0
5	EDO	D	306	-	3,3,3	0.45	0	2,2,2	0.25	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
5	EDO	A	307	-	-	0/1/1/1	-
2	16A	A	301	-	-	3/17/17/17	-
3	GOL	A	305	-	-	2/4/4/4	-
2	16A	C	301	-	-	3/17/17/17	-
2	16A	C	302	-	-	3/17/17/17	-
3	GOL	C	306[B]	-	-	0/4/4/4	-
3	GOL	C	305	-	-	3/4/4/4	-
2	16A	B	302	-	-	4/17/17/17	-
2	16A	D	302	-	-	6/17/17/17	-
3	GOL	D	304	-	-	4/4/4/4	-
3	GOL	D	305	-	-	3/4/4/4	-
3	GOL	B	303	-	-	4/4/4/4	-
3	GOL	D	303	-	-	0/4/4/4	-
2	16A	C	303	-	-	7/9/9/17	-
2	16A	A	302	-	-	5/17/17/17	-
3	GOL	A	304	-	-	2/4/4/4	-
5	EDO	B	305	-	-	0/1/1/1	-
3	GOL	C	306[A]	-	-	0/4/4/4	-
5	EDO	B	304	-	-	1/1/1/1	-
2	16A	B	301	-	-	5/17/17/17	-
2	16A	D	301	-	-	3/17/17/17	-
3	GOL	C	304	-	-	2/4/4/4	-
2	16A	A	303	-	-	7/8/8/17	-
5	EDO	B	306	-	-	0/1/1/1	-
5	EDO	D	306	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	306[B]	GOL	O2-C2	-3.13	1.34	1.43
3	D	304	GOL	O3-C3	-2.93	1.30	1.42
3	D	303	GOL	C1-C2	2.17	1.60	1.51
3	D	304	GOL	C1-C2	2.03	1.60	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	306[A]	GOL	O3-C3-C2	-2.80	96.76	110.20
3	A	305	GOL	C3-C2-C1	-2.55	101.79	111.70
2	A	302	16A	C12-C11-C10	-2.41	102.17	114.42
2	B	301	16A	C9-C8-C7	-2.29	102.81	114.42
3	D	305	GOL	C3-C2-C1	-2.22	103.07	111.70
2	C	301	16A	C18-N1-C16	-2.21	100.87	109.92
2	C	302	16A	C10-C9-C8	-2.14	103.55	114.42
2	D	301	16A	C17-N1-C16	2.03	118.23	109.92
2	B	301	16A	C19-N1-C17	2.01	114.13	108.97

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	304	GOL	O1-C1-C2-C3
3	A	305	GOL	O1-C1-C2-C3
3	B	303	GOL	O1-C1-C2-O2
3	B	303	GOL	C1-C2-C3-O3
3	D	304	GOL	O1-C1-C2-C3
2	C	303	16A	C7-C8-C9-C10
2	A	303	16A	C2-C3-C4-C5
2	A	301	16A	C2-C3-C4-C5
3	A	305	GOL	O1-C1-C2-O2
3	B	303	GOL	O2-C2-C3-O3
2	A	302	16A	C14-C15-C16-N1
2	C	301	16A	C11-C10-C9-C8
3	B	303	GOL	O1-C1-C2-C3
3	C	304	GOL	O1-C1-C2-C3
3	C	305	GOL	C1-C2-C3-O3
3	D	304	GOL	C1-C2-C3-O3
3	D	305	GOL	O1-C1-C2-C3
2	B	302	16A	C6-C7-C8-C9
2	A	302	16A	C12-C13-C14-C15
2	B	302	16A	C7-C8-C9-C10
2	A	301	16A	C6-C7-C8-C9
2	D	302	16A	C7-C8-C9-C10
2	B	301	16A	C11-C10-C9-C8
2	A	303	16A	C7-C8-C9-C10
2	C	301	16A	C7-C8-C9-C10
3	D	304	GOL	O1-C1-C2-O2
3	D	305	GOL	O1-C1-C2-O2
2	C	303	16A	C4-C5-C6-C7
2	A	302	16A	C13-C14-C15-C16

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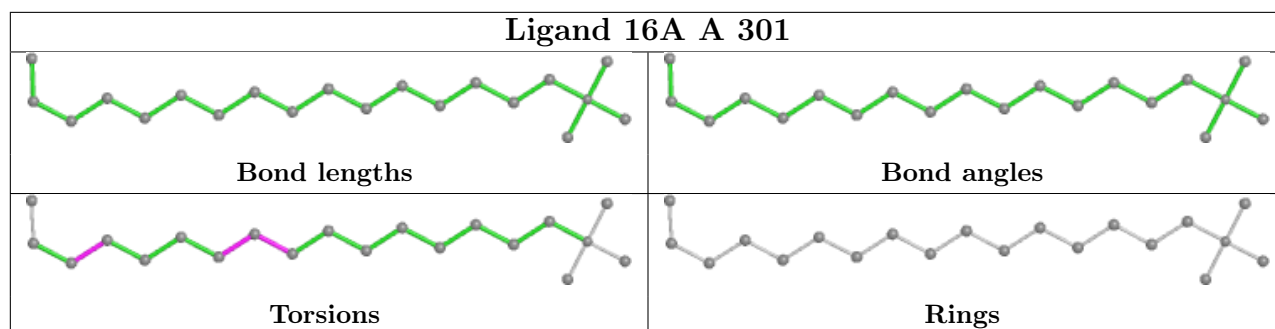
Mol	Chain	Res	Type	Atoms
2	A	303	16A	C6-C7-C8-C9
2	D	302	16A	C3-C4-C5-C6
2	C	303	16A	C2-C3-C4-C5
2	D	301	16A	C11-C10-C9-C8
2	C	303	16A	C5-C6-C7-C8
2	C	303	16A	C3-C4-C5-C6
2	C	302	16A	C11-C10-C9-C8
3	A	304	GOL	O1-C1-C2-O2
3	D	304	GOL	O2-C2-C3-O3
2	A	301	16A	C7-C8-C9-C10
2	B	301	16A	C2-C3-C4-C5
2	C	302	16A	C6-C7-C8-C9
2	B	301	16A	C3-C4-C5-C6
2	A	303	16A	C5-C6-C7-C8
2	D	302	16A	C15-C16-N1-C18
2	D	301	16A	C2-C3-C4-C5
3	C	304	GOL	O1-C1-C2-O2
2	C	302	16A	C10-C11-C12-C13
2	B	302	16A	C2-C3-C4-C5
2	B	302	16A	C5-C6-C7-C8
5	B	304	EDO	O1-C1-C2-O2
2	A	302	16A	C3-C4-C5-C6
2	D	302	16A	C15-C16-N1-C17
2	A	303	16A	C11-C10-C9-C8
2	B	301	16A	C6-C7-C8-C9
2	D	302	16A	C12-C13-C14-C15
2	A	303	16A	C3-C4-C5-C6
2	A	303	16A	C4-C5-C6-C7
2	B	301	16A	C1-C2-C3-C4
2	D	302	16A	C15-C16-N1-C19
3	C	305	GOL	O1-C1-C2-C3
3	D	305	GOL	C1-C2-C3-O3
3	C	305	GOL	O2-C2-C3-O3
2	D	301	16A	C1-C2-C3-C4
2	C	301	16A	C2-C3-C4-C5
2	C	303	16A	C9-C10-C11-C12
2	C	303	16A	C11-C10-C9-C8
2	A	302	16A	C1-C2-C3-C4

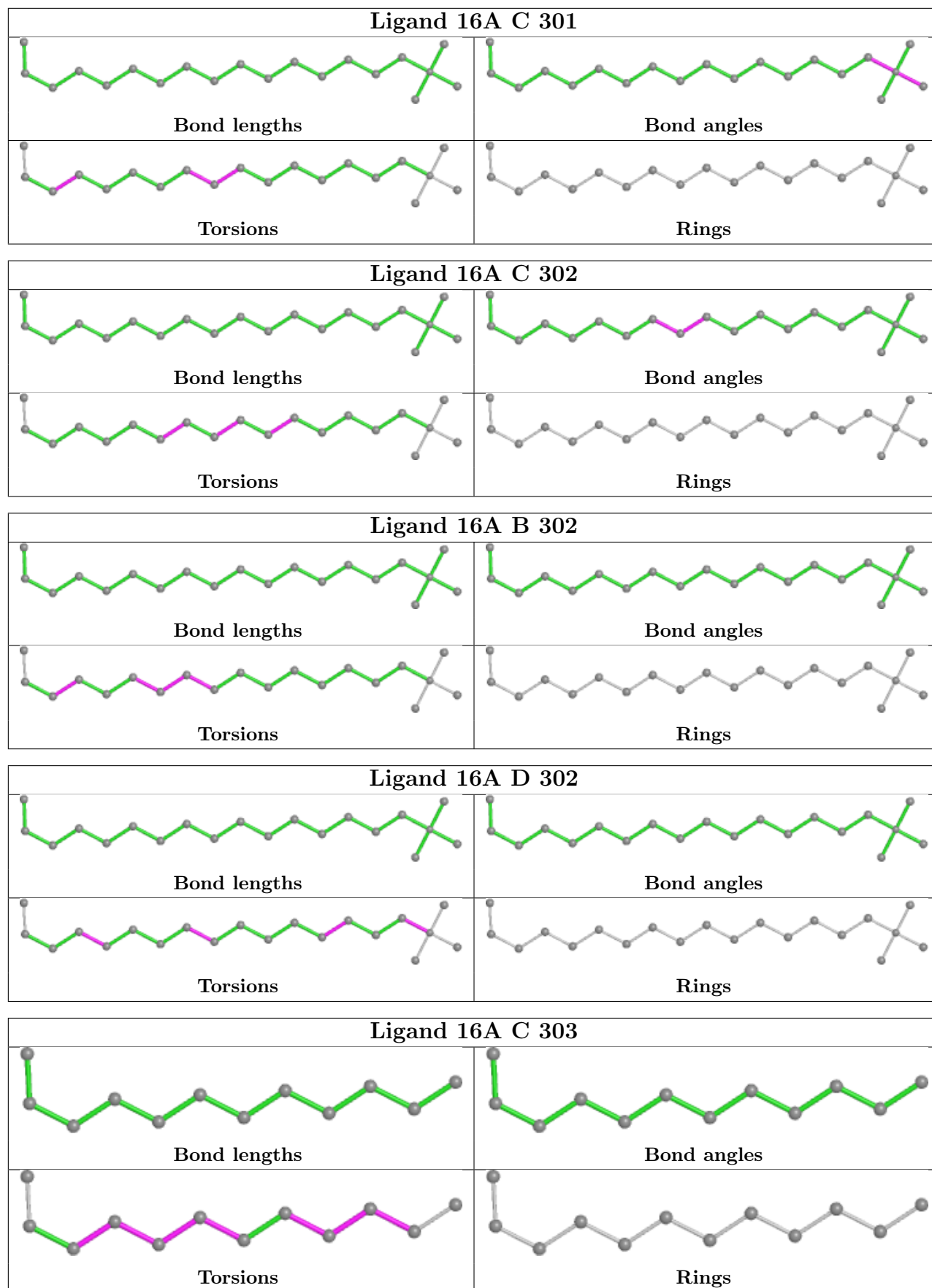
There are no ring outliers.

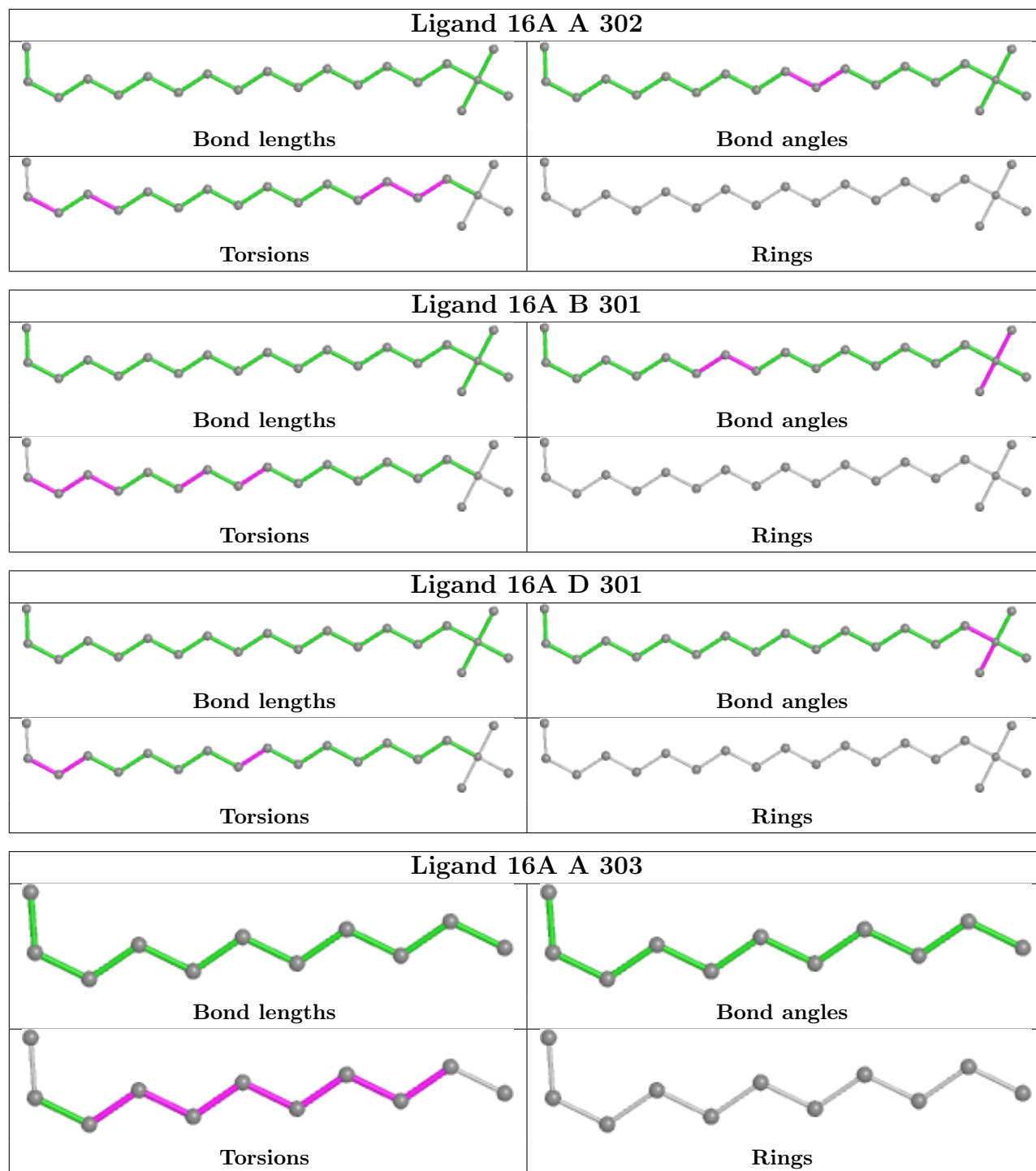
15 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	307	EDO	1	0
2	C	301	16A	7	0
2	C	302	16A	4	0
3	C	306[B]	GOL	8	0
3	C	305	GOL	1	0
2	B	302	16A	2	0
3	D	305	GOL	2	0
3	D	303	GOL	1	0
2	C	303	16A	6	0
2	A	302	16A	1	0
3	A	304	GOL	1	0
5	B	305	EDO	1	0
3	C	306[A]	GOL	8	0
3	C	304	GOL	3	0
2	A	303	16A	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, 95th 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 ²)	Q<0.9
1	A	158/159 (99%)	0.20	7 (4%) 34 34	14, 21, 43, 56	0
1	B	158/159 (99%)	0.13	4 (2%) 57 57	13, 21, 40, 54	0
1	C	158/159 (99%)	0.28	8 (5%) 28 27	9, 15, 32, 56	0
1	D	158/159 (99%)	0.23	3 (1%) 66 67	10, 15, 30, 53	0
All	All	632/636 (99%)	0.21	22 (3%) 44 43	9, 18, 38, 56	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	155[A]	PRO	4.5
1	B	113	LEU	4.2
1	A	155	PRO	4.2
1	D	155	PRO	4.1
1	B	112	MET	3.9
1	D	113	LEU	3.6
1	C	112	MET	3.3
1	A	112	MET	3.2
1	A	190	PHE	3.1
1	A	113	LEU	3.0
1	C	190[A]	PHE	3.0
1	A	152	LYS	2.9
1	A	192	LYS	2.9
1	C	152	LYS	2.9
1	D	112	MET	2.8
1	C	192	LYS	2.3
1	A	172	LYS	2.2
1	B	196	ASN	2.1
1	C	113	LEU	2.1
1	C	194	GLU	2.0
1	C	156[A]	GLY	2.0
1	B	236	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

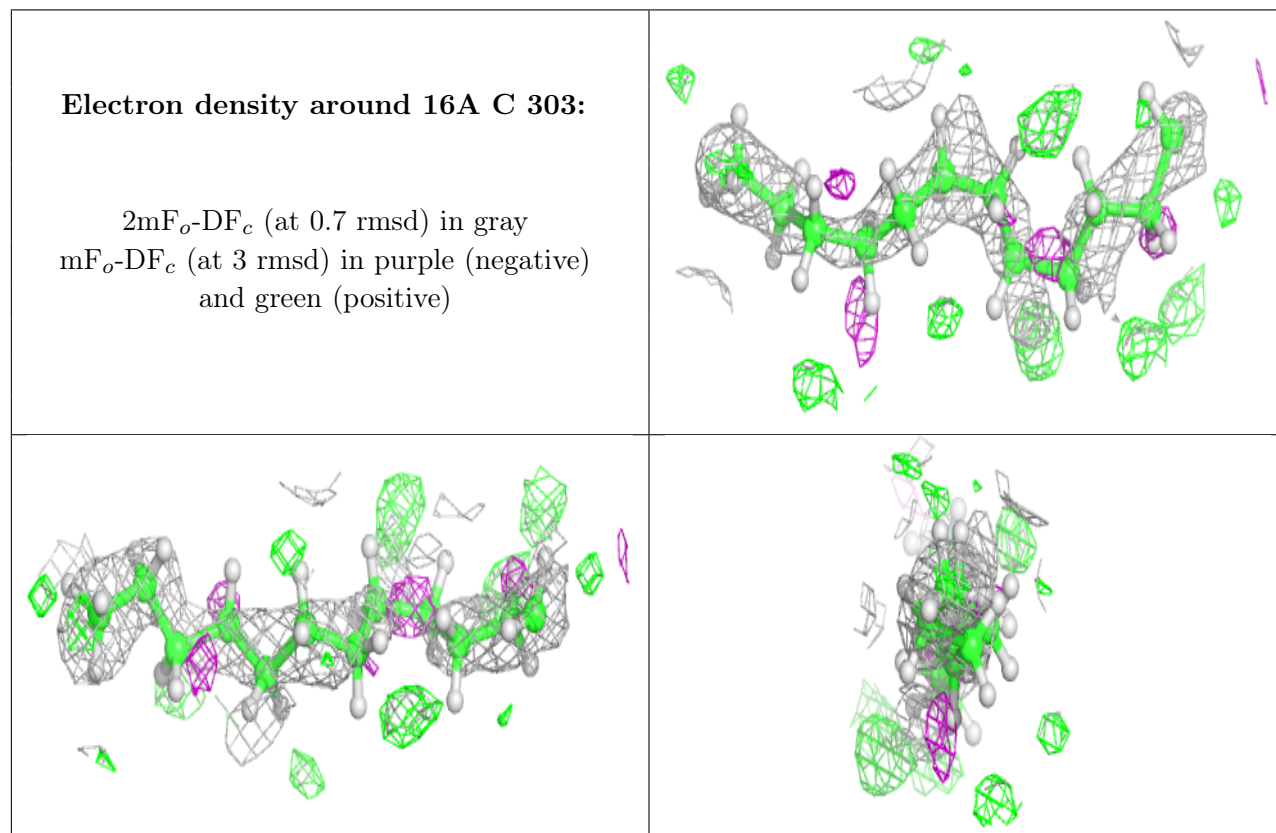
There are no monosaccharides in this entry.

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, 95th 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.

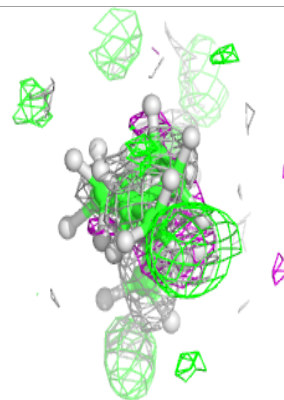
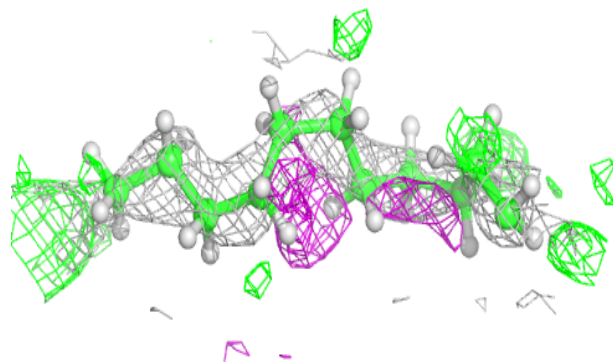
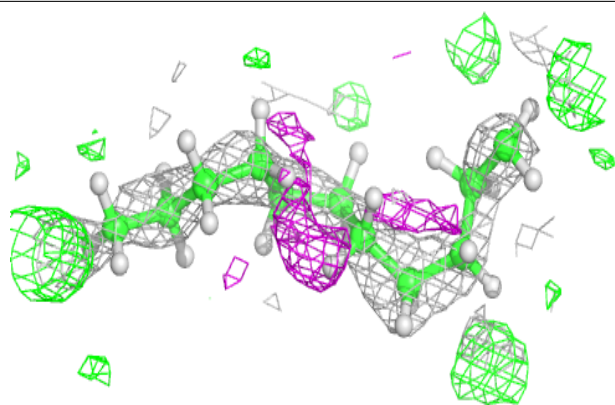
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	16A	C	303	12/20	0.69	0.32	37,50,58,58	0
3	GOL	A	304	6/6	0.71	0.36	44,53,56,58	0
3	GOL	B	303	6/6	0.73	0.23	59,70,82,85	0
2	16A	A	303	11/20	0.78	0.31	44,53,61,62	0
3	GOL	C	304	6/6	0.79	0.35	37,44,50,53	0
5	EDO	B	306	4/4	0.83	0.21	36,44,48,48	0
3	GOL	D	303	6/6	0.84	0.27	26,39,46,47	0
5	EDO	B	305	4/4	0.84	0.25	39,47,50,55	0
3	GOL	A	305	6/6	0.84	0.34	44,53,60,65	0
3	GOL	C	305	6/6	0.85	0.31	36,48,58,58	0
3	GOL	D	305	6/6	0.86	0.24	38,52,60,62	0
5	EDO	A	307	4/4	0.86	0.23	40,48,52,52	0
3	GOL	D	304	6/6	0.87	0.23	20,30,36,38	0
2	16A	C	301	20/20	0.89	0.17	19,34,62,68	0
5	EDO	B	304	4/4	0.89	0.21	38,48,51,58	0
2	16A	A	302	20/20	0.90	0.18	30,41,60,63	0
2	16A	B	302	20/20	0.90	0.16	31,42,53,54	0
2	16A	C	302	20/20	0.91	0.15	28,39,56,58	0
2	16A	A	301	20/20	0.92	0.15	23,37,67,68	0
2	16A	D	302	20/20	0.92	0.17	27,38,51,52	0
2	16A	B	301	20/20	0.95	0.14	21,40,64,65	0
5	EDO	D	306	4/4	0.95	0.14	23,31,38,38	0
3	GOL	C	306[B]	6/6	0.96	0.34	27,27,30,35	6
2	16A	D	301	20/20	0.96	0.13	16,32,60,61	0
3	GOL	C	306[A]	6/6	0.96	0.34	25,29,30,31	6
4	CL	A	306	1/1	0.99	0.04	48,48,48,48	0
4	CL	C	307	1/1	1.00	0.07	26,26,26,26	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.

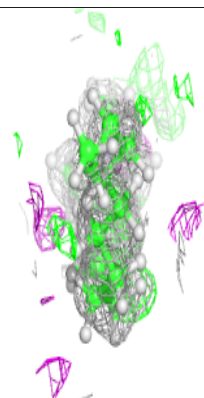
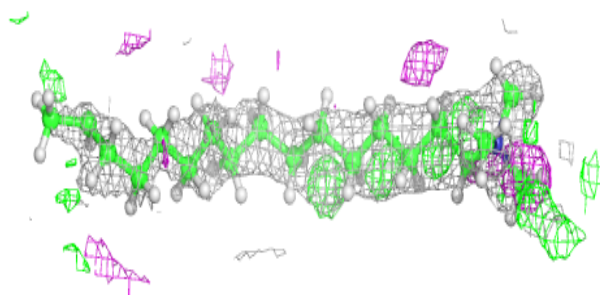
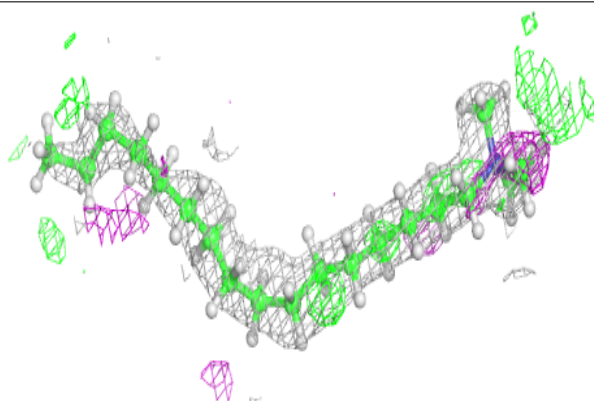


Electron density around 16A A 303:

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

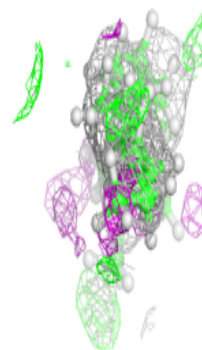
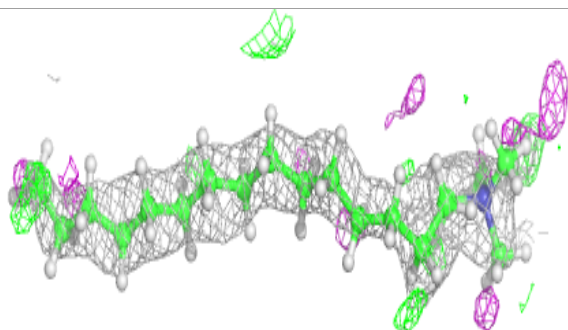
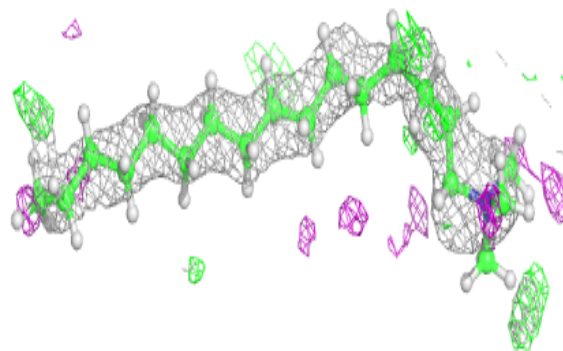
**Electron density around 16A C 301:**

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

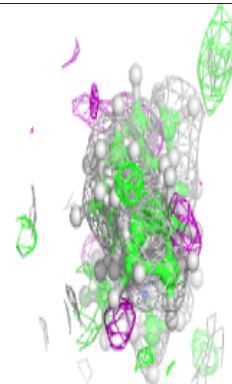
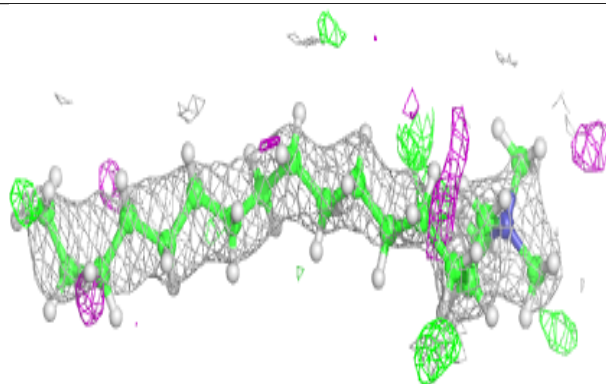
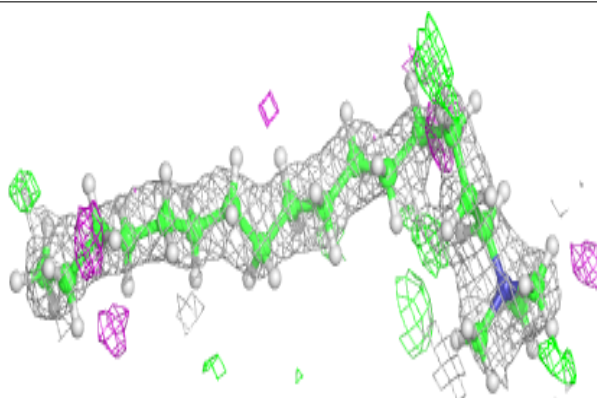


Electron density around 16A A 302:

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

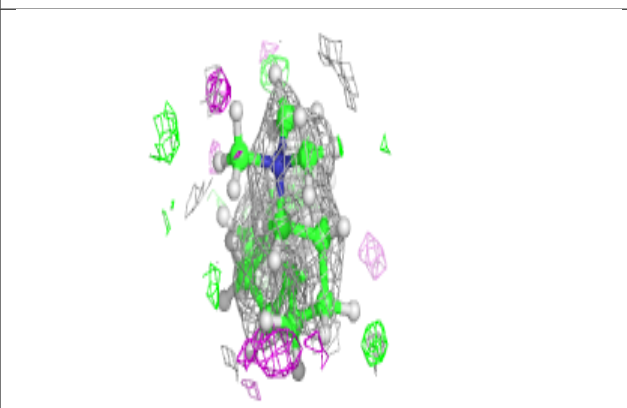
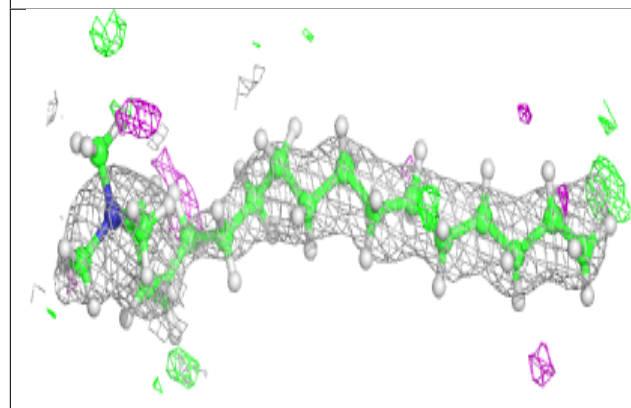
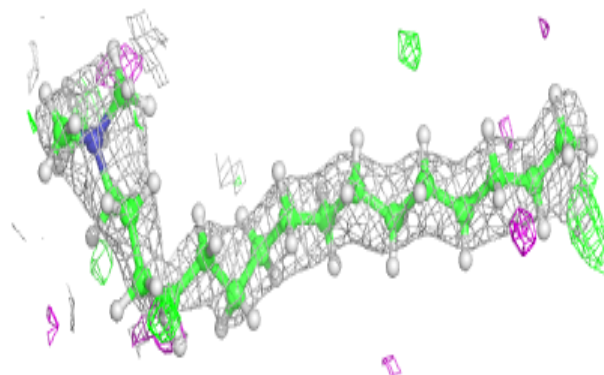
**Electron density around 16A B 302:**

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

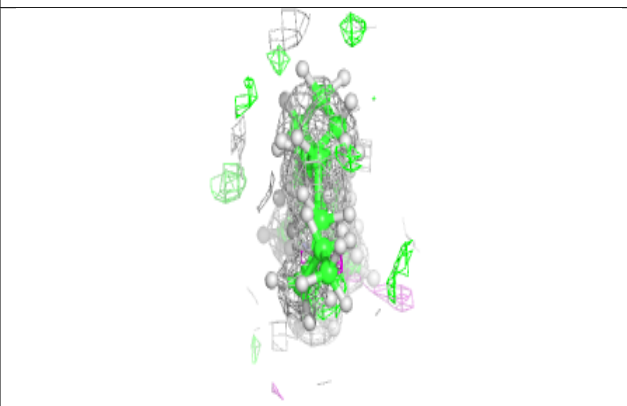
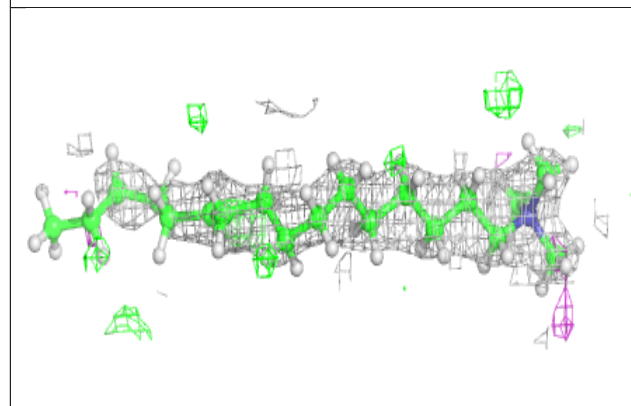
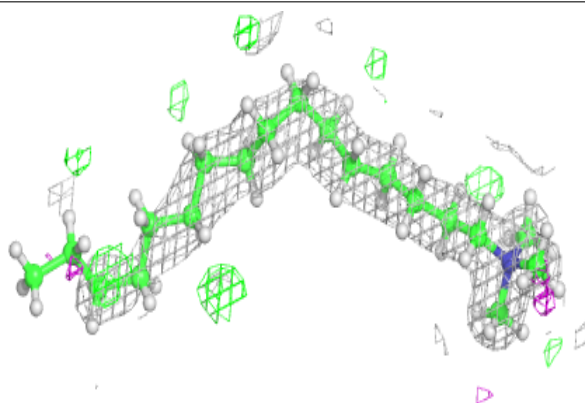


Electron density around 16A C 302:

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

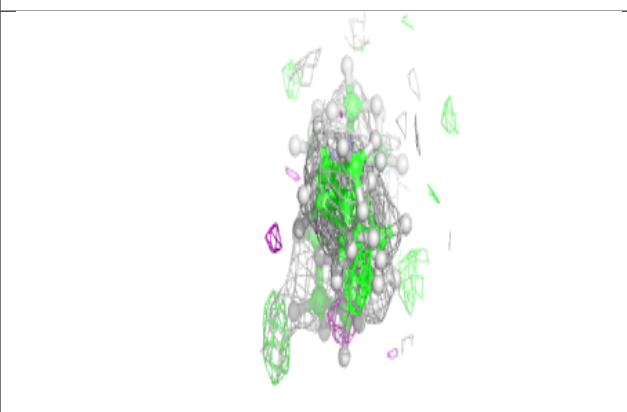
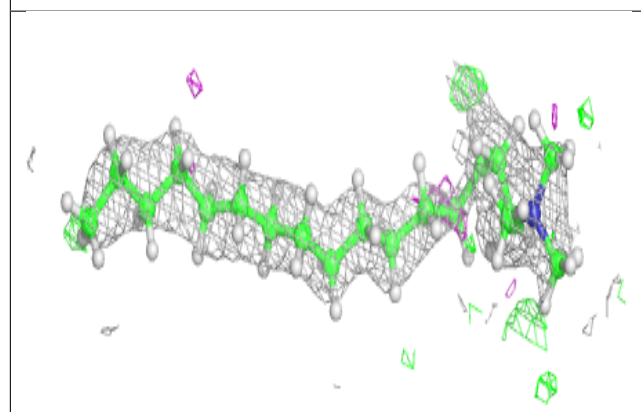
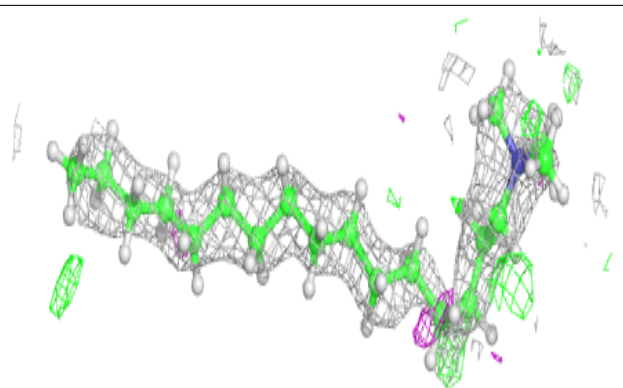
**Electron density around 16A A 301:**

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

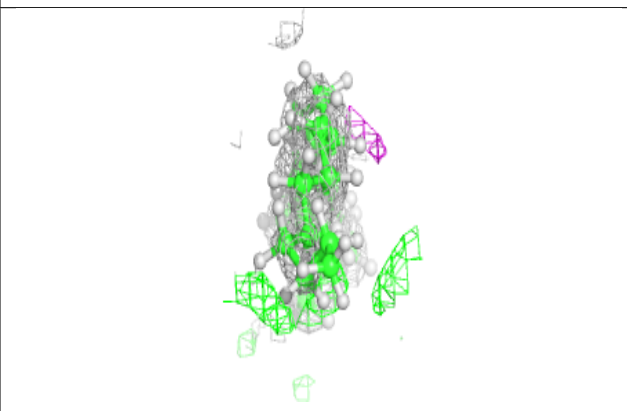
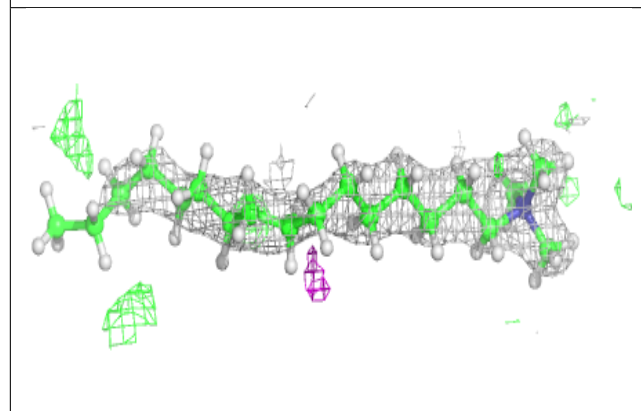
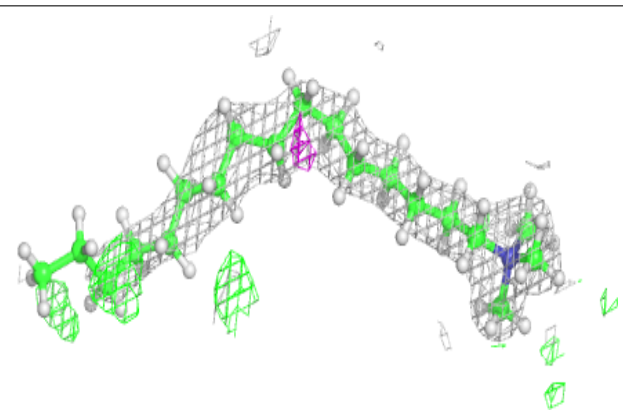


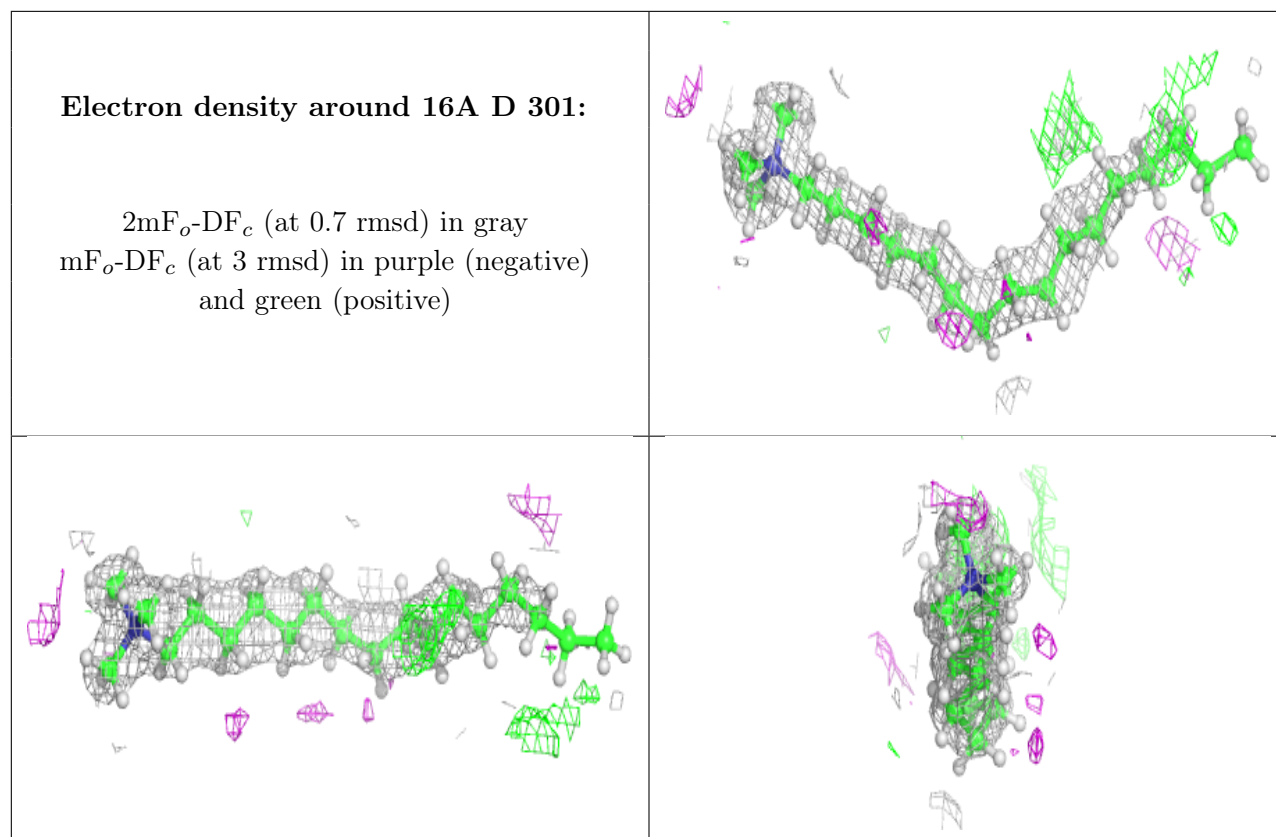
Electron density around 16A D 302:

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

**Electron density around 16A B 301:**

$2mF_o-DF_c$ (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.