



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:28 PM UTC

PDB ID : 6YBZ / pdb_00006ybz
Title : Crystal structure of the D116N mutant of the light-driven sodium pump KR2 in the pentameric form, pH 8.0
Authors : Kovalev, K.; Gushchin, I.; Gordeliy, V.
Deposited on : 2020-03-18
Resolution : 2.35 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

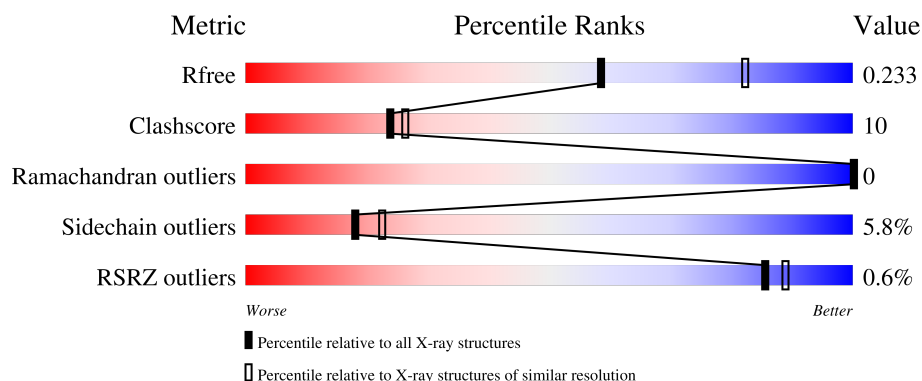
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	273	78% 19% ..
1	B	273	77% 20% ..
1	C	273	78% 18% ..
1	D	273	82% 15% ..
1	E	273	81% 16% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11574 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 Sodium pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	4	0
			2153	1435	327	382	9			
1	B	269	Total	C	N	O	S	0	3	0
			2137	1424	326	378	9			
1	C	269	Total	C	N	O	S	0	3	0
			2151	1435	327	380	9			
1	D	271	Total	C	N	O	S	0	3	0
			2159	1439	329	382	9			
1	E	269	Total	C	N	O	S	0	4	0
			2154	1434	327	384	9			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ASN	ASP	engineered mutation	UNP N0DKS8
B	116	ASN	ASP	engineered mutation	UNP N0DKS8
C	116	ASN	ASP	engineered mutation	UNP N0DKS8
D	116	ASN	ASP	engineered mutation	UNP N0DKS8
E	116	ASN	ASP	engineered mutation	UNP N0DKS8

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

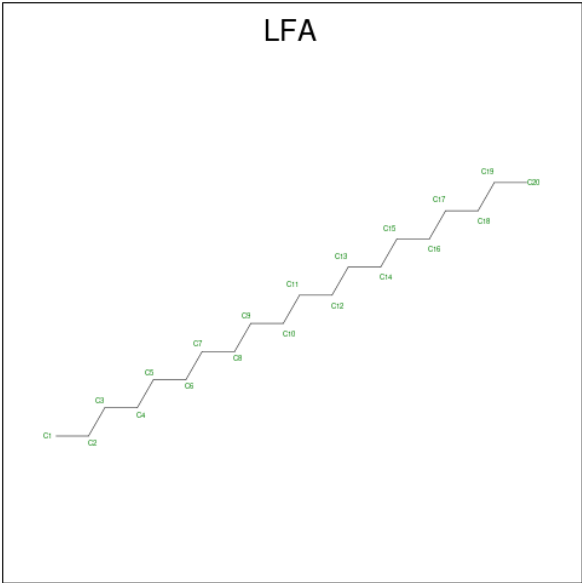
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Na	0	0
			1	1		

- Molecule 3 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



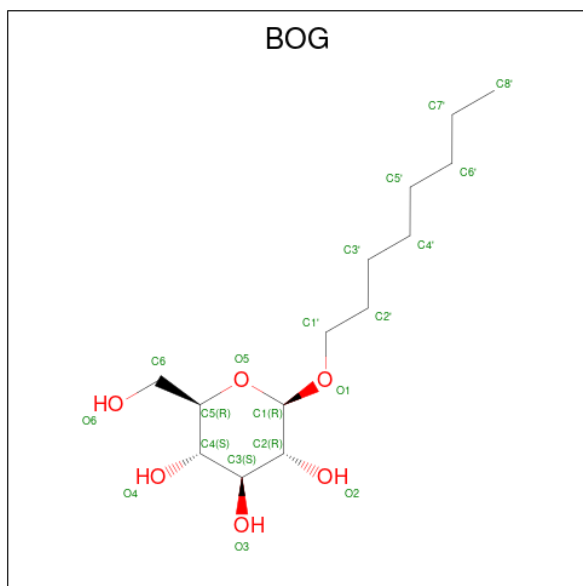
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			10	10		
3	A	1	Total	C	0	0
			6	6		
3	A	1	Total	C	0	0
			16	16		
3	A	1	Total	C	0	0
			18	18		
3	A	1	Total	C	0	0
			14	14		
3	B	1	Total	C	0	0
			12	12		
3	B	1	Total	C	0	0
			18	18		
3	B	1	Total	C	0	0
			6	6		
3	B	1	Total	C	0	0
			15	15		
3	C	1	Total	C	0	0
			15	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C 5 5	0	0
3	C	1	Total C 19 19	0	0
3	D	1	Total C 11 11	0	0
3	D	1	Total C 14 14	0	0
3	D	1	Total C 18 18	0	0
3	D	1	Total C 6 6	0	0
3	E	1	Total C 16 16	0	0
3	E	1	Total C 18 18	0	0
3	E	1	Total C 6 6	0	0

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



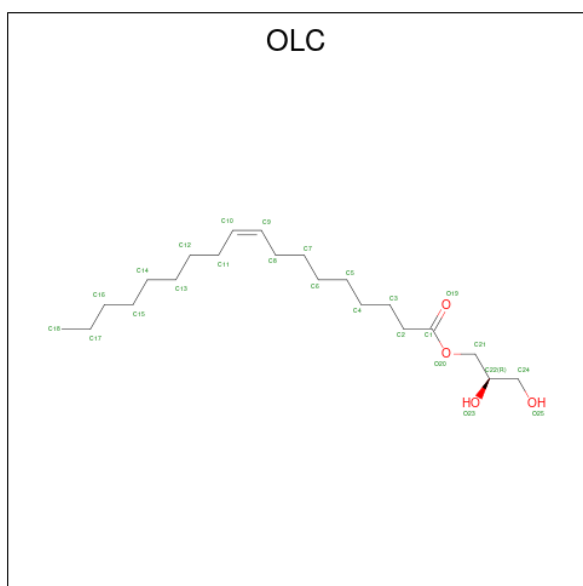
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 14 6	0	0
4	B	1	Total C O 20 14 6	0	0

Continued on next page...

Continued from previous page...

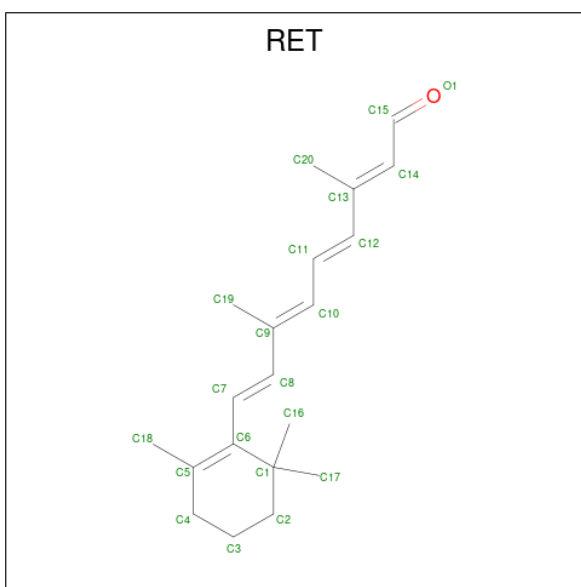
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			20	14	6		
4	D	1	Total	C	O	0	0
			20	14	6		
4	E	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			15	11	4		
5	B	1	Total	C	O	0	0
			15	11	4		
5	C	1	Total	C	O	0	0
			21	17	4		
5	C	1	Total	C	O	0	0
			16	12	4		
5	D	1	Total	C	O	0	0
			15	11	4		
5	E	1	Total	C	O	0	0
			15	11	4		

- Molecule 6 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 40 40	0	1
6	B	1	Total C 40 40	0	1
6	C	1	Total C 40 40	0	1
6	D	1	Total C 40 40	0	1
6	E	1	Total C 40 40	0	1

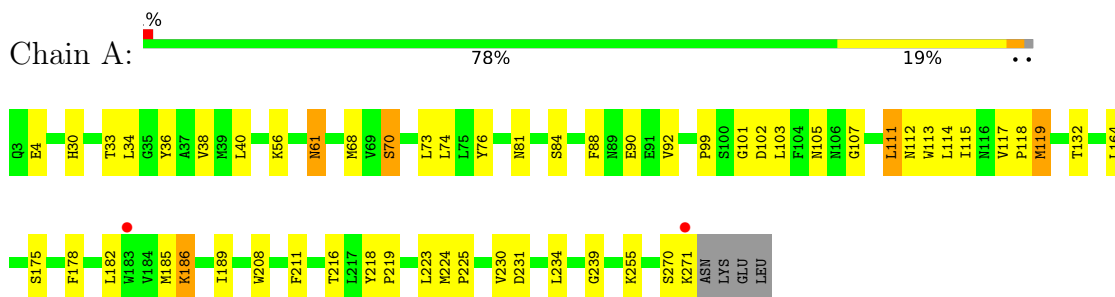
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	36	Total O 36 36	0	0
7	B	30	Total O 30 30	0	0
7	C	34	Total O 34 34	0	0
7	D	39	Total O 39 39	0	0
7	E	36	Total O 36 36	0	0

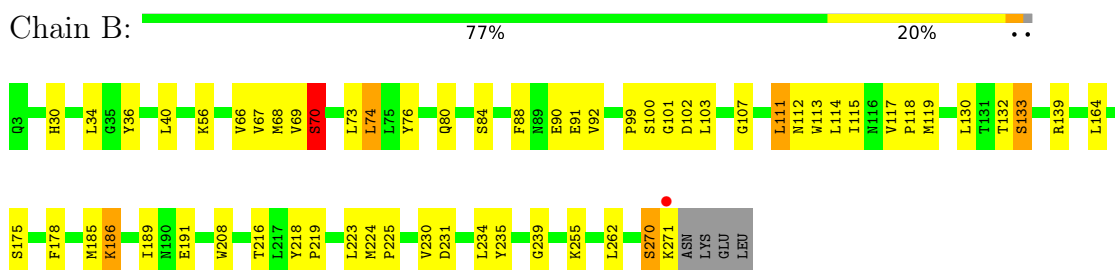
3 Residue-property plots [i](#)

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.

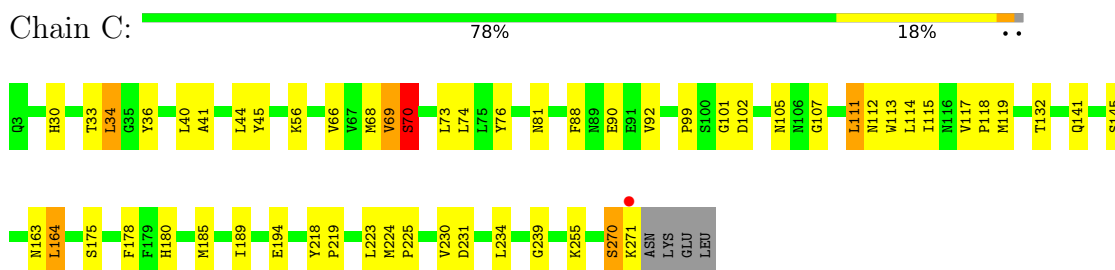
- Molecule 1: Sodium pumping rhodopsin



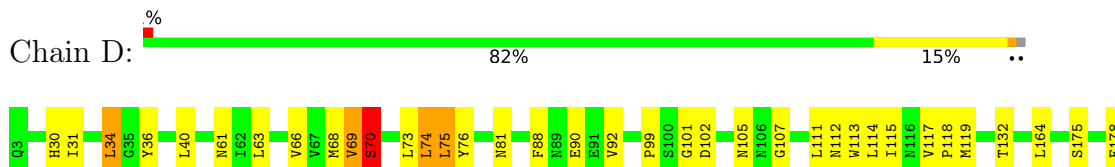
- Molecule 1: Sodium pumping rhodopsin

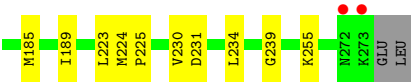


- Molecule 1: Sodium pumping rhodopsin

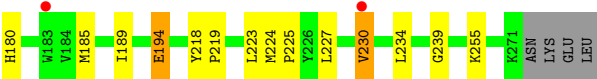
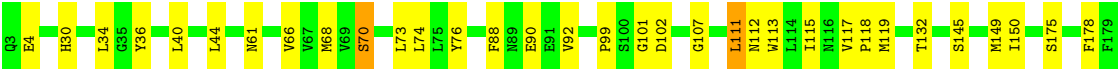
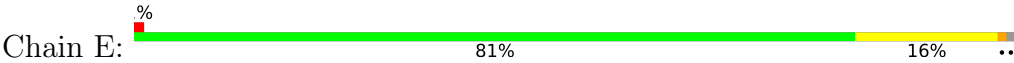


- Molecule 1: Sodium pumping rhodopsin





● Molecule 1: Sodium pumping rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	131.34Å 240.48Å 135.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.35) 99.7 (20.00-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.196 , 0.217 0.210 , 0.233	Depositor DCC
R_{free} test set	4470 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11574	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET, NA, LFA, OLC, BOG

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	0.94	0/2210	1.50	0/3005
1	B	1.61	4/2195 (0.2%)	1.53	1/2989 (0.0%)
1	C	1.49	4/2209 (0.2%)	1.52	1/3004 (0.0%)
1	D	1.24	3/2217 (0.1%)	1.52	1/3016 (0.0%)
1	E	0.94	0/2212	1.49	0/3010
All	All	1.27	11/11043 (0.1%)	1.51	3/15024 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	SER	C-N	46.15	1.98	1.33
1	C	270	SER	C-N	43.97	1.95	1.33
1	B	70[A]	SER	C-N	-27.94	0.97	1.33
1	B	70[B]	SER	C-N	-27.94	0.97	1.33
1	D	70[A]	SER	C-N	-26.48	0.99	1.33
1	D	70[B]	SER	C-N	-26.48	0.99	1.33
1	C	70[A]	SER	C-N	-21.04	1.06	1.33
1	C	70[B]	SER	C-N	-21.04	1.06	1.33
1	C	69	VAL	C-N	11.02	1.47	1.33
1	D	69	VAL	C-N	8.30	1.44	1.33
1	B	69	VAL	C-N	8.05	1.44	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	VAL	O-C-N	11.96	134.26	121.94
1	D	69	VAL	O-C-N	11.18	133.46	121.94
1	C	69	VAL	O-C-N	10.97	133.24	121.94

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	69	VAL	Mainchain
1	D	69	VAL	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2153	0	2113	56	0
1	B	2137	0	2093	65	0
1	C	2151	0	2120	53	0
1	D	2159	0	2121	45	0
1	E	2154	0	2112	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	64	0	123	2	0
3	B	51	0	98	0	0
3	C	39	0	75	1	0
3	D	49	0	94	0	0
3	E	40	0	77	0	0
4	A	20	0	28	1	0
4	B	20	0	28	6	0
4	C	20	0	28	2	0
4	D	20	0	28	1	0
4	E	20	0	28	1	0
5	A	15	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	15	0	19	0	0
5	C	37	0	50	5	0
5	D	15	0	19	0	0
5	E	15	0	19	0	0
6	A	40	0	54	8	0
6	B	40	0	54	12	0
6	C	40	0	54	8	0
6	D	40	0	54	8	0
6	E	40	0	54	8	0
7	A	36	0	0	5	0
7	B	30	0	0	3	0
7	C	34	0	0	2	0
7	D	39	0	0	2	0
7	E	36	0	0	2	0
All	All	11574	0	11562	233	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (233) 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:C:270:SER:C	1:C:271:LYS:N	1.94	1.25
1:B:270:SER:C	1:B:271:LYS:N	1.98	1.21
6:E:307[B]:RET:H161	6:E:307[B]:RET:H8	1.40	1.03
1:A:270:SER:C	1:A:271:LYS:N	2.19	1.00
1:A:34:LEU:CD1	1:B:115:ILE:HD11	1.91	0.99
1:C:66:VAL:HG12	1:C:119:MET:HE1	1.45	0.98
1:D:30:HIS:HB3	1:E:111:LEU:HD22	1.43	0.97
6:D:308[B]:RET:H8	6:D:308[B]:RET:H161	1.46	0.97
6:B:308[B]:RET:H8	6:B:308[B]:RET:H161	1.47	0.96
6:B:308[A]:RET:H161	6:B:308[A]:RET:H8	1.48	0.95
1:D:61:ASN:ND2	7:D:401:HOH:O	1.99	0.95
1:E:66:VAL:HG12	1:E:119:MET:HE1	1.47	0.95
1:A:30:HIS:HB3	1:B:111:LEU:HD22	1.48	0.94
1:B:30:HIS:HB3	1:C:111:LEU:HD22	1.51	0.92
1:B:66:VAL:CG1	1:B:119:MET:HE1	2.00	0.92
1:A:111:LEU:HD22	1:E:30:HIS:HB3	1.50	0.91
6:D:308[A]:RET:H8	6:D:308[A]:RET:H161	1.51	0.91
6:C:307[A]:RET:H8	6:C:307[A]:RET:H161	1.52	0.90
6:E:307[A]:RET:H8	6:E:307[A]:RET:H161	1.50	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:VAL:HG12	1:B:119:MET:HE1	1.54	0.89
6:C:307[B]:RET:H8	6:C:307[B]:RET:H161	1.54	0.89
6:A:307[A]:RET:H161	6:A:307[A]:RET:H8	1.52	0.88
6:A:307[B]:RET:H8	6:A:307[B]:RET:H161	1.52	0.87
1:A:61:ASN:OD1	7:A:401:HOH:O	1.90	0.87
1:C:66:VAL:CG1	1:C:119:MET:HE1	2.05	0.87
1:B:34:LEU:HD12	1:C:115:ILE:HD11	1.58	0.86
1:A:115:ILE:HD11	1:E:34:LEU:HD12	1.56	0.85
1:D:30:HIS:HB3	1:E:111:LEU:CD2	2.06	0.85
1:A:34:LEU:HD13	1:B:115:ILE:HD11	1.58	0.84
1:C:70[A]:SER:HB2	7:C:408:HOH:O	1.80	0.81
1:A:70[A]:SER:HB2	7:A:425:HOH:O	1.81	0.80
1:C:163:ASN:HD22	5:C:306:OLC:C24	1.97	0.77
1:C:163:ASN:HD22	5:C:306:OLC:H24	1.50	0.76
1:B:30:HIS:HB3	1:C:111:LEU:CD2	2.16	0.74
1:E:70[B]:SER:HB2	7:E:419:HOH:O	1.88	0.74
1:A:34:LEU:HD12	1:B:115:ILE:HD11	1.70	0.73
6:B:308[B]:RET:H161	6:B:308[B]:RET:C8	2.20	0.71
1:A:111:LEU:CD2	1:E:30:HIS:HB3	2.20	0.71
6:B:308[A]:RET:H161	6:B:308[A]:RET:C8	2.20	0.71
1:B:70[A]:SER:HB2	7:B:417:HOH:O	1.89	0.70
1:B:68:MET:HE1	1:B:255[A]:LYS:HB3	1.73	0.70
1:C:113:TRP:CD1	6:C:307[A]:RET:H14	2.27	0.69
6:A:307[A]:RET:H161	6:A:307[A]:RET:C8	2.22	0.69
1:B:68:MET:HE1	1:B:255[B]:LYS:HB3	1.74	0.69
6:E:307[A]:RET:H161	6:E:307[A]:RET:C8	2.22	0.69
6:A:307[B]:RET:H161	6:A:307[B]:RET:C8	2.23	0.69
1:B:113:TRP:CD1	6:B:308[A]:RET:H14	2.28	0.68
1:A:34:LEU:CD1	1:B:115:ILE:CD1	2.71	0.68
1:A:113:TRP:CD1	6:A:307[B]:RET:H14	2.29	0.68
1:D:70[A]:SER:HB2	7:D:421:HOH:O	1.92	0.68
1:E:113:TRP:CD1	6:E:307[A]:RET:H14	2.29	0.67
1:E:66:VAL:CG1	1:E:119:MET:HE1	2.24	0.66
1:A:81:ASN:HD21	1:A:105:ASN:H	1.43	0.66
1:A:113:TRP:CD1	6:A:307[A]:RET:H14	2.30	0.66
6:E:307[B]:RET:H161	6:E:307[B]:RET:C8	2.15	0.66
1:B:80:GLN:NE2	7:B:401:HOH:O	2.29	0.66
1:C:145:SER:OG	1:C:180:HIS:HD2	1.79	0.65
1:A:70[B]:SER:HB3	7:A:425:HOH:O	1.97	0.64
1:B:66:VAL:HG12	1:B:119:MET:CE	2.27	0.63
6:D:308[B]:RET:H161	6:D:308[B]:RET:C8	2.20	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:SER:OG	1:E:180:HIS:HD2	1.81	0.63
1:C:163:ASN:ND2	5:C:306:OLC:H24	2.14	0.63
1:E:70[A]:SER:HB3	7:E:419:HOH:O	1.99	0.62
1:B:66:VAL:HG11	1:B:119:MET:HE1	1.82	0.61
1:A:30:HIS:HB3	1:B:111:LEU:CD2	2.28	0.61
1:A:115:ILE:CD1	1:E:34:LEU:HD12	2.28	0.61
1:B:231:ASP:H	4:B:304:BOG:HO6	1.48	0.61
6:D:308[A]:RET:H161	6:D:308[A]:RET:C8	2.22	0.61
6:C:307[A]:RET:H161	6:C:307[A]:RET:C8	2.23	0.61
1:B:218:TYR:HB2	1:B:219:PRO:HD3	1.82	0.61
1:D:113:TRP:CD1	6:D:308[A]:RET:H14	2.36	0.61
6:C:307[B]:RET:H161	6:C:307[B]:RET:C8	2.24	0.60
1:C:234:LEU:O	1:C:239:GLY:HA3	2.02	0.60
1:B:231:ASP:N	4:B:304:BOG:O6	2.23	0.59
1:D:81:ASN:HD21	1:D:105:ASN:H	1.47	0.59
1:B:234:LEU:O	1:B:239:GLY:HA3	2.02	0.59
1:A:119:MET:HE1	3:A:309:LFA:H182	1.83	0.59
1:B:235:TYR:CG	4:B:304:BOG:H62	2.37	0.59
1:A:84[B]:SER:OG	7:A:402:HOH:O	2.17	0.59
6:E:307[B]:RET:H8	6:E:307[B]:RET:C16	2.24	0.59
1:B:164:LEU:HD11	4:B:304:BOG:H1'1	1.83	0.58
1:C:34:LEU:HD12	1:D:115:ILE:HD11	1.84	0.58
1:C:81:ASN:HD21	1:C:105:ASN:H	1.51	0.58
1:E:234:LEU:O	1:E:239:GLY:HA3	2.03	0.58
1:B:70[B]:SER:HB3	7:B:417:HOH:O	2.03	0.58
1:C:163:ASN:ND2	5:C:306:OLC:C24	2.67	0.58
1:C:224:MET:N	1:C:225:PRO:HD2	2.19	0.58
1:B:40:LEU:HD23	1:C:73:LEU:HD11	1.85	0.57
1:A:224:MET:N	1:A:225:PRO:HD2	2.19	0.57
1:D:224:MET:N	1:D:225:PRO:HD2	2.19	0.57
1:D:234:LEU:O	1:D:239:GLY:HA3	2.03	0.57
1:E:224:MET:N	1:E:225:PRO:HD2	2.20	0.57
1:C:163:ASN:HD22	5:C:306:OLC:H24A	1.70	0.57
7:A:431:HOH:O	1:B:100:SER:HA	2.05	0.56
1:B:224:MET:N	1:B:225:PRO:HD2	2.20	0.56
1:A:234:LEU:O	1:A:239:GLY:HA3	2.04	0.56
1:B:34:LEU:HD12	1:C:115:ILE:CD1	2.34	0.56
1:A:99:PRO:HG2	1:E:90:GLU:OE1	2.06	0.56
1:B:186:LYS:HG2	1:B:208:TRP:CZ2	2.41	0.56
1:E:230:VAL:HG12	4:E:304:BOG:O1	2.05	0.56
1:C:68:MET:HE1	1:C:255[A]:LYS:HB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HD13	1:B:115:ILE:CD1	2.34	0.55
1:E:68:MET:HE1	1:E:255[A]:LYS:HB3	1.89	0.55
1:C:68:MET:HE1	1:C:255[B]:LYS:HB3	1.87	0.55
1:D:113:TRP:CD1	6:D:308[B]:RET:H14	2.41	0.55
1:B:185:MET:O	1:B:189:ILE:HG12	2.08	0.53
1:B:133:SER:OG	1:B:191:GLU:OE2	2.27	0.52
1:C:113:TRP:CD1	6:C:307[B]:RET:H14	2.43	0.52
1:B:30:HIS:CE1	1:C:107:GLY:HA3	2.45	0.52
1:C:90:GLU:CG	1:D:99:PRO:HG2	2.40	0.52
1:C:164:LEU:HD21	4:C:304:BOG:H1'1	1.92	0.51
1:C:66:VAL:HG12	1:C:119:MET:CE	2.30	0.51
1:A:90:GLU:CG	1:B:99:PRO:HG2	2.40	0.51
1:B:90:GLU:HG2	1:C:99:PRO:HG2	1.92	0.50
1:A:231:ASP:H	4:A:303:BOG:HO6	1.59	0.50
1:D:66:VAL:HG11	1:D:119:MET:HE1	1.94	0.50
1:E:149:MET:HE3	1:E:150:ILE:CD1	2.42	0.50
1:A:68:MET:HE1	1:A:255[A]:LYS:HB3	1.93	0.50
1:B:88:PHE:CD2	1:C:99:PRO:HB3	2.47	0.49
1:D:185:MET:O	1:D:189:ILE:HG12	2.12	0.49
1:A:40:LEU:HD23	1:B:73:LEU:HD11	1.94	0.49
1:A:68:MET:HE1	1:A:255[B]:LYS:HB3	1.93	0.49
1:A:111:LEU:CD2	1:E:30:HIS:C	2.86	0.49
1:C:30:HIS:CE1	1:D:107:GLY:HA3	2.47	0.49
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.94	0.49
1:A:107:GLY:HA3	1:E:30:HIS:CE1	2.47	0.49
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.95	0.49
1:C:231:ASP:H	4:C:304:BOG:HO6	1.58	0.49
1:A:34:LEU:CD1	1:B:115:ILE:CG1	2.91	0.48
1:E:185:MET:O	1:E:189:ILE:HG12	2.13	0.48
6:D:308[A]:RET:H8	6:D:308[A]:RET:C16	2.32	0.48
1:A:185:MET:O	1:A:189:ILE:HG12	2.13	0.48
1:A:99:PRO:HB3	1:E:88:PHE:CD2	2.49	0.48
1:C:185:MET:O	1:C:189:ILE:HG12	2.13	0.48
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.96	0.47
1:A:111:LEU:HD23	1:E:30:HIS:O	2.13	0.47
1:A:223:LEU:C	1:A:225:PRO:HD2	2.39	0.47
1:C:90:GLU:HG2	1:D:99:PRO:HG2	1.96	0.47
1:D:88:PHE:CD2	1:E:99:PRO:HB3	2.50	0.47
1:C:40:LEU:HD23	1:D:73:LEU:HD11	1.96	0.47
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.96	0.47
1:D:30:HIS:CE1	1:E:107:GLY:HA3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:GLN:HE21	1:C:180:HIS:CE1	2.32	0.47
1:B:30:HIS:O	1:C:111:LEU:HD23	2.15	0.47
1:C:88:PHE:CD2	1:D:99:PRO:HB3	2.50	0.47
1:E:175:SER:O	1:E:178:PHE:HB3	2.15	0.47
1:A:175:SER:O	1:A:178:PHE:HB3	2.15	0.46
1:B:40:LEU:CD2	1:C:73:LEU:HD11	2.45	0.46
1:B:113:TRP:CD1	6:B:308[B]:RET:H14	2.51	0.46
1:B:175:SER:O	1:B:178:PHE:HB3	2.16	0.46
1:C:223:LEU:C	1:C:225:PRO:HD2	2.41	0.46
1:A:30:HIS:CE1	1:B:107:GLY:HA3	2.49	0.46
1:C:33:THR:HG22	1:D:74:LEU:CD1	2.46	0.46
1:D:223:LEU:C	1:D:225:PRO:HD2	2.41	0.46
1:A:88:PHE:CD2	1:B:99:PRO:HB3	2.51	0.45
1:B:30:HIS:C	1:C:111:LEU:CD2	2.90	0.45
1:C:175:SER:O	1:C:178:PHE:HB3	2.17	0.45
1:C:90:GLU:OE1	1:D:99:PRO:HG2	2.17	0.45
1:D:40:LEU:HD23	1:E:73:LEU:HD11	1.99	0.45
1:E:194:GLU:H	1:E:194:GLU:HG2	1.57	0.45
1:B:223:LEU:C	1:B:225:PRO:HD2	2.42	0.45
6:B:308[B]:RET:H8	6:B:308[B]:RET:C16	2.29	0.45
1:E:223:LEU:C	1:E:225:PRO:HD2	2.42	0.45
1:D:175:SER:O	1:D:178:PHE:HB3	2.16	0.44
1:E:36:TYR:CD2	1:E:76:TYR:HA	2.52	0.44
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.99	0.44
1:A:36:TYR:CD2	1:A:76:TYR:HA	2.53	0.44
1:E:68:MET:HE1	1:E:255[B]:LYS:HB3	2.00	0.44
1:C:70[B]:SER:HB3	7:C:408:HOH:O	2.17	0.44
1:D:31:ILE:HD12	1:D:31:ILE:HA	1.91	0.44
6:B:308[A]:RET:H8	6:B:308[A]:RET:C16	2.30	0.44
1:B:67:VAL:HG12	1:B:68:MET:HE2	1.99	0.43
1:A:186:LYS:HD2	1:A:208:TRP:CZ2	2.53	0.43
1:D:231:ASP:N	4:D:305:BOG:O6	2.33	0.43
1:A:34:LEU:HD11	1:B:115:ILE:HG12	2.00	0.43
1:A:30:HIS:C	1:B:111:LEU:CD2	2.92	0.43
1:B:164:LEU:HD11	4:B:304:BOG:C1'	2.47	0.43
1:E:101:GLY:O	1:E:102:ASP:HB2	2.19	0.43
1:A:73:LEU:HD11	1:E:40:LEU:HD23	2.01	0.43
1:C:45:TYR:CE1	3:C:302:LFA:H101	2.54	0.43
1:C:101:GLY:O	1:C:102:ASP:HB2	2.18	0.43
1:A:101:GLY:O	1:A:102:ASP:HB2	2.19	0.42
1:B:219:PRO:HG3	6:B:308[B]:RET:H183	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLY:O	1:B:102:ASP:HB2	2.20	0.42
1:E:227:LEU:HD23	1:E:227:LEU:HA	1.92	0.42
1:A:33:THR:HG22	1:B:74:LEU:CD1	2.49	0.42
1:A:111:LEU:CD2	1:E:30:HIS:O	2.67	0.42
1:B:219:PRO:HG3	6:B:308[A]:RET:H183	1.99	0.42
1:C:88:PHE:HD2	1:D:99:PRO:HB3	1.85	0.42
1:D:34:LEU:HD12	1:E:115:ILE:HD11	2.02	0.42
1:A:40:LEU:CD2	1:B:73:LEU:HD11	2.49	0.42
1:A:182:LEU:HD23	1:A:211:PHE:HE1	1.85	0.42
1:B:90:GLU:CG	1:C:99:PRO:HG2	2.49	0.42
1:B:216:THR:O	1:B:219:PRO:HD2	2.19	0.42
1:D:40:LEU:CD2	1:E:73:LEU:HD11	2.49	0.42
1:A:30:HIS:O	1:B:111:LEU:HD23	2.20	0.42
6:B:308[A]:RET:H7	6:B:308[A]:RET:H181	1.85	0.41
1:C:33:THR:HG22	1:D:74:LEU:HD11	2.01	0.41
6:E:307[B]:RET:C8	6:E:307[B]:RET:C16	2.89	0.41
1:C:41:ALA:HB1	1:D:66:VAL:HG13	2.02	0.41
1:D:68:MET:HE1	1:D:255[A]:LYS:HB3	2.00	0.41
1:D:164:LEU:HD12	1:D:164:LEU:HA	1.80	0.41
1:D:66:VAL:CG1	1:D:119:MET:CE	2.98	0.41
6:B:308[B]:RET:H7	6:B:308[B]:RET:H181	1.85	0.41
1:D:74:LEU:HD12	1:D:74:LEU:HA	1.94	0.41
1:D:90:GLU:OE1	1:E:99:PRO:HG2	2.20	0.41
1:A:34:LEU:HD12	1:A:38:VAL:HG23	2.02	0.41
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.93	0.41
1:E:218:TYR:N	1:E:219:PRO:HD2	2.36	0.41
6:A:307[A]:RET:H181	6:A:307[A]:RET:H7	1.85	0.41
1:D:68:MET:HE1	1:D:255[B]:LYS:HB3	2.01	0.41
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.87	0.41
6:C:307[B]:RET:H181	6:C:307[B]:RET:H7	1.84	0.41
1:D:30:HIS:O	1:E:111:LEU:HD23	2.20	0.41
6:A:307[B]:RET:H181	6:A:307[B]:RET:H7	1.86	0.41
1:B:36:TYR:CD2	1:B:76:TYR:HA	2.55	0.41
1:B:235:TYR:CD1	4:B:304:BOG:H62	2.55	0.41
6:C:307[A]:RET:H181	6:C:307[A]:RET:H7	1.85	0.41
1:D:63:LEU:HD23	1:D:63:LEU:HA	1.91	0.41
1:A:99:PRO:HB3	1:E:88:PHE:HD2	1.86	0.41
1:A:216:THR:O	1:A:219:PRO:HG2	2.21	0.41
1:D:36:TYR:HB3	1:D:75:LEU:HB3	2.02	0.41
6:E:307[B]:RET:H181	6:E:307[B]:RET:H7	1.81	0.41
1:C:36:TYR:CD2	1:C:76:TYR:HA	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:GLY:O	1:D:102:ASP:HB2	2.22	0.40
1:D:36:TYR:CD2	1:D:76:TYR:HA	2.56	0.40
1:D:88:PHE:HD2	1:E:99:PRO:HB3	1.84	0.40
1:D:90:GLU:HG2	1:E:99:PRO:HG2	2.03	0.40
6:D:308[A]:RET:H11	6:D:308[A]:RET:H191	1.95	0.40
1:A:119:MET:HE1	3:A:309:LFA:C18	2.50	0.40
1:A:218:TYR:N	1:A:219:PRO:HD2	2.35	0.40
1:C:218:TYR:N	1:C:219:PRO:HD2	2.35	0.40
1:A:33:THR:HA	1:A:36:TYR:CE2	2.57	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	270/273 (99%)	264 (98%)	6 (2%)	0	100	100
1	B	270/273 (99%)	265 (98%)	5 (2%)	0	100	100
1	C	270/273 (99%)	265 (98%)	5 (2%)	0	100	100
1	D	272/273 (100%)	265 (97%)	7 (3%)	0	100	100
1	E	271/273 (99%)	266 (98%)	5 (2%)	0	100	100
All	All	1353/1365 (99%)	1325 (98%)	28 (2%)	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	226/234 (97%)	210 (93%)	16 (7%)	13	15
1	B	224/234 (96%)	207 (92%)	17 (8%)	12	13
1	C	226/234 (97%)	212 (94%)	14 (6%)	16	19
1	D	226/234 (97%)	215 (95%)	11 (5%)	22	28
1	E	227/234 (97%)	215 (95%)	12 (5%)	20	25
All	All	1129/1170 (96%)	1059 (94%)	70 (6%)	18	19

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	56	LYS
1	A	61	ASN
1	A	70[A]	SER
1	A	70[B]	SER
1	A	74	LEU
1	A	92	VAL
1	A	103	LEU
1	A	111	LEU
1	A	112	ASN
1	A	114	LEU
1	A	119	MET
1	A	132	THR
1	A	164	LEU
1	A	186	LYS
1	A	230	VAL
1	B	56	LYS
1	B	70[A]	SER
1	B	70[B]	SER
1	B	74	LEU
1	B	84	SER
1	B	91	GLU
1	B	92	VAL
1	B	103	LEU
1	B	111	LEU
1	B	112	ASN
1	B	114	LEU
1	B	130	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	132	THR
1	B	133	SER
1	B	139	ARG
1	B	186	LYS
1	B	230	VAL
1	C	34	LEU
1	C	44	LEU
1	C	56	LYS
1	C	70[A]	SER
1	C	70[B]	SER
1	C	74	LEU
1	C	92	VAL
1	C	111	LEU
1	C	112	ASN
1	C	114	LEU
1	C	132	THR
1	C	164	LEU
1	C	194	GLU
1	C	230	VAL
1	D	34	LEU
1	D	70[A]	SER
1	D	70[B]	SER
1	D	74	LEU
1	D	75	LEU
1	D	92	VAL
1	D	111	LEU
1	D	112	ASN
1	D	114	LEU
1	D	132	THR
1	D	230	VAL
1	E	4	GLU
1	E	44	LEU
1	E	61	ASN
1	E	70[A]	SER
1	E	70[B]	SER
1	E	74	LEU
1	E	92	VAL
1	E	111	LEU
1	E	112	ASN
1	E	132	THR
1	E	194	GLU
1	E	230	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	78	GLN
1	A	81	ASN
1	B	7	ASN
1	B	80	GLN
1	C	7	ASN
1	C	78	GLN
1	C	81	ASN
1	C	141	GLN
1	C	163	ASN
1	C	180	HIS
1	D	7	ASN
1	D	81	ASN
1	E	180	HIS

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](#)

Of 45 ligands modelled in this entry, 5 are monoatomic - leaving 40 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
6	RET	B	308[A]	1	20,20,21	1.57	3 (15%)	27,27,28	1.01	1 (3%)
4	BOG	C	304	-	20,20,20	1.10	1 (5%)	25,25,25	0.83	0
4	BOG	A	303	-	20,20,20	1.08	1 (5%)	25,25,25	0.87	0
4	BOG	E	304	-	20,20,20	1.10	1 (5%)	25,25,25	0.98	1 (4%)
3	LFA	A	305	-	15,15,19	0.07	0	14,14,18	0.07	0
3	LFA	A	309	-	13,13,19	0.10	0	12,12,18	0.08	0
3	LFA	B	306	-	14,14,19	0.08	0	13,13,18	0.07	0
3	LFA	A	304	-	5,5,19	0.12	0	4,4,18	0.09	0
5	OLC	D	307	-	14,14,24	1.25	1 (7%)	15,15,25	0.95	1 (6%)
3	LFA	B	302	-	11,11,19	0.09	0	10,10,18	0.10	0
3	LFA	C	308	-	18,18,19	0.06	0	17,17,18	0.08	0
6	RET	C	307[A]	1	20,20,21	1.50	3 (15%)	27,27,28	1.08	2 (7%)
6	RET	E	307[A]	1	20,20,21	1.52	3 (15%)	27,27,28	1.05	2 (7%)
3	LFA	E	305	-	5,5,19	0.14	0	4,4,18	0.11	0
3	LFA	A	308	-	17,17,19	0.08	0	16,16,18	0.07	0
4	BOG	B	304	-	20,20,20	1.12	1 (5%)	25,25,25	0.79	0
4	BOG	D	305	-	20,20,20	1.09	1 (5%)	25,25,25	0.83	0
6	RET	A	307[A]	1	20,20,21	1.51	3 (15%)	27,27,28	1.01	2 (7%)
6	RET	B	308[B]	1	20,20,21	1.63	3 (15%)	27,27,28	1.01	1 (3%)
6	RET	D	308[A]	1	20,20,21	1.57	3 (15%)	27,27,28	1.03	1 (3%)
3	LFA	D	304	-	17,17,19	0.08	0	16,16,18	0.07	0
3	LFA	C	302	-	14,14,19	0.08	0	13,13,18	0.07	0
3	LFA	B	303	-	17,17,19	0.08	0	16,16,18	0.05	0
5	OLC	A	306	-	14,14,24	1.22	1 (7%)	15,15,25	1.04	2 (13%)
3	LFA	C	305	-	4,4,19	0.13	0	3,3,18	0.22	0
5	OLC	C	306	-	15,15,24	1.14	1 (6%)	16,16,25	1.00	2 (12%)
5	OLC	E	306	-	14,14,24	1.22	1 (7%)	15,15,25	1.07	2 (13%)
3	LFA	D	306	-	5,5,19	0.13	0	4,4,18	0.11	0
6	RET	C	307[B]	1	20,20,21	1.53	3 (15%)	27,27,28	1.07	2 (7%)
3	LFA	E	303	-	17,17,19	0.08	0	16,16,18	0.07	0
6	RET	E	307[B]	1	20,20,21	1.62	3 (15%)	27,27,28	1.04	2 (7%)
3	LFA	D	302	-	10,10,19	0.09	0	9,9,18	0.10	0
5	OLC	B	307	-	14,14,24	1.21	1 (7%)	15,15,25	1.02	2 (13%)
6	RET	A	307[B]	1	20,20,21	1.59	3 (15%)	27,27,28	1.01	1 (3%)
6	RET	D	308[B]	1	20,20,21	1.61	3 (15%)	27,27,28	1.03	1 (3%)
3	LFA	E	302	-	15,15,19	0.08	0	14,14,18	0.07	0
3	LFA	B	305	-	5,5,19	0.12	0	4,4,18	0.14	0
5	OLC	C	303	-	20,20,24	1.07	1 (5%)	21,21,25	1.03	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LFA	A	302	-	9,9,19	0.11	0	8,8,18	0.12	0
3	LFA	D	303	-	13,13,19	0.09	0	12,12,18	0.08	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
6	RET	B	308[A]	1	-	0/13/30/31	0/1/1/1
4	BOG	C	304	-	-	7/11/31/31	0/1/1/1
4	BOG	A	303	-	-	5/11/31/31	0/1/1/1
4	BOG	E	304	-	-	5/11/31/31	0/1/1/1
3	LFA	A	305	-	-	9/13/13/17	-
3	LFA	A	309	-	-	3/11/11/17	-
3	LFA	B	306	-	-	8/12/12/17	-
3	LFA	A	304	-	-	2/3/3/17	-
5	OLC	D	307	-	-	6/14/14/24	-
3	LFA	B	302	-	-	3/9/9/17	-
3	LFA	C	308	-	-	11/16/16/17	-
6	RET	C	307[A]	1	-	0/13/30/31	0/1/1/1
6	RET	E	307[A]	1	-	0/13/30/31	0/1/1/1
3	LFA	E	305	-	-	2/3/3/17	-
3	LFA	A	308	-	-	9/15/15/17	-
4	BOG	B	304	-	-	9/11/31/31	0/1/1/1
4	BOG	D	305	-	-	3/11/31/31	0/1/1/1
6	RET	A	307[A]	1	-	0/13/30/31	0/1/1/1
6	RET	B	308[B]	1	-	2/13/30/31	0/1/1/1
6	RET	D	308[A]	1	-	0/13/30/31	0/1/1/1
3	LFA	D	304	-	-	8/15/15/17	-
3	LFA	C	302	-	-	6/12/12/17	-
3	LFA	B	303	-	-	8/15/15/17	-
5	OLC	A	306	-	-	7/14/14/24	-
3	LFA	C	305	-	-	0/2/2/17	-
5	OLC	C	306	-	-	8/15/15/24	-
5	OLC	E	306	-	-	6/14/14/24	-
3	LFA	D	306	-	-	3/3/3/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	RET	C	307[B]	1	-	1/13/30/31	0/1/1/1
3	LFA	E	303	-	-	7/15/15/17	-
6	RET	E	307[B]	1	-	4/13/30/31	0/1/1/1
3	LFA	D	302	-	-	5/8/8/17	-
5	OLC	B	307	-	-	6/14/14/24	-
6	RET	A	307[B]	1	-	0/13/30/31	0/1/1/1
6	RET	D	308[B]	1	-	2/13/30/31	0/1/1/1
3	LFA	E	302	-	-	6/13/13/17	-
3	LFA	B	305	-	-	1/3/3/17	-
5	OLC	C	303	-	-	8/20/20/24	-
3	LFA	A	302	-	-	0/7/7/17	-
3	LFA	D	303	-	-	5/11/11/17	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	308[B]	RET	C14-C13	4.95	1.37	1.33
6	E	307[B]	RET	C14-C13	4.91	1.37	1.33
6	D	308[B]	RET	C14-C13	4.79	1.37	1.33
6	A	307[B]	RET	C14-C13	4.77	1.37	1.33
5	C	303	OLC	O20-C1	4.56	1.46	1.33
6	B	308[A]	RET	C14-C13	4.52	1.36	1.33
5	D	307	OLC	O20-C1	4.46	1.46	1.33
6	D	308[A]	RET	C14-C13	4.44	1.36	1.33
5	E	306	OLC	O20-C1	4.33	1.46	1.33
5	A	306	OLC	O20-C1	4.33	1.46	1.33
6	C	307[B]	RET	C14-C13	4.33	1.36	1.33
6	E	307[A]	RET	C14-C13	4.32	1.36	1.33
5	B	307	OLC	O20-C1	4.29	1.45	1.33
6	C	307[A]	RET	C14-C13	4.13	1.36	1.33
5	C	306	OLC	O20-C1	4.13	1.45	1.33
6	A	307[A]	RET	C14-C13	4.13	1.36	1.33
4	B	304	BOG	O5-C1	3.73	1.51	1.41
4	C	304	BOG	O5-C1	3.70	1.51	1.41
4	E	304	BOG	O5-C1	3.70	1.51	1.41
4	A	303	BOG	O5-C1	3.61	1.51	1.41
4	D	305	BOG	O5-C1	3.59	1.51	1.41
6	B	308[A]	RET	C8-C9	-2.79	1.40	1.46
6	A	307[A]	RET	C8-C9	-2.75	1.40	1.46
6	B	308[B]	RET	C8-C9	-2.73	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	307[B]	RET	C8-C9	-2.69	1.40	1.46
6	D	308[A]	RET	C8-C9	-2.65	1.40	1.46
6	D	308[B]	RET	C8-C9	-2.61	1.40	1.46
6	E	307[A]	RET	C8-C9	-2.61	1.40	1.46
6	E	307[B]	RET	C8-C9	-2.59	1.40	1.46
6	C	307[A]	RET	C8-C9	-2.48	1.40	1.46
6	C	307[B]	RET	C8-C9	-2.46	1.40	1.46
6	D	308[B]	RET	C10-C9	2.33	1.41	1.35
6	D	308[A]	RET	C10-C9	2.31	1.41	1.35
6	E	307[B]	RET	C10-C9	2.31	1.41	1.35
6	C	307[B]	RET	C10-C9	2.30	1.41	1.35
6	A	307[B]	RET	C10-C9	2.28	1.41	1.35
6	C	307[A]	RET	C10-C9	2.25	1.41	1.35
6	B	308[B]	RET	C10-C9	2.25	1.41	1.35
6	A	307[A]	RET	C10-C9	2.20	1.40	1.35
6	B	308[A]	RET	C10-C9	2.18	1.40	1.35
6	E	307[A]	RET	C10-C9	2.14	1.40	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	307[A]	RET	C19-C9-C10	-3.60	116.99	122.82
6	E	307[B]	RET	C19-C9-C10	-3.55	117.06	122.82
6	E	307[A]	RET	C19-C9-C10	-3.52	117.11	122.82
6	C	307[B]	RET	C19-C9-C10	-3.51	117.13	122.82
6	D	308[A]	RET	C19-C9-C10	-3.41	117.29	122.82
6	B	308[A]	RET	C19-C9-C10	-3.39	117.32	122.82
6	A	307[A]	RET	C19-C9-C10	-3.36	117.36	122.82
6	D	308[B]	RET	C19-C9-C10	-3.34	117.41	122.82
6	A	307[B]	RET	C19-C9-C10	-3.33	117.43	122.82
6	B	308[B]	RET	C19-C9-C10	-3.30	117.46	122.82
5	C	303	OLC	O20-C1-C2	3.30	121.91	111.83
5	E	306	OLC	O20-C1-C2	2.94	120.81	111.83
5	A	306	OLC	O20-C1-C2	2.82	120.42	111.83
5	B	307	OLC	O20-C1-C2	2.79	120.34	111.83
5	C	306	OLC	O20-C1-C2	2.69	120.04	111.83
5	D	307	OLC	O20-C1-C2	2.55	119.61	111.83
5	A	306	OLC	O20-C1-O19	-2.30	117.87	123.63
6	E	307[B]	RET	C8-C9-C10	2.29	122.61	119.01
5	C	306	OLC	O20-C1-O19	-2.26	117.96	123.63
4	E	304	BOG	C1-C2-C3	2.22	114.68	110.01
5	E	306	OLC	O20-C1-O19	-2.16	118.22	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	307[B]	RET	C19-C9-C8	2.13	121.35	118.09
6	E	307[A]	RET	C19-C9-C8	2.09	121.28	118.09
6	C	307[A]	RET	C19-C9-C8	2.07	121.24	118.09
5	B	307	OLC	O20-C1-O19	-2.04	118.54	123.63
6	A	307[A]	RET	C19-C9-C8	2.01	121.15	118.09

There are no chirality outliers.

All (175) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	304	BOG	C2-C1-O1-C1'
4	C	304	BOG	O5-C1-O1-C1'
5	A	306	OLC	C21-C22-C24-O25
5	B	307	OLC	O20-C21-C22-O23
5	C	303	OLC	O20-C21-C22-O23
5	C	306	OLC	O20-C21-C22-C24
5	C	306	OLC	O20-C21-C22-O23
6	B	308[B]	RET	C20-C13-C14-C15
6	D	308[B]	RET	C20-C13-C14-C15
6	E	307[B]	RET	C11-C12-C13-C14
6	E	307[B]	RET	C12-C13-C14-C15
6	E	307[B]	RET	C20-C13-C14-C15
5	E	306	OLC	O19-C1-O20-C21
5	A	306	OLC	C2-C1-O20-C21
5	E	306	OLC	C2-C1-O20-C21
5	B	307	OLC	O19-C1-O20-C21
5	B	307	OLC	C2-C1-O20-C21
4	E	304	BOG	O5-C5-C6-O6
5	A	306	OLC	O19-C1-O20-C21
4	B	304	BOG	O5-C1-O1-C1'
5	C	303	OLC	O20-C21-C22-C24
5	E	306	OLC	O20-C21-C22-C24
4	B	304	BOG	C2-C1-O1-C1'
6	E	307[B]	RET	C11-C12-C13-C20
4	E	304	BOG	C4-C5-C6-O6
4	A	303	BOG	O5-C5-C6-O6
4	A	303	BOG	O1-C1'-C2'-C3'
4	A	303	BOG	C4-C5-C6-O6
4	C	304	BOG	C4-C5-C6-O6
4	C	304	BOG	O5-C5-C6-O6
5	E	306	OLC	O20-C21-C22-O23
3	D	304	LFA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	308	LFA	C15-C16-C17-C18
5	D	307	OLC	C21-C22-C24-O25
3	A	308	LFA	C12-C13-C14-C15
4	D	305	BOG	O1-C1'-C2'-C3'
3	A	308	LFA	C11-C10-C9-C8
3	B	303	LFA	C3-C4-C5-C6
3	D	303	LFA	C15-C16-C17-C18
5	A	306	OLC	C3-C4-C5-C6
3	C	308	LFA	C11-C10-C9-C8
5	A	306	OLC	O23-C22-C24-O25
3	D	304	LFA	C13-C14-C15-C16
3	A	305	LFA	C9-C10-C11-C12
3	D	304	LFA	C2-C3-C4-C5
5	C	306	OLC	C2-C3-C4-C5
4	D	305	BOG	C1'-C2'-C3'-C4'
4	E	304	BOG	C1'-C2'-C3'-C4'
4	C	304	BOG	C2'-C3'-C4'-C5'
3	E	303	LFA	C12-C13-C14-C15
3	A	308	LFA	C9-C10-C11-C12
5	D	307	OLC	C2-C1-O20-C21
3	C	308	LFA	C7-C8-C9-C10
5	C	306	OLC	C3-C4-C5-C6
3	C	308	LFA	C2-C3-C4-C5
3	D	302	LFA	C2-C3-C4-C5
3	E	303	LFA	C4-C5-C6-C7
3	B	306	LFA	C5-C6-C7-C8
5	C	306	OLC	C2-C1-O20-C21
3	E	302	LFA	C3-C4-C5-C6
3	D	304	LFA	C14-C15-C16-C17
3	E	303	LFA	C10-C11-C12-C13
3	B	303	LFA	C5-C6-C7-C8
3	B	306	LFA	C2-C3-C4-C5
4	A	303	BOG	C1'-C2'-C3'-C4'
3	A	305	LFA	C5-C6-C7-C8
3	E	303	LFA	C3-C4-C5-C6
3	C	308	LFA	C6-C7-C8-C9
3	A	305	LFA	C12-C13-C14-C15
3	D	306	LFA	C2-C3-C4-C5
4	C	304	BOG	C3'-C4'-C5'-C6'
3	B	303	LFA	C4-C5-C6-C7
3	B	306	LFA	C4-C5-C6-C7
5	C	306	OLC	O19-C1-O20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	307	OLC	O19-C1-O20-C21
3	B	306	LFA	C10-C11-C12-C13
4	B	304	BOG	C2'-C3'-C4'-C5'
5	C	303	OLC	C10-C11-C12-C13
5	A	306	OLC	C4-C5-C6-C7
3	A	308	LFA	C3-C4-C5-C6
3	B	303	LFA	C11-C10-C9-C8
6	B	308[B]	RET	C12-C13-C14-C15
6	D	308[B]	RET	C12-C13-C14-C15
3	A	308	LFA	C5-C6-C7-C8
3	A	308	LFA	C14-C15-C16-C17
3	B	303	LFA	C14-C15-C16-C17
3	C	302	LFA	C6-C7-C8-C9
3	A	308	LFA	C15-C16-C17-C18
3	B	305	LFA	C3-C4-C5-C6
3	A	309	LFA	C14-C15-C16-C17
4	A	303	BOG	C3'-C4'-C5'-C6'
3	B	302	LFA	C10-C11-C12-C13
4	E	304	BOG	O1-C1'-C2'-C3'
4	C	304	BOG	C2'-C1'-O1-C1
5	D	307	OLC	C2-C3-C4-C5
5	B	307	OLC	C5-C6-C7-C8
3	D	302	LFA	C1-C2-C3-C4
4	D	305	BOG	C5'-C6'-C7'-C8'
3	C	302	LFA	C10-C11-C12-C13
4	B	304	BOG	C3'-C4'-C5'-C6'
3	D	304	LFA	C4-C5-C6-C7
3	A	305	LFA	C1-C2-C3-C4
4	B	304	BOG	C1'-C2'-C3'-C4'
3	D	303	LFA	C17-C18-C19-C20
3	B	303	LFA	C9-C10-C11-C12
3	B	306	LFA	C11-C10-C9-C8
3	E	305	LFA	C2-C3-C4-C5
3	B	303	LFA	C7-C8-C9-C10
3	A	305	LFA	C10-C11-C12-C13
3	A	304	LFA	C2-C3-C4-C5
3	A	305	LFA	C13-C14-C15-C16
3	A	308	LFA	C11-C12-C13-C14
3	E	302	LFA	C11-C12-C13-C14
5	C	306	OLC	C4-C5-C6-C7
4	E	304	BOG	C5'-C6'-C7'-C8'
3	E	303	LFA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	304	BOG	C4-C5-C6-O6
3	D	303	LFA	C9-C10-C11-C12
3	D	303	LFA	C13-C14-C15-C16
3	E	302	LFA	C5-C6-C7-C8
3	A	308	LFA	C10-C11-C12-C13
5	E	306	OLC	C3-C4-C5-C6
3	D	303	LFA	C7-C8-C9-C10
3	E	302	LFA	C2-C3-C4-C5
5	B	307	OLC	C4-C5-C6-C7
3	B	303	LFA	C11-C12-C13-C14
3	C	302	LFA	C7-C8-C9-C10
3	D	306	LFA	C1-C2-C3-C4
3	A	309	LFA	C11-C12-C13-C14
3	C	302	LFA	C12-C13-C14-C15
3	B	306	LFA	C6-C7-C8-C9
3	E	302	LFA	C4-C5-C6-C7
5	D	307	OLC	O23-C22-C24-O25
3	A	305	LFA	C6-C7-C8-C9
3	A	304	LFA	C3-C4-C5-C6
5	B	307	OLC	O20-C21-C22-C24
3	A	309	LFA	C15-C16-C17-C18
6	C	307[B]	RET	C12-C13-C14-C15
3	C	308	LFA	C1-C2-C3-C4
3	E	305	LFA	C3-C4-C5-C6
5	D	307	OLC	C5-C6-C7-C8
5	A	306	OLC	C2-C3-C4-C5
3	A	305	LFA	C2-C3-C4-C5
3	D	302	LFA	C3-C4-C5-C6
5	E	306	OLC	C2-C3-C4-C5
3	D	304	LFA	C5-C6-C7-C8
4	B	304	BOG	C2'-C1'-O1-C1
4	B	304	BOG	O5-C5-C6-O6
3	C	308	LFA	C9-C10-C11-C12
5	C	303	OLC	C2-C1-O20-C21
3	B	306	LFA	C11-C12-C13-C14
3	E	303	LFA	C11-C10-C9-C8
3	C	308	LFA	C12-C13-C14-C15
3	C	308	LFA	C5-C6-C7-C8
5	C	303	OLC	O19-C1-O20-C21
3	E	302	LFA	C1-C2-C3-C4
5	C	303	OLC	C3-C4-C5-C6
3	C	308	LFA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	302	LFA	C11-C10-C9-C8
3	D	304	LFA	C9-C10-C11-C12
3	E	303	LFA	C1-C2-C3-C4
3	D	306	LFA	C3-C4-C5-C6
4	B	304	BOG	C4'-C5'-C6'-C7'
3	D	304	LFA	C12-C13-C14-C15
5	C	303	OLC	C21-C22-C24-O25
3	B	302	LFA	C15-C16-C17-C18
3	D	302	LFA	C7-C8-C9-C10
3	B	306	LFA	C3-C4-C5-C6
5	C	306	OLC	C6-C7-C8-C9
5	C	303	OLC	O23-C22-C24-O25
3	C	302	LFA	C3-C4-C5-C6
3	B	302	LFA	C9-C10-C11-C12
3	D	302	LFA	C5-C6-C7-C8
3	C	308	LFA	C13-C14-C15-C16
3	A	305	LFA	C3-C4-C5-C6

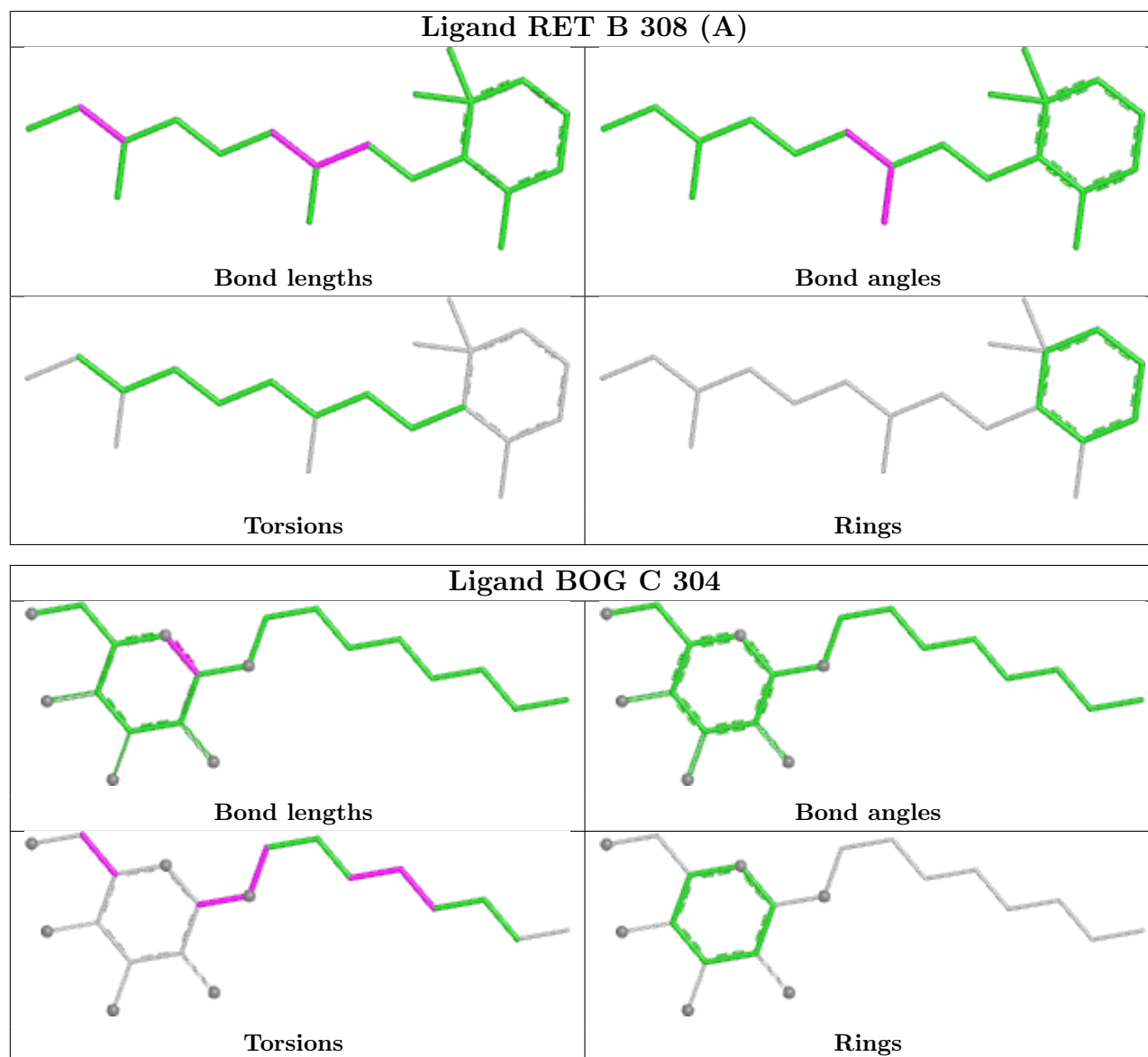
There are no ring outliers.

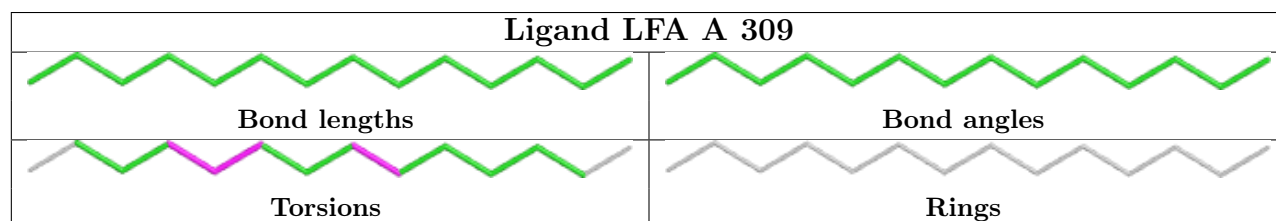
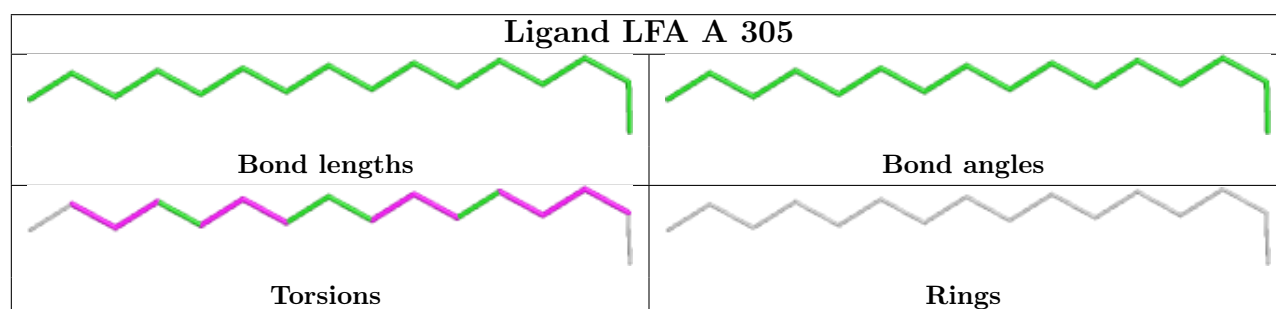
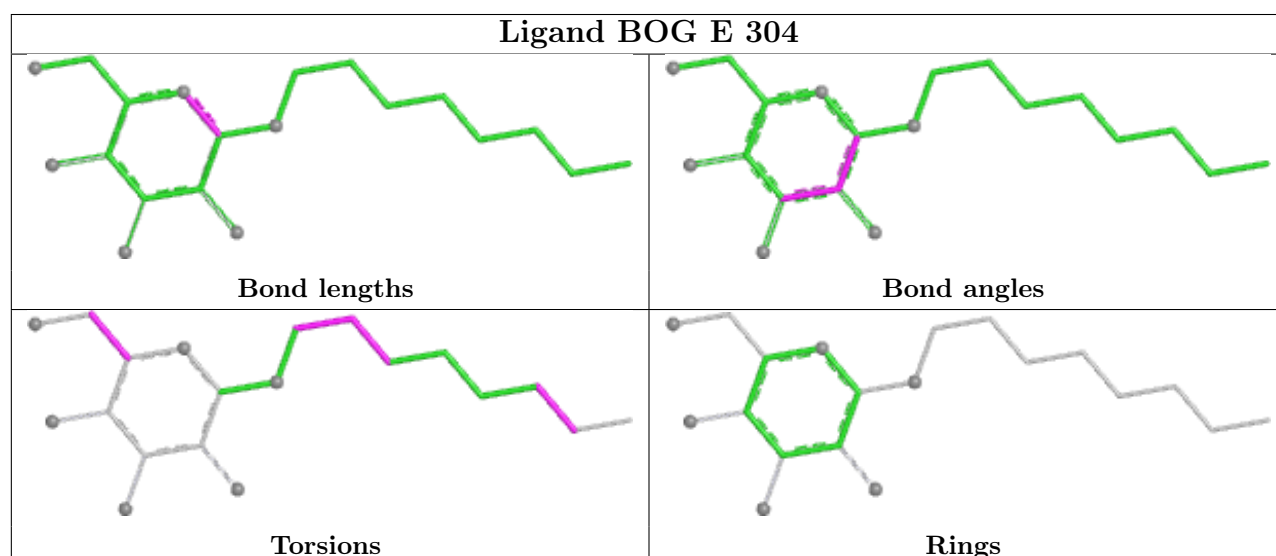
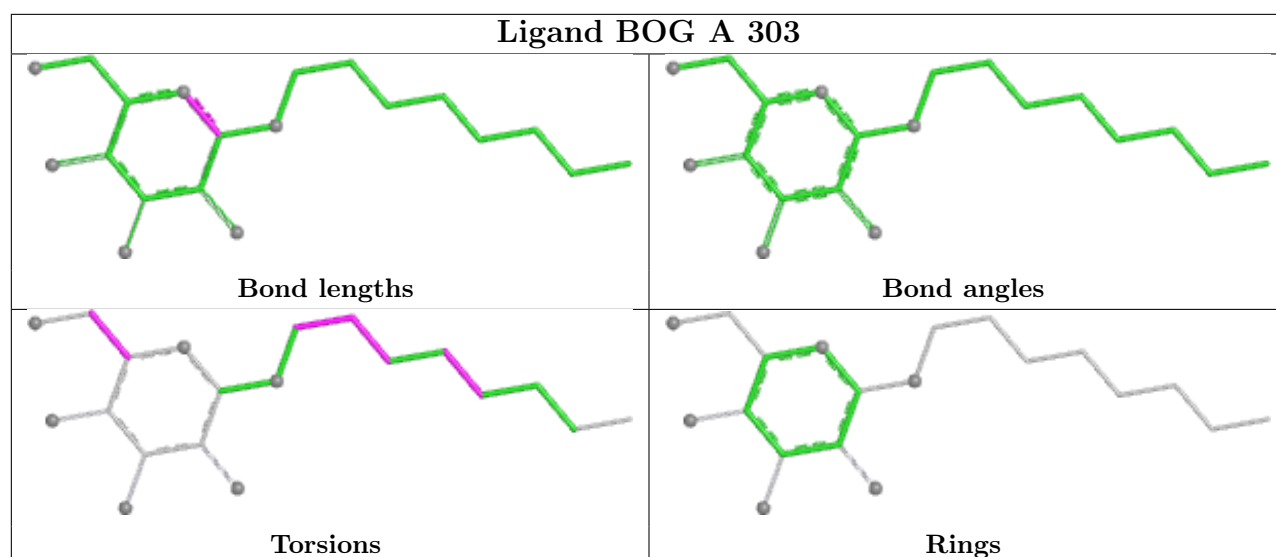
18 monomers are involved in 63 short contacts:

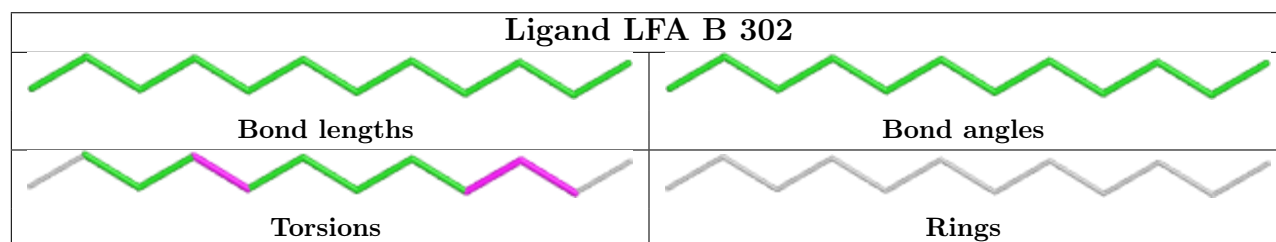
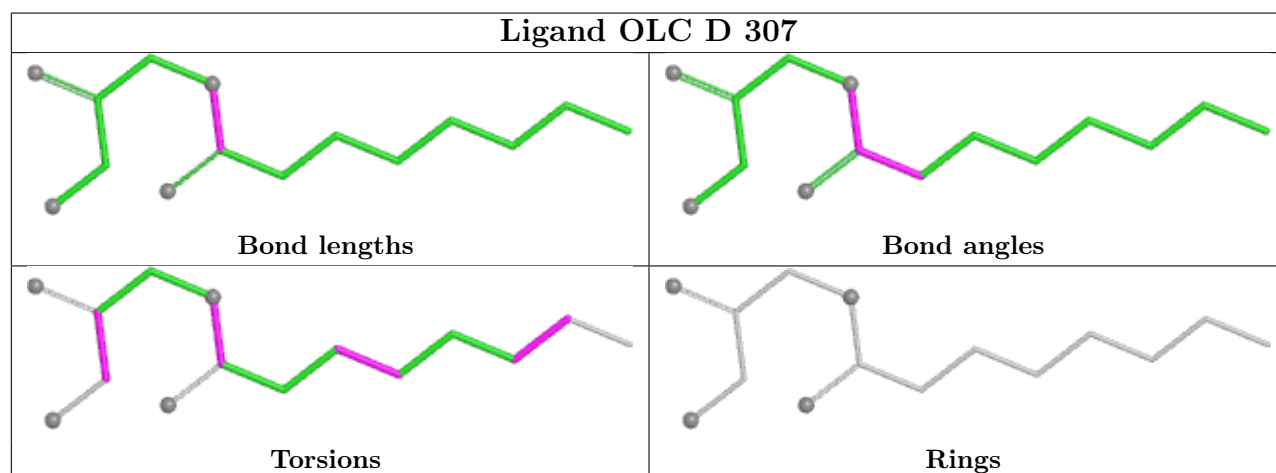
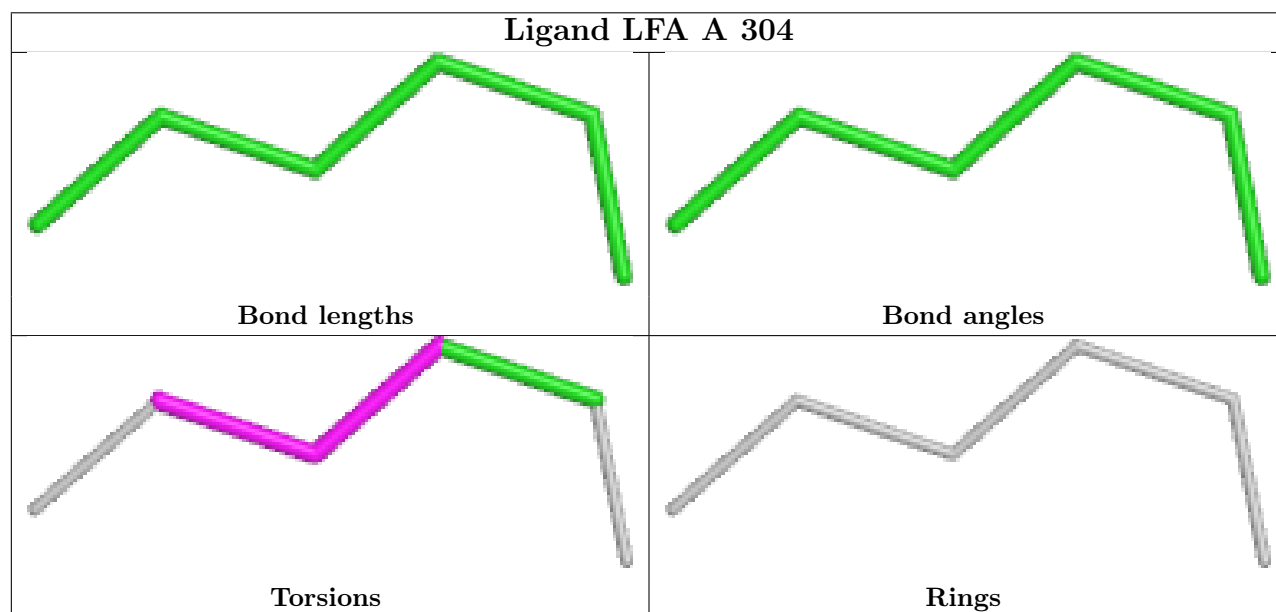
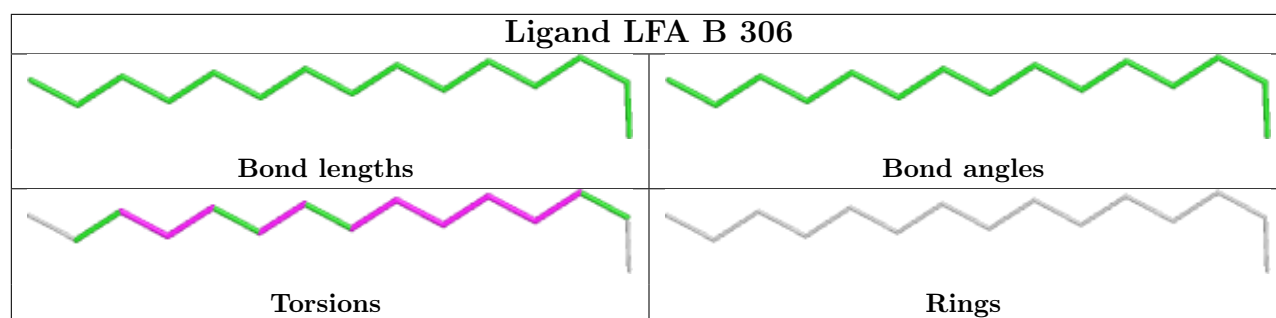
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	308[A]	RET	6	0
4	C	304	BOG	2	0
4	A	303	BOG	1	0
4	E	304	BOG	1	0
3	A	309	LFA	2	0
6	C	307[A]	RET	4	0
6	E	307[A]	RET	3	0
4	B	304	BOG	6	0
4	D	305	BOG	1	0
6	A	307[A]	RET	4	0
6	B	308[B]	RET	6	0
6	D	308[A]	RET	5	0
3	C	302	LFA	1	0
5	C	306	OLC	5	0
6	C	307[B]	RET	4	0
6	E	307[B]	RET	5	0
6	A	307[B]	RET	4	0
6	D	308[B]	RET	3	0

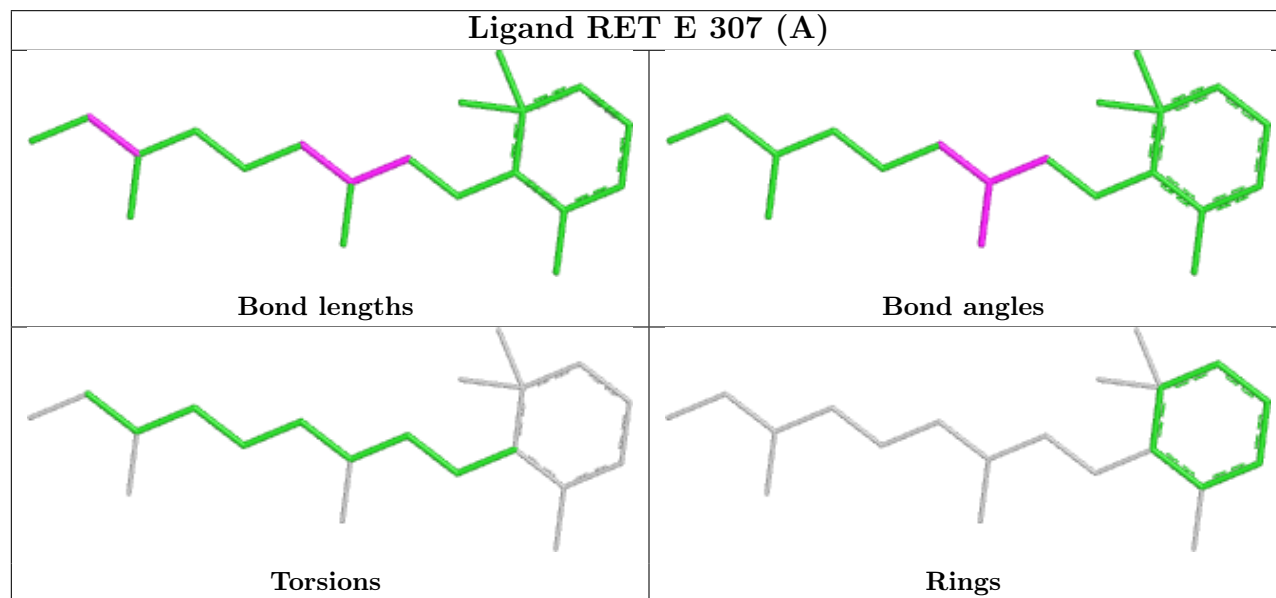
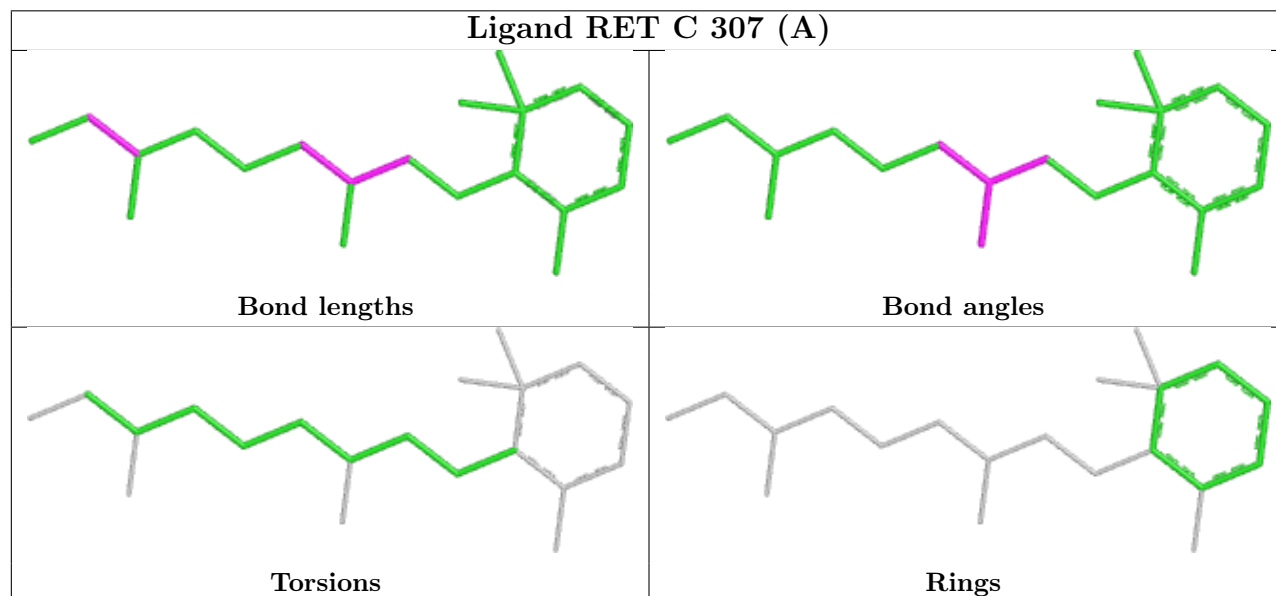
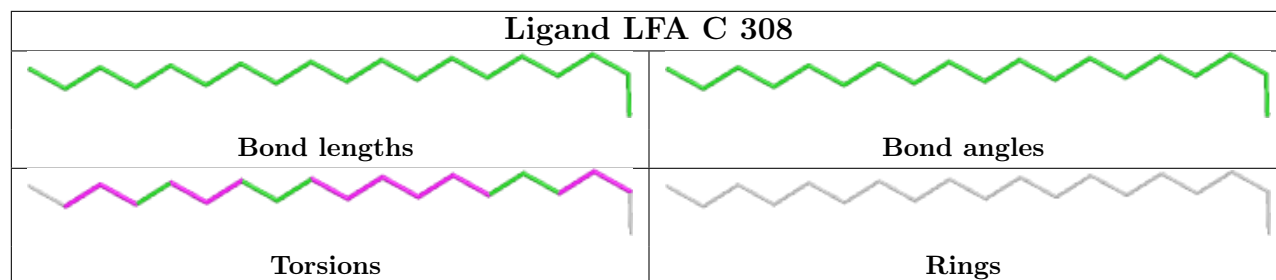
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

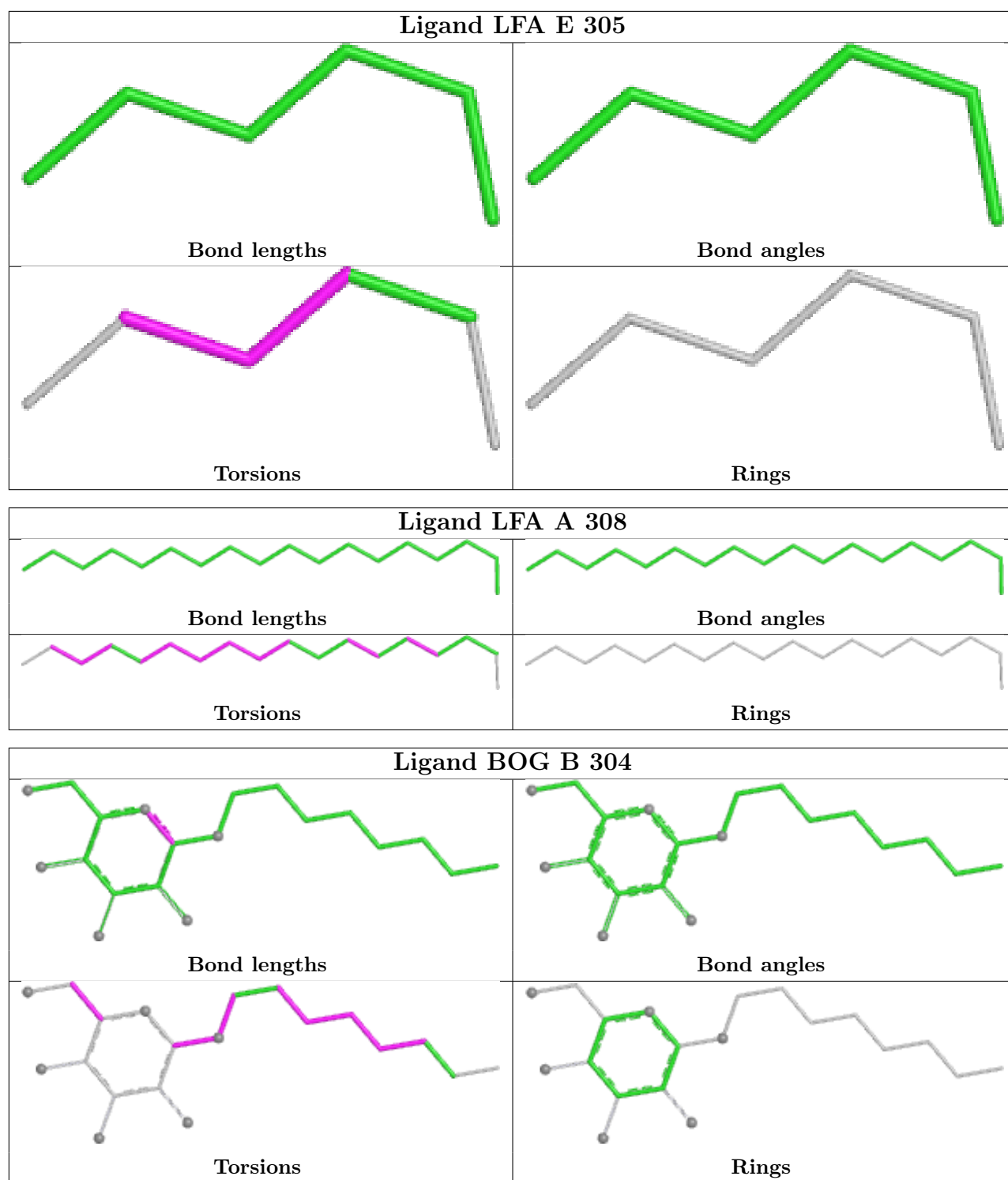
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

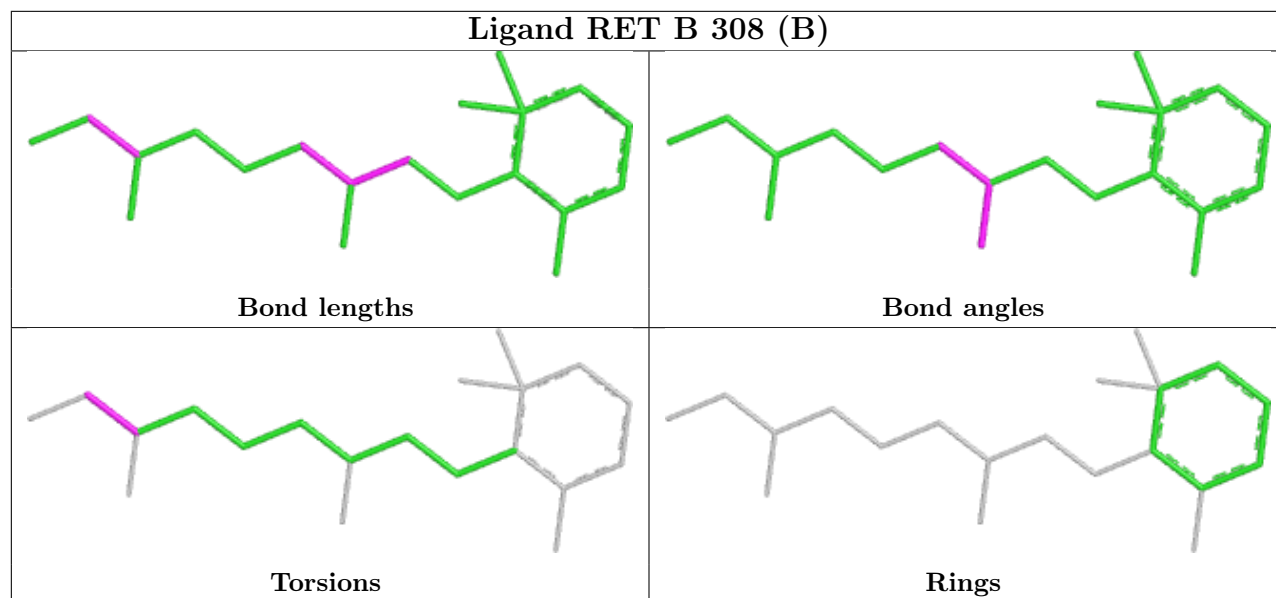
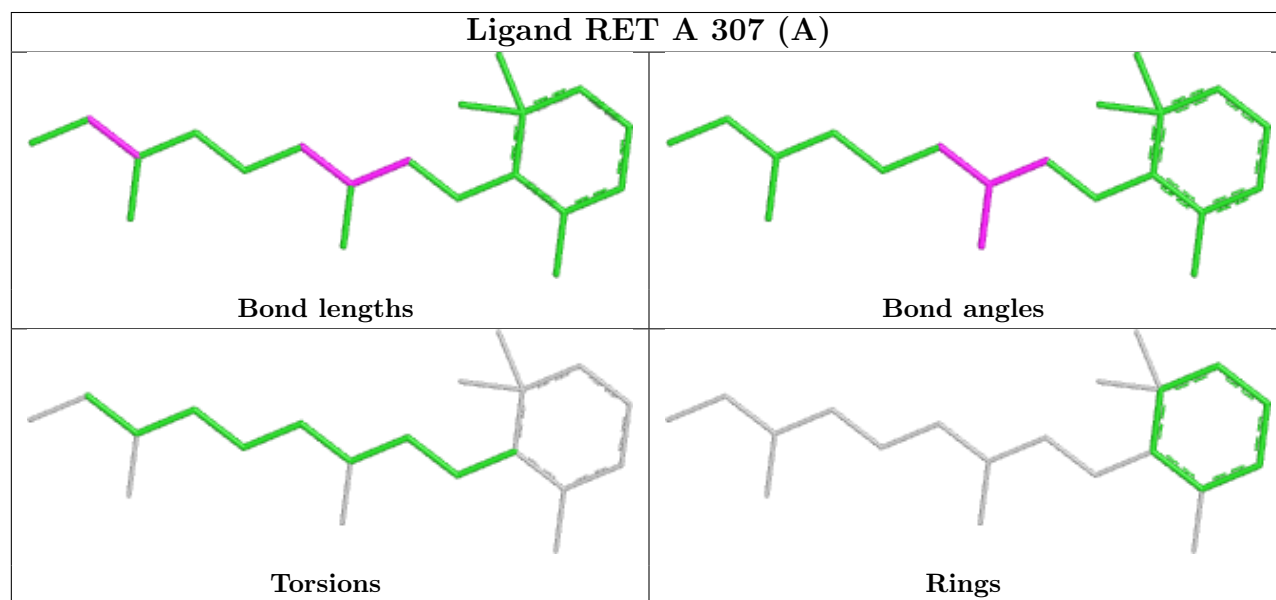
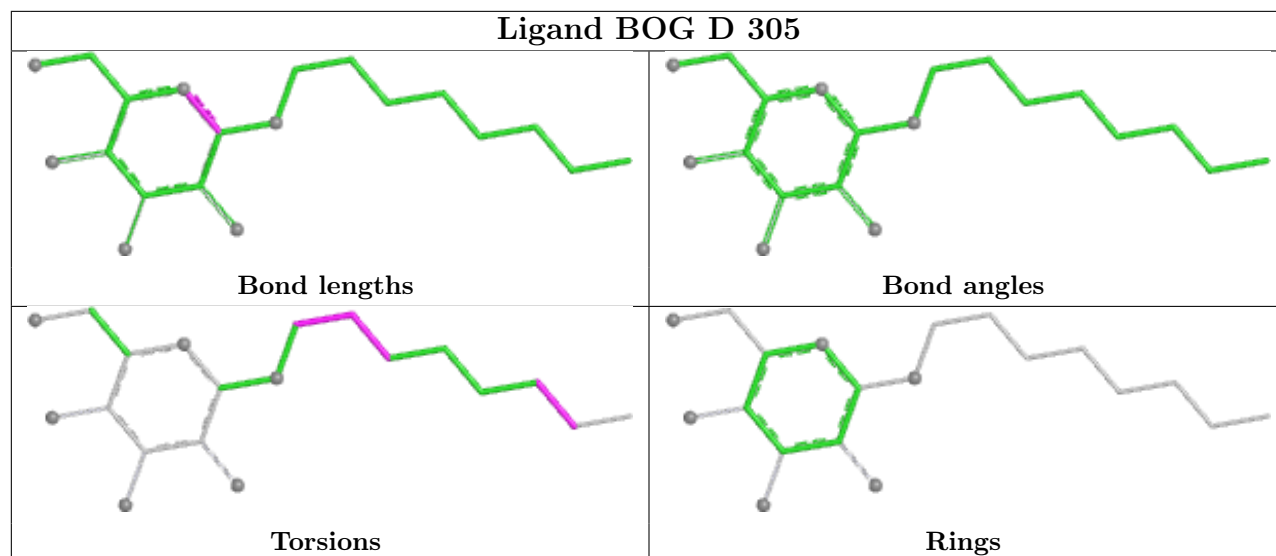


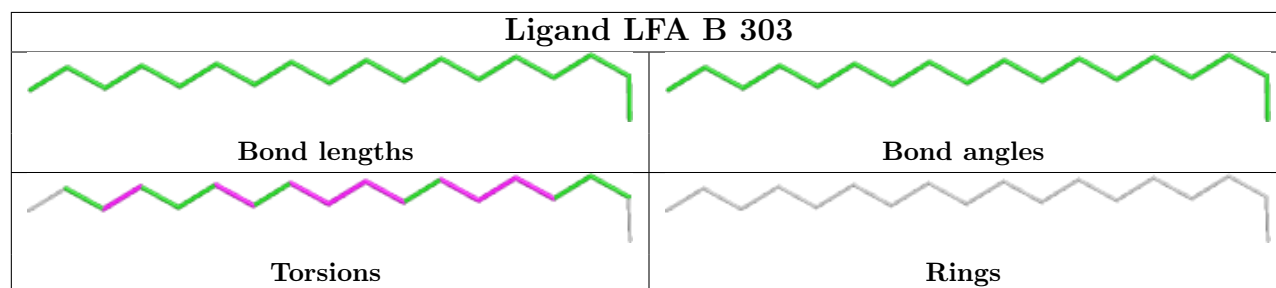
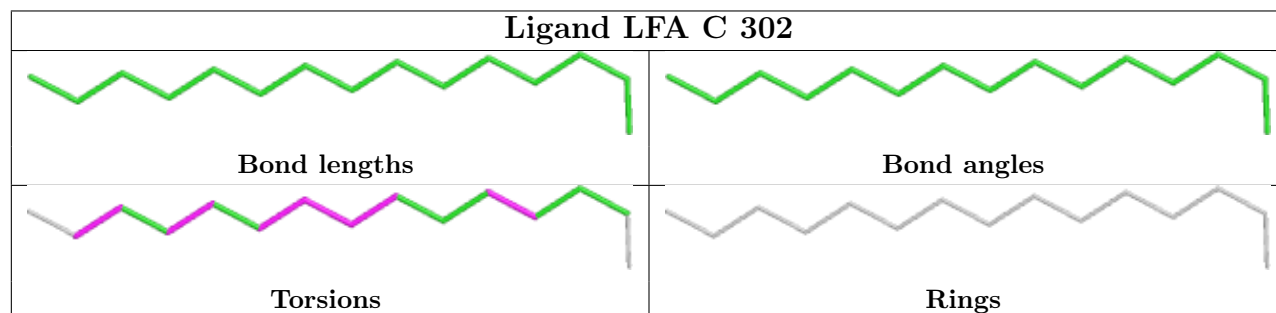
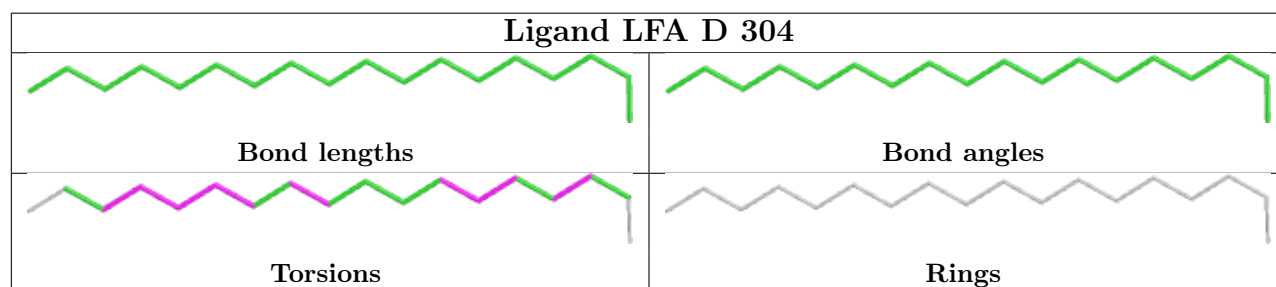
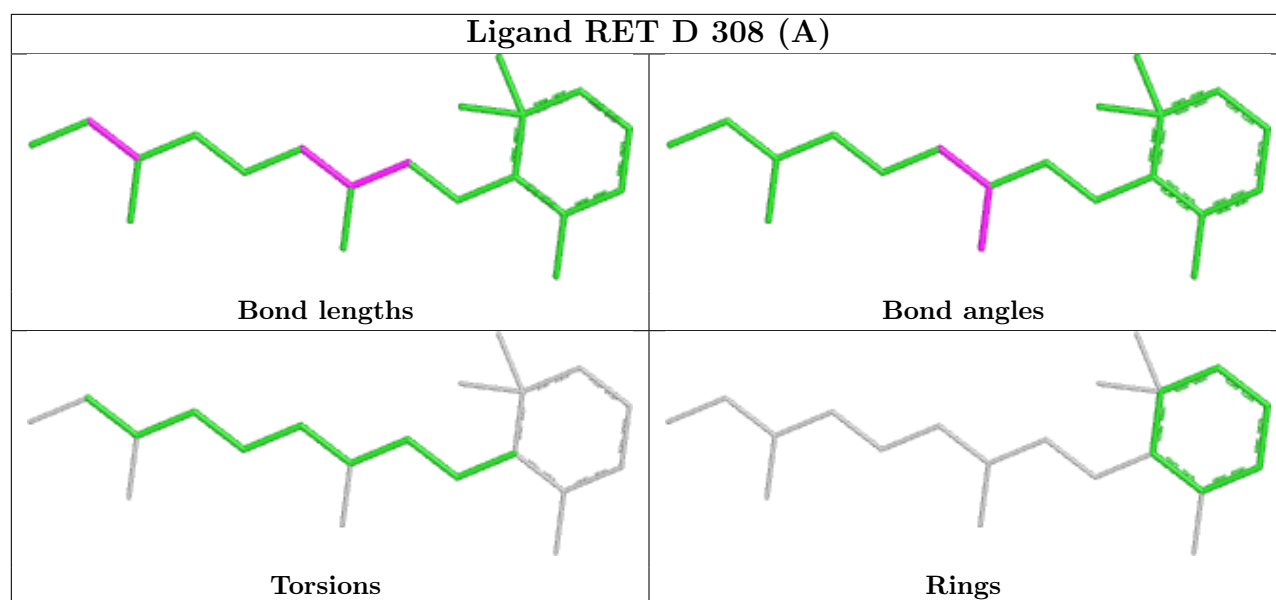


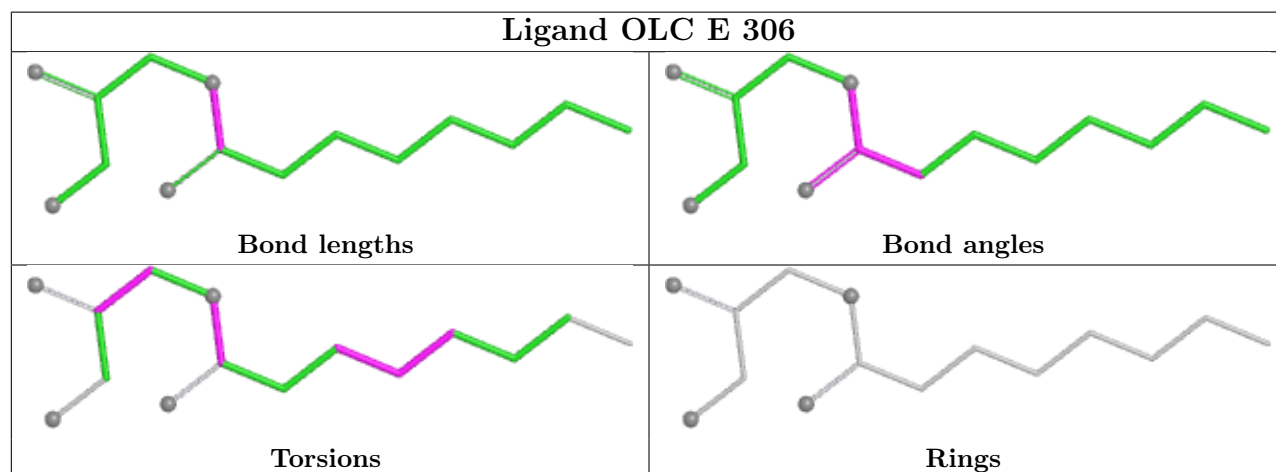
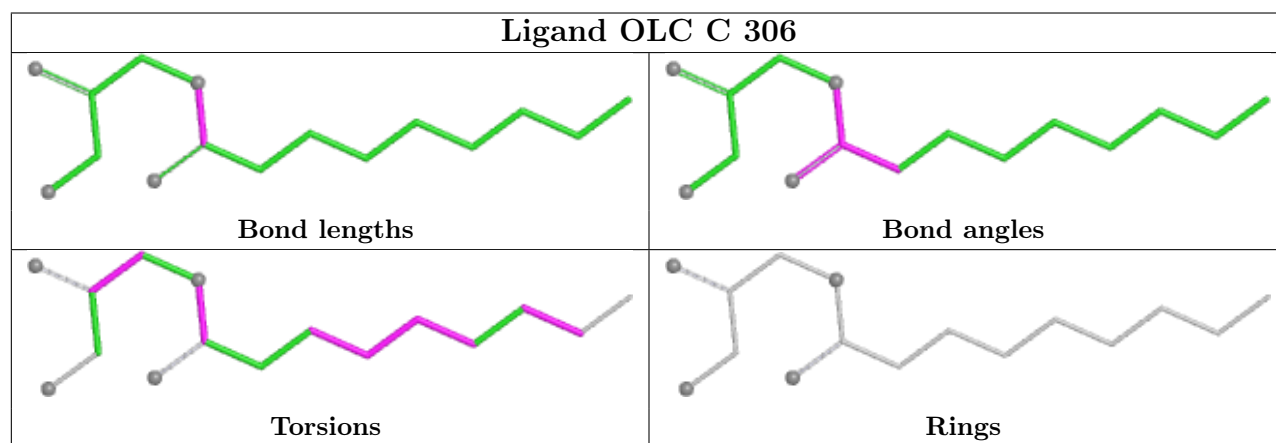
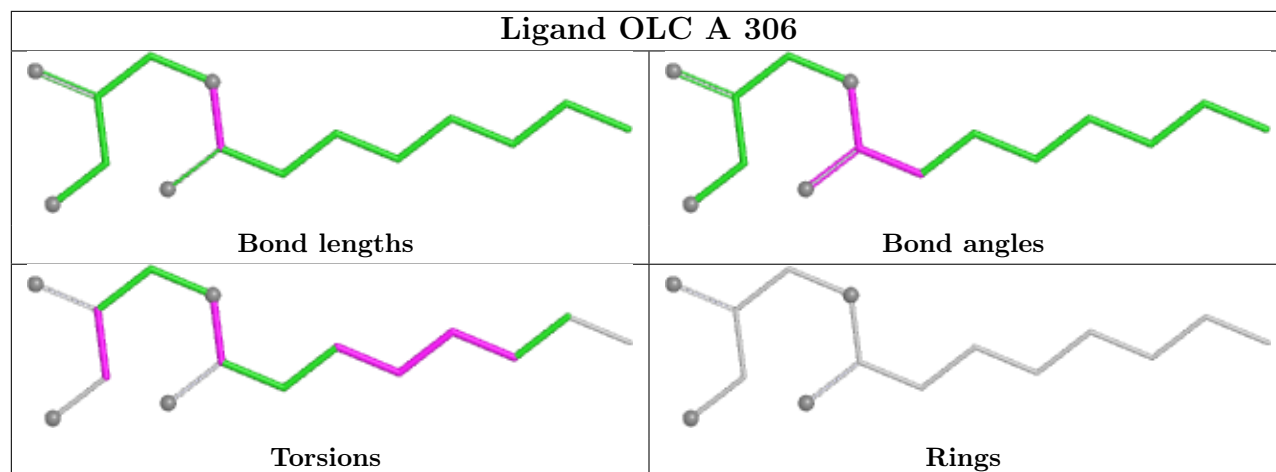


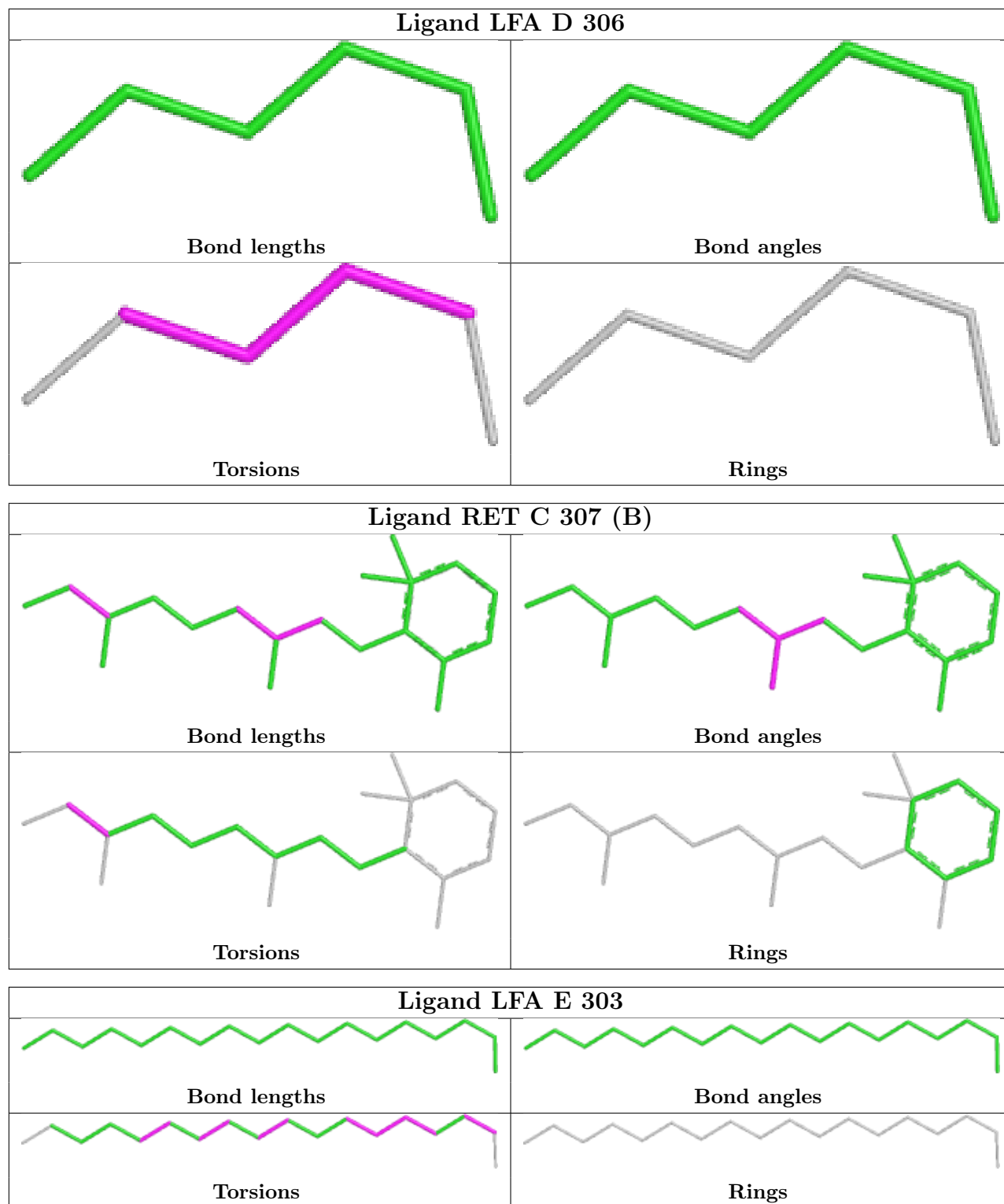


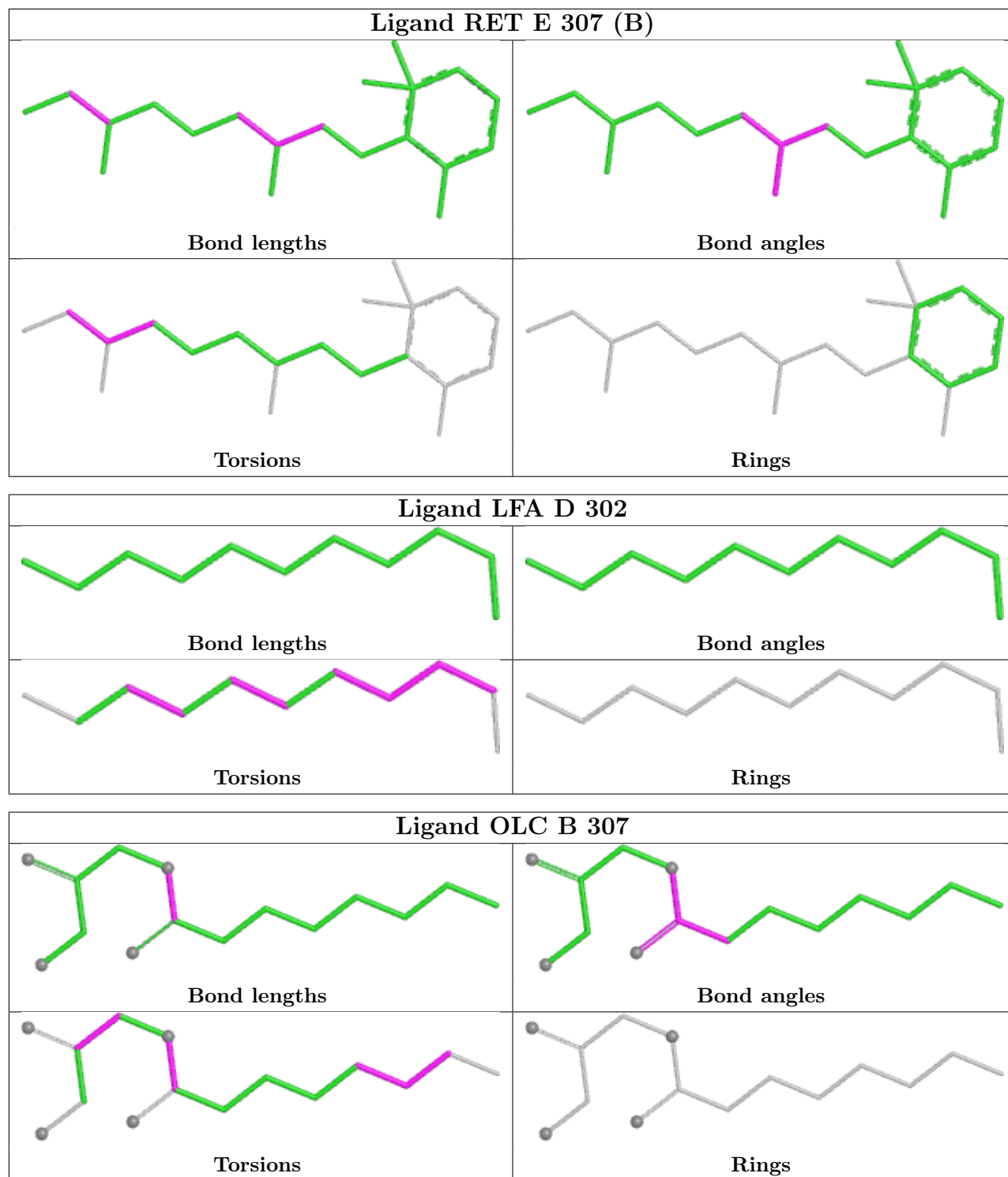


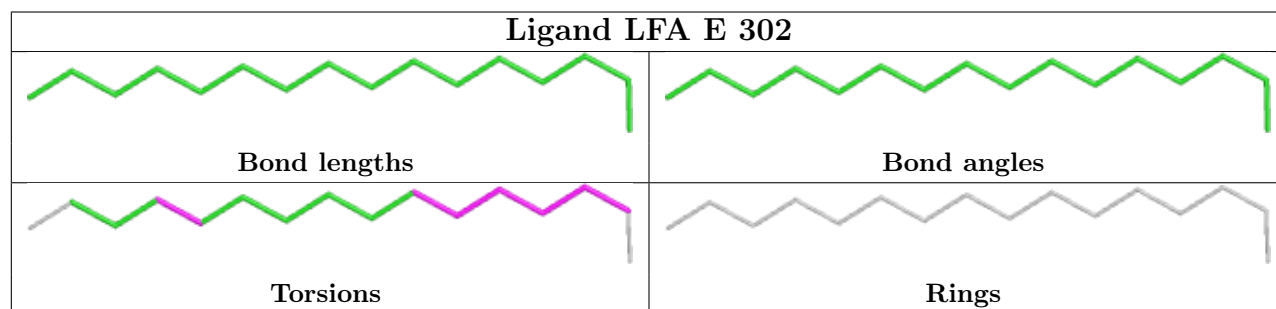
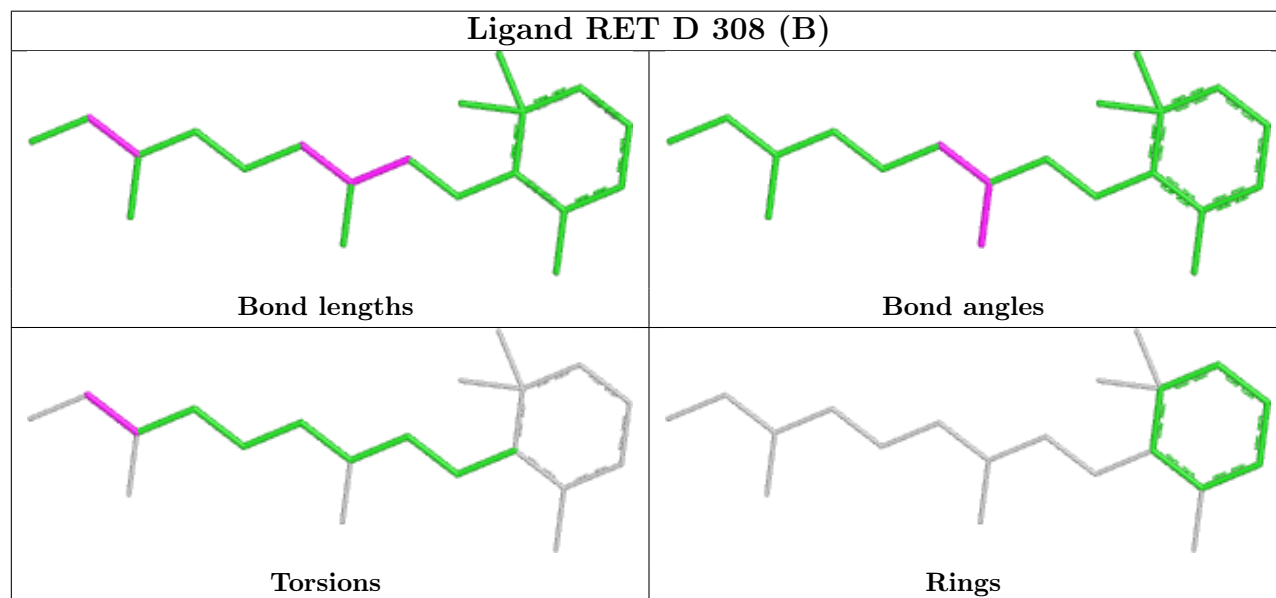
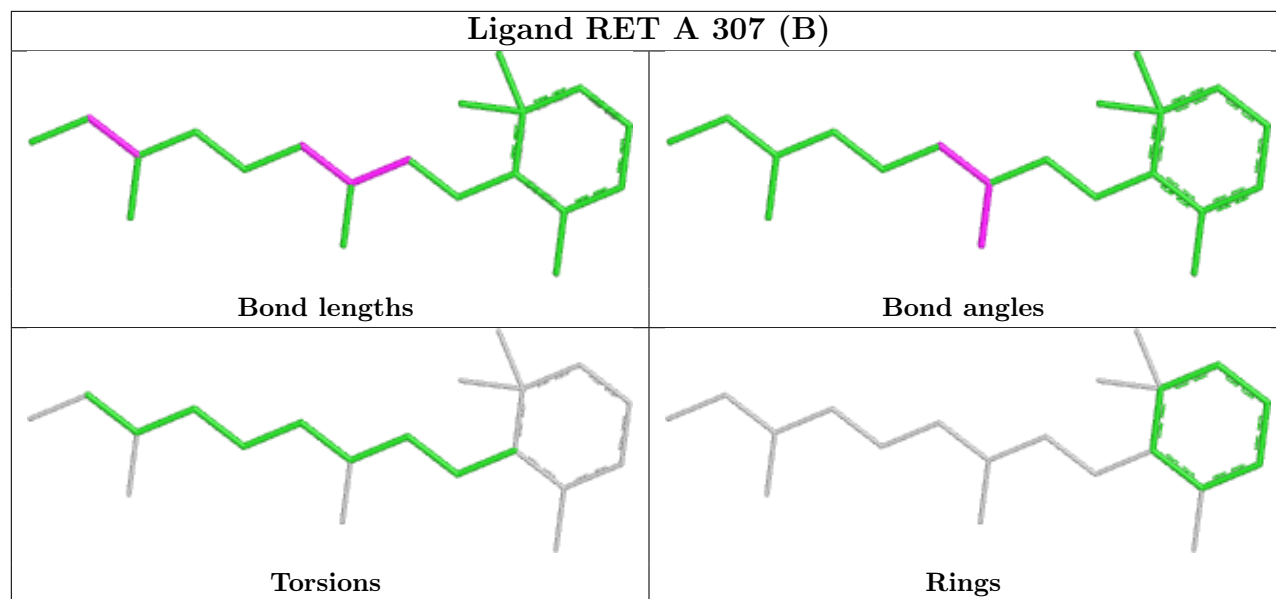


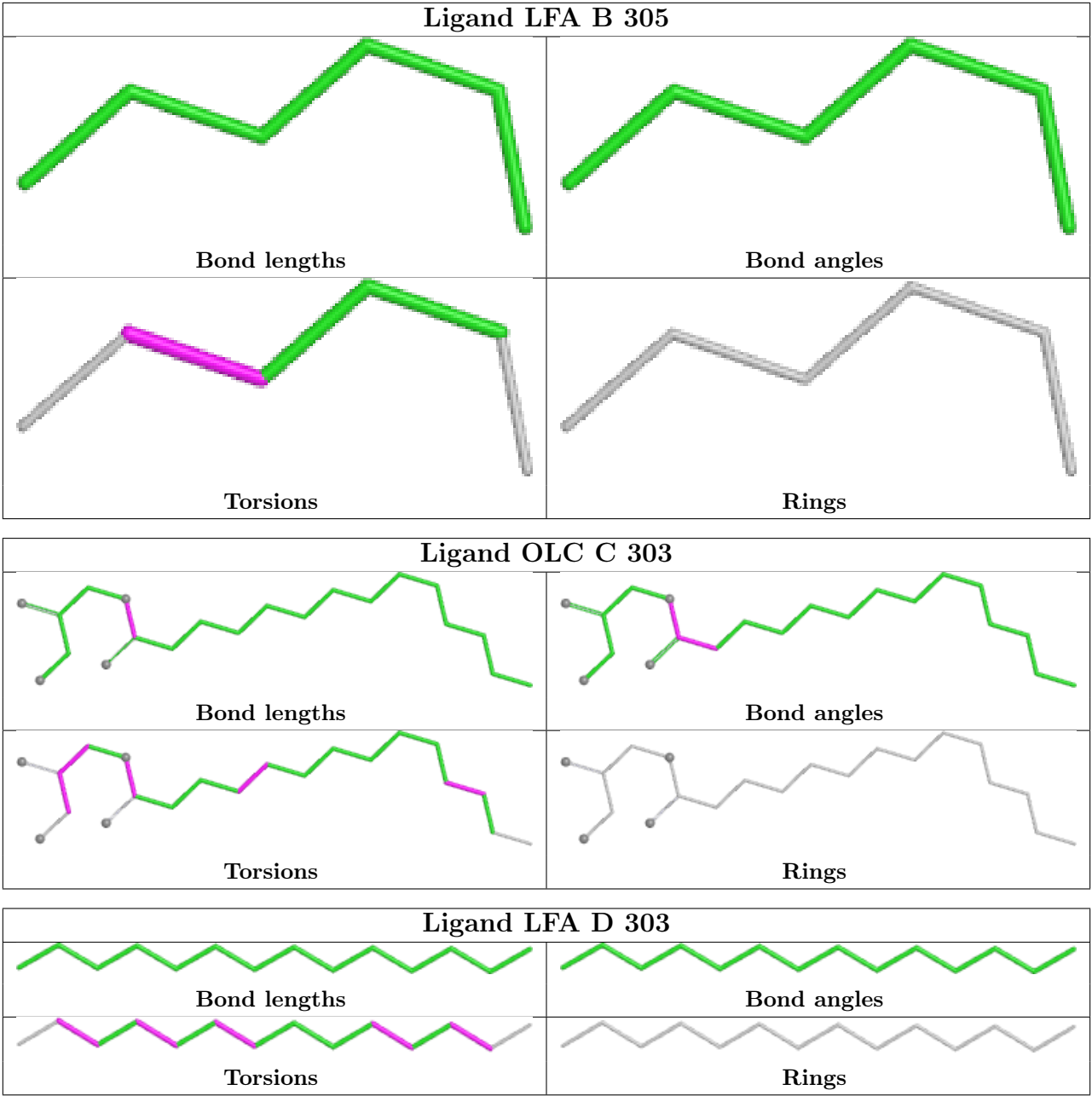












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	C	3
1	D	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	270:SER	C	271:LYS	N	2.19
1	B	270:SER	C	271:LYS	N	1.98
1	C	270:SER	C	271:LYS	N	1.94
1	C	70[B]:SER	C	71:ALA	N	1.06
1	D	70[B]:SER	C	71:ALA	N	0.99
1	B	70[B]:SER	C	71:ALA	N	0.97
1	C	70[A]:SER	C	71:ALA	N	0.97
1	B	70[A]:SER	C	71:ALA	N	0.92
1	D	70[A]:SER	C	71:ALA	N	0.90

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	269/273 (98%)	-0.29	2 (0%) 84 87	12, 32, 50, 79	4 (1%)
1	B	269/273 (98%)	-0.26	1 (0%) 88 91	13, 32, 56, 90	3 (1%)
1	C	269/273 (98%)	-0.28	1 (0%) 88 91	12, 32, 52, 80	3 (1%)
1	D	271/273 (99%)	-0.28	2 (0%) 84 87	12, 31, 53, 116	3 (1%)
1	E	269/273 (98%)	-0.32	2 (0%) 84 87	12, 32, 50, 78	4 (1%)
All	All	1347/1365 (98%)	-0.29	8 (0%) 85 89	12, 32, 53, 116	17 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	TRP	3.8
1	D	272	ASN	3.7
1	D	273	LYS	3.4
1	B	271	LYS	3.3
1	A	271	LYS	3.3
1	E	230	VAL	2.4
1	E	183	TRP	2.4
1	C	271	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	LFA	E	305	6/20	0.66	0.26	50,58,64,66	0
3	LFA	D	304	18/20	0.67	0.13	53,63,68,70	0
3	LFA	E	302	16/20	0.71	0.22	52,64,73,74	0
4	BOG	E	304	20/20	0.71	0.16	63,74,91,93	0
3	LFA	A	302	10/20	0.72	0.20	47,54,56,57	0
4	BOG	C	304	20/20	0.74	0.14	58,75,93,95	0
3	LFA	D	306	6/20	0.74	0.17	44,49,52,54	0
5	OLC	A	306	15/25	0.74	0.13	47,55,71,77	0
4	BOG	D	305	20/20	0.75	0.15	69,81,88,92	0
3	LFA	C	308	19/20	0.75	0.13	53,63,67,69	0
3	LFA	A	304	6/20	0.75	0.21	45,55,61,61	0
5	OLC	D	307	15/25	0.76	0.14	47,60,72,84	0
3	LFA	A	308	18/20	0.77	0.11	44,51,63,66	0
3	LFA	E	303	18/20	0.77	0.11	43,53,59,62	0
3	LFA	D	302	11/20	0.78	0.16	45,50,59,59	0
5	OLC	E	306	15/25	0.79	0.11	54,61,66,67	0
3	LFA	B	306	15/20	0.80	0.15	47,54,66,67	0
3	LFA	B	303	18/20	0.81	0.11	49,59,66,67	0
3	LFA	A	305	16/20	0.82	0.14	43,52,60,61	0
4	BOG	A	303	20/20	0.82	0.11	56,68,76,76	0
3	LFA	C	305	5/20	0.83	0.18	46,51,56,59	0
3	LFA	A	309	14/20	0.83	0.16	47,52,57,57	0
5	OLC	C	303	21/25	0.83	0.15	52,72,83,90	0
3	LFA	C	302	15/20	0.83	0.13	36,42,52,52	0
3	LFA	D	303	14/20	0.83	0.14	43,46,53,56	0
2	NA	B	301	1/1	0.84	0.07	30,30,30,30	0
3	LFA	B	305	6/20	0.84	0.19	47,48,52,54	0
3	LFA	B	302	12/20	0.84	0.16	52,57,72,73	0
4	BOG	B	304	20/20	0.85	0.11	53,65,79,79	0
5	OLC	C	306	16/25	0.85	0.12	42,56,65,67	0
2	NA	E	301	1/1	0.88	0.07	33,33,33,33	0
2	NA	C	301	1/1	0.90	0.06	30,30,30,30	0
5	OLC	B	307	15/25	0.91	0.10	45,58,70,84	0
6	RET	C	307[A]	20/21	0.91	0.09	25,29,31,31	20
6	RET	C	307[B]	20/21	0.91	0.09	29,32,33,33	20
6	RET	A	307[B]	20/21	0.93	0.09	28,30,32,33	20
2	NA	A	301	1/1	0.93	0.07	31,31,31,31	0

Continued on next page...

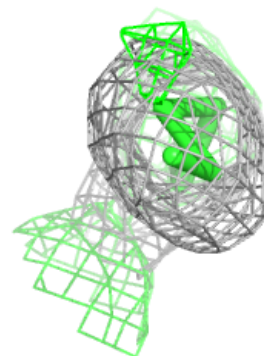
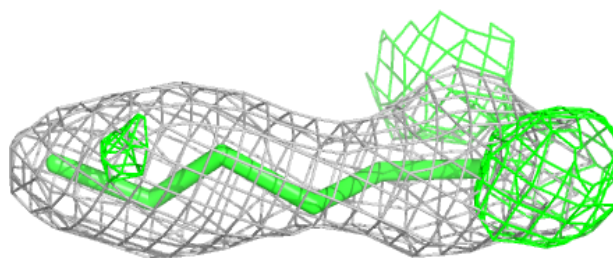
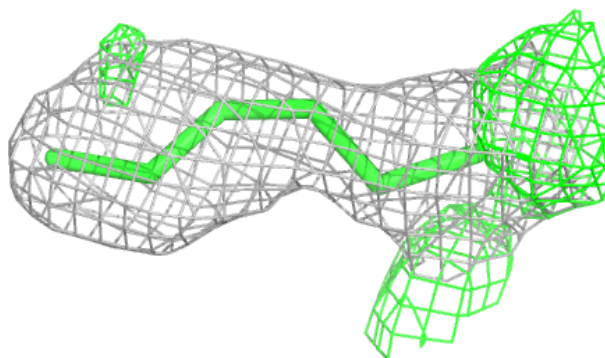
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	RET	A	307[A]	20/21	0.93	0.09	30,33,37,38	20
6	RET	B	308[B]	20/21	0.94	0.08	30,31,34,37	20
2	NA	D	301	1/1	0.94	0.08	33,33,33,33	0
6	RET	B	308[A]	20/21	0.94	0.08	28,30,32,33	20
6	RET	D	308[A]	20/21	0.95	0.08	31,33,36,38	20
6	RET	D	308[B]	20/21	0.95	0.08	24,28,32,34	20
6	RET	E	307[A]	20/21	0.95	0.08	27,31,34,35	20
6	RET	E	307[B]	20/21	0.95	0.08	30,33,37,37	20

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.

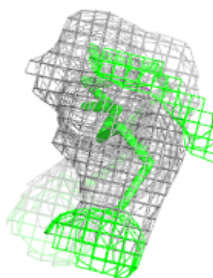
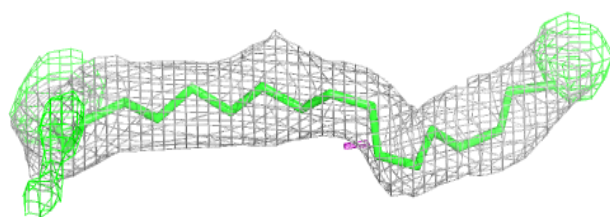
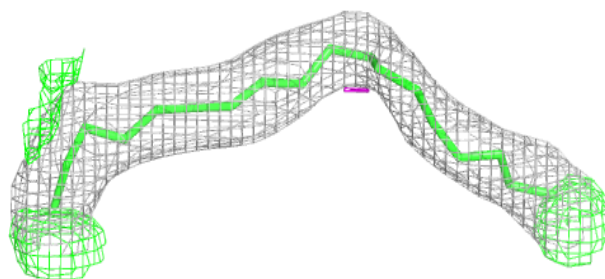
Electron density around LFA E 305:

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

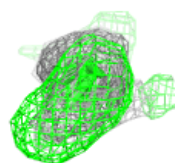
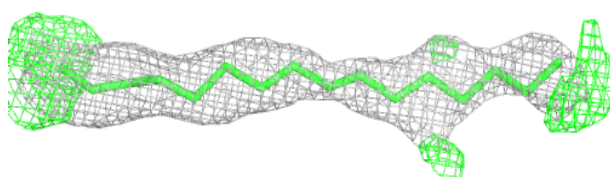
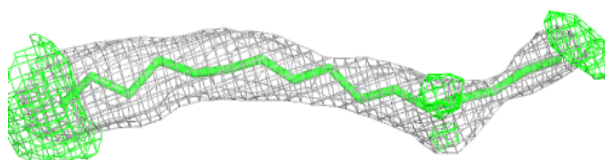


Electron density around LFA D 304:

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

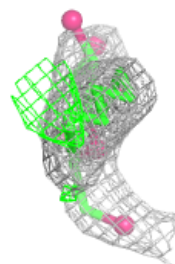
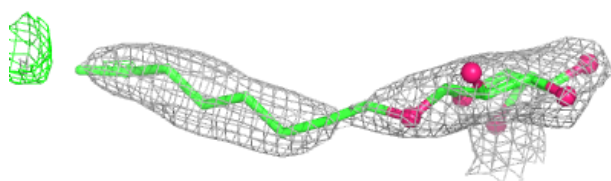
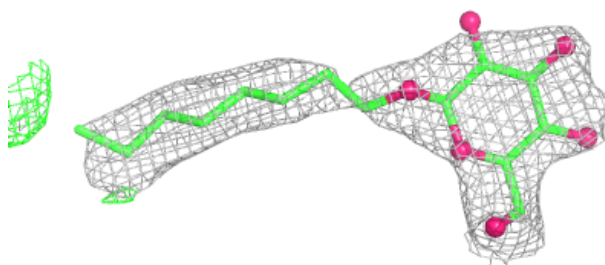
**Electron density around LFA E 302:**

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

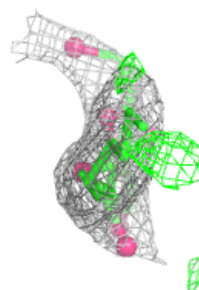
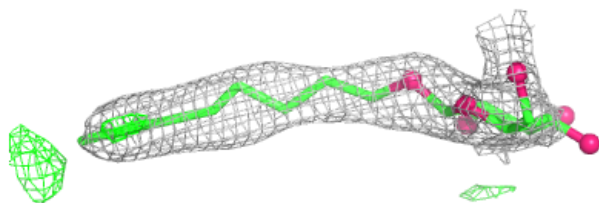
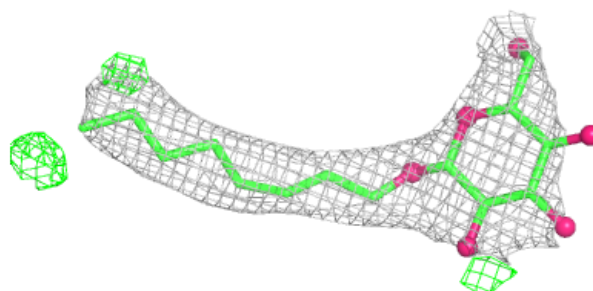


Electron density around BOG E 304:

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

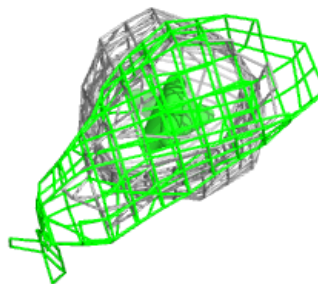
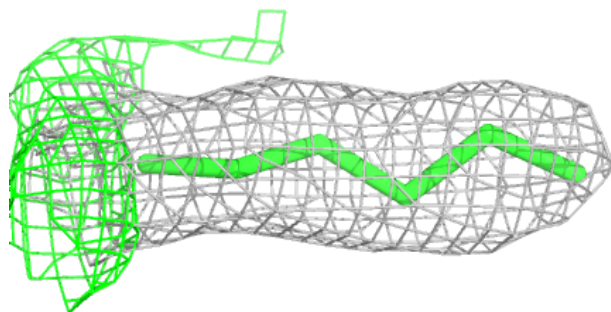
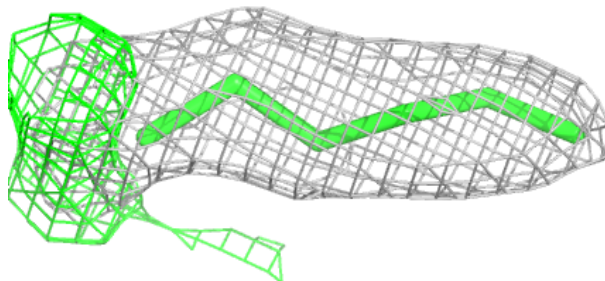
**Electron density around BOG C 304:**

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

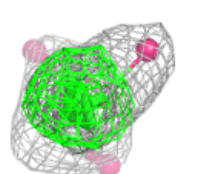
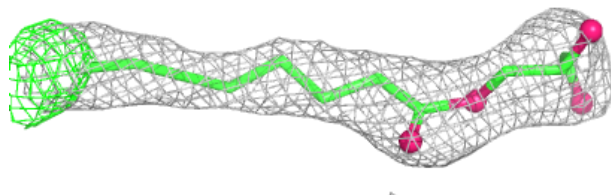
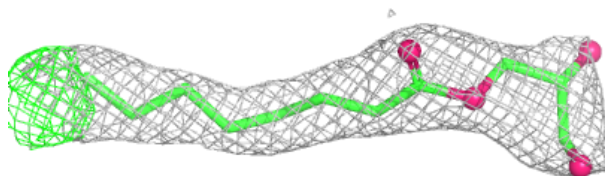


Electron density around LFA D 306:

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

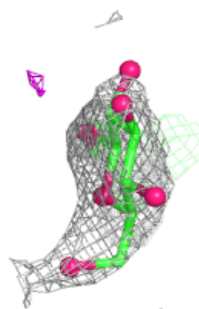
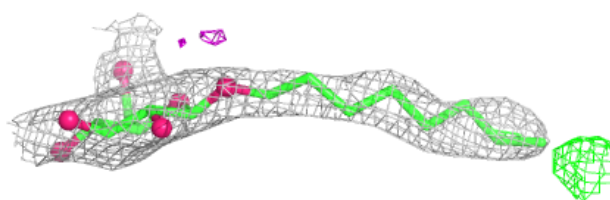
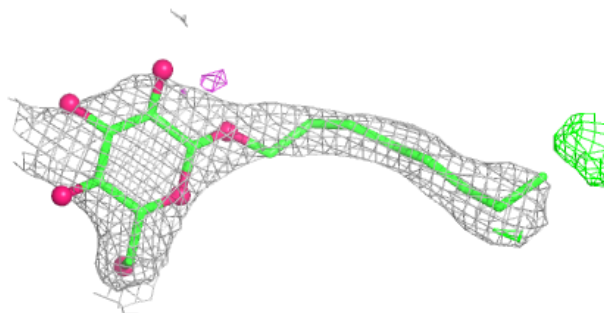
**Electron density around OLC A 306:**

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

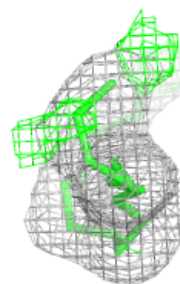
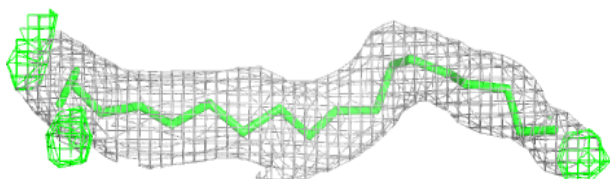
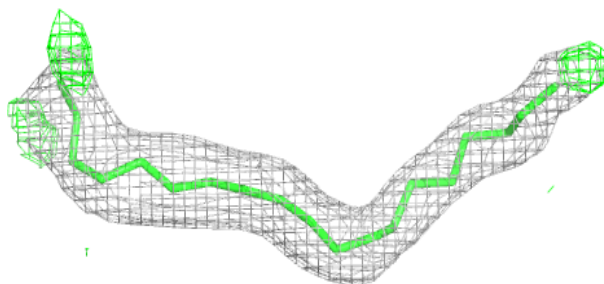


Electron density around BOG D 305:

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

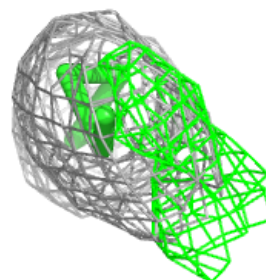
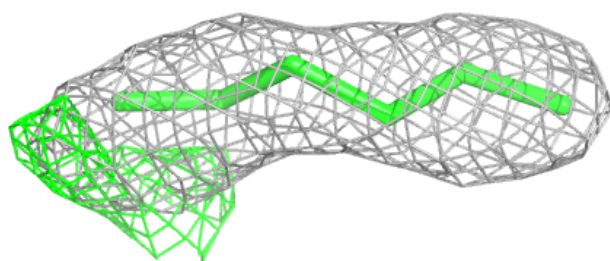
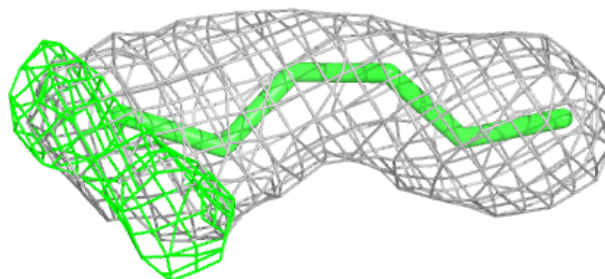
**Electron density around LFA C 308:**

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

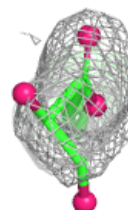
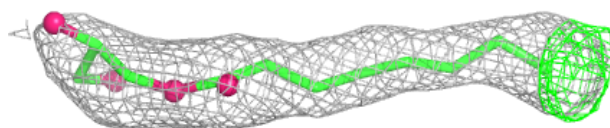
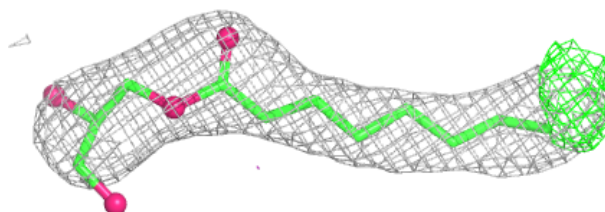


Electron density around LFA A 304:

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

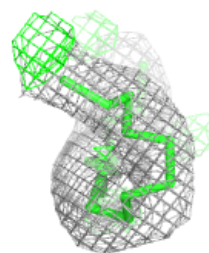
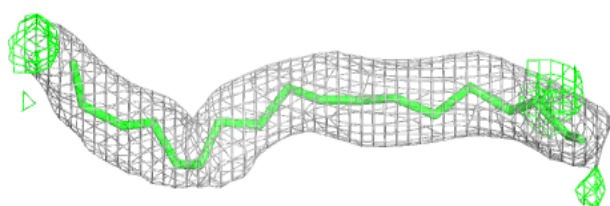
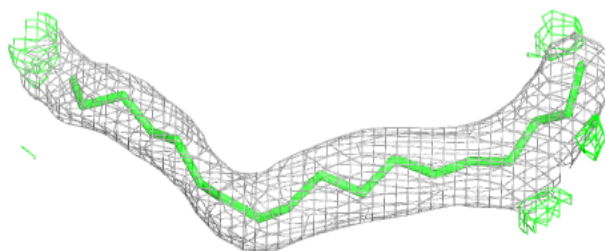
**Electron density around OLC D 307:**

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

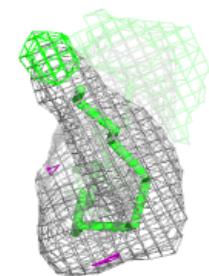
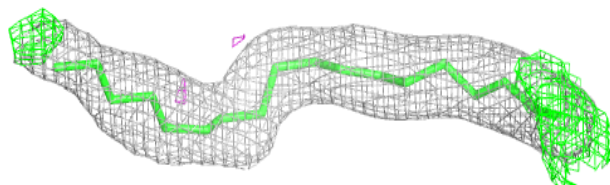
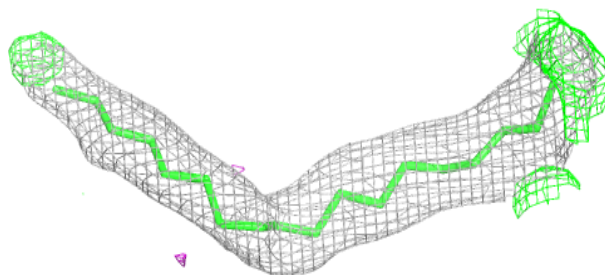


Electron density around LFA A 308:

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

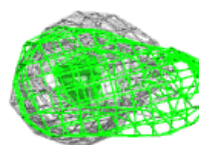
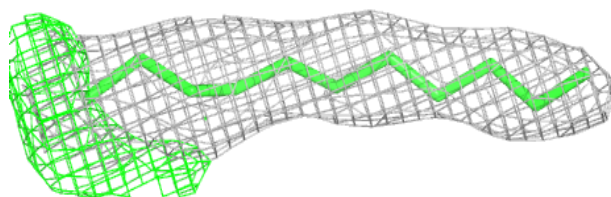
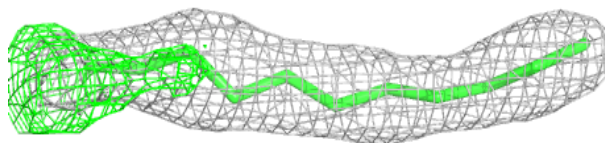
**Electron density around LFA E 303:**

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

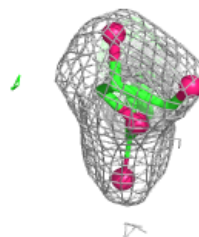
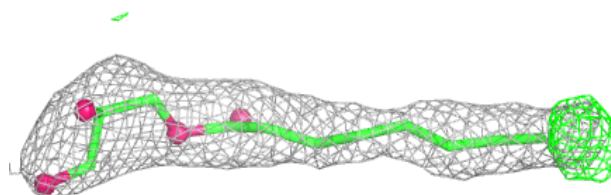
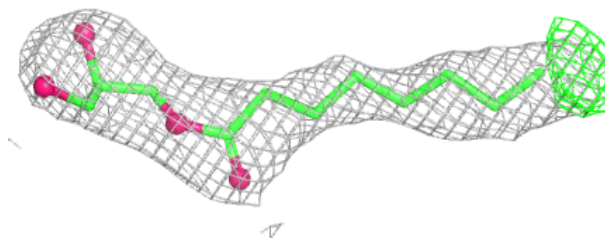


Electron density around LFA D 302:

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

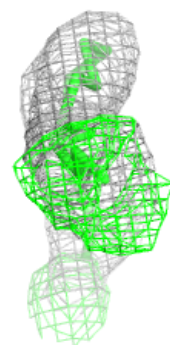
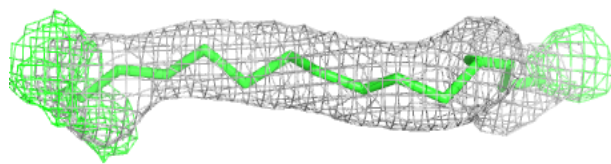
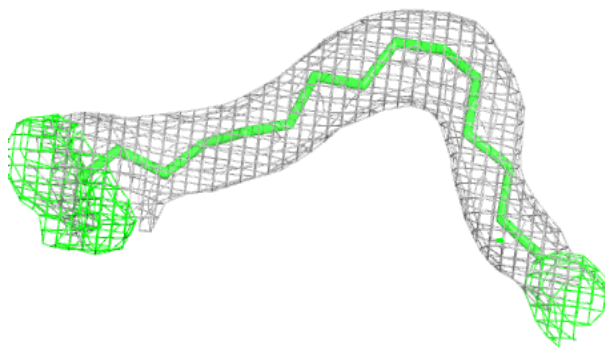
**Electron density around OLC E 306:**

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

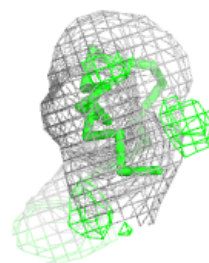
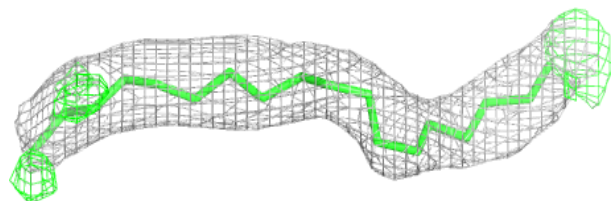
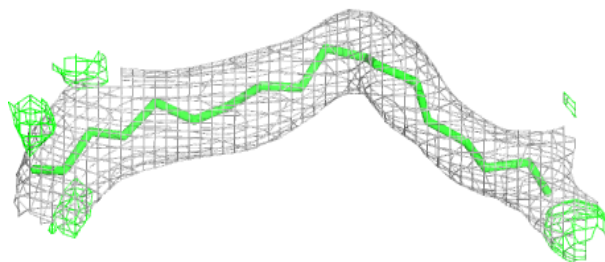


Electron density around LFA B 306:

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

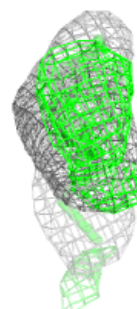
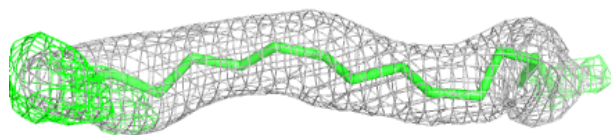
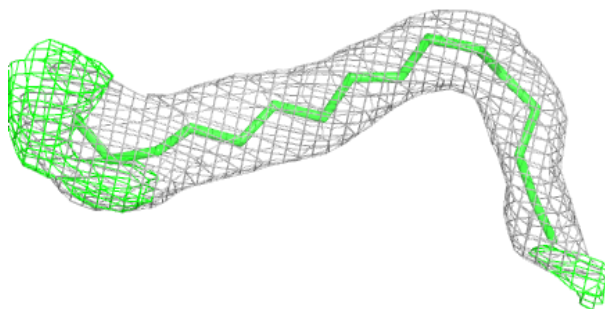
**Electron density around LFA B 303:**

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

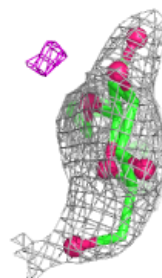
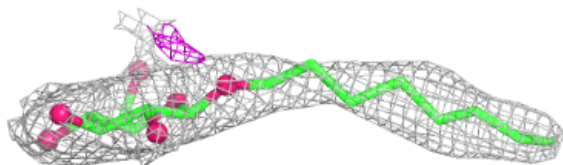
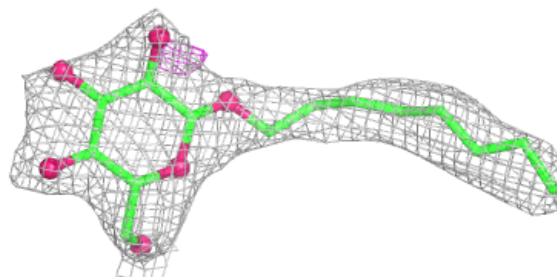


Electron density around LFA A 305:

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

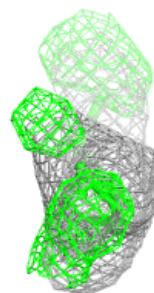
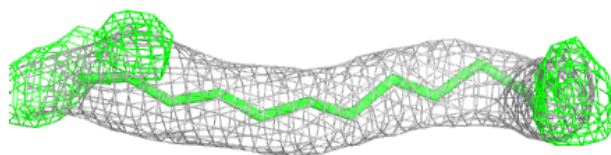
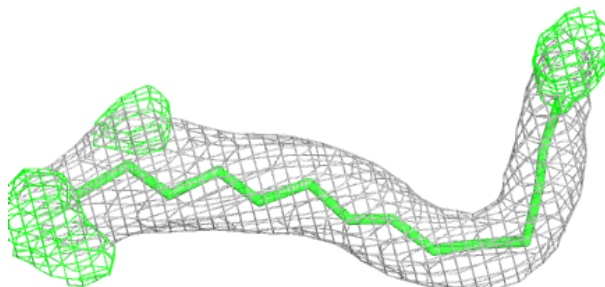
**Electron density around BOG A 303:**

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

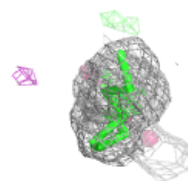
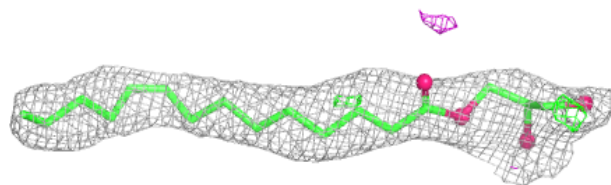
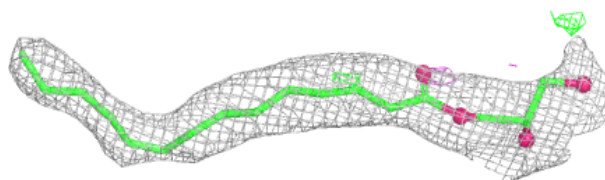


Electron density around LFA A 309:

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

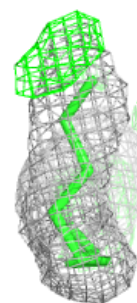
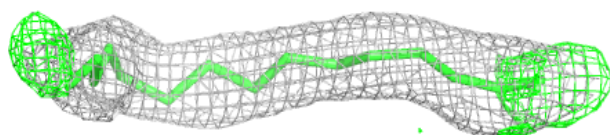
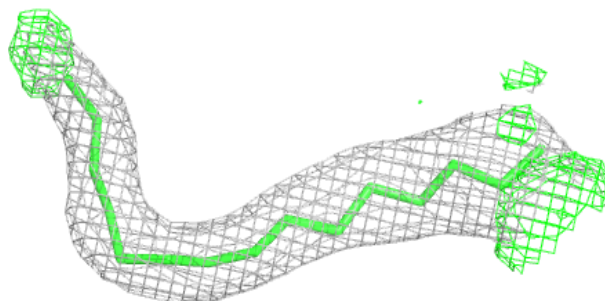
**Electron density around OLC C 303:**

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

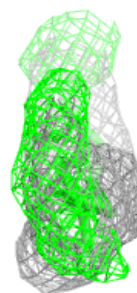
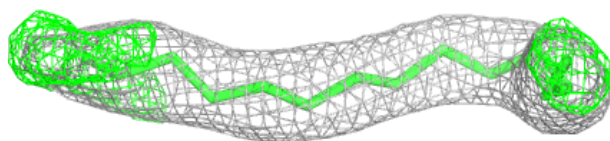
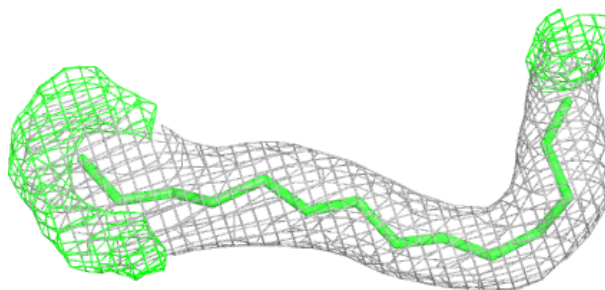


Electron density around LFA C 302:

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

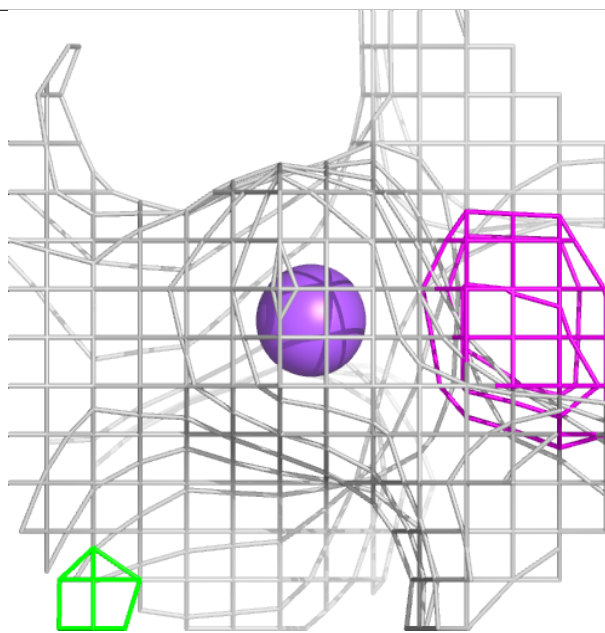
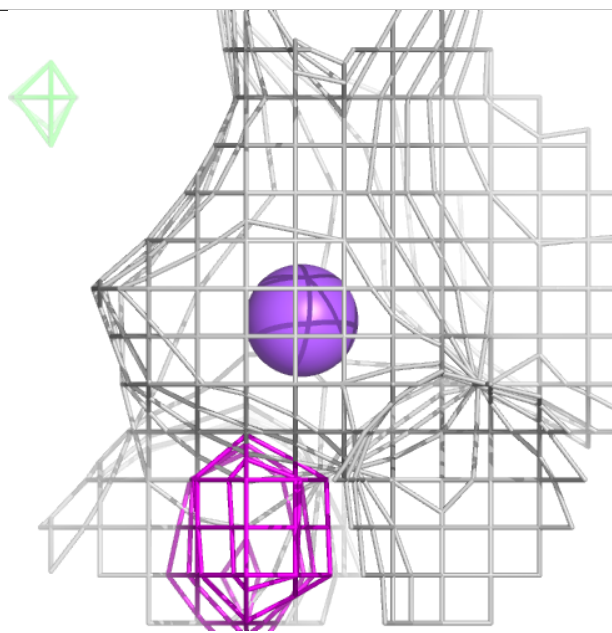
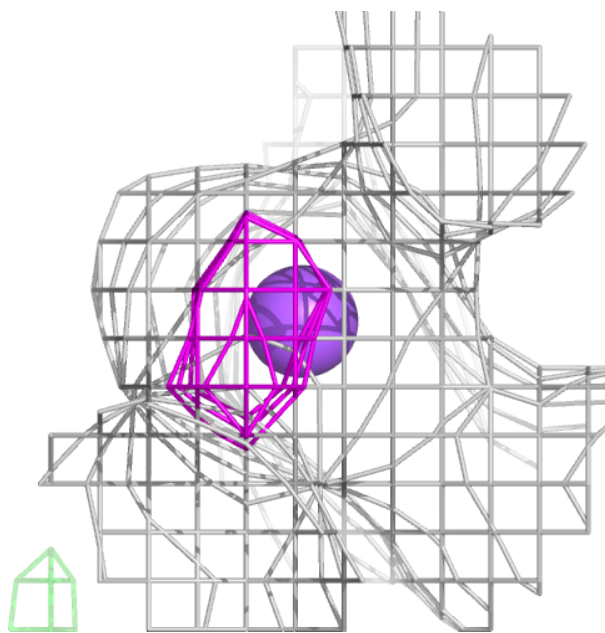
**Electron density around LFA D 303:**

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



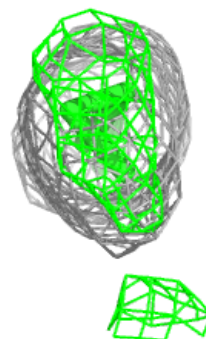
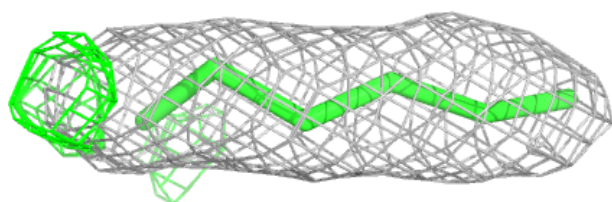
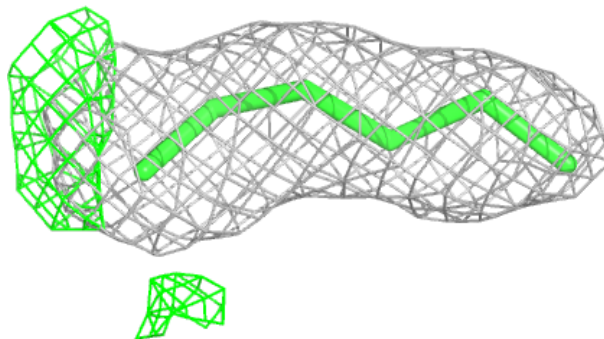
Electron density around NA B 301:

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

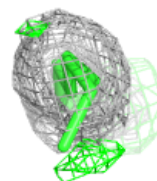
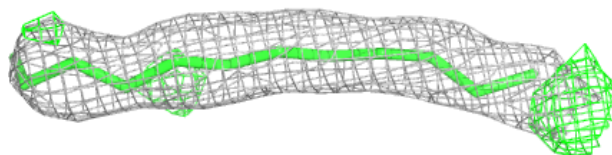
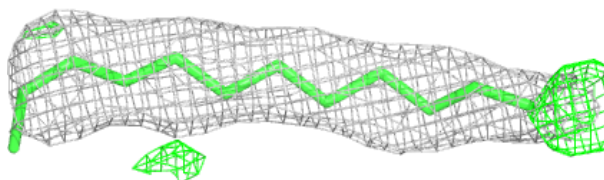


Electron density around LFA B 305:

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

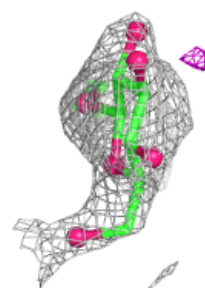
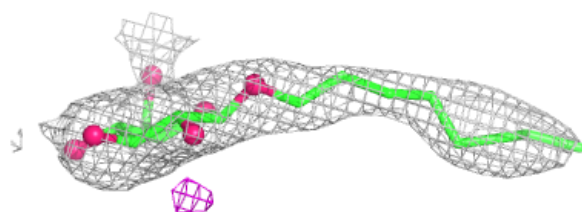
**Electron density around LFA B 302:**

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

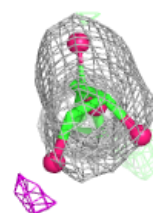
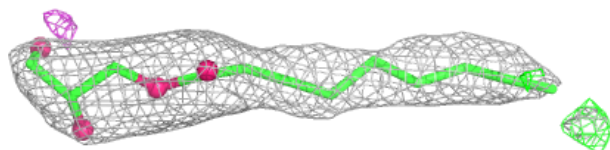
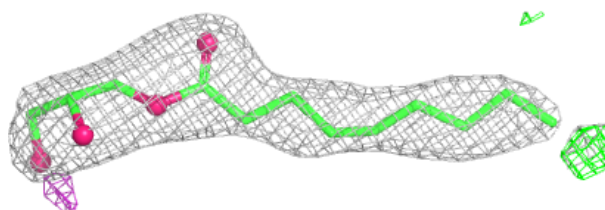


Electron density around BOG B 304:

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

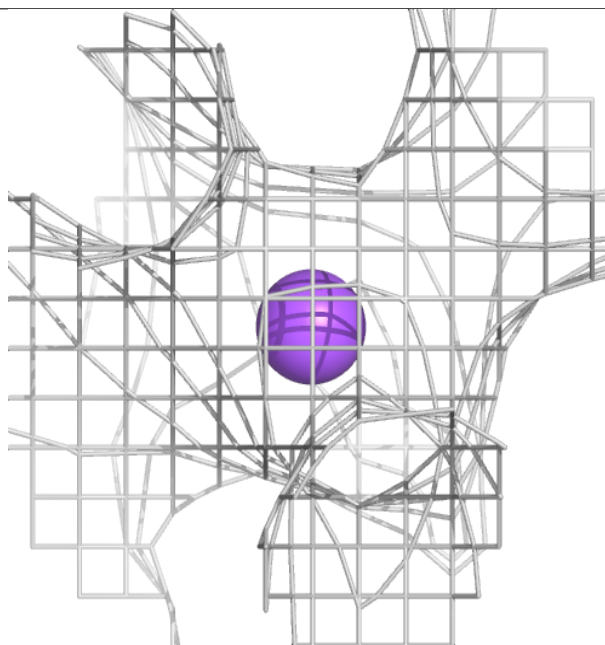
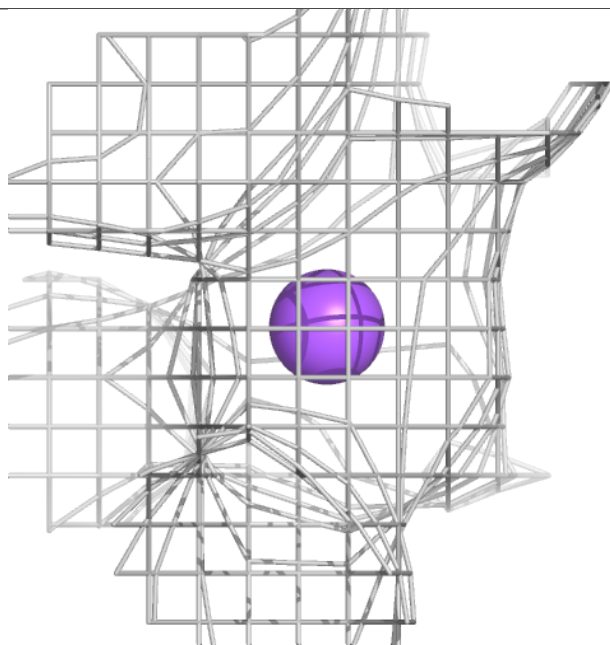
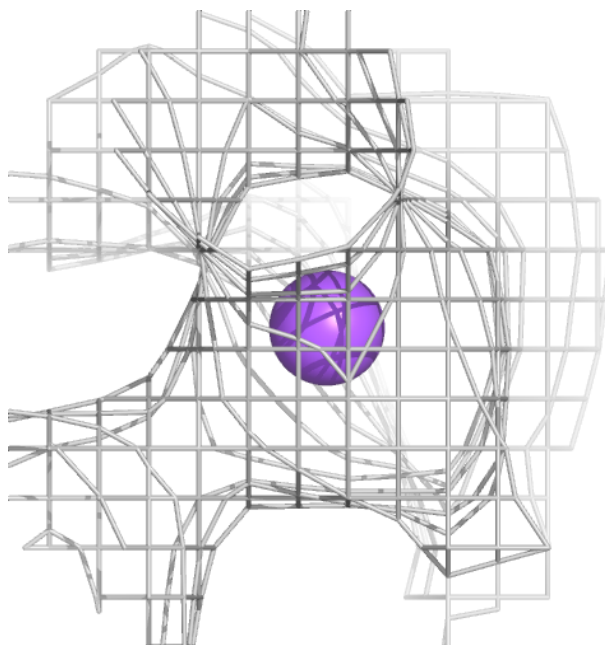
**Electron density around OLC C 306:**

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



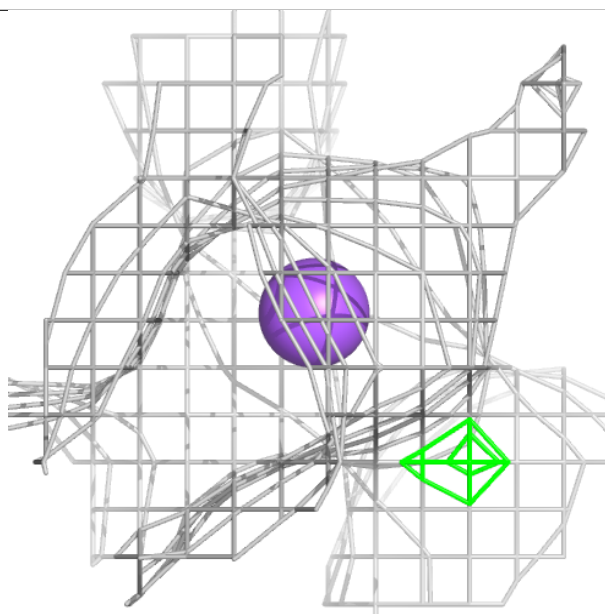
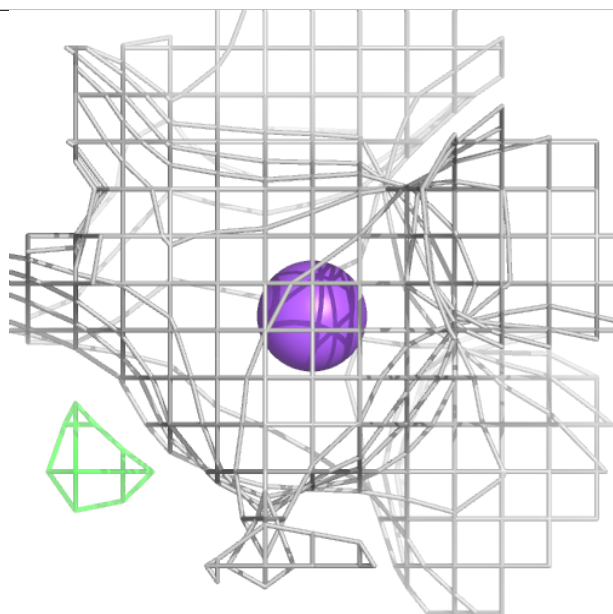
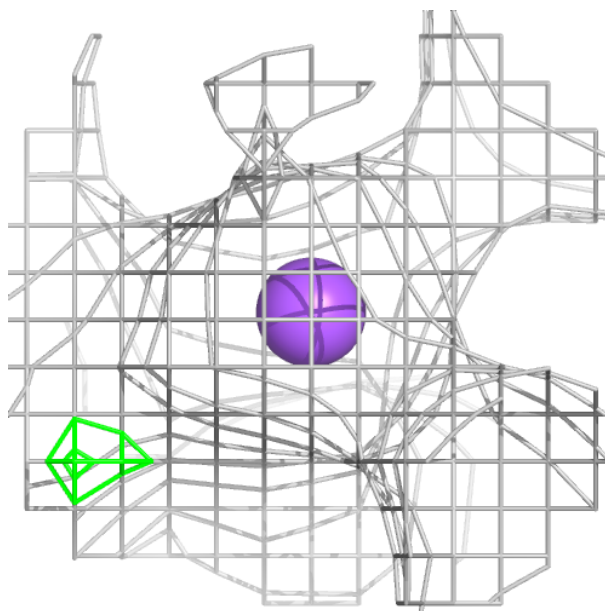
Electron density around NA E 301:

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



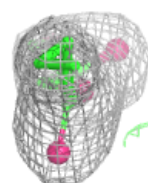
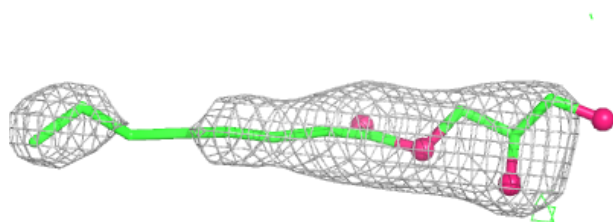
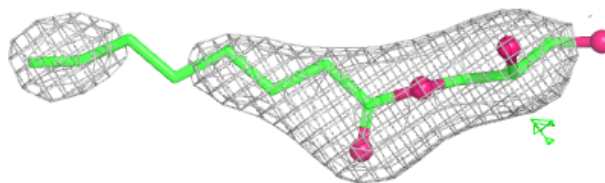
Electron density around NA C 301:

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

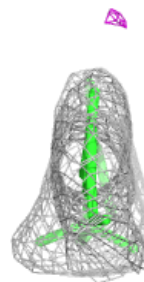
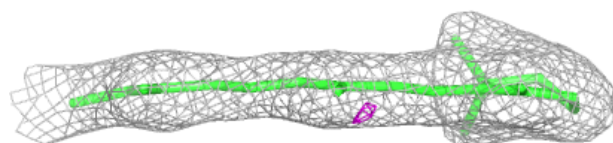
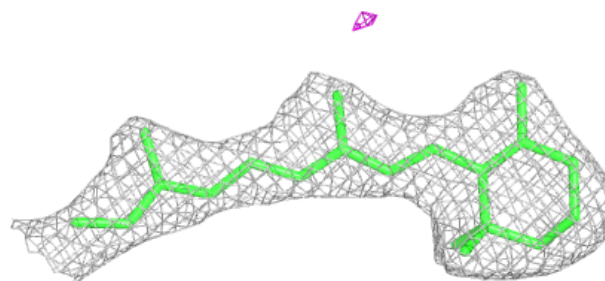


Electron density around OLC B 307:

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

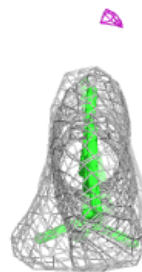
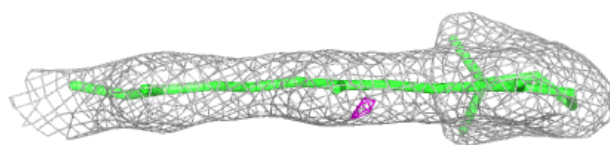
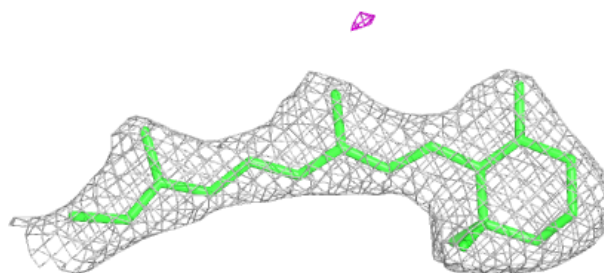
**Electron density around RET C 307 (A):**

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

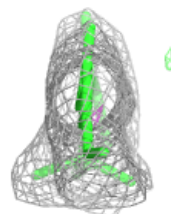
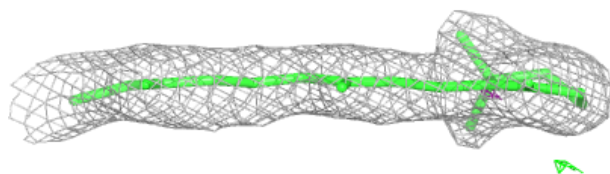
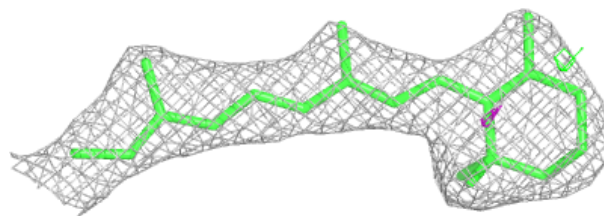


Electron density around RET C 307 (B):

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

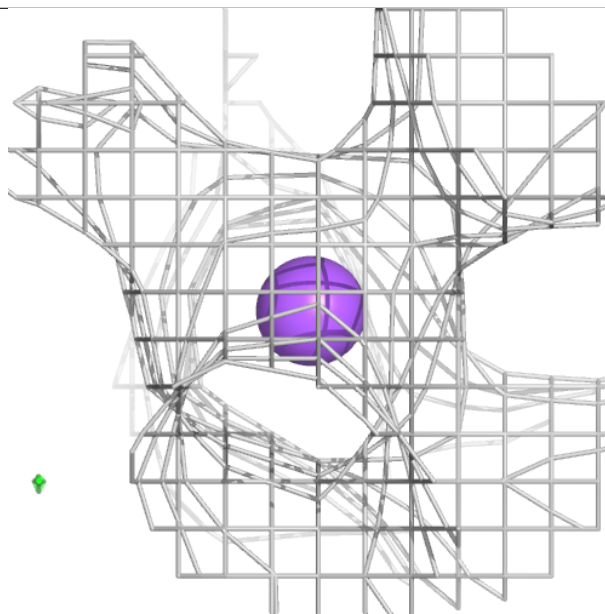
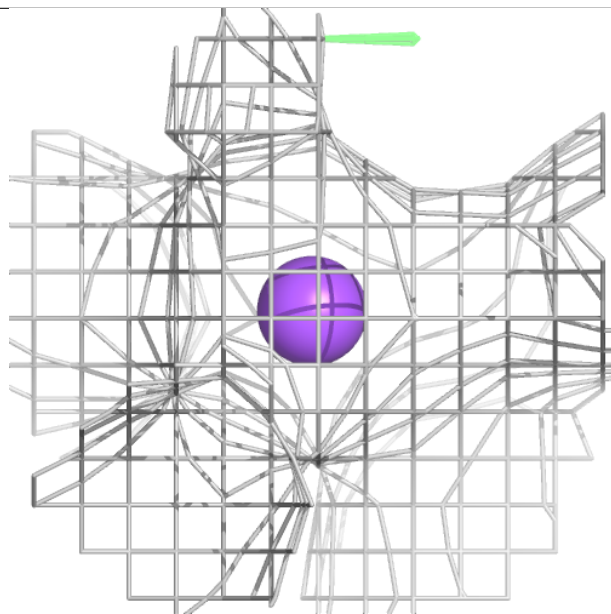
**Electron density around RET A 307 (B):**

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



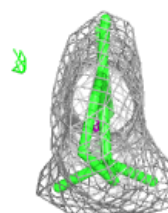
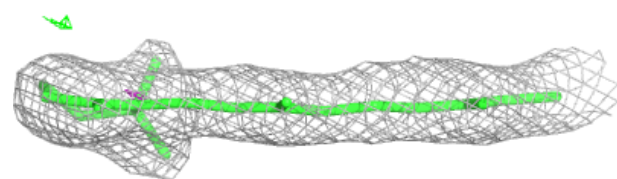
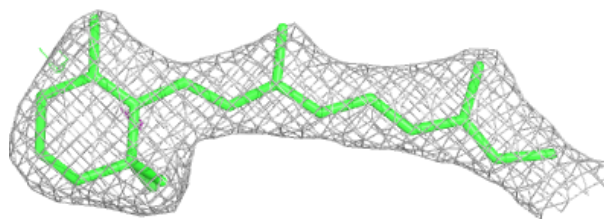
Electron density around NA A 301:

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

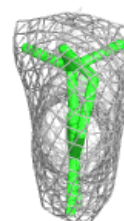
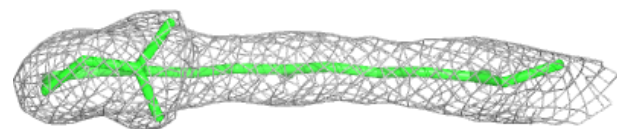
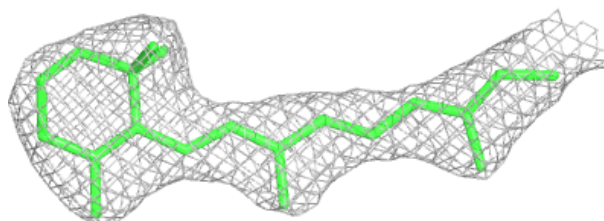


Electron density around RET A 307 (A):

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

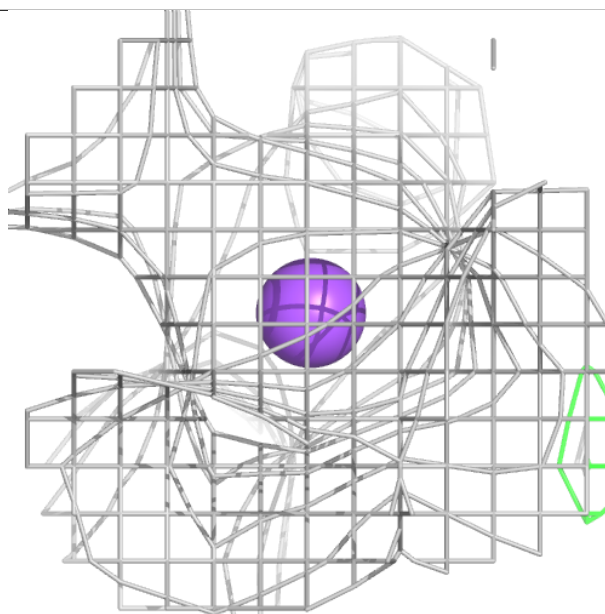
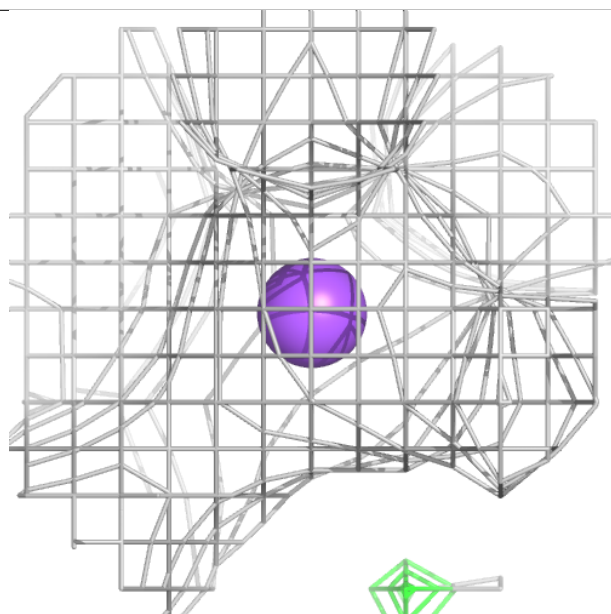
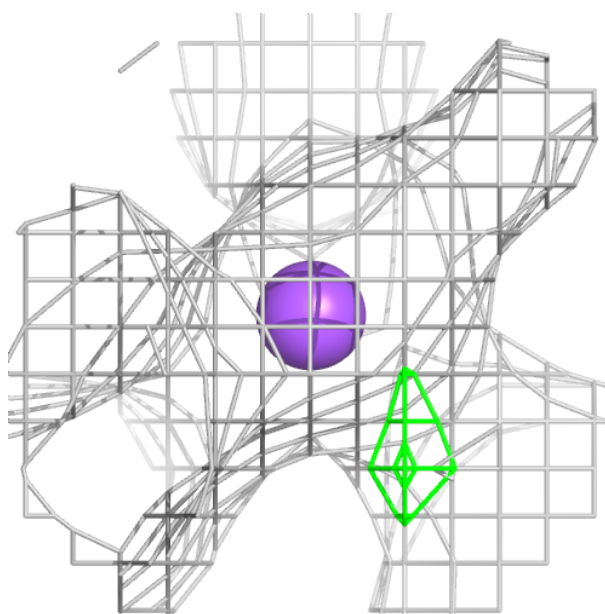
**Electron density around RET B 308 (B):**

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



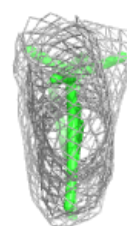
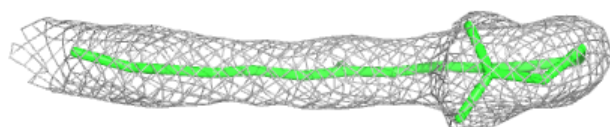
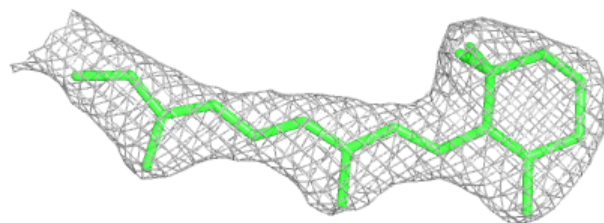
Electron density around NA D 301:

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

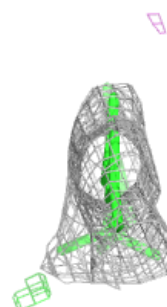
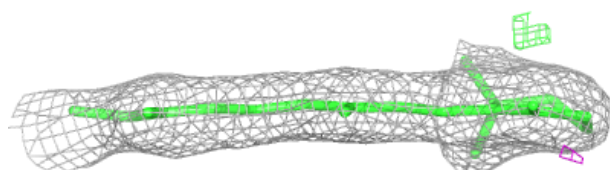
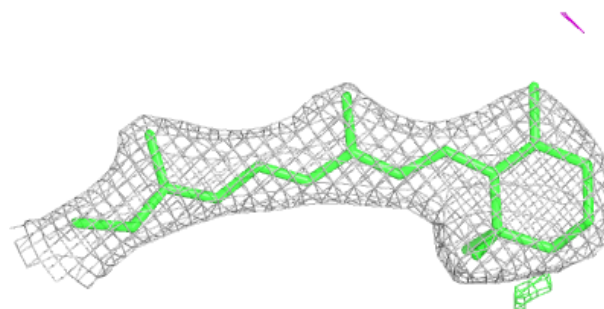


Electron density around RET B 308 (A):

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

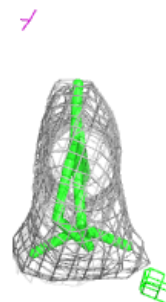
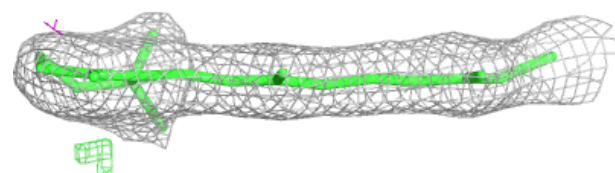
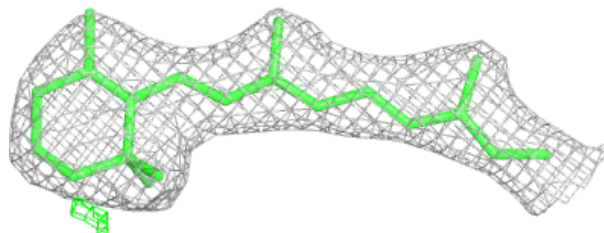
**Electron density around RET D 308 (A):**

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

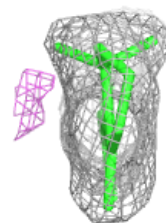
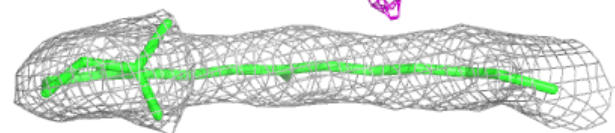
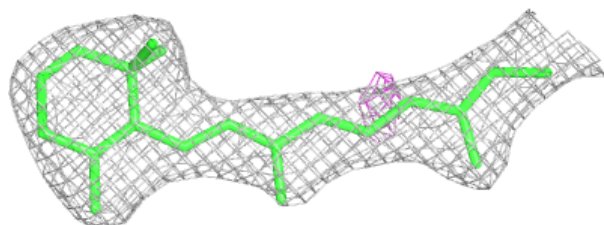


Electron density around RET D 308 (B):

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

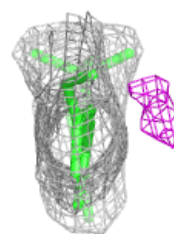
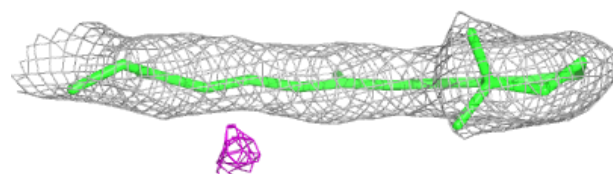
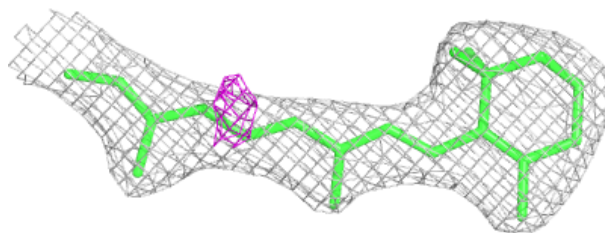
**Electron density around RET E 307 (A):**

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



Electron density around RET E 307 (B):

$2mF_o-DF_c$ (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.